



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:48 PM UTC

PDB ID : 5YIL / pdb_00005yil
Title : Hoisting-loop in bacterial multidrug exporter AcrB is a highly flexible hinge that enables the large motion of the subdomains
Authors : Zwama, M.; Sakurai, K.; Hayashi, K.; Nakashima, R.; Kitagawa, K.; Nishino, K.; Yamaguchi, A.
Deposited on : 2017-10-05
Resolution : 3.00 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

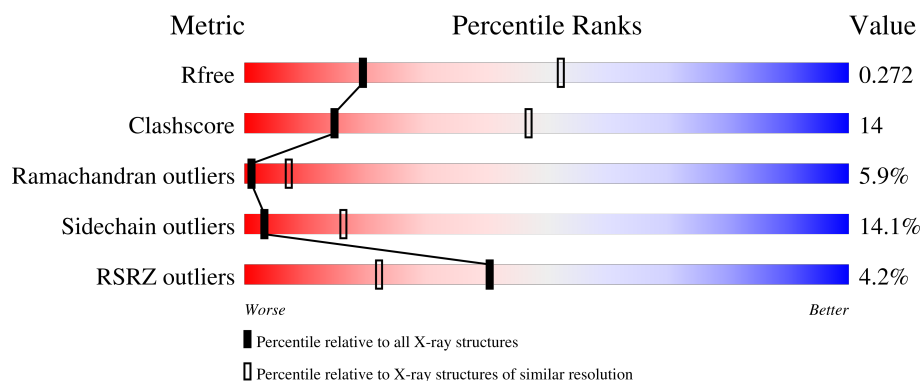
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1050	3% 69% 26% ..
1	B	1050	4% 63% 30% 5% ..
1	C	1050	6% 55% 35% 7% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23566 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1041	Total	C	N	O	S	0	0	0
			7918	5091	1310	1473	44			
1	B	1030	Total	C	N	O	S	0	0	0
			7824	5037	1290	1453	44			
1	C	1030	Total	C	N	O	S	0	0	0
			7824	5037	1290	1453	44			

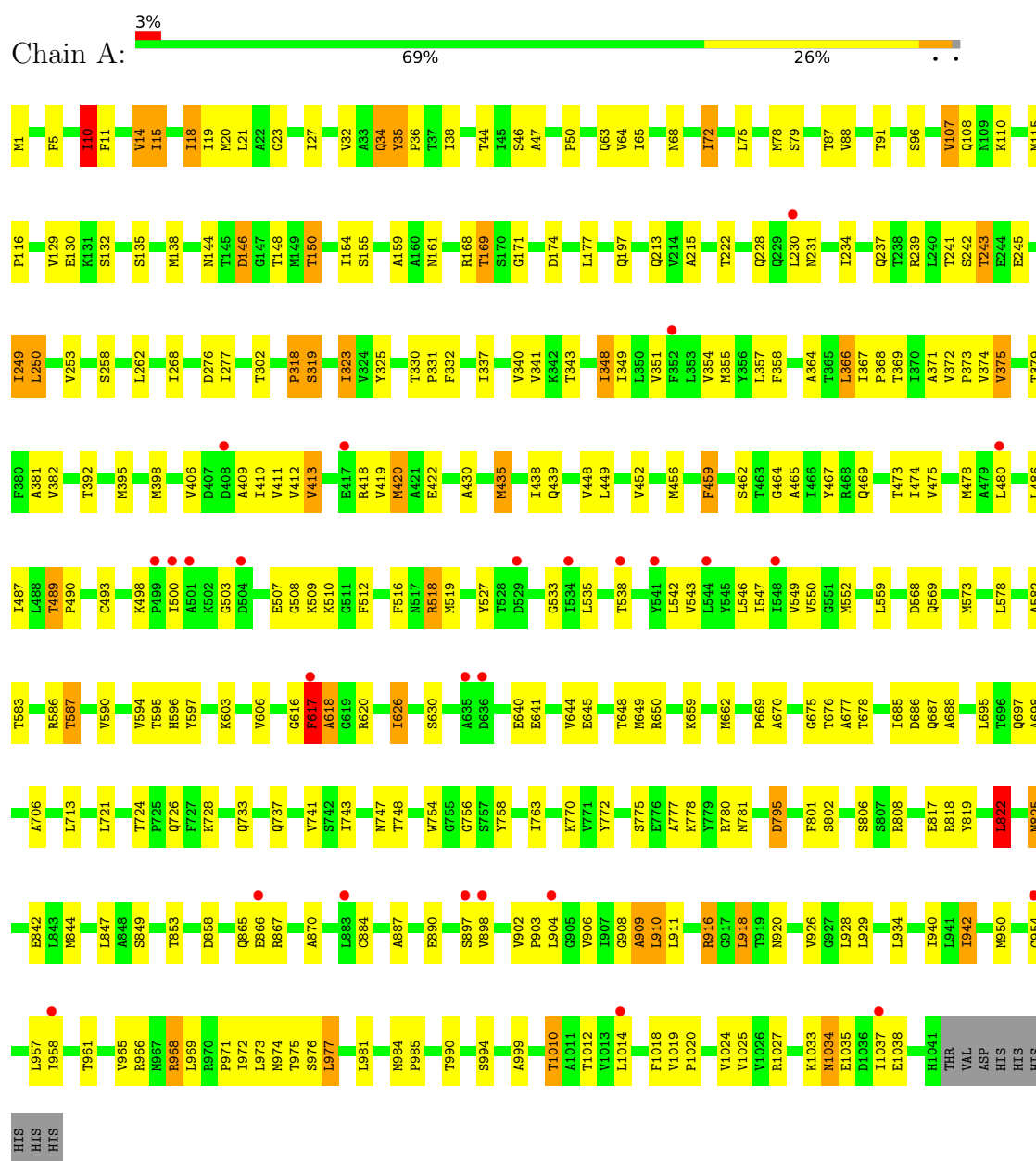
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P31224
A	1048	HIS	-	expression tag	UNP P31224
A	1049	HIS	-	expression tag	UNP P31224
A	1050	HIS	-	expression tag	UNP P31224
B	1047	HIS	-	expression tag	UNP P31224
B	1048	HIS	-	expression tag	UNP P31224
B	1049	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
C	1047	HIS	-	expression tag	UNP P31224
C	1048	HIS	-	expression tag	UNP P31224
C	1049	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224

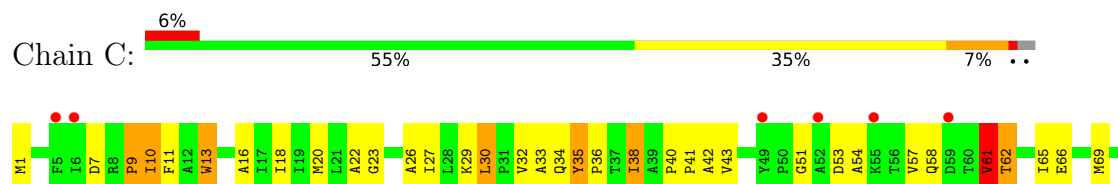
3 Residue-property plots

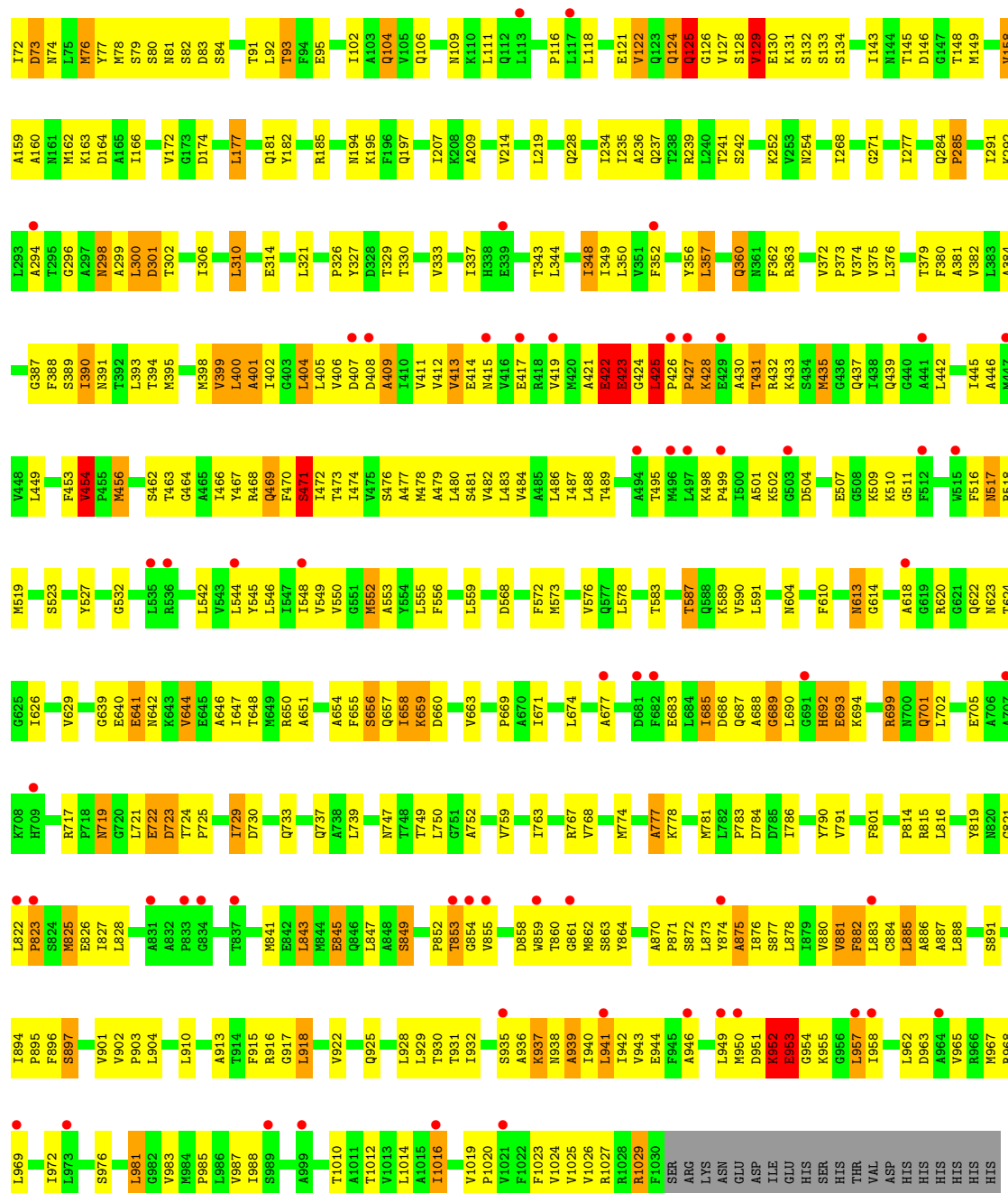
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.98Å 139.81Å 285.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00 100.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (100.00-3.00) 94.5 (100.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.224 , 0.273 0.227 , 0.272	Depositor DCC
R_{free} test set	5112 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23566	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.99	4/8070 (0.0%)	1.12	17/10957 (0.2%)
1	B	0.92	1/7974 (0.0%)	1.12	16/10829 (0.1%)
1	C	1.00	0/7974	1.15	20/10829 (0.2%)
All	All	0.97	5/24018 (0.0%)	1.13	53/32615 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	LEU	C-O	-6.12	1.18	1.24
1	A	150	THR	N-CA	-5.85	1.39	1.46
1	B	600	THR	CA-C	5.57	1.57	1.52
1	A	47	ALA	CA-C	-5.36	1.46	1.52
1	A	819	TYR	C-O	-5.02	1.18	1.24

