



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K71  
Title : Structure of integrin alphaX beta2 ectodomain  
Authors : Xie, C.; Zhu, J.; Chen, X.; Mi, L.; Nishida, N.; Springer, T.A.  
Deposited on : 2009-10-11  
Resolution : 3.95 Å(reported)

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

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

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

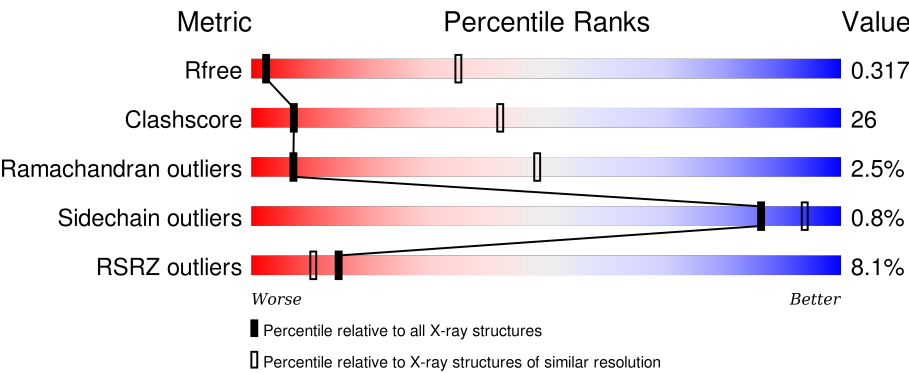
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.95 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 <sub>free</sub>	91344	1011 (4.38-3.54)
Clashscore	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)
RSRZ outliers	91569	1015 (4.38-3.54)

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 <=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	1095	<div><div>3%</div><div>42%</div><div>35%</div><div>•</div><div>20%</div></div>
1	C	1095	<div><div>3%</div><div>44%</div><div>35%</div><div>•</div><div>19%</div></div>
1	E	1095	<div><div>4%</div><div>42%</div><div>36%</div><div>•</div><div>19%</div></div>
1	G	1095	<div><div>8%</div><div>54%</div><div>42%</div><div>••</div></div>
2	B	687	<div><div>11%</div><div>64%</div><div>33%</div><div>••</div></div>

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Mol	Chain	Length	Quality of chain
2	D	687	
2	F	687	
2	H	687	

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
4	NAG	A	3373	X	-	-	-
4	MAN	A	3375	X	-	-	-
4	MAN	A	3718	X	-	-	-
4	MAN	A	3882	X	-	-	-
4	MAN	C	3718	X	-	-	-
4	NAG	E	3373	-	-	X	-
4	MAN	E	3375	X	-	-	-
4	MAN	E	3718	X	-	-	-
4	MAN	G	3718	X	-	-	-
5	NAG	D	3479	-	-	X	-
5	NAG	F	3094	-	-	-	X
7	MAN	G	3375	X	-	-	-
8	MG	G	2009	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 50191 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	880	Total	C	N	O	S	0	0	0
			6782	4284	1173	1291	34			
1	C	884	Total	C	N	O	S	0	0	0
			6814	4305	1178	1297	34			
1	E	882	Total	C	N	O	S	0	0	0
			6802	4299	1176	1293	34			
1	G	1082	Total	C	N	O	S	0	0	0
			8392	5304	1454	1596	38			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION TAG	UNP P20702
A	1094	PHE	-	EXPRESSION TAG	UNP P20702
A	1095	GLN	-	EXPRESSION TAG	UNP P20702
C	1085	GLY	-	EXPRESSION TAG	UNP P20702
C	1086	CYS	-	EXPRESSION TAG	UNP P20702
C	1087	GLY	-	EXPRESSION TAG	UNP P20702
C	1088	GLY	-	EXPRESSION TAG	UNP P20702
C	1089	LEU	-	EXPRESSION TAG	UNP P20702
C	1090	GLU	-	EXPRESSION TAG	UNP P20702
C	1091	ASN	-	EXPRESSION TAG	UNP P20702
C	1092	LEU	-	EXPRESSION TAG	UNP P20702
C	1093	TYR	-	EXPRESSION TAG	UNP P20702
C	1094	PHE	-	EXPRESSION TAG	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLN	-	EXPRESSION TAG	UNP P20702
E	1085	GLY	-	EXPRESSION TAG	UNP P20702
E	1086	CYS	-	EXPRESSION TAG	UNP P20702
E	1087	GLY	-	EXPRESSION TAG	UNP P20702
E	1088	GLY	-	EXPRESSION TAG	UNP P20702
E	1089	LEU	-	EXPRESSION TAG	UNP P20702
E	1090	GLU	-	EXPRESSION TAG	UNP P20702
E	1091	ASN	-	EXPRESSION TAG	UNP P20702
E	1092	LEU	-	EXPRESSION TAG	UNP P20702
E	1093	TYR	-	EXPRESSION TAG	UNP P20702
E	1094	PHE	-	EXPRESSION TAG	UNP P20702
E	1095	GLN	-	EXPRESSION TAG	UNP P20702
G	1085	GLY	-	EXPRESSION TAG	UNP P20702
G	1086	CYS	-	EXPRESSION TAG	UNP P20702
G	1087	GLY	-	EXPRESSION TAG	UNP P20702
G	1088	GLY	-	EXPRESSION TAG	UNP P20702
G	1089	LEU	-	EXPRESSION TAG	UNP P20702
G	1090	GLU	-	EXPRESSION TAG	UNP P20702
G	1091	ASN	-	EXPRESSION TAG	UNP P20702
G	1092	LEU	-	EXPRESSION TAG	UNP P20702
G	1093	TYR	-	EXPRESSION TAG	UNP P20702
G	1094	PHE	-	EXPRESSION TAG	UNP P20702
G	1095	GLN	-	EXPRESSION TAG	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	D	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	F	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	H	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	EXPRESSION TAG	UNP P05107
B	679	GLY	-	EXPRESSION TAG	UNP P05107
B	680	CYS	-	EXPRESSION TAG	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	GLY	-	EXPRESSION TAG	UNP P05107
B	682	GLU	-	EXPRESSION TAG	UNP P05107
B	684	LEU	-	EXPRESSION TAG	UNP P05107
B	685	TYR	-	EXPRESSION TAG	UNP P05107
B	686	PHE	-	EXPRESSION TAG	UNP P05107
B	687	GLN	-	EXPRESSION TAG	UNP P05107
D	678	ASP	-	EXPRESSION TAG	UNP P05107
D	679	GLY	-	EXPRESSION TAG	UNP P05107
D	680	CYS	-	EXPRESSION TAG	UNP P05107
D	681	GLY	-	EXPRESSION TAG	UNP P05107
D	682	GLU	-	EXPRESSION TAG	UNP P05107
D	684	LEU	-	EXPRESSION TAG	UNP P05107
D	685	TYR	-	EXPRESSION TAG	UNP P05107
D	686	PHE	-	EXPRESSION TAG	UNP P05107
D	687	GLN	-	EXPRESSION TAG	UNP P05107
F	678	ASP	-	EXPRESSION TAG	UNP P05107
F	679	GLY	-	EXPRESSION TAG	UNP P05107
F	680	CYS	-	EXPRESSION TAG	UNP P05107
F	681	GLY	-	EXPRESSION TAG	UNP P05107
F	682	GLU	-	EXPRESSION TAG	UNP P05107
F	684	LEU	-	EXPRESSION TAG	UNP P05107
F	685	TYR	-	EXPRESSION TAG	UNP P05107
F	686	PHE	-	EXPRESSION TAG	UNP P05107
F	687	GLN	-	EXPRESSION TAG	UNP P05107
H	678	ASP	-	EXPRESSION TAG	UNP P05107
H	679	GLY	-	EXPRESSION TAG	UNP P05107
H	680	CYS	-	EXPRESSION TAG	UNP P05107
H	681	GLY	-	EXPRESSION TAG	UNP P05107
H	682	GLU	-	EXPRESSION TAG	UNP P05107
H	684	LEU	-	EXPRESSION TAG	UNP P05107
H	685	TYR	-	EXPRESSION TAG	UNP P05107
H	686	PHE	-	EXPRESSION TAG	UNP P05107
H	687	GLN	-	EXPRESSION TAG	UNP P05107

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

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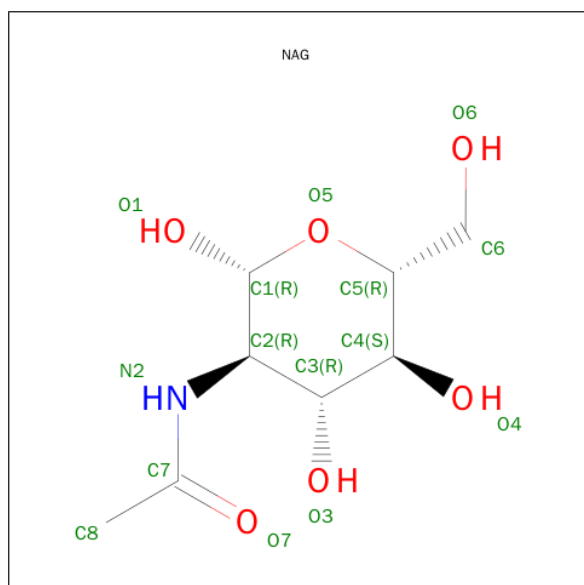
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	G	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	E	1	Total C N O 14 8 1 5	0	0
5	E	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	H	1	Total C N O 14 8 1 5	0	0
5	H	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	3	Total Ca 3 3	0	0
6	D	1	Total Ca 1 1	0	0
6	E	3	Total Ca 3 3	0	0
6	H	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	3	Total 3	Ca 3	0	0
6	A	3	Total 3	Ca 3	0	0
6	F	1	Total 1	Ca 1	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	4	Total 50	C 28	N 2	O 20	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total 1	Mg 1	0	0

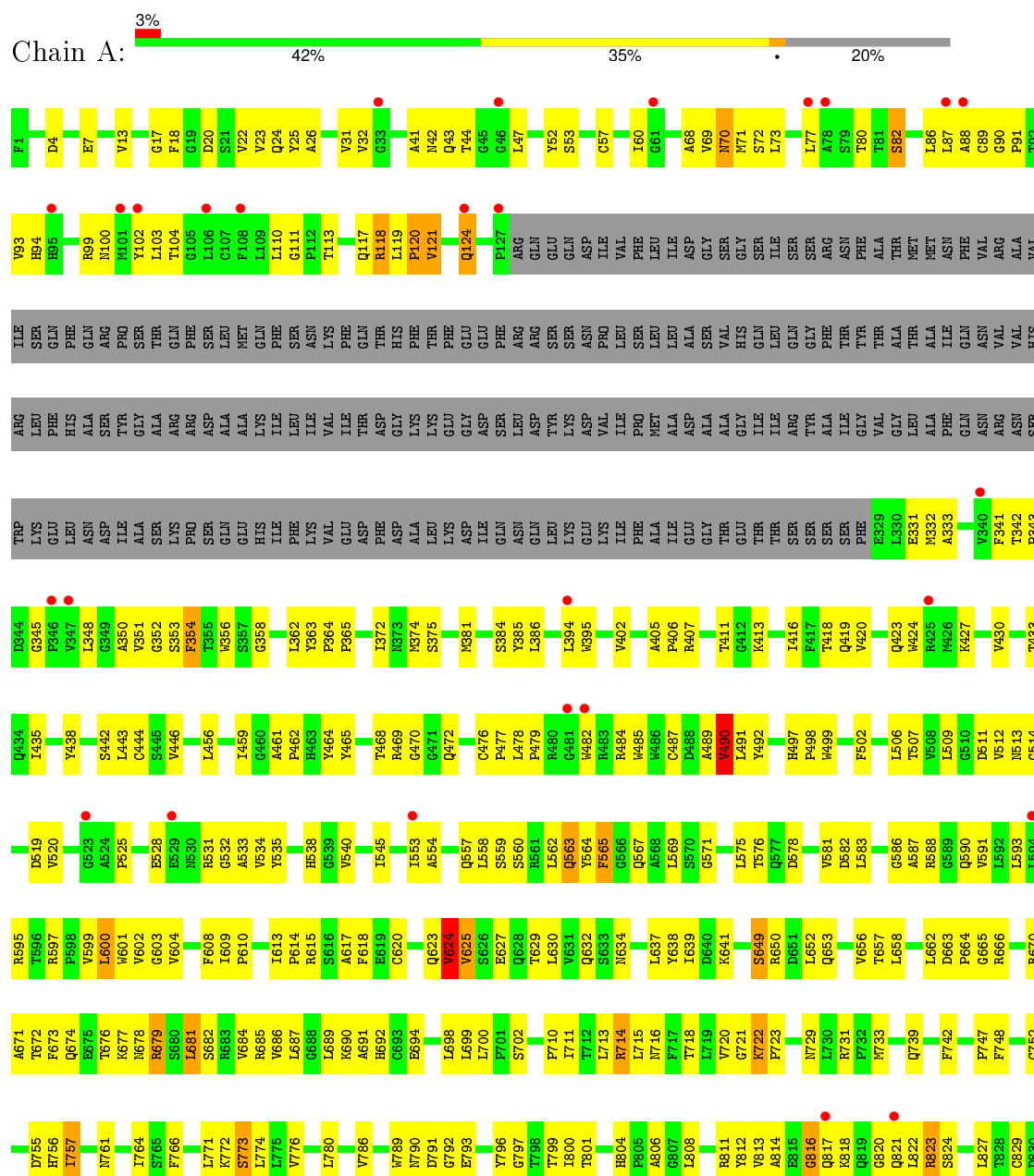
- Molecule 9 is water.

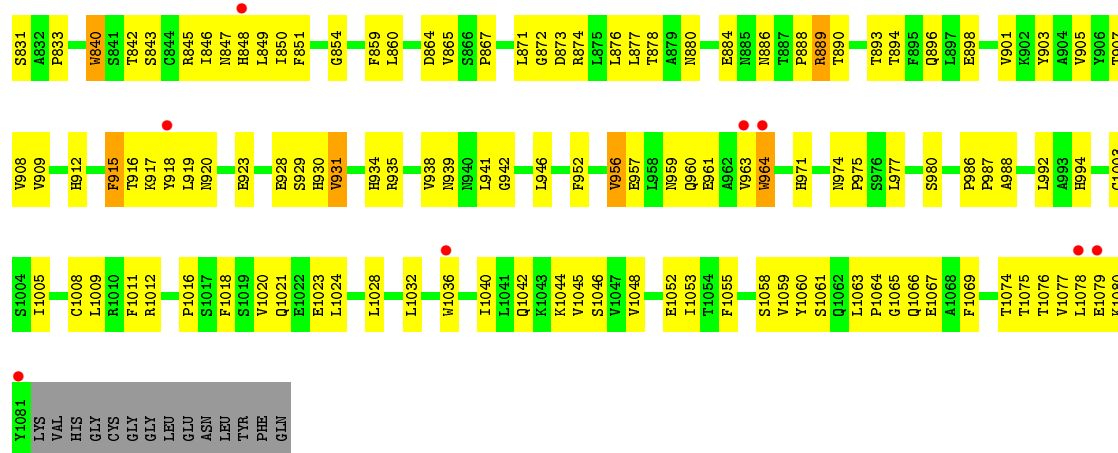
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	3	Total 3	O 3	0	0

### 3 Residue-property plots

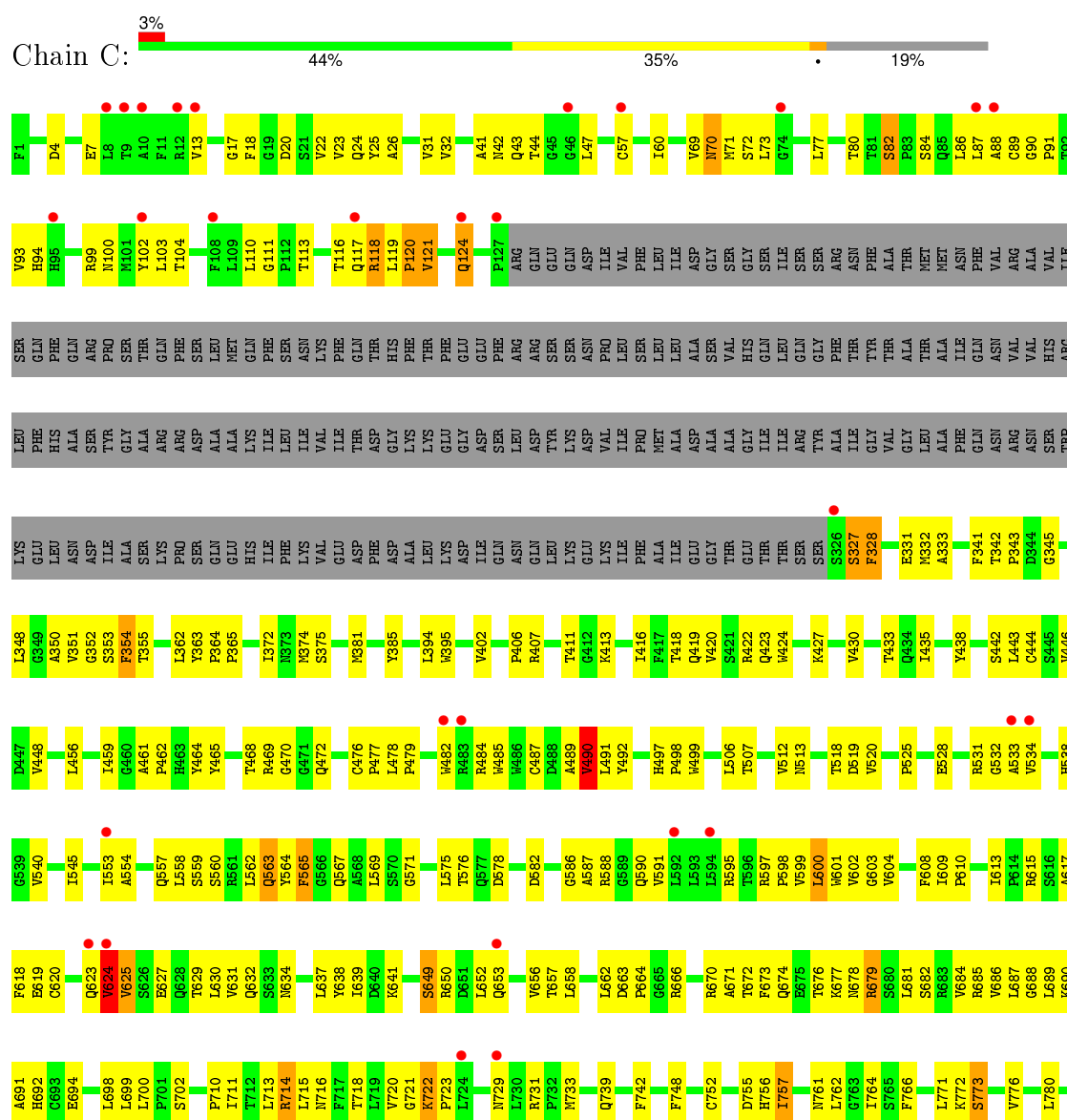
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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.

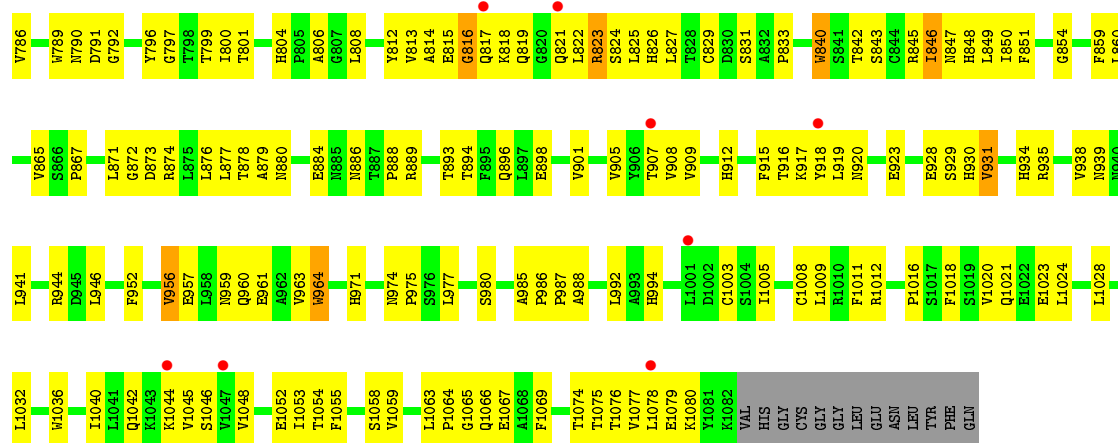
#### • Molecule 1: Integrin alpha-X



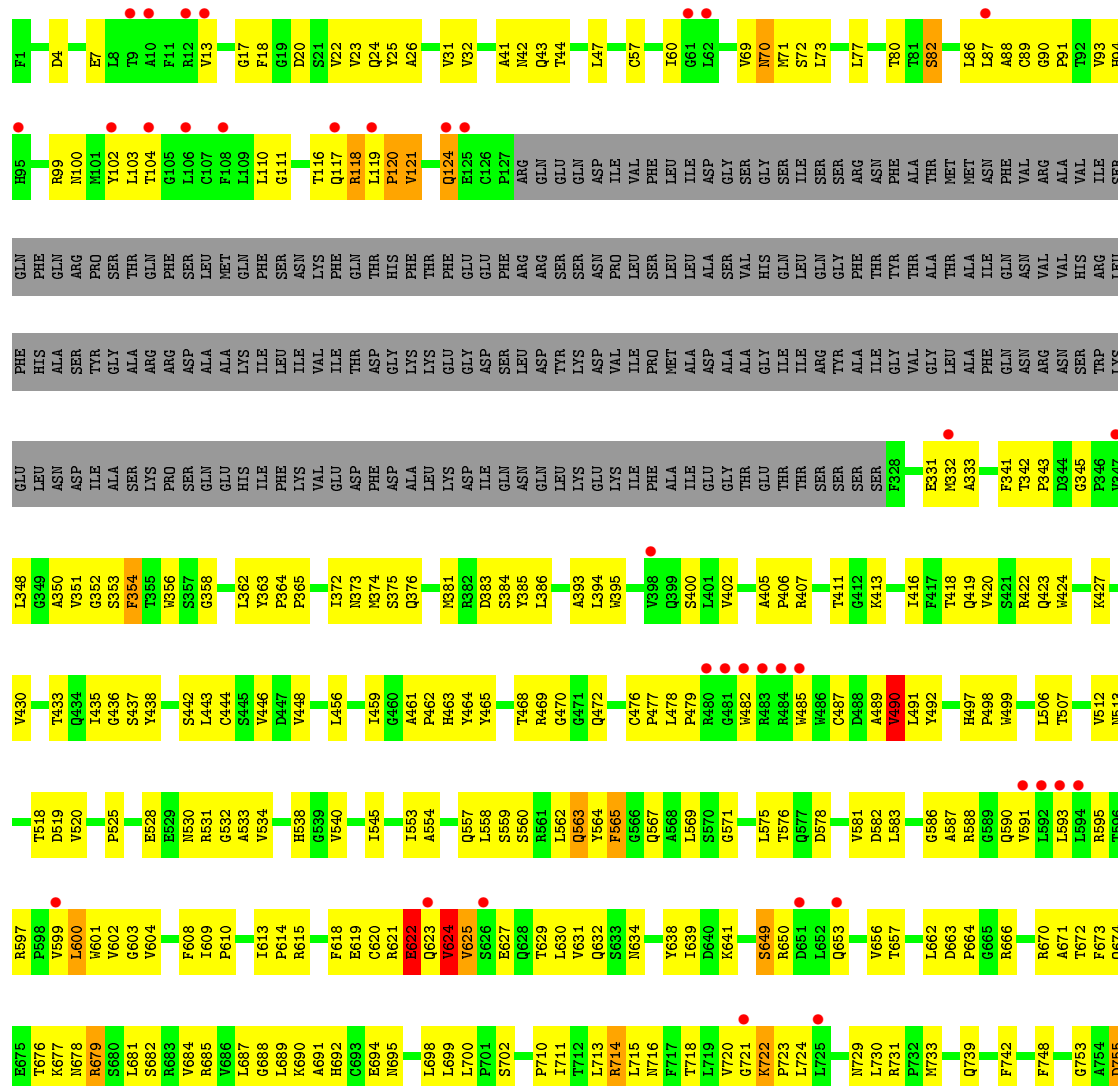


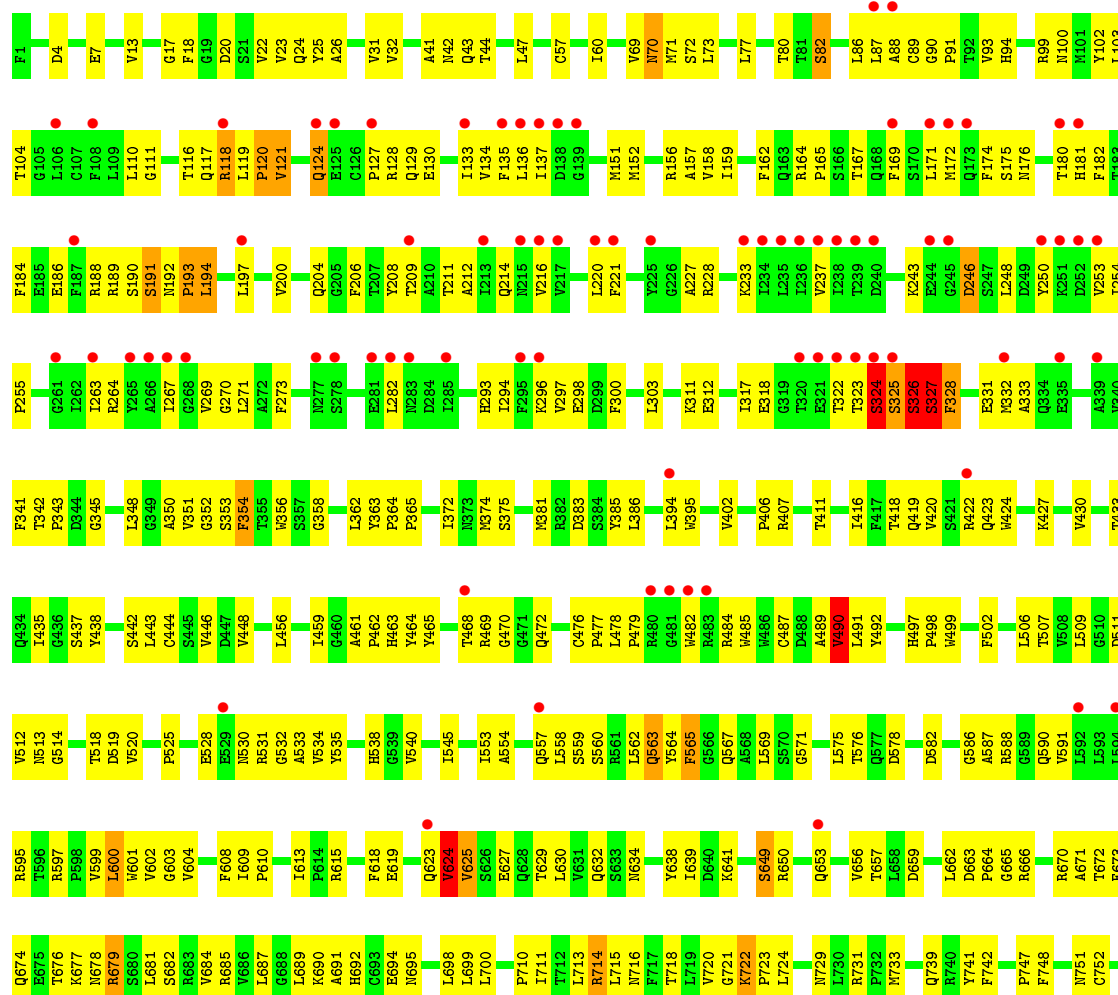
### • Molecule 1: Integrin alpha-X

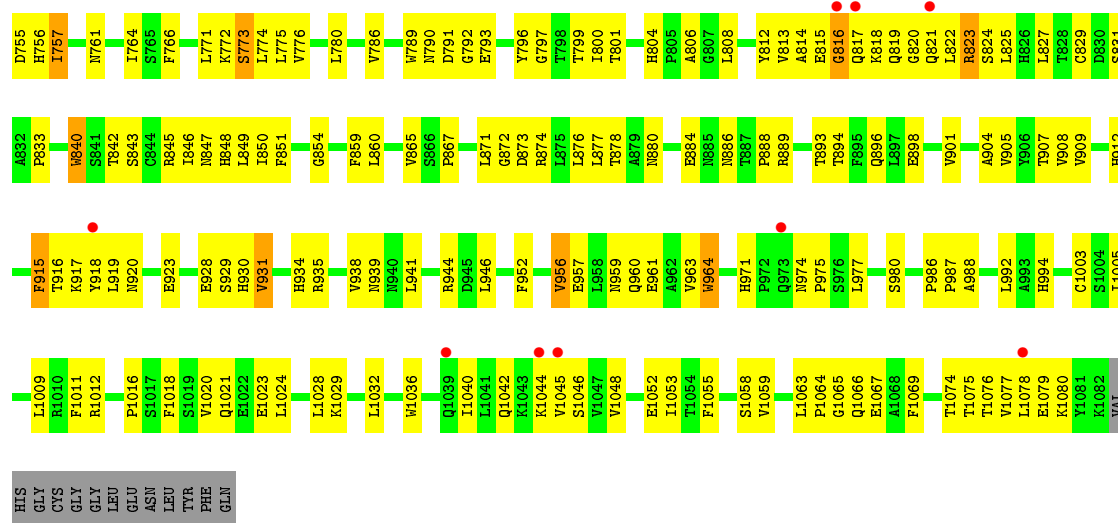




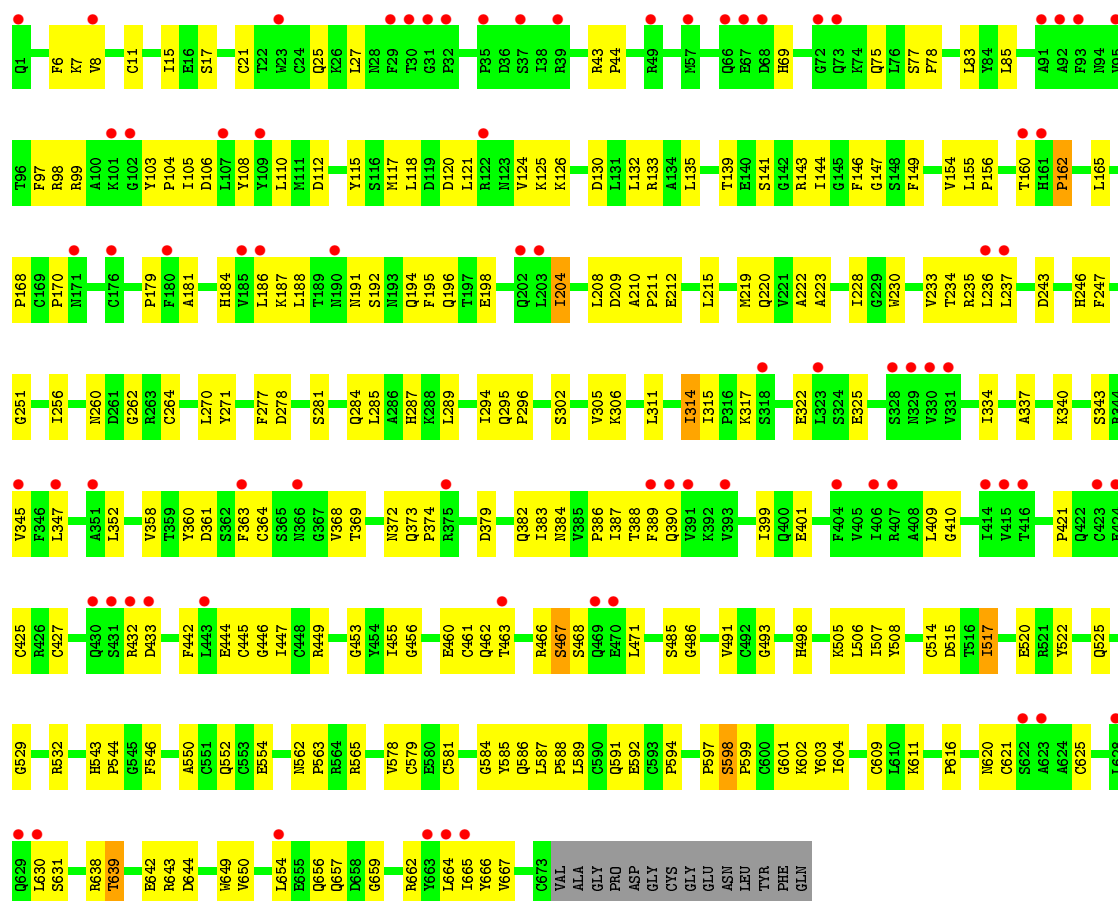
### • Molecule 1: Integrin alpha-X





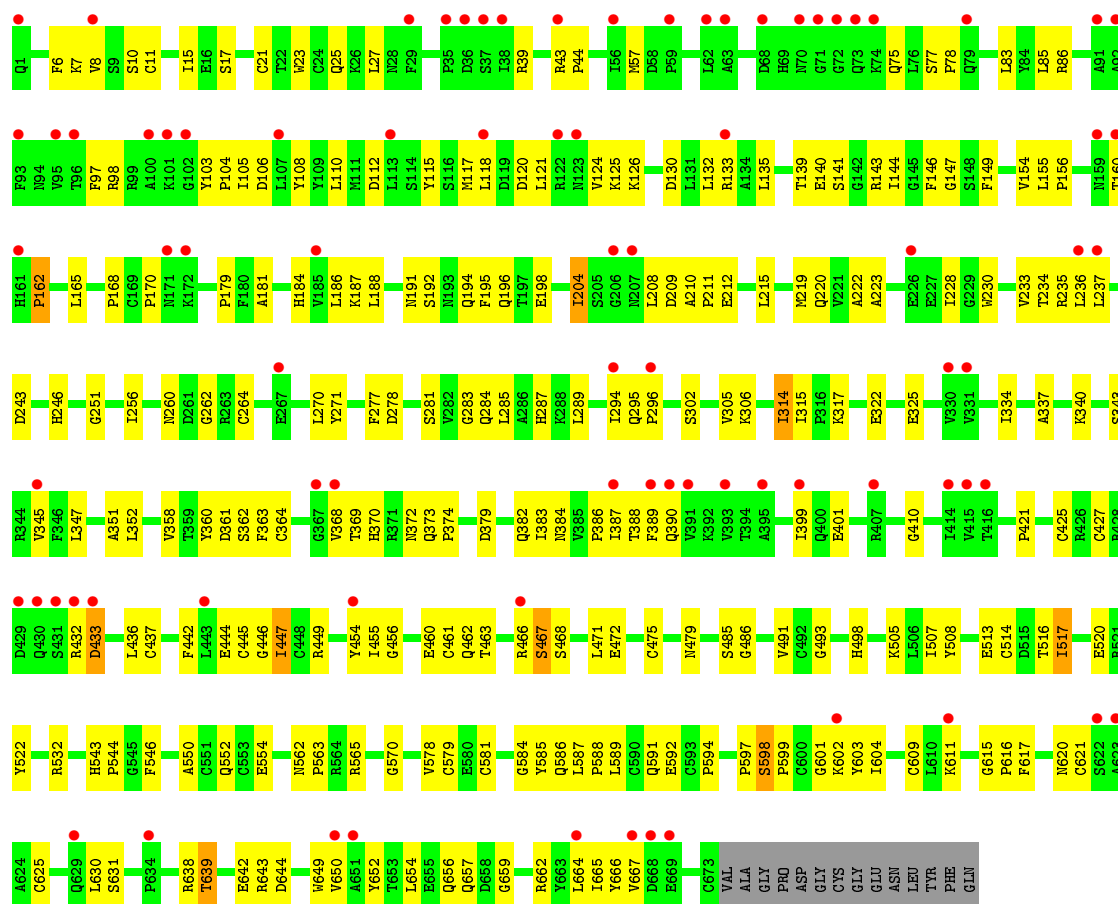


• Molecule 2: Integrin beta-2

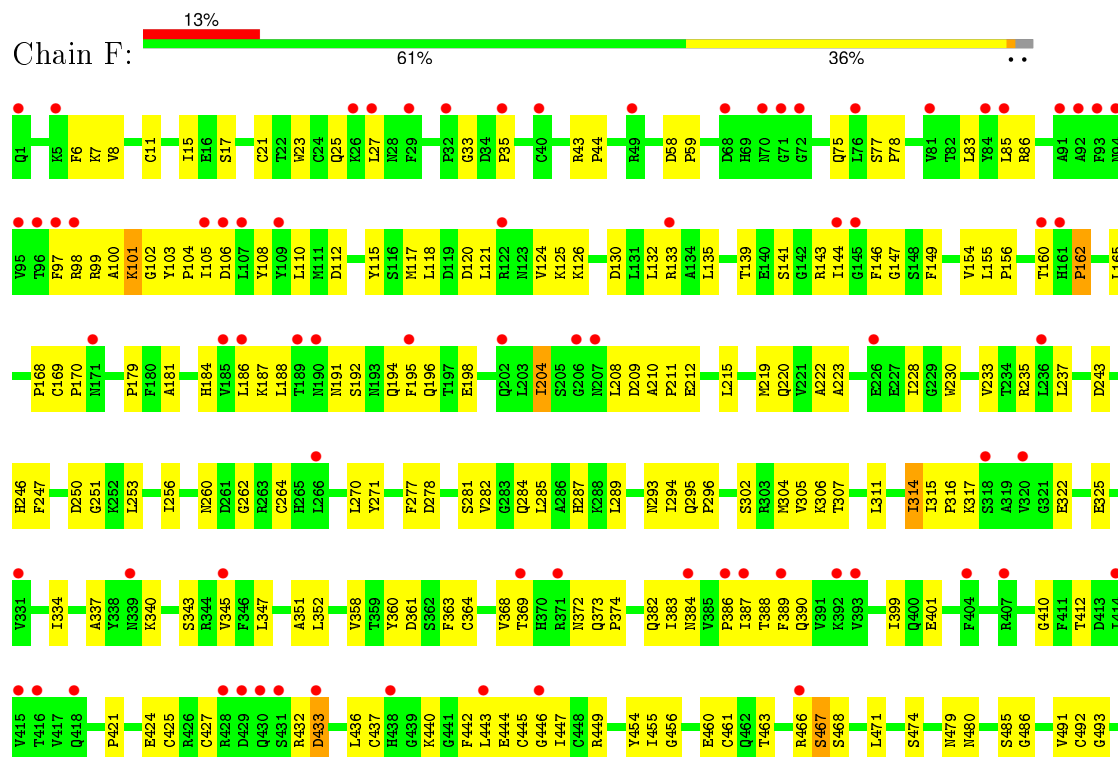


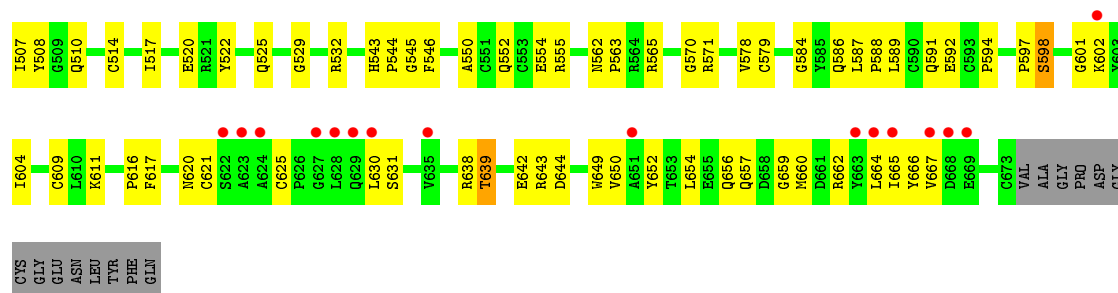
• Molecule 2: Integrin beta-2



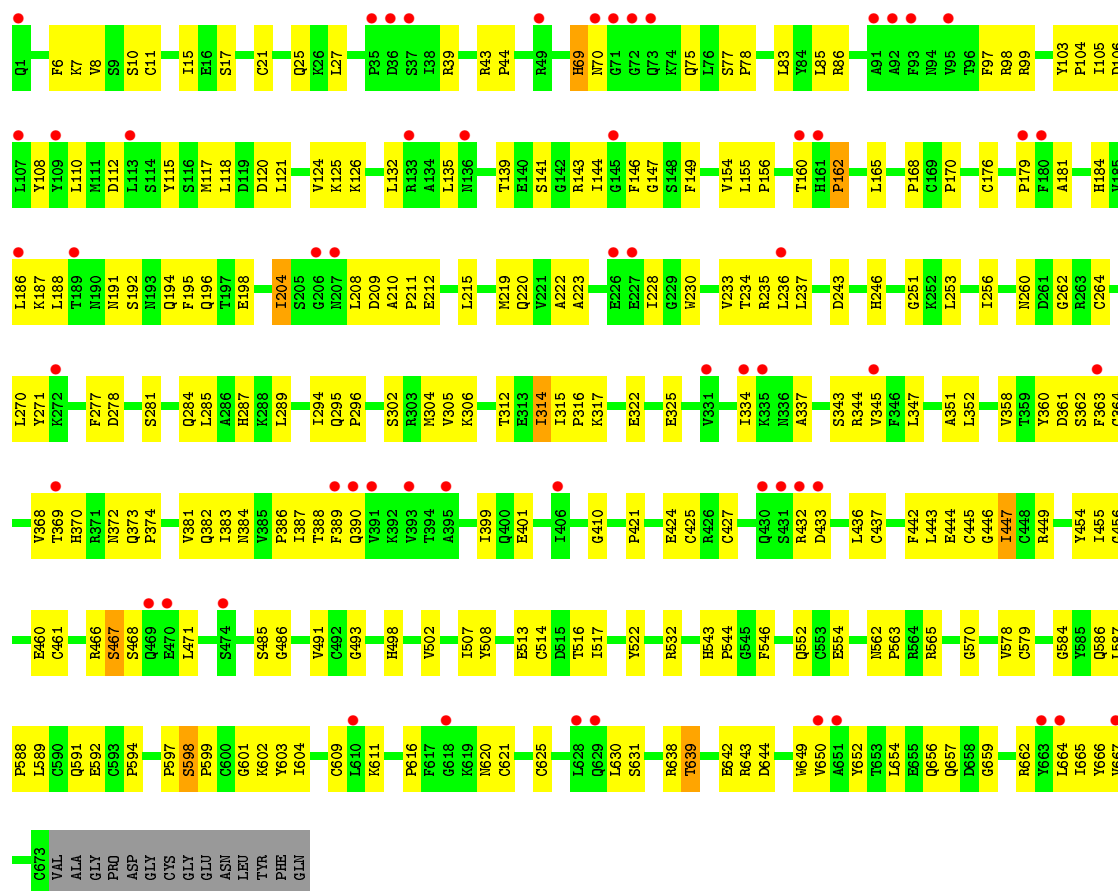


• Molecule 2: Integrin beta-2





# Molecule 2: Integrin beta-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.66Å 165.75Å 537.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.95 49.67 – 3.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.67-3.95) 99.4 (49.67-3.95)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.350 , 0.373 0.304 , 0.317	Depositor DCC
$R_{free}$ test set	1020 reflections (0.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 130.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	4 of 117372 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	50191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MAN, CA, NAG

