



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:23 PM GMT

PDB ID : 1T36
Title : Crystal structure of E. coli carbamoyl phosphate synthetase small subunit mutant C248D complexed with uridine 5'-monophosphate
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 2004-04-24
Resolution : 2.10 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

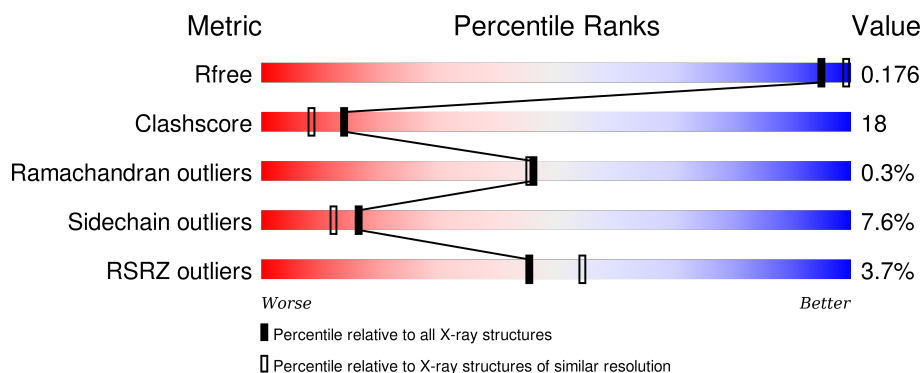
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 ≥ 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	A	1073	 2% 62% 30% 7% •
1	C	1073	 3% 58% 32% 7% ••
1	E	1073	 2% 65% 27% 6% ••
1	G	1073	 4% 52% 37% 9% ••
2	B	382	 4% 54% 35% 8% ••

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Mol	Chain	Length	Quality of chain
2	D	382	
2	F	382	
2	H	382	

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
6	CL	H	384	-	-	-	X
8	ORN	A	1089	-	-	-	X
8	ORN	C	1091	-	-	-	X
8	ORN	E	1091	-	-	-	X
8	ORN	G	1091	-	-	-	X
9	NET	E	1092	-	-	-	X
9	NET	G	1092	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48757 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 Carbamoyl-phosphate synthase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	9	0
			8212	5155	1436	1575	46			
1	C	1058	Total	C	N	O	S	0	8	0
			8197	5146	1426	1579	46			
1	E	1058	Total	C	N	O	S	0	5	0
			8182	5137	1425	1575	45			
1	G	1058	Total	C	N	O	S	0	8	0
			8206	5152	1432	1577	45			

- Molecule 2 is a protein called Carbamoyl-phosphate synthase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			
2	D	379	Total	C	N	O	S	0	1	0
			2904	1830	511	554	9			
2	F	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			
2	H	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	248	ASP	CYS	ENGINEERED	UNP P00907
D	248	ASP	CYS	ENGINEERED	UNP P00907
F	248	ASP	CYS	ENGINEERED	UNP P00907
H	248	ASP	CYS	ENGINEERED	UNP P00907

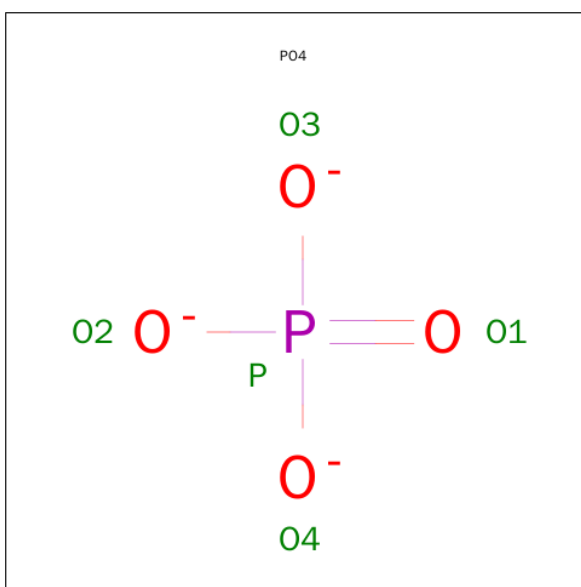
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Mn 3 3	0	0
3	A	3	Total Mn 3 3	0	0
3	C	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	5	Total K 5 5	0	0
4	D	1	Total K 1 1	0	0
4	E	5	Total K 5 5	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	4	Total K 4 4	0	0
4	A	4	Total K 4 4	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

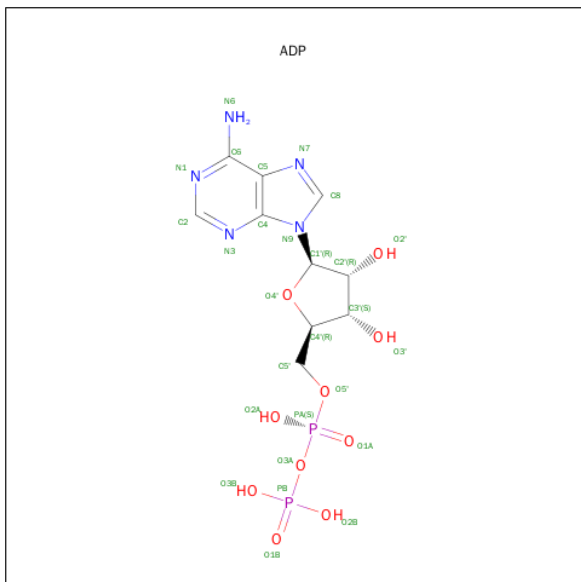


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

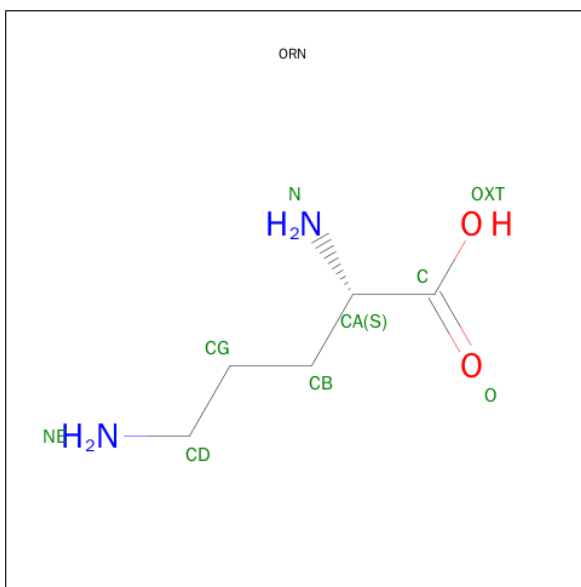
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	6	Total	Cl	0	0
			6	6		
6	D	1	Total	Cl	0	0
			1	1		
6	E	6	Total	Cl	0	0
			6	6		
6	H	2	Total	Cl	0	0
			2	2		
6	C	6	Total	Cl	0	0
			6	6		
6	A	5	Total	Cl	0	0
			5	5		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



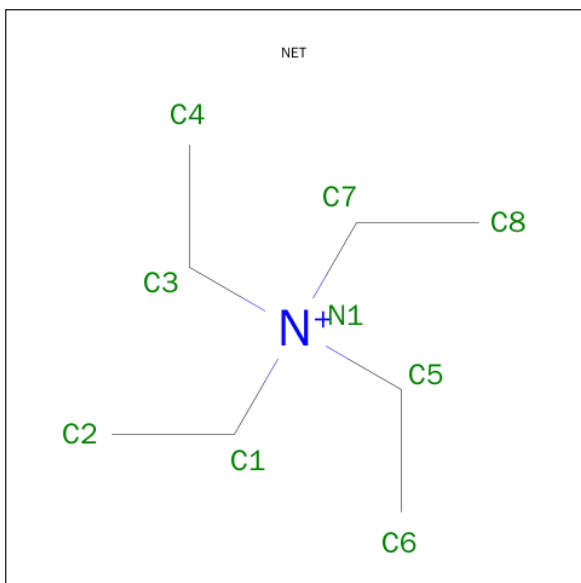
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 8 is L-ORNITHINE (three-letter code: ORN) (formula: $\text{C}_5\text{H}_{12}\text{N}_2\text{O}_2$).



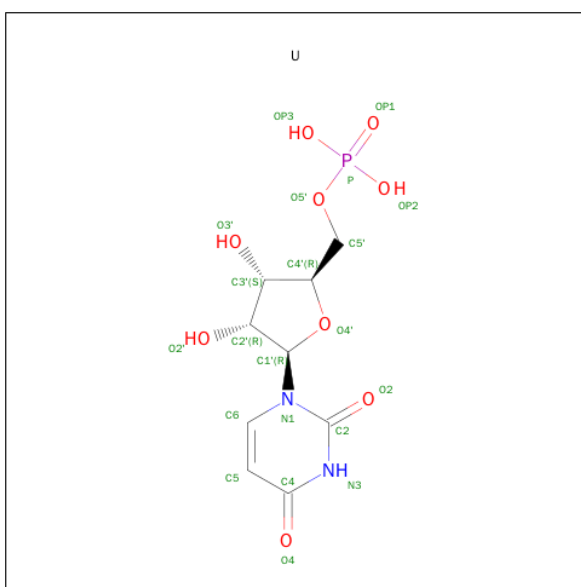
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N 9 8 1	0	0
9	C	1	Total C N 9 8 1	0	0
9	E	1	Total C N 9 8 1	0	0
9	G	1	Total C N 9 8 1	0	0

- Molecule 10 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U) (formula: $C_9H_{13}N_2O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O P 21 9 2 9 1	0	0
10	C	1	Total C N O P 21 9 2 9 1	0	0
10	E	1	Total C N O P 21 9 2 9 1	0	0
10	G	1	Total C N O P 21 9 2 9 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	851	Total O 851 851	0	0

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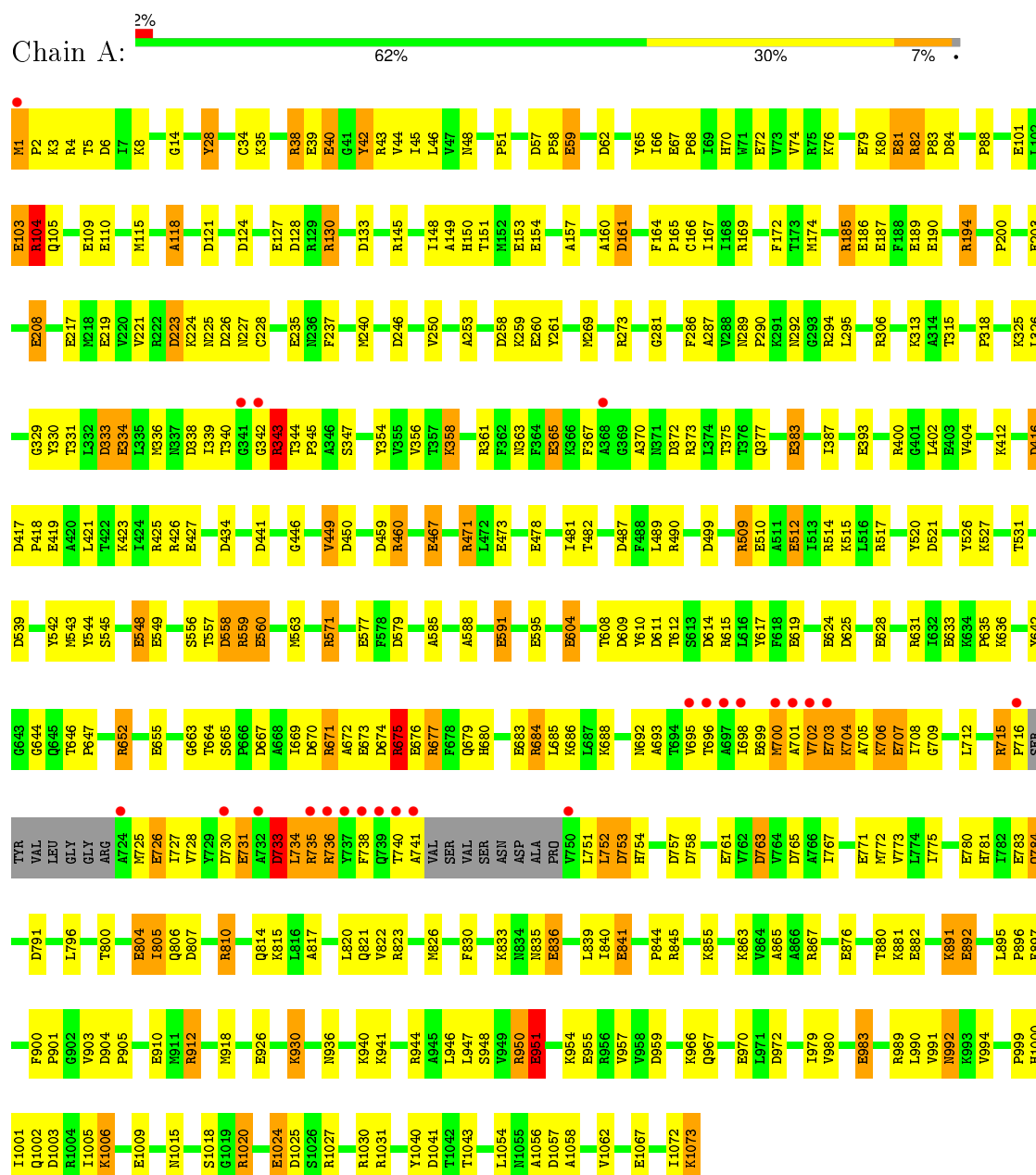
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	161	Total 161	O 161	0	0
11	C	819	Total 819	O 819	0	0
11	D	221	Total 221	O 221	0	0
11	E	832	Total 832	O 832	0	0
11	F	200	Total 200	O 200	0	0
11	G	705	Total 705	O 705	0	0
11	H	118	Total 118	O 118	0	0

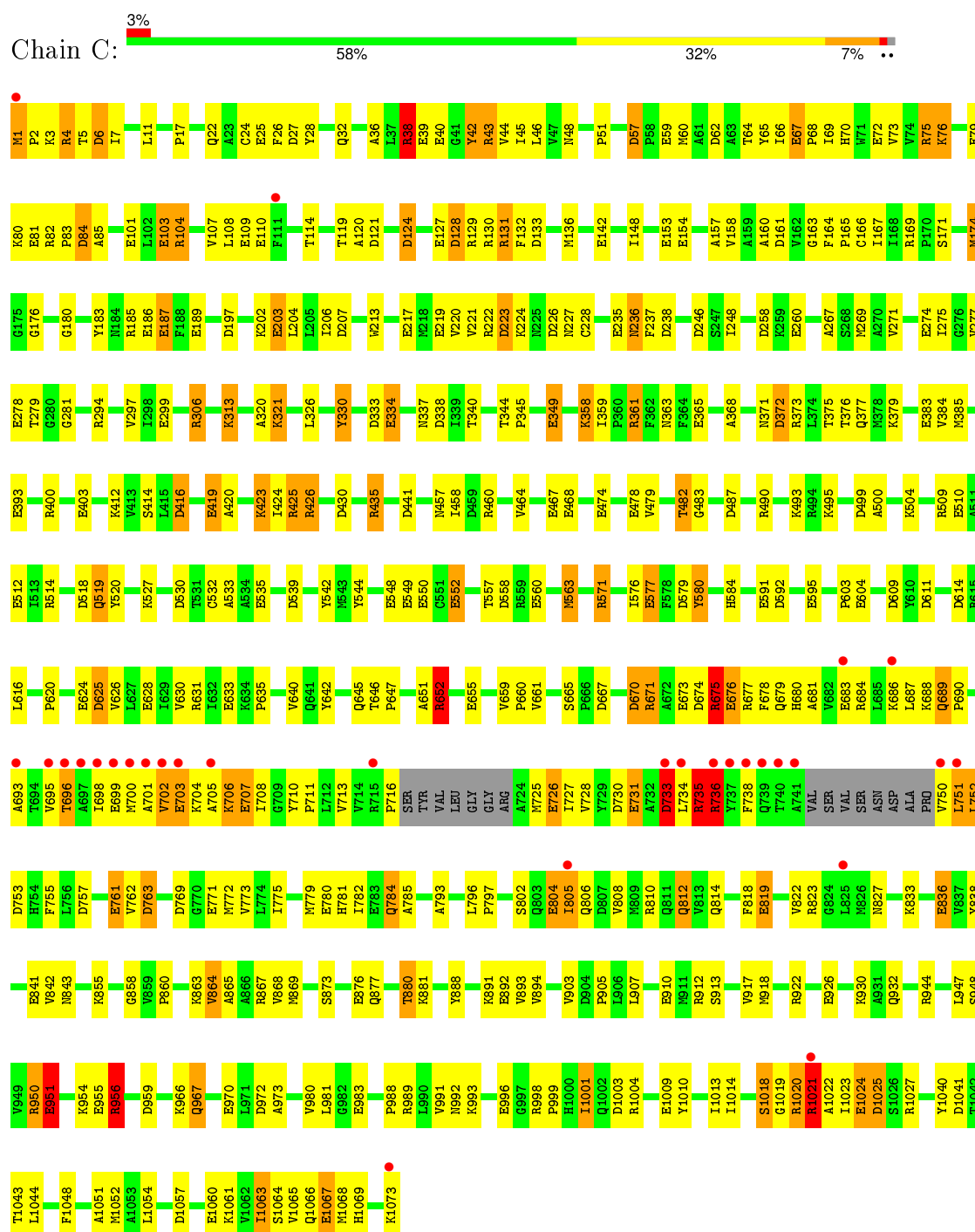
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

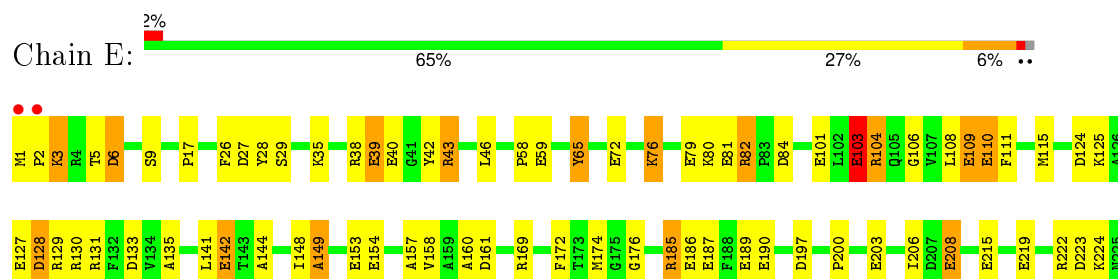
- Molecule 1: Carbamoyl-phosphate synthase large chain

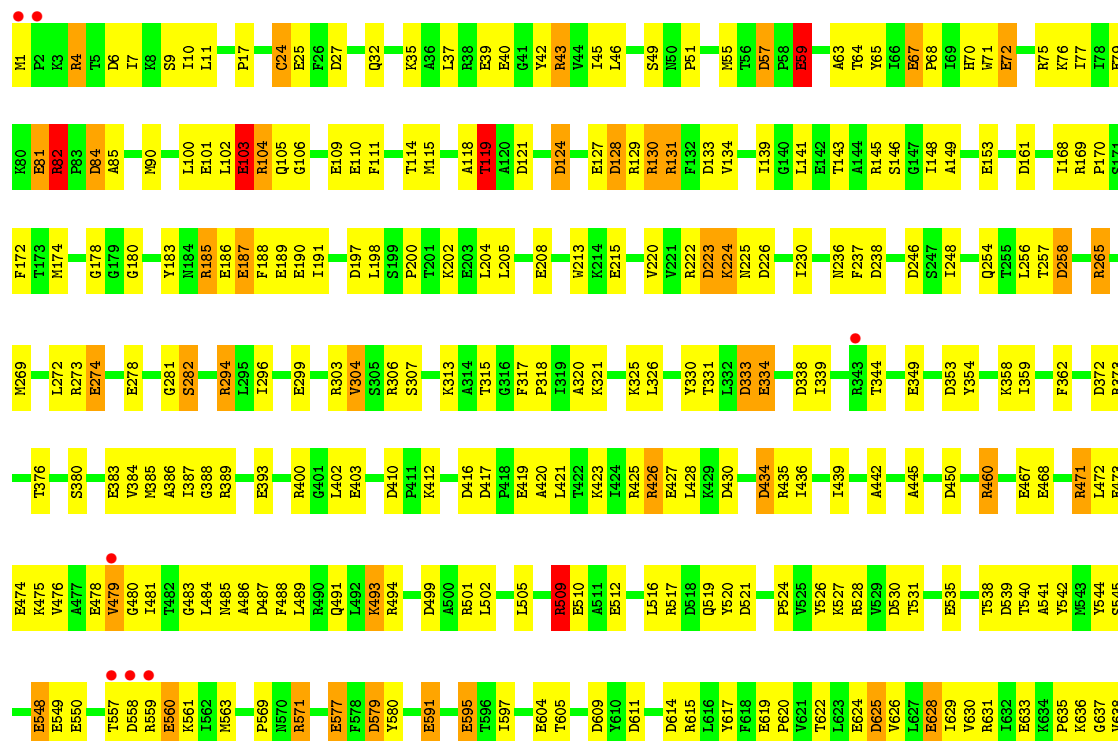


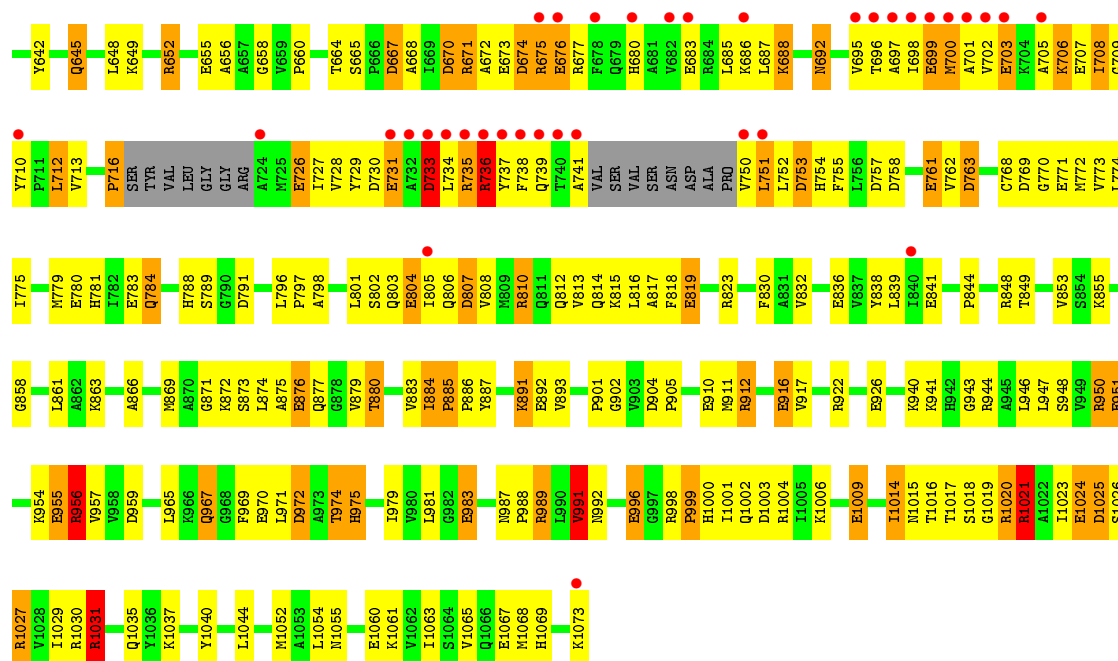
- Molecule 1: Carbamoyl-phosphate synthase large chain



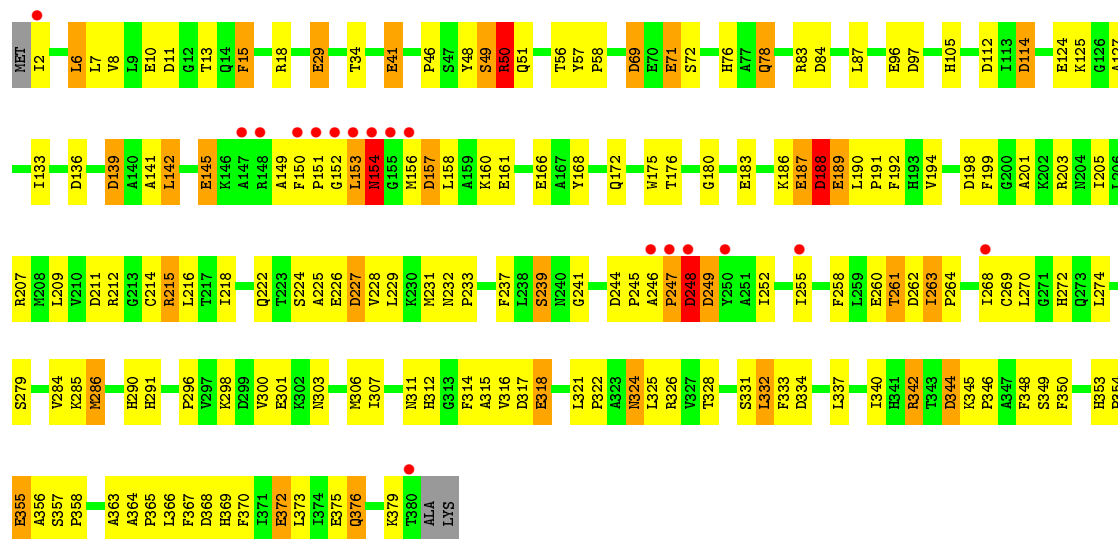
• Molecule 1: Carbamoyl-phosphate synthase large chain



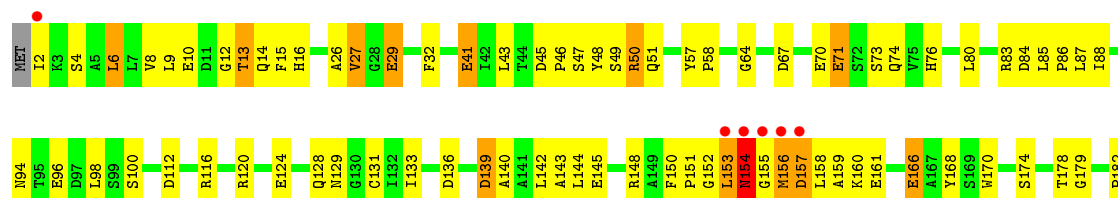


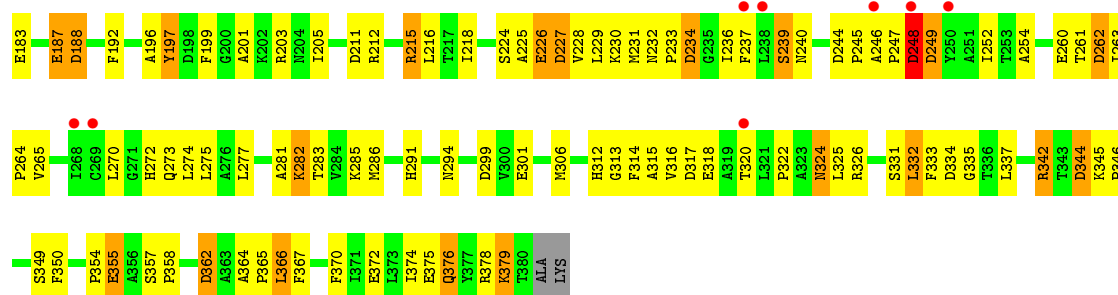


• Molecule 2: Carbamoyl-phosphate synthase small chain

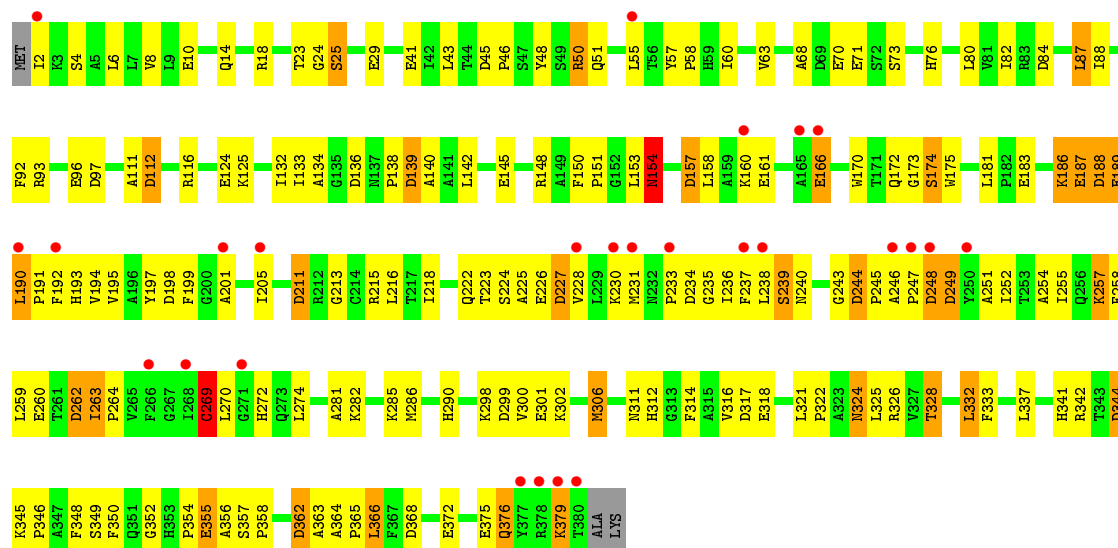


• Molecule 2: Carbamoyl-phosphate synthase small chain

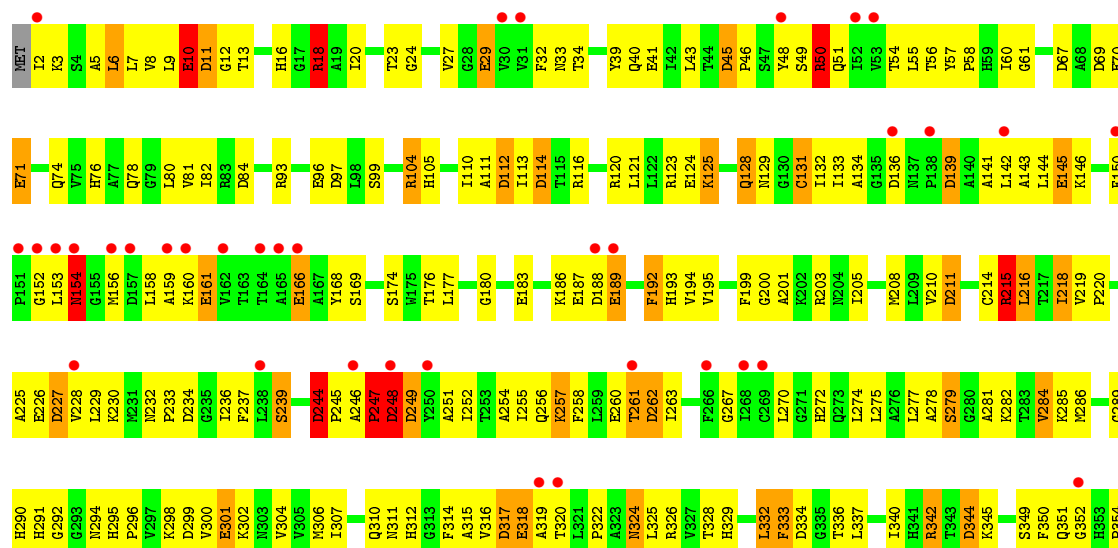




• Molecule 2: Carbamoyl-phosphate synthase small chain



• Molecule 2: Carbamoyl-phosphate synthase small chain



E355	
H361	
D362	
A363	
A364	
P365	
L366	
F367	
D368	
H369	
F370	
L371	
E372	
L373	
I374	
E375	
Q376	
Y377	
R378	
K379	
T380	
ALA	
LYS	