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	LYS	N-CA-C	-8.06	96.18	108.67
1	A	675	GLY	N-CA-C	7.84	120.04	112.04
1	C	104	GLN	N-CA-C	-7.71	102.00	111.40
1	B	382	VAL	N-CA-C	-7.40	103.31	110.42
1	A	756	GLY	N-CA-C	-7.17	104.26	112.29
1	C	360	GLN	N-CA-C	7.13	121.31	112.47
1	B	72	ILE	N-CA-C	-6.99	98.29	108.71
1	C	132	SER	N-CA-C	6.99	121.42	110.17
1	C	507	GLU	N-CA-C	6.78	121.30	112.89
1	C	128	SER	CB-CA-C	-6.76	97.73	110.51
1	B	608	SER	N-CA-C	6.68	119.22	109.07
1	B	118	LEU	CA-C-N	-6.37	114.07	120.31
1	B	118	LEU	C-N-CA	-6.37	114.07	120.31
1	B	404	LEU	N-CA-C	-6.30	103.71	111.33
1	C	163	LYS	N-CA-C	6.27	118.12	111.28
1	C	897	SER	N-CA-C	6.24	117.78	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ILE	CB-CA-C	-6.11	104.14	111.97
1	B	180	SER	N-CA-C	6.06	118.04	107.49
1	C	164	ASP	N-CA-C	-6.01	104.35	111.03
1	C	163	LYS	CB-CA-C	-5.97	100.87	110.79
1	B	273	GLU	N-CA-C	-5.91	104.76	111.14
1	A	65	ILE	N-CA-CB	5.90	117.45	110.55
1	A	817	GLU	CB-CA-C	5.86	120.25	109.71
1	C	35	TYR	CA-C-N	-5.74	112.66	119.84
1	C	35	TYR	C-N-CA	-5.74	112.66	119.84
1	B	644	VAL	N-CA-C	5.74	121.27	109.34
1	A	169	THR	N-CA-CB	5.66	119.09	109.87
1	B	907	ILE	N-CA-CB	5.64	116.77	110.62
1	A	34	GLN	N-CA-C	-5.62	101.15	109.86
1	C	658	ILE	N-CA-C	5.49	116.88	108.71
1	C	589	LYS	N-CA-C	-5.45	105.23	111.07
1	A	357	LEU	N-CA-C	-5.40	107.25	112.97
1	A	276	ASP	N-CA-C	5.37	117.83	111.33
1	A	10	ILE	N-CA-C	-5.33	106.60	111.67
1	A	1025	VAL	N-CA-C	5.31	115.52	110.53
1	B	894	ILE	CA-C-N	5.30	126.47	119.84
1	B	894	ILE	C-N-CA	5.30	126.47	119.84
1	B	208	LYS	N-CA-C	-5.30	104.29	111.55
1	C	133	SER	N-CA-C	-5.26	101.44	109.65
1	B	351	VAL	N-CA-C	-5.21	107.68	111.90
1	A	617	PHE	N-CA-C	-5.20	100.03	108.41
1	B	754	TRP	N-CA-C	5.16	119.28	112.89
1	C	777	ALA	N-CA-C	5.15	117.30	111.02
1	A	748	THR	N-CA-C	5.15	117.56	111.33
1	C	330	THR	CA-C-N	-5.13	113.75	119.19
1	C	330	THR	C-N-CA	-5.13	113.75	119.19
1	B	688	ALA	N-CA-C	5.09	116.97	110.61
1	A	1012	THR	N-CA-C	-5.07	105.33	112.12
1	A	772	TYR	N-CA-C	5.05	117.72	109.59
1	A	146	ASP	N-CA-C	5.03	118.73	112.59
1	C	294	ALA	N-CA-C	5.02	118.55	112.93
1	C	719	ASN	N-CA-C	-5.02	103.78	110.55
1	A	64	VAL	N-CA-CB	5.01	117.35	110.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7918	0	8059	140	0
1	B	7824	0	7976	238	0
1	C	7824	0	7976	300	0
All	All	23566	0	24011	654	0

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 14.

