



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:06 pm BST

PDB ID : 3S4Z
Title : Structure of a Y DNA-FANCI complex
Authors : Pavletich, N.P.
Deposited on : 2011-05-20
Resolution : 7.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

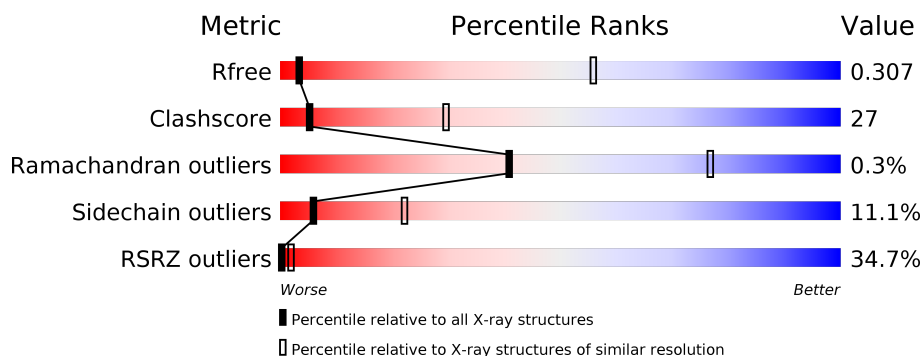
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1308	
1	B	1308	
1	C	1308	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26814 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 dna repair 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1131	Total	C	N	O	S	0	0	0
			8938	5748	1485	1652	53			
1	B	1131	Total	C	N	O	S	0	0	0
			8938	5748	1485	1652	53			
1	C	1131	Total	C	N	O	S	0	0	0
			8938	5748	1485	1652	53			

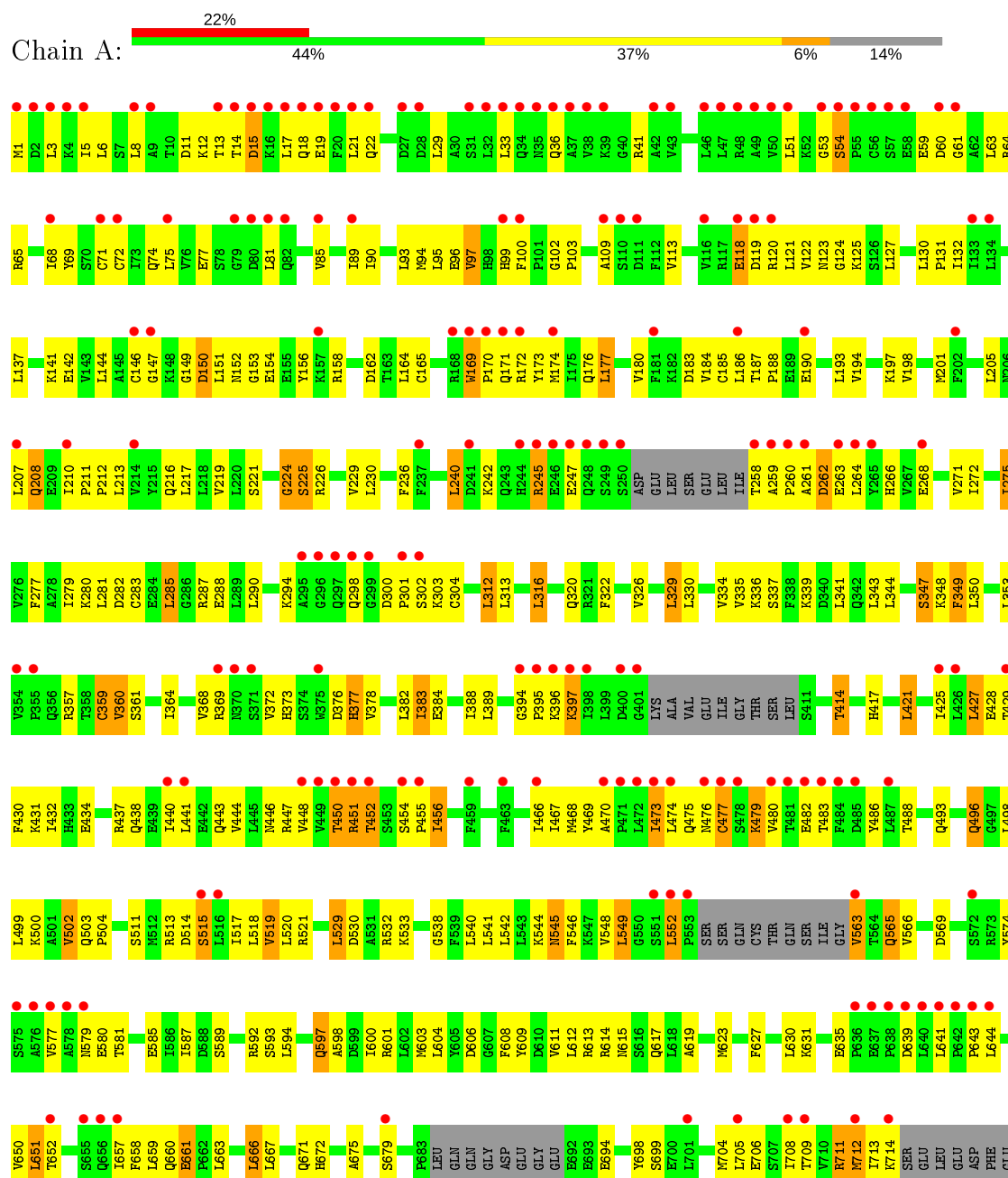
There are 18 discrepancies between the modelled and reference sequences:

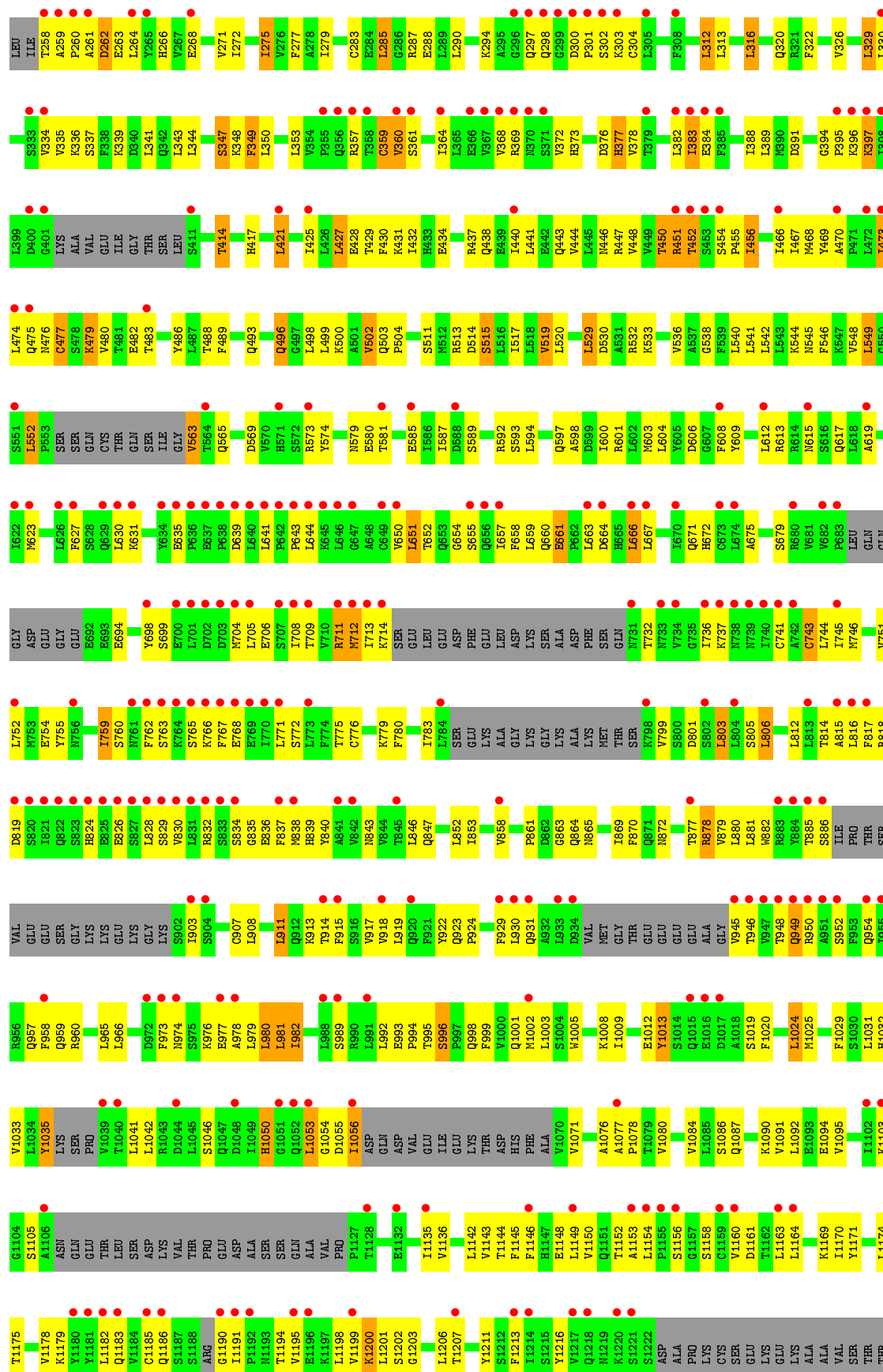
Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1308	HIS	-	EXPRESSION TAG	UNP Q8K368

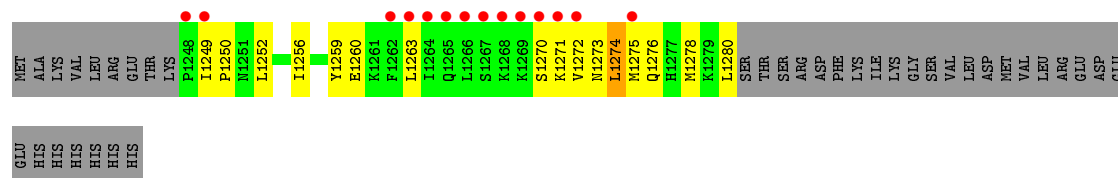
3 Residue-property plots

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

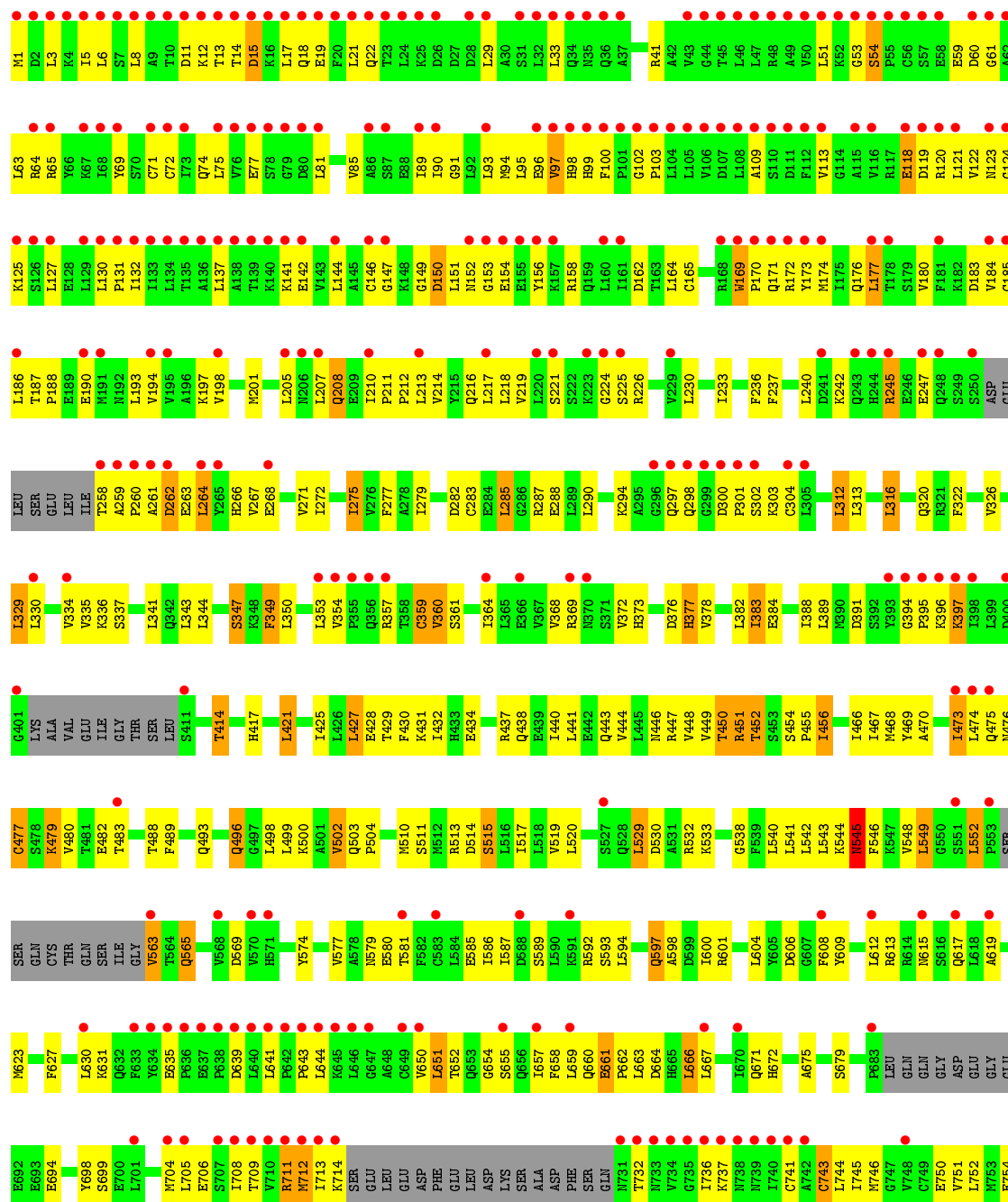
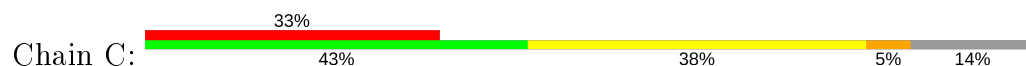
• Molecule 1: dna repair 1







• Molecule 1: dna repair 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	235.20 Å 307.90 Å 375.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 7.80 50.02 – 7.80	Depositor EDS
% Data completeness (in resolution range)	85.3 (33.00-7.80) 85.2 (50.02-7.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 7.37 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.310 , 0.324 0.303 , 0.307	Depositor DCC
R_{free} test set	604 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	473.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 619.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	26814	wwPDB-VP
Average B, all atoms (Å ²)	413.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.42	4/9075 (0.0%)	0.62	6/12252 (0.0%)
1	B	0.26	2/9073 (0.0%)	0.46	0/12246
1	C	0.27	3/9074 (0.0%)	0.48	3/12249 (0.0%)
All	All	0.33	9/27222 (0.0%)	0.52	9/36747 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	GLY	C-N	25.03	1.91	1.34
1	A	545	ASN	C-N	18.55	1.76	1.34
1	B	320	GLN	CD-NE2	-6.82	1.15	1.32
1	A	320	GLN	CD-NE2	-6.82	1.15	1.32
1	C	320	GLN	CD-NE2	-6.80	1.15	1.32
1	C	545	ASN	C-N	6.53	1.49	1.34
1	C	320	GLN	CD-OE1	-6.04	1.10	1.24
1	B	320	GLN	CD-OE1	-6.04	1.10	1.24
1	A	320	GLN	CD-OE1	-5.98	1.10	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLY	O-C-N	-34.14	68.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLY	CA-C-N	21.55	164.61	117.20
1	A	224	GLY	C-N-CA	15.07	159.37	121.70
1	C	545	ASN	C-N-CA	-11.18	93.76	121.70
1	A	545	ASN	O-C-N	10.27	139.13	122.70
1	C	545	ASN	O-C-N	9.38	137.70	122.70
1	C	545	ASN	CA-C-N	-9.15	97.06	117.20
1	A	545	ASN	C-N-CA	-7.93	101.87	121.70
1	A	545	ASN	CA-C-N	-7.63	100.41	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	LEU	Peptide
1	B	1053	LEU	Peptide
1	C	1053	LEU	Peptide
1	C	545	ASN	Mainchain

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	8938	0	9247	507	13
1	B	8938	0	9247	452	0
1	C	8938	0	9248	527	0
All	All	26814	0	27742	1452	13

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 27.