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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.50 Å 164.90 Å 333.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.10) 88.6 (29.70-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.10 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.176 , 0.209 0.175 , 0.176	Depositor DCC
R_{free} test set	42730 reflections (11.03%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 119.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 430082 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48757	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ADP, CL, K, MN, ORN, NET, PO4

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	A	1.05	68/8374 (0.8%)	1.50	137/11315 (1.2%)
1	C	1.06	81/8355 (1.0%)	1.48	127/11293 (1.1%)
1	E	1.06	74/8328 (0.9%)	1.50	128/11257 (1.1%)
1	G	1.05	74/8368 (0.9%)	1.50	148/11308 (1.3%)
2	B	0.94	19/2959 (0.6%)	1.46	43/4019 (1.1%)
2	D	0.97	17/2970 (0.6%)	1.48	45/4033 (1.1%)
2	F	0.97	19/2959 (0.6%)	1.45	41/4019 (1.0%)
2	H	0.94	20/2959 (0.7%)	1.42	37/4019 (0.9%)
All	All	1.03	372/45272 (0.8%)	1.49	706/61263 (1.2%)

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
2	B	1	0
2	D	1	0
2	F	1	0
All	All	3	0

All (372) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	372	GLU	CD-OE2	8.39	1.34	1.25
2	H	166	GLU	CD-OE2	8.34	1.34	1.25
2	D	145	GLU	CD-OE2	8.28	1.34	1.25
1	G	1009[A]	GLU	CD-OE2	8.21	1.34	1.25
1	G	1009[B]	GLU	CD-OE2	8.21	1.34	1.25
1	E	349	GLU	CD-OE2	8.21	1.34	1.25
2	F	355	GLU	CD-OE2	8.16	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	183	GLU	CD-OE2	7.96	1.34	1.25
1	E	190	GLU	CD-OE2	7.95	1.34	1.25
1	A	109	GLU	CD-OE2	7.87	1.34	1.25
1	E	655	GLU	CD-OE2	7.82	1.34	1.25
2	H	145	GLU	CD-OE2	7.81	1.34	1.25
1	E	1024	GLU	CD-OE2	7.80	1.34	1.25
1	G	804	GLU	CD-OE2	7.73	1.34	1.25
1	C	1024	GLU	CD-OE2	7.72	1.34	1.25
2	H	226	GLU	CD-OE2	7.71	1.34	1.25
1	A	1009	GLU	CD-OE2	7.63	1.34	1.25
1	A	699	GLU	CD-OE2	7.62	1.34	1.25
2	F	166	GLU	CD-OE2	7.60	1.34	1.25
2	H	372	GLU	CD-OE2	7.59	1.34	1.25
1	C	910	GLU	CD-OE2	7.59	1.34	1.25
2	D	166	GLU	CD-OE2	7.55	1.33	1.25
2	B	166	GLU	CD-OE2	7.54	1.33	1.25
2	F	145	GLU	CD-OE2	7.54	1.33	1.25
1	A	955	GLU	CD-OE2	7.53	1.33	1.25
1	A	217	GLU	CD-OE2	7.49	1.33	1.25
1	E	153	GLU	CD-OE2	7.44	1.33	1.25
2	F	183	GLU	CD-OE2	7.41	1.33	1.25
1	G	983	GLU	CD-OE2	7.40	1.33	1.25
2	B	226	GLU	CD-OE2	7.38	1.33	1.25
1	A	707	GLU	CD-OE2	7.36	1.33	1.25
1	E	591	GLU	CD-OE2	7.32	1.33	1.25
1	A	478	GLU	CD-OE2	7.29	1.33	1.25
1	E	419	GLU	CD-OE2	7.28	1.33	1.25
1	G	1024	GLU	CD-OE2	7.28	1.33	1.25
1	E	983	GLU	CD-OE2	7.27	1.33	1.25
1	C	771	GLU	CD-OE2	7.26	1.33	1.25
1	C	217	GLU	CD-OE2	7.20	1.33	1.25
1	E	1009	GLU	CD-OE2	7.17	1.33	1.25
1	E	707	GLU	CD-OE2	7.14	1.33	1.25
1	A	910	GLU	CD-OE2	7.13	1.33	1.25
1	E	365	GLU	CD-OE2	7.13	1.33	1.25
1	C	676	GLU	CD-OE2	7.12	1.33	1.25
2	H	183	GLU	CD-OE2	7.12	1.33	1.25
1	C	109	GLU	CD-OE2	7.10	1.33	1.25
1	C	703	GLU	CD-OE2	7.09	1.33	1.25
2	D	183	GLU	CD-OE2	7.08	1.33	1.25
1	C	39	GLU	CD-OE2	7.08	1.33	1.25
1	C	127	GLU	CD-OE2	7.08	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	59	GLU	CD-OE2	7.08	1.33	1.25
1	G	703	GLU	CD-OE2	7.07	1.33	1.25
1	A	676	GLU	CD-OE2	7.06	1.33	1.25
1	G	427	GLU	CD-OE2	7.04	1.33	1.25
2	D	372	GLU	CD-OE2	7.02	1.33	1.25
1	E	780	GLU	CD-OE2	6.98	1.33	1.25
1	A	951	GLU	CD-OE2	6.97	1.33	1.25
2	H	301	GLU	CD-OE2	6.97	1.33	1.25
1	E	804	GLU	CD-OE2	6.97	1.33	1.25
1	C	876	GLU	CD-OE2	6.96	1.33	1.25
1	G	731	GLU	CD-OE2	6.96	1.33	1.25
1	C	699	GLU	CD-OE2	6.96	1.33	1.25
1	E	703	GLU	CD-OE2	6.95	1.33	1.25
1	A	186	GLU	CD-OE2	6.93	1.33	1.25
1	A	473	GLU	CD-OE2	6.89	1.33	1.25
2	H	187	GLU	CD-OE2	6.87	1.33	1.25
1	A	591	GLU	CD-OE2	6.87	1.33	1.25
1	C	550	GLU	CD-OE2	6.86	1.33	1.25
2	H	318	GLU	CD-OE2	6.86	1.33	1.25
1	E	955	GLU	CD-OE2	6.86	1.33	1.25
1	C	577	GLU	CD-OE2	6.84	1.33	1.25
1	E	550	GLU	CD-OE2	6.83	1.33	1.25
1	C	512	GLU	CD-OE2	6.83	1.33	1.25
2	F	260	GLU	CD-OE2	6.82	1.33	1.25
2	F	226	GLU	CD-OE2	6.81	1.33	1.25
2	B	372	GLU	CD-OE2	6.79	1.33	1.25
1	A	726	GLU	CD-OE2	6.79	1.33	1.25
1	E	771	GLU	CD-OE2	6.78	1.33	1.25
1	A	683	GLU	CD-OE2	6.77	1.33	1.25
1	G	510	GLU	CD-OE2	6.77	1.33	1.25
2	F	161	GLU	CD-OE2	6.76	1.33	1.25
1	E	726	GLU	CD-OE2	6.76	1.33	1.25
2	B	260	GLU	CD-OE2	6.75	1.33	1.25
1	E	699	GLU	CD-OE2	6.74	1.33	1.25
2	H	70	GLU	CD-OE2	6.74	1.33	1.25
1	A	512[A]	GLU	CD-OE2	6.73	1.33	1.25
1	A	512[B]	GLU	CD-OE2	6.73	1.33	1.25
1	G	110	GLU	CD-OE2	6.73	1.33	1.25
1	C	604	GLU	CD-OE2	6.71	1.33	1.25
2	F	375	GLU	CD-OE2	6.70	1.33	1.25
1	G	676	GLU	CD-OE2	6.67	1.32	1.25
2	B	145	GLU	CD-OE2	6.67	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	355	GLU	CD-OE2	6.65	1.32	1.25
1	A	467	GLU	CD-OE2	6.64	1.32	1.25
1	A	780	GLU	CD-OE2	6.64	1.32	1.25
1	G	215	GLU	CD-OE2	6.64	1.32	1.25
2	D	96	GLU	CD-OE2	6.63	1.32	1.25
2	D	226	GLU	CD-OE2	6.63	1.32	1.25
1	E	836	GLU	CD-OE2	6.63	1.32	1.25
1	G	699	GLU	CD-OE2	6.63	1.32	1.25
1	G	683	GLU	CD-OE2	6.63	1.32	1.25
1	E	951	GLU	CD-OE2	6.62	1.32	1.25
1	E	783	GLU	CD-OE2	6.62	1.32	1.25
1	A	203	GLU	CD-OE2	6.62	1.32	1.25
1	C	560	GLU	CD-OE2	6.61	1.32	1.25
1	G	673	GLU	CD-OE2	6.61	1.32	1.25
2	D	355	GLU	CD-OE2	6.61	1.32	1.25
1	E	683	GLU	CD-OE2	6.61	1.32	1.25
1	G	109	GLU	CD-OE1	-6.60	1.18	1.25
1	E	910	GLU	CD-OE2	6.60	1.32	1.25
1	G	771	GLU	CD-OE2	6.60	1.32	1.25
1	C	349	GLU	CD-OE2	6.59	1.32	1.25
1	C	1009	GLU	CD-OE2	6.59	1.32	1.25
1	E	761	GLU	CD-OE2	6.59	1.32	1.25
1	G	512	GLU	CD-OE2	6.58	1.32	1.25
1	A	783	GLU	CD-OE2	6.57	1.32	1.25
2	H	161	GLU	CD-OE2	6.55	1.32	1.25
1	A	876	GLU	CD-OE2	6.54	1.32	1.25
1	A	72	GLU	CD-OE2	6.54	1.32	1.25
1	C	731	GLU	CD-OE2	6.53	1.32	1.25
1	E	478	GLU	CD-OE2	6.53	1.32	1.25
1	C	383	GLU	CD-OE2	6.52	1.32	1.25
1	C	683	GLU	CD-OE2	6.51	1.32	1.25
1	G	926	GLU	CD-OE2	6.51	1.32	1.25
1	E	970	GLU	CD-OE2	6.51	1.32	1.25
1	E	577	GLU	CD-OE2	6.49	1.32	1.25
1	G	474	GLU	CD-OE2	6.48	1.32	1.25
1	G	655	GLU	CD-OE2	6.47	1.32	1.25
1	A	365	GLU	CD-OE2	6.47	1.32	1.25
1	C	707	GLU	CD-OE2	6.47	1.32	1.25
1	E	186	GLU	CD-OE2	6.46	1.32	1.25
2	B	301	GLU	CD-OE2	6.45	1.32	1.25
1	E	926	GLU	CD-OE2	6.45	1.32	1.25
1	C	186	GLU	CD-OE2	6.44	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	955	GLU	CD-OE2	6.44	1.32	1.25
1	C	478	GLU	CD-OE2	6.42	1.32	1.25
1	C	951	GLU	CD-OE2	6.42	1.32	1.25
1	G	383	GLU	CD-OE2	6.41	1.32	1.25
1	G	103	GLU	CD-OE2	6.41	1.32	1.25
1	A	983	GLU	CD-OE2	6.39	1.32	1.25
1	A	771	GLU	CD-OE2	6.39	1.32	1.25
1	G	955	GLU	CD-OE2	6.39	1.32	1.25
1	G	190	GLU	CD-OE2	6.37	1.32	1.25
1	A	153	GLU	CD-OE2	6.36	1.32	1.25
1	C	72	GLU	CD-OE2	6.36	1.32	1.25
1	E	110	GLU	CD-OE2	6.36	1.32	1.25
1	G	467	GLU	CD-OE2	6.35	1.32	1.25
1	A	219	GLU	CD-OE2	6.35	1.32	1.25
1	A	804	GLU	CD-OE2	6.35	1.32	1.25
1	A	334	GLU	CD-OE2	6.34	1.32	1.25
1	C	419	GLU	CD-OE2	6.33	1.32	1.25
1	A	577	GLU	CD-OE2	6.33	1.32	1.25
1	C	110	GLU	CD-OE2	6.31	1.32	1.25
1	C	274	GLU	CD-OE2	6.31	1.32	1.25
1	E	189	GLU	CD-OE2	6.27	1.32	1.25
1	G	334	GLU	CD-OE2	6.27	1.32	1.25
1	E	549	GLU	CD-OE2	6.26	1.32	1.25
1	E	731	GLU	CD-OE2	6.26	1.32	1.25
1	G	591	GLU	CD-OE2	6.25	1.32	1.25
2	B	375	GLU	CD-OE2	6.25	1.32	1.25
1	A	633	GLU	CD-OE2	6.24	1.32	1.25
1	C	260	GLU	CD-OE2	6.23	1.32	1.25
2	F	189	GLU	CD-OE2	6.23	1.32	1.25
1	G	153[A]	GLU	CD-OE2	6.21	1.32	1.25
1	G	153[B]	GLU	CD-OE2	6.21	1.32	1.25
1	G	186	GLU	CD-OE2	6.21	1.32	1.25
1	C	624	GLU	CD-OE2	6.21	1.32	1.25
1	E	676	GLU	CD-OE2	6.20	1.32	1.25
1	C	299	GLU	CD-OE2	6.19	1.32	1.25
1	A	970	GLU	CD-OE2	6.19	1.32	1.25
1	E	72	GLU	CD-OE2	6.18	1.32	1.25
1	C	726	GLU	CD-OE2	6.18	1.32	1.25
1	E	876	GLU	CD-OE2	6.15	1.32	1.25
1	G	633	GLU	CD-OE2	6.14	1.32	1.25
1	G	707	GLU	CD-OE2	6.14	1.32	1.25
1	C	467	GLU	CD-OE2	6.13	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	187	GLU	CD-OE2	6.13	1.32	1.25
1	G	419	GLU	CD-OE2	6.12	1.32	1.25
1	A	110	GLU	CD-OE2	6.12	1.32	1.25
2	B	161	GLU	CD-OE2	6.12	1.32	1.25
2	D	29	GLU	CD-OE2	6.12	1.32	1.25
1	C	841	GLU	CD-OE2	6.12	1.32	1.25
1	C	996	GLU	CD-OE2	6.11	1.32	1.25
1	E	215	GLU	CD-OE2	6.11	1.32	1.25
2	H	375	GLU	CD-OE2	6.09	1.32	1.25
1	C	983	GLU	CD-OE2	6.08	1.32	1.25
2	F	96	GLU	CD-OE2	6.07	1.32	1.25
1	C	474	GLU	CD-OE2	6.07	1.32	1.25
1	A	510	GLU	CD-OE2	6.07	1.32	1.25
1	A	703	GLU	CD-OE2	6.07	1.32	1.25
1	G	187	GLU	CD-OE2	6.06	1.32	1.25
1	G	892	GLU	CD-OE2	6.05	1.32	1.25
2	D	318	GLU	CD-OE2	6.03	1.32	1.25
1	G	208	GLU	CD-OE2	6.03	1.32	1.25
1	C	655	GLU	CD-OE2	6.02	1.32	1.25
1	E	208	GLU	CD-OE2	6.02	1.32	1.25
1	A	624	GLU	CD-OE2	6.01	1.32	1.25
2	H	124	GLU	CD-OE2	6.01	1.32	1.25
2	F	70	GLU	CD-OE2	6.00	1.32	1.25
2	F	301	GLU	CD-OE2	6.00	1.32	1.25
1	G	478	GLU	CD-OE2	5.98	1.32	1.25
1	G	274	GLU	CD-OE2	5.98	1.32	1.25
1	G	549	GLU	CD-OE2	5.98	1.32	1.25
1	C	403	GLU	CD-OE2	5.97	1.32	1.25
1	E	109	GLU	CD-OE2	5.96	1.32	1.25
1	E	103	GLU	CD-OE2	5.95	1.32	1.25
1	A	892	GLU	CD-OE2	5.95	1.32	1.25
1	C	549	GLU	CD-OE2	5.95	1.32	1.25
1	G	836	GLU	CD-OE2	5.95	1.32	1.25
2	B	318	GLU	CD-OE2	5.94	1.32	1.25
1	C	468	GLU	CD-OE2	5.94	1.32	1.25
1	G	560	GLU	CD-OE2	5.93	1.32	1.25
1	G	876	GLU	CD-OE2	5.93	1.32	1.25
1	G	577	GLU	CD-OE2	5.92	1.32	1.25
1	C	510	GLU	CD-OE2	5.92	1.32	1.25
1	E	673	GLU	CD-OE2	5.92	1.32	1.25
1	A	655	GLU	CD-OE2	5.91	1.32	1.25
1	E	474	GLU	CD-OE2	5.90	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	10	GLU	CD-OE2	5.89	1.32	1.25
2	B	41	GLU	CD-OE2	5.89	1.32	1.25
2	B	189	GLU	CD-OE2	5.88	1.32	1.25
1	A	1024	GLU	CD-OE2	5.86	1.32	1.25
1	G	299	GLU	CD-OE2	5.85	1.32	1.25
1	E	154	GLU	CD-OE2	5.85	1.32	1.25
2	D	260	GLU	CD-OE2	5.83	1.32	1.25
1	G	628	GLU	CD-OE2	5.83	1.32	1.25
1	A	59	GLU	CD-OE2	5.82	1.32	1.25
2	F	29	GLU	CD-OE2	5.80	1.32	1.25
1	C	628	GLU	CD-OE2	5.80	1.32	1.25
2	H	10	GLU	CD-OE2	5.79	1.32	1.25
1	G	189	GLU	CD-OE2	5.79	1.32	1.25
1	A	1067	GLU	CD-OE2	5.79	1.32	1.25
1	C	633	GLU	CD-OE2	5.79	1.32	1.25
2	B	71	GLU	CD-OE2	5.78	1.32	1.25
2	D	375	GLU	CD-OE2	5.78	1.32	1.25
1	A	549[A]	GLU	CD-OE2	5.78	1.32	1.25
1	A	549[B]	GLU	CD-OE2	5.78	1.32	1.25
1	E	39[A]	GLU	CD-OE2	5.77	1.31	1.25
1	E	39[B]	GLU	CD-OE2	5.77	1.31	1.25
1	C	535	GLU	CD-OE2	5.77	1.31	1.25
1	C	1067	GLU	CD-OE2	5.76	1.31	1.25
1	C	1060	GLU	CD-OE2	5.76	1.31	1.25
1	G	726	GLU	CD-OE2	5.76	1.31	1.25
1	G	783	GLU	CD-OE2	5.76	1.31	1.25
2	F	187	GLU	CD-OE2	5.75	1.31	1.25
1	G	996	GLU	CD-OE2	5.75	1.31	1.25
1	A	841	GLU	CD-OE2	5.74	1.31	1.25
1	E	996	GLU	CD-OE2	5.74	1.31	1.25
1	A	731	GLU	CD-OE2	5.74	1.31	1.25
2	D	70	GLU	CD-OE2	5.73	1.31	1.25
2	H	260	GLU	CD-OE2	5.71	1.31	1.25
1	A	628	GLU	CD-OE2	5.71	1.31	1.25
1	C	79	GLU	CD-OE2	5.70	1.31	1.25
1	E	512	GLU	CD-OE2	5.68	1.31	1.25
1	C	780	GLU	CD-OE2	5.67	1.31	1.25
1	C	101	GLU	CD-OE2	5.67	1.31	1.25
1	E	467	GLU	CD-OE2	5.67	1.31	1.25
1	G	127	GLU	CD-OE2	5.66	1.31	1.25
1	E	560	GLU	CD-OE2	5.64	1.31	1.25
1	E	819	GLU	CD-OE2	5.64	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	535	GLU	CD-OE1	-5.63	1.19	1.25
1	A	560	GLU	CD-OE2	5.63	1.31	1.25
2	H	96	GLU	CD-OE2	5.62	1.31	1.25
2	H	71	GLU	CD-OE2	5.60	1.31	1.25
1	G	67	GLU	CD-OE2	5.60	1.31	1.25
1	G	1060	GLU	CD-OE2	5.59	1.31	1.25
1	G	535	GLU	CD-OE2	5.58	1.31	1.25
1	E	628	GLU	CD-OE2	5.55	1.31	1.25
1	E	40	GLU	CD-OE2	5.55	1.31	1.25
1	E	299	GLU	CD-OE2	5.54	1.31	1.25
1	C	59	GLU	CD-OE2	5.54	1.31	1.25
1	A	836	GLU	CD-OE2	5.53	1.31	1.25
1	C	219	GLU	CD-OE2	5.53	1.31	1.25
1	A	673	GLU	CD-OE2	5.52	1.31	1.25
1	A	190	GLU	CD-OE2	5.52	1.31	1.25
1	A	189	GLU	CD-OE2	5.52	1.31	1.25
1	A	926	GLU	CD-OE2	5.52	1.31	1.25
1	C	153	GLU	CD-OE2	5.52	1.31	1.25
1	G	841	GLU	CD-OE2	5.51	1.31	1.25
2	D	41	GLU	CD-OE2	5.51	1.31	1.25
1	A	419	GLU	CD-OE2	5.51	1.31	1.25
1	G	39	GLU	CD-OE2	5.51	1.31	1.25
2	B	355	GLU	CD-OE2	5.51	1.31	1.25
2	F	10	GLU	CD-OE2	5.50	1.31	1.25
1	E	260	GLU	CD-OE2	5.49	1.31	1.25
1	C	673	GLU	CD-OE2	5.49	1.31	1.25
1	E	473	GLU	CD-OE2	5.49	1.31	1.25
2	H	189	GLU	CD-OE2	5.49	1.31	1.25
1	A	260	GLU	CD-OE2	5.47	1.31	1.25
1	C	550	GLU	CD-OE1	-5.45	1.19	1.25
1	C	67	GLU	CD-OE2	5.44	1.31	1.25
1	G	951	GLU	CD-OE2	5.43	1.31	1.25
1	A	187	GLU	CD-OE2	5.42	1.31	1.25
1	E	219	GLU	CD-OE2	5.42	1.31	1.25
1	C	591[A]	GLU	CD-OE2	5.42	1.31	1.25
1	C	591[B]	GLU	CD-OE2	5.42	1.31	1.25
1	E	892	GLU	CD-OE2	5.41	1.31	1.25
2	D	301	GLU	CD-OE2	5.41	1.31	1.25
1	A	393	GLU	CD-OE2	5.40	1.31	1.25
1	E	548	GLU	CD-OE2	5.40	1.31	1.25
1	A	127	GLU	CD-OE2	5.39	1.31	1.25
2	D	71	GLU	CD-OE2	5.39	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	203	GLU	CD-OE2	5.39	1.31	1.25
1	E	79	GLU	CD-OE2	5.39	1.31	1.25
1	A	619	GLU	CD-OE2	5.36	1.31	1.25
1	C	334	GLU	CD-OE2	5.36	1.31	1.25
1	C	804[A]	GLU	CD-OE2	5.35	1.31	1.25
1	C	804[B]	GLU	CD-OE2	5.35	1.31	1.25
2	B	96	GLU	CD-OE2	5.35	1.31	1.25
1	C	926	GLU	CD-OE2	5.35	1.31	1.25
1	A	103	GLU	CD-OE2	5.34	1.31	1.25
1	G	624	GLU	CD-OE2	5.34	1.31	1.25
1	A	79	GLU	CD-OE2	5.34	1.31	1.25
1	C	819	GLU	CD-OE2	5.33	1.31	1.25
1	C	142	GLU	CD-OE2	5.33	1.31	1.25
1	E	142	GLU	CD-OE2	5.33	1.31	1.25
2	B	29	GLU	CD-OE2	5.32	1.31	1.25
1	C	836	GLU	CD-OE2	5.32	1.31	1.25
1	G	468	GLU	CD-OE2	5.31	1.31	1.25
1	C	187	GLU	CD-OE2	5.31	1.31	1.25
1	G	619	GLU	CD-OE2	5.31	1.31	1.25
1	E	383	GLU	CD-OE1	-5.31	1.19	1.25
2	B	124	GLU	CD-OE2	5.30	1.31	1.25
1	E	278	GLU	CD-OE2	5.30	1.31	1.25
1	A	383	GLU	CD-OE2	5.29	1.31	1.25
1	A	81	GLU	CD-OE2	5.28	1.31	1.25
1	G	761	GLU	CD-OE2	5.28	1.31	1.25
1	E	624	GLU	CD-OE2	5.27	1.31	1.25
1	C	189	GLU	CD-OE2	5.26	1.31	1.25
1	C	39	GLU	CD-OE1	-5.26	1.19	1.25
1	G	278	GLU	CD-OE2	5.26	1.31	1.25
1	G	550	GLU	CD-OE2	5.25	1.31	1.25
1	E	1067	GLU	CD-OE2	5.25	1.31	1.25
1	A	604	GLU	CD-OE2	5.23	1.31	1.25
2	F	124	GLU	CD-OE2	5.22	1.31	1.25
1	C	154	GLU	CD-OE2	5.22	1.31	1.25
1	C	278	GLU	CD-OE2	5.21	1.31	1.25
1	C	552	GLU	CD-OE1	-5.20	1.20	1.25
1	G	819	GLU	CD-OE2	5.20	1.31	1.25
1	G	595	GLU	CD-OE2	5.19	1.31	1.25
2	D	187	GLU	CD-OE2	5.19	1.31	1.25
2	H	41	GLU	CD-OE2	5.19	1.31	1.25
2	F	318	GLU	CD-OE2	5.19	1.31	1.25
1	C	235	GLU	CD-OE2	5.15	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	127	GLU	CD-OE2	5.14	1.31	1.25
2	D	124	GLU	CD-OE2	5.14	1.31	1.25
1	C	970	GLU	CD-OE2	5.14	1.31	1.25
2	H	29	GLU	CD-OE2	5.12	1.31	1.25
1	G	780	GLU	CD-OE2	5.12	1.31	1.25
1	C	365	GLU	CD-OE2	5.11	1.31	1.25
1	E	203	GLU	CD-OE2	5.11	1.31	1.25
1	G	970	GLU	CD-OE2	5.11	1.31	1.25
1	C	761	GLU	CD-OE2	5.11	1.31	1.25
1	E	882	GLU	CD-OE2	5.11	1.31	1.25
1	A	427	GLU	CD-OE2	5.10	1.31	1.25
1	C	393	GLU	CD-OE2	5.09	1.31	1.25
1	G	910	GLU	CD-OE2	5.09	1.31	1.25
1	A	39	GLU	CD-OE2	5.08	1.31	1.25
1	G	25	GLU	CD-OE2	5.08	1.31	1.25
1	E	624	GLU	CD-OE1	-5.07	1.20	1.25
1	G	393	GLU	CD-OE2	5.06	1.31	1.25
1	G	916	GLU	CD-OE2	5.06	1.31	1.25
1	E	403	GLU	CD-OE2	5.06	1.31	1.25
1	A	208	GLU	CD-OE2	5.06	1.31	1.25
1	E	633	GLU	CD-OE2	5.06	1.31	1.25
1	E	841	GLU	CD-OE2	5.05	1.31	1.25
2	F	71	GLU	CD-OE2	5.05	1.31	1.25
1	G	72	GLU	CD-OE2	5.04	1.31	1.25
1	E	101	GLU	CD-OE2	5.04	1.31	1.25
1	G	101	GLU	CD-OE2	5.03	1.31	1.25
1	C	595	GLU	CD-OE2	5.02	1.31	1.25
1	A	595	GLU	CD-OE2	5.02	1.31	1.25
2	B	187	GLU	CD-OE2	5.00	1.31	1.25