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	0.24	0/6936	0.45	0/9437
1	C	0.24	0/6969	0.45	0/9480
1	E	0.27	1/6957 (0.0%)	0.46	0/9464
1	G	0.26	0/8579	0.46	0/11652
2	B	0.25	0/5273	0.41	0/7119
2	D	0.24	0/5273	0.41	0/7119
2	F	0.25	0/5273	0.42	0/7119
2	H	0.24	0/5273	0.40	0/7119
All	All	0.25	1/50533 (0.0%)	0.44	0/68509

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
1	A	0	9
1	C	0	10
1	E	0	10
1	G	0	14
2	B	0	1
2	D	0	1
2	F	0	2
2	H	0	1
4	A	4	0
4	C	1	0
4	E	2	0
4	G	1	0
7	G	1	0
All	All	9	48

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	622	GLU	CG-CD	-8.81	1.38	1.51

There are no bond angle outliers.

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3373	NAG	C1
4	A	3375	MAN	C1
4	A	3718	MAN	C1
4	A	3882	MAN	C1
4	C	3718	MAN	C1
4	E	3375	MAN	C1
4	E	3718	MAN	C1
7	G	3375	MAN	C1
4	G	3718	MAN	C1

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Peptide
1	A	490	VAL	Peptide
1	A	624	VAL	Peptide
1	A	625	VAL	Peptide
1	A	816	GLY	Peptide
1	A	82	SER	Peptide
1	A	821	GLN	Peptide
1	A	824	SER	Peptide
1	A	889	ARG	Peptide
2	B	425	CYS	Peptide
1	C	118	ARG	Peptide
1	C	327	SER	Peptide
1	C	490	VAL	Peptide
1	C	624	VAL	Peptide
1	C	625	VAL	Peptide
1	C	816	GLY	Peptide
1	C	82	SER	Peptide
1	C	821	GLN	Peptide
1	C	824	SER	Peptide
1	C	889	ARG	Peptide
2	D	425	CYS	Peptide
1	E	118	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	E	490	VAL	Peptide
1	E	622	GLU	Peptide
1	E	624	VAL	Peptide
1	E	625	VAL	Peptide
1	E	816	GLY	Peptide
1	E	82	SER	Peptide
1	E	821	GLN	Peptide
1	E	824	SER	Peptide
1	E	889	ARG	Peptide
2	F	100	ALA	Peptide
2	F	425	CYS	Peptide
1	G	118	ARG	Peptide
1	G	127	PRO	Peptide
1	G	324	SER	Peptide
1	G	325	SER	Peptide
1	G	326	SER	Peptide
1	G	327	SER	Peptide
1	G	490	VAL	Peptide
1	G	624	VAL	Peptide
1	G	625	VAL	Peptide
1	G	816	GLY	Peptide
1	G	82	SER	Peptide
1	G	821	GLN	Peptide
1	G	824	SER	Peptide
1	G	889	ARG	Peptide
2	H	425	CYS	Peptide

## 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	6782	0	6641	427	0
1	C	6814	0	6672	418	0
1	E	6802	0	6662	428	2
1	G	8392	0	8229	492	2
2	B	5177	0	4966	214	0
2	D	5177	0	4966	246	0
2	F	5177	0	4966	249	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	5177	0	4966	234	0
3	A	28	0	25	0	0
3	C	56	0	50	0	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
4	A	117	0	102	3	0
4	C	39	0	34	0	0
4	E	78	0	68	8	0
4	G	39	0	34	1	0
5	A	14	0	13	0	0
5	B	28	0	26	0	0
5	C	28	0	26	1	0
5	D	28	0	26	8	0
5	E	28	0	26	1	0
5	F	28	0	26	3	0
5	G	28	0	26	0	0
5	H	28	0	26	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
6	H	1	0	0	0	0
7	G	50	0	43	2	0
8	G	1	0	0	0	0
9	G	3	0	0	0	0
All	All	50191	0	48669	2584	2

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 26.

