



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:12 PM UTC

PDB ID : 3S4Z / pdb_00003s4z
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

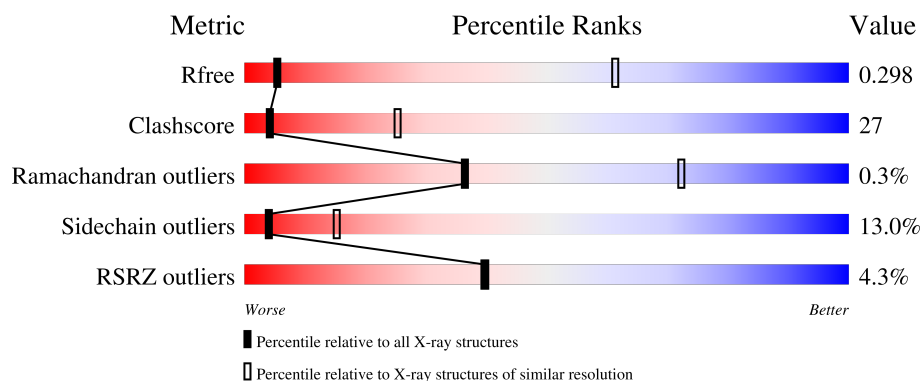
1 Overall quality at a glance

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}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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 of 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	4% 43% 37% 7% 14%
1	B	1308	3% 43% 37% 6% 14%
1	C	1308	4% 43% 37% 7% 14%

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			

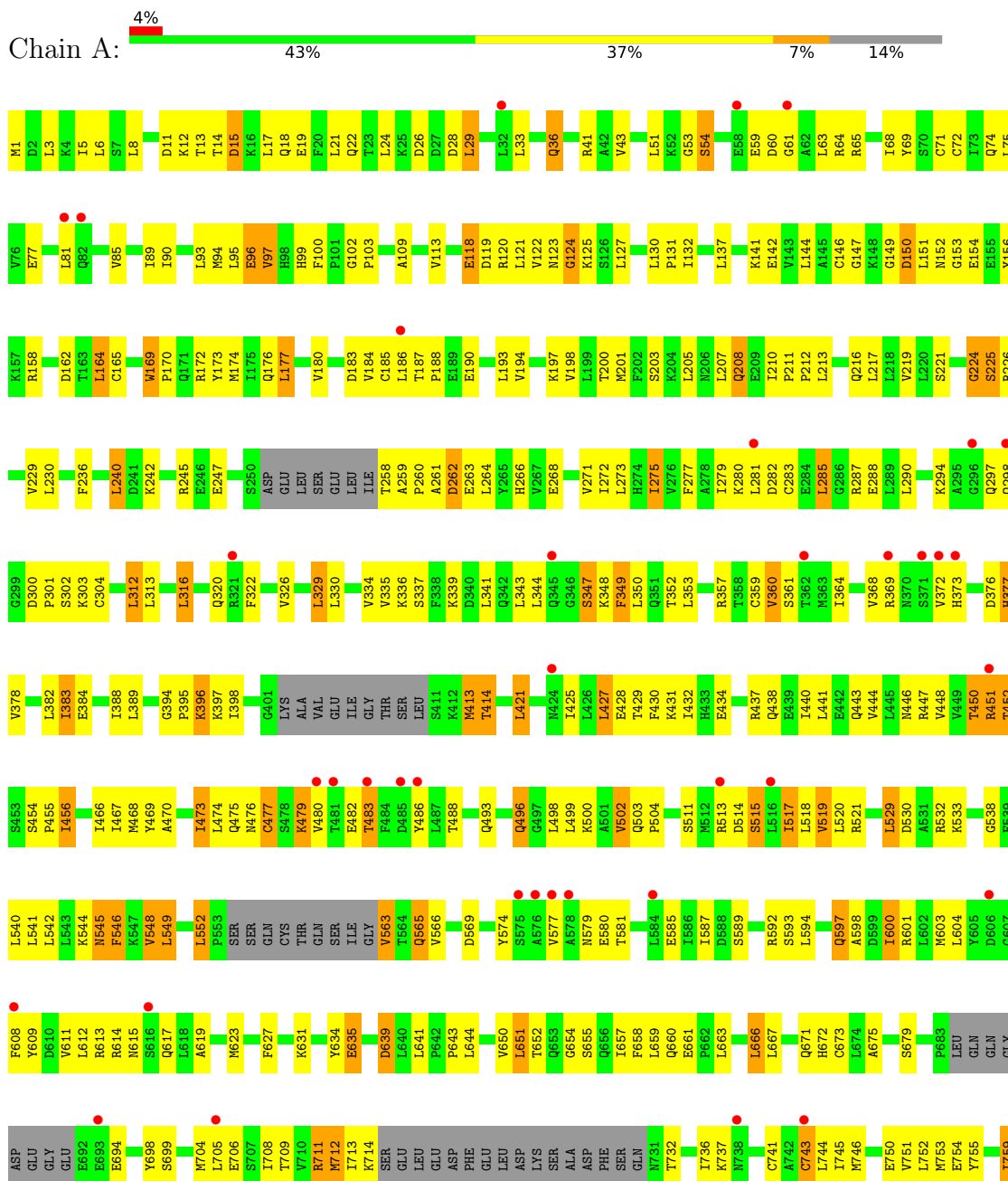
There are 18 discrepancies between the modelled and reference sequences:

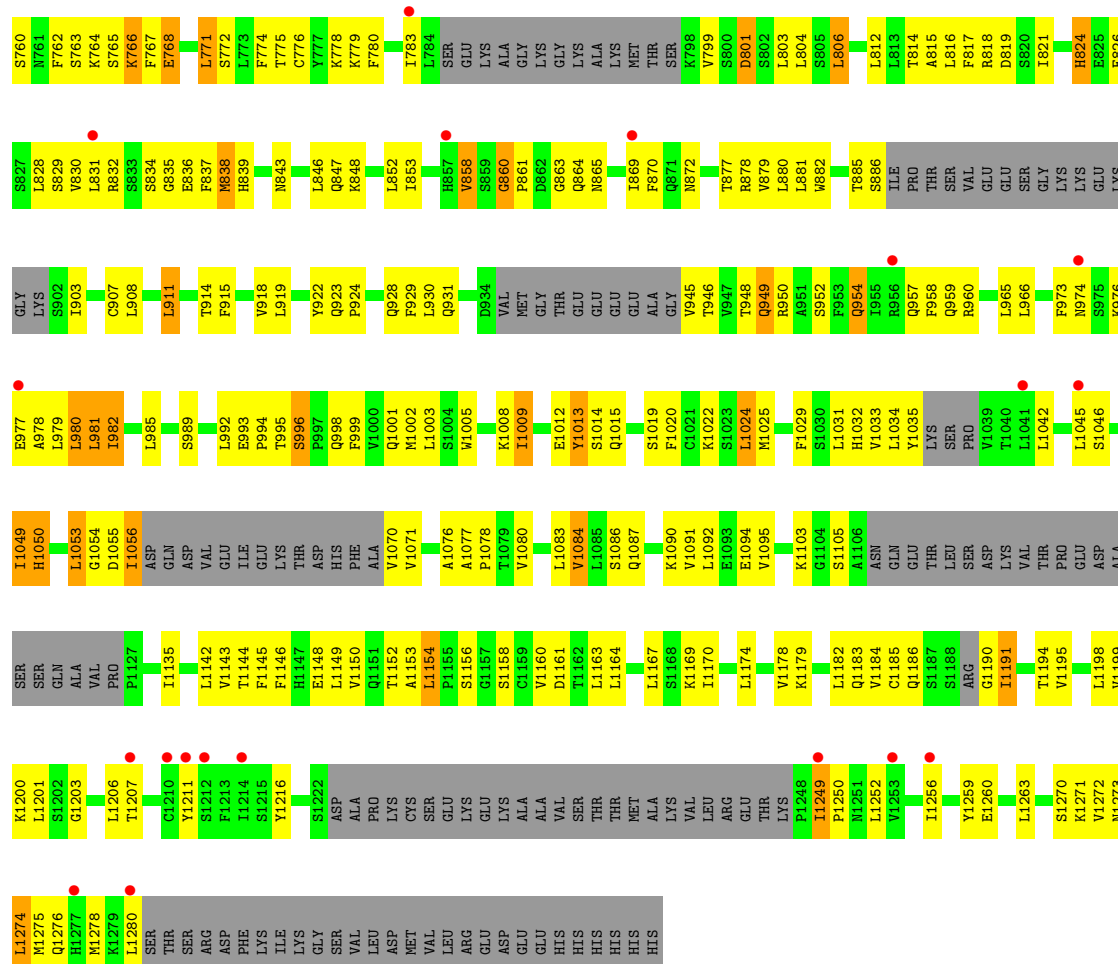
Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	expression tag	UNP Q8K368
A	1304	HIS	-	expression tag	UNP Q8K368
A	1305	HIS	-	expression tag	UNP Q8K368
A	1306	HIS	-	expression tag	UNP Q8K368
A	1307	HIS	-	expression tag	UNP Q8K368
A	1308	HIS	-	expression tag	UNP Q8K368
B	1303	HIS	-	expression 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

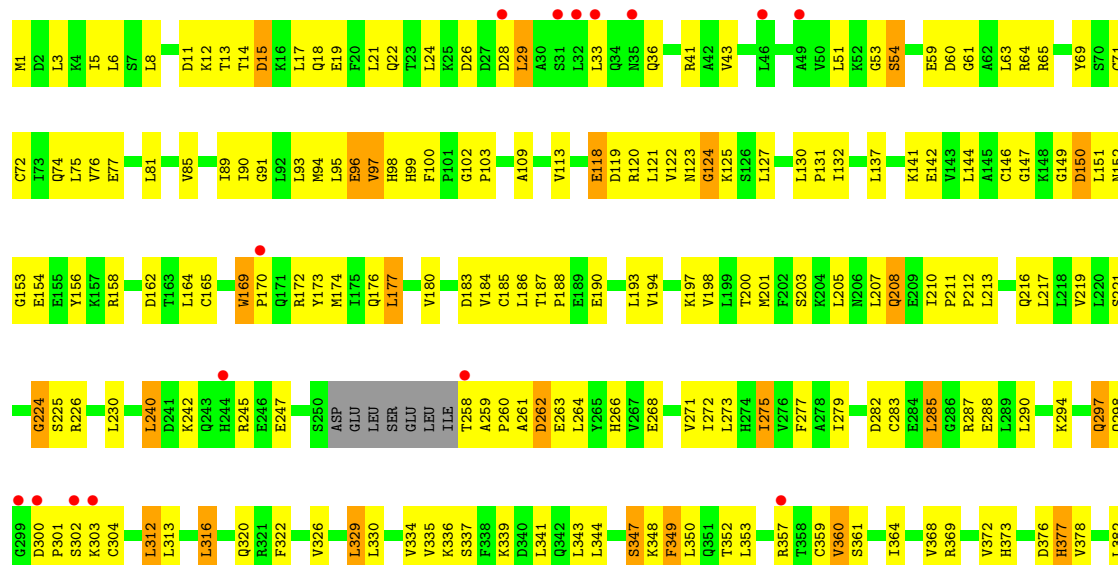
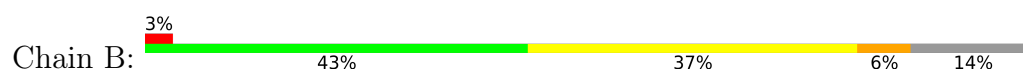
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