All (706) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	514	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	944	ARG	NE-CZ-NH1	14.25	127.42	120.30
1	C	514	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	A	104	ARG	NE-CZ-NH1	13.43	127.02	120.30
1	A	652	ARG	NE-CZ-NH1	13.13	126.87	120.30
1	E	810	ARG	NE-CZ-NH1	12.83	126.72	120.30
1	C	43	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	G	82	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	G	75	ARG	NE-CZ-NH1	11.24	125.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	514	ARG	NE-CZ-NH1	11.07	125.84	120.30
1	G	42	TYR	CB-CG-CD1	-10.98	114.41	121.00
1	A	104	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	E	400	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	A	471	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	E	104	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	E	517	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	C	425	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	C	514	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	736	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	G	389	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	A	400	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	G	265	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	C	518	ASP	CB-CG-OD2	-9.92	109.37	118.30
1	A	677	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	A	130[A]	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	130[B]	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	736	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	43	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	G	671	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	684	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	652	ARG	CD-NE-CZ	9.35	136.69	123.60
1	E	1021	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	C	769	ASP	CB-CG-OD2	-9.24	109.99	118.30
1	E	38	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	G	75	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	C	838	TYR	CB-CG-CD1	-9.10	115.54	121.00
2	H	93	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	G	670	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	E	912	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	E	912	ARG	NE-CZ-NH2	-8.94	115.83	120.30
2	H	342	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	E	1020	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	G	625	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	A	579	ASP	CB-CG-OD1	8.86	126.27	118.30
1	E	956	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	G	460	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	C	518	ASP	CB-CG-OD1	8.79	126.21	118.30
1	G	671	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	E	131	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	G	131	ARG	NE-CZ-NH1	8.60	124.60	120.30
2	F	188	ASP	CB-CG-OD1	8.59	126.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	509	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	C	128	ASP	CB-CG-OD2	-8.57	110.59	118.30
2	B	112	ASP	CB-CG-OD1	8.56	126.00	118.30
1	E	1020	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	G	972	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	C	43	ARG	NE-CZ-NH2	-8.51	116.05	120.30
2	H	97	ASP	CB-CG-OD2	-8.46	110.68	118.30
1	G	956	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	A	43	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	A	373	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	G	517	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	652	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	C	128	ASP	CB-CG-OD1	8.35	125.82	118.30
2	B	262	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	A	579	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	C	425	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	C	972	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	C	609	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	E	372	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	E	944	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	G	579	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	E	223	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	E	810	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	G	416	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	E	753	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	A	416	ASP	CB-CG-OD1	8.23	125.71	118.30
1	A	611	ASP	CB-CG-OD2	-8.22	110.91	118.30
1	G	104	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	G	223	ASP	CB-CG-OD1	8.16	125.64	118.30
2	B	136	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	A	42	TYR	CB-CG-CD1	-8.10	116.14	121.00
2	D	342	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	G	222	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	E	558	ASP	N-CA-CB	-8.04	96.12	110.60
1	E	671	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	C	1004	ARG	NE-CZ-NH1	7.99	124.30	120.30
2	D	136	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	C	733	ASP	CB-CG-OD2	-7.96	111.13	118.30
1	A	223	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	C	6	ASP	CB-CG-OD2	-7.94	111.15	118.30
2	D	248	ASP	N-CA-CB	-7.94	96.31	110.60
1	G	6	ASP	CB-CG-OD2	-7.93	111.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	306	ARG	NE-CZ-NH1	7.93	124.27	120.30
2	H	50	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	G	6	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	128	ASP	CB-CG-OD1	7.90	125.41	118.30
2	B	227	ASP	CB-CG-OD1	7.89	125.40	118.30
1	E	459	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	E	670	ASP	CB-CG-OD1	7.86	125.38	118.30
2	H	378	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	E	609	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	E	223	ASP	CB-CG-OD1	7.86	125.37	118.30
1	G	57	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	C	1021	ARG	NE-CZ-NH1	7.85	124.23	120.30
2	B	50	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	E	998	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	867	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	D	248	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	G	223	ASP	CB-CG-OD2	-7.82	111.26	118.30
2	D	112	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	E	558	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	E	631	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	E	38	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	F	326	ARG	NE-CZ-NH2	-7.75	116.42	120.30
2	F	188	ASP	CB-CG-OD2	-7.75	111.33	118.30
2	B	211	ASP	CB-CG-OD2	-7.74	111.34	118.30
2	D	227	ASP	CB-CG-OD2	-7.74	111.34	118.30
2	H	342	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	G	912	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	G	372	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	E	674	ASP	CB-CG-OD2	-7.71	111.37	118.30
2	B	212	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	42	TYR	CB-CG-CD2	7.69	125.62	121.00
1	C	736	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	G	579	ASP	CB-CG-OD1	7.69	125.22	118.30
1	E	459	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	611	ASP	CB-CG-OD1	7.66	125.19	118.30
1	E	1054	LEU	N-CA-CB	-7.66	95.08	110.40
2	F	249	ASP	CB-CG-OD2	-7.65	111.42	118.30
2	H	112	ASP	CB-CG-OD2	-7.64	111.42	118.30
2	B	11	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	C	631	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	D	317	ASP	CB-CG-OD1	7.59	125.14	118.30
1	G	1021	ARG	NE-CZ-NH1	7.59	124.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	959	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	C	306	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	E	609	ASP	CB-CG-OD1	7.57	125.11	118.30
1	C	922	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	959	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	G	753	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	E	736	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	C	490	ARG	NE-CZ-NH1	7.51	124.05	120.30
2	B	262	ASP	CB-CG-OD1	7.50	125.05	118.30
1	G	736	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	730	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	G	922	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	E	579	ASP	CB-CG-OD2	-7.47	111.57	118.30
1	E	1021	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	161	ASP	CB-CG-OD2	-7.47	111.58	118.30
2	H	317	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	A	124	ASP	CB-CG-OD1	7.45	125.01	118.30
1	A	520	TYR	CB-CG-CD2	-7.44	116.54	121.00
2	D	15	PHE	CB-CG-CD2	7.43	126.00	120.80
1	E	807	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	E	959	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	C	989	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	E	6	ASP	CB-CG-OD1	7.41	124.97	118.30
2	H	211	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	609	ASP	CB-CG-OD1	7.39	124.96	118.30
1	A	487	ASP	CB-CG-OD2	-7.39	111.65	118.30
2	B	227	ASP	CB-CG-OD2	-7.35	111.69	118.30
2	F	136	ASP	CB-CG-OD2	-7.34	111.69	118.30
2	F	227	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	E	579	ASP	CB-CG-OD1	7.34	124.90	118.30
1	G	128	ASP	CB-CG-OD1	7.33	124.90	118.30
1	C	558	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	G	944	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	867	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	652	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	E	197	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	G	614	ASP	CB-CG-OD2	-7.32	111.72	118.30
2	F	248	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	G	226	ASP	CB-CG-OD1	7.31	124.88	118.30
1	G	959	ASP	CB-CG-OD2	-7.28	111.75	118.30
2	D	136	ASP	CB-CG-OD1	7.27	124.84	118.30
1	E	6	ASP	CB-CG-OD2	-7.27	111.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	611	ASP	CB-CG-OD1	7.26	124.84	118.30
1	A	558	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	194	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	C	530	ASP	CB-CG-OD2	-7.24	111.78	118.30
2	H	116	ARG	NE-CZ-NH1	7.24	123.92	120.30
2	D	362	ASP	CB-CG-OD2	-7.23	111.79	118.30
2	F	326	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	E	611	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	C	487	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	G	558	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	E	27	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	1030	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	G	84	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	G	124	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	E	416	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	670	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	769	ASP	CB-CG-OD1	7.14	124.73	118.30
1	E	765	ASP	CB-CG-OD1	7.14	124.73	118.30
2	H	249	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	C	838	TYR	CB-CG-CD2	7.14	125.28	121.00
1	E	333	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	E	675	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	C	361	ARG	NE-CZ-NH1	7.13	123.86	120.30
2	F	50	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	223	ASP	CB-CG-OD1	7.09	124.68	118.30
1	G	501	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	G	667	ASP	CB-CG-OD2	-7.07	111.93	118.30
1	G	471	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	G	246	ASP	CB-CG-OD1	7.06	124.65	118.30
2	B	97	ASP	CB-CG-OD2	-7.05	111.96	118.30
2	F	262	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	C	490	ARG	NE-CZ-NH2	-7.05	116.78	120.30
2	B	114	ASP	CB-CG-OD2	-7.04	111.96	118.30
2	D	83	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	237	PHE	CB-CG-CD1	-7.03	115.88	120.80
1	A	845	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	G	333	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	A	82	ARG	NE-CZ-NH1	-7.00	116.80	120.30
2	D	15	PHE	CB-CG-CD1	-6.99	115.91	120.80
1	G	509	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	E	129	ARG	NE-CZ-NH1	6.99	123.79	120.30
2	B	188	ASP	CB-CG-OD1	6.98	124.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	262	ASP	CB-CG-OD1	6.96	124.56	118.30
2	B	342	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	675	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	G	43	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	E	625	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	715	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	B	212	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	G	43	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	471	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	460	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	558	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	G	733	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	C	223	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	670	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	G	131	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	F	97	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	E	82	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	490[A]	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	490[B]	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	956	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	H	215	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	E	435	ARG	NE-CZ-NH2	-6.81	116.89	120.30
2	H	67	ASP	CB-CG-OD1	6.81	124.43	118.30
2	F	50	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	E	517	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	F	317	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	C	757	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	124	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	C	330	TYR	CB-CG-CD2	-6.73	116.96	121.00
2	H	227	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	G	848	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	763	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	G	460	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	G	133	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	223	ASP	CB-CG-OD2	-6.71	112.26	118.30
2	F	211	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	609	ASP	CB-CG-OD1	6.68	124.32	118.30
1	E	490	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	B	97	ASP	CB-CG-OD1	6.67	124.31	118.30
2	D	334	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	G	434	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	333	ASP	CB-CG-OD2	-6.67	112.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	330	TYR	CB-CG-CD2	-6.67	117.00	121.00
2	F	198	ASP	CB-CG-OD1	6.66	124.30	118.30
1	G	238	ASP	CB-CG-OD2	-6.66	112.31	118.30
2	B	342	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	810	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	C	84	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	G	625	ASP	CB-CG-OD1	6.64	124.28	118.30
1	E	246	ASP	CB-CG-OD1	6.62	124.26	118.30
1	C	124	ASP	CB-CG-OD2	-6.62	112.35	118.30
1	E	128	ASP	CB-CG-OD1	6.62	124.25	118.30
1	C	104	ARG	NE-CZ-NH1	6.61	123.61	120.30
2	B	188	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	C	579	ASP	CB-CG-OD2	-6.61	112.36	118.30
2	D	262	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	E	372	ASP	CB-CG-OD1	6.60	124.24	118.30
2	F	139	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	128	ASP	CB-CG-OD2	-6.59	112.37	118.30
2	F	227	ASP	CB-CG-OD1	6.59	124.23	118.30
2	D	148[A]	ARG	NE-CZ-NH1	6.59	123.59	120.30
2	D	148[B]	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	E	471	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	G	246	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	530	ASP	CB-CG-OD1	6.58	124.22	118.30
1	E	715	ARG	NE-CZ-NH2	6.57	123.58	120.30
2	F	269	CYS	CA-CB-SG	6.55	125.79	114.00
1	G	426[A]	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	G	426[B]	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	169	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	C	1027	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	459	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	287	ALA	N-CA-CB	6.54	119.26	110.10
1	A	343	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	G	258	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	G	294	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	G	757	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	667	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	460	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	D	67	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	G	226	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	B	317	ASP	CB-CG-OD1	6.50	124.15	118.30
1	C	57	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	258	ASP	CB-CG-OD1	6.49	124.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	670	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	614	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	1041	ASP	CB-CG-OD1	6.48	124.13	118.30
2	F	317	ASP	CB-CG-OD1	6.47	124.13	118.30
1	G	642	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	G	539	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	G	258	ASP	CB-CG-OD1	6.46	124.12	118.30
1	G	410	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	944	ARG	NH1-CZ-NH2	-6.45	112.30	119.40
1	E	1025	ASP	CB-CG-OD1	6.45	124.10	118.30
2	H	84	ASP	CB-CG-OD1	6.45	124.10	118.30
1	E	791	ASP	CB-CG-OD1	6.44	124.10	118.30
1	E	373	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	D	84	ASP	CB-CG-OD2	-6.43	112.51	118.30
2	D	50	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	E	410	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	736	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	D	84	ASP	CB-CG-OD1	6.41	124.07	118.30
2	D	192	PHE	CB-CG-CD1	-6.41	116.31	120.80
1	E	972	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	G	991	VAL	CA-CB-CG1	6.41	120.51	110.90
1	A	631	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	G	1025	ASP	CB-CG-OD1	6.38	124.04	118.30
1	E	592	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	E	124	ASP	CB-CG-OD1	6.36	124.03	118.30
1	E	43	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	294	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	G	989	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	C	944	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	E	333	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	763	ASP	CB-CG-OD1	6.34	124.01	118.30
2	H	188	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	57	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	E	1025	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	G	757	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	E	494	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	667	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	C	753	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	E	733	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	C	735	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	E	149	ALA	N-CA-CB	6.28	118.90	110.10
1	C	57	ASP	CB-CG-OD1	6.28	123.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	161	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	C	226	ASP	CB-CG-OD1	6.28	123.95	118.30
2	B	317	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	H	262	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	D	112	ASP	CB-CG-OD1	6.26	123.94	118.30
2	D	249	ASP	CB-CG-OD2	-6.26	112.67	118.30
2	F	249	ASP	CB-CG-OD1	6.26	123.93	118.30
1	G	434	ASP	CB-CG-OD1	6.26	123.93	118.30
1	G	807	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	441	ASP	CB-CG-OD1	6.25	123.92	118.30
1	C	460	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	521	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	C	169	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	E	807	ASP	CB-CG-OD1	6.21	123.89	118.30
1	G	27	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	D	211	ASP	CB-CG-OD1	6.19	123.88	118.30
1	A	261	TYR	CB-CG-CD2	-6.19	117.28	121.00
1	A	609	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	C	539	ASP	CB-CG-OD2	-6.19	112.73	118.30
2	D	227	ASP	CB-CG-OD1	6.18	123.86	118.30
1	G	130	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	G	956	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	G	674	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	A	757	ASP	CB-CG-OD1	6.17	123.85	118.30
2	B	249	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	6	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	416	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	C	460	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	F	148	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	D	211	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	670	ASP	CB-CG-OD1	6.12	123.81	118.30
1	E	161	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	G	716	PRO	N-CA-CB	6.11	110.64	103.30
1	G	991	VAL	CA-CB-CG2	6.11	120.07	110.90
1	G	959	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	6	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	197	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	416	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	G	769	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	959	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	400	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	C	558	ASP	N-CA-CB	-6.08	99.65	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	197	ASP	CB-CG-OD1	6.08	123.77	118.30
1	C	592	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	E	539	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	246	ASP	CB-CG-OD2	-6.07	112.84	118.30
2	B	211	ASP	CB-CG-OD1	6.07	123.76	118.30
1	E	128	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	E	539	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	G	197	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	294	ARG	NE-CZ-NH2	-6.05	117.28	120.30
2	B	69	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	758	ASP	CB-CG-OD1	6.04	123.74	118.30
1	E	671	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	333	ASP	CB-CG-OD1	6.04	123.73	118.30
1	C	238	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	652	ARG	CD-NE-CZ	6.02	132.03	123.60
1	C	670	ASP	CB-CG-OD1	6.02	123.72	118.30
1	G	169	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	757	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	G	42	TYR	CB-CG-CD2	6.00	124.60	121.00
1	A	28	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	333	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	487	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	1010	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	C	810	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	G	559	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	499	ASP	CB-CG-OD1	5.95	123.65	118.30
2	B	105	HIS	CA-CB-CG	-5.95	103.49	113.60
1	A	1057	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	499	ASP	CB-CG-OD2	-5.94	112.95	118.30
2	F	136	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	539	ASP	CB-CG-OD2	-5.93	112.96	118.30
2	H	139	ASP	CB-CG-OD2	-5.93	112.96	118.30
2	H	114	ASP	CB-CG-OD1	5.92	123.63	118.30
2	D	299	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	G	82	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	G	758	ASP	CB-CG-OD1	5.92	123.62	118.30
2	F	344	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	E	84	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	517	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	810	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	E	823	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	B	344	ASP	CB-CG-OD2	-5.89	113.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	128	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	42	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	E	974	THR	CA-CB-CG2	-5.88	104.16	112.40
1	C	441	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	C	557	THR	C-N-CA	5.88	136.41	121.70
1	G	338	ASP	CB-CG-OD2	-5.88	113.01	118.30
2	D	299	ASP	CB-CG-OD1	5.88	123.59	118.30
1	G	1025	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	G	238	ASP	CB-CG-OD1	5.87	123.58	118.30
2	H	215	ARG	N-CA-CB	-5.87	100.04	110.60
2	F	84	ASP	CB-CG-OD1	5.86	123.58	118.30
1	G	521	ASP	CB-CG-OD1	5.86	123.58	118.30
1	E	959	ASP	CB-CG-OD1	5.85	123.57	118.30
1	C	161	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	449	VAL	CA-CB-CG2	-5.83	102.15	110.90
1	E	944	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	C	1025	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	372	ASP	CB-CG-OD2	-5.83	113.06	118.30
2	F	211	ASP	CB-CG-OD1	5.83	123.54	118.30
1	G	57	ASP	CB-CG-OD1	5.83	123.54	118.30
1	C	226	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	674	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	4	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	E	334	GLU	CB-CA-C	-5.81	98.78	110.40
1	E	251	ALA	N-CA-CB	5.81	118.23	110.10
2	F	248	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	1057	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	E	791	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	E	730	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	G	430	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	430	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	131	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	C	716	PRO	N-CA-CB	5.77	110.23	103.30
1	A	441	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	G	758	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	G	807	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	G	904	ASP	CB-CG-OD1	5.76	123.49	118.30
1	C	207	ASP	CB-CG-OD2	-5.76	113.12	118.30
2	H	112	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	625	ASP	CB-CG-OD1	5.75	123.48	118.30
1	G	974	THR	CA-CB-CG2	-5.75	104.35	112.40
1	A	684	ARG	NE-CZ-NH1	5.75	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	128	GLN	CB-CA-C	-5.75	98.91	110.40
1	C	642	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	H	136	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	E	131	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	H	244	ASP	CB-CG-OD1	5.72	123.45	118.30
2	D	362	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	912	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	677	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	G	129	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	G	950	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	434	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	E	1020	ARG	CD-NE-CZ	5.69	131.57	123.60
1	G	912	ARG	CD-NE-CZ	5.69	131.57	123.60
1	A	84	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	B	154	ASN	N-CA-CB	5.67	120.81	110.60
1	C	129	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	674	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	G	373	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	E	730	ASP	CB-CG-OD1	5.65	123.38	118.30
1	G	558	ASP	CB-CG-OD1	5.64	123.38	118.30
1	G	133	ASP	CB-CG-OD1	5.64	123.38	118.30
1	E	133	ASP	CB-CG-OD1	5.64	123.38	118.30
1	G	273	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	H	67	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	667	ASP	CB-CG-OD1	5.64	123.37	118.30
2	B	127	ALA	N-CA-CB	5.63	117.99	110.10
2	F	198	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	F	362	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	E	998	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	G	501	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	G	558	ASP	N-CA-CB	-5.62	100.48	110.60
1	A	121	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	E	716	PRO	N-CA-CB	5.61	110.04	103.30
2	B	84	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	579	ASP	CB-CG-OD1	5.61	123.35	118.30
1	G	609	ASP	CB-CG-OD2	-5.61	113.25	118.30
2	B	154	ASN	CB-CA-C	5.60	121.61	110.40
1	A	716	PRO	N-CA-CB	5.60	110.02	103.30
1	G	373	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	133	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	G	82	ARG	CD-NE-CZ	5.59	131.42	123.60
2	D	45	ASP	CB-CG-OD2	-5.58	113.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	487	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	169	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	D	249	ASP	CB-CG-OD1	5.58	123.32	118.30
1	E	386	ALA	N-CA-CB	5.58	117.91	110.10
1	A	625	ASP	CB-CG-OD1	5.57	123.32	118.30
1	E	684	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	G	119	THR	CA-CB-CG2	-5.57	104.60	112.40
2	D	159	ALA	CB-CA-C	5.56	118.44	110.10
1	A	557	THR	C-N-CA	5.56	135.59	121.70
1	G	609	ASP	CB-CG-OD1	5.54	123.29	118.30
2	H	139	ASP	CB-CG-OD1	5.54	123.29	118.30
1	E	625	ASP	CB-CG-OD2	-5.54	113.31	118.30
2	H	344	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	258	ASP	CB-CG-OD1	5.54	123.28	118.30
2	B	326	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	B	139	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	G	39	GLU	CB-CA-C	-5.53	99.35	110.40
2	H	378	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	121	ASP	CB-CG-OD1	5.52	123.27	118.30
2	B	368	ASP	CB-CG-OD1	5.52	123.26	118.30
1	C	625	ASP	CB-CG-OD2	-5.52	113.34	118.30
1	E	410	ASP	CB-CG-OD2	-5.50	113.34	118.30
2	B	198	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	H	377	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	C	84	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	435	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	1025	ASP	CB-CG-OD1	5.50	123.25	118.30
2	D	197	TYR	CB-CG-CD2	5.50	124.30	121.00
1	G	972	ASP	CB-CG-OD1	5.50	123.25	118.30
2	D	13	THR	CA-CB-CG2	-5.50	104.70	112.40
2	F	97	ASP	CB-CG-OD1	5.49	123.24	118.30
1	G	338	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	133	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	867	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	520	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	G	631	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	478	GLU	CB-CG-CD	-5.47	99.42	114.20
1	E	594	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	1025	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	G	521	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	237	PHE	CB-CG-CD2	5.46	124.63	120.80
1	C	888	TYR	CB-CG-CD1	-5.46	117.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	93	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	667	ASP	CB-CG-OD1	5.46	123.22	118.30
1	E	457	ASN	N-CA-CB	5.46	120.43	110.60
2	F	344	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	118	ALA	N-CA-CB	5.45	117.73	110.10
1	C	38	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	B	248	ASP	CB-CG-OD1	5.44	123.20	118.30
2	F	362	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	459	ASP	CB-CG-OD1	5.44	123.19	118.30
2	D	234	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	G	121	ASP	CB-CG-OD2	-5.43	113.41	118.30
2	D	247	PRO	C-N-CA	5.43	135.28	121.70
1	G	471	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	G	791	ASP	CB-CG-OD1	5.43	123.19	118.30
1	G	389	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	338	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	130[A]	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	130[B]	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	F	157	ASP	CB-CG-OD1	5.42	123.18	118.30
1	G	922	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	H	45	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	1003	ASP	CB-CG-OD2	-5.41	113.44	118.30
2	D	139	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	C	361	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	H	18	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	887	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	A	82	ARG	CD-NE-CZ	-5.38	116.07	123.60
2	B	157	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	757	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	A	904	ASP	CB-CG-OD1	5.37	123.13	118.30
1	E	763	ASP	CB-CA-C	-5.37	99.66	110.40
1	G	416	ASP	CB-CG-OD1	5.37	123.13	118.30
1	G	494	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	G	330	TYR	CB-CG-CD1	5.37	124.22	121.00
1	C	763	ASP	CB-CG-OD2	-5.37	113.47	118.30
2	B	286	MET	CG-SD-CE	-5.36	91.62	100.20
2	H	362	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	G	1031	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	E	972	ASP	N-CA-CB	5.34	120.22	110.60
1	A	614	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	C	400	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	G	674	ASP	CB-CG-OD1	5.33	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	VAL	CA-CB-CG1	-5.33	102.91	110.90
1	E	1003	ASP	CB-CG-OD2	-5.33	113.51	118.30
2	D	344	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	G	559	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	830	PHE	CB-CA-C	-5.31	99.78	110.40
1	C	922	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	C	1003	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	333	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	E	124	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	75	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	G	372	ASP	CB-CG-OD1	5.29	123.06	118.30
2	D	197	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	E	652	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	E	27	ASP	CB-CG-OD2	-5.29	113.54	118.30
2	H	216	LEU	CA-C-N	-5.29	105.57	117.20
1	A	57	ASP	CB-CG-OD1	5.28	123.05	118.30
2	B	136	ASP	CB-CG-OD1	5.28	123.05	118.30
1	E	226	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	733	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	G	353	ASP	CB-CG-OD1	5.28	123.05	118.30
2	D	157	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	204	LEU	CB-CA-C	-5.27	100.19	110.20
2	F	244	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	G	487	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	608	THR	CA-CB-CG2	-5.25	105.05	112.40
1	A	807	ASP	CB-CG-OD2	-5.25	113.58	118.30
2	B	247	PRO	C-N-CA	5.24	134.79	121.70
1	E	757	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	807	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	614	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	758	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	675	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	333	ASP	CB-CG-OD1	5.22	123.00	118.30
1	G	27	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	371	ASN	O-C-N	-5.21	114.36	122.70
2	D	154	ASN	N-CA-C	5.21	125.07	111.00
1	A	40	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	C	1041	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	1025	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	F	112	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	730	ASP	CB-CG-OD1	5.21	122.98	118.30
1	E	757	ASP	CB-CG-OD1	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	F	157	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	864	VAL	CA-CB-CG2	-5.20	103.11	110.90
1	E	667	ASP	CB-CG-OD1	5.19	122.97	118.30
1	E	133	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	E	677	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	E	758	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	81	GLU	CG-CD-OE2	-5.18	107.94	118.30
2	H	247	PRO	C-N-CA	5.18	134.65	121.70
1	C	1057	ASP	CB-CG-OD1	5.17	122.95	118.30
2	B	50	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	E	989	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	G	24	CYS	CA-CB-SG	-5.16	104.71	114.00
1	C	539	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	306	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	A	615	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	G	450	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	C	580	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	C	684	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	G	528	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	517	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	E	65	TYR	CB-CG-CD1	-5.12	117.92	121.00
1	C	959	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	765	ASP	CB-CG-OD1	5.12	122.90	118.30
1	A	904	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	G	294	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	D	188	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	D	326	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	H	154	ASN	CB-CA-C	5.10	120.60	110.40
2	B	15	PHE	CB-CG-CD1	-5.09	117.24	120.80
2	B	50	ARG	CB-CA-C	-5.09	100.22	110.40
1	C	1057	ASP	N-CA-CB	5.09	119.77	110.60
2	F	84	ASP	CB-CG-OD2	-5.08	113.72	118.30
2	H	97	ASP	CB-CG-OD1	5.08	122.88	118.30
2	F	154	ASN	N-CA-CB	5.08	119.75	110.60
1	A	372	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	559	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	B	306	MET	CG-SD-CE	-5.08	92.08	100.20
2	D	6	LEU	N-CA-CB	-5.07	100.25	110.40
1	E	104	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	E	416	ASP	CB-CG-OD1	5.07	122.86	118.30
1	G	557	THR	C-N-CA	5.07	134.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	885	PRO	N-CA-CB	5.07	109.38	103.30
1	A	402	LEU	CB-CG-CD2	-5.06	102.39	111.00
1	C	27	ASP	CB-CG-OD1	5.06	122.86	118.30
1	E	530	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	E	1054	LEU	CB-CA-C	-5.06	100.59	110.20
2	F	88	ILE	CB-CA-C	-5.06	101.49	111.60
2	F	269	CYS	N-CA-CB	5.05	119.70	110.60
1	C	614	ASP	CB-CG-OD1	5.05	122.85	118.30
1	E	1000	HIS	CA-CB-CG	-5.05	105.01	113.60
1	E	471	ARG	NE-CZ-NH1	5.05	122.82	120.30
2	F	328	THR	N-CA-CB	5.05	119.89	110.30
1	G	161	ASP	CB-CG-OD1	5.05	122.84	118.30
1	G	386	ALA	N-CA-CB	5.05	117.17	110.10
1	E	278	GLU	CB-CA-C	-5.04	100.32	110.40
1	G	304	VAL	CA-CB-CG1	-5.04	103.34	110.90
2	B	344	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	912	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	C	279	THR	CA-CB-CG2	-5.03	105.36	112.40
1	C	338	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	E	818	PHE	CB-CG-CD1	5.02	124.32	120.80
2	H	248	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	226	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	791	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	E	657	ALA	C-N-CA	-5.00	111.80	122.30
1	E	1057	ASP	CB-CG-OD1	5.00	122.80	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	154	ASN	CA
2	D	154	ASN	CA
2	F	154	ASN	CA

There are no planarity outliers.

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	A	8212	0	8255	231	0
1	C	8197	0	8225	254	0
1	E	8182	0	8216	209	0
1	G	8206	0	8247	340	0
2	B	2897	0	2860	147	0
2	D	2904	0	2869	133	0
2	F	2897	0	2860	128	0
2	H	2897	0	2860	213	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	5	0	0	0	0
4	F	1	0	0	0	0
4	G	5	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	0	0
5	C	10	0	0	1	0
5	E	5	0	0	0	0
5	G	5	0	0	0	0
6	A	5	0	0	1	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
6	E	6	0	0	1	0
6	F	1	0	0	0	0
6	G	6	0	0	2	0
6	H	2	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	0	0
7	E	54	0	24	3	0
7	G	54	0	24	0	0
8	A	9	0	11	0	0
8	C	9	0	11	1	0
8	E	9	0	11	2	0
8	G	9	0	11	1	0
9	A	9	0	20	1	0
9	C	9	0	20	1	0
9	E	9	0	20	2	0
9	G	9	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	21	0	11	1	0
10	C	21	0	11	2	0
10	E	21	0	11	2	0
10	G	21	0	11	1	0
11	A	851	0	0	29	1
11	B	161	0	0	5	0
11	C	819	0	0	23	1
11	D	221	0	0	5	0
11	E	832	0	0	24	0
11	F	200	0	0	2	0
11	G	705	0	0	28	0
11	H	118	0	0	5	0
All	All	48757	0	44656	1643	1

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 18.