All (654) 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:B:344:LEU:HD23	1:B:402:ILE:CD1	1.46	1.45
1:B:449:LEU:HB3	1:B:478:MET:CE	1.52	1.37
1:B:344:LEU:CD2	1:B:402:ILE:CD1	2.18	1.20
1:B:344:LEU:CD2	1:B:402:ILE:HD11	1.79	1.12
1:B:449:LEU:CB	1:B:478:MET:HE2	1.79	1.11
1:C:568:ASP:OD1	1:C:644:VAL:HG23	1.52	1.07
1:B:449:LEU:CB	1:B:478:MET:CE	2.33	1.06
1:B:404:LEU:H	1:B:404:LEU:HD12	1.22	1.02
1:B:449:LEU:HB3	1:B:478:MET:HE2	1.04	1.01
1:B:344:LEU:HD23	1:B:402:ILE:HD13	0.98	0.97
1:B:445:ILE:HG23	1:B:449:LEU:HG	1.47	0.94
1:B:449:LEU:CD1	1:B:478:MET:HE2	1.96	0.94
1:B:731:ILE:HD13	1:B:731:ILE:H	1.30	0.93
1:B:180:SER:O	1:B:181:GLN:O	1.87	0.92
1:B:344:LEU:HD21	1:B:402:ILE:HD11	1.51	0.92
1:C:130:GLU:OE1	1:C:174:ASP:OD2	1.89	0.90
1:B:449:LEU:HD13	1:B:478:MET:HE2	1.54	0.90
1:B:379:THR:OG1	1:B:398:MET:HE1	1.71	0.88
1:C:446:ALA:HB2	1:C:482:VAL:HG11	1.52	0.88
1:C:940:ILE:O	1:C:944:GLU:HB2	1.76	0.86
1:C:885:LEU:HD12	1:C:886:ALA:N	1.89	0.86
1:C:951:ASP:HB3	1:C:952:LYS:HZ2	1.44	0.83
1:B:344:LEU:CD2	1:B:402:ILE:HD13	1.93	0.82
1:B:375:VAL:O	1:B:379:THR:HG23	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ILE:O	1:B:449:LEU:HB2	1.80	0.80
1:A:410:ILE:HD11	1:A:975:THR:HG23	1.61	0.80
1:C:149:MET:HE1	1:C:321:LEU:HD13	1.61	0.80
1:A:38:ILE:HD13	1:A:465:ALA:HB3	1.62	0.80
1:B:449:LEU:HB3	1:B:478:MET:HE1	1.62	0.78
1:B:445:ILE:CG2	1:B:449:LEU:HG	2.13	0.78
1:B:449:LEU:CD1	1:B:478:MET:CE	2.63	0.77
1:C:881:VAL:HA	1:C:884:CYS:SG	2.27	0.75
1:A:420:MET:HE3	1:A:500:ILE:HG22	1.68	0.75
1:B:174:ASP:C	1:B:175:VAL:HG13	2.11	0.75
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.22	0.75
1:C:872:SER:O	1:C:876:ILE:HG12	1.87	0.75
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.69	0.74
1:B:180:SER:O	1:B:181:GLN:C	2.30	0.73
1:B:445:ILE:O	1:B:449:LEU:N	2.19	0.73
1:C:422:GLU:OE2	1:C:423:GLU:N	2.21	0.73
1:C:30:LEU:HD22	1:C:390:ILE:HG13	1.71	0.73
1:C:641:GLU:O	1:C:650:ARG:NH2	2.22	0.73
1:B:449:LEU:CB	1:B:478:MET:HE1	2.15	0.73
1:C:952:LYS:HE3	1:C:952:LYS:HA	1.69	0.73
1:B:449:LEU:CG	1:B:478:MET:HE2	2.19	0.72
1:C:104:GLN:NE2	1:C:129:VAL:O	2.22	0.72
1:C:952:LYS:O	1:C:954:GLY:N	2.23	0.72
1:B:174:ASP:C	1:B:175:VAL:CG1	2.64	0.71
1:B:454:VAL:O	1:B:456:MET:N	2.23	0.71
1:C:940:ILE:O	1:C:944:GLU:CB	2.37	0.71
1:B:401:ALA:HA	1:B:404:LEU:CD1	2.21	0.71
1:B:454:VAL:HB	1:B:455:PRO:HD3	1.71	0.71
1:C:27:ILE:HD11	1:C:380:PHE:CD2	2.26	0.71
1:B:404:LEU:HD12	1:B:404:LEU:N	2.03	0.70
1:B:889:TYR:O	1:B:891:SER:N	2.24	0.70
1:B:641:GLU:O	1:B:650:ARG:NH1	2.25	0.70
1:C:36:PRO:O	1:C:38:ILE:N	2.25	0.69
1:C:61:VAL:O	1:C:62:THR:OG1	2.08	0.69
1:C:425:LEU:HB2	1:C:426:PRO:HD2	1.74	0.69
1:C:885:LEU:HD11	1:C:895:PRO:HG3	1.73	0.69
1:B:401:ALA:C	1:B:403:GLY:H	2.02	0.68
1:B:449:LEU:HD13	1:B:478:MET:CE	2.23	0.68
1:C:427:PRO:O	1:C:430:ALA:N	2.27	0.67
1:A:44:THR:HG22	1:A:91:THR:HG23	1.76	0.67
1:A:348:ILE:HD11	1:A:372:VAL:HG11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PRO:O	1:C:38:ILE:HG23	1.93	0.67
1:C:298:ASN:O	1:C:301:ASP:N	2.28	0.67
1:C:901:VAL:HG21	1:C:939:ALA:HB2	1.76	0.67
1:A:249:ILE:O	1:A:250:LEU:HB3	1.95	0.67
1:A:695:LEU:HD23	1:A:825:MET:SD	2.36	0.66
1:B:174:ASP:O	1:B:175:VAL:CG1	2.43	0.66
1:B:234:ILE:HD11	1:C:729:ILE:HG21	1.78	0.66
1:C:976:SER:HB3	1:C:1012:THR:HG21	1.77	0.66
1:C:692:HIS:O	1:C:694:LYS:N	2.29	0.65
1:C:882:PHE:CE2	1:C:883:LEU:HD21	2.32	0.65
1:A:412:VAL:HG12	1:A:438:ILE:HD12	1.77	0.65
1:B:444:GLY:O	1:B:448:VAL:N	2.25	0.65
1:A:573:MET:HE2	1:A:626:ILE:HD11	1.77	0.65
1:B:898:VAL:HG11	1:B:940:ILE:HG13	1.79	0.65
1:B:990:THR:HG23	1:B:998:ASN:HD21	1.62	0.65
1:C:940:ILE:O	1:C:944:GLU:N	2.30	0.65
1:B:372:VAL:HG12	1:B:373:PRO:HD3	1.80	0.64
1:C:376:LEU:HD22	1:C:398:MET:HG2	1.80	0.64
1:B:174:ASP:O	1:B:175:VAL:HG12	1.98	0.64
1:B:478:MET:O	1:B:481:SER:N	2.30	0.64
1:B:379:THR:HG21	1:B:477:ALA:HA	1.78	0.63
1:B:236:ALA:HB2	1:C:729:ILE:HG23	1.81	0.63
1:C:134:SER:O	1:C:292:LYS:HE2	1.98	0.63