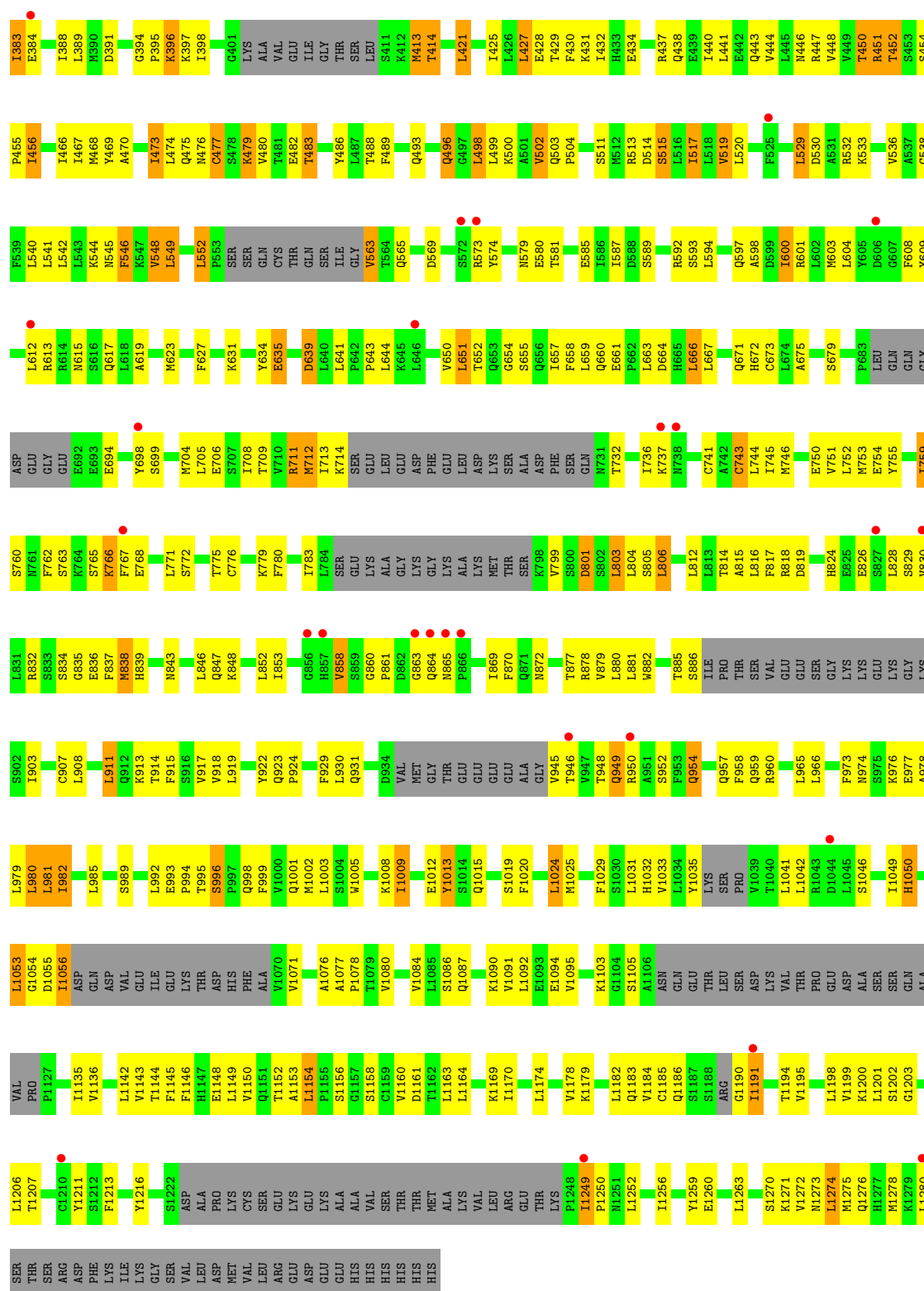
• Molecule 1: dna repair 1





• 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	235.20Å 307.90Å 375.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 7.80 33.00 – 7.80	Depositor EDS
% Data completeness (in resolution range)	85.3 (33.00-7.80) 84.0 (33.00-7.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 7.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.310 , 0.324 0.295 , 0.298	Depositor DCC
R_{free} test set	604 reflections (3.78%)	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)	0.41 , 710.2	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	0.65	4/9075 (0.0%)	0.94	15/12252 (0.1%)
1	B	0.34	2/9073 (0.0%)	0.79	10/12246 (0.1%)
1	C	0.37	3/9074 (0.0%)	0.82	12/12249 (0.1%)
All	All	0.47	9/27222 (0.0%)	0.85	37/36747 (0.1%)

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	41.38	1.91	1.33
1	A	545	ASN	C-N	32.24	1.76	1.33
1	C	545	ASN	C-N	11.91	1.49	1.33
1	B	320	GLN	CD-NE2	-8.31	1.15	1.33
1	A	320	GLN	CD-NE2	-8.30	1.15	1.33
1	C	320	GLN	CD-NE2	-8.28	1.15	1.33
1	C	320	GLN	CD-OE1	-6.78	1.10	1.23
1	B	320	GLN	CD-OE1	-6.78	1.10	1.23
1	A	320	GLN	CD-OE1	-6.71	1.10	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLY	O-C-N	-42.02	68.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLY	CA-C-N	19.81	159.37	121.54
1	A	224	GLY	C-N-CA	19.81	159.37	121.54
1	C	545	ASN	CA-C-N	-16.17	93.76	121.89
1	C	545	ASN	C-N-CA	-16.17	93.76	121.89
1	A	545	ASN	CA-C-N	-14.98	101.87	122.99
1	A	545	ASN	C-N-CA	-14.98	101.87	122.99
1	A	545	ASN	O-C-N	12.76	139.13	122.42
1	C	545	ASN	O-C-N	12.48	137.70	122.35
1	C	860	GLY	CA-C-N	7.71	127.76	119.90
1	C	860	GLY	C-N-CA	7.71	127.76	119.90
1	B	224	GLY	N-CA-C	7.70	123.61	112.60
1	B	860	GLY	CA-C-N	7.70	127.75	119.90
1	B	860	GLY	C-N-CA	7.70	127.75	119.90
1	A	860	GLY	CA-C-N	7.69	127.75	119.90
1	A	860	GLY	C-N-CA	7.69	127.75	119.90
1	A	28	ASP	N-CA-C	-6.78	104.63	113.17
1	C	28	ASP	N-CA-C	-6.73	104.69	113.17
1	B	28	ASP	N-CA-C	-6.70	104.73	113.17
1	B	546	PHE	N-CA-C	5.83	117.88	108.32
1	C	635	GLU	CA-C-N	5.63	125.16	119.19
1	C	635	GLU	C-N-CA	5.63	125.16	119.19
1	A	635	GLU	CA-C-N	5.62	125.15	119.19
1	A	635	GLU	C-N-CA	5.62	125.15	119.19
1	B	635	GLU	CA-C-N	5.58	125.11	119.19
1	B	635	GLU	C-N-CA	5.58	125.11	119.19
1	A	546	PHE	N-CA-C	5.55	117.94	108.90
1	B	1191	ILE	CA-C-N	5.43	125.73	119.92
1	B	1191	ILE	C-N-CA	5.43	125.73	119.92
1	A	1191	ILE	CA-C-N	5.40	125.70	119.92
1	A	1191	ILE	C-N-CA	5.40	125.70	119.92
1	C	1191	ILE	CA-C-N	5.38	125.68	119.92
1	C	1191	ILE	C-N-CA	5.38	125.68	119.92
1	C	546	PHE	N-CA-C	5.24	117.91	108.48
1	B	124	GLY	N-CA-C	-5.19	107.57	115.66
1	A	124	GLY	N-CA-C	-5.18	107.58	115.66
1	C	124	GLY	N-CA-C	-5.18	107.58	115.66