All (1452) 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)
1:A:208:GLN:HE22	1:A:263:GLU:CG	1.18	1.57
1:C:210:ILE:CD1	1:C:236:PHE:CE2	1.90	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HD22	1:C:237:PHE:CE2	1.48	1.46
1:A:545:ASN:C	1:A:546:PHE:N	1.76	1.37
1:A:208:GLN:NE2	1:A:263:GLU:HG2	1.38	1.34
1:C:210:ILE:HD12	1:C:236:PHE:CE2	1.60	1.27
1:A:764:LYS:HB3	1:A:824:HIS:NE2	1.50	1.25
1:C:214:VAL:CG2	1:C:233:ILE:CD1	2.15	1.24
1:A:224:GLY:C	1:A:225:SER:N	1.91	1.20
1:C:207:LEU:CD2	1:C:237:PHE:CE2	2.25	1.19
1:A:208:GLN:NE2	1:A:263:GLU:CG	1.97	1.18
1:C:214:VAL:CG2	1:C:233:ILE:HD11	1.72	1.16
1:B:208:GLN:HE22	1:B:263:GLU:CG	1.57	1.15
1:A:207:LEU:HD21	1:A:240:LEU:HD11	1.26	1.15
1:B:208:GLN:HE22	1:B:263:GLU:HG2	1.01	1.14
1:C:214:VAL:HG21	1:C:233:ILE:CD1	1.76	1.14
1:B:450:THR:HG21	1:C:489:PHE:HB3	1.12	1.12
1:C:210:ILE:HD11	1:C:236:PHE:CE2	1.71	1.11
1:C:210:ILE:HD11	1:C:236:PHE:CZ	1.85	1.11
1:B:208:GLN:NE2	1:B:263:GLU:HG2	1.66	1.10
1:A:208:GLN:HE22	1:A:263:GLU:CD	1.56	1.09
1:C:214:VAL:HG21	1:C:233:ILE:HD13	1.23	1.09
1:A:771:LEU:CD1	1:A:830:VAL:O	2.01	1.09
1:C:208:GLN:HE22	1:C:263:GLU:CA	1.67	1.08
1:A:224:GLY:O	1:A:225:SER:N	1.85	1.08
1:C:214:VAL:HG22	1:C:233:ILE:HD11	1.22	1.08
1:A:799:VAL:O	1:A:847:GLN:NE2	1.87	1.07
1:C:799:VAL:O	1:C:847:GLN:NE2	1.87	1.07
1:C:672:HIS:ND1	1:C:861:PRO:HG3	1.70	1.06
1:C:354:VAL:HG21	1:C:1101:LYS:HZ2	1.18	1.06
1:A:208:GLN:NE2	1:A:263:GLU:CD	2.00	1.06
1:B:799:VAL:O	1:B:847:GLN:NE2	1.87	1.06
1:B:545:ASN:C	1:B:546:PHE:N	2.09	1.06
1:C:207:LEU:HD23	1:C:236:PHE:HE2	1.22	1.05
1:B:489:PHE:HB3	1:C:450:THR:CG2	1.87	1.04
1:B:489:PHE:CB	1:C:450:THR:HG21	1.87	1.02
1:B:1032:HIS:CE1	1:B:1041:LEU:HD11	1.95	1.02
1:A:1012:GLU:CD	1:B:1008:LYS:HE3	1.80	1.02
1:C:207:LEU:HD23	1:C:236:PHE:CE2	1.95	1.02
1:C:218:LEU:HD22	1:C:285:LEU:HD11	1.35	1.02
1:B:259:ALA:HB3	1:B:260:PRO:HD3	1.43	0.99
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.43	0.99
1:C:354:VAL:HG22	1:C:1101:LYS:HZ3	1.24	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ALA:HB3	1:C:260:PRO:HD3	1.43	0.98
1:A:208:GLN:HE22	1:A:263:GLU:HG2	0.81	0.97
1:C:354:VAL:CG2	1:C:1101:LYS:NZ	2.26	0.97
1:C:210:ILE:CD1	1:C:236:PHE:CD2	2.48	0.96
1:C:214:VAL:HG22	1:C:233:ILE:CD1	1.88	0.96
1:A:1012:GLU:OE1	1:B:1008:LYS:HE3	1.67	0.95
1:A:778:LYS:HE2	1:A:836:GLU:OE1	1.66	0.95
1:C:1029:PHE:CE2	1:C:1087:GLN:HG2	2.03	0.93
1:C:211:PRO:HD3	1:C:271:VAL:CG2	1.98	0.92
1:A:1008:LYS:HE3	1:B:1012:GLU:OE1	1.68	0.92
1:B:489:PHE:HB3	1:C:450:THR:HG21	0.95	0.92
1:A:764:LYS:HB3	1:A:824:HIS:CE1	2.05	0.91
1:B:713:ILE:O	1:B:714:LYS:HG2	1.70	0.91
1:C:210:ILE:HD12	1:C:236:PHE:HE2	1.09	0.91
1:A:713:ILE:O	1:A:714:LYS:HG2	1.70	0.90
1:C:713:ILE:O	1:C:714:LYS:HG2	1.70	0.90
1:C:207:LEU:HD22	1:C:237:PHE:CD2	2.05	0.90
1:A:771:LEU:HD12	1:A:830:VAL:CG1	2.02	0.90
1:A:1014:SER:HB3	1:A:1070:VAL:HG12	1.54	0.89
1:C:354:VAL:HG22	1:C:1101:LYS:NZ	1.86	0.88
1:A:1008:LYS:HE3	1:B:1012:GLU:CD	1.94	0.88
1:C:29:LEU:O	1:C:33:LEU:HG	1.74	0.88
1:B:29:LEU:O	1:B:33:LEU:HG	1.74	0.87
1:C:354:VAL:CG2	1:C:1101:LYS:HZ2	1.83	0.87
1:A:764:LYS:CB	1:A:824:HIS:NE2	2.37	0.86
1:A:1012:GLU:OE2	1:B:1008:LYS:HE3	1.73	0.86
1:A:29:LEU:O	1:A:33:LEU:HG	1.74	0.86
1:A:774:PHE:CG	1:A:837:PHE:HD2	1.93	0.86
1:A:771:LEU:HD12	1:A:830:VAL:HG13	1.58	0.85
1:C:208:GLN:HE22	1:C:263:GLU:HA	1.39	0.85
1:A:774:PHE:CE2	1:A:837:PHE:HB2	2.10	0.85
1:C:207:LEU:CD2	1:C:236:PHE:CE2	2.60	0.85
1:C:207:LEU:HD22	1:C:237:PHE:HE2	1.05	0.85
1:A:771:LEU:HD12	1:A:830:VAL:O	1.76	0.84
1:C:598:ALA:HB2	1:C:660:GLN:HA	1.59	0.84
1:A:1055:ASP:H	1:A:1152:THR:HA	1.42	0.84
1:B:598:ALA:HB2	1:B:660:GLN:HA	1.59	0.84
1:B:1055:ASP:H	1:B:1152:THR:HA	1.42	0.84
1:C:1055:ASP:H	1:C:1152:THR:HA	1.42	0.84
1:A:641:LEU:O	1:A:643:PRO:HD3	1.78	0.84
1:C:354:VAL:HG21	1:C:1101:LYS:NZ	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ALA:HB2	1:A:660:GLN:HA	1.59	0.83
1:B:301:PRO:HA	1:B:304:CYS:HB2	1.60	0.83
1:B:641:LEU:O	1:B:643:PRO:HD3	1.78	0.83
1:B:1077:ALA:HB3	1:B:1078:PRO:HD3	1.61	0.83
1:A:1077:ALA:HB3	1:A:1078:PRO:HD3	1.61	0.83
1:B:208:GLN:NE2	1:B:263:GLU:CG	2.33	0.82
1:B:450:THR:CG2	1:C:489:PHE:HB3	2.03	0.82
1:C:641:LEU:O	1:C:643:PRO:HD3	1.78	0.82
1:A:301:PRO:HA	1:A:304:CYS:HB2	1.60	0.81
1:A:258:THR:N	1:A:261:ALA:HB3	1.96	0.81
1:C:301:PRO:HA	1:C:304:CYS:HB2	1.60	0.81
1:A:207:LEU:HD21	1:A:240:LEU:CD1	2.10	0.81
1:C:258:THR:N	1:C:261:ALA:HB3	1.96	0.81
1:B:207:LEU:HD21	1:B:240:LEU:HD11	1.63	0.80
1:C:350:LEU:HD22	1:C:1097:TRP:HZ3	1.46	0.80
1:A:771:LEU:HD11	1:A:830:VAL:O	1.79	0.80
1:B:258:THR:N	1:B:261:ALA:HB3	1.96	0.80
1:C:1056:ILE:HG12	1:C:1153:ALA:HB2	1.64	0.80
1:A:774:PHE:CD2	1:A:837:PHE:HB2	2.17	0.79
1:C:1077:ALA:HB3	1:C:1078:PRO:HD3	1.61	0.79
1:B:427:LEU:HD22	1:B:431:LYS:HD2	1.65	0.79
1:B:65:ARG:HB3	1:B:100:PHE:HZ	1.48	0.79
1:C:65:ARG:HB3	1:C:100:PHE:HZ	1.48	0.79
1:A:545:ASN:C	1:A:546:PHE:CA	2.51	0.79
1:A:65:ARG:HB3	1:A:100:PHE:HZ	1.48	0.78
1:C:208:GLN:NE2	1:C:263:GLU:HA	1.98	0.78
1:C:208:GLN:HA	1:C:267:VAL:CG1	2.13	0.78
1:A:1056:ILE:HG12	1:A:1153:ALA:HB2	1.64	0.78
1:C:427:LEU:HD22	1:C:431:LYS:HD2	1.65	0.78
1:A:302:SER:HB2	1:A:357:ARG:HG2	1.66	0.78
1:C:302:SER:HB2	1:C:357:ARG:HG2	1.66	0.77
1:A:210:ILE:HD13	1:A:236:PHE:CZ	2.19	0.77
1:B:208:GLN:NE2	1:B:263:GLU:CD	2.37	0.77
1:A:348:LYS:NZ	1:A:994:PRO:HB2	2.00	0.77
1:A:427:LEU:HD22	1:A:431:LYS:HD2	1.65	0.77
1:B:671:GLN:HE21	1:B:755:TYR:HA	1.50	0.77
1:A:671:GLN:HE21	1:A:755:TYR:HA	1.50	0.77
1:C:671:GLN:HE21	1:C:755:TYR:HA	1.50	0.77
1:B:1056:ILE:HG12	1:B:1153:ALA:HB2	1.64	0.76
1:B:302:SER:HB2	1:B:357:ARG:HG2	1.66	0.76
1:C:210:ILE:HD13	1:C:236:PHE:CD2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:CYS:HB3	1:C:197:LYS:HG3	1.67	0.76
1:C:207:LEU:CD2	1:C:237:PHE:CD2	2.64	0.76
1:B:208:GLN:HE22	1:B:263:GLU:CD	1.88	0.76
1:C:218:LEU:CD2	1:C:285:LEU:HD11	2.14	0.76
1:C:208:GLN:HE22	1:C:263:GLU:C	1.88	0.76
1:A:452:THR:HB	1:A:454:SER:H	1.51	0.76
1:B:1032:HIS:ND1	1:B:1041:LEU:HD11	2.00	0.76
1:B:470:ALA:O	1:B:473:ILE:HG13	1.86	0.76
1:B:259:ALA:CB	1:B:260:PRO:HD3	2.17	0.75
1:C:545:ASN:C	1:C:546:PHE:CG	2.59	0.75
1:B:165:CYS:HB3	1:B:197:LYS:HG3	1.67	0.75
1:C:349:PHE:H	1:C:349:PHE:HD2	1.32	0.75
1:C:377:HIS:H	1:C:377:HIS:CD2	2.04	0.75
1:A:165:CYS:HB3	1:A:197:LYS:HG3	1.67	0.75
1:C:211:PRO:CD	1:C:271:VAL:CG2	2.64	0.75
1:C:208:GLN:NE2	1:C:263:GLU:CA	2.47	0.75
1:A:470:ALA:O	1:A:473:ILE:HG13	1.86	0.75
1:A:377:HIS:H	1:A:377:HIS:CD2	2.04	0.75
1:B:1054:GLY:O	1:B:1055:ASP:HB2	1.87	0.75
1:B:349:PHE:HD2	1:B:349:PHE:H	1.33	0.75
1:C:1054:GLY:O	1:C:1055:ASP:HB2	1.87	0.75
1:C:470:ALA:O	1:C:473:ILE:HG13	1.86	0.75
1:A:1054:GLY:O	1:A:1055:ASP:HB2	1.87	0.74
1:C:452:THR:HB	1:C:454:SER:H	1.51	0.74
1:A:349:PHE:H	1:A:349:PHE:HD2	1.33	0.74
1:B:474:LEU:O	1:B:477:CYS:HB2	1.88	0.74
1:B:377:HIS:H	1:B:377:HIS:CD2	2.04	0.74
1:B:452:THR:HB	1:B:454:SER:H	1.51	0.74
1:C:208:GLN:HA	1:C:267:VAL:HG11	1.69	0.74
1:C:474:LEU:O	1:C:477:CYS:HB2	1.88	0.74
1:A:1146:PHE:CD1	1:A:1170:ILE:HD11	2.23	0.73
1:C:1146:PHE:CD1	1:C:1170:ILE:HD11	2.23	0.73
1:A:946:THR:O	1:A:950:ARG:HG2	1.88	0.73
1:A:474:LEU:O	1:A:477:CYS:HB2	1.88	0.73
1:A:521:ARG:NH2	1:A:577:VAL:HG13	2.03	0.73
1:C:214:VAL:CG1	1:C:233:ILE:CD1	2.65	0.73
1:B:946:THR:O	1:B:950:ARG:HG2	1.88	0.73
1:C:946:THR:O	1:C:950:ARG:HG2	1.88	0.73
1:A:544:LYS:O	1:A:614:ARG:HD2	1.89	0.72
1:C:259:ALA:CB	1:C:260:PRO:HD3	2.17	0.72
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:LYS:HB3	1:A:824:HIS:CD2	2.25	0.72
1:B:548:VAL:O	1:B:549:LEU:HB3	1.89	0.72
1:B:1146:PHE:CD1	1:B:1170:ILE:HD11	2.24	0.72
1:C:214:VAL:CG1	1:C:233:ILE:HD11	2.20	0.72
1:A:1008:LYS:HG3	1:B:1012:GLU:OE2	1.90	0.71
1:B:483:THR:HG21	1:B:498:LEU:HD21	1.73	0.71
1:A:1012:GLU:OE1	1:B:1008:LYS:CE	2.38	0.71
1:C:211:PRO:CB	1:C:271:VAL:HG22	2.20	0.71
1:B:1143:VAL:HG13	1:B:1206:LEU:HG	1.73	0.71
1:C:389:LEU:HD13	1:C:421:LEU:HD23	1.72	0.71
1:A:545:ASN:CA	1:A:546:PHE:N	2.54	0.71
1:A:548:VAL:O	1:A:549:LEU:HB3	1.89	0.71
1:C:548:VAL:O	1:C:549:LEU:HB3	1.89	0.71
1:A:389:LEU:HD13	1:A:421:LEU:HD23	1.72	0.70
1:A:1012:GLU:OE2	1:B:1008:LYS:HG3	1.91	0.70
1:C:483:THR:HG21	1:C:498:LEU:HD21	1.72	0.70
1:B:149:GLY:O	1:B:151:LEU:N	2.24	0.70
1:A:451:ARG:HB3	1:A:456:ILE:HD11	1.73	0.70
1:A:483:THR:HG21	1:A:498:LEU:HD21	1.73	0.70
1:C:149:GLY:O	1:C:151:LEU:N	2.24	0.70
1:C:451:ARG:HB3	1:C:456:ILE:HD11	1.73	0.70
1:B:389:LEU:HD13	1:B:421:LEU:HD23	1.72	0.70
1:B:451:ARG:HB3	1:B:456:ILE:HD11	1.73	0.70
1:C:1143:VAL:HG13	1:C:1206:LEU:HG	1.73	0.70
1:A:149:GLY:O	1:A:151:LEU:N	2.24	0.69
1:C:542:LEU:O	1:C:546:PHE:HD2	1.74	0.69
1:A:518:LEU:HD21	1:A:577:VAL:CG2	2.23	0.69
1:A:1143:VAL:HG13	1:A:1206:LEU:HG	1.73	0.69
1:A:1008:LYS:HE3	1:B:1012:GLU:OE2	1.92	0.69
1:C:1054:GLY:HA3	1:C:1153:ALA:H	1.56	0.69
1:C:946:THR:HG22	1:C:950:ARG:HE	1.57	0.69
1:A:946:THR:HG22	1:A:950:ARG:HE	1.57	0.69
1:C:760:SER:HB2	1:C:766:LYS:HE2	1.75	0.69
1:A:513:ARG:HD3	1:A:546:PHE:CE1	2.28	0.69
1:A:1054:GLY:HA3	1:A:1153:ALA:H	1.56	0.68
1:A:448:VAL:HA	1:A:456:ILE:HD13	1.74	0.68
1:B:760:SER:HB2	1:B:766:LYS:HE2	1.75	0.68
1:B:1054:GLY:HA3	1:B:1153:ALA:H	1.56	0.68
1:B:1190:GLY:N	1:B:1271:LYS:HZ2	1.91	0.68
1:C:448:VAL:HA	1:C:456:ILE:HD13	1.74	0.68
1:C:1190:GLY:N	1:C:1271:LYS:HZ2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ILE:HG22	1:A:760:SER:N	2.09	0.68
1:C:1154:LEU:HD11	1:C:1163:LEU:HD12	1.76	0.68
1:A:1154:LEU:HD11	1:A:1163:LEU:HD12	1.76	0.68
1:B:470:ALA:HB3	1:B:473:ILE:HD11	1.77	0.67
1:B:448:VAL:HA	1:B:456:ILE:HD13	1.74	0.67
1:A:221:SER:HB2	1:A:229:VAL:HG21	1.77	0.67
1:C:428:GLU:O	1:C:432:ILE:HG12	1.94	0.67
1:C:759:ILE:HG22	1:C:760:SER:N	2.09	0.67
1:C:369:ARG:O	1:C:372:VAL:HG23	1.95	0.67
1:A:1008:LYS:CE	1:B:1012:GLU:OE1	2.42	0.67
1:A:760:SER:HB2	1:A:766:LYS:HE2	1.75	0.67
1:A:771:LEU:HB2	1:A:830:VAL:HG12	1.77	0.67
1:B:1154:LEU:HD11	1:B:1163:LEU:HD12	1.76	0.67
1:B:1195:VAL:O	1:B:1199:VAL:HG23	1.95	0.67
1:B:369:ARG:O	1:B:372:VAL:HG23	1.95	0.67
1:B:428:GLU:O	1:B:432:ILE:HG12	1.94	0.67
1:C:275:ILE:HD11	1:C:312:LEU:HD11	1.77	0.67
1:A:517:ILE:HG21	1:A:577:VAL:HG11	1.77	0.67
1:B:475:GLN:HG3	1:B:476:ASN:H	1.61	0.67
1:A:428:GLU:O	1:A:432:ILE:HG12	1.94	0.66
1:A:475:GLN:HG3	1:A:476:ASN:H	1.61	0.66
1:A:275:ILE:HD11	1:A:312:LEU:HD11	1.77	0.66
1:B:330:LEU:O	1:B:334:VAL:HG23	1.95	0.66
1:C:211:PRO:CA	1:C:271:VAL:HG22	2.25	0.66
1:C:475:GLN:HG3	1:C:476:ASN:H	1.61	0.66
1:A:347:SER:HB2	1:A:349:PHE:CE2	2.30	0.66
1:A:65:ARG:HB3	1:A:100:PHE:CZ	2.30	0.66
1:A:959:GLN:HB2	1:A:1005:TRP:CZ2	2.31	0.66
1:B:946:THR:HG22	1:B:950:ARG:HE	1.58	0.66
1:B:863:GLY:O	1:B:869:ILE:HD11	1.94	0.66
1:C:863:GLY:O	1:C:869:ILE:HD11	1.94	0.66
1:A:369:ARG:O	1:A:372:VAL:HG23	1.95	0.66
1:A:768:GLU:OE1	1:A:830:VAL:HG21	1.95	0.66
1:A:1190:GLY:N	1:A:1271:LYS:HZ2	1.94	0.66
1:A:330:LEU:O	1:A:334:VAL:HG23	1.95	0.66
1:B:959:GLN:HB2	1:B:1005:TRP:CZ2	2.30	0.66
1:C:208:GLN:HE22	1:C:263:GLU:CB	2.08	0.66
1:C:347:SER:HB2	1:C:349:PHE:CE2	2.30	0.66
1:B:446:ASN:HB3	1:C:489:PHE:CE1	2.30	0.66
1:B:347:SER:HB2	1:B:349:PHE:CE2	2.30	0.66
1:A:863:GLY:O	1:A:869:ILE:HD11	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:672:HIS:ND1	1:C:861:PRO:CG	2.56	0.66
1:C:350:LEU:HD22	1:C:1097:TRP:CZ3	2.30	0.66
1:C:470:ALA:HB3	1:C:473:ILE:HD11	1.77	0.66
1:C:959:GLN:HB2	1:C:1005:TRP:CZ2	2.31	0.66
1:C:1195:VAL:O	1:C:1199:VAL:HG23	1.95	0.65
1:A:1195:VAL:O	1:A:1199:VAL:HG23	1.95	0.65
1:B:275:ILE:HD11	1:B:312:LEU:HD11	1.77	0.65
1:C:330:LEU:O	1:C:334:VAL:HG23	1.95	0.65
1:C:33:LEU:HD23	1:C:75:LEU:HD11	1.78	0.65
1:A:1259:TYR:CZ	1:A:1263:LEU:HD11	2.32	0.65
1:A:470:ALA:HB3	1:A:473:ILE:HD11	1.77	0.65
1:B:1259:TYR:CZ	1:B:1263:LEU:HD11	2.32	0.65
1:B:759:ILE:HG22	1:B:760:SER:N	2.09	0.65
1:C:377:HIS:H	1:C:377:HIS:HD2	1.45	0.65
1:C:1164:LEU:HB3	1:C:1252:LEU:HD21	1.79	0.65
1:C:65:ARG:HB3	1:C:100:PHE:CZ	2.30	0.65
1:B:1164:LEU:HB3	1:B:1252:LEU:HD21	1.79	0.64
1:C:907:CYS:O	1:C:911:LEU:HB2	1.97	0.64
1:A:545:ASN:O	1:A:566:VAL:N	2.26	0.64
1:A:907:CYS:O	1:A:911:LEU:HB2	1.97	0.64
1:C:1259:TYR:CZ	1:C:1263:LEU:HD11	2.32	0.64
1:B:33:LEU:HD23	1:B:75:LEU:HD11	1.78	0.64
1:C:211:PRO:CD	1:C:271:VAL:HG22	2.28	0.64
1:C:298:GLN:HE21	1:C:336:LYS:HG2	1.63	0.64
1:A:1164:LEU:HB3	1:A:1252:LEU:HD21	1.78	0.64
1:B:65:ARG:HB3	1:B:100:PHE:CZ	2.30	0.64
1:C:335:VAL:HG13	1:C:414:THR:HG21	1.79	0.64
1:A:33:LEU:HD23	1:A:75:LEU:HD11	1.78	0.64
1:B:120:ARG:HG2	1:B:172:ARG:NH1	2.13	0.64
1:A:120:ARG:HG2	1:A:172:ARG:NH1	2.13	0.64
1:A:672:HIS:ND1	1:A:861:PRO:HG3	2.13	0.64
1:A:335:VAL:HG13	1:A:414:THR:HG21	1.79	0.64
1:A:431:LYS:HE3	1:A:469:TYR:CE1	2.33	0.64
1:B:907:CYS:O	1:B:911:LEU:HB2	1.97	0.64
1:C:120:ARG:HG2	1:C:172:ARG:NH1	2.13	0.64
1:B:298:GLN:HE21	1:B:336:LYS:HG2	1.63	0.63
1:A:348:LYS:HD3	1:A:1034:LEU:O	1.98	0.63
1:B:446:ASN:HB2	1:C:489:PHE:CZ	2.33	0.63
1:B:335:VAL:HG13	1:B:414:THR:HG21	1.79	0.63
1:A:1160:VAL:O	1:A:1164:LEU:HG	1.98	0.63
1:C:1160:VAL:O	1:C:1164:LEU:HG	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:HIS:N	1:A:377:HIS:CD2	2.67	0.63
1:B:1160:VAL:O	1:B:1164:LEU:HG	1.98	0.63
1:B:1198:LEU:HD22	1:B:1201:LEU:HD13	1.81	0.63
1:B:431:LYS:HE3	1:B:469:TYR:CE1	2.33	0.63
1:A:518:LEU:HD21	1:A:577:VAL:HG22	1.81	0.63
1:C:169:TRP:N	1:C:169:TRP:CD1	2.66	0.63
1:C:948:THR:HG23	1:C:992:LEU:HA	1.81	0.63
1:A:169:TRP:N	1:A:169:TRP:CD1	2.67	0.63
1:A:948:THR:HG23	1:A:992:LEU:HA	1.81	0.63
1:B:708:ILE:O	1:B:712:MET:HB2	1.99	0.63
1:B:948:THR:HG23	1:B:992:LEU:HA	1.81	0.63
1:A:521:ARG:CZ	1:A:577:VAL:HG13	2.28	0.62
1:C:545:ASN:HB2	1:C:546:PHE:CE2	2.34	0.62
1:A:1046:SER:O	1:A:1050:HIS:HB3	1.99	0.62
1:C:169:TRP:HD1	1:C:169:TRP:H	1.47	0.62
1:A:713:ILE:HG21	1:A:772:SER:HB3	1.81	0.62
1:C:672:HIS:CE1	1:C:861:PRO:HG3	2.34	0.62
1:A:771:LEU:HD12	1:A:830:VAL:HG12	1.79	0.62
1:C:1055:ASP:N	1:C:1152:THR:HA	2.13	0.62
1:C:431:LYS:HE3	1:C:469:TYR:CE1	2.33	0.62
1:A:708:ILE:O	1:A:712:MET:HB2	1.99	0.62
1:B:609:TYR:CZ	1:B:613:ARG:HD2	2.35	0.62
1:A:298:GLN:HE21	1:A:336:LYS:HG2	1.63	0.62
1:B:290:LEU:O	1:B:294:LYS:HG3	2.00	0.62
1:C:377:HIS:N	1:C:377:HIS:CD2	2.67	0.62
1:A:208:GLN:CD	1:A:263:GLU:CG	2.64	0.62
1:A:290:LEU:O	1:A:294:LYS:HG3	2.00	0.62
1:B:1046:SER:O	1:B:1050:HIS:HB3	1.99	0.62
1:B:377:HIS:H	1:B:377:HIS:HD2	1.45	0.62
1:B:377:HIS:N	1:B:377:HIS:CD2	2.67	0.62
1:C:713:ILE:HG21	1:C:772:SER:HB3	1.81	0.62
1:C:609:TYR:CZ	1:C:613:ARG:HD2	2.34	0.62
1:A:1179:LYS:HA	1:A:1182:LEU:HD12	1.82	0.62
1:A:1198:LEU:HD22	1:A:1201:LEU:HD13	1.81	0.62
1:A:1203:GLY:HA3	1:A:1278:MET:CG	2.30	0.62
1:B:190:GLU:O	1:B:194:VAL:HG23	2.00	0.62
1:C:672:HIS:CE1	1:C:805:SER:HB3	2.35	0.61
1:B:1203:GLY:HA3	1:B:1278:MET:CG	2.31	0.61
1:C:190:GLU:O	1:C:194:VAL:HG23	2.00	0.61
1:B:169:TRP:CD1	1:B:169:TRP:N	2.66	0.61
1:C:33:LEU:HD22	1:C:75:LEU:HD21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:TYR:CZ	1:A:613:ARG:HD2	2.35	0.61
1:C:1198:LEU:HD22	1:C:1201:LEU:HD13	1.81	0.61
1:C:397:LYS:HD3	1:C:397:LYS:H	1.65	0.61
1:C:708:ILE:O	1:C:712:MET:HB2	1.99	0.61
1:C:475:GLN:HG3	1:C:476:ASN:N	2.15	0.61
1:A:187:THR:HG22	1:A:188:PRO:HD2	1.83	0.61
1:B:499:LEU:HB3	1:B:541:LEU:HD13	1.82	0.61
1:B:877:THR:OG1	1:B:914:THR:HG21	2.00	0.61
1:C:1179:LYS:HA	1:C:1182:LEU:HD12	1.82	0.61
1:C:214:VAL:CG2	1:C:233:ILE:HD13	1.96	0.61
1:C:499:LEU:HB3	1:C:541:LEU:HD13	1.82	0.61
1:A:397:LYS:HD3	1:A:397:LYS:H	1.65	0.61
1:A:877:THR:OG1	1:A:914:THR:HG21	2.00	0.61
1:B:187:THR:HG22	1:B:188:PRO:HD2	1.83	0.61
1:B:397:LYS:HD3	1:B:397:LYS:H	1.65	0.61
1:A:169:TRP:HD1	1:A:169:TRP:H	1.47	0.61
1:A:475:GLN:HG3	1:A:476:ASN:N	2.15	0.61
1:A:499:LEU:HB3	1:A:541:LEU:HD13	1.82	0.61
1:B:475:GLN:HG3	1:B:476:ASN:N	2.15	0.61
1:C:1076:ALA:HA	1:C:1080:VAL:HB	1.83	0.61
1:C:187:THR:HG22	1:C:188:PRO:HD2	1.83	0.61
1:C:290:LEU:O	1:C:294:LYS:HG3	1.99	0.61
1:B:779:LYS:O	1:B:783:ILE:HG13	2.01	0.60
1:B:1032:HIS:CE1	1:B:1041:LEU:CD1	2.79	0.60
1:B:713:ILE:HG21	1:B:772:SER:HB3	1.81	0.60
1:C:1203:GLY:HA3	1:C:1278:MET:CG	2.31	0.60
1:A:13:THR:HA	1:A:17:LEU:HD12	1.84	0.60
1:A:33:LEU:HD22	1:A:75:LEU:HD21	1.81	0.60
1:B:169:TRP:H	1:B:169:TRP:HD1	1.47	0.60
1:C:1046:SER:O	1:C:1050:HIS:HB3	1.99	0.60
1:C:877:THR:OG1	1:C:914:THR:HG21	2.00	0.60
1:A:1076:ALA:HA	1:A:1080:VAL:HB	1.83	0.60
1:A:210:ILE:CD1	1:A:236:PHE:CZ	2.83	0.60
1:B:33:LEU:HD22	1:B:75:LEU:HD21	1.81	0.60
1:B:989:SER:HB2	1:B:1031:LEU:HD21	1.83	0.60
1:A:1055:ASP:N	1:A:1152:THR:HA	2.13	0.60
1:A:377:HIS:HD2	1:A:377:HIS:H	1.45	0.60
1:C:1249:ILE:N	1:C:1250:PRO:HD2	2.16	0.60
1:C:989:SER:HB2	1:C:1031:LEU:HD21	1.83	0.60
1:A:989:SER:HB2	1:A:1031:LEU:HD21	1.83	0.60
1:B:13:THR:HA	1:B:17:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:779:LYS:O	1:C:783:ILE:HG13	2.01	0.60
1:A:548:VAL:HG11	1:A:580:GLU:O	2.01	0.60
1:B:1179:LYS:HA	1:B:1182:LEU:HD12	1.82	0.60
1:A:982:ILE:HD11	1:A:1024:LEU:HG	1.84	0.60
1:A:190:GLU:O	1:A:194:VAL:HG23	2.00	0.60
1:B:124:GLY:O	1:B:127:LEU:N	2.35	0.60
1:C:13:THR:HA	1:C:17:LEU:HD12	1.84	0.60
1:C:349:PHE:N	1:C:349:PHE:CD2	2.68	0.60
1:A:11:ASP:O	1:A:12:LYS:HG2	2.02	0.60
1:A:545:ASN:C	1:A:546:PHE:HA	2.21	0.60
1:A:779:LYS:O	1:A:783:ILE:HG13	2.01	0.60
1:B:121:LEU:C	1:B:123:ASN:H	2.06	0.60
1:B:1076:ALA:HA	1:B:1080:VAL:HB	1.83	0.60
1:C:480:VAL:O	1:C:483:THR:HB	2.02	0.60
1:A:121:LEU:C	1:A:123:ASN:H	2.06	0.59
1:A:210:ILE:CD1	1:A:236:PHE:HZ	2.15	0.59
1:B:1055:ASP:N	1:B:1152:THR:HA	2.13	0.59
1:B:1249:ILE:N	1:B:1250:PRO:HD2	2.16	0.59
1:C:211:PRO:HB3	1:C:271:VAL:CG2	2.31	0.59
1:A:545:ASN:C	1:A:565:GLN:HB3	2.22	0.59
1:B:982:ILE:HD11	1:B:1024:LEU:HG	1.84	0.59
1:C:982:ILE:HD11	1:C:1024:LEU:HG	1.84	0.59
1:A:533:LYS:HG3	1:A:603:MET:CE	2.33	0.59
1:B:102:GLY:HA3	1:B:144:LEU:HD22	1.85	0.59
1:B:480:VAL:O	1:B:483:THR:HB	2.02	0.59
1:C:121:LEU:C	1:C:123:ASN:H	2.05	0.59
1:C:211:PRO:HD3	1:C:271:VAL:HG21	1.81	0.59
1:C:548:VAL:HG11	1:C:580:GLU:O	2.01	0.59
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.16	0.59
1:A:124:GLY:O	1:A:127:LEU:N	2.35	0.59
1:B:11:ASP:O	1:B:12:LYS:HG2	2.01	0.59
1:B:18:GLN:HG2	1:B:53:GLY:O	2.03	0.59
1:B:548:VAL:HG11	1:B:580:GLU:O	2.01	0.59
1:A:480:VAL:O	1:A:483:THR:HB	2.03	0.59
1:C:214:VAL:HG13	1:C:233:ILE:HD11	1.84	0.59
1:C:214:VAL:CB	1:C:233:ILE:HD11	2.33	0.59
1:B:741:CYS:O	1:B:745:ILE:HG13	2.03	0.59
1:C:11:ASP:O	1:C:12:LYS:HG2	2.02	0.59
1:C:741:CYS:O	1:C:745:ILE:HG13	2.03	0.59
1:B:672:HIS:ND1	1:B:861:PRO:HG3	2.17	0.59
1:C:18:GLN:HG2	1:C:53:GLY:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1200:LYS:HB3	1:B:1274:LEU:HD21	1.85	0.58
1:C:672:HIS:HE1	1:C:805:SER:HB3	1.68	0.58
1:A:348:LYS:CD	1:A:1034:LEU:O	2.52	0.58
1:A:650:VAL:HG21	1:A:737:LYS:HG3	1.86	0.58
1:B:446:ASN:CB	1:C:489:PHE:CZ	2.86	0.58
1:C:211:PRO:CB	1:C:271:VAL:CG2	2.81	0.58
1:A:544:LYS:HD3	1:A:614:ARG:HH21	1.68	0.58
1:B:72:CYS:HB2	1:B:93:LEU:HD11	1.85	0.58
1:C:72:CYS:HB2	1:C:93:LEU:HD11	1.85	0.58
1:C:517:ILE:HG21	1:C:577:VAL:HG11	1.84	0.58
1:A:102:GLY:HA3	1:A:144:LEU:HD22	1.85	0.58
1:A:72:CYS:HB2	1:A:93:LEU:HD11	1.85	0.58
1:B:446:ASN:CB	1:C:489:PHE:CE1	2.87	0.58
1:B:650:VAL:HG21	1:B:737:LYS:HG3	1.86	0.58
1:A:18:GLN:HG2	1:A:53:GLY:O	2.03	0.58
1:C:124:GLY:O	1:C:127:LEU:N	2.35	0.58
1:A:771:LEU:HG	1:A:831:LEU:HD23	1.86	0.58
1:C:211:PRO:CG	1:C:271:VAL:HG23	2.34	0.58
1:A:1203:GLY:HA3	1:A:1278:MET:HG2	1.86	0.58
1:A:348:LYS:HZ3	1:A:994:PRO:HB2	1.69	0.58
1:B:1203:GLY:HA3	1:B:1278:MET:HG2	1.86	0.58
1:A:771:LEU:CG	1:A:830:VAL:O	2.51	0.58
1:B:446:ASN:HB3	1:C:489:PHE:CD1	2.39	0.58
1:C:1200:LYS:HB3	1:C:1274:LEU:HD21	1.85	0.57
1:A:741:CYS:O	1:A:745:ILE:HG13	2.03	0.57
1:A:496:GLN:O	1:A:500:LYS:HG2	2.05	0.57
1:A:712:MET:HA	1:A:712:MET:HE2	1.87	0.57
1:A:131:PRO:HA	1:A:184:VAL:HG22	1.87	0.57
1:C:870:PHE:HD1	1:C:922:TYR:HD2	1.53	0.57
1:C:350:LEU:HD13	1:C:1097:TRP:CZ3	2.40	0.57
1:C:214:VAL:CG2	1:C:233:ILE:CG1	2.81	0.57
1:A:1200:LYS:HB3	1:A:1274:LEU:HD21	1.85	0.57
1:A:977:GLU:O	1:A:981:LEU:HB2	2.05	0.57
1:C:102:GLY:HA3	1:C:144:LEU:HD22	1.85	0.57
1:A:313:LEU:HB3	1:A:326:VAL:HG13	1.87	0.57
1:B:131:PRO:HA	1:B:184:VAL:HG22	1.87	0.57
1:C:1087:GLN:O	1:C:1091:VAL:HG23	2.04	0.57
1:C:300:ASP:O	1:C:304:CYS:N	2.38	0.57
1:C:1029:PHE:CD2	1:C:1087:GLN:HG2	2.40	0.57
1:C:713:ILE:C	1:C:714:LYS:HG2	2.25	0.57
1:A:1087:GLN:O	1:A:1091:VAL:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:CD1	1:A:312:LEU:HD11	2.35	0.56
1:B:300:ASP:O	1:B:304:CYS:N	2.38	0.56
1:C:131:PRO:HA	1:C:184:VAL:HG22	1.87	0.56
1:C:313:LEU:HB3	1:C:326:VAL:HG13	1.87	0.56
1:C:496:GLN:O	1:C:500:LYS:HG2	2.05	0.56
1:A:760:SER:HB2	1:A:766:LYS:HZ1	1.70	0.56
1:C:21:LEU:HD13	1:C:64:ARG:HD3	1.87	0.56
1:C:208:GLN:HA	1:C:267:VAL:CG2	2.35	0.56
1:C:650:VAL:HG21	1:C:737:LYS:HG3	1.85	0.56
1:B:102:GLY:N	1:B:103:PRO:HD2	2.21	0.56
1:C:211:PRO:HB3	1:C:271:VAL:HA	1.86	0.56
1:C:430:PHE:CE2	1:C:466:ILE:HG23	2.40	0.56
1:C:977:GLU:O	1:C:981:LEU:HB2	2.05	0.56
1:A:349:PHE:HE2	1:A:1033:VAL:CG1	2.18	0.56
1:C:102:GLY:N	1:C:103:PRO:HD2	2.21	0.56
1:A:542:LEU:O	1:A:546:PHE:N	2.39	0.56
1:A:713:ILE:C	1:A:714:LYS:HG2	2.25	0.56
1:A:835:GLY:HA2	1:A:838:MET:HB2	1.87	0.56
1:B:713:ILE:C	1:B:714:LYS:HG2	2.25	0.56
1:B:977:GLU:O	1:B:981:LEU:HB2	2.05	0.56
1:C:1146:PHE:CE1	1:C:1170:ILE:HD11	2.41	0.56
1:A:430:PHE:CE2	1:A:466:ILE:HG23	2.40	0.56
1:A:533:LYS:CG	1:A:603:MET:SD	2.93	0.56
1:B:615:ASN:OD1	1:B:617:GLN:HG2	2.06	0.56
1:B:870:PHE:HD1	1:B:922:TYR:HD2	1.53	0.56
1:C:211:PRO:HB3	1:C:271:VAL:HG22	1.86	0.56
1:C:214:VAL:HG11	1:C:233:ILE:CD1	2.34	0.56
1:C:835:GLY:HA2	1:C:838:MET:HB2	1.87	0.56