All (2584) 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:F:317:LYS:HE3	2:F:410:GLY:HA3	1.42	1.01
1:G:103:LEU:HD11	2:H:155:LEU:HD13	1.49	0.95
1:C:119:LEU:N	1:C:120:PRO:HA	1.83	0.94
1:A:119:LEU:N	1:A:120:PRO:HA	1.84	0.93
2:H:27:LEU:HG	2:H:446:GLY:HA2	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:LEU:HD11	2:F:155:LEU:HD13	1.51	0.92
1:C:94:HIS:NE2	2:D:155:LEU:HD21	1.84	0.92
1:E:119:LEU:N	1:E:120:PRO:HA	1.84	0.92
1:E:623:GLN:O	1:E:624:VAL:HG22	1.69	0.92
2:F:15:ILE:HG23	2:F:86:ARG:NH2	1.85	0.92
2:F:35:PRO:HG2	2:F:510:GLN:CD	1.90	0.92
1:G:119:LEU:N	1:G:120:PRO:HA	1.83	0.90
1:A:484:ARG:NH1	2:B:586:GLN:HG3	1.88	0.87
2:F:15:ILE:HD12	2:F:86:ARG:HH22	1.39	0.87
1:A:756:HIS:HA	1:C:1052:GLU:OE1	1.75	0.87
1:A:772:LYS:HA	1:C:789:TRP:CZ2	2.10	0.86
1:A:789:TRP:CZ2	1:C:772:LYS:HA	2.11	0.86
2:F:317:LYS:HE3	2:F:410:GLY:CA	2.04	0.86
1:G:99:ARG:HH12	1:G:318:GLU:HG3	1.41	0.86
1:C:103:LEU:HD11	2:D:155:LEU:HD13	1.57	0.84
2:D:479:ASN:HD21	5:D:3479:NAG:H82	1.40	0.84
2:F:15:ILE:HD12	2:F:86:ARG:NH2	1.92	0.84
2:H:25:GLN:OE1	2:H:427:CYS:SG	2.36	0.83
2:H:532:ARG:HD3	2:H:554:GLU:CD	1.97	0.83
2:F:570:GLY:HA2	2:F:659:GLY:HA2	1.61	0.83
1:A:94:HIS:NE2	2:B:155:LEU:HD21	1.93	0.83
2:F:293:ASN:OD1	2:F:412:THR:HG22	1.79	0.82
1:G:99:ARG:NH1	1:G:318:GLU:HG3	1.94	0.82
1:C:625:VAL:HG21	1:C:627:GLU:HG3	1.59	0.82
1:C:113:THR:HG22	1:E:1029:LYS:CE	2.10	0.82
1:A:625:VAL:HG21	1:A:627:GLU:HG3	1.61	0.81
1:E:625:VAL:HG21	1:E:627:GLU:HG3	1.60	0.81
1:G:625:VAL:HG21	1:G:627:GLU:HG3	1.62	0.81
2:D:479:ASN:ND2	5:D:3479:NAG:C7	2.44	0.81
1:E:1064:PRO:HG3	1:E:1067:GLU:CD	2.01	0.81
2:B:532:ARG:HD3	2:B:554:GLU:CD	2.01	0.81
2:D:570:GLY:HA2	2:D:659:GLY:HA2	1.64	0.80
1:E:1063:LEU:HD12	1:E:1064:PRO:CA	2.12	0.80
1:E:1063:LEU:HD12	1:E:1064:PRO:N	1.96	0.80
2:F:479:ASN:HD22	5:F:3479:NAG:C1	1.95	0.80
1:G:1063:LEU:HD12	1:G:1064:PRO:CA	2.12	0.80
1:C:1064:PRO:HG3	1:C:1067:GLU:CD	2.01	0.80
2:D:532:ARG:HD3	2:D:554:GLU:CD	2.02	0.80
1:C:1063:LEU:HD12	1:C:1064:PRO:N	1.96	0.80
1:A:923:GLU:HB2	1:A:1080:LYS:HB3	1.63	0.80
1:C:1063:LEU:HD12	1:C:1064:PRO:CA	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:570:GLY:HA2	2:H:659:GLY:HA2	1.64	0.79
1:G:1063:LEU:HD12	1:G:1064:PRO:N	1.97	0.79
1:E:923:GLU:HB2	1:E:1080:LYS:HB3	1.63	0.79
1:E:1052:GLU:OE1	1:G:756:HIS:HA	1.83	0.79
1:A:1063:LEU:HD12	1:A:1064:PRO:CA	2.12	0.79
1:A:1064:PRO:HG3	1:A:1067:GLU:CD	2.03	0.79
1:C:923:GLU:HB2	1:C:1080:LYS:HB3	1.64	0.79
1:G:923:GLU:HB2	1:G:1080:LYS:HB3	1.63	0.78
1:A:1063:LEU:HD12	1:A:1064:PRO:N	1.97	0.78
1:E:772:LYS:HA	1:G:789:TRP:CZ2	2.18	0.78
1:G:1064:PRO:HG3	1:G:1067:GLU:CD	2.04	0.78
1:G:623:GLN:O	1:G:624:VAL:HG22	1.84	0.78
1:G:99:ARG:NH1	1:G:318:GLU:CG	2.47	0.77
1:E:789:TRP:CZ2	1:G:772:LYS:HA	2.20	0.77
2:F:155:LEU:HB2	2:F:156:PRO:HA	1.67	0.77
2:B:155:LEU:HB2	2:B:156:PRO:HA	1.67	0.77
1:E:756:HIS:HA	1:G:1052:GLU:OE1	1.84	0.77
1:G:119:LEU:H	1:G:120:PRO:HA	1.50	0.76
2:D:155:LEU:HB2	2:D:156:PRO:HA	1.67	0.75
1:C:623:GLN:O	1:C:624:VAL:HG22	1.87	0.75
2:D:210:ALA:HB3	2:D:211:PRO:HD3	1.69	0.75
2:H:155:LEU:HB2	2:H:156:PRO:HA	1.67	0.75
1:E:94:HIS:NE2	2:F:155:LEU:HD21	2.02	0.74
1:C:113:THR:HG22	1:E:1029:LYS:HE3	1.67	0.74
1:G:756:HIS:O	1:G:757:ILE:HG22	1.87	0.74
1:A:623:GLN:O	1:A:624:VAL:HG22	1.87	0.74
2:B:210:ALA:HB3	2:B:211:PRO:HD3	1.69	0.74
2:H:27:LEU:CG	2:H:446:GLY:HA2	2.17	0.74
2:D:10:SER:CB	2:D:449:ARG:CZ	2.65	0.74
2:F:15:ILE:HG23	2:F:86:ARG:CZ	2.17	0.74
2:F:461:CYS:HB3	2:F:466:ARG:HD2	1.68	0.74
2:H:210:ALA:HB3	2:H:211:PRO:HD3	1.69	0.73
1:G:662:LEU:HD11	1:G:673:PHE:CZ	2.24	0.73
2:D:10:SER:HB3	2:D:449:ARG:CZ	2.18	0.73
1:C:756:HIS:O	1:C:757:ILE:HG22	1.89	0.73
1:E:848:HIS:HB2	2:F:485:SER:HB3	1.70	0.73
1:E:119:LEU:H	1:E:120:PRO:HA	1.50	0.73
1:A:119:LEU:H	1:A:120:PRO:HA	1.50	0.73
1:A:756:HIS:O	1:A:757:ILE:HG22	1.89	0.73
1:C:662:LEU:HD11	1:C:673:PHE:CZ	2.24	0.73
2:F:210:ALA:HB3	2:F:211:PRO:HD3	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LEU:HD11	1:A:673:PHE:CZ	2.24	0.72
1:C:119:LEU:H	1:C:120:PRO:HA	1.50	0.72
2:D:25:GLN:HB3	2:D:445:CYS:HB3	1.72	0.72
1:G:484:ARG:NH1	2:H:586:GLN:HG3	2.03	0.72
1:E:756:HIS:O	1:E:757:ILE:HG22	1.90	0.72
1:G:273:PHE:HB2	1:G:296:LYS:HD2	1.72	0.72
2:F:461:CYS:SG	2:F:466:ARG:CD	2.78	0.72
1:E:721:GLY:C	1:E:723:PRO:HD3	2.10	0.72
1:E:1064:PRO:CG	1:E:1067:GLU:HG3	2.20	0.71
4:E:3373:NAG:H3	4:E:3374:NAG:N2	2.05	0.71
1:E:662:LEU:HD11	1:E:673:PHE:CZ	2.24	0.71
1:G:1064:PRO:CG	1:G:1067:GLU:HG3	2.20	0.71
2:D:25:GLN:CB	2:D:445:CYS:HB3	2.20	0.71
1:E:817:GLN:N	1:E:818:LYS:HA	2.05	0.71
1:G:721:GLY:C	1:G:723:PRO:HD3	2.10	0.71
1:C:653:GLN:HB2	1:G:630:LEU:HD21	1.72	0.71
1:C:1064:PRO:CG	1:C:1067:GLU:HG3	2.20	0.71
1:A:721:GLY:C	1:A:723:PRO:HD3	2.11	0.71
2:H:27:LEU:HD21	2:H:446:GLY:O	1.91	0.71
1:A:1064:PRO:CG	1:A:1067:GLU:HG3	2.20	0.71
1:C:817:GLN:N	1:C:818:LYS:HA	2.06	0.70
1:C:94:HIS:CD2	2:D:155:LEU:HD21	2.25	0.70
1:C:721:GLY:C	1:C:723:PRO:HD3	2.11	0.70
1:A:731:ARG:O	1:A:731:ARG:HG3	1.92	0.70
1:C:731:ARG:O	1:C:731:ARG:HG3	1.92	0.70
1:G:328:PHE:O	1:G:354:PHE:HA	1.91	0.70
1:C:332:MET:SD	2:D:208:LEU:HD13	2.32	0.69
1:E:623:GLN:O	1:E:624:VAL:CG2	2.39	0.69
1:E:491:LEU:HD11	1:E:545:ILE:HG12	1.75	0.69
1:C:484:ARG:NH1	2:D:586:GLN:HG3	2.08	0.69
2:B:460:GLU:HG2	2:B:461:CYS:SG	2.32	0.69
1:C:812:TYR:CD2	1:C:814:ALA:HB2	2.28	0.69
2:D:25:GLN:OE1	2:D:427:CYS:SG	2.50	0.69
1:E:43:GLN:HA	1:E:70:ASN:H	1.58	0.69
1:A:812:TYR:CD2	1:A:814:ALA:HB2	2.27	0.69
1:A:817:GLN:N	1:A:818:LYS:HA	2.07	0.69
1:C:919:LEU:HB2	1:C:1079:GLU:HB3	1.75	0.69
1:C:491:LEU:HD11	1:C:545:ILE:HG12	1.75	0.69
1:E:919:LEU:HB2	1:E:1079:GLU:HB3	1.75	0.69
1:C:43:GLN:HA	1:C:70:ASN:H	1.58	0.69
2:F:455:ILE:HG13	2:F:463:THR:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:GLN:HB2	1:E:630:LEU:HD21	1.75	0.68
2:B:317:LYS:HE3	2:B:410:GLY:HA3	1.74	0.68
2:F:546:PHE:HA	2:F:554:GLU:O	1.93	0.68
1:A:1032:LEU:HD21	1:A:1078:LEU:HD21	1.75	0.68
1:A:919:LEU:HB2	1:A:1079:GLU:HB3	1.75	0.68
1:E:1032:LEU:HD21	1:E:1078:LEU:HD21	1.75	0.68
2:D:39:ARG:NE	2:D:447:ILE:CG2	2.57	0.68
1:A:491:LEU:HD11	1:A:545:ILE:HG12	1.76	0.68
2:F:317:LYS:CE	2:F:410:GLY:HA3	2.21	0.68
1:G:919:LEU:HB2	1:G:1079:GLU:HB3	1.75	0.68
1:A:912:HIS:ND1	1:A:935:ARG:HD2	2.09	0.68
1:A:513:ASN:HA	1:A:599:VAL:CG2	2.23	0.68
1:G:1032:LEU:HD21	1:G:1078:LEU:HD21	1.76	0.68
1:C:406:PRO:HB3	1:C:438:TYR:CE2	2.29	0.68
1:E:731:ARG:O	1:E:731:ARG:HG3	1.91	0.68
1:G:491:LEU:HD11	1:G:545:ILE:HG12	1.75	0.68
2:D:103:TYR:HB3	2:D:104:PRO:HD2	1.76	0.68
1:G:374:MET:HG3	1:G:381:MET:SD	2.34	0.68
1:E:912:HIS:ND1	1:E:935:ARG:HD2	2.09	0.67
1:C:328:PHE:O	1:C:354:PHE:HA	1.94	0.67
1:G:912:HIS:ND1	1:G:935:ARG:HD2	2.08	0.67
2:F:479:ASN:ND2	5:F:3479:NAG:C1	2.56	0.67
2:B:220:GLN:HA	2:B:264:CYS:HB3	1.76	0.67
1:E:374:MET:HG3	1:E:381:MET:SD	2.34	0.67
1:A:406:PRO:HB3	1:A:438:TYR:CE2	2.29	0.67
1:G:817:GLN:N	1:G:818:LYS:HA	2.08	0.67
1:G:731:ARG:O	1:G:731:ARG:HG3	1.92	0.67
1:C:912:HIS:ND1	1:C:935:ARG:HD2	2.09	0.67
2:H:597:PRO:O	2:H:598:SER:HB2	1.95	0.67
2:D:220:GLN:HA	2:D:264:CYS:HB3	1.76	0.67
1:A:374:MET:HG3	1:A:381:MET:SD	2.35	0.67
2:B:103:TYR:HB3	2:B:104:PRO:HD2	1.76	0.67
1:G:406:PRO:HB3	1:G:438:TYR:CE2	2.29	0.67
1:G:164:ARG:HB2	1:G:165:PRO:HA	1.76	0.67
1:E:406:PRO:HB3	1:E:438:TYR:CE2	2.29	0.67
2:H:25:GLN:CB	2:H:445:CYS:HB3	2.25	0.67
2:D:27:LEU:HG	2:D:446:GLY:HA2	1.75	0.67
1:C:1032:LEU:HD21	1:C:1078:LEU:HD21	1.75	0.67
2:H:27:LEU:CD2	2:H:446:GLY:HA2	2.25	0.67
1:C:812:TYR:CE2	1:C:814:ALA:HB2	2.29	0.67
2:H:220:GLN:HA	2:H:264:CYS:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:PRO:CG	2:F:510:GLN:CD	2.63	0.66
1:E:812:TYR:CE2	1:E:814:ALA:HB2	2.31	0.66
2:F:220:GLN:HA	2:F:264:CYS:HB3	1.77	0.66
1:C:374:MET:HG3	1:C:381:MET:SD	2.35	0.66
1:G:43:GLN:HA	1:G:70:ASN:H	1.58	0.66
1:A:609:ILE:HB	1:A:610:PRO:HD3	1.77	0.66
1:E:812:TYR:CD2	1:E:814:ALA:HB2	2.29	0.66
1:G:513:ASN:HA	1:G:599:VAL:HG21	1.77	0.66
2:H:15:ILE:HG23	2:H:86:ARG:CZ	2.25	0.66
2:H:103:TYR:HB3	2:H:104:PRO:HD2	1.77	0.66
1:G:364:PRO:CB	1:G:365:PRO:HD2	2.26	0.66
1:A:484:ARG:NH1	2:B:586:GLN:CG	2.59	0.66
2:F:23:TRP:HE1	2:F:445:CYS:HB3	1.61	0.66
2:H:522:TYR:CD1	2:H:552:GLN:HA	2.31	0.66
1:A:43:GLN:HA	1:A:70:ASN:H	1.59	0.66
1:C:1064:PRO:HG2	1:C:1067:GLU:HG3	1.78	0.66
1:C:848:HIS:HB2	2:D:485:SER:HB3	1.78	0.65
1:E:562:LEU:HD11	1:E:590:GLN:HG2	1.79	0.65
1:G:181:HIS:CE1	1:G:200:VAL:HG13	2.31	0.65
1:G:513:ASN:HA	1:G:599:VAL:CG2	2.25	0.65
1:G:322:THR:O	1:G:325:SER:HB2	1.96	0.65
1:G:609:ILE:HB	1:G:610:PRO:HD3	1.77	0.65
1:G:562:LEU:HD11	1:G:590:GLN:HG2	1.78	0.65
1:G:194:LEU:HD22	1:G:197:LEU:HD12	1.77	0.65
2:D:479:ASN:HD21	5:D:3479:NAG:C8	2.08	0.65
1:A:1064:PRO:HG2	1:A:1067:GLU:HG3	1.79	0.65
1:E:364:PRO:CB	1:E:365:PRO:HD2	2.26	0.65
1:C:609:ILE:HB	1:C:610:PRO:HD3	1.78	0.65
2:H:39:ARG:NE	2:H:447:ILE:CG2	2.59	0.65
1:A:599:VAL:O	1:A:599:VAL:HG23	1.95	0.65
1:A:630:LEU:HD21	1:E:653:GLN:HB2	1.77	0.65
1:C:364:PRO:CB	1:C:365:PRO:HD2	2.26	0.65
2:D:23:TRP:CZ2	2:D:447:ILE:HD13	2.31	0.65
1:A:364:PRO:CB	1:A:365:PRO:HD2	2.26	0.65
1:C:562:LEU:HD11	1:C:590:GLN:HG2	1.79	0.65
2:F:27:LEU:HD21	2:F:443:LEU:HD11	1.78	0.65
1:A:562:LEU:HD11	1:A:590:GLN:HG2	1.79	0.65
2:F:103:TYR:HB3	2:F:104:PRO:HD2	1.77	0.65
1:E:609:ILE:HB	1:E:610:PRO:HD3	1.77	0.65
1:C:103:LEU:CD1	2:D:155:LEU:HD13	2.26	0.64
1:G:812:TYR:CD2	1:G:814:ALA:HB2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:HIS:NE2	2:H:155:LEU:HD21	2.13	0.64
1:G:103:LEU:CD1	2:H:155:LEU:HD13	2.25	0.64
1:G:1064:PRO:HG2	1:G:1067:GLU:HG3	1.79	0.64
1:E:1064:PRO:HG2	1:E:1067:GLU:HG3	1.78	0.64
1:A:513:ASN:HA	1:A:599:VAL:HG21	1.78	0.64
2:F:101:LYS:HG2	2:F:102:GLY:H	1.62	0.64
1:G:659:ASP:OD2	4:G:3716:NAG:H82	1.97	0.64
2:B:104:PRO:HD2	2:B:233:VAL:HG11	1.78	0.64
2:F:104:PRO:HD2	2:F:233:VAL:HG11	1.78	0.64
1:A:812:TYR:CE2	1:A:814:ALA:HB2	2.33	0.64
2:D:104:PRO:HD2	2:D:233:VAL:HG11	1.78	0.64
1:E:599:VAL:HG23	1:E:599:VAL:O	1.98	0.64
2:B:471:LEU:O	2:B:493:GLY:HA2	1.98	0.64
1:G:194:LEU:CD2	1:G:197:LEU:HD12	2.28	0.64
1:G:871:LEU:HD11	1:G:901:VAL:HG21	1.80	0.64
1:E:121:VAL:O	1:E:121:VAL:HG12	1.98	0.64
2:D:10:SER:HB3	2:D:449:ARG:NE	2.13	0.64
1:A:673:PHE:CG	1:A:681:LEU:HD23	2.33	0.64
1:A:871:LEU:HD11	1:A:901:VAL:HG21	1.80	0.64
1:C:118:ARG:HA	1:C:120:PRO:HA	1.80	0.63
1:E:332:MET:SD	2:F:208:LEU:HD13	2.38	0.63
1:E:673:PHE:CG	1:E:681:LEU:HD23	2.33	0.63
2:H:104:PRO:HD2	2:H:233:VAL:HG11	1.78	0.63
1:G:121:VAL:HG12	1:G:121:VAL:O	1.98	0.63
2:H:39:ARG:NE	2:H:447:ILE:HG23	2.13	0.63
2:B:597:PRO:O	2:B:598:SER:HB2	1.98	0.63
1:C:673:PHE:CG	1:C:681:LEU:HD23	2.33	0.63
1:G:269:VAL:HG11	1:G:300:PHE:CE2	2.34	0.63
1:C:513:ASN:HA	1:C:599:VAL:CG2	2.29	0.63
2:F:35:PRO:HG2	2:F:510:GLN:NE2	2.12	0.63
1:G:673:PHE:CG	1:G:681:LEU:HD23	2.33	0.63
1:A:722:LYS:N	1:A:723:PRO:CD	2.62	0.63
1:A:121:VAL:HG12	1:A:121:VAL:O	1.98	0.63
2:F:35:PRO:HG2	2:F:510:GLN:OE1	1.98	0.63
1:A:118:ARG:HA	1:A:120:PRO:HA	1.81	0.63
2:F:461:CYS:CB	2:F:466:ARG:HD2	2.29	0.63
2:B:27:LEU:HG	2:B:446:GLY:HA2	1.81	0.63
1:A:797:GLY:CA	1:A:884:GLU:HB2	2.29	0.63
1:G:662:LEU:HD11	1:G:673:PHE:CE1	2.34	0.62
1:G:797:GLY:CA	1:G:884:GLU:HB2	2.29	0.62
2:F:461:CYS:HB3	2:F:466:ARG:CD	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:LEU:HD11	1:C:673:PHE:CE1	2.34	0.62
1:A:662:LEU:HD11	1:A:673:PHE:CE1	2.34	0.62
2:D:597:PRO:O	2:D:598:SER:HB2	1.98	0.62
1:C:119:LEU:HD21	1:C:124:GLN:HE21	1.64	0.62
1:C:722:LYS:N	1:C:723:PRO:CD	2.63	0.62
1:C:121:VAL:HG12	1:C:121:VAL:O	1.98	0.62
1:C:797:GLY:CA	1:C:884:GLU:HB2	2.30	0.62
1:E:797:GLY:CA	1:E:884:GLU:HB2	2.29	0.62
1:C:625:VAL:CG2	1:C:627:GLU:HG3	2.28	0.62
1:C:599:VAL:O	1:C:599:VAL:HG23	1.99	0.62
1:C:871:LEU:HD11	1:C:901:VAL:HG21	1.82	0.62
1:E:625:VAL:CG2	1:E:627:GLU:HG3	2.29	0.62
1:C:1064:PRO:HG3	1:C:1067:GLU:CG	2.30	0.62
1:E:722:LYS:N	1:E:723:PRO:CD	2.62	0.62
2:F:546:PHE:CE2	2:F:554:GLU:HG2	2.35	0.62
1:G:599:VAL:O	1:G:599:VAL:HG23	1.99	0.62
1:E:662:LEU:HD11	1:E:673:PHE:CE1	2.34	0.62
1:G:722:LYS:N	1:G:723:PRO:CD	2.62	0.62
1:G:327:SER:O	1:G:328:PHE:O	2.18	0.62
1:A:971:HIS:CE1	1:A:974:ASN:HB2	2.35	0.62
1:A:739:GLN:HB2	1:A:742:PHE:CZ	2.35	0.62
1:G:119:LEU:HD21	1:G:124:GLN:HE21	1.64	0.61
2:F:460:GLU:HG2	2:F:461:CYS:SG	2.40	0.61
1:A:519:ASP:CG	1:A:538:HIS:HD1	2.03	0.61
1:G:118:ARG:HA	1:G:120:PRO:HA	1.81	0.61
1:C:364:PRO:HB3	1:C:365:PRO:HD2	1.83	0.61
1:E:871:LEU:HD11	1:E:901:VAL:HG21	1.80	0.61
1:C:630:LEU:HD21	1:G:653:GLN:HB2	1.82	0.61
1:C:513:ASN:HA	1:C:599:VAL:HG21	1.82	0.61
1:E:364:PRO:HB3	1:E:365:PRO:HD2	1.83	0.61
2:H:295:GLN:HG3	2:H:317:LYS:HE2	1.82	0.61
2:B:295:GLN:HG3	2:B:317:LYS:HE2	1.82	0.61
1:E:963:VAL:HA	1:E:1036:TRP:CD1	2.35	0.61
2:B:597:PRO:O	2:B:598:SER:CB	2.48	0.61
2:D:597:PRO:O	2:D:598:SER:CB	2.48	0.61
1:E:739:GLN:HB2	1:E:742:PHE:CZ	2.35	0.61
1:E:1064:PRO:HG3	1:E:1067:GLU:CG	2.30	0.61
2:D:295:GLN:HG3	2:D:317:LYS:HE2	1.82	0.61
1:E:971:HIS:CE1	1:E:974:ASN:HB2	2.35	0.61
1:G:625:VAL:CG2	1:G:627:GLU:HG3	2.30	0.61
1:G:364:PRO:HB3	1:G:365:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:LEU:CD2	2:F:446:GLY:HA2	2.30	0.61
1:A:80:THR:HB	1:A:341:PHE:CG	2.35	0.61
1:A:119:LEU:HD21	1:A:124:GLN:HE21	1.65	0.61
1:E:118:ARG:HA	1:E:120:PRO:HA	1.81	0.61
1:E:119:LEU:HD21	1:E:124:GLN:HE21	1.64	0.61
2:B:154:VAL:HA	2:B:160:THR:HG22	1.83	0.61
1:A:1064:PRO:HG3	1:A:1067:GLU:HG3	1.83	0.61
1:A:364:PRO:HB3	1:A:365:PRO:HD2	1.83	0.61
1:A:1064:PRO:HG3	1:A:1067:GLU:CG	2.31	0.61
2:F:260:ASN:HA	2:F:277:PHE:CE2	2.36	0.61
1:C:44:THR:HG22	1:C:71:MET:HG2	1.83	0.61
1:C:739:GLN:HB2	1:C:742:PHE:CZ	2.36	0.60
1:E:103:LEU:CD1	2:F:155:LEU:HD13	2.26	0.60
2:D:479:ASN:ND2	5:D:3479:NAG:H82	2.15	0.60
1:G:1064:PRO:HG3	1:G:1067:GLU:CG	2.31	0.60
1:A:963:VAL:HA	1:A:1036:TRP:CD1	2.36	0.60
1:G:80:THR:HB	1:G:341:PHE:CG	2.36	0.60
1:C:80:THR:HB	1:C:341:PHE:CG	2.36	0.60
1:E:80:THR:HB	1:E:341:PHE:CG	2.36	0.60
1:A:928:GLU:HG3	1:A:929:SER:N	2.17	0.60
2:D:546:PHE:CD2	2:D:554:GLU:O	2.54	0.60
1:G:623:GLN:O	1:G:624:VAL:CG2	2.49	0.60
1:G:656:VAL:HG21	1:G:687:LEU:CD1	2.32	0.60
1:G:739:GLN:HB2	1:G:742:PHE:CZ	2.35	0.60
2:B:260:ASN:HA	2:B:277:PHE:CE2	2.37	0.60
1:C:928:GLU:HG3	1:C:929:SER:N	2.17	0.60
1:C:971:HIS:CE1	1:C:974:ASN:HB2	2.36	0.60
1:A:119:LEU:N	1:A:120:PRO:CA	2.60	0.60
1:E:373:ASN:OD1	4:E:3373:NAG:H2	2.02	0.60
1:A:513:ASN:CA	1:A:599:VAL:HG21	2.31	0.60
2:H:597:PRO:O	2:H:598:SER:CB	2.49	0.60
1:G:468:THR:HG23	1:G:498:PRO:HG3	1.84	0.60
1:G:1064:PRO:HG3	1:G:1067:GLU:HG3	1.83	0.60
1:C:1064:PRO:HG3	1:C:1067:GLU:HG3	1.83	0.60
1:G:971:HIS:CE1	1:G:974:ASN:HB2	2.36	0.60
1:E:928:GLU:HG3	1:E:929:SER:N	2.17	0.60
1:C:963:VAL:HA	1:C:1036:TRP:CD1	2.36	0.60
1:C:519:ASP:CG	1:C:538:HIS:HD1	2.05	0.60
2:D:462:GLN:HG2	2:D:463:THR:N	2.17	0.60
2:D:471:LEU:O	2:D:493:GLY:HA2	2.01	0.60
2:D:587:LEU:HB3	2:D:588:PRO:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:505:LYS:HA	2:D:517:ILE:HG21	1.84	0.60
2:F:295:GLN:HG3	2:F:317:LYS:HE2	1.82	0.60
2:H:154:VAL:HA	2:H:160:THR:HG22	1.83	0.60
1:A:1052:GLU:OE1	1:C:756:HIS:HA	2.01	0.60
2:D:25:GLN:HA	2:D:445:CYS:O	2.02	0.60
2:B:115:TYR:CD1	2:B:170:PRO:HD2	2.37	0.60
2:F:587:LEU:HB3	2:F:588:PRO:HA	1.84	0.60
1:G:963:VAL:HA	1:G:1036:TRP:CD1	2.37	0.60
1:E:44:THR:HG22	1:E:71:MET:HG2	1.83	0.60
1:E:469:ARG:NH2	2:F:287:HIS:HB2	2.15	0.60
1:G:519:ASP:CG	1:G:538:HIS:HD1	2.03	0.60
1:A:656:VAL:HG21	1:A:687:LEU:CD1	2.32	0.60
2:H:562:ASN:HB2	2:H:563:PRO:HD2	1.84	0.60
1:E:519:ASP:CG	1:E:538:HIS:HD1	2.05	0.60
2:D:154:VAL:HA	2:D:160:THR:HG22	1.83	0.59
1:A:625:VAL:CG2	1:A:627:GLU:HG3	2.29	0.59
2:F:546:PHE:CD2	2:F:554:GLU:HG2	2.36	0.59
1:C:604:VAL:HG11	1:C:742:PHE:CD2	2.37	0.59
2:F:115:TYR:CD1	2:F:170:PRO:HD2	2.37	0.59
1:C:833:PRO:HA	1:C:840:TRP:HB2	1.84	0.59
2:H:260:ASN:HA	2:H:277:PHE:CE2	2.37	0.59
2:D:260:ASN:HA	2:D:277:PHE:CE2	2.37	0.59
2:F:154:VAL:HA	2:F:160:THR:HG22	1.83	0.59
2:D:562:ASN:HB2	2:D:563:PRO:HD2	1.84	0.59
1:E:615:ARG:HA	1:E:618:PHE:HB2	1.85	0.59
2:F:562:ASN:HB2	2:F:563:PRO:HD2	1.84	0.59
1:C:653:GLN:CB	1:G:630:LEU:HD21	2.32	0.59
2:F:289:LEU:HD21	2:F:296:PRO:CD	2.33	0.59
2:H:289:LEU:HD21	2:H:296:PRO:CD	2.33	0.59
1:E:604:VAL:HG11	1:E:742:PHE:CD2	2.38	0.59
1:G:615:ARG:HA	1:G:618:PHE:HB2	1.83	0.59
2:H:184:HIS:CE1	2:H:228:ILE:HG23	2.38	0.59
2:B:184:HIS:CE1	2:B:228:ILE:HG23	2.37	0.59
2:B:347:LEU:HD22	2:B:389:PHE:CD1	2.38	0.59
1:A:118:ARG:HG2	1:A:120:PRO:HB3	1.85	0.59
1:A:468:THR:HG23	1:A:498:PRO:HG3	1.84	0.59
1:C:490:VAL:HG12	1:C:491:LEU:N	2.18	0.59
2:F:27:LEU:HD23	2:F:446:GLY:HA2	1.83	0.59
1:G:362:LEU:HD23	1:G:363:TYR:N	2.18	0.59
1:G:44:THR:HG22	1:G:71:MET:HG2	1.83	0.59
1:G:118:ARG:HG2	1:G:120:PRO:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:812:TYR:CE2	1:G:814:ALA:HB2	2.38	0.59
2:H:587:LEU:HB3	2:H:588:PRO:HA	1.85	0.59
2:D:115:TYR:CD1	2:D:170:PRO:HD2	2.37	0.59
1:A:623:GLN:O	1:A:624:VAL:CG2	2.50	0.59
2:F:532:ARG:HD3	2:F:554:GLU:CD	2.22	0.59
2:D:115:TYR:HA	2:D:204:ILE:HD13	1.85	0.59
2:D:289:LEU:HD21	2:D:296:PRO:CD	2.33	0.59
1:A:362:LEU:HD23	1:A:363:TYR:N	2.18	0.59
2:B:317:LYS:HE3	2:B:410:GLY:CA	2.33	0.59
1:G:137:ILE:HD13	1:G:152:MET:SD	2.42	0.59
1:E:813:VAL:HB	1:E:823:ARG:HH21	1.66	0.59
2:F:571:ARG:HH21	2:F:660:MET:CG	2.16	0.59
1:G:928:GLU:HG3	1:G:929:SER:N	2.17	0.59
2:H:471:LEU:O	2:H:493:GLY:HA2	2.03	0.59
1:C:119:LEU:N	1:C:120:PRO:CA	2.60	0.59
1:G:721:GLY:C	1:G:723:PRO:CD	2.72	0.59
1:A:444:CYS:HB2	1:A:506:LEU:CD1	2.33	0.59
1:E:656:VAL:HG21	1:E:687:LEU:CD1	2.32	0.59
1:E:362:LEU:HD23	1:E:363:TYR:N	2.18	0.59
2:H:115:TYR:HA	2:H:204:ILE:HD13	1.85	0.59
2:F:15:ILE:HG23	2:F:86:ARG:HH21	1.66	0.58
2:B:592:GLU:O	2:B:594:PRO:HD3	2.02	0.58
1:G:490:VAL:HG12	1:G:491:LEU:N	2.18	0.58
1:A:490:VAL:HG12	1:A:491:LEU:N	2.18	0.58
2:B:289:LEU:HD21	2:B:296:PRO:CD	2.33	0.58
2:F:562:ASN:HB3	2:F:589:LEU:HD13	1.86	0.58
2:H:115:TYR:CD1	2:H:170:PRO:HD2	2.37	0.58
1:E:446:VAL:HG21	1:E:520:VAL:CG1	2.33	0.58
2:B:115:TYR:HA	2:B:204:ILE:HD13	1.85	0.58
1:A:44:THR:HG22	1:A:71:MET:HG2	1.83	0.58
2:B:587:LEU:HB3	2:B:588:PRO:HA	1.85	0.58
1:C:18:PHE:CE2	1:C:32:VAL:HG21	2.38	0.58
1:G:385:TYR:CZ	2:H:253:LEU:HD11	2.39	0.58
1:C:362:LEU:HD23	1:C:363:TYR:N	2.18	0.58
2:F:184:HIS:CE1	2:F:228:ILE:HG23	2.38	0.58
1:A:18:PHE:CE2	1:A:32:VAL:HG21	2.38	0.58
1:E:1064:PRO:HG3	1:E:1067:GLU:HG3	1.83	0.58
2:D:442:PHE:CZ	2:D:449:ARG:HB2	2.39	0.58
2:B:295:GLN:CG	2:B:317:LYS:HE2	2.34	0.58
1:C:444:CYS:HB2	1:C:506:LEU:CD1	2.34	0.58
2:F:442:PHE:CZ	2:F:449:ARG:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:LEU:HG	1:A:823:ARG:H	1.69	0.58
2:F:597:PRO:O	2:F:598:SER:HB2	2.04	0.58
1:E:118:ARG:HG2	1:E:120:PRO:HB3	1.85	0.58
2:B:562:ASN:HB2	2:B:563:PRO:HD2	1.84	0.58
1:G:710:PRO:HG3	1:G:884:GLU:OE2	2.02	0.58
1:G:813:VAL:HB	1:G:823:ARG:HH21	1.68	0.58
2:D:184:HIS:CE1	2:D:228:ILE:HG23	2.38	0.58
1:C:623:GLN:O	1:C:624:VAL:CG2	2.51	0.58
1:C:721:GLY:C	1:C:723:PRO:CD	2.72	0.58
1:A:604:VAL:HG11	1:A:742:PHE:CD2	2.39	0.58
1:G:604:VAL:HG11	1:G:742:PHE:CD2	2.38	0.58
2:F:115:TYR:HA	2:F:204:ILE:HD13	1.85	0.58
1:E:621:ARG:HG2	1:E:622:GLU:H	1.68	0.58
1:E:468:THR:HG23	1:E:498:PRO:HG3	1.84	0.58
1:C:468:THR:HG23	1:C:498:PRO:HG3	1.85	0.58
1:C:656:VAL:HG21	1:C:687:LEU:CD1	2.32	0.58
1:A:666:ARG:HB3	2:B:498:HIS:CD2	2.39	0.58
1:G:986:PRO:CB	1:G:987:PRO:HD2	2.34	0.58
1:C:446:VAL:HG21	1:C:520:VAL:CG1	2.33	0.58
2:F:295:GLN:CG	2:F:317:LYS:HE2	2.34	0.57
2:B:461:CYS:HB3	2:B:466:ARG:HD3	1.85	0.57
1:E:18:PHE:CE2	1:E:32:VAL:HG21	2.39	0.57
2:B:442:PHE:CZ	2:B:449:ARG:HB2	2.39	0.57
1:C:994:HIS:CG	1:C:1005:ILE:HD11	2.39	0.57
1:G:332:MET:SD	2:H:208:LEU:HD13	2.44	0.57
1:E:444:CYS:HB2	1:E:506:LEU:CD1	2.34	0.57
1:E:833:PRO:HA	1:E:840:TRP:HB2	1.84	0.57
2:D:347:LEU:HD22	2:D:389:PHE:CD1	2.39	0.57
1:E:721:GLY:C	1:E:723:PRO:CD	2.72	0.57
1:E:364:PRO:CB	1:E:365:PRO:CD	2.83	0.57
2:D:295:GLN:CG	2:D:317:LYS:HE2	2.34	0.57
1:G:446:VAL:HG21	1:G:520:VAL:CG1	2.34	0.57
2:D:15:ILE:HG23	2:D:86:ARG:CZ	2.34	0.57
1:A:721:GLY:C	1:A:723:PRO:CD	2.72	0.57
2:H:562:ASN:HB3	2:H:589:LEU:HD13	1.86	0.57
1:A:575:LEU:HD12	1:A:576:THR:N	2.20	0.57
1:G:364:PRO:CB	1:G:365:PRO:CD	2.82	0.57
1:A:446:VAL:HG21	1:A:520:VAL:CG1	2.34	0.57
1:C:822:LEU:HG	1:C:823:ARG:H	1.69	0.57
1:E:986:PRO:CB	1:E:987:PRO:HD2	2.34	0.57
2:B:562:ASN:HB3	2:B:589:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:444:CYS:HB2	1:G:506:LEU:CD1	2.34	0.57
1:G:186:GLU:HA	1:G:189:ARG:HG2	1.85	0.57
2:H:592:GLU:O	2:H:594:PRO:HD3	2.04	0.57
2:D:23:TRP:CZ2	2:D:447:ILE:CD1	2.88	0.57
2:H:442:PHE:CZ	2:H:449:ARG:HB2	2.39	0.57
1:G:18:PHE:CE2	1:G:32:VAL:HG21	2.39	0.57
2:D:39:ARG:CD	2:D:447:ILE:CG2	2.82	0.57
2:D:562:ASN:HB3	2:D:589:LEU:HD13	1.86	0.57
1:E:490:VAL:HG12	1:E:491:LEU:N	2.18	0.57
2:F:444:GLU:OE2	2:F:445:CYS:SG	2.63	0.57
1:E:407:ARG:HG2	2:F:247:PHE:CZ	2.40	0.57
1:A:653:GLN:CB	1:E:630:LEU:HD21	2.35	0.56
1:A:32:VAL:HG11	1:A:591:VAL:HG11	1.87	0.56
2:B:285:LEU:O	2:B:289:LEU:HB3	2.06	0.56
2:H:295:GLN:CG	2:H:317:LYS:HE2	2.34	0.56
2:D:340:LYS:HD2	2:D:379:ASP:OD1	2.05	0.56
1:E:479:PRO:HD2	1:E:485:TRP:CD1	2.40	0.56
2:D:479:ASN:HD22	5:D:3479:NAG:C1	2.19	0.56
1:G:513:ASN:CA	1:G:599:VAL:HG21	2.34	0.56
1:A:364:PRO:CB	1:A:365:PRO:CD	2.83	0.56
1:G:666:ARG:HB3	2:H:498:HIS:NE2	2.20	0.56
2:D:460:GLU:HG2	2:D:461:CYS:SG	2.46	0.56
1:A:986:PRO:CB	1:A:987:PRO:HD2	2.35	0.56
1:A:833:PRO:HA	1:A:840:TRP:HB2	1.85	0.56
1:C:575:LEU:HD12	1:C:576:THR:N	2.21	0.56
4:A:3374:NAG:O3	4:A:3375:MAN:H2	2.05	0.56
2:D:479:ASN:ND2	5:D:3479:NAG:C8	2.69	0.56
1:C:364:PRO:CB	1:C:365:PRO:CD	2.83	0.56
1:G:833:PRO:HA	1:G:840:TRP:HB2	1.86	0.56
1:C:602:VAL:HG23	1:C:638:TYR:O	2.06	0.56
1:C:118:ARG:HG2	1:C:120:PRO:HB3	1.85	0.56
2:F:399:ILE:HG13	2:F:421:PRO:HG3	1.88	0.56
2:F:340:LYS:HA	2:F:343:SER:HB2	1.85	0.56
1:E:831:SER:CB	1:E:842:THR:HG22	2.36	0.56
1:G:831:SER:CB	1:G:842:THR:HG22	2.36	0.56
1:A:602:VAL:HG23	1:A:638:TYR:O	2.05	0.56
1:A:831:SER:CB	1:A:842:THR:HG22	2.35	0.56
2:B:162:PRO:O	2:B:165:LEU:HB3	2.06	0.56
1:A:578:ASP:OD2	1:A:595:ARG:HD2	2.06	0.56
1:G:602:VAL:HG23	1:G:638:TYR:O	2.04	0.56
1:E:575:LEU:HD12	1:E:576:THR:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:LEU:HD11	1:G:88:ALA:CB	2.36	0.56
1:C:103:LEU:HD13	2:D:156:PRO:HG3	1.87	0.56
2:D:162:PRO:O	2:D:165:LEU:HB3	2.06	0.56
2:D:285:LEU:O	2:D:289:LEU:HB3	2.06	0.56
1:C:831:SER:CB	1:C:842:THR:HG22	2.36	0.56
1:A:479:PRO:HD2	1:A:485:TRP:CD1	2.41	0.56
2:H:399:ILE:HG13	2:H:421:PRO:HG3	1.88	0.56
2:H:27:LEU:HD11	2:H:443:LEU:HD11	1.88	0.56
2:D:479:ASN:ND2	5:D:3479:NAG:N2	2.54	0.56
1:G:662:LEU:CD1	1:G:673:PHE:CE1	2.89	0.56
2:F:597:PRO:O	2:F:598:SER:CB	2.54	0.56
1:E:602:VAL:HG23	1:E:638:TYR:O	2.05	0.56
2:H:609:CYS:SG	2:H:616:PRO:HB3	2.46	0.56
1:C:479:PRO:HD2	1:C:485:TRP:CD1	2.41	0.56
2:B:609:CYS:SG	2:B:616:PRO:HB3	2.46	0.56
2:F:592:GLU:O	2:F:594:PRO:HD3	2.05	0.56
1:E:907:THR:CG2	1:E:1053:ILE:HD13	2.36	0.56
1:A:928:GLU:HG3	1:A:929:SER:H	1.71	0.56
1:G:214:GLN:CD	1:G:253:VAL:HG12	2.27	0.56
1:G:907:THR:CG2	1:G:1053:ILE:HD13	2.36	0.56
2:D:592:GLU:O	2:D:594:PRO:HD3	2.05	0.56
2:D:609:CYS:SG	2:D:616:PRO:HB3	2.46	0.56
2:D:616:PRO:HB2	2:D:620:ASN:HA	1.88	0.56
1:G:575:LEU:HD12	1:G:576:THR:N	2.20	0.56
1:E:578:ASP:OD2	1:E:595:ARG:HD2	2.06	0.55
1:G:747:PRO:HB3	1:G:884:GLU:HG2	1.88	0.55
1:G:32:VAL:HG11	1:G:591:VAL:HG11	1.88	0.55
2:F:616:PRO:HB2	2:F:620:ASN:HA	1.88	0.55
1:C:565:PHE:HB2	1:C:587:ALA:HB2	1.88	0.55
1:E:32:VAL:HG11	1:E:591:VAL:HG11	1.87	0.55
1:G:876:LEU:HD12	1:G:876:LEU:C	2.27	0.55
2:F:508:TYR:CZ	2:F:514:CYS:HB3	2.41	0.55
1:E:876:LEU:C	1:E:876:LEU:HD12	2.26	0.55
2:H:460:GLU:HG2	2:H:461:CYS:SG	2.47	0.55
1:C:662:LEU:CD1	1:C:673:PHE:CE1	2.89	0.55
2:H:591:GLN:HG2	2:H:592:GLU:N	2.22	0.55
2:F:285:LEU:O	2:F:289:LEU:HB3	2.06	0.55
2:B:103:TYR:HB3	2:B:104:PRO:CD	2.36	0.55
1:E:418:THR:HG21	1:E:482:TRP:CZ2	2.42	0.55
2:H:616:PRO:HB2	2:H:620:ASN:HA	1.88	0.55
2:B:616:PRO:HB2	2:B:620:ASN:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:666:ARG:HB3	2:D:498:HIS:CD2	2.41	0.55
1:A:876:LEU:HD12	1:A:876:LEU:C	2.27	0.55
2:B:399:ILE:HG13	2:B:421:PRO:HG3	1.88	0.55
1:E:103:LEU:CD1	2:F:156:PRO:HG3	2.37	0.55
2:F:461:CYS:SG	2:F:466:ARG:NE	2.79	0.55
1:E:662:LEU:CD1	1:E:673:PHE:CE1	2.90	0.55
1:A:565:PHE:HB2	1:A:587:ALA:HB2	1.89	0.55
2:H:162:PRO:O	2:H:165:LEU:HB3	2.06	0.55
1:A:662:LEU:CD1	1:A:673:PHE:CE1	2.90	0.55
1:C:484:ARG:NH1	2:D:586:GLN:CG	2.69	0.55
1:C:876:LEU:C	1:C:876:LEU:HD12	2.27	0.55
1:E:94:HIS:CD2	2:F:155:LEU:HD21	2.41	0.55
1:E:822:LEU:HG	1:E:823:ARG:H	1.72	0.55
1:G:822:LEU:HG	1:G:823:ARG:H	1.70	0.55
1:G:479:PRO:HD2	1:G:485:TRP:CD1	2.41	0.55
1:A:907:THR:CG2	1:A:1053:ILE:HD13	2.36	0.55
1:G:578:ASP:OD2	1:G:595:ARG:HD2	2.06	0.55
2:D:103:TYR:HB3	2:D:104:PRO:CD	2.36	0.55
1:G:418:THR:HG21	1:G:482:TRP:CZ2	2.41	0.55
2:D:399:ILE:HG13	2:D:421:PRO:HG3	1.88	0.55
1:E:47:LEU:HD11	1:E:88:ALA:CB	2.37	0.55
1:C:986:PRO:CB	1:C:987:PRO:HD2	2.36	0.55
1:C:907:THR:CG2	1:C:1053:ILE:HD13	2.36	0.55
2:B:6:PHE:O	2:B:8:VAL:HG23	2.07	0.55
1:C:941:LEU:HD12	1:C:941:LEU:N	2.22	0.55
2:H:285:LEU:O	2:H:289:LEU:HB3	2.06	0.55
2:F:103:TYR:HB3	2:F:104:PRO:CD	2.37	0.55
1:A:47:LEU:HB2	1:A:60:ILE:HG21	1.88	0.55
1:A:333:ALA:HB1	1:A:350:ALA:HB1	1.89	0.55
1:A:1065:GLY:C	1:A:1066:GLN:HG3	2.27	0.55
1:C:333:ALA:HB1	1:C:350:ALA:HB1	1.89	0.55
1:E:435:ILE:HD13	2:F:311:LEU:HB2	1.87	0.55
2:F:162:PRO:O	2:F:165:LEU:HB3	2.06	0.55
1:G:119:LEU:N	1:G:120:PRO:CA	2.60	0.55
1:C:32:VAL:HG11	1:C:591:VAL:HG11	1.87	0.55
1:A:47:LEU:HD11	1:A:88:ALA:CB	2.37	0.55
1:E:905:VAL:HG11	1:E:946:LEU:HD21	1.89	0.55
1:E:941:LEU:N	1:E:941:LEU:HD12	2.22	0.55
1:A:772:LYS:HG3	1:A:772:LYS:O	2.07	0.55
1:C:578:ASP:OD2	1:C:595:ARG:HD2	2.06	0.55
1:A:822:LEU:CG	1:A:823:ARG:H	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ILE:HG13	1:A:689:LEU:HA	1.88	0.55
1:E:639:ILE:HG13	1:E:689:LEU:HA	1.88	0.55
1:C:418:THR:HG21	1:C:482:TRP:CZ2	2.42	0.55
1:E:47:LEU:HB2	1:E:60:ILE:HG21	1.89	0.55
1:C:47:LEU:HD11	1:C:88:ALA:CB	2.37	0.55
1:E:565:PHE:HB2	1:E:587:ALA:HB2	1.89	0.55
1:E:786:VAL:HG11	1:E:859:PHE:CZ	2.42	0.55
2:F:347:LEU:HD22	2:F:389:PHE:CD1	2.42	0.55
1:C:1065:GLY:C	1:C:1066:GLN:HG3	2.27	0.55
2:H:444:GLU:OE2	2:H:445:CYS:SG	2.65	0.54
1:E:513:ASN:HA	1:E:599:VAL:CG2	2.36	0.54
1:G:639:ILE:HG13	1:G:689:LEU:HA	1.89	0.54
1:G:1065:GLY:C	1:G:1066:GLN:HG3	2.28	0.54
1:G:941:LEU:HD12	1:G:941:LEU:N	2.22	0.54
2:H:103:TYR:HB3	2:H:104:PRO:CD	2.37	0.54
1:A:418:THR:HG21	1:A:482:TRP:CZ2	2.41	0.54
2:H:6:PHE:O	2:H:8:VAL:HG23	2.07	0.54
2:H:522:TYR:CE1	2:H:552:GLN:HA	2.42	0.54
2:F:609:CYS:SG	2:F:616:PRO:HB3	2.48	0.54
1:A:905:VAL:HG11	1:A:946:LEU:HD21	1.89	0.54
2:F:604:ILE:HD11	2:F:642:GLU:HB2	1.89	0.54
1:G:772:LYS:O	1:G:772:LYS:HG3	2.08	0.54
2:D:6:PHE:O	2:D:8:VAL:HG23	2.07	0.54
1:G:174:PHE:CE1	1:G:209:THR:HA	2.42	0.54
1:G:136:LEU:HD13	1:G:216:VAL:HG21	1.89	0.54
1:G:311:LYS:HG3	1:G:312:GLU:N	2.20	0.54
1:C:103:LEU:HD21	2:D:155:LEU:CD2	2.38	0.54
2:D:23:TRP:HZ2	2:D:447:ILE:CD1	2.21	0.54
1:C:327:SER:O	1:C:328:PHE:O	2.26	0.54
1:E:928:GLU:HG3	1:E:929:SER:H	1.72	0.54
1:G:47:LEU:HB2	1:G:60:ILE:HG21	1.89	0.54
1:A:941:LEU:HD12	1:A:941:LEU:N	2.22	0.54
1:C:113:THR:HG22	1:E:1029:LYS:HE2	1.89	0.54
1:G:928:GLU:HG3	1:G:929:SER:H	1.72	0.54
1:G:565:PHE:HB2	1:G:587:ALA:HB2	1.88	0.54
1:C:815:GLU:HB3	1:C:819:GLN:NE2	2.23	0.54
2:B:591:GLN:HG2	2:B:592:GLU:N	2.22	0.54
2:B:468:SER:HB2	2:B:471:LEU:HG	1.90	0.54
1:G:665:GLY:HA3	2:H:498:HIS:HB3	1.88	0.54
1:G:766:PHE:CZ	1:G:877:LEU:CD1	2.91	0.54
1:G:786:VAL:HG11	1:G:859:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:ALA:HB1	1:G:350:ALA:HB1	1.90	0.54
1:A:615:ARG:HA	1:A:618:PHE:HB2	1.89	0.54
2:B:599:PRO:HB2	2:B:603:TYR:HE2	1.73	0.54
2:B:444:GLU:OE2	2:B:445:CYS:SG	2.66	0.54
1:C:905:VAL:HG11	1:C:946:LEU:HD21	1.90	0.54
1:G:905:VAL:HG11	1:G:946:LEU:HD21	1.90	0.54
1:C:93:VAL:O	1:C:103:LEU:HA	2.08	0.54
1:E:772:LYS:HG3	1:E:772:LYS:O	2.07	0.54
1:A:652:LEU:HD21	1:E:609:ILE:HG22	1.89	0.54
2:B:112:ASP:O	2:B:117:MET:HG3	2.07	0.54
1:C:615:ARG:HA	1:C:618:PHE:HB2	1.90	0.54
1:C:531:ARG:HA	1:C:563:GLN:O	2.08	0.54
2:F:112:ASP:O	2:F:117:MET:HG3	2.07	0.54
1:E:1065:GLY:C	1:E:1066:GLN:HG3	2.27	0.54
1:E:93:VAL:O	1:E:103:LEU:HA	2.08	0.54
1:G:681:LEU:HD12	1:G:682:SER:N	2.23	0.54
1:E:964:TRP:CB	1:E:1032:LEU:HA	2.38	0.54
1:C:928:GLU:HG3	1:C:929:SER:H	1.72	0.54
2:H:468:SER:HB2	2:H:471:LEU:HG	1.90	0.54
1:G:506:LEU:HA	1:G:569:LEU:HD11	1.90	0.54
2:B:212:GLU:HG2	2:B:243:ASP:HB2	1.89	0.54
2:B:455:ILE:HG22	2:B:456:GLY:N	2.23	0.54
2:F:35:PRO:HB3	2:F:510:GLN:HG2	1.90	0.54
1:C:755:ASP:O	1:C:756:HIS:HB3	2.07	0.54
2:D:444:GLU:OE2	2:D:445:CYS:SG	2.66	0.54
1:C:822:LEU:CG	1:C:823:ARG:H	2.20	0.54
1:G:243:LYS:HD3	1:G:250:TYR:CE2	2.43	0.54
2:H:212:GLU:HG2	2:H:243:ASP:HB2	1.89	0.54
2:D:112:ASP:O	2:D:117:MET:HG3	2.07	0.54
2:D:212:GLU:HG2	2:D:243:ASP:HB2	1.89	0.54
2:F:471:LEU:O	2:F:493:GLY:HA2	2.08	0.54
1:E:671:ALA:O	1:E:672:THR:HG23	2.08	0.54
2:F:58:ASP:N	2:F:59:PRO:HD3	2.23	0.54
1:C:420:VAL:HB	1:C:423:GLN:HB2	1.91	0.54
2:B:295:GLN:CD	2:B:317:LYS:HE2	2.28	0.53
2:F:295:GLN:CD	2:F:317:LYS:HE2	2.28	0.53
1:C:772:LYS:O	1:C:772:LYS:HG3	2.08	0.53
2:F:546:PHE:CD2	2:F:554:GLU:CG	2.91	0.53
2:H:289:LEU:HD21	2:H:296:PRO:HD3	1.89	0.53
2:H:295:GLN:CD	2:H:317:LYS:HE2	2.29	0.53
1:C:506:LEU:HA	1:C:569:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:VAL:HB	1:C:823:ARG:HH21	1.72	0.53
2:D:591:GLN:HG2	2:D:592:GLU:N	2.23	0.53
2:F:468:SER:HB2	2:F:471:LEU:HG	1.90	0.53
2:F:6:PHE:O	2:F:8:VAL:HG23	2.07	0.53
1:E:994:HIS:CG	1:E:1005:ILE:HD11	2.43	0.53
2:H:112:ASP:O	2:H:117:MET:HG3	2.08	0.53
1:G:600:LEU:O	1:G:600:LEU:HD12	2.08	0.53
1:G:184:PHE:CD2	1:G:227:ALA:HB2	2.43	0.53
1:E:103:LEU:HD13	2:F:156:PRO:HG3	1.90	0.53
1:A:964:TRP:CB	1:A:1032:LEU:HA	2.39	0.53
2:H:317:LYS:HE3	2:H:410:GLY:HA3	1.90	0.53
2:D:295:GLN:CD	2:D:317:LYS:HE2	2.28	0.53
2:D:468:SER:HB2	2:D:471:LEU:HG	1.90	0.53
1:C:47:LEU:HB2	1:C:60:ILE:HG21	1.89	0.53
1:C:786:VAL:HG11	1:C:859:PHE:CZ	2.44	0.53
2:D:604:ILE:HD11	2:D:642:GLU:HB2	1.90	0.53
1:C:639:ILE:HG13	1:C:689:LEU:HA	1.89	0.53
1:E:491:LEU:HD11	1:E:545:ILE:CG1	2.38	0.53
1:C:465:TYR:HB3	1:C:469:ARG:HA	1.91	0.53
1:A:506:LEU:HA	1:A:569:LEU:HD11	1.90	0.53
2:H:347:LEU:HD22	2:H:389:PHE:CD1	2.43	0.53
1:G:93:VAL:O	1:G:103:LEU:HA	2.08	0.53
1:A:94:HIS:CD2	2:B:155:LEU:HD21	2.43	0.53
1:G:666:ARG:HB3	2:H:498:HIS:CD2	2.44	0.53
1:A:420:VAL:HB	1:A:423:GLN:HB2	1.91	0.53
1:C:103:LEU:CD1	2:D:156:PRO:HG3	2.39	0.53
1:C:964:TRP:CB	1:C:1032:LEU:HA	2.38	0.53
2:B:562:ASN:HB2	2:B:563:PRO:CD	2.39	0.53
1:E:476:CYS:CB	1:E:487:CYS:HA	2.38	0.53
2:H:604:ILE:HD11	2:H:642:GLU:HB2	1.90	0.53
1:A:681:LEU:HD12	1:A:682:SER:N	2.23	0.53
1:E:465:TYR:HB3	1:E:469:ARG:HA	1.91	0.53
2:F:289:LEU:HD21	2:F:296:PRO:HD3	1.89	0.53
2:H:289:LEU:HD23	2:H:315:ILE:HD11	1.91	0.53
1:C:833:PRO:HA	1:C:840:TRP:CB	2.39	0.53
1:G:243:LYS:O	1:G:243:LYS:HG3	2.08	0.53
1:G:174:PHE:HB2	1:G:212:ALA:HB2	1.91	0.53
2:F:212:GLU:HG2	2:F:243:ASP:HB2	1.89	0.53
1:A:766:PHE:CZ	1:A:877:LEU:CD1	2.92	0.53
1:G:531:ARG:HA	1:G:563:GLN:O	2.09	0.53
2:D:121:LEU:O	2:D:125:LYS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:O	1:A:103:LEU:HA	2.08	0.53
4:E:3373:NAG:C3	4:E:3374:NAG:N2	2.72	0.53
2:B:289:LEU:HD21	2:B:296:PRO:HD3	1.89	0.53
1:G:964:TRP:CB	1:G:1032:LEU:HA	2.38	0.53
1:A:823:ARG:HD3	1:A:860:LEU:H	1.74	0.53
1:G:211:THR:HA	1:G:248:LEU:HD12	1.91	0.53
2:H:121:LEU:O	2:H:125:LYS:HB3	2.09	0.53
1:C:761:ASN:ND2	1:C:791:ASP:HB2	2.24	0.53
1:A:761:ASN:ND2	1:A:791:ASP:HB2	2.24	0.53
2:B:546:PHE:CE2	2:B:554:GLU:HG2	2.44	0.53
1:G:491:LEU:HD12	1:G:492:TYR:N	2.24	0.53
2:F:562:ASN:HB2	2:F:563:PRO:CD	2.39	0.53
1:G:476:CYS:CB	1:G:487:CYS:HA	2.38	0.53
1:E:766:PHE:CZ	1:E:877:LEU:CD1	2.92	0.53
2:B:604:ILE:HD11	2:B:642:GLU:HB2	1.90	0.53
2:F:121:LEU:O	2:F:125:LYS:HB3	2.09	0.53
1:C:1063:LEU:HD12	1:C:1064:PRO:HA	1.90	0.53
2:D:57:MET:SD	2:D:427:CYS:SG	3.07	0.53
1:E:436:GLY:C	2:F:282:VAL:HG11	2.30	0.53
1:A:692:HIS:ND1	1:E:694:GLU:HA	2.24	0.53
1:E:952:PHE:HB2	1:E:1011:PHE:HB2	1.91	0.53
1:C:766:PHE:CZ	1:C:877:LEU:CD1	2.92	0.53
1:A:531:ARG:HA	1:A:563:GLN:O	2.09	0.53
1:C:652:LEU:HD21	1:G:609:ILE:HG22	1.90	0.52
2:D:289:LEU:HD21	2:D:296:PRO:HD3	1.90	0.52
1:A:416:ILE:HD11	1:A:485:TRP:CZ2	2.45	0.52
1:A:786:VAL:HG11	1:A:859:PHE:CZ	2.44	0.52
2:B:508:TYR:CZ	2:B:514:CYS:HB3	2.44	0.52
1:C:917:LYS:HE3	1:C:1077:VAL:CG2	2.39	0.52
1:A:499:TRP:CZ2	2:B:284:GLN:HG3	2.43	0.52
1:E:848:HIS:O	1:E:849:LEU:HB3	2.10	0.52
1:G:491:LEU:HD12	1:G:491:LEU:C	2.30	0.52
1:G:325:SER:OG	1:G:326:SER:N	2.42	0.52
1:C:952:PHE:HB2	1:C:1011:PHE:HB2	1.91	0.52
1:G:952:PHE:HB2	1:G:1011:PHE:HB2	1.91	0.52
1:E:420:VAL:HB	1:E:423:GLN:HB2	1.91	0.52
1:A:671:ALA:O	1:A:672:THR:HG23	2.08	0.52
2:H:546:PHE:CD2	2:H:554:GLU:O	2.62	0.52
1:G:159:ILE:HD12	1:G:197:LEU:HD11	1.89	0.52
2:D:562:ASN:HB2	2:D:563:PRO:CD	2.39	0.52
2:D:289:LEU:HD23	2:D:315:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:CYS:CB	1:A:487:CYS:HA	2.38	0.52
1:C:25:TYR:CD1	1:C:86:LEU:HB2	2.44	0.52
1:A:994:HIS:CG	1:A:1005:ILE:HD11	2.45	0.52
1:A:25:TYR:CD1	1:A:86:LEU:HB2	2.45	0.52
1:C:600:LEU:HD12	1:C:600:LEU:O	2.10	0.52
1:G:1063:LEU:HD12	1:G:1064:PRO:HA	1.90	0.52
1:C:681:LEU:HD12	1:C:682:SER:N	2.24	0.52
1:G:484:ARG:NH1	2:H:586:GLN:CG	2.73	0.52
1:G:465:TYR:HB3	1:G:469:ARG:HA	1.91	0.52
1:A:813:VAL:HB	1:A:823:ARG:HH21	1.75	0.52
1:A:333:ALA:HA	1:A:352:GLY:H	1.74	0.52
1:E:333:ALA:HB1	1:E:350:ALA:HB1	1.90	0.52
2:F:432:ARG:O	2:F:433:ASP:HB2	2.10	0.52
2:H:135:LEU:HD11	2:H:139:THR:HB	1.90	0.52
1:G:671:ALA:O	1:G:672:THR:HG23	2.10	0.52
1:E:761:ASN:ND2	1:E:791:ASP:HB2	2.24	0.52
1:C:476:CYS:CB	1:C:487:CYS:HA	2.39	0.52
1:C:634:ASN:ND2	1:G:690:LYS:HG3	2.24	0.52
1:G:221:PHE:CD1	1:G:233:LYS:HD2	2.44	0.52
1:A:491:LEU:HD12	1:A:492:TYR:N	2.24	0.52
2:B:289:LEU:HD23	2:B:315:ILE:HD11	1.91	0.52
2:H:562:ASN:HB2	2:H:563:PRO:CD	2.39	0.52
1:A:71:MET:HG3	1:A:90:GLY:HA3	1.92	0.52
1:G:420:VAL:HB	1:G:423:GLN:HB2	1.90	0.52
1:G:848:HIS:O	1:G:849:LEU:HB3	2.09	0.52
1:G:761:ASN:ND2	1:G:791:ASP:HB2	2.24	0.52
1:G:180:THR:CG2	1:G:220:LEU:HD21	2.39	0.52
1:C:491:LEU:HD12	1:C:492:TYR:N	2.24	0.52
1:A:18:PHE:CZ	1:A:32:VAL:HG21	2.45	0.52
1:E:833:PRO:HA	1:E:840:TRP:CB	2.40	0.52
1:G:595:ARG:HB2	1:G:597:ARG:HH12	1.75	0.52
1:E:333:ALA:HA	1:E:352:GLY:H	1.74	0.52
1:A:917:LYS:HE3	1:A:1077:VAL:CG2	2.39	0.52
1:E:600:LEU:HD12	1:E:600:LEU:O	2.09	0.52
1:E:119:LEU:HD21	1:E:124:GLN:NE2	2.25	0.52
1:A:103:LEU:HD11	2:B:155:LEU:HD13	1.91	0.52
1:A:1063:LEU:HD12	1:A:1064:PRO:HA	1.90	0.52
2:D:25:GLN:HB2	2:D:445:CYS:CA	2.39	0.52
1:C:513:ASN:CA	1:C:599:VAL:HG21	2.39	0.52
1:A:491:LEU:HD12	1:A:491:LEU:C	2.30	0.52
2:F:591:GLN:HG2	2:F:592:GLU:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:532:GLY:HA3	1:G:565:PHE:HD2	1.75	0.52
2:F:644:ASP:HB3	2:F:650:VAL:HG23	1.92	0.52
2:D:135:LEU:HD11	2:D:139:THR:HB	1.90	0.52
2:B:364:CYS:HB2	2:B:368:VAL:HB	1.92	0.52
1:E:917:LYS:HE3	1:E:1077:VAL:CG2	2.39	0.52
1:A:600:LEU:O	1:A:600:LEU:HD12	2.09	0.52
2:F:155:LEU:H	2:F:160:THR:CG2	2.23	0.52
2:D:155:LEU:H	2:D:160:THR:CG2	2.23	0.52
1:C:491:LEU:HD12	1:C:491:LEU:C	2.30	0.52
1:G:873:ASP:C	1:G:901:VAL:HG12	2.30	0.52
1:E:531:ARG:HA	1:E:563:GLN:O	2.09	0.52
2:F:638:ARG:HB2	2:F:654:LEU:O	2.10	0.52
2:H:155:LEU:H	2:H:160:THR:CG2	2.23	0.52
2:H:532:ARG:CD	2:H:554:GLU:HG3	2.40	0.52
2:B:155:LEU:H	2:B:160:THR:CG2	2.23	0.52
1:E:1063:LEU:HD12	1:E:1064:PRO:HA	1.90	0.52
2:D:211:PRO:HB2	2:D:246:HIS:CE1	2.45	0.52
1:C:595:ARG:HB2	1:C:597:ARG:HH12	1.75	0.52
2:D:23:TRP:CH2	2:D:447:ILE:HD13	2.45	0.52
2:B:27:LEU:CD2	2:B:446:GLY:HA2	2.39	0.52
1:C:117:GLN:CB	1:C:121:VAL:HG21	2.40	0.52
1:E:815:GLU:HB3	1:E:819:GLN:NE2	2.25	0.52
1:G:18:PHE:CZ	1:G:32:VAL:HG21	2.45	0.52
1:C:525:PRO:HA	1:C:532:GLY:HA2	1.92	0.52
1:C:25:TYR:CE1	1:C:86:LEU:HB2	2.44	0.52
2:D:522:TYR:CD1	2:D:552:GLN:HA	2.44	0.52
1:G:25:TYR:CD1	1:G:86:LEU:HB2	2.44	0.52
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.91	0.52
2:F:83:LEU:HD13	2:F:85:LEU:HB2	1.92	0.52
1:G:99:ARG:NH1	1:G:318:GLU:CD	2.63	0.52
1:E:71:MET:HG3	1:E:90:GLY:HA3	1.92	0.52
1:C:416:ILE:HD11	1:C:485:TRP:CZ2	2.45	0.52
1:A:525:PRO:HA	1:A:532:GLY:HA2	1.92	0.52
1:A:532:GLY:HA3	1:A:565:PHE:HD2	1.75	0.52
1:C:333:ALA:HA	1:C:352:GLY:H	1.74	0.52
1:G:333:ALA:HA	1:G:352:GLY:H	1.74	0.52
2:D:644:ASP:HB3	2:D:650:VAL:HG23	1.92	0.52
1:G:917:LYS:HE3	1:G:1077:VAL:CG2	2.39	0.52
7:G:3374:NAG:O3	7:G:3375:MAN:H2	2.10	0.52
1:A:755:ASP:O	1:A:756:HIS:HB3	2.10	0.51
2:B:211:PRO:HB2	2:B:246:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:SER:HB2	2:B:471:LEU:CG	2.41	0.51
1:C:71:MET:HG3	1:C:90:GLY:HA3	1.92	0.51
1:A:528:GLU:HB2	1:A:531:ARG:HB2	1.92	0.51
1:E:528:GLU:HB2	1:E:531:ARG:HB2	1.92	0.51
1:G:25:TYR:CE1	1:G:86:LEU:HB2	2.44	0.51
2:B:121:LEU:O	2:B:125:LYS:HB3	2.09	0.51
1:C:685:ARG:NH2	1:G:685:ARG:CZ	2.73	0.51
2:D:546:PHE:CE2	2:D:554:GLU:HG2	2.44	0.51
1:G:71:MET:HG3	1:G:90:GLY:HA3	1.92	0.51
1:E:430:VAL:HG21	1:E:487:CYS:SG	2.50	0.51
1:E:766:PHE:CZ	1:E:877:LEU:HD12	2.46	0.51
1:G:766:PHE:CZ	1:G:877:LEU:HD12	2.45	0.51
2:D:638:ARG:HB2	2:D:654:LEU:O	2.10	0.51
1:E:491:LEU:HD12	1:E:491:LEU:C	2.30	0.51
1:G:491:LEU:HD11	1:G:545:ILE:CG1	2.39	0.51
1:C:848:HIS:O	1:C:849:LEU:HB3	2.10	0.51
1:A:873:ASP:C	1:A:901:VAL:HG12	2.30	0.51
1:G:822:LEU:CG	1:G:823:ARG:H	2.22	0.51
1:E:506:LEU:HA	1:E:569:LEU:HD11	1.90	0.51
1:G:430:VAL:HG21	1:G:487:CYS:SG	2.51	0.51
1:C:430:VAL:HG21	1:C:487:CYS:SG	2.50	0.51
2:F:25:GLN:OE1	2:F:427:CYS:SG	2.68	0.51
1:E:25:TYR:CD1	1:E:86:LEU:HB2	2.44	0.51
2:H:83:LEU:HD13	2:H:85:LEU:HB2	1.93	0.51
1:G:394:LEU:HD23	1:G:395:TRP:N	2.26	0.51
2:F:211:PRO:HB2	2:F:246:HIS:CE1	2.45	0.51
1:G:469:ARG:NH2	2:H:287:HIS:HB2	2.26	0.51
1:E:117:GLN:CB	1:E:121:VAL:HG21	2.41	0.51
1:E:18:PHE:CZ	1:E:32:VAL:HG21	2.45	0.51
1:E:532:GLY:HA3	1:E:565:PHE:HD2	1.75	0.51
1:C:671:ALA:O	1:C:672:THR:HG23	2.11	0.51
1:G:254:ILE:N	1:G:255:PRO:CD	2.73	0.51