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	LEU	Peptide

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Mol	Chain	Res	Type	Group
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	518	13
1	B	8938	0	9247	466	0
1	C	8938	0	9248	540	0
All	All	26814	0	27742	1490	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 (1490) 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
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	1.41
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:224:GLY:C	1:A:225:SER:N	1.91	1.25
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:C:207:LEU:CD2	1:C:237:PHE:CE2	2.25	1.19
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:A:208:GLN:HE22	1:A:263:GLU:CD	1.56	1.14
1:B:450:THR:HG21	1:C:489:PHE:HB3	1.12	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ILE:HD11	1:C:236:PHE:CE2	1.71	1.11
1:A:208:GLN:NE2	1:A:263:GLU:CD	2.00	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:B:545:ASN:C	1:B:546:PHE:N	2.09	1.10
1:A:208:GLN:NE2	1:A:263:GLU:CG	1.97	1.09
1:A:771:LEU:CD1	1:A:830:VAL:O	2.01	1.09
1:C:214:VAL:HG21	1:C:233:ILE:HD13	1.23	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:A:1012:GLU:CD	1:B:1008:LYS:HE3	1.80	1.06
1:C:354:VAL:HG21	1:C:1101:LYS:HZ2	1.18	1.06
1:C:672:HIS:ND1	1:C:861:PRO:HG3	1.70	1.06
1:B:799:VAL:O	1:B:847:GLN:NE2	1.87	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: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
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:A:1008:LYS:HE3	1:B:1012:GLU:CD	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD22	1:C:237:PHE:HE2	1.05	0.85
1:C:207:LEU:CD2	1:C:236:PHE:CE2	2.60	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:545:ASN:C	1:A:546:PHE:CA	2.51	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
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:208:GLN:NE2	1:B:263:GLU:CD	2.37	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:B:816:LEU:HD13	1:B:838:MET:HE1	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:THR:N	1:C:261:ALA:HB3	1.96	0.81
1:C:816:LEU:HD13	1:C:838:MET:HE1	1.62	0.81
1:B:208:GLN:HE22	1:B:263:GLU:CD	1.88	0.81
1:C:208:GLN:HE22	1:C:263:GLU:C	1.88	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:A:816:LEU:HD13	1:A:838:MET:HE1	1.62	0.80
1:C:545:ASN:C	1:C:546:PHE:CG	2.59	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:623:MET:HE1	1:B:673:CYS:HB3	1.65	0.79
1:A:623:MET:HE1	1:A:673:CYS:HB3	1.65	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:B:536:VAL:HG11	1:B:603:MET:HE3	1.65	0.79
1:C:65:ARG:HB3	1:C:100:PHE:HZ	1.48	0.79
1:C:623:MET:HE1	1:C:673:CYS:HB3	1.65	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: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:302:SER:HB2	1:B:357:ARG:HG2	1.66	0.76
1:B:1056:ILE:HG12	1:B:1153:ALA:HB2	1.64	0.76
1:C:210:ILE:HD13	1:C:236:PHE:CD2	2.20	0.76
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:C:218:LEU:CD2	1:C:285:LEU:HD11	2.14	0.76
1:A:452:THR:HB	1:A:454:SER:H	1.51	0.76
1:B:470:ALA:O	1:B:473:ILE:HG13	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1032:HIS:ND1	1:B:1041:LEU:HD11	2.00	0.76
1:B:259:ALA:CB	1:B:260:PRO:HD3	2.17	0.75
1:B:165:CYS:HB3	1:B:197:LYS:HG3	1.67	0.75
1:C:349:PHE:HD2	1:C:349:PHE:H	1.32	0.75
1:C:377:HIS:CD2	1:C:377:HIS:H	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:CD2	1:A:377:HIS:H	2.04	0.75
1:B:349:PHE:H	1:B:349:PHE:HD2	1.33	0.75
1:B:1054:GLY:O	1:B:1055:ASP:HB2	1.87	0.75
1:C:470:ALA:O	1:C:473:ILE:HG13	1.86	0.75
1:C:1054:GLY:O	1:C:1055:ASP:HB2	1.87	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:94:MET:HE3	1:C:132:ILE:HD11	1.71	0.72
1:C:259:ALA:CB	1:C:260:PRO:HD3	2.17	0.72
1:A:94:MET:HE3	1:A:132:ILE:HD11	1.71	0.72
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.17	0.72
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:94:MET:HE3	1:B:132:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:750:GLU:HA	1:C:753:MET:HE3	1.73	0.70
1:A:149:GLY:O	1:A:151:LEU:N	2.24	0.69
1:A:1025:MET:HA	1:A:1025:MET:HE2	1.74	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:1008:LYS:HE3	1:B:1012:GLU:OE2	1.92	0.69
1:A:1143:VAL:HG13	1:A:1206:LEU:HG	1.73	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:C:946:THR:HG22	1:C:950:ARG:HE	1.57	0.69
1:C:1054:GLY:HA3	1:C:1153:ALA:H	1.56	0.69
1:A:513:ARG:HD3	1:A:546:PHE:CE1	2.28	0.69
1:A:448:VAL:HA	1:A:456:ILE:HD13	1.74	0.68
1:A:1054:GLY:HA3	1:A:1153:ALA:H	1.56	0.68
1:B:750:GLU:HA	1:B:753:MET:HE3	1.73	0.68
1:B:760:SER:HB2	1:B:766:LYS:HE2	1.75	0.68
1:A:750:GLU:HA	1:A:753:MET:HE3	1.73	0.68
1:B:1054:GLY:HA3	1:B:1153:ALA:H	1.56	0.68
1:C:448:VAL:HA	1:C:456:ILE:HD13	1.74	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1025:MET:HA	1:C:1025:MET:HE2	1.74	0.67
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:B:1025:MET:HE2	1:B:1025:MET:HA	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:208:GLN:CD	1:A:263:GLU:CG	2.64	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:A:1008:LYS:CE	1:B:1012:GLU:OE1	2.42	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: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:C:275:ILE:HD11	1:C:312:LEU:HD11	1.77	0.67
1:C:838:MET:HE2	1:C:838:MET:HA	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:838:MET:HA	1:A:838:MET:HE2	1.77	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:65:ARG:HB3	1:A:100:PHE:CZ	2.30	0.66
1:A:347:SER:HB2	1:A:349:PHE:CE2	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:330:LEU:O	1:A:334:VAL:HG23	1.95	0.66
1:A:1190:GLY:N	1:A:1271:LYS:HZ1	1.94	0.66
1:B:446:ASN:HB3	1:C:489:PHE:CE1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:672:HIS:ND1	1:C:861:PRO:CG	2.56	0.66
1:C:712:MET:HA	1:C:712:MET:HE2	1.78	0.66
1:B:712:MET:HE2	1:B:712:MET:HA	1.78	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:A:545:ASN:C	1:A:546:PHE:HA	2.21	0.65
1:A:169:TRP:CD1	1:A:169:TRP:H	2.15	0.65
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:33:LEU:HD23	1:C:75:LEU:HD11	1.78	0.65
1:C:330:LEU:O	1:C:334:VAL:HG23	1.95	0.65
1:A:470:ALA:HB3	1:A:473:ILE:HD11	1.77	0.65
1:A:1259:TYR:CZ	1:A:1263:LEU:HD11	2.32	0.65
1:B:838:MET:HE2	1:B:838:MET:HA	1.77	0.65
1:A:712:MET:HA	1:A:712:MET:HE2	1.78	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:121:LEU:C	1:B:123:ASN:H	2.06	0.64
1:B:169:TRP:H	1:B:169:TRP:CD1	2.15	0.64
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:169:TRP:H	1:C:169:TRP:CD1	2.14	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:A:545:ASN:C	1:A:565:GLN:HB3	2.22	0.64
1:C:121:LEU:C	1:C:123:ASN:H	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:121:LEU:C	1:A:123:ASN:H	2.06	0.63
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:1012:GLU:CD	1:B:1008:LYS:CE	2.67	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
1:A:377:HIS:CD2	1:A:377:HIS:N	2.67	0.63
1:B:431:LYS:HE3	1:B:469:TYR:CE1	2.33	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:A:518:LEU:HD21	1:A:577:VAL:HG22	1.81	0.63
1:C:169:TRP:CD1	1:C:169:TRP:N	2.66	0.63
1:C:948:THR:HG23	1:C:992:LEU:HA	1.81	0.63
1:A:169:TRP:CD1	1:A:169:TRP:N	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:H	1:C:169:TRP:HD1	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:413:MET:HA	1:C:413:MET:HE2	1.81	0.62
1:C:431:LYS:HE3	1:C:469:TYR:CE1	2.33	0.62
1:C:1055:ASP:N	1:C:1152:THR:HA	2.13	0.62
1:B:413:MET:HE2	1:B:413:MET:HA	1.81	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:A:413:MET:HE2	1:A:413:MET:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LEU:O	1:B:294:LYS:HG3	2.00	0.62
1:C:377:HIS:CD2	1:C:377:HIS:N	2.67	0.62
1:A:290:LEU:O	1:A:294:LYS:HG3	2.00	0.62
1:B:377:HIS:H	1:B:377:HIS:HD2	1.45	0.62
1:B:377:HIS:CD2	1:B:377:HIS:N	2.67	0.62
1:B:1046:SER:O	1:B:1050:HIS:HB3	1.99	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:1190:GLY:N	1:C:1271:LYS:HZ1	1.97	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:C:713:ILE:C	1:C:714:LYS:HG2	2.25	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
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:H	1:C:397:LYS:HD3	1.65	0.61
1:C:708:ILE:O	1:C:712:MET:HB2	1.99	0.61
1:A:174:MET:HE1	1:A:205:LEU:HD11	1.83	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: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:C:1179:LYS:HA	1:C:1182:LEU:HD12	1.82	0.61
1:A:397:LYS:HD3	1:A:397:LYS:H	1.65	0.61
1:A:713:ILE:C	1:A:714:LYS:HG2	2.25	0.61
1:A:877:THR:OG1	1:A:914:THR:HG21	2.00	0.61
1:B:174:MET:HE1	1:B:205:LEU:HD11	1.83	0.61
1:B:187:THR:HG22	1:B:188:PRO:HD2	1.83	0.61
1:B:397:LYS:H	1:B:397:LYS:HD3	1.65	0.61
1:B:713:ILE:C	1:B:714:LYS:HG2	2.25	0.61
1:A:169:TRP:H	1:A:169:TRP:HD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:GLN:HG3	1:B:476:ASN:N	2.15	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:C:1076:ALA:HA	1:C:1080:VAL:HB	1.83	0.61
1:B:779:LYS:O	1:B:783:ILE:HG13	2.01	0.60
1:B:713:ILE:HG21	1:B:772:SER:HB3	1.81	0.60
1:B:1032:HIS:CE1	1:B:1041:LEU:CD1	2.79	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:877:THR:OG1	1:C:914:THR:HG21	2.00	0.60
1:C:1046:SER:O	1:C:1050:HIS:HB3	1.99	0.60
1:A:210:ILE:CD1	1:A:236:PHE:CZ	2.83	0.60
1:A:348:LYS:HZ1	1:A:994:PRO:HB2	1.66	0.60
1:A:1076:ALA:HA	1:A:1080:VAL:HB	1.83	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:377:HIS:H	1:A:377:HIS:HD2	1.45	0.60
1:A:1055:ASP:N	1:A:1152:THR:HA	2.13	0.60
1:C:174:MET:HE1	1:C:205:LEU:HD11	1.83	0.60
1:C:989:SER:HB2	1:C:1031:LEU:HD21	1.83	0.60
1:C:1249:ILE:N	1:C:1250:PRO:HD2	2.16	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
1:B:1190:GLY:N	1:B:1271:LYS:HZ1	1.98	0.60
1:C:779:LYS:O	1:C:783:ILE:HG13	2.01	0.60