1:A:1146:PHE:CE1	1:A:1170:ILE:HD11	2.41	0.56
1:A:300:ASP:O	1:A:304:CYS:N	2.38	0.56
1:A:870:PHE:HD1	1:A:922:TYR:HD2	1.53	0.56
1:B:275:ILE:CD1	1:B:312:LEU:HD11	2.36	0.56
1:B:1087:GLN:O	1:B:1091:VAL:HG23	2.05	0.56
1:C:1203:GLY:HA3	1:C:1278:MET:HG2	1.86	0.56
1:C:187:THR:CG2	1:C:188:PRO:HD2	2.36	0.56
1:C:979:LEU:HD11	1:C:1019:SER:HB2	1.88	0.56
1:C:211:PRO:CG	1:C:271:VAL:CG2	2.84	0.56
1:A:542:LEU:HD23	1:A:546:PHE:CE2	2.41	0.56
1:A:544:LYS:HB3	1:A:614:ARG:HE	1.71	0.56
1:B:1146:PHE:CE1	1:B:1170:ILE:HD11	2.41	0.56
1:B:430:PHE:CE2	1:B:466:ILE:HG23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ARG:HB3	1:B:456:ILE:CD1	2.36	0.56
1:C:593:SER:HB2	1:C:600:ILE:HG21	1.88	0.56
1:A:103:PRO:HA	1:A:146:CYS:SG	2.46	0.56
1:A:774:PHE:CZ	1:A:837:PHE:HA	2.41	0.56
1:B:187:THR:CG2	1:B:188:PRO:HD2	2.36	0.56
1:B:760:SER:HB2	1:B:766:LYS:CE	2.36	0.56
1:C:275:ILE:CD1	1:C:312:LEU:HD11	2.35	0.56
1:A:518:LEU:HD21	1:A:577:VAL:HG21	1.89	0.55
1:A:615:ASN:OD1	1:A:617:GLN:HG2	2.06	0.55
1:B:207:LEU:HD21	1:B:240:LEU:CD1	2.35	0.55
1:B:496:GLN:O	1:B:500:LYS:HG2	2.05	0.55
1:B:593:SER:HB2	1:B:600:ILE:HG21	1.88	0.55
1:C:712:MET:HA	1:C:712:MET:HE2	1.86	0.55
1:A:187:THR:CG2	1:A:188:PRO:HD2	2.36	0.55
1:B:1146:PHE:O	1:B:1150:VAL:HG23	2.06	0.55
1:C:150:ASP:OD1	1:C:151:LEU:HG	2.06	0.55
1:B:313:LEU:HB3	1:B:326:VAL:HG13	1.87	0.55
1:B:835:GLY:HA2	1:B:838:MET:HB2	1.88	0.55
1:C:654:GLY:O	1:C:655:SER:OG	2.23	0.55
1:B:150:ASP:OD1	1:B:151:LEU:HG	2.06	0.55
1:A:21:LEU:HD13	1:A:64:ARG:HD3	1.87	0.55
1:C:194:VAL:O	1:C:198:VAL:HG23	2.06	0.55
1:A:102:GLY:N	1:A:103:PRO:HD2	2.21	0.55
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.07	0.55
1:B:103:PRO:HA	1:B:146:CYS:SG	2.46	0.55
1:A:1146:PHE:O	1:A:1150:VAL:HG23	2.06	0.55
1:A:150:ASP:OD1	1:A:151:LEU:HG	2.06	0.55
1:B:979:LEU:HD11	1:B:1019:SER:HB2	1.87	0.55
1:C:103:PRO:HA	1:C:146:CYS:SG	2.46	0.55
1:C:661:GLU:OE1	1:C:666:LEU:HD12	2.06	0.55
1:C:760:SER:HB2	1:C:766:LYS:CE	2.36	0.55
1:A:979:LEU:HD11	1:A:1019:SER:HB2	1.87	0.55
1:B:21:LEU:HD13	1:B:64:ARG:HD3	1.87	0.55
1:A:65:ARG:HD3	1:A:100:PHE:CE1	2.42	0.55
1:C:451:ARG:HB3	1:C:456:ILE:CD1	2.36	0.55
1:B:118:GLU:OE1	1:B:118:GLU:HA	2.07	0.55
1:B:446:ASN:O	1:B:450:THR:HB	2.07	0.55
1:C:446:ASN:O	1:C:450:THR:HB	2.07	0.55
1:C:543:LEU:HD11	1:C:586:ILE:CG2	2.37	0.55
1:C:615:ASN:OD1	1:C:617:GLN:HG2	2.06	0.55
1:A:194:VAL:O	1:A:198:VAL:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:SER:HB2	1:A:600:ILE:HG21	1.88	0.54
1:B:1185:CYS:SG	1:B:1191:ILE:HG12	2.47	0.54
1:B:704:MET:O	1:B:708:ILE:HG13	2.08	0.54
1:A:760:SER:HB2	1:A:766:LYS:CE	2.36	0.54
1:B:434:GLU:HA	1:B:437:ARG:HG3	1.89	0.54
1:C:1185:CYS:SG	1:C:1191:ILE:HG12	2.47	0.54
1:A:150:ASP:O	1:A:151:LEU:HD23	2.07	0.54
1:B:661:GLU:OE1	1:B:666:LEU:HD12	2.06	0.54
1:C:176:GLN:O	1:C:180:VAL:HG23	2.07	0.54
1:C:214:VAL:HG22	1:C:233:ILE:CG1	2.37	0.54
1:C:826:GLU:O	1:C:830:VAL:HG23	2.08	0.54
1:A:451:ARG:HB3	1:A:456:ILE:CD1	2.36	0.54
1:A:826:GLU:O	1:A:830:VAL:HG23	2.08	0.54
1:C:1146:PHE:O	1:C:1150:VAL:HG23	2.06	0.54
1:A:479:LYS:HE2	1:A:482:GLU:OE1	2.08	0.54
1:A:704:MET:O	1:A:708:ILE:HG13	2.08	0.54
1:A:713:ILE:O	1:A:714:LYS:CG	2.52	0.54
1:B:65:ARG:HD3	1:B:100:PHE:CE1	2.42	0.54
1:A:774:PHE:CG	1:A:837:PHE:CD2	2.85	0.54
1:B:826:GLU:O	1:B:830:VAL:HG23	2.08	0.54
1:C:150:ASP:O	1:C:151:LEU:HD23	2.08	0.54
1:C:593:SER:OG	1:C:604:LEU:HD22	2.08	0.54
1:C:704:MET:O	1:C:708:ILE:HG13	2.08	0.54
1:C:760:SER:HB2	1:C:766:LYS:HZ1	1.73	0.54
1:A:661:GLU:OE1	1:A:666:LEU:HD12	2.06	0.54
1:B:194:VAL:O	1:B:198:VAL:HG23	2.06	0.54
1:C:1029:PHE:O	1:C:1033:VAL:HG23	2.08	0.54
1:C:434:GLU:HA	1:C:437:ARG:HG3	1.89	0.54
1:C:65:ARG:HD3	1:C:100:PHE:CE1	2.42	0.54
1:A:544:LYS:HB3	1:A:614:ARG:NE	2.22	0.54
1:A:593:SER:OG	1:A:604:LEU:HD22	2.08	0.54
1:B:150:ASP:O	1:B:151:LEU:HD23	2.07	0.54
1:B:479:LYS:HE2	1:B:482:GLU:OE1	2.08	0.54
1:A:1185:CYS:SG	1:A:1191:ILE:HG12	2.47	0.54
1:A:771:LEU:HB2	1:A:830:VAL:CG1	2.38	0.54
1:B:176:GLN:O	1:B:180:VAL:HG23	2.07	0.54
1:B:593:SER:OG	1:B:604:LEU:HD22	2.08	0.54
1:C:118:GLU:OE1	1:C:118:GLU:HA	2.07	0.54
1:B:766:LYS:NZ	1:B:766:LYS:HB2	2.23	0.54
1:A:533:LYS:HG3	1:A:603:MET:SD	2.48	0.53
1:B:483:THR:CG2	1:B:498:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:PRO:HG3	1:C:271:VAL:HG23	1.90	0.53
1:A:176:GLN:O	1:A:180:VAL:HG23	2.07	0.53
1:B:452:THR:HA	1:C:452:THR:HA	1.90	0.53
1:A:434:GLU:HA	1:A:437:ARG:HG3	1.89	0.53
1:C:384:GLU:O	1:C:388:ILE:HG13	2.08	0.53
1:C:946:THR:HA	1:C:949:GLN:HB2	1.91	0.53
1:A:533:LYS:HG2	1:A:603:MET:SD	2.49	0.53
1:B:384:GLU:O	1:B:388:ILE:HG13	2.08	0.53
1:B:389:LEU:CD1	1:B:421:LEU:HD23	2.37	0.53
1:B:542:LEU:O	1:B:546:PHE:HD2	1.92	0.53
1:B:712:MET:HE2	1:B:712:MET:HA	1.90	0.53
1:C:85:VAL:O	1:C:89:ILE:HG13	2.09	0.53
1:A:384:GLU:O	1:A:388:ILE:HG13	2.08	0.53
1:A:499:LEU:HD13	1:A:538:GLY:HA2	1.90	0.53
1:B:1029:PHE:O	1:B:1033:VAL:HG23	2.08	0.53
1:B:545:ASN:C	1:B:546:PHE:CD2	2.82	0.53
1:B:85:VAL:O	1:B:89:ILE:HG13	2.09	0.53
1:C:389:LEU:CD1	1:C:421:LEU:HD23	2.37	0.53
1:C:479:LYS:HE2	1:C:482:GLU:OE1	2.08	0.53
1:C:763:SER:O	1:C:767:PHE:HD1	1.92	0.53
1:A:446:ASN:O	1:A:450:THR:HB	2.07	0.53
1:B:763:SER:O	1:B:767:PHE:HD1	1.92	0.53
1:C:483:THR:CG2	1:C:498:LEU:HD21	2.38	0.53
1:B:760:SER:HB2	1:B:766:LYS:HZ1	1.74	0.53
1:C:651:LEU:HD23	1:C:658:PHE:HB2	1.91	0.53
1:C:766:LYS:NZ	1:C:766:LYS:HB2	2.23	0.53
1:C:337:SER:OG	1:C:359:CYS:HB2	2.08	0.53
1:A:574:TYR:CD2	1:A:574:TYR:N	2.76	0.53
1:B:383:ILE:HG22	1:B:429:THR:HG21	1.91	0.53
1:C:757:PHE:CG	1:C:808:PHE:HE1	2.27	0.53
1:C:828:LEU:HB3	1:C:832:ARG:HD3	1.91	0.53
1:A:383:ILE:HG22	1:A:429:THR:HG21	1.91	0.53
1:A:766:LYS:HB2	1:A:766:LYS:NZ	2.24	0.53
1:B:467:ILE:HG12	1:B:474:LEU:HD12	1.91	0.52
1:B:755:TYR:CZ	1:B:759:ILE:HD11	2.44	0.52
1:C:832:ARG:HA	1:C:838:MET:HG2	1.91	0.52
1:B:456:ILE:O	1:B:456:ILE:HG23	2.09	0.52
1:B:499:LEU:HD13	1:B:538:GLY:HA2	1.91	0.52
1:B:651:LEU:HD23	1:B:658:PHE:HB2	1.91	0.52
1:C:499:LEU:HD13	1:C:538:GLY:HA2	1.91	0.52
1:C:755:TYR:CZ	1:C:759:ILE:HD11	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:CD1	1:A:421:LEU:HD23	2.37	0.52
1:A:467:ILE:HG12	1:A:474:LEU:HD12	1.90	0.52
1:A:865:ASN:O	1:A:869:ILE:HG13	2.09	0.52
1:C:208:GLN:CA	1:C:267:VAL:HG21	2.34	0.52
1:C:208:GLN:NE2	1:C:263:GLU:CB	2.72	0.52
1:A:54:SER:HB2	1:A:61:GLY:O	2.10	0.52
1:A:755:TYR:CZ	1:A:759:ILE:HD11	2.44	0.52
1:A:760:SER:HB3	1:A:762:PHE:HD1	1.73	0.52
1:A:832:ARG:HA	1:A:838:MET:HG2	1.91	0.52
1:B:337:SER:OG	1:B:359:CYS:HB2	2.08	0.52
1:B:713:ILE:O	1:B:714:LYS:CG	2.52	0.52
1:B:760:SER:HB3	1:B:762:PHE:HD1	1.73	0.52
1:B:828:LEU:HB3	1:B:832:ARG:HD3	1.91	0.52
1:B:832:ARG:HA	1:B:838:MET:HG2	1.91	0.52
1:C:1149:LEU:HB3	1:C:1163:LEU:HD11	1.92	0.52
1:C:54:SER:HB2	1:C:61:GLY:O	2.10	0.52
1:C:865:ASN:O	1:C:869:ILE:HG13	2.09	0.52
1:A:959:GLN:HB2	1:A:1005:TRP:CE2	2.45	0.52
1:A:1029:PHE:O	1:A:1033:VAL:HG23	2.08	0.52
1:A:210:ILE:N	1:A:211:PRO:HD2	2.25	0.52
1:A:349:PHE:N	1:A:349:PHE:CD2	2.68	0.52
1:A:517:ILE:CG2	1:A:577:VAL:HG11	2.38	0.52
1:A:828:LEU:HB3	1:A:832:ARG:HD3	1.91	0.52
1:B:54:SER:HB2	1:B:61:GLY:O	2.10	0.52
1:A:1200:LYS:HB3	1:A:1274:LEU:CD2	2.39	0.52
1:A:337:SER:OG	1:A:359:CYS:HB2	2.08	0.52
1:A:815:ALA:O	1:A:819:ASP:HB3	2.09	0.52
1:A:923:GLN:HB3	1:A:924:PRO:HD3	1.92	0.52
1:B:1033:VAL:HG21	1:B:1087:GLN:NE2	2.25	0.52
1:B:654:GLY:O	1:B:655:SER:OG	2.22	0.52
1:C:207:LEU:HD13	1:C:264:LEU:CD2	2.39	0.52
1:A:545:ASN:N	1:A:546:PHE:N	2.58	0.52
1:A:651:LEU:HD23	1:A:658:PHE:HB2	1.91	0.52
1:A:85:VAL:O	1:A:89:ILE:HG13	2.09	0.52
1:C:959:GLN:HB2	1:C:1005:TRP:CE2	2.45	0.52
1:C:713:ILE:O	1:C:714:LYS:CG	2.52	0.52
1:A:395:PRO:O	1:A:455:PRO:HG2	2.10	0.52
1:A:517:ILE:HG21	1:A:577:VAL:CG1	2.39	0.52
1:A:750:GLU:HG2	1:A:804:LEU:CD2	2.39	0.52
1:B:1200:LYS:HB3	1:B:1274:LEU:CD2	2.39	0.52
1:C:1200:LYS:HB3	1:C:1274:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ILE:HG12	1:C:474:LEU:HD12	1.90	0.52
1:C:545:ASN:C	1:C:546:PHE:CD2	2.83	0.52
1:B:224:GLY:C	1:B:225:SER:N	2.63	0.52
1:B:815:ALA:O	1:B:819:ASP:HB3	2.09	0.52
1:B:946:THR:HA	1:B:949:GLN:HB2	1.91	0.52
1:B:489:PHE:HE2	1:C:447:ARG:HG3	1.74	0.52
1:C:750:GLU:OE2	1:C:802:SER:HA	2.09	0.52
1:C:815:ALA:O	1:C:819:ASP:HB3	2.09	0.52
1:C:613:ARG:NH2	1:C:862:ASP:OD1	2.43	0.52
1:B:959:GLN:HB2	1:B:1005:TRP:CE2	2.45	0.52
1:B:1056:ILE:HD12	1:B:1216:TYR:CG	2.45	0.52
1:C:1056:ILE:HD12	1:C:1216:TYR:CG	2.45	0.52
1:B:489:PHE:CE1	1:C:446:ASN:HB3	2.45	0.52
1:B:210:ILE:N	1:B:211:PRO:HD2	2.25	0.51
1:C:383:ILE:HG22	1:C:429:THR:HG21	1.91	0.51
1:C:760:SER:HB3	1:C:762:PHE:HD1	1.73	0.51
1:A:1056:ILE:HD12	1:A:1216:TYR:CG	2.45	0.51
1:A:763:SER:O	1:A:767:PHE:HD1	1.92	0.51
1:A:946:THR:HA	1:A:949:GLN:HB2	1.91	0.51
1:B:395:PRO:O	1:B:455:PRO:HG2	2.10	0.51
1:B:574:TYR:N	1:B:574:TYR:CD2	2.76	0.51
1:B:1054:GLY:CA	1:B:1152:THR:HG23	2.41	0.51
1:C:1095:VAL:HG13	1:C:1135:ILE:HG23	1.93	0.51
1:A:483:THR:CG2	1:A:498:LEU:HD21	2.38	0.51
1:B:923:GLN:HB3	1:B:924:PRO:HD3	1.92	0.51
1:B:865:ASN:O	1:B:869:ILE:HG13	2.09	0.51
1:A:542:LEU:O	1:A:546:PHE:HD2	1.94	0.51
1:B:966:LEU:HB3	1:B:1013:TYR:CZ	2.46	0.51
1:B:1149:LEU:HB3	1:B:1163:LEU:HD11	1.92	0.51
1:C:210:ILE:N	1:C:211:PRO:HD2	2.25	0.51
1:A:456:ILE:HG23	1:A:456:ILE:O	2.09	0.51
1:C:275:ILE:O	1:C:279:ILE:HG13	2.11	0.51
1:A:72:CYS:CB	1:A:93:LEU:HD11	2.41	0.51
1:C:743:CYS:HA	1:C:746:MET:HB2	1.93	0.51
1:C:764:LYS:HD3	1:C:826:GLU:OE1	2.11	0.51
1:A:652:THR:OG1	1:A:657:ILE:HG12	2.11	0.50
1:B:275:ILE:O	1:B:279:ILE:HG13	2.11	0.50
1:C:923:GLN:HB3	1:C:924:PRO:HD3	1.92	0.50
1:A:1032:HIS:O	1:A:1035:TYR:N	2.37	0.50
1:B:536:VAL:HG11	1:B:603:MET:HE3	1.92	0.50
1:C:456:ILE:O	1:C:456:ILE:HG23	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1095:VAL:HG13	1:B:1135:ILE:HG23	1.93	0.50
1:B:303:LYS:HG2	1:B:357:ARG:NH2	2.26	0.50
1:C:395:PRO:O	1:C:455:PRO:HG2	2.10	0.50
1:B:72:CYS:CB	1:B:93:LEU:HD11	2.41	0.50
1:C:1054:GLY:CA	1:C:1152:THR:HG23	2.41	0.50
1:C:303:LYS:HG2	1:C:357:ARG:NH2	2.26	0.50
1:C:652:THR:OG1	1:C:657:ILE:HG12	2.11	0.50
1:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.93	0.50
1:A:216:GLN:O	1:A:219:VAL:HG22	2.11	0.50
1:A:221:SER:CB	1:A:229:VAL:HG21	2.41	0.50
1:A:839:HIS:HB3	1:A:903:ILE:HG13	1.93	0.50
1:B:230:LEU:HD21	1:B:285:LEU:HD21	1.94	0.50
1:C:1092:LEU:HD13	1:C:1169:LYS:HG2	1.93	0.50
1:C:1273:ASN:O	1:C:1276:GLN:N	2.45	0.50
1:C:187:THR:HG22	1:C:188:PRO:CD	2.41	0.50
1:C:995:THR:O	1:C:996:SER:O	2.30	0.50
1:A:349:PHE:HE2	1:A:1033:VAL:HG12	1.76	0.50
1:A:268:GLU:O	1:A:272:ILE:HG13	2.12	0.50
1:A:513:ARG:O	1:A:517:ILE:HD12	2.12	0.50
1:B:1252:LEU:O	1:B:1256:ILE:HG13	2.12	0.50
1:B:94:MET:HG2	1:B:132:ILE:HD13	1.94	0.50
1:B:743:CYS:HA	1:B:746:MET:HB2	1.94	0.50
1:B:839:HIS:HB3	1:B:903:ILE:HG13	1.93	0.50
1:B:995:THR:O	1:B:996:SER:O	2.29	0.50
1:A:966:LEU:HB3	1:A:1013:TYR:CZ	2.46	0.50
1:A:187:THR:HG22	1:A:188:PRO:CD	2.41	0.50
1:B:652:THR:OG1	1:B:657:ILE:HG12	2.11	0.50
1:B:838:MET:HA	1:B:838:MET:CE	2.42	0.50
1:C:930:LEU:HD13	1:C:950:ARG:HB2	1.94	0.50
1:B:1054:GLY:O	1:B:1055:ASP:CB	2.59	0.50
1:B:635:GLU:O	1:B:711:ARG:NH2	2.40	0.50
1:C:230:LEU:HD21	1:C:285:LEU:HD21	1.94	0.50
1:C:341:LEU:CD1	1:C:359:CYS:HB3	2.42	0.50
1:C:839:HIS:HB3	1:C:903:ILE:HG13	1.93	0.50
1:A:1086:SER:O	1:A:1090:LYS:HG2	2.12	0.50
1:A:397:LYS:N	1:A:397:LYS:HD3	2.27	0.50
1:C:72:CYS:CB	1:C:93:LEU:HD11	2.41	0.50
1:C:966:LEU:HB3	1:C:1013:TYR:CZ	2.46	0.50
1:A:1252:LEU:O	1:A:1256:ILE:HG13	2.12	0.49
1:A:394:GLY:O	1:A:396:LYS:HE3	2.12	0.49
1:A:750:GLU:HG2	1:A:804:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:PHE:CB	1:A:837:PHE:HD2	2.25	0.49
1:B:1033:VAL:HG21	1:B:1087:GLN:HE22	1.77	0.49
1:B:1086:SER:O	1:B:1090:LYS:HG2	2.12	0.49
1:B:513:ARG:O	1:B:517:ILE:HD12	2.12	0.49
1:A:1092:LEU:HD13	1:A:1169:LYS:HG2	1.93	0.49
1:B:187:THR:HG22	1:B:188:PRO:CD	2.41	0.49
1:B:397:LYS:HD3	1:B:397:LYS:N	2.27	0.49
1:C:268:GLU:O	1:C:272:ILE:HG13	2.12	0.49
1:C:672:HIS:CE1	1:C:861:PRO:CG	2.95	0.49
1:A:1054:GLY:CA	1:A:1152:THR:HG23	2.41	0.49
1:A:1149:LEU:HB3	1:A:1163:LEU:HD11	1.92	0.49
1:A:995:THR:O	1:A:996:SER:O	2.30	0.49
1:B:1050:HIS:HA	1:B:1152:THR:OG1	2.12	0.49
1:B:843:ASN:O	1:B:847:GLN:HB2	2.13	0.49
1:C:1086:SER:O	1:C:1090:LYS:HG2	2.12	0.49
1:C:639:ASP:H	1:C:711:ARG:HE	1.60	0.49
1:A:262:ASP:O	1:A:266:HIS:ND1	2.44	0.49
1:A:303:LYS:HG2	1:A:357:ARG:NH2	2.26	0.49
1:B:1092:LEU:HD13	1:B:1169:LYS:HG2	1.93	0.49
1:B:216:GLN:O	1:B:219:VAL:HG22	2.11	0.49
1:C:216:GLN:O	1:C:219:VAL:HG22	2.11	0.49
1:A:230:LEU:HD21	1:A:285:LEU:HD21	1.94	0.49
1:B:262:ASP:O	1:B:266:HIS:ND1	2.44	0.49
1:B:268:GLU:O	1:B:272:ILE:HG13	2.12	0.49
1:B:341:LEU:CD1	1:B:359:CYS:HB3	2.43	0.49
1:C:1050:HIS:HA	1:C:1152:THR:OG1	2.13	0.49
1:C:208:GLN:NE2	1:C:263:GLU:O	2.46	0.49
1:A:1012:GLU:CD	1:B:1008:LYS:CE	2.67	0.49
1:A:838:MET:HA	1:A:838:MET:CE	2.42	0.49
1:B:1273:ASN:O	1:B:1276:GLN:N	2.45	0.49
1:C:201:MET:O	1:C:205:LEU:HD12	2.13	0.49
1:C:322:PHE:O	1:C:326:VAL:HG23	2.13	0.49
1:A:275:ILE:O	1:A:279:ILE:HG13	2.11	0.49
1:B:973:PHE:HD1	1:B:974:ASN:H	1.57	0.49
1:C:94:MET:HG2	1:C:132:ILE:HD13	1.94	0.49
1:C:394:GLY:O	1:C:396:LYS:HE3	2.12	0.49
1:C:545:ASN:HB2	1:C:546:PHE:CD2	2.48	0.49
1:C:760:SER:HB2	1:C:766:LYS:NZ	2.28	0.49
1:C:843:ASN:O	1:C:847:GLN:HB2	2.13	0.49
1:A:843:ASN:O	1:A:847:GLN:HB2	2.12	0.49
1:B:511:SER:O	1:B:515:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:HIS:HA	1:A:1152:THR:OG1	2.13	0.49
1:A:760:SER:HB2	1:A:766:LYS:NZ	2.28	0.49
1:A:826:GLU:HA	1:A:829:SER:OG	2.13	0.49
1:B:589:SER:O	1:B:592:ARG:HG2	2.13	0.49
1:C:1252:LEU:O	1:C:1256:ILE:HG13	2.12	0.49
1:C:1:MET:O	1:C:5:ILE:HG13	2.13	0.49
1:C:21:LEU:HB3	1:C:64:ARG:NE	2.28	0.49
1:C:397:LYS:N	1:C:397:LYS:HD3	2.27	0.49
1:A:1091:VAL:HA	1:A:1094:GLU:HG3	1.95	0.49
1:A:341:LEU:CD1	1:A:359:CYS:HB3	2.42	0.49
1:A:448:VAL:HA	1:A:456:ILE:CD1	2.43	0.49
1:B:1032:HIS:O	1:B:1035:TYR:N	2.37	0.49
1:B:799:VAL:O	1:B:847:GLN:CD	2.49	0.49
1:B:930:LEU:HD13	1:B:950:ARG:HB2	1.94	0.49
1:C:137:LEU:O	1:C:153:GLY:HA3	2.13	0.49
1:C:207:LEU:HD21	1:C:236:PHE:CE2	2.45	0.49
1:C:976:LYS:O	1:C:980:LEU:HD22	2.13	0.49
1:A:201:MET:O	1:A:205:LEU:HD12	2.13	0.48
1:A:743:CYS:HA	1:A:746:MET:HB2	1.94	0.48
1:B:201:MET:O	1:B:205:LEU:HD12	2.13	0.48
1:C:1014:SER:HB3	1:C:1070:VAL:HG12	1.95	0.48
1:A:94:MET:HG2	1:A:132:ILE:HD13	1.94	0.48
1:A:511:SER:O	1:A:515:SER:HB2	2.13	0.48
1:A:799:VAL:O	1:A:847:GLN:CD	2.49	0.48
1:B:137:LEU:O	1:B:153:GLY:HA3	2.13	0.48
1:B:322:PHE:O	1:B:326:VAL:HG23	2.13	0.48
1:B:870:PHE:CD1	1:B:922:TYR:HD2	2.32	0.48
1:C:448:VAL:HA	1:C:456:ILE:CD1	2.43	0.48
1:C:838:MET:HA	1:C:838:MET:CE	2.42	0.48
1:A:1054:GLY:HA3	1:A:1152:THR:HG23	1.95	0.48
1:A:339:LYS:HD2	1:A:339:LYS:HA	1.67	0.48
1:B:1054:GLY:HA3	1:B:1152:THR:HG23	1.95	0.48
1:B:141:LYS:O	1:B:142:GLU:HG3	2.13	0.48
1:B:1:MET:O	1:B:5:ILE:HG13	2.13	0.48
1:B:394:GLY:O	1:B:396:LYS:HE3	2.12	0.48
1:B:639:ASP:H	1:B:711:ARG:HE	1.60	0.48
1:B:826:GLU:HA	1:B:829:SER:OG	2.13	0.48
1:B:828:LEU:O	1:B:832:ARG:HG3	2.13	0.48
1:C:1054:GLY:O	1:C:1055:ASP:CB	2.59	0.48
1:C:589:SER:O	1:C:592:ARG:HG2	2.13	0.48
1:A:137:LEU:O	1:A:153:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:LEU:HD21	1:B:1077:ALA:HB2	1.95	0.48
1:B:1091:VAL:HA	1:B:1094:GLU:HG3	1.95	0.48
1:B:74:GLN:HA	1:B:77:GLU:OE2	2.14	0.48
1:C:208:GLN:HA	1:C:267:VAL:HG21	1.94	0.48
1:C:513:ARG:O	1:C:517:ILE:HD12	2.12	0.48
1:C:574:TYR:CD2	1:C:574:TYR:N	2.76	0.48
1:A:1053:LEU:HD21	1:A:1077:ALA:HB2	1.95	0.48
1:A:21:LEU:HB3	1:A:64:ARG:NE	2.28	0.48
1:A:828:LEU:O	1:A:832:ARG:HG3	2.13	0.48
1:B:259:ALA:CB	1:B:260:PRO:CD	2.91	0.48
1:B:775:THR:O	1:B:779:LYS:HB2	2.13	0.48
1:B:976:LYS:O	1:B:980:LEU:HD22	2.13	0.48
1:C:826:GLU:HA	1:C:829:SER:OG	2.13	0.48
1:A:141:LYS:O	1:A:142:GLU:HG3	2.13	0.48
1:A:908:LEU:HD11	1:A:981:LEU:HG	1.96	0.48
1:B:1033:VAL:CG2	1:B:1087:GLN:NE2	2.76	0.48
1:B:732:THR:O	1:B:736:ILE:HG13	2.14	0.48
1:C:1022:LYS:HA	1:C:1083:LEU:HD11	1.94	0.48
1:A:1054:GLY:O	1:A:1055:ASP:CB	2.59	0.48
1:A:322:PHE:O	1:A:326:VAL:HG23	2.13	0.48
1:A:639:ASP:H	1:A:711:ARG:HE	1.60	0.48
1:A:930:LEU:HD13	1:A:950:ARG:HB2	1.94	0.48
1:C:1054:GLY:HA3	1:C:1152:THR:HG23	1.95	0.48
1:C:775:THR:O	1:C:779:LYS:HB2	2.13	0.48
1:A:589:SER:O	1:A:592:ARG:HG2	2.13	0.48
1:A:732:THR:O	1:A:736:ILE:HG13	2.14	0.48
1:A:771:LEU:HG	1:A:830:VAL:O	2.13	0.48
1:A:672:HIS:CE1	1:A:861:PRO:HG3	2.49	0.48
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.96	0.48
1:A:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
1:B:1055:ASP:O	1:B:1056:ILE:C	2.52	0.48
1:B:1171:TYR:O	1:B:1175:THR:OG1	2.23	0.48
1:B:776:CYS:O	1:B:780:PHE:HD1	1.97	0.48
1:C:732:THR:O	1:C:736:ILE:HG13	2.14	0.48
1:A:170:PRO:HG2	1:A:173:TYR:HD1	1.79	0.48
1:A:1:MET:O	1:A:5:ILE:HG13	2.13	0.48
1:B:908:LEU:HD11	1:B:981:LEU:HG	1.96	0.48
1:C:908:LEU:HD11	1:C:981:LEU:HG	1.96	0.48
1:A:533:LYS:HA	1:A:603:MET:HE1	1.96	0.48
1:A:635:GLU:O	1:A:711:ARG:NH2	2.40	0.48
1:C:170:PRO:HG2	1:C:173:TYR:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:THR:O	1:A:779:LYS:HB2	2.13	0.47
1:B:1207:THR:O	1:B:1211:TYR:HD1	1.97	0.47
1:C:141:LYS:O	1:C:142:GLU:HG3	2.13	0.47
1:C:74:GLN:HA	1:C:77:GLU:OE2	2.13	0.47
1:C:818:ARG:NH1	1:C:878:ARG:HD2	2.29	0.47
1:A:801:ASP:OD1	1:A:801:ASP:N	2.47	0.47
1:A:768:GLU:OE1	1:A:830:VAL:CG2	2.60	0.47
1:B:1080:VAL:HG12	1:B:1080:VAL:O	2.14	0.47
1:B:8:LEU:HD13	1:B:17:LEU:HA	1.96	0.47
1:C:1055:ASP:O	1:C:1056:ILE:C	2.52	0.47
1:A:818:ARG:NH1	1:A:878:ARG:HD2	2.29	0.47
1:B:21:LEU:HB3	1:B:64:ARG:NE	2.29	0.47
1:C:776:CYS:O	1:C:780:PHE:HD1	1.97	0.47
1:C:806:LEU:CD2	1:C:872:ASN:HB3	2.44	0.47
1:C:672:HIS:CE1	1:C:861:PRO:CD	2.97	0.47
1:A:1055:ASP:O	1:A:1056:ILE:C	2.52	0.47
1:A:1080:VAL:HG12	1:A:1080:VAL:O	2.14	0.47
1:A:174:MET:HA	1:A:177:LEU:HB2	1.97	0.47
1:A:74:GLN:HA	1:A:77:GLU:OE2	2.13	0.47
1:B:174:MET:HA	1:B:177:LEU:HB2	1.97	0.47
1:B:259:ALA:HB3	1:B:260:PRO:CD	2.29	0.47
1:B:360:VAL:O	1:B:364:ILE:HG13	2.15	0.47
1:B:486:TYR:HE2	1:C:449:VAL:CG2	2.27	0.47
1:B:760:SER:HB2	1:B:766:LYS:NZ	2.28	0.47
1:C:259:ALA:HB3	1:C:260:PRO:CD	2.29	0.47
1:C:353:LEU:HD12	1:C:1098:LEU:HD21	1.95	0.47
1:C:918:VAL:HG21	1:C:929:PHE:CE2	2.50	0.47
1:A:774:PHE:CZ	1:A:837:PHE:CA	2.98	0.47
1:A:1280:LEU:HD12	1:B:1280:LEU:HB3	1.10	0.47
1:C:1171:TYR:O	1:C:1175:THR:OG1	2.23	0.47
1:C:1207:THR:O	1:C:1211:TYR:HD1	1.97	0.47
1:C:511:SER:O	1:C:515:SER:HB2	2.13	0.47
1:C:594:LEU:HG	1:C:604:LEU:HD23	1.96	0.47
1:C:609:TYR:CE2	1:C:861:PRO:HB3	2.49	0.47
1:C:908:LEU:HD22	1:C:980:LEU:HG	1.96	0.47
1:A:1012:GLU:OE1	1:B:1008:LYS:NZ	2.47	0.47
1:A:1273:ASN:O	1:A:1276:GLN:N	2.45	0.47
1:A:630:LEU:HD13	1:A:704:MET:HE1	1.97	0.47
1:C:1029:PHE:CZ	1:C:1087:GLN:HG2	2.48	0.47
1:C:360:VAL:O	1:C:364:ILE:HG13	2.15	0.47
1:C:604:LEU:HG	1:C:608:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:PHE:CD1	1:C:922:TYR:HD2	2.32	0.47
1:A:1207:THR:O	1:A:1211:TYR:HD1	1.97	0.47
1:B:922:TYR:N	1:B:922:TYR:CD1	2.83	0.47
1:B:918:VAL:HG21	1:B:929:PHE:CE2	2.50	0.47
1:C:1053:LEU:HD21	1:C:1077:ALA:HB2	1.95	0.47
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.50	0.47
1:A:922:TYR:CD1	1:A:922:TYR:N	2.83	0.47
1:B:1145:PHE:HD2	1:B:1146:PHE:CD1	2.33	0.47
1:B:806:LEU:CD2	1:B:872:ASN:HB3	2.44	0.47
1:C:1091:VAL:HA	1:C:1094:GLU:HG3	1.95	0.47
1:C:630:LEU:HD13	1:C:704:MET:HE1	1.96	0.47
1:C:8:LEU:HD13	1:C:17:LEU:HA	1.96	0.47
1:A:360:VAL:O	1:A:364:ILE:HG13	2.15	0.47
1:A:513:ARG:HD3	1:A:546:PHE:CZ	2.50	0.47
1:B:581:THR:HB	1:B:585:GLU:HG3	1.96	0.47
1:B:94:MET:HG2	1:B:132:ILE:CD1	2.45	0.47
1:C:1145:PHE:HD2	1:C:1146:PHE:CD1	2.33	0.47
1:A:259:ALA:CB	1:A:260:PRO:CD	2.91	0.47
1:A:598:ALA:HA	1:A:601:ARG:HD3	1.97	0.47
1:B:15:ASP:N	1:B:15:ASP:OD1	2.47	0.47
1:B:359:CYS:SG	1:B:361:SER:HB2	2.55	0.47
1:C:214:VAL:HG21	1:C:233:ILE:CG1	2.42	0.47
1:C:543:LEU:CD2	1:C:586:ILE:HD12	2.45	0.47
1:C:828:LEU:O	1:C:832:ARG:HG3	2.14	0.47
1:C:816:LEU:HD13	1:C:838:MET:HE1	1.96	0.47
1:A:1145:PHE:HD2	1:A:1146:PHE:CD1	2.33	0.47
1:A:918:VAL:HG21	1:A:929:PHE:CE2	2.50	0.47
1:A:94:MET:HG2	1:A:132:ILE:CD1	2.45	0.47
1:B:349:PHE:CD2	1:B:349:PHE:N	2.68	0.47
1:B:818:ARG:NH1	1:B:878:ARG:HD2	2.30	0.47
1:C:1080:VAL:HG12	1:C:1080:VAL:O	2.14	0.47
1:C:174:MET:HA	1:C:177:LEU:HB2	1.97	0.47
1:C:359:CYS:SG	1:C:361:SER:HB2	2.55	0.47
1:C:503:GLN:HB2	1:C:504:PRO:HD3	1.97	0.47
1:C:911:LEU:CD2	1:C:915:PHE:HE1	2.28	0.47
1:A:594:LEU:HG	1:A:604:LEU:HD23	1.96	0.46
1:A:778:LYS:HE2	1:A:836:GLU:CD	2.34	0.46
1:A:806:LEU:CD2	1:A:872:ASN:HB3	2.44	0.46
1:C:1249:ILE:N	1:C:1250:PRO:CD	2.79	0.46
1:B:594:LEU:HG	1:B:604:LEU:HD23	1.96	0.46
1:C:581:THR:HB	1:C:585:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLN:HB2	1:A:504:PRO:HD3	1.97	0.46
1:A:542:LEU:CD2	1:A:546:PHE:CE2	2.99	0.46
1:A:776:CYS:O	1:A:780:PHE:HD1	1.97	0.46
1:A:1280:LEU:HB3	1:B:1280:LEU:HD12	1.64	0.46
1:B:170:PRO:HG2	1:B:173:TYR:HD1	1.79	0.46
1:B:446:ASN:HD22	1:C:489:PHE:HE1	1.62	0.46
1:B:911:LEU:CD2	1:B:915:PHE:HE1	2.29	0.46
1:B:908:LEU:HD22	1:B:980:LEU:HG	1.96	0.46
1:C:623:MET:HE2	1:C:623:MET:HB2	1.84	0.46
1:C:69:TYR:CE2	1:C:97:VAL:HG23	2.51	0.46
1:A:109:ALA:O	1:A:113:VAL:HG23	2.16	0.46
1:A:1249:ILE:N	1:A:1250:PRO:CD	2.79	0.46
1:A:359:CYS:SG	1:A:361:SER:HB2	2.55	0.46
1:B:121:LEU:C	1:B:123:ASN:N	2.69	0.46
1:B:59:GLU:O	1:B:63:LEU:HG	2.16	0.46
1:B:604:LEU:HG	1:B:608:PHE:CE1	2.50	0.46
1:C:973:PHE:HD1	1:C:974:ASN:H	1.57	0.46
1:A:207:LEU:CD2	1:A:240:LEU:HD11	2.19	0.46
1:A:581:THR:HB	1:A:585:GLU:HG3	1.96	0.46
1:A:908:LEU:HD22	1:A:980:LEU:HG	1.96	0.46