1:C:36:PRO:HG2	1:C:469:GLN:NE2	2.14	0.63
1:C:129:VAL:O	1:C:129:VAL:HG12	1.97	0.63
1:C:613:ASN:C	1:C:613:ASN:HD22	2.06	0.63
1:C:478:MET:HA	1:C:478:MET:HE2	1.80	0.63
1:B:478:MET:SD	1:B:479:ALA:N	2.72	0.62
1:C:415:ASN:OD1	1:C:968:ARG:NH2	2.32	0.62
1:C:54:ALA:CB	1:C:816:LEU:HD12	2.29	0.62
1:C:425:LEU:HB2	1:C:426:PRO:CD	2.29	0.62
1:A:228:GLN:O	1:B:583:THR:HG21	1.99	0.61
1:C:843:LEU:HD23	1:C:847:LEU:HD13	1.82	0.61
1:A:72:ILE:N	1:A:72:ILE:HD12	2.15	0.61
1:B:38:ILE:HG22	1:B:462:SER:OG	2.01	0.61
1:C:877:SER:O	1:C:881:VAL:HG22	2.00	0.61
1:B:444:GLY:O	1:B:448:VAL:HB	1.99	0.61
1:B:583:THR:HG22	1:B:586:ARG:HG3	1.81	0.61
1:C:885:LEU:HD11	1:C:895:PRO:CB	2.29	0.61
1:C:613:ASN:HD22	1:C:614:GLY:N	1.99	0.61
1:B:548:ILE:HD12	1:B:904:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ILE:HD12	1:C:38:ILE:C	2.26	0.60
1:C:885:LEU:HD12	1:C:885:LEU:C	2.26	0.60
1:B:443:VAL:O	1:B:443:VAL:HG12	2.01	0.60
1:B:449:LEU:CD1	1:B:478:MET:SD	2.90	0.60
1:B:643:LYS:O	1:B:645:GLU:N	2.34	0.60
1:C:655:PHE:O	1:C:658:ILE:HG13	2.02	0.60
1:C:969:LEU:HA	1:C:972:ILE:HG22	1.83	0.60
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.84	0.60
1:A:277:ILE:HD11	1:A:620:ARG:HD2	1.84	0.60
1:B:403:GLY:O	1:B:404:LEU:C	2.45	0.60
1:C:143:ILE:HD12	1:C:284:GLN:HE22	1.67	0.60
1:B:77:TYR:HA	1:B:820:ASN:HD21	1.66	0.60
1:C:423:GLU:O	1:C:425:LEU:HD12	2.02	0.60
1:C:425:LEU:HD22	1:C:426:PRO:HD2	1.82	0.60
1:B:158:VAL:CG1	1:B:289:LEU:HD13	2.32	0.59
1:C:424:GLY:C	1:C:425:LEU:HD12	2.27	0.59
1:C:885:LEU:HD11	1:C:895:PRO:CG	2.31	0.59
1:B:139:VAL:HG13	1:B:178:PHE:HE2	1.67	0.59
1:B:599:LEU:O	1:B:599:LEU:HD12	2.03	0.59
1:C:431:THR:O	1:C:433:LYS:N	2.35	0.59
1:C:722:GLU:O	1:C:723:ASP:O	2.19	0.59
1:B:350:LEU:HD23	1:B:981:LEU:HB3	1.85	0.59
1:C:957:LEU:HD23	1:C:958:ILE:HG13	1.83	0.59
1:C:54:ALA:HB3	1:C:816:LEU:HD12	1.85	0.59
1:C:35:TYR:CE2	1:C:671:ILE:HG22	2.37	0.59
1:C:641:GLU:O	1:C:646:ALA:HB3	2.02	0.59
1:C:427:PRO:O	1:C:428:LYS:C	2.45	0.58
1:B:20:MET:HA	1:B:377:LEU:HD21	1.86	0.58
1:C:724:THR:HG22	1:C:814:PRO:HD3	1.86	0.58
1:C:901:VAL:HG22	1:C:1019:VAL:HG22	1.85	0.58
1:B:452:VAL:HG13	1:B:453:PHE:N	2.19	0.58
1:B:963:ASP:HA	1:B:966:ARG:HB3	1.86	0.58
1:B:403:GLY:O	1:B:406:VAL:N	2.37	0.57
1:B:337:ILE:HG12	1:B:395:MET:HE1	1.85	0.57
1:B:379:THR:CG2	1:B:477:ALA:HA	2.34	0.57
1:C:699:ARG:HG3	1:C:827:ILE:HD11	1.85	0.57
1:C:121:GLU:O	1:C:125:GLN:NE2	2.38	0.57
1:C:124:GLN:O	1:C:125:GLN:C	2.48	0.57
1:C:298:ASN:ND2	1:C:301:ASP:OD2	2.37	0.57
1:C:456:MET:HE1	1:C:470:PHE:HB2	1.86	0.57
1:C:692:HIS:O	1:C:693:GLU:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:HG22	1:B:402:ILE:O	2.05	0.57
1:B:403:GLY:O	1:B:406:VAL:HG12	2.04	0.57
1:B:449:LEU:HD13	1:B:478:MET:SD	2.45	0.56
1:C:425:LEU:HD13	1:C:426:PRO:O	2.05	0.56
1:C:641:GLU:HG2	1:C:642:ASN:N	2.20	0.56
1:B:730:ASP:OD1	1:B:730:ASP:N	2.38	0.56
1:C:111:LEU:HD21	1:C:127:VAL:HG21	1.86	0.56
1:C:542:LEU:HD21	1:C:1025:VAL:HG11	1.86	0.56
1:C:875:ALA:O	1:C:878:LEU:N	2.35	0.56
1:C:877:SER:C	1:C:880:VAL:HG12	2.30	0.56
1:B:441:ALA:C	1:B:443:VAL:H	2.14	0.56
1:C:390:ILE:HG22	1:C:390:ILE:O	2.06	0.56
1:B:399:VAL:HA	1:B:402:ILE:HG13	1.86	0.56
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.86	0.56
1:C:641:GLU:O	1:C:646:ALA:CB	2.54	0.56
1:C:876:ILE:O	1:C:880:VAL:HG12	2.05	0.56
1:C:699:ARG:CG	1:C:827:ILE:HD11	2.36	0.56
1:C:149:MET:CE	1:C:321:LEU:HD13	2.33	0.56
1:C:470:PHE:O	1:C:471:SER:C	2.49	0.56
1:B:354:VAL:HG12	1:B:974:MET:HB2	1.87	0.56
1:B:383:LEU:HD11	1:B:473:THR:HG22	1.87	0.56
1:C:76:MET:CG	1:C:95:GLU:HG3	2.36	0.56
1:A:527:TYR:CD2	1:A:969:LEU:HD22	2.41	0.56
1:C:61:VAL:HG11	1:C:122:VAL:HG21	1.88	0.56
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.88	0.55
1:A:583:THR:HG22	1:A:586:ARG:HG3	1.87	0.55
1:A:1010:THR:HG23	1:A:1014:LEU:HD13	1.86	0.55
1:C:880:VAL:O	1:C:884:CYS:HB3	2.06	0.55
1:B:5:PHE:CD2	1:B:487:ILE:HG23	2.40	0.55