1:A:533:LYS:HG3	1:A:603:MET:HE1	1.83	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:190:GLU:O	1:A:194:VAL:HG23	2.00	0.60
1:A:982:ILE:HD11	1:A:1024:LEU:HG	1.84	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:CD2	1:C:349:PHE:N	2.68	0.60
1:A:11:ASP:O	1:A:12:LYS:HG2	2.02	0.60
1:A:779:LYS:O	1:A:783:ILE:HG13	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:124:GLY:O	1:A:127:LEU:N	2.35	0.59
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.16	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
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:72:CYS:HB2	1:A:93:LEU:HD11	1.85	0.58
1:A:102:GLY:HA3	1:A:144:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ASN:C	1:B:546:PHE:CD2	2.82	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: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:214:VAL:CG2	1:C:233:ILE:CG1	2.81	0.57
1:C:350:LEU:HD13	1:C:1097:TRP:CZ3	2.40	0.57
1:A:977:GLU:O	1:A:981:LEU:HB2	2.05	0.57
1:A:1200:LYS:HB3	1:A:1274:LEU:HD21	1.85	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:300:ASP:O	1:C:304:CYS:N	2.38	0.57
1:C:1087:GLN:O	1:C:1091:VAL:HG23	2.04	0.57
1:C:1029:PHE:CD2	1:C:1087:GLN:HG2	2.40	0.57
1:A:275:ILE:CD1	1:A:312:LEU:HD11	2.35	0.56
1:A:1087:GLN:O	1:A:1091:VAL:HG23	2.04	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: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:A:349:PHE:HE2	1:A:1033:VAL:CG1	2.18	0.56
1:B:102:GLY:N	1:B:103:PRO:HD2	2.21	0.56
1:B:224:GLY:C	1:B:225:SER:N	2.63	0.56
1:C:102:GLY:N	1:C: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:545:ASN:C	1:C:546:PHE:CD2	2.83	0.56
1:C:977:GLU:O	1:C:981:LEU:HB2	2.05	0.56
1:A:542:LEU:O	1:A:546:PHE:N	2.39	0.56
1:A:835:GLY:HA2	1:A:838:MET:HB2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1146:PHE:CE1	1:A:1170:ILE:HD11	2.41	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: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:1203:GLY:HA3	1:C:1278:MET:HG2	1.86	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:430:PHE:CE2	1:B:466:ILE:HG23	2.40	0.56
1:B:451:ARG:HB3	1:B:456:ILE:CD1	2.36	0.56
1:B:1146:PHE:CE1	1:B:1170:ILE:HD11	2.41	0.56
1:C:593:SER:HB2	1:C:600:ILE:HG21	1.88	0.56
1:C:799:VAL:O	1:C:847:GLN:CD	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:N	1:A:103:PRO:HD2	2.21	0.55
1:A:118:GLU:HA	1:A:118:GLU:OE1	2.07	0.55
1:B:103:PRO:HA	1:B:146:CYS:SG	2.46	0.55
1:A:150:ASP:OD1	1:A:151:LEU:HG	2.06	0.55
1:A:1146:PHE:O	1:A:1150:VAL:HG23	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
1:A:593:SER:HB2	1:A:600:ILE:HG21	1.88	0.54
1:B:704:MET:O	1:B:708:ILE:HG13	2.08	0.54
1:B:799:VAL:O	1:B:847:GLN:CD	2.49	0.54
1:B:1185:CYS:SG	1:B:1191:ILE:HG12	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:65:ARG:HD3	1:C:100:PHE:CE1	2.42	0.54
1:C:434:GLU:HA	1:C:437:ARG:HG3	1.89	0.54
1:C:1029:PHE:O	1:C:1033:VAL:HG23	2.08	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:771:LEU:HB2	1:A:830:VAL:CG1	2.38	0.54
1:A:1185:CYS:SG	1:A:1191:ILE:HG12	2.47	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:HA	1:C:118:GLU:OE1	2.07	0.54
1:B:766:LYS:HB2	1:B:766:LYS:NZ	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
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:A:799:VAL:O	1:A:847:GLN:CD	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: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:85:VAL:O	1:B:89:ILE:HG13	2.09	0.53
1:B:1029:PHE:O	1:B:1033:VAL:HG23	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:574:TYR:CD2	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:1055:ASP:O	1:B:1056:ILE:C	2.52	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:A:654:GLY:O	1:A:655:SER:OG	2.23	0.52
1:B:456:ILE:HG23	1:B:456:ILE:O	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
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:NE2	1:C:263:GLU:CB	2.72	0.52
1:C:208:GLN:CA	1:C:267:VAL:HG21	2.34	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: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:C:1055:ASP:O	1:C:1056:ILE:C	2.52	0.52
1:C:1149:LEU:HB3	1:C:1163:LEU:HD11	1.92	0.52
1:A:210:ILE:N	1:A:211:PRO:HD2	2.25	0.52
1:A:349:PHE:CD2	1:A:349:PHE:N	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:54:SER:HB2	1:B:61:GLY:O	2.10	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:A:1055:ASP:O	1:A:1056:ILE:C	2.52	0.52
1:A:1200:LYS:HB3	1:A:1274:LEU:CD2	2.39	0.52
1:B:654:GLY:O	1:B:655:SER:OG	2.22	0.52
1:B:1033:VAL:HG21	1:B:1087:GLN:NE2	2.25	0.52
1:C:207:LEU:HD13	1:C:264:LEU:CD2	2.39	0.52
1:A:85:VAL:O	1:A:89:ILE:HG13	2.09	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:C:713:ILE:O	1:C:714:LYS:CG	2.52	0.52
1:C:959:GLN:HB2	1:C:1005:TRP:CE2	2.45	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:467:ILE:HG12	1:C:474:LEU:HD12	1.90	0.52
1:C:1200:LYS:HB3	1:C:1274:LEU:CD2	2.39	0.52
1:B:489:PHE:HE2	1:C:447:ARG:HG3	1.74	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:C:613:ARG:NH2	1:C:862:ASP:OD1	2.43	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:B:489:PHE:CE1	1:C:446:ASN:HB3	2.45	0.52
1:B:826:GLU:HA	1:B:829:SER:HG	1.75	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: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:763:SER:O	1:A:767:PHE:HD1	1.92	0.51
1:A:1056:ILE:HD12	1:A:1216:TYR:CG	2.45	0.51
1:A:946:THR:HA	1:A:949:GLN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:778:LYS:HE2	1:A:836:GLU:CD	2.34	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:A:766:LYS:HB2	1:A:766:LYS:HZ2	1.75	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:121:LEU:C	1:A:123:ASN:N	2.69	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:146:CYS:O	1:B:147:GLY:C	2.54	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:C:456:ILE:HG23	1:C:456:ILE:O	2.09	0.50
1:B:303:LYS:HG2	1:B:357:ARG:NH2	2.26	0.50
1:B:1095:VAL:HG13	1:B:1135:ILE:HG23	1.93	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:B:993:GLU:CD	1:B:994:PRO:HD2	2.37	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:C:1054:GLY:CA	1:C:1152:THR:HG23	2.41	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:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.93	0.50
1:B:230:LEU:HD21	1:B:285:LEU:HD21	1.94	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:C:1092:LEU:HD13	1:C:1169:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1273:ASN:O	1:C:1276:GLN:N	2.45	0.50
1:A:268:GLU:O	1:A:272:ILE:HG13	2.12	0.50
1:A:349:PHE:HE2	1:A:1033:VAL:HG12	1.76	0.50
1:A:513:ARG:O	1:A:517:ILE:HD12	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:B:1252:LEU:O	1:B:1256:ILE:HG13	2.12	0.50
1:A:187:THR:HG22	1:A:188:PRO:CD	2.41	0.50
1:A:966:LEU:HB3	1:A:1013:TYR:CZ	2.46	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:146:CYS:O	1:C:147:GLY:C	2.54	0.50
1:C:930:LEU:HD13	1:C:950:ARG:HB2	1.94	0.50
1:A:993:GLU:CD	1:A:994:PRO:HD2	2.37	0.50
1:B:635:GLU:O	1:B:711:ARG:NH2	2.40	0.50
1:B:1054:GLY:O	1:B:1055:ASP:CB	2.59	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:C:993:GLU:CD	1:C:994:PRO:HD2	2.37	0.50
1:A:397:LYS:HD3	1:A:397:LYS:N	2.27	0.50
1:A:1086:SER:O	1:A:1090:LYS:HG2	2.12	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: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
1:A:774:PHE:CB	1:A:837:PHE:HD2	2.25	0.49
1:A:1252:LEU:O	1:A:1256:ILE:HG13	2.12	0.49
1:B:513:ARG:O	1:B:517:ILE:HD12	2.12	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: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:995:THR:O	1:A:996:SER:O	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:ASN:O	1:B:847:GLN:HB2	2.13	0.49
1:B:1050:HIS:HA	1:B:1152:THR:OG1	2.12	0.49
1:C:121:LEU:C	1:C:123:ASN:N	2.69	0.49
1:C:639:ASP:H	1:C:711:ARG:HE	1.60	0.49
1:C:1086:SER:O	1:C:1090:LYS:HG2	2.12	0.49
1:A:146:CYS:O	1:A:147:GLY:C	2.54	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:A:623:MET:HE1	1:A:673:CYS:CB	2.40	0.49
1:B:216:GLN:O	1:B:219:VAL:HG22	2.11	0.49
1:B:1092:LEU:HD13	1:B:1169:LYS:HG2	1.93	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:208:GLN:NE2	1:C:263:GLU:O	2.46	0.49
1:C:552:LEU:C	1:C:552:LEU:HD23	2.38	0.49
1:C:1050:HIS:HA	1:C:1152:THR:OG1	2.13	0.49
1:A:545:ASN:C	1:A:565:GLN:CB	2.85	0.49
1:A:552:LEU:C	1:A:552:LEU:HD23	2.38	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:14:THR:O	1:A:15:ASP:C	2.56	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
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:A:1050:HIS:HA	1:A:1152:THR:OG1	2.13	0.49
1:B:589:SER:O	1:B:592:ARG:HG2	2.13	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:HD3	1:C:397:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:LEU:O	1:C:1256:ILE:HG13	2.12	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:A:533:LYS:HA	1:A:603:MET:HE1	1.95	0.49
1:A:1091:VAL:HA	1:A:1094:GLU:HG3	1.95	0.49
1:B:298:GLN:C	1:B:301:PRO:HD2	2.38	0.49
1:B:930:LEU:HD13	1:B:950:ARG:HB2	1.94	0.49
1:B:1032:HIS:O	1:B:1035:TYR:N	2.37	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: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:816:LEU:CD1	1:B:838:MET:HE1	2.39	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:A:339:LYS:HA	1:A:339:LYS:HD2	1.67	0.48
1:A:1054:GLY:HA3	1:A:1152:THR:HG23	1.95	0.48
1:B:1:MET:O	1:B:5:ILE:HG13	2.13	0.48
1:B:141:LYS:O	1:B:142:GLU:HG3	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:B:1054:GLY:HA3	1:B:1152:THR:HG23	1.95	0.48
1:C:298:GLN:C	1:C:301:PRO:HD2	2.37	0.48
1:C:589:SER:O	1:C:592:ARG:HG2	2.13	0.48
1:C:1054:GLY:O	1:C:1055:ASP:CB	2.59	0.48
1:A:137:LEU:O	1:A:153:GLY:HA3	2.13	0.48
1:B:74:GLN:HA	1:B:77:GLU:OE2	2.14	0.48