All (1643) 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)
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.13	1.10
2:D:227:ASP:HA	2:D:230:LYS:HD2	1.25	1.07
1:G:784:GLN:NE2	1:G:784:GLN:H	1.53	1.05
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.41	1.03
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.25	1.00
2:H:354:PRO:HG3	2:H:366:LEU:HD22	1.45	0.99
2:H:324:ASN:HD22	2:H:324:ASN:N	1.55	0.98
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.44	0.98
2:H:245:PRO:HD3	2:H:270:LEU:HD11	1.46	0.97
2:B:245:PRO:HD3	2:B:270:LEU:HD11	1.47	0.97
2:H:324:ASN:HD22	2:H:324:ASN:H	0.96	0.95
2:D:324:ASN:HD22	2:D:324:ASN:H	0.99	0.94
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.50	0.94
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.49	0.93
1:G:1:MET:HB2	1:G:224:LYS:HZ2	1.33	0.93
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.50	0.92
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.52	0.92
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.33	0.92
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.33	0.91
1:G:784:GLN:N	1:G:784:GLN:HE21	1.67	0.91
2:F:245:PRO:HD3	2:F:270:LEU:HD11	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:PRO:HD3	2:D:270:LEU:HD11	1.51	0.91
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.35	0.91
1:E:1002:GLN:HE22	1:E:1006:LYS:HE3	1.34	0.91
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.87	0.90
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.54	0.90
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.87	0.90
1:G:1:MET:HB2	1:G:224:LYS:NZ	1.86	0.90
2:H:324:ASN:H	2:H:324:ASN:ND2	1.65	0.89
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.08	0.89
1:G:339:ILE:HD12	1:G:530:ASP:HA	1.55	0.88
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.55	0.87
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.05	0.87
1:C:670:ASP:HB3	1:C:677:ARG:HH21	1.39	0.86
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.57	0.86
2:H:245:PRO:CD	2:H:270:LEU:HD11	2.05	0.86
2:B:50:ARG:HH11	2:B:50:ARG:HG3	1.40	0.86
2:D:285:LYS:HG3	2:D:314:PHE:CE1	2.12	0.85
2:D:324:ASN:HD22	2:D:324:ASN:N	1.67	0.85
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.57	0.85
1:G:509:ARG:HB2	1:G:509:ARG:HH11	1.42	0.84
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.57	0.84
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.13	0.84
1:G:708:ILE:HG22	1:G:712:LEU:HD11	1.59	0.83
1:C:728:VAL:CG1	1:C:733:ASP:HB3	2.08	0.83
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.59	0.83
1:E:698:ILE:H	1:E:698:ILE:HD12	1.42	0.83
1:G:784:GLN:HE21	1:G:784:GLN:H	0.86	0.83
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.60	0.83
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.07	0.83
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.58	0.83
2:D:324:ASN:ND2	2:D:324:ASN:H	1.77	0.83
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.08	0.83
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.58	0.83
2:H:27:VAL:CG2	2:H:131:CYS:HB2	2.05	0.83
1:A:130[A]:ARG:HB2	1:A:148:ILE:HG13	1.60	0.82
2:D:227:ASP:HA	2:D:230:LYS:CD	2.08	0.82
2:F:322:PRO:HD2	2:F:325:LEU:HD12	1.62	0.82
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.62	0.82
2:H:247:PRO:HA	2:H:252:ILE:HD13	1.61	0.82
1:G:475[B]:LYS:HD2	1:G:488:PHE:CZ	2.14	0.82
1:G:563:MET:CE	1:G:635:PRO:HG3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:ALA:HB2	1:C:708:ILE:HD11	1.61	0.81
1:E:967[B]:GLN:HE21	1:E:1054:LEU:HD13	1.43	0.81
1:G:768:CYS:HB2	1:G:773:VAL:HG22	1.63	0.80
2:H:272:HIS:HA	2:H:349:SER:HB2	1.63	0.80
1:G:872:LYS:HG2	1:G:877:GLN:HG2	1.64	0.80
2:D:228:VAL:HA	2:D:231:MET:CE	2.11	0.80
1:A:130[B]:ARG:HB2	1:A:148:ILE:HG13	1.64	0.80
1:A:1073:LYS:N	1:A:1073:LYS:HD2	1.95	0.80
1:G:708:ILE:CG2	1:G:712:LEU:HD11	2.12	0.79
1:G:991:VAL:HB	11:G:1721:HOH:O	1.83	0.79
1:G:225:ASN:ND2	1:G:331:THR:HG21	1.97	0.79
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.64	0.78
1:E:509:ARG:HH11	1:E:509:ARG:CB	1.97	0.78
2:F:263:ILE:HG22	2:F:264:PRO:HD2	1.65	0.78
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.19	0.78
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.66	0.77
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.14	0.77
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.99	0.77
1:G:479:VAL:CG2	1:G:483:GLY:HA3	2.14	0.77
1:G:726:GLU:HG3	1:G:727:ILE:N	2.00	0.77
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.15	0.77
1:G:563:MET:HE1	1:G:635:PRO:HG3	1.66	0.77
1:A:784:GLN:HE21	1:A:784:GLN:H	1.33	0.77
1:A:1020:ARG:O	1:A:1024:GLU:HG3	1.85	0.77
1:A:725:MET:HE3	11:A:1609:HOH:O	1.84	0.77
2:B:194:VAL:HB	2:B:216:LEU:HD23	1.65	0.77
1:C:652:ARG:HH11	1:C:652:ARG:HG2	1.47	0.76
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.19	0.76
1:G:1020:ARG:O	1:G:1024:GLU:HG3	1.85	0.76
2:D:27:VAL:HG13	2:D:131:CYS:HB2	1.68	0.76
2:F:154:ASN:HD21	2:F:314:PHE:HZ	1.34	0.76
1:G:1001:ILE:HD12	1:G:1029:ILE:HG12	1.67	0.76
2:B:324:ASN:N	2:B:324:ASN:HD22	1.81	0.76
2:F:259:LEU:O	2:F:345:LYS:HE3	1.86	0.76
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.65	0.76
2:F:324:ASN:H	2:F:324:ASN:HD22	1.34	0.76
1:C:967[A]:GLN:HG3	1:C:1054:LEU:HD13	1.68	0.76
1:E:157:ALA:HA	11:E:1237:HOH:O	1.84	0.76
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.85	0.76
1:A:228:CYS:SG	1:A:269:MET:HG2	2.26	0.76
2:D:345:LYS:HB3	2:D:346:PRO:HD2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:215:ARG:HH11	2:H:215:ARG:HG2	1.51	0.76
1:E:103:GLU:HG3	1:E:104:ARG:N	2.01	0.76
1:E:3:LYS:HB2	1:E:42:TYR:OH	1.85	0.75
2:H:71:GLU:O	2:H:203:ARG:HG3	1.87	0.75
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.21	0.75
1:G:57:ASP:HB3	1:G:59:GLU:OE1	1.86	0.75
2:B:322:PRO:HG2	2:B:324:ASN:HD21	1.51	0.75
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.22	0.75
2:D:227:ASP:CA	2:D:230:LYS:HD2	2.12	0.75
1:E:693:ALA:HB3	1:E:708:ILE:HD11	1.68	0.75
1:C:675:ARG:CD	1:C:675:ARG:H	1.99	0.75
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.69	0.74
1:A:726:GLU:HG3	1:A:727:ILE:N	2.00	0.74
2:D:50:ARG:HD2	2:D:50:ARG:N	2.01	0.74
9:E:1092:NET:H22	9:E:1092:NET:H42	1.66	0.74
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.16	0.74
1:C:1020:ARG:O	1:C:1024:GLU:HG3	1.87	0.74
2:B:324:ASN:H	2:B:324:ASN:HD22	1.36	0.74
2:D:8:VAL:HG22	2:D:14:GLN:HG2	1.70	0.74
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.69	0.74
2:D:228:VAL:HA	2:D:231:MET:HE2	1.68	0.74
2:D:282:LYS:HG3	2:D:320:THR:HG21	1.68	0.74
1:A:675:ARG:H	1:A:675:ARG:CD	1.99	0.73
1:A:1001:ILE:HD12	1:A:1002:GLN:N	2.03	0.73
2:B:139:ASP:OD2	2:B:142:LEU:HB2	1.89	0.73
1:G:64:THR:O	1:G:1065:VAL:HG23	1.88	0.73
2:D:226:GLU:O	2:D:230:LYS:HG3	1.87	0.73
2:H:16:HIS:O	2:H:113:ILE:HG22	1.88	0.73
1:A:449:VAL:N	11:A:1435:HOH:O	2.21	0.73
1:C:967[B]:GLN:HG2	1:C:1054:LEU:HD13	1.69	0.73
2:D:150:PHE:CE1	2:D:152:GLY:HA2	2.24	0.73
1:G:423:LYS:HB3	11:G:1397:HOH:O	1.89	0.73
2:H:50:ARG:HG3	2:H:50:ARG:HH11	1.52	0.73
2:F:154:ASN:ND2	2:F:285:LYS:HE2	2.04	0.72
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.24	0.72
1:E:331:THR:OG1	1:E:334:GLU:HG3	1.89	0.72
1:E:734:LEU:O	1:E:734:LEU:HD12	1.89	0.72
1:A:344:THR:HB	1:A:345:PRO:HD2	1.71	0.72
1:C:698:ILE:H	1:C:698:ILE:HD12	1.53	0.72
1:C:38:ARG:NH1	1:C:38:ARG:HG3	2.03	0.72
2:B:316:VAL:HG12	2:B:337:LEU:HD23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:THR:OG1	2:B:263:ILE:HG13	1.89	0.72
1:C:772:MET:SD	1:C:880:THR:HG22	2.30	0.72
2:H:33:ASN:HA	2:H:291:HIS:O	1.90	0.72
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.90	0.72
2:B:50:ARG:HG3	2:B:50:ARG:NH1	2.03	0.72
2:D:263:ILE:HG22	2:D:264:PRO:HD2	1.72	0.72
2:B:324:ASN:H	2:B:324:ASN:ND2	1.87	0.71
2:H:299:ASP:OD1	2:H:302:LYS:HD2	1.91	0.71
1:G:1004:ARG:HD3	1:G:1009[B]:GLU:OE2	1.91	0.71
1:G:1001:ILE:HD12	1:G:1029:ILE:CG1	2.21	0.71
2:B:286:MET:HE1	2:B:315:ALA:HB2	1.73	0.71
1:E:967[B]:GLN:NE2	1:E:1054:LEU:HB3	2.06	0.70
2:B:246:ALA:HB1	2:B:248:ASP:CG	2.12	0.70
2:F:376:GLN:HA	2:F:379:LYS:HZ2	1.56	0.70
2:F:286:MET:HG2	11:F:1893:HOH:O	1.91	0.70
1:C:321:LYS:HE3	11:C:1621:HOH:O	1.91	0.70
1:C:670:ASP:HB3	1:C:677:ARG:NH2	2.05	0.70
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.06	0.70
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.72	0.70
2:B:205:ILE:HG13	2:B:355:GLU:HG3	1.74	0.70
1:E:1:MET:HB2	1:E:224:LYS:NZ	2.07	0.70
1:E:734:LEU:HD11	1:E:738:PHE:CE2	2.27	0.70
1:C:1:MET:HB2	1:C:224:LYS:NZ	2.05	0.70
1:G:668:ALA:O	1:G:671:ARG:HB2	1.92	0.69
1:A:930:LYS:HE3	11:A:1156:HOH:O	1.92	0.69
1:C:873:SER:O	1:C:877:GLN:HG3	1.93	0.69
1:A:38:ARG:NH1	1:A:38:ARG:HG3	2.00	0.69
2:B:190:LEU:HD13	2:B:214:CYS:O	1.91	0.69
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.27	0.69
1:G:726:GLU:HG3	1:G:727:ILE:H	1.57	0.69
2:F:324:ASN:O	2:F:342:ARG:HD2	1.93	0.69
2:B:324:ASN:O	2:B:342:ARG:HD2	1.91	0.69
2:H:326:ARG:O	2:H:340:ILE:HG22	1.93	0.69
2:B:279:SER:O	2:B:322:PRO:HG3	1.93	0.69
1:C:1063:ILE:HG12	1:C:1067:GLU:OE2	1.93	0.69
2:F:254:ALA:O	2:F:257:LYS:HB2	1.92	0.68
1:G:901:PRO:HD2	6:G:1086:CL:CL	2.30	0.68
1:E:644:GLY:O	1:E:647:PRO:HD2	1.92	0.68
1:E:726:GLU:HG3	1:E:727:ILE:H	1.56	0.68
2:H:334:ASP:OD2	2:H:336:THR:HG23	1.94	0.68
1:A:784:GLN:NE2	1:A:784:GLN:H	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:PHE:CE1	2:H:152:GLY:HA2	2.27	0.68
1:G:652[A]:ARG:NH1	1:G:667:ASP:HA	2.09	0.68
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.76	0.68
1:C:833:LYS:O	1:C:836:GLU:HB2	1.94	0.68
2:H:133:ILE:HD12	2:H:143:ALA:CB	2.22	0.67
1:C:228:CYS:SG	1:C:269:MET:HG2	2.34	0.67
1:G:1027:ARG:HE	1:G:1031:ARG:HD3	1.59	0.67
1:C:43:ARG:NH2	1:C:81:GLU:OE2	2.28	0.67
1:A:1:MET:HG3	1:A:2:PRO:HD2	1.75	0.67
1:G:967[A]:GLN:HG3	1:G:1054:LEU:HD13	1.76	0.67
2:D:227:ASP:O	2:D:230:LYS:HB2	1.95	0.67
2:B:322:PRO:CG	2:B:324:ASN:HD21	2.08	0.67
1:A:703:GLU:O	1:A:706:LYS:HB2	1.94	0.67
2:F:157:ASP:HB3	2:F:160:LYS:HE2	1.76	0.67
1:A:343:ARG:HD3	11:A:1715:HOH:O	1.92	0.67
2:B:50:ARG:N	2:B:50:ARG:HD2	1.99	0.67
2:D:50:ARG:HH11	2:D:50:ARG:HG3	1.58	0.67
1:E:1021:ARG:HD3	1:E:1025:ASP:OD2	1.94	0.67
1:C:1:MET:HG3	1:C:2:PRO:HD2	1.77	0.67
1:G:716:PRO:HA	1:G:750:VAL:HG22	1.77	0.67
1:A:40:GLU:HG2	1:A:325:LYS:HE2	1.77	0.67
2:B:225:ALA:O	2:B:228:VAL:HB	1.94	0.67
2:B:228:VAL:HA	2:B:231:MET:CE	2.25	0.67
1:E:905:PRO:HB2	1:E:1040:TYR:OH	1.95	0.67
2:B:322:PRO:HB2	2:B:324:ASN:ND2	2.09	0.67
2:H:192:PHE:O	2:H:215:ARG:HB3	1.95	0.67
2:D:282:LYS:HG3	2:D:320:THR:CG2	2.24	0.67
2:B:263:ILE:HG22	2:B:264:PRO:HD2	1.77	0.67
1:G:479:VAL:HG23	1:G:483:GLY:HA3	1.77	0.66
2:B:222:GLN:HB2	11:B:3567:HOH:O	1.95	0.66
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.77	0.66
1:G:687:LEU:HD13	1:G:812:GLN:HG2	1.76	0.66
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.76	0.66
2:B:228:VAL:HA	2:B:231:MET:HE2	1.77	0.66
1:G:863:LYS:O	1:G:866:ALA:HB3	1.94	0.66
1:C:726:GLU:HG3	1:C:727:ILE:H	1.59	0.66
2:B:228:VAL:HG11	2:B:258:PHE:CE1	2.30	0.66
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.77	0.66
2:B:153:LEU:O	2:B:156:MET:HB2	1.95	0.66
1:C:419:GLU:HG2	11:C:1718:HOH:O	1.95	0.66
2:D:139:ASP:OD2	2:D:142:LEU:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.76	0.66
1:G:735:ARG:O	1:G:738:PHE:N	2.29	0.66
2:B:286:MET:HG2	11:B:3570:HOH:O	1.94	0.66
1:E:757:ASP:O	1:E:833:LYS:NZ	2.28	0.66
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.23	0.66
2:D:50:ARG:NH1	2:D:50:ARG:HG3	2.11	0.66
1:C:482:THR:HB	11:C:1747:HOH:O	1.96	0.66
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.78	0.66
1:G:803:GLN:HG3	1:G:807:ASP:OD1	1.96	0.66
1:E:698:ILE:CD1	1:E:698:ILE:H	2.09	0.66
1:E:907:LEU:HD11	8:E:1091:ORN:HD3	1.76	0.66
2:H:40:GLN:OE1	2:H:69:ASP:HB2	1.95	0.66
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.27	0.65
2:F:244:ASP:OD2	2:F:245:PRO:HD2	1.97	0.65
2:B:228:VAL:HG12	2:B:229:LEU:N	2.10	0.65
1:G:873:SER:O	1:G:877:GLN:HG3	1.97	0.65
1:E:43:ARG:NH2	1:E:81:GLU:OE2	2.30	0.65
1:G:475[C]:LYS:HD3	1:G:488:PHE:CZ	2.32	0.65
1:C:703:GLU:O	1:C:706:LYS:HB2	1.97	0.65
1:A:735:ARG:O	1:A:738:PHE:N	2.29	0.65
1:C:671:ARG:NH2	1:C:819:GLU:O	2.30	0.65
1:A:509:ARG:NH1	1:A:512[A]:GLU:OE1	2.29	0.65
1:A:814:GLN:NE2	11:A:1532:HOH:O	2.30	0.65
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.79	0.65
1:G:24:CYS:HB2	1:G:604:GLU:HB2	1.79	0.65
1:A:289:ASN:HB3	1:A:292:ASN:OD1	1.97	0.65
2:H:33:ASN:OD1	2:H:292:GLY:HA2	1.97	0.65
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.96	0.65
1:E:726:GLU:OE1	1:E:1020:ARG:NE	2.30	0.64
1:G:475[A]:LYS:HD3	1:G:488:PHE:CZ	2.32	0.64
2:H:262:ASP:OD1	2:H:345:LYS:NZ	2.31	0.64
2:D:228:VAL:HG22	2:D:231:MET:CE	2.27	0.64
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.32	0.64
1:G:954:LYS:O	1:G:957:VAL:HG12	1.96	0.64
1:A:696:THR:HB	1:A:700:MET:SD	2.37	0.64
1:E:703:GLU:O	1:E:706:LYS:HB2	1.97	0.64
2:H:139:ASP:OD2	2:H:142:LEU:HB2	1.97	0.64
1:G:417:ASP:OD1	1:G:423:LYS:NZ	2.29	0.64
2:H:34:THR:HA	2:H:56:THR:OG1	1.97	0.64
1:G:4:ARG:HD3	1:G:7:ILE:HD12	1.79	0.64
2:B:71:GLU:O	2:B:203:ARG:HG3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:THR:HB	1:A:345:PRO:CD	2.27	0.64
2:B:228:VAL:HG11	2:B:258:PHE:CZ	2.33	0.64
9:G:1092:NET:H42	9:G:1092:NET:H22	1.79	0.64
1:G:781:HIS:CE1	1:G:789:SER:HB2	2.33	0.64
1:G:738:PHE:O	1:G:741:ALA:HB3	1.97	0.64
2:H:248:ASP:N	2:H:248:ASP:OD2	2.29	0.64
1:A:946:LEU:C	1:A:947:LEU:HD12	2.18	0.64
1:G:702:VAL:HG11	1:G:735:ARG:NH2	2.13	0.64
1:E:1:MET:HB2	1:E:224:LYS:HE3	1.80	0.64
1:G:321:LYS:NZ	1:G:611:ASP:OD1	2.30	0.64
2:H:286:MET:HE1	2:H:312:HIS:HE1	1.62	0.64
2:D:158:LEU:O	2:D:161:GLU:HB2	1.98	0.64
1:G:1:MET:HB2	1:G:224:LYS:CE	2.28	0.64
1:G:950:ARG:NH1	11:G:1675:HOH:O	2.31	0.64
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.78	0.64
1:G:339:ILE:HD11	1:G:531:THR:HG23	1.79	0.63
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.27	0.63
2:H:215:ARG:HG2	2:H:215:ARG:NH1	2.13	0.63
1:A:425[B]:ARG:NH2	11:A:1745:HOH:O	2.31	0.63
1:E:321:LYS:NZ	1:E:611:ASP:OD1	2.30	0.63
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.61	0.63
2:D:120:ARG:NH2	11:D:2337:HOH:O	2.29	0.63
2:D:201:ALA:HB2	2:D:239:SER:CB	2.28	0.63
2:B:344:ASP:O	2:B:345:LYS:HD3	1.99	0.63
1:A:1001:ILE:HD12	1:A:1002:GLN:HB2	1.79	0.63
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.79	0.63
2:F:194:VAL:HG13	2:F:235:GLY:O	1.98	0.63
1:A:375:THR:HG23	1:A:377:GLN:H	1.63	0.63
1:C:693:ALA:HB1	1:C:704:LYS:HG2	1.81	0.63
1:E:1:MET:N	11:E:1623:HOH:O	2.30	0.63
2:F:8:VAL:HG22	2:F:14:GLN:HG2	1.80	0.63
1:A:698:ILE:H	1:A:698:ILE:HD12	1.63	0.63
2:H:46:PRO:HG2	2:H:200:GLY:O	1.99	0.63
1:E:698:ILE:O	1:E:702:VAL:HG23	1.98	0.63
1:E:1:MET:HB2	1:E:224:LYS:CE	2.29	0.63
2:H:74:GLN:HA	11:H:475:HOH:O	1.98	0.63
1:C:495:LYS:NZ	11:C:1740:HOH:O	2.27	0.63
1:C:32:GLN:OE1	1:C:320:ALA:HB3	1.98	0.62
2:F:195:VAL:HG23	2:F:233:PRO:HB3	1.81	0.62
2:D:286:MET:HB2	2:D:313:GLY:O	1.98	0.62
2:D:153:LEU:O	2:D:156:MET:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:HIS:ND1	2:B:355:GLU:OE1	2.30	0.62
1:E:812:GLN:NE2	11:E:1791:HOH:O	2.27	0.62
1:E:493:LYS:HE2	1:E:517:ARG:HD3	1.82	0.62
2:F:324:ASN:HD22	2:F:324:ASN:N	1.97	0.62
2:D:228:VAL:HA	2:D:231:MET:HE3	1.80	0.62
1:G:974:THR:O	1:G:975:HIS:C	2.38	0.62
2:H:46:PRO:HA	2:H:76:HIS:CG	2.35	0.62
1:C:65:TYR:OH	1:C:80:LYS:HE2	1.99	0.62
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.33	0.62
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.30	0.62
1:C:698:ILE:O	1:C:702:VAL:HG23	1.99	0.62
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.13	0.62
1:G:1037:LYS:HE2	11:G:1756:HOH:O	1.98	0.62
1:G:762:VAL:HG13	1:G:779:MET:O	2.00	0.62
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.82	0.62
2:H:5:ALA:CB	2:H:110:ILE:HG13	2.30	0.62
2:H:27:VAL:HG22	2:H:131:CYS:CB	2.08	0.62
2:F:251:ALA:O	2:F:252:ILE:C	2.38	0.62
1:E:997:GLY:O	1:E:1000:HIS:HB3	2.00	0.62
1:G:488:PHE:O	1:G:491:GLN:N	2.33	0.62
1:A:563:MET:CE	1:A:635:PRO:HG3	2.30	0.62
2:H:286:MET:CE	2:H:315:ALA:HB2	2.29	0.62
2:H:5:ALA:HB3	2:H:110:ILE:HG13	1.82	0.62
2:B:245:PRO:HD3	2:B:270:LEU:CD1	2.27	0.62
2:D:228:VAL:O	2:D:231:MET:HG3	2.00	0.62
2:D:26:ALA:O	2:D:131:CYS:HA	2.00	0.62
1:E:675:ARG:CD	1:E:675:ARG:H	2.12	0.62
1:E:698:ILE:N	1:E:698:ILE:HD12	2.14	0.61
1:G:76:LYS:HE3	11:G:1740:HOH:O	1.99	0.61
1:G:400:ARG:HD3	11:G:1373:HOH:O	2.00	0.61
1:E:784:GLN:H	1:E:784:GLN:NE2	1.98	0.61
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.35	0.61
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.34	0.61
2:B:247:PRO:HA	2:B:252:ILE:CD1	2.30	0.61
2:H:144:LEU:O	2:H:144:LEU:HD12	2.00	0.61
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.63	0.61
1:G:1063:ILE:HG13	1:G:1067:GLU:OE2	1.99	0.61
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.29	0.61
1:A:738:PHE:O	1:A:741:ALA:HB3	2.01	0.61
1:E:967[B]:GLN:HE21	1:E:1054:LEU:CD1	2.13	0.61
1:G:354:TYR:HB2	1:G:388:GLY:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:236:ILE:HD12	2:H:263:ILE:HG21	1.82	0.61
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.28	0.61
1:C:698:ILE:N	1:C:698:ILE:HD12	2.14	0.61
1:C:44:VAL:N	1:C:62:ASP:OD2	2.29	0.61
1:G:65:TYR:CG	1:G:77:ILE:HD13	2.36	0.61
1:G:617:TYR:CG	1:G:629:ILE:HD13	2.35	0.61
1:C:998:ARG:CB	1:C:999:PRO:HA	2.30	0.61
1:E:1002:GLN:NE2	1:E:1006:LYS:HE3	2.12	0.61
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.19	0.60
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.19	0.60
2:H:324:ASN:N	2:H:324:ASN:ND2	2.30	0.60
1:G:804:GLU:O	1:G:808:VAL:HG23	2.00	0.60
2:H:342:ARG:HB3	2:H:344:ASP:OD2	2.01	0.60
1:G:946:LEU:CD1	1:G:991:VAL:HG11	2.31	0.60
1:E:509:ARG:HH11	1:E:509:ARG:HB3	1.66	0.60
1:C:17:PRO:HG3	1:C:917:VAL:HG13	1.83	0.60
1:C:1020:ARG:O	1:C:1020:ARG:HG3	2.01	0.60
1:C:956:ARG:HB3	1:C:1044:LEU:HD21	1.82	0.60
1:G:471:ARG:HD2	11:G:1643:HOH:O	2.00	0.60
1:G:1021:ARG:HG3	1:G:1021:ARG:HH11	1.66	0.60
2:B:34:THR:HA	2:B:56:THR:OG1	2.02	0.60
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.48	0.60
1:C:822:VAL:O	1:C:823:ARG:HD3	2.01	0.60
1:E:527:LYS:HD2	2:F:116:ARG:HD3	1.84	0.60
2:B:246:ALA:HB1	2:B:248:ASP:OD2	2.01	0.60
2:D:178:THR:HG22	2:D:179:GLY:N	2.15	0.60
2:B:237:PHE:HE1	2:B:268:ILE:HG13	1.66	0.60
2:B:245:PRO:CG	2:B:274:LEU:HD21	2.32	0.60
2:F:247:PRO:HA	2:F:252:ILE:HD13	1.82	0.60
2:B:232:ASN:N	2:B:233:PRO:HD3	2.16	0.60
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.36	0.60
2:H:367:PHE:O	2:H:370:PHE:HB3	2.01	0.60
1:C:907:LEU:HD11	8:C:1091:ORN:HD3	1.84	0.60
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.84	0.60
1:G:772:MET:HE2	1:G:880:THR:HA	1.82	0.60
1:E:257:THR:HG22	2:F:63:VAL:HG21	1.84	0.60
1:A:948:SER:OG	10:A:1091:U:H5"	2.01	0.60
2:H:232:ASN:N	2:H:233:PRO:HD3	2.17	0.59
1:A:994:VAL:HG23	1:A:1001:ILE:HD11	1.82	0.59
2:H:29:GLU:CD	2:H:153:LEU:HD22	2.22	0.59
2:H:50:ARG:HD2	2:H:50:ARG:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:THR:HB	1:E:345:PRO:HD2	1.83	0.59
2:F:300:VAL:HG22	2:F:328:THR:O	2.01	0.59
1:C:698:ILE:H	1:C:698:ILE:CD1	2.14	0.59
1:E:1021:ARG:CG	1:E:1021:ARG:HH11	2.15	0.59
1:G:620:PRO:HB2	1:G:622:THR:HG23	1.83	0.59
1:A:695:VAL:CG1	1:A:700:MET:HB3	2.30	0.59
1:E:1073:LYS:HD2	1:E:1073:LYS:N	2.17	0.59
2:D:282:LYS:HG3	2:D:320:THR:CB	2.32	0.59
2:B:78:GLN:HG2	11:B:3896:HOH:O	2.03	0.59
1:C:552:GLU:HB3	11:C:1775:HOH:O	2.01	0.59
2:F:41:GLU:CB	2:F:358:PRO:HD3	2.33	0.59
1:C:519:GLN:NE2	11:C:1768:HOH:O	2.32	0.59
2:D:157:ASP:OD2	2:D:160:LYS:HG2	2.03	0.59
2:B:269:CYS:O	2:B:272:HIS:HB3	2.02	0.59
1:C:237:PHE:CE2	1:C:458:ILE:HD13	2.38	0.59
1:G:905:PRO:HB2	1:G:1040:TYR:OH	2.02	0.59
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.49	0.59
1:A:693:ALA:HB2	1:A:708:ILE:HD11	1.84	0.59
1:C:784:GLN:H	1:C:784:GLN:HE21	1.50	0.59
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.68	0.59
1:G:734:LEU:O	1:G:734:LEU:HD12	2.02	0.59
2:H:215:ARG:HH11	2:H:215:ARG:CG	2.16	0.59
1:G:597:ILE:HG12	1:G:615:ARG:HB2	1.85	0.59
1:A:115:MET:HG2	1:A:118:ALA:O	2.01	0.59
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.85	0.58
1:E:904:ASP:O	1:E:906:LEU:N	2.36	0.58
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.39	0.58
1:C:713:VAL:HG23	1:C:755:PHE:HB2	1.84	0.58
1:C:1:MET:N	1:C:224:LYS:HE3	2.17	0.58
1:C:1021:ARG:HH11	1:C:1021:ARG:HG3	1.67	0.58
2:B:245:PRO:HG2	2:B:274:LEU:CD2	2.34	0.58
1:G:698:ILE:O	1:G:702:VAL:HG23	2.03	0.58
2:F:376:GLN:HA	2:F:379:LYS:NZ	2.18	0.58
2:F:322:PRO:CD	2:F:325:LEU:HD12	2.33	0.58
2:H:247:PRO:HA	2:H:252:ILE:CD1	2.31	0.58
1:C:17:PRO:HG3	1:C:917:VAL:CG1	2.33	0.58
2:F:92:PHE:CE1	2:F:93:ARG:HG2	2.38	0.58
1:A:417:ASP:OD1	1:A:423:LYS:NZ	2.30	0.58
2:H:153:LEU:O	2:H:156:MET:HB2	2.03	0.58
1:G:761:GLU:HG2	1:G:781:HIS:CE1	2.39	0.58
1:G:676:GLU:O	1:G:680:HIS:ND1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.38	0.58
1:G:773:VAL:HG21	1:G:817:ALA:CB	2.33	0.58
2:B:272:HIS:ND1	2:B:349:SER:OG	2.32	0.58
1:C:646:THR:HB	1:C:647:PRO:HD3	1.86	0.58
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.19	0.58
1:E:440:ALA:O	1:E:444:ARG:HG3	2.03	0.58
1:G:79:GLU:HG2	1:G:111:PHE:CE2	2.38	0.58
1:G:481:ILE:HA	1:G:484:LEU:HD12	1.86	0.58
2:B:345:LYS:HB3	2:B:346:PRO:HD2	1.84	0.58
1:C:1:MET:H3	1:C:224:LYS:HE3	1.69	0.58
2:F:186:LYS:HB2	2:F:189:GLU:OE2	2.04	0.58
2:D:275:LEU:HD23	2:D:349:SER:OG	2.04	0.58
1:G:784:GLN:N	1:G:784:GLN:NE2	2.36	0.58
1:E:735:ARG:O	1:E:738:PHE:N	2.37	0.58
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.85	0.58
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.38	0.57
2:B:46:PRO:HA	2:B:76:HIS:CG	2.39	0.57
1:C:60[B]:MET:HE3	11:C:1146:HOH:O	2.04	0.57
2:H:201:ALA:HB2	2:H:239:SER:CB	2.34	0.57
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.34	0.57
1:E:340:THR:O	1:E:343:ARG:HB2	2.04	0.57
1:C:814:GLN:HG3	1:C:818:PHE:HE2	1.69	0.57
1:G:118:ALA:HA	11:G:1763:HOH:O	2.03	0.57
1:G:702:VAL:O	1:G:706:LYS:HD2	2.05	0.57
1:G:902:GLY:O	1:G:1027:ARG:NH2	2.38	0.57
1:G:32:GLN:OE1	1:G:320:ALA:HB3	2.04	0.57
2:H:272:HIS:HA	2:H:349:SER:CB	2.32	0.57
1:A:1072:ILE:C	1:A:1073:LYS:HD2	2.24	0.57
1:A:726:GLU:HG3	1:A:727:ILE:H	1.67	0.57
1:G:1021:ARG:CG	1:G:1021:ARG:HH11	2.17	0.57
11:G:1440:HOH:O	2:H:123:ARG:HD2	2.02	0.57
1:C:678:PHE:CE1	1:C:842:VAL:HG23	2.40	0.57
1:G:168:ILE:CG2	1:G:204:LEU:HD22	2.34	0.57
1:C:157:ALA:O	1:C:160:ALA:HB3	2.05	0.57
2:H:361:HIS:ND1	11:H:399:HOH:O	2.30	0.57
2:H:142:LEU:O	2:H:146:LYS:HG3	2.05	0.57
1:C:419:GLU:HB3	1:C:423[B]:LYS:NZ	2.18	0.57
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.19	0.57
2:H:369:HIS:O	2:H:372:GLU:HB2	2.05	0.57
1:E:1006:LYS:O	1:E:1006:LYS:HG3	2.04	0.57
1:G:702:VAL:HG13	1:G:731:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:225:ALA:HB2	2:D:254:ALA:HB1	1.87	0.57
1:C:24:CYS:SG	1:C:576:ILE:HD12	2.44	0.57
1:G:516:LEU:HD11	1:G:520:TYR:CZ	2.40	0.57
1:G:105:GLN:HA	1:G:105:GLN:NE2	2.20	0.57
1:G:965:LEU:HG	1:G:971:LEU:HD11	1.87	0.57
1:E:947:LEU:N	1:E:947:LEU:HD12	2.20	0.57
1:A:460:ARG:HG3	11:A:1299:HOH:O	2.04	0.57
1:A:936:ASN:HB2	11:A:1109:HOH:O	2.04	0.57
1:G:695:VAL:CG1	1:G:700:MET:HB3	2.34	0.57
2:H:286:MET:HE2	2:H:315:ALA:HB2	1.87	0.56
1:E:158:VAL:HG11	1:E:206:ILE:HB	1.86	0.56
2:B:324:ASN:N	2:B:324:ASN:ND2	2.45	0.56
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.69	0.56
1:A:1001:ILE:O	1:A:1005:ILE:HG13	2.06	0.56
2:D:201:ALA:HA	2:D:240:ASN:OD1	2.05	0.56
2:B:237:PHE:CE1	2:B:268:ILE:HG13	2.41	0.56
1:C:814:GLN:HG3	1:C:818:PHE:CE2	2.39	0.56
2:B:150:PHE:CE1	2:B:152:GLY:HA2	2.40	0.56
1:C:51:PRO:HG3	1:C:918:MET:HB2	1.86	0.56
1:E:417:ASP:OD2	1:E:418:PRO:HD2	2.04	0.56
2:H:342:ARG:NH2	2:H:344:ASP:OD1	2.33	0.56
1:A:730:ASP:H	1:A:733:ASP:HB2	1.71	0.56
1:E:503:ALA:HB1	1:E:508:VAL:O	2.06	0.56
2:F:290:HIS:HB2	2:F:312:HIS:CD2	2.40	0.56
1:E:950:ARG:HD3	11:E:1593:HOH:O	2.04	0.56
2:H:133:ILE:HD11	2:H:143:ALA:HA	1.87	0.56
1:C:423[A]:LYS:HE2	11:C:1420:HOH:O	2.04	0.56
1:E:142:GLU:OE2	1:E:294:ARG:NH2	2.38	0.56
1:G:695:VAL:HG11	1:G:701:ALA:N	2.21	0.56
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.87	0.56
1:G:698:ILE:N	1:G:698:ILE:HD12	2.20	0.56
1:A:698:ILE:O	1:A:702:VAL:HG23	2.06	0.56
2:H:295:HIS:HD2	2:H:296:PRO:O	1.89	0.56
1:G:703:GLU:HA	1:G:706:LYS:HD3	1.88	0.56
1:E:1057:ASP:HB3	1:E:1060:GLU:HB2	1.87	0.56
1:C:695:VAL:HG21	1:C:701:ALA:CA	2.28	0.55
1:G:223:ASP:OD1	1:G:225:ASN:N	2.39	0.55
2:D:345:LYS:HB3	2:D:346:PRO:CD	2.35	0.55
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.70	0.55
1:E:995:HIS:ND1	11:E:1847:HOH:O	2.33	0.55
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ARG:HD3	1:C:571:ARG:N	2.21	0.55
1:A:40:GLU:HG3	1:A:325:LYS:HE2	1.88	0.55
1:E:967[B]:GLN:NE2	1:E:1054:LEU:HD13	2.17	0.55
1:E:703:GLU:HA	1:E:706:LYS:HD3	1.89	0.55
2:D:201:ALA:HB2	2:D:239:SER:HB2	1.87	0.55
2:H:363:ALA:O	2:H:366:LEU:HD13	2.06	0.55
1:G:874:LEU:HB3	1:G:879:VAL:O	2.05	0.55
1:E:494:ARG:HG2	1:E:547:TYR:HB2	1.89	0.55
2:H:218:ILE:N	2:H:218:ILE:HD13	2.21	0.55
1:G:950:ARG:HG2	1:G:1016:THR:OG1	2.07	0.55
2:B:298:LYS:HE2	2:B:303:ASN:OD1	2.06	0.55
1:E:956:ARG:HB3	1:E:1044:LEU:CD2	2.36	0.55
2:F:153:LEU:HG	2:F:158:LEU:HD11	1.88	0.55
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.72	0.55
1:C:423[B]:LYS:NZ	11:C:1420:HOH:O	2.38	0.55
1:G:802:SER:O	1:G:806:GLN:HG3	2.07	0.55
1:E:108:LEU:HB2	11:E:1179:HOH:O	2.07	0.55
1:G:274:GLU:HB2	11:G:1205:HOH:O	2.06	0.55
2:B:168:TYR:O	2:B:218:ILE:N	2.29	0.55
1:E:1061:LYS:NZ	11:E:1828:HOH:O	2.39	0.55
1:A:130[A]:ARG:NE	11:A:1197:HOH:O	2.38	0.55
1:G:645[A]:GLN:HG3	1:G:649:LYS:HE3	1.89	0.55
2:F:224:SER:OG	2:F:227:ASP:HB2	2.07	0.55
2:B:263:ILE:CG2	2:B:264:PRO:HD2	2.36	0.55
1:C:1:MET:HB2	1:C:224:LYS:HZ1	1.72	0.55
1:A:76:LYS:HD3	11:A:1163:HOH:O	2.07	0.55
1:C:509:ARG:HD3	11:C:1763:HOH:O	2.07	0.55
1:E:3:LYS:NZ	11:E:1094:HOH:O	2.39	0.55
1:A:1001:ILE:HD12	1:A:1002:GLN:H	1.69	0.55
1:G:948:SER:OG	10:G:1093:U:H5"	2.07	0.55
2:B:172:GLN:O	2:B:207:ARG:HA	2.07	0.55
1:G:128:ASP:CG	1:G:131:ARG:HG3	2.27	0.55
1:C:64:THR:O	1:C:1065:VAL:HG23	2.07	0.54
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.89	0.54
1:A:446:GLY:O	1:E:447:LEU:HD23	2.07	0.54
1:G:213:TRP:CZ3	1:G:296:ILE:HD12	2.42	0.54
2:H:350:PHE:CG	2:H:366:LEU:HD21	2.42	0.54
1:C:321:LYS:NZ	1:C:611:ASP:OD1	2.40	0.54
2:H:186:LYS:O	2:H:189:GLU:HB2	2.06	0.54
1:A:701:ALA:O	1:A:705:ALA:N	2.30	0.54
1:E:1:MET:N	1:E:224:LYS:HE3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:788:HIS:ND1	1:G:911:MET:HB2	2.23	0.54
2:D:205:ILE:HG13	2:D:355:GLU:HG3	1.89	0.54
1:A:588:ALA:HB2	1:A:863:LYS:HG2	1.90	0.54
1:C:46:LEU:HD12	1:C:46:LEU:C	2.28	0.54
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.89	0.54
1:G:1001:ILE:HD11	11:G:1537:HOH:O	2.07	0.54
2:H:334:ASP:CG	2:H:336:THR:HG23	2.28	0.54
1:C:661:VAL:HB	11:C:1801:HOH:O	2.08	0.54
1:A:646:THR:HB	1:A:647:PRO:HD3	1.88	0.54
2:F:342:ARG:HB3	2:F:345:LYS:H	1.71	0.54
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.21	0.54
1:A:167:ILE:N	1:A:167:ILE:HD12	2.21	0.54
1:G:294:ARG:HD2	6:G:1085:CL:CL	2.45	0.54
2:D:324:ASN:N	2:D:324:ASN:ND2	2.41	0.54
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.89	0.54
2:F:228:VAL:O	2:F:231:MET:HG3	2.08	0.54
1:A:833:LYS:O	1:A:836:GLU:HB2	2.08	0.54
1:G:991:VAL:HG21	1:G:1001:ILE:HG22	1.89	0.54
2:B:355:GLU:OE2	2:B:355:GLU:N	2.30	0.54
2:F:50:ARG:N	2:F:50:ARG:HD2	2.21	0.54
2:B:201:ALA:HB2	2:B:239:SER:CB	2.38	0.54
2:H:257:LYS:O	2:H:261:THR:HG23	2.06	0.54
1:E:670:ASP:HB2	11:E:1785:HOH:O	2.08	0.54
2:B:364:ALA:N	2:B:365:PRO:HD2	2.23	0.54
2:H:132:ILE:HG22	2:H:133:ILE:N	2.23	0.54
1:C:905:PRO:HB2	1:C:1040:TYR:HH	1.70	0.54
1:G:967[B]:GLN:HG2	1:G:1054:LEU:HD13	1.90	0.54
1:E:185:ARG:NH2	11:E:1238:HOH:O	2.40	0.54
1:C:762:VAL:HG13	1:C:779:MET:O	2.08	0.54
2:D:10:GLU:OE2	2:D:129:ASN:N	2.29	0.54
1:C:43:ARG:HA	1:C:62:ASP:OD2	2.08	0.54
2:H:69:ASP:HA	11:H:500:HOH:O	2.07	0.54
2:F:50:ARG:HG2	2:F:158:LEU:HD22	1.90	0.54
1:E:901:PRO:HD2	6:E:1086:CL:CL	2.45	0.54
1:E:125:LYS:NZ	11:E:1188:HOH:O	2.41	0.54
1:E:144:ALA:HB1	1:E:208:GLU:CG	2.38	0.54
2:D:277:LEU:HD23	2:D:281:ALA:O	2.08	0.54
1:G:1067:GLU:O	1:G:1068:MET:C	2.46	0.53
2:H:363:ALA:C	2:H:365:PRO:HD2	2.28	0.53
2:H:275:LEU:HD23	2:H:349:SER:CB	2.39	0.53
1:G:698:ILE:HD12	1:G:698:ILE:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:HB2	1:E:224:LYS:HZ2	1.73	0.53
2:D:272:HIS:HA	2:D:349:SER:HB2	1.88	0.53
1:C:827:ASN:HB3	1:C:843:ASN:HB2	1.90	0.53
2:B:6:LEU:HD12	2:B:7:LEU:N	2.23	0.53
9:A:1090:NET:H82	9:A:1090:NET:H62	1.91	0.53
2:D:262:ASP:HB2	11:D:2882:HOH:O	2.08	0.53
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.44	0.53
1:E:1051:ALA:O	1:E:1054:LEU:HB2	2.08	0.53
1:G:622:THR:O	1:G:626:VAL:HG23	2.08	0.53
1:A:941:LYS:NZ	1:A:1056:ALA:O	2.33	0.53
1:E:734:LEU:C	1:E:734:LEU:HD12	2.28	0.53
1:G:139:ILE:HD11	1:G:141:LEU:HD12	1.90	0.53
2:F:350:PHE:HB2	2:F:366:LEU:CD2	2.39	0.53
1:E:482:THR:HB	11:E:1442:HOH:O	2.08	0.53
1:A:772[B]:MET:SD	1:A:880:THR:HG22	2.49	0.53
2:F:43:LEU:HD21	2:F:80:LEU:HD13	1.90	0.53
2:H:45:ASP:HB3	2:H:48:TYR:HD2	1.74	0.53
1:E:675:ARG:HD3	1:E:675:ARG:H	1.72	0.53
2:H:236:ILE:HD12	2:H:263:ILE:CG2	2.38	0.53
1:C:1019:GLY:O	1:C:1023:ILE:HD12	2.08	0.53
1:E:954:LYS:O	1:E:980:VAL:HG11	2.09	0.53
1:C:171:SER:HB2	1:C:203:GLU:HB3	1.90	0.53
1:G:710:TYR:HB3	1:G:729:TYR:O	2.07	0.53
1:A:709:GLY:O	1:A:754:HIS:ND1	2.41	0.53
2:H:275:LEU:HD23	2:H:349:SER:OG	2.09	0.53
1:G:946:LEU:HD11	1:G:991:VAL:HG11	1.89	0.53
2:B:322:PRO:HG2	2:B:324:ASN:ND2	2.21	0.53
1:G:423:LYS:HA	1:G:426[B]:ARG:NH2	2.24	0.53
2:H:236:ILE:CD1	2:H:263:ILE:HG21	2.39	0.53
2:F:41:GLU:HB2	2:F:358:PRO:HD3	1.91	0.53
1:A:70:HIS:O	1:A:74:VAL:HG23	2.09	0.53
2:H:8:VAL:HG12	2:H:9:LEU:N	2.24	0.53
2:F:201:ALA:HB2	2:F:239:SER:CB	2.38	0.53
2:H:205:ILE:HG13	2:H:355:GLU:HG3	1.90	0.53
2:H:279:SER:OG	2:H:342:ARG:NH1	2.30	0.53
2:B:49:SER:O	2:B:50:ARG:HB2	2.08	0.53
1:C:1051:ALA:O	1:C:1054:LEU:HB2	2.07	0.53
1:A:979:ILE:O	1:A:983:GLU:HG3	2.08	0.53
1:G:272:LEU:HD21	1:G:282:SER:HB2	1.89	0.53
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.91	0.53
1:C:1:MET:CG	1:C:2:PRO:HD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.08	0.53
2:B:367:PHE:O	2:B:370:PHE:HB3	2.08	0.53
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.08	0.53
1:A:665:SER:O	1:A:669:ILE:HG13	2.09	0.53
2:D:188:ASP:N	2:D:188:ASP:OD2	2.31	0.53
1:G:100:LEU:HD12	1:G:100:LEU:N	2.24	0.53
1:G:751:LEU:O	1:G:752:LEU:HD12	2.08	0.52
2:B:50:ARG:HH11	2:B:50:ARG:CG	2.18	0.52
2:B:247:PRO:HA	2:B:252:ILE:HD12	1.90	0.52
1:A:695:VAL:HG12	1:A:696:THR:N	2.22	0.52
2:H:48:TYR:O	2:H:51:GLN:HB2	2.09	0.52
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.90	0.52
2:F:41:GLU:HB3	2:F:358:PRO:HD3	1.92	0.52
1:G:237:PHE:HB3	1:G:248:ILE:HB	1.91	0.52
1:G:17:PRO:HG3	1:G:917:VAL:HG13	1.90	0.52
1:C:992:ASN:ND2	1:E:975:HIS:NE2	2.57	0.52
1:G:1:MET:HB2	1:G:224:LYS:HE3	1.90	0.52
1:E:726:GLU:HG3	1:E:727:ILE:N	2.24	0.52
1:E:278:GLU:HG2	11:E:1310:HOH:O	2.09	0.52
1:G:178:GLY:HA3	1:G:198:LEU:HD23	1.91	0.52
1:C:419:GLU:CB	1:C:423[B]:LYS:NZ	2.73	0.52
2:F:193:HIS:O	2:F:234:ASP:HB2	2.10	0.52
1:A:28:TYR:CZ	1:A:313:LYS:HE3	2.43	0.52
2:H:176:THR:O	2:H:180:GLY:N	2.37	0.52
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.40	0.52
1:G:384:VAL:HG22	1:G:385:MET:N	2.24	0.52
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.24	0.52
1:C:420:ALA:HA	1:C:423[B]:LYS:HD2	1.91	0.52
1:G:1035:GLN:NE2	11:G:1544:HOH:O	2.43	0.52
1:A:822:VAL:O	1:A:823:ARG:HD3	2.10	0.52
1:C:542:TYR:CD1	1:C:616:LEU:HD23	2.45	0.52
1:A:685:LEU:O	1:A:686:LYS:HB2	2.09	0.52
1:C:3:LYS:HB3	1:C:330:TYR:CZ	2.44	0.52
1:A:954:LYS:O	1:A:957:VAL:HG12	2.10	0.52
2:D:245:PRO:HD3	2:D:270:LEU:CD1	2.33	0.52
1:G:708:ILE:HG21	1:G:712:LEU:HD11	1.92	0.52
2:D:228:VAL:HG22	2:D:231:MET:HE1	1.91	0.52
2:D:282:LYS:HG3	2:D:320:THR:HB	1.92	0.52
2:H:54:THR:HG23	2:H:81:VAL:HG12	1.90	0.52
1:C:998:ARG:HB3	1:C:999:PRO:HA	1.91	0.52
1:A:671:ARG:HG3	1:A:677:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:199:PHE:HB3	2:F:270:LEU:HD23	1.92	0.52
2:B:316:VAL:CG1	2:B:337:LEU:HD23	2.38	0.52
2:B:50:ARG:HG2	2:B:158:LEU:CD2	2.40	0.52
1:E:517:ARG:HG2	1:E:522:LEU:HD23	1.91	0.52
2:D:46:PRO:HA	2:D:76:HIS:CG	2.45	0.52
1:A:891:LYS:HG2	1:A:892:GLU:N	2.25	0.52
1:A:370:ALA:HB2	1:A:903:VAL:CG2	2.40	0.52
2:F:247:PRO:HD2	2:F:248:ASP:OD1	2.10	0.51
1:A:223:ASP:OD1	1:A:227:ASN:HB2	2.10	0.51
1:G:10:ILE:HD13	1:G:37:LEU:HD13	1.90	0.51
2:D:362:ASP:OD2	2:D:362:ASP:N	2.41	0.51
1:G:701:ALA:O	1:G:705:ALA:N	2.33	0.51
2:D:196:ALA:HA	2:D:237:PHE:O	2.10	0.51
2:H:160:LYS:HE3	2:H:161:GLU:OE2	2.09	0.51
2:B:340:ILE:O	2:B:348:PHE:HB2	2.10	0.51
1:E:873:SER:O	1:E:877:GLN:HG3	2.09	0.51
1:C:174:MET:HB2	5:C:1078:PO4:O1	2.09	0.51
1:G:784:GLN:HB3	11:G:1480:HOH:O	2.11	0.51
1:E:967[B]:GLN:NE2	1:E:1054:LEU:CB	2.74	0.51
2:H:286:MET:HE1	2:H:312:HIS:CE1	2.44	0.51
2:H:317:ASP:HB3	2:H:320:THR:HG23	1.92	0.51
1:A:663:GLY:O	1:A:664:THR:C	2.48	0.51
1:E:998:ARG:CB	1:E:999:PRO:HA	2.40	0.51
1:C:426:ARG:C	1:C:426:ARG:HD3	2.30	0.51
2:B:83:ARG:HG3	2:B:83:ARG:HH11	1.75	0.51
1:G:225:ASN:ND2	11:G:1296:HOH:O	2.42	0.51
1:A:450:ASP:N	11:A:1435:HOH:O	2.27	0.51
2:H:50:ARG:HG3	2:H:50:ARG:NH1	2.16	0.51
1:A:224:LYS:HE2	1:A:329:GLY:O	2.10	0.51
1:G:762:VAL:HG12	1:G:763:ASP:N	2.25	0.51
2:H:317:ASP:OD2	2:H:319:ALA:HB3	2.09	0.51
1:C:998:ARG:HA	1:C:999:PRO:C	2.28	0.51
1:C:344:THR:HB	1:C:345:PRO:HD2	1.93	0.51
2:H:6:LEU:HD12	2:H:7:LEU:N	2.25	0.51
1:C:784:GLN:NE2	1:C:784:GLN:H	2.08	0.51
1:C:7:ILE:HG23	1:C:84:ASP:HB2	1.91	0.51
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.46	0.51
1:E:500:ALA:O	1:E:504:LYS:HG3	2.10	0.51
1:G:773:VAL:HG21	1:G:817:ALA:HB3	1.91	0.51
1:A:228:CYS:HB2	1:A:273:ARG:NH2	2.26	0.51
2:F:255:ILE:HA	2:F:258:PHE:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.28	0.51
1:E:361:ARG:CZ	1:E:571:ARG:HG2	2.41	0.51
1:C:973:ALA:O	1:C:991:VAL:HG12	2.10	0.51
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.90	0.51
1:C:167:ILE:HD12	1:C:167:ILE:N	2.25	0.51
1:E:796:LEU:C	1:E:796:LEU:HD23	2.31	0.51
1:G:695:VAL:CG2	1:G:752:LEU:HD22	2.40	0.51
1:C:69:ILE:HG22	1:C:69:ILE:O	2.10	0.51
1:A:730:ASP:OD2	1:A:733:ASP:HB2	2.11	0.51
1:A:991:VAL:HG22	1:A:992:ASN:N	2.26	0.51
9:E:1092:NET:C2	9:E:1092:NET:H42	2.33	0.51
2:B:248:ASP:OD2	2:B:248:ASP:N	2.41	0.51
1:A:948:SER:O	1:A:1015:ASN:HA	2.11	0.51
2:D:277:LEU:HD21	2:D:283:THR:HG23	1.93	0.51
1:E:526:TYR:CE1	1:E:545:SER:HB3	2.46	0.51
1:C:385:MET:HB2	1:C:603:PRO:HG3	1.92	0.51
1:E:258:ASP:O	1:E:262:GLN:HG2	2.10	0.51
1:G:479:VAL:HG21	1:G:483:GLY:HA3	1.92	0.51
1:G:143:THR:HA	1:G:296:ILE:HG23	1.93	0.51
1:A:772[A]:MET:SD	1:A:880:THR:HG22	2.51	0.51
1:G:146:SER:HB2	1:G:205:LEU:HD11	1.93	0.51
1:G:891:LYS:NZ	11:G:1678:HOH:O	2.43	0.51
1:E:973:ALA:O	1:E:991:VAL:HG12	2.10	0.51
1:A:1027[B]:ARG:HB3	1:A:1027[B]:ARG:CZ	2.40	0.51
2:D:174:SER:O	2:D:182:PRO:HD3	2.11	0.51
2:H:244:ASP:OD2	2:H:245:PRO:HD2	2.11	0.50
2:B:194:VAL:HB	2:B:216:LEU:CD2	2.38	0.50
1:G:119:THR:HG23	11:G:1763:HOH:O	2.11	0.50
2:B:72:SER:HB2	11:B:3543:HOH:O	2.10	0.50
2:F:190:LEU:HD23	2:F:213:GLY:HA2	1.93	0.50
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.39	0.50
2:H:9:LEU:O	2:H:10:GLU:C	2.49	0.50
2:H:141:ALA:O	2:H:145:GLU:N	2.39	0.50
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.26	0.50
1:C:1048:PHE:O	1:C:1052:MET:HG3	2.11	0.50
1:G:1:MET:O	1:G:334:GLU:OE1	2.29	0.50
2:D:116:ARG:O	2:D:120:ARG:HG3	2.11	0.50
2:F:306:MET:HB3	2:F:362:ASP:HB3	1.92	0.50
1:A:951:GLU:OE1	1:A:951:GLU:HA	2.06	0.50
2:H:82:ILE:O	2:H:111:ALA:HA	2.12	0.50
2:B:245:PRO:HG2	2:B:274:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:SER:O	2:H:50:ARG:HB2	2.11	0.50
2:H:316:VAL:HG12	2:H:337:LEU:HD23	1.93	0.50
2:D:246:ALA:HB1	2:D:248:ASP:HB2	1.94	0.50
1:G:577:GLU:O	1:G:580:TYR:HB3	2.12	0.50
1:A:333:ASP:N	1:A:333:ASP:OD1	2.44	0.50
2:H:10:GLU:HB2	2:H:128:GLN:HG2	1.94	0.50
2:B:6:LEU:HD11	2:B:8:VAL:CG2	2.41	0.50
2:H:121:LEU:CD1	2:H:125:LYS:HD3	2.42	0.50
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.93	0.50
2:B:318:GLU:HA	2:B:321:LEU:HD13	1.91	0.50
1:A:715:ARG:NH2	7:A:1088:ADP:O1A	2.44	0.50
1:G:814:GLN:CG	1:G:818:PHE:HE2	2.25	0.50
2:H:225:ALA:HA	2:H:258:PHE:CZ	2.47	0.50
2:D:316:VAL:CG1	2:D:337:LEU:HD23	2.41	0.50
2:F:246:ALA:C	2:F:248:ASP:H	2.13	0.50
2:B:6:LEU:HD11	2:B:8:VAL:HG23	1.94	0.50
1:G:796:LEU:HD23	1:G:797:PRO:N	2.27	0.50
1:G:40:GLU:OE1	1:G:325:LYS:HE2	2.12	0.50
2:D:12:GLY:HA2	2:D:144:LEU:HD13	1.92	0.50
1:C:948:SER:OG	10:C:1093:U:H5"	2.11	0.50
2:H:324:ASN:O	2:H:342:ARG:HA	2.10	0.50
2:B:285:LYS:HG3	2:B:314:PHE:CD1	2.47	0.50
1:C:675:ARG:HD3	1:C:675:ARG:H	1.77	0.50
1:C:1:MET:HB2	1:C:224:LYS:HZ2	1.76	0.50
1:E:682:VAL:CG1	1:E:687:LEU:HB2	2.42	0.50
1:G:358:LYS:HG2	1:G:359:ILE:N	2.19	0.50
1:A:467:GLU:O	1:A:471:ARG:HG2	2.12	0.50
1:C:802:SER:O	1:C:806:GLN:HG3	2.12	0.50
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.41	0.50
1:G:339:ILE:CD1	1:G:530:ASP:HA	2.36	0.50
2:F:154:ASN:ND2	2:F:314:PHE:HZ	2.08	0.50
1:C:372:ASP:N	11:C:1371:HOH:O	2.30	0.50
1:G:579:ASP:OD1	1:G:605:THR:HB	2.12	0.50
1:E:425:ARG:HD3	11:E:1422:HOH:O	2.11	0.50
2:F:342:ARG:NE	2:F:344:ASP:OD2	2.45	0.50
2:H:32:PHE:HA	2:H:54:THR:O	2.11	0.50
2:H:161:GLU:OE1	2:H:161:GLU:HA	2.12	0.50
2:F:23:THR:HG22	2:F:24:GLY:N	2.25	0.50
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.46	0.50
1:C:349:GLU:O	2:D:294:ASN:HB2	2.12	0.50
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:281:ALA:HB2	2:F:322:PRO:HD3	1.94	0.49
2:D:9:LEU:HD12	2:D:13:THR:HB	1.94	0.49