1:E:852:ARG:HD2	2:F:480:ASN:CG	2.30	0.51
2:H:638:ARG:HB2	2:H:654:LEU:O	2.11	0.51
1:A:491:LEU:HD11	1:A:545:ILE:CG1	2.39	0.51
1:G:117:GLN:CB	1:G:121:VAL:HG21	2.40	0.51
1:E:822:LEU:CG	1:E:823:ARG:H	2.24	0.51
1:G:986:PRO:HB3	1:G:987:PRO:HD2	1.92	0.51
1:G:416:ILE:HD11	1:G:485:TRP:CZ2	2.45	0.51
1:A:25:TYR:CE1	1:A:86:LEU:HB2	2.45	0.51
1:G:133:ILE:O	1:G:169:PHE:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LEU:HD23	1:C:395:TRP:N	2.26	0.51
2:F:364:CYS:HB2	2:F:368:VAL:HB	1.92	0.51
2:H:343:SER:HA	2:H:381:VAL:O	2.11	0.51
2:B:363:PHE:CE2	2:B:369:THR:HG23	2.46	0.51
1:G:119:LEU:HD21	1:G:124:GLN:NE2	2.25	0.51
2:F:466:ARG:O	2:F:467:SER:HB3	2.11	0.51
1:A:117:GLN:CB	1:A:121:VAL:HG21	2.40	0.51
1:G:815:GLU:HB3	1:G:819:GLN:NE2	2.26	0.51
1:G:553:ILE:HG23	1:G:557:GLN:HG3	1.92	0.51
2:H:364:CYS:HB2	2:H:368:VAL:HB	1.93	0.51
1:A:848:HIS:O	1:A:849:LEU:HB3	2.10	0.51
1:A:394:LEU:HD23	1:A:395:TRP:N	2.26	0.51
1:E:755:ASP:O	1:E:756:HIS:HB3	2.10	0.51
1:E:383:ASP:OD2	2:F:211:PRO:HD3	2.11	0.51
1:C:873:ASP:C	1:C:901:VAL:HG12	2.31	0.51
2:D:468:SER:HB2	2:D:471:LEU:CG	2.40	0.51
2:D:587:LEU:N	2:D:587:LEU:HD12	2.26	0.51
1:G:833:PRO:HA	1:G:840:TRP:CB	2.40	0.51
1:G:77:LEU:HD23	1:G:88:ALA:HA	1.93	0.51
1:E:907:THR:HG21	1:E:1053:ILE:HD13	1.93	0.51
2:F:347:LEU:HD22	2:F:389:PHE:CG	2.46	0.51
2:D:466:ARG:O	2:D:467:SER:HB3	2.11	0.51
2:B:83:LEU:HD13	2:B:85:LEU:HB2	1.93	0.51
1:C:553:ILE:HG23	1:C:557:GLN:HG3	1.93	0.51
2:D:364:CYS:HB2	2:D:368:VAL:HB	1.93	0.51
1:E:698:LEU:N	1:E:698:LEU:HD12	2.26	0.51
1:E:491:LEU:HD12	1:E:492:TYR:N	2.25	0.51
1:A:465:TYR:HB3	1:A:469:ARG:HA	1.91	0.51
2:H:468:SER:HB2	2:H:471:LEU:CG	2.41	0.51
1:E:416:ILE:HD11	1:E:485:TRP:CZ2	2.45	0.51
2:H:466:ARG:O	2:H:467:SER:HB3	2.11	0.51
1:C:766:PHE:CZ	1:C:877:LEU:HD12	2.46	0.51
1:E:394:LEU:HD23	1:E:395:TRP:N	2.26	0.51
2:F:363:PHE:CE2	2:F:369:THR:HG23	2.46	0.51
1:G:994:HIS:CG	1:G:1005:ILE:HD11	2.45	0.51
2:B:644:ASP:HB3	2:B:650:VAL:HG23	1.92	0.51
2:H:211:PRO:HB2	2:H:246:HIS:CE1	2.45	0.51
1:C:465:TYR:CG	1:C:469:ARG:HG3	2.46	0.51
2:B:347:LEU:HD22	2:B:389:PHE:CG	2.45	0.51
2:D:347:LEU:HD22	2:D:389:PHE:CG	2.46	0.51
1:A:77:LEU:HD23	1:A:88:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:TYR:CE1	1:E:86:LEU:HB2	2.45	0.51
2:H:508:TYR:HE2	2:H:516:THR:HG23	1.75	0.51
2:B:638:ARG:HB2	2:B:654:LEU:O	2.11	0.51
1:G:698:LEU:HD12	1:G:698:LEU:N	2.26	0.51
1:E:465:TYR:CG	1:E:469:ARG:HG3	2.46	0.51
1:C:491:LEU:HD11	1:C:545:ILE:CG1	2.39	0.51
1:G:1044:LYS:HA	1:G:1079:GLU:HB2	1.93	0.51
1:G:385:TYR:CE1	2:H:253:LEU:HD11	2.46	0.51
1:C:528:GLU:HB2	1:C:531:ARG:HB2	1.93	0.51
1:A:766:PHE:CZ	1:A:877:LEU:HD12	2.46	0.51
1:G:848:HIS:O	1:G:848:HIS:ND1	2.44	0.51
2:D:83:LEU:HD13	2:D:85:LEU:HB2	1.92	0.51
1:G:499:TRP:CZ2	2:H:284:GLN:HG3	2.46	0.51
1:A:1044:LYS:HA	1:A:1079:GLU:HB2	1.93	0.50
1:A:833:PRO:HA	1:A:840:TRP:CB	2.40	0.50
1:C:907:THR:HG21	1:C:1053:ILE:HD13	1.93	0.50
2:H:212:GLU:HG2	2:H:243:ASP:CB	2.41	0.50
2:F:468:SER:HB2	2:F:471:LEU:CG	2.41	0.50
1:E:553:ILE:HG23	1:E:557:GLN:HG3	1.92	0.50
1:C:119:LEU:HD21	1:C:124:GLN:NE2	2.25	0.50
2:D:154:VAL:HG23	2:D:160:THR:HG21	1.94	0.50
2:F:289:LEU:HD23	2:F:315:ILE:HD11	1.91	0.50
2:H:587:LEU:HD12	2:H:587:LEU:N	2.26	0.50
1:A:89:CYS:O	1:A:91:PRO:HD3	2.11	0.50
1:G:528:GLU:HB2	1:G:531:ARG:HB2	1.93	0.50
1:A:634:ASN:ND2	1:E:690:LYS:HG3	2.26	0.50
2:D:432:ARG:O	2:D:433:ASP:HB2	2.11	0.50
2:H:644:ASP:HB3	2:H:650:VAL:HG23	1.92	0.50
2:B:154:VAL:HG23	2:B:160:THR:HG21	1.94	0.50
1:C:18:PHE:CZ	1:C:32:VAL:HG21	2.45	0.50
1:E:385:TYR:CE1	2:F:253:LEU:HD11	2.46	0.50
1:A:430:VAL:HG21	1:A:487:CYS:SG	2.50	0.50
1:E:77:LEU:HD23	1:E:88:ALA:HA	1.93	0.50
1:E:436:GLY:HA3	2:F:282:VAL:CB	2.41	0.50
1:C:77:LEU:HD23	1:C:88:ALA:HA	1.93	0.50
1:C:31:VAL:HG21	1:C:86:LEU:HD13	1.94	0.50
1:C:692:HIS:ND1	1:G:694:GLU:HA	2.27	0.50
2:H:363:PHE:CE2	2:H:369:THR:HG23	2.46	0.50
1:G:674:GLN:HB2	1:G:699:LEU:HD11	1.94	0.50
1:E:848:HIS:ND1	1:E:848:HIS:O	2.45	0.50
1:E:681:LEU:HD12	1:E:682:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:ARG:O	2:B:467:SER:HB3	2.11	0.50
2:H:10:SER:HB3	2:H:449:ARG:CZ	2.41	0.50
1:E:436:GLY:HA3	2:F:282:VAL:HB	1.93	0.50
1:E:525:PRO:HA	1:E:532:GLY:HA2	1.92	0.50
2:D:146:PHE:HB2	2:D:195:PHE:CZ	2.47	0.50
1:G:801:THR:HG22	1:G:843:SER:CB	2.41	0.50
1:G:715:LEU:O	1:G:715:LEU:HD12	2.12	0.50
1:A:681:LEU:C	1:A:681:LEU:HD12	2.32	0.50
1:E:595:ARG:HB2	1:E:597:ARG:HH12	1.77	0.50
1:G:987:PRO:O	1:G:988:ALA:HB3	2.11	0.50
1:C:446:VAL:HG12	1:C:456:LEU:CD1	2.42	0.50
1:C:532:GLY:HA3	1:C:565:PHE:HD2	1.75	0.50
1:C:764:ILE:CD1	1:C:800:ILE:HD11	2.41	0.50
2:D:77:SER:HA	2:D:78:PRO:C	2.32	0.50
1:C:698:LEU:N	1:C:698:LEU:HD12	2.25	0.50
1:C:89:CYS:O	1:C:91:PRO:HD3	2.12	0.50
1:G:656:VAL:HG21	1:G:687:LEU:HD11	1.94	0.50
1:A:820:GLY:N	1:A:822:LEU:HB3	2.26	0.50
1:E:986:PRO:HB3	1:E:987:PRO:HD2	1.92	0.50
1:E:908:VAL:O	1:E:938:VAL:HG23	2.12	0.50
2:B:505:LYS:HA	2:B:517:ILE:HG21	1.92	0.50
2:F:222:ALA:CB	2:F:294:ILE:HD12	2.42	0.50
1:A:920:ASN:OD1	1:A:1080:LYS:HE2	2.12	0.50
1:E:373:ASN:OD1	4:E:3373:NAG:C2	2.58	0.50
1:E:89:CYS:O	1:E:91:PRO:HD3	2.12	0.50
1:G:89:CYS:O	1:G:91:PRO:HD3	2.12	0.50
2:B:587:LEU:HD12	2:B:587:LEU:N	2.26	0.50
1:A:907:THR:HG21	1:A:1053:ILE:HD13	1.93	0.50
1:G:4:ASP:CG	1:G:597:ARG:NH2	2.65	0.50
1:G:525:PRO:HA	1:G:532:GLY:HA2	1.92	0.50
1:A:553:ILE:HG23	1:A:557:GLN:HG3	1.93	0.50
2:B:462:GLN:HG2	2:B:463:THR:N	2.26	0.50
1:A:597:ARG:HB3	1:A:731:ARG:O	2.12	0.50
2:F:587:LEU:HD12	2:F:587:LEU:N	2.27	0.50
1:A:656:VAL:HG21	1:A:687:LEU:HD11	1.94	0.50
2:D:212:GLU:HG2	2:D:243:ASP:CB	2.42	0.50
1:C:685:ARG:CZ	1:G:685:ARG:NH2	2.75	0.50
2:B:222:ALA:CB	2:B:294:ILE:HD12	2.42	0.50
2:B:546:PHE:HA	2:B:554:GLU:O	2.12	0.50
1:A:465:TYR:CG	1:A:469:ARG:HG3	2.46	0.50
1:G:465:TYR:CG	1:G:469:ARG:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:873:ASP:C	1:E:901:VAL:HG12	2.32	0.50
1:G:569:LEU:HD12	1:G:569:LEU:O	2.12	0.50
1:C:908:VAL:O	1:C:938:VAL:HG23	2.11	0.50
1:C:461:ALA:N	1:C:462:PRO:HD3	2.27	0.50
2:D:363:PHE:CE2	2:D:369:THR:HG23	2.46	0.50
1:E:461:ALA:N	1:E:462:PRO:HD3	2.27	0.50
1:G:267:ILE:HG21	1:G:303:LEU:HD11	1.93	0.50
2:F:77:SER:HA	2:F:78:PRO:C	2.32	0.50
1:A:119:LEU:HD21	1:A:124:GLN:NE2	2.25	0.49
2:H:546:PHE:CE2	2:H:554:GLU:HG2	2.47	0.49
1:E:1044:LYS:HA	1:E:1079:GLU:HB2	1.93	0.49
2:F:212:GLU:HG2	2:F:243:ASP:CB	2.42	0.49
2:H:77:SER:HA	2:H:78:PRO:C	2.32	0.49
2:D:222:ALA:CB	2:D:294:ILE:HD12	2.42	0.49
1:C:886:ASN:O	1:C:888:PRO:HD3	2.12	0.49
2:B:340:LYS:HA	2:B:343:SER:HB2	1.92	0.49
1:G:70:ASN:HB3	1:G:94:HIS:ND1	2.27	0.49
1:C:920:ASN:OD1	1:C:1080:LYS:HE2	2.13	0.49
1:E:674:GLN:HB2	1:E:699:LEU:HD11	1.94	0.49
1:G:4:ASP:HB2	1:G:597:ARG:CZ	2.42	0.49
1:G:886:ASN:O	1:G:888:PRO:HD3	2.12	0.49
1:A:886:ASN:O	1:A:888:PRO:HD3	2.12	0.49
2:D:75:GLN:O	2:D:97:PHE:CD1	2.65	0.49
1:A:461:ALA:N	1:A:462:PRO:HD3	2.27	0.49
2:H:222:ALA:CB	2:H:294:ILE:HD12	2.42	0.49
1:G:908:VAL:O	1:G:938:VAL:HG23	2.12	0.49
1:G:755:ASP:O	1:G:756:HIS:HB3	2.12	0.49
1:A:513:ASN:HA	1:A:599:VAL:HG22	1.92	0.49
1:G:174:PHE:O	1:G:174:PHE:CG	2.65	0.49
1:A:908:VAL:O	1:A:938:VAL:HG23	2.12	0.49
1:A:595:ARG:HB2	1:A:597:ARG:HH12	1.77	0.49
1:C:848:HIS:O	1:C:848:HIS:ND1	2.45	0.49
1:A:31:VAL:HG21	1:A:86:LEU:HD13	1.95	0.49
1:A:848:HIS:ND1	1:A:848:HIS:O	2.45	0.49
2:F:33:GLY:O	2:F:474:SER:CB	2.59	0.49
1:G:461:ALA:N	1:G:462:PRO:HD3	2.27	0.49
1:A:698:LEU:HD12	1:A:698:LEU:N	2.26	0.49
1:E:513:ASN:HA	1:E:599:VAL:HG21	1.93	0.49
1:G:325:SER:O	1:G:326:SER:HB3	2.13	0.49
1:A:666:ARG:HB3	2:B:498:HIS:NE2	2.28	0.49
1:G:446:VAL:HG12	1:G:456:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:VAL:HG12	1:A:456:LEU:CD1	2.43	0.49
2:D:110:LEU:HD11	2:D:237:LEU:HD23	1.95	0.49
1:A:780:LEU:O	1:A:865:VAL:HG12	2.12	0.49
2:H:146:PHE:HB2	2:H:195:PHE:CZ	2.47	0.49
1:A:801:THR:HG22	1:A:843:SER:CB	2.42	0.49
1:A:893:THR:HG23	1:A:893:THR:O	2.12	0.49
1:A:715:LEU:HD12	1:A:715:LEU:O	2.12	0.49
1:A:674:GLN:HB2	1:A:699:LEU:HD11	1.95	0.49
2:D:39:ARG:NE	2:D:447:ILE:HG23	2.28	0.49
1:A:797:GLY:HA3	1:A:884:GLU:HB2	1.95	0.49
1:A:362:LEU:C	1:A:362:LEU:HD23	2.33	0.49
2:B:212:GLU:HG2	2:B:243:ASP:CB	2.42	0.49
2:D:135:LEU:CD1	2:D:139:THR:HB	2.43	0.49
1:G:938:VAL:HG12	1:G:1024:LEU:O	2.13	0.49
1:E:886:ASN:O	1:E:888:PRO:HD3	2.12	0.49
2:F:132:LEU:HA	2:F:135:LEU:HB3	1.95	0.49
1:C:1063:LEU:HG	1:C:1064:PRO:HD3	1.95	0.49
1:G:920:ASN:OD1	1:G:1080:LYS:HE2	2.13	0.49
1:E:446:VAL:HG12	1:E:456:LEU:CD1	2.42	0.49
2:H:105:ILE:HG21	2:H:135:LEU:HD13	1.95	0.49
1:C:938:VAL:HG12	1:C:1024:LEU:O	2.12	0.49
2:H:186:LEU:HD13	2:H:195:PHE:CD1	2.48	0.49
2:F:105:ILE:HG21	2:F:135:LEU:HD13	1.95	0.49
1:E:801:THR:HG22	1:E:843:SER:CB	2.43	0.49
1:C:801:THR:HG22	1:C:843:SER:CB	2.42	0.49
2:B:75:GLN:O	2:B:97:PHE:CD1	2.66	0.49
2:F:186:LEU:HD13	2:F:195:PHE:CD1	2.48	0.49
2:F:251:GLY:HA3	2:F:278:ASP:OD1	2.13	0.49
1:C:362:LEU:C	1:C:362:LEU:HD23	2.33	0.49
2:F:75:GLN:O	2:F:97:PHE:CD1	2.66	0.49
1:E:827:LEU:CD1	1:E:829:CYS:SG	3.01	0.49
1:C:1058:SER:O	1:C:1059:VAL:HB	2.13	0.49
1:C:827:LEU:CD1	1:C:829:CYS:SG	3.00	0.49
1:C:681:LEU:HD12	1:C:681:LEU:C	2.33	0.49
1:C:1044:LYS:HA	1:C:1079:GLU:HB2	1.93	0.49
1:A:609:ILE:CB	1:A:610:PRO:HD3	2.43	0.49
2:F:146:PHE:HB2	2:F:195:PHE:CZ	2.47	0.49
1:G:776:VAL:HG12	1:G:867:PRO:O	2.13	0.49
2:H:154:VAL:HG23	2:H:160:THR:HG21	1.94	0.49
1:A:484:ARG:HH11	2:B:594:PRO:HG2	1.77	0.49
1:A:771:LEU:O	1:C:789:TRP:CZ2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:681:LEU:HD12	1:G:681:LEU:C	2.32	0.49
1:A:469:ARG:NH2	2:B:287:HIS:HB2	2.27	0.49
1:G:137:ILE:HB	1:G:151:MET:HE1	1.95	0.49
1:A:986:PRO:CB	1:A:987:PRO:CD	2.90	0.49
1:E:47:LEU:HB2	1:E:60:ILE:CG2	2.43	0.49
1:C:47:LEU:HB2	1:C:60:ILE:CG2	2.43	0.49
2:D:186:LEU:HD13	2:D:195:PHE:CD1	2.48	0.49
1:E:1058:SER:O	1:E:1059:VAL:HB	2.13	0.49
1:E:70:ASN:HB3	1:E:94:HIS:ND1	2.28	0.48
1:E:920:ASN:OD1	1:E:1080:LYS:HE2	2.13	0.48
1:E:31:VAL:HG21	1:E:86:LEU:HD13	1.94	0.48
2:B:110:LEU:HD11	2:B:237:LEU:HD23	1.95	0.48
2:H:110:LEU:HD11	2:H:237:LEU:HD23	1.95	0.48
2:B:146:PHE:HB2	2:B:195:PHE:CZ	2.47	0.48
1:A:764:ILE:CD1	1:A:800:ILE:HD11	2.43	0.48
1:G:827:LEU:CD1	1:G:829:CYS:SG	3.01	0.48
1:A:827:LEU:CD1	1:A:829:CYS:SG	3.01	0.48
1:A:70:ASN:HB3	1:A:94:HIS:ND1	2.28	0.48
1:A:657:THR:HG23	1:A:720:VAL:HB	1.95	0.48
2:D:251:GLY:HA3	2:D:278:ASP:OD1	2.13	0.48
1:E:385:TYR:CZ	2:F:253:LEU:HD11	2.48	0.48
1:G:907:THR:HG21	1:G:1053:ILE:HD13	1.93	0.48
1:G:780:LEU:O	1:G:865:VAL:HG12	2.13	0.48
1:A:411:THR:HG22	1:A:435:ILE:HA	1.96	0.48
1:E:780:LEU:O	1:E:865:VAL:HG12	2.14	0.48
2:B:656:GLN:HG2	2:B:657:GLN:N	2.28	0.48
1:E:1063:LEU:HG	1:E:1064:PRO:HD3	1.95	0.48
1:G:657:THR:HG23	1:G:720:VAL:HB	1.95	0.48
1:E:797:GLY:HA3	1:E:884:GLU:HB2	1.94	0.48
1:E:986:PRO:HG3	1:E:1003:CYS:O	2.13	0.48
1:C:986:PRO:HB3	1:C:987:PRO:HD2	1.95	0.48
1:A:47:LEU:HB2	1:A:60:ILE:CG2	2.43	0.48
2:F:121:LEU:HD23	2:F:121:LEU:O	2.14	0.48
2:H:135:LEU:CD1	2:H:139:THR:HB	2.43	0.48
2:H:132:LEU:HA	2:H:135:LEU:HB3	1.95	0.48
2:B:186:LEU:HD13	2:B:195:PHE:CD1	2.48	0.48
2:B:77:SER:HA	2:B:78:PRO:C	2.32	0.48
2:F:154:VAL:HG23	2:F:160:THR:HG21	1.93	0.48
2:H:532:ARG:HD3	2:H:554:GLU:CG	2.43	0.48
1:E:657:THR:HG23	1:E:720:VAL:HB	1.94	0.48
1:E:362:LEU:HD23	1:E:362:LEU:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:PRO:HG2	1:C:489:ALA:HB2	1.96	0.48
1:E:569:LEU:HD12	1:E:569:LEU:O	2.14	0.48
1:A:576:THR:HG23	1:A:582:ASP:OD2	2.14	0.48
1:G:47:LEU:HB2	1:G:60:ILE:CG2	2.43	0.48
1:G:31:VAL:HG21	1:G:86:LEU:HD13	1.95	0.48
2:H:75:GLN:O	2:H:97:PHE:CD1	2.66	0.48
2:D:656:GLN:HG2	2:D:657:GLN:N	2.28	0.48
1:A:894:THR:O	1:C:874:ARG:NH2	2.47	0.48
2:F:656:GLN:HG2	2:F:657:GLN:N	2.28	0.48
1:A:776:VAL:HG12	1:A:867:PRO:O	2.13	0.48
2:D:270:LEU:HD23	2:D:271:TYR:O	2.14	0.48
1:E:715:LEU:HD12	1:E:715:LEU:O	2.13	0.48
1:C:70:ASN:HB3	1:C:94:HIS:ND1	2.28	0.48
1:G:362:LEU:HD23	1:G:362:LEU:C	2.33	0.48
1:C:986:PRO:HG3	1:C:1003:CYS:O	2.14	0.48
1:E:470:GLY:HA2	1:E:497:HIS:O	2.13	0.48
1:C:657:THR:HG23	1:C:720:VAL:HB	1.95	0.48
1:G:797:GLY:HA3	1:G:884:GLU:HB2	1.95	0.48
1:C:797:GLY:HA3	1:C:884:GLU:HB2	1.95	0.48
1:E:656:VAL:HG21	1:E:687:LEU:HD11	1.95	0.48
1:G:477:PRO:HG2	1:G:489:ALA:HB2	1.96	0.48
1:G:806:ALA:HA	1:G:840:TRP:NE1	2.29	0.48
1:E:1009:LEU:HD22	1:E:1011:PHE:CE1	2.49	0.48
2:B:105:ILE:HG21	2:B:135:LEU:HD13	1.95	0.48
1:G:676:THR:HG23	1:G:678:ASN:H	1.79	0.48
1:E:119:LEU:N	1:E:120:PRO:CA	2.60	0.48
1:C:674:GLN:HB2	1:C:699:LEU:HD11	1.95	0.48
2:D:39:ARG:CD	2:D:447:ILE:HG23	2.42	0.48
1:C:117:GLN:HB2	1:C:121:VAL:HG21	1.95	0.48
1:G:656:VAL:HG13	1:G:718:THR:O	2.14	0.48
2:B:251:GLY:HA3	2:B:278:ASP:OD1	2.14	0.48
1:E:477:PRO:HG2	1:E:489:ALA:HB2	1.96	0.48
1:E:986:PRO:CB	1:E:987:PRO:CD	2.90	0.48
1:C:25:TYR:CG	1:C:26:ALA:N	2.82	0.48
2:D:105:ILE:HG21	2:D:135:LEU:HD13	1.95	0.48
2:D:105:ILE:HG12	2:D:106:ASP:N	2.29	0.48
1:A:1009:LEU:HD22	1:A:1011:PHE:CE1	2.48	0.48
1:E:938:VAL:HG12	1:E:1024:LEU:O	2.13	0.48
2:F:105:ILE:HG12	2:F:106:ASP:N	2.29	0.48
1:E:827:LEU:HD13	1:E:829:CYS:SG	2.54	0.48
2:B:105:ILE:HG12	2:B:106:ASP:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:270:LEU:HD23	2:H:271:TYR:O	2.13	0.48
1:A:1063:LEU:HG	1:A:1064:PRO:HD3	1.96	0.48
1:A:4:ASP:CG	1:A:597:ARG:NH2	2.67	0.48
2:F:546:PHE:HD2	2:F:554:GLU:HG3	1.78	0.48
1:C:656:VAL:HG21	1:C:687:LEU:HD11	1.95	0.48
1:A:575:LEU:HD12	1:A:576:THR:CG2	2.44	0.48
1:C:986:PRO:CB	1:C:987:PRO:CD	2.92	0.48
2:H:105:ILE:HG12	2:H:106:ASP:N	2.28	0.48
1:A:880:ASN:OD1	1:A:894:THR:HG22	2.14	0.48
2:D:43:ARG:HB3	2:D:44:PRO:HD3	1.96	0.48
1:A:470:GLY:HA2	1:A:497:HIS:O	2.14	0.48
2:H:659:GLY:O	2:H:662:ARG:HG2	2.14	0.48
2:F:532:ARG:HD3	2:F:554:GLU:OE1	2.14	0.48
1:E:117:GLN:HB2	1:E:121:VAL:HG21	1.95	0.48
1:A:569:LEU:HD12	1:A:569:LEU:O	2.13	0.48
1:C:569:LEU:HD12	1:C:569:LEU:O	2.14	0.48
1:A:665:GLY:HA3	2:B:498:HIS:HB3	1.96	0.48
1:A:477:PRO:HG2	1:A:489:ALA:HB2	1.96	0.48
1:C:565:PHE:HB2	1:C:587:ALA:CB	2.44	0.48
1:C:1009:LEU:HD22	1:C:1011:PHE:CE1	2.49	0.48
2:D:363:PHE:HB2	2:D:388:THR:HB	1.96	0.48
1:E:764:ILE:CD1	1:E:800:ILE:HD11	2.43	0.48
2:F:43:ARG:HB3	2:F:44:PRO:HD3	1.96	0.48
1:E:716:ASN:OD1	1:E:716:ASN:C	2.52	0.48
1:C:715:LEU:HD12	1:C:715:LEU:O	2.13	0.48
1:C:806:ALA:HA	1:C:840:TRP:NE1	2.29	0.48
1:G:986:PRO:CB	1:G:987:PRO:CD	2.91	0.48
1:G:575:LEU:HD12	1:G:576:THR:CG2	2.44	0.48
2:D:222:ALA:HB2	2:D:294:ILE:CD1	2.44	0.48
1:G:908:VAL:HG13	1:G:1069:PHE:HB3	1.96	0.48
1:C:827:LEU:HD13	1:C:829:CYS:SG	2.53	0.48
2:B:132:LEU:HA	2:B:135:LEU:HB3	1.95	0.48
2:F:461:CYS:SG	2:F:466:ARG:HD2	2.54	0.47
1:A:731:ARG:NH2	1:A:733:MET:SD	2.87	0.47
1:G:121:VAL:CG1	1:G:121:VAL:O	2.62	0.47
1:G:739:GLN:HB2	1:G:742:PHE:CE1	2.49	0.47
1:G:71:MET:CG	1:G:90:GLY:HA3	2.44	0.47
1:G:986:PRO:HG3	1:G:1003:CYS:O	2.13	0.47
1:G:478:LEU:HA	1:G:485:TRP:HE1	1.79	0.47
1:A:25:TYR:CG	1:A:26:ALA:N	2.82	0.47
1:E:86:LEU:HD23	1:E:87:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LEU:HD11	2:B:139:THR:HB	1.95	0.47
1:A:110:LEU:HD12	1:A:110:LEU:N	2.29	0.47
1:A:4:ASP:HB2	1:A:597:ARG:CZ	2.44	0.47
2:B:27:LEU:CG	2:B:446:GLY:HA2	2.43	0.47
1:A:739:GLN:HB2	1:A:742:PHE:CE1	2.49	0.47
1:E:739:GLN:HB2	1:E:742:PHE:CE1	2.50	0.47
1:G:961:GLU:HG2	1:G:1036:TRP:HA	1.96	0.47
1:A:73:LEU:HA	1:A:90:GLY:HA2	1.96	0.47
1:G:565:PHE:HB2	1:G:587:ALA:CB	2.44	0.47
1:G:1009:LEU:HD22	1:G:1011:PHE:CE1	2.49	0.47
2:D:132:LEU:HA	2:D:135:LEU:HB3	1.95	0.47
1:G:25:TYR:CG	1:G:26:ALA:N	2.82	0.47
2:F:222:ALA:HB2	2:F:294:ILE:CD1	2.45	0.47
2:F:110:LEU:HD11	2:F:237:LEU:HD23	1.95	0.47
1:A:827:LEU:HD13	1:A:829:CYS:SG	2.54	0.47
2:F:270:LEU:HD23	2:F:271:TYR:O	2.14	0.47
1:E:650:ARG:HD3	1:E:729:ASN:HB3	1.96	0.47
1:G:741:TYR:CD2	2:H:502:VAL:HG22	2.49	0.47
1:G:470:GLY:HA2	1:G:497:HIS:O	2.14	0.47
1:E:893:THR:O	1:E:893:THR:HG23	2.13	0.47
1:G:273:PHE:CB	1:G:296:LYS:HD2	2.42	0.47
1:E:73:LEU:HA	1:E:90:GLY:HA2	1.96	0.47
2:H:251:GLY:HA3	2:H:278:ASP:OD1	2.14	0.47
1:E:444:CYS:CB	1:E:506:LEU:CD1	2.93	0.47
2:D:340:LYS:HA	2:D:343:SER:HB2	1.96	0.47
1:A:986:PRO:HB3	1:A:987:PRO:HD2	1.94	0.47
1:A:831:SER:HB3	1:A:842:THR:HG22	1.95	0.47
1:C:478:LEU:HA	1:C:485:TRP:HE1	1.80	0.47
2:D:616:PRO:HB3	2:D:621:CYS:SG	2.54	0.47
1:A:876:LEU:HB3	1:A:898:GLU:HG3	1.96	0.47
1:A:565:PHE:HB2	1:A:587:ALA:CB	2.44	0.47
1:E:905:VAL:CG1	1:E:946:LEU:HD21	2.44	0.47
1:A:905:VAL:CG1	1:A:946:LEU:HD21	2.44	0.47
1:C:905:VAL:HG21	1:C:946:LEU:HD22	1.97	0.47
2:H:121:LEU:O	2:H:121:LEU:HD23	2.14	0.47
2:F:630:LEU:HD12	2:F:665:ILE:HB	1.97	0.47
1:E:908:VAL:HG13	1:E:1069:PHE:HB3	1.96	0.47
1:C:780:LEU:O	1:C:865:VAL:HG12	2.14	0.47
1:G:724:LEU:HD12	1:G:729:ASN:ND2	2.30	0.47
1:G:293:HIS:O	1:G:294:ILE:HG13	2.14	0.47
1:G:764:ILE:CD1	1:G:800:ILE:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:893:THR:HG23	1:C:893:THR:O	2.14	0.47
1:A:789:TRP:CZ2	1:C:771:LEU:O	2.66	0.47
1:G:117:GLN:HB2	1:G:121:VAL:HG21	1.95	0.47
1:E:961:GLU:HG2	1:E:1036:TRP:HA	1.96	0.47
2:D:11:CYS:O	2:D:15:ILE:HG12	2.14	0.47
1:E:478:LEU:HA	1:E:485:TRP:HE1	1.79	0.47
1:G:831:SER:HB3	1:G:842:THR:HG22	1.96	0.47
2:B:616:PRO:HB3	2:B:621:CYS:SG	2.54	0.47
1:G:86:LEU:HD23	1:G:87:LEU:N	2.30	0.47
2:H:630:LEU:HD12	2:H:665:ILE:HB	1.96	0.47
2:F:135:LEU:HD11	2:F:139:THR:HB	1.95	0.47
1:A:1058:SER:O	1:A:1059:VAL:HB	2.14	0.47
1:E:980:SER:HB3	1:E:1012:ARG:HB3	1.96	0.47
1:C:110:LEU:N	1:C:110:LEU:HD12	2.30	0.47
2:H:165:LEU:HD12	2:H:179:PRO:HG2	1.96	0.47
1:E:465:TYR:CG	1:E:469:ARG:CG	2.98	0.47
1:E:731:ARG:NH2	1:E:733:MET:SD	2.87	0.47
1:G:609:ILE:CB	1:G:610:PRO:HD3	2.42	0.47
1:C:609:ILE:CB	1:C:610:PRO:HD3	2.44	0.47
1:C:961:GLU:HG2	1:C:1036:TRP:HA	1.96	0.47
1:E:89:CYS:C	1:E:91:PRO:HD3	2.35	0.47
2:H:508:TYR:CE2	2:H:516:THR:HG23	2.50	0.47
2:B:222:ALA:HB2	2:B:294:ILE:CD1	2.44	0.47
1:A:975:PRO:HG2	1:A:977:LEU:HD11	1.97	0.47
1:C:676:THR:HG23	1:C:678:ASN:H	1.79	0.47
1:C:776:VAL:HG12	1:C:867:PRO:O	2.14	0.47
2:B:149:PHE:HA	2:B:181:ALA:O	2.14	0.47
1:A:657:THR:HG22	1:A:684:VAL:HG22	1.97	0.47
1:C:731:ARG:NH2	1:C:733:MET:SD	2.88	0.47
2:D:39:ARG:NE	2:D:447:ILE:HG22	2.30	0.47
2:H:39:ARG:CZ	2:H:447:ILE:HG23	2.43	0.47
1:C:71:MET:CG	1:C:90:GLY:HA3	2.44	0.47
1:G:822:LEU:HG	1:G:823:ARG:N	2.30	0.47
1:E:806:ALA:HA	1:E:840:TRP:NE1	2.30	0.47
1:C:575:LEU:HD12	1:C:576:THR:CG2	2.44	0.47
1:E:831:SER:HA	1:E:842:THR:HG22	1.97	0.47
1:E:905:VAL:HG21	1:E:946:LEU:HD22	1.96	0.47
2:D:522:TYR:CE1	2:D:552:GLN:HA	2.49	0.47
2:B:121:LEU:O	2:B:121:LEU:HD23	2.14	0.47
1:C:980:SER:HB3	1:C:1012:ARG:HB3	1.96	0.47
1:G:1058:SER:O	1:G:1059:VAL:HB	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:THR:HG22	1:C:435:ILE:HA	1.97	0.47
2:B:43:ARG:HB3	2:B:44:PRO:HD3	1.96	0.47
1:G:893:THR:O	1:G:893:THR:HG23	2.15	0.47
2:D:659:GLY:O	2:D:662:ARG:HG2	2.15	0.47
1:C:512:VAL:HG23	1:C:513:ASN:N	2.30	0.47
1:C:465:TYR:CG	1:C:469:ARG:CG	2.98	0.47
2:D:23:TRP:HZ2	2:D:447:ILE:HD13	1.76	0.47
1:E:4:ASP:CG	1:E:597:ARG:NH2	2.68	0.47
1:A:117:GLN:HB2	1:A:121:VAL:HG21	1.95	0.47
1:A:121:VAL:CG1	1:A:121:VAL:O	2.62	0.47
1:C:121:VAL:O	1:C:121:VAL:CG1	2.62	0.47
2:F:277:PHE:CE1	2:F:278:ASP:O	2.68	0.47
1:A:89:CYS:C	1:A:91:PRO:HD3	2.34	0.47
1:C:444:CYS:CB	1:C:506:LEU:CD1	2.93	0.47
1:E:831:SER:HB3	1:E:842:THR:HG22	1.96	0.47
1:G:831:SER:HA	1:G:842:THR:HG22	1.96	0.47
1:A:478:LEU:HA	1:A:485:TRP:HE1	1.80	0.47
1:C:831:SER:HB3	1:C:842:THR:HG22	1.96	0.47
2:D:630:LEU:HD12	2:D:665:ILE:HB	1.97	0.47
1:C:908:VAL:HG13	1:C:1069:PHE:HB3	1.97	0.47
2:H:222:ALA:HB2	2:H:294:ILE:CD1	2.45	0.47
1:A:938:VAL:HG12	1:A:1024:LEU:O	2.14	0.47
1:G:827:LEU:HD13	1:G:829:CYS:SG	2.54	0.47
2:D:43:ARG:N	2:D:44:PRO:CD	2.78	0.47
2:F:43:ARG:N	2:F:44:PRO:CD	2.78	0.47
2:B:270:LEU:HD23	2:B:271:TYR:O	2.14	0.47
2:H:656:GLN:HG2	2:H:657:GLN:N	2.29	0.47
2:B:382:GLN:HG3	2:B:383:ILE:H	1.80	0.47
1:A:676:THR:HG23	1:A:678:ASN:H	1.79	0.47
2:F:424:GLU:HA	2:F:424:GLU:OE1	2.14	0.47
1:G:110:LEU:N	1:G:110:LEU:HD12	2.29	0.47
1:C:470:GLY:HA2	1:C:497:HIS:O	2.14	0.47
1:A:980:SER:HB3	1:A:1012:ARG:HB3	1.96	0.47
1:A:13:VAL:HG21	1:A:57:CYS:HB2	1.96	0.47
2:H:43:ARG:HB3	2:H:44:PRO:HD3	1.96	0.47
1:C:650:ARG:HD3	1:C:729:ASN:HB3	1.97	0.47
2:H:155:LEU:HD12	2:H:155:LEU:C	2.35	0.47
2:F:461:CYS:CB	2:F:466:ARG:CD	2.92	0.47
1:G:657:THR:HG22	1:G:684:VAL:HG22	1.97	0.47
1:C:89:CYS:C	1:C:91:PRO:HD3	2.35	0.47
1:G:444:CYS:CB	1:G:506:LEU:CD1	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:444:CYS:HB2	1:G:506:LEU:HD12	1.97	0.47
1:A:986:PRO:HG3	1:A:1003:CYS:O	2.14	0.47
1:E:565:PHE:HB2	1:E:587:ALA:CB	2.44	0.47
1:C:86:LEU:HD23	1:C:87:LEU:N	2.30	0.47
1:E:25:TYR:CG	1:E:26:ALA:N	2.82	0.47
2:B:363:PHE:HB2	2:B:388:THR:HB	1.97	0.47
2:H:363:PHE:HB2	2:H:388:THR:HB	1.96	0.47
1:A:908:VAL:HG13	1:A:1069:PHE:HB3	1.96	0.47
2:F:372:ASN:O	2:F:373:GLN:HG3	2.15	0.47
2:F:382:GLN:HG3	2:F:383:ILE:H	1.79	0.47
1:C:657:THR:HG22	1:C:684:VAL:HG22	1.97	0.47
1:G:181:HIS:CE1	1:G:200:VAL:CG1	2.97	0.47
1:A:630:LEU:HD21	1:E:653:GLN:CB	2.44	0.47
1:A:822:LEU:HG	1:A:823:ARG:N	2.29	0.47
2:F:616:PRO:HB3	2:F:621:CYS:SG	2.55	0.47
1:G:876:LEU:HB3	1:G:898:GLU:HG3	1.97	0.47
2:D:121:LEU:HD23	2:D:121:LEU:O	2.14	0.47
2:F:135:LEU:CD1	2:F:139:THR:HB	2.45	0.47
2:D:372:ASN:O	2:D:373:GLN:HG3	2.15	0.47
2:D:345:VAL:HG11	2:D:387:ILE:CD1	2.45	0.47
1:G:411:THR:HG22	1:G:435:ILE:HA	1.96	0.47
2:H:372:ASN:O	2:H:373:GLN:HG3	2.15	0.47
1:C:716:ASN:C	1:C:716:ASN:OD1	2.54	0.47
2:F:155:LEU:C	2:F:155:LEU:HD12	2.35	0.47
2:D:165:LEU:HD12	2:D:179:PRO:HG2	1.97	0.47
2:B:155:LEU:HD12	2:B:155:LEU:C	2.35	0.47
1:G:1063:LEU:HG	1:G:1064:PRO:HD3	1.95	0.47
1:E:512:VAL:HG23	1:E:513:ASN:N	2.30	0.47
1:G:156:ARG:HB3	1:G:197:LEU:HD13	1.97	0.47
1:E:609:ILE:CB	1:E:610:PRO:HD3	2.43	0.47
2:B:118:LEU:HD21	2:B:204:ILE:CD1	2.45	0.47
1:G:89:CYS:C	1:G:91:PRO:HD3	2.34	0.47
1:A:444:CYS:HB2	1:A:506:LEU:HD12	1.97	0.47
1:C:656:VAL:HG13	1:C:718:THR:O	2.15	0.47
1:C:822:LEU:HG	1:C:823:ARG:N	2.29	0.47
1:C:576:THR:HG23	1:C:582:ASP:OD2	2.15	0.47
2:H:347:LEU:HD22	2:H:389:PHE:CG	2.49	0.47
1:C:761:ASN:HB3	1:C:792:GLY:HA3	1.97	0.47
2:D:466:ARG:HB2	2:D:491:VAL:HG13	1.96	0.47
2:D:143:ARG:C	2:D:144:ILE:HD12	2.36	0.47
2:D:362:SER:HB2	2:D:370:HIS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:776:VAL:HG12	1:E:867:PRO:O	2.14	0.47
2:H:455:ILE:HG22	2:H:456:GLY:N	2.30	0.47
1:C:752:CYS:O	1:C:752:CYS:SG	2.72	0.47
1:E:110:LEU:HD12	1:E:110:LEU:N	2.30	0.47
1:A:103:LEU:CD1	2:B:156:PRO:HG3	2.45	0.46
1:E:681:LEU:HD12	1:E:681:LEU:C	2.35	0.46
1:A:512:VAL:HG23	1:A:513:ASN:N	2.31	0.46
1:C:71:MET:SD	1:C:90:GLY:HA3	2.55	0.46
1:E:71:MET:SD	1:E:90:GLY:HA3	2.55	0.46
1:A:444:CYS:CB	1:A:506:LEU:CD1	2.92	0.46
2:H:118:LEU:HD21	2:H:204:ILE:CD1	2.45	0.46
1:G:385:TYR:CZ	2:H:253:LEU:CD1	2.98	0.46
1:A:806:ALA:HA	1:A:840:TRP:NE1	2.29	0.46
2:B:340:LYS:HD2	2:B:379:ASP:OD1	2.15	0.46
2:D:149:PHE:HA	2:D:181:ALA:O	2.14	0.46
1:A:650:ARG:HD3	1:A:729:ASN:HB3	1.97	0.46
1:A:41:ALA:O	1:A:42:ASN:C	2.54	0.46
1:C:714:ARG:C	1:C:714:ARG:HD2	2.36	0.46
2:F:659:GLY:O	2:F:662:ARG:HG2	2.15	0.46
1:C:739:GLN:HB2	1:C:742:PHE:CE1	2.50	0.46
2:F:118:LEU:HD21	2:F:204:ILE:CD1	2.46	0.46
1:A:71:MET:CG	1:A:90:GLY:HA3	2.44	0.46
2:D:6:PHE:CG	2:D:7:LYS:N	2.84	0.46
1:G:905:VAL:CG1	1:G:946:LEU:HD21	2.45	0.46
2:H:149:PHE:HA	2:H:181:ALA:O	2.14	0.46
2:H:43:ARG:N	2:H:44:PRO:CD	2.78	0.46
1:G:135:PHE:HZ	1:G:158:VAL:HB	1.80	0.46
1:E:850:ILE:HG22	1:E:851:PHE:N	2.30	0.46
2:F:345:VAL:HG11	2:F:387:ILE:CD1	2.45	0.46
1:A:685:ARG:NH2	1:E:685:ARG:CZ	2.78	0.46
1:G:714:ARG:C	1:G:714:ARG:HD2	2.36	0.46
2:F:11:CYS:O	2:F:15:ILE:HG12	2.15	0.46
2:B:165:LEU:HD12	2:B:179:PRO:HG2	1.97	0.46
2:D:659:GLY:O	2:D:662:ARG:CG	2.63	0.46
2:D:532:ARG:CD	2:D:554:GLU:HG3	2.45	0.46
2:F:460:GLU:OE2	2:F:461:CYS:SG	2.74	0.46
1:G:406:PRO:HB3	1:G:438:TYR:CZ	2.51	0.46
1:C:73:LEU:HA	1:C:90:GLY:HA2	1.97	0.46
1:E:71:MET:CG	1:E:90:GLY:HA3	2.44	0.46
1:E:575:LEU:HD12	1:E:576:THR:CG2	2.44	0.46
2:H:616:PRO:HB3	2:H:621:CYS:SG	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:876:LEU:HB3	1:E:898:GLU:HG3	1.97	0.46
1:G:905:VAL:HG21	1:G:946:LEU:HD22	1.98	0.46
1:A:86:LEU:HD23	1:A:87:LEU:N	2.30	0.46
2:B:453:GLY:O	2:B:462:GLN:HG3	2.16	0.46
2:D:382:GLN:HG3	2:D:383:ILE:H	1.79	0.46
1:G:13:VAL:HG21	1:G:57:CYS:HB2	1.96	0.46
1:C:975:PRO:HG2	1:C:977:LEU:HD11	1.97	0.46
1:C:13:VAL:HG21	1:C:57:CYS:HB2	1.96	0.46
1:E:13:VAL:HG21	1:E:57:CYS:HB2	1.96	0.46
2:D:334:ILE:HA	2:D:337:ALA:CB	2.45	0.46
1:G:93:VAL:HB	1:G:104:THR:CG2	2.45	0.46
1:A:103:LEU:HD13	2:B:156:PRO:HG3	1.97	0.46
1:A:93:VAL:HB	1:A:104:THR:CG2	2.45	0.46
2:H:277:PHE:CE1	2:H:278:ASP:O	2.68	0.46
2:H:6:PHE:CG	2:H:7:LYS:N	2.83	0.46
2:B:143:ARG:C	2:B:144:ILE:HD12	2.36	0.46
1:E:780:LEU:C	1:E:780:LEU:HD23	2.36	0.46
1:G:41:ALA:O	1:G:42:ASN:C	2.54	0.46
1:E:93:VAL:HB	1:E:104:THR:CG2	2.44	0.46
1:C:597:ARG:HB3	1:C:731:ARG:O	2.15	0.46
1:G:731:ARG:NH2	1:G:733:MET:SD	2.88	0.46
2:D:277:PHE:CE1	2:D:278:ASP:O	2.68	0.46
1:G:73:LEU:HA	1:G:90:GLY:HA2	1.97	0.46
1:G:71:MET:SD	1:G:90:GLY:HA3	2.55	0.46
1:E:823:ARG:HD3	1:E:860:LEU:H	1.80	0.46
1:E:576:THR:HG23	1:E:582:ASP:OD2	2.15	0.46
1:G:576:THR:HG23	1:G:582:ASP:OD2	2.14	0.46
2:F:363:PHE:HB2	2:F:388:THR:HB	1.96	0.46
1:C:780:LEU:C	1:C:780:LEU:HD23	2.36	0.46
2:B:25:GLN:OE1	2:B:427:CYS:SG	2.73	0.46
1:A:714:ARG:C	1:A:714:ARG:HD2	2.36	0.46
2:H:659:GLY:O	2:H:662:ARG:CG	2.63	0.46
1:A:831:SER:HA	1:A:842:THR:HG22	1.96	0.46
1:C:663:ASP:N	1:C:664:PRO:HD3	2.31	0.46
2:F:149:PHE:HA	2:F:181:ALA:O	2.15	0.46
1:A:649:SER:O	1:A:650:ARG:HB3	2.16	0.46
2:B:522:TYR:CE1	2:B:552:GLN:HA	2.50	0.46
1:E:676:THR:HG23	1:E:678:ASN:H	1.79	0.46
2:H:362:SER:HB2	2:H:370:HIS:HB2	1.98	0.46
1:G:175:SER:CB	1:G:204:GLN:O	2.64	0.46
1:C:93:VAL:HB	1:C:104:THR:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PRO:HB3	1:A:438:TYR:CZ	2.51	0.46
2:D:118:LEU:HD21	2:D:204:ILE:CD1	2.46	0.46
1:A:71:MET:SD	1:A:90:GLY:HA3	2.55	0.46
1:E:411:THR:HG22	1:E:435:ILE:HA	1.96	0.46
1:A:905:VAL:HG21	1:A:946:LEU:HD22	1.97	0.46
2:H:507:ILE:HG22	2:H:508:TYR:N	2.31	0.46
2:H:143:ARG:C	2:H:144:ILE:HD12	2.36	0.46
2:B:43:ARG:N	2:B:44:PRO:CD	2.78	0.46
2:F:98:ARG:HG2	2:F:98:ARG:O	2.15	0.46
2:D:508:TYR:CZ	2:D:514:CYS:HB3	2.51	0.46
1:G:850:ILE:HG22	1:G:851:PHE:N	2.30	0.46
2:D:155:LEU:C	2:D:155:LEU:HD12	2.36	0.46
1:G:772:LYS:O	1:G:773:SER:HB3	2.16	0.46
4:E:3373:NAG:O3	4:E:3374:NAG:C7	2.64	0.46
1:A:465:TYR:CG	1:A:469:ARG:CG	2.99	0.46
1:G:465:TYR:CG	1:G:469:ARG:CG	2.98	0.46
1:G:221:PHE:CE1	1:G:233:LYS:HD2	2.51	0.46
2:B:630:LEU:HD12	2:B:665:ILE:HB	1.97	0.46
1:E:41:ALA:O	1:E:42:ASN:C	2.54	0.46
2:B:659:GLY:O	2:B:662:ARG:HG2	2.15	0.46
2:B:334:ILE:HA	2:B:337:ALA:CB	2.46	0.46
1:A:22:VAL:HG22	1:A:23:VAL:N	2.31	0.46
2:H:345:VAL:HG11	2:H:387:ILE:CD1	2.46	0.46
1:G:980:SER:HB3	1:G:1012:ARG:HB3	1.97	0.46
1:E:975:PRO:HG2	1:E:977:LEU:HD11	1.98	0.46
1:G:716:ASN:OD1	1:G:716:ASN:C	2.53	0.46
1:C:601:TRP:HZ2	1:C:641:LYS:HD3	1.81	0.46
1:E:657:THR:HG22	1:E:684:VAL:HG22	1.97	0.46
2:H:219:MET:HE2	2:H:262:GLY:HA2	1.98	0.46
1:E:710:PRO:HG3	1:E:884:GLU:OE2	2.16	0.46
1:A:345:GLY:HA3	1:A:363:TYR:O	2.16	0.46
1:E:823:ARG:NH1	1:E:825:LEU:O	2.49	0.46
1:E:656:VAL:HG13	1:E:718:THR:O	2.16	0.46
2:F:6:PHE:CG	2:F:7:LYS:N	2.83	0.46
2:F:143:ARG:C	2:F:144:ILE:HD12	2.36	0.46
2:B:659:GLY:O	2:B:662:ARG:CG	2.63	0.46
1:G:878:THR:HG22	1:G:896:GLN:HB3	1.98	0.46
2:B:432:ARG:O	2:B:433:ASP:HB2	2.16	0.46
2:B:11:CYS:O	2:B:15:ILE:HG12	2.16	0.46
2:F:165:LEU:HD12	2:F:179:PRO:HG2	1.97	0.46
1:G:99:ARG:HG3	1:G:100:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:479:ASN:HD21	5:D:3479:NAG:C7	2.21	0.46
4:E:3373:NAG:H3	4:E:3374:NAG:HN2	1.77	0.46
2:H:643:ARG:NH2	2:H:649:TRP:CZ2	2.84	0.46
1:C:406:PRO:HB3	1:C:438:TYR:CD2	2.51	0.46
1:E:406:PRO:HB3	1:E:438:TYR:CZ	2.51	0.46
1:A:656:VAL:HG13	1:A:718:THR:O	2.15	0.46
2:B:6:PHE:CG	2:B:7:LYS:N	2.83	0.46
2:B:135:LEU:CD1	2:B:139:THR:HB	2.45	0.46
1:E:790:ASN:O	1:E:854:GLY:HA2	2.15	0.46
2:H:334:ILE:HA	2:H:337:ALA:CB	2.46	0.46
1:G:939:ASN:HB3	1:G:1023:GLU:HA	1.98	0.46
2:H:27:LEU:CD2	2:H:446:GLY:CA	2.93	0.45
2:D:168:PRO:CG	2:D:179:PRO:HG3	2.47	0.45
2:F:659:GLY:O	2:F:662:ARG:CG	2.64	0.45
2:D:209:ASP:OD2	2:D:246:HIS:CE1	2.70	0.45
1:E:465:TYR:HB3	1:E:469:ARG:HG2	1.98	0.45
1:C:575:LEU:HD12	1:C:576:THR:HG23	1.99	0.45
1:A:939:ASN:HB3	1:A:1023:GLU:HA	1.98	0.45
2:H:98:ARG:O	2:H:98:ARG:HG2	2.15	0.45
1:G:649:SER:O	1:G:650:ARG:HB3	2.15	0.45
1:C:939:ASN:HB3	1:C:1023:GLU:HA	1.98	0.45
1:A:878:THR:HG22	1:A:896:GLN:HB3	1.99	0.45
2:D:652:TYR:HB3	2:D:667:VAL:HA	1.98	0.45
1:G:533:ALA:HA	1:G:554:ALA:HA	1.98	0.45
1:G:130:GLU:HB3	1:G:228:ARG:CZ	2.45	0.45
1:A:597:ARG:HD2	1:A:731:ARG:O	2.16	0.45
2:F:571:ARG:HH21	2:F:660:MET:HG3	1.81	0.45
1:C:345:GLY:HA3	1:C:363:TYR:O	2.16	0.45
1:G:820:GLY:N	1:G:822:LEU:HB3	2.31	0.45
1:E:444:CYS:HB2	1:E:506:LEU:HD12	1.98	0.45
1:A:575:LEU:HD12	1:A:576:THR:HG23	1.99	0.45
2:H:461:CYS:HB3	2:H:466:ARG:HD3	1.98	0.45
2:B:98:ARG:HB2	2:B:386:PRO:HG3	1.98	0.45
1:A:23:VAL:HG22	1:A:24:GLN:N	2.31	0.45
1:E:601:TRP:HZ2	1:E:641:LYS:HD3	1.82	0.45
2:F:191:ASN:ND2	2:F:194:GLN:HB3	2.31	0.45
2:H:432:ARG:O	2:H:433:ASP:HB2	2.16	0.45
1:A:1020:VAL:HG12	1:A:1021:GLN:HG3	1.98	0.45
1:E:4:ASP:HB2	1:E:597:ARG:CZ	2.46	0.45
1:A:710:PRO:HG3	1:A:884:GLU:OE2	2.17	0.45
1:E:820:GLY:N	1:E:822:LEU:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:822:LEU:HG	1:E:823:ARG:N	2.31	0.45
2:H:118:LEU:HD21	2:H:204:ILE:HD13	1.98	0.45
1:E:446:VAL:CG1	1:E:456:LEU:HD11	2.47	0.45
1:G:804:HIS:CE1	1:G:840:TRP:NE1	2.85	0.45
1:C:525:PRO:HB3	1:C:564:TYR:HB2	1.99	0.45
1:G:766:PHE:HZ	1:G:877:LEU:HD12	1.80	0.45
1:G:282:LEU:O	1:G:294:ILE:HD11	2.17	0.45
1:C:649:SER:O	1:C:650:ARG:HB3	2.16	0.45
1:E:790:ASN:HB2	1:E:851:PHE:CE1	2.52	0.45
2:B:305:VAL:HG13	2:B:306:LYS:N	2.32	0.45
2:F:643:ARG:NH2	2:F:649:TRP:CZ2	2.85	0.45
2:D:108:TYR:CE2	2:D:147:GLY:HA3	2.52	0.45
2:H:382:GLN:HG3	2:H:383:ILE:H	1.79	0.45
1:A:850:ILE:HG22	1:A:851:PHE:N	2.32	0.45
1:A:716:ASN:OD1	1:A:716:ASN:C	2.54	0.45
2:B:546:PHE:CD2	2:B:554:GLU:HG2	2.50	0.45
4:E:3373:NAG:N2	4:E:3374:NAG:H82	2.31	0.45
2:D:39:ARG:HD2	2:D:447:ILE:HG21	1.98	0.45
1:G:823:ARG:HD3	1:G:860:LEU:H	1.81	0.45
1:C:446:VAL:CG1	1:C:456:LEU:HD11	2.47	0.45
1:E:987:PRO:O	1:E:988:ALA:HB3	2.16	0.45
1:C:905:VAL:CG1	1:C:946:LEU:HD21	2.45	0.45
2:B:98:ARG:O	2:B:98:ARG:HG2	2.15	0.45
1:G:780:LEU:HD23	1:G:780:LEU:C	2.36	0.45
1:A:676:THR:O	1:A:677:LYS:CB	2.64	0.45
1:A:685:ARG:CZ	1:E:685:ARG:NH2	2.79	0.45
1:C:880:ASN:OD1	1:C:894:THR:HG22	2.17	0.45
1:G:323:THR:O	1:G:324:SER:C	2.54	0.45
1:C:850:ILE:HG22	1:C:851:PHE:N	2.31	0.45
2:B:631:SER:HB3	2:B:664:LEU:HD11	1.97	0.45
1:C:41:ALA:O	1:C:42:ASN:C	2.55	0.45
1:E:1020:VAL:HG12	1:E:1021:GLN:HG3	1.98	0.45
2:F:652:TYR:HB3	2:F:667:VAL:HA	1.99	0.45
1:C:619:GLU:O	1:C:620:CYS:SG	2.74	0.45
2:B:372:ASN:O	2:B:373:GLN:HG3	2.16	0.45
1:A:772:LYS:O	1:A:773:SER:HB3	2.16	0.45
2:F:479:ASN:ND2	5:F:3479:NAG:N2	2.62	0.45
1:G:919:LEU:O	2:H:643:ARG:NH1	2.47	0.45
1:A:406:PRO:HB3	1:A:438:TYR:CD2	2.52	0.45
2:H:11:CYS:O	2:H:15:ILE:HG12	2.15	0.45
1:G:663:ASP:N	1:G:664:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:575:LEU:HD12	1:E:576:THR:HG23	1.99	0.45
1:C:670:ARG:HG2	1:C:711:ILE:CG2	2.46	0.45
2:D:98:ARG:HG2	2:D:98:ARG:O	2.15	0.45
2:H:98:ARG:HB2	2:H:386:PRO:HG3	1.98	0.45
2:D:181:ALA:HB3	2:D:271:TYR:CZ	2.52	0.45
1:C:790:ASN:HB2	1:C:851:PHE:CE1	2.51	0.45
2:F:334:ILE:HA	2:F:337:ALA:CB	2.46	0.45
1:E:533:ALA:HA	1:E:554:ALA:HA	1.99	0.45
2:H:631:SER:HB3	2:H:664:LEU:HD11	1.97	0.45
1:G:916:THR:O	1:G:1076:THR:HG23	2.17	0.45
1:A:772:LYS:HB3	1:C:789:TRP:NE1	2.32	0.45
2:B:168:PRO:CG	2:B:179:PRO:HG3	2.47	0.45
1:C:919:LEU:HD11	2:D:643:ARG:NH1	2.32	0.45
1:G:465:TYR:HB3	1:G:469:ARG:HG2	1.98	0.45
1:C:964:TRP:HB3	1:C:1032:LEU:HA	1.98	0.45
1:C:652:LEU:HD21	1:G:609:ILE:CG2	2.47	0.45
1:E:121:VAL:O	1:E:121:VAL:CG1	2.62	0.45
2:B:277:PHE:CE1	2:B:278:ASP:O	2.69	0.45
1:C:876:LEU:HB3	1:C:898:GLU:HG3	1.98	0.45
1:A:848:HIS:O	1:A:849:LEU:CB	2.65	0.45
1:A:780:LEU:HD23	1:A:780:LEU:C	2.36	0.45
1:G:419:GLN:HA	1:G:424:TRP:HA	1.99	0.45
1:G:975:PRO:HG2	1:G:977:LEU:HD11	1.97	0.45
1:G:17:GLY:O	1:G:20:ASP:HB2	2.17	0.45
2:F:631:SER:HB3	2:F:664:LEU:HD11	1.97	0.45
2:D:455:ILE:HG22	2:D:456:GLY:N	2.32	0.45
2:F:168:PRO:CG	2:F:179:PRO:HG3	2.47	0.45
1:C:69:VAL:HG12	1:C:70:ASN:N	2.32	0.45
1:C:1064:PRO:HG3	1:C:1067:GLU:OE2	2.16	0.45
1:A:662:LEU:HD21	1:A:698:LEU:HD23	1.99	0.45
1:E:964:TRP:HB3	1:E:1032:LEU:HA	1.99	0.45
1:G:345:GLY:HA3	1:G:363:TYR:O	2.15	0.45
1:E:345:GLY:HA3	1:E:363:TYR:O	2.16	0.45
1:A:670:ARG:HG2	1:A:711:ILE:CG2	2.46	0.45
1:G:456:LEU:HA	1:G:477:PRO:HA	1.99	0.45
1:A:446:VAL:CG1	1:A:456:LEU:HD11	2.47	0.45
1:G:670:ARG:HG2	1:G:711:ILE:CG2	2.47	0.45
1:A:1003:CYS:HB3	1:A:1008:CYS:HB2	1.85	0.45
1:A:804:HIS:CE1	1:A:840:TRP:NE1	2.85	0.45
4:A:3374:NAG:C3	4:A:3375:MAN:H2	2.46	0.45
1:G:243:LYS:HD2	1:G:246:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:416:ILE:HG22	1:G:427:LYS:HD3	1.99	0.45
1:G:476:CYS:HB3	1:G:487:CYS:HA	1.98	0.45
2:B:665:ILE:HD12	2:B:665:ILE:N	2.32	0.45
2:H:181:ALA:HB3	2:H:271:TYR:CZ	2.52	0.45
1:E:724:LEU:HD12	1:E:729:ASN:ND2	2.32	0.45
2:F:99:ARG:O	2:F:383:ILE:O	2.35	0.45
2:D:345:VAL:HG11	2:D:387:ILE:HD11	1.98	0.45
1:E:23:VAL:HG22	1:E:24:GLN:N	2.32	0.45
1:G:317:ILE:HG23	1:G:317:ILE:O	2.17	0.45
1:A:686:VAL:CG1	1:E:695:ASN:O	2.64	0.45
2:F:305:VAL:HG13	2:F:306:LYS:N	2.32	0.45
1:C:23:VAL:HG22	1:C:24:GLN:N	2.31	0.45
1:C:22:VAL:HG22	1:C:23:VAL:N	2.32	0.45
1:E:714:ARG:HD2	1:E:714:ARG:C	2.36	0.45
2:B:215:LEU:HD12	2:B:246:HIS:O	2.17	0.45
1:C:599:VAL:HG12	1:C:733:MET:HG3	1.99	0.45
1:G:406:PRO:HB3	1:G:438:TYR:CD2	2.52	0.45
1:A:961:GLU:HG2	1:A:1036:TRP:HA	1.97	0.45
1:C:804:HIS:CE1	1:C:840:TRP:NE1	2.85	0.45
1:C:831:SER:HA	1:C:842:THR:HG22	1.98	0.45
2:H:466:ARG:HB2	2:H:491:VAL:HG13	1.98	0.45
1:E:435:ILE:O	2:F:282:VAL:HG21	2.16	0.45
1:C:766:PHE:HZ	1:C:877:LEU:HD12	1.82	0.45
2:H:665:ILE:N	2:H:665:ILE:HD12	2.32	0.45
2:B:83:LEU:O	2:B:83:LEU:HD12	2.16	0.45
1:C:676:THR:O	1:C:677:LYS:CB	2.65	0.45
2:B:181:ALA:HB3	2:B:271:TYR:CZ	2.52	0.45
1:A:790:ASN:HB2	1:A:851:PHE:CE1	2.51	0.45
1:A:419:GLN:HA	1:A:424:TRP:HA	1.99	0.45
2:B:506:LEU:O	2:B:515:ASP:HA	2.17	0.45
1:C:99:ARG:HG3	1:C:100:ASN:OD1	2.17	0.45
1:A:99:ARG:HG3	1:A:100:ASN:OD1	2.17	0.45
1:A:713:LEU:HD23	1:A:713:LEU:C	2.38	0.45
1:G:69:VAL:HG12	1:G:70:ASN:N	2.32	0.45
1:C:772:LYS:O	1:C:773:SER:HB3	2.16	0.45
2:B:219:MET:HE2	2:B:262:GLY:HA2	1.99	0.45
1:E:599:VAL:HG12	1:E:733:MET:HG3	1.98	0.45
1:A:652:LEU:HD21	1:E:609:ILE:CG2	2.46	0.45
1:A:971:HIS:CE1	1:A:974:ASN:CB	3.00	0.45
2:D:118:LEU:HD21	2:D:204:ILE:HD13	1.98	0.45
1:G:446:VAL:CG1	1:G:456:LEU:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:ILE:HG22	1:E:427:LYS:HD3	1.99	0.45
1:G:848:HIS:O	1:G:849:LEU:CB	2.65	0.45
2:D:644:ASP:HB3	2:D:650:VAL:CG2	2.47	0.45
1:C:1024:LEU:C	1:C:1024:LEU:HD23	2.37	0.45
1:E:649:SER:O	1:E:650:ARG:HB3	2.16	0.45
2:B:383:ILE:HG22	2:B:384:ASN:N	2.32	0.45
1:G:158:VAL:O	1:G:158:VAL:HG12	2.17	0.45
1:G:507:THR:HG21	1:G:571:GLY:N	2.32	0.45
1:C:686:VAL:CG1	1:G:695:ASN:O	2.65	0.45
1:G:171:LEU:HB3	1:G:182:PHE:CE1	2.51	0.45
1:A:69:VAL:HG12	1:A:70:ASN:N	2.32	0.45
1:E:1064:PRO:HG3	1:E:1067:GLU:OE2	2.16	0.45
1:E:772:LYS:O	1:E:773:SER:HB3	2.17	0.45
2:F:215:LEU:HD12	2:F:246:HIS:O	2.17	0.45
2:B:643:ARG:NH2	2:B:649:TRP:CZ2	2.85	0.45
2:B:260:ASN:ND2	2:B:277:PHE:HZ	2.15	0.45
1:G:137:ILE:CD1	1:G:152:MET:SD	3.05	0.45
1:E:525:PRO:HB3	1:E:564:TYR:HB2	1.99	0.45
1:G:174:PHE:O	1:G:174:PHE:CD1	2.70	0.45
1:G:212:ALA:O	1:G:216:VAL:HG23	2.16	0.45
2:F:665:ILE:HD12	2:F:665:ILE:N	2.32	0.45
2:D:665:ILE:HG22	2:D:666:TYR:N	2.32	0.45
1:E:348:LEU:HD12	1:E:348:LEU:N	2.32	0.45
1:G:188:ARG:NH2	1:G:228:ARG:HD3	2.32	0.45
2:H:383:ILE:HG22	2:H:384:ASN:N	2.32	0.45
1:A:694:GLU:HA	1:E:692:HIS:ND1	2.32	0.45
2:H:305:VAL:HG13	2:H:306:LYS:N	2.32	0.45
2:D:191:ASN:ND2	2:D:194:GLN:HB3	2.32	0.45
2:B:120:ASP:O	2:B:124:VAL:HB	2.17	0.45
2:D:305:VAL:HG13	2:D:306:LYS:N	2.32	0.45
1:G:297:VAL:HG12	1:G:298:GLU:N	2.32	0.45
1:A:992:LEU:C	1:A:992:LEU:HD23	2.37	0.45
2:H:168:PRO:CG	2:H:179:PRO:HG3	2.47	0.44
1:C:118:ARG:HA	1:C:120:PRO:CA	2.47	0.44
2:H:209:ASP:OD2	2:H:246:HIS:CE1	2.70	0.44
1:C:662:LEU:HD21	1:C:698:LEU:HD23	1.98	0.44
2:F:209:ASP:OD2	2:F:246:HIS:CE1	2.70	0.44
2:D:25:GLN:HB2	2:D:445:CYS:HA	1.99	0.44
1:C:4:ASP:HB2	1:C:597:ARG:CZ	2.46	0.44
2:F:219:MET:HE2	2:F:262:GLY:HA2	1.99	0.44
1:G:512:VAL:HG23	1:G:513:ASN:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HA	1:A:477:PRO:HA	1.99	0.44
1:E:476:CYS:HB3	1:E:487:CYS:HA	1.98	0.44
1:A:987:PRO:O	1:A:988:ALA:HB3	2.17	0.44
1:G:575:LEU:HD12	1:G:576:THR:HG23	1.99	0.44
1:A:613:ILE:HD12	1:A:748:PHE:CD2	2.52	0.44
1:A:25:TYR:OH	1:A:111:GLY:HA2	2.17	0.44
2:F:644:ASP:HB3	2:F:650:VAL:CG2	2.47	0.44
2:F:665:ILE:HG22	2:F:666:TYR:N	2.32	0.44
1:A:435:ILE:HD13	2:B:311:LEU:HB2	1.98	0.44
2:D:508:TYR:HE2	2:D:516:THR:HG23	1.82	0.44
1:A:1045:VAL:HG22	1:A:1046:SER:N	2.32	0.44
1:C:533:ALA:HA	1:C:554:ALA:HA	1.99	0.44
2:D:631:SER:HB3	2:D:664:LEU:HD11	1.97	0.44
1:C:4:ASP:CG	1:C:597:ARG:NH2	2.70	0.44
1:A:465:TYR:HB3	1:A:469:ARG:HG2	1.99	0.44
1:E:406:PRO:HB3	1:E:438:TYR:CD2	2.52	0.44
1:E:507:THR:HG21	1:E:571:GLY:N	2.33	0.44
1:C:761:ASN:O	1:C:762:LEU:HD23	2.17	0.44
1:C:1020:VAL:HG12	1:C:1021:GLN:HG3	1.99	0.44
2:H:108:TYR:CE2	2:H:147:GLY:HA3	2.52	0.44
1:C:419:GLN:HA	1:C:424:TRP:HA	1.99	0.44
1:E:878:THR:HG22	1:E:896:GLN:HB3	1.98	0.44
2:D:360:TYR:HD1	2:D:374:PRO:HA	1.82	0.44
2:F:120:ASP:O	2:F:124:VAL:HB	2.17	0.44
2:D:215:LEU:HD12	2:D:246:HIS:O	2.17	0.44
2:B:209:ASP:OD2	2:B:246:HIS:CE1	2.70	0.44
2:D:219:MET:CE	2:D:262:GLY:HA2	2.47	0.44
1:C:456:LEU:HA	1:C:477:PRO:HA	1.99	0.44
1:G:666:ARG:CZ	1:G:670:ARG:HH21	2.31	0.44
1:G:603:GLY:O	1:G:638:TYR:CD2	2.71	0.44
1:C:1003:CYS:HB3	1:C:1008:CYS:HB2	1.85	0.44
1:C:348:LEU:HD12	1:C:348:LEU:N	2.32	0.44
2:F:654:LEU:HD13	2:F:665:ILE:HG13	2.00	0.44
1:E:1024:LEU:HD23	1:E:1024:LEU:C	2.38	0.44