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: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:N	1:C:574:TYR:CD2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HB3	1:A:64:ARG:NE	2.28	0.48
1:A:298:GLN:C	1:A:301:PRO:HD2	2.38	0.48
1:A:828:LEU:O	1:A:832:ARG:HG3	2.13	0.48
1:A:1053:LEU:HD21	1:A:1077:ALA:HB2	1.95	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:623:MET:HE1	1:B:673:CYS:CB	2.40	0.48
1:B:732:THR:O	1:B:736:ILE:HG13	2.14	0.48
1:B:1033:VAL:CG2	1:B:1087:GLN:NE2	2.76	0.48
1:C:1022:LYS:HA	1:C:1083:LEU:HD11	1.94	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:A:1054:GLY:O	1:A:1055:ASP:CB	2.59	0.48
1:C:775:THR:O	1:C:779:LYS:HB2	2.13	0.48
1:C:1054:GLY:HA3	1:C:1152:THR:HG23	1.95	0.48
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.96	0.48
1:A:589:SER:O	1:A:592:ARG:HG2	2.13	0.48
1:A:672:HIS:CE1	1:A:861:PRO:HG3	2.49	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:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
1:B:552:LEU:HD23	1:B:552:LEU:C	2.38	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:1:MET:O	1:A:5:ILE:HG13	2.13	0.48
1:A:170:PRO:HG2	1:A:173:TYR:HD1	1.79	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:635:GLU:O	1:A:711:ARG:NH2	2.40	0.48
1:B:14:THR:O	1:B:15:ASP:C	2.56	0.48
1:C:170:PRO:HG2	1:C:173:TYR:HD1	1.79	0.48
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:74:GLN:HA	1:C:77:GLU:OE2	2.13	0.47
1:C:141:LYS:O	1:C:142:GLU:HG3	2.13	0.47
1:C:818:ARG:NH1	1:C:878:ARG:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLU:OE1	1:A:830:VAL:CG2	2.60	0.47
1:B:8:LEU:HD13	1:B:17:LEU:HA	1.96	0.47
1:B:1080:VAL:HG12	1:B:1080:VAL:O	2.14	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:672:HIS:CE1	1:C:861:PRO:CD	2.97	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:A:74:GLN:HA	1:A:77:GLU:OE2	2.13	0.47
1:A:174:MET:HA	1:A:177:LEU:HB2	1.97	0.47
1:A:1080:VAL:HG12	1:A:1080:VAL:O	2.14	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:B:985:LEU:HB3	1:B:1002:MET:HE1	1.96	0.47
1:C:14:THR:O	1:C:15:ASP:C	2.56	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:348:LYS:HD3	1:A:1034:LEU:C	2.38	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: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:C:1207:THR:O	1:C:1211:TYR:HD1	1.97	0.47
1:A:225:SER:O	1:A:226:ARG:C	2.57	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: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
1:C:870:PHE:CD1	1:C:922:TYR:HD2	2.32	0.47
1:C:1029:PHE:CZ	1:C:1087:GLN:HG2	2.48	0.47
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.50	0.47
1:A:838:MET:HA	1:A:838:MET:CE	2.42	0.47
1:A:922:TYR:N	1:A:922:TYR:CD1	2.83	0.47
1:A:1207:THR:O	1:A:1211:TYR:HD1	1.97	0.47
1:B:806:LEU:CD2	1:B:872:ASN:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:VAL:HG21	1:B:929:PHE:CE2	2.50	0.47
1:B:922:TYR:N	1:B:922:TYR:CD1	2.83	0.47
1:B:1145:PHE:HD2	1:B:1146:PHE:CD1	2.33	0.47
1:C:8:LEU:HD13	1:C:17:LEU:HA	1.96	0.47
1:C:225:SER:O	1:C:226:ARG:C	2.57	0.47
1:C:826:GLU:HA	1:C:829:SER:HG	1.79	0.47
1:C:1053:LEU:HD21	1:C:1077:ALA:HB2	1.95	0.47
1:C:1091:VAL:HA	1:C:1094:GLU:HG3	1.95	0.47
1:A:360:VAL:O	1:A:364:ILE:HG13	2.15	0.47
1:A:474:LEU:O	1:A:475:GLN:C	2.57	0.47
1:A:513:ARG:HD3	1:A:546:PHE:CZ	2.50	0.47
1:B:94:MET:HG2	1:B:132:ILE:CD1	2.45	0.47
1:B:383:ILE:C	1:B:383:ILE:HD12	2.40	0.47
1:B:581:THR:HB	1:B:585:GLU:HG3	1.96	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:383:ILE:C	1:A:383:ILE:HD12	2.40	0.47
1:A:598:ALA:HA	1:A:601:ARG:HD3	1.97	0.47
1:B:15:ASP:OD1	1:B:15:ASP:N	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:474:LEU:O	1:C:475:GLN:C	2.57	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:A:94:MET:HG2	1:A:132:ILE:CD1	2.45	0.47
1:A:918:VAL:HG21	1:A:929:PHE:CE2	2.50	0.47
1:A:1145:PHE:HD2	1:A:1146:PHE:CD1	2.33	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: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:C:1080:VAL:HG12	1:C:1080:VAL:O	2.14	0.47
1:A:594:LEU:HG	1:A:604:LEU:HD23	1.96	0.46
1:A:806:LEU:CD2	1:A:872:ASN:HB3	2.44	0.46
1:A:985:LEU:HB3	1:A:1002:MET:HE1	1.96	0.46
1:C:1249:ILE:N	1:C:1250:PRO:CD	2.79	0.46
1:B:225:SER:O	1:B:226:ARG:C	2.57	0.46
1:B:594:LEU:HG	1:B:604:LEU:HD23	1.96	0.46
1:C:383:ILE:HD12	1:C:383:ILE:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:THR:HB	1:C:585:GLU:HG3	1.96	0.46
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:474:LEU:O	1:B:475:GLN:C	2.57	0.46
1:A:801:ASP:OD1	1:A:801:ASP:N	2.47	0.46
1:B:446:ASN:HD22	1:C:489:PHE:HE1	1.62	0.46
1:B:908:LEU:HD22	1:B:980:LEU:HG	1.96	0.46
1:B:911:LEU:CD2	1:B:915:PHE:HE1	2.29	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:359:CYS:SG	1:A:361:SER:HB2	2.55	0.46
1:A:1249:ILE:N	1:A:1250:PRO:CD	2.79	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:870:PHE:CD1	1:A:922:TYR:HD2	2.32	0.46
1:A:911:LEU:CD2	1:A:915:PHE:HE1	2.28	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:C:985:LEU:HB3	1:C:1002:MET:HE1	1.96	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:C:51:LEU:HD13	1:C:96:GLU:HG2	1.98	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: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:C:598:ALA:HA	1:C:601:ARG:HD3	1.97	0.46
1:C:816:LEU:CD1	1:C:838:MET:HE1	2.39	0.46
1:C:1154:LEU:CD1	1:C:1163:LEU:HD12	2.46	0.46
1:A:529:LEU:HA	1:A:532:ARG:NH2	2.31	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:GLN:HB2	1:B:504:PRO:HD3	1.97	0.46
1:B:922:TYR:N	1:B:922:TYR:HD1	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:816:LEU:CD1	1:A:838:MET:HE1	2.39	0.45
1:A:922:TYR:N	1:A:922:TYR:HD1	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: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: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:372:VAL:HG22	1:A:432:ILE:CG2	2.46	0.45
1:A:671:GLN:C	1:A:671:GLN:OE1	2.59	0.45
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.17	0.45
1:B:121:LEU:C	1:B:123:ASN:N	2.69	0.45
1:B:529:LEU:HA	1:B:532:ARG:NH2	2.31	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:C:510:MET:HE1	1:C:574:TYR:HB2	1.98	0.45
1:A:151:LEU:HD12	1:A:156:TYR:CZ	2.52	0.45
1:A:226:ARG:HH12	1:A:282:ASP:CG	2.25	0.45
1:A:1103:LYS:HB3	1:A:1103:LYS:HE2	1.80	0.45
1:B:51:LEU:HD13	1:B:96:GLU:HG2	1.98	0.45
1:B:266:HIS:CE1	1:B:373:HIS:HB3	2.51	0.45
1:B:372:VAL:HG22	1:B:432:ILE:CG2	2.46	0.45
1:B:441:LEU:HD13	1:B:474:LEU:HD22	1.98	0.45
1:B:671:GLN:C	1:B:671:GLN:OE1	2.59	0.45
1:C:59:GLU:O	1:C:63:LEU:HG	2.16	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:675:ALA:O	1:C:679:SER:HB3	2.17	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:B:1154:LEU:CD1	1:B:1163:LEU:HD12	2.46	0.45
1:C:226:ARG:HH12	1:C:282:ASP:CG	2.25	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:671:GLN:OE1	1:A:672:HIS:CD2	2.70	0.45
1:A:1174:LEU:O	1:A:1178:VAL:HG23	2.17	0.45
1:B:708:ILE:HG22	1:B:752:LEU:HD11	1.99	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:C:1174:LEU:O	1:C:1178:VAL:HG23	2.17	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: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: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:B:1249:ILE:N	1:B:1250:PRO:CD	2.79	0.45
1:C:441:LEU:HD13	1:C:474:LEU:HD22	1.99	0.45
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:41:ARG:N	1:C:41:ARG:HD3	2.32	0.44
1:C:120:ARG:HG2	1:C:172:ARG:HH12	1.82	0.44
1:C:671:GLN:OE1	1:C:671:GLN:C	2.60	0.44
1:C:922:TYR:N	1:C:922:TYR:HD1	2.14	0.44
1:A:22:GLN:HG2	1:A:60:ASP:OD2	2.18	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: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
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:B:120:ARG:HG2	1:B:172:ARG:HH12	1.82	0.44
1:B:1144:THR:O	1:B:1148:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:LEU:HD23	1:C:744:LEU:HA	1.87	0.44
1:C:801:ASP:OD1	1:C:801:ASP:N	2.47	0.44
1:C:838:MET:HA	1:C:838:MET:CE	2.42	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: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: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:C:1144:THR:O	1:C:1148:GLU:HG2	2.17	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:208:GLN:NE2	1:C:263:GLU:C	2.66	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:852:LEU:HD13	1:C:858:VAL:HG23	1.98	0.44
1:C:1199:VAL:O	1:C:1202:SER:OG	2.30	0.44
1:A:476:ASN:N	1:A:476:ASN:OD1	2.50	0.44
1:A:644:LEU:HD21	1:A:708:ILE:HD13	1.99	0.44
1:A:1002:MET:HG3	1:A:1031:LEU:CD1	2.47	0.44
1:B:151:LEU:HD12	1:B:156:TYR:CZ	2.52	0.44
1:B:978:ALA:HB1	1:B:1020:PHE:CE1	2.53	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: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:A:1053:LEU:HD11	1:A:1077:ALA:HA	1.99	0.44
1:B:226:ARG:HH12	1:B:282:ASP:CG	2.25	0.44
1:B:1164:LEU:HD22	1:B:1252:LEU:CD1	2.48	0.44
1:B:1260:GLU:HA	1:B: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:542:LEU:HD23	1:A:546:PHE:HE2	1.82	0.44
1:A:1056:ILE:HD12	1:A:1216:TYR:CD1	2.52	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:C:1056:ILE:HD12	1:C:1216:TYR:CD1	2.53	0.44
1:A:226:ARG:H	1:A:226:ARG:HG2	1.54	0.44
1:B:540:LEU:O	1:B:544:LYS:HG3	2.17	0.44
1:B:1002:MET:HG3	1:B:1031:LEU:CD1	2.47	0.44
1:C:466:ILE:O	1:C:469:TYR:HB3	2.18	0.44
1:C:1002:MET:HG3	1:C:1031:LEU:CD1	2.47	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:973:PHE:CD1	1:B:974:ASN:N	2.72	0.43
1:C:973:PHE:CD1	1:C:974:ASN:N	2.72	0.43
1:A:549:LEU:O	1:A:549:LEU:HG	2.19	0.43
1:B:217:LEU:HD23	1:B:217:LEU:O	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: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:O	1:A:217:LEU:HD23	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
1:B:41:ARG:N	1:B:41:ARG:HD3	2.32	0.43
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:671:GLN:CG	1:B:755:TYR:HB2	2.47	0.43