1:C:94:MET:HG2	1:C:132:ILE:CD1	2.45	0.46
1:C:922:TYR:N	1:C:922:TYR:CD1	2.83	0.46
1:A:759:ILE:CG2	1:A:760:SER:N	2.79	0.46
1:A:911:LEU:CD2	1:A:915:PHE:HE1	2.28	0.46
1:A:870:PHE:CD1	1:A:922:TYR:HD2	2.32	0.46
1:B:361:SER:HG	1:B:417:HIS:CE1	2.34	0.46
1:C:635:GLU:O	1:C:711:ARG:NH2	2.40	0.46
1:C:771:LEU:HD12	1:C:830:VAL:O	2.15	0.46
1:A:266:HIS:CE1	1:A:373:HIS:HB3	2.51	0.46
1:A:316:LEU:O	1:A:316:LEU:HD22	2.16	0.46
1:B:146:CYS:O	1:B:147:GLY:C	2.54	0.46
1:C:109:ALA:O	1:C:113:VAL:HG23	2.16	0.46
1:C:207:LEU:HD21	1:C:237:PHE:CD2	2.48	0.46
1:C:51:LEU:HD13	1:C:96:GLU:HG2	1.98	0.46
1:A:259:ALA:HB3	1:A:260:PRO:CD	2.29	0.46
1:B:271:VAL:O	1:B:275:ILE:HG23	2.16	0.46
1:B:630:LEU:HD13	1:B:704:MET:HE1	1.97	0.46
1:C:1154:LEU:CD1	1:C:1163:LEU:HD12	2.46	0.46
1:C:121:LEU:C	1:C:123:ASN:N	2.69	0.46
1:C:598:ALA:HA	1:C:601:ARG:HD3	1.97	0.46
1:A:529:LEU:HA	1:A:532:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:LEU:HD13	1:A:858:VAL:HG23	1.98	0.46
1:B:489:PHE:CE2	1:C:447:ARG:HG3	2.51	0.46
1:B:503:GLN:HB2	1:B:504:PRO:HD3	1.97	0.46
1:B:922:TYR:HD1	1:B:922:TYR:N	2.14	0.46
1:C:158:ARG:O	1:C:162:ASP:HB2	2.16	0.46
1:C:316:LEU:O	1:C:316:LEU:HD22	2.16	0.46
1:C:529:LEU:HA	1:C:532:ARG:NH2	2.31	0.46
1:A:69:TYR:CE2	1:A:97:VAL:HG23	2.51	0.45
1:A:744:LEU:HD23	1:A:744:LEU:HA	1.87	0.45
1:A:764:LYS:HD3	1:A:824:HIS:CE1	2.51	0.45
1:B:69:TYR:CE2	1:B:97:VAL:HG23	2.51	0.45
1:A:158:ARG:O	1:A:162:ASP:HB2	2.16	0.45
1:A:922:TYR:HD1	1:A:922:TYR:N	2.14	0.45
1:B:109:ALA:O	1:B:113:VAL:HG23	2.16	0.45
1:B:316:LEU:HD22	1:B:316:LEU:O	2.16	0.45
1:B:993:GLU:CD	1:B:994:PRO:HD2	2.37	0.45
1:C:372:VAL:HG22	1:C:432:ILE:CG2	2.46	0.45
1:C:644:LEU:HD21	1:C:708:ILE:HD13	1.98	0.45
1:A:1199:VAL:O	1:A:1202:SER:OG	2.30	0.45
1:A:59:GLU:O	1:A:63:LEU:HG	2.16	0.45
1:B:158:ARG:O	1:B:162:ASP:HB2	2.16	0.45
1:C:271:VAL:O	1:C:275:ILE:HG23	2.16	0.45
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.17	0.45
1:A:372:VAL:HG22	1:A:432:ILE:CG2	2.46	0.45
1:B:529:LEU:HA	1:B:532:ARG:NH2	2.31	0.45
1:C:146:CYS:O	1:C:147:GLY:C	2.54	0.45
1:C:993:GLU:CD	1:C:994:PRO:HD2	2.37	0.45
1:A:335:VAL:HG13	1:A:414:THR:CG2	2.46	0.45
1:A:675:ALA:O	1:A:679:SER:HB3	2.17	0.45
1:A:881:LEU:HG	1:A:911:LEU:HD21	1.99	0.45
1:C:262:ASP:O	1:C:266:HIS:ND1	2.44	0.45
1:C:266:HIS:CE1	1:C:373:HIS:HB3	2.51	0.45
1:A:1103:LYS:HE2	1:A:1103:LYS:HB3	1.80	0.45
1:A:151:LEU:HD12	1:A:156:TYR:CZ	2.52	0.45
1:A:993:GLU:CD	1:A:994:PRO:HD2	2.37	0.45
1:B:372:VAL:HG22	1:B:432:ILE:CG2	2.46	0.45
1:B:266:HIS:CE1	1:B:373:HIS:HB3	2.51	0.45
1:B:441:LEU:HD13	1:B:474:LEU:HD22	1.98	0.45
1:B:51:LEU:HD13	1:B:96:GLU:HG2	1.98	0.45
1:C:335:VAL:HG13	1:C:414:THR:CG2	2.46	0.45
1:C:540:LEU:O	1:C:544:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLU:O	1:C:63:LEU:HG	2.16	0.45
1:C:675:ALA:O	1:C:679:SER:HB3	2.17	0.45
1:B:1154:LEU:CD1	1:B:1163:LEU:HD12	2.46	0.45
1:B:598:ALA:HA	1:B:601:ARG:HD3	1.97	0.45
1:B:644:LEU:HD21	1:B:708:ILE:HD13	1.98	0.45
1:C:259:ALA:CB	1:C:260:PRO:CD	2.91	0.45
1:C:708:ILE:HG22	1:C:752:LEU:HD11	1.99	0.45
1:A:1174:LEU:O	1:A:1178:VAL:HG23	2.17	0.45
1:A:671:GLN:OE1	1:A:672:HIS:CD2	2.70	0.45
1:B:708:ILE:HG22	1:B:752:LEU:HD11	1.99	0.45
1:C:1174:LEU:O	1:C:1178:VAL:HG23	2.17	0.45
1:C:671:GLN:OE1	1:C:672:HIS:CD2	2.70	0.45
1:C:764:LYS:CD	1:C:826:GLU:OE1	2.65	0.45
1:A:51:LEU:HD13	1:A:96:GLU:HG2	1.98	0.45
1:A:708:ILE:HG22	1:A:752:LEU:HD11	1.99	0.45
1:B:801:ASP:N	1:B:801:ASP:OD1	2.47	0.45
1:C:671:GLN:CG	1:C:755:TYR:HB2	2.47	0.45
1:A:121:LEU:C	1:A:123:ASN:N	2.69	0.45
1:A:540:LEU:O	1:A:544:LYS:HG3	2.17	0.45
1:A:671:GLN:CG	1:A:755:TYR:HB2	2.47	0.45
1:B:1249:ILE:N	1:B:1250:PRO:CD	2.79	0.45
1:B:298:GLN:HE21	1:B:336:LYS:CG	2.29	0.45
1:B:675:ALA:O	1:B:679:SER:HB3	2.17	0.45
1:C:441:LEU:HD13	1:C:474:LEU:HD22	1.99	0.45
1:C:799:VAL:O	1:C:847:GLN:CD	2.49	0.45
1:A:146:CYS:O	1:A:147:GLY:C	2.54	0.44
1:A:361:SER:HG	1:A:417:HIS:CE1	2.34	0.44
1:A:945:VAL:O	1:A:949:GLN:HB2	2.17	0.44
1:B:448:VAL:HA	1:B:456:ILE:CD1	2.43	0.44
1:B:852:LEU:HD13	1:B:858:VAL:HG23	1.99	0.44
1:C:120:ARG:HG2	1:C:172:ARG:HH12	1.82	0.44
1:C:41:ARG:HD3	1:C:41:ARG:N	2.32	0.44
1:C:552:LEU:HD23	1:C:552:LEU:C	2.38	0.44
1:C:922:TYR:N	1:C:922:TYR:HD1	2.14	0.44
1:A:271:VAL:O	1:A:275:ILE:HG23	2.16	0.44
1:A:430:PHE:CZ	1:A:466:ILE:HG23	2.52	0.44
1:A:513:ARG:NH1	1:A:514:ASP:OD1	2.51	0.44
1:A:22:GLN:HG2	1:A:60:ASP:OD2	2.18	0.44
1:B:349:PHE:O	1:B:353:LEU:HG	2.17	0.44
1:B:430:PHE:CZ	1:B:466:ILE:HG23	2.52	0.44
1:B:945:VAL:O	1:B:949:GLN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:SER:HB2	1:A:1148:GLU:HB2	2.00	0.44
1:A:1164:LEU:HD22	1:A:1252:LEU:CD1	2.48	0.44
1:A:552:LEU:C	1:A:552:LEU:HD23	2.38	0.44
1:B:1144:THR:O	1:B:1148:GLU:HG2	2.17	0.44
1:B:120:ARG:HG2	1:B:172:ARG:HH12	1.82	0.44
1:C:744:LEU:HA	1:C:744:LEU:HD23	1.87	0.44
1:C:801:ASP:OD1	1:C:801:ASP:N	2.47	0.44
1:A:14:THR:O	1:A:15:ASP:C	2.56	0.44
1:B:1103:LYS:HE2	1:B:1103:LYS:HB3	1.79	0.44
1:B:1174:LEU:O	1:B:1178:VAL:HG23	2.17	0.44
1:B:671:GLN:OE1	1:B:672:HIS:CD2	2.70	0.44
1:B:881:LEU:HG	1:B:911:LEU:HD21	1.99	0.44
1:C:1144:THR:O	1:C:1148:GLU:HG2	2.17	0.44
1:C:211:PRO:N	1:C:212:PRO:HD2	2.33	0.44
1:C:650:VAL:HG13	1:C:657:ILE:HG23	2.00	0.44
1:C:881:LEU:HG	1:C:911:LEU:HD21	1.99	0.44
1:A:441:LEU:HD13	1:A:474:LEU:HD22	1.99	0.44
1:A:540:LEU:CD2	1:A:611:VAL:HG21	2.47	0.44
1:A:650:VAL:HG13	1:A:657:ILE:HG23	2.00	0.44
1:B:1053:LEU:HD11	1:B:1077:ALA:HA	1.99	0.44
1:B:1056:ILE:HD12	1:B:1216:TYR:CD1	2.53	0.44
1:C:1199:VAL:O	1:C:1202:SER:OG	2.30	0.44
1:C:214:VAL:CB	1:C:233:ILE:CD1	2.91	0.44
1:C:298:GLN:HE21	1:C:336:LYS:CG	2.28	0.44
1:C:361:SER:HG	1:C:417:HIS:CE1	2.34	0.44
1:C:852:LEU:HD13	1:C:858:VAL:HG23	1.98	0.44
1:A:1002:MET:HG3	1:A:1031:LEU:CD1	2.47	0.44
1:A:476:ASN:OD1	1:A:476:ASN:N	2.50	0.44
1:A:644:LEU:HD21	1:A:708:ILE:HD13	1.99	0.44
1:B:978:ALA:HB1	1:B:1020:PHE:CE1	2.53	0.44
1:B:151:LEU:HD12	1:B:156:TYR:CZ	2.52	0.44
1:B:298:GLN:C	1:B:301:PRO:HD2	2.38	0.44
1:C:349:PHE:O	1:C:353:LEU:HG	2.17	0.44
1:C:430:PHE:CZ	1:C:466:ILE:HG23	2.52	0.44
1:C:476:ASN:N	1:C:476:ASN:OD1	2.50	0.44
1:C:513:ARG:NH1	1:C:514:ASP:OD1	2.51	0.44
1:C:945:VAL:O	1:C:949:GLN:HB2	2.17	0.44
1:A:1053:LEU:HD11	1:A:1077:ALA:HA	1.99	0.44
1:A:120:ARG:HG2	1:A:172:ARG:HH12	1.82	0.44
1:A:542:LEU:O	1:A:546:PHE:CD2	2.71	0.44
1:B:1164:LEU:HD22	1:B:1252:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1260:GLU:HA	1:B:1263:LEU:HD12	2.00	0.44
1:C:1046:SER:HB2	1:C:1148:GLU:HB2	2.00	0.44
1:C:1260:GLU:HA	1:C:1263:LEU:HD12	2.00	0.44
1:C:151:LEU:HD12	1:C:156:TYR:CZ	2.52	0.44
1:C:211:PRO:HB3	1:C:271:VAL:CA	2.48	0.44
1:C:214:VAL:CG2	1:C:233:ILE:HG12	2.47	0.44
1:C:664:ASP:HB2	1:C:803:LEU:CD1	2.48	0.44
1:A:1056:ILE:HD12	1:A:1216:TYR:CD1	2.52	0.44
1:A:542:LEU:HD23	1:A:546:PHE:HE2	1.82	0.44
1:C:1056:ILE:HD12	1:C:1216:TYR:CD1	2.53	0.44
1:C:217:LEU:O	1:C:217:LEU:HD23	2.18	0.44
1:C:563:VAL:O	1:C:563:VAL:HG13	2.17	0.44
1:C:667:LEU:HB3	1:C:751:VAL:HG11	2.00	0.44
1:C:996:SER:HB3	1:C:999:PHE:CB	2.48	0.44
1:A:226:ARG:H	1:A:226:ARG:HG2	1.54	0.44
1:A:545:ASN:C	1:A:565:GLN:CB	2.85	0.44
1:B:1002:MET:HG3	1:B:1031:LEU:CD1	2.47	0.44
1:B:14:THR:O	1:B:15:ASP:C	2.56	0.44
1:B:540:LEU:O	1:B:544:LYS:HG3	2.17	0.44
1:C:1002:MET:HG3	1:C:1031:LEU:CD1	2.47	0.44
1:C:466:ILE:O	1:C:469:TYR:HB3	2.18	0.44
1:A:349:PHE:O	1:A:353:LEU:HG	2.17	0.43
1:A:431:LYS:HG2	1:A:469:TYR:CE1	2.53	0.43
1:B:193:LEU:O	1:B:197:LYS:HG2	2.18	0.43
1:B:440:ILE:O	1:B:444:VAL:HG23	2.18	0.43
1:B:552:LEU:HD23	1:B:552:LEU:C	2.38	0.43
1:B:973:PHE:CD1	1:B:974:ASN:N	2.72	0.43
1:C:298:GLN:C	1:C:301:PRO:HD2	2.37	0.43
1:C:973:PHE:CD1	1:C:974:ASN:N	2.72	0.43
1:A:298:GLN:C	1:A:301:PRO:HD2	2.38	0.43
1:A:549:LEU:HG	1:A:549:LEU:O	2.19	0.43
1:B:217:LEU:O	1:B:217:LEU:HD23	2.18	0.43
1:B:283:CYS:O	1:B:287:ARG:HG3	2.18	0.43
1:B:341:LEU:HD11	1:B:359:CYS:HB3	2.00	0.43
1:B:563:VAL:O	1:B:563:VAL:HG13	2.17	0.43
1:C:14:THR:O	1:C:15:ASP:C	2.56	0.43
1:C:22:GLN:HG2	1:C:60:ASP:OD2	2.17	0.43
1:A:193:LEU:O	1:A:197:LYS:HG2	2.18	0.43
1:A:217:LEU:HD23	1:A:217:LEU:O	2.18	0.43
1:A:563:VAL:O	1:A:563:VAL:HG13	2.17	0.43
1:A:973:PHE:CD1	1:A:974:ASN:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:CYS:O	1:B:186:LEU:HD23	2.18	0.43
1:B:382:LEU:HD22	1:B:425:ILE:HG23	2.00	0.43
1:B:41:ARG:HD3	1:B:41:ARG:N	2.32	0.43
1:B:671:GLN:CG	1:B:755:TYR:HB2	2.47	0.43
1:C:1077:ALA:CB	1:C:1078:PRO:HD3	2.40	0.43
1:C:474:LEU:HB3	1:C:477:CYS:SG	2.58	0.43
1:A:283:CYS:O	1:A:287:ARG:HG3	2.18	0.43
1:B:221:SER:O	1:B:224:GLY:N	2.51	0.43
1:B:513:ARG:NH1	1:B:514:ASP:OD1	2.51	0.43
1:B:706:GLU:O	1:B:709:THR:HB	2.19	0.43
1:B:762:PHE:CD1	1:B:762:PHE:N	2.87	0.43
1:B:995:THR:HB	1:B:996:SER:H	1.66	0.43
1:C:1053:LEU:HD11	1:C:1077:ALA:HA	1.99	0.43
1:C:297:GLN:HG2	1:C:297:GLN:H	1.62	0.43
1:C:341:LEU:HD11	1:C:359:CYS:HB3	2.00	0.43
1:A:1014:SER:HB3	1:A:1070:VAL:CG1	2.35	0.43
1:A:211:PRO:N	1:A:212:PRO:HD2	2.33	0.43
1:B:211:PRO:N	1:B:212:PRO:HD2	2.33	0.43
1:B:667:LEU:HB3	1:B:751:VAL:HG11	2.00	0.43
1:C:1164:LEU:HD22	1:C:1252:LEU:CD1	2.48	0.43
1:B:447:ARG:HG3	1:C:489:PHE:HE2	1.84	0.43
1:C:706:GLU:O	1:C:709:THR:HB	2.19	0.43
1:A:90:ILE:CD1	1:A:125:LYS:HB3	2.49	0.43
1:A:344:LEU:HD23	1:A:350:LEU:HB3	2.00	0.43
1:A:466:ILE:O	1:A:469:TYR:HB3	2.18	0.43
1:B:431:LYS:HG2	1:B:469:TYR:CE1	2.53	0.43
1:B:474:LEU:HD22	1:B:477:CYS:SG	2.59	0.43
1:B:996:SER:HB3	1:B:999:PHE:CB	2.48	0.43
1:C:762:PHE:N	1:C:762:PHE:CD1	2.87	0.43
1:A:1156:SER:HA	1:A:1160:VAL:HG21	2.01	0.43
1:A:341:LEU:HD11	1:A:359:CYS:HB3	2.00	0.43
1:A:440:ILE:O	1:A:444:VAL:HG23	2.18	0.43
1:A:667:LEU:HB3	1:A:751:VAL:HG11	2.00	0.43
1:A:996:SER:HB3	1:A:999:PHE:CB	2.48	0.43
1:B:1046:SER:HB2	1:B:1148:GLU:HB2	2.00	0.43
1:B:1145:PHE:CD2	1:B:1146:PHE:CD1	3.07	0.43
1:B:650:VAL:HG13	1:B:657:ILE:HG23	2.00	0.43
1:C:221:SER:O	1:C:224:GLY:N	2.51	0.43
1:C:440:ILE:O	1:C:444:VAL:HG23	2.18	0.43
1:A:978:ALA:HB1	1:A:1020:PHE:CE1	2.53	0.43
1:A:1154:LEU:CD1	1:A:1163:LEU:HD12	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:HB3	1:A:477:CYS:SG	2.58	0.43
1:A:619:ALA:O	1:A:623:MET:HB2	2.18	0.43
1:B:446:ASN:HB3	1:C:489:PHE:CZ	2.52	0.43
1:B:466:ILE:O	1:B:469:TYR:HB3	2.18	0.43
1:B:474:LEU:HB3	1:B:477:CYS:SG	2.59	0.43
1:B:619:ALA:O	1:B:623:MET:HB2	2.19	0.43
1:C:283:CYS:O	1:C:287:ARG:HG3	2.18	0.43
1:C:549:LEU:HG	1:C:549:LEU:O	2.18	0.43
1:C:978:ALA:HB1	1:C:1020:PHE:CE1	2.53	0.43
1:A:1260:GLU:HA	1:A:1263:LEU:HD12	2.00	0.43
1:A:706:GLU:O	1:A:709:THR:HB	2.19	0.43
1:A:762:PHE:CD1	1:A:762:PHE:N	2.87	0.43
1:B:22:GLN:HG2	1:B:60:ASP:OD2	2.18	0.43
1:C:193:LEU:O	1:C:197:LYS:HG2	2.18	0.43
1:C:210:ILE:HD12	1:C:236:PHE:CD2	2.29	0.43
1:C:431:LYS:HG2	1:C:469:TYR:CE1	2.54	0.43
1:C:619:ALA:O	1:C:623:MET:HB2	2.18	0.43
1:A:1145:PHE:CD2	1:A:1146:PHE:CD1	3.07	0.43
1:A:225:SER:O	1:A:226:ARG:C	2.57	0.43
1:A:519:VAL:HG12	1:A:520:LEU:N	2.34	0.43
1:A:597:GLN:HG2	1:A:597:GLN:H	1.44	0.43
1:A:821:ILE:H	1:A:821:ILE:HG13	1.52	0.43
1:B:519:VAL:HG12	1:B:520:LEU:N	2.34	0.43
1:B:957:GLN:HG3	1:B:960:ARG:NH2	2.34	0.43
1:C:185:CYS:O	1:C:186:LEU:HD23	2.19	0.43
1:C:474:LEU:HD22	1:C:477:CYS:SG	2.59	0.43
1:A:185:CYS:O	1:A:186:LEU:HD23	2.19	0.42
1:A:3:LEU:HD23	1:A:6:LEU:HD12	2.01	0.42
1:A:957:GLN:HG3	1:A:960:ARG:NH2	2.34	0.42
1:B:502:VAL:HG13	1:B:502:VAL:O	2.19	0.42
1:B:549:LEU:HG	1:B:549:LEU:O	2.19	0.42
1:C:1145:PHE:CD2	1:C:1146:PHE:CD1	3.07	0.42
1:C:60:ASP:O	1:C:64:ARG:HB2	2.19	0.42
1:A:348:LYS:HD3	1:A:1034:LEU:C	2.38	0.42
1:A:60:ASP:O	1:A:64:ARG:HB2	2.19	0.42
1:B:1156:SER:HA	1:B:1160:VAL:HG21	2.01	0.42
1:B:335:VAL:HG13	1:B:414:THR:CG2	2.46	0.42
1:B:447:ARG:O	1:B:456:ILE:HD11	2.19	0.42
1:B:744:LEU:HD23	1:B:744:LEU:HA	1.87	0.42
1:C:1103:LYS:HB3	1:C:1103:LYS:HE2	1.80	0.42
1:C:165:CYS:HB3	1:C:197:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:LEU:HD22	1:C:425:ILE:HG23	2.00	0.42
1:B:242:LYS:HA	1:B:245:ARG:HE	1.84	0.42
1:B:344:LEU:HD23	1:B:350:LEU:HB3	2.00	0.42
1:B:456:ILE:O	1:B:456:ILE:CG2	2.67	0.42
1:B:60:ASP:O	1:B:64:ARG:HB2	2.19	0.42
1:B:90:ILE:CD1	1:B:125:LYS:HB3	2.49	0.42
1:C:65:ARG:HD3	1:C:100:PHE:CZ	2.54	0.42
1:C:885:THR:O	1:C:886:SER:HB2	2.20	0.42
1:C:880:LEU:HD22	1:C:907:CYS:HA	2.02	0.42
1:A:447:ARG:O	1:A:456:ILE:HD11	2.19	0.42
1:A:502:VAL:HG13	1:A:502:VAL:O	2.19	0.42
1:A:816:LEU:HD13	1:A:838:MET:HE1	2.01	0.42
1:B:3:LEU:HD23	1:B:6:LEU:HD12	2.01	0.42
1:B:880:LEU:HD22	1:B:907:CYS:HA	2.01	0.42
1:C:1005:TRP:O	1:C:1009:ILE:HG13	2.19	0.42
1:C:225:SER:O	1:C:226:ARG:C	2.57	0.42
1:C:447:ARG:O	1:C:456:ILE:HD11	2.19	0.42
1:C:545:ASN:O	1:C:546:PHE:CG	2.73	0.42
1:C:661:GLU:HA	1:C:662:PRO:HD2	1.92	0.42
1:C:957:GLN:HG3	1:C:960:ARG:NH2	2.34	0.42
1:A:1249:ILE:HG13	1:A:1249:ILE:H	1.68	0.42
1:A:860:GLY:HA3	1:A:861:PRO:HD2	1.77	0.42
1:A:954:GLN:O	1:A:958:PHE:HD1	2.03	0.42
1:A:952:SER:HB3	1:A:998:GLN:HB3	2.00	0.42
1:C:517:ILE:HG21	1:C:577:VAL:CG1	2.49	0.42
1:C:954:GLN:O	1:C:958:PHE:HD1	2.03	0.42
1:A:1158:SER:O	1:A:1161:ASP:N	2.53	0.42
1:A:1270:SER:OG	1:A:1271:LYS:N	2.51	0.42
1:A:221:SER:O	1:A:224:GLY:N	2.51	0.42
1:A:41:ARG:N	1:A:41:ARG:HD3	2.32	0.42
1:B:165:CYS:HB3	1:B:197:LYS:HE3	2.01	0.42
1:B:383:ILE:C	1:B:383:ILE:HD12	2.40	0.42
1:B:476:ASN:OD1	1:B:476:ASN:N	2.50	0.42
1:B:952:SER:HB3	1:B:998:GLN:HB3	2.01	0.42
1:A:1182:LEU:O	1:A:1186:GLN:HG3	2.19	0.42
1:A:15:ASP:N	1:A:15:ASP:OD1	2.47	0.42
1:A:242:LYS:HA	1:A:245:ARG:HE	1.84	0.42
1:A:474:LEU:O	1:A:475:GLN:C	2.57	0.42
1:A:816:LEU:HD13	1:A:838:MET:CE	2.50	0.42
1:B:694:GLU:O	1:B:698:TYR:HD1	2.03	0.42
1:C:90:ILE:CD1	1:C:125:LYS:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ILE:O	1:C:456:ILE:CG2	2.67	0.42
1:C:474:LEU:O	1:C:475:GLN:C	2.57	0.42
1:A:382:LEU:HD22	1:A:425:ILE:HG23	2.00	0.42
1:A:474:LEU:HD22	1:A:477:CYS:SG	2.59	0.42
1:B:954:GLN:O	1:B:958:PHE:HD1	2.03	0.42
1:C:214:VAL:HG11	1:C:233:ILE:HD13	2.01	0.42
1:A:383:ILE:C	1:A:383:ILE:HD12	2.40	0.42
1:A:880:LEU:HD22	1:A:907:CYS:HA	2.02	0.42
1:B:65:ARG:HD3	1:B:100:PHE:CZ	2.55	0.42
1:B:1053:LEU:HA	1:B:1053:LEU:HD23	1.85	0.42
1:B:1158:SER:O	1:B:1161:ASP:N	2.53	0.42
1:C:1249:ILE:H	1:C:1249:ILE:HG13	1.68	0.42
1:C:344:LEU:HD23	1:C:350:LEU:HB3	2.00	0.42
1:C:705:LEU:HB3	1:C:755:TYR:CE2	2.55	0.42
1:A:65:ARG:HD3	1:A:100:PHE:CZ	2.55	0.42
1:A:456:ILE:O	1:A:456:ILE:CG2	2.67	0.42
1:A:565:GLN:H	1:A:565:GLN:HG2	1.54	0.42
1:B:1182:LEU:O	1:B:1186:GLN:HG3	2.20	0.42
1:B:225:SER:O	1:B:226:ARG:C	2.57	0.42
1:B:573:ARG:HE	1:B:573:ARG:HB2	1.70	0.42
1:B:816:LEU:HD13	1:B:838:MET:HE1	2.01	0.42
1:B:834:SER:OG	1:B:837:PHE:HB3	2.20	0.42
1:C:1182:LEU:O	1:C:1186:GLN:HG3	2.19	0.42
1:C:383:ILE:C	1:C:383:ILE:HD12	2.41	0.42
1:C:834:SER:OG	1:C:837:PHE:HB3	2.20	0.42
1:A:368:VAL:HG11	1:A:428:GLU:HB3	2.02	0.41
1:B:297:GLN:HG2	1:B:297:GLN:H	1.62	0.41
1:B:368:VAL:HG11	1:B:428:GLU:HB3	2.02	0.41
1:B:474:LEU:O	1:B:475:GLN:C	2.57	0.41
1:B:667:LEU:HD23	1:B:667:LEU:HA	1.80	0.41
1:B:816:LEU:HD13	1:B:838:MET:CE	2.50	0.41
1:C:226:ARG:HG2	1:C:226:ARG:H	1.54	0.41
1:C:242:LYS:HA	1:C:245:ARG:HE	1.84	0.41
1:C:597:GLN:H	1:C:597:GLN:HG2	1.44	0.41
1:A:694:GLU:O	1:A:698:TYR:HD1	2.03	0.41
1:A:816:LEU:HD22	1:A:838:MET:HE3	2.03	0.41
1:A:995:THR:HB	1:A:996:SER:H	1.66	0.41
1:B:1005:TRP:CZ2	1:B:1009:ILE:HD11	2.55	0.41
1:B:90:ILE:HG13	1:B:90:ILE:H	1.72	0.41
1:B:996:SER:HB3	1:B:999:PHE:HB3	2.03	0.41
1:C:1156:SER:HA	1:C:1160:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1150:VAL:O	1:C:1213:PHE:HD1	2.03	0.41
1:C:763:SER:O	1:C:767:PHE:CD1	2.72	0.41
1:C:816:LEU:HD13	1:C:838:MET:CE	2.50	0.41
1:C:996:SER:HB3	1:C:999:PHE:HB3	2.02	0.41
1:A:165:CYS:HB3	1:A:197:LYS:HE3	2.01	0.41
1:A:713:ILE:CG2	1:A:772:SER:HB3	2.49	0.41
1:A:774:PHE:CE2	1:A:837:PHE:CB	2.95	0.41
1:A:814:THR:OG1	1:A:879:VAL:HG21	2.20	0.41
1:B:226:ARG:H	1:B:226:ARG:HG2	1.54	0.41
1:B:672:HIS:HE1	1:B:805:SER:HB3	1.85	0.41
1:C:1042:LEU:O	1:C:1145:PHE:HD1	2.04	0.41
1:C:174:MET:HE1	1:C:205:LEU:HD11	2.02	0.41
1:C:3:LEU:HD23	1:C:6:LEU:HD12	2.01	0.41
1:C:96:GLU:HA	1:C:96:GLU:OE1	2.20	0.41
1:A:329:LEU:HD12	1:A:329:LEU:O	2.20	0.41
1:A:372:VAL:HG22	1:A:432:ILE:HG21	2.03	0.41
1:A:705:LEU:HB3	1:A:755:TYR:CE2	2.55	0.41
1:A:96:GLU:HA	1:A:96:GLU:OE1	2.20	0.41
1:B:339:LYS:HD2	1:B:339:LYS:HA	1.67	0.41
1:C:502:VAL:HG13	1:C:502:VAL:O	2.19	0.41
1:C:694:GLU:O	1:C:698:TYR:HD1	2.03	0.41
1:C:713:ILE:CG2	1:C:772:SER:HB3	2.49	0.41
1:C:952:SER:HB3	1:C:998:GLN:HB3	2.01	0.41
1:A:1005:TRP:O	1:A:1009:ILE:HG13	2.19	0.41
1:A:1042:LEU:O	1:A:1145:PHE:HD1	2.04	0.41
1:A:763:SER:O	1:A:767:PHE:CD1	2.72	0.41
1:A:817:PHE:HB3	1:A:882:TRP:CZ3	2.55	0.41
1:A:996:SER:HB3	1:A:999:PHE:HB3	2.03	0.41
1:C:519:VAL:HG12	1:C:520:LEU:N	2.34	0.41
1:C:817:PHE:HB3	1:C:882:TRP:CZ3	2.55	0.41
1:C:90:ILE:O	1:C:94:MET:HG3	2.21	0.41
1:A:1022:LYS:HA	1:A:1083:LEU:HD11	2.03	0.41
1:A:152:ASN:HB2	1:A:154:GLU:HG2	2.02	0.41
1:A:503:GLN:HG2	1:A:541:LEU:HD21	2.03	0.41
1:B:814:THR:OG1	1:B:879:VAL:HG21	2.20	0.41
1:C:1005:TRP:CE2	1:C:1009:ILE:HD11	2.56	0.41
1:C:169:TRP:CZ3	1:C:177:LEU:HB3	2.56	0.41
1:B:486:TYR:CE2	1:C:449:VAL:CG2	3.03	0.41
1:C:529:LEU:HD22	1:C:533:LYS:HE3	2.03	0.41
1:C:671:GLN:HG2	1:C:755:TYR:HB2	2.03	0.41
1:C:814:THR:OG1	1:C:879:VAL:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:LEU:CB	1:A:830:VAL:HG12	2.46	0.41
1:B:1042:LEU:O	1:B:1145:PHE:HD1	2.04	0.41
1:B:1199:VAL:O	1:B:1202:SER:OG	2.30	0.41
1:B:152:ASN:HB2	1:B:154:GLU:HG2	2.03	0.41
1:B:372:VAL:HG22	1:B:432:ILE:HG21	2.03	0.41
1:C:503:GLN:HG2	1:C:541:LEU:HD21	2.03	0.41
1:A:298:GLN:HE21	1:A:336:LYS:CG	2.29	0.41
1:A:885:THR:O	1:A:886:SER:HB2	2.20	0.41
1:B:329:LEU:O	1:B:329:LEU:HD12	2.21	0.41
1:B:817:PHE:HB3	1:B:882:TRP:CZ3	2.55	0.41
1:B:885:THR:O	1:B:886:SER:HB2	2.20	0.41
1:C:1042:LEU:CD2	1:C:1084:VAL:HG12	2.51	0.41
1:C:368:VAL:HG11	1:C:428:GLU:HB3	2.02	0.41
1:C:95:LEU:O	1:C:98:HIS:CE1	2.74	0.41
1:A:1042:LEU:CD2	1:A:1084:VAL:HG12	2.51	0.41
1:A:113:VAL:HG22	1:A:164:LEU:HG	2.02	0.41
1:A:302:SER:CB	1:A:357:ARG:HG2	2.46	0.41
1:A:931:GLN:HG2	1:A:950:ARG:NH1	2.36	0.41
1:B:529:LEU:HD22	1:B:533:LYS:HE3	2.02	0.41
1:C:372:VAL:HG22	1:C:432:ILE:HG21	2.03	0.41
1:A:1272:VAL:HG12	1:A:1273:ASN:N	2.36	0.41
1:A:667:LEU:HA	1:A:667:LEU:HD23	1.80	0.41
1:B:1025:MET:CE	1:B:1025:MET:HA	2.51	0.41
1:B:350:LEU:HG	1:B:1094:GLU:OE1	2.21	0.41
1:B:1150:VAL:O	1:B:1213:PHE:HD1	2.03	0.41
1:B:169:TRP:CZ3	1:B:177:LEU:HB3	2.56	0.41
1:B:391:ASP:OD2	1:B:447:ARG:NH1	2.54	0.41
1:B:664:ASP:OD1	1:B:664:ASP:N	2.54	0.41
1:C:113:VAL:HG22	1:C:164:LEU:HG	2.03	0.41
1:C:1158:SER:O	1:C:1161:ASP:N	2.53	0.41
1:C:152:ASN:HB2	1:C:154:GLU:HG2	2.03	0.41
1:C:329:LEU:O	1:C:329:LEU:HD12	2.21	0.41
1:C:391:ASP:OD2	1:C:447:ARG:NH1	2.54	0.41
1:A:1005:TRP:CZ2	1:A:1009:ILE:HD11	2.56	0.41
1:A:127:LEU:HB3	1:A:180:VAL:HG21	2.03	0.41
1:A:623:MET:HE2	1:A:623:MET:HB2	1.85	0.41
1:B:1005:TRP:CE2	1:B:1009:ILE:HD11	2.56	0.41
1:B:1005:TRP:O	1:B:1009:ILE:HG13	2.20	0.41
1:B:641:LEU:O	1:B:643:PRO:CD	2.61	0.41
1:B:705:LEU:HB3	1:B:755:TYR:CE2	2.55	0.41
1:B:91:GLY:O	1:B:95:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:O	1:B:98:HIS:CE1	2.74	0.41
1:C:1136:VAL:CG1	1:C:1198:LEU:HD12	2.51	0.41
1:C:1272:VAL:HG12	1:C:1273:ASN:N	2.36	0.41
1:A:177:LEU:O	1:A:180:VAL:HB	2.21	0.40
1:A:529:LEU:HD22	1:A:533:LYS:HE3	2.03	0.40
1:A:671:GLN:C	1:A:671:GLN:OE1	2.59	0.40
1:A:68:ILE:H	1:A:68:ILE:HG13	1.73	0.40
1:B:1272:VAL:HG12	1:B:1273:ASN:N	2.36	0.40
1:B:836:GLU:HA	1:B:839:HIS:NE2	2.37	0.40
1:B:931:GLN:HG2	1:B:950:ARG:NH1	2.36	0.40
1:C:1032:HIS:O	1:C:1035:TYR:N	2.37	0.40
1:C:127:LEU:HB3	1:C:180:VAL:HG21	2.03	0.40
1:C:383:ILE:HG13	1:C:384:GLU:N	2.37	0.40
1:A:169:TRP:CZ3	1:A:177:LEU:HB3	2.56	0.40
1:A:627:PHE:CE2	1:A:631:LYS:HD2	2.56	0.40
1:B:486:TYR:CE2	1:C:449:VAL:HG21	2.56	0.40
1:C:430:PHE:HB2	1:C:440:ILE:HD12	2.03	0.40
1:C:565:GLN:HG2	1:C:565:GLN:H	1.54	0.40
1:C:91:GLY:O	1:C:95:LEU:HG	2.21	0.40
1:A:1005:TRP:CE2	1:A:1009:ILE:HD11	2.56	0.40
1:A:1025:MET:HA	1:A:1025:MET:CE	2.51	0.40
1:A:1150:VAL:HG22	1:A:1167:LEU:HD11	2.04	0.40
1:A:226:ARG:HH12	1:A:282:ASP:CG	2.25	0.40
1:A:383:ILE:HG13	1:A:384:GLU:N	2.37	0.40
1:B:348:LYS:HA	1:B:348:LYS:HD2	1.97	0.40
1:B:503:GLN:HG2	1:B:541:LEU:HD21	2.03	0.40
1:B:671:GLN:OE1	1:B:671:GLN:C	2.59	0.40
1:B:817:PHE:HB3	1:B:882:TRP:CE3	2.56	0.40
1:C:1025:MET:HA	1:C:1025:MET:CE	2.51	0.40
1:C:510:MET:HE1	1:C:574:TYR:HB2	2.03	0.40
1:C:542:LEU:O	1:C:546:PHE:CD2	2.64	0.40
1:C:667:LEU:HA	1:C:667:LEU:HD23	1.79	0.40
1:C:757:PHE:CB	1:C:808:PHE:HE1	2.35	0.40
1:A:430:PHE:HB2	1:A:440:ILE:HD12	2.03	0.40
1:A:836:GLU:HA	1:A:839:HIS:NE2	2.37	0.40
1:A:928:GLN:H	1:A:928:GLN:HG2	1.60	0.40
1:A:980:LEU:HD23	1:A:981:LEU:N	2.37	0.40
1:B:664:ASP:OD2	1:B:803:LEU:HD11	2.21	0.40
1:C:1005:TRP:CZ2	1:C:1009:ILE:HD11	2.56	0.40
1:C:1045:LEU:O	1:C:1049:ILE:HG13	2.22	0.40
1:C:177:LEU:O	1:C:180:VAL:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:PHE:CE2	1:C:631:LYS:HD2	2.56	0.40
1:A:1045:LEU:O	1:A:1049:ILE:HG13	2.22	0.40
1:A:834:SER:OG	1:A:837:PHE:HB3	2.20	0.40
1:A:36:GLN:HG3	1:A:85:VAL:HG11	2.04	0.40
1:B:1136:VAL:CG1	1:B:1198:LEU:HD12	2.51	0.40
1:B:1270:SER:OG	1:B:1271:LYS:N	2.51	0.40
1:B:177:LEU:O	1:B:180:VAL:HB	2.21	0.40
1:B:430:PHE:HB2	1:B:440:ILE:HD12	2.04	0.40
1:B:627:PHE:CE2	1:B:631:LYS:HD2	2.56	0.40
1:B:76:VAL:HG11	1:B:90:ILE:HD11	2.03	0.40
1:B:913:LYS:O	1:B:917:VAL:HG23	2.22	0.40
1:B:95:LEU:HA	1:B:98:HIS:HE1	1.87	0.40
1:C:226:ARG:HH12	1:C:282:ASP:CG	2.25	0.40
1:C:774:PHE:HE2	1:C:836:GLU:HG3	1.86	0.40
1:C:95:LEU:HA	1:C:98:HIS:HE1	1.87	0.40