1:C:424:GLY:O	1:C:425:LEU:HB3	2.06	0.55
1:B:988:ILE:O	1:B:990:THR:N	2.38	0.55
1:B:447:MET:HB3	1:B:884:CYS:SG	2.47	0.55
1:C:76:MET:HG2	1:C:95:GLU:HG3	1.89	0.55
1:B:178:PHE:CZ	1:B:290:GLY:N	2.75	0.55
1:B:180:SER:C	1:B:181:GLN:O	2.49	0.55
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.88	0.55
1:B:83:ASP:C	1:B:83:ASP:OD1	2.50	0.55
1:B:702:LEU:HD13	1:B:851:LEU:HD11	1.89	0.55
1:C:404:LEU:HD23	1:C:478:MET:HE3	1.89	0.55
1:B:177:LEU:O	1:B:179:GLY:N	2.38	0.55
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:PRO:HB2	1:C:10:ILE:HD12	1.88	0.54
1:A:159:ALA:HB2	1:A:177:LEU:HD21	1.88	0.54
1:B:818:ARG:NH1	1:B:821:GLY:O	2.38	0.54
1:C:686:ASP:HB2	1:C:823:PRO:O	2.07	0.54
1:A:904:LEU:O	1:A:1010:THR:O	2.25	0.54
1:C:38:ILE:HD13	1:C:462:SER:HB3	1.88	0.54
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.90	0.54
1:C:104:GLN:CG	1:C:129:VAL:HG12	2.36	0.54
1:C:412:VAL:HG22	1:C:442:LEU:HD11	1.88	0.54
1:A:1:MET:HE2	1:A:486:LEU:HD23	1.88	0.54
1:B:987:VAL:HG21	1:B:1005:MET:CG	2.37	0.54
1:C:752:ALA:O	1:C:774:MET:HA	2.08	0.54
1:B:454:VAL:HB	1:B:455:PRO:CD	2.38	0.54
1:B:444:GLY:O	1:B:448:VAL:CB	2.55	0.54
1:C:146:ASP:OD1	1:C:148:THR:HG23	2.08	0.54
1:C:425:LEU:CD2	1:C:426:PRO:HD2	2.37	0.54
1:B:150:THR:OG1	1:B:151:GLN:N	2.40	0.54
1:B:449:LEU:HD12	1:B:478:MET:SD	2.48	0.54
1:A:733:GLN:HE22	1:A:743:ILE:HD13	1.73	0.54
1:C:38:ILE:HD12	1:C:38:ILE:O	2.08	0.54
1:C:38:ILE:CD1	1:C:462:SER:HB3	2.38	0.54
1:C:127:VAL:O	1:C:127:VAL:HG23	2.08	0.54
1:C:688:ALA:O	1:C:689:GLY:C	2.51	0.54
1:A:348:ILE:HD11	1:A:372:VAL:CG1	2.38	0.53
1:B:398:MET:O	1:B:402:ILE:HG13	2.08	0.53
1:C:878:LEU:HA	1:C:881:VAL:HG23	1.90	0.53
1:B:980:ILE:O	1:B:984:MET:HG2	2.08	0.53
1:C:30:LEU:HD21	1:C:388:PHE:O	2.07	0.53
1:C:348:ILE:HG22	1:C:402:ILE:HG21	1.90	0.53
1:C:376:LEU:HD22	1:C:398:MET:CG	2.38	0.53
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.90	0.53
1:B:731:ILE:H	1:B:731:ILE:CD1	2.02	0.53
1:B:138:MET:HE2	1:B:140:VAL:HG12	1.89	0.53
1:C:1023:PHE:O	1:C:1027:ARG:HB2	2.09	0.53
1:C:57:VAL:HG13	1:C:61:VAL:HG23	1.91	0.52
1:A:20:MET:SD	1:A:374:VAL:HG12	2.50	0.52
1:A:63:GLN:HE22	1:C:767:ARG:HA	1.75	0.52
1:C:57:VAL:O	1:C:61:VAL:O	2.27	0.52
1:A:5:PHE:CD2	1:A:487:ILE:HG22	2.45	0.52
1:B:520:PHE:O	1:B:524:THR:HG22	2.10	0.52
1:C:885:LEU:CD1	1:C:895:PRO:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:HIS:O	1:A:597:TYR:C	2.52	0.52
1:A:961:THR:HG21	1:A:1024:VAL:HG13	1.91	0.52
1:C:721:LEU:O	1:C:722:GLU:C	2.52	0.52
1:B:210:GLN:HB2	1:B:249:ILE:HD12	1.92	0.52
1:C:699:ARG:CD	1:C:827:ILE:HD11	2.40	0.52
1:B:582:ALA:HB3	1:B:623:ASN:HB3	1.91	0.52
1:C:858:ASP:O	1:C:860:THR:N	2.43	0.52
1:A:583:THR:HG22	1:A:586:ARG:CG	2.39	0.51
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.91	0.51
1:C:298:ASN:ND2	1:C:301:ASP:HB2	2.25	0.51
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.92	0.51
1:B:53:ASP:O	1:B:54:ALA:C	2.53	0.51
1:B:986:LEU:HD22	1:B:997:GLN:HE21	1.75	0.51
1:C:946:ALA:HB1	1:C:1023:PHE:CE2	2.44	0.51
1:C:425:LEU:HD22	1:C:426:PRO:CD	2.41	0.51
1:A:243:THR:HG22	1:A:268:ILE:HG22	1.91	0.51
1:A:590:VAL:O	1:A:594:VAL:HG23	2.11	0.51
1:A:743:ILE:HD12	1:C:209:ALA:HB1	1.92	0.51
1:C:641:GLU:HG2	1:C:642:ASN:H	1.75	0.51
1:C:644:VAL:O	1:C:648:THR:HG23	2.10	0.51
1:C:40:PRO:CD	1:C:674:LEU:HD11	2.41	0.51
1:A:583:THR:HG22	1:A:586:ARG:HD3	1.93	0.51
1:A:890:GLU:C	1:C:10:ILE:HD13	2.36	0.51
1:C:42:ALA:HB2	1:C:93:THR:HG23	1.93	0.51
1:C:453:PHE:CD2	1:C:474:ILE:HG21	2.45	0.51
1:A:942:ILE:HD11	1:A:965:VAL:HG22	1.92	0.50
1:A:72:ILE:HD13	1:A:75:LEU:HD22	1.93	0.50
1:A:420:MET:HE3	1:A:500:ILE:CG2	2.38	0.50
1:A:687:GLN:O	1:A:688:ALA:HB2	2.12	0.50
1:B:371:ALA:HB1	1:B:488:LEU:HD23	1.93	0.50
1:B:762:PHE:CZ	1:B:764:ASP:HB2	2.47	0.50
1:C:480:LEU:O	1:C:484:VAL:HG23	2.12	0.50
1:C:952:LYS:C	1:C:954:GLY:H	2.19	0.50
1:B:902:VAL:HG23	1:B:903:PRO:HD3	1.93	0.50
1:B:211:ASN:ND2	1:B:761:ASP:O	2.43	0.50
1:B:246:PHE:O	1:B:249:ILE:HG12	2.10	0.50
