



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:55 PM GMT

PDB ID : 4V8R  
Title : The crystal structures of the eukaryotic chaperonin CCT reveal its functional partitioning  
Authors : Kalisman, N.; Schroder, G.F.; Levitt, M.  
Deposited on : 2012-03-28  
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

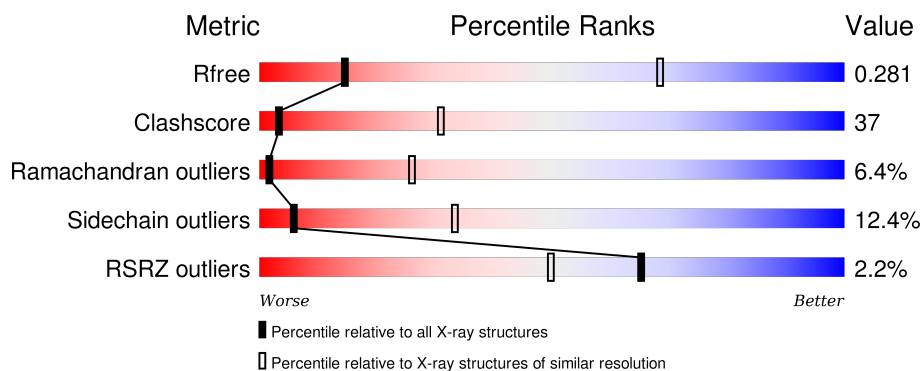
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






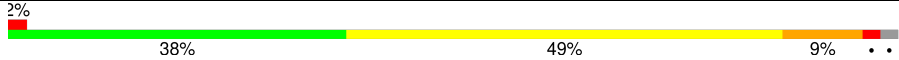
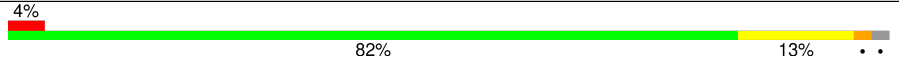
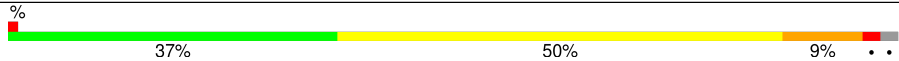
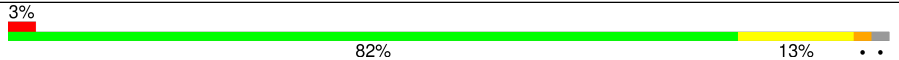
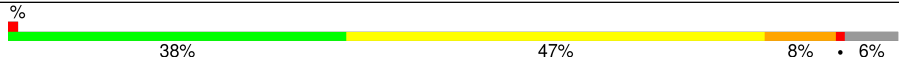
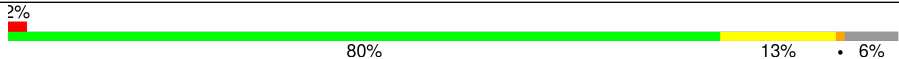
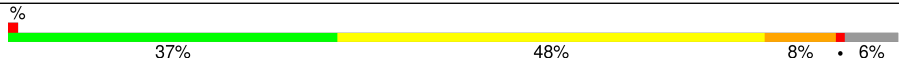
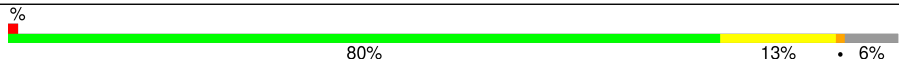
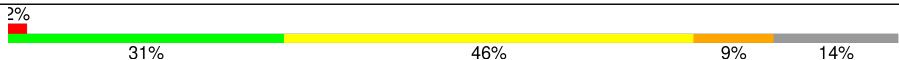

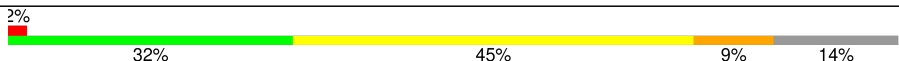
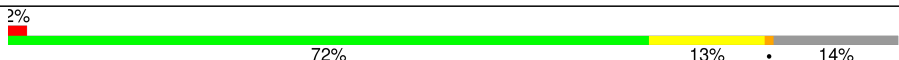
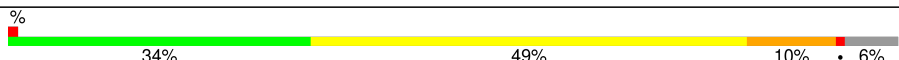
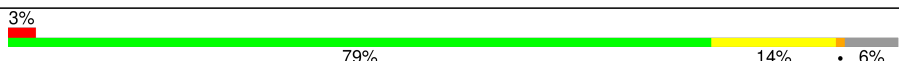
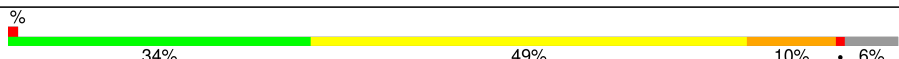
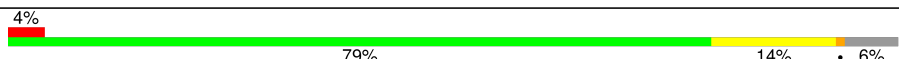
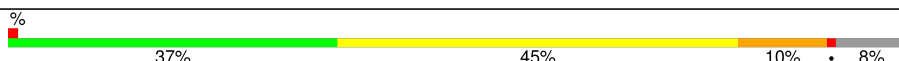
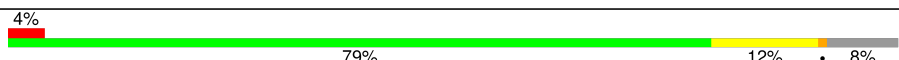
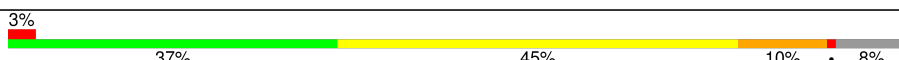
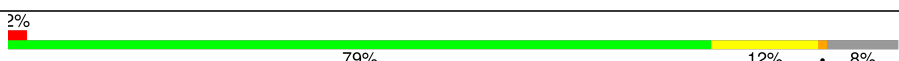
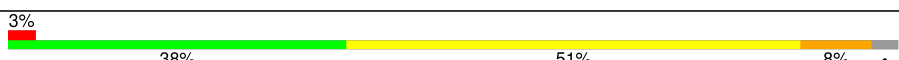
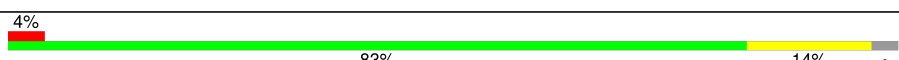
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	559	<div> <div>33%</div> <div>53%</div> <div>10%</div> <div>..</div> </div>
1	Aa	559	<div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	BA	559	<div> <div>33%</div> <div>53%</div> <div>10%</div> <div>..</div> </div>
1	Ba	559	<div> <div>3%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
2	AB	527	<div> <div>33%</div> <div>52%</div> <div>12%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	Ab	527	
2	BB	527	
2	Bb	527	
3	AD	528	
3	Ad	528	
3	BD	528	
3	Bd	528	
4	AE	562	
4	Ae	562	
4	BE	562	
4	Be	562	
5	AG	590	
5	Ag	590	
5	BG	590	
5	Bg	590	
6	AH	550	
6	Ah	550	
6	BH	550	
6	Bh	550	
7	AQ	568	
7	Aq	568	
7	BQ	568	
7	Bq	568	
8	AZ	546	
8	Az	546	

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Mol	Chain	Length	Quality of chain
8	BZ	546	
8	Bz	546	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BEF	AG	1002	-	-	X	-
10	BEF	BG	4002	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 128780 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	Aa	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	BA	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	Ba	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			

- Molecule 2 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	Ab	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	BB	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	Bb	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			

- Molecule 3 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	Ad	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	BD	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	Bd	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AD	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
Ad	1345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
BD	3345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
Bd	4345	ASP	GLY	ENGINEERED MUTATION	UNP P39078

- Molecule 4 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT EPSILON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	Ae	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	BE	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	Be	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			

- Molecule 5 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AG	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	Ag	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	BG	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	Bg	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	901	GLY	-	INSERTION	UNP P39077
AG	902	SER	-	INSERTION	UNP P39077
AG	903	GLY	-	INSERTION	UNP P39077
AG	904	SER	-	INSERTION	UNP P39077
AG	905	GLY	-	INSERTION	UNP P39077
AG	906	TRP	-	INSERTION	UNP P39077
AG	907	SER	-	INSERTION	UNP P39077
AG	908	HIS	-	INSERTION	UNP P39077
AG	909	PRO	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
AG	910	GLN	-	INSERTION	UNP P39077
AG	911	PHE	-	INSERTION	UNP P39077
AG	912	GLU	-	INSERTION	UNP P39077
AG	913	LYS	-	INSERTION	UNP P39077
AG	914	GLY	-	INSERTION	UNP P39077
AG	915	SER	-	INSERTION	UNP P39077
AG	916	GLY	-	INSERTION	UNP P39077
AG	917	LYS	-	INSERTION	UNP P39077
AG	918	ARG	-	INSERTION	UNP P39077
AG	919	ARG	-	INSERTION	UNP P39077
AG	920	TRP	-	INSERTION	UNP P39077
AG	921	LYS	-	INSERTION	UNP P39077
AG	922	LYS	-	INSERTION	UNP P39077
AG	923	ASN	-	INSERTION	UNP P39077
AG	924	PHE	-	INSERTION	UNP P39077
AG	925	ILE	-	INSERTION	UNP P39077
AG	926	ALA	-	INSERTION	UNP P39077
AG	927	VAL	-	INSERTION	UNP P39077
AG	928	SER	-	INSERTION	UNP P39077
AG	929	ALA	-	INSERTION	UNP P39077
AG	930	ALA	-	INSERTION	UNP P39077
AG	931	ASN	-	INSERTION	UNP P39077
AG	932	ARG	-	INSERTION	UNP P39077
AG	933	PHE	-	INSERTION	UNP P39077
AG	934	LYS	-	INSERTION	UNP P39077
AG	935	LYS	-	INSERTION	UNP P39077
AG	936	ILE	-	INSERTION	UNP P39077
AG	937	SER	-	INSERTION	UNP P39077
AG	938	SER	-	INSERTION	UNP P39077
AG	939	SER	-	INSERTION	UNP P39077
AG	940	GLY	-	INSERTION	UNP P39077
AG	941	ALA	-	INSERTION	UNP P39077
AG	942	LEU	-	INSERTION	UNP P39077
AG	943	GLY	-	INSERTION	UNP P39077
AG	944	SER	-	INSERTION	UNP P39077
AG	945	GLY	-	INSERTION	UNP P39077
AG	946	HIS	-	INSERTION	UNP P39077
AG	947	HIS	-	INSERTION	UNP P39077
AG	948	HIS	-	INSERTION	UNP P39077
AG	949	HIS	-	INSERTION	UNP P39077
AG	950	HIS	-	INSERTION	UNP P39077
AG	951	HIS	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
AG	952	HIS	-	INSERTION	UNP P39077
AG	953	HIS	-	INSERTION	UNP P39077
AG	954	GLY	-	INSERTION	UNP P39077
AG	955	SER	-	INSERTION	UNP P39077
AG	956	GLY	-	INSERTION	UNP P39077
Ag	1901	GLY	-	INSERTION	UNP P39077
Ag	1902	SER	-	INSERTION	UNP P39077
Ag	1903	GLY	-	INSERTION	UNP P39077
Ag	1904	SER	-	INSERTION	UNP P39077
Ag	1905	GLY	-	INSERTION	UNP P39077
Ag	1906	TRP	-	INSERTION	UNP P39077
Ag	1907	SER	-	INSERTION	UNP P39077
Ag	1908	HIS	-	INSERTION	UNP P39077
Ag	1909	PRO	-	INSERTION	UNP P39077
Ag	1910	GLN	-	INSERTION	UNP P39077
Ag	1911	PHE	-	INSERTION	UNP P39077
Ag	1912	GLU	-	INSERTION	UNP P39077
Ag	1913	LYS	-	INSERTION	UNP P39077
Ag	1914	GLY	-	INSERTION	UNP P39077
Ag	1915	SER	-	INSERTION	UNP P39077
Ag	1916	GLY	-	INSERTION	UNP P39077
Ag	1917	LYS	-	INSERTION	UNP P39077
Ag	1918	ARG	-	INSERTION	UNP P39077
Ag	1919	ARG	-	INSERTION	UNP P39077
Ag	1920	TRP	-	INSERTION	UNP P39077
Ag	1921	LYS	-	INSERTION	UNP P39077
Ag	1922	LYS	-	INSERTION	UNP P39077
Ag	1923	ASN	-	INSERTION	UNP P39077
Ag	1924	PHE	-	INSERTION	UNP P39077
Ag	1925	ILE	-	INSERTION	UNP P39077
Ag	1926	ALA	-	INSERTION	UNP P39077
Ag	1927	VAL	-	INSERTION	UNP P39077
Ag	1928	SER	-	INSERTION	UNP P39077
Ag	1929	ALA	-	INSERTION	UNP P39077
Ag	1930	ALA	-	INSERTION	UNP P39077
Ag	1931	ASN	-	INSERTION	UNP P39077
Ag	1932	ARG	-	INSERTION	UNP P39077
Ag	1933	PHE	-	INSERTION	UNP P39077
Ag	1934	LYS	-	INSERTION	UNP P39077
Ag	1935	LYS	-	INSERTION	UNP P39077
Ag	1936	ILE	-	INSERTION	UNP P39077
Ag	1937	SER	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Ag	1938	SER	-	INSERTION	UNP P39077
Ag	1939	SER	-	INSERTION	UNP P39077
Ag	1940	GLY	-	INSERTION	UNP P39077
Ag	1941	ALA	-	INSERTION	UNP P39077
Ag	1942	LEU	-	INSERTION	UNP P39077
Ag	1943	GLY	-	INSERTION	UNP P39077
Ag	1944	SER	-	INSERTION	UNP P39077
Ag	1945	GLY	-	INSERTION	UNP P39077
Ag	1946	HIS	-	INSERTION	UNP P39077
Ag	1947	HIS	-	INSERTION	UNP P39077
Ag	1948	HIS	-	INSERTION	UNP P39077
Ag	1949	HIS	-	INSERTION	UNP P39077
Ag	1950	HIS	-	INSERTION	UNP P39077
Ag	1951	HIS	-	INSERTION	UNP P39077
Ag	1952	HIS	-	INSERTION	UNP P39077
Ag	1953	HIS	-	INSERTION	UNP P39077
Ag	1954	GLY	-	INSERTION	UNP P39077
Ag	1955	SER	-	INSERTION	UNP P39077
Ag	1956	GLY	-	INSERTION	UNP P39077
BG	3901	GLY	-	INSERTION	UNP P39077
BG	3902	SER	-	INSERTION	UNP P39077
BG	3903	GLY	-	INSERTION	UNP P39077
BG	3904	SER	-	INSERTION	UNP P39077
BG	3905	GLY	-	INSERTION	UNP P39077
BG	3906	TRP	-	INSERTION	UNP P39077
BG	3907	SER	-	INSERTION	UNP P39077
BG	3908	HIS	-	INSERTION	UNP P39077
BG	3909	PRO	-	INSERTION	UNP P39077
BG	3910	GLN	-	INSERTION	UNP P39077
BG	3911	PHE	-	INSERTION	UNP P39077
BG	3912	GLU	-	INSERTION	UNP P39077
BG	3913	LYS	-	INSERTION	UNP P39077
BG	3914	GLY	-	INSERTION	UNP P39077
BG	3915	SER	-	INSERTION	UNP P39077
BG	3916	GLY	-	INSERTION	UNP P39077
BG	3917	LYS	-	INSERTION	UNP P39077
BG	3918	ARG	-	INSERTION	UNP P39077
BG	3919	ARG	-	INSERTION	UNP P39077
BG	3920	TRP	-	INSERTION	UNP P39077
BG	3921	LYS	-	INSERTION	UNP P39077
BG	3922	LYS	-	INSERTION	UNP P39077
BG	3923	ASN	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
BG	3924	PHE	-	INSERTION	UNP P39077
BG	3925	ILE	-	INSERTION	UNP P39077
BG	3926	ALA	-	INSERTION	UNP P39077
BG	3927	VAL	-	INSERTION	UNP P39077
BG	3928	SER	-	INSERTION	UNP P39077
BG	3929	ALA	-	INSERTION	UNP P39077
BG	3930	ALA	-	INSERTION	UNP P39077
BG	3931	ASN	-	INSERTION	UNP P39077
BG	3932	ARG	-	INSERTION	UNP P39077
BG	3933	PHE	-	INSERTION	UNP P39077
BG	3934	LYS	-	INSERTION	UNP P39077
BG	3935	LYS	-	INSERTION	UNP P39077
BG	3936	ILE	-	INSERTION	UNP P39077
BG	3937	SER	-	INSERTION	UNP P39077
BG	3938	SER	-	INSERTION	UNP P39077
BG	3939	SER	-	INSERTION	UNP P39077
BG	3940	GLY	-	INSERTION	UNP P39077
BG	3941	ALA	-	INSERTION	UNP P39077
BG	3942	LEU	-	INSERTION	UNP P39077
BG	3943	GLY	-	INSERTION	UNP P39077
BG	3944	SER	-	INSERTION	UNP P39077
BG	3945	GLY	-	INSERTION	UNP P39077
BG	3946	HIS	-	INSERTION	UNP P39077
BG	3947	HIS	-	INSERTION	UNP P39077
BG	3948	HIS	-	INSERTION	UNP P39077
BG	3949	HIS	-	INSERTION	UNP P39077
BG	3950	HIS	-	INSERTION	UNP P39077
BG	3951	HIS	-	INSERTION	UNP P39077
BG	3952	HIS	-	INSERTION	UNP P39077
BG	3953	HIS	-	INSERTION	UNP P39077
BG	3954	GLY	-	INSERTION	UNP P39077
BG	3955	SER	-	INSERTION	UNP P39077
BG	3956	GLY	-	INSERTION	UNP P39077
Bg	4901	GLY	-	INSERTION	UNP P39077
Bg	4902	SER	-	INSERTION	UNP P39077
Bg	4903	GLY	-	INSERTION	UNP P39077
Bg	4904	SER	-	INSERTION	UNP P39077
Bg	4905	GLY	-	INSERTION	UNP P39077
Bg	4906	TRP	-	INSERTION	UNP P39077
Bg	4907	SER	-	INSERTION	UNP P39077
Bg	4908	HIS	-	INSERTION	UNP P39077
Bg	4909	PRO	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Bg	4910	GLN	-	INSERTION	UNP P39077
Bg	4911	PHE	-	INSERTION	UNP P39077
Bg	4912	GLU	-	INSERTION	UNP P39077
Bg	4913	LYS	-	INSERTION	UNP P39077
Bg	4914	GLY	-	INSERTION	UNP P39077
Bg	4915	SER	-	INSERTION	UNP P39077
Bg	4916	GLY	-	INSERTION	UNP P39077
Bg	4917	LYS	-	INSERTION	UNP P39077
Bg	4918	ARG	-	INSERTION	UNP P39077
Bg	4919	ARG	-	INSERTION	UNP P39077
Bg	4920	TRP	-	INSERTION	UNP P39077
Bg	4921	LYS	-	INSERTION	UNP P39077
Bg	4922	LYS	-	INSERTION	UNP P39077
Bg	4923	ASN	-	INSERTION	UNP P39077
Bg	4924	PHE	-	INSERTION	UNP P39077
Bg	4925	ILE	-	INSERTION	UNP P39077
Bg	4926	ALA	-	INSERTION	UNP P39077
Bg	4927	VAL	-	INSERTION	UNP P39077
Bg	4928	SER	-	INSERTION	UNP P39077
Bg	4929	ALA	-	INSERTION	UNP P39077
Bg	4930	ALA	-	INSERTION	UNP P39077
Bg	4931	ASN	-	INSERTION	UNP P39077
Bg	4932	ARG	-	INSERTION	UNP P39077
Bg	4933	PHE	-	INSERTION	UNP P39077
Bg	4934	LYS	-	INSERTION	UNP P39077
Bg	4935	LYS	-	INSERTION	UNP P39077
Bg	4936	ILE	-	INSERTION	UNP P39077
Bg	4937	SER	-	INSERTION	UNP P39077
Bg	4938	SER	-	INSERTION	UNP P39077
Bg	4939	SER	-	INSERTION	UNP P39077
Bg	4940	GLY	-	INSERTION	UNP P39077
Bg	4941	ALA	-	INSERTION	UNP P39077
Bg	4942	LEU	-	INSERTION	UNP P39077
Bg	4943	GLY	-	INSERTION	UNP P39077
Bg	4944	SER	-	INSERTION	UNP P39077
Bg	4945	GLY	-	INSERTION	UNP P39077
Bg	4946	HIS	-	INSERTION	UNP P39077
Bg	4947	HIS	-	INSERTION	UNP P39077
Bg	4948	HIS	-	INSERTION	UNP P39077
Bg	4949	HIS	-	INSERTION	UNP P39077
Bg	4950	HIS	-	INSERTION	UNP P39077
Bg	4951	HIS	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Bg	4952	HIS	-	INSERTION	UNP P39077
Bg	4953	HIS	-	INSERTION	UNP P39077
Bg	4954	GLY	-	INSERTION	UNP P39077
Bg	4955	SER	-	INSERTION	UNP P39077
Bg	4956	GLY	-	INSERTION	UNP P39077

- Molecule 6 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AH	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	Ah	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	BH	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	Bh	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			

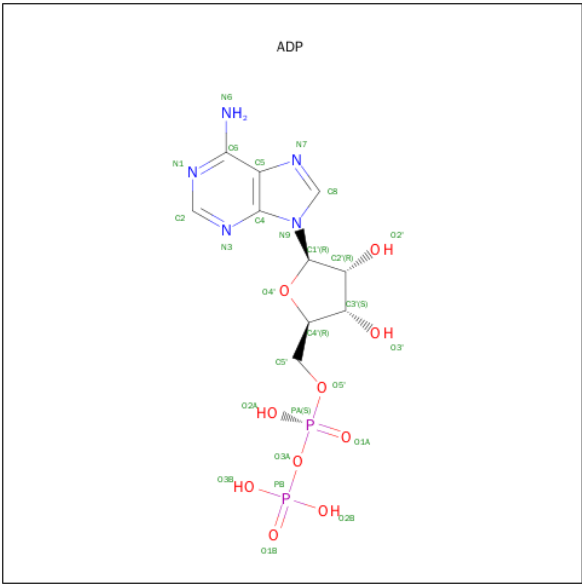
- Molecule 7 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT THETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AQ	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	Aq	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	BQ	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	Bq	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			

- Molecule 8 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ZETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AZ	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	Az	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	BZ	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	Bz	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



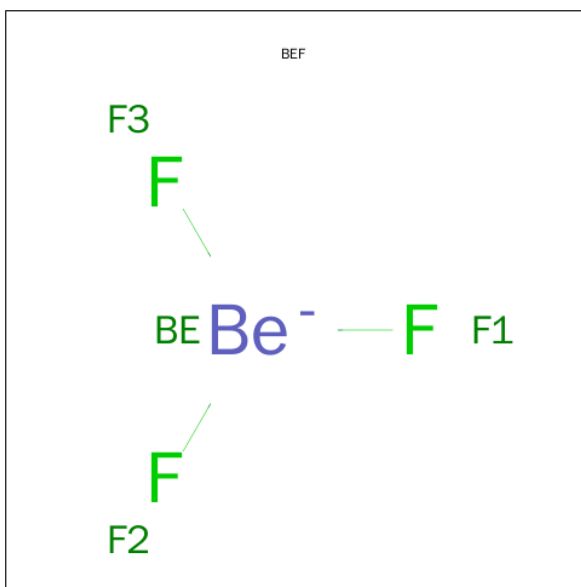
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AA	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AB	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AD	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AE	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AG	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AH	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AQ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AZ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Aa	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ab	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ad	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ae	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Ag	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Ah	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Aq	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Az	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	BA	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	BB	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	BD	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	BE	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	BG	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	BH	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	BQ	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	BZ	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Ba	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Bb	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Bd	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Be	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Bg	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Bh	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Bq	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	Bz	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	AA	1	Total	Be	F	0	0
			4	1	3		
10	AB	1	Total	Be	F	0	0
			4	1	3		
10	AD	1	Total	Be	F	0	0
			4	1	3		
10	AE	1	Total	Be	F	0	0
			4	1	3		
10	AG	1	Total	Be	F	0	0
			4	1	3		
10	AH	1	Total	Be	F	0	0
			4	1	3		
10	AQ	1	Total	Be	F	0	0
			4	1	3		
10	AZ	1	Total	Be	F	0	0
			4	1	3		
10	Aa	1	Total	Be	F	0	0
			4	1	3		
10	Ab	1	Total	Be	F	0	0
			4	1	3		
10	Ad	1	Total	Be	F	0	0
			4	1	3		
10	Ae	1	Total	Be	F	0	0
			4	1	3		
10	Ag	1	Total	Be	F	0	0
			4	1	3		
10	Ah	1	Total	Be	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	Aq	1	Total 4	Be 1	F 3	0	0
10	Az	1	Total 4	Be 1	F 3	0	0
10	BA	1	Total 4	Be 1	F 3	0	0
10	BB	1	Total 4	Be 1	F 3	0	0
10	BD	1	Total 4	Be 1	F 3	0	0
10	BE	1	Total 4	Be 1	F 3	0	0
10	BG	1	Total 4	Be 1	F 3	0	0
10	BH	1	Total 4	Be 1	F 3	0	0
10	BQ	1	Total 4	Be 1	F 3	0	0
10	BZ	1	Total 4	Be 1	F 3	0	0
10	Ba	1	Total 4	Be 1	F 3	0	0
10	Bb	1	Total 4	Be 1	F 3	0	0
10	Bd	1	Total 4	Be 1	F 3	0	0
10	Be	1	Total 4	Be 1	F 3	0	0
10	Bg	1	Total 4	Be 1	F 3	0	0
10	Bh	1	Total 4	Be 1	F 3	0	0
10	Bq	1	Total 4	Be 1	F 3	0	0
10	Bz	1	Total 4	Be 1	F 3	0	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	Ag	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	Aq	1	Total 1	Mg 1	0	0
11	BA	1	Total 1	Mg 1	0	0
11	Ah	1	Total 1	Mg 1	0	0
11	Bz	1	Total 1	Mg 1	0	0
11	AB	1	Total 1	Mg 1	0	0
11	BE	1	Total 1	Mg 1	0	0
11	Bd	1	Total 1	Mg 1	0	0
11	Bh	1	Total 1	Mg 1	0	0
11	BB	1	Total 1	Mg 1	0	0
11	Ba	1	Total 1	Mg 1	0	0
11	AE	1	Total 1	Mg 1	0	0
11	Ab	1	Total 1	Mg 1	0	0
11	Be	1	Total 1	Mg 1	0	0
11	AA	1	Total 1	Mg 1	0	0
11	BQ	1	Total 1	Mg 1	0	0
11	Bb	1	Total 1	Mg 1	0	0
11	AD	1	Total 1	Mg 1	0	0
11	Ae	1	Total 1	Mg 1	0	0
11	BG	1	Total 1	Mg 1	0	0
11	AZ	1	Total 1	Mg 1	0	0
11	Aa	1	Total 1	Mg 1	0	0

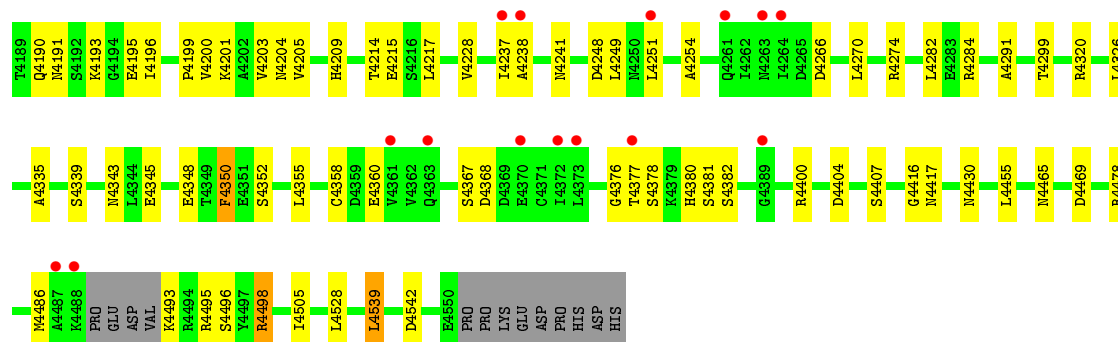
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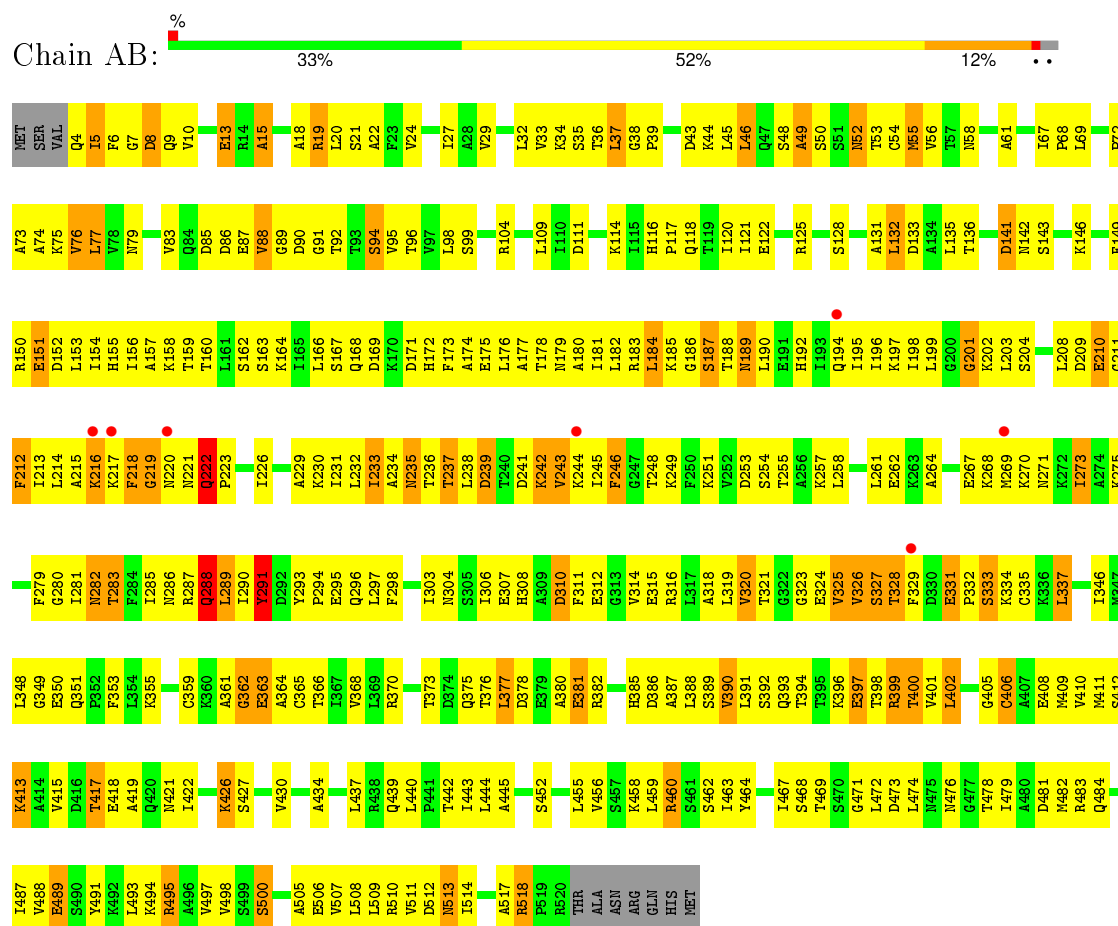
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	Bq	1	Total 1	Mg 1	0	0
11	AG	1	Total 1	Mg 1	0	0
11	AQ	1	Total 1	Mg 1	0	0
11	Ad	1	Total 1	Mg 1	0	0
11	AH	1	Total 1	Mg 1	0	0
11	BZ	1	Total 1	Mg 1	0	0
11	Bg	1	Total 1	Mg 1	0	0
11	Az	1	Total 1	Mg 1	0	0
11	BD	1	Total 1	Mg 1	0	0
11	BH	1	Total 1	Mg 1	0	0



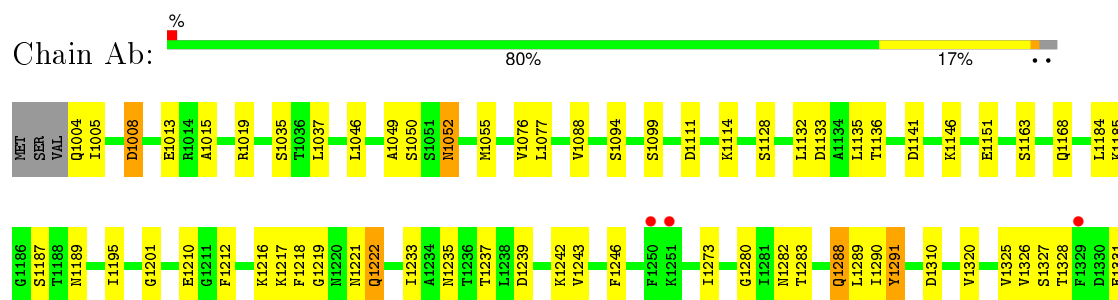


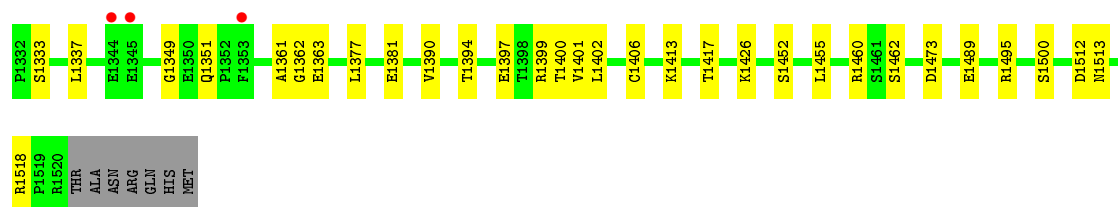


• Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA

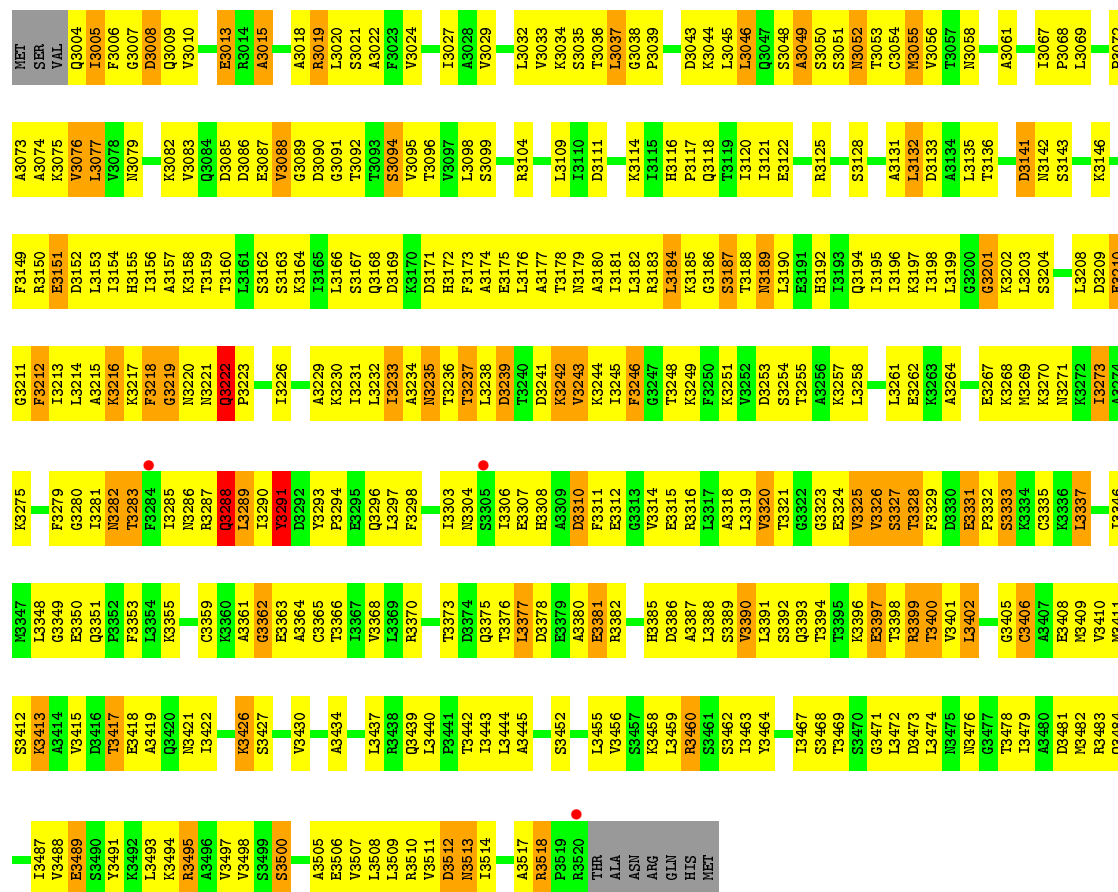


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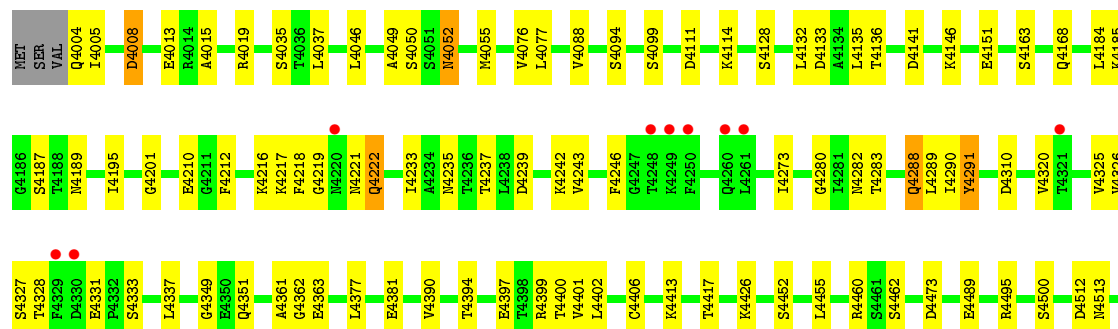
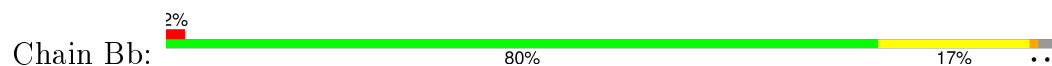




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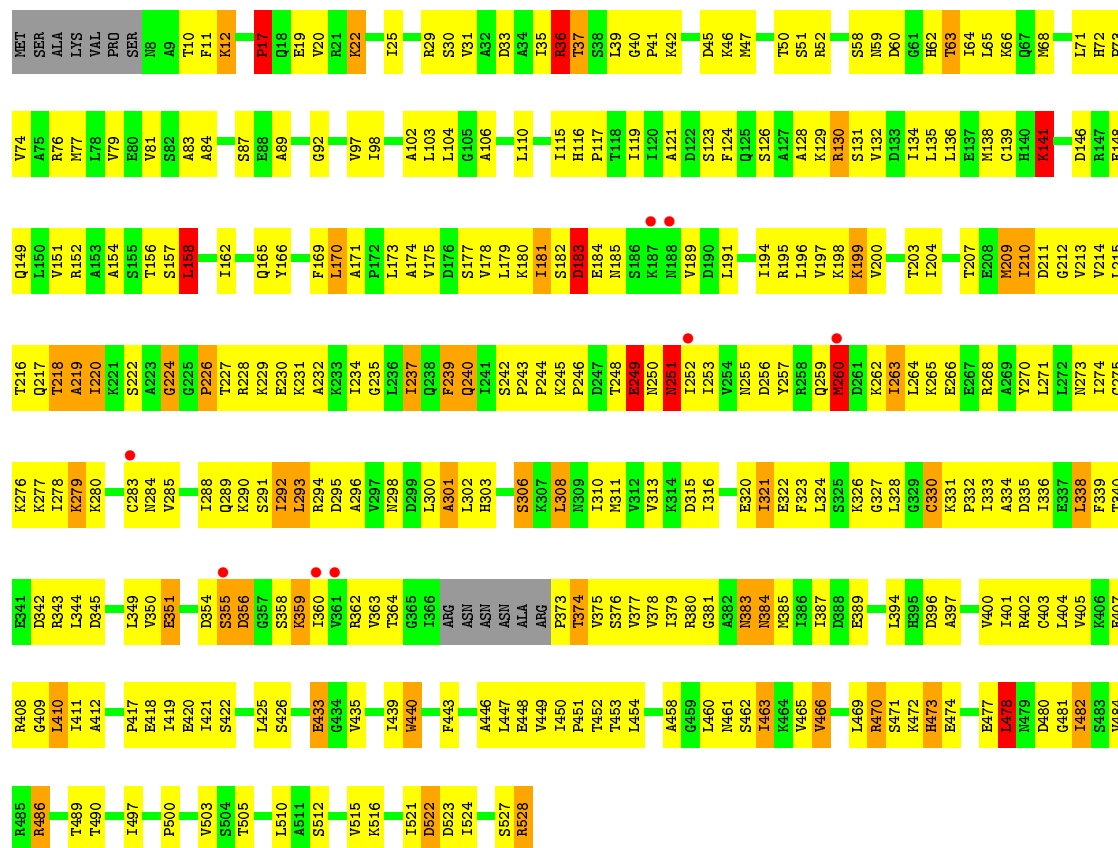
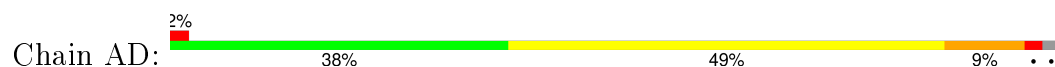


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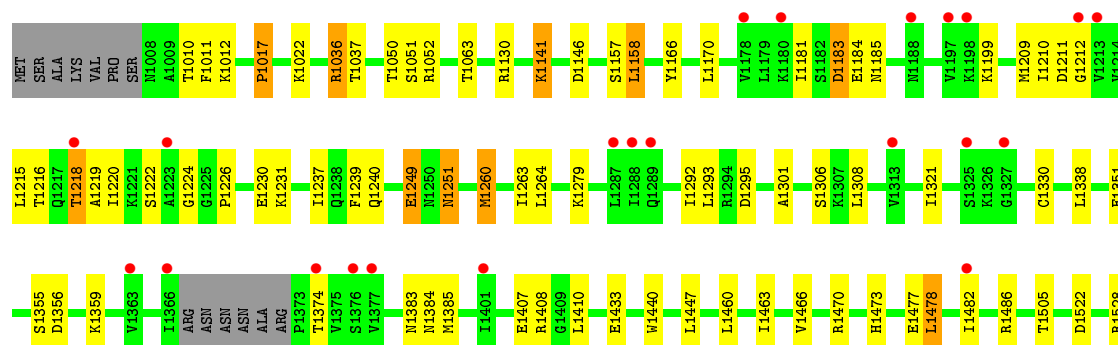
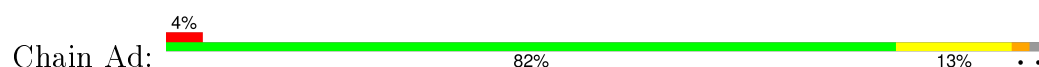




• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

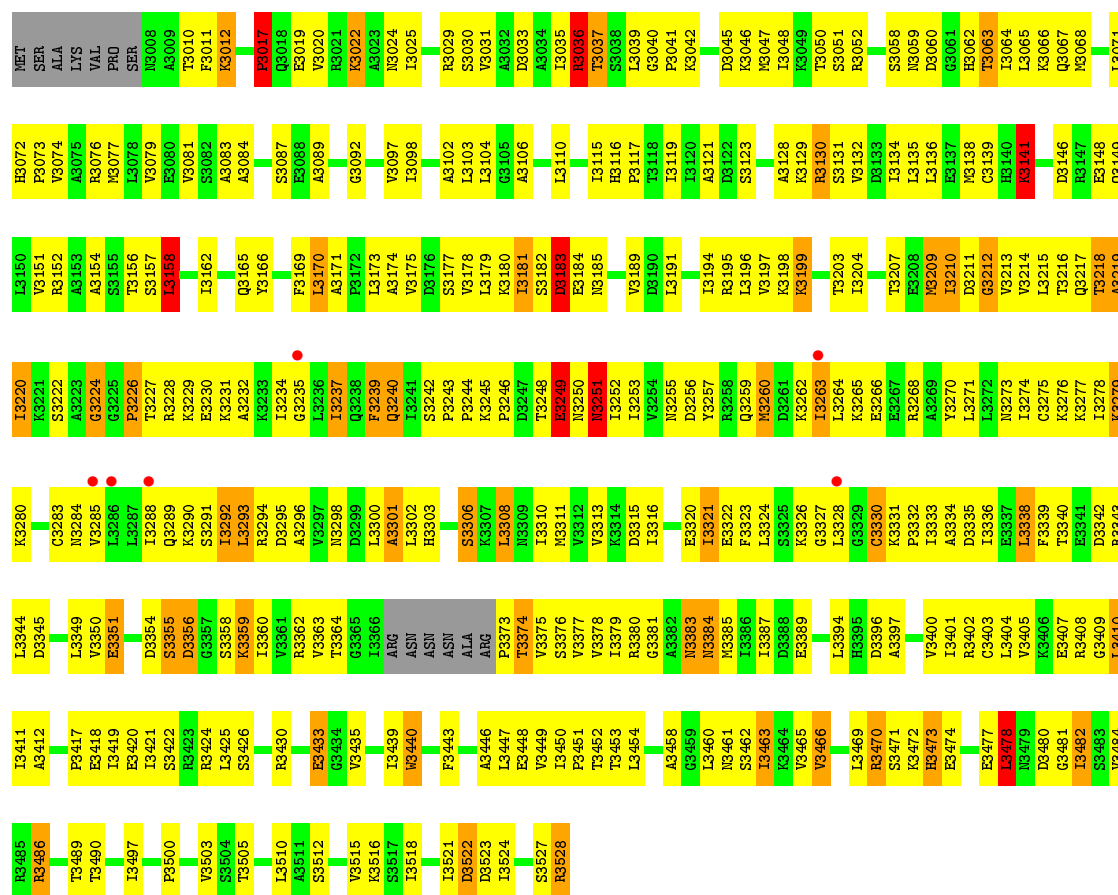


• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

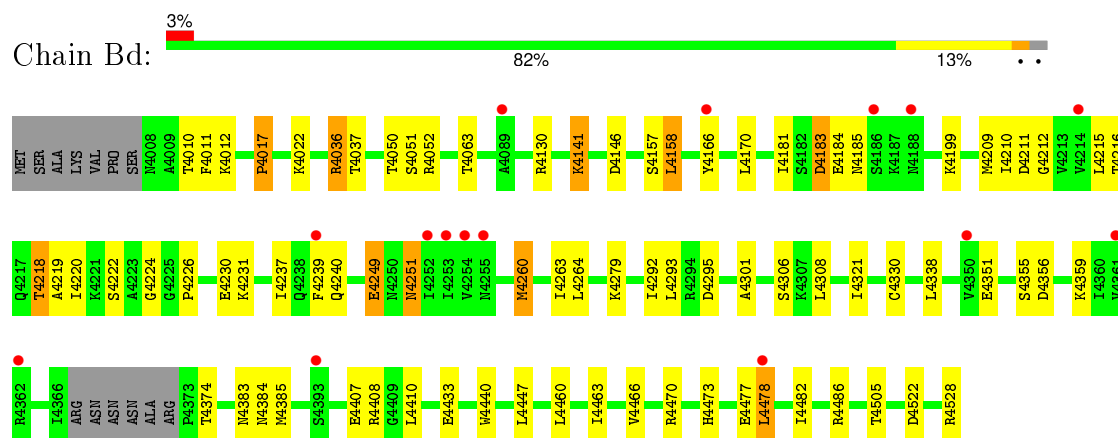


• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

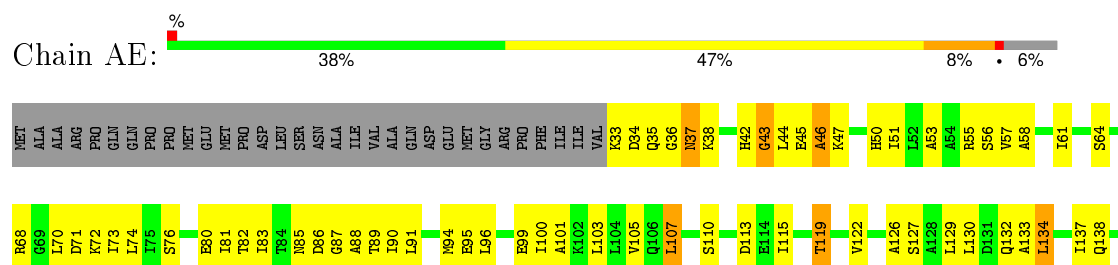




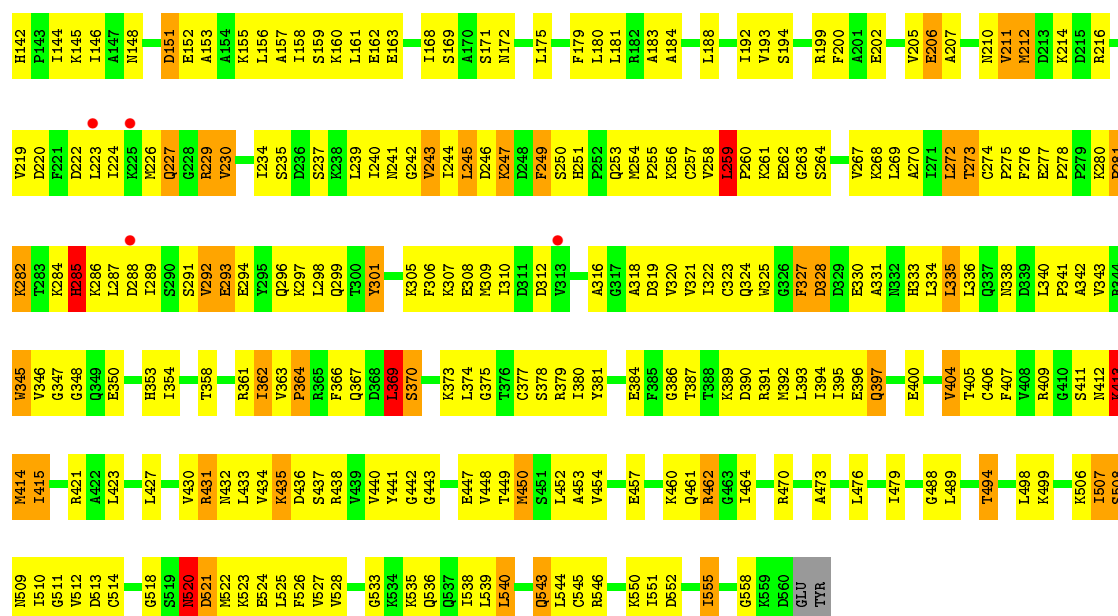
• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA



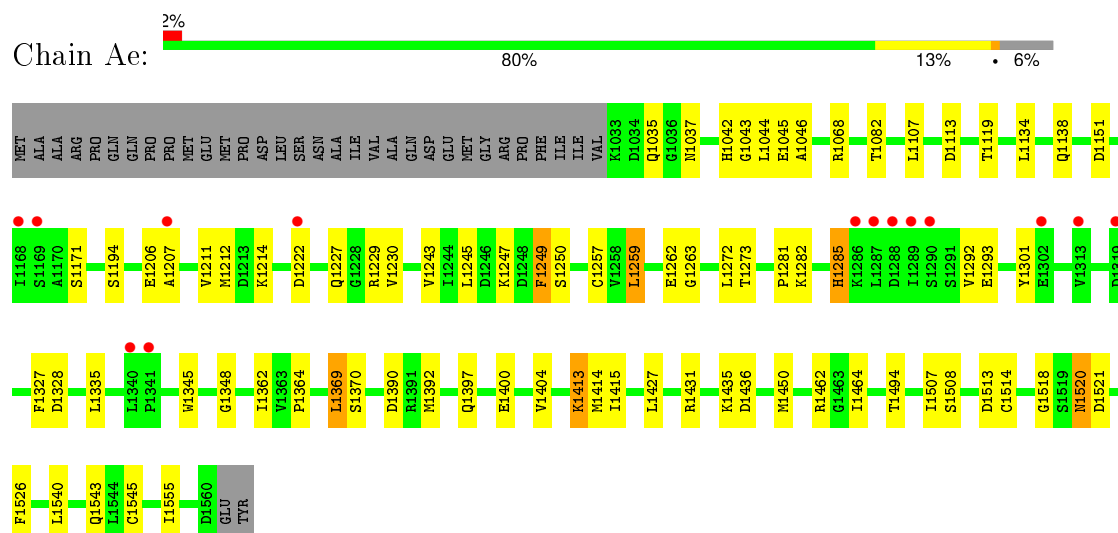
• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON



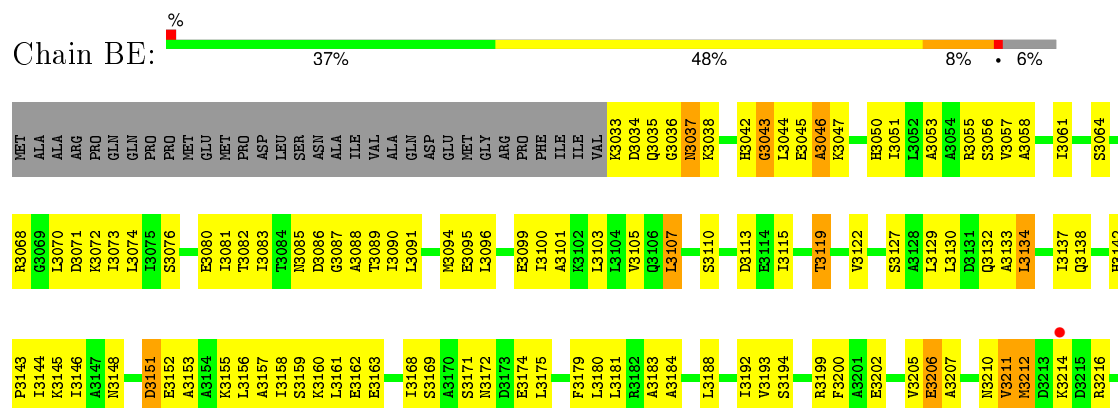


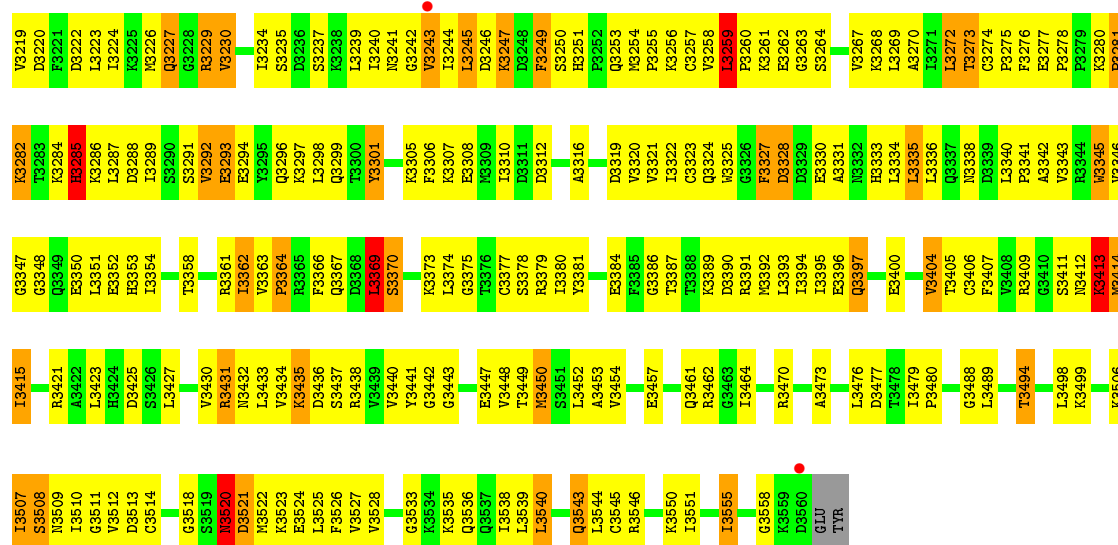


### • Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

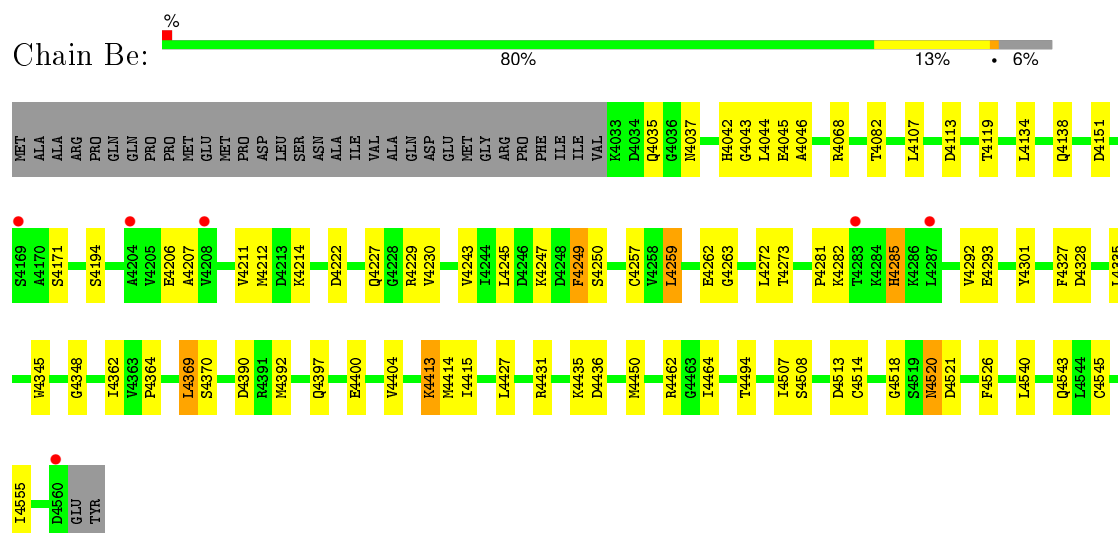


### • Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

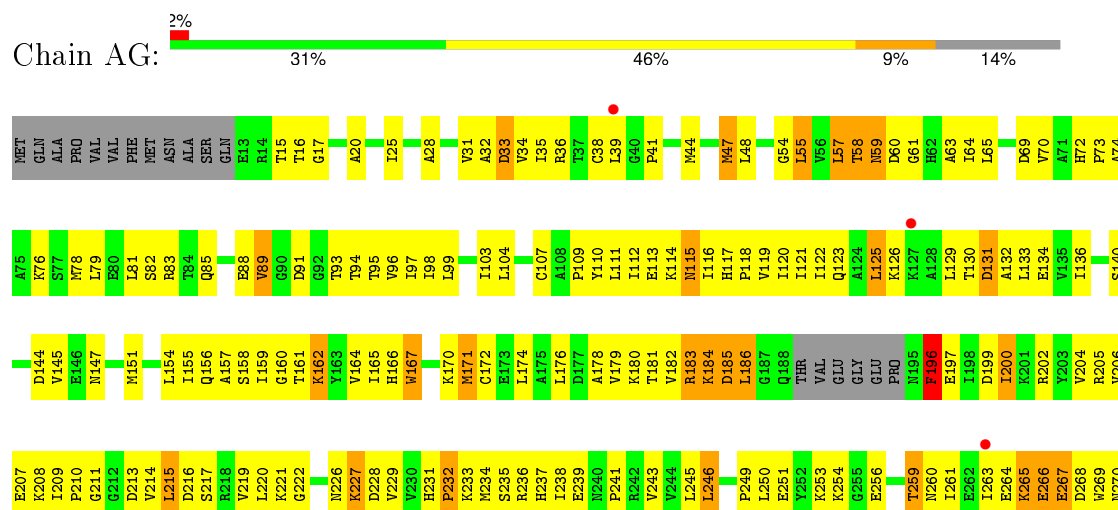


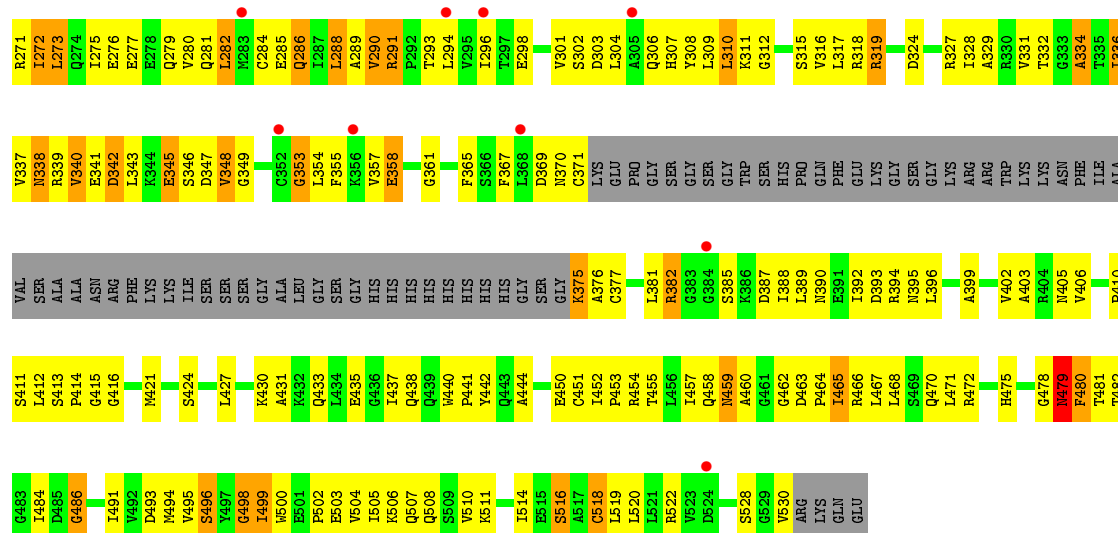


• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

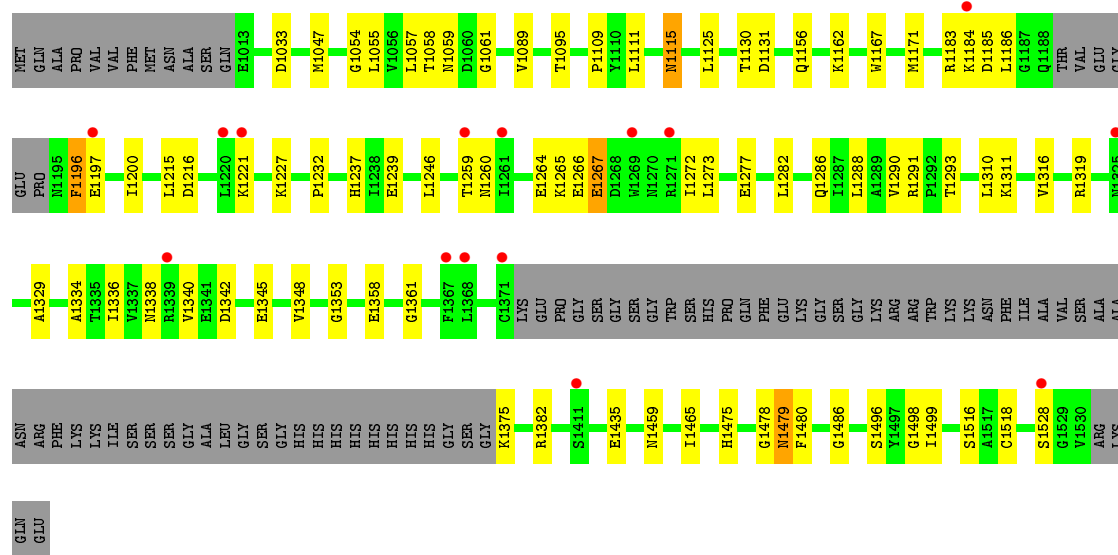
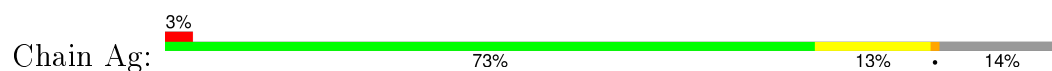


● Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

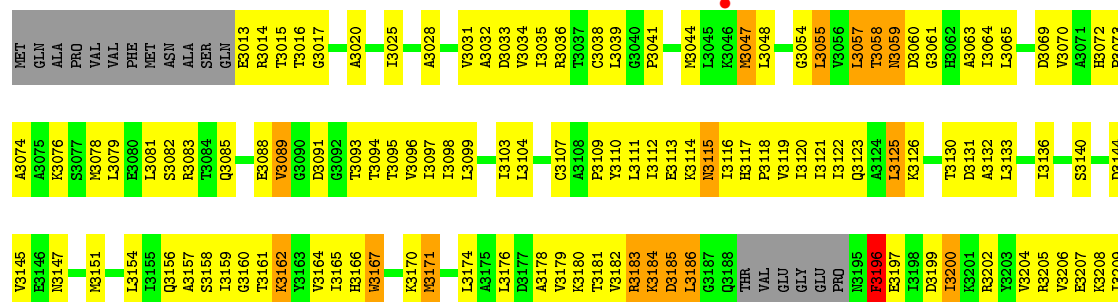


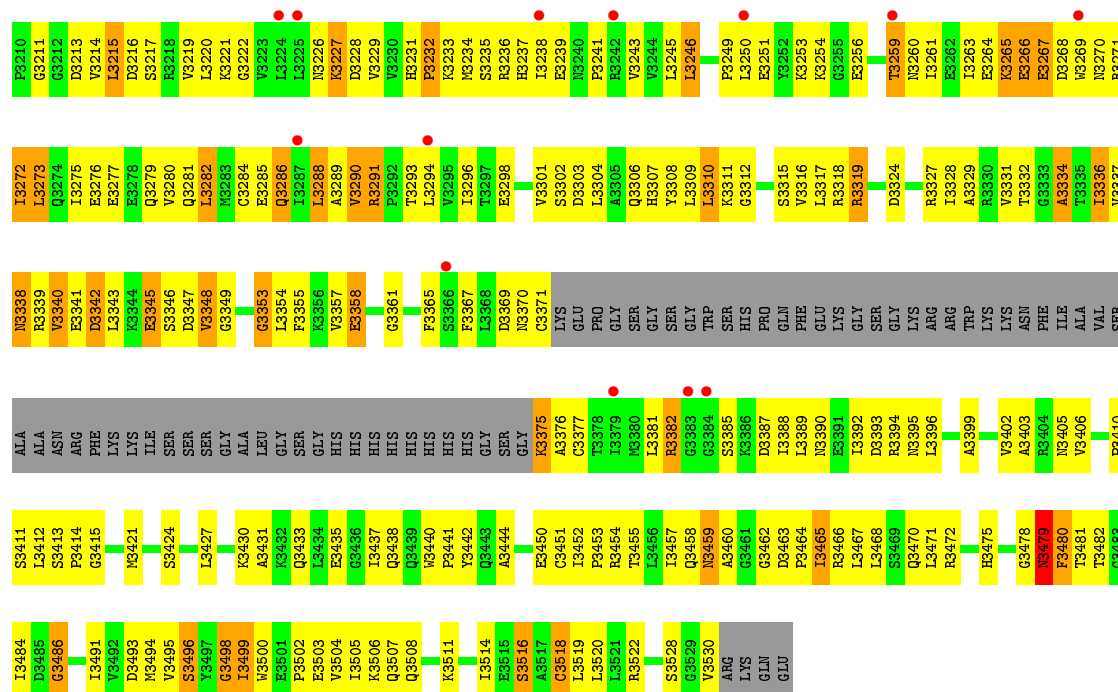


• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

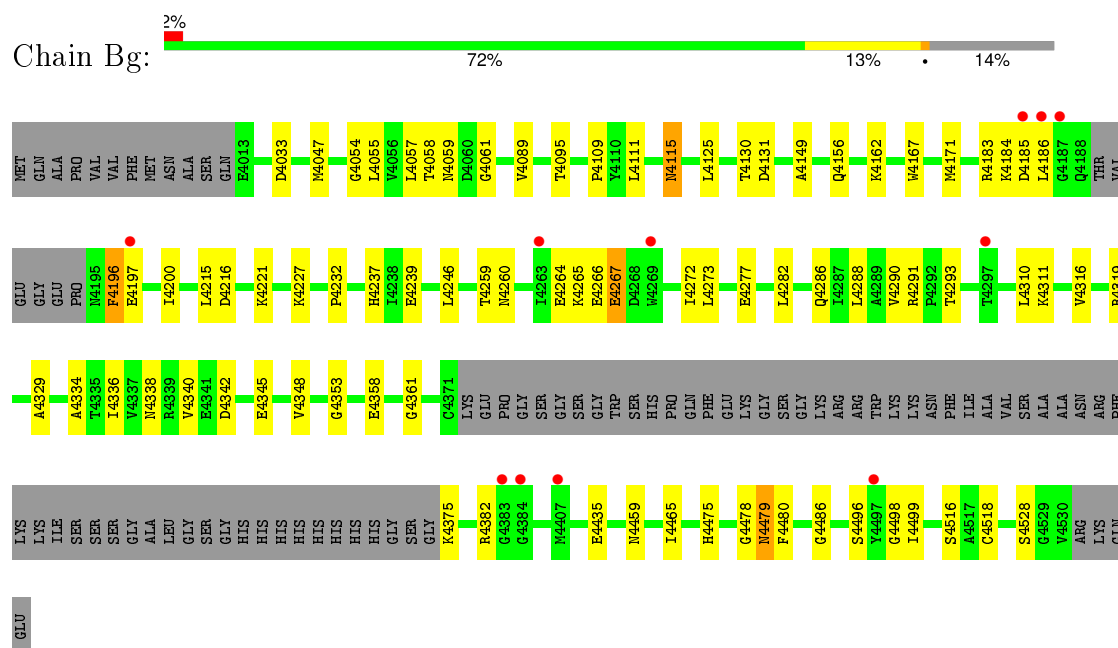


• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

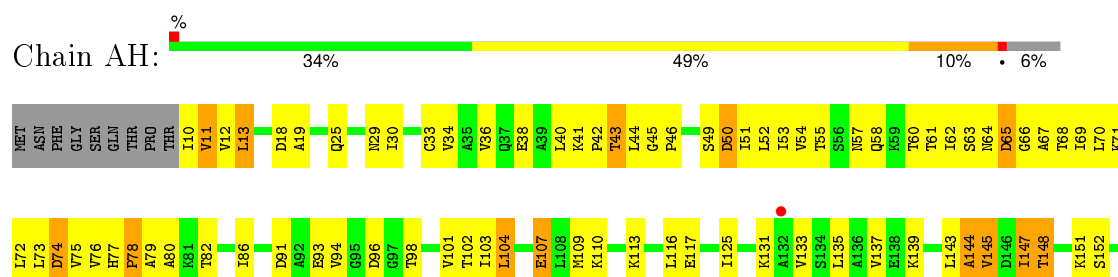




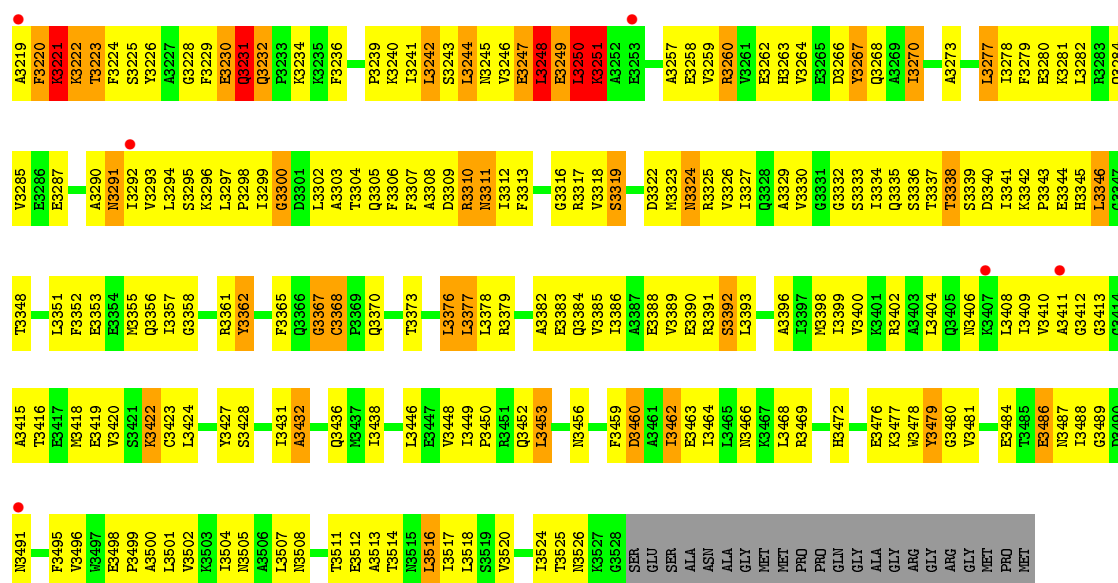
• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA



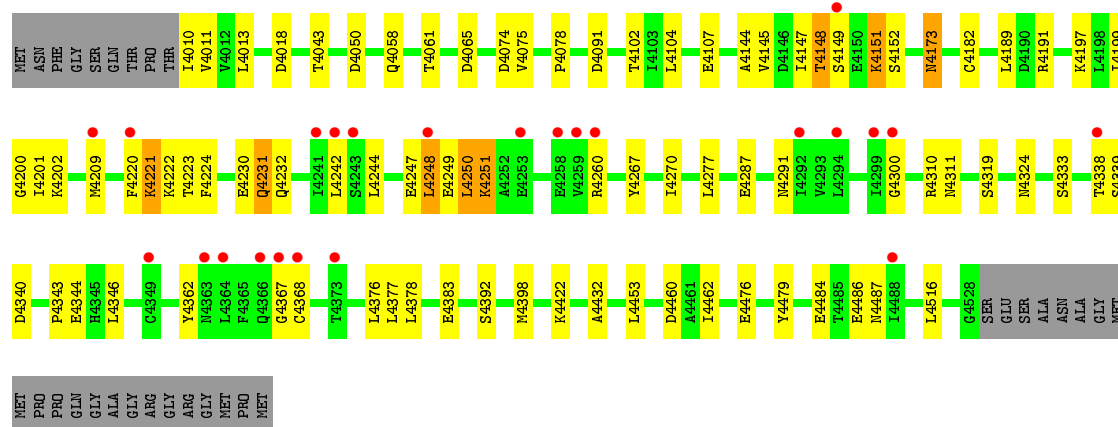
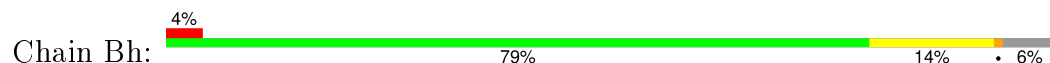
• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA



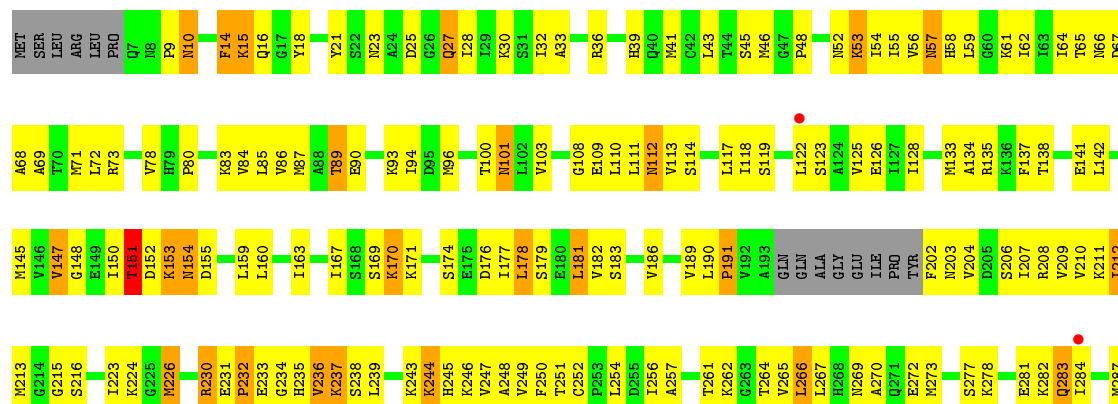


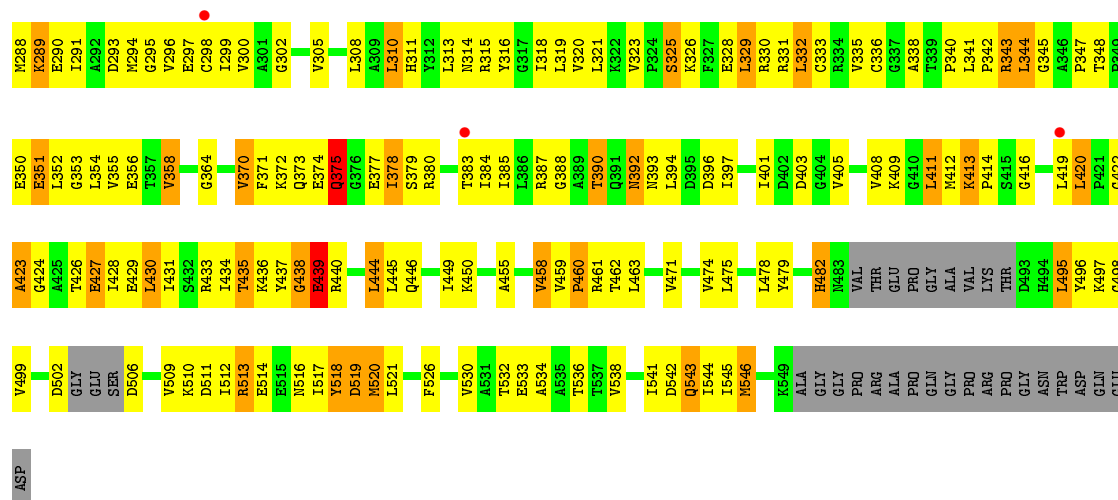


### • Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

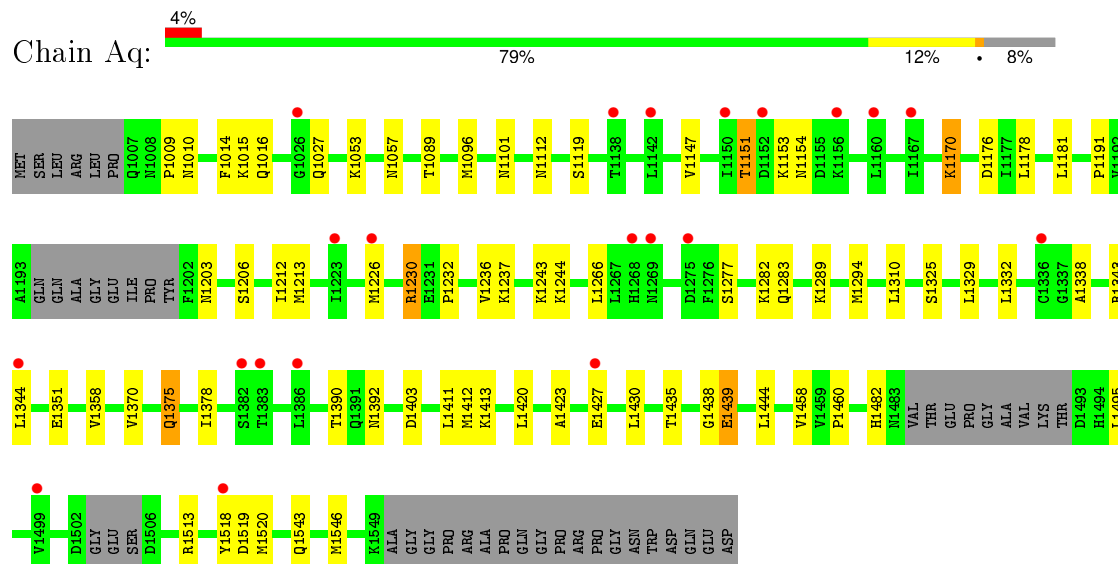


### • Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

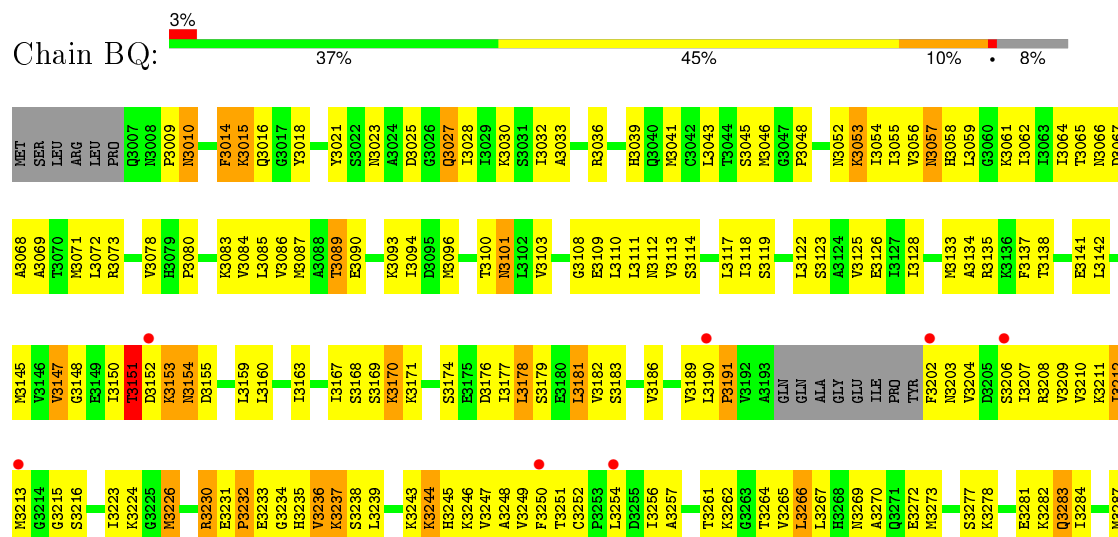


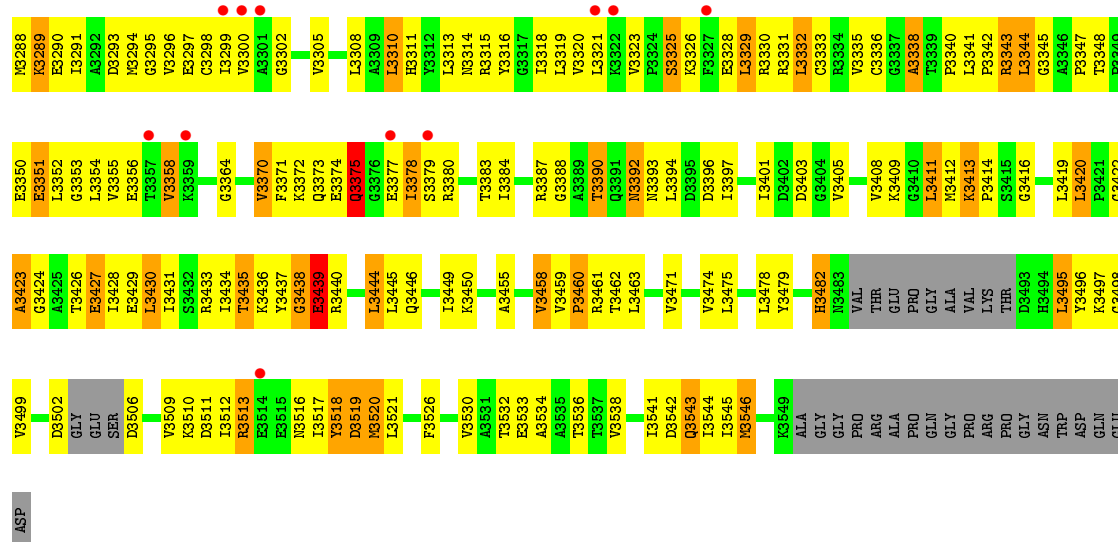


- Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

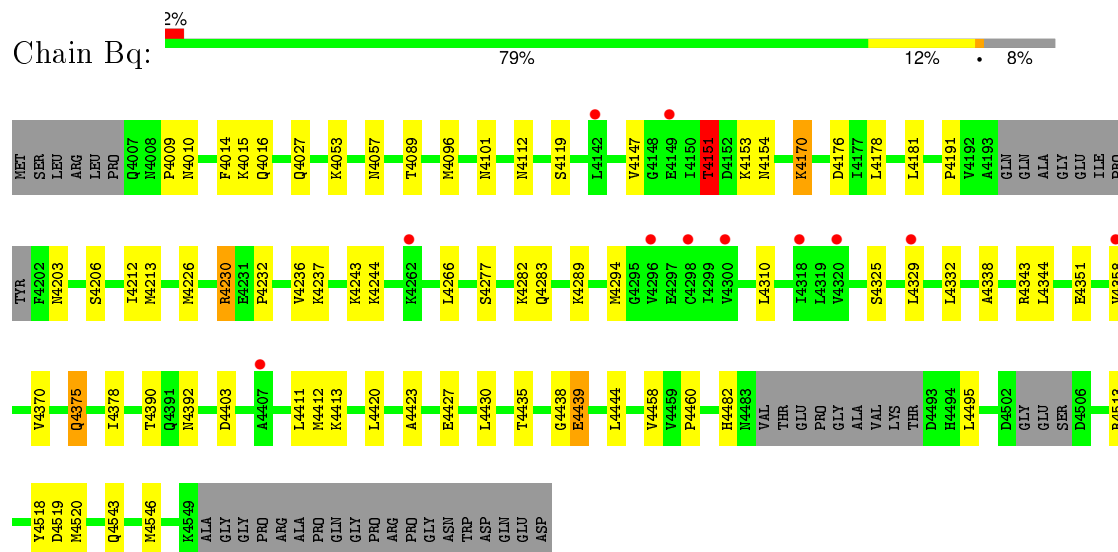


- Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

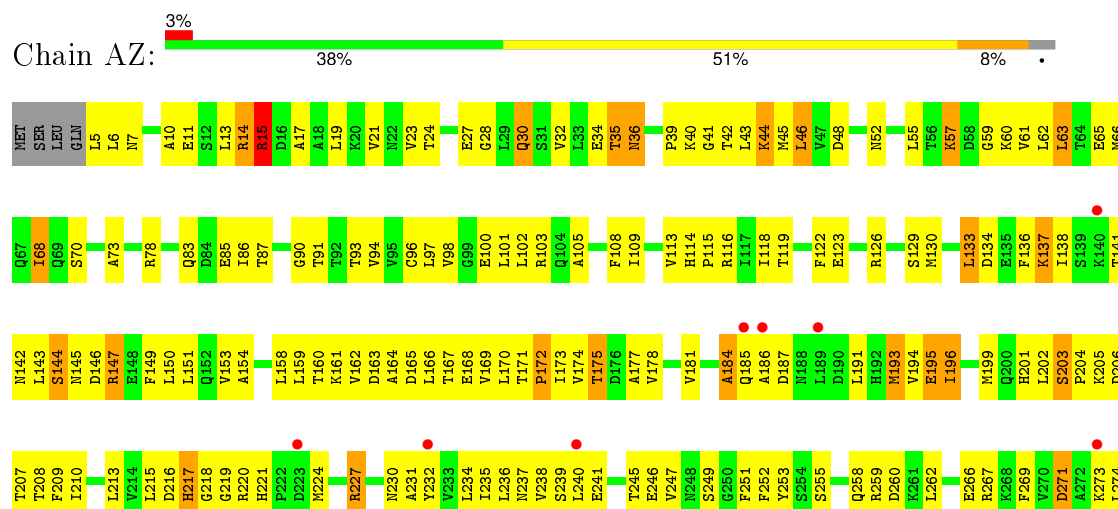




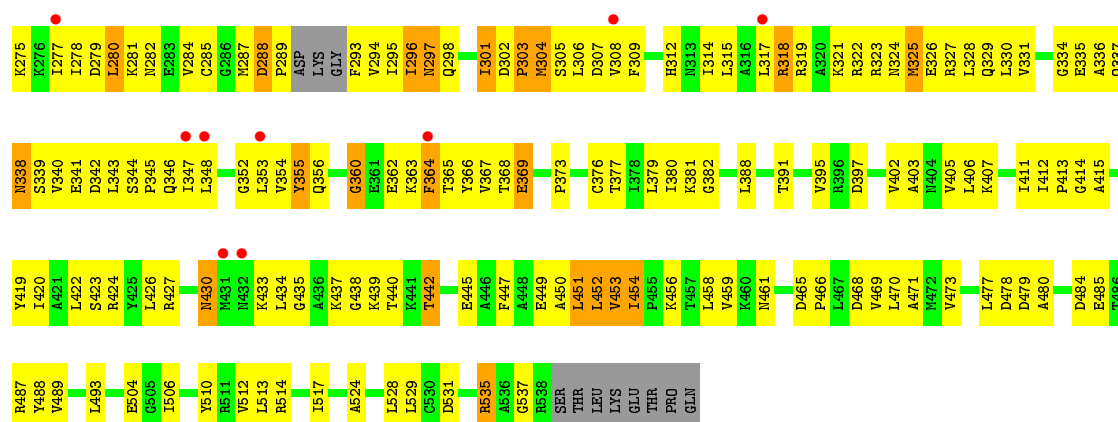
• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA



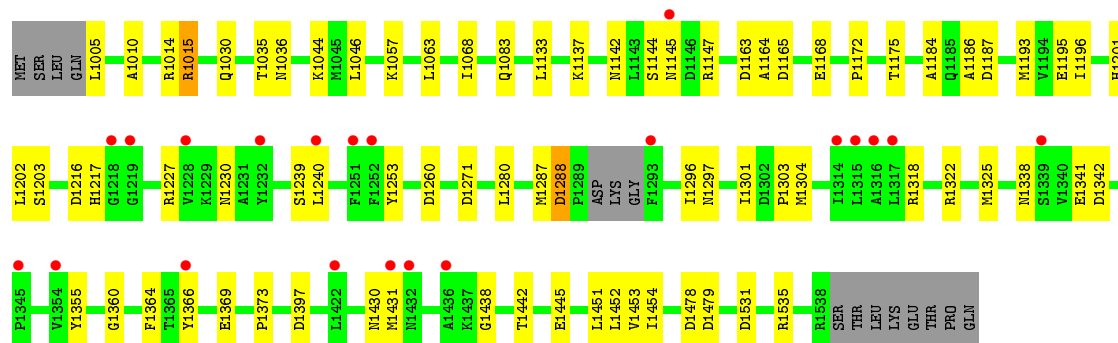
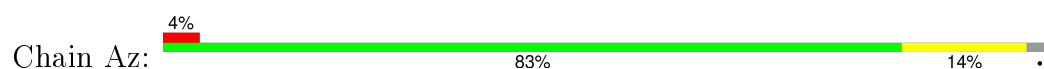
• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA



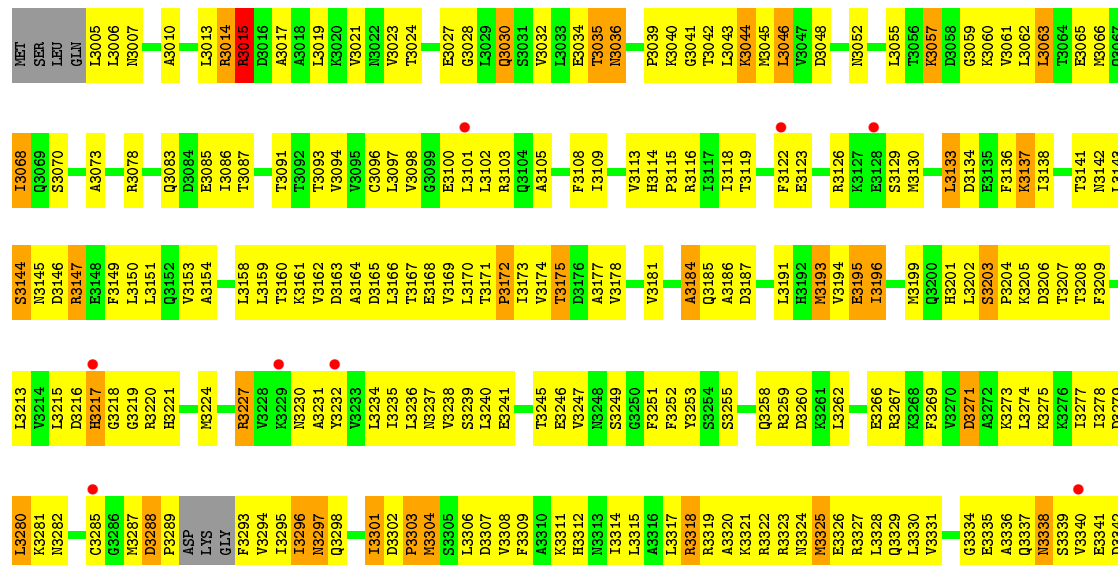


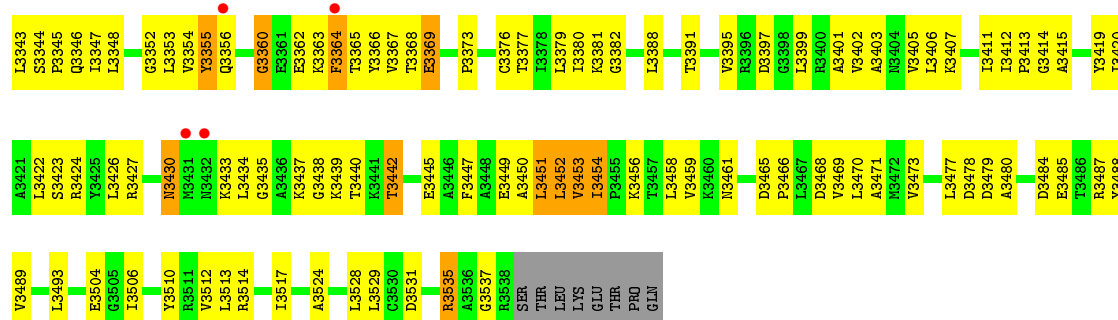


• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA

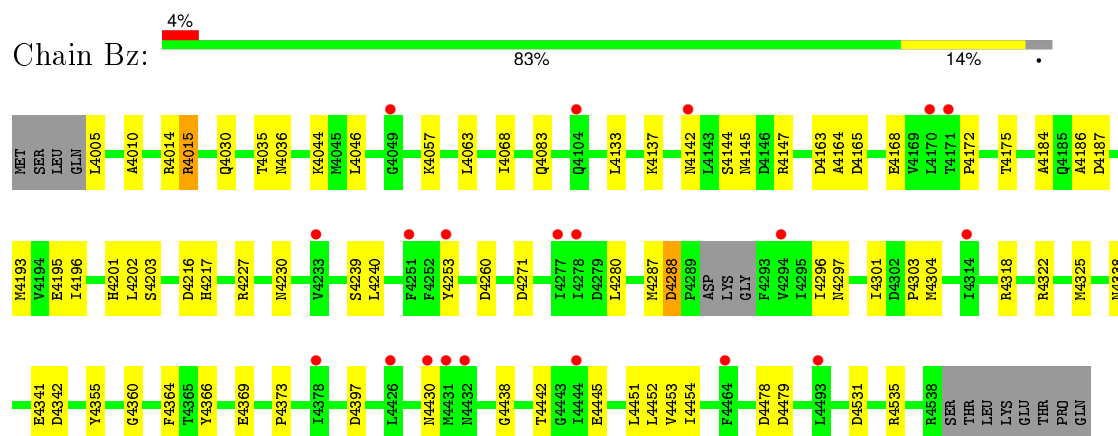


• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA





- Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17°	Depositor
Resolution (Å)	89.95 – 3.80 89.95 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.5 (89.95-3.80) 91.2 (89.95-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.78Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.248 , 0.284 0.248 , 0.281	Depositor DCC
$R_{free}$ test set	10483 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	112.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 121.3	EDS
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 209673 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	128780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.64	0/4095	0.78	2/5521 (0.0%)
1	Aa	0.64	0/4095	0.78	2/5521 (0.0%)
1	BA	0.64	0/4095	0.78	2/5521 (0.0%)
1	Ba	0.64	0/4095	0.78	2/5521 (0.0%)
2	AB	0.69	0/3966	0.80	1/5344 (0.0%)
2	Ab	0.69	0/3966	0.80	1/5344 (0.0%)
2	BB	0.69	0/3966	0.80	1/5344 (0.0%)
2	Bb	0.69	0/3966	0.80	1/5344 (0.0%)
3	AD	0.61	0/3974	0.77	1/5355 (0.0%)
3	Ad	0.61	0/3974	0.77	1/5355 (0.0%)
3	BD	0.61	0/3974	0.77	1/5355 (0.0%)
3	Bd	0.61	0/3974	0.77	1/5355 (0.0%)
4	AE	0.67	0/4117	0.78	2/5539 (0.0%)
4	Ae	0.67	0/4117	0.78	2/5539 (0.0%)
4	BE	0.67	0/4117	0.78	2/5539 (0.0%)
4	Be	0.67	0/4117	0.78	2/5539 (0.0%)
5	AG	0.60	0/3957	0.74	0/5340
5	Ag	0.60	0/3957	0.74	0/5340
5	BG	0.60	0/3957	0.74	0/5340
5	Bg	0.60	0/3957	0.74	0/5340
6	AH	0.66	1/4010 (0.0%)	0.78	2/5412 (0.0%)
6	Ah	0.66	1/4010 (0.0%)	0.78	2/5412 (0.0%)
6	BH	0.66	1/4010 (0.0%)	0.78	2/5412 (0.0%)
6	Bh	0.66	1/4010 (0.0%)	0.78	2/5412 (0.0%)
7	AQ	0.62	0/4025	0.75	1/5426 (0.0%)
7	Aq	0.62	0/4025	0.75	1/5426 (0.0%)
7	BQ	0.62	0/4025	0.75	1/5426 (0.0%)
7	Bq	0.62	0/4025	0.75	1/5426 (0.0%)
8	AZ	0.65	0/4140	0.72	0/5594
8	Az	0.65	0/4140	0.72	0/5594
8	BZ	0.65	0/4140	0.72	0/5594
8	Bz	94.13	3/4140 (0.1%)	1.43	3/5594 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	16.87	7/129136 (0.0%)	0.80	39/174124 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	AZ	0	1
8	Az	0	1
8	BZ	0	1
8	Bz	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Bz	4287	MET	CG-SD	4418.85	116.70	1.81
8	Bz	4287	MET	CB-CG	3613.95	117.16	1.51
8	Bz	4287	MET	SD-CE	2023.56	115.09	1.77
6	BH	3010	ILE	CA-CB	5.25	1.67	1.54
6	AH	10	ILE	CA-CB	5.25	1.67	1.54
6	Bh	4010	ILE	CA-CB	5.25	1.67	1.54
6	Ah	1010	ILE	CA-CB	5.24	1.67	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Bz	4287	MET	CG-SD-CE	-61.94	1.09	100.20
8	Bz	4287	MET	CA-CB-CG	-57.26	15.96	113.30
8	Bz	4287	MET	CB-CG-SD	-37.01	1.38	112.40
3	BD	3017	PRO	N-CA-C	-7.14	93.54	112.10
3	AD	17	PRO	N-CA-C	-7.14	93.55	112.10
3	Ad	1017	PRO	N-CA-C	-7.13	93.56	112.10
3	Bd	4017	PRO	N-CA-C	-7.12	93.58	112.10
6	AH	231	GLN	N-CA-C	-7.04	91.98	111.00
6	Ah	1231	GLN	N-CA-C	-7.04	92.00	111.00
6	BH	3231	GLN	N-CA-C	-7.03	92.01	111.00
6	Bh	4231	GLN	N-CA-C	-7.03	92.02	111.00
1	BA	3073	LEU	CA-CB-CG	5.95	128.99	115.30
1	Aa	1073	LEU	CA-CB-CG	5.95	128.98	115.30
1	AA	73	LEU	CA-CB-CG	5.94	128.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ba	4073	LEU	CA-CB-CG	5.94	128.97	115.30
4	BE	3043	GLY	N-CA-C	5.56	127.00	113.10
4	AE	43	GLY	N-CA-C	5.55	126.97	113.10
4	Ae	1043	GLY	N-CA-C	5.55	126.97	113.10
4	Be	4043	GLY	N-CA-C	5.53	126.93	113.10
6	BH	3244	LEU	CA-CB-CG	5.45	127.83	115.30
6	AH	244	LEU	CA-CB-CG	5.44	127.81	115.30
6	Bh	4244	LEU	CA-CB-CG	5.44	127.81	115.30
6	Ah	1244	LEU	CA-CB-CG	5.43	127.80	115.30
2	Bb	4402	LEU	CB-CG-CD2	-5.29	102.01	111.00
2	AB	402	LEU	CB-CG-CD2	-5.28	102.02	111.00
2	Ab	1402	LEU	CB-CG-CD2	-5.28	102.02	111.00
4	BE	3259	LEU	CA-CB-CG	5.28	127.44	115.30
4	Ae	1259	LEU	CA-CB-CG	5.27	127.43	115.30
4	AE	259	LEU	CA-CB-CG	5.26	127.40	115.30
2	BB	3402	LEU	CB-CG-CD2	-5.26	102.06	111.00
4	Be	4259	LEU	CA-CB-CG	5.26	127.40	115.30
1	AA	539	LEU	CA-CB-CG	5.24	127.35	115.30
1	BA	3539	LEU	CA-CB-CG	5.24	127.35	115.30
1	Aa	1539	LEU	CA-CB-CG	5.23	127.34	115.30
1	Ba	4539	LEU	CA-CB-CG	5.23	127.34	115.30
7	AQ	15	LYS	CD-CE-NZ	5.08	123.38	111.70
7	Aq	1015	LYS	CD-CE-NZ	5.08	123.38	111.70
7	Bq	4015	LYS	CD-CE-NZ	5.08	123.38	111.70
7	BQ	3015	LYS	CD-CE-NZ	5.06	123.33	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	AZ	366	TYR	Sidechain
8	Az	1366	TYR	Sidechain
8	BZ	3366	TYR	Sidechain
8	Bz	4366	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	4060	0	4220	345	0
1	Aa	4060	0	4220	0	0
1	BA	4060	0	4220	343	0
1	Ba	4060	0	4220	0	0
2	AB	3927	0	4030	361	0
2	Ab	3927	0	4030	0	0
2	BB	3927	0	4030	353	0
2	Bb	3927	0	4030	0	0
3	AD	3938	0	4109	292	0
3	Ad	3938	0	4109	0	0
3	BD	3938	0	4109	294	0
3	Bd	3938	0	4109	0	0
4	AE	4068	0	4163	363	5
4	Ae	4068	0	4163	0	0
4	BE	4068	0	4163	359	2
4	Be	4068	0	4163	0	0
5	AG	3914	0	4057	297	0
5	Ag	3914	0	4057	0	0
5	BG	3914	0	4057	295	0
5	Bg	3914	0	4057	0	1
6	AH	3962	0	4045	357	0
6	Ah	3962	0	4045	0	1
6	BH	3962	0	4045	351	0
6	Bh	3962	0	4045	0	5
7	AQ	3981	0	4120	319	1
7	Aq	3981	0	4120	0	0
7	BQ	3981	0	4120	319	0
7	Bq	3981	0	4120	0	2
8	AZ	4089	0	4183	307	0
8	Az	4089	0	4183	0	1
8	BZ	4089	0	4183	302	0
8	Bz	4089	0	4183	0	0
9	AA	27	0	12	1	0
9	AB	27	0	12	2	0
9	AD	27	0	12	4	0
9	AE	27	0	12	2	0
9	AG	27	0	12	2	0
9	AH	27	0	12	0	0
9	AQ	27	0	12	1	0
9	AZ	27	0	12	3	0
9	Aa	27	0	12	0	0
9	Ab	27	0	12	0	0
9	Ad	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Ae	27	0	12	0	0
9	Ag	27	0	12	0	0
9	Ah	27	0	12	0	0
9	Aq	27	0	12	0	0
9	Az	27	0	12	0	0
9	BA	27	0	12	1	0
9	BB	27	0	12	2	0
9	BD	27	0	12	4	0
9	BE	27	0	12	2	0
9	BG	27	0	12	2	0
9	BH	27	0	12	0	0
9	BQ	27	0	12	1	0
9	BZ	27	0	12	2	0
9	Ba	27	0	12	0	0
9	Bb	27	0	12	0	0
9	Bd	27	0	12	0	0
9	Be	27	0	12	0	0
9	Bg	27	0	12	0	0
9	Bh	27	0	12	0	0
9	Bq	27	0	12	0	0
9	Bz	27	0	12	0	0
10	AA	4	0	0	0	0
10	AB	4	0	0	0	0
10	AD	4	0	0	0	0
10	AE	4	0	0	0	0
10	AG	4	0	0	2	0
10	AH	4	0	0	0	0
10	AQ	4	0	0	0	0
10	AZ	4	0	0	0	0
10	Aa	4	0	0	0	0
10	Ab	4	0	0	0	0
10	Ad	4	0	0	0	0
10	Ae	4	0	0	0	0
10	Ag	4	0	0	0	0
10	Ah	4	0	0	0	0
10	Aq	4	0	0	0	0
10	Az	4	0	0	0	0
10	BA	4	0	0	0	0
10	BB	4	0	0	0	0
10	BD	4	0	0	0	0
10	BE	4	0	0	0	0
10	BG	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BH	4	0	0	0	0
10	BQ	4	0	0	0	0
10	BZ	4	0	0	0	0
10	Ba	4	0	0	0	0
10	Bb	4	0	0	0	0
10	Bd	4	0	0	0	0
10	Be	4	0	0	0	0
10	Bg	4	0	0	0	0
10	Bh	4	0	0	0	0
10	Bq	4	0	0	0	0
10	Bz	4	0	0	0	0
11	AA	1	0	0	0	0
11	AB	1	0	0	0	0
11	AD	1	0	0	0	0
11	AE	1	0	0	0	0
11	AG	1	0	0	0	0
11	AH	1	0	0	0	0
11	AQ	1	0	0	0	0
11	AZ	1	0	0	0	0
11	Aa	1	0	0	0	0
11	Ab	1	0	0	0	0
11	Ad	1	0	0	0	0
11	Ae	1	0	0	0	0
11	Ag	1	0	0	0	0
11	Ah	1	0	0	0	0
11	Aq	1	0	0	0	0
11	Az	1	0	0	0	0
11	BA	1	0	0	0	0
11	BB	1	0	0	0	0
11	BD	1	0	0	0	0
11	BE	1	0	0	0	0
11	BG	1	0	0	0	0
11	BH	1	0	0	0	0
11	BQ	1	0	0	0	0
11	BZ	1	0	0	0	0
11	Ba	1	0	0	0	0
11	Bb	1	0	0	0	0
11	Bd	1	0	0	0	0
11	Be	1	0	0	0	0
11	Bg	1	0	0	0	0
11	Bh	1	0	0	0	0
11	Bq	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Bz	1	0	0	0	0
All	All	128780	0	132092	4783	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (4783) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:3413:LYS:HE3	4:BE:3413:LYS:H	1.17	1.09
7:BQ:3257:ALA:HB2	7:BQ:3343:ARG:HH22	1.18	1.08
3:AD:141:LYS:HA	3:AD:409:GLY:HA2	1.39	1.05
7:AQ:257:ALA:HB2	7:AQ:343:ARG:HH22	1.18	1.03
4:AE:413:LYS:HE3	4:AE:413:LYS:H	1.17	1.03
1:BA:3162:THR:HG21	1:BA:3517:VAL:HA	1.40	1.01
3:BD:3141:LYS:HA	3:BD:3409:GLY:HA2	1.39	1.00
1:AA:162:THR:HG21	1:AA:517:VAL:HA	1.40	0.99
3:AD:265:LYS:HA	3:AD:268:ARG:HD3	1.43	0.98
8:AZ:207:THR:HG22	8:AZ:381:LYS:H	1.28	0.98
3:BD:3265:LYS:HA	3:BD:3268:ARG:HD3	1.43	0.97
7:BQ:3513:ARG:HA	7:BQ:3513:ARG:HH11	1.28	0.97
2:BB:3273:ILE:HG21	2:BB:3297:LEU:HD13	1.47	0.96
2:AB:273:ILE:HG21	2:AB:297:LEU:HD13	1.47	0.96
8:BZ:3013:LEU:HD13	8:BZ:3021:VAL:HG21	1.48	0.96
7:AQ:513:ARG:HH11	7:AQ:513:ARG:HA	1.28	0.96
8:BZ:3207:THR:HG22	8:BZ:3381:LYS:H	1.27	0.95
3:AD:338:LEU:HD22	3:AD:343:ARG:HH22	1.30	0.95
2:AB:197:LYS:HD3	2:AB:377:LEU:HB3	1.48	0.94
7:BQ:3356:GLU:HB2	7:BQ:3373:GLN:HA	1.49	0.94
7:BQ:3256:ILE:HG21	8:BZ:3259:ARG:HD3	1.50	0.94
2:BB:3197:LYS:HD3	2:BB:3377:LEU:HB3	1.48	0.94
7:BQ:3151:THR:HG23	7:BQ:3153:LYS:HB2	1.48	0.94
7:AQ:256:ILE:HG21	8:AZ:259:ARG:HD3	1.50	0.94
3:BD:3338:LEU:HD22	3:BD:3343:ARG:HH22	1.30	0.93
2:BB:3230:LYS:H	2:BB:3282:ASN:HD21	1.16	0.93
7:AQ:151:THR:HG23	7:AQ:153:LYS:HB2	1.48	0.93
5:AG:58:THR:HG23	5:AG:60:ASP:H	1.35	0.92
3:AD:229:LYS:HD2	3:AD:284:ASN:HD21	1.33	0.92
3:BD:3229:LYS:HD2	3:BD:3284:ASN:HD21	1.33	0.92
4:BE:3180:LEU:HD12	4:BE:3205:VAL:HG13	1.52	0.92
2:AB:159:THR:HG21	2:AB:487:ILE:HA	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:179:MET:HG3	1:AA:218:LEU:HD12	1.50	0.91
8:AZ:13:LEU:HD13	8:AZ:21:VAL:HG21	1.48	0.91
1:BA:3179:MET:HG3	1:BA:3218:LEU:HD12	1.50	0.91
7:AQ:356:GLU:HB2	7:AQ:373:GLN:HA	1.49	0.91
4:BE:3181:LEU:HD11	4:BE:3202:GLU:HG2	1.51	0.90
2:BB:3159:THR:HG21	2:BB:3487:ILE:HA	1.52	0.90
4:AE:180:LEU:HD12	4:AE:205:VAL:HG13	1.52	0.90
4:AE:181:LEU:HD11	4:AE:202:GLU:HG2	1.51	0.90
1:AA:487:ALA:HB1	1:AA:493:LYS:HA	1.53	0.90
2:AB:230:LYS:H	2:AB:282:ASN:HD21	1.16	0.90
1:BA:3487:ALA:HB1	1:BA:3493:LYS:HA	1.53	0.90
6:BH:3250:LEU:HA	6:BH:3278:ILE:HG12	1.54	0.89
6:BH:3054:VAL:HG22	6:BH:3060:THR:HG23	1.53	0.89
2:BB:3402:LEU:HD21	2:BB:3483:ARG:HB2	1.53	0.89
4:AE:161:LEU:HB2	4:AE:450:MET:HE1	1.52	0.89
1:AA:327:ARG:HA	1:AA:337:LEU:HD11	1.55	0.89
1:BA:3327:ARG:HA	1:BA:3337:LEU:HD11	1.55	0.89
4:BE:3161:LEU:HB2	4:BE:3450:MET:HE1	1.53	0.89
5:AG:41:PRO:HG3	5:AG:486:GLY:HA3	1.53	0.89
8:BZ:3129:SER:HA	8:BZ:3422:LEU:HD21	1.55	0.89
5:BG:3041:PRO:HG3	5:BG:3486:GLY:HA3	1.53	0.88
5:BG:3058:THR:HG23	5:BG:3060:ASP:H	1.35	0.88
6:AH:54:VAL:HG22	6:AH:60:THR:HG23	1.54	0.88
6:AH:250:LEU:HA	6:AH:278:ILE:HG12	1.54	0.88
3:BD:3290:LYS:HB2	3:BD:3315:ASP:HA	1.56	0.88
1:BA:3109:LEU:HD11	1:BA:3538:ILE:HG21	1.54	0.88
8:BZ:3102:LEU:HD22	8:BZ:3528:LEU:HD21	1.54	0.88
4:AE:72:LYS:HD2	4:AE:90:ILE:HD13	1.56	0.88
8:BZ:3430:ASN:HA	8:BZ:3433:LYS:HB3	1.54	0.88
1:AA:140:ILE:HD11	1:AA:429:LEU:HD11	1.55	0.88
3:BD:3065:LEU:HB3	3:BD:3079:VAL:HG22	1.54	0.88
2:AB:402:LEU:HD21	2:AB:483:ARG:HB2	1.53	0.87
8:AZ:102:LEU:HD22	8:AZ:528:LEU:HD21	1.54	0.87
8:AZ:430:ASN:HA	8:AZ:433:LYS:HB3	1.54	0.87
6:BH:3260:ARG:HH11	6:BH:3260:ARG:HB3	1.38	0.87
2:AB:98:LEU:HD21	2:AB:437:LEU:HD12	1.57	0.87
2:AB:233:ILE:H	2:AB:233:ILE:HD13	1.37	0.87
3:AD:65:LEU:HB3	3:AD:79:VAL:HG22	1.54	0.87
2:AB:242:LYS:HB3	2:AB:245:ILE:HD11	1.56	0.87
3:AD:156:THR:HG21	3:AD:497:ILE:HA	1.57	0.87
2:AB:230:LYS:H	2:AB:282:ASN:ND2	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:329:ILE:HD12	1:AA:374:ILE:HD12	1.57	0.87
8:AZ:452:LEU:HD22	8:AZ:470:LEU:HD11	1.56	0.86
8:AZ:129:SER:HA	8:AZ:422:LEU:HD21	1.55	0.86
3:BD:3156:THR:HG21	3:BD:3497:ILE:HA	1.57	0.86
2:BB:3242:LYS:HB3	2:BB:3245:ILE:HD11	1.56	0.86
2:BB:3233:ILE:H	2:BB:3233:ILE:HD13	1.37	0.86
1:AA:109:LEU:HD11	1:AA:538:ILE:HG21	1.55	0.86
2:BB:3230:LYS:H	2:BB:3282:ASN:ND2	1.73	0.86
2:AB:249:LYS:HD3	4:AE:286:LYS:HG3	1.56	0.86
4:AE:172:ASN:HB3	4:AE:175:LEU:HB3	1.57	0.86
4:AE:33:LYS:HB2	6:AH:76:VAL:HG23	1.56	0.86
4:BE:3033:LYS:HB2	6:BH:3076:VAL:HG23	1.56	0.86
8:BZ:3452:LEU:HD22	8:BZ:3470:LEU:HD11	1.56	0.86
1:BA:3140:ILE:HD11	1:BA:3429:LEU:HD11	1.55	0.86
1:AA:506:ARG:HD3	1:AA:508:LYS:HE2	1.58	0.86
6:AH:260:ARG:HB3	6:AH:260:ARG:HH11	1.38	0.86
1:BA:3329:ILE:HD12	1:BA:3374:ILE:HD12	1.57	0.86
6:BH:3068:THR:HG21	6:BH:3391:ARG:HD2	1.57	0.86
3:AD:290:LYS:HB2	3:AD:315:ASP:HA	1.56	0.85
1:AA:545:ILE:HD13	3:AD:68:MET:HG3	1.58	0.85
8:BZ:3043:LEU:HD11	8:BZ:3055:LEU:HB3	1.57	0.85
2:BB:3249:LYS:HD3	4:BE:3286:LYS:HG3	1.56	0.85
6:AH:68:THR:HG21	6:AH:391:ARG:HD2	1.57	0.85
2:BB:3098:LEU:HD21	2:BB:3437:LEU:HD12	1.56	0.85
8:AZ:271:ASP:HA	8:AZ:274:LEU:HB3	1.57	0.85
4:BE:3072:LYS:HD2	4:BE:3090:ILE:HD13	1.56	0.85
8:AZ:43:LEU:HD11	8:AZ:55:LEU:HB3	1.57	0.85
1:BA:3506:ARG:HD3	1:BA:3508:LYS:HE2	1.58	0.85
3:BD:3271:LEU:HD23	3:BD:3301:ALA:HB2	1.58	0.85
6:BH:3241:ILE:HG13	6:BH:3330:VAL:HG11	1.59	0.85
4:BE:3172:ASN:HB3	4:BE:3175:LEU:HB3	1.57	0.84
2:AB:6:PHE:HB3	2:AB:10:VAL:HG21	1.59	0.84
5:AG:494:MET:SD	5:AG:499:ILE:HG22	2.17	0.84
2:AB:258:LEU:HD23	3:AD:244:PRO:HB2	1.58	0.84
8:BZ:3271:ASP:HA	8:BZ:3274:LEU:HB3	1.57	0.84
2:BB:3258:LEU:HD23	3:BD:3244:PRO:HB2	1.58	0.84
3:AD:256:ASP:HB2	3:AD:259:GLN:HB2	1.60	0.84
5:BG:3494:MET:SD	5:BG:3499:ILE:HG22	2.17	0.84
1:BA:3545:ILE:HD13	3:BD:3068:MET:HG3	1.58	0.84
3:AD:271:LEU:HD23	3:AD:301:ALA:HB2	1.58	0.83
7:BQ:3436:LYS:HE3	7:BQ:3440:ARG:HH12	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:431:ARG:HH11	4:AE:431:ARG:HB3	1.44	0.83
2:AB:67:ILE:HD13	3:AD:527:SER:HB2	1.59	0.83
6:AH:241:ILE:HG13	6:AH:330:VAL:HG11	1.59	0.83
2:BB:3067:ILE:HD13	3:BD:3527:SER:HB2	1.59	0.83
4:BE:3431:ARG:HB3	4:BE:3431:ARG:HH11	1.44	0.83
2:AB:255:THR:HG23	3:AD:263:ILE:HG22	1.61	0.83
8:BZ:3181:VAL:HG11	8:BZ:3194:VAL:HG22	1.62	0.82
2:BB:3255:THR:HG23	3:BD:3263:ILE:HG22	1.61	0.82
2:BB:3006:PHE:HB3	2:BB:3010:VAL:HG21	1.59	0.82
5:BG:3103:ILE:HD13	5:BG:3514:ILE:HD13	1.61	0.82
1:AA:256:MET:HB3	1:AA:260:VAL:HG11	1.61	0.82
4:AE:380:ILE:HG12	4:AE:395:ILE:HG12	1.61	0.82
7:AQ:444:LEU:HD23	7:AQ:444:LEU:H	1.44	0.82
4:BE:3380:ILE:HG12	4:BE:3395:ILE:HG12	1.61	0.82
4:AE:550:LYS:HG2	6:AH:50:ASP:HB2	1.62	0.82
7:AQ:436:LYS:HE3	7:AQ:440:ARG:HH12	1.43	0.82
7:BQ:3444:LEU:H	7:BQ:3444:LEU:HD23	1.44	0.82
7:BQ:3057:ASN:HD22	7:BQ:3061:LYS:HB3	1.44	0.82
7:AQ:57:ASN:HD22	7:AQ:61:LYS:HB3	1.44	0.82
8:AZ:181:VAL:HG11	8:AZ:194:VAL:HG22	1.62	0.82
4:AE:180:LEU:HD11	4:AE:430:VAL:HG13	1.63	0.81
4:BE:3498:LEU:HD21	4:BE:3512:VAL:HG22	1.62	0.81
3:BD:3256:ASP:HB2	3:BD:3259:GLN:HB2	1.60	0.81
8:BZ:3295:ILE:HD12	8:BZ:3309:PHE:HE2	1.44	0.81
4:BE:3180:LEU:HD11	4:BE:3430:VAL:HG13	1.63	0.81
3:BD:3292:ILE:HD13	3:BD:3292:ILE:H	1.46	0.81
5:AG:103:ILE:HD13	5:AG:514:ILE:HD13	1.61	0.81
2:BB:3507:VAL:HG22	4:BE:3192:ILE:HD13	1.63	0.81
3:AD:384:ASN:HA	3:AD:387:ILE:HD12	1.63	0.81
1:BA:3256:MET:HB3	1:BA:3260:VAL:HG11	1.61	0.81
4:AE:494:THR:HG21	4:AE:512:VAL:HG13	1.63	0.80
2:AB:507:VAL:HG22	4:AE:192:ILE:HD13	1.63	0.80
3:BD:3384:ASN:HA	3:BD:3387:ILE:HD12	1.63	0.80
2:BB:3495:ARG:HB3	2:BB:3495:ARG:HH11	1.46	0.80
8:AZ:295:ILE:HD12	8:AZ:309:PHE:HE2	1.44	0.80
4:BE:3494:THR:HG21	4:BE:3512:VAL:HG13	1.63	0.80
4:AE:498:LEU:HD21	4:AE:512:VAL:HG22	1.62	0.80
4:BE:3550:LYS:HG2	6:BH:3050:ASP:HB2	1.62	0.80
3:BD:3220:ILE:HD13	3:BD:3226:PRO:HD2	1.64	0.80
4:AE:361:ARG:HD2	4:AE:373:LYS:HG2	1.64	0.80
3:BD:3210:ILE:HD12	3:BD:3362:ARG:HD3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AD:210:ILE:HD12	3:AD:362:ARG:HD3	1.62	0.80
1:AA:352:SER:HA	1:AA:355:LEU:HB2	1.63	0.80
5:BG:3182:VAL:HG12	5:BG:3376:ALA:HA	1.62	0.80
4:BE:3452:LEU:HD11	4:BE:3499:LYS:HG2	1.63	0.80
5:AG:182:VAL:HG12	5:AG:376:ALA:HA	1.62	0.79
6:AH:307:PHE:HB3	6:AH:312:ILE:HB	1.63	0.79
3:AD:292:ILE:H	3:AD:292:ILE:HD13	1.46	0.79
4:BE:3361:ARG:HD2	4:BE:3373:LYS:HG2	1.64	0.79
6:AH:164:THR:HG21	6:AH:496:VAL:HA	1.65	0.79
4:AE:247:LYS:NZ	4:AE:393:LEU:HB3	1.97	0.79
6:BH:3164:THR:HG21	6:BH:3496:VAL:HA	1.65	0.79
2:AB:495:ARG:HH11	2:AB:495:ARG:HB3	1.46	0.79
5:AG:382:ARG:HH11	5:AG:382:ARG:HB3	1.48	0.79
4:BE:3546:ARG:HH22	6:BH:3173:ASN:H	1.30	0.79
5:AG:405:ASN:HB3	5:AG:504:VAL:HG21	1.64	0.79
5:BG:3382:ARG:HB3	5:BG:3382:ARG:HH11	1.48	0.79
4:AE:546:ARG:HH22	6:AH:173:ASN:H	1.30	0.78
6:BH:3094:VAL:HG12	6:BH:3096:ASP:H	1.48	0.78
1:BA:3212:SER:HB2	1:BA:3215:GLU:HG3	1.65	0.78
6:BH:3307:PHE:HB3	6:BH:3312:ILE:HB	1.63	0.78
2:AB:285:ILE:HG23	2:AB:306:ILE:HG23	1.65	0.78
3:AD:226:PRO:HB2	3:AD:311:MET:HB2	1.65	0.78
4:BE:3157:ALA:HB1	4:BE:3450:MET:HB3	1.65	0.78
4:BE:3247:LYS:NZ	4:BE:3393:LEU:HB3	1.97	0.78
1:AA:212:SER:HB2	1:AA:215:GLU:HG3	1.65	0.78
3:BD:3226:PRO:HB2	3:BD:3311:MET:HB2	1.65	0.78
3:AD:220:ILE:HD13	3:AD:226:PRO:HD2	1.64	0.78
1:BA:3274:ARG:HH22	5:BG:3279:GLN:HE22	1.31	0.78
6:AH:94:VAL:HG12	6:AH:96:ASP:H	1.48	0.78
4:AE:452:LEU:HD11	4:AE:499:LYS:HG2	1.63	0.78
7:BQ:3348:THR:HB	7:BQ:3351:GLU:HG2	1.66	0.78
2:BB:3285:ILE:HG23	2:BB:3306:ILE:HG23	1.65	0.78
1:BA:3430:ASN:HD21	1:BA:3478:ARG:CZ	1.98	0.77
2:BB:3459:LEU:HD22	2:BB:3472:LEU:HD11	1.65	0.77
8:AZ:236:LEU:HD23	8:AZ:238:VAL:H	1.49	0.77
4:AE:157:ALA:HB1	4:AE:450:MET:HB3	1.65	0.77
1:AA:430:ASN:HD21	1:AA:478:ARG:CZ	1.97	0.77
5:BG:3405:ASN:HB3	5:BG:3504:VAL:HG21	1.65	0.77
1:BA:3352:SER:HA	1:BA:3355:LEU:HB2	1.63	0.77
5:BG:3041:PRO:HA	5:BG:3161:THR:HG22	1.66	0.77
7:BQ:3171:LYS:HE2	7:BQ:3397:ILE:HG12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:41:PRO:HA	5:AG:161:THR:HG22	1.66	0.77
5:AG:266:GLU:HA	8:AZ:262:LEU:HD23	1.67	0.77
6:BH:3131:LYS:HE3	6:BH:3135:LEU:HD21	1.67	0.77
1:BA:3243:LYS:HB3	1:BA:3355:LEU:HD12	1.67	0.77
7:AQ:348:THR:HB	7:AQ:351:GLU:HG2	1.66	0.77
7:AQ:171:LYS:HE2	7:AQ:397:ILE:HG12	1.67	0.76
1:BA:3189:THR:HG22	1:BA:3190:GLN:H	1.51	0.76
8:BZ:3236:LEU:HD23	8:BZ:3238:VAL:H	1.49	0.76
4:BE:3316:ALA:HB2	4:BE:3369:LEU:HB2	1.67	0.76
5:BG:3266:GLU:HA	8:BZ:3262:LEU:HD23	1.67	0.76
5:AG:243:VAL:H	5:AG:349:GLY:HA3	1.49	0.76
3:BD:3350:VAL:HG22	3:BD:3363:VAL:HG22	1.67	0.76
2:AB:459:LEU:HD22	2:AB:472:LEU:HD11	1.65	0.76
2:AB:239:ASP:OD1	2:AB:291:TYR:HB2	1.86	0.76
7:AQ:461:ARG:HG3	7:AQ:471:VAL:HG11	1.67	0.76
3:BD:3017:PRO:O	3:BD:3020:VAL:HG12	1.86	0.76
7:BQ:3254:LEU:HD13	7:BQ:3305:VAL:HG22	1.67	0.76
5:BG:3243:VAL:H	5:BG:3349:GLY:HA3	1.48	0.76
6:BH:3259:VAL:HG22	7:BQ:3267:LEU:HD12	1.67	0.76
1:AA:189:THR:HG22	1:AA:190:GLN:H	1.51	0.76
1:AA:243:LYS:HB3	1:AA:355:LEU:HD12	1.67	0.76
4:BE:3284:LYS:HG3	4:BE:3285:HIS:H	1.51	0.76
2:BB:3239:ASP:OD1	2:BB:3291:TYR:HB2	1.86	0.76
7:AQ:541:ILE:HD12	8:AZ:45:MET:HB2	1.68	0.76
8:AZ:321:LYS:HZ1	8:AZ:323:ARG:HH12	1.34	0.76
1:AA:75:VAL:HG21	1:AA:84:VAL:HG21	1.67	0.76
1:BA:3252:GLN:HA	1:BA:3303:ASP:HB2	1.68	0.76
7:BQ:3461:ARG:HG3	7:BQ:3471:VAL:HG11	1.67	0.76
8:AZ:255:SER:HB2	8:AZ:258:GLN:HB2	1.66	0.76
1:AA:274:ARG:HH22	5:AG:279:GLN:HE22	1.31	0.76
3:AD:198:LYS:HB2	3:AD:387:ILE:HG22	1.68	0.75
1:AA:252:GLN:HA	1:AA:303:ASP:HB2	1.68	0.75
4:AE:316:ALA:HB2	4:AE:369:LEU:HB2	1.67	0.75
1:BA:3350:PHE:HB3	1:BA:3353:SER:HB2	1.67	0.75
5:BG:3389:LEU:HD23	5:BG:3392:ILE:HD12	1.68	0.75
8:BZ:3255:SER:HB2	8:BZ:3258:GLN:HB2	1.66	0.75
4:BE:3282:LYS:HD2	6:BH:3251:LYS:HD2	1.68	0.75
1:AA:541:ILE:HD13	3:AD:47:MET:HE2	1.68	0.75
1:BA:3541:ILE:HD13	3:BD:3047:MET:HE2	1.68	0.75
1:BA:3529:LYS:HG3	3:BD:3203:THR:HG21	1.69	0.75
4:AE:381:TYR:CE1	4:AE:394:ILE:HB	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3218:PHE:HB3	2:BB:3306:ILE:HB	1.68	0.75
3:AD:350:VAL:HG22	3:AD:363:VAL:HG22	1.66	0.75
4:AE:61:ILE:HD13	4:AE:91:LEU:HD21	1.68	0.75
6:AH:189:LEU:H	6:AH:189:LEU:HD23	1.51	0.75
1:AA:350:PHE:HB3	1:AA:353:SER:HB2	1.67	0.75
5:AG:389:LEU:HD23	5:AG:392:ILE:HD12	1.68	0.75
5:BG:3336:ILE:HD12	5:BG:3336:ILE:H	1.52	0.75
6:BH:3189:LEU:HD23	6:BH:3189:LEU:H	1.51	0.75
1:BA:3257:ALA:O	1:BA:3260:VAL:HG12	1.86	0.75
6:AH:131:LYS:HE3	6:AH:135:LEU:HD21	1.67	0.75
7:AQ:254:LEU:HD13	7:AQ:305:VAL:HG22	1.67	0.75
4:AE:284:LYS:HG3	4:AE:285:HIS:H	1.51	0.75
6:AH:259:VAL:HG22	7:AQ:267:LEU:HD12	1.67	0.75
4:BE:3381:TYR:CE1	4:BE:3394:ILE:HB	2.22	0.75
1:AA:529:LYS:HG3	3:AD:203:THR:HG21	1.69	0.75
1:BA:3333:THR:HG22	1:BA:3377:THR:HG21	1.69	0.74
3:AD:17:PRO:O	3:AD:20:VAL:HG12	1.86	0.74
1:AA:512:GLU:HB3	1:AA:517:VAL:HB	1.69	0.74
2:AB:218:PHE:HB3	2:AB:306:ILE:HB	1.68	0.74
1:BA:3075:VAL:HG21	1:BA:3084:VAL:HG21	1.66	0.74
1:BA:3512:GLU:HB3	1:BA:3517:VAL:HB	1.69	0.74
2:AB:328:THR:HG21	4:AE:334:LEU:HD21	1.70	0.74
1:AA:257:ALA:O	1:AA:260:VAL:HG12	1.86	0.74
8:AZ:150:LEU:HD21	8:AZ:406:LEU:HD11	1.69	0.74
8:BZ:3150:LEU:HD21	8:BZ:3406:LEU:HD11	1.69	0.74
7:AQ:291:ILE:HG22	7:AQ:296:VAL:HG11	1.69	0.74
3:BD:3198:LYS:HB2	3:BD:3387:ILE:HG22	1.68	0.74
4:AE:245:LEU:HD11	4:AE:346:VAL:HG13	1.70	0.74
7:BQ:3291:ILE:HG22	7:BQ:3296:VAL:HG11	1.69	0.74
8:AZ:207:THR:HG22	8:AZ:381:LYS:N	2.02	0.74
1:AA:333:THR:HG22	1:AA:377:THR:HG21	1.69	0.74
4:AE:546:ARG:NH2	6:AH:173:ASN:H	1.85	0.74
5:AG:336:ILE:H	5:AG:336:ILE:HD12	1.52	0.74
7:BQ:3541:ILE:HD12	8:BZ:3045:MET:HB2	1.68	0.74
4:BE:3546:ARG:NH2	6:BH:3173:ASN:H	1.85	0.74
1:AA:264:ILE:HB	5:AG:261:ILE:HG12	1.70	0.74
1:BA:3082:ILE:HG22	1:BA:3083:LEU:HD23	1.70	0.74
3:BD:3065:LEU:HD11	3:BD:3097:VAL:HG21	1.68	0.74
6:BH:3139:LYS:HG3	6:BH:3423:CYS:SG	2.28	0.74
3:AD:65:LEU:HD11	3:AD:97:VAL:HG21	1.68	0.74
1:AA:82:ILE:HG22	1:AA:83:LEU:HD23	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:247:LYS:HZ2	4:AE:393:LEU:HB3	1.51	0.74
4:BE:3245:LEU:HD11	4:BE:3346:VAL:HG13	1.70	0.74
3:AD:196:LEU:HD23	3:AD:377:VAL:HB	1.70	0.74
8:AZ:273:LYS:HB3	8:AZ:340:VAL:HG11	1.70	0.74
1:BA:3184:LEU:HD21	1:BA:3198:TYR:HB3	1.70	0.74
8:BZ:3207:THR:HG22	8:BZ:3381:LYS:N	2.02	0.73
2:BB:3328:THR:HG21	4:BE:3334:LEU:HD21	1.70	0.73
7:AQ:244:LYS:HG3	7:AQ:354:LEU:HD11	1.70	0.73
2:BB:3315:GLU:O	2:BB:3319:LEU:HG	1.88	0.73
3:AD:207:THR:HG22	3:AD:379:ILE:HA	1.69	0.73
1:BA:3473:LEU:HD23	1:BA:3502:LEU:HD22	1.70	0.73
1:AA:473:LEU:HD23	1:AA:502:LEU:HD22	1.70	0.73
6:BH:3505:ASN:HD21	7:BQ:3215:GLY:H	1.36	0.73
8:BZ:3354:VAL:HG22	8:BZ:3367:VAL:HA	1.70	0.73
7:AQ:354:LEU:HB3	7:AQ:377:GLU:HG2	1.70	0.73
1:BA:3310:PHE:HA	1:BA:3315:ILE:HD12	1.70	0.73
4:AE:282:LYS:HD2	6:AH:251:LYS:HD2	1.68	0.73
2:BB:3406:CYS:O	2:BB:3410:VAL:HG23	1.88	0.73
4:BE:3061:ILE:HD13	4:BE:3091:LEU:HD21	1.68	0.73
8:BZ:3280:LEU:HD11	8:BZ:3345:PRO:HA	1.69	0.73
8:AZ:354:VAL:HG22	8:AZ:367:VAL:HA	1.70	0.73
2:BB:3244:LYS:HB2	4:BE:3278:PRO:HD2	1.71	0.73
2:AB:244:LYS:HB2	4:AE:278:PRO:HD2	1.71	0.73
1:AA:184:LEU:HD21	1:AA:198:TYR:HB3	1.70	0.73
1:AA:310:PHE:HA	1:AA:315:ILE:HD12	1.70	0.73
2:BB:3190:LEU:H	4:BE:3389:LYS:HZ1	1.36	0.73
8:AZ:280:LEU:HD11	8:AZ:345:PRO:HA	1.69	0.73
7:AQ:435:THR:HG23	7:AQ:450:LYS:HG3	1.71	0.73
5:BG:3065:LEU:HD23	5:BG:3079:LEU:HD12	1.71	0.73
8:BZ:3273:LYS:HB3	8:BZ:3340:VAL:HG11	1.70	0.73
3:BD:3207:THR:HG22	3:BD:3379:ILE:HA	1.69	0.72
6:AH:216:ASN:HD22	6:AH:367:GLY:HA2	1.53	0.72
7:AQ:154:ASN:HD22	7:AQ:190:LEU:HD13	1.54	0.72
4:BE:3412:ASN:N	4:BE:3415:ILE:HD12	2.04	0.72
8:BZ:3294:VAL:HG23	8:BZ:3315:LEU:HB3	1.70	0.72
1:BA:3055:ASP:HB2	5:BG:3530:VAL:HG22	1.71	0.72
7:BQ:3435:THR:HG23	7:BQ:3450:LYS:HG3	1.71	0.72
2:AB:406:CYS:O	2:AB:410:VAL:HG23	1.88	0.72
4:AE:412:ASN:N	4:AE:415:ILE:HD12	2.04	0.72
8:AZ:109:ILE:HD12	8:AZ:115:PRO:HG3	1.72	0.72
2:AB:315:GLU:O	2:AB:319:LEU:HG	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3020:LEU:O	2:BB:3024:VAL:HG23	1.89	0.72
5:BG:3290:VAL:HG12	5:BG:3345:GLU:HG2	1.71	0.72
8:BZ:3274:LEU:HD21	8:BZ:3308:VAL:HG11	1.69	0.72
6:AH:139:LYS:HG3	6:AH:423:CYS:SG	2.28	0.72
1:AA:34:MET:HE3	1:AA:110:LYS:HB2	1.71	0.72
8:BZ:3109:ILE:HD12	8:BZ:3115:PRO:HG3	1.72	0.72
8:BZ:3068:ILE:H	8:BZ:3068:ILE:HD13	1.55	0.72
1:BA:3264:ILE:HB	5:BG:3261:ILE:HG12	1.70	0.72
6:AH:505:ASN:HD21	7:AQ:215:GLY:H	1.36	0.72
6:AH:460:ASP:O	6:AH:464:ILE:HG22	1.90	0.72
5:AG:290:VAL:HG12	5:AG:345:GLU:HG2	1.71	0.72
6:BH:3460:ASP:O	6:BH:3464:ILE:HG22	1.90	0.72
2:AB:34:LYS:HB3	2:AB:443:ILE:HD11	1.70	0.72
1:BA:3394:SER:HB3	5:BG:3519:LEU:HD22	1.72	0.72
7:BQ:3154:ASN:HD22	7:BQ:3190:LEU:HD13	1.54	0.72
7:AQ:48:PRO:HA	7:AQ:169:SER:HA	1.71	0.72
1:AA:269:GLN:HG3	3:AD:255:ASN:O	1.90	0.72
4:BE:3107:LEU:HG	4:BE:3544:LEU:HD22	1.72	0.72
1:AA:394:SER:HB3	5:AG:519:LEU:HD22	1.72	0.72
6:BH:3216:ASN:HD22	6:BH:3367:GLY:HA2	1.53	0.72
8:AZ:274:LEU:HD21	8:AZ:308:VAL:HG11	1.69	0.72
4:AE:107:LEU:HG	4:AE:544:LEU:HD22	1.72	0.72
7:BQ:3048:PRO:HA	7:BQ:3169:SER:HA	1.71	0.72
1:BA:3269:GLN:HG3	3:BD:3255:ASN:O	1.90	0.72
3:BD:3141:LYS:HA	3:BD:3409:GLY:CA	2.19	0.71
5:AG:65:LEU:HD23	5:AG:79:LEU:HD12	1.71	0.71
8:BZ:3173:ILE:HG23	8:BZ:3209:PHE:HB2	1.72	0.71
7:BQ:3244:LYS:HG3	7:BQ:3354:LEU:HD11	1.70	0.71
7:BQ:3354:LEU:HB3	7:BQ:3377:GLU:HG2	1.70	0.71
2:AB:20:LEU:O	2:AB:24:VAL:HG23	1.89	0.71
8:AZ:294:VAL:HG23	8:AZ:315:LEU:HB3	1.70	0.71
3:BD:3196:LEU:HD23	3:BD:3377:VAL:HB	1.70	0.71
1:AA:419:VAL:HG23	1:AA:521:THR:HG22	1.72	0.71
2:AB:190:LEU:H	4:AE:389:LYS:HZ1	1.38	0.71
2:AB:293:TYR:HA	3:AD:334:ALA:HB1	1.71	0.71
2:BB:3034:LYS:HB3	2:BB:3443:ILE:HD11	1.70	0.71
1:BA:3419:VAL:HG23	1:BA:3521:THR:HG22	1.72	0.71
4:BE:3110:SER:HB2	6:BH:3206:GLY:HA2	1.73	0.71
1:BA:3253:LYS:HA	1:BA:3281:VAL:HG21	1.72	0.71
7:BQ:3388:GLY:HA3	7:BQ:3394:LEU:HD13	1.72	0.71
1:BA:3281:VAL:HA	1:BA:3284:ARG:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:183:ARG:NH1	2:AB:210:GLU:HA	2.06	0.71
4:AE:110:SER:HB2	6:AH:206:GLY:HA2	1.72	0.71
2:BB:3293:TYR:HA	3:BD:3334:ALA:HB1	1.71	0.71
8:BZ:3433:LYS:HG2	8:BZ:3435:GLY:H	1.55	0.71
4:BE:3282:LYS:HB3	6:BH:3251:LYS:HB3	1.73	0.71
5:AG:78:MET:HA	5:AG:81:LEU:HD12	1.73	0.71
8:AZ:68:ILE:H	8:AZ:68:ILE:HD13	1.55	0.71
3:AD:246:PRO:HD2	3:AD:250:ASN:ND2	2.06	0.71
8:AZ:153:VAL:HG11	8:AZ:405:VAL:HG21	1.72	0.71
7:AQ:388:GLY:HA3	7:AQ:394:LEU:HD13	1.72	0.71
6:BH:3356:GLN:HE22	6:BH:3361:ARG:HD3	1.55	0.71
6:AH:356:GLN:HE22	6:AH:361:ARG:HD3	1.55	0.71
2:BB:3294:PRO:HA	2:BB:3297:LEU:HD12	1.73	0.71
1:AA:55:ASP:HB2	5:AG:530:VAL:HG22	1.71	0.70
4:BE:3188:LEU:HD22	4:BE:3193:VAL:HG11	1.73	0.70
3:AD:141:LYS:HA	3:AD:409:GLY:CA	2.19	0.70
3:BD:3246:PRO:HD2	3:BD:3250:ASN:ND2	2.06	0.70
1:AA:281:VAL:HA	1:AA:284:ARG:HG3	1.72	0.70
2:BB:3005:ILE:HG22	2:BB:3006:PHE:H	1.56	0.70
6:BH:3216:ASN:ND2	6:BH:3368:CYS:H	1.88	0.70
6:BH:3137:VAL:HG13	6:BH:3504:ILE:HG13	1.73	0.70
4:AE:284:LYS:HG2	6:AH:259:VAL:H	1.56	0.70
1:AA:301:GLY:HA2	1:AA:320:ARG:H	1.56	0.70
5:BG:3233:LYS:HB2	8:BZ:3329:GLN:HE22	1.56	0.70
4:AE:307:LYS:HA	4:AE:310:ILE:HG22	1.74	0.70
7:AQ:209:VAL:HG22	7:AQ:384:ILE:HB	1.72	0.70
2:BB:3320:VAL:HA	2:BB:3362:GLY:HA2	1.74	0.70
4:BE:3284:LYS:HG2	6:BH:3259:VAL:H	1.56	0.70
6:AH:216:ASN:ND2	6:AH:368:CYS:H	1.88	0.70
4:AE:362:ILE:H	4:AE:362:ILE:HD12	1.57	0.70
1:BA:3301:GLY:HA2	1:BA:3320:ARG:H	1.56	0.70
6:AH:137:VAL:HG13	6:AH:504:ILE:HG13	1.73	0.70
2:BB:3183:ARG:NH1	2:BB:3210:GLU:HA	2.06	0.70
4:BE:3033:LYS:HD3	6:BH:3074:ASP:HB3	1.74	0.70
2:AB:5:ILE:HG22	2:AB:6:PHE:H	1.56	0.70
8:AZ:36:ASN:HB3	8:AZ:44:LYS:HE2	1.74	0.70
7:BQ:3420:LEU:HD12	7:BQ:3426:THR:HG21	1.74	0.70
7:BQ:3010:ASN:N	7:BQ:3010:ASN:HD22	1.90	0.70
8:BZ:3153:VAL:HG11	8:BZ:3405:VAL:HG21	1.72	0.70
4:BE:3307:LYS:HA	4:BE:3310:ILE:HG22	1.74	0.70
7:BQ:3100:THR:O	7:BQ:3103:VAL:HG12	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:188:LEU:HD22	4:AE:193:VAL:HG11	1.73	0.70
7:AQ:420:LEU:HD12	7:AQ:426:THR:HG21	1.74	0.70
2:BB:3072:PRO:HA	4:BE:3081:ILE:HD13	1.73	0.70
7:BQ:3209:VAL:HG22	7:BQ:3384:ILE:HB	1.72	0.70
5:BG:3078:MET:HA	5:BG:3081:LEU:HD12	1.73	0.70
5:AG:233:LYS:HB2	8:AZ:329:GLN:HE22	1.56	0.70
1:AA:141:ASN:HA	1:AA:144:LEU:HG	1.73	0.70
8:AZ:173:ILE:HG23	8:AZ:209:PHE:HB2	1.73	0.70
8:AZ:215:LEU:HD21	8:AZ:324:ASN:ND2	2.07	0.69
6:AH:161:CYS:SG	6:AH:499:PRO:HD3	2.32	0.69
5:BG:3120:ILE:HG23	5:BG:3438:GLN:HE21	1.57	0.69
3:BD:3121:ALA:HB1	3:BD:3516:LYS:HG3	1.74	0.69
8:BZ:3215:LEU:HD21	8:BZ:3324:ASN:ND2	2.07	0.69
2:AB:72:PRO:HA	4:AE:81:ILE:HD13	1.73	0.69
8:AZ:321:LYS:NZ	8:AZ:323:ARG:HH12	1.90	0.69
1:AA:127:THR:HG22	3:AD:165:GLN:NE2	2.08	0.69
7:AQ:100:THR:O	7:AQ:103:VAL:HG12	1.92	0.69
4:AE:282:LYS:HB3	6:AH:251:LYS:HB3	1.73	0.69
7:AQ:325:SER:HB2	7:AQ:328:GLU:HB2	1.75	0.69
4:BE:3412:ASN:H	4:BE:3415:ILE:HD12	1.58	0.69
1:BA:3141:ASN:HA	1:BA:3144:LEU:HG	1.73	0.69
6:BH:3247:GLU:HG3	6:BH:3248:LEU:H	1.58	0.69
2:AB:320:VAL:HA	2:AB:362:GLY:HA2	1.74	0.69
4:AE:33:LYS:HD3	6:AH:74:ASP:HB3	1.74	0.69
2:AB:325:VAL:HB	4:AE:251:HIS:CE1	2.28	0.69
2:BB:3325:VAL:HB	4:BE:3251:HIS:CE1	2.28	0.69
1:BA:3274:ARG:NH2	5:BG:3279:GLN:HE22	1.91	0.69
1:AA:253:LYS:HA	1:AA:281:VAL:HG21	1.72	0.69
6:BH:3161:CYS:SG	6:BH:3499:PRO:HD3	2.32	0.69
1:AA:202:ALA:HA	1:AA:328:ARG:NH1	2.08	0.69
6:AH:338:THR:HA	6:AH:341:ILE:HD11	1.73	0.69
5:BG:3249:PRO:HG2	5:BG:3253:LYS:HE3	1.75	0.69
4:AE:247:LYS:HD2	4:AE:393:LEU:HD22	1.74	0.69
3:AD:110:LEU:HB3	3:AD:115:ILE:HD12	1.75	0.69
1:BA:3202:ALA:HA	1:BA:3328:ARG:NH1	2.07	0.69
1:BA:3034:MET:HE3	1:BA:3110:LYS:HB2	1.74	0.69
3:BD:3110:LEU:HB3	3:BD:3115:ILE:HD12	1.75	0.69
4:BE:3362:ILE:H	4:BE:3362:ILE:HD12	1.57	0.69
2:AB:294:PRO:HA	2:AB:297:LEU:HD12	1.74	0.69
1:AA:46:PRO:HD2	1:AA:504:LEU:HD12	1.74	0.69
8:BZ:3093:THR:HG23	8:BZ:3454:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:69:ASP:HB2	8:AZ:537:GLY:HA2	1.74	0.68
3:AD:121:ALA:HB1	3:AD:516:LYS:HG3	1.74	0.68
7:AQ:10:ASN:N	7:AQ:10:ASN:HD22	1.90	0.68
1:AA:296:VAL:HG21	1:AA:310:PHE:CE1	2.28	0.68
4:AE:543:GLN:HG3	4:AE:544:LEU:H	1.57	0.68
2:BB:3049:ALA:HA	3:BD:3528:ARG:NE	2.08	0.68
1:BA:3460:LYS:O	1:BA:3464:VAL:HG23	1.93	0.68
6:AH:247:GLU:HG3	6:AH:248:LEU:H	1.58	0.68
8:AZ:433:LYS:HG2	8:AZ:435:GLY:H	1.55	0.68
2:BB:3230:LYS:N	2:BB:3282:ASN:HD21	1.91	0.68
4:BE:3247:LYS:HD2	4:BE:3393:LEU:HD22	1.74	0.68
1:AA:460:LYS:O	1:AA:464:VAL:HG23	1.93	0.68
8:AZ:93:THR:HG23	8:AZ:454:ILE:HD12	1.74	0.68
5:AG:249:PRO:HG2	5:AG:253:LYS:HE3	1.75	0.68
6:BH:3338:THR:HA	6:BH:3341:ILE:HD11	1.73	0.68
5:AG:120:ILE:HG23	5:AG:438:GLN:HE21	1.57	0.68
2:AB:49:ALA:HA	3:AD:528:ARG:NE	2.08	0.68
2:AB:199:LEU:H	2:AB:199:LEU:HD12	1.57	0.68
4:AE:412:ASN:H	4:AE:415:ILE:HD12	1.58	0.68
7:BQ:3343:ARG:HG3	7:BQ:3344:LEU:H	1.59	0.68
1:BA:3296:VAL:HG21	1:BA:3310:PHE:CE1	2.28	0.68
8:BZ:3321:LYS:NZ	8:BZ:3323:ARG:HH12	1.90	0.68
1:BA:3046:PRO:HD2	1:BA:3504:LEU:HD12	1.74	0.68
2:AB:79:ASN:HB3	4:AE:413:LYS:HZ2	1.58	0.68
6:BH:3299:ILE:HD13	6:BH:3316:GLY:HA2	1.76	0.68
4:BE:3086:ASP:CG	4:BE:3421:ARG:HE	1.97	0.68
5:AG:454:ARG:HA	5:AG:457:ILE:HG22	1.76	0.68
2:BB:3173:PHE:HA	2:BB:3176:LEU:HD12	1.76	0.68
7:BQ:3028:ILE:O	7:BQ:3032:ILE:HG12	1.94	0.68
2:AB:242:LYS:O	2:AB:245:ILE:HG13	1.94	0.68
2:BB:3199:LEU:H	2:BB:3199:LEU:HD12	1.57	0.68
7:AQ:28:ILE:O	7:AQ:32:ILE:HG12	1.94	0.68
5:AG:41:PRO:HG3	5:AG:486:GLY:CA	2.24	0.68
4:BE:3543:GLN:HG3	4:BE:3544:LEU:H	1.57	0.68
8:BZ:3036:ASN:HB3	8:BZ:3044:LYS:HE2	1.74	0.68
4:AE:86:ASP:CG	4:AE:421:ARG:HE	1.97	0.68
1:BA:3127:THR:HG22	3:BD:3165:GLN:NE2	2.08	0.67
8:BZ:3337:GLN:NE2	8:BZ:3347:ILE:HG21	2.09	0.67
3:AD:243:PRO:HD3	3:AD:298:ASN:HD22	1.59	0.67
4:AE:297:LYS:HB3	6:AH:264:VAL:HG21	1.76	0.67
6:BH:3220:PHE:HB2	6:BH:3322:ASP:OD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:3426:GLU:HG2	1:BA:3458:ILE:HB	1.76	0.67
2:BB:3045:LEU:HD12	3:BD:3521:ILE:HD13	1.76	0.67
4:BE:3322:ILE:HD13	4:BE:3354:ILE:HD13	1.75	0.67
4:AE:322:ILE:HD13	4:AE:354:ILE:HD13	1.75	0.67
2:BB:3242:LYS:O	2:BB:3245:ILE:HG13	1.94	0.67
4:BE:3297:LYS:HB3	6:BH:3264:VAL:HG21	1.76	0.67
2:AB:183:ARG:CZ	2:AB:365:CYS:HB3	2.25	0.67
7:BQ:3142:LEU:HD21	7:BQ:3430:LEU:HD11	1.75	0.67
8:AZ:414:GLY:HA3	8:AZ:506:ILE:HG22	1.77	0.67
7:AQ:142:LEU:HD21	7:AQ:430:LEU:HD11	1.75	0.67
3:BD:3326:LYS:HD2	3:BD:3373:PRO:HD2	1.77	0.67
2:AB:45:LEU:HD12	3:AD:521:ILE:HD13	1.76	0.67
5:AG:160:GLY:HA2	5:AG:165:ILE:HD12	1.75	0.67
3:BD:3243:PRO:HD3	3:BD:3298:ASN:HD22	1.59	0.67
5:BG:3069:ASP:HB2	8:BZ:3537:GLY:HA2	1.74	0.67
2:AB:173:PHE:HA	2:AB:176:LEU:HD12	1.76	0.67
1:BA:3211:LYS:HD3	1:BA:3215:GLU:OE1	1.95	0.67
5:BG:3041:PRO:HG3	5:BG:3486:GLY:CA	2.24	0.67
8:AZ:337:GLN:NE2	8:AZ:347:ILE:HG21	2.09	0.67
8:BZ:3414:GLY:HA3	8:BZ:3506:ILE:HG22	1.77	0.67
6:AH:78:PRO:HB3	7:AQ:54:ILE:HG21	1.77	0.67
1:BA:3291:ALA:HB1	1:BA:3351:GLU:HA	1.77	0.67
8:BZ:3352:GLY:HA3	8:BZ:3369:GLU:HB2	1.75	0.67
7:BQ:3325:SER:HB2	7:BQ:3328:GLU:HB2	1.75	0.67
6:AH:299:ILE:HD13	6:AH:316:GLY:HA2	1.76	0.67
2:AB:215:ALA:O	2:AB:216:LYS:HB3	1.93	0.67
1:AA:274:ARG:NH2	5:AG:279:GLN:HE22	1.91	0.67
4:BE:3272:LEU:HD12	4:BE:3274:CYS:SG	2.35	0.67
8:AZ:352:GLY:HA3	8:AZ:369:GLU:HB2	1.76	0.67
3:AD:259:GLN:HG2	3:AD:263:ILE:HD11	1.77	0.67
1:AA:86:LEU:HD21	1:AA:531:ALA:HA	1.77	0.67
7:AQ:343:ARG:HG3	7:AQ:344:LEU:H	1.59	0.67
1:BA:3053:LEU:HD12	1:BA:3072:LEU:HD13	1.77	0.67
6:BH:3078:PRO:HB3	7:BQ:3054:ILE:HG21	1.77	0.67
1:AA:247:LEU:HB2	1:AA:298:THR:HA	1.77	0.66
6:AH:220:PHE:HB2	6:AH:322:ASP:OD2	1.94	0.66
2:BB:3183:ARG:CZ	2:BB:3365:CYS:HB3	2.25	0.66
1:BA:3308:LYS:HD3	5:BG:3337:VAL:HG13	1.77	0.66
7:AQ:83:LYS:O	7:AQ:87:MET:HG2	1.95	0.66
8:AZ:329:GLN:HE21	8:AZ:335:GLU:HA	1.61	0.66
4:AE:272:LEU:HD12	4:AE:274:CYS:SG	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3157:LEU:HD11	6:BH:3409:ILE:HD13	1.77	0.66
5:AG:227:LYS:HD3	5:AG:318:ARG:O	1.96	0.66
1:AA:308:LYS:HD3	5:AG:337:VAL:HG13	1.77	0.66
6:AH:334:ILE:HB	7:AQ:235:HIS:HE2	1.60	0.66
5:BG:3454:ARG:HA	5:BG:3457:ILE:HG22	1.76	0.66
6:BH:3213:LEU:HB2	6:BH:3377:LEU:HD23	1.77	0.66
2:AB:43:ASP:OD1	2:AB:58:ASN:HB2	1.95	0.66
5:BG:3160:GLY:HA2	5:BG:3165:ILE:HD12	1.75	0.66
4:AE:284:LYS:HG3	4:AE:285:HIS:N	2.09	0.66
1:AA:426:GLU:HG2	1:AA:458:ILE:HB	1.76	0.66
6:AH:243:SER:O	6:AH:334:ILE:HA	1.96	0.66
5:BG:3232:PRO:HG2	8:BZ:3325:MET:HB3	1.78	0.66
1:BA:3288:ILE:HG12	1:BA:3349:THR:HB	1.77	0.66
2:BB:3152:ASP:OD2	2:BB:3400:THR:HG21	1.96	0.66
6:AH:144:ALA:HB1	6:AH:408:LEU:HB3	1.77	0.66
2:BB:3346:ILE:HD13	2:BB:3355:LYS:HE3	1.76	0.66
5:AG:47:MET:HB2	5:AG:57:LEU:HD13	1.78	0.66
6:AH:25:GLN:HE22	6:AH:29:ASN:HD21	1.44	0.66
4:AE:506:LYS:HG3	4:AE:508:SER:OG	1.95	0.66
2:BB:3215:ALA:O	2:BB:3216:LYS:HB3	1.93	0.66
3:BD:3217:GLN:NE2	3:BD:3316:ILE:HA	2.11	0.66
1:BA:3086:LEU:HD21	1:BA:3531:ALA:HA	1.77	0.66
6:BH:3144:ALA:HB1	6:BH:3408:LEU:HB3	1.77	0.66
3:AD:326:LYS:HD2	3:AD:373:PRO:HD2	1.77	0.66
6:BH:3310:ARG:O	6:BH:3312:ILE:HG13	1.96	0.66
8:BZ:3215:LEU:HD21	8:BZ:3324:ASN:HD21	1.61	0.66
6:BH:3158:LEU:HB3	6:BH:3400:VAL:HG13	1.76	0.66
1:AA:288:ILE:HG12	1:AA:349:THR:HB	1.77	0.66
2:AB:5:ILE:HG22	2:AB:6:PHE:N	2.11	0.66
4:BE:3247:LYS:HZ2	4:BE:3393:LEU:HB3	1.58	0.66
8:AZ:215:LEU:HD21	8:AZ:324:ASN:HD21	1.61	0.66
1:BA:3247:LEU:HB2	1:BA:3298:THR:HA	1.77	0.66
6:AH:419:GLU:HB2	6:AH:472:HIS:NE2	2.11	0.66
1:AA:53:LEU:HD12	1:AA:72:LEU:HD13	1.77	0.66
1:AA:291:ALA:HB1	1:AA:351:GLU:HA	1.77	0.66
2:AB:346:ILE:HD13	2:AB:355:LYS:HE3	1.76	0.66
4:BE:3284:LYS:HG3	4:BE:3285:HIS:N	2.09	0.66
4:AE:384:GLU:OE2	4:AE:391:ARG:HD3	1.96	0.66
3:AD:278:ILE:HA	3:AD:339:PHE:HE2	1.60	0.66
6:BH:3419:GLU:HB2	6:BH:3472:HIS:NE2	2.11	0.66
5:BG:3164:VAL:HB	5:BG:3395:ASN:HD22	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3275:CYS:HA	3:BD:3278:ILE:HD12	1.78	0.66
6:BH:3327:ILE:HD11	6:BH:3334:ILE:H	1.61	0.66
3:BD:3259:GLN:HG2	3:BD:3263:ILE:HD11	1.77	0.66
2:BB:3005:ILE:HG22	2:BB:3006:PHE:N	2.11	0.66
1:AA:211:LYS:HD3	1:AA:215:GLU:OE1	1.95	0.66
8:AZ:219:GLY:H	8:AZ:356:GLN:NE2	1.93	0.66
5:BG:3227:LYS:HD3	5:BG:3318:ARG:O	1.96	0.66
8:AZ:344:SER:HB2	8:AZ:346:GLN:HE21	1.61	0.66
4:BE:3384:GLU:OE2	4:BE:3391:ARG:HD3	1.96	0.66
7:AQ:513:ARG:NH1	7:AQ:513:ARG:HA	2.06	0.65
8:BZ:3219:GLY:H	8:BZ:3356:GLN:NE2	1.93	0.65
4:BE:3310:ILE:HD11	4:BE:3335:LEU:HA	1.78	0.65
3:BD:3278:ILE:HA	3:BD:3339:PHE:HE2	1.60	0.65
7:BQ:3083:LYS:O	7:BQ:3087:MET:HG2	1.95	0.65
7:AQ:498:GLY:O	7:AQ:509:VAL:HB	1.95	0.65
2:BB:3043:ASP:OD1	2:BB:3058:ASN:HB2	1.95	0.65
7:BQ:3498:GLY:O	7:BQ:3509:VAL:HB	1.95	0.65
6:BH:3198:LEU:O	6:BH:3373:THR:HG23	1.96	0.65
1:BA:3229:ALA:HB1	1:BA:3307:LEU:HD11	1.78	0.65
8:BZ:3162:VAL:HG11	8:BZ:3167:THR:HG23	1.79	0.65
6:AH:213:LEU:HB2	6:AH:377:LEU:HD23	1.77	0.65
2:BB:3079:ASN:HB3	4:BE:3413:LYS:HZ2	1.61	0.65
2:AB:230:LYS:N	2:AB:282:ASN:HD21	1.91	0.65
6:BH:3163:ARG:HH11	6:BH:3179:VAL:HG11	1.61	0.65
6:AH:190:ASP:HB2	6:AH:192:ASN:ND2	2.11	0.65
1:BA:3329:ILE:O	1:BA:3333:THR:HG23	1.97	0.65
3:AD:275:CYS:HA	3:AD:278:ILE:HD12	1.78	0.65
8:BZ:3154:ALA:HB3	8:BZ:3171:THR:HG23	1.78	0.65
6:AH:157:LEU:HD11	6:AH:409:ILE:HD13	1.77	0.65
5:AG:164:VAL:HB	5:AG:395:ASN:HD22	1.61	0.65
6:AH:158:LEU:HB3	6:AH:400:VAL:HG13	1.76	0.65
2:AB:152:ASP:OD2	2:AB:400:THR:HG21	1.96	0.65
8:BZ:3321:LYS:HZ1	8:BZ:3323:ARG:HH12	1.42	0.65
6:BH:3051:ILE:HD12	6:BH:3069:ILE:HD13	1.79	0.65
4:BE:3506:LYS:HG3	4:BE:3508:SER:OG	1.95	0.65
6:AH:51:ILE:HD12	6:AH:69:ILE:HD13	1.78	0.65
3:AD:60:ASP:HB3	3:AD:63:THR:OG1	1.97	0.65
2:AB:234:ALA:HA	2:AB:325:VAL:O	1.97	0.65
6:AH:402:ARG:HB3	6:AH:501:LEU:HD23	1.78	0.65
5:BG:3123:GLN:HA	5:BG:3126:LYS:HE2	1.79	0.65
6:BH:3402:ARG:HB3	6:BH:3501:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BQ:3150:ILE:HD11	7:BQ:3411:LEU:HD13	1.78	0.65
6:AH:310:ARG:O	6:AH:312:ILE:HG13	1.96	0.65
5:AG:228:ASP:CG	5:AG:229:VAL:H	2.01	0.65
8:AZ:315:LEU:HD11	8:AZ:356:GLN:NE2	2.12	0.65
6:AH:327:ILE:HD11	6:AH:334:ILE:H	1.61	0.65
5:BG:3463:ASP:OD1	5:BG:3465:ILE:HG13	1.97	0.65
8:AZ:162:VAL:HG11	8:AZ:167:THR:HG23	1.79	0.65
3:AD:217:GLN:NE2	3:AD:316:ILE:HA	2.11	0.65
6:AH:198:LEU:O	6:AH:373:THR:HG23	1.96	0.65
4:AE:310:ILE:HD11	4:AE:335:LEU:HA	1.78	0.65
1:AA:301:GLY:N	1:AA:320:ARG:HG3	2.12	0.65
1:BA:3065:ASP:HB3	1:BA:3068:THR:OG1	1.97	0.65
1:AA:65:ASP:HB3	1:AA:68:THR:OG1	1.97	0.65
5:AG:463:ASP:OD1	5:AG:465:ILE:HG13	1.97	0.65
3:BD:3060:ASP:HB3	3:BD:3063:THR:OG1	1.97	0.65
7:BQ:3348:THR:HG22	7:BQ:3350:GLU:H	1.63	0.65
6:BH:3243:SER:O	6:BH:3334:ILE:HA	1.96	0.65
6:BH:3334:ILE:HB	7:BQ:3235:HIS:HE2	1.60	0.65
5:AG:226:ASN:HA	5:AG:365:PHE:HA	1.80	0.65
3:AD:276:LYS:HE2	3:AD:280:LYS:HD3	1.79	0.65
7:BQ:3014:PHE:HB2	8:BZ:3070:SER:HB2	1.79	0.65
8:BZ:3267:ARG:HG3	8:BZ:3304:MET:SD	2.37	0.65
5:AG:232:PRO:HG2	8:AZ:325:MET:HB3	1.78	0.64
5:BG:3228:ASP:CG	5:BG:3229:VAL:H	2.01	0.64
8:BZ:3329:GLN:HE21	8:BZ:3335:GLU:HA	1.61	0.64
8:AZ:267:ARG:HG3	8:AZ:304:MET:SD	2.37	0.64
6:AH:86:ILE:HD12	6:AH:101:VAL:HG22	1.79	0.64
1:AA:329:ILE:O	1:AA:333:THR:HG23	1.97	0.64
7:AQ:348:THR:HG22	7:AQ:350:GLU:H	1.62	0.64
8:AZ:166:LEU:HD13	8:AZ:205:LYS:HA	1.79	0.64
8:BZ:3344:SER:HB2	8:BZ:3346:GLN:HE21	1.61	0.64
3:BD:3486:ARG:HH11	3:BD:3486:ARG:HB2	1.63	0.64
6:BH:3190:ASP:HB2	6:BH:3192:ASN:ND2	2.11	0.64
5:BG:3250:LEU:HD12	5:BG:3301:VAL:HG22	1.79	0.64
6:BH:3025:GLN:HE22	6:BH:3029:ASN:HD21	1.44	0.64
1:AA:229:ALA:HB1	1:AA:307:LEU:HD11	1.78	0.64
1:BA:3301:GLY:N	1:BA:3320:ARG:HG3	2.12	0.64
7:BQ:3278:LYS:O	7:BQ:3281:GLU:HB2	1.98	0.64
6:AH:163:ARG:HH11	6:AH:179:VAL:HG11	1.61	0.64
3:AD:418:GLU:HG2	3:AD:450:ILE:HB	1.79	0.64
5:AG:286:GLN:HB2	5:AG:340:VAL:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BQ:3208:ARG:HD3	7:BQ:3331:ARG:HH22	1.62	0.64
8:AZ:17:ALA:O	8:AZ:21:VAL:HG23	1.97	0.64
1:AA:361:VAL:HG22	1:AA:374:ILE:HG12	1.78	0.64
2:AB:233:ILE:H	2:AB:233:ILE:CD1	2.10	0.64
5:AG:174:LEU:HD22	5:AG:219:VAL:HG23	1.79	0.64
7:AQ:57:ASN:HB2	7:AQ:61:LYS:H	1.63	0.64
7:AQ:123:SER:HB3	7:AQ:126:GLU:HG3	1.79	0.64
6:BH:3086:ILE:HD12	6:BH:3101:VAL:HG22	1.79	0.64
5:BG:3286:GLN:HB2	5:BG:3340:VAL:HB	1.79	0.64
2:BB:3095:VAL:HA	2:BB:3497:VAL:HG13	1.80	0.64
2:BB:3153:LEU:HD22	2:BB:3178:THR:HG23	1.78	0.64
2:BB:3229:ALA:HA	2:BB:3282:ASN:OD1	1.98	0.64
7:BQ:3266:LEU:O	7:BQ:3267:LEU:HD23	1.98	0.64
7:AQ:266:LEU:O	7:AQ:267:LEU:HD23	1.98	0.64
7:BQ:3057:ASN:HB2	7:BQ:3061:LYS:H	1.63	0.64
8:BZ:3166:LEU:HD13	8:BZ:3205:LYS:HA	1.79	0.64
2:AB:95:VAL:HA	2:AB:497:VAL:HG13	1.80	0.64
4:BE:3156:LEU:HD11	4:BE:3457:GLU:HG3	1.80	0.64
5:AG:123:GLN:HA	5:AG:126:LYS:HE2	1.79	0.64
8:BZ:3315:LEU:HD11	8:BZ:3356:GLN:NE2	2.12	0.64
8:BZ:3017:ALA:O	8:BZ:3021:VAL:HG23	1.97	0.64
8:BZ:3422:LEU:HD13	8:BZ:3426:LEU:HG	1.80	0.64
2:AB:382:ARG:HE	2:AB:386:ASP:CG	2.01	0.64
1:AA:113:ASN:ND2	1:AA:117:LYS:HE3	2.13	0.64
7:AQ:150:ILE:HD11	7:AQ:411:LEU:HD13	1.78	0.64
4:BE:3043:GLY:H	4:BE:3046:ALA:HB3	1.62	0.64
5:BG:3174:LEU:HD22	5:BG:3219:VAL:HG23	1.79	0.64
5:BG:3047:MET:HB2	5:BG:3057:LEU:HD13	1.77	0.64
1:BA:3113:ASN:ND2	1:BA:3117:LYS:HE3	2.13	0.64
7:BQ:3513:ARG:HA	7:BQ:3513:ARG:NH1	2.06	0.64
1:BA:3361:VAL:HG22	1:BA:3374:ILE:HG12	1.78	0.64
6:AH:251:LYS:HD3	6:AH:251:LYS:H	1.63	0.64
7:AQ:278:LYS:O	7:AQ:281:GLU:HB2	1.98	0.64
4:BE:3043:GLY:N	4:BE:3046:ALA:HB3	2.13	0.64
7:AQ:208:ARG:HD3	7:AQ:331:ARG:HH22	1.62	0.64
4:AE:43:GLY:N	4:AE:46:ALA:HB3	2.13	0.64
2:AB:482:MET:SD	2:AB:487:ILE:HD12	2.38	0.64
7:BQ:3123:SER:HB3	7:BQ:3126:GLU:HG3	1.79	0.64
7:AQ:39:HIS:HD2	7:AQ:108:GLY:HA3	1.62	0.64
2:BB:3350:GLU:HG2	3:BD:3402:ARG:HH12	1.63	0.64
1:AA:277:GLU:HA	1:AA:280:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:483:ALA:O	1:AA:486:MET:HB2	1.98	0.64
3:AD:486:ARG:HB2	3:AD:486:ARG:HH11	1.63	0.64
4:BE:3162:GLU:HG3	4:BE:3438:ARG:NH1	2.13	0.64
8:AZ:422:LEU:HD13	8:AZ:426:LEU:HG	1.80	0.64
6:BH:3251:LYS:HD3	6:BH:3251:LYS:H	1.63	0.63
2:AB:153:LEU:HD22	2:AB:178:THR:HG23	1.78	0.63
5:AG:250:LEU:HD12	5:AG:301:VAL:HG22	1.80	0.63
3:BD:3418:GLU:HG2	3:BD:3450:ILE:HB	1.79	0.63
4:AE:268:LYS:HB3	4:AE:374:LEU:HD13	1.80	0.63
7:BQ:3533:GLU:O	7:BQ:3536:THR:HG22	1.98	0.63
5:BG:3226:ASN:HA	5:BG:3365:PHE:HA	1.80	0.63
2:BB:3233:ILE:H	2:BB:3233:ILE:CD1	2.10	0.63
7:AQ:14:PHE:HB2	8:AZ:70:SER:HB2	1.79	0.63
1:BA:3126:ILE:HD13	1:BA:3536:VAL:HG13	1.80	0.63
4:BE:3251:HIS:HB3	4:BE:3254:MET:HG3	1.80	0.63
5:BG:3402:VAL:HA	5:BG:3405:ASN:ND2	2.14	0.63
1:AA:233:MET:HB2	1:AA:234:PRO:HD2	1.81	0.63
6:AH:300:GLY:O	6:AH:304:THR:HG22	1.98	0.63
2:BB:3033:VAL:O	2:BB:3036:THR:HG22	1.99	0.63
7:AQ:533:GLU:O	7:AQ:536:THR:HG22	1.98	0.63
5:AG:288:LEU:HD13	5:AG:309:LEU:HD23	1.81	0.63
7:BQ:3039:HIS:HD2	7:BQ:3108:GLY:HA3	1.62	0.63
1:BA:3013:LEU:HG	1:BA:3015:LEU:HD13	1.80	0.63
7:AQ:513:ARG:HH12	7:AQ:516:ASN:HA	1.64	0.63
2:AB:229:ALA:HA	2:AB:282:ASN:OD1	1.98	0.63
2:AB:68:PRO:O	2:AB:69:LEU:HD23	1.99	0.63
5:BG:3288:LEU:HD13	5:BG:3309:LEU:HD23	1.81	0.63
5:AG:208:LYS:HD3	5:AG:393:ASP:HB2	1.80	0.63
1:BA:3184:LEU:HD12	1:BA:3409:VAL:HG12	1.80	0.63
8:AZ:160:THR:O	8:AZ:161:LYS:HG3	1.99	0.63
2:AB:287:ARG:HB2	2:AB:314:VAL:HG11	1.81	0.63
4:BE:3073:ILE:HG12	4:BE:3083:ILE:HG12	1.80	0.63
2:BB:3201:GLY:H	3:BD:3510:LEU:HD21	1.63	0.63
1:BA:3483:ALA:O	1:BA:3486:MET:HB2	1.98	0.63
6:BH:3300:GLY:O	6:BH:3304:THR:HG22	1.98	0.63
5:BG:3208:LYS:HD3	5:BG:3393:ASP:HB2	1.79	0.63
1:BA:3277:GLU:HA	1:BA:3280:ILE:HD12	1.79	0.63
8:AZ:154:ALA:HB3	8:AZ:171:THR:HG23	1.78	0.63
4:AE:43:GLY:H	4:AE:46:ALA:HB3	1.62	0.63
5:BG:3110:TYR:HE2	5:BG:3444:ALA:HB2	1.63	0.63
1:BA:3485:GLN:HA	1:BA:3488:LYS:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3382:ARG:HE	2:BB:3386:ASP:CG	2.01	0.63
3:BD:3039:LEU:HD13	3:BD:3098:ILE:HD12	1.81	0.63
3:BD:3276:LYS:HE2	3:BD:3280:LYS:HD3	1.79	0.63
2:AB:268:LYS:HZ1	4:AE:299:GLN:HB2	1.63	0.63
2:BB:3006:PHE:HB3	2:BB:3010:VAL:CG2	2.28	0.63
6:BH:3342:LYS:H	6:BH:3345:HIS:HD2	1.46	0.63
6:BH:3257:ALA:HB1	7:BQ:3265:VAL:O	1.99	0.63
2:BB:3482:MET:SD	2:BB:3487:ILE:HD12	2.38	0.63
1:AA:126:ILE:HD13	1:AA:536:VAL:HG13	1.80	0.63
2:BB:3234:ALA:HA	2:BB:3325:VAL:O	1.97	0.63
2:AB:350:GLU:HG2	3:AD:402:ARG:HH12	1.63	0.63
1:BA:3487:ALA:HB1	1:BA:3493:LYS:CA	2.29	0.62
5:AG:402:VAL:HA	5:AG:405:ASN:ND2	2.14	0.62
2:BB:3216:LYS:HE2	2:BB:3307:GLU:O	1.99	0.62
5:BG:3457:ILE:HB	5:BG:3484:ILE:HD13	1.81	0.62
2:BB:3150:ARG:HD3	2:BB:3182:LEU:HD21	1.80	0.62
3:AD:74:VAL:HA	3:AD:77:MET:HG3	1.80	0.62
7:BQ:3117:LEU:HB3	7:BQ:3122:LEU:HD12	1.80	0.62
1:AA:242:VAL:HA	1:AA:294:GLN:HE22	1.63	0.62
4:AE:251:HIS:HB3	4:AE:254:MET:HG3	1.80	0.62
3:BD:3198:LYS:HB2	3:BD:3387:ILE:CG2	2.29	0.62
2:AB:132:LEU:HD23	2:AB:498:VAL:HG12	1.80	0.62
6:AH:396:ALA:O	6:AH:399:ILE:HG22	2.00	0.62
2:AB:33:VAL:O	2:AB:36:THR:HG22	1.99	0.62
4:AE:162:GLU:HG3	4:AE:438:ARG:NH1	2.13	0.62
8:AZ:281:LYS:HD2	8:AZ:293:PHE:HA	1.81	0.62
2:AB:6:PHE:HB3	2:AB:10:VAL:CG2	2.28	0.62
4:BE:3254:MET:SD	4:BE:3341:PRO:HA	2.39	0.62
7:AQ:436:LYS:HE3	7:AQ:440:ARG:NH1	2.13	0.62
5:AG:507:GLN:HB3	5:AG:511:LYS:HE2	1.80	0.62
6:AH:342:LYS:H	6:AH:345:HIS:HD2	1.46	0.62
7:AQ:526:PHE:O	7:AQ:530:VAL:HG23	2.00	0.62
1:BA:3242:VAL:HA	1:BA:3294:GLN:HE22	1.63	0.62
2:AB:216:LYS:HE2	2:AB:307:GLU:O	1.99	0.62
5:BG:3243:VAL:N	5:BG:3349:GLY:HA3	2.14	0.62
7:BQ:3502:ASP:O	7:BQ:3506:ASP:HB2	2.00	0.62
7:AQ:117:LEU:HB3	7:AQ:122:LEU:HD12	1.80	0.62
3:BD:3042:LYS:HG3	3:BD:3458:ALA:HA	1.82	0.62
2:BB:3132:LEU:HD23	2:BB:3498:VAL:HG12	1.80	0.62
2:BB:3087:GLU:HA	4:BE:3386:GLY:HA3	1.82	0.62
5:BG:3039:LEU:HD22	5:BG:3098:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:201:GLY:H	3:AD:510:LEU:HD21	1.63	0.62
7:AQ:248:ALA:HB3	7:AQ:299:ILE:HG22	1.80	0.62
1:AA:184:LEU:HD12	1:AA:409:VAL:HG12	1.80	0.62
7:AQ:54:ILE:HG12	7:AQ:64:ILE:HG12	1.82	0.62
7:BQ:3054:ILE:HG12	7:BQ:3064:ILE:HG12	1.82	0.62
5:AG:39:LEU:HD22	5:AG:98:ILE:HD12	1.81	0.62
3:AD:39:LEU:HD13	3:AD:98:ILE:HD12	1.81	0.62
8:BZ:3459:VAL:HG21	8:BZ:3466:PRO:HA	1.82	0.62
4:AE:156:LEU:HD11	4:AE:457:GLU:HG3	1.80	0.62
1:AA:13:LEU:HG	1:AA:15:LEU:HD13	1.81	0.62
6:AH:257:ALA:HB1	7:AQ:265:VAL:O	1.99	0.62
1:BA:3183:ALA:HB2	1:BA:3218:LEU:HD11	1.81	0.62
1:AA:274:ARG:HH22	5:AG:279:GLN:NE2	1.97	0.62
3:BD:3217:GLN:NE2	3:BD:3316:ILE:HD13	2.15	0.62
1:BA:3476:LYS:HD3	1:BA:3509:ILE:HD13	1.80	0.62
7:AQ:41:MET:HE2	7:AQ:71:MET:HB3	1.81	0.62
5:AG:110:TYR:HE2	5:AG:444:ALA:HB2	1.63	0.62
7:AQ:257:ALA:HB2	7:AQ:343:ARG:NH2	2.03	0.62
5:BG:3451:CYS:SG	5:BG:3452:ILE:HD12	2.40	0.62
4:AE:366:PHE:O	4:AE:369:LEU:HD23	2.00	0.62
8:AZ:227:ARG:NH2	8:AZ:353:LEU:HD21	2.15	0.62
1:BA:3121:HIS:HE2	3:BD:3042:LYS:HB3	1.65	0.62
2:BB:3411:MET:SD	2:BB:3498:VAL:HG21	2.40	0.62
8:AZ:60:LYS:H	8:AZ:91:THR:HG21	1.65	0.62
2:AB:223:PRO:HD2	2:AB:304:ASN:OD1	1.99	0.62
3:BD:3237:ILE:HG23	3:BD:3239:PHE:HB3	1.81	0.62
6:BH:3396:ALA:O	6:BH:3399:ILE:HG22	2.00	0.62
5:AG:385:SER:HB3	5:AG:388:ILE:HG13	1.82	0.62
3:AD:237:ILE:HG23	3:AD:239:PHE:HB3	1.81	0.62
4:AE:254:MET:SD	4:AE:341:PRO:HA	2.39	0.62
5:AG:243:VAL:N	5:AG:349:GLY:HA3	2.14	0.62
4:BE:3086:ASP:HB3	4:BE:3089:THR:OG1	2.00	0.62
7:BQ:3513:ARG:HH12	7:BQ:3516:ASN:HA	1.64	0.62
1:AA:476:LYS:HD3	1:AA:509:ILE:HD13	1.80	0.62
2:BB:3223:PRO:HD2	2:BB:3304:ASN:OD1	1.99	0.62
4:BE:3259:LEU:HD13	4:BE:3261:LYS:H	1.64	0.62
4:BE:3268:LYS:HB3	4:BE:3374:LEU:HD13	1.80	0.62
4:AE:413:LYS:CE	4:AE:413:LYS:H	2.04	0.62
2:BB:3234:ALA:O	2:BB:3286:ASN:HA	2.00	0.62
8:BZ:3227:ARG:NH2	8:BZ:3353:LEU:HD21	2.15	0.62
2:BB:3268:LYS:HZ1	4:BE:3299:GLN:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:3385:SER:HB3	5:BG:3388:ILE:HG13	1.82	0.62
5:BG:3507:GLN:HB3	5:BG:3511:LYS:HE2	1.80	0.62
4:BE:3158:ILE:HG12	4:BE:3539:LEU:HD11	1.82	0.62
4:AE:280:LYS:HG3	6:AH:267:TYR:OH	2.00	0.62
2:BB:3068:PRO:O	2:BB:3069:LEU:HD23	1.99	0.62
3:AD:198:LYS:HB2	3:AD:387:ILE:CG2	2.29	0.62
4:AE:86:ASP:HB3	4:AE:89:THR:OG1	2.00	0.62
8:BZ:3160:THR:O	8:BZ:3161:LYS:HG3	1.99	0.62
2:AB:150:ARG:HD3	2:AB:182:LEU:HD21	1.80	0.62
3:BD:3213:VAL:HG11	3:BD:3327:GLY:HA3	1.82	0.62
1:AA:136:ALA:O	1:AA:140:ILE:HG12	2.00	0.61
8:AZ:61:VAL:O	8:AZ:65:GLU:HB2	2.00	0.61
4:AE:73:ILE:HG12	4:AE:83:ILE:HG12	1.80	0.61
1:BA:3431:ILE:HG12	1:BA:3482:ALA:HA	1.81	0.61
8:BZ:3329:GLN:NE2	8:BZ:3336:ALA:H	1.98	0.61
8:BZ:3061:VAL:O	8:BZ:3065:GLU:HB2	2.00	0.61
8:AZ:14:ARG:HB3	8:AZ:14:ARG:NH1	2.15	0.61
3:AD:412:ALA:O	3:AD:417:PRO:HD3	2.00	0.61
2:BB:3083:VAL:HG23	4:BE:3413:LYS:HZ1	1.65	0.61
7:BQ:3436:LYS:HE3	7:BQ:3440:ARG:NH1	2.13	0.61
2:AB:234:ALA:O	2:AB:286:ASN:HA	2.00	0.61
4:BE:3366:PHE:O	4:BE:3369:LEU:HD23	2.00	0.61
7:AQ:420:LEU:HD21	7:AQ:521:LEU:HA	1.83	0.61
5:AG:457:ILE:HB	5:AG:484:ILE:HD13	1.81	0.61
4:AE:158:ILE:HG12	4:AE:539:LEU:HD11	1.82	0.61
3:BD:3412:ALA:O	3:BD:3417:PRO:HD3	2.00	0.61
7:BQ:3257:ALA:HB2	7:BQ:3343:ARG:NH2	2.03	0.61
2:AB:83:VAL:HG23	4:AE:413:LYS:HZ1	1.66	0.61
7:BQ:3248:ALA:HB3	7:BQ:3299:ILE:HG22	1.80	0.61
1:BA:3233:MET:HB2	1:BA:3234:PRO:HD2	1.81	0.61
3:BD:3246:PRO:HB2	3:BD:3250:ASN:HB3	1.82	0.61
7:BQ:3041:MET:HE2	7:BQ:3071:MET:HB3	1.82	0.61
3:AD:42:LYS:HG3	3:AD:458:ALA:HA	1.82	0.61
1:AA:485:GLN:HA	1:AA:488:LYS:HB3	1.81	0.61
1:AA:498:ARG:H	1:AA:498:ARG:HD3	1.64	0.61
2:AB:411:MET:SD	2:AB:498:VAL:HG21	2.40	0.61
1:AA:431:ILE:HG12	1:AA:482:ALA:HA	1.81	0.61
3:BD:3360:ILE:HD13	3:BD:3380:ARG:HH21	1.65	0.61
6:BH:3133:VAL:O	6:BH:3137:VAL:HG23	2.01	0.61
7:BQ:3420:LEU:HD21	7:BQ:3521:LEU:HA	1.83	0.61
2:AB:76:VAL:HG12	2:AB:77:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3074:VAL:HA	3:BD:3077:MET:HG3	1.80	0.61
1:AA:183:ALA:HB2	1:AA:218:LEU:HD11	1.81	0.61
1:AA:380:HIS:C	1:AA:382:SER:H	2.04	0.61
1:BA:3136:ALA:O	1:BA:3140:ILE:HG12	2.00	0.61
2:AB:254:SER:OG	2:AB:257:LYS:HD3	2.01	0.61
2:BB:3287:ARG:HB2	2:BB:3314:VAL:HG11	1.81	0.61
6:AH:240:LYS:HB2	6:AH:290:ALA:HA	1.82	0.61
8:BZ:3014:ARG:NH1	8:BZ:3014:ARG:HB3	2.15	0.61
5:AG:58:THR:HG23	5:AG:60:ASP:N	2.13	0.61
1:AA:326:LEU:HB3	1:AA:337:LEU:HD21	1.83	0.61
4:BE:3320:VAL:HG12	4:BE:3341:PRO:HB2	1.82	0.61
5:BG:3232:PRO:HB2	8:BZ:3329:GLN:OE1	2.00	0.61
5:BG:3208:LYS:HB3	5:BG:3389:LEU:HD13	1.82	0.61
5:AG:208:LYS:HB3	5:AG:389:LEU:HD13	1.82	0.61
5:BG:3117:HIS:CE1	5:BG:3119:VAL:HG23	2.35	0.61
1:BA:3498:ARG:HD3	1:BA:3498:ARG:H	1.64	0.61
8:BZ:3103:ARG:HB2	8:BZ:3103:ARG:NH1	2.16	0.61
3:AD:246:PRO:HB2	3:AD:250:ASN:HB3	1.82	0.61
4:BE:3346:VAL:CG1	4:BE:3350:GLU:HB3	2.31	0.61
1:AA:187:VAL:HB	1:AA:199:PRO:HG3	1.83	0.61
3:BD:3041:PRO:HB2	3:BD:3484:VAL:HG21	1.82	0.61
2:AB:231:ILE:HG22	2:AB:283:THR:OG1	2.00	0.61
4:AE:521:ASP:OD2	4:AE:524:GLU:HB2	2.01	0.61
4:BE:3521:ASP:OD2	4:BE:3524:GLU:HB2	2.01	0.61
2:AB:32:LEU:HD12	2:AB:44:LYS:HE2	1.82	0.61
4:BE:3413:LYS:CE	4:BE:3413:LYS:H	2.04	0.61
4:AE:320:VAL:HG12	4:AE:341:PRO:HB2	1.83	0.61
1:BA:3233:MET:HE3	1:BA:3307:LEU:HD22	1.83	0.61
1:AA:68:THR:HG21	1:AA:400:ARG:NH1	2.16	0.61
5:AG:117:HIS:CE1	5:AG:119:VAL:HG23	2.35	0.61
3:BD:3025:ILE:HG23	3:BD:3104:LEU:HB3	1.83	0.61
7:BQ:3526:PHE:O	7:BQ:3530:VAL:HG23	2.00	0.61
4:AE:168:ILE:HD13	4:AE:179:PHE:HB3	1.83	0.61
3:AD:195:ARG:HH22	3:AD:320:GLU:HG2	1.65	0.61
8:BZ:3281:LYS:HD2	8:BZ:3293:PHE:HA	1.81	0.61
4:BE:3168:ILE:HD13	4:BE:3179:PHE:HB3	1.83	0.61
7:BQ:3154:ASN:ND2	7:BQ:3190:LEU:HD13	2.16	0.61
7:BQ:3239:LEU:HD12	7:BQ:3358:VAL:HG11	1.83	0.61
7:AQ:502:ASP:O	7:AQ:506:ASP:HB2	2.00	0.61
1:AA:161:LYS:HA	1:AA:164:MET:HE2	1.81	0.61
4:AE:244:ILE:HG12	4:AE:405:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3202:LYS:HD2	3:BD:3129:LYS:HE2	1.83	0.60
2:AB:87:GLU:HA	4:AE:386:GLY:HA3	1.82	0.60
2:BB:3032:LEU:HD12	2:BB:3044:LYS:HE2	1.82	0.60
5:AG:58:THR:HG21	5:AG:63:ALA:HB3	1.83	0.60
4:BE:3280:LYS:HG3	6:BH:3267:TYR:OH	2.00	0.60
1:BA:3326:LEU:HB3	1:BA:3337:LEU:HD21	1.83	0.60
3:AD:217:GLN:NE2	3:AD:316:ILE:HD13	2.15	0.60
5:AG:303:ASP:HA	5:AG:306:GLN:NE2	2.16	0.60
5:BG:3303:ASP:HA	5:BG:3306:GLN:NE2	2.16	0.60
5:AG:199:ASP:OD2	5:AG:202:ARG:HB2	2.01	0.60
6:BH:3169:LYS:HB3	6:BH:3392:SER:OG	2.02	0.60
3:BD:3173:LEU:HD21	3:BD:3377:VAL:HG21	1.83	0.60
6:AH:133:VAL:O	6:AH:137:VAL:HG23	2.01	0.60
8:BZ:3060:LYS:H	8:BZ:3091:THR:HG21	1.65	0.60
2:BB:3076:VAL:HG12	2:BB:3077:LEU:HD23	1.82	0.60
5:BG:3199:ASP:OD2	5:BG:3202:ARG:HB2	2.01	0.60
5:AG:451:CYS:SG	5:AG:452:ILE:HD12	2.40	0.60
5:BG:3058:THR:HG21	5:BG:3063:ALA:HB3	1.83	0.60
4:AE:320:VAL:HG21	4:AE:380:ILE:HD12	1.83	0.60
8:AZ:236:LEU:O	8:AZ:297:ASN:HA	2.02	0.60
8:AZ:329:GLN:NE2	8:AZ:336:ALA:H	1.98	0.60
3:AD:360:ILE:HD13	3:AD:380:ARG:HH21	1.65	0.60
2:AB:248:THR:HG22	4:AE:287:LEU:HD22	1.84	0.60
4:AE:259:LEU:HD13	4:AE:261:LYS:H	1.65	0.60
5:AG:48:LEU:HD21	5:AG:64:ILE:HG23	1.83	0.60
1:BA:3243:LYS:H	1:BA:3294:GLN:NE2	1.99	0.60
8:AZ:459:VAL:HG21	8:AZ:466:PRO:HA	1.82	0.60
8:AZ:105:ALA:O	8:AZ:109:ILE:HG12	2.01	0.60
3:BD:3278:ILE:HA	3:BD:3339:PHE:CE2	2.36	0.60
3:AD:41:PRO:HB2	3:AD:484:VAL:HG21	1.82	0.60
1:AA:121:HIS:HE2	3:AD:42:LYS:HB3	1.65	0.60
6:BH:3181:MET:SD	6:BH:3376:LEU:HD12	2.41	0.60
6:AH:181:MET:SD	6:AH:376:LEU:HD12	2.41	0.60
3:BD:3355:SER:O	3:BD:3356:ASP:HB2	2.02	0.60
1:BA:3419:VAL:CG2	1:BA:3521:THR:HG22	2.31	0.60
1:BA:3068:THR:HG21	1:BA:3400:ARG:NH1	2.16	0.60
3:BD:3245:LYS:HD2	3:BD:3294:ARG:HB3	1.84	0.60
3:AD:25:ILE:HG23	3:AD:104:LEU:HB3	1.83	0.60
1:BA:3206:LEU:HD21	1:BA:3225:ASN:HD22	1.67	0.60
6:BH:3240:LYS:HB2	6:BH:3290:ALA:HA	1.82	0.60
7:AQ:257:ALA:CB	7:AQ:343:ARG:HH22	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:251:HIS:HD2	4:AE:253:GLN:H	1.50	0.60
5:AG:232:PRO:HB2	8:AZ:329:GLN:OE1	2.00	0.60
8:BZ:3321:LYS:O	8:BZ:3324:ASN:HB2	2.02	0.60
7:BQ:3234:GLY:HA2	7:BQ:3310:LEU:HD21	1.83	0.60
8:AZ:340:VAL:HG23	8:AZ:343:LEU:HD13	1.83	0.60
5:AG:82:SER:HB2	5:AG:97:ILE:HD11	1.84	0.60
4:BE:3551:ILE:HD11	6:BH:3062:ILE:HD13	1.84	0.60
7:BQ:3204:VAL:HG23	7:BQ:3405:VAL:CG1	2.32	0.60
8:AZ:103:ARG:NH1	8:AZ:103:ARG:HB2	2.15	0.60
3:AD:245:LYS:HD2	3:AD:294:ARG:HB3	1.84	0.60
4:BE:3244:ILE:HG12	4:BE:3405:THR:HG21	1.82	0.60
4:BE:3292:VAL:O	4:BE:3296:GLN:HB2	2.01	0.60
8:BZ:3006:LEU:C	8:BZ:3007:ASN:HD22	2.05	0.60
4:BE:3200:PHE:HD1	4:BE:3423:LEU:HD13	1.67	0.60
1:AA:533:GLU:OE2	3:AD:204:ILE:HG13	2.02	0.60
3:AD:338:LEU:CD2	3:AD:343:ARG:HH22	2.11	0.60
3:BD:3338:LEU:CD2	3:BD:3343:ARG:HH22	2.11	0.60
7:BQ:3429:GLU:HG2	7:BQ:3482:HIS:HD2	1.67	0.60
1:AA:419:VAL:CG2	1:AA:521:THR:HG22	2.31	0.60
4:BE:3362:ILE:HB	6:BH:3305:GLN:HE21	1.66	0.60
4:AE:362:ILE:HB	6:AH:305:GLN:HE21	1.66	0.60
7:BQ:3226:MET:HE1	7:BQ:3332:LEU:HB2	1.84	0.60
5:BG:3450:GLU:O	5:BG:3453:PRO:HD2	2.02	0.60
7:BQ:3308:LEU:O	7:BQ:3311:HIS:HB3	2.02	0.60
2:BB:3489:GLU:HG2	2:BB:3493:LEU:HD23	1.83	0.60
3:AD:219:ALA:HA	3:AD:313:VAL:HG22	1.84	0.60
7:AQ:341:LEU:HD21	7:AQ:351:GLU:HB3	1.83	0.60
7:AQ:154:ASN:ND2	7:AQ:190:LEU:HD13	2.16	0.60
5:AG:28:ALA:HA	5:AG:78:MET:HG3	1.83	0.60
6:AH:229:PHE:HA	6:AH:232:GLN:HE21	1.67	0.60
1:AA:476:LYS:HG2	1:AA:480:TYR:HE1	1.66	0.60
6:AH:169:LYS:HB3	6:AH:392:SER:OG	2.02	0.60
7:AQ:234:GLY:HA2	7:AQ:310:LEU:HD21	1.83	0.59
4:BE:3323:CYS:HB3	4:BE:3327:PHE:HE1	1.66	0.59
8:BZ:3236:LEU:O	8:BZ:3297:ASN:HA	2.02	0.59
3:BD:3217:GLN:HE21	3:BD:3316:ILE:HA	1.67	0.59
3:AD:278:ILE:HA	3:AD:339:PHE:CE2	2.36	0.59
8:AZ:344:SER:CB	8:AZ:346:GLN:HE21	2.15	0.59
1:BA:3476:LYS:HG2	1:BA:3480:TYR:HE1	1.66	0.59
8:AZ:221:HIS:HB3	8:AZ:224:MET:CG	2.32	0.59
5:BG:3479:ASN:ND2	5:BG:3480:PHE:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:202:LYS:HD2	3:AD:129:LYS:HE2	1.83	0.59
5:AG:479:ASN:ND2	5:AG:480:PHE:H	2.00	0.59
1:AA:243:LYS:H	1:AA:294:GLN:NE2	1.99	0.59
5:AG:183:ARG:HH11	5:AG:183:ARG:HB3	1.67	0.59
1:AA:206:LEU:HD21	1:AA:225:ASN:HD22	1.67	0.59
3:AD:213:VAL:HG11	3:AD:327:GLY:HA3	1.82	0.59
7:AQ:247:VAL:HG12	7:AQ:298:CYS:HB3	1.83	0.59
4:AE:200:PHE:HD1	4:AE:423:LEU:HD13	1.67	0.59
2:BB:3143:SER:HA	2:BB:3398:THR:HG21	1.84	0.59
4:AE:346:VAL:CG1	4:AE:350:GLU:HB3	2.31	0.59
4:AE:323:CYS:HB3	4:AE:327:PHE:HE1	1.66	0.59
3:AD:173:LEU:HD21	3:AD:377:VAL:HG21	1.83	0.59
1:BA:3187:VAL:HB	1:BA:3199:PRO:HG3	1.83	0.59
7:BQ:3236:VAL:CG2	7:BQ:3319:LEU:HA	2.32	0.59
7:AQ:226:MET:HE1	7:AQ:332:LEU:HB2	1.84	0.59
2:BB:3231:ILE:HG22	2:BB:3283:THR:OG1	2.00	0.59
2:BB:3413:LYS:HD3	2:BB:3464:TYR:HA	1.84	0.59
7:AQ:308:LEU:O	7:AQ:311:HIS:HB3	2.02	0.59
7:AQ:239:LEU:HD12	7:AQ:358:VAL:HG11	1.83	0.59
6:AH:385:VAL:O	6:AH:389:VAL:HG23	2.03	0.59
4:BE:3333:HIS:O	4:BE:3336:LEU:HB3	2.03	0.59
4:AE:281:PRO:HD3	6:AH:267:TYR:HE1	1.68	0.59
4:BE:3320:VAL:HG21	4:BE:3380:ILE:HD12	1.83	0.59
1:BA:3136:ALA:HB2	1:BA:3433:LEU:HD11	1.85	0.59
7:AQ:204:VAL:HG23	7:AQ:405:VAL:HG11	1.83	0.59
3:BD:3195:ARG:HH22	3:BD:3320:GLU:HG2	1.65	0.59
5:AG:291:ARG:NH1	5:AG:291:ARG:HB2	2.18	0.59
2:BB:3254:SER:OG	2:BB:3257:LYS:HD3	2.01	0.59
1:BA:3238:ALA:HB2	1:BA:3242:VAL:HB	1.85	0.59
6:BH:3094:VAL:HG11	6:BH:3502:VAL:HG22	1.85	0.59
1:BA:3274:ARG:HH22	5:BG:3279:GLN:NE2	1.97	0.59
5:AG:229:VAL:HG21	5:AG:234:MET:HB3	1.84	0.59
8:AZ:321:LYS:O	8:AZ:324:ASN:HB2	2.02	0.59
5:AG:389:LEU:HA	5:AG:392:ILE:HD12	1.85	0.59
1:BA:3270:LEU:HD13	5:BG:3261:ILE:HD11	1.83	0.59
6:BH:3229:PHE:HA	6:BH:3232:GLN:HE21	1.67	0.59
2:AB:489:GLU:HG2	2:AB:493:LEU:HD23	1.83	0.59
2:BB:3500:SER:HA	4:BE:3411:SER:OG	2.03	0.59
3:BD:3219:ALA:HA	3:BD:3313:VAL:HG22	1.84	0.59
1:BA:3276:ARG:O	1:BA:3280:ILE:HG13	2.02	0.59
7:BQ:3204:VAL:HG23	7:BQ:3405:VAL:HG11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:143:SER:HA	2:AB:398:THR:HG21	1.83	0.59
8:BZ:3133:LEU:HD13	8:BZ:3510:TYR:CE1	2.37	0.59
4:AE:301:TYR:O	4:AE:305:LYS:HB2	2.02	0.59
3:AD:262:LYS:O	3:AD:266:GLU:HB2	2.02	0.59
3:BD:3262:LYS:O	3:BD:3266:GLU:HB2	2.02	0.59
1:AA:270:LEU:HD13	5:AG:261:ILE:HD11	1.83	0.59
8:BZ:3105:ALA:O	8:BZ:3109:ILE:HG12	2.01	0.59
6:AH:512:GLU:OE2	7:AQ:390:THR:HG23	2.03	0.59
8:AZ:133:LEU:HD13	8:AZ:510:TYR:CE1	2.37	0.59
3:AD:420:GLU:HG2	3:AD:478:LEU:HD12	1.84	0.59
1:AA:519:GLU:OE1	1:AA:524:LYS:HE3	2.03	0.59
8:BZ:3221:HIS:HB3	8:BZ:3224:MET:CG	2.32	0.59
4:AE:324:GLN:O	4:AE:345:TRP:HA	2.02	0.59
6:BH:3218:VAL:HG11	6:BH:3325:ARG:O	2.03	0.59
1:BA:3380:HIS:C	1:BA:3382:SER:H	2.04	0.59
1:AA:276:ARG:O	1:AA:280:ILE:HG13	2.02	0.59
6:BH:3012:VAL:HG22	6:BH:3013:LEU:N	2.18	0.59
4:AE:521:ASP:O	4:AE:525:LEU:HD23	2.03	0.59
7:AQ:204:VAL:HG23	7:AQ:405:VAL:CG1	2.32	0.59
2:BB:3348:LEU:HD23	2:BB:3353:PHE:CD2	2.38	0.59
4:AE:551:ILE:HD11	6:AH:62:ILE:HD13	1.84	0.59
7:BQ:3247:VAL:HG12	7:BQ:3298:CYS:HB3	1.83	0.59
7:BQ:3023:ASN:HA	7:BQ:3027:GLN:HB2	1.85	0.59
2:AB:348:LEU:HD23	2:AB:353:PHE:CD2	2.37	0.59
3:AD:224:GLY:O	3:AD:226:PRO:HD3	2.03	0.59
4:AE:292:VAL:O	4:AE:296:GLN:HB2	2.01	0.59
5:AG:93:THR:O	5:AG:96:VAL:HG12	2.03	0.59
1:BA:3161:LYS:HA	1:BA:3164:MET:HE2	1.83	0.59
3:BD:3420:GLU:HG2	3:BD:3478:LEU:HD12	1.84	0.59
3:BD:3102:ALA:CB	3:BD:3449:VAL:HG11	2.33	0.59
6:BH:3512:GLU:OE2	7:BQ:3390:THR:HG23	2.03	0.59
8:AZ:19:LEU:O	8:AZ:23:VAL:HG23	2.03	0.59
7:BQ:3341:LEU:HD21	7:BQ:3351:GLU:HB3	1.83	0.59
7:AQ:236:VAL:CG2	7:AQ:319:LEU:HA	2.32	0.59
8:BZ:3296:ILE:HD13	8:BZ:3328:LEU:HD21	1.85	0.59
8:BZ:3036:ASN:ND2	8:BZ:3036:ASN:H	2.01	0.59
1:BA:3400:ARG:HG3	1:BA:3400:ARG:HH11	1.68	0.59
4:AE:333:HIS:O	4:AE:336:LEU:HB3	2.03	0.59
1:BA:3533:GLU:OE2	3:BD:3204:ILE:HG13	2.02	0.59
6:BH:3385:VAL:O	6:BH:3389:VAL:HG23	2.03	0.59
5:AG:450:GLU:O	5:AG:453:PRO:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AQ:290:GLU:OE2	7:AQ:345:GLY:HA2	2.03	0.58
7:AQ:429:GLU:HG2	7:AQ:482:HIS:HD2	1.67	0.58
2:BB:3220:ASN:O	3:BD:3322:GLU:HG3	2.03	0.58
1:AA:111:ARG:HD2	1:AA:450:GLU:OE1	2.03	0.58
1:BA:3357:LEU:HB2	1:BA:3378:SER:HB3	1.84	0.58
4:AE:284:LYS:HD3	6:AH:258:GLU:HG2	1.86	0.58
1:AA:136:ALA:HB2	1:AA:433:LEU:HD11	1.85	0.58
3:BD:3224:GLY:O	3:BD:3226:PRO:HD3	2.03	0.58
6:AH:12:VAL:HG22	6:AH:13:LEU:N	2.18	0.58
1:AA:400:ARG:NH1	1:AA:400:ARG:HG3	2.18	0.58
5:AG:159:ILE:HD11	5:AG:399:ALA:HB2	1.86	0.58
4:BE:3158:ILE:HG23	4:BE:3535:LYS:HG3	1.85	0.58
4:BE:3521:ASP:O	4:BE:3525:LEU:HD23	2.03	0.58
4:BE:3543:GLN:HG3	4:BE:3544:LEU:N	2.19	0.58
4:BE:3378:SER:HB2	4:BE:3397:GLN:HA	1.85	0.58
1:BA:3111:ARG:HD2	1:BA:3450:GLU:OE1	2.03	0.58
4:BE:3183:ALA:HA	4:BE:3528:VAL:HG23	1.86	0.58
2:AB:500:SER:HA	4:AE:411:SER:OG	2.03	0.58
1:AA:487:ALA:HB1	1:AA:493:LYS:CA	2.29	0.58
8:AZ:296:ILE:HD13	8:AZ:328:LEU:HD21	1.85	0.58
1:AA:233:MET:HE3	1:AA:307:LEU:HD22	1.85	0.58
2:AB:311:PHE:O	2:AB:314:VAL:HG22	2.03	0.58
2:BB:3248:THR:HG22	4:BE:3287:LEU:HD22	1.84	0.58
8:BZ:3344:SER:CB	8:BZ:3346:GLN:HE21	2.15	0.58
9:AG:1001:ADP:O1B	10:AG:1002:BEF:F1	2.11	0.58
2:AB:220:ASN:O	3:AD:322:GLU:HG3	2.03	0.58
4:BE:3324:GLN:O	4:BE:3345:TRP:HA	2.02	0.58
8:AZ:6:LEU:C	8:AZ:7:ASN:HD22	2.05	0.58
7:BQ:3257:ALA:CB	7:BQ:3343:ARG:HH22	2.05	0.58
6:BH:3297:LEU:HB3	6:BH:3298:PRO:HD2	1.85	0.58
4:AE:284:LYS:HG2	6:AH:259:VAL:N	2.17	0.58
8:AZ:217:HIS:O	8:AZ:317:LEU:HG	2.04	0.58
7:BQ:3290:GLU:OE2	7:BQ:3345:GLY:HA2	2.03	0.58
8:BZ:3340:VAL:HG23	8:BZ:3343:LEU:HD13	1.83	0.58
7:AQ:191:PRO:HB3	7:AQ:380:ARG:HH22	1.68	0.58
4:AE:224:ILE:HG23	4:AE:404:VAL:HG23	1.85	0.58
5:BG:3093:THR:O	5:BG:3096:VAL:HG12	2.03	0.58
4:BE:3115:ILE:HG23	4:BE:3432:ASN:ND2	2.18	0.58
4:AE:115:ILE:HG23	4:AE:432:ASN:ND2	2.18	0.58
7:BQ:3289:LYS:HA	7:BQ:3316:TYR:HE2	1.68	0.58
7:AQ:289:LYS:HA	7:AQ:316:TYR:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3015:ALA:HB1	2:BB:3019:ARG:HH22	1.69	0.58
1:BA:3495:ARG:HD2	1:BA:3495:ARG:O	2.04	0.58
4:AE:284:LYS:CG	6:AH:259:VAL:H	2.16	0.58
2:BB:3311:PHE:O	2:BB:3314:VAL:HG22	2.03	0.58
5:BG:3183:ARG:HB3	5:BG:3183:ARG:HH11	1.67	0.58
4:BE:3284:LYS:HG2	6:BH:3259:VAL:N	2.17	0.58
5:BG:3159:ILE:HD11	5:BG:3399:ALA:HB2	1.86	0.58
4:AE:158:ILE:HG23	4:AE:535:LYS:HG3	1.85	0.58
4:BE:3226:MET:SD	4:BE:3423:LEU:HD23	2.44	0.58
9:BG:4001:ADP:O1B	10:BG:4002:BEF:F1	2.11	0.58
8:AZ:423:SER:O	8:AZ:427:ARG:HG3	2.04	0.58
1:BA:3519:GLU:OE1	1:BA:3524:LYS:HE3	2.03	0.58
1:AA:495:ARG:HD2	1:AA:495:ARG:O	2.04	0.58
5:BG:3048:LEU:HD21	5:BG:3064:ILE:HG23	1.83	0.58
4:AE:413:LYS:HB2	4:AE:414:MET:HE3	1.86	0.58
4:BE:3284:LYS:HD3	6:BH:3258:GLU:HG2	1.86	0.58
4:BE:3281:PRO:HD3	6:BH:3267:TYR:HE1	1.68	0.58
8:AZ:234:LEU:HB3	8:AZ:295:ILE:HG12	1.86	0.58
4:BE:3301:TYR:O	4:BE:3305:LYS:HB2	2.02	0.58
6:AH:218:VAL:HG11	6:AH:325:ARG:O	2.03	0.58
2:AB:413:LYS:HD3	2:AB:464:TYR:HA	1.84	0.58
8:AZ:85:GLU:O	8:AZ:86:ILE:HD12	2.04	0.58
3:BD:3396:ASP:O	3:BD:3400:VAL:HG23	2.04	0.58
2:BB:3203:LEU:HD11	2:BB:3376:THR:HG21	1.86	0.58
4:BE:3251:HIS:CD2	4:BE:3253:GLN:HB2	2.38	0.58
4:BE:3294:GLU:OE2	6:BH:3263:HIS:HA	2.04	0.58
5:BG:3028:ALA:HA	5:BG:3078:MET:HG3	1.83	0.58
5:AG:69:ASP:CB	8:AZ:537:GLY:HA2	2.34	0.58
3:AD:102:ALA:CB	3:AD:449:VAL:HG11	2.33	0.58
6:AH:19:ALA:HB2	6:AH:524:ILE:HG23	1.86	0.58
2:BB:3388:LEU:O	2:BB:3392:SER:HB3	2.03	0.58
1:AA:357:LEU:HB2	1:AA:378:SER:HB3	1.84	0.58
2:AB:255:THR:OG1	3:AD:266:GLU:HB3	2.04	0.58
6:BH:3164:THR:O	6:BH:3167:SER:HB3	2.04	0.58
8:AZ:236:LEU:HD23	8:AZ:237:ASN:N	2.19	0.58
5:BG:3229:VAL:HG21	5:BG:3234:MET:HB3	1.84	0.58
1:AA:184:LEU:CD2	1:AA:198:TYR:HB3	2.34	0.58
3:AD:217:GLN:HE21	3:AD:316:ILE:HA	1.67	0.58
3:AD:355:SER:O	3:AD:356:ASP:HB2	2.02	0.58
5:AG:259:THR:HG22	8:AZ:247:VAL:HG11	1.86	0.58
1:BA:3540:ARG:HD3	3:BD:3162:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:332:GLY:HA2	6:AH:346:LEU:O	2.04	0.58
7:AQ:251:THR:HB	7:AQ:342:PRO:HA	1.85	0.58
2:AB:15:ALA:HB1	2:AB:19:ARG:HH22	1.69	0.58
1:BA:3184:LEU:CD2	1:BA:3198:TYR:HB3	2.34	0.58
2:AB:244:LYS:CB	4:AE:278:PRO:HD2	2.33	0.58
6:AH:229:PHE:C	6:AH:231:GLN:H	2.07	0.58
6:AH:281:LYS:O	6:AH:284:GLN:HB2	2.04	0.58
1:AA:238:ALA:HB2	1:AA:242:VAL:HB	1.85	0.58
5:BG:3479:ASN:HD22	5:BG:3480:PHE:H	1.52	0.58
6:BH:3019:ALA:HB2	6:BH:3524:ILE:HG23	1.85	0.58
6:AH:412:GLY:HA3	6:AH:498:GLU:OE1	2.04	0.58
4:AE:378:SER:HB2	4:AE:397:GLN:HA	1.84	0.58
2:AB:388:LEU:O	2:AB:392:SER:HB3	2.03	0.58
6:AH:152:SER:O	6:AH:156:GLU:HB2	2.04	0.58
4:BE:3224:ILE:HG23	4:BE:3404:VAL:HG23	1.85	0.58
4:BE:3284:LYS:CG	6:BH:3259:VAL:H	2.16	0.58
8:BZ:3423:SER:O	8:BZ:3427:ARG:HG3	2.04	0.58
7:BQ:3191:PRO:HB3	7:BQ:3380:ARG:HH22	1.68	0.58
6:AH:229:PHE:HD1	6:AH:230:GLU:H	1.51	0.58
1:AA:400:ARG:HH11	1:AA:400:ARG:HG3	1.68	0.58
3:AD:195:ARG:NH2	3:AD:320:GLU:HG2	2.19	0.58
4:AE:229:ARG:O	4:AE:409:ARG:HD2	2.04	0.58
5:BG:3082:SER:HB2	5:BG:3097:ILE:HD11	1.84	0.58
3:AD:180:LYS:HD3	3:AD:375:VAL:HB	1.86	0.58
3:BD:3045:ASP:OD1	3:BD:3059:ASN:HB2	2.04	0.58
6:AH:526:ASN:HB2	7:AQ:56:VAL:O	2.04	0.58
1:BA:3217:LEU:HD23	1:BA:3217:LEU:H	1.69	0.58
8:BZ:3301:ILE:HG22	8:BZ:3306:LEU:HG	1.86	0.58
5:BG:3259:THR:HG22	8:BZ:3247:VAL:HG11	1.86	0.58
8:BZ:3217:HIS:O	8:BZ:3317:LEU:HG	2.04	0.57
2:AB:45:LEU:HB3	3:AD:524:ILE:HG12	1.86	0.57
8:BZ:3019:LEU:O	8:BZ:3023:VAL:HG23	2.03	0.57
1:AA:205:VAL:O	1:AA:206:LEU:HD12	2.03	0.57
3:BD:3195:ARG:NH2	3:BD:3320:GLU:HG2	2.19	0.57
6:AH:109:MET:HG2	6:AH:514:THR:HG23	1.86	0.57
6:BH:3109:MET:HG2	6:BH:3514:THR:HG23	1.86	0.57
8:BZ:3085:GLU:O	8:BZ:3086:ILE:HD12	2.04	0.57
2:BB:3255:THR:OG1	3:BD:3266:GLU:HB3	2.04	0.57
8:BZ:3236:LEU:HD23	8:BZ:3237:ASN:N	2.19	0.57
4:BE:3331:ALA:O	4:BE:3335:LEU:HD12	2.04	0.57
2:BB:3244:LYS:CB	4:BE:3278:PRO:HD2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3229:PHE:HD1	6:BH:3230:GLU:H	1.51	0.57
8:AZ:36:ASN:ND2	8:AZ:36:ASN:H	2.01	0.57
2:BB:3045:LEU:HB3	3:BD:3524:ILE:HG12	1.86	0.57
7:AQ:137:PHE:HE2	7:AQ:434:ILE:HA	1.69	0.57
2:AB:268:LYS:NZ	4:AE:299:GLN:HB2	2.19	0.57
2:AB:513:ASN:HD22	2:AB:514:ILE:N	2.03	0.57
8:BZ:3285:CYS:SG	8:BZ:3289:PRO:HG3	2.44	0.57
1:BA:3205:VAL:O	1:BA:3206:LEU:HD12	2.03	0.57
4:AE:226:MET:SD	4:AE:423:LEU:HD23	2.44	0.57
5:BG:3358:GLU:HG3	5:BG:3367:PHE:CE1	2.40	0.57
3:AD:45:ASP:OD1	3:AD:59:ASN:HB2	2.04	0.57
1:AA:67:ALA:HB2	1:AA:98:THR:HG21	1.87	0.57
2:AB:421:ASN:O	2:AB:422:ILE:HG23	2.04	0.57
7:AQ:223:ILE:CG2	7:AQ:372:LYS:HB3	2.33	0.57
5:BG:3296:ILE:HG12	5:BG:3317:LEU:HB2	1.86	0.57
4:AE:331:ALA:O	4:AE:335:LEU:HD12	2.04	0.57
7:BQ:3138:THR:HG23	7:BQ:3430:LEU:HD21	1.86	0.57
6:AH:297:LEU:HB3	6:AH:298:PRO:HD2	1.85	0.57
6:BH:3171:ILE:HD11	6:BH:3178:PHE:CE1	2.39	0.57
8:AZ:285:CYS:SG	8:AZ:289:PRO:HG3	2.44	0.57
5:BG:3337:VAL:HG21	5:BG:3347:ASP:OD2	2.05	0.57
6:BH:3332:GLY:HA2	6:BH:3346:LEU:O	2.04	0.57
6:BH:3152:SER:O	6:BH:3156:GLU:HB2	2.04	0.57
5:BG:3291:ARG:NH1	5:BG:3291:ARG:HB2	2.18	0.57
1:BA:3067:ALA:HB2	1:BA:3098:THR:HG21	1.87	0.57
6:AH:324:ASN:N	6:AH:324:ASN:HD22	2.03	0.57
7:BQ:3223:ILE:CG2	7:BQ:3372:LYS:HB3	2.34	0.57
4:AE:443:GLY:O	4:AE:512:VAL:HG23	2.05	0.57
7:AQ:246:LYS:HD2	7:AQ:295:GLY:HA3	1.86	0.57
1:BA:3400:ARG:NH1	1:BA:3400:ARG:HG3	2.18	0.57
7:AQ:23:ASN:HA	7:AQ:27:GLN:HB2	1.85	0.57
5:AG:358:GLU:HG3	5:AG:367:PHE:CE1	2.40	0.57
1:BA:3052:MET:SD	5:BG:3073:PRO:HB2	2.45	0.57
8:BZ:3275:LYS:HA	8:BZ:3278:ILE:HG12	1.86	0.57
4:AE:251:HIS:CD2	4:AE:253:GLN:HB2	2.38	0.57
4:BE:3346:VAL:HG12	4:BE:3350:GLU:HB3	1.87	0.57
8:AZ:219:GLY:H	8:AZ:356:GLN:HE22	1.53	0.57
6:AH:229:PHE:HA	6:AH:232:GLN:NE2	2.20	0.57
7:AQ:138:THR:HG23	7:AQ:430:LEU:HD21	1.86	0.57
4:BE:3051:ILE:HG13	4:BE:3134:LEU:HB2	1.86	0.57
3:AD:396:ASP:O	3:AD:400:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:64:SER:OG	4:AE:72:LYS:HE2	2.04	0.57
2:BB:3232:LEU:HB2	2:BB:3281:ILE:HG21	1.87	0.57
2:BB:3495:ARG:HB3	2:BB:3495:ARG:NH1	2.19	0.57
4:BE:3088:ALA:H	4:BE:3119:THR:HB	1.70	0.57
7:BQ:3347:PRO:HB2	7:BQ:3352:LEU:HD11	1.87	0.57
6:BH:3229:PHE:HA	6:BH:3232:GLN:NE2	2.20	0.57
7:BQ:3014:PHE:CD1	7:BQ:3015:LYS:HG3	2.40	0.57
5:AG:286:GLN:O	5:AG:343:LEU:HD23	2.05	0.57
2:AB:458:LYS:HB3	2:AB:479:ILE:HD13	1.86	0.57
4:AE:51:ILE:HG13	4:AE:134:LEU:HB2	1.86	0.57
8:AZ:141:THR:HG22	8:AZ:143:LEU:H	1.69	0.57
6:BH:3324:ASN:N	6:BH:3324:ASN:HD22	2.03	0.57
7:BQ:3010:ASN:N	7:BQ:3010:ASN:ND2	2.53	0.57
4:AE:284:LYS:CG	4:AE:285:HIS:H	2.18	0.57
4:AE:294:GLU:OE2	6:AH:263:HIS:HA	2.04	0.57
4:AE:281:PRO:HD3	6:AH:267:TYR:CE1	2.39	0.57
8:AZ:275:LYS:HA	8:AZ:278:ILE:HG12	1.86	0.57
8:BZ:3234:LEU:HB3	8:BZ:3295:ILE:HG12	1.86	0.57
5:AG:269:TRP:CD1	8:AZ:266:GLU:HA	2.40	0.57
7:AQ:347:PRO:HB2	7:AQ:352:LEU:HD11	1.86	0.57
2:AB:49:ALA:HA	3:AD:528:ARG:CZ	2.35	0.57
3:AD:326:LYS:HZ1	3:AD:373:PRO:HG2	1.68	0.57
3:BD:3180:LYS:HD3	3:BD:3375:VAL:HB	1.85	0.57
3:AD:465:VAL:O	3:AD:469:LEU:HB2	2.04	0.57
8:AZ:208:THR:HG23	8:AZ:379:LEU:HB3	1.87	0.57
4:BE:3064:SER:OG	4:BE:3072:LYS:HE2	2.04	0.57
6:AH:94:VAL:HG11	6:AH:502:VAL:HG22	1.84	0.57
1:AA:279:GLY:HA2	1:AA:282:LEU:HB3	1.86	0.57
1:BA:3494:ARG:HG3	1:BA:3495:ARG:HG3	1.87	0.57
1:AA:52:MET:SD	5:AG:73:PRO:HB2	2.45	0.57
2:BB:3421:ASN:O	2:BB:3422:ILE:HG23	2.04	0.57
4:AE:183:ALA:HA	4:AE:528:VAL:HG23	1.86	0.57
8:BZ:3208:THR:HG23	8:BZ:3379:LEU:HB3	1.87	0.57
7:AQ:10:ASN:N	7:AQ:10:ASN:ND2	2.53	0.57
5:BG:3263:ILE:O	8:BZ:3251:PHE:HA	2.05	0.57
7:BQ:3288:MET:SD	7:BQ:3313:LEU:HG	2.45	0.57
5:AG:337:VAL:HG21	5:AG:347:ASP:OD2	2.05	0.57
1:AA:288:ILE:HA	1:AA:349:THR:CG2	2.35	0.57
6:AH:171:ILE:HD11	6:AH:178:PHE:CE1	2.40	0.57
4:AE:543:GLN:HG3	4:AE:544:LEU:N	2.19	0.57
4:AE:521:ASP:OD1	4:AE:523:LYS:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3141:THR:HG22	8:BZ:3143:LEU:H	1.69	0.57
4:BE:3251:HIS:HD2	4:BE:3253:GLN:H	1.50	0.57
6:BH:3222:LYS:HD3	6:BH:3222:LYS:O	2.05	0.57
4:AE:346:VAL:HG12	4:AE:350:GLU:HB3	1.87	0.57
5:BG:3389:LEU:HA	5:BG:3392:ILE:HD12	1.85	0.57
7:AQ:288:MET:SD	7:AQ:313:LEU:HG	2.45	0.57
5:AG:296:ILE:HG12	5:AG:317:LEU:HB2	1.86	0.57
4:BE:3335:LEU:HD23	4:BE:3340:LEU:HB3	1.86	0.57
2:AB:75:LYS:HD2	4:AE:81:ILE:HD12	1.87	0.57
7:BQ:3137:PHE:HE2	7:BQ:3434:ILE:HA	1.70	0.57
7:BQ:3251:THR:HB	7:BQ:3342:PRO:HA	1.85	0.57
4:AE:449:THR:HG23	4:AE:507:ILE:HG13	1.87	0.57
7:BQ:3141:GLU:O	7:BQ:3145:MET:HG2	2.05	0.56
2:BB:3069:LEU:HD13	2:BB:3074:ALA:HB1	1.87	0.56
4:AE:88:ALA:H	4:AE:119:THR:HB	1.70	0.56
7:AQ:236:VAL:HG21	7:AQ:319:LEU:HA	1.87	0.56
4:AE:335:LEU:HD23	4:AE:340:LEU:HB3	1.86	0.56
8:BZ:3405:VAL:HG13	8:BZ:3411:ILE:HD13	1.87	0.56
3:AD:207:THR:HG22	3:AD:380:ARG:H	1.70	0.56
8:AZ:207:THR:HA	8:AZ:381:LYS:HG3	1.87	0.56
1:BA:3288:ILE:HA	1:BA:3349:THR:CG2	2.35	0.56
3:AD:237:ILE:HD12	3:AD:239:PHE:HB3	1.87	0.56
2:AB:373:THR:HG22	3:AD:81:VAL:HG22	1.87	0.56
1:BA:3340:SER:HB3	3:BD:3303:HIS:ND1	2.20	0.56
1:AA:340:SER:HB3	3:AD:303:HIS:ND1	2.20	0.56
4:BE:3284:LYS:CG	4:BE:3285:HIS:H	2.18	0.56
2:AB:69:LEU:HD13	2:AB:74:ALA:HB1	1.87	0.56
6:AH:164:THR:O	6:AH:167:SER:HB3	2.04	0.56
5:AG:263:ILE:O	8:AZ:251:PHE:HA	2.05	0.56
8:AZ:295:ILE:HD12	8:AZ:309:PHE:CE2	2.34	0.56
6:AH:319:SER:O	6:AH:322:ASP:HB2	2.05	0.56
6:BH:3156:GLU:O	6:BH:3160:ARG:HB2	2.06	0.56
4:AE:142:HIS:HB3	4:AE:145:LYS:HB2	1.87	0.56
2:AB:442:THR:HA	2:AB:456:VAL:HG21	1.87	0.56
3:BD:3232:ALA:HB1	3:BD:3284:ASN:HB3	1.87	0.56
1:AA:243:LYS:HD2	1:AA:292:GLY:HA3	1.87	0.56
3:BD:3256:ASP:HB2	3:BD:3259:GLN:CB	2.33	0.56
5:BG:3269:TRP:CD1	8:BZ:3266:GLU:HA	2.40	0.56
1:BA:3279:GLY:HA2	1:BA:3282:LEU:HB3	1.86	0.56
6:BH:3526:ASN:HB2	7:BQ:3056:VAL:O	2.04	0.56
6:BH:3229:PHE:C	6:BH:3231:GLN:H	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3281:LYS:O	6:BH:3284:GLN:HB2	2.04	0.56
5:BG:3069:ASP:CB	8:BZ:3537:GLY:HA2	2.34	0.56
6:BH:3011:VAL:HG12	6:BH:3012:VAL:H	1.70	0.56
7:AQ:14:PHE:CD1	7:AQ:15:LYS:HG3	2.40	0.56
4:BE:3521:ASP:OD1	4:BE:3523:LYS:HB3	2.05	0.56
5:AG:479:ASN:HD22	5:AG:480:PHE:H	1.52	0.56
4:AE:239:LEU:HD21	4:AE:404:VAL:HB	1.88	0.56
6:BH:3412:GLY:HA3	6:BH:3498:GLU:OE1	2.04	0.56
4:BE:3142:HIS:HB3	4:BE:3145:LYS:HB2	1.87	0.56
1:AA:540:ARG:HD3	3:AD:162:ILE:HG12	1.86	0.56
1:AA:207:LYS:HE2	1:AA:396:ASP:OD1	2.06	0.56
7:BQ:3495:LEU:H	7:BQ:3495:LEU:HD22	1.71	0.56
4:AE:94:MET:O	4:AE:96:LEU:HG	2.05	0.56
7:BQ:3433:ARG:HH21	7:BQ:3436:LYS:HE2	1.70	0.56
2:AB:232:LEU:HB2	2:AB:281:ILE:HG21	1.86	0.56
8:BZ:3207:THR:HA	8:BZ:3381:LYS:HG3	1.87	0.56
8:BZ:3219:GLY:H	8:BZ:3356:GLN:HE22	1.53	0.56
8:BZ:3321:LYS:HZ3	8:BZ:3327:ARG:HH22	1.52	0.56
4:BE:3281:PRO:HD3	6:BH:3267:TYR:CE1	2.39	0.56
3:AD:452:THR:HG23	3:AD:462:SER:OG	2.06	0.56
7:AQ:495:LEU:H	7:AQ:495:LEU:HD22	1.71	0.56
2:BB:3373:THR:HG22	3:BD:3081:VAL:HG22	1.87	0.56
3:BD:3465:VAL:O	3:BD:3469:LEU:HB2	2.04	0.56
7:AQ:433:ARG:HH21	7:AQ:436:LYS:HE2	1.70	0.56
4:BE:3443:GLY:O	4:BE:3512:VAL:HG23	2.05	0.56
7:AQ:291:ILE:HG23	7:AQ:347:PRO:HG3	1.88	0.56
6:BH:3319:SER:O	6:BH:3322:ASP:HB2	2.05	0.56
6:AH:222:LYS:O	6:AH:222:LYS:HD3	2.05	0.56
2:BB:3199:LEU:HB3	3:BD:3084:ALA:HB2	1.88	0.56
6:AH:78:PRO:HA	7:AQ:62:ILE:HD13	1.88	0.56
5:BG:3286:GLN:O	5:BG:3343:LEU:HD23	2.05	0.56
2:BB:3513:ASN:HD22	2:BB:3514:ILE:N	2.03	0.56
4:BE:3229:ARG:O	4:BE:3409:ARG:HD2	2.04	0.56
4:AE:55:ARG:O	4:AE:58:ALA:HB3	2.06	0.56
1:BA:3380:HIS:CD2	1:BA:3381:SER:H	2.24	0.56
2:AB:10:VAL:HG12	2:AB:517:ALA:HA	1.88	0.56
4:AE:276:PHE:HB2	4:AE:327:PHE:HB3	1.88	0.56
6:BH:3292:ILE:HG21	6:BH:3365:PHE:CE2	2.41	0.56
6:BH:3277:LEU:O	6:BH:3281:LYS:HG3	2.06	0.56
6:AH:11:VAL:HG12	6:AH:12:VAL:H	1.70	0.56
8:BZ:3221:HIS:HB3	8:BZ:3224:MET:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:3055:ARG:O	4:BE:3058:ALA:HB3	2.06	0.56
1:BA:3207:LYS:HE2	1:BA:3396:ASP:OD1	2.06	0.56
2:AB:293:TYR:HA	3:AD:334:ALA:CB	2.35	0.56
2:BB:3010:VAL:HG12	2:BB:3517:ALA:HA	1.88	0.56
5:AG:182:VAL:HA	5:AG:375:LYS:O	2.06	0.56
2:BB:3216:LYS:HG3	2:BB:3306:ILE:HD11	1.88	0.56
2:BB:3049:ALA:HA	3:BD:3528:ARG:CZ	2.35	0.56
7:BQ:3246:LYS:HD2	7:BQ:3295:GLY:HA3	1.86	0.56
1:BA:3200:VAL:HG22	1:BA:3200:VAL:O	2.06	0.56
1:BA:3397:GLU:HA	1:BA:3400:ARG:HB3	1.88	0.56
8:BZ:3420:ILE:O	8:BZ:3424:ARG:HG3	2.06	0.56
2:AB:203:LEU:HD11	2:AB:376:THR:HG21	1.86	0.56
2:BB:3251:LYS:HB2	4:BE:3288:ASP:OD1	2.05	0.56
4:BE:3449:THR:HG23	4:BE:3507:ILE:HG13	1.87	0.56
5:AG:60:ASP:CG	5:AG:394:ARG:HE	2.09	0.56
2:BB:3254:SER:HB2	3:BD:3266:GLU:OE1	2.06	0.56
4:AE:441:TYR:HB2	4:AE:509:ASN:HB2	1.87	0.56
4:AE:443:GLY:HA2	9:AE:601:ADP:N3	2.21	0.56
4:BE:3276:PHE:HB2	4:BE:3327:PHE:HB3	1.88	0.56
1:AA:200:VAL:HG22	1:AA:200:VAL:O	2.06	0.56
8:AZ:504:GLU:HB2	8:AZ:506:ILE:HG12	1.88	0.56
8:BZ:3504:GLU:HB2	8:BZ:3506:ILE:HG12	1.88	0.56
5:BG:3454:ARG:HB2	5:BG:3468:LEU:HD11	1.88	0.56
2:AB:268:LYS:HA	2:AB:271:ASN:HD22	1.70	0.56
2:BB:3411:MET:O	2:BB:3415:VAL:HG23	2.06	0.56
3:BD:3237:ILE:HD12	3:BD:3239:PHE:HB3	1.87	0.56
3:BD:3245:LYS:HE3	3:BD:3294:ARG:HG2	1.88	0.56
8:AZ:420:ILE:O	8:AZ:424:ARG:HG3	2.06	0.56
8:AZ:301:ILE:HG22	8:AZ:306:LEU:HG	1.86	0.56
1:AA:217:LEU:H	1:AA:217:LEU:HD23	1.70	0.56
7:BQ:3512:ILE:HG23	7:BQ:3517:ILE:O	2.06	0.56
1:AA:380:HIS:CD2	1:AA:381:SER:H	2.24	0.56
1:AA:33:THR:HG21	1:AA:109:LEU:HD12	1.87	0.56
4:BE:3443:GLY:HA2	9:BE:3601:ADP:N3	2.21	0.56
2:AB:495:ARG:NH1	2:AB:495:ARG:HB3	2.19	0.56
4:AE:540:LEU:HA	4:AE:543:GLN:HG2	1.88	0.56
1:AA:427:ALA:O	1:AA:430:ASN:HB3	2.06	0.56
4:AE:362:ILE:HD11	6:AH:231:GLN:HE21	1.71	0.56
5:AG:454:ARG:HB2	5:AG:468:LEU:HD11	1.88	0.56
4:BE:3281:PRO:O	4:BE:3282:LYS:HG2	2.06	0.56
2:BB:3415:VAL:HB	2:BB:3434:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3116:HIS:ND1	3:BD:3117:PRO:HD2	2.20	0.56
2:BB:3442:THR:HA	2:BB:3456:VAL:HG21	1.87	0.56
3:AD:116:HIS:ND1	3:AD:117:PRO:HD2	2.20	0.56
5:BG:3144:ASP:OD2	5:BG:3147:ASN:HB2	2.06	0.56
4:BE:3094:MET:O	4:BE:3096:LEU:HG	2.05	0.56
2:AB:254:SER:HB2	3:AD:266:GLU:OE1	2.06	0.56
7:AQ:141:GLU:O	7:AQ:145:MET:HG2	2.05	0.56
3:BD:3219:ALA:HB1	3:BD:3220:ILE:HD12	1.88	0.56
2:AB:415:VAL:HB	2:AB:434:ALA:HB2	1.87	0.56
4:BE:3540:LEU:HA	4:BE:3543:GLN:HG2	1.88	0.56
1:BA:3189:THR:HG22	1:BA:3190:GLN:N	2.20	0.56
7:BQ:3236:VAL:HG21	7:BQ:3319:LEU:HA	1.87	0.56
1:BA:3188:LYS:HB3	1:BA:3198:TYR:CE2	2.41	0.56
7:BQ:3419:LEU:HD13	7:BQ:3518:TYR:CD1	2.41	0.56
2:BB:3458:LYS:HB3	2:BB:3479:ILE:HD13	1.86	0.56
7:BQ:3208:ARG:HD3	7:BQ:3331:ARG:NH2	2.20	0.56
8:BZ:3046:LEU:HD21	8:BZ:3062:LEU:HD12	1.87	0.56
6:BH:3197:LYS:H	6:BH:3197:LYS:HD2	1.71	0.56
3:BD:3452:THR:HG23	3:BD:3462:SER:OG	2.06	0.56
7:AQ:46:MET:HG3	9:AQ:601:ADP:O5'	2.06	0.56
5:AG:171:MET:HG3	5:AG:396:LEU:HD13	1.88	0.56
1:AA:357:LEU:O	1:AA:377:THR:HG22	2.06	0.55
1:BA:3243:LYS:HD2	1:BA:3292:GLY:HA3	1.87	0.55
2:BB:3293:TYR:HB3	2:BB:3294:PRO:HD3	1.88	0.55
5:AG:382:ARG:NH1	5:AG:382:ARG:HB3	2.19	0.55
5:BG:3382:ARG:HB3	5:BG:3382:ARG:NH1	2.19	0.55
8:BZ:3326:GLU:O	8:BZ:3330:LEU:HD13	2.06	0.55
7:BQ:3291:ILE:HG23	7:BQ:3347:PRO:HG3	1.88	0.55
5:BG:3060:ASP:CG	5:BG:3394:ARG:HE	2.09	0.55
7:AQ:208:ARG:HD3	7:AQ:331:ARG:NH2	2.20	0.55
5:AG:110:TYR:HB3	5:AG:116:ILE:HD12	1.88	0.55
7:AQ:72:LEU:HD13	7:AQ:86:VAL:HG22	1.89	0.55
8:AZ:41:GLY:HA3	8:AZ:57:LYS:HE2	1.88	0.55
8:AZ:46:LEU:HD21	8:AZ:62:LEU:HD12	1.87	0.55
2:AB:162:SER:HA	2:AB:167:SER:OG	2.06	0.55
8:AZ:97:LEU:O	8:AZ:101:LEU:HB2	2.06	0.55
5:AG:495:VAL:HA	5:AG:500:TRP:CH2	2.40	0.55
4:BE:3362:ILE:HD11	6:BH:3231:GLN:HE21	1.71	0.55
5:AG:89:VAL:HG12	5:AG:405:ASN:CG	2.27	0.55
6:BH:3263:HIS:HB2	6:BH:3266:ASP:OD2	2.06	0.55
2:AB:199:LEU:HB3	3:AD:84:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3097:LEU:O	8:BZ:3101:LEU:HB2	2.06	0.55
2:AB:251:LYS:HB2	4:AE:288:ASP:OD1	2.05	0.55
6:AH:260:ARG:CD	7:AQ:266:LEU:HD21	2.37	0.55
1:BA:3427:ALA:O	1:BA:3430:ASN:HB3	2.06	0.55
1:AA:188:LYS:HB3	1:AA:198:TYR:CE2	2.41	0.55
2:BB:3268:LYS:NZ	4:BE:3299:GLN:HB2	2.19	0.55
4:BE:3239:LEU:HD21	4:BE:3404:VAL:HB	1.87	0.55
6:AH:208:ALA:HB3	6:AH:211:GLU:HB2	1.88	0.55
5:BG:3495:VAL:HA	5:BG:3500:TRP:CH2	2.40	0.55
2:AB:293:TYR:HB3	2:AB:294:PRO:HD3	1.88	0.55
2:AB:216:LYS:HG3	2:AB:306:ILE:HD11	1.88	0.55
2:AB:117:PRO:O	2:AB:121:ILE:HG13	2.06	0.55
2:BB:3075:LYS:HD2	4:BE:3081:ILE:HD12	1.87	0.55
4:BE:3268:LYS:HA	4:BE:3375:GLY:O	2.07	0.55
6:AH:30:ILE:HD12	6:AH:109:MET:HB3	1.88	0.55
6:BH:3418:MET:HE2	6:BH:3468:LEU:HD23	1.87	0.55
2:BB:3162:SER:HA	2:BB:3167:SER:OG	2.06	0.55
1:AA:220:PRO:HG2	1:AA:375:LYS:HB2	1.87	0.55
8:BZ:3136:PHE:HE1	8:BZ:3413:PRO:HD2	1.71	0.55
3:AD:232:ALA:HB1	3:AD:284:ASN:HB3	1.87	0.55
3:AD:219:ALA:HB1	3:AD:220:ILE:HD12	1.88	0.55
8:AZ:326:GLU:O	8:AZ:330:LEU:HD13	2.06	0.55
6:BH:3260:ARG:CD	7:BQ:3266:LEU:HD21	2.37	0.55
7:AQ:419:LEU:HD13	7:AQ:518:TYR:CD1	2.41	0.55
7:AQ:137:PHE:CZ	7:AQ:437:TYR:HB2	2.41	0.55
4:AE:162:GLU:HG3	4:AE:438:ARG:HH12	1.71	0.55
5:BG:3093:THR:HG22	10:BG:4002:BEF:F3	1.97	0.55
6:BH:3296:LYS:CG	6:BH:3323:MET:HG3	2.37	0.55
1:BA:3220:PRO:HG2	1:BA:3375:LYS:HB2	1.87	0.55
3:AD:151:VAL:HG22	3:AD:175:VAL:HG21	1.88	0.55
5:BG:3179:VAL:HG21	5:BG:3403:ALA:HB3	1.88	0.55
8:AZ:136:PHE:HE1	8:AZ:413:PRO:HD2	1.71	0.55
6:AH:292:ILE:HG21	6:AH:365:PHE:CE2	2.41	0.55
8:AZ:275:LYS:HA	8:AZ:278:ILE:CG1	2.37	0.55
4:AE:284:LYS:CB	6:AH:259:VAL:H	2.20	0.55
2:BB:3255:THR:HG22	3:BD:3252:ILE:HD13	1.88	0.55
5:AG:263:ILE:HD11	5:AG:269:TRP:HE3	1.71	0.55
8:BZ:3195:GLU:HG2	8:BZ:3327:ARG:NH1	2.22	0.55
4:BE:3284:LYS:CB	6:BH:3259:VAL:H	2.20	0.55
7:BQ:3072:LEU:HD13	7:BQ:3086:VAL:HG22	1.89	0.55
1:AA:494:ARG:HG3	1:AA:495:ARG:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:156:GLU:O	6:AH:160:ARG:HB2	2.06	0.55
2:AB:198:ILE:HG23	2:AB:370:ARG:NE	2.22	0.55
3:BD:3135:LEU:HD22	3:BD:3411:ILE:HD13	1.88	0.55
2:BB:3507:VAL:HG21	4:BE:3415:ILE:HG12	1.89	0.55
2:BB:3293:TYR:HA	3:BD:3334:ALA:CB	2.35	0.55
4:AE:522:MET:HB3	4:AE:527:VAL:HB	1.89	0.55
8:AZ:405:VAL:HG13	8:AZ:411:ILE:HD13	1.87	0.55
5:AG:122:ILE:HG23	5:AG:518:CYS:SG	2.47	0.55
5:BG:3171:MET:HG3	5:BG:3396:LEU:HD13	1.89	0.55
6:AH:296:LYS:CG	6:AH:323:MET:HG3	2.37	0.55
7:AQ:262:LYS:HG2	7:AQ:264:THR:HG23	1.89	0.55
8:BZ:3275:LYS:HA	8:BZ:3278:ILE:CG1	2.37	0.55
2:BB:3117:PRO:O	2:BB:3121:ILE:HG13	2.07	0.55
2:BB:3005:ILE:HD11	4:BE:3056:SER:OG	2.07	0.55
7:BQ:3058:HIS:C	7:BQ:3059:LEU:HD22	2.28	0.55
3:BD:3292:ILE:CD1	3:BD:3292:ILE:H	2.19	0.55
3:BD:3207:THR:HG22	3:BD:3380:ARG:H	1.70	0.55
1:AA:168:ILE:HG21	1:AA:397:GLU:HG3	1.88	0.55
8:BZ:3103:ARG:HH11	8:BZ:3103:ARG:HB2	1.71	0.55
6:BH:3311:ASN:H	6:BH:3311:ASN:HD22	1.55	0.55
8:BZ:3355:TYR:HD1	8:BZ:3355:TYR:H	1.55	0.55
3:BD:3151:VAL:HG22	3:BD:3175:VAL:HG21	1.88	0.55
3:BD:3171:ALA:O	3:BD:3175:VAL:HG23	2.07	0.55
6:AH:263:HIS:HB2	6:AH:266:ASP:OD2	2.06	0.55
1:AA:82:ILE:HG21	1:AA:538:ILE:HD11	1.89	0.55
7:AQ:58:HIS:C	7:AQ:59:LEU:HD22	2.28	0.55
1:BA:3357:LEU:O	1:BA:3377:THR:HG22	2.06	0.55
7:BQ:3137:PHE:CZ	7:BQ:3437:TYR:HB2	2.41	0.55
6:BH:3078:PRO:HA	7:BQ:3062:ILE:HD13	1.88	0.55
6:AH:53:ILE:HD11	6:AH:69:ILE:HG23	1.89	0.55
3:AD:245:LYS:HE3	3:AD:294:ARG:HG2	1.87	0.55
5:AG:133:LEU:HD23	5:AG:136:ILE:HD12	1.87	0.55
5:AG:144:ASP:OD2	5:AG:147:ASN:HB2	2.06	0.55
5:BG:3133:LEU:HD23	5:BG:3136:ILE:HD12	1.88	0.55
6:BH:3036:VAL:HG21	6:BH:3080:ALA:HB1	1.89	0.55
8:BZ:3041:GLY:HA3	8:BZ:3057:LYS:HE2	1.88	0.55
4:BE:3275:PRO:HB2	4:BE:3277:GLU:HG2	1.88	0.55
2:AB:255:THR:HG22	3:AD:252:ILE:HD13	1.88	0.55
7:BQ:3254:LEU:HD21	7:BQ:3299:ILE:HD12	1.89	0.55
7:AQ:254:LEU:HD21	7:AQ:299:ILE:HD12	1.89	0.55
8:BZ:3149:PHE:HD2	8:BZ:3150:LEU:HD12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3280:LEU:HD21	8:BZ:3345:PRO:HG3	1.89	0.55
4:BE:3287:LEU:HD22	4:BE:3298:LEU:HD11	1.89	0.55
6:AH:221:LYS:HD3	6:AH:319:SER:OG	2.07	0.55
5:AG:159:ILE:HG23	5:AG:164:VAL:HG13	1.89	0.55
4:BE:3162:GLU:HG3	4:BE:3438:ARG:HH12	1.71	0.55
8:BZ:3231:ALA:HB1	8:BZ:3293:PHE:HB2	1.88	0.55
3:AD:171:ALA:O	3:AD:175:VAL:HG23	2.07	0.55
6:AH:204:ILE:HD11	6:AH:362:TYR:CZ	2.42	0.55
6:BH:3204:ILE:HD11	6:BH:3362:TYR:CZ	2.42	0.55
4:AE:277:GLU:HB3	4:AE:328:ASP:OD1	2.07	0.55
4:AE:287:LEU:HD22	4:AE:298:LEU:HD11	1.89	0.54
4:BE:3522:MET:HB3	4:BE:3527:VAL:HB	1.89	0.54
5:BG:3182:VAL:HA	5:BG:3375:LYS:O	2.06	0.54
8:BZ:3327:ARG:O	8:BZ:3331:VAL:HG23	2.07	0.54
1:AA:144:LEU:HB3	1:AA:419:VAL:HG22	1.89	0.54
1:BA:3168:ILE:HG21	1:BA:3397:GLU:HG3	1.88	0.54
1:AA:397:GLU:HA	1:AA:400:ARG:HB3	1.88	0.54
2:BB:3268:LYS:HZ2	4:BE:3299:GLN:HG2	1.72	0.54
8:AZ:103:ARG:HH11	8:AZ:103:ARG:HB2	1.71	0.54
6:BH:3030:ILE:HD12	6:BH:3109:MET:HB3	1.87	0.54
5:AG:15:THR:O	5:AG:20:ALA:HB2	2.07	0.54
5:AG:179:VAL:HG21	5:AG:403:ALA:HB3	1.88	0.54
2:BB:3289:LEU:HD12	2:BB:3289:LEU:H	1.72	0.54
4:AE:412:ASN:HB3	4:AE:415:ILE:HD11	1.89	0.54
4:AE:281:PRO:O	4:AE:282:LYS:HG2	2.06	0.54
1:BA:3082:ILE:HG21	1:BA:3538:ILE:HD11	1.89	0.54
2:AB:5:ILE:HD11	4:AE:56:SER:OG	2.07	0.54
8:AZ:327:ARG:O	8:AZ:331:VAL:HG23	2.07	0.54
5:BG:3154:LEU:HD21	5:BG:3406:VAL:HG21	1.89	0.54
5:BG:3263:ILE:HD11	5:BG:3269:TRP:HE3	1.71	0.54
1:AA:156:LEU:HD21	1:AA:409:VAL:HG13	1.88	0.54
1:BA:3144:LEU:HB3	1:BA:3419:VAL:HG22	1.89	0.54
6:BH:3295:SER:HB3	6:BH:3299:ILE:HD11	1.89	0.54
5:BG:3122:ILE:HG23	5:BG:3518:CYS:SG	2.47	0.54
4:AE:457:GLU:O	4:AE:461:GLN:HG2	2.08	0.54
7:BQ:3085:LEU:HD22	7:BQ:3534:ALA:HB1	1.89	0.54
2:AB:236:THR:HG23	2:AB:238:LEU:HD23	1.89	0.54
6:AH:197:LYS:HD2	6:AH:197:LYS:H	1.71	0.54
7:BQ:3046:MET:HG3	9:BQ:3601:ADP:O5'	2.06	0.54
2:BB:3013:GLU:O	2:BB:3018:ALA:HB2	2.07	0.54
7:AQ:250:PHE:HE2	7:AQ:344:LEU:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:507:VAL:HG21	4:AE:415:ILE:HG12	1.89	0.54
2:AB:273:ILE:CG2	2:AB:297:LEU:HD13	2.29	0.54
1:BA:3033:THR:HG21	1:BA:3109:LEU:HD12	1.88	0.54
5:AG:154:LEU:HD11	5:AG:406:VAL:HG21	1.89	0.54
8:AZ:280:LEU:HD21	8:AZ:345:PRO:HG3	1.89	0.54
6:AH:232:GLN:HG2	6:AH:308:ALA:HA	1.89	0.54
6:AH:277:LEU:O	6:AH:281:LYS:HG3	2.06	0.54
5:AG:119:VAL:O	5:AG:123:GLN:HG2	2.07	0.54
2:BB:3268:LYS:HA	2:BB:3271:ASN:HD22	1.70	0.54
4:AE:241:ASN:O	4:AE:397:GLN:HB2	2.07	0.54
4:AE:275:PRO:HB2	4:AE:277:GLU:HG2	1.88	0.54
7:AQ:85:LEU:HD22	7:AQ:534:ALA:HB1	1.89	0.54
1:BA:3186:ALA:HB1	1:BA:3381:SER:O	2.08	0.54
4:AE:272:LEU:HD21	4:AE:321:VAL:HG13	1.90	0.54
6:BH:3221:LYS:HD3	6:BH:3319:SER:OG	2.07	0.54
6:AH:247:GLU:O	6:AH:248:LEU:HB2	2.07	0.54
6:AH:295:SER:HB3	6:AH:299:ILE:HD11	1.89	0.54
4:AE:259:LEU:HD13	4:AE:261:LYS:HA	1.89	0.54
8:AZ:221:HIS:HB3	8:AZ:224:MET:HG2	1.88	0.54
4:AE:229:ARG:HG2	4:AE:230:VAL:H	1.72	0.54
4:AE:234:ILE:HA	4:AE:409:ARG:O	2.08	0.54
5:AG:93:THR:HG22	10:AG:1002:BEF:F3	1.97	0.54
7:AQ:429:GLU:HG2	7:AQ:482:HIS:CD2	2.43	0.54
8:AZ:424:ARG:NH2	8:AZ:477:LEU:HG	2.22	0.54
2:BB:3122:GLU:HB3	2:BB:3426:LYS:NZ	2.22	0.54
3:BD:3279:LYS:HG2	3:BD:3310:ILE:HD11	1.90	0.54
2:AB:289:LEU:H	2:AB:289:LEU:HD12	1.72	0.54
1:AA:238:ALA:CB	1:AA:242:VAL:HB	2.38	0.54
3:BD:3226:PRO:HB2	3:BD:3311:MET:CB	2.37	0.54
5:AG:154:LEU:HD21	5:AG:406:VAL:HG21	1.89	0.54
3:AD:170:LEU:HD12	3:AD:394:LEU:HD13	1.89	0.54
3:AD:207:THR:CG2	3:AD:379:ILE:HA	2.37	0.54
4:BE:3272:LEU:HD21	4:BE:3321:VAL:HG13	1.90	0.54
2:AB:48:SER:C	3:AD:528:ARG:HG2	2.27	0.54
8:BZ:3100:GLU:HG2	8:BZ:3453:VAL:HG22	1.89	0.54
8:BZ:3289:PRO:HD3	8:BZ:3293:PHE:CZ	2.43	0.54
2:BB:3413:LYS:HD3	2:BB:3464:TYR:CA	2.38	0.54
3:BD:3446:ALA:O	3:BD:3449:VAL:HG13	2.07	0.54
7:AQ:512:ILE:HD12	7:AQ:517:ILE:O	2.08	0.54
7:AQ:512:ILE:HG23	7:AQ:517:ILE:O	2.06	0.54
5:BG:3015:THR:O	5:BG:3020:ALA:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:506:LYS:HA	5:AG:506:LYS:HE2	1.89	0.54
2:BB:3378:ASP:O	2:BB:3381:GLU:HB3	2.08	0.54
4:BE:3284:LYS:HB3	6:BH:3259:VAL:H	1.73	0.54
4:BE:3258:VAL:HG21	4:BE:3320:VAL:HG11	1.90	0.54
4:BE:3441:TYR:HB2	4:BE:3509:ASN:HB2	1.87	0.54
1:BA:3456:LEU:HD11	1:BA:3478:ARG:HE	1.73	0.54
1:AA:456:LEU:HD11	1:AA:478:ARG:HE	1.73	0.54
2:AB:409:MET:HE3	2:AB:412:SER:HB3	1.89	0.54
8:AZ:149:PHE:HD2	8:AZ:150:LEU:HD12	1.72	0.54
7:BQ:3249:VAL:HG21	7:BQ:3333:CYS:SG	2.48	0.54
8:AZ:231:ALA:HB1	8:AZ:293:PHE:HB2	1.88	0.54
5:AG:110:TYR:CE2	5:AG:444:ALA:HB2	2.43	0.54
1:AA:498:ARG:HG2	1:AA:499:ASN:N	2.23	0.54
3:BD:3135:LEU:HG	3:BD:3421:ILE:HD11	1.90	0.54
3:AD:135:LEU:HG	3:AD:421:ILE:HD11	1.90	0.54
2:BB:3079:ASN:HB3	4:BE:3413:LYS:NZ	2.23	0.54
2:AB:411:MET:O	2:AB:415:VAL:HG23	2.06	0.54
4:BE:3245:LEU:HD23	4:BE:3246:ASP:H	1.73	0.54
2:BB:3409:MET:HE3	2:BB:3412:SER:HB3	1.89	0.54
8:BZ:3215:LEU:HD22	8:BZ:3217:HIS:HE1	1.72	0.54
7:BQ:3310:LEU:HD12	7:BQ:3320:VAL:HG21	1.90	0.54
2:BB:3273:ILE:CG2	2:BB:3297:LEU:HD13	2.29	0.54
4:BE:3241:ASN:O	4:BE:3397:GLN:HB2	2.07	0.54
3:AD:446:ALA:O	3:AD:449:VAL:HG13	2.07	0.54
4:BE:3277:GLU:HB3	4:BE:3328:ASP:OD1	2.07	0.54
3:AD:135:LEU:HD22	3:AD:411:ILE:HD13	1.89	0.54
2:BB:3243:VAL:HG11	4:BE:3330:GLU:OE1	2.08	0.54
3:BD:3454:LEU:HD21	9:BD:3601:ADP:H4'	1.90	0.54
5:BG:3055:LEU:HD22	5:BG:3055:LEU:H	1.73	0.54
4:BE:3412:ASN:HB3	4:BE:3415:ILE:HD11	1.89	0.54
7:AQ:223:ILE:HD12	7:AQ:372:LYS:HD3	1.90	0.54
1:BA:3493:LYS:O	1:BA:3493:LYS:HE3	2.08	0.54
4:AE:268:LYS:HA	4:AE:375:GLY:O	2.07	0.54
4:AE:381:TYR:O	4:AE:393:LEU:HG	2.08	0.54
8:AZ:280:LEU:CD2	8:AZ:345:PRO:HG3	2.38	0.54
1:BA:3269:GLN:O	1:BA:3273:ILE:HG12	2.08	0.54
7:BQ:3420:LEU:O	7:BQ:3518:TYR:HB2	2.08	0.54
1:AA:127:THR:HG22	3:AD:165:GLN:HE22	1.71	0.54
5:BG:3159:ILE:HG23	5:BG:3164:VAL:HG13	1.89	0.54
5:BG:3119:VAL:O	5:BG:3123:GLN:HG2	2.07	0.54
6:BH:3208:ALA:HB3	6:BH:3211:GLU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:3229:ARG:HG2	4:BE:3230:VAL:H	1.72	0.54
2:BB:3198:ILE:HG23	2:BB:3370:ARG:NE	2.22	0.54
7:BQ:3422:GLY:HA2	7:BQ:3519:ASP:OD2	2.08	0.54
3:AD:182:SER:O	3:AD:183:ASP:HB3	2.08	0.54
4:BE:3071:ASP:OD1	4:BE:3085:ASN:HB2	2.07	0.54
5:BG:3222:GLY:HA2	5:BG:3331:VAL:HG11	1.90	0.54
1:BA:3260:VAL:O	1:BA:3260:VAL:HG13	2.07	0.54
4:AE:245:LEU:HD23	4:AE:246:ASP:H	1.73	0.54
5:AG:154:LEU:HD12	5:AG:412:LEU:HD11	1.90	0.54
8:AZ:195:GLU:HG2	8:AZ:327:ARG:NH1	2.22	0.54
1:BA:3156:LEU:HD21	1:BA:3409:VAL:HG13	1.88	0.54
2:AB:45:LEU:HD23	2:AB:46:LEU:N	2.23	0.54
4:BE:3457:GLU:O	4:BE:3461:GLN:HG2	2.08	0.54
7:BQ:3429:GLU:HG2	7:BQ:3482:HIS:CD2	2.43	0.54
6:BH:3242:LEU:HD23	6:BH:3244:LEU:HB2	1.90	0.54
3:AD:288:ILE:HG21	3:AD:296:ALA:HB1	1.89	0.54
1:AA:260:VAL:O	1:AA:260:VAL:HG13	2.07	0.54
5:BG:3089:VAL:HG12	5:BG:3405:ASN:CG	2.27	0.54
5:BG:3154:LEU:HD12	5:BG:3412:LEU:HD11	1.90	0.54
1:BA:3156:LEU:CD2	1:BA:3409:VAL:HG13	2.38	0.54
4:BE:3298:LEU:O	4:BE:3301:TYR:HB3	2.08	0.54
7:BQ:3533:GLU:OE2	8:BZ:3203:SER:HB3	2.08	0.54
2:BB:3048:SER:C	3:BD:3528:ARG:HG2	2.27	0.54
6:BH:3218:VAL:HG13	6:BH:3329:ALA:HB2	1.90	0.54
7:BQ:3223:ILE:HG23	7:BQ:3372:LYS:HD3	1.89	0.54
7:BQ:3065:THR:HG22	7:BQ:3067:ASP:N	2.23	0.54
2:BB:3513:ASN:HD22	2:BB:3514:ILE:H	1.56	0.54
4:BE:3234:ILE:HA	4:BE:3409:ARG:O	2.08	0.54
8:AZ:430:ASN:HD22	8:AZ:434:LEU:H	1.56	0.54
6:AH:292:ILE:HG21	6:AH:365:PHE:HE2	1.72	0.54
6:AH:36:VAL:HG21	6:AH:80:ALA:HB1	1.89	0.54
2:BB:3175:GLU:HG3	2:BB:3179:ASN:HD21	1.73	0.54
8:AZ:355:TYR:H	8:AZ:355:TYR:HD1	1.55	0.54
6:BH:3226:TYR:HE1	6:BH:3317:ARG:NH2	2.06	0.54
7:AQ:223:ILE:HG23	7:AQ:372:LYS:HB3	1.90	0.53
1:AA:493:LYS:O	1:AA:493:LYS:HE3	2.08	0.53
7:BQ:3262:LYS:HG2	7:BQ:3264:THR:HG23	1.89	0.53
7:BQ:3250:PHE:HE2	7:BQ:3344:LEU:HA	1.73	0.53
5:AG:411:SER:O	5:AG:412:LEU:HD23	2.08	0.53
5:BG:3089:VAL:HG12	5:BG:3405:ASN:ND2	2.23	0.53
5:AG:272:ILE:HA	5:AG:275:ILE:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3232:GLN:HG2	6:BH:3308:ALA:HA	1.89	0.53
1:BA:3127:THR:HG22	3:BD:3165:GLN:HE22	1.71	0.53
2:AB:46:LEU:N	2:AB:46:LEU:HD12	2.23	0.53
6:AH:218:VAL:HG13	6:AH:329:ALA:HB2	1.90	0.53
1:BA:3082:ILE:HG12	3:BD:3383:ASN:ND2	2.23	0.53
7:AQ:423:ALA:O	7:AQ:499:VAL:HG23	2.08	0.53
2:BB:3236:THR:HG23	2:BB:3238:LEU:HD23	1.89	0.53
6:AH:311:ASN:H	6:AH:311:ASN:HD22	1.55	0.53
1:BA:3242:VAL:HG12	1:BA:3358:CYS:O	2.07	0.53
5:BG:3058:THR:HG23	5:BG:3060:ASP:N	2.13	0.53
2:AB:233:ILE:HD11	2:AB:324:GLU:H	1.73	0.53
2:AB:7:GLY:H	2:AB:10:VAL:CG2	2.21	0.53
5:BG:3499:ILE:HG23	5:BG:3499:ILE:O	2.09	0.53
4:AE:258:VAL:HG21	4:AE:320:VAL:HG11	1.90	0.53
4:BE:3393:LEU:HD23	4:BE:3394:ILE:N	2.23	0.53
8:AZ:215:LEU:HD22	8:AZ:217:HIS:HE1	1.72	0.53
5:BG:3411:SER:O	5:BG:3412:LEU:HD23	2.08	0.53
6:AH:247:GLU:CG	6:AH:248:LEU:H	2.21	0.53
6:BH:3198:LEU:HB3	6:BH:3373:THR:OG1	2.08	0.53
7:BQ:3125:VAL:HA	7:BQ:3128:ILE:HD12	1.90	0.53
1:BA:3083:LEU:HB3	1:BA:3102:VAL:HG13	1.90	0.53
2:AB:32:LEU:HD12	2:AB:32:LEU:O	2.08	0.53
7:AQ:289:LYS:HA	7:AQ:316:TYR:CE2	2.43	0.53
1:BA:3540:ARG:CD	3:BD:3162:ILE:HG12	2.39	0.53
8:AZ:100:GLU:HG2	8:AZ:453:VAL:HG22	1.89	0.53
3:BD:3288:ILE:HG21	3:BD:3296:ALA:HB1	1.89	0.53
3:AD:279:LYS:HG2	3:AD:310:ILE:HD11	1.90	0.53
4:AE:71:ASP:OD1	4:AE:85:ASN:HB2	2.07	0.53
1:AA:242:VAL:HG12	1:AA:358:CYS:O	2.07	0.53
4:AE:393:LEU:HD23	4:AE:394:ILE:N	2.23	0.53
5:BG:3089:VAL:HG11	5:BG:3505:ILE:HG13	1.89	0.53
5:BG:3272:ILE:HA	5:BG:3275:ILE:HG13	1.89	0.53
5:BG:3110:TYR:HB3	5:BG:3116:ILE:HD12	1.88	0.53
8:AZ:232:TYR:CD2	8:AZ:348:LEU:HD12	2.43	0.53
3:BD:3170:LEU:HD12	3:BD:3394:LEU:HD13	1.89	0.53
3:BD:3207:THR:CG2	3:BD:3379:ILE:HA	2.37	0.53
1:BA:3141:ASN:HA	1:BA:3144:LEU:CG	2.38	0.53
7:AQ:65:THR:HG22	7:AQ:67:ASP:N	2.23	0.53
1:AA:540:ARG:CD	3:AD:162:ILE:HG12	2.39	0.53
1:AA:207:LYS:HB2	1:AA:395:LEU:HG	1.90	0.53
8:BZ:3046:LEU:H	8:BZ:3046:LEU:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:226:TYR:HE1	6:AH:317:ARG:NH2	2.06	0.53
1:BA:3219:VAL:HG11	1:BA:3373:LEU:HD22	1.91	0.53
5:AG:55:LEU:H	5:AG:55:LEU:HD22	1.73	0.53
2:AB:122:GLU:HB3	2:AB:426:LYS:NZ	2.22	0.53
3:AD:454:LEU:HD21	9:AD:601:ADP:H4'	1.90	0.53
7:BQ:3223:ILE:HD12	7:BQ:3372:LYS:HD3	1.90	0.53
8:BZ:3295:ILE:HD12	8:BZ:3309:PHE:CE2	2.34	0.53
4:BE:3381:TYR:O	4:BE:3393:LEU:HG	2.08	0.53
1:AA:141:ASN:HA	1:AA:144:LEU:CG	2.38	0.53
1:AA:144:LEU:HD13	1:AA:417:ASN:OD1	2.08	0.53
1:AA:417:ASN:C	1:AA:521:THR:HG23	2.29	0.53
2:BB:3046:LEU:HD12	2:BB:3046:LEU:N	2.23	0.53
6:BH:3355:MET:O	6:BH:3361:ARG:HA	2.09	0.53
4:BE:3322:ILE:CD1	4:BE:3354:ILE:HG21	2.38	0.53
6:AH:198:LEU:HB3	6:AH:373:THR:OG1	2.08	0.53
7:BQ:3123:SER:HB3	7:BQ:3126:GLU:CG	2.39	0.53
7:AQ:125:VAL:HA	7:AQ:128:ILE:HD12	1.90	0.53
2:AB:513:ASN:HD22	2:AB:514:ILE:H	1.56	0.53
4:BE:3115:ILE:HG12	4:BE:3533:GLY:HA2	1.90	0.53
7:BQ:3289:LYS:HA	7:BQ:3316:TYR:CE2	2.43	0.53
8:BZ:3424:ARG:NH2	8:BZ:3477:LEU:HG	2.22	0.53
3:AD:462:SER:O	3:AD:466:VAL:HG23	2.09	0.53
6:AH:242:LEU:HD23	6:AH:244:LEU:HB2	1.90	0.53
3:BD:3062:HIS:O	3:BD:3066:LYS:HB2	2.09	0.53
7:AQ:455:ALA:O	7:AQ:458:VAL:HG22	2.09	0.53
2:AB:79:ASN:HB3	4:AE:413:LYS:NZ	2.23	0.53
1:AA:82:ILE:HG12	3:AD:383:ASN:ND2	2.23	0.53
6:AH:63:SER:HB2	6:AH:391:ARG:HH21	1.74	0.53
8:BZ:3279:ASP:HA	8:BZ:3282:ASN:HD22	1.74	0.53
4:BE:3053:ALA:O	4:BE:3057:VAL:HG23	2.08	0.53
5:AG:89:VAL:HG11	5:AG:505:ILE:HG13	1.89	0.53
5:AG:89:VAL:HG12	5:AG:405:ASN:ND2	2.23	0.53
7:AQ:420:LEU:O	7:AQ:518:TYR:HB2	2.08	0.53
6:AH:377:LEU:H	6:AH:377:LEU:HD22	1.73	0.53
6:BH:3063:SER:HB2	6:BH:3391:ARG:HH21	1.74	0.53
2:BB:3032:LEU:O	2:BB:3032:LEU:HD12	2.08	0.53
2:AB:243:VAL:HG11	4:AE:330:GLU:OE1	2.08	0.53
2:AB:378:ASP:O	2:AB:381:GLU:HB3	2.08	0.53
1:AA:365:LYS:HA	1:AA:370:GLU:HA	1.91	0.53
2:AB:175:GLU:HG3	2:AB:179:ASN:HD21	1.73	0.53
4:BE:3273:THR:HG21	6:BH:3305:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:186:ALA:HB1	1:AA:381:SER:O	2.08	0.53
2:AB:242:LYS:CB	2:AB:245:ILE:HD11	2.35	0.53
1:BA:3019:LYS:HG3	1:BA:3545:ILE:HG12	1.91	0.53
3:BD:3349:LEU:HB3	3:BD:3364:THR:HG23	1.90	0.53
1:AA:199:PRO:C	1:AA:201:LYS:H	2.12	0.53
3:BD:3196:LEU:CD2	3:BD:3377:VAL:HB	2.38	0.53
1:BA:3144:LEU:HD13	1:BA:3417:ASN:OD1	2.08	0.53
8:AZ:35:THR:HB	8:AZ:42:THR:OG1	2.09	0.53
1:BA:3238:ALA:CB	1:BA:3242:VAL:HB	2.38	0.53
2:AB:413:LYS:HD3	2:AB:464:TYR:CA	2.38	0.53
6:BH:3063:SER:HB2	6:BH:3391:ARG:NH2	2.24	0.53
2:BB:3175:GLU:HG3	2:BB:3179:ASN:ND2	2.24	0.53
2:AB:175:GLU:HG3	2:AB:179:ASN:ND2	2.24	0.53
2:AB:13:GLU:O	2:AB:18:ALA:HB2	2.07	0.53
3:AD:248:THR:O	3:AD:250:ASN:N	2.41	0.53
1:AA:19:LYS:HG3	1:AA:545:ILE:HG12	1.91	0.53
4:AE:53:ALA:O	4:AE:57:VAL:HG23	2.08	0.53
4:BE:3443:GLY:HA3	4:BE:3522:MET:SD	2.49	0.53
7:BQ:3455:ALA:O	7:BQ:3458:VAL:HG22	2.09	0.53
8:BZ:3232:TYR:CD2	8:BZ:3348:LEU:HD12	2.43	0.53
1:BA:3417:ASN:C	1:BA:3521:THR:HG23	2.29	0.53
6:BH:3377:LEU:H	6:BH:3377:LEU:HD22	1.73	0.53
2:AB:268:LYS:HZ2	4:AE:299:GLN:HG2	1.72	0.53
5:AG:503:GLU:O	5:AG:507:GLN:HG2	2.09	0.53
6:BH:3178:PHE:HD2	6:BH:3393:LEU:HD21	1.74	0.53
8:BZ:3430:ASN:HD22	8:BZ:3434:LEU:H	1.56	0.53
6:BH:3033:CYS:SG	6:BH:3080:ALA:HA	2.49	0.53
6:AH:33:CYS:SG	6:AH:80:ALA:HA	2.49	0.53
1:AA:208:ALA:O	1:AA:388:ARG:HA	2.08	0.53
5:BG:3184:LYS:O	5:BG:3186:LEU:HD13	2.09	0.53
5:AG:121:ILE:O	5:AG:125:LEU:HD12	2.09	0.53
5:BG:3459:ASN:HD22	5:BG:3459:ASN:N	2.07	0.53
7:AQ:223:ILE:HG23	7:AQ:372:LYS:HD3	1.89	0.53
8:AZ:94:VAL:O	8:AZ:98:VAL:HG12	2.09	0.53
2:BB:3233:ILE:CD1	2:BB:3323:GLY:HA3	2.38	0.53
1:BA:3136:ALA:HB1	1:BA:3429:LEU:HD22	1.91	0.53
6:AH:63:SER:HB2	6:AH:391:ARG:NH2	2.24	0.53
2:BB:3517:ALA:HB1	4:BE:3095:GLU:OE1	2.09	0.53
3:AD:292:ILE:H	3:AD:292:ILE:CD1	2.19	0.53
4:BE:3301:TYR:OH	6:BH:3268:GLN:HB2	2.09	0.53
8:AZ:356:GLN:HB2	8:AZ:365:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:3199:PRO:C	1:BA:3201:LYS:H	2.12	0.53
1:AA:269:GLN:O	1:AA:273:ILE:HG12	2.08	0.53
7:AQ:93:LYS:HD3	7:AQ:100:THR:HG21	1.91	0.53
4:AE:322:ILE:CD1	4:AE:354:ILE:HG21	2.38	0.53
6:AH:178:PHE:HD2	6:AH:393:LEU:HD21	1.74	0.53
7:AQ:249:VAL:HG21	7:AQ:333:CYS:SG	2.48	0.53
8:AZ:289:PRO:HD3	8:AZ:293:PHE:CZ	2.43	0.53
3:BD:3469:LEU:O	3:BD:3473:HIS:HB2	2.09	0.53
7:BQ:3512:ILE:HD12	7:BQ:3517:ILE:O	2.08	0.53
3:BD:3148:GLU:O	3:BD:3152:ARG:HG3	2.08	0.53
8:BZ:3484:ASP:O	8:BZ:3485:GLU:HB3	2.09	0.53
5:AG:184:LYS:O	5:AG:186:LEU:HD13	2.09	0.53
5:BG:3506:LYS:HA	5:BG:3506:LYS:HE2	1.89	0.53
5:AG:459:ASN:N	5:AG:459:ASN:HD22	2.07	0.53
5:AG:70:VAL:HG23	5:AG:76:LYS:HG3	1.91	0.53
2:BB:3270:LYS:HD3	2:BB:3293:TYR:OH	2.09	0.53
7:BQ:3223:ILE:HG23	7:BQ:3372:LYS:HB3	1.90	0.53
4:AE:301:TYR:OH	6:AH:268:GLN:HB2	2.09	0.53
2:BB:3233:ILE:HD11	2:BB:3324:GLU:H	1.73	0.53
5:AG:499:ILE:HG23	5:AG:499:ILE:O	2.09	0.53
5:AG:263:ILE:HG21	5:AG:272:ILE:HD11	1.90	0.53
5:BG:3263:ILE:HG21	5:BG:3272:ILE:HD11	1.90	0.53
7:AQ:310:LEU:HD12	7:AQ:320:VAL:HG21	1.90	0.53
1:AA:156:LEU:CD2	1:AA:409:VAL:HG13	2.38	0.53
3:BD:3207:THR:CG2	3:BD:3380:ARG:H	2.21	0.53
6:BH:3356:GLN:HE22	6:BH:3361:ARG:CD	2.22	0.53
7:BQ:3093:LYS:HD3	7:BQ:3100:THR:HG21	1.91	0.53
6:BH:3247:GLU:CG	6:BH:3248:LEU:H	2.21	0.53
2:BB:3045:LEU:HD23	2:BB:3046:LEU:N	2.23	0.53
3:BD:3326:LYS:HZ1	3:BD:3373:PRO:HG2	1.74	0.53
7:AQ:123:SER:HB3	7:AQ:126:GLU:CG	2.39	0.53
7:AQ:533:GLU:OE2	8:AZ:203:SER:HB3	2.08	0.53
5:AG:288:LEU:HD11	5:AG:312:GLY:HA3	1.91	0.53
5:BG:3288:LEU:HD21	5:BG:3312:GLY:HA3	1.91	0.53
8:BZ:3098:VAL:O	8:BZ:3102:LEU:HG	2.09	0.53
3:BD:3355:SER:HB2	3:BD:3358:SER:OG	2.09	0.53
8:BZ:3035:THR:HB	8:BZ:3042:THR:OG1	2.09	0.53
6:AH:244:LEU:HD23	6:AH:245:ASN:N	2.24	0.53
1:BA:3137:ILE:CD1	1:BA:3525:VAL:HG13	2.39	0.53
7:BQ:3423:ALA:O	7:BQ:3499:VAL:HG23	2.08	0.53
2:BB:3241:ASP:O	2:BB:3242:LYS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:241:ASP:O	2:AB:242:LYS:HB2	2.09	0.53
2:BB:3325:VAL:HB	4:BE:3251:HIS:NE2	2.24	0.53
5:AG:145:VAL:HG13	5:AG:410:PRO:HB3	1.91	0.53
8:BZ:3315:LEU:HD11	8:BZ:3356:GLN:HE22	1.74	0.53
6:BH:3247:GLU:O	6:BH:3248:LEU:HB2	2.07	0.53
6:BH:3053:ILE:HD11	6:BH:3069:ILE:HG23	1.89	0.53
6:BH:3292:ILE:HG21	6:BH:3365:PHE:HE2	1.72	0.53
7:BQ:3372:LYS:O	7:BQ:3373:GLN:HG3	2.09	0.53
3:AD:179:LEU:HA	3:AD:182:SER:OG	2.09	0.53
7:AQ:134:ALA:HB2	7:AQ:449:ILE:HG23	1.91	0.53
7:AQ:422:GLY:HA2	7:AQ:519:ASP:OD2	2.08	0.53
4:AE:284:LYS:HB3	6:AH:259:VAL:H	1.73	0.52
2:AB:233:ILE:CD1	2:AB:323:GLY:HA3	2.38	0.52
8:AZ:279:ASP:HA	8:AZ:282:ASN:HD22	1.74	0.52
3:AD:256:ASP:HB2	3:AD:259:GLN:CB	2.34	0.52
4:AE:443:GLY:HA3	4:AE:522:MET:SD	2.49	0.52
5:BG:3154:LEU:HD11	5:BG:3406:VAL:HG21	1.89	0.52
1:AA:229:ALA:HB3	1:AA:233:MET:HE3	1.91	0.52
8:BZ:3422:LEU:HD12	8:BZ:3451:LEU:CD1	2.40	0.52
3:AD:207:THR:CG2	3:AD:380:ARG:H	2.21	0.52
8:BZ:3280:LEU:CD2	8:BZ:3345:PRO:HG3	2.38	0.52
6:AH:355:MET:O	6:AH:361:ARG:HA	2.09	0.52
8:BZ:3036:ASN:H	8:BZ:3036:ASN:HD22	1.57	0.52
8:AZ:227:ARG:CZ	8:AZ:353:LEU:HD11	2.39	0.52
6:AH:12:VAL:HG22	6:AH:13:LEU:H	1.74	0.52
2:AB:514:ILE:HG12	4:AE:73:ILE:HB	1.91	0.52
1:AA:136:ALA:HB1	1:AA:429:LEU:HD22	1.91	0.52
3:AD:300:LEU:HA	3:AD:303:HIS:CE1	2.45	0.52
6:AH:125:ILE:HA	6:AH:438:ILE:HD13	1.90	0.52
3:AD:62:HIS:O	3:AD:66:LYS:HB2	2.09	0.52
3:BD:3182:SER:O	3:BD:3183:ASP:HB3	2.08	0.52
6:AH:55:THR:C	6:AH:57:ASN:H	2.13	0.52
4:BE:3555:ILE:CD1	6:BH:3053:ILE:HG12	2.39	0.52
8:AZ:422:LEU:HD12	8:AZ:451:LEU:CD1	2.39	0.52
1:BA:3156:LEU:HB3	1:BA:3181:VAL:HG11	1.91	0.52
2:BB:3190:LEU:HD21	2:BB:3389:SER:HA	1.91	0.52
3:BD:3248:THR:O	3:BD:3250:ASN:N	2.41	0.52
5:BG:3288:LEU:HD11	5:BG:3312:GLY:HA3	1.91	0.52
5:AG:93:THR:HG23	5:AG:94:THR:N	2.25	0.52
3:BD:3179:LEU:HA	3:BD:3182:SER:OG	2.09	0.52
2:AB:142:ASN:O	2:AB:149:PHE:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AD:148:GLU:O	3:AD:152:ARG:HG3	2.08	0.52
4:AE:298:LEU:O	4:AE:301:TYR:HB3	2.08	0.52
1:AA:83:LEU:HB3	1:AA:102:VAL:HG13	1.90	0.52
2:AB:517:ALA:HB1	4:AE:95:GLU:OE1	2.09	0.52
4:AE:242:GLY:HA3	4:AE:395:ILE:O	2.10	0.52
4:AE:550:LYS:HE3	6:AH:50:ASP:OD1	2.09	0.52
5:BG:3088:GLU:HG3	5:BG:3508:GLN:NE2	2.25	0.52
6:AH:139:LYS:O	6:AH:143:LEU:HD12	2.10	0.52
1:AA:273:ILE:O	1:AA:276:ARG:HB3	2.09	0.52
2:AB:125:ARG:HD3	2:AB:506:GLU:OE1	2.10	0.52
4:AE:555:ILE:CD1	6:AH:53:ILE:HG12	2.39	0.52
8:AZ:154:ALA:O	8:AZ:158:LEU:HB2	2.09	0.52
7:BQ:3117:LEU:HD22	7:BQ:3122:LEU:HD12	1.90	0.52
7:AQ:117:LEU:HD22	7:AQ:122:LEU:HD12	1.90	0.52
4:BE:3259:LEU:HD13	4:BE:3261:LYS:HA	1.89	0.52
4:AE:115:ILE:HG12	4:AE:533:GLY:HA2	1.90	0.52
8:BZ:3318:ARG:HD3	8:BZ:3319:ARG:HG2	1.91	0.52
3:BD:3462:SER:O	3:BD:3466:VAL:HG23	2.09	0.52
1:AA:344:LEU:HB3	1:AA:345:GLU:OE2	2.09	0.52
2:AB:467:ILE:O	2:AB:469:THR:HG22	2.09	0.52
7:AQ:372:LYS:O	7:AQ:373:GLN:HG3	2.09	0.52
8:BZ:3094:VAL:O	8:BZ:3098:VAL:HG12	2.09	0.52
8:BZ:3356:GLN:HB2	8:BZ:3365:THR:HG22	1.91	0.52
8:BZ:3153:VAL:HG11	8:BZ:3405:VAL:CG2	2.39	0.52
2:AB:190:LEU:HD21	2:AB:389:SER:HA	1.91	0.52
1:BA:3498:ARG:HG2	1:BA:3499:ASN:N	2.23	0.52
1:BA:3207:LYS:HB2	1:BA:3395:LEU:HG	1.90	0.52
8:AZ:46:LEU:HD12	8:AZ:46:LEU:H	1.73	0.52
5:AG:222:GLY:HA2	5:AG:331:VAL:HG11	1.90	0.52
2:AB:166:LEU:HD21	2:AB:380:ALA:HA	1.91	0.52
7:BQ:3283:GLN:O	7:BQ:3287:MET:HG3	2.09	0.52
2:AB:61:ALA:HB2	2:AB:92:THR:HB	1.90	0.52
7:BQ:3134:ALA:HB2	7:BQ:3449:ILE:HG23	1.91	0.52
1:BA:3208:ALA:O	1:BA:3388:ARG:HA	2.09	0.52
5:BG:3332:THR:C	5:BG:3334:ALA:H	2.13	0.52
2:BB:3007:GLY:H	2:BB:3010:VAL:CG2	2.21	0.52
4:BE:3242:GLY:HA3	4:BE:3395:ILE:O	2.10	0.52
8:AZ:235:ILE:CG2	8:AZ:336:ALA:HA	2.40	0.52
1:AA:156:LEU:HB3	1:AA:181:VAL:HG11	1.91	0.52
2:BB:3508:LEU:O	2:BB:3511:VAL:HG23	2.10	0.52
3:BD:3354:ASP:OD2	3:BD:3359:LYS:HE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3125:ILE:HA	6:BH:3438:ILE:HD13	1.90	0.52
2:BB:3261:LEU:O	2:BB:3264:ALA:HB3	2.09	0.52
7:AQ:68:ALA:HB2	7:AQ:101:ASN:ND2	2.25	0.52
8:AZ:102:LEU:HD22	8:AZ:528:LEU:CD2	2.34	0.52
8:AZ:98:VAL:O	8:AZ:102:LEU:HG	2.09	0.52
4:BE:3550:LYS:HE3	6:BH:3050:ASP:OD1	2.09	0.52
3:AD:226:PRO:HB2	3:AD:311:MET:CB	2.37	0.52
8:AZ:321:LYS:HZ3	8:AZ:327:ARG:HH22	1.56	0.52
5:BG:3145:VAL:HG13	5:BG:3410:PRO:HB3	1.91	0.52
3:AD:199:LYS:HG3	3:AD:380:ARG:HH12	1.74	0.52
6:AH:464:ILE:HD11	6:AH:481:VAL:HG12	1.92	0.52
8:AZ:36:ASN:HD22	8:AZ:36:ASN:H	1.57	0.52
2:BB:3166:LEU:HD21	2:BB:3380:ALA:HA	1.91	0.52
2:AB:55:MET:HA	2:AB:375:GLN:OE1	2.10	0.52
8:BZ:3154:ALA:O	8:BZ:3158:LEU:HB2	2.09	0.52
2:BB:3153:LEU:HG	2:BB:3391:LEU:HD22	1.92	0.52
2:AB:157:ALA:HB2	2:AB:391:LEU:HD11	1.92	0.52
7:AQ:128:ILE:HG23	7:AQ:536:THR:OG1	2.10	0.52
5:BG:3503:GLU:O	5:BG:3507:GLN:HG2	2.09	0.52
5:BG:3093:THR:HG23	5:BG:3094:THR:N	2.25	0.52
4:AE:115:ILE:HG23	4:AE:432:ASN:HD21	1.74	0.52
4:AE:536:GLN:HE22	6:AH:207:GLY:HA2	1.74	0.52
6:BH:3244:LEU:HD23	6:BH:3245:ASN:N	2.24	0.52
6:BH:3042:PRO:HA	6:BH:3456:ASN:OD1	2.09	0.52
2:BB:3426:LYS:HB3	2:BB:3426:LYS:NZ	2.25	0.52
8:AZ:480:ALA:CB	8:AZ:487:ARG:HD2	2.40	0.52
5:AG:353:GLY:HA3	5:AG:370:ASN:HA	1.92	0.52
7:BQ:3068:ALA:HB2	7:BQ:3101:ASN:ND2	2.25	0.52
5:BG:3286:GLN:NE2	5:BG:3341:GLU:HA	2.24	0.52
4:BE:3247:LYS:HD2	4:BE:3393:LEU:HD13	1.91	0.52
4:BE:3536:GLN:HE22	6:BH:3207:GLY:HA2	1.74	0.52
8:AZ:153:VAL:HG11	8:AZ:405:VAL:CG2	2.39	0.52
1:BA:3055:ASP:CB	5:BG:3530:VAL:HG22	2.39	0.52
2:AB:190:LEU:H	2:AB:190:LEU:HD12	1.74	0.52
6:AH:280:GLU:O	6:AH:284:GLN:HG3	2.10	0.52
2:BB:3055:MET:HA	2:BB:3375:GLN:OE1	2.10	0.52
6:BH:3012:VAL:HG22	6:BH:3013:LEU:H	1.74	0.52
1:AA:499:ASN:HB3	1:AA:513:ILE:HG13	1.92	0.52
6:AH:42:PRO:HA	6:AH:456:ASN:OD1	2.09	0.52
7:AQ:109:GLU:O	7:AQ:113:VAL:HG22	2.10	0.52
5:BG:3238:ILE:HB	5:BG:3241:PRO:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:3344:LEU:HB3	1:BA:3345:GLU:OE2	2.09	0.52
5:BG:3025:ILE:HD13	5:BG:3104:LEU:HD22	1.91	0.52
3:AD:349:LEU:HB3	3:AD:364:THR:HG23	1.90	0.52
4:BE:3244:ILE:HG23	4:BE:3394:ILE:HG12	1.91	0.52
8:BZ:3235:ILE:CG2	8:BZ:3336:ALA:HA	2.40	0.52
1:AA:473:LEU:HB3	1:AA:502:LEU:HD22	1.92	0.52
1:AA:272:GLN:HB3	3:AD:257:TYR:CD1	2.44	0.52
1:BA:3273:ILE:O	1:BA:3276:ARG:HB3	2.09	0.52
4:BE:3288:ASP:HB3	6:BH:3262:GLU:HG3	1.91	0.52
3:BD:3243:PRO:HD3	3:BD:3298:ASN:ND2	2.24	0.52
8:BZ:3158:LEU:HB3	8:BZ:3167:THR:HG23	1.92	0.52
5:AG:286:GLN:NE2	5:AG:341:GLU:HA	2.24	0.52
2:BB:3467:ILE:O	2:BB:3469:THR:HG22	2.09	0.52
3:AD:355:SER:HB2	3:AD:358:SER:OG	2.09	0.52
4:AE:449:THR:HG23	4:AE:507:ILE:CG1	2.40	0.52
3:BD:3300:LEU:HA	3:BD:3303:HIS:CE1	2.45	0.52
5:AG:238:ILE:HB	5:AG:241:PRO:HB3	1.92	0.52
7:BQ:3329:LEU:HD23	7:BQ:3330:ARG:N	2.25	0.52
2:BB:3142:ASN:O	2:BB:3149:PHE:HB2	2.09	0.52
5:AG:25:ILE:HD13	5:AG:104:LEU:HD22	1.91	0.52
7:AQ:212:ILE:HD13	7:AQ:387:ARG:NE	2.25	0.52
1:AA:242:VAL:HA	1:AA:294:GLN:NE2	2.24	0.52
1:AA:245:ALA:HB3	1:AA:296:VAL:HA	1.92	0.52
4:AE:270:ALA:HB1	4:AE:272:LEU:HD22	1.92	0.52
1:BA:3299:THR:O	1:BA:3320:ARG:HA	2.10	0.52
8:AZ:158:LEU:HB3	8:AZ:167:THR:HG23	1.92	0.52
7:BQ:3128:ILE:HG23	7:BQ:3536:THR:OG1	2.10	0.52
5:AG:288:LEU:HD21	5:AG:312:GLY:HA3	1.91	0.52
4:BE:3115:ILE:HG23	4:BE:3432:ASN:HD21	1.74	0.52
3:AD:469:LEU:O	3:AD:473:HIS:HB2	2.09	0.52
7:BQ:3109:GLU:O	7:BQ:3113:VAL:HG22	2.10	0.52
5:BG:3072:HIS:HD2	5:BG:3074:ALA:H	1.58	0.52
5:AG:72:HIS:HD2	5:AG:74:ALA:H	1.58	0.52
1:AA:137:ILE:CD1	1:AA:525:VAL:HG13	2.39	0.52
8:AZ:28:GLY:O	8:AZ:32:VAL:HG23	2.10	0.52
4:BE:3413:LYS:HB2	4:BE:3414:MET:HE3	1.90	0.52
3:AD:336:ILE:C	3:AD:338:LEU:H	2.14	0.52
1:AA:333:THR:OG1	1:AA:356:GLY:HA3	2.10	0.52
1:BA:3245:ALA:HB3	1:BA:3296:VAL:HA	1.92	0.52
6:AH:259:VAL:CG2	7:AQ:267:LEU:HD12	2.39	0.52
5:AG:231:HIS:CE1	8:AZ:336:ALA:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AZ:236:LEU:CD2	8:AZ:238:VAL:H	2.21	0.52
6:BH:3139:LYS:O	6:BH:3143:LEU:HD12	2.10	0.52
1:BA:3473:LEU:HB3	1:BA:3502:LEU:HD22	1.92	0.52
6:AH:413:GLY:O	6:AH:481:VAL:HG22	2.10	0.52
6:BH:3413:GLY:O	6:BH:3481:VAL:HG22	2.10	0.52
2:BB:3180:ALA:O	2:BB:3184:LEU:HD12	2.10	0.52
7:BQ:3411:LEU:HA	7:BQ:3416:GLY:HA3	1.91	0.52
3:BD:3138:MET:CB	3:BD:3478:LEU:HD13	2.40	0.52
8:AZ:318:ARG:HD3	8:AZ:319:ARG:HG2	1.91	0.52
1:AA:51:LYS:O	1:AA:62:VAL:HA	2.10	0.52
2:BB:3459:LEU:HD22	2:BB:3472:LEU:CD1	2.39	0.51
8:BZ:3294:VAL:HG11	8:BZ:3354:VAL:HG11	1.92	0.51
5:BG:3208:LYS:HD2	5:BG:3389:LEU:HB3	1.92	0.51
4:BE:3338:ASN:O	4:BE:3340:LEU:HD13	2.10	0.51
2:AB:244:LYS:O	4:AE:278:PRO:HB2	2.10	0.51
3:BD:3199:LYS:HG3	3:BD:3380:ARG:HH12	1.74	0.51
6:BH:3481:VAL:H	6:BH:3491:ASN:HD21	1.57	0.51
7:AQ:411:LEU:HA	7:AQ:416:GLY:HA3	1.91	0.51
3:AD:354:ASP:OD2	3:AD:359:LYS:HE2	2.10	0.51
6:BH:3245:ASN:OD1	6:BH:3246:VAL:HG13	2.10	0.51
3:AD:40:GLY:N	9:AD:601:ADP:H5'1	2.25	0.51
5:BG:3070:VAL:HG23	5:BG:3076:LYS:HG3	1.91	0.51
7:AQ:321:LEU:O	7:AQ:323:VAL:HG23	2.11	0.51
1:BA:3365:LYS:HA	1:BA:3370:GLU:HA	1.91	0.51
5:BG:3036:ARG:NH1	5:BG:3036:ARG:HB3	2.25	0.51
8:BZ:3028:GLY:O	8:BZ:3032:VAL:HG23	2.10	0.51
8:BZ:3480:ALA:CB	8:BZ:3487:ARG:HD2	2.40	0.51
8:AZ:196:ILE:HD12	8:AZ:196:ILE:H	1.76	0.51
2:AB:261:LEU:O	2:AB:264:ALA:HB3	2.09	0.51
1:BA:3014:PHE:N	1:BA:3014:PHE:CD1	2.78	0.51
3:BD:3336:ILE:C	3:BD:3338:LEU:H	2.14	0.51
5:AG:88:GLU:HG3	5:AG:508:GLN:NE2	2.25	0.51
1:BA:3333:THR:OG1	1:BA:3356:GLY:HA3	2.10	0.51
1:BA:3288:ILE:HA	1:BA:3349:THR:HG22	1.92	0.51
2:BB:3157:ALA:HB2	2:BB:3391:LEU:HD11	1.92	0.51
2:BB:3178:THR:O	2:BB:3182:LEU:HD13	2.10	0.51
7:BQ:3239:LEU:HD12	7:BQ:3358:VAL:CG1	2.41	0.51
4:BE:3449:THR:HG23	4:BE:3507:ILE:CG1	2.40	0.51
4:AE:288:ASP:HB3	6:AH:262:GLU:HG3	1.91	0.51
2:AB:426:LYS:NZ	2:AB:426:LYS:HB3	2.25	0.51
5:BG:3353:GLY:H	5:BG:3370:ASN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3061:ALA:HB2	2:BB:3092:THR:HB	1.90	0.51
2:BB:3125:ARG:HD3	2:BB:3506:GLU:OE1	2.10	0.51
5:BG:3181:THR:HG21	5:BG:3377:CYS:HB3	1.93	0.51
4:BE:3151:ASP:O	4:BE:3155:LYS:HG3	2.10	0.51
4:BE:3287:LEU:HD21	4:BE:3289:ILE:HD11	1.93	0.51
6:AH:222:LYS:HB2	6:AH:361:ARG:O	2.11	0.51
7:AQ:64:ILE:HD12	7:AQ:392:ASN:HB3	1.93	0.51
8:AZ:227:ARG:HH22	8:AZ:353:LEU:HD21	1.75	0.51
7:BQ:3064:ILE:HD12	7:BQ:3392:ASN:HB3	1.93	0.51
6:AH:25:GLN:NE2	6:AH:29:ASN:HD21	2.09	0.51
5:BG:3215:LEU:HD22	5:BG:3215:LEU:H	1.75	0.51
7:AQ:15:LYS:HD2	8:AZ:66:MET:CE	2.41	0.51
5:BG:3121:ILE:O	5:BG:3125:LEU:HD12	2.09	0.51
3:BD:3040:GLY:N	9:BD:3601:ADP:H5'1	2.25	0.51
5:AG:353:GLY:H	5:AG:370:ASN:HA	1.75	0.51
1:AA:219:VAL:HG11	1:AA:373:LEU:HD22	1.91	0.51
7:BQ:3335:VAL:HA	7:BQ:3379:SER:OG	2.11	0.51
2:BB:3156:ILE:HG12	2:BB:3488:VAL:HG23	1.93	0.51
1:AA:162:THR:CG2	1:AA:517:VAL:HA	2.28	0.51
2:AB:296:GLN:HB2	3:AD:334:ALA:HB2	1.92	0.51
6:BH:3260:ARG:HB3	6:BH:3260:ARG:NH1	2.17	0.51
6:BH:3270:ILE:HD11	7:BQ:3273:MET:SD	2.51	0.51
1:AA:296:VAL:O	1:AA:297:LEU:HD23	2.11	0.51
1:BA:3242:VAL:HA	1:BA:3294:GLN:NE2	2.24	0.51
2:AB:253:ASP:HB3	3:AD:259:GLN:NE2	2.25	0.51
2:AB:325:VAL:HB	4:AE:251:HIS:NE2	2.24	0.51
4:AE:244:ILE:HG23	4:AE:394:ILE:HG12	1.91	0.51
4:BE:3151:ASP:OD1	4:BE:3546:ARG:HD2	2.10	0.51
5:AG:402:VAL:HA	5:AG:405:ASN:HD22	1.75	0.51
5:BG:3231:HIS:CE1	8:BZ:3336:ALA:HB3	2.45	0.51
1:BA:3200:VAL:CG1	1:BA:3201:LYS:HE3	2.41	0.51
6:BH:3280:GLU:O	6:BH:3284:GLN:HG3	2.10	0.51
8:BZ:3227:ARG:CZ	8:BZ:3353:LEU:HD11	2.39	0.51
1:AA:291:ALA:CB	1:AA:351:GLU:HA	2.40	0.51
8:AZ:7:ASN:HD22	8:AZ:7:ASN:N	2.09	0.51
3:BD:3397:ALA:O	3:BD:3400:VAL:HB	2.11	0.51
8:BZ:3424:ARG:HA	8:BZ:3427:ARG:HD2	1.93	0.51
7:BQ:3427:GLU:HG2	7:BQ:3459:VAL:HB	1.92	0.51
1:BA:3051:LYS:O	1:BA:3062:VAL:HA	2.10	0.51
2:AB:270:LYS:HD3	2:AB:293:TYR:OH	2.09	0.51
7:BQ:3212:ILE:HD13	7:BQ:3387:ARG:NE	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AZ:30:GLN:O	8:AZ:34:GLU:HG3	2.11	0.51
7:AQ:283:GLN:O	7:AQ:287:MET:HG3	2.09	0.51
6:BH:3055:THR:C	6:BH:3057:ASN:H	2.12	0.51
4:AE:287:LEU:HD21	4:AE:289:ILE:HD11	1.93	0.51
4:AE:151:ASP:OD1	4:AE:546:ARG:HD2	2.10	0.51
5:BG:3402:VAL:HA	5:BG:3405:ASN:HD22	1.75	0.51
1:AA:189:THR:HG22	1:AA:190:GLN:N	2.21	0.51
6:AH:419:GLU:OE2	6:AH:477:LYS:HG2	2.10	0.51
1:BA:3127:THR:HG22	3:BD:3165:GLN:CD	2.31	0.51
8:BZ:3337:GLN:HE21	8:BZ:3347:ILE:HG21	1.75	0.51
8:BZ:3352:GLY:CA	8:BZ:3369:GLU:HB2	2.41	0.51
4:AE:151:ASP:O	4:AE:155:LYS:HG3	2.10	0.51
5:BG:3250:LEU:HB2	5:BG:3301:VAL:HA	1.93	0.51
2:BB:3157:ALA:HA	2:BB:3160:THR:HG22	1.92	0.51
6:AH:270:ILE:HD11	7:AQ:273:MET:SD	2.51	0.51
2:AB:508:LEU:O	2:AB:511:VAL:HG23	2.10	0.51
8:BZ:3021:VAL:O	8:BZ:3024:THR:HB	2.10	0.51
1:BA:3209:HIS:HE1	5:BG:3083:ARG:HH21	1.59	0.51
7:BQ:3321:LEU:O	7:BQ:3323:VAL:HG23	2.11	0.51
6:BH:3107:GLU:HG2	6:BH:3448:VAL:HB	1.93	0.51
2:AB:156:ILE:HG12	2:AB:488:VAL:HG23	1.93	0.51
8:AZ:433:LYS:HG2	8:AZ:435:GLY:N	2.25	0.51
8:AZ:294:VAL:HG11	8:AZ:354:VAL:HG11	1.92	0.51
1:AA:70:LEU:HB3	1:AA:84:VAL:HG22	1.92	0.51
4:AE:312:ASP:O	4:AE:369:LEU:HD22	2.10	0.51
6:AH:189:LEU:HD23	6:AH:189:LEU:N	2.24	0.51
2:BB:3190:LEU:H	2:BB:3190:LEU:HD12	1.74	0.51
1:AA:299:THR:O	1:AA:320:ARG:HA	2.10	0.51
1:BA:3291:ALA:CB	1:BA:3351:GLU:HA	2.40	0.51
7:BQ:3015:LYS:HD2	8:BZ:3066:MET:CE	2.41	0.51
3:AD:397:ALA:O	3:AD:400:VAL:HB	2.11	0.51
6:AH:116:LEU:HD11	6:AH:518:LEU:CD2	2.41	0.51
7:AQ:147:VAL:HG12	7:AQ:148:GLY:N	2.26	0.51
1:BA:3041:LYS:HE2	1:BA:3103:ILE:HG23	1.93	0.51
8:AZ:315:LEU:HD11	8:AZ:356:GLN:HE22	1.74	0.51
4:BE:3312:ASP:O	4:BE:3369:LEU:HD22	2.10	0.51
4:AE:272:LEU:HD23	4:AE:272:LEU:H	1.76	0.51
8:BZ:3102:LEU:HD22	8:BZ:3528:LEU:CD2	2.34	0.51
3:AD:169:PHE:O	3:AD:173:LEU:HB2	2.10	0.51
4:AE:273:THR:HG21	6:AH:305:GLN:HE22	1.74	0.51
1:AA:127:THR:HG22	3:AD:165:GLN:CD	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:458:GLN:C	5:AG:460:ALA:H	2.13	0.51
2:BB:3046:LEU:O	2:BB:3054:CYS:HA	2.11	0.51
1:AA:63:THR:OG1	1:AA:400:ARG:HD3	2.11	0.51
6:AH:245:ASN:HD22	6:AH:296:LYS:HD3	1.75	0.51
7:AQ:427:GLU:HG2	7:AQ:459:VAL:HB	1.92	0.51
2:BB:3253:ASP:HB3	3:BD:3259:GLN:NE2	2.25	0.51
4:AE:276:PHE:CD2	4:AE:335:LEU:HD11	2.45	0.51
4:BE:3270:ALA:HB1	4:BE:3272:LEU:HD22	1.92	0.51
1:BA:3272:GLN:HB3	3:BD:3257:TYR:CD1	2.44	0.51
2:AB:48:SER:HA	3:AD:528:ARG:HA	1.92	0.51
2:BB:3296:GLN:HB2	3:BD:3334:ALA:HB2	1.92	0.51
2:AB:157:ALA:HA	2:AB:160:THR:HG22	1.92	0.51
2:BB:3514:ILE:HG12	4:BE:3073:ILE:HB	1.91	0.51
2:AB:350:GLU:OE1	3:AD:87:SER:HA	2.11	0.51
4:AE:520:ASN:O	4:AE:521:ASP:HB3	2.10	0.51
7:AQ:311:HIS:O	7:AQ:314:ASN:HB2	2.11	0.51
4:BE:3142:HIS:O	4:BE:3146:ILE:HG13	2.11	0.51
3:BD:3469:LEU:HD13	3:BD:3489:THR:CG2	2.41	0.51
6:AH:245:ASN:OD1	6:AH:246:VAL:HG13	2.10	0.51
8:AZ:484:ASP:O	8:AZ:485:GLU:HB3	2.09	0.51
5:AG:181:THR:HG21	5:AG:377:CYS:HB3	1.93	0.51
8:AZ:59:GLY:O	8:AZ:63:LEU:HB2	2.10	0.51
7:AQ:335:VAL:HA	7:AQ:379:SER:OG	2.11	0.51
6:AH:449:ILE:HB	6:AH:450:PRO:HD3	1.93	0.51
7:BQ:3114:SER:O	7:BQ:3118:ILE:HG13	2.11	0.51
6:AH:260:ARG:HH11	6:AH:260:ARG:CB	2.17	0.51
4:AE:247:LYS:HD2	4:AE:393:LEU:HD13	1.91	0.51
8:AZ:193:MET:HA	8:AZ:193:MET:HE3	1.91	0.51
8:AZ:193:MET:CE	8:AZ:327:ARG:HG3	2.41	0.51
4:AE:338:ASN:O	4:AE:340:LEU:HD13	2.10	0.51
2:AB:180:ALA:O	2:AB:184:LEU:HD12	2.10	0.51
5:BG:3281:GLN:O	5:BG:3285:GLU:HG2	2.11	0.51
1:BA:3063:THR:OG1	1:BA:3400:ARG:HD3	2.11	0.51
6:BH:3218:VAL:HG21	6:BH:3326:VAL:HA	1.93	0.51
4:AE:55:ARG:HA	4:AE:127:SER:OG	2.11	0.51
4:BE:3055:ARG:HA	4:BE:3127:SER:OG	2.11	0.51
5:BG:3353:GLY:HA3	5:BG:3370:ASN:HA	1.92	0.51
8:BZ:3059:GLY:O	8:BZ:3063:LEU:HB2	2.10	0.51
5:AG:215:LEU:HD22	5:AG:215:LEU:H	1.76	0.51
7:AQ:114:SER:O	7:AQ:118:ILE:HG13	2.11	0.51
6:BH:3449:ILE:HB	6:BH:3450:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:281:GLN:O	5:AG:285:GLU:HG2	2.11	0.51
6:AH:107:GLU:HG2	6:AH:448:VAL:HB	1.93	0.51
5:AG:36:ARG:NH1	5:AG:36:ARG:HB3	2.25	0.51
7:BQ:3057:ASN:HB2	7:BQ:3061:LYS:N	2.26	0.51
8:BZ:3206:ASP:HB3	8:BZ:3381:LYS:HD2	1.92	0.51
8:BZ:3213:LEU:HD21	8:BZ:3215:LEU:HG	1.93	0.51
8:BZ:3296:ILE:HG13	8:BZ:3317:LEU:HD22	1.93	0.51
5:AG:208:LYS:HD2	5:AG:389:LEU:HB3	1.92	0.51
4:BE:3276:PHE:CD2	4:BE:3335:LEU:HD11	2.45	0.51
1:AA:200:VAL:CG1	1:AA:201:LYS:HE3	2.41	0.51
3:BD:3169:PHE:O	3:BD:3173:LEU:HB2	2.10	0.51
6:AH:419:GLU:HB2	6:AH:472:HIS:HE2	1.75	0.51
6:AH:356:GLN:HE22	6:AH:361:ARG:CD	2.22	0.51
1:BA:3202:ALA:HA	1:BA:3328:ARG:HH11	1.76	0.51
7:AQ:138:THR:HG23	7:AQ:430:LEU:CD2	2.41	0.51
7:BQ:3147:VAL:HG12	7:BQ:3148:GLY:N	2.26	0.51
8:BZ:3096:CYS:HB3	8:BZ:3453:VAL:HG11	1.93	0.51
6:BH:3025:GLN:NE2	6:BH:3029:ASN:HD21	2.09	0.51
1:BA:3499:ASN:HB3	1:BA:3513:ILE:HG13	1.92	0.51
3:BD:3025:ILE:HG22	3:BD:3029:ARG:HD2	1.93	0.51
2:BB:3203:LEU:HA	2:BB:3370:ARG:O	2.11	0.51
7:AQ:224:LYS:HE3	7:AQ:378:ILE:HA	1.92	0.50
1:AA:41:LYS:HE2	1:AA:103:ILE:HG23	1.93	0.50
1:AA:90:GLN:HE22	1:AA:527:SER:HB2	1.76	0.50
6:AH:67:ALA:O	6:AH:71:LYS:HG3	2.12	0.50
1:BA:3090:GLN:HE22	1:BA:3527:SER:HB2	1.77	0.50
7:AQ:231:GLU:HA	7:AQ:231:GLU:OE1	2.11	0.50
8:AZ:174:VAL:HG13	8:AZ:175:THR:N	2.26	0.50
7:BQ:3436:LYS:O	7:BQ:3440:ARG:HB2	2.11	0.50
1:BA:3474:VAL:O	1:BA:3478:ARG:HB2	2.11	0.50
3:AD:196:LEU:CD2	3:AD:377:VAL:HB	2.38	0.50
2:BB:3208:LEU:HD11	2:BB:3365:CYS:HB2	1.92	0.50
6:BH:3247:GLU:OE2	6:BH:3249:GLU:HB2	2.11	0.50
2:BB:3048:SER:HA	3:BD:3528:ARG:HA	1.92	0.50
5:BG:3185:ASP:HA	5:BG:3196:PHE:HA	1.92	0.50
2:BB:3350:GLU:OE1	3:BD:3087:SER:HA	2.11	0.50
2:AB:178:THR:O	2:AB:182:LEU:HD13	2.10	0.50
4:BE:3520:ASN:O	4:BE:3521:ASP:HB3	2.10	0.50
3:AD:138:MET:CB	3:AD:478:LEU:HD13	2.40	0.50
8:AZ:424:ARG:HA	8:AZ:427:ARG:HD2	1.93	0.50
6:BH:3245:ASN:HD22	6:BH:3296:LYS:HD3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BQ:3224:LYS:HE3	7:BQ:3378:ILE:HA	1.92	0.50
6:AH:418:MET:HE2	6:AH:468:LEU:HD23	1.92	0.50
1:AA:14:PHE:N	1:AA:14:PHE:CD1	2.79	0.50
7:BQ:3231:GLU:HA	7:BQ:3231:GLU:OE1	2.11	0.50
8:AZ:21:VAL:O	8:AZ:24:THR:HB	2.10	0.50
6:BH:3466:ASN:HA	6:BH:3469:ARG:HD3	1.92	0.50
8:AZ:206:ASP:HB3	8:AZ:381:LYS:HD2	1.92	0.50
5:AG:273:LEU:HD13	8:AZ:269:PHE:CG	2.46	0.50
1:BA:3070:LEU:HB3	1:BA:3084:VAL:HG22	1.92	0.50
2:BB:3244:LYS:O	4:BE:3278:PRO:HB2	2.10	0.50
4:AE:278:PRO:HD3	4:AE:306:PHE:CE1	2.47	0.50
2:BB:3190:LEU:H	4:BE:3389:LYS:NZ	2.08	0.50
3:BD:3244:PRO:O	3:BD:3246:PRO:HD3	2.11	0.50
1:BA:3457:ILE:O	1:BA:3461:THR:HG23	2.11	0.50
6:AH:178:PHE:CD2	6:AH:393:LEU:HD11	2.46	0.50
5:BG:3284:CYS:O	5:BG:3288:LEU:HB2	2.11	0.50
2:AB:151:GLU:O	2:AB:154:ILE:HG22	2.10	0.50
5:AG:332:THR:C	5:AG:334:ALA:H	2.13	0.50
5:BG:3236:ARG:HD2	5:BG:3357:VAL:HG11	1.92	0.50
1:AA:367:SER:O	1:AA:368:ASP:HB3	2.11	0.50
3:AD:244:PRO:O	3:AD:246:PRO:HD3	2.11	0.50
8:BZ:3236:LEU:CD2	8:BZ:3238:VAL:H	2.21	0.50
8:AZ:213:LEU:HD21	8:AZ:215:LEU:HG	1.93	0.50
6:BH:3464:ILE:HD11	6:BH:3481:VAL:HG12	1.92	0.50
2:AB:190:LEU:H	4:AE:389:LYS:NZ	2.08	0.50
6:BH:3222:LYS:HB2	6:BH:3361:ARG:O	2.10	0.50
6:AH:247:GLU:OE2	6:AH:249:GLU:HB2	2.11	0.50
6:AH:327:ILE:HD11	6:AH:334:ILE:HD13	1.93	0.50
1:BA:3289:ILE:HG23	1:BA:3315:ILE:HD11	1.93	0.50
6:BH:3178:PHE:CD2	6:BH:3393:LEU:HD11	2.46	0.50
2:AB:153:LEU:HG	2:AB:391:LEU:HD22	1.92	0.50
5:AG:284:CYS:O	5:AG:288:LEU:HB2	2.11	0.50
4:BE:3229:ARG:HG2	4:BE:3230:VAL:N	2.27	0.50
4:BE:3200:PHE:HE2	4:BE:3234:ILE:HD12	1.77	0.50
8:BZ:3030:GLN:O	8:BZ:3034:GLU:HG3	2.11	0.50
7:AQ:224:LYS:HE3	7:AQ:379:SER:H	1.76	0.50
6:AH:203:LYS:HB3	6:AH:386:ILE:HG21	1.93	0.50
1:AA:289:ILE:HG23	1:AA:315:ILE:HD11	1.94	0.50
1:BA:3296:VAL:O	1:BA:3297:LEU:HD23	2.11	0.50
4:AE:276:PHE:CE2	4:AE:335:LEU:HD11	2.47	0.50
4:BE:3276:PHE:CE2	4:BE:3335:LEU:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:481:VAL:H	6:AH:491:ASN:HD21	1.58	0.50
1:AA:145:SER:O	1:AA:417:ASN:HA	2.11	0.50
2:AB:46:LEU:O	2:AB:54:CYS:HA	2.11	0.50
8:BZ:3368:THR:HG22	8:BZ:3369:GLU:H	1.77	0.50
5:BG:3458:GLN:C	5:BG:3460:ALA:H	2.14	0.50
1:AA:113:ASN:O	1:AA:116:VAL:HG23	2.12	0.50
4:AE:229:ARG:O	4:AE:409:ARG:HA	2.12	0.50
1:BA:3367:SER:O	1:BA:3368:ASP:HB3	2.11	0.50
2:AB:245:ILE:HD13	2:AB:248:THR:CG2	2.41	0.50
8:AZ:96:CYS:HB3	8:AZ:453:VAL:HG11	1.93	0.50
5:AG:185:ASP:HA	5:AG:196:PHE:HA	1.92	0.50
4:BE:3269:LEU:HB3	4:BE:3320:VAL:HG23	1.94	0.50
1:AA:457:ILE:O	1:AA:461:THR:HG23	2.11	0.50
5:BG:3273:LEU:HD13	8:BZ:3269:PHE:CG	2.46	0.50
1:AA:288:ILE:HA	1:AA:349:THR:HG22	1.92	0.50
8:AZ:166:LEU:HD12	8:AZ:169:VAL:HB	1.93	0.50
8:AZ:27:GLU:HG2	8:AZ:103:ARG:HH11	1.76	0.50
1:BA:3494:ARG:HG3	1:BA:3495:ARG:NE	2.27	0.50
6:AH:466:ASN:HA	6:AH:469:ARG:HD3	1.92	0.50
6:BH:3043:THR:HA	6:BH:3049:SER:O	2.11	0.50
1:AA:228:VAL:HG13	1:AA:372:ILE:HD11	1.94	0.50
8:BZ:3174:VAL:HG13	8:BZ:3175:THR:N	2.26	0.50
7:BQ:3266:LEU:HD12	8:BZ:3252:PHE:HB3	1.94	0.50
7:AQ:329:LEU:HD23	7:AQ:330:ARG:N	2.25	0.50
5:BG:3182:VAL:HG11	5:BG:3204:VAL:HG22	1.94	0.50
2:AB:459:LEU:HD22	2:AB:472:LEU:CD1	2.39	0.50
5:BG:3159:ILE:HD12	5:BG:3164:VAL:HG11	1.94	0.50
5:AG:159:ILE:HD12	5:AG:164:VAL:HG11	1.94	0.50
5:AG:122:ILE:O	5:AG:126:LYS:HG2	2.12	0.50
7:AQ:150:ILE:C	7:AQ:152:ASP:H	2.15	0.50
5:AG:289:ALA:C	5:AG:291:ARG:H	2.15	0.50
4:BE:3267:VAL:HG13	4:BE:3319:ASP:OD2	2.12	0.50
8:BZ:3048:ASP:OD2	8:BZ:3052:ASN:HB2	2.12	0.50
5:AG:236:ARG:HD2	5:AG:357:VAL:HG11	1.92	0.50
1:BA:3295:VAL:HA	1:BA:3316:MET:O	2.12	0.50
4:AE:316:ALA:HB2	4:AE:370:SER:H	1.77	0.50
4:BE:3272:LEU:HD23	4:BE:3272:LEU:H	1.76	0.50
6:AH:480:GLY:HA3	6:AH:491:ASN:HD22	1.76	0.50
3:AD:110:LEU:HD13	3:AD:439:ILE:HD13	1.94	0.50
7:AQ:208:ARG:HB2	7:AQ:331:ARG:NH1	2.26	0.50
5:BG:3110:TYR:CE2	5:BG:3444:ALA:HB2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BQ:3311:HIS:O	7:BQ:3314:ASN:HB2	2.11	0.50
4:AE:260:PRO:HA	4:AE:267:VAL:HG22	1.94	0.50
8:BZ:3007:ASN:N	8:BZ:3007:ASN:HD22	2.09	0.50
3:AD:469:LEU:HD13	3:AD:489:THR:CG2	2.41	0.50
2:BB:3151:GLU:O	2:BB:3154:ILE:HG22	2.10	0.50
8:BZ:3196:ILE:H	8:BZ:3196:ILE:HD12	1.76	0.50
8:AZ:48:ASP:OD2	8:AZ:52:ASN:HB2	2.12	0.50
1:AA:295:VAL:HA	1:AA:316:MET:O	2.12	0.50
6:AH:260:ARG:HB3	6:AH:260:ARG:NH1	2.17	0.50
7:AQ:266:LEU:HD12	8:AZ:252:PHE:HB3	1.94	0.50
6:BH:3480:GLY:HA3	6:BH:3491:ASN:HD22	1.76	0.50
7:BQ:3190:LEU:HD23	7:BQ:3191:PRO:HD2	1.94	0.50
2:AB:180:ALA:HB2	2:AB:208:LEU:HD22	1.93	0.50
3:AD:326:LYS:NZ	3:AD:373:PRO:HG2	2.27	0.50
6:AH:218:VAL:HG21	6:AH:326:VAL:HA	1.93	0.50
4:AE:229:ARG:HG2	4:AE:230:VAL:N	2.27	0.50
7:AQ:239:LEU:HD12	7:AQ:358:VAL:CG1	2.41	0.50
3:AD:209:MET:CE	3:AD:375:VAL:HG23	2.41	0.50
3:BD:3209:MET:CE	3:BD:3375:VAL:HG23	2.41	0.50
6:AH:43:THR:HA	6:AH:49:SER:O	2.12	0.50
2:AB:264:ALA:O	2:AB:267:GLU:HB2	2.12	0.50
3:BD:3308:LEU:HD23	3:BD:3308:LEU:N	2.27	0.50
8:AZ:360:GLY:C	8:AZ:362:GLU:H	2.15	0.50
3:AD:89:ALA:HA	3:AD:403:CYS:SG	2.52	0.50
5:AG:145:VAL:HG12	5:AG:406:VAL:HG12	1.94	0.50
8:BZ:3329:GLN:HG2	8:BZ:3334:GLY:O	2.12	0.50
7:BQ:3236:VAL:O	7:BQ:3319:LEU:HD12	2.11	0.50
6:BH:3419:GLU:OE2	6:BH:3477:LYS:HG2	2.10	0.50
1:AA:55:ASP:CB	5:AG:530:VAL:HG22	2.39	0.50
4:BE:3267:VAL:HB	4:BE:3377:CYS:SG	2.52	0.50
2:AB:413:LYS:CD	2:AB:464:TYR:HA	2.42	0.50
4:AE:142:HIS:O	4:AE:146:ILE:HG13	2.11	0.50
1:BA:3228:VAL:HG13	1:BA:3372:ILE:HD11	1.94	0.49
6:BH:3116:LEU:HD11	6:BH:3518:LEU:CD2	2.41	0.49
2:AB:169:ASP:OD2	2:AB:204:SER:HB3	2.12	0.49
4:BE:3180:LEU:O	4:BE:3180:LEU:HD13	2.12	0.49
7:AQ:436:LYS:O	7:AQ:440:ARG:HB2	2.11	0.49
1:AA:474:VAL:O	1:AA:478:ARG:HB2	2.11	0.49
8:BZ:3193:MET:HA	8:BZ:3193:MET:HE3	1.93	0.49
4:BE:3316:ALA:HB2	4:BE:3370:SER:H	1.77	0.49
7:AQ:236:VAL:O	7:AQ:319:LEU:HD12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3110:LEU:HD13	3:BD:3439:ILE:HD13	1.94	0.49