1:C:474:LEU:HB3	1:C:477:CYS:SG	2.58	0.43
1:C:1077:ALA:CB	1:C:1078:PRO:HD3	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:995:THR:HB	1:B:996:SER:H	1.66	0.43
1:C:297:GLN:H	1:C:297:GLN:HG2	1.62	0.43
1:C:341:LEU:HD11	1:C:359:CYS:HB3	2.00	0.43
1:C:1053:LEU:HD11	1:C:1077:ALA:HA	1.99	0.43
1:A:211:PRO:N	1:A:212:PRO:HD2	2.33	0.43
1:A:1014:SER:HB3	1:A:1070:VAL:CG1	2.35	0.43
1:B:211:PRO:N	1:B:212:PRO:HD2	2.33	0.43
1:B:447:ARG:HG3	1:C:489:PHE:HE2	1.84	0.43
1:B:667:LEU:HB3	1:B:751:VAL:HG11	2.00	0.43
1:C:706:GLU:O	1:C:709:THR:HB	2.19	0.43
1:C:1164:LEU:HD22	1:C:1252:LEU:CD1	2.48	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:CD1	1:C:762:PHE:N	2.87	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:A:1156:SER:HA	1:A:1160:VAL:HG21	2.01	0.43
1:B:650:VAL:HG13	1:B:657:ILE:HG23	2.00	0.43
1:B:804:LEU:O	1:B:848:LYS:NZ	2.51	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: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: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: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
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:O	1:C:549:LEU:HG	2.18	0.43
1:C:978:ALA:HB1	1:C:1020:PHE:CE1	2.53	0.43
1:A:706:GLU:O	1:A:709:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:PHE:CD1	1:A:762:PHE:N	2.87	0.43
1:A:1260:GLU:HA	1:A:1263:LEU:HD12	2.00	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:519:VAL:HG12	1:A:520:LEU:N	2.34	0.43
1:A:597:GLN:H	1:A:597:GLN:HG2	1.44	0.43
1:A:821:ILE:H	1:A:821:ILE:HG13	1.52	0.43
1:A:1145:PHE:CD2	1:A:1146:PHE:CD1	3.07	0.43
1:B:519:VAL:HG12	1:B:520:LEU:N	2.34	0.43
1:B:623:MET:HE3	1:B:698:TYR:OH	2.19	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:C:623:MET:HE1	1:C:673:CYS:CB	2.40	0.43
1:A:3:LEU:HD23	1:A:6:LEU:HD12	2.01	0.42
1:A:185:CYS:O	1:A:186:LEU:HD23	2.19	0.42
1:A:804:LEU:O	1:A:848:LYS:NZ	2.51	0.42
1:A:957:GLN:HG3	1:A:960:ARG:NH2	2.34	0.42
1:B:502:VAL:O	1:B:502:VAL:HG13	2.19	0.42
1:B:549:LEU:O	1:B:549:LEU:HG	2.19	0.42
1:C:60:ASP:O	1:C:64:ARG:HB2	2.19	0.42
1:C:1145:PHE:CD2	1:C:1146:PHE:CD1	3.07	0.42
1:A:60:ASP:O	1:A:64:ARG:HB2	2.19	0.42
1:A:623:MET:HE3	1:A:698:TYR:OH	2.20	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:B:1156:SER:HA	1:B:1160:VAL:HG21	2.01	0.42
1:C:165:CYS:HB3	1:C:197:LYS:HE3	2.01	0.42
1:C:382:LEU:HD22	1:C:425:ILE:HG23	2.00	0.42
1:C:1103:LYS:HB3	1:C:1103:LYS:HE2	1.80	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: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:C:65:ARG:HD3	1:C:100:PHE:CZ	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:VAL:O	1:A:502:VAL:HG13	2.19	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: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:885:THR:O	1:C:886:SER:HB2	2.20	0.42
1:C:957:GLN:HG3	1:C:960:ARG:NH2	2.34	0.42
1:C:1005:TRP:O	1:C:1009:ILE:HG13	2.19	0.42
1:A:860:GLY:HA3	1:A:861:PRO:HD2	1.77	0.42
1:A:952:SER:HB3	1:A:998:GLN:HB3	2.00	0.42
1:A:954:GLN:O	1:A:958:PHE:HD1	2.03	0.42
1:A:1249:ILE:H	1:A:1249:ILE:HG13	1.68	0.42
1:C:517:ILE:HG21	1:C:577:VAL:CG1	2.49	0.42
1:C:623:MET:HE3	1:C:698:TYR:OH	2.19	0.42
1:C:634:TYR:CG	1:C:704:MET:HE3	2.54	0.42
1:C:954:GLN:O	1:C:958:PHE:HD1	2.03	0.42
1:A:41:ARG:N	1:A:41:ARG:HD3	2.32	0.42
1:A:221:SER:O	1:A:224:GLY:N	2.51	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:B:165:CYS:HB3	1:B:197:LYS:HE3	2.01	0.42
1:B:476:ASN:N	1:B:476:ASN:OD1	2.50	0.42
1:B:536:VAL:CG1	1:B:603:MET:HE3	2.43	0.42
1:B:952:SER:HB3	1:B:998:GLN:HB3	2.01	0.42
1:A:15:ASP:OD1	1:A:15:ASP:N	2.47	0.42
1:A:242:LYS:HA	1:A:245:ARG:HE	1.84	0.42
1:A:634:TYR:CG	1:A:704:MET:HE3	2.54	0.42
1:A:760:SER:HB2	1:A:766:LYS:HZ1	1.84	0.42
1:A:1182:LEU:O	1:A:1186:GLN:HG3	2.19	0.42
1:B:545:ASN:C	1:B:546:PHE:CG	2.98	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
1:C:456:ILE:O	1:C:456:ILE:CG2	2.67	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: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:HD23	1:B:1053:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1158:SER:O	1:B:1161:ASP:N	2.53	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:C:1249:ILE:H	1:C:1249:ILE:HG13	1.68	0.42
1:A:65:ARG:HD3	1:A:100:PHE:CZ	2.55	0.42
1:A:565:GLN:H	1:A:565:GLN:HG2	1.54	0.42
1:B:573:ARG:HE	1:B:573:ARG:HB2	1.70	0.42
1:B:834:SER:OG	1:B:837:PHE:HB3	2.20	0.42
1:B:1182:LEU:O	1:B:1186:GLN:HG3	2.20	0.42
1:C:834:SER:OG	1:C:837:PHE:HB3	2.20	0.42
1:C:1182:LEU:O	1:C:1186:GLN:HG3	2.19	0.42
1:A:368:VAL:HG11	1:A:428:GLU:HB3	2.02	0.41
1:B:297:GLN:H	1:B:297:GLN:HG2	1.62	0.41
1:B:368:VAL:HG11	1:B:428:GLU:HB3	2.02	0.41
1:B:667:LEU:HD23	1:B:667:LEU:HA	1.80	0.41
1:C:226:ARG:H	1:C:226:ARG:HG2	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:329:LEU:HD12	1:A:329:LEU:C	2.45	0.41
1:A:694:GLU:O	1:A:698:TYR:HD1	2.03	0.41
1:A:995:THR:HB	1:A:996:SER:H	1.66	0.41
1:B:90:ILE:H	1:B:90:ILE:HG13	1.72	0.41
1:B:996:SER:HB3	1:B:999:PHE:HB3	2.03	0.41
1:B:1005:TRP:CZ2	1:B:1009:ILE:HD11	2.55	0.41
1:C:329:LEU:HD12	1:C:329:LEU:C	2.45	0.41
1:C:763:SER:O	1:C:767:PHE:CD1	2.72	0.41
1:C:996:SER:HB3	1:C:999:PHE:HB3	2.02	0.41
1:C:1150:VAL:O	1:C:1213:PHE:HD1	2.03	0.41
1:C:1156:SER:HA	1:C:1160:VAL:HG21	2.01	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:329:LEU:C	1:B:329:LEU:HD12	2.45	0.41
1:B:634:TYR:CG	1:B:704:MET:HE3	2.55	0.41
1:B:672:HIS:HE1	1:B:805:SER:HB3	1.85	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:C:1042:LEU:O	1:C:1145:PHE:HD1	2.04	0.41
1:A:96:GLU:OE1	1:A:96:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:339:LYS:HD2	1:B:339:LYS:HA	1.67	0.41
1:C:502:VAL:O	1:C:502:VAL:HG13	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: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: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:C:90:ILE:O	1:C:94:MET:HG3	2.21	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: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:A:623:MET:HE3	1:A:698:TYR:CE2	2.55	0.41
1:A:1022:LYS:HA	1:A:1083:LEU:HD11	2.03	0.41
1:B:486:TYR:CE2	1:C:449:VAL:CG2	3.03	0.41
1:B:814:THR:OG1	1:B:879:VAL:HG21	2.20	0.41
1:C:169:TRP:CZ3	1:C:177:LEU:HB3	2.56	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
1:C:1005:TRP:CE2	1:C:1009:ILE:HD11	2.56	0.41
1:A:771:LEU:CB	1:A:830:VAL:HG12	2.46	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: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:C:503:GLN:HG2	1:C:541:LEU:HD21	2.03	0.41
1:C:623:MET:HE3	1:C:698:TYR:CE2	2.55	0.41
1:C:1029:PHE:CG	1:C:1087:GLN:CD	2.99	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:HD12	1:B:329:LEU:O	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:95:LEU:O	1:C:98:HIS:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:VAL:HG11	1:C:428:GLU:HB3	2.02	0.41
1:C:1042:LEU:CD2	1:C: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:667:LEU:HA	1:A:667:LEU:HD23	1.80	0.41
1:A:931:GLN:HG2	1:A:950:ARG:NH1	2.36	0.41
1:A:1042:LEU:CD2	1:A:1084:VAL:HG12	2.51	0.41
1:A:1272:VAL:HG12	1:A:1273:ASN:N	2.36	0.41
1:B:169:TRP:CZ3	1:B:177:LEU:HB3	2.56	0.41
1:B:350:LEU:HG	1:B:1094:GLU:OE1	2.21	0.41
1:B:391:ASP:OD2	1:B:447:ARG:NH1	2.54	0.41
1:B:529:LEU:HD22	1:B:533:LYS:HE3	2.02	0.41
1:B:664:ASP:OD1	1:B:664:ASP:N	2.54	0.41
1:B:1150:VAL:O	1:B:1213:PHE:HD1	2.03	0.41
1:C:113:VAL:HG22	1:C:164:LEU:HG	2.03	0.41
1:C:152:ASN:HB2	1:C:154:GLU:HG2	2.03	0.41
1:C:201:MET:O	1:C:202:PHE:C	2.64	0.41
1:C:329:LEU:HD12	1:C:329:LEU:O	2.21	0.41
1:C:372:VAL:HG22	1:C:432:ILE:HG21	2.03	0.41
1:C:391:ASP:OD2	1:C:447:ARG:NH1	2.54	0.41
1:C:1158:SER:O	1:C:1161:ASP:N	2.53	0.41
1:A:127:LEU:HB3	1:A:180:VAL:HG21	2.03	0.41
1:A:1005:TRP:CZ2	1:A:1009:ILE:HD11	2.56	0.41
1:B:91:GLY:O	1:B:95:LEU:HG	2.21	0.41
1:B:95:LEU:O	1:B:98:HIS:CE1	2.74	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: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:C:1136:VAL:CG1	1:C:1198:LEU:HD12	2.51	0.41
1:A:68:ILE:H	1:A:68:ILE:HG13	1.73	0.40
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: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:B:1272:VAL:HG12	1:B:1273:ASN:N	2.36	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:C:1032:HIS:O	1:C:1035:TYR:N	2.37	0.40
1:A:24:LEU:C	1:A:26:ASP:H	2.29	0.40
1:A:169:TRP:CZ3	1:A:177:LEU:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:GLY:O	1:C:95:LEU:HG	2.21	0.40
1:C:430:PHE:HB2	1:C:440:ILE:HD12	2.03	0.40
1:C:565:GLN:H	1:C:565:GLN:HG2	1.54	0.40
1:A:383:ILE:HG13	1:A:384:GLU:N	2.37	0.40
1:A:1005:TRP:CE2	1:A:1009:ILE:HD11	2.56	0.40
1:A:1150:VAL:HG22	1:A:1167:LEU:HD11	2.04	0.40
1:B:24:LEU:C	1:B:26:ASP:H	2.30	0.40
1:B:348:LYS:HD2	1:B:348:LYS:HA	1.97	0.40
1:B:503:GLN:HG2	1:B:541:LEU:HD21	2.03	0.40
1:B:817:PHE:HB3	1:B:882:TRP:CE3	2.56	0.40
1:C:542:LEU:O	1:C:546:PHE:CD2	2.64	0.40
1:C:667:LEU:HD23	1:C:667:LEU:HA	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:24:LEU:C	1:C:26:ASP:H	2.30	0.40
1:C:177:LEU:O	1:C:180:VAL:HB	2.21	0.40
1:C:627:PHE:CE2	1:C:631:LYS:HD2	2.56	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:A:36:GLN:HG3	1:A:85:VAL:HG11	2.04	0.40
1:A:834:SER:OG	1:A:837:PHE:HB3	2.20	0.40
1:A:1045:LEU:O	1:A:1049:ILE:HG13	2.22	0.40
1:B:76:VAL:HG11	1:B:90:ILE:HD11	2.03	0.40
1:B:95:LEU:HA	1:B:98:HIS:HE1	1.87	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:913:LYS:O	1:B:917:VAL:HG23	2.22	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:C:95:LEU:HA	1:C:98:HIS:HE1	1.87	0.40
1:C:774:PHE:HE2	1:C:836:GLU:HG3	1.86	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%)	30	67
1	B	1099/1308 (84%)	1016 (92%)	80 (7%)	3 (0%)	36	72
1	C	1101/1308 (84%)	1019 (93%)	79 (7%)	3 (0%)	36	72
All	All	3303/3924 (84%)	3054 (92%)	239 (7%)	10 (0%)	36	72