1:B:649:MET:O	1:B:652:THR:HG22	2.10	0.50
1:B:375:VAL:HG22	1:B:484:VAL:HG11	1.94	0.50
1:B:379:THR:C	1:B:381:ALA:N	2.69	0.50
1:B:696:THR:O	1:B:699:ARG:HB3	2.10	0.50
1:C:435:MET:HE1	1:C:439:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HG12	1:A:493:CYS:SG	2.51	0.50
1:C:352:PHE:CG	1:C:352:PHE:O	2.65	0.50
1:C:422:GLU:O	1:C:424:GLY:N	2.44	0.50
1:A:456:MET:HE1	1:A:926:VAL:HG12	1.94	0.50
1:A:573:MET:CE	1:A:626:ILE:HD11	2.41	0.50
1:B:65:ILE:O	1:B:66:GLU:C	2.53	0.49
1:B:406:VAL:HG22	1:B:410:ILE:HD12	1.93	0.49
1:A:818:ARG:NH1	1:A:822:LEU:HA	2.27	0.49
1:A:222:THR:HG21	1:B:276:ASP:CG	2.37	0.49
1:B:137:LEU:HD12	1:B:329:THR:HG22	1.94	0.49
1:C:393:LEU:CD1	1:C:466:ILE:HG23	2.41	0.49
1:C:874:TYR:O	1:C:878:LEU:N	2.46	0.49
1:A:754:TRP:CE3	1:C:234:ILE:HD11	2.47	0.49
1:B:441:ALA:O	1:B:443:VAL:N	2.44	0.49
1:A:908:GLY:O	1:A:909:ALA:HB2	2.12	0.49
1:C:937:LYS:HD3	1:C:938:ASN:HD22	1.77	0.49
1:B:120:GLN:O	1:B:123:GLN:HB3	2.11	0.49
1:B:401:ALA:O	1:B:405:LEU:HB2	2.12	0.49
1:B:449:LEU:HB2	1:B:478:MET:HE1	1.91	0.49
1:C:411:VAL:HG21	1:C:941:LEU:HD23	1.95	0.49
1:C:519:MET:O	1:C:523:SER:OG	2.27	0.49
1:C:885:LEU:CD1	1:C:895:PRO:CB	2.91	0.49
1:A:241:THR:HG22	1:A:245:GLU:OE1	2.13	0.49
1:A:518:ARG:HE	1:A:518:ARG:HA	1.78	0.49
1:B:454:VAL:CB	1:B:455:PRO:HD3	2.38	0.49
1:B:898:VAL:HG13	1:B:939:ALA:HB3	1.93	0.49
1:C:425:LEU:HD22	1:C:426:PRO:O	2.12	0.49
1:C:862:MET:HE3	1:C:862:MET:HA	1.95	0.49
1:C:343:THR:O	1:C:344:LEU:C	2.56	0.49
1:A:330:THR:O	1:A:331:PRO:C	2.55	0.49
1:B:111:LEU:HD21	1:B:127:VAL:CG1	2.43	0.49
1:C:478:MET:O	1:C:479:ALA:C	2.56	0.49
1:C:882:PHE:O	1:C:885:LEU:HG	2.13	0.49
1:A:237:GLN:HG3	1:B:731:ILE:HD11	1.95	0.49
1:B:38:ILE:HG22	1:B:462:SER:HG	1.78	0.48
1:C:885:LEU:HD13	1:C:895:PRO:HB3	1.95	0.48
1:A:318:PRO:O	1:A:319:SER:C	2.56	0.48
1:B:158:VAL:HG11	1:B:289:LEU:HD13	1.96	0.48
1:B:375:VAL:HG21	1:B:481:SER:HA	1.95	0.48
1:B:448:VAL:O	1:B:452:VAL:HG12	2.12	0.48
1:B:874:TYR:CE2	1:B:878:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:MET:SD	1:C:373:PRO:HB2	2.53	0.48
1:C:552:MET:HE3	1:C:553:ALA:N	2.28	0.48
1:C:943:VAL:HA	1:C:946:ALA:HB3	1.93	0.48
1:A:332:PHE:C	1:A:332:PHE:CD2	2.90	0.48
1:B:20:MET:HA	1:B:377:LEU:CD2	2.43	0.48
1:B:478:MET:SD	1:B:478:MET:C	2.96	0.48
1:B:655:PHE:O	1:B:656:SER:C	2.56	0.48
1:C:23:GLY:CA	1:C:381:ALA:HB2	2.42	0.48
1:C:578:LEU:HD13	1:C:587:THR:HB	1.94	0.48
1:A:354:VAL:O	1:A:354:VAL:HG12	2.13	0.48
1:A:685:ILE:CG2	1:A:822:LEU:HD13	2.43	0.48
1:B:143:ILE:HG22	1:B:286:ALA:HB1	1.94	0.48
1:C:424:GLY:O	1:C:425:LEU:CB	2.61	0.48
1:C:950:MET:HE1	1:C:1027:ARG:HE	1.79	0.48
1:C:104:GLN:CG	1:C:129:VAL:CG1	2.91	0.48
1:C:16:ALA:HB1	1:C:374:VAL:HG21	1.96	0.48
1:B:142:VAL:HG12	1:B:154:ILE:CG2	2.43	0.48
1:C:13:TRP:HA	1:C:13:TRP:CE3	2.49	0.48
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.95	0.48
1:C:343:THR:HG23	1:C:985:PRO:HB2	1.96	0.48
1:A:410:ILE:HA	1:A:413:VAL:HG22	1.96	0.48
1:C:69:MET:HE2	1:C:92:LEU:HD21	1.95	0.48
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.47	0.48
1:A:984:MET:N	1:A:985:PRO:HD2	2.29	0.48
1:C:421:ALA:O	1:C:422:GLU:O	2.30	0.48
1:C:425:LEU:HD13	1:C:425:LEU:C	2.39	0.48
1:A:1:MET:HE3	1:A:486:LEU:HB3	1.96	0.47
1:A:168:ARG:HG2	1:B:69:MET:O	2.14	0.47
1:C:298:ASN:O	1:C:300:LEU:N	2.48	0.47
1:B:1022:PHE:O	1:B:1026:VAL:HG22	2.14	0.47
1:C:27:ILE:HG23	1:C:390:ILE:CD1	2.44	0.47
1:C:382:VAL:HG11	1:C:476:SER:OG	2.15	0.47
1:A:902:VAL:HB	1:A:903:PRO:HD3	1.97	0.47
1:C:388:PHE:CE2	1:C:472:ILE:HG21	2.49	0.47
1:A:11:PHE:CE1	1:B:887:ALA:HB1	2.49	0.47
1:A:957:LEU:HD23	1:A:958:ILE:HD13	1.96	0.47
1:C:214:VAL:HG23	1:C:236:ALA:HB3	1.95	0.47
1:B:396:PHE:O	1:B:400:LEU:HG	2.14	0.47
1:A:410:ILE:HD13	1:A:974:MET:CB	2.44	0.47
1:A:686:ASP:HB2	1:A:695:LEU:HD13	1.95	0.47
1:A:918:LEU:HD21	1:A:999:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:MET:N	1:B:116:PRO:CD	2.78	0.47
1:B:382:VAL:HG21	1:B:480:LEU:HD13	1.96	0.47