6:BH:3013:LEU:HA	7:BQ:3078:VAL:HG12	1.94	0.49
8:BZ:3166:LEU:HD12	8:BZ:3169:VAL:HB	1.93	0.49
4:AE:267:VAL:HB	4:AE:377:CYS:SG	2.52	0.49
2:AB:402:LEU:HD11	2:AB:483:ARG:HE	1.77	0.49
4:AE:180:LEU:O	4:AE:180:LEU:HD13	2.12	0.49
4:AE:269:LEU:HB3	4:AE:320:VAL:HG23	1.94	0.49
6:BH:3185:ALA:HB2	6:BH:3214:PHE:HE1	1.77	0.49
8:BZ:3294:VAL:HG23	8:BZ:3315:LEU:O	2.12	0.49
5:BG:3345:GLU:O	5:BG:3348:VAL:HG13	2.12	0.49
1:BA:3145:SER:O	1:BA:3417:ASN:HA	2.11	0.49
3:AD:243:PRO:HD3	3:AD:298:ASN:ND2	2.24	0.49
7:BQ:3208:ARG:HB2	7:BQ:3331:ARG:NH1	2.26	0.49
7:AQ:411:LEU:HD12	7:AQ:411:LEU:O	2.13	0.49
3:AD:25:ILE:HG22	3:AD:29:ARG:HD2	1.93	0.49
4:AE:200:PHE:HE2	4:AE:234:ILE:HD12	1.77	0.49
2:BB:3413:LYS:CD	2:BB:3464:TYR:HA	2.42	0.49
8:BZ:3294:VAL:CG2	8:BZ:3315:LEU:HB3	2.40	0.49
3:AD:308:LEU:HD23	3:AD:308:LEU:N	2.27	0.49
2:BB:3245:ILE:HD13	2:BB:3248:THR:CG2	2.41	0.49
4:AE:287:LEU:CD2	4:AE:298:LEU:HD11	2.42	0.49
8:BZ:3524:ALA:O	8:BZ:3528:LEU:HG	2.12	0.49
5:AG:182:VAL:HG11	5:AG:204:VAL:HG22	1.94	0.49
8:AZ:329:GLN:HG2	8:AZ:334:GLY:O	2.12	0.49
6:BH:3505:ASN:HD21	7:BQ:3215:GLY:N	2.08	0.49
2:BB:3180:ALA:HB2	2:BB:3208:LEU:HD22	1.93	0.49
5:BG:3081:LEU:HD11	5:BG:3516:SER:HB2	1.94	0.49
4:BE:3322:ILE:HA	4:BE:3343:VAL:HB	1.94	0.49
3:BD:3326:LYS:NZ	3:BD:3373:PRO:HG2	2.27	0.49
6:BH:3406:ASN:C	6:BH:3408:LEU:H	2.15	0.49
5:BG:3122:ILE:O	5:BG:3126:LYS:HG2	2.12	0.49
5:AG:250:LEU:HB2	5:AG:301:VAL:HA	1.93	0.49
2:BB:3346:ILE:CD1	2:BB:3355:LYS:HB2	2.42	0.49
1:AA:494:ARG:HG3	1:AA:495:ARG:NE	2.27	0.49
5:AG:179:VAL:HG21	5:AG:403:ALA:CB	2.42	0.49
2:BB:3264:ALA:O	2:BB:3267:GLU:HB2	2.12	0.49
3:BD:3128:ALA:C	3:BD:3130:ARG:H	2.15	0.49
5:AG:430:LYS:HD2	5:AG:442:TYR:OH	2.12	0.49
3:AD:404:LEU:HD21	3:AD:410:LEU:HD23	1.93	0.49
2:AB:233:ILE:HD11	2:AB:323:GLY:HA3	1.94	0.49
7:BQ:3439:GLU:HA	7:BQ:3446:GLN:CD	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3310:ASP:O	2:BB:3314:VAL:HG13	2.12	0.49
7:AQ:439:GLU:HA	7:AQ:446:GLN:CD	2.33	0.49
1:BA:3229:ALA:HB3	1:BA:3233:MET:HE3	1.93	0.49
4:BE:3278:PRO:HD3	4:BE:3306:PHE:CE1	2.47	0.49
5:AG:345:GLU:O	5:AG:348:VAL:HG13	2.12	0.49
5:BG:3282:LEU:O	5:BG:3286:GLN:HG2	2.12	0.49
6:AH:13:LEU:HA	7:AQ:78:VAL:HG12	1.94	0.49
6:AH:406:ASN:C	6:AH:408:LEU:H	2.15	0.49
5:AG:162:LYS:HG2	5:AG:395:ASN:OD1	2.12	0.49
8:BZ:3027:GLU:HG2	8:BZ:3103:ARG:HH11	1.76	0.49
4:BE:3324:GLN:NE2	4:BE:3325:TRP:HE1	2.11	0.49
4:AE:206:GLU:HG2	4:AE:239:LEU:CD1	2.42	0.49
4:AE:260:PRO:O	4:AE:264:SER:HB3	2.13	0.49
2:AB:154:ILE:O	2:AB:158:LYS:HG3	2.12	0.49
7:BQ:3153:LYS:HG3	7:BQ:3155:ASP:HB2	1.94	0.49
6:BH:3067:ALA:O	6:BH:3071:LYS:HG3	2.12	0.49
1:AA:204:ASN:HB2	1:AA:222:TYR:CZ	2.48	0.49
2:BB:3402:LEU:HD11	2:BB:3483:ARG:HE	1.77	0.49
4:AE:161:LEU:HB2	4:AE:450:MET:CE	2.35	0.49
1:AA:503:ASP:OD2	1:AA:506:ARG:HB2	2.13	0.49
2:AB:285:ILE:HA	2:AB:306:ILE:HG23	1.93	0.49
8:AZ:294:VAL:HG23	8:AZ:315:LEU:O	2.12	0.49
8:AZ:296:ILE:HG13	8:AZ:317:LEU:HD22	1.93	0.49
4:AE:316:ALA:CB	4:AE:370:SER:H	2.25	0.49
3:AD:207:THR:HG22	3:AD:380:ARG:N	2.27	0.49
2:AB:208:LEU:HD11	2:AB:365:CYS:HB2	1.92	0.49
1:AA:202:ALA:HA	1:AA:328:ARG:HH11	1.76	0.49
8:AZ:368:THR:HG22	8:AZ:369:GLU:H	1.77	0.49
7:AQ:23:ASN:C	7:AQ:25:ASP:H	2.15	0.49
6:BH:3327:ILE:HD11	6:BH:3334:ILE:HD13	1.93	0.49
7:BQ:3023:ASN:C	7:BQ:3025:ASP:H	2.15	0.49
7:AQ:302:GLY:HA2	7:AQ:323:VAL:O	2.12	0.49
5:AG:215:LEU:C	5:AG:217:SER:H	2.16	0.49
2:BB:3169:ASP:OD2	2:BB:3204:SER:HB3	2.12	0.49
1:AA:520:PRO:HB2	1:AA:522:ILE:HG23	1.94	0.49
4:BE:3287:LEU:O	4:BE:3287:LEU:HD23	2.12	0.49
7:AQ:153:LYS:C	7:AQ:155:ASP:H	2.15	0.49
4:AE:543:GLN:O	4:AE:546:ARG:HB3	2.13	0.49
5:BG:3508:GLN:OE1	5:BG:3508:GLN:HA	2.13	0.49
7:BQ:3137:PHE:CE2	7:BQ:3434:ILE:HA	2.47	0.49
1:BA:3168:ILE:CG2	1:BA:3397:GLU:HG3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:168:ILE:CG2	1:AA:397:GLU:HG3	2.43	0.49
2:AB:346:ILE:CD1	2:AB:355:LYS:HB2	2.42	0.49
5:AG:282:LEU:O	5:AG:286:GLN:HG2	2.12	0.49
4:BE:3296:GLN:O	4:BE:3299:GLN:HB3	2.13	0.49
4:BE:3229:ARG:O	4:BE:3409:ARG:HA	2.12	0.49
4:AE:324:GLN:NE2	4:AE:325:TRP:HE1	2.11	0.49
6:BH:3292:ILE:HD13	6:BH:3313:PHE:HB3	1.94	0.49
2:AB:203:LEU:HA	2:AB:370:ARG:O	2.11	0.49
6:AH:292:ILE:HD13	6:AH:313:PHE:HB3	1.94	0.49
6:BH:3041:LYS:HD3	6:BH:3452:GLN:OE1	2.12	0.49
2:BB:3154:ILE:O	2:BB:3158:LYS:HG3	2.12	0.49
7:BQ:3302:GLY:HA2	7:BQ:3323:VAL:O	2.12	0.49
5:BG:3215:LEU:C	5:BG:3217:SER:H	2.16	0.49
7:BQ:3153:LYS:C	7:BQ:3155:ASP:H	2.15	0.49
1:AA:54:VAL:HA	1:AA:60:PHE:HB3	1.94	0.49
6:AH:185:ALA:HB2	6:AH:214:PHE:HE1	1.78	0.49
1:AA:209:HIS:HE1	5:AG:83:ARG:HH21	1.59	0.49
8:BZ:3191:LEU:O	8:BZ:3194:VAL:HG23	2.13	0.49
1:BA:3520:PRO:HB2	1:BA:3522:ILE:HG23	1.94	0.49
4:BE:3543:GLN:O	4:BE:3546:ARG:HB3	2.13	0.49
5:AG:508:GLN:HA	5:AG:508:GLN:OE1	2.13	0.49
5:BG:3502:PRO:HD2	5:BG:3505:ILE:HD12	1.95	0.49
8:BZ:3193:MET:CE	8:BZ:3327:ARG:HG3	2.41	0.49
1:AA:253:LYS:HG3	1:AA:303:ASP:OD2	2.13	0.49
3:BD:3207:THR:HG22	3:BD:3380:ARG:N	2.28	0.49
6:AH:480:GLY:HA3	6:AH:491:ASN:ND2	2.27	0.49
6:BH:3198:LEU:O	6:BH:3325:ARG:HD2	2.13	0.49
3:BD:3450:ILE:HB	3:BD:3451:PRO:HD3	1.95	0.49
3:AD:178:VAL:O	3:AD:181:ILE:HD12	2.12	0.49
5:BG:3289:ALA:C	5:BG:3291:ARG:H	2.15	0.49
4:BE:3260:PRO:O	4:BE:3264:SER:HB3	2.13	0.49
8:AZ:459:VAL:CG2	8:AZ:466:PRO:HA	2.43	0.49
4:BE:3206:GLU:HG2	4:BE:3239:LEU:CD1	2.42	0.49
8:BZ:3403:ALA:O	8:BZ:3407:LYS:HG3	2.13	0.49
3:AD:244:PRO:C	3:AD:246:PRO:HD3	2.33	0.49
1:BA:3503:ASP:OD2	1:BA:3506:ARG:HB2	2.13	0.49
4:AE:255:PRO:O	4:AE:256:LYS:HE2	2.12	0.49
3:BD:3234:ILE:HG12	3:BD:3285:VAL:HB	1.94	0.49
5:AG:402:VAL:O	5:AG:406:VAL:HG23	2.13	0.49
7:BQ:3236:VAL:HG11	7:BQ:3318:ILE:C	2.33	0.49
7:AQ:236:VAL:HG11	7:AQ:318:ILE:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3123:SER:HG	3:BD:3440:TRP:HZ3	1.60	0.49
4:BE:3287:LEU:CD2	4:BE:3298:LEU:HD11	2.42	0.49
7:BQ:3138:THR:HG23	7:BQ:3430:LEU:CD2	2.41	0.49
3:AD:283:CYS:SG	3:AD:339:PHE:HZ	2.36	0.49
3:BD:3448:GLU:C	3:BD:3451:PRO:HD2	2.33	0.49
1:BA:3120:ILE:HG23	1:BA:3443:ARG:HD3	1.94	0.49
2:AB:289:LEU:HD12	2:AB:289:LEU:N	2.27	0.49
8:AZ:403:ALA:O	8:AZ:407:LYS:HG3	2.13	0.49
5:AG:339:ARG:HB3	5:AG:339:ARG:NH1	2.28	0.49
6:AH:267:TYR:O	6:AH:270:ILE:HG22	2.13	0.49
6:AH:241:ILE:HG21	6:AH:330:VAL:HG21	1.95	0.49
7:BQ:3444:LEU:H	7:BQ:3444:LEU:CD2	2.18	0.49
7:BQ:3069:ALA:HB2	7:BQ:3089:THR:HG22	1.95	0.49
5:AG:158:SER:OG	5:AG:402:VAL:HG21	2.13	0.49
2:BB:3285:ILE:HA	2:BB:3306:ILE:HG23	1.93	0.49
8:AZ:294:VAL:CG2	8:AZ:315:LEU:HB3	2.40	0.49
5:AG:273:LEU:HD22	8:AZ:269:PHE:CE2	2.48	0.49
8:BZ:3213:LEU:HD11	8:BZ:3324:ASN:OD1	2.13	0.49
2:AB:310:ASP:O	2:AB:314:VAL:HG13	2.12	0.49
6:BH:3480:GLY:HA3	6:BH:3491:ASN:ND2	2.27	0.49
2:AB:183:ARG:NH2	2:AB:365:CYS:HB3	2.27	0.49
7:AQ:137:PHE:CE2	7:AQ:434:ILE:HA	2.47	0.49
8:BZ:3227:ARG:HH22	8:BZ:3353:LEU:HD21	1.75	0.49
1:AA:485:GLN:HG3	1:AA:488:LYS:HD2	1.95	0.49
4:BE:3260:PRO:HA	4:BE:3267:VAL:HG22	1.94	0.49
7:BQ:3224:LYS:HE3	7:BQ:3379:SER:H	1.76	0.49
7:AQ:69:ALA:HB2	7:AQ:89:THR:HG22	1.95	0.49
6:BH:3267:TYR:O	6:BH:3270:ILE:HG22	2.12	0.49
4:AE:287:LEU:HD23	4:AE:287:LEU:O	2.12	0.49
6:BH:3241:ILE:HG21	6:BH:3330:VAL:HG21	1.95	0.49
8:BZ:3360:GLY:C	8:BZ:3362:GLU:H	2.15	0.49
3:BD:3404:LEU:HD21	3:BD:3410:LEU:HD23	1.93	0.49
6:BH:3203:LYS:HB3	6:BH:3386:ILE:HG21	1.94	0.49
3:AD:234:ILE:HG12	3:AD:285:VAL:HB	1.94	0.49
5:BG:3158:SER:OG	5:BG:3402:VAL:HG21	2.13	0.49
5:BG:3402:VAL:O	5:BG:3406:VAL:HG23	2.13	0.49
5:BG:3273:LEU:HD22	8:BZ:3269:PHE:CE2	2.48	0.49
1:AA:156:LEU:HD22	1:AA:181:VAL:HG12	1.95	0.49
2:BB:3183:ARG:NH2	2:BB:3365:CYS:HB3	2.27	0.49
4:AE:322:ILE:HA	4:AE:343:VAL:HB	1.94	0.49
1:AA:476:LYS:HG2	1:AA:480:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:259:THR:HG22	8:AZ:247:VAL:CG1	2.43	0.49
7:BQ:3458:VAL:O	7:BQ:3462:THR:HG23	2.13	0.49
1:BA:3162:THR:CG2	1:BA:3517:VAL:HA	2.28	0.48
1:BA:3020:ILE:HB	1:BA:3025:ILE:HB	1.95	0.48
3:AD:128:ALA:C	3:AD:130:ARG:H	2.15	0.48
7:AQ:264:THR:O	8:AZ:252:PHE:HA	2.13	0.48
1:AA:532:LEU:O	1:AA:536:VAL:HG23	2.13	0.48
5:AG:415:GLY:HA3	5:AG:499:ILE:O	2.12	0.48
5:BG:3415:GLY:HA3	5:BG:3499:ILE:O	2.12	0.48
5:BG:3214:VAL:HA	5:BG:3382:ARG:O	2.13	0.48
7:AQ:190:LEU:HD23	7:AQ:191:PRO:HD2	1.94	0.48
7:BQ:3264:THR:O	8:BZ:3252:PHE:HA	2.13	0.48
6:AH:281:LYS:O	6:AH:338:THR:HG21	2.13	0.48
2:AB:172:HIS:CE1	2:AB:176:LEU:HD11	2.48	0.48
7:AQ:23:ASN:HA	7:AQ:27:GLN:CB	2.43	0.48
7:BQ:3411:LEU:HD12	7:BQ:3411:LEU:O	2.12	0.48
3:AD:450:ILE:HB	3:AD:451:PRO:HD3	1.95	0.48
3:BD:3178:VAL:O	3:BD:3181:ILE:HD12	2.12	0.48
2:BB:3350:GLU:HG2	3:BD:3402:ARG:NH1	2.27	0.48
8:BZ:3174:VAL:HG13	8:BZ:3175:THR:H	1.78	0.48
2:AB:413:LYS:HG2	2:AB:464:TYR:HA	1.95	0.48
2:BB:3289:LEU:N	2:BB:3289:LEU:HD12	2.27	0.48
6:BH:3449:ILE:O	6:BH:3453:LEU:HB2	2.13	0.48
5:BG:3414:PRO:HG3	5:BG:3481:THR:HG22	1.94	0.48
1:BA:3316:MET:SD	1:BA:3361:VAL:HG12	2.53	0.48
1:BA:3377:THR:HB	1:BA:3380:HIS:HB3	1.95	0.48
1:BA:3532:LEU:O	1:BA:3536:VAL:HG23	2.13	0.48
4:AE:33:LYS:CD	6:AH:74:ASP:HB3	2.42	0.48
4:BE:3255:PRO:O	4:BE:3256:LYS:HE2	2.12	0.48
7:AQ:57:ASN:HB2	7:AQ:61:LYS:N	2.26	0.48
2:BB:3298:PHE:HD2	2:BB:3303:ILE:HB	1.78	0.48
5:BG:3339:ARG:NH1	5:BG:3339:ARG:HB3	2.28	0.48
2:BB:3232:LEU:HD21	2:BB:3326:VAL:HG21	1.95	0.48
1:BA:3189:THR:O	1:BA:3196:ILE:HA	2.14	0.48
4:BE:3278:PRO:HD3	4:BE:3306:PHE:CZ	2.48	0.48
2:AB:75:LYS:HD2	4:AE:81:ILE:CD1	2.43	0.48
7:AQ:32:ILE:O	7:AQ:36:ARG:HB2	2.13	0.48
2:BB:3476:ASN:HB2	2:BB:3478:THR:HG22	1.94	0.48
1:BA:3113:ASN:O	1:BA:3116:VAL:HG23	2.12	0.48
5:BG:3110:TYR:HA	5:BG:3114:LYS:HB2	1.95	0.48
2:AB:268:LYS:HD2	4:AE:299:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:350:GLU:HG2	3:AD:402:ARG:NH1	2.27	0.48
2:BB:3268:LYS:HD2	4:BE:3299:GLN:OE1	2.13	0.48
8:BZ:3027:GLU:HG2	8:BZ:3103:ARG:NH1	2.28	0.48
4:BE:3378:SER:O	4:BE:3379:ARG:HB2	2.13	0.48
7:BQ:3545:ILE:HB	8:BZ:3046:LEU:HB3	1.95	0.48
5:BG:3179:VAL:HG21	5:BG:3403:ALA:CB	2.42	0.48
4:AE:413:LYS:HE3	4:AE:413:LYS:N	2.02	0.48
5:AG:166:HIS:CD2	8:AZ:123:GLU:HG2	2.49	0.48
2:AB:109:LEU:HB2	2:AB:120:ILE:HD11	1.95	0.48
7:AQ:177:ILE:O	7:AQ:181:LEU:HB2	2.13	0.48
1:AA:377:THR:HB	1:AA:380:HIS:HB3	1.95	0.48
8:BZ:3194:VAL:HG13	8:BZ:3376:CYS:SG	2.53	0.48
8:AZ:191:LEU:O	8:AZ:194:VAL:HG23	2.13	0.48
5:AG:214:VAL:HA	5:AG:382:ARG:O	2.13	0.48
3:BD:3030:SER:O	3:BD:3033:ASP:HB2	2.13	0.48
1:BA:3204:ASN:HB2	1:BA:3222:TYR:CZ	2.48	0.48
2:BB:3188:THR:CG2	2:BB:3396:LYS:HG3	2.44	0.48
5:BG:3145:VAL:HG12	5:BG:3406:VAL:HG12	1.94	0.48
8:BZ:3317:LEU:HD11	8:BZ:3365:THR:HG21	1.95	0.48
1:BA:3253:LYS:HG3	1:BA:3303:ASP:OD2	2.13	0.48
5:BG:3519:LEU:O	5:BG:3522:ARG:HB2	2.13	0.48
5:BG:3307:HIS:CD2	8:BZ:3339:SER:HB3	2.48	0.48
7:BQ:3202:PHE:HD2	7:BQ:3409:LYS:HA	1.78	0.48
5:BG:3162:LYS:HG2	5:BG:3395:ASN:OD1	2.13	0.48
6:BH:3012:VAL:HG13	7:BQ:3078:VAL:HG11	1.95	0.48
3:BD:3178:VAL:HG21	3:BD:3401:ILE:HB	1.94	0.48
4:AE:267:VAL:HG13	4:AE:319:ASP:OD2	2.12	0.48
8:AZ:101:LEU:HD22	8:AZ:122:PHE:CZ	2.49	0.48
6:AH:41:LYS:HD3	6:AH:452:GLN:OE1	2.12	0.48
3:AD:149:GLN:NE2	3:AD:152:ARG:HD2	2.28	0.48
5:AG:307:HIS:CD2	8:AZ:339:SER:HB3	2.48	0.48
1:BA:3054:VAL:HA	1:BA:3060:PHE:HB3	1.94	0.48
6:AH:513:ALA:O	6:AH:517:ILE:HG12	2.14	0.48
5:BG:3430:LYS:HD2	5:BG:3442:TYR:OH	2.12	0.48
8:AZ:194:VAL:HG13	8:AZ:376:CYS:SG	2.53	0.48
8:AZ:213:LEU:HD11	8:AZ:324:ASN:OD1	2.13	0.48
4:AE:278:PRO:HD3	4:AE:306:PHE:CZ	2.48	0.48
8:BZ:3277:ILE:HG23	8:BZ:3340:VAL:CG2	2.44	0.48
6:AH:222:LYS:NZ	6:AH:361:ARG:HH21	2.11	0.48
6:BH:3281:LYS:O	6:BH:3338:THR:HG21	2.13	0.48
6:AH:12:VAL:HG13	7:AQ:78:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3283:CYS:SG	3:BD:3339:PHE:HZ	2.36	0.48
8:BZ:3158:LEU:O	8:BZ:3162:VAL:HG12	2.14	0.48
3:AD:448:GLU:C	3:AD:451:PRO:HD2	2.33	0.48
7:BQ:3208:ARG:HD3	7:BQ:3331:ARG:HH12	1.78	0.48
1:AA:498:ARG:N	1:AA:498:ARG:HD3	2.28	0.48
6:AH:428:SER:O	6:AH:436:GLN:HG3	2.13	0.48
1:AA:316:MET:SD	1:AA:361:VAL:HG12	2.53	0.48
1:BA:3335:ALA:HB2	1:BA:3356:GLY:HA3	1.96	0.48
8:AZ:524:ALA:O	8:AZ:528:LEU:HG	2.12	0.48
4:AE:550:LYS:HE3	6:AH:50:ASP:CG	2.34	0.48
4:BE:3550:LYS:HE3	6:BH:3050:ASP:CG	2.34	0.48
2:BB:3075:LYS:HD2	4:BE:3081:ILE:CD1	2.43	0.48
2:BB:3172:HIS:CE1	2:BB:3176:LEU:HD11	2.48	0.48
2:BB:3375:GLN:HA	2:BB:3375:GLN:OE1	2.14	0.48
3:BD:3486:ARG:HD2	3:BD:3490:THR:HG21	1.95	0.48
3:AD:486:ARG:HD2	3:AD:490:THR:HG21	1.96	0.48
4:AE:99:GLU:OE1	6:AH:60:THR:HG21	2.13	0.48
7:AQ:545:ILE:HB	8:AZ:46:LEU:HB3	1.95	0.48
7:AQ:224:LYS:HG2	7:AQ:379:SER:HB3	1.95	0.48
3:BD:3089:ALA:HA	3:BD:3403:CYS:SG	2.53	0.48
6:AH:279:PHE:O	6:AH:282:LEU:HB3	2.14	0.48
1:BA:3545:ILE:CD1	3:BD:3068:MET:HG3	2.38	0.48
2:BB:3233:ILE:HD11	2:BB:3323:GLY:HA3	1.94	0.48
7:AQ:153:LYS:HG3	7:AQ:155:ASP:HB2	1.94	0.48
4:BE:3316:ALA:CB	4:BE:3370:SER:H	2.25	0.48
6:AH:388:GLU:HA	6:AH:391:ARG:NH2	2.29	0.48
1:BA:3156:LEU:HD22	1:BA:3181:VAL:HG12	1.95	0.48
1:AA:268:GLU:CG	1:AA:269:GLN:H	2.26	0.48
5:AG:519:LEU:O	5:AG:522:ARG:HB2	2.13	0.48
6:BH:3011:VAL:HG22	7:BQ:3021:TYR:CE2	2.48	0.48
6:AH:186:VAL:HG21	6:AH:400:VAL:HB	1.95	0.48
3:AD:178:VAL:HG21	3:AD:401:ILE:HB	1.94	0.48
2:AB:476:ASN:HB2	2:AB:478:THR:HG22	1.94	0.48
8:BZ:3014:ARG:HH11	8:BZ:3014:ARG:HB3	1.78	0.48
3:BD:3138:MET:HB2	3:BD:3478:LEU:HD13	1.96	0.48
6:AH:296:LYS:HG3	6:AH:323:MET:HG3	1.96	0.48
2:BB:3155:HIS:HB2	2:BB:3488:VAL:HG22	1.96	0.48
2:AB:155:HIS:HB2	2:AB:488:VAL:HG22	1.96	0.48
8:AZ:174:VAL:HG13	8:AZ:175:THR:H	1.78	0.48
4:BE:3211:VAL:HG11	4:BE:3223:LEU:HB3	1.96	0.48
7:BQ:3160:LEU:O	7:BQ:3160:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:17:GLY:HA2	1:AA:548:ASP:OD1	2.13	0.48
1:AA:335:ALA:HB2	1:AA:356:GLY:HA3	1.96	0.48
1:BA:3295:VAL:HG22	1:BA:3316:MET:HB3	1.96	0.48
2:AB:254:SER:HB3	3:AD:262:LYS:HE2	1.96	0.48
7:BQ:3438:GLY:C	7:BQ:3440:ARG:H	2.17	0.48
5:BG:3166:HIS:CD2	8:BZ:3123:GLU:HG2	2.48	0.48
3:BD:3311:MET:HE2	3:BD:3311:MET:HB3	1.64	0.48
6:BH:3259:VAL:CG2	7:BQ:3267:LEU:HD12	2.39	0.48
1:AA:295:VAL:HG22	1:AA:316:MET:HB3	1.96	0.48
8:AZ:337:GLN:HE21	8:AZ:347:ILE:HG21	1.75	0.48
6:AH:299:ILE:HD13	6:AH:316:GLY:CA	2.43	0.48
1:BA:3498:ARG:HG2	1:BA:3499:ASN:H	1.79	0.48
4:AE:296:GLN:O	4:AE:299:GLN:HB3	2.13	0.48
4:AE:406:CYS:HB3	4:AE:423:LEU:HD21	1.96	0.48
6:AH:336:SER:HB3	7:AQ:311:HIS:CG	2.48	0.48
8:BZ:3101:LEU:HD22	8:BZ:3122:PHE:CZ	2.48	0.48
7:BQ:3224:LYS:HG2	7:BQ:3379:SER:HB3	1.95	0.48
5:BG:3121:ILE:HG23	5:BG:3441:PRO:HB3	1.95	0.48
3:AD:30:SER:O	3:AD:33:ASP:HB2	2.13	0.48
1:AA:120:ILE:HG23	1:AA:443:ARG:HD3	1.94	0.48
7:AQ:374:GLU:O	7:AQ:375:GLN:HB2	2.13	0.48
6:BH:3411:ALA:O	6:BH:3415:ALA:HB3	2.14	0.48
6:BH:3513:ALA:O	6:BH:3517:ILE:HG12	2.13	0.48
2:AB:216:LYS:HE2	2:AB:307:GLU:HG3	1.96	0.48
4:AE:101:ALA:O	4:AE:105:VAL:HG23	2.13	0.48
8:AZ:277:ILE:HG23	8:AZ:340:VAL:CG2	2.44	0.48
8:AZ:232:TYR:HD2	8:AZ:348:LEU:HB2	1.78	0.48
8:AZ:115:PRO:O	8:AZ:119:THR:HG23	2.14	0.48
8:BZ:3115:PRO:O	8:BZ:3119:THR:HG23	2.14	0.48
5:AG:81:LEU:HD11	5:AG:516:SER:HB2	1.94	0.48
6:BH:3299:ILE:HD13	6:BH:3316:GLY:CA	2.43	0.48
5:AG:457:ILE:CD1	5:AG:467:LEU:HG	2.44	0.48
6:AH:11:VAL:HG22	7:AQ:21:TYR:CE2	2.48	0.48
6:AH:198:LEU:O	6:AH:325:ARG:HD2	2.13	0.48
7:AQ:208:ARG:HD3	7:AQ:331:ARG:HH12	1.78	0.48
1:BA:3485:GLN:HG3	1:BA:3488:LYS:HD2	1.95	0.48
5:AG:110:TYR:HA	5:AG:114:LYS:HB2	1.95	0.48
6:AH:242:LEU:HD22	6:AH:285:VAL:HG13	1.96	0.48
5:AG:121:ILE:HG23	5:AG:441:PRO:HB3	1.95	0.48
7:AQ:202:PHE:HD2	7:AQ:409:LYS:HA	1.78	0.48
7:BQ:3177:ILE:O	7:BQ:3181:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:45:GLY:O	6:AH:168:SER:HB2	2.14	0.48
2:AB:232:LEU:HD21	2:AB:326:VAL:HG21	1.95	0.48
5:AG:502:PRO:HD2	5:AG:505:ILE:HD12	1.95	0.48
5:BG:3235:SER:HB3	5:BG:3315:SER:OG	2.14	0.48
5:BG:3231:HIS:HD2	8:BZ:3338:ASN:HD22	1.62	0.48
3:AD:169:PHE:HZ	3:AD:207:THR:HG1	1.61	0.48
1:BA:3268:GLU:CG	1:BA:3269:GLN:H	2.26	0.48
6:BH:3222:LYS:NZ	6:BH:3361:ARG:HH21	2.11	0.48
8:BZ:3093:THR:HG23	8:BZ:3454:ILE:CD1	2.43	0.48
6:AH:243:SER:HB3	6:AH:334:ILE:HD12	1.96	0.48
6:BH:3178:PHE:CE2	6:BH:3393:LEU:HD11	2.48	0.48
7:BQ:3150:ILE:C	7:BQ:3152:ASP:H	2.15	0.48
2:BB:3216:LYS:HE2	2:BB:3307:GLU:HG3	1.96	0.48
7:BQ:3023:ASN:HA	7:BQ:3027:GLN:CB	2.43	0.48
2:BB:3122:GLU:HB3	2:BB:3426:LYS:HZ3	1.77	0.48
3:AD:62:HIS:CE1	3:AD:83:ALA:HA	2.49	0.48
6:AH:411:ALA:O	6:AH:415:ALA:HB3	2.14	0.48
7:AQ:160:LEU:O	7:AQ:160:LEU:HD23	2.14	0.48
1:AA:510:VAL:HG22	1:AA:511:ASP:N	2.28	0.48
3:AD:60:ASP:O	3:AD:64:ILE:HG13	2.14	0.48
2:AB:216:LYS:NZ	2:AB:307:GLU:HG3	2.29	0.48
2:BB:3188:THR:HG22	2:BB:3396:LYS:HG3	1.96	0.48
1:AA:189:THR:O	1:AA:196:ILE:HA	2.14	0.48
6:BH:3220:PHE:HE2	6:BH:3318:VAL:HG22	1.78	0.48
4:AE:322:ILE:HD12	4:AE:354:ILE:HG21	1.96	0.48
1:BA:3072:LEU:HD23	1:BA:3072:LEU:O	2.14	0.48
6:AH:178:PHE:CE2	6:AH:393:LEU:HD11	2.48	0.48
7:BQ:3150:ILE:HD12	7:BQ:3152:ASP:H	1.79	0.48
8:AZ:158:LEU:O	8:AZ:162:VAL:HG12	2.14	0.48
6:BH:3257:ALA:HB2	7:BQ:3265:VAL:HB	1.96	0.48
4:BE:3259:LEU:HD13	4:BE:3261:LYS:N	2.29	0.48
8:AZ:27:GLU:HG2	8:AZ:103:ARG:NH1	2.29	0.48
4:AE:324:GLN:HE21	4:AE:325:TRP:HE1	1.61	0.48
4:BE:3324:GLN:HE21	4:BE:3325:TRP:HE1	1.61	0.48
3:BD:3149:GLN:NE2	3:BD:3152:ARG:HD2	2.28	0.48
5:BG:3032:ALA:O	5:BG:3036:ARG:HG3	2.14	0.47
5:AG:16:THR:HG22	5:AG:17:GLY:H	1.79	0.47
2:AB:298:PHE:HD2	2:AB:303:ILE:HB	1.78	0.47
1:BA:3017:GLY:HA2	1:BA:3548:ASP:OD1	2.13	0.47
5:AG:206:VAL:HG12	5:AG:207:GLU:H	1.80	0.47
8:AZ:317:LEU:HD11	8:AZ:365:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3045:GLY:O	6:BH:3168:SER:HB2	2.14	0.47
1:BA:3156:LEU:HD11	1:BA:3413:LEU:HD11	1.96	0.47
7:BQ:3267:LEU:HA	7:BQ:3272:GLU:OE1	2.14	0.47
3:BD:3123:SER:HB3	3:BD:3439:ILE:HG21	1.96	0.47
2:AB:375:GLN:HA	2:AB:375:GLN:OE1	2.14	0.47
8:AZ:352:GLY:CA	8:AZ:369:GLU:HB2	2.41	0.47
1:BA:3498:ARG:HD3	1:BA:3498:ARG:N	2.28	0.47
2:AB:226:ILE:HD11	2:AB:304:ASN:ND2	2.29	0.47
6:BH:3464:ILE:HD12	6:BH:3488:ILE:HG23	1.96	0.47
4:BE:3406:CYS:HB3	4:BE:3423:LEU:HD21	1.96	0.47
8:AZ:98:VAL:HG23	8:AZ:524:ALA:HB2	1.96	0.47
7:BQ:3534:ALA:O	7:BQ:3538:VAL:HG23	2.14	0.47
5:AG:55:LEU:HD22	5:AG:55:LEU:N	2.29	0.47
3:BD:3471:SER:O	3:BD:3474:GLU:HB2	2.13	0.47
2:BB:3427:SER:O	2:BB:3430:VAL:HB	2.14	0.47
4:BE:3488:GLY:O	4:BE:3489:LEU:HD23	2.14	0.47
2:AB:481:ASP:HB3	2:AB:484:GLN:HB3	1.97	0.47
3:BD:3324:LEU:O	3:BD:3328:LEU:HB2	2.14	0.47
6:BH:3459:PHE:CD1	6:BH:3486:GLU:HB3	2.49	0.47
1:AA:327:ARG:O	1:AA:331:ARG:HG3	2.15	0.47
2:AB:242:LYS:HE2	3:AD:248:THR:OG1	2.14	0.47
5:BG:3167:TRP:HH2	8:BZ:3126:ARG:CZ	2.27	0.47
5:AG:270:ASN:OD1	8:AZ:269:PHE:HA	2.14	0.47
2:BB:3109:LEU:HB2	2:BB:3120:ILE:HD11	1.95	0.47
8:BZ:3232:TYR:HD2	8:BZ:3348:LEU:HB2	1.78	0.47
2:BB:3242:LYS:CB	2:BB:3245:ILE:HD11	2.35	0.47
2:BB:3242:LYS:HE2	3:BD:3248:THR:OG1	2.14	0.47
7:BQ:3032:ILE:O	7:BQ:3036:ARG:HB2	2.13	0.47
5:AG:282:LEU:HD21	5:AG:341:GLU:OE2	2.15	0.47
8:BZ:3459:VAL:CG2	8:BZ:3466:PRO:HA	2.43	0.47
4:AE:259:LEU:HD13	4:AE:261:LYS:N	2.29	0.47
7:BQ:3252:CYS:HB2	7:BQ:3342:PRO:O	2.14	0.47
6:BH:3242:LEU:HD22	6:BH:3285:VAL:HG13	1.96	0.47
2:AB:122:GLU:HB3	2:AB:426:LYS:HZ3	1.79	0.47
2:AB:467:ILE:HG23	2:AB:469:THR:HG22	1.96	0.47
2:BB:3298:PHE:HB3	2:BB:3303:ILE:O	2.14	0.47
5:AG:414:PRO:HG3	5:AG:481:THR:HG22	1.94	0.47
3:AD:471:SER:O	3:AD:474:GLU:HB2	2.13	0.47
4:BE:3099:GLU:OE1	6:BH:3060:THR:HG21	2.13	0.47
5:BG:3167:TRP:CE2	5:BG:3214:VAL:HG21	2.49	0.47
2:BB:3216:LYS:NZ	2:BB:3307:GLU:HG3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AQ:460:PRO:HG2	7:AQ:461:ARG:H	1.79	0.47
7:BQ:3313:LEU:HD22	7:BQ:3318:ILE:HG21	1.95	0.47
7:BQ:3374:GLU:O	7:BQ:3375:GLN:HB2	2.13	0.47
2:AB:88:VAL:HG13	2:AB:90:ASP:H	1.79	0.47
4:BE:3363:VAL:O	4:BE:3363:VAL:HG23	2.14	0.47
5:BG:3457:ILE:CD1	5:BG:3467:LEU:HG	2.44	0.47
7:AQ:39:HIS:CD2	7:AQ:108:GLY:HA3	2.47	0.47
1:BA:3476:LYS:HG2	1:BA:3480:TYR:CE1	2.46	0.47
2:BB:3226:ILE:HD11	2:BB:3304:ASN:ND2	2.29	0.47
8:AZ:133:LEU:HD21	8:AZ:412:ILE:HD13	1.96	0.47
7:AQ:252:CYS:HB2	7:AQ:342:PRO:O	2.14	0.47
6:BH:3296:LYS:HG3	6:BH:3323:MET:HG3	1.96	0.47
2:AB:236:THR:HG21	2:AB:329:PHE:HE2	1.79	0.47
6:BH:3428:SER:O	6:BH:3436:GLN:HG3	2.13	0.47
7:BQ:3133:MET:SD	7:BQ:3445:LEU:HD22	2.54	0.47
1:BA:3510:VAL:HG22	1:BA:3511:ASP:N	2.28	0.47
7:BQ:3269:ASN:ND2	7:BQ:3270:ALA:H	2.13	0.47
5:BG:3016:THR:HG22	5:BG:3017:GLY:H	1.79	0.47
6:AH:351:LEU:HD12	6:AH:352:PHE:N	2.29	0.47
6:AH:459:PHE:CD1	6:AH:486:GLU:HB3	2.49	0.47
1:AA:377:THR:HG1	1:AA:380:HIS:CG	2.32	0.47
4:AE:281:PRO:HD2	4:AE:285:HIS:NE2	2.29	0.47
7:AQ:267:LEU:HA	7:AQ:272:GLU:OE1	2.14	0.47
3:AD:35:ILE:HG13	3:AD:65:LEU:HD21	1.96	0.47
4:BE:3033:LYS:CD	6:BH:3074:ASP:HB3	2.42	0.47
1:AA:257:ALA:HB3	1:AA:260:VAL:HB	1.96	0.47
4:BE:3441:TYR:HB3	4:BE:3522:MET:HB2	1.96	0.47
7:AQ:189:VAL:HG23	7:AQ:380:ARG:HA	1.96	0.47
6:BH:3220:PHE:CE2	6:BH:3318:VAL:HG22	2.49	0.47
6:AH:220:PHE:HE2	6:AH:318:VAL:HG22	1.78	0.47
2:AB:312:GLU:O	2:AB:316:ARG:HG3	2.14	0.47
6:BH:3520:VAL:HG11	7:BQ:3054:ILE:HG13	1.97	0.47
6:BH:3186:VAL:HG21	6:BH:3400:VAL:HB	1.95	0.47
7:AQ:332:LEU:HD23	7:AQ:333:CYS:N	2.30	0.47
2:AB:511:VAL:HG21	4:AE:73:ILE:HD11	1.97	0.47
3:BD:3356:ASP:C	3:BD:3358:SER:H	2.17	0.47
2:BB:3413:LYS:HG2	2:BB:3464:TYR:HA	1.95	0.47
8:BZ:3133:LEU:HD21	8:BZ:3412:ILE:HD13	1.96	0.47
7:AQ:534:ALA:O	7:AQ:538:VAL:HG23	2.14	0.47
5:BG:3055:LEU:HD22	5:BG:3055:LEU:N	2.29	0.47
7:AQ:458:VAL:O	7:AQ:462:THR:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:3044:LEU:HD12	9:BA:3601:ADP:O2A	2.14	0.47
8:BZ:3040:LYS:O	8:BZ:3461:ASN:HB3	2.15	0.47
7:AQ:428:ILE:HG13	7:AQ:478:LEU:HG	1.96	0.47
5:AG:167:TRP:CE2	5:AG:214:VAL:HG21	2.49	0.47
3:AD:311:MET:HE2	3:AD:311:MET:HB3	1.63	0.47
8:BZ:3329:GLN:O	8:BZ:3330:LEU:HD12	2.15	0.47
1:AA:298:THR:HG21	1:AA:302:ILE:HG13	1.96	0.47
4:BE:3270:ALA:HB3	4:BE:3321:VAL:HA	1.96	0.47
6:AH:464:ILE:HD12	6:AH:488:ILE:HG23	1.96	0.47
6:AH:229:PHE:CE1	6:AH:234:LYS:HE2	2.50	0.47
2:AB:212:PHE:HE1	2:AB:214:LEU:HD13	1.80	0.47
6:BH:3163:ARG:HG3	6:BH:3179:VAL:HG21	1.96	0.47
1:AA:72:LEU:O	1:AA:72:LEU:HD23	2.14	0.47
3:BD:3331:LYS:HZ3	3:BD:3332:PRO:HD2	1.80	0.47
2:BB:3079:ASN:HB3	4:BE:3412:ASN:OD1	2.15	0.47
1:AA:389:GLY:HA3	1:AA:395:LEU:HD13	1.97	0.47
6:AH:449:ILE:O	6:AH:453:LEU:HB2	2.13	0.47
1:AA:44:LEU:HD12	9:AA:601:ADP:O2A	2.14	0.47
2:AB:188:THR:HG22	2:AB:396:LYS:HG3	1.96	0.47
8:AZ:40:LYS:O	8:AZ:461:ASN:HB3	2.15	0.47
2:AB:427:SER:O	2:AB:430:VAL:HB	2.14	0.47
4:BE:3285:HIS:HB3	4:BE:3286:LYS:H	1.58	0.47
6:BH:3260:ARG:HH11	6:BH:3260:ARG:CB	2.17	0.47
1:AA:335:ALA:HB2	1:AA:356:GLY:CA	2.45	0.47
4:BE:3033:LYS:HB3	6:BH:3074:ASP:CB	2.45	0.47
6:BH:3098:THR:O	6:BH:3101:VAL:HG12	2.15	0.47
7:AQ:438:GLY:C	7:AQ:440:ARG:H	2.17	0.47
7:AQ:438:GLY:O	7:AQ:446:GLN:HG3	2.14	0.47
1:BA:3257:ALA:HB3	1:BA:3260:VAL:HB	1.96	0.47
5:AG:235:SER:HB3	5:AG:315:SER:OG	2.14	0.47
6:BH:3189:LEU:HD23	6:BH:3189:LEU:N	2.24	0.47
7:AQ:313:LEU:HD22	7:AQ:318:ILE:HG21	1.95	0.47
1:AA:156:LEU:HD11	1:AA:413:LEU:HD11	1.96	0.47
6:BH:3273:ALA:HB3	7:BQ:3273:MET:HE2	1.96	0.47
6:AH:190:ASP:C	6:AH:192:ASN:H	2.18	0.47
6:AH:162:ALA:HB2	6:AH:400:VAL:HG22	1.97	0.47
8:BZ:3456:LYS:O	8:BZ:3459:VAL:HG22	2.15	0.47
1:AA:498:ARG:HG2	1:AA:499:ASN:H	1.79	0.47
1:AA:169:ILE:HD11	1:AA:176:PHE:HB3	1.96	0.47
2:AB:141:ASP:HB2	2:AB:399:ARG:HA	1.97	0.47
1:BA:3169:ILE:HD11	1:BA:3176:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3210:GLU:C	6:BH:3212:SER:H	2.16	0.47
5:AG:32:ALA:O	5:AG:36:ARG:HG3	2.14	0.47
1:BA:3226:CYS:O	1:BA:3372:ILE:HG12	2.15	0.47
7:BQ:3174:SER:O	7:BQ:3178:LEU:HB2	2.15	0.47
6:BH:3432:ALA:HA	6:BH:3436:GLN:NE2	2.30	0.47
2:AB:188:THR:CG2	2:AB:396:LYS:HG3	2.44	0.47
6:BH:3279:PHE:O	6:BH:3282:LEU:HB3	2.14	0.47
3:AD:324:LEU:O	3:AD:328:LEU:HB2	2.14	0.47
4:BE:3101:ALA:O	4:BE:3105:VAL:HG23	2.13	0.47
1:AA:132:ALA:HB2	1:AA:448:ILE:HG23	1.97	0.47
3:BD:3244:PRO:C	3:BD:3246:PRO:HD3	2.34	0.47
4:BE:3294:GLU:OE2	6:BH:3264:VAL:HG23	2.15	0.47
1:AA:333:THR:HG22	1:AA:377:THR:CG2	2.42	0.47
1:AA:327:ARG:CA	1:AA:337:LEU:HD11	2.38	0.47
1:BA:3327:ARG:O	1:BA:3331:ARG:HG3	2.15	0.47
4:AE:305:LYS:O	4:AE:308:GLU:HB2	2.14	0.47
8:BZ:3274:LEU:O	8:BZ:3278:ILE:HG12	2.14	0.47
7:BQ:3438:GLY:O	7:BQ:3446:GLN:HG3	2.14	0.47
5:BG:3099:LEU:O	5:BG:3103:ILE:HG13	2.15	0.47
4:AE:494:THR:O	4:AE:498:LEU:HD13	2.15	0.47
8:AZ:329:GLN:O	8:AZ:330:LEU:HD12	2.15	0.47
1:AA:451:PHE:CE1	1:AA:455:LEU:HD11	2.50	0.47
5:BG:3270:ASN:OD1	8:BZ:3269:PHE:HA	2.14	0.47
7:BQ:3460:PRO:HG2	7:BQ:3461:ARG:H	1.79	0.47
4:AE:270:ALA:HB3	4:AE:321:VAL:HA	1.96	0.47
5:BG:3494:MET:O	5:BG:3498:GLY:N	2.42	0.47
7:BQ:3189:VAL:HG23	7:BQ:3380:ARG:HA	1.96	0.47
6:BH:3229:PHE:CE1	6:BH:3234:LYS:HE2	2.50	0.47
1:BA:3451:PHE:CE1	1:BA:3455:LEU:HD11	2.50	0.47
7:BQ:3208:ARG:O	7:BQ:3383:THR:HA	2.15	0.47
6:AH:342:LYS:O	6:AH:345:HIS:HB2	2.14	0.47
2:BB:3481:ASP:HB3	2:BB:3484:GLN:HB3	1.97	0.47
6:AH:257:ALA:HB2	7:AQ:265:VAL:HB	1.96	0.47
8:BZ:3289:PRO:HD3	8:BZ:3293:PHE:CE2	2.50	0.47
8:AZ:221:HIS:HB3	8:AZ:224:MET:HG3	1.96	0.47
2:BB:3141:ASP:HB2	2:BB:3399:ARG:HA	1.97	0.47
4:AE:378:SER:O	4:AE:379:ARG:HB2	2.13	0.47
4:BE:3239:LEU:HD23	4:BE:3240:ILE:N	2.30	0.47
2:BB:3251:LYS:HD2	4:BE:3288:ASP:OD2	2.15	0.47
3:BD:3062:HIS:CE1	3:BD:3083:ALA:HA	2.49	0.47
6:AH:432:ALA:HA	6:AH:436:GLN:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3351:LEU:HD12	6:BH:3352:PHE:N	2.29	0.47
2:BB:3088:VAL:HG13	2:BB:3090:ASP:H	1.79	0.47
4:AE:285:HIS:HB3	4:AE:286:LYS:H	1.58	0.47
4:AE:431:ARG:O	4:AE:434:VAL:HG22	2.15	0.47
2:BB:3235:ASN:HA	2:BB:3286:ASN:OD1	2.15	0.47
4:BE:3281:PRO:HD2	4:BE:3285:HIS:NE2	2.29	0.47
2:BB:3312:GLU:O	2:BB:3316:ARG:HG3	2.14	0.47
6:BH:3162:ALA:HB2	6:BH:3400:VAL:HG22	1.97	0.47
7:AQ:150:ILE:HD12	7:AQ:152:ASP:H	1.79	0.47
6:BH:3342:LYS:H	6:BH:3345:HIS:CD2	2.31	0.47
1:AA:164:MET:HB3	1:AA:169:ILE:HG23	1.97	0.47
6:BH:3336:SER:HB3	7:BQ:3311:HIS:CG	2.48	0.47
9:AG:1001:ADP:O1A	9:AG:1001:ADP:O2B	2.33	0.47
8:BZ:3433:LYS:HG2	8:BZ:3435:GLY:N	2.25	0.47
2:BB:3402:LEU:HD23	2:BB:3482:MET:HB2	1.97	0.47
7:AQ:133:MET:SD	7:AQ:445:LEU:HD22	2.54	0.47
1:BA:3335:ALA:HB2	1:BA:3356:GLY:CA	2.45	0.47
3:BD:3035:ILE:HG13	3:BD:3065:LEU:HD21	1.96	0.47
4:AE:33:LYS:HB3	6:AH:74:ASP:CB	2.45	0.47
7:BQ:3433:ARG:O	7:BQ:3436:LYS:HB3	2.15	0.47
4:BE:3431:ARG:O	4:BE:3434:VAL:HG22	2.15	0.47
5:AG:167:TRP:HH2	8:AZ:126:ARG:CZ	2.27	0.47
1:BA:3211:LYS:H	5:BG:3508:GLN:NE2	2.13	0.47
7:AQ:461:ARG:CG	7:AQ:471:VAL:HG11	2.43	0.47
1:AA:133:LEU:HD21	1:AA:529:LYS:HA	1.96	0.47
4:AE:321:VAL:HG21	4:AE:335:LEU:HD21	1.96	0.47
5:BG:3065:LEU:H	5:BG:3065:LEU:HD12	1.80	0.47
2:BB:3212:PHE:HE1	2:BB:3214:LEU:HD13	1.80	0.47
3:AD:123:SER:HG	3:AD:440:TRP:HZ3	1.62	0.47
6:BH:3243:SER:HB3	6:BH:3334:ILE:HD12	1.96	0.47
1:BA:3333:THR:HG22	1:BA:3377:THR:CG2	2.43	0.47
2:BB:3458:LYS:HB3	2:BB:3479:ILE:CD1	2.45	0.47
6:AH:163:ARG:HG3	6:AH:179:VAL:HG21	1.96	0.47
4:BE:3555:ILE:HD11	6:BH:3053:ILE:HG12	1.96	0.47
6:BH:3263:HIS:O	6:BH:3266:ASP:HB2	2.15	0.47
2:BB:3467:ILE:HG23	2:BB:3469:THR:CG2	2.45	0.47
2:AB:79:ASN:HB3	4:AE:412:ASN:OD1	2.15	0.47
5:AG:416:GLY:HA3	5:AG:494:MET:HE1	1.97	0.47
3:AD:342:ASP:C	3:AD:344:LEU:H	2.19	0.47
4:AE:488:GLY:O	4:AE:489:LEU:HD23	2.14	0.47
4:AE:76:SER:HB3	4:AE:80:GLU:HB2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:20:ILE:HB	1:AA:25:ILE:HB	1.95	0.47
2:AB:171:ASP:O	2:AB:174:ALA:HB3	2.14	0.47
1:AA:332:ALA:O	1:AA:380:HIS:HB3	2.16	0.47
2:AB:233:ILE:HD11	2:AB:324:GLU:N	2.30	0.47
1:AA:112:ALA:HB3	1:AA:539:LEU:HD21	1.97	0.47
2:BB:3235:ASN:O	2:BB:3327:SER:HB3	2.15	0.47
4:AE:441:TYR:HB3	4:AE:522:MET:HB2	1.96	0.47
1:BA:3133:LEU:HD21	1:BA:3529:LYS:HA	1.96	0.47
3:BD:3060:ASP:O	3:BD:3064:ILE:HG13	2.14	0.47
1:BA:3184:LEU:HD12	1:BA:3409:VAL:CG1	2.45	0.47
7:AQ:135:ARG:HG3	7:AQ:532:THR:HG21	1.96	0.47
1:BA:3269:GLN:OE1	3:BD:3257:TYR:N	2.48	0.47
7:BQ:3420:LEU:N	7:BQ:3420:LEU:HD23	2.30	0.47
3:BD:3435:VAL:O	3:BD:3439:ILE:HG12	2.15	0.47
4:AE:294:GLU:OE2	6:AH:264:VAL:HG23	2.15	0.47
2:BB:3467:ILE:HG23	2:BB:3469:THR:HG22	1.96	0.47
2:BB:3236:THR:HG21	2:BB:3329:PHE:HE2	1.79	0.47
2:AB:467:ILE:HG23	2:AB:469:THR:CG2	2.45	0.46
7:AQ:110:LEU:O	7:AQ:114:SER:HB2	2.15	0.46
2:AB:242:LYS:HB2	2:AB:242:LYS:NZ	2.29	0.46
6:AH:263:HIS:O	6:AH:266:ASP:HB2	2.15	0.46
8:AZ:274:LEU:O	8:AZ:278:ILE:HG12	2.14	0.46
2:BB:3171:ASP:O	2:BB:3174:ALA:HB3	2.14	0.46
1:AA:269:GLN:OE1	3:AD:257:TYR:N	2.48	0.46
6:BH:3221:LYS:HB2	6:BH:3222:LYS:H	1.52	0.46
3:AD:435:VAL:O	3:AD:439:ILE:HG12	2.15	0.46
5:BG:3421:MET:HG2	5:BG:3471:LEU:HD12	1.96	0.46
6:AH:190:ASP:HB2	6:AH:192:ASN:HD21	1.81	0.46
4:AE:555:ILE:HD11	6:AH:53:ILE:HG12	1.96	0.46
8:AZ:289:PRO:HD3	8:AZ:293:PHE:CE2	2.50	0.46
3:BD:3077:MET:HE2	3:BD:3518:ILE:HG12	1.96	0.46
5:BG:3259:THR:HG22	8:BZ:3247:VAL:CG1	2.43	0.46
1:BA:3137:ILE:HD12	1:BA:3525:VAL:HG13	1.97	0.46
5:AG:213:ASP:OD1	5:AG:215:LEU:HD22	2.15	0.46
5:AG:298:GLU:O	5:AG:319:ARG:HA	2.15	0.46
6:AH:215:ILE:HG13	6:AH:219:ALA:HB2	1.96	0.46
3:AD:273:ASN:O	3:AD:277:LYS:HG3	2.16	0.46
1:AA:438:THR:HG23	1:AA:445:GLN:NE2	2.30	0.46
1:BA:3244:ILE:HG12	1:BA:3295:VAL:CG1	2.46	0.46
6:AH:250:LEU:HB3	6:AH:251:LYS:HD3	1.97	0.46
2:BB:3254:SER:HB3	3:BD:3262:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:402:LEU:HD23	2:AB:482:MET:HB2	1.97	0.46
5:AG:231:HIS:HD2	8:AZ:338:ASN:HD22	1.62	0.46
5:AG:265:LYS:O	5:AG:268:ASP:HB2	2.15	0.46
5:BG:3269:TRP:NE1	5:BG:3273:LEU:HD12	2.30	0.46
4:AE:363:VAL:O	4:AE:363:VAL:HG23	2.14	0.46
6:AH:505:ASN:HD21	7:AQ:215:GLY:N	2.08	0.46
2:BB:3320:VAL:O	2:BB:3359:CYS:HB3	2.15	0.46
7:AQ:420:LEU:N	7:AQ:420:LEU:HD23	2.30	0.46
4:BE:3305:LYS:O	4:BE:3308:GLU:HB2	2.14	0.46
1:BA:3423:GLY:HA2	1:BA:3426:GLU:OE1	2.15	0.46
4:BE:3322:ILE:HD12	4:BE:3354:ILE:HG21	1.96	0.46
6:BH:3408:LEU:N	6:BH:3408:LEU:HD12	2.31	0.46
5:AG:284:CYS:SG	5:AG:308:TYR:HB2	2.56	0.46
3:AD:189:VAL:HG11	3:AD:405:VAL:HG21	1.98	0.46
4:BE:3247:LYS:HZ3	4:BE:3393:LEU:HB3	1.75	0.46
4:BE:3200:PHE:CE2	4:BE:3234:ILE:HD12	2.51	0.46
8:BZ:3221:HIS:HB3	8:BZ:3224:MET:HG3	1.96	0.46
3:AD:356:ASP:C	3:AD:358:SER:H	2.17	0.46
1:BA:3438:THR:HG23	1:BA:3445:GLN:NE2	2.30	0.46
4:AE:37:ASN:ND2	4:AE:558:GLY:H	2.13	0.46
1:AA:89:GLN:HA	1:AA:92:ARG:NH2	2.31	0.46
7:AQ:269:ASN:ND2	7:AQ:270:ALA:H	2.13	0.46
4:AE:211:VAL:HG11	4:AE:223:LEU:HB3	1.96	0.46
2:BB:3242:LYS:HB2	2:BB:3242:LYS:NZ	2.29	0.46
4:BE:3494:THR:O	4:BE:3498:LEU:HD13	2.15	0.46
3:AD:224:GLY:HA3	3:AD:306:SER:OG	2.16	0.46
8:BZ:3237:ASN:HB3	8:BZ:3338:ASN:HA	1.96	0.46
4:BE:3321:VAL:HG21	4:BE:3335:LEU:HD21	1.96	0.46
8:BZ:3419:TYR:CZ	8:BZ:3454:ILE:HG13	2.51	0.46
1:AA:397:GLU:HA	1:AA:400:ARG:CB	2.45	0.46
7:BQ:3332:LEU:HD23	7:BQ:3333:CYS:N	2.30	0.46
2:AB:150:ARG:HH11	2:AB:150:ARG:HG3	1.80	0.46
7:BQ:3065:THR:CG2	7:BQ:3067:ASP:HB3	2.45	0.46
1:BA:3206:LEU:HB2	1:BA:3386:ILE:HG12	1.96	0.46
1:BA:3164:MET:HB3	1:BA:3169:ILE:HG23	1.97	0.46
2:AB:251:LYS:HD2	4:AE:288:ASP:OD2	2.15	0.46
6:AH:210:GLU:C	6:AH:212:SER:H	2.16	0.46
4:BE:3412:ASN:O	4:BE:3415:ILE:HG13	2.16	0.46
2:BB:3155:HIS:O	2:BB:3158:LYS:HB2	2.16	0.46
4:AE:412:ASN:O	4:AE:415:ILE:HG13	2.15	0.46
2:AB:298:PHE:HB3	2:AB:303:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3037:LEU:HD21	2:BB:3444:LEU:HD12	1.97	0.46
5:AG:421:MET:HG2	5:AG:471:LEU:HD12	1.96	0.46
2:BB:3279:PHE:CZ	2:BB:3332:PRO:HA	2.51	0.46
7:AQ:80:PRO:O	7:AQ:84:VAL:HG23	2.16	0.46
5:AG:387:ASP:HA	5:AG:390:ASN:ND2	2.30	0.46
6:BH:3250:LEU:HB3	6:BH:3251:LYS:HD3	1.97	0.46
1:BA:3332:ALA:O	1:BA:3380:HIS:HB3	2.16	0.46
6:BH:3388:GLU:HA	6:BH:3391:ARG:NH2	2.29	0.46
5:BG:3091:ASP:HB3	5:BG:3505:ILE:HD11	1.98	0.46
5:BG:3265:LYS:O	5:BG:3268:ASP:HB2	2.15	0.46
5:BG:3245:LEU:O	5:BG:3336:ILE:HA	2.16	0.46
6:BH:3215:ILE:HG13	6:BH:3219:ALA:HB2	1.96	0.46
2:BB:3245:ILE:HD12	2:BB:3246:PHE:N	2.31	0.46
6:AH:220:PHE:CE2	6:AH:318:VAL:HG22	2.49	0.46
7:BQ:3135:ARG:HG3	7:BQ:3532:THR:HG21	1.96	0.46
3:BD:3119:ILE:HG21	3:BD:3435:VAL:HG11	1.97	0.46
7:AQ:208:ARG:O	7:AQ:383:THR:HA	2.15	0.46
6:BH:3342:LYS:O	6:BH:3345:HIS:HB2	2.14	0.46
7:AQ:67:ASP:O	7:AQ:71:MET:HG3	2.16	0.46
3:BD:3072:HIS:HE1	3:BD:3074:VAL:HG23	1.80	0.46
4:AE:239:LEU:HD23	4:AE:240:ILE:N	2.30	0.46
8:AZ:298:GLN:O	8:AZ:319:ARG:HA	2.16	0.46
5:BG:3282:LEU:HD21	5:BG:3341:GLU:OE2	2.15	0.46
4:BE:3294:GLU:CD	6:BH:3264:VAL:HG23	2.36	0.46
1:AA:244:ILE:HG12	1:AA:295:VAL:CG1	2.46	0.46
1:AA:211:LYS:H	5:AG:508:GLN:NE2	2.13	0.46
8:BZ:3213:LEU:HA	8:BZ:3377:THR:OG1	2.15	0.46
1:AA:233:MET:CE	1:AA:307:LEU:HD22	2.46	0.46
6:BH:3422:LYS:HZ3	6:BH:3477:LYS:HE2	1.81	0.46
1:AA:184:LEU:HD12	1:AA:409:VAL:CG1	2.45	0.46
6:BH:3216:ASN:HB3	6:BH:3367:GLY:H	1.81	0.46
5:BG:3294:LEU:HD11	5:BG:3355:PHE:CZ	2.51	0.46
3:BD:3342:ASP:C	3:BD:3344:LEU:H	2.19	0.46
2:AB:72:PRO:HA	4:AE:81:ILE:CD1	2.45	0.46
3:AD:119:ILE:HG21	3:AD:435:VAL:HG11	1.97	0.46
3:AD:123:SER:HB3	3:AD:439:ILE:HG21	1.97	0.46
7:AQ:542:ASP:OD1	8:AZ:42:THR:HB	2.16	0.46
2:AB:58:ASN:HB3	2:AB:164:LYS:HD3	1.97	0.46
8:BZ:3304:MET:O	8:BZ:3307:ASP:HB2	2.16	0.46
2:BB:3511:VAL:HG21	4:BE:3073:ILE:HD11	1.97	0.46
8:AZ:293:PHE:O	8:AZ:314:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BQ:3289:LYS:HG2	7:BQ:3316:TYR:OH	2.15	0.46
2:BB:3203:LEU:HD11	2:BB:3376:THR:CG2	2.46	0.46
6:BH:3042:PRO:HB2	6:BH:3049:SER:HB3	1.98	0.46
7:BQ:3428:ILE:HG13	7:BQ:3478:LEU:HG	1.96	0.46
8:BZ:3480:ALA:HB3	8:BZ:3487:ARG:HD2	1.97	0.46
7:BQ:3110:LEU:O	7:BQ:3114:SER:HB2	2.15	0.46
1:BA:3261:GLN:HB2	3:BD:3253:ILE:HD13	1.98	0.46
8:AZ:138:ILE:HD11	8:AZ:488:TYR:CE2	2.51	0.46
2:AB:279:PHE:CZ	2:AB:332:PRO:HA	2.51	0.46
7:AQ:413:LYS:HB3	7:AQ:414:PRO:CD	2.45	0.46
5:AG:99:LEU:O	5:AG:103:ILE:HG13	2.15	0.46
3:BD:3224:GLY:HA3	3:BD:3306:SER:OG	2.16	0.46
5:AG:269:TRP:NE1	5:AG:273:LEU:HD12	2.30	0.46
6:BH:3223:THR:O	6:BH:3225:SER:N	2.49	0.46
6:AH:223:THR:O	6:AH:225:SER:N	2.49	0.46
6:AH:408:LEU:HD12	6:AH:408:LEU:N	2.31	0.46
1:BA:3236:ARG:C	1:BA:3316:MET:HE1	2.36	0.46
7:BQ:3542:ASP:OD1	8:BZ:3042:THR:HB	2.16	0.46
8:AZ:456:LYS:O	8:AZ:459:VAL:HG22	2.15	0.46
6:BH:3160:ARG:HD2	6:BH:3495:PHE:CD2	2.51	0.46
1:BA:3389:GLY:HA3	1:BA:3395:LEU:HD13	1.97	0.46
1:BA:3331:ARG:HB2	1:BA:3331:ARG:CZ	2.45	0.46
7:AQ:433:ARG:O	7:AQ:436:LYS:HB3	2.15	0.46
1:BA:3431:ILE:HD13	1:BA:3478:ARG:NH1	2.31	0.46
1:AA:451:PHE:O	1:AA:455:LEU:HD12	2.16	0.46
3:BD:3199:LYS:O	3:BD:3380:ARG:HG2	2.16	0.46
2:BB:3478:THR:OG1	2:BB:3479:ILE:N	2.49	0.46
8:AZ:304:MET:O	8:AZ:307:ASP:HB2	2.16	0.46
8:AZ:382:GLY:HA3	8:AZ:388:LEU:HD13	1.98	0.46
6:AH:257:ALA:CB	7:AQ:265:VAL:HB	2.46	0.46
7:AQ:65:THR:CG2	7:AQ:67:ASP:HB3	2.45	0.46
8:BZ:3098:VAL:HG23	8:BZ:3524:ALA:HB2	1.96	0.46
1:AA:206:LEU:HB2	1:AA:386:ILE:HG12	1.96	0.46
6:AH:160:ARG:HD2	6:AH:495:PHE:CD2	2.51	0.46
8:BZ:3136:PHE:CE1	8:BZ:3413:PRO:HD2	2.50	0.46
6:AH:42:PRO:HB2	6:AH:49:SER:HB3	1.98	0.46
2:AB:155:HIS:O	2:AB:158:LYS:HB2	2.16	0.46
3:AD:234:ILE:HB	3:AD:345:ASP:OD2	2.16	0.46
1:BA:3218:LEU:HD21	1:BA:3383:SER:HB2	1.97	0.46
7:AQ:174:SER:O	7:AQ:178:LEU:HB2	2.15	0.46
5:AG:307:HIS:O	5:AG:310:LEU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:3387:ASP:HA	5:BG:3390:ASN:ND2	2.30	0.46
5:AG:294:LEU:HD11	5:AG:355:PHE:CZ	2.51	0.46
5:BG:3206:VAL:HG12	5:BG:3207:GLU:H	1.80	0.46
8:BZ:3138:ILE:HD11	8:BZ:3488:TYR:CE2	2.51	0.46
4:AE:294:GLU:CD	6:AH:264:VAL:HG23	2.36	0.46
2:BB:3233:ILE:HD11	2:BB:3324:GLU:N	2.30	0.46
4:BE:3033:LYS:HE2	4:BE:3034:ASP:OD2	2.16	0.46
7:AQ:356:GLU:HG3	7:AQ:373:GLN:HG2	1.98	0.46
5:AG:234:MET:HG2	5:AG:315:SER:HA	1.98	0.46
1:BA:3298:THR:HG21	1:BA:3302:ILE:HG13	1.96	0.46
5:AG:245:LEU:O	5:AG:336:ILE:HA	2.16	0.46
2:BB:3072:PRO:HA	4:BE:3081:ILE:CD1	2.45	0.46
1:BA:3132:ALA:HB2	1:BA:3448:ILE:HG23	1.97	0.46
5:BG:3433:GLN:HG3	5:BG:3433:GLN:O	2.15	0.46
1:AA:464:VAL:C	1:AA:466:ALA:H	2.19	0.46
6:AH:520:VAL:HG11	7:AQ:54:ILE:HG13	1.96	0.46
1:BA:3397:GLU:HA	1:BA:3400:ARG:CB	2.45	0.46
6:AH:98:THR:O	6:AH:101:VAL:HG12	2.15	0.46
6:BH:3190:ASP:C	6:BH:3192:ASN:H	2.18	0.46
6:BH:3190:ASP:HB2	6:BH:3192:ASN:HD21	1.81	0.46
2:BB:3511:VAL:HG12	2:BB:3513:ASN:H	1.81	0.46
3:AD:174:ALA:O	3:AD:178:VAL:HG23	2.16	0.46
2:AB:511:VAL:HG12	2:AB:513:ASN:H	1.81	0.46
7:AQ:289:LYS:HG2	7:AQ:316:TYR:OH	2.15	0.46
8:AZ:480:ALA:HB3	8:AZ:487:ARG:HD2	1.97	0.46
5:BG:3307:HIS:O	5:BG:3310:LEU:HB3	2.16	0.46
2:BB:3258:LEU:HG	3:BD:3246:PRO:HG2	1.98	0.46
6:BH:3260:ARG:HD2	7:BQ:3266:LEU:HD21	1.98	0.46
3:AD:58:SER:HA	3:AD:389:GLU:OE2	2.16	0.46
6:BH:3082:THR:HG21	6:BH:3516:LEU:HD13	1.98	0.46
2:AB:245:ILE:HD12	2:AB:246:PHE:N	2.31	0.46
2:AB:258:LEU:HG	3:AD:246:PRO:HG2	1.98	0.46
3:AD:37:THR:HG21	3:AD:46:LYS:HZ1	1.81	0.46
5:AG:91:ASP:HB3	5:AG:505:ILE:HD11	1.98	0.46
1:BA:3230:SER:O	1:BA:3233:MET:HG2	2.16	0.46
1:BA:3302:ILE:HG22	1:BA:3303:ASP:O	2.15	0.46
7:AQ:354:LEU:CB	7:AQ:377:GLU:HG2	2.44	0.46
2:AB:287:ARG:O	2:AB:308:HIS:HA	2.16	0.46
7:AQ:179:SER:HA	7:AQ:182:VAL:HG12	1.98	0.46
5:BG:3457:ILE:O	5:BG:3460:ALA:HB3	2.16	0.46
7:BQ:3459:VAL:O	7:BQ:3463:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3257:ALA:CB	7:BQ:3265:VAL:HB	2.46	0.46
3:AD:72:HIS:HE1	3:AD:74:VAL:HG23	1.80	0.46
4:AE:200:PHE:CE2	4:AE:234:ILE:HD12	2.51	0.46
3:BD:3058:SER:HA	3:BD:3389:GLU:OE2	2.16	0.46
2:AB:37:LEU:HD21	2:AB:444:LEU:HD12	1.97	0.46
6:BH:3370:GLN:OE1	6:BH:3370:GLN:HA	2.16	0.46
8:AZ:184:ALA:O	8:AZ:185:GLN:HB3	2.16	0.46
7:BQ:3413:LYS:HB3	7:BQ:3414:PRO:CD	2.46	0.46
6:AH:260:ARG:HD2	7:AQ:266:LEU:HD21	1.98	0.46
4:BE:3442:GLY:O	4:BE:3522:MET:HG3	2.16	0.46
5:BG:3211:GLY:C	5:BG:3382:ARG:HH12	2.19	0.46
5:AG:85:GLN:OE1	5:AG:508:GLN:HB3	2.16	0.46
8:AZ:237:ASN:HB3	8:AZ:338:ASN:HA	1.96	0.46
8:AZ:213:LEU:HA	8:AZ:377:THR:OG1	2.15	0.46
3:AD:170:LEU:HD13	3:AD:173:LEU:HD13	1.98	0.46
6:AH:216:ASN:HB3	6:AH:367:GLY:H	1.81	0.46
6:AH:505:ASN:ND2	7:AQ:215:GLY:HA2	2.31	0.46
1:AA:277:GLU:OE1	5:AG:256:GLU:HB2	2.17	0.46
4:AE:216:ARG:NH2	6:AH:355:MET:HE3	2.30	0.46
6:BH:3248:LEU:HD23	6:BH:3303:ALA:HB1	1.98	0.46
8:BZ:3184:ALA:O	8:BZ:3185:GLN:HB3	2.16	0.46
6:BH:3298:PRO:O	6:BH:3299:ILE:HD12	2.16	0.46
5:BG:3162:LYS:HB3	5:BG:3395:ASN:ND2	2.31	0.46
6:AH:196:ASP:O	6:AH:198:LEU:N	2.48	0.46
2:AB:458:LYS:HB3	2:AB:479:ILE:CD1	2.45	0.46
1:BA:3112:ALA:HB3	1:BA:3539:LEU:HD21	1.97	0.46
6:AH:335:GLN:HE22	7:AQ:315:ARG:NH1	2.14	0.46
3:AD:138:MET:HB2	3:AD:478:LEU:HD13	1.96	0.46
8:BZ:3298:GLN:O	8:BZ:3319:ARG:HA	2.16	0.46
1:BA:3391:ASN:O	1:BA:3395:LEU:HB2	2.16	0.46
2:BB:3237:THR:O	2:BB:3238:LEU:HD22	2.16	0.46
1:AA:137:ILE:HD12	1:AA:525:VAL:HG13	1.97	0.46
5:BG:3213:ASP:OD1	5:BG:3215:LEU:HD22	2.15	0.45
2:BB:3037:LEU:HG	2:BB:3038:GLY:H	1.81	0.45
4:BE:3282:LYS:HG3	6:BH:3250:LEU:HD21	1.98	0.45
1:AA:236:ARG:C	1:AA:316:MET:HE1	2.36	0.45
1:AA:331:ARG:CZ	1:AA:331:ARG:HB2	2.45	0.45
4:AE:33:LYS:HE2	4:AE:34:ASP:OD2	2.16	0.45
1:AA:545:ILE:CD1	3:AD:68:MET:HG3	2.38	0.45
8:BZ:3177:ALA:HA	8:BZ:3376:CYS:SG	2.57	0.45
2:AB:235:ASN:O	2:AB:327:SER:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:442:GLY:O	4:AE:522:MET:HG3	2.16	0.45
2:BB:3445:ALA:HB2	2:BB:3472:LEU:CD2	2.46	0.45
5:AG:231:HIS:HB3	5:AG:234:MET:CE	2.46	0.45
8:BZ:3235:ILE:HG21	8:BZ:3336:ALA:HA	1.97	0.45
4:BE:3369:LEU:O	4:BE:3370:SER:HB3	2.16	0.45
7:AQ:234:GLY:C	7:AQ:236:VAL:H	2.19	0.45
3:BD:3046:LYS:HB2	3:BD:3064:ILE:HD13	1.99	0.45
5:AG:65:LEU:HD12	5:AG:65:LEU:H	1.80	0.45
6:BH:3221:LYS:HD2	6:BH:3221:LYS:H	1.82	0.45
6:AH:221:LYS:O	6:AH:222:LYS:HB2	2.17	0.45
8:BZ:3113:VAL:HG22	8:BZ:3439:LYS:HD3	1.98	0.45
5:BG:3298:GLU:O	5:BG:3319:ARG:HA	2.15	0.45
6:AH:427:TYR:OH	6:AH:431:ILE:HD11	2.16	0.45
8:BZ:3108:PHE:HD2	8:BZ:3442:THR:HB	1.81	0.45
5:AG:205:ARG:HB2	5:AG:327:ARG:CZ	2.46	0.45
8:AZ:14:ARG:HB3	8:AZ:14:ARG:HH11	1.78	0.45
2:AB:399:ARG:HB3	2:AB:491:TYR:HB3	1.99	0.45
2:AB:237:THR:O	2:AB:238:LEU:HD22	2.16	0.45
8:AZ:275:LYS:NZ	8:AZ:279:ASP:HB3	2.31	0.45
1:AA:226:CYS:O	1:AA:372:ILE:HG12	2.15	0.45
7:BQ:3356:GLU:HG3	7:BQ:3373:GLN:HG2	1.98	0.45
1:AA:218:LEU:HD21	1:AA:383:SER:HB2	1.98	0.45
3:AD:328:LEU:C	3:AD:330:CYS:H	2.19	0.45
2:AB:213:ILE:HB	2:AB:366:THR:HG21	1.98	0.45
3:BD:3103:LEU:HD11	3:BD:3443:PHE:CD2	2.51	0.45
2:AB:235:ASN:HA	2:AB:286:ASN:OD1	2.15	0.45
8:BZ:3325:MET:HE2	8:BZ:3325:MET:HA	1.97	0.45
1:AA:302:ILE:HG22	1:AA:303:ASP:O	2.15	0.45
4:AE:369:LEU:O	4:AE:370:SER:HB3	2.16	0.45
3:AD:199:LYS:O	3:AD:380:ARG:HG2	2.16	0.45
6:BH:3107:GLU:O	6:BH:3110:LYS:HB3	2.16	0.45
7:BQ:3210:VAL:HG12	7:BQ:3211:LYS:N	2.31	0.45
6:AH:221:LYS:HD2	6:AH:221:LYS:H	1.82	0.45
4:BE:3188:LEU:HD22	4:BE:3193:VAL:CG1	2.45	0.45
2:AB:320:VAL:O	2:AB:359:CYS:HB3	2.15	0.45
8:AZ:113:VAL:HG22	8:AZ:439:LYS:HD3	1.98	0.45
4:AE:450:MET:O	4:AE:454:VAL:HG23	2.16	0.45
5:AG:433:GLN:O	5:AG:433:GLN:HG3	2.15	0.45
4:BE:3169:SER:H	4:BE:3437:SER:HB3	1.82	0.45
6:AH:298:PRO:O	6:AH:299:ILE:HD12	2.16	0.45
6:BH:3196:ASP:O	6:BH:3198:LEU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3070:SER:HB3	8:BZ:3073:ALA:HB3	1.98	0.45
6:AH:273:ALA:HB3	7:AQ:273:MET:HE2	1.98	0.45
7:BQ:3067:ASP:O	7:BQ:3071:MET:HG3	2.16	0.45
5:BG:3284:CYS:SG	5:BG:3308:TYR:HB2	2.56	0.45
7:AQ:284:ILE:HD12	7:AQ:308:LEU:HD12	1.98	0.45
9:BG:4001:ADP:O1A	9:BG:4001:ADP:O2B	2.33	0.45
1:BA:3340:SER:HB3	3:BD:3303:HIS:CE1	2.51	0.45
1:AA:340:SER:HB3	3:AD:303:HIS:CE1	2.51	0.45
6:AH:204:ILE:HB	6:AH:379:ARG:HD3	1.99	0.45
4:BE:3282:LYS:HG3	6:BH:3250:LEU:CD2	2.46	0.45
4:BE:3037:ASN:ND2	4:BE:3558:GLY:H	2.13	0.45
4:AE:282:LYS:HG3	6:AH:250:LEU:CD2	2.46	0.45
7:BQ:3461:ARG:CG	7:BQ:3471:VAL:HG11	2.43	0.45
2:AB:5:ILE:HD13	4:AE:57:VAL:HG22	1.99	0.45
2:AB:67:ILE:HG22	2:AB:69:LEU:HD21	1.98	0.45
4:BE:3160:LYS:HG3	4:BE:3453:ALA:HB1	1.98	0.45
4:BE:3320:VAL:HG12	4:BE:3341:PRO:HD2	1.98	0.45
3:AD:12:LYS:O	3:AD:12:LYS:HD2	2.17	0.45
5:AG:211:GLY:C	5:AG:382:ARG:HH12	2.19	0.45
5:BG:3231:HIS:HB3	5:BG:3234:MET:CE	2.46	0.45
8:BZ:3356:GLN:HA	8:BZ:3365:THR:HA	1.98	0.45
4:AE:270:ALA:HB1	4:AE:272:LEU:CD2	2.47	0.45
1:AA:34:MET:HE3	1:AA:110:LYS:CB	2.45	0.45
8:BZ:3114:HIS:ND1	8:BZ:3115:PRO:HD2	2.32	0.45
5:BG:3044:MET:HE1	8:BZ:3529:LEU:HA	1.98	0.45
7:AQ:420:LEU:CD1	7:AQ:426:THR:HG21	2.44	0.45
8:AZ:419:TYR:CZ	8:AZ:454:ILE:HG13	2.51	0.45
6:AH:190:ASP:N	6:AH:190:ASP:OD1	2.48	0.45
2:BB:3150:ARG:HG3	2:BB:3150:ARG:HH11	1.80	0.45
3:BD:3174:ALA:O	3:BD:3178:VAL:HG23	2.15	0.45
7:AQ:247:VAL:HG22	7:AQ:353:GLY:O	2.16	0.45
2:BB:3399:ARG:HB3	2:BB:3491:TYR:HB3	1.99	0.45
7:AQ:545:ILE:N	7:AQ:545:ILE:HD12	2.32	0.45
8:AZ:136:PHE:CE1	8:AZ:413:PRO:HD2	2.50	0.45
3:BD:3234:ILE:HA	3:BD:3285:VAL:O	2.16	0.45
3:AD:234:ILE:HA	3:AD:285:VAL:O	2.16	0.45
5:AG:387:ASP:OD1	8:AZ:78:ARG:NH2	2.49	0.45
6:AH:508:ASN:HB3	7:AQ:216:SER:HB3	1.99	0.45
8:AZ:204:PRO:HA	8:AZ:381:LYS:O	2.17	0.45
7:AQ:496:TYR:CE2	7:AQ:513:ARG:HD3	2.51	0.45
2:BB:3216:LYS:HG3	2:BB:3306:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:3200:VAL:HA	1:BA:3410:LYS:HD3	1.99	0.45
8:AZ:93:THR:HG23	8:AZ:454:ILE:CD1	2.43	0.45
4:BE:3450:MET:O	4:BE:3454:VAL:HG23	2.16	0.45
3:BD:3189:VAL:HG11	3:BD:3405:VAL:HG21	1.98	0.45
2:BB:3201:GLY:N	3:BD:3510:LEU:HD21	2.30	0.45
2:BB:3219:GLY:HA3	2:BB:3222:GLN:CD	2.37	0.45
1:AA:121:HIS:NE2	3:AD:42:LYS:HB3	2.31	0.45
8:BZ:3293:PHE:O	8:BZ:3314:ILE:HG23	2.16	0.45
7:BQ:3284:ILE:HD12	7:BQ:3308:LEU:HD12	1.98	0.45
6:BH:3525:THR:HA	7:BQ:3056:VAL:HB	1.99	0.45
7:BQ:3545:ILE:N	7:BQ:3545:ILE:HD12	2.32	0.45
1:AA:261:GLN:HB2	3:AD:253:ILE:HD13	1.98	0.45
8:AZ:302:ASP:HB2	8:AZ:303:PRO:CD	2.47	0.45
1:AA:167:LYS:HD2	1:AA:401:SER:HB3	1.99	0.45
4:AE:227:GLN:HE21	4:AE:227:GLN:HB3	1.61	0.45
4:AE:282:LYS:HG3	6:AH:250:LEU:HD21	1.98	0.45
3:AD:331:LYS:HZ3	3:AD:332:PRO:HD2	1.81	0.45
5:AG:157:ALA:HA	5:AG:499:ILE:HD11	1.99	0.45
8:AZ:177:ALA:HA	8:AZ:376:CYS:SG	2.57	0.45
1:BA:3456:LEU:HD11	1:BA:3478:ARG:NE	2.31	0.45
8:AZ:356:GLN:HA	8:AZ:365:THR:HA	1.98	0.45
1:AA:423:GLY:HA2	1:AA:426:GLU:OE1	2.16	0.45
1:AA:200:VAL:HA	1:AA:410:LYS:HD3	1.99	0.45
5:BG:3035:ILE:HG21	5:BG:3065:LEU:HD11	1.98	0.45
2:BB:3034:LYS:HB3	2:BB:3443:ILE:CD1	2.43	0.45
7:AQ:210:VAL:HG12	7:AQ:211:LYS:N	2.31	0.45
6:BH:3221:LYS:O	6:BH:3222:LYS:HB2	2.17	0.45
6:BH:3508:ASN:HB3	7:BQ:3216:SER:HB3	1.99	0.45
2:BB:3183:ARG:NH1	2:BB:3365:CYS:HB3	2.32	0.45
4:AE:184:ALA:O	4:AE:188:LEU:HD12	2.17	0.45
4:AE:188:LEU:HD22	4:AE:193:VAL:CG1	2.45	0.45
5:AG:162:LYS:HB3	5:AG:395:ASN:ND2	2.31	0.45
2:BB:3329:PHE:C	2:BB:3331:GLU:H	2.20	0.45
5:AG:107:CYS:SG	5:AG:125:LEU:HD11	2.56	0.45
2:AB:155:HIS:CB	2:AB:488:VAL:HG22	2.47	0.45
6:BH:3044:LEU:HD22	6:BH:3103:ILE:CD1	2.47	0.45
5:AG:324:ASP:O	5:AG:328:ILE:HG13	2.17	0.45
3:AD:103:LEU:HD11	3:AD:443:PHE:CD2	2.51	0.45
7:BQ:3145:MET:CE	7:BQ:3433:ARG:HH11	2.29	0.45
2:BB:3281:ILE:HG22	2:BB:3337:LEU:HD21	1.99	0.45
7:AQ:145:MET:CE	7:AQ:433:ARG:HH11	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3328:LEU:C	3:BD:3330:CYS:H	2.19	0.45
3:BD:3169:PHE:HZ	3:BD:3207:THR:HG1	1.65	0.45
7:AQ:278:LYS:HA	7:AQ:281:GLU:HB2	1.98	0.45
1:BA:3464:VAL:C	1:BA:3466:ALA:H	2.19	0.45
2:AB:48:SER:HB3	2:AB:53:THR:HG21	1.98	0.45
5:AG:457:ILE:O	5:AG:460:ALA:HB3	2.16	0.45
1:BA:3451:PHE:O	1:BA:3455:LEU:HD12	2.16	0.45
6:BH:3335:GLN:HE22	7:BQ:3315:ARG:NH1	2.14	0.45
2:BB:3058:ASN:HB3	2:BB:3164:LYS:HD3	1.97	0.45
1:AA:171:ALA:HB1	5:AG:126:LYS:HD3	1.99	0.45
8:AZ:70:SER:HB3	8:AZ:73:ALA:HB3	1.98	0.45
2:AB:219:GLY:HA3	2:AB:222:GLN:CD	2.37	0.45
3:AD:461:ASN:OD1	3:AD:463:ILE:HG13	2.17	0.45
4:BE:3076:SER:HB3	4:BE:3080:GLU:HB2	1.97	0.45
5:BG:3107:CYS:SG	5:BG:3125:LEU:HD11	2.56	0.45
6:AH:44:LEU:HD22	6:AH:103:ILE:CD1	2.47	0.45
2:AB:419:ALA:HB2	2:AB:430:VAL:HG12	1.99	0.45
2:AB:387:ALA:O	2:AB:390:VAL:HG23	2.17	0.45
8:BZ:3382:GLY:HA3	8:BZ:3388:LEU:HD13	1.98	0.45
5:BG:3493:ASP:O	5:BG:3496:SER:HB2	2.17	0.45
4:AE:367:GLN:CD	4:AE:367:GLN:H	2.20	0.45
3:BD:3273:ASN:O	3:BD:3277:LYS:HG3	2.16	0.45
4:BE:3161:LEU:HB2	4:BE:3450:MET:CE	2.35	0.45
1:BA:3112:ALA:CB	1:BA:3539:LEU:HD21	2.47	0.45
7:AQ:141:GLU:O	7:AQ:145:MET:N	2.50	0.45
3:BD:3234:ILE:HB	3:BD:3345:ASP:OD2	2.16	0.45
1:BA:3233:MET:CE	1:BA:3307:LEU:HD22	2.45	0.45
4:AE:307:LYS:HA	4:AE:310:ILE:CG2	2.46	0.45
2:AB:34:LYS:HB3	2:AB:443:ILE:CD1	2.43	0.45
4:BE:3216:ARG:NH2	6:BH:3355:MET:HE3	2.31	0.45
6:BH:3133:VAL:HG21	6:BH:3511:THR:HG21	1.99	0.45
7:BQ:3321:LEU:HD23	7:BQ:3323:VAL:CG2	2.46	0.45
3:AD:110:LEU:HD11	3:AD:439:ILE:HA	1.99	0.45
3:BD:3110:LEU:HD11	3:BD:3439:ILE:HA	1.99	0.45
2:BB:3296:GLN:HE22	3:BD:3331:LYS:NZ	2.15	0.45
5:AG:286:GLN:CB	5:AG:340:VAL:HB	2.47	0.45
2:AB:382:ARG:HD2	2:AB:385:HIS:HB3	1.98	0.45
6:BH:3427:TYR:OH	6:BH:3431:ILE:HD11	2.16	0.45
8:AZ:133:LEU:HD13	8:AZ:510:TYR:HE1	1.80	0.45
7:BQ:3247:VAL:HG22	7:BQ:3353:GLY:O	2.16	0.45
1:AA:391:ASN:O	1:AA:395:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:381:LEU:HD21	5:AG:396:LEU:CD2	2.47	0.45
5:BG:3381:LEU:HD21	5:BG:3396:LEU:CD2	2.47	0.45
5:BG:3254:LYS:HE2	8:BZ:3246:GLU:O	2.17	0.45
2:AB:194:GLN:NE2	2:AB:196:ILE:HD11	2.31	0.45
6:BH:3093:GLU:OE1	7:BQ:3364:GLY:HA2	2.17	0.45
1:BA:3440:VAL:HG11	1:BA:3444:GLU:CD	2.37	0.45
2:BB:3387:ALA:O	2:BB:3390:VAL:HG23	2.17	0.45
8:AZ:108:PHE:HD2	8:AZ:442:THR:HB	1.81	0.45
2:AB:281:ILE:CG2	2:AB:337:LEU:HD11	2.47	0.45
2:BB:3281:ILE:CG2	2:BB:3337:LEU:HD11	2.47	0.45
2:BB:3287:ARG:O	2:BB:3308:HIS:HA	2.16	0.45
4:AE:546:ARG:HH11	4:AE:546:ARG:HG3	1.82	0.45
1:AA:431:ILE:HD13	1:AA:478:ARG:NH1	2.31	0.45
5:BG:3324:ASP:O	5:BG:3328:ILE:HG13	2.17	0.45
2:AB:445:ALA:HB2	2:AB:472:LEU:CD2	2.46	0.45
7:BQ:3291:ILE:HG12	7:BQ:3347:PRO:HG3	1.99	0.45
4:BE:3270:ALA:HB1	4:BE:3272:LEU:CD2	2.47	0.45
7:BQ:3211:LYS:HB2	7:BQ:3394:LEU:HD21	1.98	0.45
4:BE:3184:ALA:O	4:BE:3188:LEU:HD12	2.17	0.45
2:AB:346:ILE:HD13	2:AB:355:LYS:HB2	1.99	0.45
3:AD:270:TYR:CE1	3:AD:274:ILE:HD11	2.52	0.45
3:AD:76:ARG:HB2	3:AD:76:ARG:NH1	2.32	0.45
8:AZ:119:THR:HG21	8:AZ:529:LEU:HG	1.99	0.45
8:AZ:231:ALA:CB	8:AZ:293:PHE:HB2	2.47	0.45
3:BD:3237:ILE:HD12	3:BD:3239:PHE:CB	2.47	0.45
2:BB:3271:ASN:O	2:BB:3275:LYS:HG3	2.17	0.45
3:BD:3461:ASN:OD1	3:BD:3463:ILE:HG13	2.16	0.45
6:AH:160:ARG:HG2	6:AH:495:PHE:HB3	1.99	0.45
3:BD:3040:GLY:HA2	9:BD:3601:ADP:O4'	2.17	0.45
7:AQ:424:GLY:HA2	7:AQ:427:GLU:OE2	2.17	0.45
5:AG:32:ALA:O	5:AG:34:VAL:N	2.50	0.45
6:AH:462:ILE:HG22	6:AH:463:GLU:N	2.32	0.45
6:AH:411:ALA:HB3	6:AH:478:TRP:CE3	2.52	0.45
2:BB:3419:ALA:HB2	2:BB:3430:VAL:HG12	1.99	0.45
5:AG:421:MET:HG2	5:AG:471:LEU:CD1	2.47	0.45
5:AG:254:LYS:HE2	8:AZ:246:GLU:O	2.17	0.45
5:AG:280:VAL:CG1	5:AG:304:LEU:HD12	2.47	0.45
2:BB:3213:ILE:HB	2:BB:3366:THR:HG21	1.98	0.45
4:BE:3470:ARG:HH11	4:BE:3470:ARG:HG3	1.81	0.45
6:AH:93:GLU:OE1	7:AQ:364:GLY:HA2	2.17	0.45
2:AB:281:ILE:HG22	2:AB:337:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:3234:MET:HG2	5:BG:3315:SER:HA	1.98	0.45
3:BD:3170:LEU:HD13	3:BD:3173:LEU:HD13	1.98	0.45
6:BH:3221:LYS:HG3	6:BH:3223:THR:HG23	1.99	0.45
6:AH:133:VAL:HG21	6:AH:511:THR:HG21	1.99	0.45
7:BQ:3073:ARG:HH22	7:BQ:3093:LYS:HG2	1.82	0.45
7:BQ:3496:TYR:CE2	7:BQ:3513:ARG:HD3	2.51	0.45
7:BQ:3150:ILE:O	7:BQ:3150:ILE:HD12	2.17	0.45
5:BG:3205:ARG:HB2	5:BG:3327:ARG:CZ	2.46	0.45
7:AQ:208:ARG:HD3	7:AQ:331:ARG:NH1	2.32	0.45
2:BB:3382:ARG:HD2	2:BB:3385:HIS:HB3	1.98	0.45
2:AB:329:PHE:C	2:AB:331:GLU:H	2.20	0.45
7:AQ:111:LEU:O	7:AQ:114:SER:HB3	2.17	0.45
2:BB:3269:MET:SD	2:BB:3294:PRO:HG3	2.56	0.45
2:AB:270:LYS:O	2:AB:273:ILE:HG22	2.17	0.45
1:AA:249:LEU:HD23	1:AA:339:SER:O	2.17	0.45
1:BA:3231:GLN:HE21	1:BA:3235:LYS:HZ1	1.65	0.45
3:AD:36:ARG:HD2	3:AD:453:THR:HG22	1.99	0.45
4:AE:435:LYS:HB3	4:AE:435:LYS:NZ	2.31	0.45
1:AA:27:ASN:O	1:AA:31:LEU:HG	2.16	0.45
5:AG:493:ASP:O	5:AG:496:SER:HB2	2.17	0.45
8:BZ:3275:LYS:NZ	8:BZ:3279:ASP:HB3	2.31	0.45
2:BB:3067:ILE:HG22	2:BB:3069:LEU:HD21	1.98	0.45
3:AD:349:LEU:HD11	3:AD:351:GLU:HG2	1.98	0.45
5:AG:234:MET:SD	5:AG:315:SER:HA	2.58	0.45
8:AZ:325:MET:HA	8:AZ:325:MET:HE2	1.99	0.45
7:AQ:290:GLU:OE2	7:AQ:291:ILE:HG13	2.17	0.45
6:AH:249:GLU:OE2	6:AH:300:GLY:HA3	2.16	0.45
5:AG:457:ILE:HB	5:AG:484:ILE:CD1	2.46	0.45
8:BZ:3337:GLN:OE1	8:BZ:3337:GLN:HA	2.17	0.45
3:AD:278:ILE:HG12	3:AD:339:PHE:CE2	2.53	0.45
6:BH:3190:ASP:OD1	6:BH:3190:ASP:N	2.48	0.45
7:BQ:3039:HIS:CD2	7:BQ:3108:GLY:HA3	2.47	0.45
2:AB:271:ASN:O	2:AB:275:LYS:HG3	2.17	0.45
8:BZ:3105:ALA:HB1	8:BZ:3118:ILE:HG21	1.99	0.45
4:BE:3536:GLN:NE2	6:BH:3207:GLY:HA2	2.32	0.45
1:BA:3067:ALA:HB2	1:BA:3098:THR:CG2	2.47	0.45
6:BH:3244:LEU:HD21	6:BH:3246:VAL:O	2.17	0.45
2:BB:3155:HIS:CB	2:BB:3488:VAL:HG22	2.47	0.44
7:AQ:459:VAL:O	7:AQ:463:LEU:HD13	2.16	0.44
6:AH:107:GLU:O	6:AH:110:LYS:HB3	2.16	0.44
3:BD:3130:ARG:O	3:BD:3134:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AQ:80:PRO:HG2	7:AQ:546:MET:SD	2.57	0.44
8:BZ:3138:ILE:HD11	8:BZ:3488:TYR:HE2	1.82	0.44
4:AE:160:LYS:HG3	4:AE:453:ALA:HB1	1.98	0.44
8:AZ:134:ASP:HA	8:AZ:137:LYS:HE2	1.99	0.44
2:AB:209:ASP:C	2:AB:211:GLY:H	2.19	0.44
4:AE:470:ARG:HH11	4:AE:470:ARG:HG3	1.81	0.44
2:AB:7:GLY:O	2:AB:10:VAL:HG22	2.17	0.44
5:AG:494:MET:O	5:AG:498:GLY:N	2.42	0.44
2:BB:3007:GLY:O	2:BB:3010:VAL:HG22	2.17	0.44
5:BG:3183:ARG:O	5:BG:3375:LYS:HE3	2.17	0.44
2:BB:3216:LYS:HE3	2:BB:3306:ILE:HD12	1.99	0.44
7:AQ:351:GLU:HG2	7:AQ:351:GLU:H	1.56	0.44
7:BQ:3234:GLY:C	7:BQ:3236:VAL:H	2.20	0.44
1:BA:3251:LEU:N	1:BA:3251:LEU:HD23	2.32	0.44
6:BH:3143:LEU:O	6:BH:3145:VAL:N	2.50	0.44
5:BG:3032:ALA:O	5:BG:3034:VAL:N	2.50	0.44
1:BA:3276:ARG:HA	1:BA:3276:ARG:HD2	1.85	0.44
7:BQ:3179:SER:HA	7:BQ:3182:VAL:HG12	1.98	0.44
7:BQ:3212:ILE:HD13	7:BQ:3387:ARG:CZ	2.47	0.44
7:AQ:211:LYS:HB2	7:AQ:394:LEU:HD21	1.98	0.44
4:AE:362:ILE:HD11	6:AH:231:GLN:NE2	2.32	0.44
6:BH:3500:ALA:O	6:BH:3504:ILE:HG22	2.18	0.44
8:AZ:337:GLN:OE1	8:AZ:337:GLN:HA	2.17	0.44
1:BA:3171:ALA:HB1	5:BG:3126:LYS:HD3	1.99	0.44
4:BE:3435:LYS:HB3	4:BE:3435:LYS:NZ	2.31	0.44
4:AE:309:MET:H	4:AE:309:MET:HG2	1.67	0.44
1:BA:3027:ASN:O	1:BA:3031:LEU:HG	2.16	0.44
3:BD:3191:LEU:HD23	3:BD:3194:ILE:HD12	2.00	0.44
2:BB:3350:GLU:CG	3:BD:3402:ARG:HH12	2.28	0.44
3:AD:237:ILE:HD12	3:AD:239:PHE:CB	2.47	0.44
1:BA:3176:PHE:O	1:BA:3180:VAL:HG23	2.17	0.44
8:AZ:477:LEU:HD22	8:AZ:489:VAL:HG11	1.98	0.44
8:BZ:3220:ARG:NH2	8:BZ:3318:ARG:HD2	2.32	0.44
3:AD:300:LEU:C	3:AD:302:LEU:H	2.21	0.44
6:AH:208:ALA:C	6:AH:210:GLU:H	2.19	0.44
6:BH:3204:ILE:HB	6:BH:3379:ARG:HD3	1.99	0.44
2:BB:3273:ILE:HD13	2:BB:3273:ILE:O	2.17	0.44
2:AB:269:MET:SD	2:AB:294:PRO:HG3	2.56	0.44
2:AB:273:ILE:HD13	2:AB:273:ILE:O	2.17	0.44
2:AB:90:ASP:CG	2:AB:91:GLY:H	2.21	0.44
5:AG:387:ASP:HA	5:AG:390:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3249:LYS:HE2	4:BE:3286:LYS:HE3	2.00	0.44
5:BG:3280:VAL:CG1	5:BG:3304:LEU:HD12	2.47	0.44
5:AG:183:ARG:O	5:AG:375:LYS:HE3	2.18	0.44
4:BE:3546:ARG:HH11	4:BE:3546:ARG:HG3	1.82	0.44
2:AB:216:LYS:HE3	2:AB:306:ILE:HD12	1.99	0.44
2:AB:216:LYS:HG3	2:AB:306:ILE:CD1	2.46	0.44
8:AZ:235:ILE:HG21	8:AZ:336:ALA:HA	1.97	0.44
1:AA:251:LEU:HD23	1:AA:251:LEU:N	2.32	0.44
6:BH:3505:ASN:ND2	7:BQ:3215:GLY:HA2	2.31	0.44
1:BA:3277:GLU:OE1	5:BG:3256:GLU:HB2	2.17	0.44
5:AG:35:ILE:HG21	5:AG:65:LEU:HD11	1.98	0.44
3:BD:3012:LYS:O	3:BD:3012:LYS:HD2	2.17	0.44
6:AH:500:ALA:O	6:AH:504:ILE:HG22	2.18	0.44
6:AH:82:THR:HG21	6:AH:516:LEU:HD13	1.98	0.44
1:BA:3464:VAL:HA	1:BA:3470:SER:OG	2.17	0.44
7:BQ:3226:MET:HA	7:BQ:3383:THR:OG1	2.18	0.44
7:BQ:3208:ARG:HD3	7:BQ:3331:ARG:NH1	2.32	0.44
7:BQ:3080:PRO:O	7:BQ:3084:VAL:HG23	2.16	0.44
1:BA:3089:GLN:HA	1:BA:3092:ARG:NH2	2.31	0.44
3:BD:3333:ILE:HG22	3:BD:3335:ASP:O	2.18	0.44
4:BE:3129:LEU:O	4:BE:3132:GLN:HB2	2.17	0.44
7:BQ:3431:ILE:HD13	7:BQ:3479:TYR:OH	2.17	0.44
2:AB:478:THR:OG1	2:AB:479:ILE:N	2.49	0.44
8:BZ:3231:ALA:CB	8:BZ:3293:PHE:HB2	2.47	0.44
8:BZ:3477:LEU:HD22	8:BZ:3489:VAL:HG11	1.98	0.44
6:BH:3160:ARG:HG2	6:BH:3495:PHE:HB3	1.99	0.44
3:BD:3062:HIS:ND1	3:BD:3083:ALA:HA	2.32	0.44
7:AQ:321:LEU:HD23	7:AQ:323:VAL:CG2	2.46	0.44
8:BZ:3204:PRO:HA	8:BZ:3381:LYS:O	2.17	0.44
3:AD:130:ARG:O	3:AD:134:ILE:HG13	2.17	0.44
2:BB:3090:ASP:CG	2:BB:3091:GLY:H	2.21	0.44
4:AE:169:SER:H	4:AE:437:SER:HB3	1.82	0.44
3:BD:3349:LEU:HD11	3:BD:3351:GLU:HG2	1.98	0.44
7:BQ:3474:VAL:HG11	7:BQ:3499:VAL:HG13	1.99	0.44
1:BA:3282:LEU:O	1:BA:3285:VAL:HB	2.17	0.44
1:AA:230:SER:O	1:AA:233:MET:HG2	2.16	0.44
7:BQ:3290:GLU:OE2	7:BQ:3291:ILE:HG13	2.17	0.44
6:AH:221:LYS:HG3	6:AH:223:THR:HG23	1.99	0.44
6:BH:3249:GLU:OE2	6:BH:3300:GLY:HA3	2.16	0.44
1:AA:464:VAL:HA	1:AA:470:SER:OG	2.17	0.44
8:BZ:3044:LYS:N	8:BZ:3044:LYS:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AQ:150:ILE:HD12	7:AQ:150:ILE:O	2.17	0.44
6:AH:370:GLN:OE1	6:AH:370:GLN:HA	2.16	0.44
6:BH:3113:LYS:O	6:BH:3117:GLU:HG3	2.17	0.44
3:BD:3270:TYR:CE1	3:BD:3274:ILE:HD11	2.52	0.44
5:BG:3387:ASP:OD1	8:BZ:3078:ARG:NH2	2.49	0.44
1:AA:488:LYS:HZ2	1:AA:498:ARG:HD2	1.82	0.44
2:BB:3397:GLU:OE1	2:BB:3399:ARG:HB2	2.18	0.44
2:AB:489:GLU:CD	2:AB:494:LYS:HE2	2.38	0.44
3:AD:400:VAL:HG13	3:AD:500:PRO:HG2	2.00	0.44
2:AB:203:LEU:HD11	2:AB:376:THR:CG2	2.46	0.44
3:AD:31:VAL:C	3:AD:33:ASP:H	2.19	0.44
1:AA:89:GLN:HG2	1:AA:526:LYS:HZ1	1.83	0.44
5:BG:3157:ALA:HA	5:BG:3499:ILE:HD11	1.99	0.44
5:BG:3266:GLU:C	5:BG:3268:ASP:H	2.21	0.44
7:BQ:3237:LYS:HG3	7:BQ:3238:SER:H	1.81	0.44
6:AH:248:LEU:HD23	6:AH:303:ALA:HB1	1.98	0.44
7:AQ:430:LEU:O	7:AQ:434:ILE:HG13	2.17	0.44
1:BA:3243:LYS:HG3	1:BA:3294:GLN:HE21	1.83	0.44
1:BA:3167:LYS:HD2	1:BA:3401:SER:HB3	1.99	0.44
4:BE:3367:GLN:CD	4:BE:3367:GLN:H	2.20	0.44
4:AE:129:LEU:O	4:AE:132:GLN:HB2	2.17	0.44
2:BB:3027:ILE:HG23	2:BB:3104:ARG:HH11	1.81	0.44
7:AQ:431:ILE:HD13	7:AQ:479:TYR:OH	2.17	0.44
4:AE:47:LYS:O	4:AE:51:ILE:HG12	2.17	0.44
8:AZ:473:VAL:O	8:AZ:477:LEU:HB2	2.18	0.44
2:AB:413:LYS:NZ	2:AB:460:ARG:NH2	2.65	0.44
8:AZ:220:ARG:NH2	8:AZ:318:ARG:HD2	2.32	0.44
7:AQ:474:VAL:HG11	7:AQ:499:VAL:HG13	2.00	0.44
4:AE:413:LYS:HB2	4:AE:414:MET:CE	2.48	0.44
7:BQ:3111:LEU:O	7:BQ:3114:SER:HB3	2.17	0.44
1:BA:3126:ILE:HD11	1:BA:3539:LEU:HB3	2.00	0.44
3:AD:46:LYS:HB2	3:AD:64:ILE:HD13	1.99	0.44
4:AE:320:VAL:HG12	4:AE:341:PRO:HD2	1.98	0.44
3:BD:3203:THR:C	3:BD:3381:GLY:HA2	2.38	0.44
3:AD:203:THR:C	3:AD:381:GLY:HA2	2.38	0.44
6:BH:3229:PHE:O	6:BH:3231:GLN:N	2.49	0.44
2:BB:3212:PHE:HB2	2:BB:3320:VAL:HG11	1.99	0.44
2:AB:212:PHE:HB2	2:AB:320:VAL:HG11	1.99	0.44
7:BQ:3278:LYS:HA	7:BQ:3281:GLU:HB2	1.98	0.44
2:BB:3189:ASN:HB2	4:BE:3391:ARG:NH1	2.33	0.44
4:BE:3036:GLY:O	4:BE:3038:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3470:ARG:HG3	3:BD:3470:ARG:HH11	1.83	0.44
5:BG:3085:GLN:OE1	5:BG:3508:GLN:HB3	2.16	0.44
7:AQ:15:LYS:HE3	7:AQ:15:LYS:HB2	1.77	0.44
1:BA:3016:GLY:N	3:BD:3071:LEU:HD21	2.33	0.44
4:BE:3473:ALA:O	4:BE:3476:LEU:HB2	2.18	0.44
8:AZ:199:MET:HB2	8:AZ:364:PHE:CZ	2.53	0.44
5:AG:140:SER:OG	5:AG:503:GLU:HG3	2.18	0.44
4:BE:3535:LYS:O	4:BE:3538:ILE:HG22	2.18	0.44
4:AE:536:GLN:NE2	6:AH:207:GLY:HA2	2.32	0.44
8:AZ:86:ILE:HG22	8:AZ:87:THR:HG23	2.00	0.44
8:AZ:141:THR:C	8:AZ:143:LEU:N	2.70	0.44
1:AA:395:LEU:HD12	1:AA:398:MET:SD	2.58	0.44
6:BH:3208:ALA:C	6:BH:3210:GLU:H	2.19	0.44
3:AD:40:GLY:HA2	9:AD:601:ADP:O4'	2.17	0.44
7:AQ:212:ILE:HD13	7:AQ:387:ARG:CZ	2.47	0.44
1:BA:3228:VAL:HG13	1:BA:3363:GLN:NE2	2.32	0.44
3:AD:154:ALA:O	3:AD:158:LEU:HG	2.17	0.44
5:BG:3132:ALA:HB2	5:BG:3427:LEU:HD11	2.00	0.44
2:AB:9:GLN:NE2	2:AB:518:ARG:HG2	2.33	0.44
2:BB:3270:LYS:O	2:BB:3273:ILE:HG22	2.17	0.44
1:AA:112:ALA:CB	1:AA:539:LEU:HD21	2.47	0.44
2:BB:3005:ILE:HD13	4:BE:3057:VAL:HG22	1.99	0.44
6:AH:173:ASN:HA	6:AH:173:ASN:HD22	1.59	0.44
8:AZ:213:LEU:HD22	8:AZ:328:LEU:HD13	1.99	0.44
8:AZ:328:LEU:C	8:AZ:330:LEU:H	2.21	0.44
1:AA:456:LEU:HD11	1:AA:478:ARG:NE	2.31	0.44
6:BH:3411:ALA:HB3	6:BH:3478:TRP:CE3	2.52	0.44
5:BG:3234:MET:SD	5:BG:3315:SER:HA	2.57	0.44
4:AE:389:LYS:HA	4:AE:389:LYS:HD3	1.88	0.44
7:AQ:73:ARG:HH22	7:AQ:93:LYS:HG2	1.82	0.44
7:BQ:3430:LEU:O	7:BQ:3434:ILE:HG13	2.17	0.44
1:BA:3068:THR:O	1:BA:3072:LEU:HB2	2.18	0.44
2:BB:3346:ILE:HD13	2:BB:3355:LYS:HB2	1.99	0.44
1:AA:68:THR:O	1:AA:72:LEU:HB2	2.18	0.44
5:BG:3437:ILE:HG12	5:BG:3440:TRP:HZ3	1.83	0.44
1:BA:3488:LYS:HZ2	1:BA:3498:ARG:HD2	1.82	0.44
7:BQ:3207:ILE:N	7:BQ:3207:ILE:HD12	2.33	0.44
1:BA:3121:HIS:CD2	3:BD:3042:LYS:HD2	2.52	0.44
1:AA:495:ARG:C	1:AA:495:ARG:HD2	2.38	0.44
2:AB:413:LYS:CG	2:AB:464:TYR:HA	2.48	0.44
1:AA:67:ALA:HB2	1:AA:98:THR:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:244:LEU:HD21	6:AH:246:VAL:O	2.17	0.44
6:BH:3040:LEU:HD21	6:BH:3070:LEU:HG	2.00	0.44
6:BH:3063:SER:CB	6:BH:3391:ARG:HH21	2.31	0.44
5:AG:104:LEU:HD11	5:AG:520:LEU:HD12	1.99	0.44
7:AQ:202:PHE:CE2	7:AQ:408:VAL:HG12	2.53	0.44
5:BG:3421:MET:HG2	5:BG:3471:LEU:CD1	2.47	0.44
4:AE:227:GLN:O	4:AE:407:PHE:HA	2.18	0.44
4:AE:36:GLY:O	4:AE:38:LYS:HG3	2.18	0.44
8:BZ:3535:ARG:O	8:BZ:3535:ARG:HD3	2.17	0.44
4:BE:3551:ILE:HD13	6:BH:3052:LEU:HB2	2.00	0.44
1:AA:282:LEU:O	1:AA:285:VAL:HB	2.17	0.44
5:AG:245:LEU:HD23	5:AG:296:ILE:HB	1.99	0.44
4:BE:3272:LEU:HB3	4:BE:3363:VAL:HG23	2.00	0.44
8:AZ:105:ALA:HB1	8:AZ:118:ILE:HG21	1.99	0.44
2:AB:184:LEU:HD21	2:AB:192:HIS:HB2	1.99	0.44
8:AZ:44:LYS:HD2	8:AZ:44:LYS:N	2.33	0.44
2:AB:56:VAL:HG11	3:AD:521:ILE:HD11	2.00	0.44
6:AH:77:HIS:CE1	6:AH:79:ALA:HB3	2.53	0.44
5:BG:3457:ILE:HB	5:BG:3484:ILE:CD1	2.46	0.44
3:AD:19:GLU:HA	3:AD:22:LYS:HG2	1.99	0.44
7:AQ:237:LYS:HG3	7:AQ:238:SER:H	1.82	0.44
3:BD:3076:ARG:NH1	3:BD:3076:ARG:HB2	2.32	0.44
8:BZ:3302:ASP:HB2	8:BZ:3303:PRO:CD	2.47	0.44
8:BZ:3178:VAL:HG21	8:BZ:3402:VAL:HB	2.00	0.44
6:AH:342:LYS:H	6:AH:345:HIS:CD2	2.31	0.44
5:BG:3140:SER:OG	5:BG:3503:GLU:HG3	2.18	0.44
4:AE:535:LYS:O	4:AE:538:ILE:HG22	2.18	0.44
8:BZ:3312:HIS:HB2	8:BZ:3314:ILE:HG12	2.00	0.44
1:AA:176:PHE:O	1:AA:180:VAL:HG23	2.17	0.44
2:BB:3413:LYS:CG	2:BB:3464:TYR:HA	2.48	0.44
4:AE:324:GLN:NE2	4:AE:325:TRP:NE1	2.66	0.44
3:BD:3400:VAL:HG13	3:BD:3500:PRO:HG2	2.00	0.44
8:BZ:3086:ILE:HG22	8:BZ:3087:THR:HG23	2.00	0.44
1:BA:3395:LEU:HD12	1:BA:3398:MET:SD	2.58	0.44
7:BQ:3424:GLY:HA2	7:BQ:3427:GLU:OE2	2.17	0.44
2:AB:270:LYS:C	2:AB:273:ILE:HG22	2.39	0.44
2:AB:296:GLN:HE22	3:AD:331:LYS:NZ	2.15	0.44
3:AD:340:THR:OG1	3:AD:343:ARG:HG2	2.18	0.44
3:BD:3340:THR:OG1	3:BD:3343:ARG:HG2	2.18	0.44
6:AH:44:LEU:HG	6:AH:45:GLY:N	2.32	0.44
3:BD:3037:THR:HG21	3:BD:3046:LYS:HZ1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:132:ALA:HB2	5:AG:427:LEU:HD11	2.00	0.44
5:BG:3059:ASN:O	5:BG:3059:ASN:ND2	2.51	0.44
8:AZ:11:GLU:H	8:AZ:11:GLU:HG2	1.63	0.44
6:AH:191:ARG:HG3	6:AH:404:LEU:HD23	2.00	0.44
1:AA:440:VAL:HG11	1:AA:444:GLU:CD	2.37	0.44
1:BA:3140:ILE:HD13	1:BA:3140:ILE:HA	1.88	0.44
7:BQ:3141:GLU:O	7:BQ:3145:MET:N	2.50	0.44
2:BB:3318:ALA:O	2:BB:3319:LEU:HD23	2.18	0.44
7:AQ:433:ARG:NH2	7:AQ:436:LYS:HE2	2.33	0.44
8:BZ:3323:ARG:HB3	8:BZ:3327:ARG:HH21	1.83	0.44
5:AG:44:MET:HE1	8:AZ:529:LEU:HA	1.99	0.44
2:BB:3048:SER:HB3	2:BB:3053:THR:HG21	1.99	0.44
2:AB:37:LEU:HG	2:AB:38:GLY:H	1.81	0.44
2:BB:3054:CYS:SG	3:BD:3073:PRO:HB3	2.58	0.44
1:BA:3155:THR:HG23	1:BA:3518:LEU:HD13	2.00	0.44
6:BH:3462:ILE:HG22	6:BH:3463:GLU:N	2.32	0.44
2:BB:3489:GLU:CD	2:BB:3494:LYS:HE2	2.38	0.44
3:BD:3465:VAL:HG11	3:BD:3482:ILE:HG23	2.00	0.44
6:BH:3070:LEU:HD23	6:BH:3073:LEU:HD12	2.00	0.44
3:AD:62:HIS:ND1	3:AD:83:ALA:HA	2.32	0.44
3:BD:3031:VAL:C	3:BD:3033:ASP:H	2.19	0.44
7:BQ:3178:LEU:O	7:BQ:3181:LEU:N	2.51	0.44
1:AA:243:LYS:CB	1:AA:355:LEU:HD12	2.43	0.44
1:BA:3243:LYS:CB	1:BA:3355:LEU:HD12	2.43	0.44
8:BZ:3513:LEU:O	8:BZ:3517:ILE:HD13	2.17	0.44
2:BB:3209:ASP:C	2:BB:3211:GLY:H	2.19	0.44
4:BE:3050:HIS:HB3	4:BE:3100:ILE:HG13	2.00	0.44
2:AB:27:ILE:HG23	2:AB:104:ARG:HH11	1.81	0.44
4:AE:473:ALA:O	4:AE:476:LEU:HB2	2.18	0.44
3:BD:3154:ALA:O	3:BD:3158:LEU:HG	2.17	0.44
5:AG:246:LEU:N	5:AG:246:LEU:HD23	2.33	0.44
8:AZ:468:ASP:O	8:AZ:471:ALA:HB3	2.18	0.44
3:AD:333:ILE:HG22	3:AD:335:ASP:O	2.18	0.44
1:AA:538:ILE:HA	1:AA:541:ILE:HD12	2.00	0.44
2:BB:3156:ILE:CG1	2:BB:3488:VAL:HG23	2.48	0.44
8:AZ:114:HIS:ND1	8:AZ:115:PRO:HD2	2.32	0.44
6:AH:229:PHE:O	6:AH:231:GLN:N	2.49	0.44
2:BB:3184:LEU:HD21	2:BB:3192:HIS:HB2	1.99	0.44
1:AA:308:LYS:HG3	5:AG:338:ASN:H	1.83	0.44
1:BA:3288:ILE:HA	1:BA:3349:THR:HG21	2.00	0.44
2:AB:350:GLU:CG	3:AD:402:ARG:HH12	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AZ:312:HIS:HB2	8:AZ:314:ILE:HG12	2.00	0.44
4:BE:3227:GLN:O	4:BE:3407:PHE:HA	2.18	0.44
4:BE:3047:LYS:O	4:BE:3051:ILE:HG12	2.17	0.44
3:AD:465:VAL:HG11	3:AD:482:ILE:HG23	2.00	0.44
4:BE:3413:LYS:HB2	4:BE:3414:MET:CE	2.48	0.43
1:AA:228:VAL:HG13	1:AA:363:GLN:NE2	2.32	0.43
2:BB:3444:LEU:HG	2:BB:3474:LEU:HD11	2.00	0.43
8:AZ:241:GLU:HB3	8:AZ:302:ASP:H	1.83	0.43
8:AZ:178:VAL:HG21	8:AZ:402:VAL:HB	2.00	0.43
1:AA:146:THR:HG22	1:AA:147:SER:N	2.33	0.43
2:BB:3194:GLN:NE2	2:BB:3196:ILE:HD11	2.31	0.43
7:AQ:207:ILE:HD12	7:AQ:207:ILE:N	2.33	0.43
4:AE:347:GLY:O	4:AE:350:GLU:HB2	2.18	0.43
8:AZ:195:GLU:HG2	8:AZ:327:ARG:CZ	2.48	0.43
8:AZ:138:ILE:HD11	8:AZ:488:TYR:HE2	1.83	0.43
7:AQ:471:VAL:O	7:AQ:475:LEU:HB2	2.19	0.43
1:AA:281:VAL:O	1:AA:285:VAL:HG23	2.18	0.43
8:BZ:3119:THR:HG21	8:BZ:3529:LEU:HG	1.98	0.43
2:AB:183:ARG:NH1	2:AB:365:CYS:HB3	2.32	0.43
6:BH:3171:ILE:HD11	6:BH:3178:PHE:CZ	2.53	0.43
4:BE:3367:GLN:NE2	4:BE:3367:GLN:H	2.16	0.43
6:AH:196:ASP:C	6:AH:198:LEU:H	2.22	0.43
1:AA:121:HIS:CD2	3:AD:42:LYS:HD2	2.52	0.43
2:AB:397:GLU:OE1	2:AB:399:ARG:HB2	2.18	0.43
8:AZ:87:THR:HB	8:AZ:512:VAL:HG22	2.00	0.43
3:BD:3300:LEU:C	3:BD:3302:LEU:H	2.21	0.43
4:BE:3142:HIS:CD2	4:BE:3144:ILE:HB	2.53	0.43
5:BG:3482:THR:HA	5:BG:3493:ASP:HA	2.01	0.43
4:AE:284:LYS:HE2	4:AE:286:LYS:HB2	1.99	0.43
3:BD:3019:GLU:HA	3:BD:3022:LYS:HG2	1.99	0.43
5:BG:3462:GLY:O	5:BG:3464:PRO:HD3	2.18	0.43
5:AG:59:ASN:ND2	5:AG:59:ASN:O	2.51	0.43
3:BD:3036:ARG:HD2	3:BD:3453:THR:HG22	1.99	0.43
2:BB:3270:LYS:C	2:BB:3273:ILE:HG22	2.39	0.43
2:AB:325:VAL:O	2:AB:326:VAL:HG22	2.18	0.43
7:BQ:3232:PRO:HG2	7:BQ:3237:LYS:O	2.18	0.43
4:BE:3088:ALA:HB2	4:BE:3119:THR:HG22	1.99	0.43
4:BE:3119:THR:O	4:BE:3122:VAL:HG12	2.18	0.43
4:AE:119:THR:O	4:AE:122:VAL:HG12	2.18	0.43
8:BZ:3195:GLU:HG2	8:BZ:3327:ARG:CZ	2.48	0.43
5:BG:3272:ILE:HA	5:BG:3275:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:3245:LEU:HD23	5:BG:3296:ILE:HB	1.99	0.43
4:AE:272:LEU:HB3	4:AE:363:VAL:HG23	2.00	0.43
7:AQ:291:ILE:HG12	7:AQ:347:PRO:HG3	1.99	0.43
6:AH:422:LYS:HZ3	6:AH:477:LYS:HE2	1.83	0.43
1:BA:3144:LEU:HD22	1:BA:3521:THR:HG21	2.00	0.43
6:BH:3305:GLN:O	6:BH:3308:ALA:HB3	2.18	0.43
1:BA:3034:MET:HE3	1:BA:3110:LYS:CB	2.46	0.43
7:AQ:14:PHE:HD1	7:AQ:15:LYS:HG3	1.82	0.43
2:AB:201:GLY:N	3:AD:510:LEU:HD21	2.30	0.43
1:BA:3249:LEU:HD23	1:BA:3339:SER:O	2.18	0.43
7:BQ:3370:VAL:HG12	7:BQ:3371:PHE:H	1.84	0.43
5:AG:220:LEU:HD11	5:AG:369:ASP:HB3	2.00	0.43
4:BE:3324:GLN:NE2	4:BE:3325:TRP:NE1	2.66	0.43
3:AD:469:LEU:HD11	3:AD:481:GLY:HA2	2.00	0.43
6:BH:3418:MET:CE	6:BH:3468:LEU:HD23	2.47	0.43
3:AD:132:VAL:O	3:AD:135:LEU:HB2	2.18	0.43
6:AH:418:MET:CE	6:AH:468:LEU:HD23	2.48	0.43
7:AQ:151:THR:C	7:AQ:153:LYS:N	2.71	0.43
7:AQ:178:LEU:O	7:AQ:181:LEU:N	2.51	0.43
2:AB:444:LEU:HG	2:AB:474:LEU:HD11	2.01	0.43
5:AG:280:VAL:HB	5:AG:304:LEU:HD12	2.01	0.43
8:BZ:3199:MET:HB2	8:BZ:3364:PHE:CZ	2.53	0.43
3:AD:191:LEU:HD23	3:AD:194:ILE:HD12	2.00	0.43
6:BH:3191:ARG:HG3	6:BH:3404:LEU:HD23	2.00	0.43
7:AQ:159:LEU:HD13	7:AQ:186:VAL:CG1	2.49	0.43
6:AH:65:ASP:O	6:AH:68:THR:N	2.52	0.43
1:BA:3253:LYS:HB3	1:BA:3253:LYS:NZ	2.33	0.43
5:BG:3104:LEU:HD11	5:BG:3520:LEU:HD12	1.99	0.43
6:BH:3355:MET:HB3	6:BH:3357:ILE:HG23	2.00	0.43
6:BH:3222:LYS:HZ2	6:BH:3361:ARG:HH21	1.66	0.43
6:AH:305:GLN:O	6:AH:308:ALA:HB3	2.18	0.43
6:BH:3077:HIS:CE1	6:BH:3079:ALA:HB3	2.53	0.43
3:BD:3278:ILE:HG12	3:BD:3339:PHE:CE2	2.53	0.43
7:BQ:3090:GLU:O	7:BQ:3094:ILE:HG13	2.19	0.43
5:AG:159:ILE:HA	5:AG:159:ILE:HD13	1.91	0.43
7:AQ:232:PRO:HG2	7:AQ:237:LYS:O	2.18	0.43
5:AG:437:ILE:HG12	5:AG:440:TRP:HZ3	1.83	0.43
7:BQ:3065:THR:HG23	7:BQ:3396:ASP:OD1	2.19	0.43
6:AH:160:ARG:CG	6:AH:495:PHE:HB3	2.48	0.43
6:AH:34:VAL:HG12	6:AH:38:GLU:HG3	1.99	0.43
6:BH:3034:VAL:HG12	6:BH:3038:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3087:THR:HB	8:BZ:3512:VAL:HG22	2.00	0.43
8:BZ:3241:GLU:HB3	8:BZ:3302:ASP:H	1.83	0.43
4:AE:33:LYS:HB3	6:AH:74:ASP:HB3	2.00	0.43
3:BD:3132:VAL:O	3:BD:3135:LEU:HB2	2.18	0.43
7:BQ:3151:THR:C	7:BQ:3153:LYS:N	2.71	0.43
7:BQ:3202:PHE:CE2	7:BQ:3408:VAL:HG12	2.53	0.43
6:AH:46:PRO:HA	6:AH:168:SER:HB3	1.99	0.43
6:BH:3046:PRO:HA	6:BH:3168:SER:HB3	1.99	0.43
8:AZ:535:ARG:O	8:AZ:535:ARG:HD3	2.17	0.43
2:BB:3249:LYS:HG2	3:BD:3249:GLU:HB3	2.01	0.43
1:AA:243:LYS:HG3	1:AA:294:GLN:HE21	1.83	0.43
1:BA:3380:HIS:C	1:BA:3382:SER:N	2.71	0.43
2:BB:3009:GLN:NE2	2:BB:3518:ARG:HG2	2.33	0.43
1:AA:126:ILE:HD11	1:AA:539:LEU:HB3	2.00	0.43
7:BQ:3080:PRO:HG2	7:BQ:3546:MET:SD	2.58	0.43
4:AE:269:LEU:HB3	4:AE:320:VAL:CG2	2.49	0.43
2:BB:3325:VAL:O	2:BB:3326:VAL:HG22	2.18	0.43
4:BE:3251:HIS:CD2	4:BE:3253:GLN:H	2.33	0.43
7:AQ:226:MET:HA	7:AQ:383:THR:OG1	2.18	0.43
4:AE:247:LYS:HZ3	4:AE:393:LEU:HB3	1.82	0.43
4:BE:3347:GLY:O	4:BE:3350:GLU:HB2	2.18	0.43
8:BZ:3213:LEU:HD22	8:BZ:3328:LEU:HD13	1.99	0.43
8:BZ:3296:ILE:HD13	8:BZ:3328:LEU:CD2	2.49	0.43
8:BZ:3193:MET:HE2	8:BZ:3327:ARG:HG3	2.00	0.43
8:BZ:3251:PHE:CD1	8:BZ:3262:LEU:HD22	2.54	0.43
6:AH:143:LEU:O	6:AH:145:VAL:N	2.50	0.43
1:AA:277:GLU:CD	5:AG:256:GLU:HB2	2.38	0.43
8:BZ:3172:PRO:HG2	8:BZ:3173:ILE:H	1.84	0.43
6:BH:3162:ALA:O	6:BH:3166:MET:HB2	2.18	0.43
6:BH:3178:PHE:CD2	6:BH:3393:LEU:HD21	2.53	0.43
2:BB:3189:ASN:HB2	4:BE:3391:ARG:HH12	1.83	0.43
6:AH:171:ILE:HD11	6:AH:178:PHE:CZ	2.53	0.43
5:BG:3117:HIS:ND1	5:BG:3118:PRO:N	2.67	0.43
2:AB:153:LEU:CD2	2:AB:178:THR:HG23	2.48	0.43
2:AB:29:VAL:O	2:AB:32:LEU:HB3	2.18	0.43
8:BZ:3134:ASP:HA	8:BZ:3137:LYS:HE2	1.99	0.43
7:BQ:3109:GLU:OE2	7:BQ:3458:VAL:HG13	2.19	0.43
5:BG:3387:ASP:HA	5:BG:3390:ASN:HD21	1.82	0.43
5:AG:176:LEU:HD22	5:AG:180:LYS:HD2	2.01	0.43
1:AA:16:GLY:N	3:AD:71:LEU:HD21	2.33	0.43
7:BQ:3145:MET:HE1	7:BQ:3433:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:3441:TYR:HB2	4:BE:3509:ASN:CB	2.49	0.43
3:BD:3227:THR:HA	3:BD:3311:MET:SD	2.59	0.43
4:BE:3087:GLY:HA3	4:BE:3119:THR:HB	2.01	0.43
8:AZ:325:MET:HA	8:AZ:325:MET:CE	2.49	0.43
8:AZ:251:PHE:CD1	8:AZ:262:LEU:HD22	2.53	0.43
7:BQ:3471:VAL:O	7:BQ:3475:LEU:HB2	2.19	0.43
7:BQ:3291:ILE:O	7:BQ:3296:VAL:HG12	2.18	0.43
1:BA:3187:VAL:HG21	1:BA:3203:VAL:CG2	2.48	0.43
2:AB:318:ALA:O	2:AB:319:LEU:HD23	2.18	0.43
2:BB:3199:LEU:N	2:BB:3199:LEU:HD12	2.30	0.43
7:AQ:90:GLU:O	7:AQ:94:ILE:HG13	2.19	0.43
5:BG:3340:VAL:C	5:BG:3342:ASP:H	2.22	0.43
4:AE:551:ILE:HD13	6:AH:52:LEU:HB2	2.00	0.43
2:AB:15:ALA:HB1	2:AB:19:ARG:NH2	2.34	0.43
6:AH:245:ASN:CG	6:AH:246:VAL:HG13	2.39	0.43
2:BB:3413:LYS:NZ	2:BB:3460:ARG:NH2	2.65	0.43
6:AH:40:LEU:HD21	6:AH:70:LEU:HG	2.00	0.43
7:AQ:109:GLU:OE2	7:AQ:458:VAL:HG13	2.19	0.43
4:BE:3074:LEU:CD1	4:BE:3090:ILE:HA	2.48	0.43
5:BG:3121:ILE:HG22	5:BG:3125:LEU:HD12	2.01	0.43
5:AG:319:ARG:HG3	5:AG:319:ARG:HH11	1.84	0.43
7:AQ:269:ASN:ND2	7:AQ:270:ALA:N	2.67	0.43
4:BE:3284:LYS:HE2	4:BE:3286:LYS:HB2	1.99	0.43
4:BE:3287:LEU:HD12	6:BH:3267:TYR:HB2	2.01	0.43
7:BQ:3266:LEU:HD23	7:BQ:3267:LEU:H	1.84	0.43
4:AE:287:LEU:HD12	6:AH:267:TYR:HB2	2.01	0.43
6:AH:113:LYS:O	6:AH:117:GLU:HG3	2.18	0.43
1:BA:3159:ILE:HG13	1:BA:3412:THR:HG21	2.00	0.43
3:AD:472:LYS:NZ	3:AD:480:ASP:HB3	2.34	0.43
4:BE:3199:ARG:HH11	4:BE:3199:ARG:CB	2.31	0.43
1:BA:3035:ALA:O	1:BA:3039:VAL:HG23	2.19	0.43
1:BA:3399:GLU:HA	1:BA:3402:LEU:HB3	2.00	0.43
7:BQ:3433:ARG:NH2	7:BQ:3436:LYS:HE2	2.33	0.43
7:AQ:145:MET:HE1	7:AQ:433:ARG:HH11	1.84	0.43
4:AE:327:PHE:CZ	4:AE:342:ALA:HB1	2.54	0.43
2:AB:287:ARG:HH12	2:AB:288:GLN:CD	2.21	0.43
2:AB:319:LEU:HB2	2:AB:364:ALA:HB2	2.00	0.43
7:BQ:3354:LEU:CB	7:BQ:3377:GLU:HG2	2.44	0.43
5:BG:3081:LEU:HD21	5:BG:3516:SER:HB2	2.01	0.43
6:BH:3337:THR:HG21	7:BQ:3281:GLU:OE1	2.18	0.43
6:AH:178:PHE:CD2	6:AH:393:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:3417:THR:HG22	2:BB:3418:GLU:N	2.33	0.43
4:BE:3033:LYS:HB3	6:BH:3074:ASP:HB3	2.00	0.43
6:BH:3245:ASN:CG	6:BH:3246:VAL:HG13	2.39	0.43
6:BH:3388:GLU:O	6:BH:3392:SER:HB2	2.18	0.43
3:AD:179:LEU:HA	3:AD:182:SER:CB	2.49	0.43
6:AH:70:LEU:HD23	6:AH:73:LEU:HD12	2.00	0.43
5:BG:3031:VAL:O	5:BG:3034:VAL:HG23	2.19	0.43
2:AB:109:LEU:HB2	2:AB:120:ILE:CD1	2.49	0.43
6:BH:3044:LEU:HG	6:BH:3045:GLY:N	2.32	0.43
4:AE:367:GLN:H	4:AE:367:GLN:NE2	2.16	0.43
4:AE:74:LEU:CD1	4:AE:90:ILE:HA	2.48	0.43
2:AB:417:THR:HG22	2:AB:418:GLU:N	2.33	0.43
8:BZ:3468:ASP:O	8:BZ:3471:ALA:HB3	2.18	0.43
3:AD:227:THR:HA	3:AD:311:MET:SD	2.59	0.43
5:AG:266:GLU:C	5:AG:268:ASP:H	2.21	0.43
8:BZ:3325:MET:CE	8:BZ:3325:MET:HA	2.49	0.43
7:BQ:3299:ILE:HG12	7:BQ:3318:ILE:CG2	2.49	0.43
6:AH:355:MET:HB3	6:AH:357:ILE:HG23	2.00	0.43
4:AE:220:ASP:OD2	6:AH:361:ARG:HD3	2.18	0.43
3:AD:242:SER:HA	3:AD:298:ASN:HB2	2.00	0.43
1:AA:288:ILE:HA	1:AA:349:THR:HG21	2.00	0.43
4:BE:3377:CYS:HA	4:BE:3397:GLN:OE1	2.19	0.43
1:BA:3498:ARG:H	1:BA:3498:ARG:CD	2.32	0.43
2:BB:3029:VAL:O	2:BB:3032:LEU:HB3	2.18	0.43
4:BE:3245:LEU:HB3	4:BE:3247:LYS:CE	2.49	0.43
3:AD:470:ARG:HG3	3:AD:470:ARG:HH11	1.83	0.43
6:AH:525:THR:HA	7:AQ:56:VAL:HB	1.98	0.43
6:AH:63:SER:CB	6:AH:391:ARG:HH21	2.31	0.43
1:BA:3179:MET:HE2	1:BA:3218:LEU:HB2	2.01	0.43
2:BB:3109:LEU:HB2	2:BB:3120:ILE:CD1	2.49	0.43
2:AB:156:ILE:CG1	2:AB:488:VAL:HG23	2.48	0.43
4:AE:450:MET:HG2	4:AE:450:MET:H	1.52	0.43
2:AB:249:LYS:HG2	3:AD:249:GLU:HB3	2.01	0.43
1:AA:159:ILE:HG13	1:AA:412:THR:HG21	2.00	0.43
8:AZ:513:LEU:O	8:AZ:517:ILE:HD13	2.17	0.43
7:BQ:3159:LEU:HD13	7:BQ:3186:VAL:CG1	2.49	0.43
1:BA:3281:VAL:O	1:BA:3285:VAL:HG23	2.18	0.43
4:BE:3307:LYS:HA	4:BE:3310:ILE:CG2	2.46	0.43
6:AH:143:LEU:HD21	6:AH:477:LYS:HD3	2.01	0.43
1:BA:3277:GLU:CD	5:BG:3256:GLU:HB2	2.38	0.43
6:AH:222:LYS:HZ2	6:AH:361:ARG:HH21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:199:LEU:N	2:AB:199:LEU:HD12	2.30	0.43
4:AE:511:GLY:O	4:AE:520:ASN:HB3	2.18	0.43
5:BG:3093:THR:HG23	5:BG:3094:THR:H	1.84	0.43
1:BA:3495:ARG:C	1:BA:3495:ARG:HD2	2.38	0.43
8:BZ:3220:ARG:O	8:BZ:3306:LEU:HD13	2.19	0.43
6:BH:3244:LEU:HD23	6:BH:3246:VAL:N	2.33	0.43
6:AH:244:LEU:HD23	6:AH:246:VAL:N	2.33	0.43
6:BH:3452:GLN:HG3	6:BH:3456:ASN:ND2	2.33	0.43
6:AH:452:GLN:HG3	6:AH:456:ASN:ND2	2.33	0.43
5:AG:421:MET:O	5:AG:424:SER:HB3	2.19	0.43
8:AZ:23:VAL:HG13	8:AZ:102:LEU:HB3	2.01	0.43
2:BB:3405:GLY:O	2:BB:3408:GLU:HG2	2.19	0.43
5:AG:462:GLY:O	5:AG:464:PRO:HD3	2.18	0.43
8:BZ:3465:ASP:O	8:BZ:3469:VAL:HG12	2.19	0.43
8:AZ:39:PRO:HG3	9:AZ:601:ADP:N6	2.34	0.43
4:AE:199:ARG:CB	4:AE:199:ARG:HH11	2.31	0.43
4:AE:219:VAL:CG2	4:AE:431:ARG:HG3	2.49	0.43
4:AE:254:MET:HB3	4:AE:255:PRO:HD2	2.01	0.43
2:BB:3287:ARG:HH12	2:BB:3288:GLN:CD	2.21	0.43
4:AE:88:ALA:HB2	4:AE:119:THR:HG22	1.99	0.43
4:AE:87:GLY:HA3	4:AE:119:THR:HB	2.01	0.43
5:AG:272:ILE:HA	5:AG:275:ILE:CD1	2.48	0.43
5:BG:3261:ILE:O	8:BZ:3249:SER:HA	2.19	0.43
2:AB:190:LEU:HD12	4:AE:389:LYS:NZ	2.34	0.43
5:AG:81:LEU:HD21	5:AG:516:SER:HB2	2.01	0.43
2:BB:3241:ASP:HB3	2:BB:3242:LYS:H	1.58	0.43
2:BB:3262:GLU:OE1	3:BD:3244:PRO:HA	2.19	0.43
8:BZ:3039:PRO:HG3	9:BZ:3601:ADP:N6	2.34	0.43
5:BG:3246:LEU:N	5:BG:3246:LEU:HD23	2.33	0.43
1:BA:3455:LEU:C	1:BA:3457:ILE:H	2.23	0.43
3:BD:3243:PRO:CD	3:BD:3298:ASN:HD22	2.29	0.43
2:AB:189:ASN:HB2	4:AE:391:ARG:NH1	2.33	0.43
7:BQ:3015:LYS:HB2	7:BQ:3015:LYS:HE3	1.77	0.43
2:AB:95:VAL:HG13	2:AB:96:THR:N	2.34	0.43
3:AD:401:ILE:O	3:AD:405:VAL:HG23	2.19	0.43
1:BA:3206:LEU:CD2	1:BA:3225:ASN:HD22	2.31	0.43
3:BD:3469:LEU:HD11	3:BD:3481:GLY:HA2	2.01	0.43
6:AH:388:GLU:O	6:AH:392:SER:HB2	2.19	0.43
7:AQ:356:GLU:H	7:AQ:373:GLN:HG3	1.84	0.43
5:BG:3421:MET:O	5:BG:3424:SER:HB3	2.19	0.43
7:AQ:266:LEU:HD23	7:AQ:267:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:3538:ILE:HA	1:BA:3541:ILE:HD12	2.00	0.43
1:BA:3146:THR:HG22	1:BA:3147:SER:N	2.33	0.43
7:AQ:151:THR:C	7:AQ:153:LYS:H	2.21	0.43
3:BD:3228:ARG:HG3	3:BD:3351:GLU:HB3	2.01	0.43
4:AE:310:ILE:HG12	4:AE:334:LEU:HB3	2.01	0.43
4:AE:310:ILE:CD1	4:AE:335:LEU:HG	2.49	0.43
2:AB:314:VAL:CG2	2:AB:315:GLU:N	2.82	0.43
1:AA:268:GLU:CG	1:AA:269:GLN:N	2.82	0.43
2:AB:54:CYS:SG	3:AD:73:PRO:HB3	2.58	0.43
6:BH:3196:ASP:C	6:BH:3198:LEU:H	2.22	0.43
3:BD:3401:ILE:O	3:BD:3405:VAL:HG23	2.19	0.43
7:AQ:65:THR:HG23	7:AQ:396:ASP:OD1	2.19	0.43
7:AQ:53:LYS:HB2	7:AQ:55:ILE:CD1	2.49	0.43
6:BH:3160:ARG:CG	6:BH:3495:PHE:HB3	2.48	0.43
4:AE:142:HIS:CD2	4:AE:144:ILE:HB	2.53	0.43
6:AH:202:LYS:HG2	6:AH:362:TYR:HE2	1.83	0.43
7:AQ:147:VAL:HG12	7:AQ:148:GLY:H	1.84	0.42
4:AE:180:LEU:HD11	4:AE:430:VAL:CG1	2.41	0.42
2:BB:3094:SER:HB2	9:BB:3601:ADP:O3B	2.19	0.42
4:AE:161:LEU:HD11	4:AE:440:VAL:HG11	2.01	0.42
1:AA:380:HIS:C	1:AA:382:SER:N	2.71	0.42
5:AG:493:ASP:HB3	5:AG:496:SER:OG	2.19	0.42
2:AB:249:LYS:HE2	4:AE:286:LYS:HE3	2.00	0.42
5:BG:3220:LEU:HD11	5:BG:3369:ASP:HB3	2.00	0.42
4:AE:50:HIS:HB3	4:AE:100:ILE:HG13	2.00	0.42
2:AB:118:GLN:HE22	2:AB:510:ARG:NH1	2.17	0.42
7:BQ:3510:LYS:HG2	7:BQ:3511:ASP:H	1.84	0.42
3:BD:3064:ILE:HG22	3:BD:3068:MET:CE	2.49	0.42
6:AH:293:VAL:HG21	6:AH:307:PHE:CE2	2.53	0.42
8:BZ:3170:LEU:O	8:BZ:3174:VAL:HG12	2.19	0.42
6:BH:3167:SER:HA	6:BH:3172:HIS:CD2	2.54	0.42
6:BH:3293:VAL:HG21	6:BH:3307:PHE:CE2	2.53	0.42
8:AZ:323:ARG:HB3	8:AZ:327:ARG:HH21	1.83	0.42
8:BZ:3328:LEU:C	8:BZ:3330:LEU:H	2.21	0.42
1:AA:187:VAL:HG21	1:AA:203:VAL:CG2	2.48	0.42
2:AB:190:LEU:HD12	4:AE:389:LYS:HZ1	1.83	0.42
4:BE:3220:ASP:OD2	6:BH:3361:ARG:HD3	2.18	0.42
2:BB:3056:VAL:HG11	3:BD:3521:ILE:HD11	2.00	0.42
1:BA:3308:LYS:HG3	5:BG:3338:ASN:H	1.83	0.42
8:AZ:151:LEU:HD22	8:AZ:171:THR:HG22	2.00	0.42
1:BA:3113:ASN:HA	1:BA:3116:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3412:ILE:HD12	8:BZ:3510:TYR:HA	2.00	0.42
5:AG:450:GLU:OE2	5:AG:472:ARG:HD2	2.19	0.42
1:BA:3268:GLU:CG	1:BA:3269:GLN:N	2.81	0.42
8:BZ:3473:VAL:O	8:BZ:3477:LEU:HB2	2.18	0.42
3:BD:3058:SER:HB2	3:BD:3389:GLU:OE1	2.19	0.42
3:BD:3103:LEU:O	3:BD:3106:ALA:HB3	2.19	0.42
1:BA:3297:LEU:HB3	1:BA:3326:LEU:HD11	2.01	0.42
1:AA:399:GLU:HA	1:AA:402:LEU:HB3	2.00	0.42
3:BD:3430:ARG:HG3	3:BD:3430:ARG:H	1.70	0.42
4:BE:3269:LEU:HB3	4:BE:3320:VAL:CG2	2.49	0.42
7:AQ:57:ASN:ND2	7:AQ:61:LYS:HD3	2.34	0.42
3:AD:228:ARG:HG3	3:AD:351:GLU:HB3	2.01	0.42
4:BE:3180:LEU:HD11	4:BE:3430:VAL:CG1	2.41	0.42
2:BB:3285:ILE:HG12	2:BB:3306:ILE:CG2	2.49	0.42
1:AA:253:LYS:HB3	1:AA:253:LYS:NZ	2.33	0.42
8:AZ:149:PHE:HE2	8:AZ:405:VAL:HG11	1.84	0.42
6:BH:3143:LEU:HD21	6:BH:3477:LYS:HD3	2.01	0.42
3:AD:170:LEU:HD13	3:AD:170:LEU:HA	1.86	0.42
5:BG:3035:ILE:O	5:BG:3038:CYS:HB2	2.19	0.42
1:AA:144:LEU:HD22	1:AA:521:THR:HG21	2.00	0.42
2:AB:199:LEU:H	2:AB:199:LEU:CD1	2.30	0.42
6:AH:166:MET:HG2	6:AH:171:ILE:HG23	2.00	0.42
2:BB:3095:VAL:HG13	2:BB:3096:THR:N	2.34	0.42
3:AD:239:PHE:CG	3:AD:240:GLN:N	2.87	0.42
4:BE:3511:GLY:O	4:BE:3520:ASN:HB3	2.18	0.42
2:BB:3220:ASN:HA	3:BD:3322:GLU:OE2	2.19	0.42
4:AE:377:CYS:HA	4:AE:397:GLN:OE1	2.19	0.42
8:BZ:3141:THR:C	8:BZ:3143:LEU:N	2.70	0.42
3:BD:3179:LEU:HA	3:BD:3182:SER:CB	2.49	0.42
1:AA:297:LEU:HB3	1:AA:326:LEU:HD11	2.01	0.42
5:AG:482:THR:HA	5:AG:493:ASP:HA	2.01	0.42
5:BG:3151:MET:CB	5:BG:3176:LEU:HD11	2.49	0.42
4:AE:364:PRO:HB3	6:AH:302:LEU:HD12	2.02	0.42
6:AH:446:LEU:HD21	6:AH:507:LEU:HD21	2.01	0.42
3:AD:291:SER:HB3	3:AD:293:LEU:HG	2.02	0.42
1:AA:497:TYR:N	1:AA:497:TYR:CD1	2.88	0.42
2:AB:333:SER:C	2:AB:335:CYS:H	2.22	0.42
4:AE:247:LYS:CG	4:AE:393:LEU:HD13	2.50	0.42
7:AQ:236:VAL:HB	7:AQ:319:LEU:HA	2.01	0.42
1:BA:3302:ILE:CG2	1:BA:3307:LEU:HG	2.50	0.42
4:AE:316:ALA:HB2	4:AE:369:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AQ:291:ILE:O	7:AQ:296:VAL:HG12	2.18	0.42
4:BE:3310:ILE:CD1	4:BE:3335:LEU:HG	2.49	0.42
2:AB:439:GLN:O	2:AB:443:ILE:HG22	2.19	0.42
4:BE:3216:ARG:NH2	6:BH:3353:GLU:OE2	2.53	0.42
3:BD:3242:SER:HA	3:BD:3298:ASN:HB2	2.00	0.42
8:BZ:3368:THR:HG22	8:BZ:3369:GLU:N	2.35	0.42
5:AG:340:VAL:C	5:AG:342:ASP:H	2.22	0.42
1:BA:3121:HIS:NE2	3:BD:3042:LYS:HB3	2.31	0.42
3:BD:3327:GLY:N	3:BD:3374:THR:HG21	2.35	0.42
7:BQ:3053:LYS:HG3	7:BQ:3071:MET:SD	2.59	0.42
8:BZ:3415:ALA:HA	9:BZ:3601:ADP:N3	2.35	0.42
4:AE:396:GLU:O	4:AE:397:GLN:HG2	2.19	0.42
6:BH:3065:ASP:O	6:BH:3068:THR:N	2.52	0.42
7:BQ:3151:THR:C	7:BQ:3153:LYS:H	2.21	0.42
3:BD:3089:ALA:HB1	3:BD:3503:VAL:HG22	2.01	0.42
6:BH:3351:LEU:HD12	6:BH:3352:PHE:H	1.84	0.42
7:BQ:3163:ILE:HD12	7:BQ:3183:SER:HB3	2.01	0.42
4:AE:245:LEU:HB3	4:AE:247:LYS:CE	2.49	0.42
6:BH:3173:ASN:HA	6:BH:3173:ASN:HD22	1.59	0.42
6:AH:351:LEU:HD12	6:AH:352:PHE:H	1.83	0.42
5:AG:35:ILE:O	5:AG:38:CYS:HB2	2.19	0.42
7:BQ:3420:LEU:CD1	7:BQ:3426:THR:HG21	2.44	0.42
8:BZ:3151:LEU:HD22	8:BZ:3171:THR:HG22	2.00	0.42
8:AZ:159:LEU:HA	8:AZ:162:VAL:HG12	2.02	0.42
5:AG:117:HIS:ND1	5:AG:118:PRO:N	2.67	0.42
1:AA:113:ASN:HA	1:AA:116:VAL:HG23	2.00	0.42
1:AA:498:ARG:CD	1:AA:498:ARG:H	2.32	0.42
7:BQ:3245:HIS:HA	7:BQ:3297:GLU:OE2	2.19	0.42
8:AZ:477:LEU:HD13	8:AZ:489:VAL:CG1	2.49	0.42
7:AQ:30:LYS:O	7:AQ:33:ALA:HB3	2.20	0.42
8:AZ:170:LEU:O	8:AZ:174:VAL:HG12	2.19	0.42
3:AD:103:LEU:O	3:AD:106:ALA:HB3	2.19	0.42
2:AB:262:GLU:OE1	3:AD:244:PRO:HA	2.19	0.42
2:AB:505:ALA:O	2:AB:509:LEU:HG	2.20	0.42
2:BB:3505:ALA:O	2:BB:3509:LEU:HG	2.20	0.42
5:BG:3112:ILE:HG13	5:BG:3113:GLU:H	1.85	0.42
2:AB:405:GLY:O	2:AB:408:GLU:HG2	2.19	0.42
1:BA:3497:TYR:CD1	1:BA:3497:TYR:N	2.88	0.42
3:AD:419:ILE:O	3:AD:422:SER:HB3	2.20	0.42
4:BE:3219:VAL:CG2	4:BE:3431:ARG:HG3	2.49	0.42
2:BB:3314:VAL:HG23	2:BB:3315:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:3107:LEU:HD13	4:BE:3122:VAL:HG22	2.01	0.42
4:BE:3546:ARG:NH2	6:BH:3173:ASN:N	2.62	0.42
2:BB:3409:MET:HG2	2:BB:3459:LEU:HG	2.01	0.42
5:AG:261:ILE:O	8:AZ:249:SER:HA	2.19	0.42
4:BE:3327:PHE:CZ	4:BE:3342:ALA:HB1	2.54	0.42
5:BG:3346:SER:C	5:BG:3348:VAL:H	2.23	0.42
6:AH:337:THR:HG21	7:AQ:281:GLU:OE1	2.19	0.42
6:AH:298:PRO:C	6:AH:299:ILE:HD12	2.39	0.42
7:BQ:3030:LYS:O	7:BQ:3033:ALA:HB3	2.20	0.42
7:BQ:3014:PHE:HD1	7:BQ:3015:LYS:HG3	1.82	0.42
7:AQ:39:HIS:CE1	7:AQ:43:LEU:HD13	2.55	0.42
7:AQ:18:TYR:HE2	8:AZ:66:MET:SD	2.43	0.42
4:BE:3510:ILE:HG23	4:BE:3520:ASN:HB2	2.02	0.42
5:BG:3450:GLU:OE2	5:BG:3472:ARG:HD2	2.19	0.42
3:AD:327:GLY:N	3:AD:374:THR:HG21	2.35	0.42
4:BE:3396:GLU:O	4:BE:3397:GLN:HG2	2.19	0.42
6:BH:3030:ILE:O	6:BH:3034:VAL:HG23	2.20	0.42
7:BQ:3543:GLN:HG2	7:BQ:3544:ILE:N	2.34	0.42
6:AH:36:VAL:HG12	6:AH:70:LEU:CD2	2.50	0.42
5:AG:121:ILE:HG22	5:AG:125:LEU:HD12	2.01	0.42
4:BE:3413:LYS:HE3	4:BE:3413:LYS:N	2.02	0.42
1:BA:3209:HIS:CD2	1:BA:3209:HIS:H	2.37	0.42
4:BE:3180:LEU:HA	4:BE:3433:LEU:HD12	2.01	0.42
7:AQ:413:LYS:HB3	7:AQ:414:PRO:HD3	2.01	0.42
5:BG:3319:ARG:HH11	5:BG:3319:ARG:HG3	1.84	0.42
6:AH:251:LYS:CD	6:AH:251:LYS:H	2.30	0.42
8:AZ:391:THR:O	8:AZ:395:VAL:HG23	2.20	0.42
2:BB:3333:SER:C	2:BB:3335:CYS:H	2.22	0.42
2:AB:22:ALA:HA	2:AB:73:ALA:HB2	2.02	0.42
3:AD:131:SER:OG	3:AD:425:LEU:HD11	2.20	0.42
8:AZ:465:ASP:O	8:AZ:469:VAL:HG12	2.19	0.42
1:AA:155:THR:HG23	1:AA:518:LEU:HD13	2.00	0.42
7:BQ:3057:ASN:ND2	7:BQ:3061:LYS:HD3	2.34	0.42
4:AE:361:ARG:HB2	4:AE:373:LYS:HB3	2.02	0.42
6:AH:167:SER:HA	6:AH:172:HIS:CD2	2.54	0.42
5:AG:382:ARG:CB	5:AG:382:ARG:HH11	2.25	0.42
7:BQ:3348:THR:HB	7:BQ:3351:GLU:CG	2.45	0.42
4:BE:3316:ALA:HB2	4:BE:3369:LEU:CD1	2.49	0.42
1:BA:3247:LEU:CD1	1:BA:3251:LEU:HD21	2.50	0.42
6:AH:222:LYS:NZ	6:AH:361:ARG:NH2	2.68	0.42
3:BD:3472:LYS:NZ	3:BD:3480:ASP:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AZ:419:TYR:CE1	8:AZ:454:ILE:HG13	2.55	0.42
6:BH:3298:PRO:C	6:BH:3299:ILE:HD12	2.39	0.42
6:BH:3162:ALA:HB3	6:BH:3179:VAL:HG23	2.02	0.42
8:BZ:3023:VAL:HG13	8:BZ:3102:LEU:HB3	2.01	0.42
2:AB:189:ASN:HB2	4:AE:391:ARG:HH12	1.83	0.42
8:BZ:3158:LEU:C	8:BZ:3160:THR:N	2.73	0.42
3:BD:3074:VAL:HG13	3:BD:3077:MET:HE2	2.01	0.42
3:BD:3358:SER:O	3:BD:3359:LYS:HB2	2.18	0.42
2:BB:3141:ASP:OD2	2:BB:3143:SER:HB3	2.19	0.42
5:AG:93:THR:HG23	5:AG:94:THR:H	1.84	0.42
2:AB:220:ASN:HA	3:AD:322:GLU:OE2	2.19	0.42
7:AQ:370:VAL:HG12	7:AQ:371:PHE:H	1.84	0.42
6:BH:3202:LYS:HG2	6:BH:3362:TYR:HE2	1.83	0.42
1:BA:3210:GLY:O	1:BA:3388:ARG:HB3	2.20	0.42
2:AB:94:SER:HB2	9:AB:601:ADP:O3B	2.19	0.42
5:AG:200:ILE:HG12	5:AG:200:ILE:H	1.49	0.42
5:AG:209:ILE:HB	5:AG:382:ARG:CD	2.49	0.42
5:BG:3209:ILE:HB	5:BG:3382:ARG:CD	2.49	0.42
2:AB:471:GLY:HA3	2:AB:482:MET:CG	2.50	0.42
4:AE:107:LEU:CD1	4:AE:122:VAL:HG22	2.50	0.42
2:AB:285:ILE:HG12	2:AB:306:ILE:CG2	2.49	0.42
4:BE:3247:LYS:CG	4:BE:3393:LEU:HD13	2.50	0.42
8:AZ:296:ILE:HG21	8:AZ:328:LEU:CD2	2.50	0.42
1:BA:3229:ALA:HB1	1:BA:3307:LEU:CD1	2.47	0.42
7:BQ:3269:ASN:ND2	7:BQ:3270:ALA:N	2.67	0.42
6:BH:3222:LYS:NZ	6:BH:3361:ARG:NH2	2.68	0.42
8:AZ:172:PRO:HG2	8:AZ:173:ILE:H	1.84	0.42
7:AQ:87:MET:O	7:AQ:90:GLU:HB2	2.20	0.42
5:BG:3457:ILE:HD11	5:BG:3467:LEU:HG	2.02	0.42
5:BG:3493:ASP:HB3	5:BG:3496:SER:OG	2.19	0.42
5:BG:3286:GLN:HB3	5:BG:3286:GLN:HE21	1.53	0.42
7:AQ:249:VAL:HG13	7:AQ:300:VAL:HG23	2.01	0.42
3:BD:3419:ILE:O	3:BD:3422:SER:HB3	2.20	0.42
6:AH:342:LYS:N	6:AH:345:HIS:HD2	2.16	0.42
3:BD:3041:PRO:CB	3:BD:3484:VAL:HG21	2.50	0.42
4:AE:158:ILE:HD11	4:AE:538:ILE:HG23	2.02	0.42
7:BQ:3239:LEU:HD13	7:BQ:3245:HIS:HD2	1.85	0.42
8:AZ:412:ILE:HD12	8:AZ:510:TYR:HA	2.00	0.42
3:BD:3136:LEU:O	3:BD:3139:CYS:HB3	2.20	0.42
2:BB:3118:GLN:HE22	2:BB:3510:ARG:NH1	2.17	0.42
4:BE:3251:HIS:HD2	4:BE:3253:GLN:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BQ:3343:ARG:HH21	7:BQ:3344:LEU:HD11	1.84	0.42
5:AG:89:VAL:HG21	5:AG:505:ILE:HA	2.02	0.42
6:BH:3410:VAL:HB	6:BH:3416:THR:OG1	2.20	0.42
8:AZ:296:ILE:HD13	8:AZ:328:LEU:CD2	2.49	0.42
1:AA:479:SER:O	1:AA:482:ALA:HB3	2.20	0.42
6:BH:3234:LYS:NZ	6:BH:3361:ARG:NH1	2.68	0.42
1:AA:302:ILE:CG2	1:AA:307:LEU:HG	2.50	0.42
2:BB:3471:GLY:HA3	2:BB:3482:MET:CG	2.50	0.42
4:AE:180:LEU:HA	4:AE:433:LEU:HD12	2.01	0.42
5:AG:346:SER:C	5:AG:348:VAL:H	2.23	0.42
2:BB:3439:GLN:O	2:BB:3443:ILE:HG22	2.19	0.42
5:AG:457:ILE:HD11	5:AG:467:LEU:HG	2.02	0.42
3:BD:3289:GLN:HA	3:BD:3316:ILE:HB	2.02	0.42
3:BD:3448:GLU:O	3:BD:3451:PRO:HD2	2.20	0.42
1:BA:3485:GLN:HG3	1:BA:3488:LYS:CE	2.50	0.42
2:BB:3226:ILE:HG13	2:BB:3283:THR:CG2	2.49	0.42
5:BG:3413:SER:OG	5:BG:3503:GLU:HA	2.19	0.42
2:AB:399:ARG:HB2	2:AB:399:ARG:HE	1.60	0.42
3:AD:358:SER:O	3:AD:359:LYS:HB2	2.18	0.42
4:AE:358:THR:CG2	4:AE:377:CYS:HB3	2.50	0.42
8:BZ:3477:LEU:HD13	8:BZ:3489:VAL:CG1	2.49	0.42
8:BZ:3130:MET:SD	8:BZ:3514:ARG:NE	2.93	0.42
2:BB:3177:ALA:O	2:BB:3181:ILE:HG12	2.20	0.42
1:AA:487:ALA:CB	1:AA:493:LYS:HA	2.37	0.42
2:BB:3270:LYS:HA	2:BB:3273:ILE:HG22	2.02	0.42
8:AZ:130:MET:SD	8:AZ:514:ARG:NE	2.93	0.42
7:AQ:163:ILE:HD12	7:AQ:183:SER:HB3	2.01	0.42
8:BZ:3391:THR:O	8:BZ:3395:VAL:HG23	2.20	0.42
1:AA:35:ALA:O	1:AA:39:VAL:HG23	2.19	0.42
2:BB:3314:VAL:CG2	2:BB:3315:GLU:N	2.82	0.42
4:BE:3153:ALA:HB1	4:BE:3454:VAL:CG1	2.50	0.42
3:BD:3210:ILE:HG21	3:BD:3214:VAL:HG22	2.02	0.42
3:BD:3214:VAL:HG21	3:BD:3378:VAL:HG23	2.02	0.42
3:AD:210:ILE:HG21	3:AD:214:VAL:HG22	2.02	0.42
4:BE:3448:VAL:HG12	4:BE:3452:LEU:HD22	2.01	0.42
5:AG:167:TRP:HH2	8:AZ:126:ARG:NH2	2.18	0.42
3:AD:220:ILE:CD1	3:AD:226:PRO:HD2	2.43	0.42
1:AA:456:LEU:C	1:AA:459:PRO:HD2	2.41	0.42
1:AA:247:LEU:CD1	1:AA:251:LEU:HD21	2.50	0.42
7:AQ:299:ILE:HG12	7:AQ:318:ILE:CG2	2.49	0.42
1:BA:3156:LEU:HD21	1:BA:3413:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:3201:LYS:N	1:BA:3410:LYS:HZ3	2.17	0.42
4:BE:3310:ILE:HG12	4:BE:3334:LEU:HB3	2.01	0.42
8:BZ:3419:TYR:CE1	8:BZ:3454:ILE:HG13	2.55	0.42
5:AG:205:ARG:HB2	5:AG:327:ARG:NE	2.35	0.42
6:AH:162:ALA:HB3	6:AH:179:VAL:HG23	2.02	0.42
5:BG:3250:LEU:HD12	5:BG:3301:VAL:HG13	2.02	0.42
5:AG:413:SER:OG	5:AG:503:GLU:HA	2.19	0.42
7:AQ:267:LEU:HD13	7:AQ:273:MET:HB2	2.02	0.42
2:BB:3231:ILE:HD11	2:BB:3321:THR:HG21	2.01	0.42
7:BQ:3053:LYS:HB2	7:BQ:3055:ILE:CD1	2.49	0.42
3:AD:320:GLU:O	3:AD:323:PHE:N	2.53	0.42
8:AZ:433:LYS:C	8:AZ:435:GLY:N	2.73	0.42
3:BD:3320:GLU:O	3:BD:3323:PHE:N	2.53	0.42
8:BZ:3133:LEU:HD13	8:BZ:3510:TYR:HE1	1.80	0.42
2:BB:3015:ALA:HB1	2:BB:3019:ARG:NH2	2.34	0.42
3:AD:375:VAL:HG22	3:AD:376:SER:N	2.35	0.42
6:BH:3236:PHE:HD2	6:BH:3292:ILE:HD11	1.85	0.42
4:BE:3133:ALA:O	4:BE:3137:ILE:HG13	2.20	0.42
2:BB:3022:ALA:HA	2:BB:3073:ALA:CB	2.49	0.42
6:AH:358:GLY:N	6:AH:379:ARG:NH2	2.68	0.42
1:BA:3422:GLY:HA3	1:BA:3512:GLU:OE2	2.20	0.42
1:AA:422:GLY:HA3	1:AA:512:GLU:OE2	2.20	0.42
2:AB:296:GLN:CB	3:AD:334:ALA:HB2	2.50	0.42
7:AQ:478:LEU:HD11	7:AQ:497:LYS:O	2.20	0.42
5:BG:3176:LEU:HD22	5:BG:3180:LYS:HD2	2.01	0.42
3:BD:3131:SER:OG	3:BD:3425:LEU:HD11	2.20	0.42
3:BD:3197:VAL:O	3:BD:3378:VAL:HA	2.20	0.42
3:AD:197:VAL:O	3:AD:378:VAL:HA	2.20	0.42
8:BZ:3217:HIS:NE2	8:BZ:3320:ALA:HA	2.35	0.42
2:BB:3190:LEU:HD12	4:BE:3389:LYS:NZ	2.34	0.42
2:AB:314:VAL:HG23	2:AB:315:GLU:N	2.35	0.42
7:BQ:3147:VAL:HG12	7:BQ:3148:GLY:H	1.84	0.42
6:AH:234:LYS:NZ	6:AH:361:ARG:NH1	2.68	0.42
2:BB:3316:ARG:O	2:BB:3320:VAL:HG22	2.20	0.42
2:AB:48:SER:HA	3:AD:528:ARG:HG2	2.02	0.42
8:AZ:458:LEU:HD22	8:AZ:493:LEU:HD11	2.02	0.42
2:AB:226:ILE:HG13	2:AB:283:THR:CG2	2.49	0.42
7:AQ:245:HIS:HA	7:AQ:297:GLU:OE2	2.19	0.42
8:AZ:412:ILE:CD1	8:AZ:510:TYR:HA	2.50	0.42
1:BA:3120:ILE:HG23	1:BA:3443:ARG:CD	2.50	0.42
6:BH:3197:LYS:H	6:BH:3197:LYS:CD	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AQ:543:GLN:NE2	7:AQ:545:ILE:HD11	2.35	0.42
6:BH:3311:ASN:HD22	6:BH:3311:ASN:N	2.16	0.42
6:BH:3358:GLY:N	6:BH:3379:ARG:NH2	2.68	0.42
5:AG:170:LYS:HE2	5:AG:215:LEU:HA	2.02	0.41
7:BQ:3167:ILE:HG23	7:BQ:3178:LEU:HD23	2.02	0.41
4:AE:153:ALA:HB1	4:AE:454:VAL:CG1	2.50	0.41
5:BG:3280:VAL:HB	5:BG:3304:LEU:HD12	2.01	0.41
5:BG:3205:ARG:HB2	5:BG:3327:ARG:NE	2.35	0.41
2:BB:3022:ALA:HA	2:BB:3073:ALA:HB2	2.02	0.41
3:AD:136:LEU:O	3:AD:139:CYS:HB3	2.20	0.41
4:AE:133:ALA:O	4:AE:137:ILE:HG13	2.20	0.41
5:AG:112:ILE:HG13	5:AG:113:GLU:H	1.85	0.41
7:AQ:57:ASN:C	7:AQ:59:LEU:H	2.23	0.41
4:AE:441:TYR:HB2	4:AE:509:ASN:CB	2.48	0.41
1:AA:193:LYS:HB2	3:AD:228:ARG:NH1	2.35	0.41
4:BE:3361:ARG:HB2	4:BE:3373:LYS:HB3	2.02	0.41
8:AZ:218:GLY:HA2	8:AZ:365:THR:CG2	2.50	0.41
1:AA:455:LEU:C	1:AA:457:ILE:H	2.23	0.41
5:BG:3231:HIS:NE2	8:BZ:3336:ALA:HB3	2.35	0.41
5:BG:3269:TRP:HH2	7:BQ:3261:THR:HG1	1.66	0.41
2:AB:409:MET:HG2	2:AB:459:LEU:HG	2.01	0.41
1:AA:190:GLN:HB3	1:AA:194:GLY:O	2.20	0.41
6:BH:3199:ILE:O	6:BH:3199:ILE:HG22	2.20	0.41
2:AB:20:LEU:O	2:AB:21:SER:C	2.58	0.41
4:BE:3362:ILE:HD11	6:BH:3231:GLN:NE2	2.32	0.41
4:AE:362:ILE:CD1	4:AE:362:ILE:H	2.23	0.41
3:AD:58:SER:HB2	3:AD:389:GLU:OE1	2.19	0.41
3:AD:243:PRO:CD	3:AD:298:ASN:HD22	2.29	0.41
6:BH:3166:MET:HG2	6:BH:3171:ILE:HG23	2.00	0.41
1:AA:397:GLU:O	1:AA:400:ARG:HB3	2.19	0.41
6:AH:162:ALA:O	6:AH:166:MET:HB2	2.18	0.41
3:AD:289:GLN:HA	3:AD:316:ILE:HB	2.02	0.41
3:AD:74:VAL:HG13	3:AD:77:MET:HE2	2.00	0.41
3:BD:3239:PHE:CG	3:BD:3240:GLN:N	2.87	0.41
1:AA:485:GLN:HG3	1:AA:488:LYS:CE	2.50	0.41
7:AQ:401:ILE:O	7:AQ:405:VAL:HG23	2.20	0.41
4:BE:3397:GLN:HE21	4:BE:3397:GLN:HB3	1.66	0.41
3:BD:3375:VAL:HG22	3:BD:3376:SER:N	2.35	0.41
7:BQ:3543:GLN:NE2	7:BQ:3545:ILE:HD11	2.35	0.41
7:AQ:343:ARG:HH21	7:AQ:344:LEU:HD11	1.84	0.41
7:AQ:153:LYS:C	7:AQ:155:ASP:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:209:HIS:H	1:AA:209:HIS:CD2	2.37	0.41
1:AA:120:ILE:HG23	1:AA:443:ARG:CD	2.50	0.41
6:BH:3044:LEU:HD22	6:BH:3103:ILE:HD13	2.02	0.41
1:BA:3487:ALA:O	1:BA:3493:LYS:HB3	2.19	0.41
7:AQ:159:LEU:HD13	7:AQ:186:VAL:HG11	2.02	0.41
5:AG:151:MET:CB	5:AG:176:LEU:HD11	2.49	0.41
6:AH:503:LYS:O	6:AH:507:LEU:HD12	2.20	0.41
4:AE:210:ASN:N	4:AE:210:ASN:HD22	2.17	0.41
3:AD:433:GLU:CD	3:AD:433:GLU:N	2.74	0.41
5:BG:3251:GLU:HA	5:BG:3302:SER:HB2	2.02	0.41
3:BD:3220:ILE:HD11	3:BD:3311:MET:HG3	2.01	0.41
3:AD:228:ARG:HA	3:AD:350:VAL:O	2.20	0.41
4:AE:107:LEU:HD13	4:AE:122:VAL:HG22	2.01	0.41
1:BA:3479:SER:O	1:BA:3482:ALA:HB3	2.20	0.41
5:BG:3089:VAL:HG21	5:BG:3505:ILE:HA	2.02	0.41
5:BG:3091:ASP:HB3	5:BG:3505:ILE:CD1	2.50	0.41
7:BQ:3326:LYS:NZ	7:BQ:3326:LYS:HB2	2.35	0.41
7:BQ:3254:LEU:HD12	7:BQ:3254:LEU:H	1.85	0.41
1:AA:284:ARG:HB3	1:AA:341:MET:HE2	2.02	0.41
6:BH:3189:LEU:HD12	6:BH:3195:ASP:H	1.85	0.41
7:AQ:254:LEU:H	7:AQ:254:LEU:HD12	1.85	0.41
8:BZ:3149:PHE:HE2	8:BZ:3405:VAL:HG11	1.84	0.41
1:BA:3184:LEU:O	1:BA:3187:VAL:HG23	2.20	0.41
8:BZ:3114:HIS:NE2	8:BZ:3116:ARG:HG3	2.35	0.41
4:BE:3421:ARG:NH2	4:BE:3425:ASP:OD1	2.54	0.41
2:BB:3054:CYS:O	2:BB:3055:MET:HB3	2.20	0.41
4:BE:3161:LEU:HD11	4:BE:3440:VAL:HG11	2.01	0.41
7:BQ:3078:VAL:HA	7:BQ:3083:LYS:HE3	2.02	0.41
5:BG:3110:TYR:CD1	5:BG:3440:TRP:HB3	2.55	0.41
4:AE:510:ILE:HG23	4:AE:520:ASN:HB2	2.02	0.41
4:BE:3047:LYS:NZ	4:BE:3551:ILE:O	2.54	0.41
5:AG:479:ASN:ND2	5:AG:480:PHE:N	2.68	0.41
2:AB:141:ASP:OD2	2:AB:143:SER:HB3	2.19	0.41
2:AB:22:ALA:HA	2:AB:73:ALA:CB	2.49	0.41
8:BZ:3447:PHE:O	8:BZ:3450:ALA:HB3	2.20	0.41
4:BE:3210:ASN:HD22	4:BE:3210:ASN:N	2.18	0.41
5:BG:3241:PRO:HD2	5:BG:3353:GLY:O	2.20	0.41
6:AH:203:LYS:HZ3	6:AH:386:ILE:CG2	2.33	0.41
7:BQ:3267:LEU:HD13	7:BQ:3273:MET:HB2	2.02	0.41
8:AZ:415:ALA:HA	9:AZ:601:ADP:N3	2.35	0.41
8:AZ:451:LEU:C	8:AZ:453:VAL:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:3013:GLU:HG3	5:BG:3014:ARG:HG3	2.03	0.41
7:AQ:520:MET:CE	7:AQ:520:MET:H	2.33	0.41
7:AQ:336:CYS:HB3	7:AQ:355:VAL:HG22	2.01	0.41
8:AZ:447:PHE:O	8:AZ:450:ALA:HB3	2.20	0.41
7:AQ:45:SER:HB3	7:AQ:66:ASN:O	2.21	0.41
2:BB:3393:GLN:HE21	4:BE:3387:THR:HG22	1.85	0.41
2:BB:3319:LEU:HB2	2:BB:3364:ALA:HB2	2.00	0.41
4:BE:3254:MET:HB3	4:BE:3255:PRO:HD2	2.01	0.41
2:AB:131:ALA:O	2:AB:411:MET:HG2	2.21	0.41
5:AG:167:TRP:CG	5:AG:214:VAL:HG11	2.56	0.41
4:BE:3107:LEU:CD1	4:BE:3122:VAL:HG22	2.50	0.41
5:BG:3167:TRP:CG	5:BG:3214:VAL:HG11	2.55	0.41
3:AD:220:ILE:HD11	3:AD:311:MET:HG3	2.01	0.41
5:BG:3228:ASP:CG	5:BG:3229:VAL:N	2.70	0.41
5:BG:3231:HIS:HB3	5:BG:3234:MET:HE1	2.02	0.41
1:AA:284:ARG:HD3	1:AA:341:MET:CE	2.50	0.41
7:AQ:293:ASP:C	7:AQ:295:GLY:H	2.24	0.41
7:BQ:3293:ASP:C	7:BQ:3295:GLY:H	2.24	0.41
8:AZ:280:LEU:HD12	8:AZ:348:LEU:HD11	2.02	0.41
6:BH:3281:LYS:NZ	7:BQ:3278:LYS:NZ	2.68	0.41
2:AB:54:CYS:O	2:AB:55:MET:HB3	2.20	0.41
8:AZ:368:THR:HG22	8:AZ:369:GLU:N	2.34	0.41
1:BA:3397:GLU:O	1:BA:3400:ARG:HB3	2.19	0.41
7:BQ:3249:VAL:HG13	7:BQ:3300:VAL:HG23	2.01	0.41
8:BZ:3116:ARG:HG2	8:BZ:3529:LEU:CD2	2.51	0.41
7:BQ:3520:MET:H	7:BQ:3520:MET:CE	2.33	0.41
7:AQ:239:LEU:HD13	7:AQ:245:HIS:HD2	1.85	0.41
4:BE:3358:THR:CG2	4:BE:3377:CYS:HB3	2.50	0.41
5:BG:3048:LEU:HD11	5:BG:3064:ILE:HG12	2.02	0.41
1:BA:3395:LEU:HA	1:BA:3395:LEU:HD12	1.86	0.41
7:AQ:543:GLN:HG2	7:AQ:544:ILE:N	2.34	0.41
5:AG:31:VAL:O	5:AG:34:VAL:HG23	2.19	0.41
2:BB:3091:GLY:HA2	9:BB:3601:ADP:O3B	2.21	0.41
1:BA:3438:THR:HA	1:BA:3445:GLN:HE21	1.85	0.41
7:BQ:3413:LYS:HB3	7:BQ:3414:PRO:HD3	2.01	0.41
1:AA:283:GLU:O	1:AA:287:LYS:HG3	2.20	0.41
1:AA:287:LYS:HD3	1:AA:347:GLU:O	2.21	0.41
6:BH:3147:ILE:N	6:BH:3147:ILE:HD13	2.36	0.41
6:AH:147:ILE:N	6:AH:147:ILE:HD13	2.36	0.41
6:BH:3239:PRO:HG2	6:BH:3241:ILE:HD11	2.02	0.41
7:BQ:3057:ASN:C	7:BQ:3059:LEU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BD:3350:VAL:HA	3:BD:3362:ARG:O	2.20	0.41
3:AD:350:VAL:HA	3:AD:362:ARG:O	2.20	0.41
5:BG:3200:ILE:HA	5:BG:3204:VAL:HG23	2.03	0.41
5:AG:209:ILE:HA	5:AG:210:PRO:HD3	1.90	0.41
2:AB:402:LEU:HD11	2:AB:483:ARG:NE	2.35	0.41
7:AQ:373:GLN:HB2	7:AQ:373:GLN:HE21	1.59	0.41
8:AZ:356:GLN:OE1	8:AZ:363:LYS:HD2	2.21	0.41
2:AB:125:ARG:HD3	2:AB:506:GLU:CD	2.41	0.41
8:AZ:353:LEU:H	8:AZ:369:GLU:HG3	1.86	0.41
3:AD:274:ILE:O	3:AD:278:ILE:HG13	2.21	0.41
8:AZ:158:LEU:C	8:AZ:160:THR:N	2.73	0.41
6:AH:199:ILE:HG22	6:AH:199:ILE:O	2.20	0.41
5:BG:3041:PRO:CA	5:BG:3161:THR:HG22	2.44	0.41
7:AQ:383:THR:HG22	7:AQ:385:ILE:HG13	2.02	0.41
2:BB:3131:ALA:O	2:BB:3411:MET:HG2	2.21	0.41
7:AQ:53:LYS:HG3	7:AQ:71:MET:SD	2.59	0.41
4:BE:3259:LEU:HD13	4:BE:3261:LYS:CA	2.50	0.41
1:AA:420:PRO:HG3	1:AA:499:ASN:OD1	2.20	0.41
5:AG:48:LEU:HD11	5:AG:64:ILE:HG12	2.02	0.41
4:AE:47:LYS:NZ	4:AE:551:ILE:O	2.54	0.41
3:BD:3177:SER:HB3	3:BD:3375:VAL:HG11	2.02	0.41
6:BH:3197:LYS:HD2	6:BH:3197:LYS:N	2.34	0.41
7:AQ:510:LYS:HG2	7:AQ:511:ASP:H	1.84	0.41
2:BB:3085:ASP:O	2:BB:3089:GLY:HA2	2.21	0.41
2:AB:85:ASP:O	2:AB:89:GLY:HA2	2.21	0.41
4:AE:291:SER:C	4:AE:293:GLU:H	2.24	0.41
3:AD:288:ILE:N	3:AD:288:ILE:HD12	2.35	0.41
4:BE:3415:ILE:HG13	4:BE:3415:ILE:H	1.49	0.41
7:BQ:3153:LYS:C	7:BQ:3155:ASP:N	2.73	0.41
1:AA:526:LYS:NZ	1:AA:530:SER:HB2	2.36	0.41
7:BQ:3018:TYR:HE2	8:BZ:3066:MET:SD	2.43	0.41
5:AG:276:GLU:O	5:AG:280:VAL:HG23	2.21	0.41
4:AE:298:LEU:HD23	6:AH:264:VAL:HG13	2.02	0.41
4:AE:100:ILE:O	4:AE:103:LEU:HB2	2.20	0.41
2:AB:510:ARG:O	4:AE:70:LEU:HB3	2.20	0.41
4:AE:291:SER:O	4:AE:293:GLU:N	2.54	0.41
2:AB:177:ALA:O	2:AB:181:ILE:HG12	2.20	0.41
3:AD:522:ASP:O	3:AD:523:ASP:HB2	2.21	0.41
5:AG:129:LEU:HD23	5:AG:510:VAL:HG12	2.03	0.41
3:BD:3251:ASN:HD22	3:BD:3251:ASN:HA	1.50	0.41
5:AG:466:ARG:HG3	5:AG:466:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:470:GLN:HG2	5:AG:491:ILE:CD1	2.51	0.41
2:AB:6:PHE:HB3	2:AB:7:GLY:H	1.62	0.41
7:AQ:444:LEU:CD2	7:AQ:444:LEU:H	2.18	0.41
9:BE:3601:ADP:H5'1	9:BE:3601:ADP:O2B	2.20	0.41
5:BG:3167:TRP:HH2	8:BZ:3126:ARG:NH2	2.18	0.41
2:AB:216:LYS:CE	2:AB:307:GLU:HG3	2.51	0.41
4:AE:448:VAL:HG12	4:AE:452:LEU:HD22	2.01	0.41
5:AG:231:HIS:NE2	8:AZ:336:ALA:HB3	2.35	0.41
1:AA:271:GLU:OE2	5:AG:275:ILE:HG22	2.20	0.41
7:BQ:3236:VAL:HB	7:BQ:3319:LEU:HA	2.01	0.41
1:BA:3284:ARG:HD3	1:BA:3341:MET:CE	2.50	0.41
7:AQ:233:GLU:HB2	7:AQ:320:VAL:HB	2.02	0.41
7:AQ:435:THR:CG2	7:AQ:450:LYS:HG3	2.46	0.41
2:AB:440:LEU:HA	2:AB:443:ILE:HG22	2.02	0.41
3:AD:326:LYS:CD	3:AD:373:PRO:HD2	2.48	0.41
2:AB:231:ILE:HD11	2:AB:321:THR:HG21	2.01	0.41
5:BG:3303:ASP:O	5:BG:3306:GLN:HB2	2.20	0.41
7:BQ:3401:ILE:O	7:BQ:3405:VAL:HG23	2.20	0.41
2:AB:202:LYS:CD	3:AD:129:LYS:HE2	2.50	0.41
1:BA:3425:VAL:HG21	1:BA:3524:LYS:HD2	2.03	0.41
6:AH:210:GLU:O	6:AH:210:GLU:HG2	2.21	0.41
6:BH:3036:VAL:HG12	6:BH:3070:LEU:CD2	2.50	0.41
2:BB:3186:GLY:O	2:BB:3187:SER:C	2.59	0.41
5:BG:3470:GLN:HG2	5:BG:3491:ILE:CD1	2.51	0.41
7:BQ:3045:SER:HB3	7:BQ:3066:ASN:O	2.21	0.41
3:BD:3522:ASP:O	3:BD:3523:ASP:HB2	2.21	0.41
6:BH:3446:LEU:HD21	6:BH:3507:LEU:HD21	2.01	0.41
8:BZ:3433:LYS:C	8:BZ:3435:GLY:N	2.73	0.41
2:BB:3402:LEU:HD11	2:BB:3483:ARG:NE	2.35	0.41
1:AA:487:ALA:O	1:AA:493:LYS:HB3	2.19	0.41
5:AG:276:GLU:OE2	8:AZ:246:GLU:HB2	2.21	0.41
4:BE:3100:ILE:O	4:BE:3103:LEU:HB2	2.20	0.41
3:AD:422:SER:O	3:AD:426:SER:HB2	2.21	0.41
5:AG:155:ILE:HG21	5:AG:172:CYS:HA	2.03	0.41
8:AZ:437:LYS:HB2	8:AZ:440:THR:HB	2.03	0.41
8:BZ:3015:ARG:NH1	8:BZ:3015:ARG:HB2	2.36	0.41
5:AG:200:ILE:HA	5:AG:204:VAL:HG23	2.03	0.41
6:BH:3229:PHE:CD1	6:BH:3234:LYS:HE2	2.56	0.41
1:BA:3190:GLN:HB3	1:BA:3194:GLY:O	2.20	0.41
5:BG:3233:LYS:HE2	8:BZ:3335:GLU:HG3	2.02	0.41
7:AQ:236:VAL:HG11	7:AQ:318:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3280:LEU:HD12	8:BZ:3348:LEU:HD11	2.02	0.41
7:BQ:3478:LEU:HD11	7:BQ:3497:LYS:O	2.20	0.41
4:AE:421:ARG:O	4:AE:421:ARG:HD2	2.21	0.41
1:BA:3457:ILE:HG23	1:BA:3458:ILE:N	2.35	0.41
7:BQ:3333:CYS:SG	7:BQ:3340:PRO:HD3	2.61	0.41
1:AA:400:ARG:HH11	1:AA:400:ARG:CG	2.33	0.41
8:AZ:147:ARG:HH21	8:AZ:151:LEU:HD11	1.85	0.41
3:AD:448:GLU:O	3:AD:451:PRO:HD2	2.20	0.41
7:BQ:3039:HIS:CE1	7:BQ:3043:LEU:HD13	2.55	0.41
1:BA:3420:PRO:HG3	1:BA:3499:ASN:OD1	2.20	0.41
5:AG:110:TYR:CD1	5:AG:440:TRP:HB3	2.55	0.41
2:AB:514:ILE:HG12	4:AE:73:ILE:HD12	2.03	0.41
8:AZ:14:ARG:H	8:AZ:14:ARG:HG2	1.69	0.41
3:AD:177:SER:HB3	3:AD:375:VAL:HG11	2.02	0.41
6:AH:236:PHE:HD2	6:AH:292:ILE:HD11	1.85	0.41
1:BA:3163:SER:HB2	1:BA:3408:VAL:HG21	2.03	0.41
2:AB:463:ILE:HD12	2:AB:468:SER:HA	2.03	0.41
5:AG:431:ALA:HB2	5:AG:442:TYR:CD1	2.56	0.41
1:BA:3020:ILE:O	1:BA:3543:THR:HA	2.21	0.41
2:AB:402:LEU:N	2:AB:402:LEU:HD12	2.36	0.41
6:AH:44:LEU:HD22	6:AH:103:ILE:HD13	2.02	0.41
2:AB:39:PRO:HD2	2:AB:474:LEU:HD12	2.03	0.41
1:AA:326:LEU:HA	1:AA:329:ILE:HB	2.03	0.41
8:AZ:207:THR:HB	8:AZ:380:ILE:HA	2.03	0.41
3:BD:3194:ILE:O	3:BD:3194:ILE:HG22	2.21	0.41
6:BH:3068:THR:O	6:BH:3072:LEU:HG	2.21	0.41
3:AD:64:ILE:HG22	3:AD:68:MET:CE	2.49	0.41
5:AG:251:GLU:HA	5:AG:302:SER:HB2	2.02	0.41
1:AA:66:GLY:HA2	1:AA:69:ILE:HD12	2.03	0.41
1:BA:3287:LYS:HD3	1:BA:3347:GLU:O	2.20	0.41
4:BE:3352:GLU:OE1	6:BH:3228:GLY:N	2.54	0.41
4:AE:212:MET:CE	4:AE:434:VAL:HG11	2.51	0.41
5:BG:3200:ILE:H	5:BG:3200:ILE:HG12	1.49	0.41
5:BG:3382:ARG:CB	5:BG:3382:ARG:HH11	2.25	0.41
8:AZ:296:ILE:HA	8:AZ:317:LEU:HB2	2.03	0.41
1:AA:457:ILE:HG23	1:AA:458:ILE:N	2.35	0.41
8:BZ:3218:GLY:HA2	8:BZ:3365:THR:CG2	2.50	0.41
2:BB:3402:LEU:N	2:BB:3402:LEU:HD12	2.36	0.41
1:AA:156:LEU:HD21	1:AA:413:LEU:CD1	2.50	0.41
8:AZ:114:HIS:NE2	8:AZ:116:ARG:HG3	2.35	0.41
2:AB:310:ASP:HB3	2:AB:311:PHE:H	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:3298:LEU:HD23	6:BH:3264:VAL:HG13	2.02	0.41
2:AB:279:PHE:CD1	2:AB:332:PRO:HG3	2.56	0.41
6:AH:12:VAL:CG2	6:AH:13:LEU:N	2.84	0.41
1:BA:3526:LYS:NZ	1:BA:3530:SER:HB2	2.36	0.41
3:BD:3326:LYS:CD	3:BD:3373:PRO:HD2	2.48	0.41
8:BZ:3169:VAL:HG11	8:BZ:3205:LYS:O	2.21	0.41
7:AQ:333:CYS:SG	7:AQ:340:PRO:HD3	2.61	0.41
3:BD:3422:SER:O	3:BD:3426:SER:HB2	2.21	0.41
4:BE:3535:LYS:O	4:BE:3539:LEU:HD13	2.20	0.41
8:BZ:3412:ILE:CD1	8:BZ:3510:TYR:HA	2.50	0.41
4:AE:115:ILE:HD12	4:AE:115:ILE:N	2.36	0.41
8:AZ:220:ARG:O	8:AZ:306:LEU:HD13	2.19	0.41
1:AA:210:GLY:O	1:AA:388:ARG:HB3	2.20	0.41
3:BD:3291:SER:HB3	3:BD:3293:LEU:HG	2.02	0.41
3:AD:89:ALA:HB1	3:AD:503:VAL:HG22	2.01	0.41
8:BZ:3458:LEU:HD22	8:BZ:3493:LEU:HD11	2.02	0.41
1:AA:438:THR:HA	1:AA:445:GLN:HE21	1.85	0.41
1:AA:237:ILE:N	1:AA:316:MET:HE1	2.36	0.41
1:AA:358:CYS:HA	1:AA:377:THR:HA	2.03	0.41
4:BE:3450:MET:HG2	4:BE:3450:MET:H	1.52	0.41
4:BE:3227:GLN:HE21	4:BE:3227:GLN:HB3	1.61	0.41
7:BQ:3159:LEU:HD13	7:BQ:3186:VAL:HG11	2.02	0.41
6:AH:68:THR:O	6:AH:72:LEU:HG	2.21	0.41
4:BE:3243:VAL:HG11	4:BE:3353:HIS:HB3	2.03	0.41
6:BH:3330:VAL:HB	6:BH:3348:THR:N	2.36	0.41
4:BE:3148:ASN:O	4:BE:3152:GLU:HG2	2.21	0.41
4:AE:243:VAL:HG11	4:AE:353:HIS:HB3	2.03	0.41
5:AG:354:LEU:HD21	5:AG:371:CYS:SG	2.60	0.41
6:AH:410:VAL:HB	6:AH:416:THR:OG1	2.20	0.41
3:AD:124:PHE:HD2	3:AD:515:VAL:HG21	1.86	0.41
6:BH:3420:VAL:O	6:BH:3424:LEU:HB2	2.21	0.41
7:BQ:3356:GLU:H	7:BQ:3373:GLN:HG3	1.84	0.41
2:BB:3006:PHE:HB3	2:BB:3007:GLY:H	1.62	0.41
3:BD:3228:ARG:HA	3:BD:3350:VAL:O	2.20	0.41
1:BA:3456:LEU:C	1:BA:3459:PRO:HD2	2.41	0.41
5:AG:228:ASP:CG	5:AG:229:VAL:N	2.70	0.41
8:AZ:323:ARG:NH1	8:AZ:327:ARG:HH22	2.19	0.41
5:AG:269:TRP:HH2	7:AQ:261:THR:HG1	1.66	0.41
8:BZ:3296:ILE:HG21	8:BZ:3328:LEU:CD2	2.50	0.41
1:BA:3271:GLU:OE2	5:BG:3275:ILE:HG22	2.20	0.41
1:AA:229:ALA:HB1	1:AA:307:LEU:CD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:406:LEU:CD2	1:AA:410:LYS:HE3	2.51	0.41
2:BB:3190:LEU:HD12	4:BE:3389:LYS:HZ1	1.86	0.41
2:BB:3020:LEU:O	2:BB:3021:SER:C	2.58	0.41
1:AA:280:ILE:H	1:AA:280:ILE:HG13	1.75	0.41
4:AE:216:ARG:NH2	6:AH:353:GLU:OE2	2.53	0.41
6:AH:229:PHE:CD1	6:AH:234:LYS:HE2	2.56	0.41
6:BH:3281:LYS:HA	6:BH:3284:GLN:NE2	2.36	0.41
2:BB:3045:LEU:HD21	2:BB:3054:CYS:HB3	2.02	0.41
6:BH:3077:HIS:O	6:BH:3078:PRO:C	2.59	0.41
5:BG:3458:GLN:C	5:BG:3460:ALA:N	2.74	0.41
1:BA:3167:LYS:HG3	1:BA:3401:SER:HB2	2.03	0.41
8:AZ:60:LYS:N	8:AZ:91:THR:HG21	2.34	0.41
5:AG:303:ASP:O	5:AG:306:GLN:HB2	2.20	0.41
4:AE:259:LEU:HD13	4:AE:261:LYS:CA	2.50	0.41
4:BE:3051:ILE:HD12	4:BE:3130:LEU:O	2.21	0.41
2:BB:3463:ILE:HD12	2:BB:3468:SER:HA	2.03	0.41
1:AA:206:LEU:CD2	1:AA:225:ASN:HD22	2.31	0.41
4:AE:551:ILE:HD11	6:AH:62:ILE:CD1	2.51	0.41
8:AZ:427:ARG:HH22	8:AZ:449:GLU:HG2	1.85	0.41
6:AH:30:ILE:O	6:AH:34:VAL:HG23	2.20	0.41
2:BB:3510:ARG:O	4:BE:3070:LEU:HB3	2.20	0.41
2:AB:331:GLU:OE2	2:AB:334:LYS:HD3	2.21	0.41
7:BQ:3046:MET:HE1	7:BQ:3459:VAL:HA	2.03	0.41
6:BH:3210:GLU:HG2	6:BH:3210:GLU:O	2.21	0.41
6:AH:40:LEU:O	6:AH:43:THR:HG23	2.20	0.41
1:BA:3267:PRO:HG3	5:BG:3271:ARG:HE	1.86	0.41
1:AA:228:VAL:HA	1:AA:318:VAL:HG22	2.03	0.41
1:BA:3228:VAL:HA	1:BA:3318:VAL:HG22	2.03	0.41
3:BD:3234:ILE:HG22	3:BD:3235:GLY:N	2.36	0.41
1:AA:437:ALA:O	1:AA:445:GLN:HG3	2.20	0.41
1:BA:3237:ILE:N	1:BA:3316:MET:HE1	2.36	0.41
4:AE:126:ALA:O	4:AE:129:LEU:HB2	2.21	0.41
2:BB:3196:ILE:O	2:BB:3368:VAL:HA	2.21	0.41
3:AD:194:ILE:O	3:AD:194:ILE:HG22	2.21	0.41
1:BA:3283:GLU:O	1:BA:3287:LYS:HG3	2.20	0.41
4:BE:3447:GLU:OE2	4:BE:3479:ILE:HG21	2.21	0.41
3:AD:251:ASN:HD22	3:AD:251:ASN:HA	1.50	0.41
6:BH:3201:ILE:HD13	6:BH:3390:GLU:HG3	2.02	0.41
4:AE:235:SER:C	4:AE:237:SER:H	2.24	0.41
2:AB:186:GLY:O	2:AB:187:SER:C	2.59	0.41
4:AE:148:ASN:O	4:AE:152:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3437:LYS:HB2	8:BZ:3440:THR:HB	2.03	0.41
1:BA:3326:LEU:HA	1:BA:3329:ILE:HB	2.03	0.41
2:BB:3116:HIS:ND1	2:BB:3117:PRO:HD2	2.36	0.41
4:BE:3212:MET:CE	4:BE:3434:VAL:HG11	2.51	0.41
8:AZ:15:ARG:HB2	8:AZ:15:ARG:NH1	2.36	0.41
5:BG:3099:LEU:HD13	5:BG:3452:ILE:HD13	2.03	0.41
7:BQ:3444:LEU:N	7:BQ:3444:LEU:HD23	2.24	0.41
9:AE:601:ADP:H5'1	9:AE:601:ADP:O2B	2.20	0.41
1:BA:3193:LYS:HB2	3:BD:3228:ARG:NH1	2.35	0.41
3:BD:3212:GLY:HA3	3:BD:3363:VAL:O	2.21	0.41
3:AD:214:VAL:HG21	3:AD:378:VAL:HG23	2.02	0.41
4:AE:546:ARG:NH2	6:AH:173:ASN:N	2.62	0.41
4:AE:540:LEU:HA	4:AE:543:GLN:CG	2.49	0.41
5:AG:233:LYS:HE2	8:AZ:335:GLU:HG3	2.02	0.41
8:BZ:3323:ARG:NH1	8:BZ:3327:ARG:HH22	2.19	0.41
5:BG:3269:TRP:CZ3	8:BZ:3245:THR:HG23	2.56	0.41
7:BQ:3236:VAL:HG11	7:BQ:3318:ILE:O	2.21	0.41
4:AE:369:LEU:O	4:AE:370:SER:CB	2.69	0.41
1:AA:229:ALA:HA	1:AA:319:ARG:HD2	2.03	0.41
6:AH:189:LEU:HD12	6:AH:195:ASP:H	1.85	0.41
4:AE:91:LEU:O	4:AE:105:VAL:HG13	2.21	0.41
6:BH:3460:ASP:C	6:BH:3464:ILE:HG22	2.41	0.41
6:AH:505:ASN:ND2	7:AQ:215:GLY:H	2.11	0.41
2:BB:3440:LEU:HA	2:BB:3443:ILE:HG22	2.02	0.41
2:AB:316:ARG:O	2:AB:320:VAL:HG22	2.20	0.41
6:AH:281:LYS:NZ	7:AQ:278:LYS:NZ	2.68	0.41
2:BB:3051:SER:C	2:BB:3053:THR:H	2.25	0.41
5:AG:458:GLN:C	5:AG:460:ALA:N	2.74	0.41
7:BQ:3341:LEU:HD21	7:BQ:3351:GLU:CB	2.51	0.41
8:BZ:3347:ILE:HA	8:BZ:3347:ILE:HD12	1.97	0.41
8:BZ:3353:LEU:H	8:BZ:3369:GLU:HG3	1.86	0.41
1:AA:308:LYS:HB3	1:AA:308:LYS:HE2	1.93	0.41
6:BH:3171:ILE:HD11	6:BH:3178:PHE:CD1	2.56	0.41
8:BZ:3159:LEU:HA	8:BZ:3162:VAL:HG12	2.02	0.41
6:AH:171:ILE:HD11	6:AH:178:PHE:CD1	2.56	0.41
6:AH:199:ILE:O	6:AH:200:GLY:C	2.59	0.41
8:BZ:3307:ASP:O	8:BZ:3311:LYS:N	2.53	0.41
5:AG:286:GLN:HB3	5:AG:286:GLN:HE21	1.53	0.41
3:AD:189:VAL:CG1	3:AD:402:ARG:HG3	2.51	0.41
7:BQ:3336:CYS:HB3	7:BQ:3355:VAL:HG22	2.01	0.41
2:BB:3202:LYS:CD	3:BD:3129:LYS:HE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:3159:SER:O	4:BE:3163:GLU:HG2	2.21	0.41
2:BB:3009:GLN:HE22	2:BB:3518:ARG:HE	1.68	0.41
6:BH:3083:LEU:HB3	6:BH:3102:THR:CG2	2.51	0.41
1:AA:425:VAL:HG21	1:AA:524:LYS:HD2	2.03	0.41
3:AD:138:MET:O	3:AD:478:LEU:HD22	2.21	0.41
4:AE:51:ILE:HD12	4:AE:130:LEU:O	2.21	0.41
4:AE:51:ILE:HD13	4:AE:130:LEU:HB3	2.03	0.41
6:BH:3030:ILE:CD1	6:BH:3109:MET:HB3	2.51	0.41
3:BD:3288:ILE:HD12	3:BD:3288:ILE:N	2.35	0.41
5:BG:3170:LYS:HE2	5:BG:3215:LEU:HA	2.02	0.41
2:BB:3155:HIS:HB2	2:BB:3488:VAL:CG2	2.51	0.41
7:AQ:112:ASN:C	7:AQ:114:SER:H	2.24	0.41
4:BE:3291:SER:C	4:BE:3293:GLU:N	2.74	0.41
6:BH:3382:ALA:C	6:BH:3384:GLN:H	2.24	0.41
1:BA:3054:VAL:HG22	1:BA:3060:PHE:HB3	2.03	0.41
5:BG:3431:ALA:HB2	5:BG:3442:TYR:CD1	2.56	0.41
2:BB:3037:LEU:HG	2:BB:3038:GLY:N	2.35	0.41
1:AA:167:LYS:HG3	1:AA:401:SER:HB2	2.03	0.41
5:BG:3276:GLU:O	5:BG:3280:VAL:HG23	2.21	0.41
4:AE:282:LYS:HD2	6:AH:251:LYS:HB3	2.02	0.41
6:AH:104:LEU:HD21	6:AH:446:LEU:HD23	2.03	0.41
8:AZ:271:ASP:O	8:AZ:275:LYS:N	2.53	0.41
8:AZ:282:ASN:C	8:AZ:284:VAL:H	2.25	0.41
5:AG:131:ASP:O	5:AG:134:GLU:HB3	2.21	0.41
5:BG:3354:LEU:HD21	5:BG:3371:CYS:SG	2.60	0.41
3:BD:3433:GLU:N	3:BD:3433:GLU:CD	2.74	0.41
8:AZ:210:ILE:HA	8:AZ:210:ILE:HD13	1.92	0.41
8:BZ:3271:ASP:CA	8:BZ:3274:LEU:HB3	2.40	0.41
5:BG:3466:ARG:HG3	5:BG:3466:ARG:HH11	1.86	0.41
8:AZ:305:SER:O	8:AZ:309:PHE:HD1	2.04	0.41
3:AD:234:ILE:HG22	3:AD:235:GLY:N	2.36	0.41
7:BQ:3246:LYS:HB3	7:BQ:3352:LEU:HD23	2.02	0.41
6:BH:3143:LEU:O	6:BH:3145:VAL:HG23	2.21	0.41
8:AZ:116:ARG:HG2	8:AZ:529:LEU:CD2	2.51	0.41
1:AA:419:VAL:HG23	1:AA:521:THR:HA	2.02	0.41
2:BB:3279:PHE:CD1	2:BB:3332:PRO:HG3	2.56	0.41
6:AH:353:GLU:HB3	6:AH:355:MET:HE3	2.03	0.41
2:BB:3048:SER:HA	3:BD:3528:ARG:HG2	2.02	0.41
7:AQ:21:TYR:O	7:AQ:27:GLN:HG3	2.21	0.41
3:BD:3419:ILE:CD1	3:BD:3451:PRO:HG2	2.51	0.41
2:AB:268:LYS:O	2:AB:271:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BZ:3207:THR:HB	8:BZ:3380:ILE:HA	2.03	0.41
2:AB:141:ASP:CB	2:AB:399:ARG:HA	2.51	0.41
7:AQ:390:THR:OG1	7:AQ:393:ASN:HB3	2.21	0.41
6:BH:3040:LEU:O	6:BH:3043:THR:HG23	2.20	0.41
3:BD:3092:GLY:HA2	9:BD:3601:ADP:PB	2.61	0.41
4:AE:552:ASP:HB3	6:AH:49:SER:OG	2.21	0.41
2:BB:3083:VAL:O	2:BB:3086:ASP:HB2	2.21	0.40
2:BB:3082:LYS:HE2	2:BB:3086:ASP:OD1	2.21	0.40
2:AB:83:VAL:O	2:AB:86:ASP:HB2	2.21	0.40
3:BD:3024:ASN:HD22	3:BD:3024:ASN:HA	1.68	0.40
7:AQ:326:LYS:NZ	7:AQ:326:LYS:HB2	2.35	0.40
2:BB:3039:PRO:HD2	2:BB:3474:LEU:HD12	2.03	0.40
8:BZ:3144:SER:C	8:BZ:3146:ASP:H	2.25	0.40
1:BA:3243:LYS:HB2	1:BA:3292:GLY:O	2.21	0.40
5:BG:3276:GLU:OE2	8:BZ:3246:GLU:HB2	2.21	0.40
2:BB:3296:GLN:CB	3:BD:3334:ALA:HB2	2.50	0.40
6:BH:3199:ILE:O	6:BH:3200:GLY:C	2.59	0.40
4:AE:291:SER:C	4:AE:293:GLU:N	2.74	0.40
4:BE:3291:SER:O	4:BE:3293:GLU:N	2.54	0.40
1:BA:3066:GLY:HA2	1:BA:3069:ILE:HD12	2.03	0.40
4:BE:3322:ILE:HG22	4:BE:3351:LEU:HD12	2.03	0.40
4:AE:251:HIS:HD2	4:AE:253:GLN:HB2	1.84	0.40
6:AH:172:HIS:O	6:AH:175:ALA:HB2	2.21	0.40
2:AB:132:LEU:HD21	2:AB:495:ARG:HG2	2.02	0.40
4:AE:543:GLN:HB3	6:AH:209:MET:SD	2.61	0.40
7:BQ:3291:ILE:HD11	7:BQ:3345:GLY:H	1.85	0.40
6:AH:422:LYS:HG2	6:AH:426:ASP:OD2	2.22	0.40
5:AG:346:SER:O	5:AG:348:VAL:HG22	2.21	0.40
2:AB:116:HIS:ND1	2:AB:117:PRO:HD2	2.36	0.40
6:BH:3353:GLU:HB3	6:BH:3355:MET:CE	2.51	0.40
6:BH:3356:GLN:NE2	6:BH:3361:ARG:HG2	2.36	0.40
2:AB:49:ALA:N	3:AD:528:ARG:HG2	2.36	0.40
2:AB:45:LEU:HD21	2:AB:54:CYS:HB3	2.02	0.40
7:AQ:23:ASN:HB2	7:AQ:542:ASP:C	2.42	0.40
1:BA:3086:LEU:HD11	1:BA:3530:SER:OG	2.21	0.40
6:BH:3162:ALA:HB2	6:BH:3400:VAL:CG2	2.51	0.40
7:BQ:3087:MET:O	7:BQ:3090:GLU:HB2	2.20	0.40
2:AB:32:LEU:CD1	2:AB:44:LYS:HE2	2.50	0.40
7:BQ:3316:TYR:CD1	7:BQ:3316:TYR:N	2.88	0.40
8:BZ:3427:ARG:HH22	8:BZ:3449:GLU:HG2	1.85	0.40
6:AH:202:LYS:HG2	6:AH:362:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:3202:LYS:HG2	6:BH:3362:TYR:CE2	2.55	0.40
5:AG:241:PRO:HD2	5:AG:353:GLY:O	2.20	0.40
2:BB:3125:ARG:HD3	2:BB:3506:GLU:CD	2.41	0.40
5:AG:33:ASP:HA	5:AG:36:ARG:CD	2.52	0.40
3:BD:3134:ILE:CG2	3:BD:3424:ARG:HD2	2.51	0.40
1:AA:179:MET:HE2	1:AA:218:LEU:HB2	2.02	0.40
7:AQ:167:ILE:HG23	7:AQ:178:LEU:HD23	2.02	0.40
3:BD:3048:ILE:HG21	3:BD:3067:GLN:O	2.21	0.40
6:BH:3266:ASP:O	6:BH:3270:ILE:HG22	2.21	0.40
1:BA:3109:LEU:HD23	1:BA:3539:LEU:HD23	2.03	0.40
8:AZ:90:GLY:HA2	9:AZ:601:ADP:PB	2.61	0.40
1:AA:109:LEU:HD23	1:AA:539:LEU:HD23	2.04	0.40
3:AD:512:SER:O	3:AD:515:VAL:HG22	2.21	0.40
6:BH:3479:TYR:HA	6:BH:3489:GLY:O	2.21	0.40
4:AE:447:GLU:OE2	4:AE:479:ILE:HG21	2.21	0.40
2:AB:393:GLN:HE21	4:AE:387:THR:HG22	1.85	0.40
1:AA:267:PRO:HG3	5:AG:271:ARG:HE	1.86	0.40
4:BE:3364:PRO:HB3	6:BH:3302:LEU:HD12	2.02	0.40
6:AH:239:PRO:HG2	6:AH:241:ILE:HD11	2.02	0.40
6:BH:3172:HIS:O	6:BH:3175:ALA:HB2	2.21	0.40
5:AG:269:TRP:CZ3	8:AZ:245:THR:HG23	2.56	0.40
1:BA:3190:GLN:H	1:BA:3190:GLN:NE2	2.19	0.40
1:BA:3198:TYR:CD2	1:BA:3413:LEU:HD23	2.57	0.40
1:BA:3406:LEU:CD2	1:BA:3410:LYS:HE3	2.51	0.40
5:AG:455:THR:HA	5:AG:458:GLN:NE2	2.35	0.40
1:AA:198:TYR:CD2	1:AA:413:LEU:HD23	2.57	0.40
2:AB:121:ILE:HG22	2:AB:125:ARG:HG3	2.03	0.40
6:AH:77:HIS:O	6:AH:78:PRO:C	2.59	0.40
5:BG:3455:THR:HA	5:BG:3458:GLN:NE2	2.35	0.40
1:AA:291:ALA:HA	1:AA:351:GLU:HB3	2.03	0.40
5:BG:3159:ILE:HD13	5:BG:3159:ILE:HA	1.91	0.40
8:AZ:169:VAL:HG11	8:AZ:205:LYS:O	2.21	0.40
3:BD:3189:VAL:CG1	3:BD:3402:ARG:HG3	2.51	0.40
7:BQ:3052:ASN:C	7:BQ:3053:LYS:HD2	2.41	0.40
4:AE:115:ILE:CD1	4:AE:536:GLN:HG2	2.52	0.40
7:AQ:495:LEU:HD13	7:AQ:495:LEU:N	2.36	0.40
6:BH:3294:LEU:HD11	6:BH:3365:PHE:CZ	2.56	0.40
3:AD:92:GLY:HA2	9:AD:601:ADP:PB	2.61	0.40
6:AH:418:MET:O	6:AH:421:SER:HB3	2.22	0.40
3:BD:3229:LYS:HD2	3:BD:3284:ASN:ND2	2.16	0.40
1:AA:20:ILE:O	1:AA:543:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:3437:ALA:O	1:BA:3445:GLN:HG3	2.20	0.40
1:BA:3332:ALA:HA	1:BA:3380:HIS:HA	2.03	0.40
2:AB:196:ILE:O	2:AB:368:VAL:HA	2.21	0.40
1:BA:3082:ILE:HA	3:BD:3383:ASN:HD21	1.86	0.40
2:BB:3512:ASP:HB3	4:BE:3070:LEU:HD22	2.04	0.40
6:AH:64:ASN:O	6:AH:66:GLY:N	2.55	0.40
6:AH:201:ILE:HD13	6:AH:390:GLU:HG3	2.02	0.40
4:AE:159:SER:O	4:AE:163:GLU:HG2	2.21	0.40
6:AH:306:PHE:O	6:AH:309:ASP:HB2	2.21	0.40
6:AH:420:VAL:O	6:AH:424:LEU:HB2	2.21	0.40
4:AE:251:HIS:CD2	4:AE:253:GLN:H	2.33	0.40
4:AE:269:LEU:CD1	4:AE:375:GLY:HA3	2.51	0.40
5:AG:91:ASP:HB3	5:AG:505:ILE:CD1	2.50	0.40
1:AA:458:ILE:HB	1:AA:459:PRO:HD3	2.03	0.40
1:BA:3229:ALA:HA	1:BA:3319:ARG:HD2	2.03	0.40
7:AQ:299:ILE:HG12	7:AQ:318:ILE:HG22	2.04	0.40
6:BH:3203:LYS:HZ1	6:BH:3386:ILE:HB	1.86	0.40
7:AQ:246:LYS:HB3	7:AQ:352:LEU:HD23	2.02	0.40
6:BH:3306:PHE:O	6:BH:3309:ASP:HB2	2.21	0.40
7:BQ:3435:THR:CG2	7:BQ:3450:LYS:HG3	2.46	0.40
7:BQ:3168:SER:O	7:BQ:3169:SER:HB3	2.21	0.40
1:BA:3419:VAL:HG23	1:BA:3521:THR:HA	2.02	0.40
4:BE:3235:SER:C	4:BE:3237:SER:H	2.24	0.40
1:BA:3046:PRO:HB3	1:BA:3165:SER:HB3	2.03	0.40
2:BB:3166:LEU:HD12	2:BB:3173:PHE:CD1	2.56	0.40
5:AG:286:GLN:HG2	5:AG:286:GLN:H	1.45	0.40
8:AZ:199:MET:HB2	8:AZ:364:PHE:HZ	1.86	0.40
5:AG:250:LEU:HD12	5:AG:301:VAL:HG13	2.02	0.40
2:BB:3511:VAL:HG11	4:BE:3073:ILE:CD1	2.51	0.40
2:BB:3514:ILE:HG12	4:BE:3073:ILE:HD12	2.03	0.40
3:BD:3042:LYS:HG2	3:BD:3484:VAL:HG11	2.03	0.40
2:BB:3268:LYS:O	2:BB:3271:ASN:HB2	2.21	0.40
7:BQ:3065:THR:HG22	7:BQ:3067:ASP:H	1.86	0.40
7:BQ:3023:ASN:HB2	7:BQ:3542:ASP:C	2.42	0.40
6:AH:346:LEU:N	6:AH:346:LEU:HD23	2.36	0.40
6:AH:30:ILE:CD1	6:AH:109:MET:HB3	2.51	0.40
6:AH:294:LEU:HD11	6:AH:365:PHE:CZ	2.56	0.40
6:AH:245:ASN:ND2	6:AH:296:LYS:HD3	2.37	0.40
6:AH:197:LYS:HD2	6:AH:197:LYS:N	2.34	0.40
5:BG:3370:ASN:HD22	5:BG:3370:ASN:N	2.20	0.40
5:BG:3370:ASN:ND2	5:BG:3370:ASN:N	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:155:HIS:HB2	2:AB:488:VAL:CG2	2.51	0.40
6:AH:67:ALA:HB1	6:AH:71:LYS:HE3	2.03	0.40
2:AB:91:GLY:HA2	9:AB:601:ADP:O3B	2.21	0.40
1:AA:325:ASP:O	1:AA:329:ILE:N	2.55	0.40
2:AB:241:ASP:HB3	2:AB:242:LYS:H	1.58	0.40
4:BE:3100:ILE:HA	4:BE:3100:ILE:HD13	1.92	0.40
5:AG:176:LEU:C	5:AG:178:ALA:H	2.25	0.40
6:AH:479:TYR:HA	6:AH:489:GLY:O	2.21	0.40
4:BE:3477:ASP:C	4:BE:3480:PRO:HD2	2.41	0.40
8:AZ:144:SER:C	8:AZ:146:ASP:H	2.25	0.40
1:AA:131:VAL:HA	1:AA:134:ARG:HD2	2.03	0.40
6:AH:291:ASN:N	6:AH:291:ASN:OD1	2.55	0.40
4:BE:3431:ARG:HB3	4:BE:3431:ARG:NH1	2.24	0.40
1:AA:256:MET:SD	3:AD:260:MET:HE2	2.62	0.40
4:AE:318:ALA:HB2	4:AE:374:LEU:HD21	2.03	0.40
7:AQ:444:LEU:HD23	7:AQ:444:LEU:N	2.24	0.40
2:BB:3235:ASN:OD1	2:BB:3287:ARG:HD3	2.21	0.40
8:BZ:3356:GLN:OE1	8:BZ:3363:LYS:HD2	2.21	0.40
7:BQ:3254:LEU:HD12	7:BQ:3254:LEU:N	2.36	0.40
7:BQ:3233:GLU:HB2	7:BQ:3320:VAL:HB	2.02	0.40
1:AA:305:LEU:C	1:AA:307:LEU:H	2.25	0.40
1:AA:184:LEU:O	1:AA:187:VAL:HG23	2.20	0.40
7:AQ:191:PRO:HB3	7:AQ:380:ARG:NH2	2.36	0.40
7:BQ:3450:LYS:HB2	7:BQ:3450:LYS:HE3	1.94	0.40
5:BG:3346:SER:O	5:BG:3348:VAL:HG22	2.21	0.40
2:AB:183:ARG:O	2:AB:363:GLU:HA	2.22	0.40
6:AH:281:LYS:HA	6:AH:284:GLN:NE2	2.36	0.40
7:BQ:3299:ILE:HG12	7:BQ:3318:ILE:HG22	2.04	0.40
1:BA:3291:ALA:HA	1:BA:3351:GLU:HB3	2.03	0.40
1:BA:3308:LYS:HB3	1:BA:3308:LYS:HE2	1.93	0.40
7:AQ:78:VAL:HA	7:AQ:83:LYS:HE3	2.02	0.40
6:AH:51:ILE:HD12	6:AH:69:ILE:HG21	2.03	0.40
6:AH:198:LEU:C	6:AH:200:GLY:H	2.25	0.40
8:AZ:70:SER:HB3	8:AZ:73:ALA:CB	2.51	0.40
2:AB:222:GLN:HG2	2:AB:304:ASN:OD1	2.22	0.40
4:BE:3158:ILE:HD11	4:BE:3538:ILE:HG23	2.02	0.40
2:AB:511:VAL:HG11	4:AE:73:ILE:CD1	2.51	0.40
3:BD:3320:GLU:O	3:BD:3321:ILE:C	2.60	0.40
3:AD:138:MET:HG3	3:AD:478:LEU:HD13	2.03	0.40
4:BE:3115:ILE:HD12	4:BE:3115:ILE:N	2.35	0.40
4:BE:3115:ILE:CD1	4:BE:3536:GLN:HG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AQ:316:TYR:N	7:AQ:316:TYR:CD1	2.88	0.40
5:BG:3176:LEU:C	5:BG:3178:ALA:H	2.25	0.40
5:BG:3381:LEU:HD21	5:BG:3396:LEU:HD22	2.03	0.40
6:BH:3452:GLN:HG3	6:BH:3456:ASN:HD21	1.86	0.40
2:AB:270:LYS:HA	2:AB:273:ILE:HG22	2.02	0.40
3:AD:126:SER:O	3:AD:130:ARG:HB2	2.22	0.40
6:AH:266:ASP:O	6:AH:270:ILE:HG22	2.21	0.40
2:AB:233:ILE:O	2:AB:233:ILE:HG12	2.22	0.40
4:BE:3172:ASN:CB	4:BE:3175:LEU:HB3	2.40	0.40
3:BD:3512:SER:O	3:BD:3515:VAL:HG22	2.21	0.40
8:BZ:3399:LEU:C	8:BZ:3401:ALA:N	2.75	0.40
6:AH:364:LEU:O	6:AH:364:LEU:HD12	2.22	0.40
6:BH:3291:ASN:N	6:BH:3291:ASN:OD1	2.55	0.40
1:BA:3358:CYS:HA	1:BA:3377:THR:HA	2.03	0.40
3:AD:200:VAL:HA	3:AD:387:ILE:HD13	2.04	0.40
8:AZ:452:LEU:HB3	8:AZ:456:LYS:HE3	2.04	0.40
1:AA:190:GLN:NE2	1:AA:190:GLN:H	2.20	0.40
7:AQ:291:ILE:HD11	7:AQ:345:GLY:H	1.85	0.40
1:AA:200:VAL:HG13	1:AA:201:LYS:HG2	2.04	0.40
2:AB:37:LEU:HG	2:AB:38:GLY:N	2.35	0.40
8:BZ:3147:ARG:HH21	8:BZ:3151:LEU:HD11	1.85	0.40
8:BZ:3451:LEU:C	8:BZ:3453:VAL:H	2.24	0.40
8:BZ:3070:SER:HB3	8:BZ:3073:ALA:CB	2.51	0.40
6:BH:3094:VAL:CG1	6:BH:3502:VAL:HG22	2.51	0.40
7:AQ:52:ASN:C	7:AQ:53:LYS:HD2	2.41	0.40
2:BB:3222:GLN:HG2	2:BB:3304:ASN:OD1	2.21	0.40
3:AD:42:LYS:HG2	3:AD:484:VAL:HG11	2.03	0.40
3:AD:320:GLU:O	3:AD:321:ILE:C	2.60	0.40
4:BE:3047:LYS:HE3	4:BE:3143:PRO:HB3	2.04	0.40
7:BQ:3247:VAL:HG23	7:BQ:3338:ALA:HB2	2.04	0.40
3:BD:3138:MET:O	3:BD:3478:LEU:HD22	2.21	0.40
7:BQ:3390:THR:OG1	7:BQ:3393:ASN:HB3	2.21	0.40
1:AA:446:LEU:O	1:AA:450:GLU:HG2	2.22	0.40
2:AB:220:ASN:ND2	2:AB:295:GLU:HG2	2.36	0.40
6:BH:3346:LEU:N	6:BH:3346:LEU:HD23	2.36	0.40
3:BD:3217:GLN:N	3:BD:3217:GLN:OE1	2.55	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:462:ARG:CD	6:Bh:4151:LYS:CE[1_465]	1.74	0.46
4:AE:460:LYS:N	6:Bh:4149:SER:O[1_465]	1.81	0.39
4:BE:3174:GLU:OE2	7:Bq:4151:THR:CB[1_465]	1.88	0.32
4:AE:462:ARG:CD	6:Bh:4151:LYS:CD[1_465]	2.01	0.19
7:AQ:514:GLU:OE2	6:Ah:1151:LYS:NZ[1_465]	2.10	0.10
4:BE:3174:GLU:OE2	7:Bq:4151:THR:CA[1_465]	2.12	0.08
4:AE:460:LYS:CD	6:Bh:4152:SER:N[1_465]	2.15	0.05
8:Az:1431:MET:O	5:Bg:4149:ALA:CB[1_466]	2.16	0.04
4:AE:462:ARG:CG	6:Bh:4151:LYS:CD[1_465]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	531/559 (95%)	388 (73%)	103 (19%)	40 (8%)	1	20
1	Aa	531/559 (95%)	388 (73%)	103 (19%)	40 (8%)	1	20
1	BA	531/559 (95%)	388 (73%)	103 (19%)	40 (8%)	1	20
1	Ba	531/559 (95%)	388 (73%)	103 (19%)	40 (8%)	1	20
2	AB	515/527 (98%)	382 (74%)	100 (19%)	33 (6%)	2	26
2	Ab	515/527 (98%)	383 (74%)	99 (19%)	33 (6%)	2	26
2	BB	515/527 (98%)	382 (74%)	100 (19%)	33 (6%)	2	26
2	Bb	515/527 (98%)	382 (74%)	100 (19%)	33 (6%)	2	26
3	AD	511/528 (97%)	391 (76%)	85 (17%)	35 (7%)	1	24
3	Ad	511/528 (97%)	391 (76%)	85 (17%)	35 (7%)	1	24
3	BD	511/528 (97%)	391 (76%)	85 (17%)	35 (7%)	1	24
3	Bd	511/528 (97%)	391 (76%)	85 (17%)	35 (7%)	1	24
4	AE	526/562 (94%)	401 (76%)	91 (17%)	34 (6%)	1	25
4	Ae	526/562 (94%)	401 (76%)	91 (17%)	34 (6%)	1	25
4	BE	526/562 (94%)	401 (76%)	91 (17%)	34 (6%)	1	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Be	526/562 (94%)	401 (76%)	91 (17%)	34 (6%)	1	25
5	AG	503/590 (85%)	387 (77%)	85 (17%)	31 (6%)	2	26
5	Ag	503/590 (85%)	387 (77%)	85 (17%)	31 (6%)	2	26
5	BG	503/590 (85%)	387 (77%)	85 (17%)	31 (6%)	2	26
5	Bg	503/590 (85%)	387 (77%)	85 (17%)	31 (6%)	2	26
6	AH	517/550 (94%)	389 (75%)	91 (18%)	37 (7%)	1	22
6	Ah	517/550 (94%)	389 (75%)	91 (18%)	37 (7%)	1	22
6	BH	517/550 (94%)	389 (75%)	91 (18%)	37 (7%)	1	22
6	Bh	517/550 (94%)	389 (75%)	91 (18%)	37 (7%)	1	22
7	AQ	515/568 (91%)	415 (81%)	73 (14%)	27 (5%)	2	30
7	Aq	515/568 (91%)	414 (80%)	74 (14%)	27 (5%)	2	30
7	BQ	515/568 (91%)	414 (80%)	74 (14%)	27 (5%)	2	30
7	Bq	515/568 (91%)	415 (81%)	73 (14%)	27 (5%)	2	30
8	AZ	527/546 (96%)	403 (76%)	97 (18%)	27 (5%)	2	31
8	Az	527/546 (96%)	403 (76%)	97 (18%)	27 (5%)	2	31
8	BZ	527/546 (96%)	403 (76%)	97 (18%)	27 (5%)	2	31
8	Bz	527/546 (96%)	403 (76%)	97 (18%)	27 (5%)	2	31
All	All	16580/17720 (94%)	12623 (76%)	2901 (18%)	1056 (6%)	2	26