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

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Mol	Chain	Res	Type
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%)	895 (87%)	134 (13%)	4	15
1	B	1029/1188 (87%)	894 (87%)	135 (13%)	4	15
1	C	1029/1188 (87%)	896 (87%)	133 (13%)	4	15
All	All	3087/3564 (87%)	2685 (87%)	402 (13%)	4	15

All (402) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	19	GLU
1	A	29	LEU
1	A	36	GLN
1	A	43	VAL
1	A	54	SER
1	A	71	CYS
1	A	81	LEU
1	A	96	GLU
1	A	97	VAL
1	A	99	HIS
1	A	118	GLU
1	A	119	ASP
1	A	130	LEU
1	A	164	LEU
1	A	169	TRP
1	A	177	LEU
1	A	183	ASP
1	A	200	THR

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Mol	Chain	Res	Type
1	A	203	SER
1	A	208	GLN
1	A	213	LEU
1	A	240	LEU
1	A	247	GLU
1	A	262	ASP
1	A	264	LEU
1	A	273	LEU
1	A	275	ILE
1	A	277	PHE
1	A	285	LEU
1	A	288	GLU
1	A	297	GLN
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	352	THR
1	A	360	VAL
1	A	376	ASP
1	A	377	HIS
1	A	378	VAL
1	A	383	ILE
1	A	396	LYS
1	A	398	ILE
1	A	413	MET
1	A	414	THR
1	A	421	LEU
1	A	427	LEU
1	A	438	GLN
1	A	443	GLN
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	483	THR

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Mol	Chain	Res	Type
1	A	488	THR
1	A	493	GLN
1	A	496	GLN
1	A	502	VAL
1	A	515	SER
1	A	517	ILE
1	A	519	VAL
1	A	529	LEU
1	A	530	ASP
1	A	548	VAL
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	600	ILE
1	A	612	LEU
1	A	639	ASP
1	A	651	LEU
1	A	659	LEU
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	766	LYS
1	A	768	GLU
1	A	771	LEU
1	A	801	ASP
1	A	803	LEU
1	A	806	LEU
1	A	812	LEU
1	A	824	HIS
1	A	838	MET
1	A	846	LEU

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Mol	Chain	Res	Type
1	A	853	ILE
1	A	858	VAL
1	A	864	GLN
1	A	911	LEU
1	A	919	LEU
1	A	949	GLN
1	A	954	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	1009	ILE
1	A	1013	TYR
1	A	1015	GLN
1	A	1024	LEU
1	A	1049	ILE
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	1154	LEU
1	A	1183	GLN
1	A	1184	VAL
1	A	1194	THR
1	A	1249	ILE
1	A	1274	LEU
1	A	1275	MET
1	B	15	ASP
1	B	19	GLU
1	B	29	LEU
1	B	36	GLN
1	B	43	VAL
1	B	54	SER
1	B	71	CYS
1	B	81	LEU
1	B	96	GLU
1	B	97	VAL
1	B	99	HIS

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Mol	Chain	Res	Type
1	B	118	GLU
1	B	119	ASP
1	B	130	LEU
1	B	164	LEU
1	B	169	TRP
1	B	177	LEU
1	B	183	ASP
1	B	200	THR
1	B	203	SER
1	B	208	GLN
1	B	213	LEU
1	B	240	LEU
1	B	247	GLU
1	B	262	ASP
1	B	264	LEU
1	B	273	LEU
1	B	275	ILE
1	B	277	PHE
1	B	285	LEU
1	B	288	GLU
1	B	297	GLN
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	352	THR
1	B	360	VAL
1	B	376	ASP
1	B	377	HIS
1	B	378	VAL
1	B	383	ILE
1	B	396	LYS
1	B	398	ILE
1	B	413	MET
1	B	414	THR
1	B	421	LEU
1	B	427	LEU
1	B	438	GLN
1	B	443	GLN
1	B	450	THR