All (13) 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:A:281:LEU:CD1	1:A:486:TYR:CZ[7_455]	0.71	1.49
1:A:281:LEU:CD1	1:A:486:TYR:CE2[7_455]	0.84	1.36
1:A:280:LYS:NZ	1:A:446:ASN:OD1[7_455]	1.39	0.81
1:A:280:LYS:NZ	1:A:446:ASN:CG[7_455]	1.47	0.73
1:A:281:LEU:CD1	1:A:486:TYR:CE1[7_455]	1.61	0.59
1:A:281:LEU:CD1	1:A:486:TYR:CD2[7_455]	1.72	0.48
1:A:281:LEU:CG	1:A:486:TYR:CZ[7_455]	1.79	0.41
1:A:95:LEU:CD2	1:A:592:ARG:NH1[7_455]	1.86	0.34
1:A:281:LEU:CG	1:A:486:TYR:CE2[7_455]	1.92	0.28
1:A:281:LEU:CD1	1:A:486:TYR:OH[7_455]	1.97	0.23
1:A:280:LYS:CE	1:A:446:ASN:OD1[7_455]	2.00	0.20
1:A:280:LYS:O	1:A:450:THR:OG1[7_455]	2.09	0.11
1:A:280:LYS:NZ	1:A:446:ASN:CB[7_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1103/1308 (84%)	1019 (92%)	80 (7%)	4 (0%)	34	72
1	B	1099/1308 (84%)	1016 (92%)	80 (7%)	3 (0%)	41	77
1	C	1101/1308 (84%)	1019 (93%)	79 (7%)	3 (0%)	41	77
All	All	3303/3924 (84%)	3054 (92%)	239 (7%)	10 (0%)	41	77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	150	ASP
1	A	225	SER
1	B	122	VAL
1	B	150	ASP
1	C	122	VAL
1	C	150	ASP
1	A	996	SER
1	B	996	SER
1	C	996	SER