All (1056) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	77	HIS
1	AA	335	ALA
1	AA	378	SER
2	AB	5	ILE
2	AB	15	ALA
2	AB	243	VAL
2	AB	310	ASP
2	AB	326	VAL
2	AB	397	GLU
3	AD	11	PHE
3	AD	141	LYS
3	AD	146	ASP
3	AD	222	SER
3	AD	249	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	AD	321	ILE
3	AD	356	ASP
4	AE	46	ALA
4	AE	119	THR
4	AE	250	SER
4	AE	262	GLU
4	AE	364	PRO
4	AE	370	SER
4	AE	520	ASN
5	AG	33	ASP
5	AG	196	PHE
5	AG	197	GLU
5	AG	266	GLU
5	AG	348	VAL
5	AG	435	GLU
5	AG	498	GLY
5	AG	499	ILE
6	AH	144	ALA
6	AH	145	VAL
6	AH	221	LYS
6	AH	222	LYS
6	AH	224	PHE
6	AH	247	GLU
6	AH	248	LEU
6	AH	250	LEU
6	AH	476	GLU
6	AH	484	GLU
7	AQ	147	VAL
7	AQ	236	VAL
7	AQ	237	LYS
7	AQ	243	LYS
7	AQ	375	GLN
7	AQ	413	LYS
8	AZ	163	ASP
8	AZ	297	ASN
1	Aa	1077	HIS
1	Aa	1335	ALA
1	Aa	1378	SER
2	Ab	1005	ILE
2	Ab	1015	ALA
2	Ab	1243	VAL
2	Ab	1310	ASP