1:A:752:CYS:HB2	1:A:793:GLU:OE2	2.18	0.44
1:G:102:TYR:CG	1:G:331:GLU:HB3	2.53	0.44
2:F:108:TYR:CE2	2:F:147:GLY:HA3	2.52	0.44
2:H:25:GLN:HB2	2:H:445:CYS:HB3	1.99	0.44
2:D:532:ARG:O	2:D:543:HIS:HB2	2.18	0.44
1:E:662:LEU:HD21	1:E:698:LEU:HD23	1.98	0.44
2:F:219:MET:CE	2:F:262:GLY:HA2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:PRO:HB3	1:C:438:TYR:CZ	2.51	0.44
1:C:971:HIS:CE1	1:C:974:ASN:CB	3.01	0.44
2:B:118:LEU:HD21	2:B:204:ILE:HD13	1.98	0.44
2:F:118:LEU:HD21	2:F:204:ILE:HD13	1.98	0.44
1:A:507:THR:HG21	1:A:571:GLY:N	2.33	0.44
1:C:823:ARG:HD3	1:C:860:LEU:H	1.82	0.44
1:G:25:TYR:OH	1:G:111:GLY:HA2	2.17	0.44
1:G:348:LEU:N	1:G:348:LEU:HD12	2.32	0.44
2:B:222:ALA:HB2	2:B:294:ILE:HD12	2.00	0.44
2:D:222:ALA:HB2	2:D:294:ILE:HD12	2.00	0.44
2:D:98:ARG:HB2	2:D:386:PRO:HG3	1.98	0.44
2:F:98:ARG:HB2	2:F:386:PRO:HG3	1.98	0.44
2:D:507:ILE:HG22	2:D:508:TYR:N	2.32	0.44
1:G:790:ASN:HB2	1:G:851:PHE:CE1	2.52	0.44
1:C:499:TRP:CZ2	2:D:284:GLN:HG3	2.53	0.44
1:E:880:ASN:OD1	1:E:894:THR:HG22	2.17	0.44
2:B:108:TYR:CE2	2:B:147:GLY:HA3	2.52	0.44
1:A:533:ALA:HA	1:A:554:ALA:HA	1.99	0.44
2:D:120:ASP:O	2:D:124:VAL:HB	2.17	0.44
1:C:916:THR:O	1:C:1076:THR:HG23	2.17	0.44
1:A:113:THR:HG22	1:G:1029:LYS:CE	2.48	0.44
2:D:565:ARG:HD3	2:D:565:ARG:HA	1.83	0.44
2:H:25:GLN:HB3	2:H:445:CYS:HB3	1.98	0.44
2:F:532:ARG:O	2:F:543:HIS:HB2	2.17	0.44
1:E:971:HIS:NE2	1:E:974:ASN:CB	2.81	0.44
2:F:260:ASN:ND2	2:F:277:PHE:HZ	2.15	0.44
1:C:444:CYS:HB2	1:C:506:LEU:HD12	1.97	0.44
1:C:507:THR:HG21	1:C:571:GLY:N	2.33	0.44
1:A:766:PHE:HZ	1:A:877:LEU:HD12	1.81	0.44
1:C:476:CYS:HB3	1:C:487:CYS:HA	1.98	0.44
2:D:83:LEU:O	2:D:83:LEU:HD12	2.17	0.44
2:H:644:ASP:HB3	2:H:650:VAL:CG2	2.48	0.44
2:F:181:ALA:HB3	2:F:271:TYR:CZ	2.52	0.44
1:A:790:ASN:O	1:A:854:GLY:HA2	2.17	0.44
1:G:323:THR:O	1:G:324:SER:O	2.36	0.44
1:E:22:VAL:HG22	1:E:23:VAL:N	2.32	0.44
1:E:663:ASP:N	1:E:664:PRO:HD3	2.32	0.44
1:G:23:VAL:HG22	1:G:24:GLN:N	2.31	0.44
1:C:17:GLY:O	1:C:20:ASP:HB2	2.18	0.44
2:B:191:ASN:ND2	2:B:194:GLN:HB3	2.32	0.44
1:A:118:ARG:HA	1:A:120:PRO:CA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:789:TRP:CZ2	1:G:771:LEU:O	2.71	0.44
2:H:285:LEU:C	2:H:287:HIS:N	2.71	0.44
1:A:351:VAL:HG23	1:A:352:GLY:N	2.33	0.44
2:B:507:ILE:HG22	2:B:508:TYR:N	2.32	0.44
1:G:761:ASN:HB3	1:G:792:GLY:HA3	1.99	0.44
2:B:237:LEU:HD13	2:B:294:ILE:HG23	1.99	0.44
2:H:222:ALA:HB2	2:H:294:ILE:HD12	2.00	0.44
1:G:676:THR:O	1:G:677:LYS:CB	2.65	0.44
2:H:454:TYR:O	2:H:455:ILE:HD13	2.18	0.44
1:C:790:ASN:O	1:C:854:GLY:HA2	2.17	0.44
1:E:670:ARG:HG2	1:E:711:ILE:CG2	2.47	0.44
2:H:120:ASP:O	2:H:124:VAL:HB	2.17	0.44
2:H:652:TYR:HB3	2:H:667:VAL:HA	1.99	0.44
1:G:934:HIS:ND1	1:G:1074:THR:CG2	2.80	0.44
1:G:1020:VAL:HG12	1:G:1021:GLN:HG3	1.98	0.44
1:E:102:TYR:CG	1:E:331:GLU:HB3	2.53	0.44
1:A:1028:LEU:O	1:A:1028:LEU:HD12	2.17	0.44
1:C:103:LEU:HD21	2:D:155:LEU:HD22	1.99	0.44
2:D:154:VAL:HG22	2:D:155:LEU:N	2.33	0.44
1:C:465:TYR:HB3	1:C:469:ARG:HG2	1.98	0.44
1:G:964:TRP:HB3	1:G:1032:LEU:HA	1.99	0.44
2:H:219:MET:CE	2:H:262:GLY:HA2	2.48	0.44
2:H:260:ASN:ND2	2:H:277:PHE:HZ	2.15	0.44
1:A:525:PRO:HB3	1:A:564:TYR:HB2	1.99	0.44
2:B:6:PHE:CD2	2:B:7:LYS:N	2.86	0.44
1:E:534:VAL:HG23	1:E:565:PHE:CZ	2.53	0.44
1:G:534:VAL:HG23	1:G:565:PHE:CE2	2.53	0.44
1:C:25:TYR:OH	1:C:111:GLY:HA2	2.18	0.44
1:G:180:THR:HG21	1:G:220:LEU:HD21	2.00	0.44
2:F:83:LEU:O	2:F:83:LEU:HD12	2.17	0.44
1:E:25:TYR:OH	1:E:111:GLY:HA2	2.18	0.44
2:H:120:ASP:OD1	2:H:325:GLU:O	2.36	0.44
1:G:342:THR:OG1	1:G:343:PRO:HD2	2.18	0.44
1:A:601:TRP:HZ2	1:A:641:LYS:HD3	1.82	0.44
2:H:191:ASN:ND2	2:H:194:GLN:HB3	2.32	0.44
2:H:256:ILE:HG13	2:H:256:ILE:O	2.17	0.44
1:C:992:LEU:HD23	1:C:992:LEU:C	2.38	0.44
1:E:69:VAL:HG12	1:E:70:ASN:N	2.32	0.44
2:H:532:ARG:O	2:H:543:HIS:HB2	2.17	0.44
1:E:848:HIS:O	1:E:849:LEU:CB	2.65	0.44
1:G:964:TRP:HB3	1:G:1032:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:505:LYS:HA	2:D:517:ILE:CG2	2.47	0.44
1:G:766:PHE:CE1	1:G:877:LEU:HD11	2.53	0.44
2:H:83:LEU:O	2:H:83:LEU:HD12	2.17	0.44
2:H:654:LEU:HD13	2:H:665:ILE:HG13	2.00	0.44
2:F:186:LEU:HD21	2:F:198:GLU:CB	2.48	0.44
1:E:676:THR:O	1:E:677:LYS:CB	2.65	0.44
2:D:120:ASP:OD1	2:D:325:GLU:O	2.36	0.44
1:G:1020:VAL:O	1:G:1021:GLN:HB2	2.17	0.44
1:A:102:TYR:CG	1:A:331:GLU:HB3	2.52	0.44
1:C:799:THR:HA	1:C:845:ARG:HA	2.00	0.44
1:A:916:THR:O	1:A:1076:THR:HG23	2.17	0.44
1:G:1028:LEU:O	1:G:1028:LEU:HD12	2.18	0.44
2:D:643:ARG:NH2	2:D:649:TRP:CZ2	2.85	0.44
1:C:433:THR:HG23	1:C:464:TYR:CE1	2.53	0.44
1:A:964:TRP:HB2	1:A:1032:LEU:HA	2.00	0.44
2:B:219:MET:CE	2:B:262:GLY:HA2	2.48	0.44
1:G:513:ASN:HA	1:G:599:VAL:HG22	1.98	0.44
1:C:804:HIS:HB2	1:C:808:LEU:HD11	1.99	0.44
1:A:73:LEU:C	1:A:73:LEU:HD12	2.38	0.44
1:A:804:HIS:HB2	1:A:808:LEU:HD11	1.99	0.44
1:C:416:ILE:HG22	1:C:427:LYS:HD3	1.99	0.44
1:G:650:ARG:HD3	1:G:729:ASN:HB3	1.99	0.44
1:G:175:SER:HB2	1:G:204:GLN:O	2.18	0.44
1:E:916:THR:O	1:E:1076:THR:HG23	2.18	0.44
1:G:1048:VAL:HG22	1:G:1075:THR:HB	2.00	0.44
1:C:1045:VAL:HG22	1:C:1046:SER:N	2.32	0.44
1:C:102:TYR:CG	1:C:331:GLU:HB3	2.53	0.44
1:E:874:ARG:NH2	1:G:894:THR:O	2.51	0.44
1:E:419:GLN:HA	1:E:424:TRP:HA	1.99	0.44
1:G:992:LEU:HD23	1:G:992:LEU:C	2.37	0.44
2:F:154:VAL:HG22	2:F:155:LEU:N	2.33	0.43
2:B:154:VAL:HG22	2:B:155:LEU:N	2.33	0.43
2:B:532:ARG:O	2:B:543:HIS:HB2	2.17	0.43
1:G:383:ASP:OD2	2:H:211:PRO:HD3	2.18	0.43
2:H:215:LEU:HD12	2:H:246:HIS:O	2.17	0.43
1:C:513:ASN:HA	1:C:599:VAL:HG22	2.00	0.43
1:G:964:TRP:HB2	1:G:1032:LEU:HA	2.00	0.43
1:A:971:HIS:NE2	1:A:974:ASN:CB	2.81	0.43
1:E:456:LEU:HA	1:E:477:PRO:HA	1.99	0.43
1:C:534:VAL:HG23	1:C:565:PHE:CZ	2.53	0.43
2:F:507:ILE:HG22	2:F:508:TYR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:LEU:HD23	1:G:237:VAL:HG22	1.99	0.43
1:G:525:PRO:HB3	1:G:564:TYR:HB2	1.99	0.43
2:D:654:LEU:HD13	2:D:665:ILE:HG13	2.00	0.43
1:E:87:LEU:HD21	1:E:348:LEU:HD11	2.00	0.43
2:H:665:ILE:HG22	2:H:666:TYR:N	2.32	0.43
2:B:665:ILE:HG22	2:B:666:TYR:N	2.33	0.43
2:F:345:VAL:HG11	2:F:387:ILE:HD11	2.00	0.43
1:E:678:ASN:ND2	5:E:3678:NAG:C7	2.78	0.43
1:G:790:ASN:O	1:G:854:GLY:HA2	2.17	0.43
1:G:22:VAL:HG22	1:G:23:VAL:N	2.31	0.43
1:E:959:ASN:O	1:E:960:GLN:HB3	2.18	0.43
2:B:455:ILE:CG2	2:B:456:GLY:N	2.80	0.43
1:A:766:PHE:CE1	1:A:877:LEU:HD11	2.54	0.43
2:D:186:LEU:HD21	2:D:198:GLU:CB	2.48	0.43
1:E:1020:VAL:O	1:E:1021:GLN:HB2	2.18	0.43
1:E:939:ASN:HB3	1:E:1023:GLU:HA	1.99	0.43
2:B:345:VAL:HG11	2:B:387:ILE:CD1	2.48	0.43
1:G:94:HIS:CD2	2:H:155:LEU:HD21	2.53	0.43
2:D:260:ASN:ND2	2:D:277:PHE:HZ	2.15	0.43
1:E:804:HIS:CE1	1:E:840:TRP:NE1	2.86	0.43
2:D:401:GLU:HA	2:D:421:PRO:HD3	2.00	0.43
2:D:188:LEU:HD12	2:D:230:TRP:HA	2.00	0.43
2:H:186:LEU:HD21	2:H:198:GLU:CB	2.48	0.43
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.53	0.43
2:H:345:VAL:HG11	2:H:387:ILE:HD11	1.99	0.43
1:C:385:TYR:CE2	1:C:407:ARG:HD3	2.53	0.43
1:A:959:ASN:O	1:A:960:GLN:HB3	2.18	0.43
1:A:1048:VAL:HG22	1:A:1075:THR:HB	2.00	0.43
1:G:959:ASN:O	1:G:960:GLN:HB3	2.18	0.43
1:A:17:GLY:O	1:A:20:ASP:HB2	2.19	0.43
1:A:354:PHE:CG	4:A:3373:NAG:H62	2.54	0.43
2:F:126:LYS:HG2	2:F:196:GLN:O	2.18	0.43
1:G:601:TRP:HZ2	1:G:641:LYS:HD3	1.82	0.43
1:E:1048:VAL:HG22	1:E:1075:THR:HB	2.00	0.43
1:C:1028:LEU:HD12	1:C:1028:LEU:O	2.19	0.43
1:C:679:ARG:HD3	1:C:679:ARG:C	2.39	0.43
1:G:662:LEU:HD21	1:G:698:LEU:HD23	1.99	0.43
1:E:464:TYR:O	1:E:465:TYR:HB3	2.18	0.43
2:F:285:LEU:C	2:F:287:HIS:N	2.71	0.43
1:A:964:TRP:HB3	1:A:1032:LEU:HA	1.99	0.43
1:E:964:TRP:HB2	1:E:1032:LEU:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:964:TRP:HB3	1:E:1032:LEU:HG	2.00	0.43
1:C:964:TRP:HB2	1:C:1032:LEU:HA	2.00	0.43
1:C:971:HIS:NE2	1:C:974:ASN:CB	2.82	0.43
1:G:73:LEU:C	1:G:73:LEU:HD12	2.38	0.43
2:D:219:MET:HE2	2:D:262:GLY:HA2	2.01	0.43
1:E:446:VAL:HG12	1:E:456:LEU:HD11	2.00	0.43
1:A:534:VAL:HG23	1:A:565:PHE:CE2	2.53	0.43
1:G:430:VAL:O	1:G:430:VAL:HG23	2.19	0.43
1:C:351:VAL:HG23	1:C:352:GLY:N	2.33	0.43
1:G:351:VAL:HG23	1:G:352:GLY:N	2.33	0.43
1:E:1065:GLY:O	1:E:1066:GLN:HG3	2.18	0.43
2:B:644:ASP:HB3	2:B:650:VAL:CG2	2.47	0.43
2:F:237:LEU:HD13	2:F:294:ILE:HG23	1.99	0.43
2:D:383:ILE:HG22	2:D:384:ASN:N	2.32	0.43
2:H:126:LYS:HG2	2:H:196:GLN:O	2.18	0.43
2:H:599:PRO:HB2	2:H:603:TYR:HE2	1.83	0.43
1:C:878:THR:HG22	1:C:896:GLN:HB3	1.99	0.43
1:C:613:ILE:HD12	1:C:748:PHE:CD2	2.53	0.43
2:B:584:GLY:O	2:B:586:GLN:HG2	2.18	0.43
1:C:465:TYR:CD1	1:C:469:ARG:HG2	2.54	0.43
1:A:964:TRP:HB3	1:A:1032:LEU:HG	2.00	0.43
1:C:964:TRP:HB3	1:C:1032:LEU:HG	2.01	0.43
2:D:317:LYS:HE3	2:D:410:GLY:HA3	2.00	0.43
1:G:956:VAL:HG12	1:G:957:GLU:N	2.34	0.43
1:A:666:ARG:CZ	1:A:670:ARG:HH21	2.31	0.43
1:G:804:HIS:HB2	1:G:808:LEU:HD11	1.99	0.43
1:A:476:CYS:HB3	1:A:487:CYS:HA	1.98	0.43
1:C:534:VAL:HG23	1:C:565:PHE:CE2	2.53	0.43
1:C:663:ASP:HB3	1:C:666:ARG:HD3	2.00	0.43
1:A:1065:GLY:O	1:A:1066:GLN:HG3	2.19	0.43
1:E:534:VAL:HG23	1:E:565:PHE:CE2	2.53	0.43
2:H:6:PHE:CD2	2:H:7:LYS:N	2.85	0.43
1:A:87:LEU:HD21	1:A:348:LEU:HD11	2.00	0.43
2:H:237:LEU:HD13	2:H:294:ILE:HG23	1.99	0.43
2:D:611:LYS:CB	2:D:667:VAL:HB	2.49	0.43
2:F:611:LYS:CB	2:F:667:VAL:HB	2.49	0.43
1:A:686:VAL:HG11	1:E:695:ASN:O	2.18	0.43
2:B:120:ASP:OD1	2:B:325:GLU:O	2.37	0.43
2:H:188:LEU:HD12	2:H:230:TRP:HA	2.01	0.43
1:E:17:GLY:O	1:E:20:ASP:HB2	2.18	0.43
1:G:713:LEU:C	1:G:713:LEU:HD23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:25:GLN:HB2	2:H:445:CYS:CB	2.49	0.43
1:A:920:ASN:O	1:A:1080:LYS:HG2	2.18	0.43
2:F:466:ARG:HB2	2:F:491:VAL:HG13	2.00	0.43
1:C:464:TYR:O	1:C:465:TYR:HB3	2.18	0.43
1:C:848:HIS:O	1:C:849:LEU:CB	2.65	0.43
1:C:956:VAL:HG12	1:C:957:GLU:N	2.34	0.43
1:E:804:HIS:HB2	1:E:808:LEU:HD11	1.99	0.43
1:G:446:VAL:HG12	1:G:456:LEU:HD11	2.00	0.43
1:A:416:ILE:HG22	1:A:427:LYS:HD3	1.99	0.43
1:C:985:ALA:HA	1:C:986:PRO:HD3	1.86	0.43
1:A:348:LEU:N	1:A:348:LEU:HD12	2.33	0.43
1:E:351:VAL:HG23	1:E:352:GLY:N	2.33	0.43
1:G:87:LEU:HD21	1:G:348:LEU:HD11	2.00	0.43
1:A:909:VAL:HG12	1:A:1069:PHE:O	2.19	0.43
2:B:144:ILE:HG22	2:B:195:PHE:CZ	2.54	0.43
1:G:1020:VAL:O	1:G:1021:GLN:CB	2.67	0.43
1:E:619:GLU:O	1:E:620:CYS:SG	2.76	0.43
2:F:360:TYR:HD1	2:F:374:PRO:HA	1.83	0.43
2:D:126:LYS:HG2	2:D:196:GLN:O	2.18	0.43
1:C:342:THR:OG1	1:C:343:PRO:HD2	2.17	0.43
1:E:1045:VAL:HG22	1:E:1046:SER:N	2.33	0.43
1:E:465:TYR:CD1	1:E:469:ARG:HG2	2.54	0.43
1:E:472:GLN:NE2	1:E:492:TYR:HB2	2.34	0.43
1:C:472:GLN:NE2	1:C:492:TYR:HB2	2.33	0.43
1:A:608:PHE:O	1:A:609:ILE:C	2.57	0.43
1:E:609:ILE:HD12	1:E:632:GLN:OE1	2.19	0.43
1:C:73:LEU:C	1:C:73:LEU:HD12	2.38	0.43
1:A:663:ASP:N	1:A:664:PRO:HD3	2.32	0.43
1:A:534:VAL:HG23	1:A:565:PHE:CZ	2.53	0.43
1:G:418:THR:HB	1:G:427:LYS:CG	2.49	0.43
2:D:6:PHE:CD2	2:D:7:LYS:N	2.87	0.43
1:G:134:VAL:HG11	1:G:216:VAL:HG13	2.01	0.43
1:G:534:VAL:HG23	1:G:565:PHE:CZ	2.53	0.43
2:F:6:PHE:CD2	2:F:7:LYS:N	2.86	0.43
1:G:254:ILE:HG23	1:G:264:ARG:NH2	2.33	0.43
2:D:237:LEU:HD13	2:D:294:ILE:HG23	1.99	0.43
2:F:144:ILE:HG22	2:F:195:PHE:CZ	2.54	0.43
1:C:1020:VAL:O	1:C:1021:GLN:HB2	2.19	0.43
1:C:930:HIS:O	1:C:931:VAL:C	2.57	0.43
1:A:342:THR:OG1	1:A:343:PRO:HD2	2.18	0.43
1:G:752:CYS:HB2	1:G:793:GLU:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:HIS:ND1	1:A:1074:THR:CG2	2.82	0.43
1:E:1028:LEU:O	1:E:1028:LEU:HD12	2.19	0.43
2:H:154:VAL:HA	2:H:160:THR:CG2	2.49	0.43
2:H:154:VAL:HG22	2:H:155:LEU:N	2.33	0.43
1:E:771:LEU:O	1:G:789:TRP:CZ2	2.71	0.43
1:A:722:LYS:N	1:A:723:PRO:HD2	2.33	0.43
1:A:464:TYR:O	1:A:465:TYR:HB3	2.19	0.43
1:E:956:VAL:HG12	1:E:957:GLU:N	2.34	0.43
1:A:663:ASP:HB3	1:A:666:ARG:HD3	2.01	0.43
2:F:621:CYS:SG	2:F:625:CYS:SG	3.17	0.43
1:C:666:ARG:CZ	1:C:670:ARG:HH21	2.31	0.43
1:G:172:MET:SD	1:G:216:VAL:CG2	3.07	0.43
1:E:761:ASN:HB3	1:E:792:GLY:HA3	2.01	0.43
2:B:654:LEU:HD13	2:B:665:ILE:HG13	2.00	0.43
2:F:383:ILE:HG22	2:F:384:ASN:N	2.32	0.43
1:G:796:TYR:CE2	1:G:850:ILE:HD13	2.54	0.43
1:A:1020:VAL:O	1:A:1021:GLN:HB2	2.19	0.43
2:H:99:ARG:O	2:H:383:ILE:O	2.37	0.43
1:A:796:TYR:CE2	1:A:850:ILE:HD13	2.54	0.43
1:E:613:ILE:HD12	1:E:748:PHE:CD2	2.54	0.43
1:C:442:SER:O	1:C:459:ILE:HA	2.19	0.43
2:F:256:ILE:HG13	2:F:256:ILE:O	2.18	0.43
2:B:256:ILE:HG13	2:B:256:ILE:O	2.19	0.43
1:C:713:LEU:C	1:C:713:LEU:HD23	2.39	0.43
2:F:601:GLY:O	2:F:602:LYS:HB2	2.19	0.43
1:E:118:ARG:HA	1:E:120:PRO:CA	2.47	0.43
1:G:1064:PRO:HG3	1:G:1067:GLU:OE2	2.19	0.43
1:E:376:GLN:HB2	4:E:3373:NAG:H61	2.01	0.43
1:G:464:TYR:O	1:G:465:TYR:HB3	2.18	0.43
1:G:472:GLN:NE2	1:G:492:TYR:HB2	2.34	0.43
1:A:609:ILE:HD12	1:A:632:GLN:OE1	2.18	0.43
1:A:586:GLY:HA2	1:A:591:VAL:HG23	2.00	0.43
1:E:418:THR:HB	1:E:427:LYS:CG	2.49	0.43
2:H:401:GLU:HA	2:H:421:PRO:HD3	2.01	0.43
1:E:603:GLY:O	1:E:638:TYR:CD2	2.72	0.43
2:D:621:CYS:SG	2:D:625:CYS:SG	3.17	0.43
1:A:1024:LEU:C	1:A:1024:LEU:HD23	2.39	0.43
2:H:601:GLY:O	2:H:602:LYS:HB2	2.19	0.43
1:E:499:TRP:CZ2	2:F:284:GLN:HG3	2.54	0.43
2:B:611:LYS:CB	2:B:667:VAL:HB	2.49	0.43
1:A:679:ARG:C	1:A:679:ARG:HD3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:433:THR:HG23	1:G:464:TYR:CE1	2.54	0.43
1:E:971:HIS:CE1	1:E:974:ASN:CB	3.00	0.43
1:E:73:LEU:C	1:E:73:LEU:HD12	2.39	0.43
1:G:385:TYR:CE2	1:G:407:ARG:HD3	2.54	0.43
1:C:822:LEU:CG	1:C:823:ARG:N	2.82	0.43
1:E:689:LEU:C	1:E:689:LEU:HD12	2.39	0.43
2:H:621:CYS:SG	2:H:625:CYS:SG	3.17	0.43
1:G:243:LYS:HB2	1:G:246:ASP:HB2	2.01	0.43
1:E:766:PHE:CE1	1:E:877:LEU:HD11	2.54	0.43
2:B:281:SER:OG	2:B:284:GLN:HB2	2.19	0.43
2:D:665:ILE:HD12	2:D:665:ILE:N	2.32	0.43
2:D:144:ILE:HG22	2:D:195:PHE:CZ	2.54	0.43
1:C:909:VAL:HG12	1:C:1069:PHE:O	2.19	0.43
1:C:676:THR:O	1:C:677:LYS:HB3	2.19	0.43
2:D:334:ILE:HA	2:D:337:ALA:HB2	2.01	0.43
1:C:934:HIS:ND1	1:C:1074:THR:CG2	2.82	0.43
1:E:99:ARG:HG3	1:E:100:ASN:OD1	2.18	0.43
1:E:799:THR:HA	1:E:845:ARG:HA	2.01	0.43
2:H:352:LEU:CD2	2:H:358:VAL:HG23	2.49	0.43
1:G:190:SER:O	1:G:193:PRO:HD3	2.19	0.43
2:B:360:TYR:HD1	2:B:374:PRO:HA	1.84	0.43
1:G:103:LEU:CD1	2:H:156:PRO:HG3	2.49	0.42
1:C:920:ASN:O	1:C:1080:LYS:HG2	2.19	0.42
1:G:971:HIS:CE1	1:G:974:ASN:CB	3.01	0.42
1:A:418:THR:HB	1:A:427:LYS:CG	2.49	0.42
2:B:401:GLU:HA	2:B:421:PRO:HD3	2.00	0.42
2:F:222:ALA:HB2	2:F:294:ILE:HD12	2.00	0.42
2:H:144:ILE:HG22	2:H:195:PHE:CZ	2.54	0.42
2:B:188:LEU:HD12	2:B:230:TRP:HA	2.00	0.42
1:A:874:ARG:NH2	1:C:894:THR:O	2.52	0.42
2:H:611:LYS:CB	2:H:667:VAL:HB	2.48	0.42
2:D:352:LEU:CD2	2:D:358:VAL:HG23	2.49	0.42
1:A:385:TYR:CE2	1:A:407:ARG:HD3	2.53	0.42
2:D:256:ILE:O	2:D:256:ILE:HG13	2.18	0.42
2:B:543:HIS:HB3	2:B:544:PRO:HD2	2.02	0.42
2:F:455:ILE:HG22	2:F:456:GLY:N	2.35	0.42
1:A:465:TYR:CD1	1:A:469:ARG:HG2	2.54	0.42
1:G:918:TYR:O	1:G:919:LEU:C	2.57	0.42
1:C:353:SER:C	1:C:354:PHE:CG	2.92	0.42
1:G:509:LEU:HB3	1:G:519:ASP:O	2.19	0.42
2:H:115:TYR:HA	2:H:204:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:GLU:HA	2:F:421:PRO:HD3	2.00	0.42
1:G:689:LEU:HD12	1:G:689:LEU:C	2.39	0.42
1:E:766:PHE:HZ	1:E:877:LEU:HD12	1.81	0.42
1:C:689:LEU:HD12	1:C:689:LEU:C	2.39	0.42
1:G:1024:LEU:HD23	1:G:1024:LEU:C	2.39	0.42
1:E:796:TYR:CE2	1:E:850:ILE:HD13	2.54	0.42
2:B:126:LYS:HG2	2:B:196:GLN:O	2.18	0.42
1:C:959:ASN:O	1:C:960:GLN:HB3	2.18	0.42
1:E:342:THR:OG1	1:E:343:PRO:HD2	2.18	0.42
1:C:84:SER:OG	1:E:968:GLU:OE1	2.32	0.42
1:E:920:ASN:O	1:E:1080:LYS:HG2	2.19	0.42
1:E:1054:THR:HG21	1:G:757:ILE:HG21	2.01	0.42
2:H:584:GLY:O	2:H:586:GLN:HG2	2.19	0.42
1:E:433:THR:HG23	1:E:464:TYR:CE1	2.53	0.42
1:E:464:TYR:HD2	1:E:472:GLN:HB2	1.85	0.42
2:D:584:GLY:O	2:D:586:GLN:HG2	2.20	0.42
1:A:918:TYR:O	1:A:919:LEU:C	2.58	0.42
1:A:464:TYR:HD2	1:A:472:GLN:HB2	1.85	0.42
1:G:464:TYR:HD2	1:G:472:GLN:HB2	1.85	0.42
1:G:608:PHE:O	1:G:609:ILE:C	2.57	0.42
1:G:267:ILE:HG21	1:G:303:LEU:CD1	2.50	0.42
1:A:676:THR:O	1:A:677:LYS:HB3	2.19	0.42
2:F:352:LEU:CD2	2:F:358:VAL:HG23	2.49	0.42
2:H:360:TYR:HD1	2:H:374:PRO:HA	1.83	0.42
2:D:639:THR:O	2:D:639:THR:HG23	2.19	0.42
2:H:639:THR:HG23	2:H:639:THR:O	2.19	0.42
1:A:7:GLU:O	1:A:595:ARG:NH2	2.53	0.42
1:A:433:THR:HG23	1:A:464:TYR:CE1	2.54	0.42
1:E:468:THR:HG23	1:E:498:PRO:CG	2.50	0.42
1:E:385:TYR:CE2	1:E:407:ARG:HD3	2.54	0.42
1:C:1065:GLY:O	1:C:1066:GLN:HG3	2.18	0.42
1:E:671:ALA:HB2	1:E:700:LEU:HD23	2.02	0.42
1:G:939:ASN:HA	1:G:1018:PHE:HZ	1.84	0.42
1:C:796:TYR:CE2	1:C:850:ILE:HD13	2.55	0.42
1:C:686:VAL:HG11	1:G:695:ASN:O	2.19	0.42
2:D:17:SER:HB2	2:D:21:CYS:SG	2.59	0.42
1:E:442:SER:O	1:E:459:ILE:HA	2.19	0.42
1:C:690:LYS:HG3	1:G:634:ASN:ND2	2.35	0.42
1:A:442:SER:O	1:A:459:ILE:HA	2.20	0.42
2:B:160:THR:O	2:B:165:LEU:HD22	2.20	0.42
1:C:464:TYR:HD2	1:C:472:GLN:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:543:HIS:HB3	2:F:544:PRO:HD2	2.01	0.42
1:G:912:HIS:ND1	1:G:935:ARG:CD	2.81	0.42
1:C:117:GLN:HB3	1:C:121:VAL:CG2	2.50	0.42
1:A:956:VAL:HG12	1:A:957:GLU:N	2.34	0.42
1:G:971:HIS:NE2	1:G:974:ASN:CB	2.82	0.42
1:A:761:ASN:HB3	1:A:792:GLY:HA3	2.00	0.42
2:B:505:LYS:HA	2:B:517:ILE:CG2	2.49	0.42
2:B:186:LEU:HD21	2:B:198:GLU:CB	2.48	0.42
1:E:676:THR:O	1:E:677:LYS:HB3	2.19	0.42
1:G:263:ILE:HD12	1:G:317:ILE:CD1	2.49	0.42
1:E:939:ASN:HA	1:E:1018:PHE:HZ	1.85	0.42
1:E:620:CYS:HB3	1:E:702:SER:O	2.19	0.42
1:E:748:PHE:N	1:E:748:PHE:CD1	2.88	0.42
1:G:162:PHE:HB3	1:G:167:THR:HG21	2.01	0.42
1:A:930:HIS:O	1:A:931:VAL:C	2.57	0.42
2:B:639:THR:HG23	2:B:639:THR:O	2.19	0.42
1:G:772:LYS:O	1:G:773:SER:CB	2.68	0.42
1:G:353:SER:C	1:G:354:PHE:CG	2.92	0.42
1:A:812:TYR:HD2	1:A:814:ALA:HB2	1.80	0.42
1:A:472:GLN:NE2	1:A:492:TYR:HB2	2.34	0.42
1:G:465:TYR:CD1	1:G:469:ARG:HG2	2.54	0.42
1:G:609:ILE:HD12	1:G:632:GLN:OE1	2.19	0.42
1:C:609:ILE:HD12	1:C:632:GLN:OE1	2.19	0.42
1:E:586:GLY:HA2	1:E:591:VAL:HG23	2.00	0.42
1:A:446:VAL:HG12	1:A:456:LEU:HD11	2.01	0.42
1:E:430:VAL:O	1:E:430:VAL:HG23	2.20	0.42
1:G:663:ASP:HB3	1:G:666:ARG:HD3	2.01	0.42
1:C:987:PRO:O	1:C:988:ALA:HB3	2.19	0.42
1:A:671:ALA:O	1:A:672:THR:CG2	2.68	0.42
1:A:939:ASN:HA	1:A:1018:PHE:HZ	1.85	0.42
1:G:1045:VAL:HG22	1:G:1046:SER:N	2.33	0.42
1:C:825:LEU:HD11	1:C:846:ILE:HG23	2.00	0.42
2:B:302:SER:HB3	2:B:322:GLU:CG	2.50	0.42
1:C:1040:ILE:CD1	1:C:1042:GLN:HB2	2.49	0.42
1:E:934:HIS:ND1	1:E:1074:THR:CG2	2.82	0.42
1:E:1040:ILE:CD1	1:E:1042:GLN:HB2	2.49	0.42
1:G:920:ASN:O	1:G:1080:LYS:HG2	2.19	0.42
1:C:720:VAL:HG22	1:C:721:GLY:N	2.35	0.42
1:E:871:LEU:CD1	1:E:901:VAL:HG11	2.50	0.42
1:C:73:LEU:HA	1:C:89:CYS:O	2.20	0.42
1:E:73:LEU:HA	1:E:89:CYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:GLY:HA2	1:C:591:VAL:HG23	2.01	0.42
1:C:446:VAL:HG12	1:C:456:LEU:HD11	2.00	0.42
1:G:586:GLY:HA2	1:G:591:VAL:HG23	2.00	0.42
1:E:407:ARG:HD2	2:F:250:ASP:OD2	2.20	0.42
1:G:250:TYR:HA	1:G:253:VAL:HG22	2.01	0.42
1:C:1065:GLY:O	1:C:1066:GLN:CG	2.68	0.42
1:C:87:LEU:HD21	1:C:348:LEU:HD11	2.00	0.42
1:E:352:GLY:HA2	1:E:356:TRP:HA	2.02	0.42
2:H:281:SER:OG	2:H:284:GLN:HB2	2.19	0.42
2:D:281:SER:OG	2:D:284:GLN:HB2	2.20	0.42
1:A:407:ARG:HG2	2:B:247:PHE:CZ	2.55	0.42
1:A:1040:ILE:CD1	1:A:1042:GLN:HB2	2.50	0.42
1:E:930:HIS:O	1:E:931:VAL:C	2.57	0.42
2:B:352:LEU:CD2	2:B:358:VAL:HG23	2.49	0.42
1:E:679:ARG:HD3	1:E:679:ARG:C	2.40	0.42
1:A:698:LEU:C	1:A:699:LEU:HD12	2.40	0.42
2:D:25:GLN:O	2:D:446:GLY:HA3	2.20	0.42
2:F:315:ILE:HA	2:F:316:PRO:HD3	1.87	0.42
1:E:629:THR:CG2	1:E:630:LEU:N	2.83	0.42
2:B:219:MET:SD	2:B:285:LEU:HD23	2.60	0.42
1:E:7:GLU:O	1:E:595:ARG:NH2	2.53	0.42
1:C:826:HIS:HB3	1:C:848:HIS:NE2	2.35	0.42
1:G:1065:GLY:O	1:G:1066:GLN:HG3	2.19	0.42
1:C:766:PHE:CE1	1:C:877:LEU:HD11	2.55	0.42
1:E:909:VAL:HG12	1:E:1069:PHE:O	2.19	0.42
2:D:98:ARG:HD3	2:D:386:PRO:HG3	2.02	0.42
2:B:187:LYS:HG2	2:B:188:LEU:N	2.35	0.42
1:G:676:THR:O	1:G:677:LYS:HB3	2.19	0.42
2:B:99:ARG:O	2:B:383:ILE:O	2.37	0.42
1:E:1020:VAL:O	1:E:1021:GLN:CB	2.68	0.42
1:A:419:GLN:CG	1:A:424:TRP:CD1	3.03	0.42
2:F:120:ASP:OD1	2:F:325:GLU:O	2.36	0.42
1:A:752:CYS:HB2	1:A:793:GLU:CD	2.40	0.42
1:C:748:PHE:CD1	1:C:748:PHE:N	2.88	0.42
1:G:774:LEU:HG	1:G:774:LEU:O	2.20	0.42
1:G:679:ARG:C	1:G:679:ARG:HD3	2.40	0.42
2:B:162:PRO:O	2:B:165:LEU:CB	2.67	0.42
1:G:722:LYS:N	1:G:723:PRO:HD2	2.33	0.42
1:G:629:THR:CG2	1:G:630:LEU:N	2.83	0.42
1:C:7:GLU:O	1:C:595:ARG:NH2	2.53	0.42
1:A:117:GLN:HB3	1:A:121:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:956:VAL:O	1:G:963:VAL:HG23	2.20	0.42
1:A:564:TYR:CZ	1:A:588:ARG:HD2	2.55	0.42
2:H:132:LEU:HD22	2:H:192:SER:HB3	2.01	0.42
1:G:909:VAL:HG12	1:G:1069:PHE:O	2.19	0.42
1:E:827:LEU:HD12	1:E:827:LEU:O	2.20	0.42
1:C:678:ASN:ND2	5:C:3678:NAG:C7	2.78	0.42
2:D:508:TYR:CE2	2:D:516:THR:HG23	2.55	0.42
2:F:334:ILE:HA	2:F:337:ALA:HB2	2.02	0.42
2:D:302:SER:HB3	2:D:322:GLU:CG	2.50	0.42
1:G:752:CYS:HB2	1:G:793:GLU:OE2	2.20	0.42
2:D:599:PRO:HB2	2:D:603:TYR:HE2	1.85	0.42
2:H:17:SER:HB2	2:H:21:CYS:SG	2.60	0.42
2:D:361:ASP:HB2	2:D:390:GLN:HB3	2.02	0.42
2:F:639:THR:HG23	2:F:639:THR:O	2.19	0.42
1:G:118:ARG:HA	1:G:120:PRO:CA	2.47	0.42
2:H:532:ARG:HD3	2:H:554:GLU:OE1	2.19	0.42
1:E:753:GLY:C	1:E:755:ASP:H	2.22	0.42
2:F:460:GLU:OE2	2:F:492:CYS:SG	2.78	0.42
1:G:698:LEU:C	1:G:699:LEU:HD12	2.40	0.42
2:H:314:ILE:HG22	2:H:315:ILE:N	2.35	0.42
1:C:328:PHE:HB2	1:C:354:PHE:O	2.20	0.42
1:G:609:ILE:HB	1:G:610:PRO:CD	2.46	0.42
1:E:117:GLN:HB3	1:E:121:VAL:CG2	2.50	0.42
1:C:629:THR:CG2	1:C:630:LEU:N	2.82	0.42
1:E:971:HIS:NE2	1:E:974:ASN:HB2	2.35	0.42
2:F:115:TYR:HA	2:F:204:ILE:CD1	2.50	0.42
2:B:334:ILE:HA	2:B:337:ALA:HB2	2.02	0.42
2:D:454:TYR:O	2:D:455:ILE:HD13	2.20	0.42
2:B:601:GLY:O	2:B:602:LYS:HB2	2.20	0.42
1:G:442:SER:O	1:G:459:ILE:HA	2.19	0.42
1:C:1048:VAL:HG22	1:C:1075:THR:HB	2.00	0.42
1:G:930:HIS:O	1:G:931:VAL:C	2.57	0.42
1:C:402:VAL:CG1	1:C:443:LEU:HD22	2.50	0.42
1:G:1040:ILE:CD1	1:G:1042:GLN:HB2	2.49	0.42
2:H:162:PRO:O	2:H:165:LEU:CB	2.67	0.41
2:D:532:ARG:HD3	2:D:554:GLU:CG	2.49	0.41
1:E:720:VAL:HG22	1:E:721:GLY:N	2.35	0.41
2:H:219:MET:SD	2:H:285:LEU:HD23	2.60	0.41
2:H:39:ARG:CD	2:H:447:ILE:HG23	2.49	0.41
1:C:603:GLY:O	1:C:638:TYR:CD2	2.73	0.41
1:G:7:GLU:O	1:G:595:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:917:LYS:HE3	1:G:1077:VAL:HG23	2.02	0.41
1:E:908:VAL:HG12	1:E:909:VAL:N	2.35	0.41
1:A:908:VAL:HG12	1:A:909:VAL:N	2.35	0.41
1:E:663:ASP:HB3	1:E:666:ARG:HD3	2.01	0.41
1:E:666:ARG:CZ	1:E:670:ARG:HH21	2.32	0.41
1:C:694:GLU:HA	1:G:692:HIS:ND1	2.35	0.41
1:G:799:THR:HA	1:G:845:ARG:HA	2.01	0.41
1:E:713:LEU:C	1:E:713:LEU:HD23	2.39	0.41
2:D:160:THR:O	2:D:165:LEU:HD22	2.20	0.41
1:C:919:LEU:CB	1:C:1079:GLU:HB3	2.47	0.41
1:C:354:PHE:HB2	1:C:355:THR:H	1.68	0.41
1:C:608:PHE:O	1:C:609:ILE:C	2.59	0.41
1:E:608:PHE:O	1:E:609:ILE:C	2.58	0.41
1:G:269:VAL:HG11	1:G:300:PHE:CZ	2.54	0.41
1:A:747:PRO:HB3	1:A:884:GLU:HG2	2.02	0.41
1:G:73:LEU:HA	1:G:89:CYS:O	2.20	0.41
1:A:71:MET:O	1:A:72:SER:C	2.58	0.41
1:A:689:LEU:C	1:A:689:LEU:HD12	2.40	0.41
1:G:602:VAL:HB	1:G:639:ILE:CG2	2.51	0.41
1:C:418:THR:HB	1:C:427:LYS:CG	2.49	0.41
1:C:564:TYR:CZ	1:C:588:ARG:HD2	2.55	0.41
2:D:132:LEU:HD22	2:D:192:SER:HB3	2.01	0.41
2:F:187:LYS:HG2	2:F:188:LEU:N	2.35	0.41
2:H:187:LYS:HG2	2:H:188:LEU:N	2.35	0.41
1:E:353:SER:C	1:E:354:PHE:CG	2.92	0.41
1:A:511:ASP:OD1	1:A:514:GLY:HA2	2.21	0.41
2:B:361:ASP:HB2	2:B:390:GLN:HB3	2.02	0.41
2:B:17:SER:HB2	2:B:21:CYS:SG	2.60	0.41
2:H:27:LEU:HD21	2:H:446:GLY:C	2.40	0.41
2:F:162:PRO:O	2:F:165:LEU:CB	2.67	0.41
2:D:162:PRO:O	2:D:165:LEU:CB	2.67	0.41
2:D:543:HIS:HB3	2:D:544:PRO:HD2	2.02	0.41
1:C:698:LEU:C	1:C:699:LEU:HD12	2.41	0.41
1:E:918:TYR:O	1:E:919:LEU:C	2.58	0.41
1:A:599:VAL:CG2	1:A:599:VAL:O	2.65	0.41
1:G:871:LEU:CD1	1:G:901:VAL:HG11	2.50	0.41
1:A:971:HIS:NE2	1:A:974:ASN:HB2	2.35	0.41
1:E:71:MET:O	1:E:72:SER:C	2.58	0.41
1:A:73:LEU:HA	1:A:89:CYS:O	2.20	0.41
1:G:385:TYR:CE1	2:H:253:LEU:CD1	3.04	0.41
1:E:985:ALA:HA	1:E:986:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1065:GLY:O	1:G:1066:GLN:CG	2.68	0.41
1:A:766:PHE:HB3	1:A:786:VAL:HG23	2.02	0.41
1:C:671:ALA:HB2	1:C:700:LEU:HD23	2.01	0.41
1:A:848:HIS:HB2	2:B:485:SER:HB3	2.02	0.41
2:F:132:LEU:HD22	2:F:192:SER:HB3	2.01	0.41
2:B:98:ARG:HD3	2:B:386:PRO:HG3	2.02	0.41
2:F:98:ARG:HD3	2:F:386:PRO:HG3	2.02	0.41
1:C:419:GLN:CG	1:C:424:TRP:CD1	3.03	0.41
2:H:302:SER:HB3	2:H:322:GLU:CG	2.50	0.41
2:F:17:SER:HB2	2:F:21:CYS:SG	2.60	0.41
1:C:448:VAL:HA	1:C:518:THR:HG22	2.03	0.41
1:G:437:SER:HA	1:G:463:HIS:O	2.20	0.41
1:A:637:LEU:HD11	1:A:658:LEU:HD21	2.03	0.41
1:G:372:ILE:HG13	1:G:372:ILE:O	2.20	0.41
2:B:565:ARG:HA	2:B:565:ARG:HD3	1.84	0.41
2:H:160:THR:O	2:H:165:LEU:HD22	2.20	0.41
1:A:772:LYS:O	1:A:773:SER:CB	2.68	0.41
1:A:720:VAL:HG22	1:A:721:GLY:N	2.35	0.41
1:A:919:LEU:O	2:B:643:ARG:NH1	2.53	0.41
1:G:117:GLN:HB3	1:G:121:VAL:CG2	2.50	0.41
1:C:871:LEU:CD1	1:C:901:VAL:HG11	2.50	0.41
1:A:956:VAL:O	1:A:963:VAL:HG23	2.20	0.41
2:D:285:LEU:C	2:D:287:HIS:N	2.71	0.41
1:A:822:LEU:CG	1:A:823:ARG:N	2.83	0.41
2:H:442:PHE:CE1	2:H:449:ARG:HD3	2.56	0.41
1:G:564:TYR:CZ	1:G:588:ARG:HD2	2.55	0.41
1:E:1065:GLY:O	1:E:1066:GLN:CG	2.68	0.41
1:E:671:ALA:O	1:E:672:THR:CG2	2.68	0.41
2:D:188:LEU:CD1	2:D:230:TRP:HA	2.51	0.41
2:D:513:GLU:HG2	2:D:514:CYS:N	2.35	0.41
1:G:915:PHE:CD1	1:G:1074:THR:CG2	3.03	0.41
1:A:353:SER:C	1:A:354:PHE:CG	2.92	0.41
2:H:230:TRP:CE3	2:H:235:ARG:HD3	2.56	0.41
1:A:1060:TYR:O	1:A:1061:SER:HB3	2.21	0.41
1:A:559:SER:O	1:A:560:SER:C	2.59	0.41
2:D:601:GLY:O	2:D:602:LYS:HB2	2.19	0.41
2:F:584:GLY:O	2:F:586:GLN:HG2	2.20	0.41
2:F:160:THR:O	2:F:165:LEU:HD22	2.20	0.41
2:H:15:ILE:HG23	2:H:86:ARG:NE	2.34	0.41
1:G:797:GLY:N	1:G:884:GLU:HB2	2.36	0.41
1:C:710:PRO:HG3	1:C:884:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:314:ILE:HG22	2:D:315:ILE:N	2.35	0.41
2:D:340:LYS:HD2	2:D:379:ASP:CG	2.41	0.41
2:B:616:PRO:HB2	2:B:620:ASN:CA	2.50	0.41
1:C:917:LYS:HE3	1:C:1077:VAL:HG23	2.02	0.41
2:F:188:LEU:HD12	2:F:230:TRP:HA	2.01	0.41
2:B:188:LEU:CD1	2:B:230:TRP:HA	2.51	0.41
2:H:334:ILE:HA	2:H:337:ALA:HB2	2.01	0.41
1:C:1020:VAL:O	1:C:1021:GLN:CB	2.69	0.41
2:F:281:SER:OG	2:F:284:GLN:HB2	2.20	0.41
2:D:352:LEU:HD22	2:D:358:VAL:HG23	2.03	0.41
2:B:234:THR:CG2	2:B:236:LEU:HD13	2.51	0.41
2:F:545:GLY:O	2:F:555:ARG:HA	2.19	0.41
2:F:522:TYR:CE1	2:F:552:GLN:HA	2.54	0.41
2:F:155:LEU:HB2	2:F:156:PRO:CA	2.46	0.41
1:A:789:TRP:NE1	1:C:772:LYS:HB3	2.35	0.41
1:C:597:ARG:HA	1:C:598:PRO:HD3	1.95	0.41
1:A:117:GLN:HB3	1:A:121:VAL:HG21	2.02	0.41
1:E:797:GLY:N	1:E:884:GLU:HB2	2.36	0.41
1:C:71:MET:O	1:C:72:SER:C	2.59	0.41
1:G:971:HIS:NE2	1:G:974:ASN:HB2	2.35	0.41
1:C:956:VAL:O	1:C:963:VAL:HG23	2.21	0.41
2:B:115:TYR:HA	2:B:204:ILE:CD1	2.50	0.41
1:A:603:GLY:O	1:A:638:TYR:CD2	2.73	0.41
1:A:831:SER:CA	1:A:842:THR:HG22	2.51	0.41
1:A:430:VAL:O	1:A:430:VAL:HG23	2.20	0.41
2:B:621:CYS:SG	2:B:625:CYS:SG	3.18	0.41
2:F:58:ASP:N	2:F:59:PRO:CD	2.84	0.41
1:G:671:ALA:HB2	1:G:700:LEU:HD23	2.02	0.41
1:A:917:LYS:HE3	1:A:1077:VAL:HG23	2.02	0.41
2:D:75:GLN:CD	2:D:98:ARG:O	2.59	0.41
1:C:939:ASN:HA	1:C:1018:PHE:HZ	1.85	0.41
2:F:305:VAL:HG13	2:F:306:LYS:HG3	2.03	0.41
2:D:305:VAL:HG13	2:D:306:LYS:HG3	2.03	0.41
2:F:520:GLU:HB3	2:F:550:ALA:HB2	2.03	0.41
1:E:402:VAL:CG1	1:E:443:LEU:HD22	2.51	0.41
1:G:206:PHE:HB2	1:G:208:TYR:HE2	1.85	0.41
1:A:774:LEU:O	1:A:774:LEU:HG	2.21	0.41
1:A:372:ILE:HG13	1:A:372:ILE:O	2.21	0.41
1:G:720:VAL:HG22	1:G:721:GLY:N	2.35	0.41
2:F:219:MET:SD	2:F:285:LEU:HD23	2.60	0.41
2:F:169:CYS:HA	2:F:170:PRO:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:TYR:HA	2:D:204:ILE:CD1	2.50	0.41
1:G:823:ARG:NH1	1:G:825:LEU:O	2.54	0.41
1:E:413:LYS:HG3	1:E:430:VAL:O	2.21	0.41
1:A:413:LYS:HG3	1:A:430:VAL:O	2.21	0.41
1:G:243:LYS:O	1:G:243:LYS:CG	2.69	0.41
1:A:352:GLY:HA2	1:A:356:TRP:HA	2.03	0.41
1:A:1065:GLY:O	1:A:1066:GLN:CG	2.68	0.41
1:G:848:HIS:HB2	2:H:485:SER:HB3	2.02	0.41
7:G:3374:NAG:C3	7:G:3375:MAN:H2	2.50	0.41
2:H:98:ARG:HD3	2:H:386:PRO:HG3	2.02	0.41
2:B:132:LEU:HD22	2:B:192:SER:HB3	2.01	0.41
2:H:234:THR:CG2	2:H:236:LEU:HD13	2.51	0.41
2:F:436:LEU:O	2:F:437:CYS:HB2	2.21	0.41
2:D:472:GLU:HA	2:D:475:CYS:CB	2.50	0.41
2:H:361:ASP:HB2	2:H:390:GLN:HB3	2.02	0.41
1:C:617:ALA:HB1	1:C:702:SER:HA	2.03	0.41
1:E:448:VAL:HA	1:E:518:THR:HG22	2.03	0.41
1:E:372:ILE:HG13	1:E:372:ILE:O	2.21	0.41
2:F:314:ILE:HG22	2:F:315:ILE:N	2.35	0.41
2:B:285:LEU:C	2:B:287:HIS:N	2.71	0.41
1:A:912:HIS:ND1	1:A:935:ARG:CD	2.82	0.41
1:A:629:THR:CG2	1:A:630:LEU:N	2.83	0.41
1:E:117:GLN:HB3	1:E:121:VAL:HG21	2.03	0.41
2:D:462:GLN:HG2	2:D:463:THR:H	1.84	0.41
1:G:665:GLY:CA	2:H:498:HIS:HB3	2.50	0.41
1:E:564:TYR:CZ	1:E:588:ARG:HD2	2.55	0.41
1:E:766:PHE:HB3	1:E:786:VAL:HG23	2.03	0.41
1:G:174:PHE:CB	1:G:212:ALA:HB2	2.50	0.41
1:A:671:ALA:HB2	1:A:700:LEU:HD23	2.02	0.41
1:A:25:TYR:O	1:A:26:ALA:C	2.59	0.41
2:F:105:ILE:HG21	2:F:135:LEU:CD1	2.51	0.41
2:B:106:ASP:OD2	2:B:188:LEU:HD13	2.21	0.41
1:G:419:GLN:CG	1:G:424:TRP:CD1	3.04	0.41
2:B:130:ASP:HA	2:B:133:ARG:HB3	2.02	0.41
1:E:437:SER:HA	1:E:463:HIS:O	2.21	0.41
1:E:559:SER:O	1:E:560:SER:C	2.59	0.41
2:H:436:LEU:O	2:H:437:CYS:HB2	2.21	0.41
2:B:520:GLU:HB3	2:B:550:ALA:HB2	2.03	0.41
1:G:270:GLY:O	1:G:271:LEU:HB3	2.20	0.41
2:D:130:ASP:HA	2:D:133:ARG:HB3	2.03	0.41
2:F:578:VAL:HG12	2:F:579:CYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:154:VAL:HA	2:F:160:THR:CG2	2.49	0.41
2:D:442:PHE:CE1	2:D:449:ARG:HD3	2.55	0.41
2:F:461:CYS:SG	2:F:466:ARG:HD3	2.60	0.41
1:E:722:LYS:N	1:E:723:PRO:HD2	2.33	0.41
1:E:698:LEU:C	1:E:699:LEU:HD12	2.41	0.41
1:C:722:LYS:N	1:C:723:PRO:HD2	2.33	0.41
1:C:919:LEU:CD1	2:D:643:ARG:NH1	2.84	0.41
1:E:919:LEU:CB	1:E:1079:GLU:HB3	2.47	0.41
2:B:317:LYS:NZ	2:B:409:LEU:HB3	2.36	0.41
1:G:562:LEU:HD23	1:G:562:LEU:HA	1.85	0.41
1:C:609:ILE:HB	1:C:610:PRO:CD	2.48	0.41
1:A:871:LEU:HD12	1:A:903:TYR:OH	2.20	0.41
1:A:871:LEU:CD1	1:A:901:VAL:HG11	2.50	0.41
1:A:797:GLY:N	1:A:884:GLU:HB2	2.35	0.41
1:C:116:THR:HG22	1:C:117:GLN:N	2.36	0.41
1:C:117:GLN:HB3	1:C:121:VAL:HG21	2.02	0.41
1:A:509:LEU:HB3	1:A:519:ASP:O	2.21	0.41
1:E:956:VAL:O	1:E:963:VAL:HG23	2.21	0.41
1:C:840:TRP:CD1	1:C:840:TRP:N	2.89	0.41
2:D:219:MET:SD	2:D:285:LEU:HD23	2.60	0.41
1:E:819:GLN:HA	1:E:820:GLY:HA2	1.80	0.41
1:C:507:THR:HG22	1:C:569:LEU:CD1	2.51	0.41
1:A:840:TRP:CD1	1:A:840:TRP:N	2.89	0.41
1:E:436:GLY:HA3	2:F:282:VAL:HG21	2.03	0.41
1:G:352:GLY:HA2	1:G:356:TRP:HA	2.03	0.41
1:G:671:ALA:O	1:G:672:THR:CG2	2.69	0.41
1:E:917:LYS:HE3	1:E:1077:VAL:HG23	2.02	0.41
1:C:908:VAL:HG12	1:C:909:VAL:N	2.35	0.41
1:G:908:VAL:HG12	1:G:909:VAL:N	2.35	0.41
2:F:188:LEU:CD1	2:F:230:TRP:HA	2.51	0.41
2:D:271:TYR:O	2:D:271:TYR:CG	2.74	0.41
2:B:105:ILE:HG21	2:B:135:LEU:CD1	2.51	0.41
1:C:422:ARG:HA	1:C:424:TRP:HZ3	1.86	0.41
1:E:422:ARG:HA	1:E:424:TRP:HZ3	1.86	0.41
2:H:352:LEU:HD22	2:H:358:VAL:HG23	2.03	0.41
1:E:915:PHE:CD1	1:E:1074:THR:CG2	3.04	0.41
2:F:525:GLN:HB3	2:F:529:GLY:N	2.36	0.41
2:D:581:CYS:HB3	2:D:585:TYR:HB2	2.03	0.41
1:A:384:SER:HB2	1:A:405:ALA:HB1	2.03	0.41
2:F:565:ARG:HA	2:F:565:ARG:HD3	1.83	0.41
2:H:565:ARG:HD3	2:H:565:ARG:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:69:HIS:HB2	2:H:70:ASN:H	1.73	0.41
1:E:358:GLY:HA3	1:E:386:LEU:HB3	2.03	0.41
2:D:234:THR:CG2	2:D:236:LEU:HD13	2.51	0.41
1:E:772:LYS:O	1:E:773:SER:CB	2.69	0.41
1:C:469:ARG:HD3	2:D:283:GLY:HA3	2.03	0.41
2:B:314:ILE:HG22	2:B:315:ILE:N	2.35	0.41
1:E:597:ARG:HD2	1:E:731:ARG:O	2.20	0.41
1:E:812:TYR:HD2	1:E:814:ALA:HB2	1.84	0.41
1:C:610:PRO:HG2	1:C:631:VAL:HA	2.03	0.41
1:E:610:PRO:HG2	1:E:631:VAL:HA	2.03	0.41
1:C:797:GLY:N	1:C:884:GLU:HB2	2.36	0.41
2:F:442:PHE:CE1	2:F:449:ARG:HD3	2.56	0.41
1:E:840:TRP:CD1	1:E:840:TRP:N	2.88	0.41
1:A:602:VAL:HB	1:A:639:ILE:CG2	2.51	0.41
1:C:413:LYS:HG3	1:C:430:VAL:O	2.21	0.41
2:D:105:ILE:HG21	2:D:135:LEU:CD1	2.51	0.41
2:D:106:ASP:OD2	2:D:188:LEU:HD13	2.21	0.41
2:B:230:TRP:CE3	2:B:235:ARG:HD3	2.56	0.41
1:A:1020:VAL:O	1:A:1021:GLN:CB	2.68	0.41
1:G:880:ASN:OD1	1:G:894:THR:HG22	2.21	0.41
1:G:448:VAL:HA	1:G:518:THR:HG22	2.03	0.41
2:H:578:VAL:HG12	2:H:579:CYS:N	2.35	0.41
1:G:613:ILE:HD12	1:G:748:PHE:CD2	2.55	0.41
2:F:302:SER:HB3	2:F:322:GLU:CG	2.50	0.41
1:G:559:SER:O	1:G:560:SER:C	2.59	0.41
1:G:358:GLY:HA3	1:G:386:LEU:HB3	2.03	0.41
2:H:424:GLU:OE1	2:H:424:GLU:HA	2.21	0.41
1:E:43:GLN:O	1:E:70:ASN:HA	2.21	0.40
1:A:484:ARG:HH12	2:B:586:GLN:HG3	1.80	0.40
1:A:1064:PRO:HG3	1:A:1067:GLU:OE2	2.18	0.40
2:F:219:MET:O	2:F:223:ALA:HB2	2.21	0.40
1:C:918:TYR:O	1:C:919:LEU:C	2.58	0.40
2:D:285:LEU:O	2:D:287:HIS:N	2.55	0.40
1:E:430:VAL:HG13	1:E:485:TRP:CE3	2.56	0.40
1:A:430:VAL:HG13	1:A:485:TRP:CE3	2.56	0.40
1:E:602:VAL:HB	1:E:639:ILE:CG2	2.51	0.40
2:F:616:PRO:HB2	2:F:620:ASN:CA	2.50	0.40
1:C:25:TYR:O	1:C:26:ALA:C	2.59	0.40
1:C:430:VAL:HG23	1:C:430:VAL:O	2.20	0.40
2:F:230:TRP:CE3	2:F:235:ARG:HD3	2.56	0.40
2:B:75:GLN:CD	2:B:98:ARG:O	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:894:THR:O	1:G:874:ARG:NH2	2.54	0.40
2:B:345:VAL:HG11	2:B:387:ILE:HD11	2.03	0.40
1:A:690:LYS:HG3	1:E:634:ASN:ND2	2.36	0.40
1:A:799:THR:HA	1:A:845:ARG:HA	2.02	0.40
2:F:361:ASP:HB2	2:F:390:GLN:HB3	2.02	0.40
2:D:520:GLU:HB3	2:D:550:ALA:HB2	2.03	0.40
1:C:43:GLN:O	1:C:70:ASN:HA	2.22	0.40
1:C:772:LYS:O	1:C:773:SER:CB	2.68	0.40
2:B:154:VAL:HA	2:B:160:THR:CG2	2.49	0.40
1:A:597:ARG:HG3	1:A:731:ARG:CG	2.51	0.40
1:C:599:VAL:O	1:C:599:VAL:CG2	2.68	0.40
2:F:223:ALA:HB1	2:F:264:CYS:H	1.86	0.40
2:D:317:LYS:HE2	2:D:317:LYS:HB2	1.93	0.40
1:E:614:PRO:O	1:E:615:ARG:HB3	2.22	0.40
1:G:618:PHE:CE2	1:G:619:GLU:HG3	2.56	0.40
2:B:442:PHE:CE1	2:B:449:ARG:HD3	2.56	0.40
1:E:507:THR:HG22	1:E:569:LEU:CD1	2.51	0.40
1:E:639:ILE:HG12	1:E:688:GLY:O	2.21	0.40
1:G:214:GLN:OE1	1:G:253:VAL:HG12	2.20	0.40
2:B:599:PRO:O	2:B:603:TYR:CD2	2.75	0.40
1:E:530:ASN:ND2	1:E:563:GLN:HG2	2.36	0.40
1:C:764:ILE:HD12	1:C:800:ILE:HD13	2.03	0.40
2:F:106:ASP:OD2	2:F:188:LEU:HD13	2.21	0.40
2:H:75:GLN:CD	2:H:98:ARG:O	2.60	0.40
1:A:975:PRO:O	1:A:977:LEU:HD13	2.22	0.40
2:H:611:LYS:HG2	2:H:667:VAL:HB	2.03	0.40
1:A:915:PHE:CD1	1:A:1074:THR:CG2	3.04	0.40
1:G:176:ASN:HB3	1:G:206:PHE:HD1	1.86	0.40
1:A:889:ARG:HB3	1:A:890:THR:H	1.74	0.40
1:C:559:SER:O	1:C:560:SER:C	2.59	0.40
2:B:578:VAL:HG12	2:B:579:CYS:N	2.36	0.40
1:C:637:LEU:HD11	1:C:658:LEU:HD21	2.03	0.40
1:E:623:GLN:C	1:E:624:VAL:HG22	2.39	0.40
2:H:543:HIS:HB3	2:H:544:PRO:HD2	2.02	0.40
1:G:484:ARG:HH11	2:H:594:PRO:HG2	1.85	0.40
2:B:466:ARG:HB2	2:B:491:VAL:HG13	2.02	0.40
2:D:223:ALA:HB1	2:D:264:CYS:H	1.86	0.40
1:E:116:THR:HG22	1:E:117:GLN:N	2.36	0.40
1:G:71:MET:O	1:G:72:SER:C	2.58	0.40
1:A:614:PRO:O	1:A:615:ARG:HB3	2.22	0.40
1:G:530:ASN:ND2	1:G:563:GLN:HG2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:LYS:HE3	1:A:1077:VAL:HG21	2.03	0.40
2:D:139:THR:HG22	2:D:140:GLU:N	2.36	0.40
1:G:827:LEU:HD12	1:G:827:LEU:O	2.21	0.40
2:F:611:LYS:HG2	2:F:667:VAL:HB	2.04	0.40
1:C:944:ARG:N	1:C:1020:VAL:HG21	2.36	0.40
1:E:419:GLN:CG	1:E:424:TRP:CD1	3.03	0.40
2:B:581:CYS:HB3	2:B:585:TYR:HB2	2.03	0.40
1:G:775:LEU:CD1	1:G:904:ALA:HB2	2.51	0.40
2:B:525:GLN:HB3	2:B:529:GLY:N	2.36	0.40
2:F:304:MET:HE3	2:F:307:THR:HG21	2.03	0.40
1:A:332:MET:SD	2:B:208:LEU:HD13	2.61	0.40
1:A:756:HIS:O	1:A:756:HIS:CG	2.74	0.40
2:B:219:MET:O	2:B:223:ALA:HB2	2.21	0.40
1:E:562:LEU:HD23	1:E:562:LEU:HA	1.85	0.40
2:H:176:CYS:HB2	2:H:204:ILE:O	2.22	0.40
1:C:468:THR:HG23	1:C:498:PRO:CG	2.50	0.40
1:G:840:TRP:N	1:G:840:TRP:CD1	2.89	0.40
2:D:615:GLY:HA2	2:D:616:PRO:HD2	1.95	0.40
1:A:613:ILE:HA	1:A:614:PRO:HD3	1.91	0.40
2:D:187:LYS:HG2	2:D:188:LEU:N	2.35	0.40
2:D:230:TRP:CE3	2:D:235:ARG:HD3	2.56	0.40
1:G:815:GLU:HB3	1:G:819:GLN:HE21	1.86	0.40
1:C:764:ILE:HD13	1:C:879:ALA:HB1	2.03	0.40
1:G:422:ARG:HA	1:G:424:TRP:HZ3	1.86	0.40
1:C:799:THR:HG22	1:C:845:ARG:HB3	2.03	0.40
2:H:188:LEU:CD1	2:H:230:TRP:HA	2.51	0.40
2:H:234:THR:HG22	2:H:235:ARG:N	2.36	0.40
2:B:611:LYS:HG2	2:B:667:VAL:HB	2.04	0.40
1:A:502:PHE:CE2	1:A:535:TYR:CD2	3.09	0.40
2:F:440:LYS:HG3	2:F:454:TYR:CZ	2.56	0.40
2:D:578:VAL:HG12	2:D:579:CYS:N	2.36	0.40
1:G:502:PHE:CE2	1:G:535:TYR:CD2	3.10	0.40
1:G:402:VAL:CG1	1:G:443:LEU:HD22	2.51	0.40
1:A:811:ARG:HD3	1:A:864:ASP:OD2	2.22	0.40
1:G:191:SER:O	1:G:192:ASN:OD1	2.40	0.40
1:E:583:LEU:O	1:E:593:LEU:HD23	2.22	0.40
1:E:393:ALA:HB3	1:E:400:SER:HB2	2.04	0.40
2:D:436:LEU:O	2:D:437:CYS:HB2	2.21	0.40
1:E:774:LEU:HG	1:E:774:LEU:O	2.21	0.40
1:A:757:ILE:HG21	1:C:1054:THR:HG21	2.03	0.40
1:A:68:ALA:HA	1:A:93:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:LEU:O	2:B:287:HIS:N	2.55	0.40
2:H:219:MET:O	2:H:223:ALA:HB2	2.21	0.40
2:H:315:ILE:HA	2:H:316:PRO:HD3	1.87	0.40
1:G:156:ARG:HG3	1:G:157:ALA:N	2.35	0.40
1:E:609:ILE:HB	1:E:610:PRO:CD	2.47	0.40
1:G:116:THR:HG22	1:G:117:GLN:N	2.36	0.40
1:G:656:VAL:HG21	1:G:687:LEU:HD12	2.04	0.40
2:B:118:LEU:HD23	2:B:204:ILE:HG21	2.04	0.40
1:G:137:ILE:HG13	1:G:137:ILE:O	2.21	0.40
1:A:507:THR:HG22	1:A:569:LEU:CD1	2.51	0.40
2:H:118:LEU:HD23	2:H:204:ILE:HG21	2.04	0.40
1:G:831:SER:CA	1:G:842:THR:HG22	2.51	0.40
1:G:430:VAL:HG13	1:G:485:TRP:CE3	2.56	0.40
1:A:748:PHE:CD1	1:A:748:PHE:N	2.88	0.40
2:H:243:ASP:O	2:H:304:MET:HE2	2.21	0.40
1:C:639:ILE:HG12	1:C:688:GLY:O	2.22	0.40
1:C:917:LYS:HE3	1:C:1077:VAL:HG21	2.03	0.40
1:A:1023:GLU:O	1:A:1024:LEU:C	2.60	0.40
2:H:271:TYR:CG	2:H:271:TYR:O	2.74	0.40
2:F:271:TYR:CG	2:F:271:TYR:O	2.74	0.40
1:G:1058:SER:O	1:G:1059:VAL:CB	2.70	0.40
2:H:305:VAL:HG13	2:H:306:LYS:HG3	2.03	0.40
2:D:302:SER:O	2:D:305:VAL:HG12	2.22	0.40
1:G:944:ARG:N	1:G:1020:VAL:HG21	2.36	0.40
1:A:679:ARG:O	1:A:679:ARG:HD3	2.22	0.40
1:G:748:PHE:N	1:G:748:PHE:CD1	2.88	0.40
1:G:511:ASP:OD1	1:G:514:GLY:HA2	2.21	0.40
1:A:617:ALA:HB1	1:A:702:SER:HA	2.03	0.40
2:H:513:GLU:HG2	2:H:514:CYS:N	2.36	0.40
1:A:402:VAL:CG1	1:A:443:LEU:HD22	2.51	0.40
2:H:312:THR:CG2	2:H:344:ARG:HH22	2.34	0.40
1:A:583:LEU:O	1:A:593:LEU:HD23	2.21	0.40
1:E:384:SER:HB2	1:E:405:ALA:HB1	2.03	0.40
1:A:358:GLY:HA3	1:A:386:LEU:HB3	2.03	0.40
1:A:52:TYR:O	1:A:53:SER:C	2.60	0.40
2:F:130:ASP:HA	2:F:133:ARG:HB3	2.02	0.40
1:C:372:ILE:O	1:C:372:ILE:HG13	2.21	0.40