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	1029/1188 (87%)	914 (89%)	115 (11%)	6	22
1	B	1029/1188 (87%)	914 (89%)	115 (11%)	6	22
1	C	1029/1188 (87%)	915 (89%)	114 (11%)	6	22
All	All	3087/3564 (87%)	2743 (89%)	344 (11%)	6	22

All (344) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	19	GLU
1	A	54	SER
1	A	71	CYS
1	A	81	LEU
1	A	97	VAL
1	A	99	HIS
1	A	118	GLU
1	A	119	ASP
1	A	130	LEU
1	A	169	TRP
1	A	171	GLN
1	A	177	LEU
1	A	183	ASP
1	A	208	GLN
1	A	213	LEU
1	A	240	LEU
1	A	245	ARG
1	A	247	GLU
1	A	262	ASP
1	A	264	LEU
1	A	275	ILE
1	A	277	PHE
1	A	285	LEU
1	A	288	GLU
1	A	312	LEU
1	A	316	LEU
1	A	329	LEU
1	A	343	LEU
1	A	347	SER
1	A	349	PHE
1	A	359	CYS
1	A	360	VAL
1	A	376	ASP
1	A	377	HIS
1	A	378	VAL
1	A	383	ILE
1	A	397	LYS
1	A	414	THR
1	A	421	LEU
1	A	427	LEU
1	A	438	GLN
1	A	443	GLN