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Mol	Chain	Res	Type
2	Ab	1326	VAL
2	Ab	1397	GLU
3	Ad	1011	PHE
3	Ad	1141	LYS
3	Ad	1146	ASP
3	Ad	1222	SER
3	Ad	1249	GLU
3	Ad	1321	ILE
3	Ad	1356	ASP
4	Ae	1046	ALA
4	Ae	1119	THR
4	Ae	1250	SER
4	Ae	1262	GLU
4	Ae	1364	PRO
4	Ae	1370	SER
4	Ae	1520	ASN
5	Ag	1033	ASP
5	Ag	1196	PHE
5	Ag	1197	GLU
5	Ag	1266	GLU
5	Ag	1348	VAL
5	Ag	1435	GLU
5	Ag	1498	GLY
5	Ag	1499	ILE
6	Ah	1144	ALA
6	Ah	1145	VAL
6	Ah	1221	LYS
6	Ah	1222	LYS
6	Ah	1224	PHE
6	Ah	1247	GLU
6	Ah	1248	LEU
6	Ah	1250	LEU
6	Ah	1476	GLU
6	Ah	1484	GLU
7	Aq	1147	VAL
7	Aq	1236	VAL
7	Aq	1237	LYS
7	Aq	1243	LYS
7	Aq	1375	GLN
7	Aq	1413	LYS
8	Az	1163	ASP
8	Az	1297	ASN