1:G:439:ILE:O	1:G:442:ALA:HB3	2.12	0.49
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.11	0.49
1:G:9:SER:O	1:G:84:ASP:HB2	2.11	0.49
2:D:6:LEU:HD13	2:D:16:HIS:CE1	2.47	0.49
1:C:930:LYS:HE3	11:C:1159:HOH:O	2.11	0.49
1:A:421:LEU:HB3	1:E:421:LEU:HD13	1.94	0.49
1:C:1066:GLN:HB2	11:C:1156:HOH:O	2.12	0.49
1:G:569:PRO:O	1:G:571:ARG:HD2	2.13	0.49
1:G:697:ALA:HB3	1:G:700:MET:HB2	1.95	0.49
2:H:48:TYR:CZ	2:H:311:ASN:ND2	2.80	0.49
1:A:416:ASP:OD2	1:A:416:ASP:N	2.34	0.49
1:E:735:ARG:O	1:E:738:PHE:HB2	2.13	0.49
1:C:702:VAL:O	1:C:706:LYS:HD3	2.12	0.49
1:A:145:ARG:HH12	1:A:161:ASP:CG	2.16	0.49
1:G:735:ARG:O	1:G:738:PHE:HB2	2.12	0.49
2:F:154:ASN:HD22	2:F:285:LYS:HE2	1.76	0.49
1:C:951:GLU:O	1:C:954:LYS:HB2	2.13	0.49
2:B:186:LYS:O	2:B:187:GLU:C	2.50	0.49
2:D:263:ILE:HG22	2:D:264:PRO:CD	2.40	0.49
1:C:1:MET:CB	1:C:2:PRO:HD2	2.43	0.49
2:F:255:ILE:HA	2:F:258:PHE:CD2	2.48	0.49
2:D:370:PHE:O	2:D:374:ILE:HG13	2.12	0.49
1:C:223:ASP:OD2	1:C:227:ASN:HB2	2.12	0.49
2:B:157:ASP:OD1	2:B:160:LYS:HD3	2.13	0.49
1:A:59:GLU:HG3	11:A:1503:HOH:O	2.13	0.49
1:G:702:VAL:CG1	1:G:731:GLU:HG3	2.43	0.49
1:E:695:VAL:HG21	1:E:701:ALA:CA	2.37	0.49
1:E:691:ALA:HB3	1:E:708:ILE:HG23	1.95	0.49
1:G:781:HIS:HE1	1:G:789:SER:HB2	1.76	0.49
2:D:2:ILE:HD11	11:D:2829:HOH:O	2.12	0.49
1:A:240:MET:HE3	7:A:1087:ADP:C4	2.46	0.49
1:E:559:ARG:NH1	11:E:1893:HOH:O	2.44	0.49
1:C:337:ASN:HB3	1:C:340:THR:OG1	2.13	0.49
1:C:686:LYS:O	1:C:687:LEU:HD23	2.13	0.49
1:G:1017:THR:HG21	1:G:1023:ILE:CA	2.40	0.49
1:E:157:ALA:O	1:E:160:ALA:HB3	2.12	0.49
1:A:1:MET:O	1:A:334:GLU:OE1	2.30	0.49
1:C:950:ARG:HD3	11:C:1583:HOH:O	2.12	0.49
1:A:767:ILE:CD1	1:A:865:ALA:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:OE2	1:A:365:GLU:N	2.39	0.49
2:H:350:PHE:HD2	2:H:354:PRO:HD3	1.77	0.49
2:B:199:PHE:O	2:B:241:GLY:HA3	2.13	0.49
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.43	0.49
2:H:310:GLN:OE1	2:H:312:HIS:NE2	2.46	0.49
1:G:79:GLU:HG2	1:G:111:PHE:CZ	2.48	0.49
1:A:358:LYS:HE3	11:A:1128:HOH:O	2.11	0.49
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.42	0.49
2:B:376:GLN:HG3	2:B:376:GLN:O	2.13	0.49
1:E:967[A]:GLN:HG3	1:E:1054:LEU:HD13	1.94	0.49
2:B:345:LYS:HB3	2:B:346:PRO:CD	2.43	0.49
1:A:675:ARG:H	1:A:675:ARG:HD3	1.76	0.49
1:A:225:ASN:ND2	1:A:331:THR:HG21	2.28	0.49
1:C:420:ALA:HA	1:C:423[A]:LYS:HD2	1.95	0.49
1:A:150:HIS:N	1:A:154:GLU:OE2	2.30	0.49
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.94	0.49
1:A:1006:LYS:O	1:A:1006:LYS:HG3	2.12	0.49
2:H:275:LEU:HD23	2:H:349:SER:HB3	1.95	0.48
1:E:693:ALA:CB	1:E:708:ILE:HD11	2.38	0.48
2:H:286:MET:HE3	2:H:315:ALA:HB2	1.95	0.48
1:E:493:LYS:HE2	1:E:517:ARG:CD	2.43	0.48
1:G:354:TYR:CD2	1:G:387:ILE:HG23	2.48	0.48
1:G:1021:ARG:O	1:G:1025:ASP:OD2	2.31	0.48
1:G:170:PRO:HA	1:G:204:LEU:HD23	1.94	0.48
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.95	0.48
1:E:58:PRO:HD2	1:E:59:GLU:OE2	2.13	0.48
1:E:110:GLU:HG2	1:E:111:PHE:CD1	2.47	0.48
1:G:315:THR:O	1:G:531:THR:HG22	2.12	0.48
6:A:1083:CL:CL	11:A:1622:HOH:O	2.57	0.48
2:H:298:LYS:O	2:H:329:HIS:HA	2.14	0.48
1:G:493:LYS:NZ	1:G:499:ASP:OD2	2.34	0.48
1:A:347:SER:O	2:B:296:PRO:HB3	2.12	0.48
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.61	0.48
2:H:355:GLU:OE2	2:H:355:GLU:N	2.42	0.48
1:C:68:PRO:HG3	1:C:930:LYS:O	2.13	0.48
1:A:515:LYS:HG3	11:A:1774:HOH:O	2.12	0.48
1:G:460:ARG:HG3	11:G:1283:HOH:O	2.11	0.48
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.48	0.48
1:A:65:TYR:OH	1:A:80[A]:LYS:HE3	2.14	0.48
1:C:479:VAL:HB	1:C:483:GLY:HA3	1.95	0.48
2:B:284:VAL:O	2:B:314:PHE:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:509:ARG:HH11	1:E:509:ARG:HB2	1.75	0.48
1:C:228:CYS:O	1:C:269:MET:HE1	2.14	0.48
1:A:101:GLU:O	1:A:105:GLN:HG2	2.13	0.48
1:E:636:LYS:HD3	11:E:1773:HOH:O	2.12	0.48
1:E:853:VAL:O	1:E:857:THR:HG23	2.13	0.48
1:C:751:LEU:O	1:C:752:LEU:HD12	2.13	0.48
1:C:772:MET:HE2	1:C:880:THR:HA	1.96	0.48
2:H:43:LEU:HD21	2:H:80:LEU:HD13	1.95	0.48
2:H:227:ASP:HA	2:H:230:LYS:HD2	1.95	0.48
1:E:1004:ARG:NH1	1:E:1009:GLU:OE1	2.41	0.48
1:G:730:ASP:O	1:G:733:ASP:HB2	2.12	0.48
1:E:2:PRO:O	1:E:3:LYS:C	2.48	0.48
1:E:1021:ARG:HG3	1:E:1021:ARG:HH11	1.79	0.48
1:C:726:GLU:HG3	1:C:727:ILE:N	2.27	0.48
1:C:361:ARG:NH2	1:C:571:ARG:HG2	2.28	0.48
1:C:174:MET:HB3	11:C:1191:HOH:O	2.13	0.48
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.96	0.48
1:E:128:ASP:OD1	1:E:130:ARG:HB3	2.14	0.48
2:F:45:ASP:OD2	2:F:46:PRO:HD2	2.13	0.48
2:D:342:ARG:NH2	2:D:344:ASP:OD1	2.30	0.48
1:E:35:LYS:O	1:E:39[B]:GLU:HB2	2.13	0.48
2:B:290:HIS:NE2	2:B:334:ASP:OD1	2.46	0.48
1:A:775:ILE:HG13	1:A:810:ARG:HG2	1.94	0.48
1:C:626:VAL:O	1:C:630:VAL:HG23	2.13	0.48
2:F:25:SER:HA	2:F:132:ILE:O	2.14	0.48
1:A:340:THR:O	1:A:343:ARG:HB2	2.14	0.48
1:C:784:GLN:O	1:C:784:GLN:HG2	2.13	0.48
2:F:158:LEU:HD12	2:F:243:GLY:HA3	1.95	0.48
1:A:151:THR:OG1	1:A:154:GLU:HG3	2.13	0.48
1:C:267:ALA:O	1:C:271:VAL:HG23	2.14	0.48
2:B:50:ARG:HG2	2:B:158:LEU:HD22	1.95	0.48
2:F:263:ILE:HG22	2:F:264:PRO:CD	2.40	0.48
2:D:153:LEU:O	2:D:155:GLY:N	2.47	0.48
2:H:295:HIS:NE2	2:H:333:PHE:HB2	2.29	0.48
2:F:6:LEU:HD21	2:F:140:ALA:HA	1.94	0.48
2:H:18:ARG:NH1	2:H:20:ILE:HG22	2.29	0.48
1:G:183:TYR:HB2	1:G:187:GLU:OE1	2.14	0.48
1:G:530:ASP:C	1:G:531:THR:HG23	2.35	0.48
2:D:154:ASN:ND2	2:D:314:PHE:HZ	2.12	0.48
2:F:342:ARG:NH2	2:F:344:ASP:OD1	2.47	0.48
1:G:563:MET:HB2	1:G:638:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1027:ARG:NE	1:G:1031:ARG:HD3	2.28	0.48
1:A:703:GLU:HA	1:A:703:GLU:OE2	2.14	0.48
1:E:950:ARG:HH11	1:E:950:ARG:HD2	1.55	0.48
1:A:704:LYS:O	1:A:707:GLU:HB2	2.13	0.48
1:A:509:ARG:HB2	1:A:509:ARG:CZ	2.44	0.47
2:F:186:LYS:HB3	2:F:188:ASP:OD2	2.13	0.47
2:H:237:PHE:CE2	2:H:239:SER:HA	2.48	0.47
1:E:494:ARG:HG2	1:E:547:TYR:CB	2.44	0.47
1:E:736:ARG:O	1:E:740:THR:HG23	2.13	0.47
1:G:563:MET:CB	1:G:638:VAL:HG22	2.44	0.47
2:H:296:PRO:HB2	2:H:332:LEU:HB2	1.97	0.47
1:A:101:GLU:OE2	1:A:101:GLU:HA	2.14	0.47
2:F:68:ALA:HA	2:F:181:LEU:HD11	1.96	0.47
1:A:315:THR:O	1:A:531:THR:HG22	2.14	0.47
1:C:772:MET:CE	1:C:880:THR:HG22	2.44	0.47
2:H:32:PHE:O	2:H:291:HIS:HB2	2.15	0.47
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.45	0.47
2:D:170:TRP:HB3	2:D:216:LEU:HB2	1.96	0.47
1:C:70:HIS:O	1:C:73:VAL:N	2.45	0.47
1:C:130:ARG:HG3	1:C:148:ILE:HG13	1.96	0.47
1:E:224:LYS:NZ	11:E:1624:HOH:O	2.42	0.47
1:A:1:MET:HB2	1:A:224:LYS:HE3	1.95	0.47
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.44	0.47
1:E:897:PHE:HB3	11:E:1557:HOH:O	2.14	0.47
1:G:49:SER:O	1:G:51:PRO:HD3	2.15	0.47
1:G:698:ILE:CD1	1:G:698:ILE:H	2.27	0.47
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.45	0.47
2:D:272:HIS:HA	2:D:349:SER:CB	2.44	0.47
1:G:168:ILE:HG23	1:G:204:LEU:HD22	1.96	0.47
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.96	0.47
1:C:860:PRO:HB2	1:C:863:LYS:HB2	1.97	0.47
1:G:349:GLU:O	2:H:294:ASN:HB2	2.15	0.47
2:H:325:LEU:HD23	2:H:325:LEU:HA	1.35	0.47
1:G:943:GLY:O	1:G:969:PHE:HA	2.14	0.47
2:D:197:TYR:HB3	2:D:199:PHE:CZ	2.50	0.47
1:A:947:LEU:N	1:A:947:LEU:HD12	2.30	0.47
2:D:286:MET:HG2	11:D:2883:HOH:O	2.13	0.47
2:H:370:PHE:CZ	2:H:374:ILE:HD11	2.49	0.47
1:G:772:MET:SD	1:G:880:THR:HG22	2.54	0.47
2:B:272:HIS:HA	2:B:349:SER:HB2	1.95	0.47
2:F:363:ALA:C	2:F:365:PRO:HD2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:VAL:HG12	2:D:337:LEU:CD2	2.44	0.47
1:E:368:ALA:HA	11:E:1708:HOH:O	2.14	0.47
2:H:251:ALA:O	2:H:255:ILE:HG13	2.15	0.47
1:A:548:GLU:OE1	2:B:114:ASP:HA	2.14	0.47
2:H:363:ALA:HB1	2:H:366:LEU:HD13	1.97	0.47
2:D:245:PRO:CG	2:D:274:LEU:HD21	2.44	0.47
1:C:676:GLU:O	1:C:680:HIS:ND1	2.48	0.47
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.15	0.47
2:H:45:ASP:OD2	2:H:46:PRO:HD2	2.14	0.47
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.49	0.47
2:F:174:SER:HB2	2:F:211:ASP:OD2	2.13	0.47
2:H:55:LEU:HD13	2:H:60:ILE:HD12	1.95	0.47
1:G:675:ARG:H	1:G:675:ARG:CD	2.26	0.47
1:C:640:VAL:HG21	1:C:651:ALA:HB2	1.97	0.47
2:B:291:HIS:HD2	2:B:311:ASN:OD1	1.98	0.47
1:A:950:ARG:HD3	11:A:1597:HOH:O	2.14	0.47
1:C:25:GLU:HG3	1:C:306:ARG:HA	1.96	0.47
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.95	0.47
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.80	0.47
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.29	0.47
2:D:205:ILE:HG21	2:D:237:PHE:CZ	2.49	0.47
1:E:144:ALA:HB1	1:E:208:GLU:HG2	1.96	0.47
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.50	0.47
1:C:124:ASP:OD1	1:C:131:ARG:HD3	2.15	0.47
2:F:298:LYS:HG2	2:F:299:ASP:N	2.30	0.47
1:G:699:GLU:OE2	1:G:699:GLU:HA	2.15	0.47
2:H:267:GLY:O	2:H:349:SER:HA	2.14	0.47
2:F:187:GLU:CG	2:F:215:ARG:HD2	2.43	0.47
1:C:702:VAL:CG1	1:C:731:GLU:HG3	2.45	0.47
1:C:773:VAL:HG23	1:C:818:PHE:CZ	2.50	0.47
2:H:111:ALA:O	2:H:112:ASP:HB2	2.15	0.47
1:A:767:ILE:HD13	1:A:865:ALA:HB2	1.97	0.47
1:C:75:ARG:HG3	1:C:107:VAL:CG1	2.45	0.47
1:C:1018:SER:O	1:C:1022:ALA:HB3	2.14	0.47
1:E:836:GLU:HB2	1:E:838:TYR:CE2	2.50	0.47
1:C:158:VAL:HG11	1:C:206:ILE:HB	1.96	0.47
1:C:695:VAL:HG23	1:C:752:LEU:HD22	1.97	0.47
1:E:1051:ALA:HA	1:E:1054:LEU:HD12	1.96	0.47
1:G:1004:ARG:O	1:G:1009[B]:GLU:HB2	2.14	0.47
1:G:185:ARG:O	1:G:188:PHE:HB3	2.14	0.47
2:F:55:LEU:HD13	2:F:60:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ASN:HA	1:A:752:LEU:O	2.15	0.47
2:H:318:GLU:O	2:H:318:GLU:HG2	2.14	0.46
1:E:1019:GLY:O	1:E:1023:ILE:HG13	2.15	0.46
2:B:209:LEU:HD23	2:B:209:LEU:HA	1.81	0.46
1:A:612:THR:O	1:A:612:THR:HG22	2.15	0.46
2:F:324:ASN:ND2	2:F:324:ASN:H	2.07	0.46
1:G:423:LYS:H	1:G:423:LYS:HG3	1.50	0.46
1:E:481:ILE:HG23	1:E:482:THR:N	2.29	0.46
1:E:109:GLU:O	1:E:110:GLU:C	2.50	0.46
1:G:90:MET:HA	1:G:304:VAL:HG22	1.96	0.46
1:G:435:ARG:O	1:G:436:ILE:C	2.52	0.46
2:D:98:LEU:O	2:D:98:LEU:HD12	2.16	0.46
1:G:131:ARG:HD2	11:G:1750:HOH:O	2.15	0.46
1:A:514:ARG:HD3	11:A:1461:HOH:O	2.14	0.46
1:C:532:CYS:O	1:C:533:ALA:HB3	2.16	0.46
1:G:103:GLU:HG3	1:G:104:ARG:N	2.19	0.46
2:H:254:ALA:O	2:H:257:LYS:HB2	2.15	0.46
2:D:252:ILE:HD13	2:D:277:LEU:HB3	1.97	0.46
2:H:301:GLU:OE1	2:H:328:THR:HG22	2.15	0.46
2:D:376:GLN:HA	2:D:379:LYS:NZ	2.30	0.46
1:G:734:LEU:HD11	1:G:738:PHE:HE2	1.79	0.46
1:A:992:ASN:HB2	1:A:999:PRO:O	2.14	0.46
2:F:379:LYS:NZ	2:F:379:LYS:HB2	2.30	0.46
1:G:486:ALA:HB2	1:G:520:TYR:CG	2.51	0.46
1:E:998:ARG:HA	1:E:999:PRO:C	2.33	0.46
1:G:484:LEU:HD22	1:G:489:LEU:HD13	1.98	0.46
1:G:726:GLU:OE1	1:G:1020:ARG:NE	2.36	0.46
2:D:263:ILE:CG2	2:D:264:PRO:HD2	2.42	0.46
1:G:124:ASP:OD1	1:G:131:ARG:HD3	2.16	0.46
1:A:972:ASP:OD1	1:A:989:ARG:HB3	2.15	0.46
1:G:665:SER:HB2	11:G:1668:HOH:O	2.16	0.46
2:B:41:GLU:HG3	2:B:69:ASP:O	2.16	0.46
2:H:10:GLU:O	2:H:12:GLY:N	2.48	0.46
1:G:685:LEU:O	1:G:686:LYS:HB2	2.15	0.46
1:E:318:PRO:HB2	1:E:321:LYS:HB2	1.97	0.46
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.45	0.46
1:E:176:GLY:N	7:E:1089:ADP:O2B	2.41	0.46
1:C:119:THR:O	1:C:120:ALA:C	2.53	0.46
1:A:805:ILE:HG22	1:A:806:GLN:N	2.29	0.46
2:B:46:PRO:HA	2:B:76:HIS:CB	2.46	0.46
2:D:286:MET:HE1	2:D:315:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:625:ASP:O	1:G:629:ILE:HG13	2.15	0.46
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.51	0.46
2:D:331:SER:O	2:D:335:GLY:HA2	2.15	0.46
1:C:236:ASN:N	1:C:236:ASN:HD22	2.14	0.46
2:H:364:ALA:O	2:H:366:LEU:N	2.48	0.46
1:G:734:LEU:CD1	1:G:738:PHE:CE2	2.99	0.46
1:A:992:ASN:ND2	1:G:975:HIS:HE2	2.14	0.46
2:B:286:MET:CE	2:B:312:HIS:ND1	2.79	0.46
1:E:783:GLU:OE1	8:E:1091:ORN:NE	2.49	0.46
2:H:45:ASP:HB3	2:H:48:TYR:CD2	2.50	0.46
2:H:169:SER:HA	2:H:216:LEU:O	2.16	0.46
1:A:157:ALA:O	1:A:160:ALA:HB3	2.16	0.46
1:C:782:ILE:HD13	1:C:793:ALA:C	2.36	0.46
8:G:1091:ORN:N	11:G:1554:HOH:O	2.36	0.46
2:H:27:VAL:O	2:H:78:GLN:HG2	2.16	0.46
2:H:344:ASP:OD2	2:H:345:LYS:N	2.48	0.46
2:D:154:ASN:ND2	2:D:314:PHE:CZ	2.84	0.46
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.97	0.46
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.98	0.46
1:G:806:GLN:HB3	1:G:810:ARG:NH1	2.31	0.46
1:A:367:PHE:HB3	1:A:903:VAL:HG21	1.98	0.46
1:E:169:ARG:HG2	11:E:1874:HOH:O	2.15	0.46
2:D:364:ALA:N	2:D:365:PRO:CD	2.79	0.46
2:B:263:ILE:HG22	2:B:264:PRO:CD	2.45	0.45
2:D:286:MET:CE	2:D:312:HIS:ND1	2.79	0.45
1:G:597:ILE:HA	1:G:615:ARG:O	2.15	0.45
2:H:218:ILE:N	2:H:218:ILE:CD1	2.79	0.45
1:C:11:LEU:HA	1:C:45:ILE:O	2.17	0.45
1:A:585:ALA:HB2	1:A:642:TYR:CE2	2.52	0.45
2:H:8:VAL:CG1	2:H:9:LEU:N	2.80	0.45
2:H:153:LEU:O	2:H:154:ASN:C	2.54	0.45
1:G:775:ILE:CD1	1:G:813:VAL:HG11	2.46	0.45
2:D:286:MET:HE1	2:D:312:HIS:ND1	2.31	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
1:C:891:LYS:HG2	1:C:892:GLU:N	2.30	0.45
2:F:222:GLN:HB2	11:F:1487:HOH:O	2.16	0.45
1:E:579:ASP:OD1	1:E:605:THR:HB	2.16	0.45
1:E:489:LEU:HD22	1:E:516:LEU:HD23	1.98	0.45
2:H:272:HIS:CA	2:H:349:SER:HB2	2.41	0.45
1:G:339:ILE:O	1:G:538:THR:OG1	2.29	0.45
2:B:205:ILE:HG13	2:B:355:GLU:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:GLU:CG	1:C:727:ILE:N	2.79	0.45
1:A:671:ARG:CG	1:A:677:ARG:NH1	2.80	0.45
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.34	0.45
2:H:11:ASP:OD2	2:H:13:THR:OG1	2.30	0.45
1:G:688:LYS:HD2	1:G:838:TYR:CE1	2.52	0.45
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.12	0.45
2:H:352:GLY:O	2:H:354:PRO:HD3	2.16	0.45
2:H:364:ALA:N	2:H:365:PRO:HD2	2.31	0.45
2:H:50:ARG:HH12	2:H:156:MET:CE	2.30	0.45
2:H:246:ALA:O	2:H:248:ASP:N	2.50	0.45
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.52	0.45
1:G:502:LEU:O	1:G:505:LEU:HB2	2.17	0.45
2:F:272:HIS:HA	2:F:349:SER:OG	2.15	0.45
1:C:220:VAL:O	1:C:281:GLY:HA2	2.16	0.45
1:A:695:VAL:CG1	1:A:696:THR:N	2.80	0.45
2:H:284:VAL:O	2:H:315:ALA:N	2.45	0.45
1:G:770:GLY:CA	1:G:823:ARG:NH1	2.80	0.45
1:A:286:PHE:CD1	1:A:295:LEU:HD11	2.51	0.45
1:G:941:LYS:HE3	11:G:1704:HOH:O	2.15	0.45
1:G:102:LEU:HA	1:G:102:LEU:HD23	1.82	0.45
2:H:350:PHE:CD1	2:H:366:LEU:HD21	2.51	0.45
1:A:947:LEU:N	1:A:947:LEU:CD1	2.80	0.45
1:A:644:GLY:O	1:A:647:PRO:HD2	2.17	0.45
2:D:316:VAL:HB	2:D:337:LEU:HD23	1.97	0.45
1:C:802:SER:OG	1:C:805:ILE:HB	2.16	0.45
1:C:103:GLU:HG3	1:C:104:ARG:N	2.31	0.45
1:C:103:GLU:HB2	1:C:108:LEU:HD12	1.99	0.45
1:C:577:GLU:O	1:C:580:TYR:HB3	2.17	0.45
1:C:865:ALA:O	1:C:869:MET:HG3	2.16	0.45
1:C:176:GLY:HA3	1:C:377:GLN:HA	1.98	0.45
1:C:1001:ILE:HD11	11:C:1576:HOH:O	2.16	0.45
1:C:695:VAL:CG1	1:C:696:THR:N	2.80	0.45
1:E:1021:ARG:O	1:E:1025:ASP:OD2	2.34	0.45
2:B:224:SER:O	2:B:225:ALA:C	2.51	0.45
1:G:813:VAL:HA	1:G:816:LEU:HD12	1.98	0.45
2:H:121:LEU:HD11	2:H:125:LYS:HD3	1.99	0.45
2:F:272:HIS:HA	2:F:349:SER:CB	2.47	0.45
1:C:1064:SER:O	1:C:1068:MET:HG3	2.17	0.45
1:E:963:LYS:O	1:E:964:LEU:C	2.53	0.45
1:E:141:LEU:HD23	1:E:141:LEU:HA	1.69	0.45
1:G:254:GLN:NE2	2:H:57:TYR:OH	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1013:ILE:O	1:C:1040:TYR:HA	2.17	0.45
2:F:223:THR:CG2	2:F:228:VAL:HG23	2.47	0.45
1:A:223:ASP:CG	1:A:227:ASN:HB2	2.36	0.45
1:C:344:THR:HB	1:C:345:PRO:CD	2.47	0.45
2:H:23:THR:HG22	2:H:24:GLY:N	2.31	0.45
1:C:213:TRP:HH2	1:C:294:ARG:HD2	1.82	0.45
2:F:82:ILE:O	2:F:111:ALA:HA	2.17	0.45
1:A:481:ILE:HG22	11:A:1762:HOH:O	2.16	0.45
2:H:274:LEU:O	2:H:275:LEU:C	2.55	0.45
1:G:703:GLU:O	1:G:706:LYS:HB2	2.17	0.45
1:E:726:GLU:CG	1:E:727:ILE:N	2.80	0.45
2:H:153:LEU:CD1	2:H:153:LEU:N	2.79	0.45
2:B:6:LEU:HD12	2:B:7:LEU:H	1.81	0.45
2:F:111:ALA:O	2:F:112:ASP:HB2	2.17	0.45
1:G:883:VAL:CG1	1:G:884:ILE:N	2.80	0.45
1:A:35:LYS:HA	11:A:1142:HOH:O	2.17	0.45
2:B:369:HIS:O	2:B:373:LEU:HG	2.16	0.45
1:G:333:ASP:N	1:G:333:ASP:OD1	2.49	0.45
2:H:232:ASN:N	2:H:233:PRO:CD	2.80	0.45
2:D:50:ARG:NH1	2:D:156:MET:CE	2.80	0.45
1:C:735:ARG:O	1:C:738:PHE:HB2	2.17	0.45
1:G:65:TYR:CE2	1:G:77:ILE:HG23	2.52	0.45
1:A:167:ILE:CD1	1:A:167:ILE:N	2.80	0.45
2:F:364:ALA:N	2:F:365:PRO:CD	2.80	0.45
1:A:882:GLU:HB3	11:A:1828:HOH:O	2.17	0.45
1:G:265:ARG:O	1:G:269:MET:HG3	2.16	0.45
1:E:282:SER:OG	1:E:302:PRO:HA	2.17	0.45
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.44
2:B:83:ARG:NH1	2:B:83:ARG:HG3	2.32	0.44
1:A:148:ILE:CG2	1:A:149:ALA:N	2.80	0.44
2:F:225:ALA:HB2	2:F:254:ALA:HB1	1.99	0.44
1:C:419:GLU:CB	1:C:423[B]:LYS:HZ3	2.29	0.44
2:D:232:ASN:N	2:D:233:PRO:HD3	2.33	0.44
1:G:561:LYS:HG2	1:G:595:GLU:OE2	2.17	0.44
2:H:281:ALA:HB2	2:H:322:PRO:HD3	2.00	0.44
2:B:199:PHE:HB3	2:B:270:LEU:HD23	1.99	0.44
1:E:730:ASP:OD2	1:E:733:ASP:HB2	2.17	0.44
1:G:866:ALA:O	1:G:869:MET:HB2	2.17	0.44
2:H:246:ALA:C	2:H:248:ASP:H	2.21	0.44
1:G:1021:ARG:NH1	1:G:1021:ARG:CG	2.80	0.44
1:A:76:LYS:HD2	1:A:76:LYS:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:PHE:CG	2:B:366:LEU:CD2	3.00	0.44
2:H:18:ARG:NH1	11:H:502:HOH:O	2.50	0.44
2:F:299:ASP:OD1	2:F:302:LYS:HD2	2.17	0.44
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.52	0.44
1:E:1028:VAL:CG1	1:E:1029:ILE:N	2.79	0.44
1:A:82:ARG:N	1:A:83:PRO:CD	2.81	0.44
1:G:730:ASP:H	1:G:733:ASP:HB2	1.83	0.44
2:H:50:ARG:NH1	2:H:156:MET:CE	2.80	0.44
2:H:286:MET:CE	2:H:312:HIS:CE1	3.00	0.44
2:B:272:HIS:HA	2:B:349:SER:CB	2.48	0.44
1:G:436:ILE:HG22	11:G:1304:HOH:O	2.16	0.44
1:A:34:CYS:SG	1:A:46:LEU:HD22	2.58	0.44
1:E:148:ILE:CG2	1:E:149:ALA:N	2.80	0.44
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.59	0.44
1:E:734:LEU:O	1:E:737:TYR:HB3	2.16	0.44
2:B:354:PRO:HB2	2:B:367:PHE:CE2	2.53	0.44
2:B:149:ALA:O	2:B:151:PRO:HD3	2.17	0.44
1:G:473:GLU:HG2	1:G:505:LEU:HD11	1.98	0.44
2:B:176:THR:O	2:B:180:GLY:N	2.39	0.44
1:E:692:ASN:HA	1:E:752:LEU:O	2.17	0.44
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.82	0.44
1:C:736:ARG:CZ	1:C:736:ARG:HB3	2.47	0.44
1:C:659:VAL:HG13	1:C:660:PRO:HD2	2.00	0.44
1:A:702:VAL:O	1:A:706:LYS:HD3	2.17	0.44
1:E:344:THR:HB	1:E:345:PRO:CD	2.46	0.44
2:D:205:ILE:HG21	2:D:237:PHE:CE2	2.52	0.44
1:G:796:LEU:HD23	1:G:797:PRO:CA	2.48	0.44
1:C:464:VAL:HG21	2:D:88:ILE:HG12	2.00	0.44
2:F:172:GLN:HG2	2:F:173:GLY:N	2.29	0.44
1:E:755:PHE:CE1	7:E:1090:ADP:C2	3.05	0.44
1:E:588:ALA:HB2	1:E:863:LYS:HG2	1.99	0.44
1:C:620:PRO:O	1:C:625:ASP:HB2	2.18	0.44
1:G:70:HIS:HE1	1:G:72:GLU:HG3	1.82	0.44
2:D:212:ARG:HH11	2:D:212:ARG:HG3	1.83	0.44
2:D:342:ARG:HE	2:D:344:ASP:CG	2.19	0.44
2:H:153:LEU:CD1	2:H:153:LEU:H	2.30	0.44
1:A:735:ARG:O	1:A:736:ARG:C	2.54	0.44
1:E:784:GLN:H	1:E:784:GLN:HE21	1.66	0.44
2:F:365:PRO:O	2:F:368:ASP:N	2.49	0.44
2:F:23:THR:CG2	2:F:24:GLY:N	2.81	0.44
2:D:6:LEU:HD21	2:D:140:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:150:PHE:HA	2:F:151:PRO:HD2	1.88	0.44
2:H:120:ARG:HD2	11:H:413:HOH:O	2.18	0.44
1:G:412:LYS:HE2	1:G:434:ASP:CG	2.37	0.44
2:F:352:GLY:O	2:F:354:PRO:HD3	2.17	0.44
1:G:45:ILE:HA	1:G:63:ALA:O	2.18	0.44
1:E:222:ARG:NE	1:E:226:ASP:OD2	2.49	0.44
2:B:342:ARG:HD2	2:B:342:ARG:HA	1.88	0.44
2:H:50:ARG:HH12	2:H:156:MET:HE1	1.82	0.44
1:C:1:MET:O	1:C:334:GLU:OE1	2.36	0.44
1:A:331:THR:OG1	1:A:334:GLU:HG3	2.18	0.44
1:A:703:GLU:OE2	1:A:706:LYS:NZ	2.36	0.44
2:B:350:PHE:CG	2:B:366:LEU:HD22	2.53	0.44
1:E:755:PHE:CD1	7:E:1090:ADP:C2	3.06	0.44
1:G:1052:MET:O	1:G:1055:ASN:HB2	2.18	0.44
1:A:560:GLU:OE1	1:A:636:LYS:HD2	2.18	0.44
2:D:332:LEU:HA	2:D:332:LEU:HD12	1.68	0.44
1:A:994:VAL:CG2	1:A:1001:ILE:HD11	2.48	0.44
2:H:50:ARG:NH1	2:H:156:MET:HE2	2.33	0.44
2:B:29:GLU:HB2	2:B:153:LEU:HD22	1.99	0.44
2:H:104:ARG:HG2	2:H:105:HIS:HD2	1.82	0.44
1:A:250:VAL:HA	1:A:356:VAL:O	2.18	0.44
1:A:900:PHE:N	1:A:901:PRO:HD3	2.33	0.44
2:H:350:PHE:CG	2:H:366:LEU:CD2	3.01	0.44
1:G:873:SER:OG	1:G:876:GLU:HB2	2.18	0.44
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.83	0.44
1:C:221:VAL:O	1:C:228:CYS:HA	2.17	0.44
1:G:1027:ARG:HE	1:G:1031:ARG:CD	2.29	0.44
1:C:60[A]:MET:HE2	11:C:1495:HOH:O	2.17	0.44
1:C:361:ARG:CZ	1:C:571:ARG:HG2	2.48	0.44
1:G:796:LEU:HD23	1:G:796:LEU:C	2.38	0.44
2:D:379:LYS:HE2	2:D:379:LYS:HB3	1.75	0.44
1:G:713:VAL:HG23	1:G:755:PHE:HB2	2.00	0.44
1:G:35:LYS:HD2	11:G:1144:HOH:O	2.17	0.44
2:H:27:VAL:HG21	2:H:146:LYS:HB3	2.00	0.43
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.18	0.43
2:F:245:PRO:CG	2:F:274:LEU:HD21	2.48	0.43
1:E:967[B]:GLN:NE2	1:E:1054:LEU:CD1	2.78	0.43
1:E:691:ALA:CB	1:E:708:ILE:HG23	2.47	0.43
1:A:1001:ILE:HD12	1:A:1002:GLN:CB	2.47	0.43
1:G:664:THR:HG22	1:G:668:ALA:HB3	2.00	0.43
2:B:228:VAL:HA	2:B:231:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:223:THR:HG22	2:F:228:VAL:HG23	1.98	0.43
1:C:82:ARG:N	1:C:83:PRO:CD	2.80	0.43
1:C:894:VAL:O	1:C:913:SER:HB2	2.17	0.43
1:C:695:VAL:HG12	1:C:696:THR:N	2.33	0.43
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.18	0.43
1:G:530:ASP:O	1:G:531:THR:OG1	2.29	0.43
1:G:738:PHE:HA	1:G:741:ALA:HB3	2.00	0.43
2:B:58:PRO:HA	2:B:83:ARG:HB3	2.00	0.43
9:G:1092:NET:C4	9:G:1092:NET:H22	2.43	0.43
1:G:762:VAL:CG1	1:G:763:ASP:N	2.81	0.43
2:F:48:TYR:HA	2:F:51:GLN:NE2	2.30	0.43
1:C:24:CYS:CB	1:C:576:ILE:HD12	2.48	0.43
1:E:711:PRO:HG2	1:E:755:PHE:HD2	1.83	0.43
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.99	0.43
1:G:560:GLU:OE1	1:G:636:LYS:HE3	2.17	0.43
2:H:270:LEU:HA	2:H:270:LEU:HD12	1.57	0.43
1:C:701:ALA:O	1:C:705:ALA:N	2.40	0.43
2:H:195:VAL:HG11	2:H:228:VAL:HG13	1.99	0.43
1:C:702:VAL:HG11	1:C:735:ARG:HH21	1.79	0.43
1:G:1000:HIS:NE2	1:G:1002:GLN:HB3	2.34	0.43
1:A:145:ARG:HB3	1:A:208:GLU:CD	2.39	0.43
1:A:571:ARG:NH2	11:A:1415:HOH:O	2.27	0.43
1:E:533:ALA:O	1:E:534:ALA:HB3	2.18	0.43
1:A:235:GLU:HB2	1:A:253:ALA:HA	2.01	0.43
1:G:257:THR:O	1:G:258:ASP:C	2.56	0.43
1:E:936:ASN:ND2	11:E:1156:HOH:O	2.52	0.43
2:D:43:LEU:HD21	2:D:80:LEU:HD13	2.00	0.43
1:A:45:ILE:HD13	1:A:81:GLU:HB3	2.01	0.43
2:B:307:ILE:HD13	2:B:307:ILE:N	2.33	0.43
2:H:132:ILE:CG2	2:H:133:ILE:N	2.81	0.43
1:C:704:LYS:O	1:C:707:GLU:HB2	2.19	0.43
1:G:692:ASN:C	1:G:708:ILE:HD11	2.39	0.43
1:G:488:PHE:O	1:G:489:LEU:C	2.55	0.43
1:C:735:ARG:O	1:C:738:PHE:N	2.50	0.43
2:F:195:VAL:HG21	2:F:231:MET:HE3	2.00	0.43
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.53	0.43
1:G:178:GLY:CA	1:G:198:LEU:HD23	2.48	0.43
2:D:364:ALA:N	2:D:365:PRO:HD2	2.34	0.43
1:G:709:GLY:O	1:G:754:HIS:ND1	2.50	0.43
2:H:193:HIS:O	2:H:234:ASP:HB2	2.18	0.43
9:C:1092:NET:H83	9:C:1092:NET:H11	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:354:PRO:HB3	2:H:363:ALA:O	2.17	0.43
2:H:199:PHE:CE2	2:H:274:LEU:CD1	3.02	0.43
1:C:693:ALA:HB3	1:C:752:LEU:HB2	2.01	0.43
2:D:199:PHE:CE2	2:D:274:LEU:HD12	2.53	0.43
2:H:16:HIS:CD2	2:H:16:HIS:N	2.86	0.43
1:E:949:VAL:O	1:E:954:LYS:NZ	2.41	0.43
2:F:190:LEU:HA	2:F:191:PRO:HD2	1.80	0.43
2:D:74:GLN:HB2	11:D:2853:HOH:O	2.18	0.43
1:E:831:ALA:HB2	1:E:840:ILE:HD11	2.01	0.43
1:C:424:ILE:HG21	1:C:424:ILE:HD13	1.83	0.43
1:A:426:ARG:HD3	1:A:426:ARG:C	2.39	0.43
2:D:354:PRO:HB2	2:D:367:PHE:CE2	2.54	0.43
2:F:342:ARG:HA	2:F:342:ARG:HD2	1.79	0.43
1:A:784:GLN:HE22	1:A:1043:THR:HB	1.83	0.43
1:G:1019:GLY:O	1:G:1023:ILE:HG13	2.18	0.43
1:E:563:MET:CE	1:E:635:PRO:HG3	2.45	0.43
2:F:364:ALA:N	2:F:365:PRO:HD2	2.32	0.43
1:E:998:ARG:HG2	1:E:999:PRO:HA	2.01	0.43
1:G:814:GLN:O	1:G:815:LYS:C	2.54	0.43
2:H:210:VAL:O	2:H:211:ASP:C	2.57	0.43
1:A:740:THR:HG23	1:A:740:THR:H	1.51	0.43
2:D:350:PHE:HB2	2:D:366:LEU:CD2	2.48	0.43
2:B:285:LYS:HG3	2:B:314:PHE:CZ	2.52	0.43
2:D:50:ARG:HH12	2:D:156:MET:CE	2.32	0.43
2:F:195:VAL:CG2	2:F:231:MET:HE3	2.49	0.43
1:G:814:GLN:HG3	1:G:818:PHE:CE2	2.53	0.43
1:E:17:PRO:HG3	1:E:917:VAL:HG13	2.00	0.43
1:E:704:LYS:O	1:E:705:ALA:C	2.56	0.43
1:G:548:GLU:OE1	2:H:114:ASP:HA	2.19	0.43
1:C:163:GLY:O	1:C:166:CYS:HB3	2.18	0.43
1:G:106:GLY:HA2	11:G:1176:HOH:O	2.18	0.43
2:D:272:HIS:HB2	2:D:349:SER:HB2	2.01	0.43
1:C:678:PHE:O	1:C:681:ALA:N	2.52	0.43
2:B:350:PHE:CD1	2:B:366:LEU:HD21	2.53	0.43
1:A:891:LYS:NZ	11:A:1825:HOH:O	2.51	0.43
2:D:6:LEU:HD13	2:D:16:HIS:ND1	2.34	0.43
2:F:46:PRO:HA	2:F:76:HIS:CG	2.53	0.43
2:H:300:VAL:HG22	2:H:328:THR:O	2.19	0.43
2:D:41:GLU:HB2	2:D:358:PRO:HD3	2.01	0.43
1:C:28:TYR:CE1	1:C:313:LYS:HE3	2.53	0.43
1:A:194:ARG:NH2	11:A:1266:HOH:O	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:761:GLU:HG2	1:E:781:HIS:CE1	2.54	0.43
2:D:168:TYR:O	2:D:218:ILE:N	2.43	0.43
1:G:472:LEU:O	1:G:476:VAL:HG23	2.18	0.43
2:D:201:ALA:CB	2:D:239:SER:HB2	2.48	0.43
2:H:201:ALA:HB2	2:H:239:SER:HB2	2.01	0.43
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.59	0.43
1:C:375:THR:HG23	1:C:377:GLN:H	1.84	0.43
1:G:883:VAL:HG12	1:G:884:ILE:N	2.33	0.43
1:C:373:ARG:O	1:C:379:LYS:NZ	2.40	0.43
1:E:885:PRO:HA	1:E:886:PRO:HD3	1.65	0.43
2:B:49:SER:HA	2:B:76:HIS:O	2.18	0.43
2:H:54:THR:HG23	2:H:81:VAL:CG1	2.48	0.43
2:B:201:ALA:HB2	2:B:239:SER:HB2	1.99	0.43
1:C:891:LYS:HE3	1:C:893:VAL:HG12	2.01	0.43
1:C:28:TYR:CZ	1:C:313:LYS:HE3	2.54	0.43
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.48	0.43
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.49	0.43
2:D:234:ASP:CG	2:D:378:ARG:HH11	2.22	0.43
1:C:358:LYS:HG2	1:C:359:ILE:N	2.32	0.43
1:G:692:ASN:HB3	1:G:753:ASP:OD2	2.19	0.42
2:B:342:ARG:NE	2:B:344:ASP:OD2	2.51	0.42
1:E:646:THR:HB	1:E:647:PRO:HD3	2.00	0.42
1:A:702:VAL:HG11	1:A:735:ARG:NH2	2.34	0.42
1:E:493:LYS:HD2	1:E:493:LYS:HA	1.74	0.42
1:E:948:SER:OG	10:E:1093:U:H5'	2.18	0.42
1:E:836:GLU:HG3	11:E:1817:HOH:O	2.18	0.42
2:H:210:VAL:HA	2:H:214:CYS:O	2.19	0.42
1:G:82:ARG:NH1	11:G:1744:HOH:O	2.52	0.42
2:F:87:LEU:HA	2:F:87:LEU:HD12	1.69	0.42
2:F:379:LYS:CB	2:F:379:LYS:NZ	2.82	0.42
1:G:652[A]:ARG:HH12	1:G:667:ASP:HA	1.81	0.42
1:E:1021:ARG:CG	1:E:1021:ARG:NH1	2.80	0.42
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	2.00	0.42
1:A:425[A]:ARG:NH1	11:A:1430:HOH:O	2.32	0.42
2:H:5:ALA:HB1	2:H:110:ILE:HG13	2.01	0.42
2:B:268:ILE:HD13	2:B:354:PRO:HD2	2.00	0.42
2:D:157:ASP:CG	2:D:160:LYS:HG2	2.40	0.42
1:C:223:ASP:CG	1:C:227:ASN:HB2	2.39	0.42
2:H:219:VAL:HG23	2:H:220:PRO:O	2.19	0.42
1:G:885:PRO:HA	1:G:886:PRO:HD3	1.66	0.42
1:E:458:ILE:O	1:E:463:LEU:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:LEU:HD23	1:A:796:LEU:C	2.40	0.42
2:B:255:ILE:HD13	2:B:274:LEU:HB3	2.01	0.42
1:G:671:ARG:NH2	1:G:819:GLU:O	2.52	0.42
1:A:67:GLU:OE1	1:A:1062:VAL:HA	2.19	0.42
1:E:26:PHE:HA	1:E:29[B]:SER:OG	2.19	0.42
2:F:139:ASP:OD2	2:F:142:LEU:HB2	2.19	0.42
1:A:840:ILE:O	1:A:841:GLU:HB3	2.19	0.42
1:C:775:ILE:HD13	1:C:775:ILE:HA	1.84	0.42
2:H:168:TYR:N	2:H:168:TYR:CD1	2.87	0.42
2:H:29:GLU:HA	2:H:129:ASN:HA	1.99	0.42
2:F:286:MET:CE	2:F:312:HIS:ND1	2.82	0.42
1:A:446:GLY:C	1:E:447:LEU:HD23	2.40	0.42
2:F:23:THR:HG23	2:F:134:ALA:O	2.19	0.42
2:B:369:HIS:O	2:B:372:GLU:HB2	2.20	0.42
1:C:864:VAL:O	1:C:868:VAL:HG23	2.19	0.42
2:H:256:GLN:HG3	2:H:278:ALA:HB1	2.01	0.42
1:C:710:TYR:HA	1:C:711:PRO:C	2.39	0.42
2:H:275:LEU:CD2	2:H:349:SER:HB3	2.48	0.42
1:G:734:LEU:O	1:G:737:TYR:HB3	2.18	0.42
1:G:479:VAL:HG23	1:G:480:GLY:O	2.19	0.42
2:D:29:GLU:CD	2:D:153:LEU:HD22	2.39	0.42
2:H:45:ASP:O	2:H:76:HIS:HB2	2.18	0.42
1:G:772:MET:CE	1:G:880:THR:HA	2.49	0.42
1:G:105:GLN:CA	1:G:105:GLN:NE2	2.82	0.42
1:G:421:LEU:HD21	1:G:445:ALA:HB1	2.00	0.42
1:C:435:ARG:HB2	11:C:1376:HOH:O	2.20	0.42
2:F:218:ILE:HD13	2:F:218:ILE:N	2.34	0.42
1:G:1:MET:CB	1:G:224:LYS:HZ2	2.17	0.42
1:G:630:VAL:HG13	1:G:635:PRO:CD	2.50	0.42
2:D:50:ARG:NH1	2:D:156:MET:HE1	2.35	0.42
1:E:1:MET:O	1:E:329:GLY:O	2.38	0.42
2:F:188:ASP:OD2	2:F:188:ASP:N	2.52	0.42
1:C:932:GLN:HG3	11:C:1554:HOH:O	2.19	0.42
1:E:434:ASP:O	1:E:435:ARG:C	2.57	0.42
1:A:1031:ARG:HE	1:A:1031:ARG:HB3	1.62	0.42
1:E:6:ASP:N	1:E:6:ASP:OD2	2.42	0.42
2:D:325:LEU:HA	2:D:325:LEU:HD23	1.52	0.42
2:B:172:GLN:HA	11:B:3559:HOH:O	2.18	0.42
2:F:6:LEU:HD23	2:F:138:PRO:HB2	2.02	0.42
2:D:71:GLU:O	2:D:203:ARG:HG3	2.20	0.42
2:F:205:ILE:HG12	2:F:355:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ARG:O	1:G:134:VAL:HG23	2.19	0.42
1:G:318:PRO:HB2	1:G:321:LYS:HB2	2.01	0.42
1:G:762:VAL:CG2	1:G:801:LEU:HD11	2.49	0.42
2:H:208:MET:SD	2:H:355:GLU:HA	2.59	0.42
1:C:980:VAL:HG13	11:C:1568:HOH:O	2.20	0.42
2:D:236:ILE:HB	2:D:265:VAL:HG22	2.00	0.42
1:E:764:VAL:HA	1:E:777:GLY:O	2.20	0.42
1:A:339:ILE:HD13	1:A:339:ILE:HG21	1.79	0.42
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.41	0.42
2:F:274:LEU:HA	2:F:274:LEU:HD23	1.61	0.42
1:A:992:ASN:HD21	1:G:975:HIS:HE2	1.68	0.42
1:E:757:ASP:O	1:E:758:ASP:C	2.58	0.42
2:F:195:VAL:HG11	2:F:231:MET:CE	2.50	0.42
1:C:689:GLN:O	1:C:690:PRO:C	2.58	0.42
1:G:948:SER:O	1:G:1015:ASN:HA	2.19	0.42
1:C:827:ASN:N	1:C:843:ASN:O	2.51	0.42
1:A:954:LYS:HB3	1:A:980:VAL:HG21	2.01	0.42
2:H:158:LEU:O	2:H:161:GLU:HB2	2.19	0.42
2:H:318:GLU:HA	2:H:337:LEU:HD22	2.01	0.42
1:C:954:LYS:HG2	1:C:980:VAL:HG21	2.01	0.42
2:D:85:LEU:HD12	2:D:86:PRO:HD2	2.02	0.42
1:C:183:TYR:N	1:C:187:GLU:OE1	2.33	0.42
2:H:272:HIS:HE1	2:H:340:ILE:HG12	1.83	0.42
1:G:698:ILE:N	1:G:698:ILE:CD1	2.83	0.42
1:G:509:ARG:HB2	1:G:509:ARG:NH1	2.23	0.42
1:A:370:ALA:HB2	1:A:903:VAL:HG23	2.00	0.42
1:G:37:LEU:HD23	1:G:37:LEU:HA	1.81	0.42
2:H:193:HIS:HD2	2:H:194:VAL:N	2.18	0.42
1:A:897:PHE:HB3	11:A:1561:HOH:O	2.20	0.42
1:C:132:PHE:O	1:C:136:MET:HG2	2.20	0.42
1:E:65:TYR:OH	1:E:80:LYS:HE3	2.20	0.42
1:G:893:VAL:HA	1:G:916:GLU:HA	2.02	0.42
1:A:44:VAL:O	1:A:62:ASP:HB2	2.20	0.42
1:G:256:LEU:HD23	1:G:256:LEU:HA	1.91	0.42
1:A:185:ARG:HD3	1:A:185:ARG:HH11	1.73	0.42
2:B:29:GLU:CB	2:B:153:LEU:HD22	2.50	0.41
1:E:677:ARG:O	1:E:680:HIS:HB2	2.20	0.41
2:F:239:SER:OG	2:F:240:ASN:O	2.38	0.41
1:G:425:ARG:NH1	11:G:1403:HOH:O	2.50	0.41
1:A:14:GLY:HA2	11:A:1098:HOH:O	2.20	0.41
1:A:804:GLU:HB3	11:A:1837:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ALA:HB2	1:A:826:MET:SD	2.60	0.41
2:H:307:ILE:O	2:H:362:ASP:HB2	2.20	0.41
2:H:289:GLY:O	2:H:290:HIS:HD2	2.03	0.41
1:E:76:LYS:HD2	1:E:76:LYS:HA	1.91	0.41
2:H:354:PRO:HA	2:H:363:ALA:HB3	2.03	0.41
2:B:190:LEU:HD12	2:B:215:ARG:HB2	2.02	0.41
1:G:735:ARG:O	1:G:736:ARG:C	2.58	0.41
2:F:345:LYS:HB3	2:F:346:PRO:CD	2.50	0.41
1:A:990:LEU:HD21	1:G:975:HIS:CE1	2.55	0.41
2:H:299:ASP:HB3	2:H:304:VAL:HG22	2.01	0.41
1:G:686:LYS:O	1:G:687:LEU:HD23	2.21	0.41
1:C:956:ARG:HD3	1:C:1044:LEU:HD23	2.02	0.41
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.34	0.41
1:C:679:GLN:HG3	1:C:689:GLN:HE22	1.84	0.41
2:B:363:ALA:C	2:B:365:PRO:HD2	2.41	0.41
1:A:318:PRO:HG3	1:A:610:TYR:OH	2.20	0.41
1:C:222:ARG:HD3	1:C:277:VAL:O	2.20	0.41
1:E:652:ARG:HD3	1:E:666:PRO:HB2	2.01	0.41
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.57	0.41
1:G:1001:ILE:CD1	1:G:1029:ILE:HD11	2.51	0.41
2:H:154:ASN:HD22	2:H:154:ASN:C	2.24	0.41
2:B:355:GLU:O	2:B:356:ALA:C	2.58	0.41
2:B:228:VAL:CG1	2:B:258:PHE:CE1	3.00	0.41
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.48	0.41
1:E:81:GLU:O	1:E:82:ARG:C	2.57	0.41
1:C:384:VAL:HG22	1:C:385:MET:N	2.35	0.41
1:C:57:ASP:OD1	1:C:584:HIS:NE2	2.46	0.41
1:E:106:GLY:HA2	11:E:1178:HOH:O	2.20	0.41
1:A:221:VAL:HA	1:A:281:GLY:HA2	2.01	0.41
1:C:6:ASP:N	1:C:6:ASP:OD2	2.43	0.41
2:H:272:HIS:HD2	2:H:351:GLN:NE2	2.19	0.41
2:D:324:ASN:O	2:D:342:ARG:HA	2.20	0.41
1:G:728:VAL:HG11	1:G:734:LEU:CA	2.49	0.41
2:D:8:VAL:HG12	2:D:9:LEU:O	2.20	0.41
1:A:563:MET:HE3	1:A:563:MET:HB2	1.90	0.41
1:E:734:LEU:CD1	1:E:738:PHE:CE2	3.00	0.41
2:F:225:ALA:HA	2:F:258:PHE:CZ	2.56	0.41
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.55	0.41
1:A:166:CYS:C	1:A:167:ILE:HD12	2.41	0.41
1:G:992:ASN:HA	1:G:996:GLU:OE1	2.19	0.41
1:G:656:ALA:C	1:G:658:GLY:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:402:LEU:O	1:G:403:GLU:HB2	2.20	0.41
2:F:270:LEU:HA	2:F:270:LEU:HD12	1.79	0.41
2:F:325:LEU:HD23	2:F:325:LEU:HA	1.83	0.41
1:E:1:MET:CB	1:E:224:LYS:NZ	2.80	0.41
1:E:671:ARG:CG	1:E:677:ARG:NH1	2.84	0.41
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.55	0.41
2:F:237:PHE:CE2	2:F:239:SER:HA	2.56	0.41
2:D:48:TYR:HA	2:D:51:GLN:NE2	2.35	0.41
1:C:180:GLY:HA2	1:C:376:THR:OG1	2.20	0.41
1:C:176:GLY:HA3	1:C:376:THR:O	2.20	0.41
1:G:992:ASN:ND2	1:G:996:GLU:HB3	2.35	0.41
1:C:493:LYS:NZ	1:C:499:ASP:OD2	2.51	0.41
1:A:895:LEU:HA	1:A:896:PRO:HD3	1.90	0.41
2:B:141:ALA:O	2:B:145:GLU:HB2	2.20	0.41
1:G:637:GLY:HA2	1:G:660:PRO:O	2.20	0.41
1:A:543:MET:CE	1:A:617:TYR:CZ	3.03	0.41
1:C:48:ASN:O	1:C:66:ILE:HA	2.20	0.41
1:C:457:ASN:ND2	11:C:1288:HOH:O	2.53	0.41
2:D:245:PRO:HG2	2:D:274:LEU:CD2	2.50	0.41
1:G:1065:VAL:O	1:G:1068:MET:HB2	2.21	0.41
1:C:761:GLU:OE2	1:C:785:ALA:HA	2.20	0.41
1:G:804:GLU:HB3	11:G:1688:HOH:O	2.21	0.41
1:E:954:LYS:NZ	10:E:1093:U:OP3	2.30	0.41
1:A:367:PHE:O	1:A:370:ALA:HB3	2.20	0.41
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.70	0.41
2:H:23:THR:HG23	2:H:134:ALA:O	2.21	0.41
2:B:357:SER:HA	2:B:358:PRO:HA	1.76	0.41
1:G:853:VAL:HG12	1:G:861:LEU:HD11	2.03	0.41
2:F:269:CYS:O	2:F:270:LEU:C	2.59	0.41
2:F:324:ASN:O	2:F:342:ARG:HA	2.21	0.41
1:A:1001:ILE:CD1	1:A:1002:GLN:N	2.80	0.41
2:H:20:ILE:O	2:H:99:SER:OG	2.35	0.41
1:C:75:ARG:HG3	1:C:107:VAL:HG11	2.02	0.41
1:A:692:ASN:HB3	1:A:753:ASP:CG	2.41	0.41
1:G:11:LEU:HA	1:G:45:ILE:O	2.21	0.41
1:E:761:GLU:HB3	1:E:781:HIS:ND1	2.36	0.41
2:B:300:VAL:HG22	2:B:328:THR:O	2.20	0.41
1:G:362:PHE:CE1	1:G:380:SER:HB3	2.55	0.41
1:G:805:ILE:HD13	1:G:832:VAL:HG11	2.02	0.41
1:C:903:VAL:HG22	11:C:1369:HOH:O	2.20	0.41
2:H:350:PHE:CD2	2:H:354:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ILE:CD1	2:B:274:LEU:HB3	2.50	0.41
1:A:130[B]:ARG:HD2	11:A:1197:HOH:O	2.19	0.41
2:H:247:PRO:CA	2:H:252:ILE:CD1	2.99	0.41
1:C:761:GLU:CG	1:C:781:HIS:CE1	3.03	0.41
2:H:374:ILE:O	2:H:378:ARG:HG3	2.20	0.41
1:G:115:MET:HG2	1:G:118:ALA:O	2.21	0.41
1:A:259:LYS:HD3	2:B:175:TRP:CD2	2.55	0.41
2:H:23:THR:CG2	2:H:24:GLY:N	2.84	0.41
1:A:164:PHE:HA	1:A:165:PRO:C	2.40	0.41
2:B:13:THR:HG22	2:B:15:PHE:CE2	2.56	0.41
2:B:332:LEU:HA	2:B:332:LEU:HD12	1.76	0.41
2:H:245:PRO:HG3	2:H:274:LEU:HG	2.02	0.41
2:B:187:GLU:O	2:B:189:GLU:N	2.53	0.41
1:C:750:VAL:HG12	1:C:752:LEU:CD1	2.51	0.41
1:G:812:GLN:O	1:G:816:LEU:HD12	2.21	0.41
1:A:773:VAL:CG2	1:A:814:GLN:HG3	2.51	0.41
2:B:350:PHE:HB2	2:B:366:LEU:HD23	2.01	0.41
1:G:187:GLU:O	1:G:191:ILE:HG13	2.20	0.41
1:E:669:ILE:HA	1:E:844:PRO:HG2	2.01	0.41
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.21	0.41
2:F:341:HIS:CD2	2:F:348:PHE:HB3	2.56	0.41
1:G:830:PHE:CE1	1:G:839:LEU:CD1	3.04	0.41
1:E:1063:ILE:CG1	1:E:1064:SER:N	2.84	0.41
2:B:133:ILE:HG21	2:B:133:ILE:HD13	1.73	0.41
1:G:875:ALA:HB2	11:G:1504:HOH:O	2.21	0.41
2:D:228:VAL:HG12	2:D:229:LEU:N	2.34	0.41
1:C:1051:ALA:HA	1:C:1054:LEU:HD12	2.03	0.41
1:A:677:ARG:HD2	11:A:1807:HOH:O	2.21	0.41
2:H:158:LEU:O	2:H:159:ALA:C	2.58	0.41
1:G:814:GLN:CG	1:G:818:PHE:CE2	3.03	0.41
1:A:361:ARG:CZ	1:A:404:VAL:HG12	2.51	0.41
1:G:947:LEU:HD12	1:G:947:LEU:N	2.36	0.41
1:G:148:ILE:HG22	1:G:149:ALA:N	2.36	0.41
2:F:356:ALA:O	2:F:357:SER:HB3	2.21	0.41
1:G:524:PRO:CG	1:G:628:GLU:HG3	2.50	0.41
1:E:570:ASN:HB2	11:E:1629:HOH:O	2.21	0.41
1:A:820:LEU:O	1:A:821:GLN:HB2	2.20	0.41
1:E:576:ILE:HG21	1:E:576:ILE:HD13	1.88	0.41
1:G:339:ILE:HG22	1:G:540:THR:OG1	2.21	0.40
1:G:1001:ILE:HD13	1:G:1001:ILE:HG21	1.69	0.40
2:D:150:PHE:HA	2:D:151:PRO:HD3	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:561:LYS:HE2	1:G:595:GLU:OE2	2.21	0.40
1:G:70:HIS:O	1:G:71:TRP:C	2.59	0.40
2:D:32:PHE:O	2:D:291:HIS:HB2	2.21	0.40
1:C:500:ALA:O	1:C:504:LYS:HG3	2.21	0.40
1:C:796:LEU:HA	1:C:797:PRO:HA	1.94	0.40
1:C:164:PHE:HA	1:C:165:PRO:C	2.42	0.40
2:H:199:PHE:CE2	2:H:274:LEU:HD12	2.56	0.40
2:D:270:LEU:O	2:D:273:GLN:HB2	2.20	0.40
1:G:734:LEU:HD12	1:G:734:LEU:C	2.41	0.40
1:A:999:PRO:HD2	1:G:983:GLU:OE1	2.20	0.40
1:G:479:VAL:HG23	1:G:483:GLY:CA	2.48	0.40
1:G:991:VAL:HG22	1:G:1001:ILE:HG23	2.03	0.40
1:G:775:ILE:HD11	1:G:813:VAL:HG11	2.02	0.40
1:E:9:SER:HA	1:E:43:ARG:O	2.20	0.40
1:C:1021:ARG:O	1:C:1025:ASP:OD2	2.39	0.40
2:D:246:ALA:CB	2:D:248:ASP:HB2	2.51	0.40
1:C:424:ILE:O	1:C:425:ARG:C	2.58	0.40
1:C:85:ALA:HA	1:C:114:THR:O	2.21	0.40
1:E:135:ALA:HB1	1:E:274:GLU:CG	2.51	0.40
1:G:67:GLU:HB3	1:G:68:PRO:HD2	2.02	0.40
1:A:48:ASN:O	1:A:66:ILE:HA	2.21	0.40
1:A:726:GLU:CG	1:A:727:ILE:N	2.79	0.40
2:B:286:MET:HE1	2:B:312:HIS:ND1	2.37	0.40
1:C:237:PHE:HB3	1:C:248:ILE:O	2.20	0.40
1:C:796:LEU:HD23	1:C:796:LEU:C	2.42	0.40
1:G:972:ASP:HA	1:G:989:ARG:O	2.21	0.40
1:A:51:PRO:HG3	1:A:918:MET:HB2	2.02	0.40
1:A:354:TYR:CD2	1:A:387:ILE:HG23	2.56	0.40
1:C:22:GLN:HG3	1:C:26:PHE:CE2	2.57	0.40
1:C:36:ALA:O	1:C:40:GLU:HG2	2.21	0.40
1:A:489:LEU:HD12	1:A:489:LEU:HA	1.87	0.40
2:B:186:LYS:HB3	2:B:188:ASP:OD2	2.22	0.40
1:G:695:VAL:HG23	1:G:752:LEU:HD22	2.03	0.40
1:G:540:THR:HG22	1:G:541:ALA:N	2.36	0.40
1:A:992:ASN:O	1:A:1000:HIS:HA	2.22	0.40
1:A:930:LYS:NZ	1:A:1058:ALA:O	2.51	0.40
2:H:176:THR:O	2:H:177:LEU:C	2.57	0.40
1:C:4:ARG:NE	1:C:7:ILE:HD12	2.37	0.40
2:H:225:ALA:O	2:H:229:LEU:HD12	2.22	0.40
1:A:58:PRO:HD2	1:A:59:GLU:OE2	2.22	0.40
2:F:316:VAL:HB	2:F:337:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:OE2	1:A:604:GLU:OE1	2.39	0.40
1:G:998:ARG:HA	1:G:999:PRO:C	2.40	0.40
1:E:765:ASP:O	1:E:776:GLY:N	2.49	0.40
1:A:1054:LEU:HD23	1:A:1054:LEU:HA	1.97	0.40
1:C:76:LYS:HD2	1:C:76:LYS:HA	1.96	0.40
2:H:277:LEU:HD23	2:H:277:LEU:HA	1.95	0.40
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.66	0.40
1:C:677:ARG:O	1:C:680:HIS:HB2	2.22	0.40
1:E:695:VAL:CG1	1:E:696:THR:N	2.84	0.40
1:A:702:VAL:CG1	1:A:731:GLU:CG	2.99	0.40
1:G:812:GLN:O	1:G:813:VAL:C	2.60	0.40
1:C:678:PHE:O	1:C:679:GLN:C	2.59	0.40
2:F:365:PRO:O	2:F:366:LEU:C	2.59	0.40
1:E:361:ARG:NH2	1:E:571:ARG:HG2	2.37	0.40
1:C:993:LYS:HG2	10:C:1093:U:C5	2.56	0.40
1:C:124:ASP:O	1:C:128:ASP:HB3	2.22	0.40
1:G:85:ALA:HA	1:G:114:THR:O	2.22	0.40
1:G:220:VAL:O	1:G:281:GLY:HA2	2.22	0.40