1:C:181:GLN:NE2	1:C:767:ARG:NH2	2.63	0.47
1:A:215:ALA:HB1	1:B:51:GLY:C	2.40	0.47
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.49	0.47
1:A:968:ARG:HB3	1:A:968:ARG:CZ	2.44	0.47
1:B:692:HIS:O	1:B:693:GLU:C	2.57	0.47
1:B:965:VAL:HG12	1:B:969:LEU:HD12	1.95	0.47
1:C:76:MET:HE2	1:C:864:TYR:CE2	2.49	0.47
1:C:158:VAL:HG23	1:C:162:MET:SD	2.54	0.47
1:C:885:LEU:C	1:C:885:LEU:CD1	2.88	0.47
1:A:249:ILE:O	1:A:250:LEU:CB	2.59	0.47
1:B:590:VAL:O	1:B:594:VAL:HG23	2.15	0.47
1:B:1009:VAL:O	1:B:1013:VAL:HG22	2.15	0.47
1:C:360:GLN:OE1	1:C:509:LYS:NZ	2.42	0.47
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.96	0.47
1:C:1020:PRO:O	1:C:1024:VAL:HG22	2.15	0.47
1:A:758:TYR:CZ	1:A:770:LYS:HD3	2.50	0.47
1:C:194:ASN:O	1:C:195:LYS:C	2.58	0.47
1:C:639:GLY:O	1:C:642:ASN:N	2.45	0.47
1:C:375:VAL:O	1:C:379:THR:HG22	2.14	0.46
1:C:719:ASN:HD22	1:C:826:GLU:HB3	1.80	0.46
1:B:198:LEU:HD23	1:B:251:LEU:HD13	1.96	0.46
1:C:578:LEU:HD11	1:C:590:VAL:HG21	1.98	0.46
1:C:655:PHE:O	1:C:657:GLN:N	2.48	0.46
1:C:965:VAL:HG21	1:C:1020:PRO:HG3	1.97	0.46
1:A:516:PHE:HA	1:A:519:MET:HB2	1.98	0.46
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.80	0.46
1:B:418:ARG:NH1	1:B:967:MET:SD	2.88	0.46
1:C:104:GLN:HG3	1:C:129:VAL:CG1	2.44	0.46
1:C:655:PHE:C	1:C:657:GLN:N	2.73	0.46
1:B:119:PRO:O	1:B:122:VAL:HG12	2.15	0.46
1:C:532:GLY:CA	1:C:962:LEU:HD21	2.45	0.46
1:C:882:PHE:CD1	1:C:882:PHE:C	2.92	0.46
1:B:563:PHE:HD2	1:B:677:ALA:HB2	1.80	0.46
1:C:1:MET:HE3	1:C:486:LEU:HD22	1.98	0.46
1:C:556:PHE:HB2	1:C:910:LEU:HD11	1.97	0.46
1:C:895:PRO:C	1:C:897:SER:N	2.73	0.46
1:A:364:ALA:HA	1:A:367:ILE:HD12	1.98	0.46
1:B:236:ALA:O	1:B:237:GLN:C	2.58	0.46
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:VAL:HG12	1:B:438:ILE:CD1	2.46	0.46
1:A:977:LEU:HD23	1:A:981:LEU:HD23	1.98	0.46
1:C:26:ALA:HB1	1:C:384:ALA:CB	2.46	0.46
1:C:390:ILE:O	1:C:390:ILE:CG2	2.64	0.46
1:A:10:ILE:HG12	1:B:890:GLU:O	2.15	0.46
1:A:754:TRP:CE3	1:C:234:ILE:CD1	2.99	0.46
1:B:393:LEU:CD2	1:B:466:ILE:HG23	2.45	0.46
1:C:13:TRP:CZ3	1:C:488:LEU:HD11	2.50	0.46
1:A:379:THR:HB	1:A:398:MET:HE1	1.98	0.46
1:B:344:LEU:CD2	1:B:402:ILE:CG1	2.91	0.46
1:C:182:TYR:HA	1:C:271:GLY:O	2.15	0.46
1:C:880:VAL:O	1:C:880:VAL:HG22	2.16	0.46
1:A:1:MET:CE	1:A:486:LEU:HD23	2.47	0.45
1:A:19:ILE:HG22	1:A:20:MET:N	2.31	0.45
1:A:72:ILE:HD12	1:A:72:ILE:H	1.79	0.45
1:A:695:LEU:CD2	1:A:825:MET:SD	3.03	0.45
1:C:298:ASN:C	1:C:300:LEU:N	2.73	0.45
1:C:777:ALA:O	1:C:781:MET:HG2	2.16	0.45
1:A:38:ILE:CG1	1:A:462:SER:O	2.64	0.45
1:B:684:LEU:HD22	1:B:699:ARG:HA	1.97	0.45
1:B:948:ASP:C	1:B:950:MET:H	2.24	0.45
1:C:327:TYR:OH	1:C:573:MET:HE3	2.16	0.45
1:C:406:VAL:O	1:C:407:ASP:C	2.58	0.45
1:C:453:PHE:CE2	1:C:474:ILE:HD13	2.52	0.45
1:C:527:TYR:OH	1:C:1016:ILE:HB	2.16	0.45
1:B:449:LEU:HD12	1:B:478:MET:CE	2.46	0.45
1:C:517:ASN:HD22	1:C:518:ARG:N	2.14	0.45
1:C:791:VAL:HG12	1:C:791:VAL:O	2.17	0.45
1:A:568:ASP:OD1	1:A:644:VAL:HG23	2.16	0.45
1:B:582:ALA:HB3	1:B:623:ASN:CB	2.46	0.45
1:C:445:ILE:HB	1:C:449:LEU:HD12	1.98	0.45
1:C:33:ALA:O	1:C:391:ASN:HA	2.17	0.45
1:B:401:ALA:C	1:B:403:GLY:N	2.68	0.45
1:C:20:MET:SD	1:C:373:PRO:CB	3.05	0.45
1:C:72:ILE:O	1:C:73:ASP:C	2.60	0.45
1:C:467:TYR:OH	1:C:925:GLN:OE1	2.30	0.45
1:A:578:LEU:HD13	1:A:587:THR:HB	1.98	0.45
1:A:972:ILE:HG22	1:A:973:LEU:HD12	1.98	0.45
1:A:171:GLY:O	1:A:302:THR:HG21	2.17	0.45
1:A:975:THR:O	1:A:976:SER:C	2.60	0.45
1:C:400:LEU:O	1:C:401:ALA:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:LEU:O	1:C:874:TYR:C	2.59	0.45
1:A:318:PRO:O	1:A:319:SER:O	2.35	0.45
1:A:549:VAL:O	1:A:549:VAL:HG12	2.15	0.45
1:B:137:LEU:HD12	1:B:329:THR:CG2	2.46	0.45
1:C:207:ILE:HG22	1:C:759:VAL:HG11	1.99	0.45
1:C:453:PHE:HA	1:C:456:MET:HG2	1.99	0.45
1:C:875:ALA:O	1:C:878:LEU:HB2	2.17	0.45
1:A:559:LEU:HD23	1:A:920:ASN:HB2	2.00	0.44
1:A:706:ALA:HB1	1:A:713:LEU:HD13	1.98	0.44
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.99	0.44