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Mol	Chain	Res	Type
1	BA	3077	HIS
1	BA	3335	ALA
1	BA	3378	SER
2	BB	3005	ILE
2	BB	3015	ALA
2	BB	3243	VAL
2	BB	3310	ASP
2	BB	3326	VAL
2	BB	3397	GLU
3	BD	3011	PHE
3	BD	3141	LYS
3	BD	3146	ASP
3	BD	3222	SER
3	BD	3249	GLU
3	BD	3321	ILE
3	BD	3356	ASP
4	BE	3046	ALA
4	BE	3119	THR
4	BE	3250	SER
4	BE	3262	GLU
4	BE	3364	PRO
4	BE	3370	SER
4	BE	3520	ASN
5	BG	3033	ASP
5	BG	3196	PHE
5	BG	3197	GLU
5	BG	3266	GLU
5	BG	3348	VAL
5	BG	3435	GLU
5	BG	3498	GLY
5	BG	3499	ILE
6	BH	3144	ALA
6	BH	3145	VAL
6	BH	3221	LYS
6	BH	3222	LYS
6	BH	3224	PHE
6	BH	3247	GLU
6	BH	3248	LEU
6	BH	3250	LEU
6	BH	3476	GLU
6	BH	3484	GLU
7	BQ	3147	VAL

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Mol	Chain	Res	Type
7	BQ	3236	VAL
7	BQ	3237	LYS
7	BQ	3243	LYS
7	BQ	3375	GLN
7	BQ	3413	LYS
8	BZ	3163	ASP
8	BZ	3297	ASN
1	Ba	4077	HIS
1	Ba	4335	ALA
1	Ba	4378	SER
2	Bb	4005	ILE
2	Bb	4015	ALA
2	Bb	4243	VAL
2	Bb	4310	ASP
2	Bb	4326	VAL
2	Bb	4397	GLU
3	Bd	4011	PHE
3	Bd	4141	LYS
3	Bd	4146	ASP
3	Bd	4222	SER
3	Bd	4249	GLU
3	Bd	4321	ILE
3	Bd	4356	ASP
4	Be	4046	ALA
4	Be	4119	THR
4	Be	4250	SER
4	Be	4262	GLU
4	Be	4364	PRO
4	Be	4370	SER
4	Be	4520	ASN
5	Bg	4033	ASP
5	Bg	4196	PHE
5	Bg	4197	GLU
5	Bg	4266	GLU
5	Bg	4348	VAL
5	Bg	4435	GLU
5	Bg	4498	GLY
5	Bg	4499	ILE
6	Bh	4144	ALA
6	Bh	4145	VAL
6	Bh	4221	LYS
6	Bh	4222	LYS

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Mol	Chain	Res	Type
6	Bh	4224	PHE
6	Bh	4247	GLU
6	Bh	4248	LEU
6	Bh	4250	LEU
6	Bh	4476	GLU
6	Bh	4484	GLU
7	Bq	4147	VAL
7	Bq	4236	VAL
7	Bq	4237	LYS
7	Bq	4243	LYS
7	Bq	4375	GLN
7	Bq	4413	LYS
8	Bz	4163	ASP
8	Bz	4297	ASN
1	AA	6	ASN
1	AA	93	GLU
1	AA	200	VAL
1	AA	201	LYS
1	AA	248	ASP
1	AA	254	ALA
1	AA	343	ASN
1	AA	350	PHE
1	AA	352	SER
1	AA	382	SER
1	AA	496	SER
1	AA	498	ARG
2	AB	219	GLY
2	AB	246	PHE
2	AB	349	GLY
2	AB	406	CYS
3	AD	17	PRO
3	AD	184	GLU
3	AD	218	THR
3	AD	224	GLY
3	AD	226	PRO
3	AD	239	PHE
3	AD	330	CYS
3	AD	478	LEU
4	AE	35	GLN
4	AE	37	ASN
4	AE	171	SER
4	AE	194	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	AE	263	GLY
4	AE	345	TRP
4	AE	369	LEU
4	AE	400	GLU
5	AG	54	GLY
5	AG	239	GLU
5	AG	259	THR
5	AG	319	ARG
5	AG	334	ALA
5	AG	338	ASN
5	AG	353	GLY
5	AG	478	GLY
6	AH	18	ASP
6	AH	197	LYS
6	AH	200	GLY
6	AH	300	GLY
6	AH	311	ASN
6	AH	339	SER
6	AH	367	GLY
6	AH	432	ALA
7	AQ	16	GLN
7	AQ	96	MET
7	AQ	151	THR
7	AQ	244	LYS
7	AQ	289	LYS
7	AQ	294	MET
8	AZ	137	LYS
8	AZ	230	ASN
8	AZ	360	GLY
8	AZ	369	GLU
8	AZ	438	GLY
1	Aa	1006	ASN
1	Aa	1093	GLU
1	Aa	1200	VAL
1	Aa	1201	LYS
1	Aa	1248	ASP
1	Aa	1254	ALA
1	Aa	1343	ASN
1	Aa	1350	PHE
1	Aa	1352	SER
1	Aa	1382	SER
1	Aa	1496	SER

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Mol	Chain	Res	Type
1	Aa	1498	ARG
2	Ab	1219	GLY
2	Ab	1246	PHE
2	Ab	1349	GLY
2	Ab	1406	CYS
3	Ad	1017	PRO
3	Ad	1184	GLU
3	Ad	1218	THR
3	Ad	1224	GLY
3	Ad	1226	PRO
3	Ad	1239	PHE
3	Ad	1330	CYS
3	Ad	1478	LEU
4	Ae	1035	GLN
4	Ae	1037	ASN
4	Ae	1171	SER
4	Ae	1194	SER
4	Ae	1263	GLY
4	Ae	1345	TRP
4	Ae	1369	LEU
4	Ae	1400	GLU
5	Ag	1054	GLY
5	Ag	1239	GLU
5	Ag	1259	THR
5	Ag	1319	ARG
5	Ag	1334	ALA
5	Ag	1338	ASN
5	Ag	1353	GLY
5	Ag	1478	GLY
6	Ah	1018	ASP
6	Ah	1197	LYS
6	Ah	1200	GLY
6	Ah	1300	GLY
6	Ah	1311	ASN
6	Ah	1339	SER
6	Ah	1367	GLY
6	Ah	1432	ALA
7	Aq	1016	GLN
7	Aq	1096	MET
7	Aq	1151	THR
7	Aq	1244	LYS
7	Aq	1289	LYS

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Mol	Chain	Res	Type
7	Aq	1294	MET
8	Az	1137	LYS
8	Az	1230	ASN
8	Az	1360	GLY
8	Az	1369	GLU
8	Az	1438	GLY
1	BA	3006	ASN
1	BA	3093	GLU
1	BA	3200	VAL
1	BA	3201	LYS
1	BA	3248	ASP
1	BA	3254	ALA
1	BA	3343	ASN
1	BA	3350	PHE
1	BA	3352	SER
1	BA	3382	SER
1	BA	3496	SER
1	BA	3498	ARG
2	BB	3219	GLY
2	BB	3246	PHE
2	BB	3349	GLY
2	BB	3406	CYS
3	BD	3017	PRO
3	BD	3184	GLU
3	BD	3218	THR
3	BD	3224	GLY
3	BD	3226	PRO
3	BD	3239	PHE
3	BD	3330	CYS
3	BD	3478	LEU
4	BE	3035	GLN
4	BE	3037	ASN
4	BE	3171	SER
4	BE	3194	SER
4	BE	3263	GLY
4	BE	3345	TRP
4	BE	3369	LEU
4	BE	3400	GLU
5	BG	3054	GLY
5	BG	3239	GLU
5	BG	3259	THR
5	BG	3319	ARG

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Mol	Chain	Res	Type
5	BG	3334	ALA
5	BG	3338	ASN
5	BG	3353	GLY
5	BG	3478	GLY
6	BH	3018	ASP
6	BH	3197	LYS
6	BH	3200	GLY
6	BH	3300	GLY
6	BH	3311	ASN
6	BH	3339	SER
6	BH	3367	GLY
6	BH	3432	ALA
7	BQ	3016	GLN
7	BQ	3096	MET
7	BQ	3151	THR
7	BQ	3244	LYS
7	BQ	3289	LYS
7	BQ	3294	MET
8	BZ	3137	LYS
8	BZ	3230	ASN
8	BZ	3360	GLY
8	BZ	3369	GLU
8	BZ	3438	GLY
1	Ba	4006	ASN
1	Ba	4093	GLU
1	Ba	4200	VAL
1	Ba	4201	LYS
1	Ba	4248	ASP
1	Ba	4254	ALA
1	Ba	4343	ASN
1	Ba	4350	PHE
1	Ba	4352	SER
1	Ba	4382	SER
1	Ba	4496	SER
1	Ba	4498	ARG
2	Bb	4219	GLY
2	Bb	4246	PHE
2	Bb	4349	GLY
2	Bb	4406	CYS
3	Bd	4017	PRO
3	Bd	4184	GLU
3	Bd	4218	THR

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Mol	Chain	Res	Type
3	Bd	4224	GLY
3	Bd	4226	PRO
3	Bd	4239	PHE
3	Bd	4330	CYS
3	Bd	4478	LEU
4	Be	4035	GLN
4	Be	4037	ASN
4	Be	4171	SER
4	Be	4194	SER
4	Be	4263	GLY
4	Be	4345	TRP
4	Be	4369	LEU
4	Be	4400	GLU
5	Bg	4054	GLY
5	Bg	4239	GLU
5	Bg	4259	THR
5	Bg	4319	ARG
5	Bg	4334	ALA
5	Bg	4338	ASN
5	Bg	4353	GLY
5	Bg	4478	GLY
6	Bh	4018	ASP
6	Bh	4197	LYS
6	Bh	4200	GLY
6	Bh	4300	GLY
6	Bh	4311	ASN
6	Bh	4339	SER
6	Bh	4367	GLY
6	Bh	4432	ALA
7	Bq	4016	GLN
7	Bq	4096	MET
7	Bq	4151	THR
7	Bq	4244	LYS
7	Bq	4289	LYS
7	Bq	4294	MET
7	Bq	4423	ALA
8	Bz	4137	LYS
8	Bz	4230	ASN
8	Bz	4360	GLY
8	Bz	4369	GLU
8	Bz	4438	GLY
1	AA	9	ARG

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Mol	Chain	Res	Type
1	AA	119	LYS
1	AA	188	LYS
1	AA	215	GLU
1	AA	238	ALA
1	AA	274	ARG
1	AA	320	ARG
1	AA	376	GLY
2	AB	49	ALA
2	AB	163	SER
2	AB	201	GLY
2	AB	280	GLY
2	AB	452	SER
3	AD	36	ARG
3	AD	50	THR
3	AD	219	ALA
3	AD	231	LYS
3	AD	295	ASP
3	AD	355	SER
4	AE	281	PRO
4	AE	285	HIS
4	AE	390	ASP
4	AE	436	ASP
4	AE	462	ARG
4	AE	514	CYS
5	AG	115	ASN
5	AG	185	ASP
5	AG	186	LEU
5	AG	216	ASP
5	AG	267	GLU
5	AG	361	GLY
5	AG	486	GLY
5	AG	496	SER
6	AH	58	GLN
6	AH	65	ASP
6	AH	75	VAL
6	AH	173	ASN
6	AH	223	THR
6	AH	251	LYS
6	AH	333	SER
6	AH	460	ASP
7	AQ	230	ARG
7	AQ	423	ALA

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Mol	Chain	Res	Type
7	AQ	438	GLY
7	AQ	543	GLN
8	AZ	15	ARG
8	AZ	57	LYS
8	AZ	184	ALA
8	AZ	186	ALA
8	AZ	187	ASP
8	AZ	202	LEU
8	AZ	217	HIS
8	AZ	341	GLU
8	AZ	373	PRO
8	AZ	451	LEU
1	Aa	1009	ARG
1	Aa	1119	LYS
1	Aa	1188	LYS
1	Aa	1215	GLU
1	Aa	1238	ALA
1	Aa	1274	ARG
1	Aa	1320	ARG
1	Aa	1376	GLY
2	Ab	1049	ALA
2	Ab	1163	SER
2	Ab	1201	GLY
2	Ab	1280	GLY
2	Ab	1452	SER
3	Ad	1036	ARG
3	Ad	1050	THR
3	Ad	1219	ALA
3	Ad	1231	LYS
3	Ad	1295	ASP
3	Ad	1355	SER
4	Ae	1281	PRO
4	Ae	1285	HIS
4	Ae	1390	ASP
4	Ae	1436	ASP
4	Ae	1462	ARG
4	Ae	1514	CYS
5	Ag	1115	ASN
5	Ag	1185	ASP
5	Ag	1186	LEU
5	Ag	1216	ASP
5	Ag	1267	GLU

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Mol	Chain	Res	Type
5	Ag	1361	GLY
5	Ag	1486	GLY
5	Ag	1496	SER
6	Ah	1058	GLN
6	Ah	1065	ASP
6	Ah	1075	VAL
6	Ah	1173	ASN
6	Ah	1223	THR
6	Ah	1251	LYS
6	Ah	1333	SER
6	Ah	1460	ASP
7	Aq	1230	ARG
7	Aq	1423	ALA
7	Aq	1438	GLY
7	Aq	1543	GLN
8	Az	1015	ARG
8	Az	1057	LYS
8	Az	1184	ALA
8	Az	1186	ALA
8	Az	1187	ASP
8	Az	1202	LEU
8	Az	1217	HIS
8	Az	1341	GLU
8	Az	1373	PRO
8	Az	1451	LEU
1	BA	3009	ARG
1	BA	3119	LYS
1	BA	3188	LYS
1	BA	3215	GLU
1	BA	3238	ALA
1	BA	3274	ARG
1	BA	3320	ARG
1	BA	3376	GLY
2	BB	3049	ALA
2	BB	3163	SER
2	BB	3201	GLY
2	BB	3280	GLY
2	BB	3452	SER
3	BD	3036	ARG
3	BD	3050	THR
3	BD	3219	ALA
3	BD	3231	LYS

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Mol	Chain	Res	Type
3	BD	3295	ASP
3	BD	3355	SER
4	BE	3281	PRO
4	BE	3285	HIS
4	BE	3390	ASP
4	BE	3436	ASP
4	BE	3462	ARG
4	BE	3514	CYS
5	BG	3115	ASN
5	BG	3185	ASP
5	BG	3186	LEU
5	BG	3216	ASP
5	BG	3267	GLU
5	BG	3361	GLY
5	BG	3486	GLY
5	BG	3496	SER
6	BH	3058	GLN
6	BH	3065	ASP
6	BH	3075	VAL
6	BH	3173	ASN
6	BH	3223	THR
6	BH	3251	LYS
6	BH	3333	SER
6	BH	3460	ASP
7	BQ	3230	ARG
7	BQ	3423	ALA
7	BQ	3438	GLY
7	BQ	3543	GLN
8	BZ	3015	ARG
8	BZ	3057	LYS
8	BZ	3184	ALA
8	BZ	3186	ALA
8	BZ	3187	ASP
8	BZ	3202	LEU
8	BZ	3217	HIS
8	BZ	3341	GLU
8	BZ	3373	PRO
8	BZ	3451	LEU
1	Ba	4009	ARG
1	Ba	4119	LYS
1	Ba	4188	LYS
1	Ba	4215	GLU

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Mol	Chain	Res	Type
1	Ba	4238	ALA
1	Ba	4274	ARG
1	Ba	4320	ARG
1	Ba	4376	GLY
2	Bb	4049	ALA
2	Bb	4163	SER
2	Bb	4201	GLY
2	Bb	4280	GLY
2	Bb	4452	SER
3	Bd	4036	ARG
3	Bd	4050	THR
3	Bd	4219	ALA
3	Bd	4295	ASP
3	Bd	4355	SER
4	Be	4281	PRO
4	Be	4285	HIS
4	Be	4390	ASP
4	Be	4436	ASP
4	Be	4462	ARG
4	Be	4514	CYS
5	Bg	4115	ASN
5	Bg	4185	ASP
5	Bg	4186	LEU
5	Bg	4216	ASP
5	Bg	4267	GLU
5	Bg	4486	GLY
5	Bg	4496	SER
6	Bh	4058	GLN
6	Bh	4065	ASP
6	Bh	4075	VAL
6	Bh	4173	ASN
6	Bh	4223	THR
6	Bh	4251	LYS
6	Bh	4333	SER
6	Bh	4383	GLU
6	Bh	4460	ASP
7	Bq	4230	ARG
7	Bq	4438	GLY
7	Bq	4543	GLN
8	Bz	4015	ARG
8	Bz	4057	LYS
8	Bz	4184	ALA

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Mol	Chain	Res	Type
8	Bz	4186	ALA
8	Bz	4187	ASP
8	Bz	4202	LEU
8	Bz	4217	HIS
8	Bz	4341	GLU
8	Bz	4373	PRO
8	Bz	4451	LEU
1	AA	143	VAL
1	AA	191	ASN
1	AA	195	GLU
1	AA	199	PRO
1	AA	270	LEU
1	AA	367	SER
1	AA	368	ASP
1	AA	430	ASN
1	AA	465	ASN
2	AB	8	ASP
2	AB	55	MET
2	AB	88	VAL
2	AB	168	GLN
2	AB	185	LYS
2	AB	212	PHE
2	AB	216	LYS
2	AB	291	TYR
3	AD	183	ASP
3	AD	211	ASP
3	AD	212	GLY
3	AD	251	ASN
3	AD	264	LEU
4	AE	45	GLU
4	AE	207	ALA
4	AE	282	LYS
4	AE	292	VAL
4	AE	293	GLU
4	AE	413	LYS
4	AE	507	ILE
4	AE	518	GLY
5	AG	47	MET
5	AG	290	VAL
5	AG	329	ALA
5	AG	479	ASN
6	AH	148	THR

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Mol	Chain	Res	Type
6	AH	230	GLU
6	AH	232	GLN
6	AH	383	GLU
6	AH	422	LYS
7	AQ	9	PRO
7	AQ	338	ALA
7	AQ	439	GLU
7	AQ	460	PRO
8	AZ	201	HIS
8	AZ	203	SER
1	Aa	1143	VAL
1	Aa	1191	ASN
1	Aa	1195	GLU
1	Aa	1199	PRO
1	Aa	1270	LEU
1	Aa	1367	SER
1	Aa	1368	ASP
1	Aa	1430	ASN
1	Aa	1465	ASN
2	Ab	1008	ASP
2	Ab	1055	MET
2	Ab	1088	VAL
2	Ab	1168	GLN
2	Ab	1185	LYS
2	Ab	1212	PHE
2	Ab	1216	LYS
2	Ab	1291	TYR
3	Ad	1183	ASP
3	Ad	1211	ASP
3	Ad	1212	GLY
3	Ad	1251	ASN
3	Ad	1264	LEU
4	Ae	1045	GLU
4	Ae	1207	ALA
4	Ae	1282	LYS
4	Ae	1292	VAL
4	Ae	1293	GLU
4	Ae	1413	LYS
4	Ae	1507	ILE
4	Ae	1518	GLY
5	Ag	1047	MET
5	Ag	1290	VAL

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Mol	Chain	Res	Type
5	Ag	1329	ALA
5	Ag	1479	ASN
6	Ah	1148	THR
6	Ah	1230	GLU
6	Ah	1232	GLN
6	Ah	1383	GLU
6	Ah	1422	LYS
7	Aq	1009	PRO
7	Aq	1338	ALA
7	Aq	1439	GLU
7	Aq	1460	PRO
8	Az	1201	HIS
8	Az	1203	SER
1	BA	3143	VAL
1	BA	3191	ASN
1	BA	3195	GLU
1	BA	3199	PRO
1	BA	3270	LEU
1	BA	3367	SER
1	BA	3368	ASP
1	BA	3430	ASN
1	BA	3465	ASN
2	BB	3008	ASP
2	BB	3055	MET
2	BB	3088	VAL
2	BB	3168	GLN
2	BB	3185	LYS
2	BB	3212	PHE
2	BB	3216	LYS
2	BB	3291	TYR
3	BD	3183	ASP
3	BD	3211	ASP
3	BD	3212	GLY
3	BD	3251	ASN
3	BD	3264	LEU
4	BE	3045	GLU
4	BE	3207	ALA
4	BE	3282	LYS
4	BE	3292	VAL
4	BE	3293	GLU
4	BE	3413	LYS
4	BE	3507	ILE

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Mol	Chain	Res	Type
4	BE	3518	GLY
5	BG	3047	MET
5	BG	3290	VAL
5	BG	3479	ASN
6	BH	3148	THR
6	BH	3230	GLU
6	BH	3232	GLN
6	BH	3383	GLU
6	BH	3422	LYS
7	BQ	3009	PRO
7	BQ	3338	ALA
7	BQ	3439	GLU
7	BQ	3460	PRO
8	BZ	3201	HIS
8	BZ	3203	SER
1	Ba	4143	VAL
1	Ba	4191	ASN
1	Ba	4195	GLU
1	Ba	4199	PRO
1	Ba	4270	LEU
1	Ba	4367	SER
1	Ba	4368	ASP
1	Ba	4430	ASN
1	Ba	4465	ASN
2	Bb	4008	ASP
2	Bb	4055	MET
2	Bb	4088	VAL
2	Bb	4168	GLN
2	Bb	4185	LYS
2	Bb	4212	PHE
2	Bb	4216	LYS
3	Bd	4183	ASP
3	Bd	4211	ASP
3	Bd	4212	GLY
3	Bd	4231	LYS
3	Bd	4251	ASN
3	Bd	4264	LEU
4	Be	4045	GLU
4	Be	4207	ALA
4	Be	4282	LYS
4	Be	4292	VAL
4	Be	4293	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	Be	4413	LYS
4	Be	4507	ILE
4	Be	4508	SER
4	Be	4518	GLY
5	Bg	4047	MET
5	Bg	4290	VAL
5	Bg	4329	ALA
5	Bg	4361	GLY
5	Bg	4479	ASN
6	Bh	4148	THR
6	Bh	4230	GLU
6	Bh	4232	GLN
6	Bh	4422	LYS
7	Bq	4009	PRO
7	Bq	4338	ALA
7	Bq	4439	GLU
7	Bq	4460	PRO
8	Bz	4201	HIS
8	Bz	4203	SER
1	AA	10	SER
1	AA	193	LYS
2	AB	52	ASN
2	AB	111	ASP
2	AB	221	ASN
2	AB	222	GLN
2	AB	288	GLN
3	AD	158	LEU
3	AD	210	ILE
3	AD	260	MET
3	AD	408	ARG
3	AD	447	LEU
3	AD	466	VAL
4	AE	348	GLY
4	AE	392	MET
4	AE	508	SER
4	AE	540	LEU
6	AH	74	ASP
6	AH	107	GLU
6	AH	191	ARG
7	AQ	170	LYS
7	AQ	191	PRO
7	AQ	206	SER

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Mol	Chain	Res	Type
7	AQ	232	PRO
7	AQ	277	SER
7	AQ	358	VAL
8	AZ	10	ALA
8	AZ	144	SER
8	AZ	288	ASP
8	AZ	452	LEU
1	Aa	1010	SER
1	Aa	1193	LYS
2	Ab	1052	ASN
2	Ab	1111	ASP
2	Ab	1221	ASN
2	Ab	1222	GLN
2	Ab	1288	GLN
3	Ad	1158	LEU
3	Ad	1210	ILE
3	Ad	1260	MET
3	Ad	1359	LYS
3	Ad	1408	ARG
3	Ad	1447	LEU
3	Ad	1466	VAL
4	Ae	1249	PHE
4	Ae	1348	GLY
4	Ae	1392	MET
4	Ae	1508	SER
4	Ae	1540	LEU
6	Ah	1074	ASP
6	Ah	1107	GLU
6	Ah	1191	ARG
7	Aq	1170	LYS
7	Aq	1191	PRO
7	Aq	1206	SER
7	Aq	1232	PRO
7	Aq	1277	SER
7	Aq	1358	VAL
8	Az	1010	ALA
8	Az	1144	SER
8	Az	1288	ASP
8	Az	1452	LEU
1	BA	3010	SER
1	BA	3193	LYS
2	BB	3052	ASN

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Mol	Chain	Res	Type
2	BB	3111	ASP
2	BB	3221	ASN
2	BB	3222	GLN
2	BB	3288	GLN
3	BD	3158	LEU
3	BD	3210	ILE
3	BD	3260	MET
3	BD	3408	ARG
3	BD	3447	LEU
4	BE	3348	GLY
4	BE	3392	MET
4	BE	3508	SER
4	BE	3540	LEU
5	BG	3329	ALA
6	BH	3074	ASP
6	BH	3107	GLU
6	BH	3191	ARG
7	BQ	3170	LYS
7	BQ	3191	PRO
7	BQ	3206	SER
7	BQ	3232	PRO
7	BQ	3277	SER
7	BQ	3358	VAL
8	BZ	3010	ALA
8	BZ	3144	SER
8	BZ	3288	ASP
8	BZ	3452	LEU
1	Ba	4010	SER
1	Ba	4193	LYS
2	Bb	4052	ASN
2	Bb	4111	ASP
2	Bb	4221	ASN
2	Bb	4222	GLN
2	Bb	4288	GLN
2	Bb	4291	TYR
3	Bd	4158	LEU
3	Bd	4210	ILE
3	Bd	4260	MET
3	Bd	4359	LYS
3	Bd	4408	ARG
3	Bd	4447	LEU
3	Bd	4466	VAL

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Mol	Chain	Res	Type
4	Be	4249	PHE
4	Be	4348	GLY
4	Be	4392	MET
4	Be	4540	LEU
6	Bh	4074	ASP
6	Bh	4107	GLU
6	Bh	4191	ARG
7	Bq	4170	LYS
7	Bq	4191	PRO
7	Bq	4206	SER
7	Bq	4232	PRO
7	Bq	4277	SER
7	Bq	4358	VAL
8	Bz	4010	ALA
8	Bz	4144	SER
8	Bz	4288	ASP
8	Bz	4452	LEU
1	AA	203	VAL
1	AA	291	ALA
2	AB	361	ALA
2	AB	518	ARG
3	AD	240	GLN
3	AD	301	ALA
3	AD	359	LYS
4	AE	249	PHE
5	AG	232	PRO
6	AH	486	GLU
7	AQ	57	ASN
8	AZ	164	ALA
1	Aa	1203	VAL
1	Aa	1291	ALA
2	Ab	1361	ALA
2	Ab	1518	ARG
3	Ad	1240	GLN
3	Ad	1301	ALA
5	Ag	1232	PRO
6	Ah	1486	GLU
7	Aq	1057	ASN
8	Az	1164	ALA
1	BA	3203	VAL
1	BA	3291	ALA
2	BB	3361	ALA

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Mol	Chain	Res	Type
2	BB	3518	ARG
3	BD	3240	GLN
3	BD	3301	ALA
3	BD	3359	LYS
3	BD	3466	VAL
4	BE	3249	PHE
5	BG	3232	PRO
6	BH	3486	GLU
7	BQ	3057	ASN
8	BZ	3164	ALA
1	Ba	4203	VAL
1	Ba	4291	ALA
2	Bb	4361	ALA
2	Bb	4518	ARG
3	Bd	4240	GLN
3	Bd	4301	ALA
5	Bg	4232	PRO
6	Bh	4486	GLU
7	Bq	4057	ASN
8	Bz	4164	ALA
1	AA	228	VAL
2	AB	290	ILE
2	AB	362	GLY
6	AH	78	PRO
1	Aa	1228	VAL
2	Ab	1290	ILE
2	Ab	1362	GLY
6	Ah	1078	PRO
1	BA	3228	VAL
2	BB	3290	ILE
2	BB	3362	GLY
6	BH	3078	PRO
1	Ba	4228	VAL
2	Bb	4290	ILE
2	Bb	4362	GLY
6	Bh	4078	PRO
5	AG	61	GLY
8	AZ	303	PRO
5	Ag	1061	GLY
8	Az	1303	PRO
5	BG	3061	GLY
8	BZ	3303	PRO

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Mol	Chain	Res	Type
5	Bg	4061	GLY
8	Bz	4303	PRO
1	AA	416	GLY
2	AB	325	VAL
6	AH	199	ILE
8	AZ	172	PRO
1	Aa	1416	GLY
2	Ab	1325	VAL
6	Ah	1199	ILE
8	Az	1172	PRO
1	BA	3416	GLY
2	BB	3325	VAL
6	BH	3199	ILE
8	BZ	3172	PRO
1	Ba	4078	PRO
1	Ba	4416	GLY
2	Bb	4325	VAL
6	Bh	4199	ILE
8	Bz	4172	PRO
1	AA	78	PRO
1	AA	196	ILE
8	AZ	301	ILE
1	Aa	1078	PRO
1	Aa	1196	ILE
8	Az	1301	ILE
1	BA	3078	PRO
1	BA	3196	ILE
8	BZ	3301	ILE
1	Ba	4196	ILE
8	Bz	4301	ILE
5	AG	109	PRO
5	Ag	1109	PRO
5	BG	3109	PRO
5	Bg	4109	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	450/471 (96%)	393 (87%)	57 (13%)	5	32
1	Aa	450/471 (96%)	393 (87%)	57 (13%)	5	32
1	BA	450/471 (96%)	393 (87%)	57 (13%)	5	32
1	Ba	450/471 (96%)	393 (87%)	57 (13%)	5	32
2	AB	431/441 (98%)	363 (84%)	68 (16%)	3	23
2	Ab	431/441 (98%)	363 (84%)	68 (16%)	3	23
2	BB	431/441 (98%)	363 (84%)	68 (16%)	3	23
2	Bb	431/441 (98%)	363 (84%)	68 (16%)	3	23
3	AD	443/454 (98%)	388 (88%)	55 (12%)	6	33
3	Ad	443/454 (98%)	388 (88%)	55 (12%)	6	33
3	BD	443/454 (98%)	388 (88%)	55 (12%)	6	33
3	Bd	443/454 (98%)	388 (88%)	55 (12%)	6	33
4	AE	454/483 (94%)	404 (89%)	50 (11%)	8	39
4	Ae	454/483 (94%)	404 (89%)	50 (11%)	8	39
4	BE	454/483 (94%)	404 (89%)	50 (11%)	8	39
4	Be	454/483 (94%)	404 (89%)	50 (11%)	8	39
5	AG	433/497 (87%)	379 (88%)	54 (12%)	6	33
5	Ag	433/497 (87%)	379 (88%)	54 (12%)	6	33
5	BG	433/497 (87%)	379 (88%)	54 (12%)	6	33
5	Bg	433/497 (87%)	379 (88%)	54 (12%)	6	33
6	AH	430/454 (95%)	379 (88%)	51 (12%)	6	35
6	Ah	430/454 (95%)	379 (88%)	51 (12%)	6	35
6	BH	430/454 (95%)	379 (88%)	51 (12%)	6	35
6	Bh	430/454 (95%)	379 (88%)	51 (12%)	6	35
7	AQ	439/473 (93%)	387 (88%)	52 (12%)	6	35
7	Aq	439/473 (93%)	387 (88%)	52 (12%)	6	35
7	BQ	439/473 (93%)	387 (88%)	52 (12%)	6	35
7	Bq	439/473 (93%)	387 (88%)	52 (12%)	6	35
8	AZ	449/463 (97%)	399 (89%)	50 (11%)	8	39
8	Az	449/463 (97%)	399 (89%)	50 (11%)	8	39
8	BZ	449/463 (97%)	399 (89%)	50 (11%)	8	39
8	Bz	449/463 (97%)	400 (89%)	49 (11%)	8	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	14116/14944 (94%)	12369 (88%)	1747 (12%)	6	33

All (1747) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	12	THR
1	AA	13	LEU
1	AA	20	ILE
1	AA	43	SER
1	AA	50	ASP
1	AA	51	LYS
1	AA	56	ASP
1	AA	61	THR
1	AA	62	VAL
1	AA	116	VAL
1	AA	130	ARG
1	AA	135	GLU
1	AA	137	ILE
1	AA	142	GLU
1	AA	156	LEU
1	AA	178	ASN
1	AA	184	LEU
1	AA	190	GLN
1	AA	204	ASN
1	AA	205	VAL
1	AA	209	HIS
1	AA	214	THR
1	AA	217	LEU
1	AA	237	ILE
1	AA	241	ASN
1	AA	249	LEU
1	AA	251	LEU
1	AA	266	ASP
1	AA	282	LEU
1	AA	284	ARG
1	AA	299	THR
1	AA	326	LEU
1	AA	339	SER
1	AA	345	GLU
1	AA	348	GLU
1	AA	350	PHE
1	AA	355	LEU

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Mol	Chain	Res	Type
1	AA	358	CYS
1	AA	360	GLU
1	AA	377	THR
1	AA	380	HIS
1	AA	381	SER
1	AA	400	ARG
1	AA	404	ASP
1	AA	407	SER
1	AA	417	ASN
1	AA	455	LEU
1	AA	469	ASP
1	AA	478	ARG
1	AA	486	MET
1	AA	493	LYS
1	AA	495	ARG
1	AA	498	ARG
1	AA	505	ILE
1	AA	528	LEU
1	AA	539	LEU
1	AA	542	ASP
2	AB	4	GLN
2	AB	8	ASP
2	AB	13	GLU
2	AB	19	ARG
2	AB	35	SER
2	AB	37	LEU
2	AB	46	LEU
2	AB	50	SER
2	AB	52	ASN
2	AB	76	VAL
2	AB	77	LEU
2	AB	94	SER
2	AB	99	SER
2	AB	114	LYS
2	AB	128	SER
2	AB	132	LEU
2	AB	133	ASP
2	AB	135	LEU
2	AB	136	THR
2	AB	141	ASP
2	AB	146	LYS
2	AB	151	GLU

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Mol	Chain	Res	Type
2	AB	184	LEU
2	AB	187	SER
2	AB	189	ASN
2	AB	195	ILE
2	AB	210	GLU
2	AB	217	LYS
2	AB	218	PHE
2	AB	222	GLN
2	AB	233	ILE
2	AB	235	ASN
2	AB	237	THR
2	AB	239	ASP
2	AB	242	LYS
2	AB	273	ILE
2	AB	282	ASN
2	AB	283	THR
2	AB	288	GLN
2	AB	289	LEU
2	AB	291	TYR
2	AB	320	VAL
2	AB	327	SER
2	AB	328	THR
2	AB	331	GLU
2	AB	333	SER
2	AB	337	LEU
2	AB	351	GLN
2	AB	363	GLU
2	AB	377	LEU
2	AB	381	GLU
2	AB	390	VAL
2	AB	394	THR
2	AB	399	ARG
2	AB	400	THR
2	AB	401	VAL
2	AB	413	LYS
2	AB	417	THR
2	AB	426	LYS
2	AB	455	LEU
2	AB	460	ARG
2	AB	462	SER
2	AB	473	ASP
2	AB	489	GLU

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Mol	Chain	Res	Type
2	AB	495	ARG
2	AB	500	SER
2	AB	512	ASP
2	AB	513	ASN
3	AD	10	THR
3	AD	12	LYS
3	AD	22	LYS
3	AD	36	ARG
3	AD	37	THR
3	AD	51	SER
3	AD	52	ARG
3	AD	63	THR
3	AD	130	ARG
3	AD	141	LYS
3	AD	157	SER
3	AD	158	LEU
3	AD	166	TYR
3	AD	170	LEU
3	AD	181	ILE
3	AD	183	ASP
3	AD	185	ASN
3	AD	199	LYS
3	AD	209	MET
3	AD	215	LEU
3	AD	216	THR
3	AD	218	THR
3	AD	220	ILE
3	AD	230	GLU
3	AD	237	ILE
3	AD	249	GLU
3	AD	251	ASN
3	AD	260	MET
3	AD	263	ILE
3	AD	279	LYS
3	AD	292	ILE
3	AD	293	LEU
3	AD	306	SER
3	AD	308	LEU
3	AD	338	LEU
3	AD	351	GLU
3	AD	374	THR
3	AD	383	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	AD	384	ASN
3	AD	385	MET
3	AD	407	GLU
3	AD	410	LEU
3	AD	433	GLU
3	AD	440	TRP
3	AD	460	LEU
3	AD	463	ILE
3	AD	470	ARG
3	AD	473	HIS
3	AD	477	GLU
3	AD	478	LEU
3	AD	482	ILE
3	AD	486	ARG
3	AD	505	THR
3	AD	522	ASP
3	AD	528	ARG
4	AE	42	HIS
4	AE	44	LEU
4	AE	68	ARG
4	AE	82	THR
4	AE	107	LEU
4	AE	113	ASP
4	AE	134	LEU
4	AE	138	GLN
4	AE	151	ASP
4	AE	206	GLU
4	AE	211	VAL
4	AE	212	MET
4	AE	214	LYS
4	AE	222	ASP
4	AE	227	GLN
4	AE	229	ARG
4	AE	230	VAL
4	AE	243	VAL
4	AE	245	LEU
4	AE	247	LYS
4	AE	249	PHE
4	AE	257	CYS
4	AE	259	LEU
4	AE	272	LEU
4	AE	273	THR

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Mol	Chain	Res	Type
4	AE	285	HIS
4	AE	301	TYR
4	AE	327	PHE
4	AE	328	ASP
4	AE	335	LEU
4	AE	362	ILE
4	AE	369	LEU
4	AE	397	GLN
4	AE	404	VAL
4	AE	413	LYS
4	AE	414	MET
4	AE	415	ILE
4	AE	427	LEU
4	AE	431	ARG
4	AE	435	LYS
4	AE	450	MET
4	AE	464	ILE
4	AE	494	THR
4	AE	513	ASP
4	AE	520	ASN
4	AE	521	ASP
4	AE	526	PHE
4	AE	543	GLN
4	AE	545	CYS
4	AE	555	ILE
5	AG	55	LEU
5	AG	57	LEU
5	AG	58	THR
5	AG	59	ASN
5	AG	89	VAL
5	AG	95	THR
5	AG	111	LEU
5	AG	115	ASN
5	AG	125	LEU
5	AG	130	THR
5	AG	131	ASP
5	AG	156	GLN
5	AG	162	LYS
5	AG	167	TRP
5	AG	171	MET
5	AG	183	ARG
5	AG	184	LYS

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Mol	Chain	Res	Type
5	AG	196	PHE
5	AG	200	ILE
5	AG	215	LEU
5	AG	221	LYS
5	AG	227	LYS
5	AG	237	HIS
5	AG	246	LEU
5	AG	260	ASN
5	AG	264	GLU
5	AG	265	LYS
5	AG	267	GLU
5	AG	272	ILE
5	AG	273	LEU
5	AG	277	GLU
5	AG	282	LEU
5	AG	286	GLN
5	AG	288	LEU
5	AG	291	ARG
5	AG	293	THR
5	AG	310	LEU
5	AG	311	LYS
5	AG	316	VAL
5	AG	336	ILE
5	AG	340	VAL
5	AG	342	ASP
5	AG	345	GLU
5	AG	358	GLU
5	AG	375	LYS
5	AG	382	ARG
5	AG	459	ASN
5	AG	465	ILE
5	AG	475	HIS
5	AG	479	ASN
5	AG	480	PHE
5	AG	516	SER
5	AG	518	CYS
5	AG	528	SER
6	AH	11	VAL
6	AH	13	LEU
6	AH	43	THR
6	AH	50	ASP
6	AH	61	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	AH	91	ASP
6	AH	102	THR
6	AH	104	LEU
6	AH	147	ILE
6	AH	148	THR
6	AH	151	LYS
6	AH	173	ASN
6	AH	182	CYS
6	AH	189	LEU
6	AH	201	ILE
6	AH	202	LYS
6	AH	209	MET
6	AH	220	PHE
6	AH	221	LYS
6	AH	231	GLN
6	AH	242	LEU
6	AH	248	LEU
6	AH	249	GLU
6	AH	250	LEU
6	AH	251	LYS
6	AH	260	ARG
6	AH	267	TYR
6	AH	270	ILE
6	AH	277	LEU
6	AH	287	GLU
6	AH	291	ASN
6	AH	310	ARG
6	AH	319	SER
6	AH	324	ASN
6	AH	338	THR
6	AH	340	ASP
6	AH	343	PRO
6	AH	344	GLU
6	AH	346	LEU
6	AH	362	TYR
6	AH	368	CYS
6	AH	376	LEU
6	AH	377	LEU
6	AH	378	LEU
6	AH	392	SER
6	AH	398	MET
6	AH	453	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	AH	462	ILE
6	AH	479	TYR
6	AH	487	ASN
6	AH	516	LEU
7	AQ	10	ASN
7	AQ	14	PHE
7	AQ	27	GLN
7	AQ	53	LYS
7	AQ	89	THR
7	AQ	101	ASN
7	AQ	112	ASN
7	AQ	119	SER
7	AQ	151	THR
7	AQ	153	LYS
7	AQ	154	ASN
7	AQ	170	LYS
7	AQ	176	ASP
7	AQ	178	LEU
7	AQ	181	LEU
7	AQ	203	ASN
7	AQ	212	ILE
7	AQ	213	MET
7	AQ	226	MET
7	AQ	230	ARG
7	AQ	266	LEU
7	AQ	282	LYS
7	AQ	283	GLN
7	AQ	310	LEU
7	AQ	325	SER
7	AQ	329	LEU
7	AQ	332	LEU
7	AQ	343	ARG
7	AQ	344	LEU
7	AQ	351	GLU
7	AQ	370	VAL
7	AQ	375	GLN
7	AQ	378	ILE
7	AQ	390	THR
7	AQ	392	ASN
7	AQ	403	ASP
7	AQ	411	LEU
7	AQ	412	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	AQ	420	LEU
7	AQ	427	GLU
7	AQ	430	LEU
7	AQ	435	THR
7	AQ	439	GLU
7	AQ	444	LEU
7	AQ	458	VAL
7	AQ	482	HIS
7	AQ	495	LEU
7	AQ	513	ARG
7	AQ	518	TYR
7	AQ	519	ASP
7	AQ	520	MET
7	AQ	546	MET
8	AZ	5	LEU
8	AZ	14	ARG
8	AZ	15	ARG
8	AZ	30	GLN
8	AZ	35	THR
8	AZ	36	ASN
8	AZ	44	LYS
8	AZ	46	LEU
8	AZ	63	LEU
8	AZ	68	ILE
8	AZ	83	GLN
8	AZ	133	LEU
8	AZ	142	ASN
8	AZ	145	ASN
8	AZ	147	ARG
8	AZ	165	ASP
8	AZ	168	GLU
8	AZ	175	THR
8	AZ	193	MET
8	AZ	195	GLU
8	AZ	196	ILE
8	AZ	216	ASP
8	AZ	227	ARG
8	AZ	239	SER
8	AZ	240	LEU
8	AZ	253	TYR
8	AZ	260	ASP
8	AZ	271	ASP

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Mol	Chain	Res	Type
8	AZ	280	LEU
8	AZ	287	MET
8	AZ	288	ASP
8	AZ	296	ILE
8	AZ	304	MET
8	AZ	318	ARG
8	AZ	322	ARG
8	AZ	325	MET
8	AZ	338	ASN
8	AZ	342	ASP
8	AZ	355	TYR
8	AZ	364	PHE
8	AZ	397	ASP
8	AZ	430	ASN
8	AZ	442	THR
8	AZ	445	GLU
8	AZ	453	VAL
8	AZ	454	ILE
8	AZ	478	ASP
8	AZ	479	ASP
8	AZ	531	ASP
8	AZ	535	ARG
1	Aa	1012	THR
1	Aa	1013	LEU
1	Aa	1020	ILE
1	Aa	1043	SER
1	Aa	1050	ASP
1	Aa	1051	LYS
1	Aa	1056	ASP
1	Aa	1061	THR
1	Aa	1062	VAL
1	Aa	1116	VAL
1	Aa	1130	ARG
1	Aa	1135	GLU
1	Aa	1137	ILE
1	Aa	1142	GLU
1	Aa	1156	LEU
1	Aa	1178	ASN
1	Aa	1184	LEU
1	Aa	1190	GLN
1	Aa	1204	ASN
1	Aa	1205	VAL

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Mol	Chain	Res	Type
1	Aa	1209	HIS
1	Aa	1214	THR
1	Aa	1217	LEU
1	Aa	1237	ILE
1	Aa	1241	ASN
1	Aa	1249	LEU
1	Aa	1251	LEU
1	Aa	1266	ASP
1	Aa	1282	LEU
1	Aa	1284	ARG
1	Aa	1299	THR
1	Aa	1326	LEU
1	Aa	1339	SER
1	Aa	1345	GLU
1	Aa	1348	GLU
1	Aa	1350	PHE
1	Aa	1355	LEU
1	Aa	1358	CYS
1	Aa	1360	GLU
1	Aa	1377	THR
1	Aa	1380	HIS
1	Aa	1381	SER
1	Aa	1400	ARG
1	Aa	1404	ASP
1	Aa	1407	SER
1	Aa	1417	ASN
1	Aa	1455	LEU
1	Aa	1469	ASP
1	Aa	1478	ARG
1	Aa	1486	MET
1	Aa	1493	LYS
1	Aa	1495	ARG
1	Aa	1498	ARG
1	Aa	1505	ILE
1	Aa	1528	LEU
1	Aa	1539	LEU
1	Aa	1542	ASP
2	Ab	1004	GLN
2	Ab	1008	ASP
2	Ab	1013	GLU
2	Ab	1019	ARG
2	Ab	1035	SER

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Mol	Chain	Res	Type
2	Ab	1037	LEU
2	Ab	1046	LEU
2	Ab	1050	SER
2	Ab	1052	ASN
2	Ab	1076	VAL
2	Ab	1077	LEU
2	Ab	1094	SER
2	Ab	1099	SER
2	Ab	1114	LYS
2	Ab	1128	SER
2	Ab	1132	LEU
2	Ab	1133	ASP
2	Ab	1135	LEU
2	Ab	1136	THR
2	Ab	1141	ASP
2	Ab	1146	LYS
2	Ab	1151	GLU
2	Ab	1184	LEU
2	Ab	1187	SER
2	Ab	1189	ASN
2	Ab	1195	ILE
2	Ab	1210	GLU
2	Ab	1217	LYS
2	Ab	1218	PHE
2	Ab	1222	GLN
2	Ab	1233	ILE
2	Ab	1235	ASN
2	Ab	1237	THR
2	Ab	1239	ASP
2	Ab	1242	LYS
2	Ab	1273	ILE
2	Ab	1282	ASN
2	Ab	1283	THR
2	Ab	1288	GLN
2	Ab	1289	LEU
2	Ab	1291	TYR
2	Ab	1320	VAL
2	Ab	1327	SER
2	Ab	1328	THR
2	Ab	1331	GLU
2	Ab	1333	SER
2	Ab	1337	LEU

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Mol	Chain	Res	Type
2	Ab	1351	GLN
2	Ab	1363	GLU
2	Ab	1377	LEU
2	Ab	1381	GLU
2	Ab	1390	VAL
2	Ab	1394	THR
2	Ab	1399	ARG
2	Ab	1400	THR
2	Ab	1401	VAL
2	Ab	1413	LYS
2	Ab	1417	THR
2	Ab	1426	LYS
2	Ab	1455	LEU
2	Ab	1460	ARG
2	Ab	1462	SER
2	Ab	1473	ASP
2	Ab	1489	GLU
2	Ab	1495	ARG
2	Ab	1500	SER
2	Ab	1512	ASP
2	Ab	1513	ASN
3	Ad	1010	THR
3	Ad	1012	LYS
3	Ad	1022	LYS
3	Ad	1036	ARG
3	Ad	1037	THR
3	Ad	1051	SER
3	Ad	1052	ARG
3	Ad	1063	THR
3	Ad	1130	ARG
3	Ad	1141	LYS
3	Ad	1157	SER
3	Ad	1158	LEU
3	Ad	1166	TYR
3	Ad	1170	LEU
3	Ad	1181	ILE
3	Ad	1183	ASP
3	Ad	1185	ASN
3	Ad	1199	LYS
3	Ad	1209	MET
3	Ad	1215	LEU
3	Ad	1216	THR

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Mol	Chain	Res	Type
3	Ad	1218	THR
3	Ad	1220	ILE
3	Ad	1230	GLU
3	Ad	1237	ILE
3	Ad	1249	GLU
3	Ad	1251	ASN
3	Ad	1260	MET
3	Ad	1263	ILE
3	Ad	1279	LYS
3	Ad	1292	ILE
3	Ad	1293	LEU
3	Ad	1306	SER
3	Ad	1308	LEU
3	Ad	1338	LEU
3	Ad	1351	GLU
3	Ad	1374	THR
3	Ad	1383	ASN
3	Ad	1384	ASN
3	Ad	1385	MET
3	Ad	1407	GLU
3	Ad	1410	LEU
3	Ad	1433	GLU
3	Ad	1440	TRP
3	Ad	1460	LEU
3	Ad	1463	ILE
3	Ad	1470	ARG
3	Ad	1473	HIS
3	Ad	1477	GLU
3	Ad	1478	LEU
3	Ad	1482	ILE
3	Ad	1486	ARG
3	Ad	1505	THR
3	Ad	1522	ASP
3	Ad	1528	ARG
4	Ae	1042	HIS
4	Ae	1044	LEU
4	Ae	1068	ARG
4	Ae	1082	THR
4	Ae	1107	LEU
4	Ae	1113	ASP
4	Ae	1134	LEU
4	Ae	1138	GLN

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Mol	Chain	Res	Type
4	Ae	1151	ASP
4	Ae	1206	GLU
4	Ae	1211	VAL
4	Ae	1212	MET
4	Ae	1214	LYS
4	Ae	1222	ASP
4	Ae	1227	GLN
4	Ae	1229	ARG
4	Ae	1230	VAL
4	Ae	1243	VAL
4	Ae	1245	LEU
4	Ae	1247	LYS
4	Ae	1249	PHE
4	Ae	1257	CYS
4	Ae	1259	LEU
4	Ae	1272	LEU
4	Ae	1273	THR
4	Ae	1285	HIS
4	Ae	1301	TYR
4	Ae	1327	PHE
4	Ae	1328	ASP
4	Ae	1335	LEU
4	Ae	1362	ILE
4	Ae	1369	LEU
4	Ae	1397	GLN
4	Ae	1404	VAL
4	Ae	1413	LYS
4	Ae	1414	MET
4	Ae	1415	ILE
4	Ae	1427	LEU
4	Ae	1431	ARG
4	Ae	1435	LYS
4	Ae	1450	MET
4	Ae	1464	ILE
4	Ae	1494	THR
4	Ae	1513	ASP
4	Ae	1520	ASN
4	Ae	1521	ASP
4	Ae	1526	PHE
4	Ae	1543	GLN
4	Ae	1545	CYS
4	Ae	1555	ILE

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Mol	Chain	Res	Type
5	Ag	1055	LEU
5	Ag	1057	LEU
5	Ag	1058	THR
5	Ag	1059	ASN
5	Ag	1089	VAL
5	Ag	1095	THR
5	Ag	1111	LEU
5	Ag	1115	ASN
5	Ag	1125	LEU
5	Ag	1130	THR
5	Ag	1131	ASP
5	Ag	1156	GLN
5	Ag	1162	LYS
5	Ag	1167	TRP
5	Ag	1171	MET
5	Ag	1183	ARG
5	Ag	1184	LYS
5	Ag	1196	PHE
5	Ag	1200	ILE
5	Ag	1215	LEU
5	Ag	1221	LYS
5	Ag	1227	LYS
5	Ag	1237	HIS
5	Ag	1246	LEU
5	Ag	1260	ASN
5	Ag	1264	GLU
5	Ag	1265	LYS
5	Ag	1267	GLU
5	Ag	1272	ILE
5	Ag	1273	LEU
5	Ag	1277	GLU
5	Ag	1282	LEU
5	Ag	1286	GLN
5	Ag	1288	LEU
5	Ag	1291	ARG
5	Ag	1293	THR
5	Ag	1310	LEU
5	Ag	1311	LYS
5	Ag	1316	VAL
5	Ag	1336	ILE
5	Ag	1340	VAL
5	Ag	1342	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	Ag	1345	GLU
5	Ag	1358	GLU
5	Ag	1375	LYS
5	Ag	1382	ARG
5	Ag	1459	ASN
5	Ag	1465	ILE
5	Ag	1475	HIS
5	Ag	1479	ASN
5	Ag	1480	PHE
5	Ag	1516	SER
5	Ag	1518	CYS
5	Ag	1528	SER
6	Ah	1011	VAL
6	Ah	1013	LEU
6	Ah	1043	THR
6	Ah	1050	ASP
6	Ah	1061	THR
6	Ah	1091	ASP
6	Ah	1102	THR
6	Ah	1104	LEU
6	Ah	1147	ILE
6	Ah	1148	THR
6	Ah	1151	LYS
6	Ah	1173	ASN
6	Ah	1182	CYS
6	Ah	1189	LEU
6	Ah	1201	ILE
6	Ah	1202	LYS
6	Ah	1209	MET
6	Ah	1220	PHE
6	Ah	1221	LYS
6	Ah	1231	GLN
6	Ah	1242	LEU
6	Ah	1248	LEU
6	Ah	1249	GLU
6	Ah	1250	LEU
6	Ah	1251	LYS
6	Ah	1260	ARG
6	Ah	1267	TYR
6	Ah	1270	ILE
6	Ah	1277	LEU
6	Ah	1287	GLU

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Mol	Chain	Res	Type
6	Ah	1291	ASN
6	Ah	1310	ARG
6	Ah	1319	SER
6	Ah	1324	ASN
6	Ah	1338	THR
6	Ah	1340	ASP
6	Ah	1343	PRO
6	Ah	1344	GLU
6	Ah	1346	LEU
6	Ah	1362	TYR
6	Ah	1368	CYS
6	Ah	1376	LEU
6	Ah	1377	LEU
6	Ah	1378	LEU
6	Ah	1392	SER
6	Ah	1398	MET
6	Ah	1453	LEU
6	Ah	1462	ILE
6	Ah	1479	TYR
6	Ah	1487	ASN
6	Ah	1516	LEU
7	Aq	1010	ASN
7	Aq	1014	PHE
7	Aq	1027	GLN
7	Aq	1053	LYS
7	Aq	1089	THR
7	Aq	1101	ASN
7	Aq	1112	ASN
7	Aq	1119	SER
7	Aq	1151	THR
7	Aq	1153	LYS
7	Aq	1154	ASN
7	Aq	1170	LYS
7	Aq	1176	ASP
7	Aq	1178	LEU
7	Aq	1181	LEU
7	Aq	1203	ASN
7	Aq	1212	ILE
7	Aq	1213	MET
7	Aq	1226	MET
7	Aq	1230	ARG
7	Aq	1266	LEU

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Mol	Chain	Res	Type
7	Aq	1282	LYS
7	Aq	1283	GLN
7	Aq	1310	LEU
7	Aq	1325	SER
7	Aq	1329	LEU
7	Aq	1332	LEU
7	Aq	1343	ARG
7	Aq	1344	LEU
7	Aq	1351	GLU
7	Aq	1370	VAL
7	Aq	1375	GLN
7	Aq	1378	ILE
7	Aq	1390	THR
7	Aq	1392	ASN
7	Aq	1403	ASP
7	Aq	1411	LEU
7	Aq	1412	MET
7	Aq	1420	LEU
7	Aq	1427	GLU
7	Aq	1430	LEU
7	Aq	1435	THR
7	Aq	1439	GLU
7	Aq	1444	LEU
7	Aq	1458	VAL
7	Aq	1482	HIS
7	Aq	1495	LEU
7	Aq	1513	ARG
7	Aq	1518	TYR
7	Aq	1519	ASP
7	Aq	1520	MET
7	Aq	1546	MET
8	Az	1005	LEU
8	Az	1014	ARG
8	Az	1015	ARG
8	Az	1030	GLN
8	Az	1035	THR
8	Az	1036	ASN
8	Az	1044	LYS
8	Az	1046	LEU
8	Az	1063	LEU
8	Az	1068	ILE
8	Az	1083	GLN

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Mol	Chain	Res	Type
8	Az	1133	LEU
8	Az	1142	ASN
8	Az	1145	ASN
8	Az	1147	ARG
8	Az	1165	ASP
8	Az	1168	GLU
8	Az	1175	THR
8	Az	1193	MET
8	Az	1195	GLU
8	Az	1196	ILE
8	Az	1216	ASP
8	Az	1227	ARG
8	Az	1239	SER
8	Az	1240	LEU
8	Az	1253	TYR
8	Az	1260	ASP
8	Az	1271	ASP
8	Az	1280	LEU
8	Az	1287	MET
8	Az	1288	ASP
8	Az	1296	ILE
8	Az	1304	MET
8	Az	1318	ARG
8	Az	1322	ARG
8	Az	1325	MET
8	Az	1338	ASN
8	Az	1342	ASP
8	Az	1355	TYR
8	Az	1364	PHE
8	Az	1397	ASP
8	Az	1430	ASN
8	Az	1442	THR
8	Az	1445	GLU
8	Az	1453	VAL
8	Az	1454	ILE
8	Az	1478	ASP
8	Az	1479	ASP
8	Az	1531	ASP
8	Az	1535	ARG
1	BA	3012	THR
1	BA	3013	LEU
1	BA	3020	ILE

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Mol	Chain	Res	Type
1	BA	3043	SER
1	BA	3050	ASP
1	BA	3051	LYS
1	BA	3056	ASP
1	BA	3061	THR
1	BA	3062	VAL
1	BA	3116	VAL
1	BA	3130	ARG
1	BA	3135	GLU
1	BA	3137	ILE
1	BA	3142	GLU
1	BA	3156	LEU
1	BA	3178	ASN
1	BA	3184	LEU
1	BA	3190	GLN
1	BA	3204	ASN
1	BA	3205	VAL
1	BA	3209	HIS
1	BA	3214	THR
1	BA	3217	LEU
1	BA	3237	ILE
1	BA	3241	ASN
1	BA	3249	LEU
1	BA	3251	LEU
1	BA	3266	ASP
1	BA	3282	LEU
1	BA	3284	ARG
1	BA	3299	THR
1	BA	3326	LEU
1	BA	3339	SER
1	BA	3345	GLU
1	BA	3348	GLU
1	BA	3350	PHE
1	BA	3355	LEU
1	BA	3358	CYS
1	BA	3360	GLU
1	BA	3377	THR
1	BA	3380	HIS
1	BA	3381	SER
1	BA	3400	ARG
1	BA	3404	ASP
1	BA	3407	SER

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Mol	Chain	Res	Type
1	BA	3417	ASN
1	BA	3455	LEU
1	BA	3469	ASP
1	BA	3478	ARG
1	BA	3486	MET
1	BA	3493	LYS
1	BA	3495	ARG
1	BA	3498	ARG
1	BA	3505	ILE
1	BA	3528	LEU
1	BA	3539	LEU
1	BA	3542	ASP
2	BB	3004	GLN
2	BB	3008	ASP
2	BB	3013	GLU
2	BB	3019	ARG
2	BB	3035	SER
2	BB	3037	LEU
2	BB	3046	LEU
2	BB	3050	SER
2	BB	3052	ASN
2	BB	3076	VAL
2	BB	3077	LEU
2	BB	3094	SER
2	BB	3099	SER
2	BB	3114	LYS
2	BB	3128	SER
2	BB	3132	LEU
2	BB	3133	ASP
2	BB	3135	LEU
2	BB	3136	THR
2	BB	3141	ASP
2	BB	3146	LYS
2	BB	3151	GLU
2	BB	3184	LEU
2	BB	3187	SER
2	BB	3189	ASN
2	BB	3195	ILE
2	BB	3210	GLU
2	BB	3217	LYS
2	BB	3218	PHE
2	BB	3222	GLN

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Mol	Chain	Res	Type
2	BB	3233	ILE
2	BB	3235	ASN
2	BB	3237	THR
2	BB	3239	ASP
2	BB	3242	LYS
2	BB	3273	ILE
2	BB	3282	ASN
2	BB	3283	THR
2	BB	3288	GLN
2	BB	3289	LEU
2	BB	3291	TYR
2	BB	3320	VAL
2	BB	3327	SER
2	BB	3328	THR
2	BB	3331	GLU
2	BB	3333	SER
2	BB	3337	LEU
2	BB	3351	GLN
2	BB	3363	GLU
2	BB	3377	LEU
2	BB	3381	GLU
2	BB	3390	VAL
2	BB	3394	THR
2	BB	3399	ARG
2	BB	3400	THR
2	BB	3401	VAL
2	BB	3413	LYS
2	BB	3417	THR
2	BB	3426	LYS
2	BB	3455	LEU
2	BB	3460	ARG
2	BB	3462	SER
2	BB	3473	ASP
2	BB	3489	GLU
2	BB	3495	ARG
2	BB	3500	SER
2	BB	3512	ASP
2	BB	3513	ASN
3	BD	3010	THR
3	BD	3012	LYS
3	BD	3022	LYS
3	BD	3036	ARG

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Mol	Chain	Res	Type
3	BD	3037	THR
3	BD	3051	SER
3	BD	3052	ARG
3	BD	3063	THR
3	BD	3130	ARG
3	BD	3141	LYS
3	BD	3157	SER
3	BD	3158	LEU
3	BD	3166	TYR
3	BD	3170	LEU
3	BD	3181	ILE
3	BD	3183	ASP
3	BD	3185	ASN
3	BD	3199	LYS
3	BD	3209	MET
3	BD	3215	LEU
3	BD	3216	THR
3	BD	3218	THR
3	BD	3220	ILE
3	BD	3230	GLU
3	BD	3237	ILE
3	BD	3249	GLU
3	BD	3251	ASN
3	BD	3260	MET
3	BD	3263	ILE
3	BD	3279	LYS
3	BD	3292	ILE
3	BD	3293	LEU
3	BD	3306	SER
3	BD	3308	LEU
3	BD	3338	LEU
3	BD	3351	GLU
3	BD	3374	THR
3	BD	3383	ASN
3	BD	3384	ASN
3	BD	3385	MET
3	BD	3407	GLU
3	BD	3410	LEU
3	BD	3433	GLU
3	BD	3440	TRP
3	BD	3460	LEU
3	BD	3463	ILE

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Mol	Chain	Res	Type
3	BD	3470	ARG
3	BD	3473	HIS
3	BD	3477	GLU
3	BD	3478	LEU
3	BD	3482	ILE
3	BD	3486	ARG
3	BD	3505	THR
3	BD	3522	ASP
3	BD	3528	ARG
4	BE	3042	HIS
4	BE	3044	LEU
4	BE	3068	ARG
4	BE	3082	THR
4	BE	3107	LEU
4	BE	3113	ASP
4	BE	3134	LEU
4	BE	3138	GLN
4	BE	3151	ASP
4	BE	3206	GLU
4	BE	3211	VAL
4	BE	3212	MET
4	BE	3214	LYS
4	BE	3222	ASP
4	BE	3227	GLN
4	BE	3229	ARG
4	BE	3230	VAL
4	BE	3243	VAL
4	BE	3245	LEU
4	BE	3247	LYS
4	BE	3249	PHE
4	BE	3257	CYS
4	BE	3259	LEU
4	BE	3272	LEU
4	BE	3273	THR
4	BE	3285	HIS
4	BE	3301	TYR
4	BE	3327	PHE
4	BE	3328	ASP
4	BE	3335	LEU
4	BE	3362	ILE
4	BE	3369	LEU
4	BE	3397	GLN

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Mol	Chain	Res	Type
4	BE	3404	VAL
4	BE	3413	LYS
4	BE	3414	MET
4	BE	3415	ILE
4	BE	3427	LEU
4	BE	3431	ARG
4	BE	3435	LYS
4	BE	3450	MET
4	BE	3464	ILE
4	BE	3494	THR
4	BE	3513	ASP
4	BE	3520	ASN
4	BE	3521	ASP
4	BE	3526	PHE
4	BE	3543	GLN
4	BE	3545	CYS
4	BE	3555	ILE
5	BG	3055	LEU
5	BG	3057	LEU
5	BG	3058	THR
5	BG	3059	ASN
5	BG	3089	VAL
5	BG	3095	THR
5	BG	3111	LEU
5	BG	3115	ASN
5	BG	3125	LEU
5	BG	3130	THR
5	BG	3131	ASP
5	BG	3156	GLN
5	BG	3162	LYS
5	BG	3167	TRP
5	BG	3171	MET
5	BG	3183	ARG
5	BG	3184	LYS
5	BG	3196	PHE
5	BG	3200	ILE
5	BG	3215	LEU
5	BG	3221	LYS
5	BG	3227	LYS
5	BG	3237	HIS
5	BG	3246	LEU
5	BG	3260	ASN