All (1) 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)
11:A:1848:HOH:O	11:C:1912:HOH:O[4_555]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	1061/1073 (99%)	1015 (96%)	44 (4%)	2 (0%)	52 53
1	C	1060/1073 (99%)	1005 (95%)	54 (5%)	1 (0%)	56 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1057/1073 (98%)	1013 (96%)	42 (4%)	2 (0%)	52	53
1	G	1061/1073 (99%)	996 (94%)	59 (6%)	6 (1%)	30	24
2	B	377/382 (99%)	348 (92%)	26 (7%)	3 (1%)	24	17
2	D	378/382 (99%)	354 (94%)	23 (6%)	1 (0%)	46	45
2	F	377/382 (99%)	355 (94%)	21 (6%)	1 (0%)	46	45
2	H	377/382 (99%)	346 (92%)	27 (7%)	4 (1%)	17	11
All	All	5748/5820 (99%)	5432 (94%)	296 (5%)	20 (0%)	46	45

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	154	ASN
2	D	154	ASN
1	E	738	PHE
1	G	485	ASN
1	G	975	HIS
2	H	11	ASP
1	A	558	ASP
2	F	311	ASN
2	H	247	PRO
1	G	798	ALA
2	B	188	ASP
1	C	368	ALA
1	E	954	LYS
1	G	739	GLN
1	G	736	ARG
2	H	10	GLU
2	H	365	PRO
1	A	88	PRO
2	B	191	PRO
1	G	871	GLY