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Mol	Chain	Res	Type
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	483	THR
1	B	488	THR
1	B	493	GLN
1	B	496	GLN
1	B	498	LEU
1	B	502	VAL
1	B	515	SER
1	B	517	ILE
1	B	519	VAL
1	B	529	LEU
1	B	530	ASP
1	B	548	VAL
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	600	ILE
1	B	612	LEU
1	B	639	ASP
1	B	651	LEU
1	B	659	LEU
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	766	LYS

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Mol	Chain	Res	Type
1	B	768	GLU
1	B	771	LEU
1	B	801	ASP
1	B	803	LEU
1	B	806	LEU
1	B	812	LEU
1	B	824	HIS
1	B	838	MET
1	B	846	LEU
1	B	853	ILE
1	B	858	VAL
1	B	864	GLN
1	B	911	LEU
1	B	919	LEU
1	B	949	GLN
1	B	954	GLN
1	B	965	LEU
1	B	980	LEU
1	B	981	LEU
1	B	982	ILE
1	B	1001	GLN
1	B	1003	LEU
1	B	1009	ILE
1	B	1013	TYR
1	B	1015	GLN
1	B	1024	LEU
1	B	1049	ILE
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	1154	LEU
1	B	1183	GLN
1	B	1184	VAL
1	B	1194	THR
1	B	1249	ILE
1	B	1274	LEU
1	B	1275	MET
1	C	15	ASP
1	C	19	GLU

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Mol	Chain	Res	Type
1	C	29	LEU
1	C	36	GLN
1	C	43	VAL
1	C	54	SER
1	C	71	CYS
1	C	81	LEU
1	C	96	GLU
1	C	97	VAL
1	C	99	HIS
1	C	118	GLU
1	C	119	ASP
1	C	130	LEU
1	C	164	LEU
1	C	169	TRP
1	C	177	LEU
1	C	183	ASP
1	C	200	THR
1	C	203	SER
1	C	208	GLN
1	C	213	LEU
1	C	240	LEU
1	C	247	GLU
1	C	262	ASP
1	C	264	LEU
1	C	273	LEU
1	C	275	ILE
1	C	277	PHE
1	C	285	LEU
1	C	288	GLU
1	C	297	GLN
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	360	VAL
1	C	376	ASP
1	C	377	HIS
1	C	378	VAL
1	C	383	ILE
1	C	396	LYS

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Mol	Chain	Res	Type
1	C	398	ILE
1	C	413	MET
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	483	THR
1	C	488	THR
1	C	493	GLN
1	C	496	GLN
1	C	502	VAL
1	C	515	SER
1	C	517	ILE
1	C	519	VAL
1	C	529	LEU
1	C	530	ASP
1	C	548	VAL
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
1	C	597	GLN
1	C	600	ILE
1	C	612	LEU
1	C	639	ASP
1	C	651	LEU
1	C	659	LEU
1	C	663	LEU
1	C	666	LEU
1	C	699	SER

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Mol	Chain	Res	Type
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	766	LYS
1	C	768	GLU
1	C	771	LEU
1	C	801	ASP
1	C	803	LEU
1	C	806	LEU
1	C	812	LEU
1	C	824	HIS
1	C	838	MET
1	C	846	LEU
1	C	853	ILE
1	C	858	VAL
1	C	864	GLN
1	C	911	LEU
1	C	919	LEU
1	C	949	GLN
1	C	954	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	1009	ILE
1	C	1013	TYR
1	C	1015	GLN
1	C	1024	LEU
1	C	1049	ILE
1	C	1050	HIS
1	C	1056	ILE
1	C	1071	VAL
1	C	1084	VAL
1	C	1105	SER
1	C	1142	LEU
1	C	1154	LEU
1	C	1183	GLN

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Mol	Chain	Res	Type
1	C	1184	VAL
1	C	1194	THR
1	C	1249	ILE
1	C	1274	LEU
1	C	1275	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	216	GLN
1	A	298	GLN
1	A	377	HIS
1	A	565	GLN
1	A	571	HIS
1	A	597	GLN
1	A	672	HIS
1	A	756	ASN
1	A	761	ASN
1	A	847	GLN
1	A	959	GLN
1	A	1251	ASN
1	B	208	GLN
1	B	274	HIS
1	B	298	GLN
1	B	351	GLN
1	B	377	HIS
1	B	565	GLN
1	B	571	HIS
1	B	597	GLN
1	B	672	HIS
1	B	756	ASN
1	B	761	ASN
1	B	847	GLN
1	B	959	GLN
1	B	1087	GLN
1	B	1251	ASN
1	B	1277	HIS
1	C	208	GLN
1	C	216	GLN
1	C	298	GLN
1	C	377	HIS

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Mol	Chain	Res	Type
1	C	565	GLN
1	C	571	HIS
1	C	597	GLN
1	C	672	HIS
1	C	756	ASN
1	C	761	ASN
1	C	847	GLN
1	C	959	GLN
1	C	1251	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	0.12	56 (4%) 34 35	267, 382, 546, 649	0
1	B	1131/1308 (86%)	0.12	41 (3%) 46 43	285, 384, 602, 757	0
1	C	1131/1308 (86%)	0.13	49 (4%) 40 40	302, 421, 620, 719	0
All	All	3393/3924 (86%)	0.12	146 (4%) 40 40	267, 397, 598, 757	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	864	GLN	9.9
1	B	32	LEU	7.9
1	B	299	GLY	7.5
1	C	248	GLN	7.2
1	C	572	SER	6.5
1	C	869	ILE	5.8
1	B	856	GLY	5.7
1	B	302	SER	5.7
1	B	31	SER	5.3
1	B	258	THR	5.1
1	B	28	ASP	4.9
1	C	320	GLN	4.6
1	C	321	ARG	4.6
1	C	242	LYS	4.6
1	C	438	GLN	4.5
1	A	451	ARG	4.5
1	A	480	VAL	4.4
1	A	1210	CYS	4.4
1	A	1249	ILE	4.4
1	C	863	GLY	4.3
1	A	483	THR	4.3
1	A	1253	VAL	4.1
1	C	393	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1211	TYR	4.1
1	A	372	VAL	4.0
1	A	577	VAL	4.0
1	C	862	ASP	3.9
1	C	922	TYR	3.9
1	C	865	ASN	3.9
1	A	516	LEU	3.8
1	A	575	SER	3.8
1	C	1006	THR	3.7
1	C	397	LYS	3.7
1	A	369	ARG	3.7
1	A	81	LEU	3.6
1	B	300	ASP	3.6
1	C	28	ASP	3.6
1	B	863	GLY	3.6
1	C	239	GLU	3.5
1	B	767	PHE	3.5
1	A	738	ASN	3.4
1	B	738	ASN	3.4
1	B	244	HIS	3.4
1	C	442	GLU	3.4
1	A	974	ASN	3.4
1	B	573	ARG	3.3
1	A	32	LEU	3.3
1	C	856	GLY	3.3
1	C	434	GLU	3.1
1	C	300	ASP	3.1
1	B	46	LEU	3.1
1	B	572	SER	3.1
1	C	864	GLN	3.1
1	B	830	VAL	3.0
1	A	485	ASP	3.0
1	B	35	ASN	3.0
1	A	1041	LEU	2.9
1	A	486	TYR	2.9
1	B	1280	LEU	2.8
1	C	395	PRO	2.8
1	B	1249	ILE	2.8
1	A	82	GLN	2.8
1	C	244	HIS	2.8
1	C	246	GLU	2.8
1	A	371	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	283	CYS	2.7
1	A	373	HIS	2.7
1	B	857	HIS	2.7
1	A	298	GLN	2.7
1	C	653	GLN	2.7
1	A	345	GLN	2.7
1	A	956	ARG	2.7
1	B	646	LEU	2.7
1	B	525	PHE	2.7
1	C	322	PHE	2.7
1	A	869	ILE	2.6
1	A	1256	ILE	2.6
1	B	946	THR	2.6
1	B	950	ARG	2.6
1	C	866	PRO	2.6
1	A	1045	LEU	2.6
1	B	612	LEU	2.6
1	C	170	PRO	2.6
1	C	597	GLN	2.6
1	B	698	TYR	2.6
1	B	865	ASN	2.5
1	B	303	LYS	2.5
1	A	58	GLU	2.5
1	A	606	ASP	2.5
1	C	307	PRO	2.5
1	C	358	THR	2.5
1	A	281	LEU	2.5
1	B	827	SER	2.5
1	A	1212	SER	2.4
1	B	1191	ILE	2.4
1	A	1280	LEU	2.4
1	A	693	GLU	2.4
1	B	384	GLU	2.4
1	B	866	PRO	2.4
1	B	33	LEU	2.4
1	A	296	GLY	2.4
1	C	809	VAL	2.4
1	B	1044	ASP	2.4
1	B	737	LYS	2.4
1	A	977	GLU	2.3
1	C	225	SER	2.3
1	A	513	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	576	ALA	2.3
1	A	584	LEU	2.3
1	C	31	SER	2.3
1	C	577	VAL	2.3
1	A	1214	ILE	2.3
1	C	50	VAL	2.2
1	B	357	ARG	2.2
1	A	608	PHE	2.2
1	B	606	ASP	2.2
1	A	831	LEU	2.2
1	A	61	GLY	2.2
1	A	362	THR	2.2
1	A	578	ALA	2.2
1	C	1010	CYS	2.2
1	C	138	ALA	2.2
1	A	616	SER	2.2
1	C	525	PHE	2.2
1	B	1210	CYS	2.2
1	A	186	LEU	2.1
1	B	49	ALA	2.1
1	A	783	ILE	2.1
1	C	319	ILE	2.1
1	A	424	ASN	2.1
1	B	170	PRO	2.1
1	C	1048	ASP	2.1
1	C	478	SER	2.1
1	C	56	CYS	2.1
1	A	857	HIS	2.1
1	A	705	LEU	2.1
1	C	654	GLY	2.1
1	C	1003	LEU	2.1
1	C	656	GLN	2.1
1	C	247	GLU	2.1
1	C	207	LEU	2.0
1	A	1277	HIS	2.0
1	A	481	THR	2.0
1	A	321	ARG	2.0
1	A	1207	THR	2.0
1	A	743	CYS	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 oligosaccharides 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.