All (2) 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)
1:E:622:GLU:OE1	1:G:194:LEU:N[4_455]	1.85	0.35
1:E:622:GLU:OE2	1:G:192:ASN:C[4_455]	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	876/1095 (80%)	660 (75%)	190 (22%)	26 (3%)	5	45
1	C	880/1095 (80%)	662 (75%)	193 (22%)	25 (3%)	6	46
1	E	878/1095 (80%)	659 (75%)	192 (22%)	27 (3%)	5	44
1	G	1080/1095 (99%)	834 (77%)	214 (20%)	32 (3%)	5	45
2	B	671/687 (98%)	511 (76%)	149 (22%)	11 (2%)	12	57
2	D	671/687 (98%)	514 (77%)	144 (22%)	13 (2%)	10	54
2	F	671/687 (98%)	512 (76%)	145 (22%)	14 (2%)	9	52
2	H	671/687 (98%)	512 (76%)	147 (22%)	12 (2%)	11	55
All	All	6398/7128 (90%)	4864 (76%)	1374 (22%)	160 (2%)	7	48

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	757	ILE
2	B	162	PRO
2	B	598	SER
1	C	82	SER
1	C	328	PHE
1	C	757	ILE
2	D	162	PRO
2	D	598	SER
1	E	82	SER
1	E	757	ILE