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	A	874/878 (100%)	811 (93%)	63 (7%)	18	14
1	C	873/878 (99%)	809 (93%)	64 (7%)	17	13
1	E	870/878 (99%)	818 (94%)	52 (6%)	24	20
1	G	874/878 (100%)	800 (92%)	74 (8%)	13	9
2	B	308/310 (99%)	283 (92%)	25 (8%)	15	10
2	D	309/310 (100%)	283 (92%)	26 (8%)	14	9
2	F	308/310 (99%)	276 (90%)	32 (10%)	9	5
2	H	308/310 (99%)	278 (90%)	30 (10%)	10	6
All	All	4724/4752 (99%)	4358 (92%)	366 (8%)	16	12

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	THR
1	A	8	LYS
1	A	38	ARG
1	A	103	GLU
1	A	104	ARG
1	A	174	MET
1	A	185	ARG
1	A	326	LEU
1	A	343	ARG
1	A	358	LYS
1	A	363	ASN
1	A	412	LYS
1	A	418	PRO
1	A	482	THR
1	A	509	ARG
1	A	542	TYR
1	A	548	GLU
1	A	556	SER
1	A	559	ARG
1	A	571	ARG
1	A	591	GLU
1	A	652	ARG
1	A	671	ARG
1	A	675	ARG
1	A	679	GLN
1	A	680	HIS

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Mol	Chain	Res	Type
1	A	684	ARG
1	A	688	LYS
1	A	700	MET
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS
1	A	712	LEU
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	751	LEU
1	A	752	LEU
1	A	753	ASP
1	A	763	ASP
1	A	784	GLN
1	A	800	THR
1	A	805	ILE
1	A	815	LYS
1	A	835	ASN
1	A	839	LEU
1	A	855	LYS
1	A	881	LYS
1	A	891	LYS
1	A	912	ARG
1	A	930	LYS
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	966	LYS
1	A	967[A]	GLN
1	A	967[B]	GLN
1	A	992	ASN
1	A	1006	LYS
1	A	1018	SER
1	A	1020	ARG
1	A	1073	LYS
2	B	2	ILE
2	B	6	LEU
2	B	18	ARG
2	B	49	SER
2	B	50	ARG
2	B	78	GLN

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Mol	Chain	Res	Type
2	B	87	LEU
2	B	125	LYS
2	B	142	LEU
2	B	153	LEU
2	B	154	ASN
2	B	192	PHE
2	B	215	ARG
2	B	227	ASP
2	B	239	SER
2	B	248	ASP
2	B	249	ASP
2	B	261	THR
2	B	263	ILE
2	B	324	ASN
2	B	331	SER
2	B	332	LEU
2	B	333	PHE
2	B	376	GLN
2	B	379	LYS
1	C	1	MET
1	C	4	ARG
1	C	5	THR
1	C	38	ARG
1	C	76	LYS
1	C	103	GLU
1	C	174	MET
1	C	185	ARG
1	C	202	LYS
1	C	236	ASN
1	C	275	ILE
1	C	313	LYS
1	C	321	LYS
1	C	326	LEU
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	414	SER
1	C	416	ASP
1	C	423[A]	LYS
1	C	423[B]	LYS
1	C	426	ARG
1	C	482	THR

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Mol	Chain	Res	Type
1	C	519	GLN
1	C	548	GLU
1	C	563	MET
1	C	571	ARG
1	C	645	GLN
1	C	652	ARG
1	C	665	SER
1	C	671	ARG
1	C	675	ARG
1	C	688	LYS
1	C	689	GLN
1	C	696	THR
1	C	702	VAL
1	C	706	LYS
1	C	725	MET
1	C	733	ASP
1	C	735	ARG
1	C	736	ARG
1	C	751	LEU
1	C	752	LEU
1	C	763	ASP
1	C	784	GLN
1	C	805	ILE
1	C	812	GLN
1	C	855	LYS
1	C	880	THR
1	C	881	LYS
1	C	912	ARG
1	C	950	ARG
1	C	951	GLU
1	C	956	ARG
1	C	966	LYS
1	C	967[A]	GLN
1	C	967[B]	GLN
1	C	1001	ILE
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1061	LYS
1	C	1063	ILE
1	C	1073	LYS
2	D	4	SER

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Mol	Chain	Res	Type
2	D	27	VAL
2	D	47	SER
2	D	49	SER
2	D	73	SER
2	D	87	LEU
2	D	100	SER
2	D	153	LEU
2	D	154	ASN
2	D	156	MET
2	D	166	GLU
2	D	215	ARG
2	D	224	SER
2	D	239	SER
2	D	248	ASP
2	D	249	ASP
2	D	261	THR
2	D	282	LYS
2	D	306	MET
2	D	324	ASN
2	D	332	LEU
2	D	333	PHE
2	D	357	SER
2	D	366	LEU
2	D	376	GLN
2	D	379	LYS
1	E	3	LYS
1	E	5	THR
1	E	46	LEU
1	E	76	LYS
1	E	103	GLU
1	E	115	MET
1	E	174	MET
1	E	185	ARG
1	E	236	ASN
1	E	275	ILE
1	E	299	GLU
1	E	326	LEU
1	E	363	ASN
1	E	412	LYS
1	E	509	ARG
1	E	518	ASP
1	E	542	TYR