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Mol	Chain	Res	Type
5	BG	3264	GLU
5	BG	3265	LYS
5	BG	3267	GLU
5	BG	3272	ILE
5	BG	3273	LEU
5	BG	3277	GLU
5	BG	3282	LEU
5	BG	3286	GLN
5	BG	3288	LEU
5	BG	3291	ARG
5	BG	3293	THR
5	BG	3310	LEU
5	BG	3311	LYS
5	BG	3316	VAL
5	BG	3336	ILE
5	BG	3340	VAL
5	BG	3342	ASP
5	BG	3345	GLU
5	BG	3358	GLU
5	BG	3375	LYS
5	BG	3382	ARG
5	BG	3459	ASN
5	BG	3465	ILE
5	BG	3475	HIS
5	BG	3479	ASN
5	BG	3480	PHE
5	BG	3516	SER
5	BG	3518	CYS
5	BG	3528	SER
6	BH	3011	VAL
6	BH	3013	LEU
6	BH	3043	THR
6	BH	3050	ASP
6	BH	3061	THR
6	BH	3091	ASP
6	BH	3102	THR
6	BH	3104	LEU
6	BH	3147	ILE
6	BH	3148	THR
6	BH	3151	LYS
6	BH	3173	ASN
6	BH	3182	CYS

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Mol	Chain	Res	Type
6	BH	3189	LEU
6	BH	3201	ILE
6	BH	3202	LYS
6	BH	3209	MET
6	BH	3220	PHE
6	BH	3221	LYS
6	BH	3231	GLN
6	BH	3242	LEU
6	BH	3248	LEU
6	BH	3249	GLU
6	BH	3250	LEU
6	BH	3251	LYS
6	BH	3260	ARG
6	BH	3267	TYR
6	BH	3270	ILE
6	BH	3277	LEU
6	BH	3287	GLU
6	BH	3291	ASN
6	BH	3310	ARG
6	BH	3319	SER
6	BH	3324	ASN
6	BH	3338	THR
6	BH	3340	ASP
6	BH	3343	PRO
6	BH	3344	GLU
6	BH	3346	LEU
6	BH	3362	TYR
6	BH	3368	CYS
6	BH	3376	LEU
6	BH	3377	LEU
6	BH	3378	LEU
6	BH	3392	SER
6	BH	3398	MET
6	BH	3453	LEU
6	BH	3462	ILE
6	BH	3479	TYR
6	BH	3487	ASN
6	BH	3516	LEU
7	BQ	3010	ASN
7	BQ	3014	PHE
7	BQ	3027	GLN
7	BQ	3053	LYS

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Mol	Chain	Res	Type
7	BQ	3089	THR
7	BQ	3101	ASN
7	BQ	3112	ASN
7	BQ	3119	SER
7	BQ	3151	THR
7	BQ	3153	LYS
7	BQ	3154	ASN
7	BQ	3170	LYS
7	BQ	3176	ASP
7	BQ	3178	LEU
7	BQ	3181	LEU
7	BQ	3203	ASN
7	BQ	3212	ILE
7	BQ	3213	MET
7	BQ	3226	MET
7	BQ	3230	ARG
7	BQ	3266	LEU
7	BQ	3282	LYS
7	BQ	3283	GLN
7	BQ	3310	LEU
7	BQ	3325	SER
7	BQ	3329	LEU
7	BQ	3332	LEU
7	BQ	3343	ARG
7	BQ	3344	LEU
7	BQ	3351	GLU
7	BQ	3370	VAL
7	BQ	3375	GLN
7	BQ	3378	ILE
7	BQ	3390	THR
7	BQ	3392	ASN
7	BQ	3403	ASP
7	BQ	3411	LEU
7	BQ	3412	MET
7	BQ	3420	LEU
7	BQ	3427	GLU
7	BQ	3430	LEU
7	BQ	3435	THR
7	BQ	3439	GLU
7	BQ	3444	LEU
7	BQ	3458	VAL
7	BQ	3482	HIS

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Mol	Chain	Res	Type
7	BQ	3495	LEU
7	BQ	3513	ARG
7	BQ	3518	TYR
7	BQ	3519	ASP
7	BQ	3520	MET
7	BQ	3546	MET
8	BZ	3005	LEU
8	BZ	3014	ARG
8	BZ	3015	ARG
8	BZ	3030	GLN
8	BZ	3035	THR
8	BZ	3036	ASN
8	BZ	3044	LYS
8	BZ	3046	LEU
8	BZ	3063	LEU
8	BZ	3068	ILE
8	BZ	3083	GLN
8	BZ	3133	LEU
8	BZ	3142	ASN
8	BZ	3145	ASN
8	BZ	3147	ARG
8	BZ	3165	ASP
8	BZ	3168	GLU
8	BZ	3175	THR
8	BZ	3193	MET
8	BZ	3195	GLU
8	BZ	3196	ILE
8	BZ	3216	ASP
8	BZ	3227	ARG
8	BZ	3239	SER
8	BZ	3240	LEU
8	BZ	3253	TYR
8	BZ	3260	ASP
8	BZ	3271	ASP
8	BZ	3280	LEU
8	BZ	3287	MET
8	BZ	3288	ASP
8	BZ	3296	ILE
8	BZ	3304	MET
8	BZ	3318	ARG
8	BZ	3322	ARG
8	BZ	3325	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	BZ	3338	ASN
8	BZ	3342	ASP
8	BZ	3355	TYR
8	BZ	3364	PHE
8	BZ	3397	ASP
8	BZ	3430	ASN
8	BZ	3442	THR
8	BZ	3445	GLU
8	BZ	3453	VAL
8	BZ	3454	ILE
8	BZ	3478	ASP
8	BZ	3479	ASP
8	BZ	3531	ASP
8	BZ	3535	ARG
1	Ba	4012	THR
1	Ba	4013	LEU
1	Ba	4020	ILE
1	Ba	4043	SER
1	Ba	4050	ASP
1	Ba	4051	LYS
1	Ba	4056	ASP
1	Ba	4061	THR
1	Ba	4062	VAL
1	Ba	4116	VAL
1	Ba	4130	ARG
1	Ba	4135	GLU
1	Ba	4137	ILE
1	Ba	4142	GLU
1	Ba	4156	LEU
1	Ba	4178	ASN
1	Ba	4184	LEU
1	Ba	4190	GLN
1	Ba	4204	ASN
1	Ba	4205	VAL
1	Ba	4209	HIS
1	Ba	4214	THR
1	Ba	4217	LEU
1	Ba	4237	ILE
1	Ba	4241	ASN
1	Ba	4249	LEU
1	Ba	4251	LEU
1	Ba	4266	ASP

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Mol	Chain	Res	Type
1	Ba	4282	LEU
1	Ba	4284	ARG
1	Ba	4299	THR
1	Ba	4326	LEU
1	Ba	4339	SER
1	Ba	4345	GLU
1	Ba	4348	GLU
1	Ba	4350	PHE
1	Ba	4355	LEU
1	Ba	4358	CYS
1	Ba	4360	GLU
1	Ba	4377	THR
1	Ba	4380	HIS
1	Ba	4381	SER
1	Ba	4400	ARG
1	Ba	4404	ASP
1	Ba	4407	SER
1	Ba	4417	ASN
1	Ba	4455	LEU
1	Ba	4469	ASP
1	Ba	4478	ARG
1	Ba	4486	MET
1	Ba	4493	LYS
1	Ba	4495	ARG
1	Ba	4498	ARG
1	Ba	4505	ILE
1	Ba	4528	LEU
1	Ba	4539	LEU
1	Ba	4542	ASP
2	Bb	4004	GLN
2	Bb	4008	ASP
2	Bb	4013	GLU
2	Bb	4019	ARG
2	Bb	4035	SER
2	Bb	4037	LEU
2	Bb	4046	LEU
2	Bb	4050	SER
2	Bb	4052	ASN
2	Bb	4076	VAL
2	Bb	4077	LEU
2	Bb	4094	SER
2	Bb	4099	SER

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Mol	Chain	Res	Type
2	Bb	4114	LYS
2	Bb	4128	SER
2	Bb	4132	LEU
2	Bb	4133	ASP
2	Bb	4135	LEU
2	Bb	4136	THR
2	Bb	4141	ASP
2	Bb	4146	LYS
2	Bb	4151	GLU
2	Bb	4184	LEU
2	Bb	4187	SER
2	Bb	4189	ASN
2	Bb	4195	ILE
2	Bb	4210	GLU
2	Bb	4217	LYS
2	Bb	4218	PHE
2	Bb	4222	GLN
2	Bb	4233	ILE
2	Bb	4235	ASN
2	Bb	4237	THR
2	Bb	4239	ASP
2	Bb	4242	LYS
2	Bb	4273	ILE
2	Bb	4282	ASN
2	Bb	4283	THR
2	Bb	4288	GLN
2	Bb	4289	LEU
2	Bb	4291	TYR
2	Bb	4320	VAL
2	Bb	4327	SER
2	Bb	4328	THR
2	Bb	4331	GLU
2	Bb	4333	SER
2	Bb	4337	LEU
2	Bb	4351	GLN
2	Bb	4363	GLU
2	Bb	4377	LEU
2	Bb	4381	GLU
2	Bb	4390	VAL
2	Bb	4394	THR
2	Bb	4399	ARG
2	Bb	4400	THR

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Mol	Chain	Res	Type
2	Bb	4401	VAL
2	Bb	4413	LYS
2	Bb	4417	THR
2	Bb	4426	LYS
2	Bb	4455	LEU
2	Bb	4460	ARG
2	Bb	4462	SER
2	Bb	4473	ASP
2	Bb	4489	GLU
2	Bb	4495	ARG
2	Bb	4500	SER
2	Bb	4512	ASP
2	Bb	4513	ASN
3	Bd	4010	THR
3	Bd	4012	LYS
3	Bd	4022	LYS
3	Bd	4036	ARG
3	Bd	4037	THR
3	Bd	4051	SER
3	Bd	4052	ARG
3	Bd	4063	THR
3	Bd	4130	ARG
3	Bd	4141	LYS
3	Bd	4157	SER
3	Bd	4158	LEU
3	Bd	4166	TYR
3	Bd	4170	LEU
3	Bd	4181	ILE
3	Bd	4183	ASP
3	Bd	4185	ASN
3	Bd	4199	LYS
3	Bd	4209	MET
3	Bd	4215	LEU
3	Bd	4216	THR
3	Bd	4218	THR
3	Bd	4220	ILE
3	Bd	4230	GLU
3	Bd	4237	ILE
3	Bd	4249	GLU
3	Bd	4251	ASN
3	Bd	4260	MET
3	Bd	4263	ILE

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Mol	Chain	Res	Type
3	Bd	4279	LYS
3	Bd	4292	ILE
3	Bd	4293	LEU
3	Bd	4306	SER
3	Bd	4308	LEU
3	Bd	4338	LEU
3	Bd	4351	GLU
3	Bd	4374	THR
3	Bd	4383	ASN
3	Bd	4384	ASN
3	Bd	4385	MET
3	Bd	4407	GLU
3	Bd	4410	LEU
3	Bd	4433	GLU
3	Bd	4440	TRP
3	Bd	4460	LEU
3	Bd	4463	ILE
3	Bd	4470	ARG
3	Bd	4473	HIS
3	Bd	4477	GLU
3	Bd	4478	LEU
3	Bd	4482	ILE
3	Bd	4486	ARG
3	Bd	4505	THR
3	Bd	4522	ASP
3	Bd	4528	ARG
4	Be	4042	HIS
4	Be	4044	LEU
4	Be	4068	ARG
4	Be	4082	THR
4	Be	4107	LEU
4	Be	4113	ASP
4	Be	4134	LEU
4	Be	4138	GLN
4	Be	4151	ASP
4	Be	4206	GLU
4	Be	4211	VAL
4	Be	4212	MET
4	Be	4214	LYS
4	Be	4222	ASP
4	Be	4227	GLN
4	Be	4229	ARG

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Mol	Chain	Res	Type
4	Be	4230	VAL
4	Be	4243	VAL
4	Be	4245	LEU
4	Be	4247	LYS
4	Be	4249	PHE
4	Be	4257	CYS
4	Be	4259	LEU
4	Be	4272	LEU
4	Be	4273	THR
4	Be	4285	HIS
4	Be	4301	TYR
4	Be	4327	PHE
4	Be	4328	ASP
4	Be	4335	LEU
4	Be	4362	ILE
4	Be	4369	LEU
4	Be	4397	GLN
4	Be	4404	VAL
4	Be	4413	LYS
4	Be	4414	MET
4	Be	4415	ILE
4	Be	4427	LEU
4	Be	4431	ARG
4	Be	4435	LYS
4	Be	4450	MET
4	Be	4464	ILE
4	Be	4494	THR
4	Be	4513	ASP
4	Be	4520	ASN
4	Be	4521	ASP
4	Be	4526	PHE
4	Be	4543	GLN
4	Be	4545	CYS
4	Be	4555	ILE
5	Bg	4055	LEU
5	Bg	4057	LEU
5	Bg	4058	THR
5	Bg	4059	ASN
5	Bg	4089	VAL
5	Bg	4095	THR
5	Bg	4111	LEU
5	Bg	4115	ASN

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Mol	Chain	Res	Type
5	Bg	4125	LEU
5	Bg	4130	THR
5	Bg	4131	ASP
5	Bg	4156	GLN
5	Bg	4162	LYS
5	Bg	4167	TRP
5	Bg	4171	MET
5	Bg	4183	ARG
5	Bg	4184	LYS
5	Bg	4196	PHE
5	Bg	4200	ILE
5	Bg	4215	LEU
5	Bg	4221	LYS
5	Bg	4227	LYS
5	Bg	4237	HIS
5	Bg	4246	LEU
5	Bg	4260	ASN
5	Bg	4264	GLU
5	Bg	4265	LYS
5	Bg	4267	GLU
5	Bg	4272	ILE
5	Bg	4273	LEU
5	Bg	4277	GLU
5	Bg	4282	LEU
5	Bg	4286	GLN
5	Bg	4288	LEU
5	Bg	4291	ARG
5	Bg	4293	THR
5	Bg	4310	LEU
5	Bg	4311	LYS
5	Bg	4316	VAL
5	Bg	4336	ILE
5	Bg	4340	VAL
5	Bg	4342	ASP
5	Bg	4345	GLU
5	Bg	4358	GLU
5	Bg	4375	LYS
5	Bg	4382	ARG
5	Bg	4459	ASN
5	Bg	4465	ILE
5	Bg	4475	HIS
5	Bg	4479	ASN

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Mol	Chain	Res	Type
5	Bg	4480	PHE
5	Bg	4516	SER
5	Bg	4518	CYS
5	Bg	4528	SER
6	Bh	4011	VAL
6	Bh	4013	LEU
6	Bh	4043	THR
6	Bh	4050	ASP
6	Bh	4061	THR
6	Bh	4091	ASP
6	Bh	4102	THR
6	Bh	4104	LEU
6	Bh	4147	ILE
6	Bh	4148	THR
6	Bh	4151	LYS
6	Bh	4173	ASN
6	Bh	4182	CYS
6	Bh	4189	LEU
6	Bh	4201	ILE
6	Bh	4202	LYS
6	Bh	4209	MET
6	Bh	4220	PHE
6	Bh	4221	LYS
6	Bh	4231	GLN
6	Bh	4242	LEU
6	Bh	4248	LEU
6	Bh	4249	GLU
6	Bh	4250	LEU
6	Bh	4251	LYS
6	Bh	4260	ARG
6	Bh	4267	TYR
6	Bh	4270	ILE
6	Bh	4277	LEU
6	Bh	4287	GLU
6	Bh	4291	ASN
6	Bh	4310	ARG
6	Bh	4319	SER
6	Bh	4324	ASN
6	Bh	4338	THR
6	Bh	4340	ASP
6	Bh	4343	PRO
6	Bh	4344	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Bh	4346	LEU
6	Bh	4362	TYR
6	Bh	4368	CYS
6	Bh	4376	LEU
6	Bh	4377	LEU
6	Bh	4378	LEU
6	Bh	4392	SER
6	Bh	4398	MET
6	Bh	4453	LEU
6	Bh	4462	ILE
6	Bh	4479	TYR
6	Bh	4487	ASN
6	Bh	4516	LEU
7	Bq	4010	ASN
7	Bq	4014	PHE
7	Bq	4027	GLN
7	Bq	4053	LYS
7	Bq	4089	THR
7	Bq	4101	ASN
7	Bq	4112	ASN
7	Bq	4119	SER
7	Bq	4151	THR
7	Bq	4153	LYS
7	Bq	4154	ASN
7	Bq	4170	LYS
7	Bq	4176	ASP
7	Bq	4178	LEU
7	Bq	4181	LEU
7	Bq	4203	ASN
7	Bq	4212	ILE
7	Bq	4213	MET
7	Bq	4226	MET
7	Bq	4230	ARG
7	Bq	4266	LEU
7	Bq	4282	LYS
7	Bq	4283	GLN
7	Bq	4310	LEU
7	Bq	4325	SER
7	Bq	4329	LEU
7	Bq	4332	LEU
7	Bq	4343	ARG
7	Bq	4344	LEU

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Mol	Chain	Res	Type
7	Bq	4351	GLU
7	Bq	4370	VAL
7	Bq	4375	GLN
7	Bq	4378	ILE
7	Bq	4390	THR
7	Bq	4392	ASN
7	Bq	4403	ASP
7	Bq	4411	LEU
7	Bq	4412	MET
7	Bq	4420	LEU
7	Bq	4427	GLU
7	Bq	4430	LEU
7	Bq	4435	THR
7	Bq	4439	GLU
7	Bq	4444	LEU
7	Bq	4458	VAL
7	Bq	4482	HIS
7	Bq	4495	LEU
7	Bq	4513	ARG
7	Bq	4518	TYR
7	Bq	4519	ASP
7	Bq	4520	MET
7	Bq	4546	MET
8	Bz	4005	LEU
8	Bz	4014	ARG
8	Bz	4015	ARG
8	Bz	4030	GLN
8	Bz	4035	THR
8	Bz	4036	ASN
8	Bz	4044	LYS
8	Bz	4046	LEU
8	Bz	4063	LEU
8	Bz	4068	ILE
8	Bz	4083	GLN
8	Bz	4133	LEU
8	Bz	4142	ASN
8	Bz	4145	ASN
8	Bz	4147	ARG
8	Bz	4165	ASP
8	Bz	4168	GLU
8	Bz	4175	THR
8	Bz	4193	MET

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Mol	Chain	Res	Type
8	Bz	4195	GLU
8	Bz	4196	ILE
8	Bz	4216	ASP
8	Bz	4227	ARG
8	Bz	4239	SER
8	Bz	4240	LEU
8	Bz	4253	TYR
8	Bz	4260	ASP
8	Bz	4271	ASP
8	Bz	4280	LEU
8	Bz	4288	ASP
8	Bz	4296	ILE
8	Bz	4304	MET
8	Bz	4318	ARG
8	Bz	4322	ARG
8	Bz	4325	MET
8	Bz	4338	ASN
8	Bz	4342	ASP
8	Bz	4355	TYR
8	Bz	4364	PHE
8	Bz	4397	ASP
8	Bz	4430	ASN
8	Bz	4442	THR
8	Bz	4445	GLU
8	Bz	4453	VAL
8	Bz	4454	ILE
8	Bz	4478	ASP
8	Bz	4479	ASP
8	Bz	4531	ASP
8	Bz	4535	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (464) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	113	ASN
1	AA	190	GLN
1	AA	204	ASN
1	AA	209	HIS
1	AA	225	ASN
1	AA	231	GLN
1	AA	261	GLN
1	AA	294	GLN

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Mol	Chain	Res	Type
1	AA	363	GLN
1	AA	380	HIS
1	AA	430	ASN
1	AA	445	GLN
2	AB	9	GLN
2	AB	47	GLN
2	AB	142	ASN
2	AB	192	HIS
2	AB	220	ASN
2	AB	271	ASN
2	AB	282	ASN
2	AB	296	GLN
2	AB	351	GLN
2	AB	385	HIS
2	AB	420	GLN
2	AB	447	ASN
2	AB	465	ASN
2	AB	476	ASN
2	AB	484	GLN
2	AB	513	ASN
3	AD	24	ASN
3	AD	112	ASN
3	AD	149	GLN
3	AD	188	ASN
3	AD	240	GLN
3	AD	251	ASN
3	AD	289	GLN
3	AD	303	HIS
3	AD	383	ASN
3	AD	499	GLN
4	AE	35	GLN
4	AE	37	ASN
4	AE	85	ASN
4	AE	138	GLN
4	AE	227	GLN
4	AE	251	HIS
4	AE	324	GLN
4	AE	333	HIS
4	AE	349	GLN
4	AE	424	HIS
4	AE	486	ASN
4	AE	509	ASN

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Mol	Chain	Res	Type
4	AE	536	GLN
4	AE	543	GLN
5	AG	72	HIS
5	AG	115	ASN
5	AG	166	HIS
5	AG	260	ASN
5	AG	279	GLN
5	AG	306	GLN
5	AG	307	HIS
5	AG	326	ASN
5	AG	370	ASN
5	AG	395	ASN
5	AG	405	ASN
5	AG	438	GLN
5	AG	458	GLN
5	AG	459	ASN
5	AG	479	ASN
6	AH	25	GLN
6	AH	31	ASN
6	AH	57	ASN
6	AH	173	ASN
6	AH	174	ASN
6	AH	216	ASN
6	AH	231	GLN
6	AH	245	ASN
6	AH	305	GLN
6	AH	311	ASN
6	AH	324	ASN
6	AH	356	GLN
6	AH	363	ASN
6	AH	366	GLN
6	AH	436	GLN
6	AH	487	ASN
6	AH	491	ASN
6	AH	505	ASN
6	AH	515	ASN
7	AQ	10	ASN
7	AQ	27	GLN
7	AQ	39	HIS
7	AQ	40	GLN
7	AQ	57	ASN
7	AQ	101	ASN

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Mol	Chain	Res	Type
7	AQ	112	ASN
7	AQ	132	ASN
7	AQ	154	ASN
7	AQ	203	ASN
7	AQ	258	ASN
7	AQ	269	ASN
7	AQ	311	HIS
7	AQ	392	ASN
7	AQ	446	GLN
7	AQ	482	HIS
7	AQ	543	GLN
8	AZ	7	ASN
8	AZ	22	ASN
8	AZ	36	ASN
8	AZ	185	GLN
8	AZ	258	GLN
8	AZ	282	ASN
8	AZ	313	ASN
8	AZ	324	ASN
8	AZ	329	GLN
8	AZ	337	GLN
8	AZ	346	GLN
8	AZ	356	GLN
8	AZ	370	ASN
8	AZ	430	ASN
1	Aa	1113	ASN
1	Aa	1190	GLN
1	Aa	1204	ASN
1	Aa	1209	HIS
1	Aa	1225	ASN
1	Aa	1231	GLN
1	Aa	1261	GLN
1	Aa	1294	GLN
1	Aa	1363	GLN
1	Aa	1380	HIS
1	Aa	1430	ASN
1	Aa	1445	GLN
2	Ab	1009	GLN
2	Ab	1047	GLN
2	Ab	1142	ASN
2	Ab	1192	HIS
2	Ab	1220	ASN

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Mol	Chain	Res	Type
2	Ab	1271	ASN
2	Ab	1282	ASN
2	Ab	1296	GLN
2	Ab	1351	GLN
2	Ab	1385	HIS
2	Ab	1420	GLN
2	Ab	1447	ASN
2	Ab	1476	ASN
2	Ab	1513	ASN
3	Ad	1024	ASN
3	Ad	1112	ASN
3	Ad	1149	GLN
3	Ad	1240	GLN
3	Ad	1251	ASN
3	Ad	1289	GLN
3	Ad	1303	HIS
3	Ad	1383	ASN
3	Ad	1499	GLN
4	Ae	1035	GLN
4	Ae	1085	ASN
4	Ae	1138	GLN
4	Ae	1227	GLN
4	Ae	1251	HIS
4	Ae	1324	GLN
4	Ae	1333	HIS
4	Ae	1349	GLN
4	Ae	1424	HIS
4	Ae	1486	ASN
4	Ae	1509	ASN
4	Ae	1536	GLN
4	Ae	1543	GLN
5	Ag	1072	HIS
5	Ag	1115	ASN
5	Ag	1166	HIS
5	Ag	1260	ASN
5	Ag	1279	GLN
5	Ag	1306	GLN
5	Ag	1307	HIS
5	Ag	1326	ASN
5	Ag	1370	ASN
5	Ag	1395	ASN
5	Ag	1405	ASN

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Mol	Chain	Res	Type
5	Ag	1438	GLN
5	Ag	1458	GLN
5	Ag	1479	ASN
5	Ag	1507	GLN
6	Ah	1025	GLN
6	Ah	1031	ASN
6	Ah	1057	ASN
6	Ah	1173	ASN
6	Ah	1174	ASN
6	Ah	1216	ASN
6	Ah	1231	GLN
6	Ah	1245	ASN
6	Ah	1305	GLN
6	Ah	1311	ASN
6	Ah	1324	ASN
6	Ah	1356	GLN
6	Ah	1363	ASN
6	Ah	1366	GLN
6	Ah	1436	GLN
6	Ah	1487	ASN
6	Ah	1491	ASN
6	Ah	1505	ASN
6	Ah	1515	ASN
7	Aq	1010	ASN
7	Aq	1027	GLN
7	Aq	1039	HIS
7	Aq	1040	GLN
7	Aq	1057	ASN
7	Aq	1079	HIS
7	Aq	1101	ASN
7	Aq	1112	ASN
7	Aq	1132	ASN
7	Aq	1154	ASN
7	Aq	1203	ASN
7	Aq	1258	ASN
7	Aq	1269	ASN
7	Aq	1311	HIS
7	Aq	1392	ASN
7	Aq	1446	GLN
7	Aq	1482	HIS
7	Aq	1543	GLN
8	Az	1007	ASN

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Mol	Chain	Res	Type
8	Az	1022	ASN
8	Az	1036	ASN
8	Az	1185	GLN
8	Az	1258	GLN
8	Az	1282	ASN
8	Az	1313	ASN
8	Az	1324	ASN
8	Az	1329	GLN
8	Az	1337	GLN
8	Az	1346	GLN
8	Az	1356	GLN
8	Az	1370	ASN
8	Az	1430	ASN
1	BA	3113	ASN
1	BA	3190	GLN
1	BA	3204	ASN
1	BA	3209	HIS
1	BA	3225	ASN
1	BA	3231	GLN
1	BA	3261	GLN
1	BA	3294	GLN
1	BA	3363	GLN
1	BA	3380	HIS
1	BA	3430	ASN
1	BA	3445	GLN
2	BB	3009	GLN
2	BB	3047	GLN
2	BB	3142	ASN
2	BB	3192	HIS
2	BB	3220	ASN
2	BB	3271	ASN
2	BB	3282	ASN
2	BB	3296	GLN
2	BB	3351	GLN
2	BB	3385	HIS
2	BB	3420	GLN
2	BB	3447	ASN
2	BB	3465	ASN
2	BB	3476	ASN
2	BB	3513	ASN
3	BD	3024	ASN
3	BD	3112	ASN

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Mol	Chain	Res	Type
3	BD	3149	GLN
3	BD	3165	GLN
3	BD	3188	ASN
3	BD	3240	GLN
3	BD	3251	ASN
3	BD	3289	GLN
3	BD	3303	HIS
3	BD	3383	ASN
3	BD	3499	GLN
4	BE	3035	GLN
4	BE	3041	GLN
4	BE	3085	ASN
4	BE	3138	GLN
4	BE	3227	GLN
4	BE	3251	HIS
4	BE	3324	GLN
4	BE	3333	HIS
4	BE	3349	GLN
4	BE	3424	HIS
4	BE	3486	ASN
4	BE	3509	ASN
4	BE	3536	GLN
4	BE	3543	GLN
5	BG	3059	ASN
5	BG	3072	HIS
5	BG	3115	ASN
5	BG	3166	HIS
5	BG	3260	ASN
5	BG	3279	GLN
5	BG	3306	GLN
5	BG	3307	HIS
5	BG	3326	ASN
5	BG	3370	ASN
5	BG	3395	ASN
5	BG	3405	ASN
5	BG	3438	GLN
5	BG	3458	GLN
5	BG	3459	ASN
5	BG	3479	ASN
6	BH	3025	GLN
6	BH	3031	ASN
6	BH	3057	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	BH	3173	ASN
6	BH	3174	ASN
6	BH	3216	ASN
6	BH	3231	GLN
6	BH	3245	ASN
6	BH	3305	GLN
6	BH	3311	ASN
6	BH	3324	ASN
6	BH	3356	GLN
6	BH	3363	ASN
6	BH	3366	GLN
6	BH	3436	GLN
6	BH	3487	ASN
6	BH	3491	ASN
6	BH	3505	ASN
6	BH	3515	ASN
7	BQ	3010	ASN
7	BQ	3027	GLN
7	BQ	3039	HIS
7	BQ	3040	GLN
7	BQ	3057	ASN
7	BQ	3079	HIS
7	BQ	3101	ASN
7	BQ	3112	ASN
7	BQ	3132	ASN
7	BQ	3154	ASN
7	BQ	3203	ASN
7	BQ	3258	ASN
7	BQ	3269	ASN
7	BQ	3311	HIS
7	BQ	3392	ASN
7	BQ	3446	GLN
7	BQ	3482	HIS
7	BQ	3543	GLN
8	BZ	3007	ASN
8	BZ	3022	ASN
8	BZ	3036	ASN
8	BZ	3185	GLN
8	BZ	3258	GLN
8	BZ	3282	ASN
8	BZ	3313	ASN
8	BZ	3329	GLN

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Mol	Chain	Res	Type
8	BZ	3337	GLN
8	BZ	3346	GLN
8	BZ	3356	GLN
8	BZ	3370	ASN
8	BZ	3430	ASN
1	Ba	4113	ASN
1	Ba	4190	GLN
1	Ba	4204	ASN
1	Ba	4209	HIS
1	Ba	4225	ASN
1	Ba	4231	GLN
1	Ba	4261	GLN
1	Ba	4294	GLN
1	Ba	4363	GLN
1	Ba	4380	HIS
1	Ba	4430	ASN
1	Ba	4445	GLN
2	Bb	4009	GLN
2	Bb	4047	GLN
2	Bb	4142	ASN
2	Bb	4192	HIS
2	Bb	4220	ASN
2	Bb	4271	ASN
2	Bb	4282	ASN
2	Bb	4296	GLN
2	Bb	4351	GLN
2	Bb	4385	HIS
2	Bb	4420	GLN
2	Bb	4447	ASN
2	Bb	4476	ASN
2	Bb	4513	ASN
3	Bd	4024	ASN
3	Bd	4112	ASN
3	Bd	4149	GLN
3	Bd	4188	ASN
3	Bd	4240	GLN
3	Bd	4251	ASN
3	Bd	4289	GLN
3	Bd	4303	HIS
3	Bd	4383	ASN
3	Bd	4499	GLN
4	Be	4035	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	Be	4085	ASN
4	Be	4138	GLN
4	Be	4227	GLN
4	Be	4251	HIS
4	Be	4324	GLN
4	Be	4333	HIS
4	Be	4349	GLN
4	Be	4424	HIS
4	Be	4486	ASN
4	Be	4509	ASN
4	Be	4536	GLN
4	Be	4543	GLN
5	Bg	4059	ASN
5	Bg	4072	HIS
5	Bg	4115	ASN
5	Bg	4166	HIS
5	Bg	4260	ASN
5	Bg	4279	GLN
5	Bg	4306	GLN
5	Bg	4307	HIS
5	Bg	4326	ASN
5	Bg	4370	ASN
5	Bg	4395	ASN
5	Bg	4405	ASN
5	Bg	4438	GLN
5	Bg	4458	GLN
5	Bg	4479	ASN
5	Bg	4507	GLN
6	Bh	4025	GLN
6	Bh	4031	ASN
6	Bh	4057	ASN
6	Bh	4173	ASN
6	Bh	4174	ASN
6	Bh	4216	ASN
6	Bh	4231	GLN
6	Bh	4245	ASN
6	Bh	4305	GLN
6	Bh	4311	ASN
6	Bh	4324	ASN
6	Bh	4356	GLN
6	Bh	4363	ASN
6	Bh	4366	GLN

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Mol	Chain	Res	Type
6	Bh	4436	GLN
6	Bh	4487	ASN
6	Bh	4491	ASN
6	Bh	4505	ASN
6	Bh	4515	ASN
7	Bq	4010	ASN
7	Bq	4027	GLN
7	Bq	4039	HIS
7	Bq	4040	GLN
7	Bq	4057	ASN
7	Bq	4101	ASN
7	Bq	4112	ASN
7	Bq	4132	ASN
7	Bq	4154	ASN
7	Bq	4203	ASN
7	Bq	4258	ASN
7	Bq	4269	ASN
7	Bq	4311	HIS
7	Bq	4373	GLN
7	Bq	4392	ASN
7	Bq	4446	GLN
7	Bq	4482	HIS
7	Bq	4543	GLN
8	Bz	4007	ASN
8	Bz	4022	ASN
8	Bz	4036	ASN
8	Bz	4185	GLN
8	Bz	4258	GLN
8	Bz	4282	ASN
8	Bz	4313	ASN
8	Bz	4329	GLN
8	Bz	4337	GLN
8	Bz	4346	GLN
8	Bz	4356	GLN
8	Bz	4370	ASN
8	Bz	4430	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
9	ADP	AA	601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.41	4 (14%)
10	BEF	AA	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AB	601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.28	4 (14%)
10	BEF	AB	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AD	601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.71	5 (18%)
10	BEF	AD	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AE	601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.39	4 (14%)
10	BEF	AE	602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AG	1001	11,10	22,29,29	2.28	5 (22%)	27,45,45	3.22	3 (11%)
10	BEF	AG	1002	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AH	601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.36	4 (14%)
10	BEF	AH	602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AQ	601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.56	5 (18%)
10	BEF	AQ	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AZ	601	11,10	22,29,29	2.25	5 (22%)	27,45,45	3.46	5 (18%)
10	BEF	AZ	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Aa	1601	11,10	22,29,29	2.28	5 (22%)	27,45,45	3.41	4 (14%)
10	BEF	Aa	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ab	1601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.28	4 (14%)
10	BEF	Ab	1602	9	0,3,3	0.00	-	0,3,3	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ADP	Ad	1601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.72	6 (22%)
10	BEF	Ad	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ae	1601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.39	4 (14%)
10	BEF	Ae	1602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ag	2001	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.21	3 (11%)
10	BEF	Ag	2002	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ah	1601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.35	4 (14%)
10	BEF	Ah	1602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Aq	1601	11,10	22,29,29	2.23	5 (22%)	27,45,45	3.55	5 (18%)
10	BEF	Aq	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Az	1601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.47	5 (18%)
10	BEF	Az	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BA	3601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.42	4 (14%)
10	BEF	BA	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BB	3601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.29	4 (14%)
10	BEF	BB	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BD	3601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.72	5 (18%)
10	BEF	BD	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BE	3601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.39	4 (14%)
10	BEF	BE	3602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BG	4001	11,10	22,29,29	2.28	5 (22%)	27,45,45	3.22	3 (11%)
10	BEF	BG	4002	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BH	3601	11,10	22,29,29	2.25	5 (22%)	27,45,45	3.35	4 (14%)
10	BEF	BH	3602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BQ	3601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.56	5 (18%)
10	BEF	BQ	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BZ	3601	11,10	22,29,29	2.25	5 (22%)	27,45,45	3.47	5 (18%)
10	BEF	BZ	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ba	4601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.40	4 (14%)
10	BEF	Ba	4602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bb	4601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.29	4 (14%)
10	BEF	Bb	4602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bd	4601	11,10	22,29,29	2.25	5 (22%)	27,45,45	3.71	5 (18%)
10	BEF	Bd	4602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Be	4601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.40	4 (14%)
10	BEF	Be	4602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bg	5001	11,10	22,29,29	2.28	5 (22%)	27,45,45	3.23	3 (11%)
10	BEF	Bg	5002	9	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ADP	Bh	4601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.36	4 (14%)
10	BEF	Bh	4602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bq	4601	11,10	22,29,29	2.22	5 (22%)	27,45,45	3.49	3 (11%)
10	BEF	Bq	4602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bz	4601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.46	5 (18%)
10	BEF	Bz	4602	9	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	AA	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AA	602	9	-	0/0/0/0	0/0/0/0
9	ADP	AB	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AB	602	9	-	0/0/0/0	0/0/0/0
9	ADP	AD	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AD	602	9	-	0/0/0/0	0/0/0/0
9	ADP	AE	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AE	602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	AG	1001	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AG	1002	9	-	0/0/0/0	0/0/0/0
9	ADP	AH	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AH	602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	AQ	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AQ	602	9	-	0/0/0/0	0/0/0/0
9	ADP	AZ	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AZ	602	9	-	0/0/0/0	0/0/0/0
9	ADP	Aa	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Aa	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	Ab	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ab	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	Ad	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ad	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	Ae	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ae	1602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	Ag	2001	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ag	2002	9	-	0/0/0/0	0/0/0/0
9	ADP	Ah	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ah	1602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	Aq	1601	11,10	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BEF	Aq	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	Az	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Az	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	BA	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BA	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	BB	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BB	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	BD	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BD	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	BE	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BE	3602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	BG	4001	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BG	4002	9	-	0/0/0/0	0/0/0/0
9	ADP	BH	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BH	3602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	BQ	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BQ	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	BZ	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BZ	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	Ba	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ba	4602	9	-	0/0/0/0	0/0/0/0
9	ADP	Bb	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bb	4602	9	-	0/0/0/0	0/0/0/0
9	ADP	Bd	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bd	4602	9	-	0/0/0/0	0/0/0/0
9	ADP	Be	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Be	4602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	Bg	5001	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bg	5002	9	-	0/0/0/0	0/0/0/0
9	ADP	Bh	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bh	4602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	Bq	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bq	4602	9	-	0/0/0/0	0/0/0/0
9	ADP	Bz	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bz	4602	9	-	0/0/0/0	0/0/0/0

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AQ	601	ADP	C5-C4	-2.95	1.33	1.40
9	Aq	1601	ADP	C5-C4	-2.94	1.33	1.40
9	Be	4601	ADP	C5-C4	-2.94	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Ae	1601	ADP	C5-C4	-2.92	1.33	1.40
9	AE	601	ADP	C5-C4	-2.92	1.33	1.40
9	Bq	4601	ADP	C5-C4	-2.92	1.33	1.40
9	BQ	3601	ADP	C5-C4	-2.91	1.33	1.40
9	BE	3601	ADP	C5-C4	-2.90	1.33	1.40
9	AD	601	ADP	C5-C4	-2.89	1.34	1.40
9	BH	3601	ADP	C5-C4	-2.88	1.34	1.40
9	Bd	4601	ADP	C5-C4	-2.88	1.34	1.40
9	BD	3601	ADP	C5-C4	-2.88	1.34	1.40
9	Ad	1601	ADP	C5-C4	-2.88	1.34	1.40
9	AH	601	ADP	C5-C4	-2.85	1.34	1.40
9	Aa	1601	ADP	C5-C4	-2.85	1.34	1.40
9	AG	1001	ADP	C5-C4	-2.85	1.34	1.40
9	Bg	5001	ADP	C5-C4	-2.85	1.34	1.40
9	Ba	4601	ADP	C5-C4	-2.85	1.34	1.40
9	BZ	3601	ADP	C5-C4	-2.85	1.34	1.40
9	Ah	1601	ADP	C5-C4	-2.84	1.34	1.40
9	Ag	2001	ADP	C5-C4	-2.84	1.34	1.40
9	Bz	4601	ADP	C5-C4	-2.84	1.34	1.40
9	AZ	601	ADP	C5-C4	-2.83	1.34	1.40
9	AA	601	ADP	C5-C4	-2.83	1.34	1.40
9	BG	4001	ADP	C5-C4	-2.83	1.34	1.40
9	Bh	4601	ADP	C5-C4	-2.82	1.34	1.40
9	Az	1601	ADP	C5-C4	-2.81	1.34	1.40
9	BA	3601	ADP	C5-C4	-2.81	1.34	1.40
9	Ab	1601	ADP	C5-C4	-2.78	1.34	1.40
9	BB	3601	ADP	C5-C4	-2.77	1.34	1.40
9	AB	601	ADP	C5-C4	-2.76	1.34	1.40
9	Bb	4601	ADP	C5-C4	-2.75	1.34	1.40
9	Bq	4601	ADP	O4'-C1'	2.06	1.43	1.41
9	Aq	1601	ADP	O4'-C1'	2.08	1.43	1.41
9	AQ	601	ADP	O4'-C1'	2.08	1.43	1.41
9	BQ	3601	ADP	O4'-C1'	2.10	1.43	1.41
9	AZ	601	ADP	O4'-C1'	2.13	1.43	1.41
9	Az	1601	ADP	O4'-C1'	2.14	1.43	1.41
9	Bz	4601	ADP	O4'-C1'	2.15	1.43	1.41
9	BZ	3601	ADP	O4'-C1'	2.17	1.43	1.41
9	Bd	4601	ADP	O4'-C1'	2.18	1.44	1.41
9	BD	3601	ADP	O4'-C1'	2.19	1.44	1.41
9	Ad	1601	ADP	O4'-C1'	2.19	1.44	1.41
9	AD	601	ADP	O4'-C1'	2.22	1.44	1.41
9	BB	3601	ADP	O4'-C1'	2.23	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Bb	4601	ADP	O4'-C1'	2.23	1.44	1.41
9	AB	601	ADP	O4'-C1'	2.24	1.44	1.41
9	Ab	1601	ADP	O4'-C1'	2.29	1.44	1.41
9	BH	3601	ADP	O4'-C1'	2.34	1.44	1.41
9	Bg	5001	ADP	O4'-C1'	2.35	1.44	1.41
9	Ah	1601	ADP	O4'-C1'	2.36	1.44	1.41
9	AH	601	ADP	O4'-C1'	2.37	1.44	1.41
9	AG	1001	ADP	O4'-C1'	2.37	1.44	1.41
9	Ag	2001	ADP	O4'-C1'	2.39	1.44	1.41
9	Bh	4601	ADP	O4'-C1'	2.39	1.44	1.41
9	BG	4001	ADP	O4'-C1'	2.40	1.44	1.41
9	BA	3601	ADP	O4'-C1'	2.45	1.44	1.41
9	Ae	1601	ADP	O4'-C1'	2.47	1.44	1.41
9	Ba	4601	ADP	O4'-C1'	2.47	1.44	1.41
9	AA	601	ADP	O4'-C1'	2.47	1.44	1.41
9	Aa	1601	ADP	O4'-C1'	2.48	1.44	1.41
9	Be	4601	ADP	O4'-C1'	2.53	1.44	1.41
9	BE	3601	ADP	O4'-C1'	2.54	1.44	1.41
9	AE	601	ADP	O4'-C1'	2.55	1.44	1.41
9	Ba	4601	ADP	C2-N1	3.28	1.40	1.33
9	AA	601	ADP	C2-N1	3.30	1.40	1.33
9	AB	601	ADP	C2-N1	3.30	1.40	1.33
9	Aa	1601	ADP	C2-N1	3.30	1.40	1.33
9	Ab	1601	ADP	C2-N1	3.31	1.40	1.33
9	BA	3601	ADP	C2-N1	3.32	1.40	1.33
9	BB	3601	ADP	C2-N1	3.32	1.40	1.33
9	BZ	3601	ADP	C2-N1	3.34	1.40	1.33
9	AH	601	ADP	C2-N1	3.34	1.40	1.33
9	Bg	5001	ADP	C2-N1	3.34	1.40	1.33
9	AZ	601	ADP	C2-N1	3.34	1.40	1.33
9	BG	4001	ADP	C2-N1	3.34	1.40	1.33
9	Bb	4601	ADP	C2-N1	3.34	1.40	1.33
9	Ah	1601	ADP	C2-N1	3.35	1.40	1.33
9	Ag	2001	ADP	C2-N1	3.35	1.40	1.33
9	AG	1001	ADP	C2-N1	3.36	1.40	1.33
9	BH	3601	ADP	C2-N1	3.36	1.40	1.33
9	Bz	4601	ADP	C2-N1	3.37	1.40	1.33
9	Bd	4601	ADP	C2-N1	3.37	1.40	1.33
9	Bh	4601	ADP	C2-N1	3.38	1.40	1.33
9	Az	1601	ADP	C2-N1	3.39	1.40	1.33
9	AD	601	ADP	C2-N1	3.39	1.40	1.33
9	BD	3601	ADP	C2-N1	3.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Aq	1601	ADP	C2-N1	3.40	1.40	1.33
9	Bq	4601	ADP	C2-N1	3.40	1.40	1.33
9	Ad	1601	ADP	C2-N1	3.41	1.40	1.33
9	AQ	601	ADP	C2-N1	3.41	1.40	1.33
9	BE	3601	ADP	C2-N1	3.41	1.40	1.33
9	BQ	3601	ADP	C2-N1	3.43	1.40	1.33
9	Ae	1601	ADP	C2-N1	3.43	1.40	1.33
9	Be	4601	ADP	C2-N1	3.44	1.40	1.33
9	AE	601	ADP	C2-N1	3.45	1.40	1.33
9	AE	601	ADP	C2-N3	4.66	1.40	1.32
9	Aq	1601	ADP	C2-N3	4.66	1.40	1.32
9	Bh	4601	ADP	C2-N3	4.68	1.40	1.32
9	Be	4601	ADP	C2-N3	4.68	1.40	1.32
9	Ah	1601	ADP	C2-N3	4.68	1.40	1.32
9	BQ	3601	ADP	C2-N3	4.69	1.40	1.32
9	Bq	4601	ADP	C2-N3	4.69	1.40	1.32
9	Ae	1601	ADP	C2-N3	4.69	1.40	1.32
9	AQ	601	ADP	C2-N3	4.70	1.40	1.32
9	AH	601	ADP	C2-N3	4.70	1.40	1.32
9	BH	3601	ADP	C2-N3	4.70	1.40	1.32
9	BE	3601	ADP	C2-N3	4.70	1.40	1.32
9	Ad	1601	ADP	C2-N3	4.71	1.40	1.32
9	Ab	1601	ADP	C2-N3	4.72	1.40	1.32
9	Bd	4601	ADP	C2-N3	4.73	1.40	1.32
9	Bb	4601	ADP	C2-N3	4.75	1.40	1.32
9	BB	3601	ADP	C2-N3	4.75	1.40	1.32
9	AD	601	ADP	C2-N3	4.75	1.40	1.32
9	AB	601	ADP	C2-N3	4.75	1.40	1.32
9	BZ	3601	ADP	C2-N3	4.75	1.40	1.32
9	AZ	601	ADP	C2-N3	4.77	1.40	1.32
9	BD	3601	ADP	C2-N3	4.77	1.40	1.32
9	AG	1001	ADP	C2-N3	4.78	1.40	1.32
9	Bz	4601	ADP	C2-N3	4.78	1.40	1.32
9	Ba	4601	ADP	C2-N3	4.79	1.40	1.32
9	Ag	2001	ADP	C2-N3	4.79	1.40	1.32
9	Bg	5001	ADP	C2-N3	4.79	1.40	1.32
9	Az	1601	ADP	C2-N3	4.80	1.40	1.32
9	BG	4001	ADP	C2-N3	4.80	1.40	1.32
9	AA	601	ADP	C2-N3	4.82	1.40	1.32
9	BA	3601	ADP	C2-N3	4.83	1.40	1.32
9	Aa	1601	ADP	C2-N3	4.85	1.40	1.32
9	Bh	4601	ADP	C8-N7	6.95	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Aq	1601	ADP	C8-N7	6.96	1.48	1.34
9	AH	601	ADP	C8-N7	6.97	1.48	1.34
9	AQ	601	ADP	C8-N7	6.98	1.48	1.34
9	Bb	4601	ADP	C8-N7	6.98	1.48	1.34
9	Ah	1601	ADP	C8-N7	6.99	1.48	1.34
9	BH	3601	ADP	C8-N7	6.99	1.48	1.34
9	AB	601	ADP	C8-N7	7.00	1.48	1.34
9	BB	3601	ADP	C8-N7	7.01	1.48	1.34
9	Bq	4601	ADP	C8-N7	7.01	1.48	1.34
9	Ab	1601	ADP	C8-N7	7.01	1.48	1.34
9	Ae	1601	ADP	C8-N7	7.01	1.48	1.34
9	AE	601	ADP	C8-N7	7.01	1.48	1.34
9	BQ	3601	ADP	C8-N7	7.02	1.48	1.34
9	BE	3601	ADP	C8-N7	7.03	1.48	1.34
9	Az	1601	ADP	C8-N7	7.04	1.48	1.34
9	BA	3601	ADP	C8-N7	7.04	1.48	1.34
9	AA	601	ADP	C8-N7	7.04	1.48	1.34
9	BZ	3601	ADP	C8-N7	7.05	1.48	1.34
9	Ag	2001	ADP	C8-N7	7.05	1.48	1.34
9	Ba	4601	ADP	C8-N7	7.05	1.48	1.34
9	AZ	601	ADP	C8-N7	7.05	1.48	1.34
9	Be	4601	ADP	C8-N7	7.05	1.48	1.34
9	Aa	1601	ADP	C8-N7	7.06	1.48	1.34
9	Bd	4601	ADP	C8-N7	7.06	1.48	1.34
9	AD	601	ADP	C8-N7	7.06	1.48	1.34
9	Ad	1601	ADP	C8-N7	7.07	1.48	1.34
9	Bz	4601	ADP	C8-N7	7.08	1.48	1.34
9	BD	3601	ADP	C8-N7	7.09	1.48	1.34
9	BG	4001	ADP	C8-N7	7.10	1.48	1.34
9	AG	1001	ADP	C8-N7	7.10	1.48	1.34
9	Bg	5001	ADP	C8-N7	7.10	1.48	1.34

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Be	4601	ADP	N3-C2-N1	-16.31	116.41	128.89
9	BE	3601	ADP	N3-C2-N1	-16.28	116.43	128.89
9	AE	601	ADP	N3-C2-N1	-16.27	116.43	128.89
9	Ae	1601	ADP	N3-C2-N1	-16.26	116.44	128.89
9	Bh	4601	ADP	N3-C2-N1	-16.16	116.52	128.89
9	BA	3601	ADP	N3-C2-N1	-16.14	116.54	128.89
9	AH	601	ADP	N3-C2-N1	-16.13	116.55	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BH	3601	ADP	N3-C2-N1	-16.11	116.56	128.89
9	Ah	1601	ADP	N3-C2-N1	-16.10	116.57	128.89
9	AA	601	ADP	N3-C2-N1	-16.10	116.57	128.89
9	Aa	1601	ADP	N3-C2-N1	-16.08	116.58	128.89
9	Ba	4601	ADP	N3-C2-N1	-16.02	116.63	128.89
9	Ad	1601	ADP	N3-C2-N1	-16.01	116.64	128.89
9	BD	3601	ADP	N3-C2-N1	-16.01	116.64	128.89
9	AD	601	ADP	N3-C2-N1	-15.99	116.65	128.89
9	Bd	4601	ADP	N3-C2-N1	-15.98	116.66	128.89
9	BQ	3601	ADP	N3-C2-N1	-15.97	116.67	128.89
9	Bq	4601	ADP	N3-C2-N1	-15.97	116.67	128.89
9	AQ	601	ADP	N3-C2-N1	-15.92	116.70	128.89
9	Aq	1601	ADP	N3-C2-N1	-15.88	116.73	128.89
9	Az	1601	ADP	N3-C2-N1	-15.68	116.89	128.89
9	BZ	3601	ADP	N3-C2-N1	-15.65	116.91	128.89
9	Bg	5001	ADP	N3-C2-N1	-15.64	116.92	128.89
9	Bb	4601	ADP	N3-C2-N1	-15.62	116.93	128.89
9	AZ	601	ADP	N3-C2-N1	-15.61	116.94	128.89
9	BB	3601	ADP	N3-C2-N1	-15.60	116.95	128.89
9	BG	4001	ADP	N3-C2-N1	-15.60	116.95	128.89
9	Bz	4601	ADP	N3-C2-N1	-15.59	116.95	128.89
9	AG	1001	ADP	N3-C2-N1	-15.59	116.96	128.89
9	Ab	1601	ADP	N3-C2-N1	-15.58	116.97	128.89
9	Ag	2001	ADP	N3-C2-N1	-15.55	116.99	128.89
9	AB	601	ADP	N3-C2-N1	-15.55	116.99	128.89
9	Bd	4601	ADP	C4'-O4'-C1'	-7.68	101.28	109.72
9	BD	3601	ADP	C4'-O4'-C1'	-7.68	101.28	109.72
9	AD	601	ADP	C4'-O4'-C1'	-7.67	101.29	109.72
9	Ad	1601	ADP	C4'-O4'-C1'	-7.66	101.30	109.72
9	Aq	1601	ADP	C4'-O4'-C1'	-7.03	101.99	109.72
9	BQ	3601	ADP	C4'-O4'-C1'	-7.03	101.99	109.72
9	AQ	601	ADP	C4'-O4'-C1'	-7.03	102.00	109.72
9	Bq	4601	ADP	C4'-O4'-C1'	-7.01	102.02	109.72
9	BZ	3601	ADP	C4'-O4'-C1'	-6.68	102.38	109.72
9	Bz	4601	ADP	C4'-O4'-C1'	-6.64	102.42	109.72
9	AZ	601	ADP	C4'-O4'-C1'	-6.63	102.44	109.72
9	Az	1601	ADP	C4'-O4'-C1'	-6.61	102.46	109.72
9	Aa	1601	ADP	PA-O3A-PB	-4.48	117.64	132.67
9	Ba	4601	ADP	PA-O3A-PB	-4.47	117.67	132.67
9	AA	601	ADP	PA-O3A-PB	-4.47	117.68	132.67
9	BA	3601	ADP	PA-O3A-PB	-4.47	117.69	132.67
9	Ad	1601	ADP	PA-O3A-PB	-3.54	120.79	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BD	3601	ADP	PA-O3A-PB	-3.54	120.80	132.67
9	AD	601	ADP	PA-O3A-PB	-3.53	120.82	132.67
9	Bd	4601	ADP	PA-O3A-PB	-3.53	120.84	132.67
9	AG	1001	ADP	PA-O3A-PB	-3.49	120.96	132.67
9	Bg	5001	ADP	PA-O3A-PB	-3.49	120.96	132.67
9	BG	4001	ADP	PA-O3A-PB	-3.49	120.98	132.67
9	Ag	2001	ADP	PA-O3A-PB	-3.48	120.99	132.67
9	AE	601	ADP	PA-O3A-PB	-3.09	122.31	132.67
9	Be	4601	ADP	PA-O3A-PB	-3.09	122.32	132.67
9	BE	3601	ADP	PA-O3A-PB	-3.08	122.33	132.67
9	Ae	1601	ADP	PA-O3A-PB	-3.08	122.35	132.67
9	Ab	1601	ADP	C4'-O4'-C1'	-3.02	106.40	109.72
9	AB	601	ADP	C4'-O4'-C1'	-3.01	106.41	109.72
9	Bb	4601	ADP	C4'-O4'-C1'	-3.00	106.42	109.72
9	BB	3601	ADP	C4'-O4'-C1'	-2.97	106.45	109.72
9	BH	3601	ADP	PA-O3A-PB	-2.92	122.89	132.67
9	Bh	4601	ADP	PA-O3A-PB	-2.91	122.91	132.67
9	Ah	1601	ADP	PA-O3A-PB	-2.91	122.91	132.67
9	AH	601	ADP	PA-O3A-PB	-2.90	122.94	132.67
9	BB	3601	ADP	PA-O3A-PB	-2.54	124.14	132.67
9	Ab	1601	ADP	PA-O3A-PB	-2.54	124.14	132.67
9	Bb	4601	ADP	PA-O3A-PB	-2.54	124.14	132.67
9	AB	601	ADP	PA-O3A-PB	-2.54	124.15	132.67
9	BZ	3601	ADP	PA-O3A-PB	-2.47	124.37	132.67
9	Bz	4601	ADP	PA-O3A-PB	-2.47	124.40	132.67
9	AZ	601	ADP	PA-O3A-PB	-2.46	124.43	132.67
9	Az	1601	ADP	PA-O3A-PB	-2.46	124.43	132.67
9	BQ	3601	ADP	PA-O3A-PB	-2.41	124.58	132.67
9	AQ	601	ADP	PA-O3A-PB	-2.41	124.59	132.67
9	Aq	1601	ADP	PA-O3A-PB	-2.40	124.64	132.67
9	Ad	1601	ADP	O3B-PB-O1B	2.00	117.03	110.58
9	AA	601	ADP	O3B-PB-O1B	2.02	117.08	110.58
9	Ba	4601	ADP	O3B-PB-O1B	2.02	117.09	110.58
9	BA	3601	ADP	O3B-PB-O1B	2.03	117.10	110.58
9	Bg	5001	ADP	O3B-PB-O2B	2.03	115.10	107.38
9	Ag	2001	ADP	O3B-PB-O2B	2.03	115.10	107.38
9	Aa	1601	ADP	O3B-PB-O1B	2.03	117.11	110.58
9	AG	1001	ADP	O3B-PB-O2B	2.03	115.12	107.38
9	BG	4001	ADP	O3B-PB-O2B	2.04	115.14	107.38
9	Az	1601	ADP	O3B-PB-O1B	2.04	117.15	110.58
9	BZ	3601	ADP	O3B-PB-O1B	2.05	117.17	110.58
9	Bh	4601	ADP	O3B-PB-O1B	2.05	117.17	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Bz	4601	ADP	O3B-PB-O1B	2.05	117.18	110.58
9	AZ	601	ADP	O3B-PB-O1B	2.06	117.20	110.58
9	BH	3601	ADP	O3B-PB-O1B	2.06	117.20	110.58
9	AH	601	ADP	O3B-PB-O1B	2.06	117.21	110.58
9	Ah	1601	ADP	O3B-PB-O1B	2.07	117.24	110.58
9	Ae	1601	ADP	O3B-PB-O1B	2.17	117.58	110.58
9	BE	3601	ADP	O3B-PB-O1B	2.18	117.59	110.58
9	AE	601	ADP	O3B-PB-O1B	2.18	117.61	110.58
9	Be	4601	ADP	O3B-PB-O1B	2.18	117.61	110.58
9	AQ	601	ADP	O3B-PB-O1B	2.25	117.84	110.58
9	Aq	1601	ADP	O3B-PB-O1B	2.26	117.86	110.58
9	BQ	3601	ADP	O3B-PB-O1B	2.27	117.89	110.58
9	Bq	4601	ADP	O3B-PB-O1B	2.34	118.12	110.58
9	Ad	1601	ADP	O4'-C1'-N9	2.56	113.45	108.10
9	Bd	4601	ADP	O4'-C1'-N9	2.56	113.46	108.10
9	AD	601	ADP	O4'-C1'-N9	2.57	113.47	108.10
9	BD	3601	ADP	O4'-C1'-N9	2.57	113.47	108.10
9	Bz	4601	ADP	O3B-PB-O2B	2.71	117.72	107.38
9	AZ	601	ADP	O3B-PB-O2B	2.72	117.73	107.38
9	Az	1601	ADP	O3B-PB-O2B	2.72	117.73	107.38
9	BZ	3601	ADP	O3B-PB-O2B	2.72	117.73	107.38
9	AQ	601	ADP	O3B-PB-O2B	2.75	117.84	107.38
9	Aq	1601	ADP	O3B-PB-O2B	2.75	117.84	107.38
9	BQ	3601	ADP	O3B-PB-O2B	2.75	117.86	107.38
9	Bb	4601	ADP	O3B-PB-O2B	2.78	117.97	107.38
9	BB	3601	ADP	O3B-PB-O2B	2.78	117.98	107.38
9	AB	601	ADP	O3B-PB-O2B	2.79	117.99	107.38
9	Ab	1601	ADP	O3B-PB-O2B	2.79	118.00	107.38
9	BH	3601	ADP	O3B-PB-O2B	2.80	118.05	107.38
9	AH	601	ADP	O3B-PB-O2B	2.81	118.08	107.38
9	BD	3601	ADP	O3B-PB-O2B	2.82	118.11	107.38
9	Ad	1601	ADP	O3B-PB-O2B	2.82	118.11	107.38
9	Bh	4601	ADP	O3B-PB-O2B	2.82	118.11	107.38
9	AD	601	ADP	O3B-PB-O2B	2.82	118.11	107.38
9	Ah	1601	ADP	O3B-PB-O2B	2.82	118.11	107.38
9	Bd	4601	ADP	O3B-PB-O2B	2.82	118.13	107.38
9	BE	3601	ADP	O3B-PB-O2B	2.84	118.21	107.38
9	AE	601	ADP	O3B-PB-O2B	2.85	118.24	107.38
9	Ae	1601	ADP	O3B-PB-O2B	2.86	118.25	107.38
9	Be	4601	ADP	O3B-PB-O2B	2.86	118.25	107.38
9	Aa	1601	ADP	O3B-PB-O2B	2.92	118.50	107.38
9	Ba	4601	ADP	O3B-PB-O2B	2.92	118.50	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
9	AA	601	ADP	O3B-PB-O2B	2.92	118.52	107.38
9	BA	3601	ADP	O3B-PB-O2B	2.93	118.55	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AA	601	ADP	1	0
9	AB	601	ADP	2	0
9	AD	601	ADP	4	0
9	AE	601	ADP	2	0
9	AG	1001	ADP	2	0
10	AG	1002	BEF	2	0
9	AQ	601	ADP	1	0
9	AZ	601	ADP	3	0
9	BA	3601	ADP	1	0
9	BB	3601	ADP	2	0
9	BD	3601	ADP	4	0
9	BE	3601	ADP	2	0
9	BG	4001	ADP	2	0
10	BG	4002	BEF	2	0
9	BQ	3601	ADP	1	0
9	BZ	3601	ADP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	537/559 (96%)	0.14	6 (1%) 82 69	71, 129, 176, 248	0
1	Aa	537/559 (96%)	0.12	8 (1%) 76 62	71, 129, 176, 248	0
1	BA	537/559 (96%)	0.07	5 (0%) 85 74	71, 129, 176, 248	0
1	Ba	537/559 (96%)	0.15	15 (2%) 56 40	71, 129, 176, 248	0
2	AB	517/527 (98%)	0.11	7 (1%) 78 63	58, 112, 163, 205	0
2	Ab	517/527 (98%)	0.04	6 (1%) 81 67	58, 112, 163, 205	0
2	BB	517/527 (98%)	0.07	3 (0%) 90 82	58, 112, 163, 205	0
2	Bb	517/527 (98%)	0.08	9 (1%) 73 58	58, 112, 163, 205	0
3	AD	515/528 (97%)	0.19	8 (1%) 74 60	60, 128, 174, 224	0
3	Ad	515/528 (97%)	0.36	22 (4%) 39 25	60, 128, 174, 224	0
3	BD	515/528 (97%)	0.09	6 (1%) 81 67	60, 128, 174, 224	0
3	Bd	515/528 (97%)	0.20	15 (2%) 55 38	60, 128, 174, 224	0
4	AE	528/562 (93%)	0.08	4 (0%) 87 77	63, 121, 173, 218	0
4	Ae	528/562 (93%)	0.18	14 (2%) 58 42	63, 121, 173, 218	0
4	BE	528/562 (93%)	0.08	3 (0%) 90 82	63, 121, 173, 218	0
4	Be	528/562 (93%)	0.07	6 (1%) 82 69	63, 121, 173, 218	0
5	AG	509/590 (86%)	0.24	12 (2%) 62 46	78, 131, 179, 233	0
5	Ag	509/590 (86%)	0.32	15 (2%) 55 38	78, 131, 179, 233	0
5	BG	509/590 (86%)	0.24	14 (2%) 56 40	78, 131, 179, 233	0
5	Bg	509/590 (86%)	0.15	11 (2%) 65 50	78, 131, 179, 233	0
6	AH	519/550 (94%)	0.13	7 (1%) 79 65	66, 131, 173, 244	0
6	Ah	519/550 (94%)	0.21	16 (3%) 52 36	66, 131, 173, 244	0
6	BH	519/550 (94%)	0.18	6 (1%) 81 67	66, 131, 173, 244	0
6	Bh	519/550 (94%)	0.28	24 (4%) 36 24	66, 131, 173, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	AQ	523/568 (92%)	0.15	5 (0%) 84 72	71, 138, 182, 249	0
7	Aq	523/568 (92%)	0.32	21 (4%) 42 28	71, 138, 182, 249	0
7	BQ	523/568 (92%)	0.26	18 (3%) 49 34	71, 138, 182, 249	0
7	Bq	523/568 (92%)	0.20	11 (2%) 67 51	71, 138, 182, 249	0
8	AZ	531/546 (97%)	0.24	17 (3%) 51 35	79, 135, 185, 261	0
8	Az	531/546 (97%)	0.21	21 (3%) 42 28	79, 135, 185, 261	0
8	BZ	531/546 (97%)	0.27	12 (2%) 64 48	79, 135, 185, 261	0
8	Bz	531/546 (97%)	0.24	20 (3%) 44 30	79, 135, 185, 261	0
All	All	16716/17720 (94%)	0.18	367 (2%) 65 50	58, 129, 177, 261	0

All (367) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ba	4488	LYS	9.6
8	Bz	4432	ASN	8.5
8	Az	1431	MET	7.3
8	Bz	4431	MET	6.7
8	Az	1316	ALA	6.7
8	Bz	4430	ASN	6.0
8	AZ	432	ASN	5.5
5	Ag	1371	CYS	5.4
6	Bh	4258	GLU	5.2
1	Ba	4238	ALA	4.8
8	Az	1432	ASN	4.7
3	Ad	1188	ASN	4.6
6	BH	3253	GLU	4.5
2	Bb	4330	ASP	4.3
8	BZ	3432	ASN	4.3
5	Ag	1261	ILE	4.2
4	BE	3560	ASP	4.2
2	Ab	1251	LYS	4.2
1	AA	264	ILE	4.2
8	Bz	4049	GLY	4.2
7	Aq	1383	THR	4.1
4	Ae	1286	LYS	4.0
3	Ad	1313	VAL	4.0
6	Ah	1260	ARG	3.9
1	Aa	1293	ALA	3.9
6	AH	209	MET	3.9

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Mol	Chain	Res	Type	RSRZ
6	Bh	4259	VAL	3.9
6	AH	480	GLY	3.8
8	BZ	3364	PHE	3.8
8	AZ	431	MET	3.8
4	Ae	1288	ASP	3.8
5	Ag	1368	LEU	3.7
8	AZ	273	LYS	3.7
6	Ah	1253	GLU	3.6
8	AZ	189	LEU	3.6
4	BE	3214	LYS	3.6
8	Az	1232	TYR	3.6
4	Ae	1287	LEU	3.6
7	BQ	3359	LYS	3.5
3	Ad	1223	ALA	3.4
2	Ab	1250	PHE	3.4
6	Bh	4253	GLU	3.4
4	Ae	1341	PRO	3.4
8	Az	1293	PHE	3.4
4	Be	4169	SER	3.4
3	Bd	4254	VAL	3.4
8	Az	1315	LEU	3.3
8	AZ	348	LEU	3.3
6	Bh	4242	LEU	3.3
7	Aq	1152	ASP	3.3
1	Ba	4389	GLY	3.2
1	Ba	4361	VAL	3.2
1	Ba	4370	GLU	3.2
5	Bg	4384	GLY	3.2
4	Be	4204	ALA	3.2
8	Az	1228	VAL	3.2
3	Bd	4350	VAL	3.2
8	Az	1218	GLY	3.1
3	BD	3286	LEU	3.1
8	Bz	4426	LEU	3.1
5	AG	352	CYS	3.1
4	Ae	1290	SER	3.1
6	Bh	4209	MET	3.1
3	Bd	4214	VAL	3.1
5	AG	356	LYS	3.1
5	Bg	4263	ILE	3.1
5	AG	384	GLY	3.0
3	Bd	4361	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
7	Bq	4320	VAL	3.0
6	Bh	4363	ASN	3.0
5	AG	263	ILE	3.0
6	Bh	4248	LEU	3.0
6	Ah	1363	ASN	3.0
7	Aq	1382	SER	3.0
2	BB	3520	ARG	3.0
2	AB	217	LYS	2.9
3	Bd	4252	ILE	2.9
6	BH	3407	LYS	2.9
2	AB	220	ASN	2.9
7	Aq	1138	THR	2.9
7	BQ	3202	PHE	2.9
3	Ad	1287	LEU	2.9
3	Ad	1482	ILE	2.9
3	Ad	1374	THR	2.9
3	AD	188	ASN	2.9
1	Aa	1262	ILE	2.9
1	BA	3352	SER	2.8
1	Ba	4237	ILE	2.8
5	Ag	1184	LYS	2.8
1	Aa	1264	ILE	2.8
6	Bh	4366	GLN	2.8
7	Aq	1142	LEU	2.8
8	AZ	308	VAL	2.8
2	Bb	4248	THR	2.8
6	BH	3491	ASN	2.8
8	AZ	277	ILE	2.8
7	Aq	1499	VAL	2.8
7	Bq	4262	LYS	2.8
8	Az	1366	TYR	2.8
2	Ab	1344	GLU	2.8
3	Bd	4255	ASN	2.8
1	AA	238	ALA	2.8
3	Ad	1327	GLY	2.8
8	BZ	3217	HIS	2.8
2	AB	329	PHE	2.8
7	BQ	3301	ALA	2.7
3	Ad	1213	VAL	2.7
5	Bg	4186	LEU	2.7
1	BA	3270	LEU	2.7
3	Ad	1197	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
7	BQ	3300	VAL	2.7
1	Ba	4363	GLN	2.7
3	Ad	1198	LYS	2.7
5	BG	3366	SER	2.7
8	Bz	4378	ILE	2.7
5	Ag	1197	GLU	2.7
5	AG	296	ILE	2.7
4	Ae	1313	VAL	2.7
1	Ba	4264	ILE	2.7
3	Bd	4186	SER	2.7
6	Bh	4364	LEU	2.7
8	BZ	3285	CYS	2.7
2	Ab	1353	PHE	2.7
2	Bb	4250	PHE	2.7
8	AZ	364	PHE	2.7
3	Ad	1377	VAL	2.7
5	AG	368	LEU	2.7
8	Az	1354	VAL	2.7
8	Bz	4233	VAL	2.7
7	BQ	3213	MET	2.7
7	Aq	1160	LEU	2.6
1	Ba	4261	GLN	2.6
5	Ag	1259	THR	2.6
8	AZ	185	GLN	2.6
8	Az	1436	ALA	2.6
2	Bb	4220	ASN	2.6
7	BQ	3152	ASP	2.6
7	BQ	3250	PHE	2.6
7	AQ	284	ILE	2.6
7	BQ	3206	SER	2.6
3	Bd	4478	LEU	2.6
4	AE	313	VAL	2.6
2	Ab	1329	PHE	2.6
6	Bh	4243	SER	2.6
8	Az	1314	ILE	2.6
1	Ba	4487	ALA	2.6
3	Bd	4362	ARG	2.6
1	AA	502	LEU	2.5
4	AE	223	LEU	2.5
3	AD	260	MET	2.5
6	Bh	4349	CYS	2.5
4	Ae	1222	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
7	BQ	3321	LEU	2.5
5	BG	3383	GLY	2.5
2	Bb	4329	PHE	2.5
8	BZ	3356	GLN	2.5
6	Bh	4300	GLY	2.5
7	Bq	4149	GLU	2.5
6	AH	381	GLY	2.5
5	Ag	1325	ASN	2.5
5	BG	3225	LEU	2.5
4	Be	4208	VAL	2.5
1	BA	3372	ILE	2.5
7	BQ	3190	LEU	2.5
5	Ag	1367	PHE	2.5
2	BB	3284	PHE	2.5
5	AG	294	LEU	2.5
7	Bq	4329	LEU	2.5
1	Ba	4372	ILE	2.5
1	BA	3488	LYS	2.5
7	Aq	1518	TYR	2.5
8	BZ	3431	MET	2.5
7	Aq	1268	HIS	2.5
3	Bd	4239	PHE	2.5
5	BG	3294	LEU	2.5
8	Az	1219	GLY	2.5
7	Bq	4300	VAL	2.5
5	AG	524	ASP	2.5
7	Aq	1275	ASP	2.5
3	Ad	1218	THR	2.5
6	Ah	1294	LEU	2.5
3	Ad	1366	ILE	2.5
6	Bh	4260	ARG	2.5
5	Bg	4407	MET	2.4
6	Bh	4220	PHE	2.4
6	Bh	4367	GLY	2.4
7	BQ	3357	THR	2.4
8	Az	1252	PHE	2.4
7	BQ	3514	GLU	2.4
1	Ba	4373	LEU	2.4
7	AQ	419	LEU	2.4
3	BD	3288	ILE	2.4
7	Bq	4318	ILE	2.4
8	Az	1422	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	Bz	4277	ILE	2.4
3	Ad	1178	VAL	2.4
7	Aq	1386	LEU	2.4
8	AZ	317	LEU	2.4
8	Bz	4170	LEU	2.4
5	Bg	4185	ASP	2.4
8	Bz	4142	ASN	2.4
5	Bg	4187	GLY	2.4
5	BG	3379	ILE	2.4
6	Ah	1171	ILE	2.4
6	Bh	4294	LEU	2.4
5	Ag	1269	TRP	2.4
6	BH	3292	ILE	2.4
6	Bh	4241	ILE	2.4
1	Aa	1281	VAL	2.4
2	Bb	4260	GLN	2.4
5	Ag	1220	LEU	2.4
2	Bb	4249	LYS	2.4
7	BQ	3377	GLU	2.4
6	Bh	4338	THR	2.4
8	BZ	3232	TYR	2.4
8	Az	1345	PRO	2.3
3	Ad	1180	LYS	2.3
6	Ah	1036	VAL	2.3
1	Aa	1258	MET	2.3
1	Aa	1270	LEU	2.3
4	AE	225	LYS	2.3
7	BQ	3254	LEU	2.3
8	AZ	186	ALA	2.3
6	AH	166	MET	2.3
7	AQ	298	CYS	2.3
3	AD	187	LYS	2.3
3	AD	355	SER	2.3
7	Aq	1223	ILE	2.3
7	Aq	1269	ASN	2.3
7	BQ	3299	ILE	2.3
8	AZ	223	ASP	2.3
8	Az	1240	LEU	2.3
3	Bd	4188	ASN	2.3
7	Bq	4298	CYS	2.3
8	Bz	4294	VAL	2.3
8	BZ	3229	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	AB	216	LYS	2.3
6	Bh	4368	CYS	2.3
7	Aq	1150	ILE	2.3
7	Aq	1156	LYS	2.3
5	BG	3250	LEU	2.3
1	Aa	1537	ALA	2.3
4	Ae	1289	ILE	2.3
2	Ab	1345	GLU	2.3
4	Ae	1169	SER	2.3
6	Ah	1293	VAL	2.3
5	Ag	1528	SER	2.3
7	BQ	3327	PHE	2.3
5	BG	3238	ILE	2.3
7	AQ	383	THR	2.3
3	Ad	1376	SER	2.2
8	AZ	353	LEU	2.2
6	Ah	1261	VAL	2.2
7	Aq	1427	GLU	2.2
8	BZ	3340	VAL	2.2
3	Ad	1363	VAL	2.2
5	BG	3242	ARG	2.2
3	Bd	4253	ILE	2.2
4	Ae	1319	ASP	2.2
6	AH	376	LEU	2.2
3	Bd	4166	TYR	2.2
2	Bb	4261	LEU	2.2
4	Ae	1302	GLU	2.2
5	Bg	4197	GLU	2.2
5	Bg	4497	TYR	2.2
3	Ad	1289	GLN	2.2
5	BG	3046	LYS	2.2
6	Ah	1356	GLN	2.2
5	Ag	1271	ARG	2.2
7	Aq	1344	LEU	2.2
8	BZ	3101	LEU	2.2
7	Bq	4296	VAL	2.2
1	Aa	1488	LYS	2.2
7	AQ	122	LEU	2.2
4	Ae	1168	ILE	2.2
1	Ba	4263	ASN	2.2
5	AG	305	ALA	2.2
6	AH	132	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	AB	244	LYS	2.2
2	BB	3305	SER	2.2
7	Aq	1167	ILE	2.2
7	Bq	4142	LEU	2.2
1	AA	256	MET	2.2
4	Be	4283	THR	2.2
4	Be	4560	ASP	2.2
3	BD	3328	LEU	2.2
7	Aq	1226	MET	2.2
7	Bq	4358	VAL	2.2
4	Be	4287	LEU	2.2
5	BG	3287	ILE	2.2
7	BQ	3379	SER	2.2
6	Ah	1337	THR	2.2
3	AD	361	VAL	2.2
5	Ag	1411	SER	2.2
5	Bg	4269	TRP	2.2
7	Aq	1026	GLY	2.2
6	Ah	1446	LEU	2.1
5	BG	3259	THR	2.1
4	Ae	1207	ALA	2.1
5	Bg	4383	GLY	2.1
1	AA	244	ILE	2.1
1	Ba	4251	LEU	2.1
2	AB	194	GLN	2.1
4	Ae	1340	LEU	2.1
7	BQ	3322	LYS	2.1
1	BA	3264	ILE	2.1
3	Ad	1401	ILE	2.1
8	BZ	3128	GLU	2.1
4	AE	288	ASP	2.1
2	Bb	4321	THR	2.1
5	Ag	1339	ARG	2.1
3	BD	3263	ILE	2.1
6	Bh	4373	THR	2.1
8	Bz	4171	THR	2.1
7	Aq	1336	CYS	2.1
8	AZ	232	TYR	2.1
5	AG	127	LYS	2.1
6	Ah	1170	LEU	2.1
5	Ag	1221	LYS	2.1
3	BD	3235	GLY	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	BG	3384	GLY	2.1
2	AB	269	MET	2.1
3	AD	283	CYS	2.1
6	Bh	4292	ILE	2.1
8	AZ	347	ILE	2.1
6	Bh	4149	SER	2.1
1	Ba	4377	THR	2.1
8	Bz	4314	ILE	2.1
6	Bh	4488	ILE	2.1
8	Bz	4444	ILE	2.1
5	AG	283	MET	2.1
8	Az	1145	ASN	2.1
8	Az	1339	SER	2.1
8	Az	1317	LEU	2.1
6	Ah	1244	LEU	2.1
6	Ah	1377	LEU	2.1
3	Bd	4089	ALA	2.1
6	AH	498	GLU	2.1
3	Ad	1212	GLY	2.1
8	Az	1251	PHE	2.1
8	AZ	240	LEU	2.0
5	BG	3269	TRP	2.0
8	Bz	4493	LEU	2.0
3	Ad	1325	SER	2.0
7	Bq	4407	ALA	2.0
5	AG	39	LEU	2.0
6	Ah	1464	ILE	2.0
8	Bz	4253	TYR	2.0
8	Bz	4464	PHE	2.0
6	Ah	1335	GLN	2.0
3	AD	360	ILE	2.0
6	BH	3411	ALA	2.0
5	BG	3224	LEU	2.0
3	Ad	1288	ILE	2.0
3	BD	3285	VAL	2.0
8	BZ	3122	PHE	2.0
3	AD	252	ILE	2.0
4	BE	3243	VAL	2.0
6	Bh	4299	ILE	2.0
8	Bz	4104	GLN	2.0
8	Bz	4278	ILE	2.0
1	AA	70	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
5	Bg	4297	THR	2.0
8	AZ	140	LYS	2.0
3	Bd	4393	SER	2.0
6	BH	3219	ALA	2.0
8	Bz	4251	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
10	BEF	Ag	2002	4/4	0.92	0.31	1.48	154,176,182,188	0
10	BEF	Ba	4602	4/4	0.97	0.19	0.53	72,141,146,155	0
10	BEF	AG	1002	4/4	0.87	0.28	0.33	154,176,182,188	0
10	BEF	BB	3602	4/4	0.98	0.23	0.29	85,91,123,141	0
11	MG	BD	3603	1/1	0.92	0.23	0.20	78,78,78,78	0
10	BEF	Bh	4602	4/4	0.92	0.23	0.19	96,148,149,170	0
9	ADP	Ag	2001	27/27	0.94	0.30	0.09	66,124,161,173	0
9	ADP	BG	4001	27/27	0.94	0.28	-0.00	66,124,161,173	0
10	BEF	Ab	1602	4/4	0.98	0.22	-0.03	85,91,123,141	0
11	MG	AA	603	1/1	0.99	0.22	-0.07	117,117,117,117	0
10	BEF	Bb	4602	4/4	0.97	0.22	-0.08	85,91,123,141	0
9	ADP	AG	1001	27/27	0.94	0.28	-0.12	66,124,161,173	0
9	ADP	Ba	4601	27/27	0.96	0.24	-0.18	32,114,157,179	0
9	ADP	BB	3601	27/27	0.97	0.25	-0.19	55,93,132,149	0
11	MG	Ba	4603	1/1	0.99	0.18	-0.20	117,117,117,117	0
9	ADP	Ab	1601	27/27	0.96	0.24	-0.20	55,93,132,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	ADP	BD	3601	27/27	0.93	0.22	-0.20	78,119,143,177	0
9	ADP	AA	601	27/27	0.93	0.26	-0.21	32,114,157,179	0
9	ADP	Ae	1601	27/27	0.95	0.25	-0.21	30,104,142,184	0
11	MG	Ad	1603	1/1	0.95	0.25	-0.25	78,78,78,78	0
10	BEF	AD	602	4/4	0.98	0.21	-0.27	103,113,151,153	0
9	ADP	Bh	4601	27/27	0.97	0.25	-0.27	29,118,145,160	0
9	ADP	Bb	4601	27/27	0.96	0.24	-0.30	55,93,132,149	0
9	ADP	AH	601	27/27	0.94	0.27	-0.32	29,118,145,160	0
9	ADP	AE	601	27/27	0.96	0.22	-0.33	30,104,142,184	0
10	BEF	AQ	602	4/4	0.96	0.21	-0.33	154,160,163,170	0
10	BEF	Bq	4602	4/4	0.96	0.21	-0.36	154,160,163,170	0
11	MG	Aq	1603	1/1	0.98	0.28	-0.37	117,117,117,117	0
9	ADP	BE	3601	27/27	0.96	0.21	-0.38	30,104,142,184	0
11	MG	Bq	4603	1/1	0.96	0.21	-0.39	117,117,117,117	0
10	BEF	BE	3602	4/4	0.97	0.20	-0.40	109,121,145,150	0
9	ADP	Ah	1601	27/27	0.96	0.26	-0.46	29,118,145,160	0
9	ADP	Aa	1601	27/27	0.95	0.24	-0.50	32,114,157,179	0
10	BEF	AE	602	4/4	0.96	0.22	-0.50	109,121,145,150	0
9	ADP	Bq	4601	27/27	0.94	0.23	-0.51	55,126,167,172	0
11	MG	AG	1003	1/1	0.94	0.25	-0.52	117,117,117,117	0
9	ADP	AD	601	27/27	0.95	0.23	-0.54	78,119,143,177	0
10	BEF	Ae	1602	4/4	0.95	0.21	-0.58	109,121,145,150	0
9	ADP	AB	601	27/27	0.98	0.25	-0.62	55,93,132,149	0
10	BEF	BA	3602	4/4	0.97	0.21	-0.64	72,141,146,155	0
9	ADP	Be	4601	27/27	0.96	0.20	-0.67	30,104,142,184	0
11	MG	AD	603	1/1	0.99	0.18	-0.69	78,78,78,78	0
9	ADP	Bg	5001	27/27	0.94	0.21	-0.74	66,124,161,173	0
10	BEF	Ah	1602	4/4	0.98	0.17	-0.75	96,148,149,170	0
9	ADP	BQ	3601	27/27	0.96	0.21	-0.76	55,126,167,172	0
9	ADP	Az	1601	27/27	0.95	0.20	-0.78	91,121,146,151	0
9	ADP	Bz	4601	27/27	0.95	0.21	-0.78	91,121,146,151	0
11	MG	BQ	3603	1/1	0.92	0.20	-0.78	117,117,117,117	0
10	BEF	BG	4002	4/4	0.95	0.18	-0.81	154,176,182,188	0
9	ADP	AQ	601	27/27	0.95	0.25	-0.82	55,126,167,172	0
9	ADP	BZ	3601	27/27	0.94	0.22	-0.84	91,121,146,151	0
9	ADP	Ad	1601	27/27	0.94	0.18	-0.84	78,119,143,177	0
10	BEF	BD	3602	4/4	0.98	0.15	-0.87	103,113,151,153	0
11	MG	Aa	1603	1/1	0.99	0.20	-0.93	117,117,117,117	0
10	BEF	Bg	5002	4/4	0.91	0.21	-0.95	154,176,182,188	0
9	ADP	BA	3601	27/27	0.96	0.20	-0.96	32,114,157,179	0
9	ADP	BH	3601	27/27	0.97	0.21	-0.98	29,118,145,160	0
10	BEF	Be	4602	4/4	0.98	0.17	-0.98	109,121,145,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	BEF	Bz	4602	4/4	0.92	0.15	-1.01	100,122,147,169	0
10	BEF	AA	602	4/4	0.96	0.15	-1.08	72,141,146,155	0
9	ADP	Bd	4601	27/27	0.97	0.21	-1.11	78,119,143,177	0
10	BEF	AB	602	4/4	0.99	0.21	-1.12	85,91,123,141	0
10	BEF	AH	602	4/4	0.92	0.19	-1.14	96,148,149,170	0
9	ADP	Aq	1601	27/27	0.96	0.20	-1.15	55,126,167,172	0
10	BEF	Az	1602	4/4	0.97	0.17	-1.24	100,122,147,169	0
9	ADP	AZ	601	27/27	0.96	0.20	-1.24	91,121,146,151	0
10	BEF	BH	3602	4/4	0.99	0.15	-1.24	96,148,149,170	0
10	BEF	BZ	3602	4/4	0.94	0.21	-1.27	100,122,147,169	0
10	BEF	BQ	3602	4/4	0.96	0.17	-1.27	154,160,163,170	0
10	BEF	Aa	1602	4/4	0.96	0.17	-1.31	72,141,146,155	0
10	BEF	Bd	4602	4/4	0.97	0.20	-1.34	103,113,151,153	0
11	MG	Bd	4603	1/1	0.99	0.17	-1.51	78,78,78,78	0
11	MG	BG	4003	1/1	0.91	0.15	-1.59	117,117,117,117	0
11	MG	AQ	603	1/1	0.97	0.15	-1.65	117,117,117,117	0
10	BEF	Aq	1602	4/4	0.98	0.10	-1.72	154,160,163,170	0
11	MG	BA	3603	1/1	0.99	0.17	-1.74	117,117,117,117	0
10	BEF	Ad	1602	4/4	0.95	0.11	-1.94	103,113,151,153	0
10	BEF	AZ	602	4/4	0.98	0.16	-1.98	100,122,147,169	0
11	MG	Ag	2003	1/1	0.98	0.18	-3.95	117,117,117,117	0
11	MG	Bg	5003	1/1	0.94	0.15	-4.66	117,117,117,117	0
11	MG	AH	603	1/1	0.99	0.23	-	112,112,112,112	0
11	MG	Be	4603	1/1	0.95	0.21	-	88,88,88,88	0
11	MG	AZ	603	1/1	0.98	0.13	-	96,96,96,96	0
11	MG	BE	3603	1/1	0.99	0.15	-	88,88,88,88	0
11	MG	BB	3603	1/1	0.95	0.28	-	79,79,79,79	0
11	MG	Bz	4603	1/1	0.96	0.15	-	96,96,96,96	0
11	MG	Bh	4603	1/1	0.99	0.10	-	112,112,112,112	0
11	MG	Az	1603	1/1	0.94	0.18	-	96,96,96,96	0
11	MG	Ah	1603	1/1	0.98	0.19	-	112,112,112,112	0
11	MG	BH	3603	1/1	0.97	0.14	-	112,112,112,112	0
11	MG	Ab	1603	1/1	0.96	0.26	-	79,79,79,79	0
11	MG	Bb	4603	1/1	0.98	0.20	-	79,79,79,79	0
11	MG	AE	603	1/1	0.99	0.21	-	88,88,88,88	0
11	MG	BZ	3603	1/1	0.97	0.12	-	96,96,96,96	0
11	MG	AB	603	1/1	0.99	0.18	-	79,79,79,79	0
11	MG	Ae	1603	1/1	0.96	0.19	-	88,88,88,88	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.