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Mol	Chain	Res	Type
2	F	162	PRO
2	F	598	SER
1	G	82	SER
1	G	324	SER
1	G	326	SER
1	G	328	PHE
1	G	757	ILE
2	H	162	PRO
2	H	598	SER
1	A	490	VAL
1	A	624	VAL
1	A	691	ALA
1	A	931	VAL
1	A	956	VAL
2	B	314	ILE
1	C	490	VAL
1	C	624	VAL
1	C	691	ALA
1	C	931	VAL
1	C	956	VAL
2	D	314	ILE
1	E	490	VAL
1	E	624	VAL
1	E	691	ALA
1	E	931	VAL
1	E	956	VAL
2	F	314	ILE
1	G	194	LEU
1	G	490	VAL
1	G	624	VAL
1	G	691	ALA
1	G	931	VAL
1	G	956	VAL
2	H	314	ILE
1	A	70	ASN
1	A	563	GLN
1	A	649	SER
1	A	722	LYS
1	A	847	ASN
2	B	467	SER
2	B	639	THR
1	C	70	ASN

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Mol	Chain	Res	Type
1	C	563	GLN
1	C	649	SER
1	C	722	LYS
1	C	847	ASN
2	D	467	SER
2	D	639	THR
1	E	70	ASN
1	E	563	GLN
1	E	649	SER
1	E	722	LYS
1	E	755	ASP
1	E	847	ASN
2	F	433	ASP
2	F	467	SER
2	F	639	THR
1	G	70	ASN
1	G	563	GLN
1	G	649	SER
1	G	722	LYS
1	G	847	ASN
2	H	69	HIS
2	H	467	SER
2	H	639	THR
1	A	124	GLN
1	A	354	PHE
1	A	773	SER
1	A	816	GLY
2	B	141	SER
1	C	124	GLN
1	C	354	PHE
1	C	773	SER
2	D	141	SER
1	E	124	GLN
1	E	354	PHE
1	E	773	SER
2	F	101	LYS
2	F	141	SER
1	G	124	GLN
1	G	327	SER
1	G	354	PHE
1	G	558	LEU
1	G	773	SER

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Mol	Chain	Res	Type
2	H	141	SER
1	A	375	SER
1	A	558	LEU
2	B	69	HIS
1	C	375	SER
1	C	558	LEU
1	C	816	GLY
2	D	433	ASP
1	E	375	SER
1	E	558	LEU
1	G	193	PRO
1	G	246	ASP
1	G	375	SER
1	G	751	ASN
1	G	816	GLY
1	A	846	ILE
1	A	872	GLY
1	C	846	ILE
1	C	872	GLY
2	D	351	ALA
2	D	617	PHE
1	E	730	LEU
1	E	816	GLY
1	E	846	ILE
1	E	872	GLY
2	F	351	ALA
2	F	617	PHE
1	G	846	ILE
1	G	872	GLY
2	H	351	ALA
1	A	121	VAL
1	C	121	VAL
1	E	121	VAL
1	G	121	VAL
1	A	1016	PRO
2	B	204	ILE
2	B	517	ILE
1	C	1016	PRO
2	D	517	ILE
1	E	1016	PRO
2	F	517	ILE
1	G	1016	PRO

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Mol	Chain	Res	Type
2	H	447	ILE
2	H	517	ILE
1	A	540	VAL
2	B	447	ILE
2	B	486	GLY
1	C	540	VAL
2	D	204	ILE
2	D	447	ILE
1	E	540	VAL
2	F	204	ILE
2	F	447	ILE
2	F	486	GLY
1	G	540	VAL
2	H	204	ILE
2	H	486	GLY
1	A	942	GLY
2	D	486	GLY
1	E	581	VAL
1	A	581	VAL
1	A	120	PRO
1	C	120	PRO
1	E	120	PRO
1	G	120	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	749/934 (80%)	737 (98%)	12 (2%)	70	89
1	C	753/934 (81%)	743 (99%)	10 (1%)	76	90
1	E	751/934 (80%)	741 (99%)	10 (1%)	76	90
1	G	924/934 (99%)	911 (99%)	13 (1%)	74	89
2	B	582/592 (98%)	582 (100%)	0	100	100
2	D	582/592 (98%)	582 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	582/592 (98%)	582 (100%)	0	100	100
2	H	582/592 (98%)	582 (100%)	0	100	100
All	All	5505/6104 (90%)	5460 (99%)	45 (1%)	86	94

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	PHE
1	A	567	GLN
1	A	600	LEU
1	A	620	CYS
1	A	679	ARG
1	A	681	LEU
1	A	714	ARG
1	A	823	ARG
1	A	840	TRP
1	A	915	PHE
1	A	964	TRP
1	A	1055	PHE
1	C	565	PHE
1	C	567	GLN
1	C	600	LEU
1	C	679	ARG
1	C	714	ARG
1	C	823	ARG
1	C	840	TRP
1	C	915	PHE
1	C	964	TRP
1	C	1055	PHE
1	E	565	PHE
1	E	567	GLN
1	E	600	LEU
1	E	679	ARG
1	E	714	ARG
1	E	823	ARG
1	E	840	TRP
1	E	915	PHE
1	E	964	TRP
1	E	1055	PHE
1	G	128	ARG
1	G	129	GLN

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Mol	Chain	Res	Type
1	G	191	SER
1	G	565	PHE
1	G	567	GLN
1	G	600	LEU
1	G	679	ARG
1	G	714	ARG
1	G	823	ARG
1	G	840	TRP
1	G	915	PHE
1	G	964	TRP
1	G	1055	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	472	GLN
1	A	495	GLN
1	A	567	GLN
1	A	692	HIS
1	A	819	GLN
2	B	159	ASN
2	B	295	GLN
1	C	334	GLN
1	C	434	GLN
1	C	472	GLN
1	C	495	GLN
1	C	567	GLN
1	C	692	HIS
1	C	819	GLN
2	D	159	ASN
2	D	295	GLN
2	D	479	ASN
1	E	334	GLN
1	E	472	GLN
1	E	495	GLN
1	E	567	GLN
1	E	692	HIS
1	E	819	GLN
2	F	159	ASN
2	F	295	GLN
2	F	479	ASN

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Mol	Chain	Res	Type
1	G	334	GLN
1	G	472	GLN
1	G	495	GLN
1	G	567	GLN
1	G	692	HIS
1	G	819	GLN
2	H	159	ASN
2	H	295	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

35 carbohydrates are modelled in this entry.