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Mol	Chain	Res	Type
1	E	548	GLU
1	E	571	ARG
1	E	591	GLU
1	E	645[A]	GLN
1	E	645[B]	GLN
1	E	671	ARG
1	E	675	ARG
1	E	677	ARG
1	E	688	LYS
1	E	696	THR
1	E	704	LYS
1	E	706	LYS
1	E	733	ASP
1	E	734	LEU
1	E	735	ARG
1	E	750	VAL
1	E	751	LEU
1	E	763	ASP
1	E	784	GLN
1	E	795	SER
1	E	805	ILE
1	E	838	TYR
1	E	849	THR
1	E	855	LYS
1	E	912	ARG
1	E	950	ARG
1	E	951	GLU
1	E	956	ARG
1	E	967[A]	GLN
1	E	967[B]	GLN
1	E	983	GLU
1	E	1018	SER
1	E	1020	ARG
1	E	1021	ARG
1	E	1073	LYS
2	F	2	ILE
2	F	4	SER
2	F	18	ARG
2	F	25	SER
2	F	73	SER
2	F	87	LEU
2	F	125	LYS

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Mol	Chain	Res	Type
2	F	154	ASN
2	F	166	GLU
2	F	174	SER
2	F	175	TRP
2	F	186	LYS
2	F	190	LEU
2	F	192	PHE
2	F	230	LYS
2	F	236	ILE
2	F	238	LEU
2	F	239	SER
2	F	249	ASP
2	F	257	LYS
2	F	262	ASP
2	F	263	ILE
2	F	269	CYS
2	F	282	LYS
2	F	306	MET
2	F	321	LEU
2	F	324	ASN
2	F	332	LEU
2	F	333	PHE
2	F	366	LEU
2	F	376	GLN
2	F	379	LYS
1	G	4	ARG
1	G	46	LEU
1	G	55	MET
1	G	59	GLU
1	G	82	ARG
1	G	103	GLU
1	G	119	THR
1	G	145	ARG
1	G	174	MET
1	G	185	ARG
1	G	202	LYS
1	G	224	LYS
1	G	230	ILE
1	G	236	ASN
1	G	282	SER
1	G	303	ARG
1	G	307	SER

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Mol	Chain	Res	Type
1	G	313	LYS
1	G	317	PHE
1	G	326	LEU
1	G	344	THR
1	G	428	LEU
1	G	479	VAL
1	G	493	LYS
1	G	509	ARG
1	G	519	GLN
1	G	542	TYR
1	G	548	GLU
1	G	571	ARG
1	G	591	GLU
1	G	645[A]	GLN
1	G	645[B]	GLN
1	G	648	LEU
1	G	652[A]	ARG
1	G	652[B]	ARG
1	G	675	ARG
1	G	688	LYS
1	G	692	ASN
1	G	696	THR
1	G	700	MET
1	G	706	LYS
1	G	708	ILE
1	G	712	LEU
1	G	733	ASP
1	G	735	ARG
1	G	751	LEU
1	G	763	ASP
1	G	774	LEU
1	G	784	GLN
1	G	810	ARG
1	G	849	THR
1	G	855	LYS
1	G	880	THR
1	G	884	ILE
1	G	891	LYS
1	G	912	ARG
1	G	940	LYS
1	G	951	GLU
1	G	955	GLU

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Mol	Chain	Res	Type
1	G	956	ARG
1	G	967[A]	GLN
1	G	967[B]	GLN
1	G	987	ASN
1	G	991	VAL
1	G	999	PRO
1	G	1006	LYS
1	G	1014	ILE
1	G	1018	SER
1	G	1020	ARG
1	G	1021	ARG
1	G	1027	ARG
1	G	1031	ARG
1	G	1061	LYS
1	G	1073	LYS
2	H	2	ILE
2	H	3	LYS
2	H	6	LEU
2	H	18	ARG
2	H	50	ARG
2	H	104	ARG
2	H	125	LYS
2	H	128	GLN
2	H	131	CYS
2	H	154	ASN
2	H	166	GLU
2	H	174	SER
2	H	192	PHE
2	H	215	ARG
2	H	218	ILE
2	H	239	SER
2	H	244	ASP
2	H	248	ASP
2	H	249	ASP
2	H	257	LYS
2	H	261	THR
2	H	279	SER
2	H	282	LYS
2	H	284	VAL
2	H	306	MET
2	H	324	ASN
2	H	332	LEU

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Mol	Chain	Res	Type
2	H	333	PHE
2	H	376	GLN
2	H	379	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	266	ASN
1	A	457	ASN
1	A	679	GLN
1	A	689	GLN
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	814	GLN
1	A	835	ASN
1	A	936	ASN
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1035	GLN
1	A	1055	ASN
1	A	1071	GLN
2	B	51	GLN
2	B	154	ASN
2	B	324	ASN
1	C	105	GLN
1	C	266	ASN
1	C	457	ASN
1	C	679	GLN
1	C	689	GLN
1	C	784	GLN
1	C	942	HIS
1	C	992	ASN
1	C	1000	HIS
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	78	GLN
2	D	291	HIS

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Mol	Chain	Res	Type
2	D	324	ASN
1	E	105	GLN
1	E	266	ASN
1	E	679	GLN
1	E	689	GLN
1	E	784	GLN
1	E	803	GLN
1	E	936	ASN
1	E	987	ASN
1	E	992	ASN
1	E	1000	HIS
1	E	1002	GLN
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	51	GLN
2	F	78	GLN
2	F	154	ASN
2	F	273	GLN
2	F	324	ASN
2	F	351	GLN
1	G	105	GLN
1	G	266	ASN
1	G	523	HIS
1	G	679	GLN
1	G	689	GLN
1	G	784	GLN
1	G	803	GLN
1	G	814	GLN
1	G	835	ASN
1	G	936	ASN
1	G	987	ASN
1	G	992	ASN
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN
1	G	1071	GLN
2	H	51	GLN
2	H	78	GLN
2	H	154	ASN
2	H	291	HIS
2	H	311	ASN

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Mol	Chain	Res	Type
2	H	324	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 86 ligands modelled in this entry, 61 are monoatomic - leaving 25 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$
5	PO4	A	1078	3	4,4,4	1.29	0	6,6,6	0.35	0
7	ADP	A	1087	3	22,29,29	1.17	2 (9%)	27,45,45	0.78	0
7	ADP	A	1088	3	22,29,29	0.98	0	27,45,45	0.95	1 (3%)
8	ORN	A	1089	-	5,8,8	0.67	0	3,9,9	1.17	0
9	NET	A	1090	-	8,8,8	0.67	0	10,10,10	0.60	0
10	U	A	1091	-	16,22,22	1.57	4 (25%)	21,33,33	3.02	2 (9%)
5	PO4	C	1078	3	4,4,4	1.65	1 (25%)	6,6,6	0.31	0
5	PO4	C	1088	-	4,4,4	1.83	1 (25%)	6,6,6	0.30	0
7	ADP	C	1089	3	22,29,29	1.26	3 (13%)	27,45,45	1.48	4 (14%)
7	ADP	C	1090	3	22,29,29	1.07	2 (9%)	27,45,45	1.11	1 (3%)
8	ORN	C	1091	-	5,8,8	0.58	0	3,9,9	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NET	C	1092	-	8,8,8	0.46	0	10,10,10	0.70	0
10	U	C	1093	-	16,22,22	1.54	3 (18%)	21,33,33	3.07	3 (14%)
5	PO4	E	1078	3	4,4,4	1.82	2 (50%)	6,6,6	0.34	0
7	ADP	E	1089	3	22,29,29	1.20	2 (9%)	27,45,45	1.15	3 (11%)
7	ADP	E	1090	3	22,29,29	1.26	3 (13%)	27,45,45	1.30	4 (14%)
8	ORN	E	1091	-	5,8,8	0.60	0	3,9,9	0.47	0
9	NET	E	1092	-	8,8,8	0.36	0	10,10,10	0.70	0
10	U	E	1093	-	16,22,22	1.62	4 (25%)	21,33,33	3.56	5 (23%)
5	PO4	G	1078	3	4,4,4	1.65	1 (25%)	6,6,6	0.31	0
7	ADP	G	1089	3	22,29,29	1.37	3 (13%)	27,45,45	1.40	4 (14%)
7	ADP	G	1090	3	22,29,29	1.26	3 (13%)	27,45,45	1.16	4 (14%)
8	ORN	G	1091	-	5,8,8	0.48	0	3,9,9	0.24	0
9	NET	G	1092	-	8,8,8	0.67	0	10,10,10	0.42	0
10	U	G	1093	-	16,22,22	1.63	4 (25%)	21,33,33	3.45	5 (23%)

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
5	PO4	A	1078	3	-	0/0/0/0	0/0/0/0
7	ADP	A	1087	3	-	0/12/32/32	0/3/3/3
7	ADP	A	1088	3	-	0/12/32/32	0/3/3/3
8	ORN	A	1089	-	-	0/4/8/8	0/0/0/0
9	NET	A	1090	-	-	0/12/12/12	0/0/0/0
10	U	A	1091	-	-	0/6/26/26	0/2/2/2
5	PO4	C	1078	3	-	0/0/0/0	0/0/0/0
5	PO4	C	1088	-	-	0/0/0/0	0/0/0/0
7	ADP	C	1089	3	-	0/12/32/32	0/3/3/3
7	ADP	C	1090	3	-	0/12/32/32	0/3/3/3
8	ORN	C	1091	-	-	0/4/8/8	0/0/0/0
9	NET	C	1092	-	-	0/12/12/12	0/0/0/0
10	U	C	1093	-	-	0/6/26/26	0/2/2/2
5	PO4	E	1078	3	-	0/0/0/0	0/0/0/0
7	ADP	E	1089	3	-	0/12/32/32	0/3/3/3
7	ADP	E	1090	3	-	0/12/32/32	0/3/3/3
8	ORN	E	1091	-	-	0/4/8/8	0/0/0/0
9	NET	E	1092	-	-	0/12/12/12	0/0/0/0
10	U	E	1093	-	-	0/6/26/26	0/2/2/2
5	PO4	G	1078	3	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	G	1089	3	-	0/12/32/32	0/3/3/3
7	ADP	G	1090	3	-	0/12/32/32	0/3/3/3
8	ORN	G	1091	-	-	0/4/8/8	0/0/0/0
9	NET	G	1092	-	-	0/12/12/12	0/0/0/0
10	U	G	1093	-	-	0/6/26/26	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1089	ADP	O4'-C1'	-3.28	1.37	1.41
10	A	1091	U	C6-C5	-2.96	1.31	1.38
10	E	1093	U	C6-C5	-2.90	1.31	1.38
10	C	1093	U	C6-C5	-2.87	1.31	1.38
10	G	1093	U	C6-C5	-2.80	1.32	1.38
7	G	1090	ADP	O4'-C1'	-2.74	1.37	1.41
5	C	1088	PO4	P-O2	-2.56	1.44	1.53
5	E	1078	PO4	P-O3	-2.40	1.44	1.53
5	G	1078	PO4	P-O2	-2.16	1.45	1.53
5	C	1078	PO4	P-O2	-2.15	1.45	1.53
5	E	1078	PO4	P-O2	-2.12	1.45	1.53
7	C	1089	ADP	O4'-C1'	-2.03	1.38	1.41
7	C	1090	ADP	O4'-C1'	-2.03	1.38	1.41
7	G	1089	ADP	C2-N1	2.11	1.37	1.33
10	E	1093	U	C6-N1	2.12	1.38	1.35
10	A	1091	U	C6-N1	2.21	1.38	1.35
7	E	1089	ADP	O2'-C2'	2.21	1.48	1.43
7	G	1090	ADP	O2'-C2'	2.28	1.48	1.43
7	E	1090	ADP	C2-N1	2.42	1.38	1.33
10	G	1093	U	C6-N1	2.47	1.39	1.35
7	C	1089	ADP	C2-N1	2.47	1.38	1.33
7	C	1090	ADP	O3'-C3'	2.52	1.49	1.43
7	A	1087	ADP	C2-N1	2.53	1.38	1.33
7	A	1087	ADP	O3'-C3'	2.71	1.49	1.43
7	E	1089	ADP	O3'-C3'	2.74	1.49	1.43
7	G	1090	ADP	O3'-C3'	2.83	1.49	1.43
10	G	1093	U	P-OP3	2.92	1.65	1.54
10	A	1091	U	P-OP3	3.03	1.65	1.54
7	G	1089	ADP	O2'-C2'	3.03	1.50	1.43
7	E	1090	ADP	O3'-C3'	3.06	1.50	1.43
7	C	1089	ADP	O2'-C2'	3.09	1.50	1.43
10	C	1093	U	P-OP3	3.13	1.65	1.54
10	E	1093	U	P-OP3	3.13	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1090	ADP	O2'-C2'	3.22	1.50	1.43
10	C	1093	U	C4-N3	3.51	1.39	1.33
10	A	1091	U	C4-N3	3.52	1.39	1.33
10	E	1093	U	C4-N3	3.52	1.39	1.33
10	G	1093	U	C4-N3	3.66	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	1093	U	OP3-P-O5'	-4.53	93.51	106.56
10	E	1093	U	C5-C4-N3	-4.08	112.66	123.12
7	E	1090	ADP	O3A-PA-O5'	-4.02	92.28	102.94
10	G	1093	U	C5-C4-N3	-3.99	112.89	123.12
10	G	1093	U	OP3-P-O5'	-3.97	95.14	106.56
10	C	1093	U	C5-C4-N3	-3.97	112.95	123.12
10	A	1091	U	C5-C4-N3	-3.65	113.76	123.12
7	G	1089	ADP	O3A-PA-O5'	-3.27	94.25	102.94
7	E	1089	ADP	C1'-N9-C4	-2.89	122.58	126.94
7	C	1089	ADP	C2'-C1'-N9	-2.64	110.26	114.29
7	C	1089	ADP	N6-C6-N1	-2.35	114.17	119.20
7	G	1090	ADP	C2'-C3'-C4'	-2.29	97.91	102.61
7	G	1090	ADP	O4'-C4'-C5'	-2.17	101.57	109.32
7	A	1088	ADP	O2'-C2'-C3'	2.01	118.37	111.83
7	E	1089	ADP	O3'-C3'-C2'	2.07	118.54	111.83
7	E	1090	ADP	C4-C5-N7	2.07	111.39	109.48
7	E	1090	ADP	O3'-C3'-C2'	2.17	118.89	111.83
7	G	1090	ADP	O2'-C2'-C3'	2.22	119.05	111.83
7	E	1089	ADP	O2A-PA-O3A	2.24	115.24	105.09
7	G	1089	ADP	O3'-C3'-C2'	2.25	119.14	111.83
7	G	1089	ADP	C4-C5-N7	2.31	111.61	109.48
10	E	1093	U	OP2-P-O5'	2.32	113.24	106.56
7	E	1090	ADP	O2A-PA-O3A	2.41	116.03	105.09
7	G	1090	ADP	C4-C5-N7	2.49	111.77	109.48
10	C	1093	U	C6-C5-C4	2.50	121.95	117.28
10	E	1093	U	O5'-P-OP1	2.58	113.71	107.14
10	G	1093	U	O4'-C1'-N1	2.62	113.61	108.08
7	C	1090	ADP	O3'-C3'-C2'	2.64	120.40	111.83
7	C	1089	ADP	O2'-C2'-C3'	2.67	120.51	111.83
7	G	1089	ADP	N6-C6-N1	2.86	125.34	119.20
10	G	1093	U	OP2-P-O5'	3.07	115.41	106.56
7	C	1089	ADP	O3A-PA-O5'	5.00	116.20	102.94
10	A	1091	U	C4-N3-C2	12.73	126.74	114.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1093	U	C4-N3-C2	12.76	126.78	114.14
10	G	1093	U	C4-N3-C2	13.48	127.50	114.14
10	E	1093	U	C4-N3-C2	13.80	127.81	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1087	ADP	1	0
7	A	1088	ADP	1	0
9	A	1090	NET	1	0
10	A	1091	U	1	0
5	C	1078	PO4	1	0
8	C	1091	ORN	1	0
9	C	1092	NET	1	0
10	C	1093	U	2	0
7	E	1089	ADP	1	0
7	E	1090	ADP	2	0
8	E	1091	ORN	2	0
9	E	1092	NET	2	0
10	E	1093	U	2	0
8	G	1091	ORN	1	0
9	G	1092	NET	2	0
10	G	1093	U	1	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, 95th 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 ²)	Q<0.9
1	A	1058/1073 (98%)	-0.37	24 (2%)	64	70	17, 33, 73, 100	0
1	C	1058/1073 (98%)	-0.24	30 (2%)	56	64	18, 35, 81, 100	0
1	E	1058/1073 (98%)	-0.31	22 (2%)	67	72	17, 31, 75, 100	0
1	G	1058/1073 (98%)	-0.06	42 (3%)	42	51	20, 42, 84, 100	0
2	B	379/382 (99%)	0.08	17 (4%)	37	46	21, 48, 87, 100	0
2	D	379/382 (99%)	0.01	14 (3%)	45	54	21, 40, 78, 100	0
2	F	379/382 (99%)	0.22	26 (6%)	20	27	20, 47, 92, 100	0
2	H	379/382 (99%)	0.54	39 (10%)	9	12	33, 63, 97, 100	0
All	All	5748/5820 (98%)	-0.12	214 (3%)	45	54	17, 38, 84, 100	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	8.6
1	E	1	MET	8.2
1	A	1	MET	7.6
1	G	1	MET	7.0
1	A	738	PHE	5.7
1	C	697	ALA	5.7
1	G	697	ALA	5.5
2	H	2	ILE	5.4
1	A	698	ILE	5.0
1	E	696	THR	5.0
2	H	380	THR	4.9
1	G	710	TYR	4.6
1	C	695	VAL	4.6
2	F	238	LEU	4.5
2	H	152	GLY	4.4
2	H	153	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	2	ILE	4.4
2	F	237	PHE	4.4
1	C	698	ILE	4.3
1	C	737	TYR	4.3
1	A	697	ALA	4.3
1	G	738	PHE	4.3
1	A	740	THR	4.3
2	F	2	ILE	4.3
2	F	268	ILE	4.3
1	A	696	THR	4.2
1	G	700	MET	4.2
1	G	740	THR	4.1
2	B	2	ILE	4.1
1	G	739	GLN	4.1
1	E	701	ALA	4.1
2	F	250	TYR	4.0
1	G	741	ALA	4.0
1	G	705	ALA	4.0
1	A	737	TYR	4.0
2	H	157	ASP	3.9
1	C	696	THR	3.9
1	G	737	TYR	3.9
2	B	250	TYR	3.9
1	C	738	PHE	3.9
1	G	724	ALA	3.8
1	E	739	GLN	3.8
1	E	741	ALA	3.8
2	H	150	PHE	3.8
1	E	697	ALA	3.7
1	G	557	THR	3.7
2	F	380	THR	3.7
1	A	750	VAL	3.7
1	G	698	ILE	3.7
1	G	680	HIS	3.7
1	A	716	PRO	3.7
1	G	702	VAL	3.6
2	D	269	CYS	3.6
1	C	701	ALA	3.6
2	F	201	ALA	3.6
2	D	268	ILE	3.5
2	H	160	LYS	3.5
2	H	31	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	246	ALA	3.5
1	A	732	ALA	3.5
1	E	2	PRO	3.4
1	A	739	GLN	3.4
1	E	738	PHE	3.4
1	A	701	ALA	3.4
1	G	734	LEU	3.3
2	D	238	LEU	3.3
2	H	165	ALA	3.3
1	A	341	GLY	3.3
2	B	152	GLY	3.3
2	F	379	LYS	3.3
2	B	156	MET	3.3
2	H	156	MET	3.3
1	C	703	GLU	3.2
1	C	741	ALA	3.1
1	E	700	MET	3.1
1	C	805	ILE	3.1
1	G	732	ALA	3.1
1	C	739	GLN	3.1
2	B	380	THR	3.1
1	G	701	ALA	3.1
2	H	151	PRO	3.1
2	B	248	ASP	3.1
1	E	750	VAL	3.1
2	F	228	VAL	3.1
1	C	740	THR	3.1
1	G	559	ARG	3.1
1	G	696	THR	3.0
1	A	342	GLY	3.0
1	G	805	ILE	3.0
2	B	155	GLY	3.0
1	C	700	MET	3.0
2	H	320	THR	2.9
1	A	724	ALA	2.9
2	B	147	ALA	2.9
2	B	246	ALA	2.9
2	H	246	ALA	2.9
2	H	136	ASP	2.9
2	H	142	LEU	2.9
1	A	702	VAL	2.9
1	G	735	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	703	GLU	2.9
2	H	138	PRO	2.9
2	D	155	GLY	2.9
2	B	153	LEU	2.9
1	G	558	ASP	2.9
1	G	695	VAL	2.8
2	F	248	ASP	2.8
2	D	250	TYR	2.8
2	H	268	ILE	2.8
1	E	675	ARG	2.8
2	B	154	ASN	2.8
1	A	703	GLU	2.8
2	H	159	ALA	2.8
2	B	150	PHE	2.8
1	G	731	GLU	2.8
2	H	53	VAL	2.8
2	F	231	MET	2.7
1	G	683	GLU	2.7
2	F	166	GLU	2.7
2	D	248	ASP	2.7
1	G	675	ARG	2.7
1	G	750	VAL	2.7
2	F	377	TYR	2.7
2	F	266	PHE	2.7
1	C	733	ASP	2.7
1	C	693	ALA	2.7
1	G	1073	LYS	2.7
2	D	156	MET	2.7
2	H	248	ASP	2.7
1	G	676	GLU	2.7
2	F	233	PRO	2.7
1	G	479	VAL	2.6
1	A	700	MET	2.6
1	E	737	TYR	2.6
2	D	154	ASN	2.6
1	E	680	HIS	2.6
2	H	250	TYR	2.5
2	F	378	ARG	2.5
1	C	750	VAL	2.5
2	H	154	ASN	2.5
1	C	736	ARG	2.5
2	H	377	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	368	ALA	2.5
1	C	702	VAL	2.5
1	E	751	LEU	2.5
1	A	735	ARG	2.5
1	E	705	ALA	2.4
2	H	266	PHE	2.4
1	E	695	VAL	2.4
1	G	682	VAL	2.4
1	G	840	ILE	2.4
2	H	269	CYS	2.4
1	C	699	GLU	2.4
2	F	165	ALA	2.4
2	H	166	GLU	2.4
2	H	189	GLU	2.4
2	H	319	ALA	2.4
2	H	188	ASP	2.4
1	G	733	ASP	2.4
2	B	148	ARG	2.4
2	F	55	LEU	2.4
2	H	164	THR	2.4
1	C	1073	LYS	2.4
2	B	255	ILE	2.3
2	D	320	THR	2.3
1	C	734	LEU	2.3
1	A	741	ALA	2.3
1	E	707	GLU	2.3
2	B	268	ILE	2.3
2	H	52	ILE	2.3
1	E	343	ARG	2.3
1	A	695	VAL	2.3
1	E	740	THR	2.3
2	D	246	ALA	2.3
1	G	678	PHE	2.3
2	F	230	LYS	2.3
2	F	271	GLY	2.2
1	C	683	GLU	2.2
2	B	151	PRO	2.2
2	F	205	ILE	2.2
1	C	751	LEU	2.2
2	H	238	LEU	2.2
1	G	2	PRO	2.2
2	H	261	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	699	GLU	2.2
2	H	162	VAL	2.2
1	A	736	ARG	2.2
2	F	192	PHE	2.2
2	H	30	VAL	2.2
1	G	686	LYS	2.2
1	G	751	LEU	2.1
1	C	111	PHE	2.1
2	H	376	GLN	2.1
2	F	247	PRO	2.1
1	E	1073	LYS	2.1
2	D	153	LEU	2.1
2	F	160	LYS	2.1
1	C	705	ALA	2.1
1	C	1021	ARG	2.1
1	G	343	ARG	2.1
1	G	736	ARG	2.1
1	E	734	LEU	2.1
1	E	825	LEU	2.1
2	H	48	TYR	2.1
1	C	715	ARG	2.0
1	C	825	LEU	2.0
2	H	228	VAL	2.0
2	F	190	LEU	2.0
1	C	686	LYS	2.0
2	D	237	PHE	2.0
2	B	247	PRO	2.0
2	H	352	GLY	2.0
1	A	730	ASP	2.0
2	D	157	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
9	NET	E	1092	9/9	0.98	0.18	4.79	15,23,27,28	0
8	ORN	C	1091	9/9	0.97	0.19	4.10	20,29,35,39	0
9	NET	G	1092	9/9	0.99	0.13	3.58	18,28,29,37	0
8	ORN	A	1089	9/9	0.95	0.18	3.37	24,29,36,37	0
6	CL	H	384	1/1	0.95	0.13	3.15	67,67,67,67	0
8	ORN	E	1091	9/9	0.97	0.13	2.97	16,25,37,40	0
8	ORN	G	1091	9/9	0.96	0.17	2.70	28,33,36,63	0
9	NET	C	1092	9/9	0.99	0.13	1.94	16,21,23,29	0
9	NET	A	1090	9/9	0.98	0.10	1.92	18,23,28,38	0
10	U	C	1093	21/21	0.95	0.12	0.21	33,51,83,89	0
10	U	G	1093	21/21	0.94	0.12	-0.06	31,57,80,85	0
7	ADP	E	1089	27/27	0.99	0.12	-0.10	15,26,34,36	0
6	CL	E	1086	1/1	0.99	0.07	-0.14	41,41,41,41	0
10	U	A	1091	21/21	0.96	0.10	-0.17	28,58,80,81	0
4	K	G	1077	1/1	0.99	0.10	-0.19	38,38,38,38	0
7	ADP	C	1089	27/27	0.99	0.10	-0.30	16,23,31,44	0
4	K	E	1077	1/1	0.99	0.12	-0.35	30,30,30,30	0
7	ADP	G	1089	27/27	0.99	0.11	-0.36	17,27,35,41	0
10	U	E	1093	21/21	0.96	0.10	-0.40	37,54,80,89	0
4	K	C	1077	1/1	0.99	0.11	-0.44	27,27,27,27	0
7	ADP	A	1087	27/27	0.99	0.09	-0.49	16,22,31,38	0
7	ADP	C	1090	27/27	0.98	0.08	-0.65	26,42,61,77	0
6	CL	F	384	1/1	1.00	0.06	-0.70	32,32,32,32	0
7	ADP	G	1090	27/27	0.98	0.09	-0.72	29,47,80,89	0
4	K	A	1080	1/1	0.99	0.08	-0.81	29,29,29,29	0
4	K	C	1080	1/1	0.99	0.08	-0.88	36,36,36,36	0
7	ADP	A	1088	27/27	0.99	0.07	-0.89	20,33,47,60	0
7	ADP	E	1090	27/27	0.99	0.06	-1.04	23,35,48,56	0
6	CL	D	384	1/1	0.99	0.07	-1.08	34,34,34,34	0
6	CL	C	1085	1/1	1.00	0.07	-1.31	39,39,39,39	0
6	CL	G	1086	1/1	0.92	0.07	-1.53	54,54,54,54	0
4	K	A	1077	1/1	0.99	0.08	-1.54	27,27,27,27	0
5	PO4	G	1078	5/5	0.99	0.07	-1.55	17,24,31,35	0
5	PO4	A	1078	5/5	0.99	0.08	-1.73	17,21,24,29	0
4	K	G	1080	1/1	0.99	0.07	-1.74	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PO4	E	1078	5/5	0.99	0.08	-1.76	19,22,26,27	0
6	CL	A	1085	1/1	0.99	0.06	-1.78	39,39,39,39	0
4	K	E	1080	1/1	0.99	0.06	-1.79	27,27,27,27	0
5	PO4	C	1078	5/5	0.99	0.09	-1.80	16,22,24,25	0
4	K	E	1076	1/1	0.99	0.09	-1.81	25,25,25,25	0
4	K	G	1076	1/1	1.00	0.09	-2.24	28,28,28,28	0
3	MN	A	1074	1/1	1.00	0.07	-2.24	25,25,25,25	0
3	MN	C	1074	1/1	1.00	0.08	-2.30	27,27,27,27	0
3	MN	G	1074	1/1	1.00	0.07	-2.30	31,31,31,31	0
3	MN	E	1074	1/1	1.00	0.09	-2.53	27,27,27,27	0
4	K	C	1076	1/1	1.00	0.07	-2.61	22,22,22,22	0
4	K	A	1076	1/1	1.00	0.07	-2.72	21,21,21,21	0
6	CL	C	1083	1/1	0.91	0.16	-	77,77,77,77	0
4	K	E	1081	1/1	0.95	0.06	-	42,42,42,42	0
4	K	B	383	1/1	0.98	0.07	-	45,45,45,45	0
6	CL	G	1087	1/1	0.98	0.08	-	81,81,81,81	0
4	K	E	1083	1/1	0.98	0.05	-	58,58,58,58	0
6	CL	G	1082	1/1	0.99	0.10	-	29,29,29,29	0
6	CL	C	1084	1/1	0.96	0.08	-	43,43,43,43	0
4	K	C	1082	1/1	0.96	0.06	-	44,44,44,44	0
3	MN	G	1079	1/1	0.99	0.05	-	47,47,47,47	0
4	K	D	383	1/1	0.99	0.03	-	34,34,34,34	0
6	CL	G	1085	1/1	0.98	0.06	-	46,46,46,46	0
4	K	G	1083	1/1	0.99	0.06	-	52,52,52,52	0
3	MN	A	1079	1/1	1.00	0.05	-	37,37,37,37	0
6	CL	G	1088	1/1	0.97	0.17	-	67,67,67,67	0
4	K	F	383	1/1	0.99	0.07	-	36,36,36,36	0
6	CL	E	1085	1/1	0.98	0.05	-	49,49,49,49	0
4	K	G	1081	1/1	0.97	0.06	-	46,46,46,46	0
3	MN	C	1079	1/1	0.99	0.05	-	46,46,46,46	0
6	CL	C	1081	1/1	0.99	0.10	-	29,29,29,29	0
6	CL	G	1084	1/1	0.83	0.22	-	72,72,72,72	0
6	CL	A	1081	1/1	0.99	0.08	-	28,28,28,28	0
3	MN	G	1075	1/1	1.00	0.08	-	28,28,28,28	0
5	PO4	C	1088	5/5	0.92	0.21	-	80,80,80,80	0
6	CL	E	1082	1/1	1.00	0.14	-	24,24,24,24	0
6	CL	E	1087	1/1	0.94	0.06	-	54,54,54,54	0
6	CL	C	1087	1/1	0.99	0.15	-	63,63,63,63	0
6	CL	A	1084	1/1	0.99	0.05	-	40,40,40,40	0
3	MN	C	1075	1/1	0.99	0.07	-	25,25,25,25	0
6	CL	E	1088	1/1	0.99	0.10	-	44,44,44,44	0
6	CL	H	385	1/1	0.84	0.07	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	K	A	1082	1/1	0.98	0.04	-	41,41,41,41	0
4	K	H	383	1/1	0.97	0.11	-	64,64,64,64	0
6	CL	A	1086	1/1	0.96	0.06	-	56,56,56,56	0
3	MN	A	1075	1/1	1.00	0.06	-	23,23,23,23	0
6	CL	A	1083	1/1	0.91	0.10	-	66,66,66,66	0
3	MN	E	1079	1/1	1.00	0.05	-	41,41,41,41	0
3	MN	E	1075	1/1	1.00	0.08	-	27,27,27,27	0
6	CL	C	1086	1/1	0.95	0.11	-	67,67,67,67	0
6	CL	E	1084	1/1	0.82	0.15	-	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.