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Mol	Chain	Res	Type
1	A	450	THR
1	A	451	ARG
1	A	452	THR
1	A	456	ILE
1	A	468	MET
1	A	473	ILE
1	A	477	CYS
1	A	479	LYS
1	A	488	THR
1	A	493	GLN
1	A	496	GLN
1	A	502	VAL
1	A	515	SER
1	A	519	VAL
1	A	529	LEU
1	A	530	ASP
1	A	549	LEU
1	A	552	LEU
1	A	563	VAL
1	A	565	GLN
1	A	569	ASP
1	A	579	ASN
1	A	587	ILE
1	A	597	GLN
1	A	606	ASP
1	A	612	LEU
1	A	651	LEU
1	A	659	LEU
1	A	661	GLU
1	A	663	LEU
1	A	666	LEU
1	A	699	SER
1	A	711	ARG
1	A	712	MET
1	A	743	CYS
1	A	754	GLU
1	A	759	ILE
1	A	765	SER
1	A	768	GLU
1	A	771	LEU
1	A	803	LEU
1	A	806	LEU

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Mol	Chain	Res	Type
1	A	812	LEU
1	A	824	HIS
1	A	840	TYR
1	A	846	LEU
1	A	853	ILE
1	A	864	GLN
1	A	878	ARG
1	A	911	LEU
1	A	919	LEU
1	A	949	GLN
1	A	965	LEU
1	A	980	LEU
1	A	981	LEU
1	A	982	ILE
1	A	1001	GLN
1	A	1003	LEU
1	A	1013	TYR
1	A	1024	LEU
1	A	1035	TYR
1	A	1050	HIS
1	A	1056	ILE
1	A	1071	VAL
1	A	1084	VAL
1	A	1105	SER
1	A	1142	LEU
1	A	1183	GLN
1	A	1194	THR
1	A	1200	LYS
1	A	1274	LEU
1	A	1275	MET
1	B	15	ASP
1	B	19	GLU
1	B	54	SER
1	B	71	CYS
1	B	81	LEU
1	B	97	VAL
1	B	99	HIS
1	B	118	GLU
1	B	119	ASP
1	B	130	LEU
1	B	169	TRP
1	B	171	GLN

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Mol	Chain	Res	Type
1	B	177	LEU
1	B	183	ASP
1	B	208	GLN
1	B	213	LEU
1	B	240	LEU
1	B	245	ARG
1	B	247	GLU
1	B	262	ASP
1	B	264	LEU
1	B	275	ILE
1	B	277	PHE
1	B	285	LEU
1	B	288	GLU
1	B	312	LEU
1	B	316	LEU
1	B	329	LEU
1	B	343	LEU
1	B	347	SER
1	B	349	PHE
1	B	359	CYS
1	B	360	VAL
1	B	376	ASP
1	B	377	HIS
1	B	378	VAL
1	B	383	ILE
1	B	397	LYS
1	B	414	THR
1	B	421	LEU
1	B	427	LEU
1	B	438	GLN
1	B	443	GLN
1	B	450	THR
1	B	451	ARG
1	B	452	THR
1	B	456	ILE
1	B	468	MET
1	B	473	ILE
1	B	477	CYS
1	B	479	LYS
1	B	488	THR
1	B	493	GLN
1	B	496	GLN

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Mol	Chain	Res	Type
1	B	502	VAL
1	B	515	SER
1	B	519	VAL
1	B	529	LEU
1	B	530	ASP
1	B	549	LEU
1	B	552	LEU
1	B	563	VAL
1	B	565	GLN
1	B	569	ASP
1	B	579	ASN
1	B	587	ILE
1	B	597	GLN
1	B	606	ASP
1	B	612	LEU
1	B	651	LEU
1	B	659	LEU
1	B	661	GLU
1	B	663	LEU
1	B	666	LEU
1	B	699	SER
1	B	711	ARG
1	B	712	MET
1	B	743	CYS
1	B	754	GLU
1	B	759	ILE
1	B	765	SER
1	B	768	GLU
1	B	771	LEU
1	B	803	LEU
1	B	806	LEU
1	B	812	LEU
1	B	824	HIS
1	B	840	TYR
1	B	846	LEU
1	B	853	ILE
1	B	864	GLN
1	B	878	ARG
1	B	911	LEU
1	B	919	LEU
1	B	949	GLN
1	B	965	LEU

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Mol	Chain	Res	Type
1	B	980	LEU
1	B	981	LEU
1	B	982	ILE
1	B	1001	GLN
1	B	1003	LEU
1	B	1013	TYR
1	B	1024	LEU
1	B	1035	TYR
1	B	1050	HIS
1	B	1056	ILE
1	B	1071	VAL
1	B	1084	VAL
1	B	1105	SER
1	B	1142	LEU
1	B	1183	GLN
1	B	1194	THR
1	B	1200	LYS
1	B	1274	LEU
1	B	1275	MET
1	C	15	ASP
1	C	19	GLU
1	C	54	SER
1	C	71	CYS
1	C	81	LEU
1	C	97	VAL
1	C	99	HIS
1	C	118	GLU
1	C	119	ASP
1	C	130	LEU
1	C	169	TRP
1	C	171	GLN
1	C	177	LEU
1	C	183	ASP
1	C	208	GLN
1	C	213	LEU
1	C	240	LEU
1	C	245	ARG
1	C	247	GLU
1	C	262	ASP
1	C	264	LEU
1	C	275	ILE
1	C	277	PHE

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Mol	Chain	Res	Type
1	C	285	LEU
1	C	288	GLU
1	C	312	LEU
1	C	316	LEU
1	C	329	LEU
1	C	343	LEU
1	C	347	SER
1	C	349	PHE
1	C	359	CYS
1	C	360	VAL
1	C	376	ASP
1	C	377	HIS
1	C	378	VAL
1	C	383	ILE
1	C	397	LYS
1	C	414	THR
1	C	421	LEU
1	C	427	LEU
1	C	438	GLN
1	C	443	GLN
1	C	450	THR
1	C	451	ARG
1	C	452	THR
1	C	456	ILE
1	C	468	MET
1	C	473	ILE
1	C	477	CYS
1	C	479	LYS
1	C	488	THR
1	C	493	GLN
1	C	496	GLN
1	C	502	VAL
1	C	515	SER
1	C	529	LEU
1	C	530	ASP
1	C	549	LEU
1	C	552	LEU
1	C	563	VAL
1	C	565	GLN
1	C	569	ASP
1	C	579	ASN
1	C	587	ILE

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Mol	Chain	Res	Type
1	C	597	GLN
1	C	606	ASP
1	C	612	LEU
1	C	651	LEU
1	C	659	LEU
1	C	661	GLU
1	C	663	LEU
1	C	666	LEU
1	C	699	SER
1	C	711	ARG
1	C	712	MET
1	C	743	CYS
1	C	754	GLU
1	C	759	ILE
1	C	765	SER
1	C	768	GLU
1	C	771	LEU
1	C	803	LEU
1	C	806	LEU
1	C	812	LEU
1	C	824	HIS
1	C	840	TYR
1	C	846	LEU
1	C	853	ILE
1	C	864	GLN
1	C	878	ARG
1	C	911	LEU
1	C	919	LEU
1	C	949	GLN
1	C	965	LEU
1	C	980	LEU
1	C	981	LEU
1	C	982	ILE
1	C	1001	GLN
1	C	1003	LEU
1	C	1013	TYR
1	C	1024	LEU
1	C	1035	TYR
1	C	1050	HIS
1	C	1056	ILE
1	C	1071	VAL
1	C	1084	VAL

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Mol	Chain	Res	Type
1	C	1105	SER
1	C	1142	LEU
1	C	1183	GLN
1	C	1194	THR
1	C	1200	LYS
1	C	1274	LEU
1	C	1275	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	298	GLN
1	A	377	HIS
1	A	597	GLN
1	A	672	HIS
1	B	208	GLN
1	B	298	GLN
1	B	377	HIS
1	B	597	GLN
1	B	672	HIS
1	B	1087	GLN
1	B	1277	HIS
1	C	208	GLN
1	C	298	GLN
1	C	377	HIS
1	C	597	GLN
1	C	672	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	224:GLY	C	225:SER	N	4.08
1	B	224:GLY	C	225:SER	N	2.63
1	B	545:ASN	C	546:PHE	N	2.09
1	A	224:GLY	C	225:SER	N	1.91
1	A	545:ASN	C	546:PHE	N	1.76

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1131/1308 (86%)	1.37	289 (25%)	0 2	267, 382, 546, 649	0
1	B	1131/1308 (86%)	2.17	453 (40%)	0 1	285, 384, 602, 757	0
1	C	1131/1308 (86%)	2.05	437 (38%)	0 1	302, 421, 620, 719	0
All	All	3393/3924 (86%)	1.87	1179 (34%)	0 2	267, 397, 598, 757	0

All (1179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	GLY	19.1
1	C	105	LEU	13.8
1	B	49	ALA	13.7
1	B	99	HIS	13.3
1	B	52	LYS	13.3
1	B	28	ASP	12.9
1	B	51	LEU	12.4
1	B	101	PRO	12.4
1	B	48	ARG	12.1
1	C	1015	GLN	12.0
1	C	140	LYS	12.0
1	C	101	PRO	12.0
1	C	138	ALA	11.4
1	B	47	LEU	11.3
1	C	137	LEU	11.2
1	B	56	CYS	11.1
1	C	102	GLY	11.0
1	C	100	PHE	10.8
1	C	56	CYS	10.7
1	C	136	ALA	10.7
1	B	54	SER	10.5
1	B	140	LYS	10.5
1	B	80	ASP	10.2

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Mol	Chain	Res	Type	RSRZ
1	B	100	PHE	10.1
1	B	50	VAL	10.1
1	B	826	GLU	10.0
1	B	103	PRO	10.0
1	B	136	ALA	9.9
1	B	65	ARG	9.8
1	B	135	THR	9.7
1	B	105	LEU	9.6
1	C	139	THR	9.5
1	C	106	VAL	9.4
1	C	170	PRO	9.3
1	B	139	THR	9.2
1	B	157	LYS	9.2
1	B	68	ILE	9.2
1	B	827	SER	9.2
1	C	642	PRO	9.1
1	B	137	LEU	9.0
1	C	644	LEU	9.0
1	B	53	GLY	8.9
1	C	134	LEU	8.8
1	B	32	LEU	8.7
1	B	185	CYS	8.7
1	B	134	LEU	8.7
1	C	99	HIS	8.6
1	C	1014	SER	8.6
1	B	31	SER	8.6
1	B	55	PRO	8.6
1	B	138	ALA	8.5
1	A	1190	GLY	8.5
1	C	98	HIS	8.5
1	C	1076	ALA	8.5
1	B	98	HIS	8.2
1	B	642	PRO	8.1
1	A	80	ASP	8.1
1	B	45	THR	8.1
1	B	106	VAL	8.1
1	C	97	VAL	8.0
1	C	133	ILE	8.0
1	C	1077	ALA	8.0
1	C	553	PRO	7.9
1	B	683	PRO	7.9
1	B	96	GLU	7.9