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	$\# Z  > 2$
3	NAG	A	3042	1,3	14,14,15	0.55	0	15,19,21	0.58	0
3	NAG	A	3043	3	14,14,15	0.64	0	15,19,21	1.09	1 (6%)
4	NAG	A	3373	1,4	14,14,15	0.50	0	15,19,21	1.01	1 (6%)
4	NAG	A	3374	4	14,14,15	0.50	0	15,19,21	2.24	1 (6%)
4	MAN	A	3375	4	11,11,12	0.53	0	14,15,17	1.06	2 (14%)
4	NAG	A	3716	1,4	14,14,15	0.70	0	15,19,21	1.22	2 (13%)
4	NAG	A	3717	4	14,14,15	0.61	0	15,19,21	0.89	1 (6%)
4	MAN	A	3718	4	11,11,12	0.61	0	14,15,17	1.43	2 (14%)
4	NAG	A	3880	1,4	14,14,15	0.68	0	15,19,21	2.05	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	3881	4	14,14,15	0.54	0	15,19,21	0.85	0
4	MAN	A	3882	4	11,11,12	0.62	0	14,15,17	1.68	2 (14%)
3	NAG	C	3042	1,3	14,14,15	0.47	0	15,19,21	0.72	0
3	NAG	C	3043	3	14,14,15	0.61	0	15,19,21	1.20	1 (6%)
3	NAG	C	3373	1,3	14,14,15	0.52	0	15,19,21	1.09	1 (6%)
3	NAG	C	3374	3	14,14,15	0.62	0	15,19,21	2.06	1 (6%)
4	NAG	C	3716	1,4	14,14,15	0.58	0	15,19,21	1.44	1 (6%)
4	NAG	C	3717	4	14,14,15	0.58	0	15,19,21	0.97	1 (6%)
4	MAN	C	3718	4	11,11,12	0.65	0	14,15,17	1.54	2 (14%)
3	NAG	E	3042	1,3	14,14,15	0.48	0	15,19,21	0.83	0
3	NAG	E	3043	3	14,14,15	0.63	0	15,19,21	1.15	1 (6%)
4	NAG	E	3373	1,4	14,14,15	0.35	0	15,19,21	0.87	1 (6%)
4	NAG	E	3374	4	14,14,15	0.71	0	15,19,21	1.84	3 (20%)
4	MAN	E	3375	4	11,11,12	0.62	0	14,15,17	1.25	2 (14%)
4	NAG	E	3716	1,4	14,14,15	0.68	0	15,19,21	1.03	1 (6%)
4	NAG	E	3717	4	14,14,15	0.58	0	15,19,21	0.95	1 (6%)
4	MAN	E	3718	4	11,11,12	0.65	0	14,15,17	1.60	2 (14%)
3	NAG	G	3042	1,3	14,14,15	0.55	0	15,19,21	0.69	0
3	NAG	G	3043	3	14,14,15	0.60	0	15,19,21	1.08	1 (6%)
7	NAG	G	3373	1,7	14,14,15	0.49	0	15,19,21	0.92	1 (6%)
7	NAG	G	3374	7	14,14,15	0.56	0	15,19,21	2.20	1 (6%)
7	MAN	G	3375	7	11,11,12	0.53	0	14,15,17	0.85	0
7	MAN	G	3377	7	11,11,12	0.61	0	14,15,17	0.58	0
4	NAG	G	3716	1,4	14,14,15	0.62	0	15,19,21	1.85	2 (13%)
4	NAG	G	3717	4	14,14,15	0.61	0	15,19,21	0.88	1 (6%)
4	MAN	G	3718	4	11,11,12	0.65	0	14,15,17	1.45	2 (14%)

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
3	NAG	A	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3043	3	-	0/6/23/26	0/1/1/1
4	NAG	A	3373	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	3374	4	-	0/6/23/26	0/1/1/1
4	MAN	A	3375	4	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	3716	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3717	4	-	0/6/23/26	0/1/1/1
4	MAN	A	3718	4	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	A	3880	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3881	4	-	0/6/23/26	0/1/1/1
4	MAN	A	3882	4	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	C	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3043	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3373	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3374	3	-	0/6/23/26	0/1/1/1
4	NAG	C	3716	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	3717	4	-	0/6/23/26	0/1/1/1
4	MAN	C	3718	4	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	E	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	3043	3	-	0/6/23/26	0/1/1/1
4	NAG	E	3373	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	3374	4	-	0/6/23/26	0/1/1/1
4	MAN	E	3375	4	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	E	3716	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	3717	4	-	0/6/23/26	0/1/1/1
4	MAN	E	3718	4	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	G	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	3043	3	-	0/6/23/26	0/1/1/1
7	NAG	G	3373	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	3374	7	-	0/6/23/26	0/1/1/1
7	MAN	G	3375	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	G	3377	7	-	0/2/19/22	0/1/1/1
4	NAG	G	3716	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	3717	4	-	0/6/23/26	0/1/1/1
4	MAN	G	3718	4	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3375	MAN	C1-O5-C5	-2.50	109.08	112.25
4	A	3375	MAN	C2-C3-C4	-2.33	107.08	111.04
4	E	3375	MAN	C1-C2-C3	-2.28	106.84	109.54
4	E	3373	NAG	C1-O5-C5	2.05	114.86	112.25
4	A	3375	MAN	O5-C5-C6	2.07	111.83	107.35
4	E	3717	NAG	O4-C4-C3	2.08	115.03	110.34
4	A	3717	NAG	O4-C4-C3	2.11	115.09	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3716	NAG	C4-C3-C2	2.13	114.55	111.23
7	G	3373	NAG	C1-O5-C5	2.28	115.14	112.25
4	G	3717	NAG	O4-C4-C3	2.31	115.54	110.34
4	E	3374	NAG	C3-C4-C5	2.32	114.25	110.20
4	C	3717	NAG	O4-C4-C3	2.39	115.72	110.34
4	A	3880	NAG	C4-C3-C2	2.45	115.04	111.23
4	E	3716	NAG	C4-C3-C2	2.53	115.16	111.23
4	A	3716	NAG	C1-O5-C5	2.71	115.68	112.25
4	A	3373	NAG	C1-O5-C5	2.85	115.86	112.25
4	A	3716	NAG	C4-C3-C2	2.85	115.66	111.23
3	G	3043	NAG	C1-O5-C5	2.93	115.96	112.25
3	A	3043	NAG	C1-O5-C5	3.12	116.21	112.25
3	C	3373	NAG	C1-O5-C5	3.15	116.25	112.25
3	E	3043	NAG	C1-O5-C5	3.31	116.45	112.25
4	C	3718	MAN	C1-O5-C5	3.34	116.49	112.25
4	A	3718	MAN	C1-O5-C5	3.39	116.55	112.25
4	G	3718	MAN	C1-O5-C5	3.39	116.55	112.25
4	A	3880	NAG	C3-C4-C5	3.55	116.39	110.20
4	A	3718	MAN	C1-C2-C3	3.60	113.80	109.54
4	G	3718	MAN	C1-C2-C3	3.64	113.84	109.54
3	C	3043	NAG	C1-O5-C5	3.68	116.92	112.25
4	E	3374	NAG	C4-C3-C2	3.77	117.08	111.23
4	A	3882	MAN	C1-C2-C3	3.95	114.21	109.54
4	E	3718	MAN	C1-O5-C5	3.97	117.28	112.25
4	C	3718	MAN	C1-C2-C3	4.03	114.31	109.54
4	E	3718	MAN	C1-C2-C3	4.06	114.35	109.54
4	A	3882	MAN	C1-O5-C5	4.28	117.68	112.25
4	E	3374	NAG	C1-O5-C5	4.71	118.22	112.25
4	C	3716	NAG	C1-O5-C5	4.73	118.25	112.25
4	A	3880	NAG	C1-O5-C5	5.71	119.49	112.25
4	G	3716	NAG	C1-O5-C5	6.35	120.31	112.25
3	C	3374	NAG	C1-O5-C5	7.49	121.76	112.25
7	G	3374	NAG	C1-O5-C5	7.86	122.23	112.25
4	A	3374	NAG	C1-O5-C5	8.01	122.42	112.25

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	3718	MAN	C1
4	A	3373	NAG	C1
4	A	3375	MAN	C1
4	A	3882	MAN	C1

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Mol	Chain	Res	Type	Atom
4	E	3375	MAN	C1
4	E	3718	MAN	C1
4	G	3718	MAN	C1
4	A	3718	MAN	C1
7	G	3375	MAN	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3373	NAG	1	0
4	A	3374	NAG	2	0
4	A	3375	MAN	2	0
4	E	3373	NAG	8	0
4	E	3374	NAG	5	0
7	G	3374	NAG	2	0
7	G	3375	MAN	2	0
4	G	3716	NAG	1	0

## 5.6 Ligand geometry

Of 32 ligands modelled in this entry, 17 are monoatomic - leaving 15 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	NAG	A	3678	1	14,14,15	0.48	0	15,19,21	0.81	1 (6%)
5	NAG	B	3094	2	14,14,15	0.44	0	15,19,21	0.95	1 (6%)
5	NAG	B	3479	-	14,14,15	0.46	0	15,19,21	0.96	1 (6%)
5	NAG	C	3678	1	14,14,15	0.49	0	15,19,21	0.66	0
5	NAG	C	3880	1	14,14,15	0.45	0	15,19,21	1.63	1 (6%)
5	NAG	D	3094	2	14,14,15	0.44	0	15,19,21	0.82	0
5	NAG	D	3479	-	14,14,15	0.44	0	15,19,21	0.92	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	3678	1	14,14,15	0.49	0	15,19,21	0.85	1 (6%)
5	NAG	E	3880	1	14,14,15	0.42	0	15,19,21	1.84	1 (6%)
5	NAG	F	3094	2	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
5	NAG	F	3479	-	14,14,15	0.53	0	15,19,21	0.88	1 (6%)
5	NAG	G	3678	1	14,14,15	0.48	0	15,19,21	0.80	1 (6%)
5	NAG	G	3880	1	14,14,15	0.46	0	15,19,21	1.72	1 (6%)
5	NAG	H	3094	2	14,14,15	0.51	0	15,19,21	0.83	1 (6%)
5	NAG	H	3479	-	14,14,15	0.47	0	15,19,21	0.98	0

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	NAG	A	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	B	3479	-	-	0/6/23/26	0/1/1/1
5	NAG	C	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3880	1	-	0/6/23/26	0/1/1/1
5	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	D	3479	-	-	0/6/23/26	0/1/1/1
5	NAG	E	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	E	3880	1	-	0/6/23/26	0/1/1/1
5	NAG	F	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	F	3479	-	-	0/6/23/26	0/1/1/1
5	NAG	G	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	G	3880	1	-	0/6/23/26	0/1/1/1
5	NAG	H	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	H	3479	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3479	NAG	C2-N2-C7	-2.46	119.88	123.04
5	A	3678	NAG	C1-O5-C5	2.21	115.05	112.25
5	E	3678	NAG	C1-O5-C5	2.26	115.11	112.25
5	G	3678	NAG	C1-O5-C5	2.33	115.20	112.25
5	F	3479	NAG	C1-O5-C5	2.45	115.36	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3094	NAG	C1-O5-C5	2.55	115.49	112.25
5	B	3094	NAG	C1-O5-C5	2.60	115.55	112.25
5	H	3094	NAG	C1-O5-C5	2.62	115.58	112.25
5	C	3880	NAG	C1-O5-C5	5.36	119.05	112.25
5	G	3880	NAG	C1-O5-C5	5.87	119.70	112.25
5	E	3880	NAG	C1-O5-C5	6.22	120.14	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3678	NAG	1	0
5	D	3479	NAG	8	0
5	E	3678	NAG	1	0
5	F	3479	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	880/1095 (80%)	0.28	35 (3%)	42	31	101, 200, 285, 359	0
1	C	884/1095 (80%)	0.25	37 (4%)	40	29	97, 199, 281, 348	0
1	E	882/1095 (80%)	0.31	47 (5%)	30	22	96, 199, 284, 352	0
1	G	1082/1095 (98%)	0.47	89 (8%)	14	10	99, 211, 324, 419	0
2	B	673/687 (97%)	0.49	79 (11%)	6	6	139, 249, 313, 389	2 (0%)
2	D	673/687 (97%)	0.66	83 (12%)	5	5	140, 249, 312, 366	2 (0%)
2	F	673/687 (97%)	0.66	91 (13%)	4	4	141, 250, 314, 382	2 (0%)
2	H	673/687 (97%)	0.41	59 (8%)	12	9	141, 249, 313, 371	2 (0%)
All	All	6420/7128 (90%)	0.43	520 (8%)	15	10	96, 225, 307, 419	8 (0%)

All (520) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	92	ALA	8.6
2	D	430	GLN	8.5
2	F	107	LEU	8.1
1	A	482	TRP	7.7
1	G	482	TRP	7.5
2	B	329	ASN	7.2
2	B	92	ALA	7.2
2	D	71	GLY	6.7
2	B	91	ALA	6.7
2	F	236	LEU	6.4
1	G	321	GLU	6.4
1	G	239	THR	6.4
1	G	322	THR	6.3
1	G	220	LEU	6.3
2	F	429	ASP	6.3
2	D	72	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
2	F	629	GLN	6.0
2	F	91	ALA	5.9
1	G	136	LEU	5.9
2	F	628	LEU	5.9
2	D	1	GLN	5.9
1	G	265	TYR	5.8
1	E	482	TRP	5.7
2	F	431	SER	5.7
1	G	238	ILE	5.6
1	G	817	GLN	5.5
1	A	124	GLN	5.5
2	B	469	GLN	5.4
2	H	469	GLN	5.4
1	G	323	THR	5.4
2	F	393	VAL	5.4
2	H	93	PHE	5.3
1	G	278	SER	5.3
1	E	821	GLN	5.3
2	F	70	ASN	5.3
1	C	482	TRP	5.2
1	A	33	GLY	5.2
2	B	73	GLN	5.1
2	D	91	ALA	5.1
1	E	124	GLN	5.1
1	G	135	PHE	5.0
1	G	234	ILE	5.0
2	H	72	GLY	5.0
2	D	161	HIS	4.9
2	F	71	GLY	4.9
2	B	318	SER	4.8
2	D	389	PHE	4.8
1	G	251	LYS	4.8
1	C	9	THR	4.8
2	D	668	ASP	4.8
1	A	1078	LEU	4.7
2	D	160	THR	4.7
2	F	386	PRO	4.7
1	A	95	HIS	4.6
1	G	108	PHE	4.6
2	B	415	VAL	4.6
1	G	266	ALA	4.6
2	H	470	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	416	THR	4.6
2	H	180	PHE	4.5
2	D	432	ARG	4.5
2	F	72	GLY	4.4
1	G	267	ILE	4.4
2	D	37	SER	4.4
2	B	32	PRO	4.4
2	F	109	TYR	4.3
2	F	664	LEU	4.3
1	A	594	LEU	4.3
1	G	483	ARG	4.3
2	B	433	ASP	4.3
2	D	367	GLY	4.3
2	B	237	LEU	4.2
2	D	237	LEU	4.2
2	H	629	GLN	4.1
2	F	160	THR	4.1
1	C	623	GLN	4.1
1	E	102	TYR	4.1
1	E	594	LEU	4.1
1	E	1044	LYS	4.1
2	D	62	LEU	4.1
2	F	144	ILE	4.0
2	B	432	ARG	4.0
2	D	236	LEU	4.0
1	A	87	LEU	4.0
1	E	95	HIS	4.0
2	F	389	PHE	4.0
1	A	821	GLN	3.9
1	A	127	PRO	3.9
1	G	217	VAL	3.9
2	F	161	HIS	3.9
2	D	433	ASP	3.9
1	C	817	GLN	3.9
1	E	817	GLN	3.9
2	D	92	ALA	3.9
1	A	106	LEU	3.9
1	A	346	PRO	3.9
2	B	389	PHE	3.9
1	A	102	TYR	3.9
1	C	13	VAL	3.9
1	G	285	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	328	SER	3.9
1	A	88	ALA	3.8
2	H	91	ALA	3.8
1	E	117	GLN	3.8
2	B	107	LEU	3.8
2	H	227	GLU	3.8
1	A	77	LEU	3.8
2	F	106	ASP	3.8
2	D	431	SER	3.8
2	D	63	ALA	3.8
1	G	127	PRO	3.7
1	G	277	ASN	3.7
2	B	629	GLN	3.7
2	F	433	ASP	3.7
2	D	622	SER	3.7
2	B	236	LEU	3.7
2	H	1	GLN	3.7
2	F	145	GLY	3.7
2	D	429	ASP	3.7
1	A	817	GLN	3.7
1	G	821	GLN	3.7
1	G	216	VAL	3.7
1	E	1078	LEU	3.7
2	B	664	LEU	3.6
1	G	250	TYR	3.6
2	F	81	VAL	3.6
2	H	37	SER	3.6
2	B	31	GLY	3.6
1	G	320	THR	3.6
2	F	416	THR	3.6
1	G	124	GLN	3.6
1	G	1045	VAL	3.6
2	B	330	VAL	3.6
2	B	463	THR	3.6
2	B	186	LEU	3.6
2	D	443	LEU	3.6
2	H	335	LYS	3.6
2	F	414	ILE	3.6
1	G	171	LEU	3.5
2	B	663	TYR	3.5
2	D	393	VAL	3.5
1	G	125	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	236	ILE	3.5
2	H	133	ARG	3.5
2	B	430	GLN	3.5
2	H	393	VAL	3.5
1	G	88	ALA	3.5
2	H	236	LEU	3.5
2	D	206	GLY	3.5
2	B	391	VAL	3.5
2	F	68	ASP	3.5
2	H	389	PHE	3.5
1	G	332	MET	3.5
1	E	918	TYR	3.5
2	B	202	GLN	3.5
2	F	428	ARG	3.4
2	H	433	ASP	3.4
2	F	266	LEU	3.4
2	D	107	LEU	3.4
1	G	106	LEU	3.4
1	G	137	ILE	3.4
1	G	221	PHE	3.4
1	G	172	MET	3.4
1	E	1045	VAL	3.4
1	G	235	LEU	3.4
1	C	483	ARG	3.4
2	F	92	ALA	3.4
1	C	124	GLN	3.4
2	B	68	ASP	3.4
2	F	97	PHE	3.3
2	F	430	GLN	3.3
2	F	133	ARG	3.3
1	A	108	PHE	3.3
2	F	665	ILE	3.3
1	G	209	THR	3.3
2	D	93	PHE	3.3
2	B	171	ASN	3.3
2	D	331	VAL	3.3
2	F	1	GLN	3.3
2	H	432	ARG	3.3
2	H	391	VAL	3.3
2	D	171	ASN	3.3
1	G	213	ILE	3.3
1	A	918	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	1078	LEU	3.2
2	F	76	LEU	3.2
2	D	669	GLU	3.2
2	F	635	VAL	3.2
1	C	821	GLN	3.2
1	E	483	ARG	3.2
2	D	122	ARG	3.2
2	F	622	SER	3.2
1	G	1078	LEU	3.2
2	H	430	GLN	3.2
1	G	87	LEU	3.2
2	D	651	ALA	3.2
2	F	29	PHE	3.2
1	C	10	ALA	3.1
2	B	23	TRP	3.1
2	B	470	GLU	3.1
2	H	650	VAL	3.1
2	B	1	GLN	3.1
2	F	93	PHE	3.1
1	E	1065	GLY	3.1
2	B	37	SER	3.1
1	G	138	ASP	3.1
2	B	72	GLY	3.1
2	B	366	ASN	3.1
2	D	634	PRO	3.1
1	G	237	VAL	3.1
1	G	233	LYS	3.1
2	H	161	HIS	3.0
1	E	9	THR	3.0
2	B	122	ARG	3.0
1	G	335	GLU	3.0
2	H	107	LEU	3.0
1	A	347	VAL	3.0
1	C	533	ALA	3.0
1	E	61	GLY	3.0
2	H	331	VAL	3.0
1	G	918	TYR	3.0
2	F	387	ILE	3.0
2	F	663	TYR	3.0
1	E	119	LEU	3.0
2	F	318	SER	3.0
2	F	371	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	71	GLY	3.0
2	B	67	GLU	3.0
2	F	369	THR	3.0
2	D	100	ALA	3.0
2	D	133	ARG	3.0
2	D	8	VAL	3.0
1	A	481	GLY	2.9
1	A	553	ILE	2.9
1	C	907	THR	2.9
2	B	323	LEU	2.9
2	B	414	ILE	2.9
1	C	108	PHE	2.9
2	F	26	LYS	2.9
1	C	624	VAL	2.9
2	F	207	ASN	2.9
2	H	664	LEU	2.9
1	C	74	GLY	2.9
1	A	46	GLY	2.9
2	D	38	ILE	2.9
2	H	207	ASN	2.9
2	H	272	LYS	2.9
2	D	602	LYS	2.9
2	D	623	ALA	2.9
2	D	415	VAL	2.9
2	F	49	ARG	2.9
2	H	651	ALA	2.9
2	H	334	ILE	2.9
1	E	13	VAL	2.9
2	B	630	LEU	2.9
1	A	529	GLU	2.9
2	H	145	GLY	2.8
1	C	594	LEU	2.8
2	F	96	THR	2.8
1	A	61	GLY	2.8
1	C	102	TYR	2.8
2	D	629	GLN	2.8
1	E	106	LEU	2.8
2	D	391	VAL	2.8
2	B	176	CYS	2.8
2	H	610	LEU	2.8
1	G	180	THR	2.8
1	G	240	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	245	GLY	2.8
2	D	296	PRO	2.8
2	F	122	ARG	2.8
2	H	206	GLY	2.8
1	E	108	PHE	2.8
2	H	667	VAL	2.8
2	F	624	ALA	2.8
2	D	267	GLU	2.7
2	D	395	ALA	2.7
2	D	43	ARG	2.7
2	B	654	LEU	2.7
2	D	399	ILE	2.7
2	F	202	GLN	2.7
1	C	729	ASN	2.7
1	G	481	GLY	2.7
2	F	206	GLY	2.7
1	G	173	GLN	2.7
2	D	667	VAL	2.7
2	B	93	PHE	2.7
1	G	529	GLU	2.7
2	B	161	HIS	2.7
2	F	320	VAL	2.7
2	H	35	PRO	2.7
1	C	553	ILE	2.7
1	E	591	VAL	2.7
2	F	95	VAL	2.7
2	F	185	VAL	2.7
2	H	628	LEU	2.7
1	A	425	ARG	2.7
1	G	816	GLY	2.7
1	E	593	LEU	2.7
2	D	95	VAL	2.7
2	D	345	VAL	2.7
2	D	96	THR	2.6
1	G	295	PHE	2.6
2	D	185	VAL	2.6
2	H	49	ARG	2.6
1	E	592	LEU	2.6
1	G	296	LYS	2.6
2	F	667	VAL	2.6
2	B	160	THR	2.6
1	C	724	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	12	ARG	2.6
1	E	907	THR	2.6
1	C	88	ALA	2.6
2	F	345	VAL	2.6
2	D	387	ILE	2.6
2	F	171	ASN	2.6
1	E	480	ARG	2.6
2	H	474	SER	2.6
1	G	480	ARG	2.5
2	B	39	ARG	2.5
2	D	56	ILE	2.5
1	C	534	VAL	2.5
2	B	347	LEU	2.5
2	B	404	PHE	2.5
1	G	1044	LYS	2.5
1	G	118	ARG	2.5
2	D	466	ARG	2.5
2	F	627	GLY	2.5
1	G	133	ILE	2.5
1	G	181	HIS	2.5
2	F	651	ALA	2.5
1	G	324	SER	2.5
2	B	30	THR	2.5
2	H	109	TYR	2.5
2	F	415	VAL	2.5
2	D	102	GLY	2.5
2	F	190	ASN	2.5
2	B	393	VAL	2.5
2	F	623	ALA	2.5
2	D	664	LEU	2.5
1	G	973	GLN	2.5
2	D	226	GLU	2.5
1	E	10	ALA	2.5
1	E	623	GLN	2.5
2	F	438	HIS	2.5
2	D	79	GLN	2.5
1	E	125	GLU	2.5
1	E	721	GLY	2.5
2	D	172	LYS	2.5
2	D	416	THR	2.4
2	F	85	LEU	2.4
2	B	407	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	390	GLN	2.4
2	B	443	LEU	2.4
2	F	602	LYS	2.4
1	G	215	ASN	2.4
1	G	261	GLY	2.4
1	E	484	ARG	2.4
2	B	424	GLU	2.4
2	H	226	GLU	2.4
2	D	123	ASN	2.4
2	D	294	ILE	2.4
2	F	339	ASN	2.4
1	A	963	VAL	2.4
2	F	407	ARG	2.4
2	B	109	TYR	2.4
2	B	406	ILE	2.4
1	E	653	GLN	2.4
1	C	326	SER	2.4
1	G	592	LEU	2.4
2	F	404	PHE	2.4
2	D	368	VAL	2.4
2	F	35	PRO	2.4
1	A	1079	GLU	2.4
2	D	68	ASP	2.4
2	F	195	PHE	2.4
2	H	369	THR	2.4
2	D	35	PRO	2.4
2	B	49	ARG	2.4
2	B	375	ARG	2.4
2	B	622	SER	2.3
1	A	101	MET	2.3
2	B	102	GLY	2.3
2	H	73	GLN	2.3
2	H	189	THR	2.3
2	D	101	LYS	2.3
2	F	418	GLN	2.3
1	E	485	TRP	2.3
1	C	653	GLN	2.3
2	B	185	VAL	2.3
2	F	669	GLU	2.3
1	G	282	LEU	2.3
1	G	594	LEU	2.3
1	G	557	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	918	TYR	2.3
1	G	281	GLU	2.3
1	G	268	GLY	2.3
2	B	95	VAL	2.3
2	F	466	ARG	2.3
1	C	592	LEU	2.3
2	B	623	ALA	2.3
1	E	104	THR	2.3
2	H	663	TYR	2.3
1	C	95	HIS	2.3
2	F	384	ASN	2.3
1	G	169	PHE	2.3
2	B	431	SER	2.3
1	E	973	GLN	2.3
2	F	105	ILE	2.3
1	G	225	TYR	2.3
2	D	74	LYS	2.3
2	H	363	PHE	2.3
1	C	46	GLY	2.3
2	D	407	ARG	2.3
2	F	446	GLY	2.2
1	A	848	HIS	2.2
2	B	628	LEU	2.2
2	H	136	ASN	2.2
2	B	423	CYS	2.2
2	B	351	ALA	2.2
2	D	330	VAL	2.2
2	F	226	GLU	2.2
2	F	443	LEU	2.2
2	H	179	PRO	2.2
1	C	57	CYS	2.2
2	B	35	PRO	2.2
2	D	73	GLN	2.2
2	B	66	GLN	2.2
1	E	332	MET	2.2
2	H	70	ASN	2.2
1	E	599	VAL	2.2
2	B	665	ILE	2.2
1	E	725	LEU	2.2
2	H	186	LEU	2.2
1	A	964	TRP	2.2
1	C	1047	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	331	VAL	2.2
2	B	345	VAL	2.2
1	E	996	GLN	2.2
2	F	189	THR	2.2
2	H	345	VAL	2.2
2	B	8	VAL	2.2
1	A	394	LEU	2.2
2	B	203	LEU	2.2
2	D	70	ASN	2.2
2	F	630	LEU	2.2
2	H	113	LEU	2.2
2	F	392	LYS	2.2
1	G	394	LEU	2.2
2	D	454	TYR	2.2
2	H	395	ALA	2.2
1	E	347	VAL	2.2
1	A	1081	TYR	2.2
2	B	331	VAL	2.2
1	C	87	LEU	2.1
1	E	62	LEU	2.1
2	D	650	VAL	2.1
2	F	32	PRO	2.1
1	C	8	LEU	2.1
1	C	1001	LEU	2.1
1	E	87	LEU	2.1
1	E	626	SER	2.1
2	B	390	GLN	2.1
2	F	40	CYS	2.1
2	H	36	ASP	2.1
1	E	481	GLY	2.1
1	C	12	ARG	2.1
2	B	101	LYS	2.1
2	H	406	ILE	2.1
1	G	252	ASP	2.1
2	F	84	TYR	2.1
2	H	618	GLY	2.1
2	B	29	PHE	2.1
1	E	651	ASP	2.1
2	D	36	ASP	2.1
2	H	431	SER	2.1
1	E	1043	LYS	2.1
1	G	422	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	611	LYS	2.1
2	F	5	LYS	2.1
2	F	27	LEU	2.1
2	B	190	ASN	2.1
1	G	653	GLN	2.1
1	C	1044	LYS	2.1
1	A	78	ALA	2.1
1	A	340	VAL	2.1
1	G	244	GLU	2.1
2	D	118	LEU	2.1
2	D	414	ILE	2.1
2	B	57	MET	2.1
1	A	523	GLY	2.1
2	D	207	ASN	2.1
2	B	363	PHE	2.1
1	G	283	ASN	2.1
2	D	159	ASN	2.1
2	H	390	GLN	2.1
1	G	139	GLY	2.0
1	G	187	PHE	2.0
2	D	29	PHE	2.0
1	C	127	PRO	2.0
2	H	95	VAL	2.0
1	C	117	GLN	2.0
1	A	1036	TRP	2.0
1	G	197	LEU	2.0
2	H	160	THR	2.0
1	G	1039	GLN	2.0
2	F	668	ASP	2.0
1	E	398	VAL	2.0
1	G	468	THR	2.0
2	B	180	PHE	2.0
2	D	59	PRO	2.0
2	D	113	LEU	2.0
2	F	186	LEU	2.0
1	G	253	VAL	2.0
1	G	263	ILE	2.0
1	G	623	GLN	2.0
2	F	94	ASN	2.0
1	G	325	SER	2.0
1	G	339	ALA	2.0
2	F	98	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	3880	14/15	0.77	0.32	1.52	140,205,251,290	0
4	NAG	E	3373	14/15	0.57	0.32	0.60	290,333,360,390	0
4	NAG	C	3716	14/15	0.90	0.19	-0.34	125,169,213,220	0
4	NAG	A	3716	14/15	0.90	0.21	-0.54	116,183,224,247	0
4	NAG	E	3716	14/15	0.94	0.16	-0.54	108,165,197,198	0
3	NAG	C	3373	14/15	0.78	0.22	-1.11	186,260,283,292	0
4	NAG	G	3716	14/15	0.93	0.15	-1.15	133,181,218,231	0
4	MAN	A	3375	11/12	0.68	0.18	-	229,283,307,312	0
3	NAG	C	3374	14/15	0.81	0.26	-	154,257,273,298	0
4	NAG	E	3374	14/15	0.53	0.52	-	286,310,336,351	0
4	MAN	C	3718	11/12	0.59	0.26	-	267,322,330,331	0
4	MAN	A	3882	11/12	0.82	0.39	-	187,257,308,323	0
4	MAN	E	3375	11/12	0.63	0.41	-	242,273,308,315	0
3	NAG	G	3042	14/15	0.84	0.24	-	184,229,251,262	0
3	NAG	G	3043	14/15	0.80	0.30	-	189,282,303,305	0
3	NAG	C	3043	14/15	0.73	0.27	-	204,296,319,331	0
4	NAG	E	3717	14/15	0.88	0.14	-	161,245,265,293	0
3	NAG	A	3042	14/15	0.81	0.18	-	216,243,262,294	0
3	NAG	C	3042	14/15	0.77	0.35	-	224,274,288,298	0
4	NAG	A	3717	14/15	0.86	0.28	-	231,265,291,318	0
4	MAN	E	3718	11/12	0.48	0.26	-	156,276,306,313	0
4	MAN	G	3718	11/12	0.67	0.24	-	266,274,284,288	0
4	MAN	A	3718	11/12	0.53	0.25	-	271,295,318,322	0
7	MAN	G	3377	11/12	0.65	0.37	-	270,291,333,336	0
4	NAG	A	3881	14/15	0.83	0.24	-	222,253,284,303	0
3	NAG	E	3042	14/15	0.73	0.28	-	182,235,257,271	0
4	NAG	A	3373	14/15	0.82	0.27	-	237,325,347,352	0
7	NAG	G	3373	14/15	0.81	0.30	-	257,281,310,318	0
4	NAG	C	3717	14/15	0.91	0.13	-	227,256,296,312	0
3	NAG	A	3043	14/15	0.66	0.33	-	190,302,317,324	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	3043	14/15	0.86	0.14	-	209,276,288,291	0
4	NAG	A	3374	14/15	0.66	0.29	-	260,301,316,331	0
4	NAG	G	3717	14/15	0.87	0.26	-	229,249,267,274	0
7	MAN	G	3375	11/12	0.48	0.28	-	286,318,328,335	0
7	NAG	G	3374	14/15	0.77	0.38	-	263,314,342,363	0

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	G	3880	14/15	0.83	0.32	1.40	158,180,199,201	0
8	MG	G	2009	1/1	0.79	0.48	0.03	414,414,414,414	0
6	CA	G	2006	1/1	0.90	0.25	-0.06	197,197,197,197	0
5	NAG	F	3094	14/15	0.56	0.54	-0.20	232,263,289,301	0
6	CA	A	2005	1/1	0.74	0.23	-0.30	235,235,235,235	0
6	CA	E	2006	1/1	0.90	0.20	-0.31	200,200,200,200	0
5	NAG	C	3880	14/15	0.86	0.22	-0.66	141,180,222,236	0
6	CA	G	2005	1/1	0.57	0.20	-0.73	228,228,228,228	0
6	CA	C	2005	1/1	0.40	0.13	-0.81	235,235,235,235	0
6	CA	E	2007	1/1	0.73	0.20	-0.93	279,279,279,279	0
6	CA	E	2005	1/1	0.63	0.14	-0.96	235,235,235,235	0
6	CA	D	2002	1/1	0.39	0.12	-1.00	533,533,533,533	0
6	CA	B	2002	1/1	0.70	0.14	-1.01	533,533,533,533	0
6	CA	F	2002	1/1	0.72	0.10	-1.03	534,534,534,534	0
6	CA	A	2006	1/1	0.66	0.16	-1.23	182,182,182,182	0
6	CA	C	2006	1/1	0.88	0.17	-1.24	201,201,201,201	0
6	CA	C	2007	1/1	0.85	0.14	-1.61	284,284,284,284	0
6	CA	A	2007	1/1	0.72	0.14	-1.64	279,279,279,279	0
6	CA	G	2007	1/1	0.80	0.16	-1.65	284,284,284,284	0
6	CA	H	2002	1/1	0.75	0.12	-1.80	532,532,532,532	0
5	NAG	D	3479	14/15	0.72	0.32	-	192,213,248,259	0
5	NAG	A	3678	14/15	0.82	0.24	-	164,238,297,317	0
5	NAG	G	3678	14/15	0.79	0.34	-	129,233,286,308	0
5	NAG	B	3479	14/15	0.76	0.26	-	232,258,304,321	0
5	NAG	F	3479	14/15	0.71	0.31	-	199,256,273,273	0
5	NAG	H	3479	14/15	0.75	0.31	-	217,264,289,289	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	3678	14/15	0.69	0.29	-	172,234,258,258	0
5	NAG	E	3880	14/15	0.81	0.35	-	117,189,224,243	0
5	NAG	H	3094	14/15	0.83	0.32	-	209,244,295,296	0
5	NAG	D	3094	14/15	0.82	0.26	-	212,265,297,302	0
5	NAG	B	3094	14/15	0.82	0.30	-	236,271,288,298	0
5	NAG	C	3678	14/15	0.80	0.28	-	212,245,268,292	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.