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Mol	Chain	Res	Type	RSRZ
1	C	109	ALA	7.8
1	A	170	PRO	7.8
1	B	57	SER	7.8
1	C	635	GLU	7.8
1	C	636	PRO	7.7
1	C	643	PRO	7.7
1	C	637	GLU	7.7
1	C	1081	CYS	7.6
1	B	64	ARG	7.6
1	C	1154	LEU	7.5
1	B	142	GLU	7.5
1	C	259	ALA	7.5
1	A	81	LEU	7.5
1	A	1185	CYS	7.4
1	B	35	ASN	7.4
1	C	1006	THR	7.4
1	C	733	ASN	7.4
1	C	1002	MET	7.4
1	B	36	GLN	7.3
1	B	154	GLU	7.3
1	C	1017	ASP	7.3
1	B	46	LEU	7.2
1	B	133	ILE	7.2
1	B	97	VAL	7.2
1	B	71	CYS	7.1
1	B	184	VAL	7.1
1	B	824	HIS	7.1
1	A	53	GLY	7.1
1	B	641	LEU	7.1
1	B	186	LEU	7.1
1	C	1075	THR	7.0
1	C	153	GLY	7.0
1	C	861	PRO	7.0
1	B	644	LEU	7.0
1	B	58	GLU	7.0
1	C	1071	VAL	6.9
1	B	13	THR	6.9
1	C	639	ASP	6.9
1	B	946	THR	6.9
1	B	141	LYS	6.9
1	C	827	SER	6.8
1	C	1080	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	641	LEU	6.8
1	A	1186	GLN	6.7
1	B	1191	ILE	6.7
1	C	1079	THR	6.7
1	B	153	GLY	6.7
1	B	643	PRO	6.7
1	C	712	MET	6.6
1	C	1016	GLU	6.6
1	C	126	SER	6.6
1	C	974	ASN	6.6
1	B	27	ASP	6.6
1	B	764	LYS	6.6
1	C	135	THR	6.5
1	B	69	TYR	6.5
1	A	2	ASP	6.5
1	A	18	GLN	6.5
1	B	109	ALA	6.5
1	A	1	MET	6.5
1	C	1190	GLY	6.4
1	B	72	CYS	6.4
1	C	634	TYR	6.4
1	A	934	ASP	6.4
1	C	972	ASP	6.4
1	B	152	ASN	6.3
1	C	57	SER	6.3
1	C	1004	SER	6.3
1	C	737	LYS	6.3
1	B	934	ASP	6.3
1	B	712	MET	6.2
1	C	645	LYS	6.2
1	B	62	ALA	6.2
1	B	302	SER	6.2
1	B	9	ALA	6.2
1	B	26	ASP	6.2
1	C	1003	LEU	6.2
1	C	1072	ASN	6.2
1	C	96	GLU	6.2
1	C	93	LEU	6.2
1	B	244	HIS	6.2
1	C	35	ASN	6.2
1	C	824	HIS	6.2
1	B	170	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	258	THR	6.1
1	C	994	PRO	6.1
1	C	157	LYS	6.0
1	C	971	ASP	6.0
1	C	999	PHE	5.9
1	B	646	LEU	5.9
1	B	974	ASN	5.9
1	C	9	ALA	5.9
1	B	767	PHE	5.9
1	B	829	SER	5.9
1	A	974	ASN	5.9
1	A	1188	SER	5.9
1	B	144	LEU	5.8
1	B	104	LEU	5.8
1	C	244	HIS	5.8
1	B	146	CYS	5.8
1	B	181	PHE	5.8
1	C	2	ASP	5.8
1	C	65	ARG	5.8
1	C	112	PHE	5.8
1	B	1155	PRO	5.8
1	B	1156	SER	5.7
1	C	32	LEU	5.7
1	A	14	THR	5.7
1	A	553	PRO	5.7
1	A	244	HIS	5.7
1	B	763	SER	5.7
1	B	401	GLY	5.7
1	A	639	ASP	5.7
1	C	954	GLN	5.7
1	C	49	ALA	5.7
1	B	43	VAL	5.7
1	A	35	ASN	5.7
1	B	18	GLN	5.7
1	B	92	LEU	5.6
1	C	1078	PRO	5.6
1	C	20	PHE	5.6
1	B	150	ASP	5.6
1	B	1270	SER	5.6
1	C	19	GLU	5.6
1	C	638	PRO	5.6
1	B	830	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	5	ILE	5.6
1	C	958	PHE	5.6
1	C	640	LEU	5.6
1	B	33	LEU	5.6
1	B	639	ASP	5.6
1	C	22	GLN	5.5
1	C	769	GLU	5.5
1	B	81	LEU	5.5
1	B	145	ALA	5.5
1	B	637	GLU	5.5
1	C	1010	CYS	5.5
1	A	17	LEU	5.5
1	A	49	ALA	5.5
1	C	47	LEU	5.5
1	B	645	LYS	5.5
1	A	1191	ILE	5.5
1	C	973	PHE	5.4
1	C	731	ASN	5.4
1	C	1007	SER	5.4
1	B	709	THR	5.4
1	B	17	LEU	5.4
1	C	863	GLY	5.4
1	C	260	PRO	5.4
1	C	68	ILE	5.4
1	A	733	ASN	5.4
1	B	635	GLU	5.4
1	B	1154	LEU	5.4
1	B	1269	LYS	5.3
1	B	299	GLY	5.3
1	B	260	PRO	5.3
1	C	69	TYR	5.3
1	A	1017	ASP	5.3
1	B	638	PRO	5.3
1	B	1265	GLN	5.3
1	C	767	PHE	5.3
1	B	817	PHE	5.2
1	C	732	THR	5.2
1	C	53	GLY	5.2
1	C	154	GLU	5.2
1	C	50	VAL	5.2
1	C	884	TYR	5.2
1	C	103	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	709	THR	5.1
1	B	112	PHE	5.1
1	C	123	ASN	5.1
1	A	401	GLY	5.1
1	C	184	VAL	5.1
1	B	126	SER	5.1
1	A	302	SER	5.1
1	C	23	THR	5.1
1	C	54	SER	5.1
1	A	50	VAL	5.1
1	C	711	ARG	5.0
1	A	36	GLN	5.0
1	A	15	ASP	5.0
1	B	14	THR	5.0
1	C	58	GLU	5.0
1	C	119	ASP	5.0
1	C	646	LEU	5.0
1	B	640	LEU	5.0
1	A	1015	GLN	5.0
1	C	18	GLN	5.0
1	B	828	LEU	5.0
1	C	141	LYS	5.0
1	C	1155	PRO	5.0
1	B	1190	GLY	5.0
1	C	761	ASN	5.0
1	C	826	GLU	5.0
1	B	737	LYS	5.0
1	C	822	GLN	4.9
1	A	638	PRO	4.9
1	C	125	LYS	4.9
1	C	46	LEU	4.9
1	B	831	LEU	4.9
1	C	55	PRO	4.8
1	C	108	LEU	4.8
1	B	5	ILE	4.8
1	B	1248	PRO	4.8
1	B	61	GLY	4.8
1	C	34	GLN	4.8
1	C	825	GLU	4.8
1	A	578	ALA	4.8
1	A	1016	GLU	4.8
1	B	44	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	1074	ARG	4.8
1	C	174	MET	4.8
1	A	5	ILE	4.7
1	B	75	LEU	4.7
1	A	299	GLY	4.7
1	C	21	LEU	4.7
1	B	73	ILE	4.7
1	B	130	LEU	4.7
1	B	825	GLU	4.7
1	C	169	TRP	4.7
1	B	704	MET	4.7
1	C	248	GLN	4.7
1	B	29	LEU	4.6
1	B	93	LEU	4.6
1	B	701	LEU	4.6
1	A	1187	SER	4.6
1	C	1191	ILE	4.6
1	B	670	ILE	4.6
1	C	571	HIS	4.6
1	A	397	LYS	4.6
1	B	473	ILE	4.6
1	B	708	ILE	4.6
1	C	186	LEU	4.6
1	A	28	ASP	4.6
1	B	37	ALA	4.6
1	C	1013	TYR	4.6
1	B	741	CYS	4.6
1	A	268	GLU	4.6
1	C	1009	ILE	4.6
1	B	259	ALA	4.6
1	C	17	LEU	4.6
1	B	816	LEU	4.6
1	B	930	LEU	4.5
1	A	551	SER	4.5
1	B	221	SER	4.5
1	B	34	GLN	4.5
1	B	634	TYR	4.5
1	A	712	MET	4.5
1	C	185	CYS	4.5
1	B	30	ALA	4.5
1	A	933	LEU	4.5
1	C	104	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	15	ASP	4.5
1	A	1270	SER	4.5
1	C	708	ILE	4.5
1	C	14	THR	4.5
1	C	860	GLY	4.5
1	B	174	MET	4.4
1	C	51	LEU	4.4
1	C	977	GLU	4.4
1	C	1153	ALA	4.4
1	B	143	VAL	4.4
1	B	369	ARG	4.4
1	B	947	VAL	4.4
1	B	673	CYS	4.4
1	B	21	LEU	4.4
1	C	52	LYS	4.4
1	B	60	ASP	4.4
1	A	54	SER	4.4
1	B	1271	LYS	4.4
1	B	705	LEU	4.4
1	B	682	VAL	4.4
1	C	28	ASP	4.4
1	C	80	ASP	4.4
1	B	127	LEU	4.4
1	C	401	GLY	4.4
1	B	59	GLU	4.4
1	C	110	SER	4.4
1	B	733	ASN	4.3
1	A	31	SER	4.3
1	B	950	ARG	4.3
1	A	32	LEU	4.3
1	C	1005	TRP	4.3
1	C	299	GLY	4.3
1	A	480	VAL	4.3
1	B	247	GLU	4.3
1	B	370	ASN	4.3
1	C	13	THR	4.3
1	C	181	PHE	4.3
1	C	171	GLN	4.3
1	C	225	SER	4.3
1	B	248	GLN	4.3
1	B	714	LYS	4.3
1	B	161	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1183	GLN	4.2
1	B	131	PRO	4.2
1	C	1163	LEU	4.2
1	A	395	PRO	4.2
1	C	7	SER	4.2
1	A	576	ALA	4.2
1	B	124	GLY	4.2
1	C	823	SER	4.2
1	B	301	PRO	4.2
1	B	1056	ILE	4.2
1	B	116	VAL	4.2
1	B	949	GLN	4.2
1	C	816	LEU	4.2
1	A	60	ASP	4.2
1	B	1048	ASP	4.2
1	C	588	ASP	4.2
1	C	31	SER	4.2
1	B	626	LEU	4.2
1	C	657	ILE	4.2
1	A	13	THR	4.2
1	B	220	LEU	4.2
1	B	630	LEU	4.2
1	B	24	LEU	4.1
1	B	1268	LYS	4.1
1	C	116	VAL	4.1
1	B	132	ILE	4.1
1	B	268	GLU	4.1
1	B	1267	SER	4.1
1	B	977	GLU	4.1
1	C	224	GLY	4.1
1	B	1040	THR	4.1
1	B	264	LEU	4.1
1	C	48	ARG	4.1
1	C	955	ILE	4.1
1	C	1070	VAL	4.1
1	C	89	ILE	4.1
1	B	66	TYR	4.1
1	A	400	ASP	4.1
1	B	738	ASN	4.1
1	C	713	ILE	4.1
1	A	247	GLU	4.1
1	A	168	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	260	PRO	4.1
1	B	169	TRP	4.1
1	C	951	ALA	4.1
1	B	168	ARG	4.0
1	B	205	LEU	4.0
1	C	64	ARG	4.0
1	A	973	PHE	4.0
1	A	1275	MET	4.0
1	C	989	SER	4.0
1	B	224	GLY	4.0
1	A	575	SER	4.0
1	C	763	SER	4.0
1	C	8	LEU	4.0
1	C	655	SER	4.0
1	B	107	ASP	4.0
1	C	111	ASP	4.0
1	A	79	GLY	4.0
1	A	21	LEU	4.0
1	C	160	LEU	4.0
1	A	4	LYS	4.0
1	A	264	LEU	4.0
1	C	24	LEU	4.0
1	C	152	ASN	4.0
1	B	250	SER	4.0
1	B	636	PRO	4.0
1	A	16	LYS	4.0
1	B	1185	CYS	3.9
1	B	647	GLY	3.9
1	A	370	ASN	3.9
1	A	732	THR	3.9
1	C	43	VAL	3.9
1	B	623	MET	3.9
1	B	711	ARG	3.9
1	A	738	ASN	3.9
1	A	57	SER	3.9
1	B	155	GLU	3.9
1	C	370	ASN	3.9
1	A	827	SER	3.9
1	C	127	LEU	3.9
1	C	60	ASP	3.9
1	C	736	ILE	3.9
1	A	248	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	6	LEU	3.9
1	B	171	GLN	3.9
1	B	551	SER	3.9
1	B	25	LYS	3.9
1	C	1084	VAL	3.9
1	C	741	CYS	3.9
1	C	992	LEU	3.9
1	C	147	GLY	3.9
1	C	16	LYS	3.9
1	C	647	GLY	3.9
1	C	570	VAL	3.9
1	C	10	THR	3.8
1	C	45	THR	3.8
1	C	770	ILE	3.8
1	B	241	ASP	3.8
1	C	959	GLN	3.8
1	C	72	CYS	3.8
1	C	206	ASN	3.8
1	C	995	THR	3.8
1	B	933	LEU	3.8
1	B	149	GLY	3.8
1	B	674	LEU	3.8
1	C	962	LEU	3.8
1	B	156	TYR	3.8
1	B	739	ASN	3.8
1	A	118	GLU	3.8
1	A	737	LYS	3.8
1	C	36	GLN	3.8
1	B	258	THR	3.8
1	C	981	LEU	3.8
1	B	649	CYS	3.8
1	B	1052	GLN	3.8
1	A	1269	LYS	3.8
1	B	147	GLY	3.8
1	A	637	GLU	3.7
1	B	82	GLN	3.7
1	B	160	LEU	3.7
1	B	762	PHE	3.7
1	C	247	GLU	3.7
1	C	241	ASP	3.7
1	A	19	GLU	3.7
1	C	1020	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	731	ASN	3.7
1	C	300	ASP	3.7
1	C	978	ALA	3.7
1	C	946	THR	3.7
1	C	1021	CYS	3.7
1	A	174	MET	3.7
1	A	169	TRP	3.7
1	B	108	LEU	3.7
1	A	1184	VAL	3.7
1	C	734	VAL	3.7
1	A	1181	TYR	3.7
1	B	1249	ILE	3.7
1	C	1160	VAL	3.7
1	A	1102	ILE	3.7
1	C	130	LEU	3.7
1	B	951	ALA	3.7
1	B	1272	VAL	3.7
1	C	397	LYS	3.7
1	C	356	GLN	3.7
1	B	663	LEU	3.7
1	C	619	ALA	3.7
1	A	642	PRO	3.7
1	A	643	PRO	3.7
1	A	20	PHE	3.7
1	B	298	GLN	3.6
1	B	79	GLY	3.6
1	C	302	SER	3.6
1	B	178	THR	3.6
1	B	770	ILE	3.6
1	A	831	LEU	3.6
1	B	70	SER	3.6
1	C	704	MET	3.6
1	C	957	GLN	3.6
1	A	451	ARG	3.6
1	B	245	ARG	3.6
1	B	1186	GLN	3.6
1	C	1249	ILE	3.6
1	C	1270	SER	3.6
1	B	954	GLN	3.6
1	C	264	LEU	3.6
1	A	483	THR	3.6
1	A	1154	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	1073	LEU	3.6
1	C	950	ARG	3.6
1	B	820	SER	3.6
1	B	1017	ASP	3.6
1	C	934	ASP	3.6
1	C	1049	ILE	3.6
1	B	564	THR	3.6
1	B	22	GLN	3.6
1	C	710	VAL	3.6
1	C	933	LEU	3.6
1	C	991	LEU	3.5
1	B	15	ASP	3.5
1	B	201	MET	3.5
1	A	1265	GLN	3.5
1	C	1018	ALA	3.5
1	C	115	ALA	3.5
1	C	1001	GLN	3.5
1	A	51	LEU	3.5
1	C	998	GLN	3.5
1	B	129	LEU	3.5
1	C	172	ARG	3.5
1	C	828	LEU	3.5
1	A	46	LEU	3.5
1	B	63	LEU	3.5
1	B	202	PHE	3.5
1	C	121	LEU	3.5
1	C	411	SER	3.5
1	C	177	LEU	3.5
1	A	1056	ILE	3.5
1	C	819	ASP	3.4
1	B	973	PHE	3.4
1	B	832	ARG	3.4
1	C	738	ASN	3.4
1	C	1164	LEU	3.4
1	B	667	LEU	3.4
1	A	245	ARG	3.4
1	B	766	LYS	3.4
1	B	12	LYS	3.4
1	A	950	ARG	3.4
1	B	765	SER	3.4
1	A	398	ILE	3.4
1	B	761	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	33	LEU	3.4
1	B	608	PHE	3.4
1	C	369	ARG	3.4
1	A	655	SER	3.4
1	C	79	GLY	3.4
1	B	265	TYR	3.4
1	C	764	LYS	3.4
1	C	988	LEU	3.4
1	B	1015	GLN	3.4
1	C	877	THR	3.4
1	B	148	LYS	3.4
1	B	397	LYS	3.4
1	C	714	LYS	3.4
1	B	382	LEU	3.3
1	B	1153	ALA	3.3
1	B	190	GLU	3.3
1	B	472	LEU	3.3
1	B	1263	LEU	3.3
1	A	296	GLY	3.3
1	C	551	SER	3.3
1	C	261	ALA	3.3
1	B	945	VAL	3.3
1	A	8	LEU	3.3
1	B	334	VAL	3.3
1	C	1000	VAL	3.3
1	C	862	ASP	3.3
1	B	769	GLU	3.3
1	B	1262	PHE	3.3
1	C	124	GLY	3.3
1	B	198	VAL	3.3
1	A	1132	GLU	3.3
1	A	250	SER	3.3
1	B	296	GLY	3.3
1	A	515	SER	3.3
1	B	357	ARG	3.3
1	A	22	GLN	3.3
1	A	34	GLN	3.3
1	C	650	VAL	3.3
1	B	989	SER	3.3
1	C	961	SER	3.3
1	B	2	ASP	3.3
1	A	454	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	258	THR	3.2
1	C	245	ARG	3.2
1	B	1182	LEU	3.2
1	A	473	ILE	3.2
1	B	822	GLN	3.2
1	A	481	THR	3.2
1	C	73	ILE	3.2
1	B	713	ILE	3.2
1	C	220	LEU	3.2
1	A	301	PRO	3.2
1	C	1008	LYS	3.2
1	C	780	PHE	3.2
1	A	147	GLY	3.2
1	A	477	CYS	3.2
1	B	151	LEU	3.2
1	B	39	LYS	3.2
1	A	1273	ASN	3.2
1	B	38	VAL	3.2
1	C	993	GLU	3.2
1	A	929	PHE	3.2
1	A	259	ALA	3.2
1	C	229	VAL	3.2
1	B	19	GLU	3.2
1	A	470	ALA	3.2
1	B	217	LEU	3.2
1	A	82	GLN	3.2
1	C	831	LEU	3.2
1	A	71	CYS	3.2
1	B	194	VAL	3.2
1	B	1214	ILE	3.2
1	A	1222	SER	3.2
1	C	146	CYS	3.2
1	A	265	TYR	3.2
1	B	1077	ALA	3.2
1	A	484	PHE	3.1
1	A	932	ALA	3.1
1	B	177	LEU	3.1
1	B	627	PHE	3.1
1	A	577	VAL	3.1
1	A	1106	ALA	3.1
1	B	10	THR	3.1
1	B	360	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	400	ASP	3.1
1	C	304	CYS	3.1
1	B	16	LYS	3.1
1	C	930	LEU	3.1
1	B	223	LYS	3.1
1	A	516	LEU	3.1
1	A	930	LEU	3.1
1	A	652	THR	3.1
1	A	954	GLN	3.1
1	A	657	ILE	3.1
1	A	1052	GLN	3.1
1	B	11	ASP	3.1
1	B	1266	LEU	3.1
1	C	90	ILE	3.1
1	A	640	LEU	3.1
1	B	183	ASP	3.1
1	C	156	TYR	3.1
1	A	1048	ASP	3.1
1	B	884	TYR	3.1
1	C	735	GLY	3.1
1	A	1249	ILE	3.1
1	A	249	SER	3.1
1	C	820	SER	3.1
1	C	829	SER	3.1
1	C	952	SER	3.1
1	A	58	GLU	3.1
1	B	8	LEU	3.1
1	C	1053	LEU	3.1
1	C	86	ALA	3.1
1	A	119	ASP	3.0
1	A	988	LEU	3.0
1	B	78	SER	3.0
1	C	268	GLU	3.0
1	A	38	VAL	3.0
1	A	972	ASP	3.0
1	C	217	LEU	3.0
1	A	679	SER	3.0
1	C	1156	SER	3.0
1	A	474	LEU	3.0
1	B	368	VAL	3.0
1	A	355	PRO	3.0
1	B	657	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1159	CYS	3.0
1	B	650	VAL	3.0
1	A	1221	SER	3.0
1	B	411	SER	3.0
1	C	207	LEU	3.0
1	A	977	GLU	3.0
1	B	74	GLN	3.0
1	C	707	SER	3.0
1	A	784	LEU	3.0
1	A	962	LEU	3.0
1	C	71	CYS	3.0
1	B	700	GLU	3.0
1	C	75	LEU	3.0
1	B	948	THR	3.0
1	A	978	ALA	3.0
1	B	110	SER	3.0
1	B	841	ALA	3.0
1	C	965	LEU	3.0
1	A	739	ASN	3.0
1	B	249	SER	3.0
1	B	474	LEU	3.0
1	A	1155	PRO	3.0
1	C	76	VAL	3.0
1	A	466	ILE	3.0
1	B	20	PHE	3.0
1	B	883	ARG	3.0
1	C	1149	LEU	3.0
1	B	698	TYR	3.0
1	B	731	ASN	3.0
1	B	1213	PHE	2.9
1	A	1180	TYR	2.9
1	B	67	LYS	2.9
1	A	478	SER	2.9
1	B	89	ILE	2.9
1	C	4	LYS	2.9
1	B	619	ALA	2.9
1	A	47	LEU	2.9
1	A	734	VAL	2.9
1	C	168	ARG	2.9
1	A	72	CYS	2.9
1	B	707	SER	2.9
1	B	914	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	113	VAL	2.9
1	C	815	ALA	2.9
1	B	756	ASN	2.9
1	C	996	SER	2.9
1	B	94	MET	2.9
1	C	129	LEU	2.9
1	C	830	VAL	2.9
1	A	172	ARG	2.9
1	B	300	ASP	2.9
1	A	965	LEU	2.9
1	A	1182	LEU	2.9
1	A	709	THR	2.9
1	A	1103	LYS	2.9
1	B	877	THR	2.9
1	B	125	LYS	2.9
1	A	455	PRO	2.9
1	C	1031	LEU	2.8
1	A	951	ALA	2.8
1	C	766	LYS	2.8
1	C	301	PRO	2.8
1	A	644	LEU	2.8
1	A	241	ASP	2.8
1	C	77	GLU	2.8
1	C	975	SER	2.8
1	A	641	LEU	2.8
1	B	915	PHE	2.8
1	A	99	HIS	2.8
1	B	588	ASP	2.8
1	B	656	GLN	2.8
1	C	630	LEU	2.8
1	C	966	LEU	2.8
1	C	739	ASN	2.8
1	A	298	GLN	2.8
1	C	740	ILE	2.8
1	C	1210	CYS	2.8
1	C	250	SER	2.8
1	C	81	LEU	2.8
1	C	178	THR	2.8
1	C	1162	THR	2.8
1	A	735	GLY	2.8
1	B	1275	MET	2.8
1	B	1183	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	633	PHE	2.8
1	C	776	CYS	2.8
1	C	142	GLU	2.8
1	C	62	ALA	2.8
1	C	817	PHE	2.8
1	B	904	SER	2.8
1	C	1024	LEU	2.8
1	B	187	THR	2.8
1	B	1102	ILE	2.8
1	B	452	THR	2.7
1	C	1	MET	2.8
1	A	830	VAL	2.7
1	C	1217	VAL	2.7
1	A	1020	PHE	2.7
1	C	296	GLY	2.7
1	B	655	SER	2.7
1	B	784	LEU	2.7
1	C	400	ASP	2.7
1	B	1106	ALA	2.7
1	A	1081	CYS	2.7
1	B	612	LEU	2.7
1	C	784	LEU	2.7
1	C	976	LYS	2.7
1	C	1052	GLN	2.7
1	B	158	ARG	2.7
1	A	552	LEU	2.7
1	B	929	PHE	2.7
1	A	354	VAL	2.7
1	A	207	LEU	2.7
1	B	1221	SER	2.7
1	A	1128	THR	2.7
1	C	25	LYS	2.7
1	B	972	ASP	2.7
1	B	1160	VAL	2.7
1	A	171	GLN	2.7
1	C	394	GLY	2.7
1	A	1266	LEU	2.7
1	B	210	ILE	2.7
1	C	198	VAL	2.7
1	B	834	SER	2.7
1	C	915	PHE	2.7
1	C	44	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	95	LEU	2.7
1	B	1217	VAL	2.7
1	B	768	GLU	2.7
1	C	223	LYS	2.7
1	A	261	ALA	2.7
1	B	115	ALA	2.7
1	B	385	PHE	2.6
1	A	463	PHE	2.6
1	B	833	SER	2.6
1	C	265	TYR	2.6
1	A	714	LYS	2.6
1	B	305	LEU	2.6
1	B	752	LEU	2.6
1	B	1195	VAL	2.6
1	A	961	SER	2.6
1	B	819	ASP	2.6
1	A	246	GLU	2.6
1	C	107	ASP	2.6
1	C	330	LEU	2.6
1	A	85	VAL	2.6
1	A	371	SER	2.6
1	B	361	SER	2.6
1	A	991	LEU	2.6
1	C	591	LYS	2.6
1	C	701	LEU	2.6
1	B	113	VAL	2.6
1	C	262	ASP	2.6
1	C	781	SER	2.6
1	A	471	PRO	2.6
1	B	1264	ILE	2.6
1	B	475	GLN	2.6
1	C	195	VAL	2.6
1	B	366	GLU	2.6
1	C	956	ARG	2.6
1	C	742	ALA	2.6
1	C	1028	PHE	2.6
1	B	1149	LEU	2.6
1	A	1272	VAL	2.6
1	C	997	PRO	2.6
1	C	357	ARG	2.6
1	A	396	LYS	2.6
1	C	1085	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1167	LEU	2.6
1	C	949	GLN	2.6
1	C	858	VAL	2.6
1	C	859	SER	2.6
1	A	120	ARG	2.6
1	A	425	ILE	2.6
1	A	33	LEU	2.6
1	A	1248	PRO	2.6
1	B	191	MET	2.6
1	C	61	GLY	2.6
1	C	161	ILE	2.6
1	C	210	ILE	2.6
1	B	581	THR	2.6
1	C	355	PRO	2.6
1	A	369	ARG	2.6
1	B	703	ASP	2.6
1	A	1149	LEU	2.6
1	B	734	VAL	2.6
1	C	173	TYR	2.6
1	C	970	GLU	2.6
1	A	452	THR	2.6
1	A	1156	SER	2.6
1	B	1207	THR	2.6
1	C	985	LEU	2.6
1	C	649	CYS	2.5
1	A	3	LEU	2.5
1	A	975	SER	2.5
1	C	1045	LEU	2.5
1	B	1039	VAL	2.5
1	A	111	ASP	2.5
1	C	67	LYS	2.5
1	C	953	PHE	2.5
1	A	863	GLY	2.5
1	B	383	ILE	2.5
1	C	1248	PRO	2.5
1	B	207	LEU	2.5
1	C	221	SER	2.5
1	B	740	ILE	2.5
1	B	745	ILE	2.5
1	A	68	ILE	2.5
1	B	297	GLN	2.5
1	A	109	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	978	ALA	2.5
1	C	144	LEU	2.5
1	B	23	THR	2.5
1	B	379	THR	2.5
1	A	426	LEU	2.5
1	A	736	ILE	2.5
1	A	828	LEU	2.5
1	B	1053	LEU	2.5
1	A	55	PRO	2.5
1	A	1076	ALA	2.5
1	A	1074	ARG	2.5
1	C	155	GLU	2.5
1	A	1195	VAL	2.5
1	B	680	ARG	2.5
1	A	146	CYS	2.5
1	B	1002	MET	2.5
1	A	89	ILE	2.5
1	A	459	PHE	2.5
1	B	1163	LEU	2.5
1	C	948	THR	2.5
1	C	1132	GLU	2.5
1	C	12	LYS	2.5
1	A	43	VAL	2.5
1	B	804	LEU	2.5
1	C	768	GLU	2.5
1	A	752	LEU	2.5
1	C	87	SER	2.5
1	C	1011	LYS	2.5
1	C	1181	TYR	2.5
1	A	952	SER	2.5
1	B	958	PHE	2.5
1	B	164	LEU	2.5
1	B	991	LEU	2.5
1	B	1159	CYS	2.4
1	B	237	PHE	2.4
1	C	762	PHE	2.4
1	A	133	ILE	2.4
1	A	958	PHE	2.4
1	C	931	GLN	2.4
1	C	1041	LEU	2.4
1	B	182	LYS	2.4
1	B	454	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	736	ILE	2.4
1	B	42	ALA	2.4
1	B	1181	TYR	2.4
1	C	474	LEU	2.4
1	B	395	PRO	2.4
1	B	585	GLU	2.4
1	C	396	LYS	2.4
1	A	448	VAL	2.4
1	A	1163	LEU	2.4
1	C	881	LEU	2.4
1	A	487	LEU	2.4
1	A	1105	SER	2.4
1	B	173	TYR	2.4
1	B	180	VAL	2.4
1	B	773	LEU	2.4
1	B	742	ALA	2.4
1	C	395	PRO	2.4
1	B	384	GLU	2.4
1	B	845	THR	2.4
1	B	1196	GLU	2.4
1	A	971	ASP	2.4
1	B	1220	LYS	2.4
1	A	482	GLU	2.4
1	B	88	GLU	2.4
1	A	989	SER	2.4
1	B	952	SER	2.4
1	A	56	CYS	2.4
1	B	364	ILE	2.4
1	C	765	SER	2.4
1	A	877	THR	2.4
1	C	670	ILE	2.4
1	C	683	PRO	2.4
1	B	367	VAL	2.4
1	A	472	LEU	2.4
1	A	705	LEU	2.4
1	B	885	THR	2.4
1	C	1161	ASP	2.4
1	C	118	GLU	2.4
1	B	303	LYS	2.4
1	A	297	GLN	2.3
1	B	453	SER	2.3
1	A	884	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	837	PHE	2.3
1	B	858	VAL	2.3
1	C	483	THR	2.3
1	A	1276	GLN	2.3
1	B	451	ARG	2.3
1	C	911	LEU	2.3
1	B	119	ASP	2.3
1	C	1202	SER	2.3
1	B	398	ILE	2.3
1	B	798	LYS	2.3
1	A	295	ALA	2.3
1	B	213	LEU	2.3
1	A	75	LEU	2.3
1	A	1014	SER	2.3
1	A	394	GLY	2.3
1	B	931	GLN	2.3
1	A	237	PHE	2.3
1	C	3	LEU	2.3
1	A	572	SER	2.3
1	B	886	SER	2.3
1	C	473	ILE	2.3
1	C	659	LEU	2.3
1	B	1044	ASP	2.3
1	A	1267	SER	2.3
1	A	946	THR	2.3
1	B	396	LYS	2.3
1	C	475	GLN	2.3
1	B	702	ASP	2.3
1	C	11	ASP	2.3
1	C	812	LEU	2.3
1	C	924	PRO	2.3
1	A	186	LEU	2.3
1	B	1051	GLY	2.3
1	A	42	ALA	2.3
1	B	920	GLN	2.3
1	C	945	VAL	2.3
1	B	1103	LYS	2.3
1	C	26	ASP	2.3
1	A	992	LEU	2.3
1	B	622	ILE	2.3
1	B	838	MET	2.3
1	A	100	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	116	VAL	2.3
1	B	842	VAL	2.3
1	B	802	SER	2.3
1	C	131	PRO	2.3
1	A	798	LYS	2.3
1	B	1	MET	2.3
1	C	190	GLU	2.3
1	C	923	GLN	2.3
1	B	571	HIS	2.3
1	A	1018	ALA	2.3
1	B	118	GLU	2.3
1	C	617	GLN	2.3
1	B	470	ALA	2.3
1	A	27	ASP	2.2
1	A	181	PHE	2.2
1	B	629	GLN	2.2
1	C	78	SER	2.2
1	C	297	GLN	2.2
1	C	608	PHE	2.2
1	A	37	ALA	2.2
1	C	929	PHE	2.2
1	B	1218	GLN	2.2
1	A	210	ILE	2.2
1	C	398	ILE	2.2
1	A	563	VAL	2.2
1	A	1002	MET	2.2
1	A	39	LYS	2.2
1	A	1279	LYS	2.2
1	B	1192	PRO	2.2
1	B	261	ALA	2.2
1	B	813	LEU	2.2
1	A	450	THR	2.2
1	B	955	ILE	2.2
1	C	364	ILE	2.2
1	C	667	LEU	2.2
1	C	581	THR	2.2
1	C	1213	PHE	2.2
1	A	1274	LEU	2.2
1	C	191	MET	2.2
1	A	636	PRO	2.2
1	B	440	ILE	2.2
1	A	134	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	988	LEU	2.2
1	C	1142	LEU	2.2
1	B	821	ILE	2.2
1	C	1127	PRO	2.2
1	A	915	PHE	2.2
1	B	308	PHE	2.2
1	B	358	THR	2.2
1	B	333	SER	2.2
1	A	579	ASN	2.2
1	B	1164	LEU	2.2
1	A	799	VAL	2.2
1	B	355	PRO	2.2
1	B	1199	VAL	2.2
1	C	213	LEU	2.2
1	C	393	TYR	2.2
1	C	583	CYS	2.2
1	A	449	VAL	2.2
1	A	110	SER	2.2
1	B	246	GLU	2.2
1	C	856	GLY	2.2
1	C	615	ASN	2.2
1	A	1135	ILE	2.2
1	A	1213	PHE	2.2
1	B	664	ASP	2.2
1	B	918	VAL	2.2
1	C	334	VAL	2.2
1	C	806	LEU	2.2
1	C	120	ARG	2.1
1	C	354	VAL	2.1
1	C	783	ILE	2.2
1	A	441	LEU	2.1
1	A	440	ILE	2.1
1	A	1214	ILE	2.1
1	C	1056	ILE	2.1
1	A	1021	CYS	2.1
1	B	631	LYS	2.1
1	C	37	ALA	2.1
1	B	330	LEU	2.1
1	C	527	SER	2.1
1	C	563	VAL	2.1
1	A	375	TRP	2.1
1	C	748	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1135	ILE	2.1
1	B	1146	PHE	2.1
1	B	1180	TYR	2.1
1	C	366	GLU	2.1
1	B	356	GLN	2.1
1	B	371	SER	2.1
1	A	1077	ALA	2.1
1	B	823	SER	2.1
1	A	429	THR	2.1
1	A	1210	CYS	2.1
1	C	705	LEU	2.1
1	A	202	PHE	2.1
1	B	1132	GLU	2.1
1	B	466	ILE	2.1
1	B	1128	THR	2.1
1	B	903	ILE	2.1
1	A	656	GLN	2.1
1	C	194	VAL	2.1
1	B	421	LEU	2.1
1	A	263	GLU	2.1
1	A	776	CYS	2.1
1	A	800	SER	2.1
1	C	1273	ASN	2.1
1	A	485	ASP	2.1
1	B	76	VAL	2.1
1	C	1025	MET	2.1
1	A	701	LEU	2.1
1	B	128	GLU	2.1
1	C	353	LEU	2.1
1	A	48	ARG	2.1
1	B	425	ILE	2.1
1	C	869	ILE	2.1
1	A	476	ASN	2.1
1	C	813	LEU	2.1
1	A	157	LYS	2.1
1	B	483	THR	2.1
1	C	568	VAL	2.1
1	B	615	ASN	2.1
1	A	845	THR	2.0
1	C	914	THR	2.0
1	C	132	ILE	2.0
1	A	1070	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	222	SER	2.0
1	C	298	GLN	2.0
1	C	821	ILE	2.0
1	C	205	LEU	2.0
1	A	1040	THR	2.0
1	B	815	ALA	2.0
1	C	918	VAL	2.0
1	B	573	ARG	2.0
1	A	9	ALA	2.0
1	C	612	LEU	2.0
1	A	708	ILE	2.0
1	A	1080	VAL	2.0
1	C	243	GLN	2.0
1	C	1102	ILE	2.0
1	B	666	LEU	2.0
1	B	1016	GLU	2.0
1	C	29	LEU	2.0
1	C	305	LEU	2.0
1	A	214	VAL	2.0
1	B	771	LEU	2.0
1	A	61	GLY	2.0
1	A	190	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.