1:B:634:TRP:CE3	1:B:992:ALA:HB2	2.52	0.44
1:B:697:GLN:O	1:B:698:ALA:C	2.58	0.44
1:B:1013:VAL:HG23	1:B:1014:LEU:HD12	1.99	0.44
1:C:207:ILE:CG2	1:C:759:VAL:HG11	2.47	0.44
1:A:777:ALA:O	1:A:781:MET:HG2	2.17	0.44
1:B:375:VAL:HG22	1:B:484:VAL:CG1	2.47	0.44
1:C:688:ALA:HB3	1:C:854:GLY:HA3	1.99	0.44
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.82	0.44
1:B:399:VAL:HA	1:B:402:ILE:CD1	2.48	0.44
1:C:545:TYR:O	1:C:548:ILE:HG13	2.17	0.44
1:C:651:ALA:O	1:C:654:ALA:N	2.50	0.44
1:A:11:PHE:HA	1:A:14:VAL:HG22	1.99	0.44
1:A:146:ASP:OD1	1:A:148:THR:HG23	2.18	0.44
1:A:409:ALA:HA	1:A:489:THR:HG21	2.00	0.44
1:C:181:GLN:NE2	1:C:767:ARG:HH22	2.15	0.44
1:B:30:LEU:HD11	1:B:380:PHE:O	2.18	0.44
1:C:124:GLN:O	1:C:126:GLY:N	2.51	0.44
1:C:372:VAL:CG2	1:C:373:PRO:HD3	2.46	0.44
1:C:498:LYS:HB2	1:C:499:PRO:CD	2.48	0.44
1:A:323:ILE:HG23	1:A:325:TYR:CE2	2.52	0.44
1:A:1019:VAL:N	1:A:1020:PRO:CD	2.81	0.44
1:B:185:ARG:HG3	1:B:187:TRP:CE2	2.53	0.44
1:A:542:LEU:CD2	1:A:546:LEU:HD21	2.48	0.44
1:B:119:PRO:O	1:B:120:GLN:C	2.61	0.44
1:B:184:MET:HB3	1:B:771:VAL:HG22	2.00	0.44
1:C:26:ALA:O	1:C:30:LEU:HB2	2.18	0.44
1:C:65:ILE:HG13	1:C:118:LEU:HD21	1.99	0.44
1:C:181:GLN:HE21	1:C:767:ARG:NH2	2.16	0.44
1:C:885:LEU:HD21	1:C:895:PRO:HB2	1.99	0.44
1:A:763:ILE:HD11	1:B:59:ASP:HB3	2.00	0.44
1:B:330:THR:HB	1:B:331:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLU:HG2	1:C:78:MET:HE1	2.00	0.44
1:A:72:ILE:HD13	1:A:75:LEU:CD2	2.47	0.44
1:A:115:MET:N	1:A:116:PRO:CD	2.80	0.44
1:B:151:GLN:NE2	1:B:278:ILE:HA	2.33	0.44
1:B:366:LEU:HD13	1:B:369:THR:HG22	1.99	0.44
1:B:403:GLY:C	1:B:405:LEU:N	2.69	0.44
1:C:34:GLN:O	1:C:35:TYR:HD1	2.01	0.44
1:B:444:GLY:O	1:B:448:VAL:HG23	2.18	0.43
1:B:876:ILE:HA	1:B:879:ILE:HG22	2.00	0.43
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.98	0.43
1:C:587:THR:HG21	1:C:623:ASN:HA	2.00	0.43
1:C:845:GLU:O	1:C:849:SER:OG	2.36	0.43
1:B:182:TYR:CD2	1:B:270:LEU:HD23	2.54	0.43
1:B:344:LEU:HD23	1:B:402:ILE:CG1	2.36	0.43
1:C:882:PHE:C	1:C:885:LEU:HG	2.43	0.43
1:B:5:PHE:CE2	1:B:487:ILE:HG23	2.53	0.43
1:C:26:ALA:HB1	1:C:384:ALA:HB3	2.00	0.43
1:B:214:VAL:HG21	1:C:747:ASN:CG	2.44	0.43
1:B:716:VAL:HG11	1:B:844:MET:HE1	2.01	0.43
1:B:997:GLN:O	1:B:1000:VAL:HG22	2.19	0.43
1:B:1013:VAL:HG23	1:B:1014:LEU:CD1	2.48	0.43
1:C:130:GLU:OE1	1:C:174:ASP:CG	2.60	0.43
1:C:399:VAL:O	1:C:401:ALA:N	2.52	0.43
1:C:639:GLY:O	1:C:641:GLU:N	2.51	0.43
1:C:873:LEU:O	1:C:877:SER:N	2.33	0.43
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.52	0.43
1:B:102:ILE:O	1:B:103:ALA:C	2.59	0.43
1:B:166:ILE:HD13	1:B:289:LEU:CD2	2.49	0.43
1:C:166:ILE:HD11	1:C:310:LEU:CD1	2.48	0.43
1:C:194:ASN:ND2	1:C:790:TYR:CG	2.86	0.43
1:C:277:ILE:N	1:C:277:ILE:CD1	2.82	0.43
1:A:23:GLY:CA	1:A:381:ALA:HB2	2.44	0.43
1:A:420:MET:SD	1:A:430:ALA:HB3	2.59	0.43
1:B:994:SER:O	1:B:998:ASN:ND2	2.52	0.43
1:C:749:THR:O	1:C:750:LEU:C	2.59	0.43
1:A:34:GLN:O	1:A:35:TYR:C	2.62	0.43
1:A:906:VAL:HG12	1:A:910:LEU:CD2	2.49	0.43
1:B:399:VAL:CA	1:B:402:ILE:HG13	2.49	0.43
1:B:866:GLU:O	1:B:867:ARG:HB2	2.18	0.43
1:C:30:LEU:HD22	1:C:390:ILE:CG1	2.46	0.43
1:C:669:PRO:HD3	1:C:677:ALA:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLN:HE21	1:C:109:ASN:HD22	1.67	0.43
1:B:403:GLY:HA2	1:B:406:VAL:HG12	2.01	0.43
1:B:449:LEU:O	1:B:453:PHE:HB2	2.19	0.43
1:C:952:LYS:HA	1:C:952:LYS:CE	2.42	0.43
1:B:731:ILE:HA	1:B:804:PHE:O	2.19	0.43
1:B:878:LEU:HA	1:B:881:VAL:HG22	2.00	0.43
1:B:964:ALA:HA	1:B:967:MET:HE3	2.00	0.43
1:C:30:LEU:HD12	1:C:384:ALA:HB2	1.99	0.43
1:A:375:VAL:O	1:A:379:THR:OG1	2.34	0.42
1:A:448:VAL:HG12	1:A:884:CYS:CB	2.49	0.42
1:A:676:THR:O	1:A:678:THR:N	2.52	0.42
1:A:961:THR:HG21	1:A:1024:VAL:CG1	2.48	0.42
1:B:102:ILE:O	1:B:105:VAL:HG12	2.19	0.42
1:C:399:VAL:HA	1:C:402:ILE:HD11	2.01	0.42
1:C:916:ARG:O	1:C:918:LEU:N	2.52	0.42
1:A:107:VAL:HG12	1:A:108:GLN:N	2.34	0.42
1:A:332:PHE:CD1	1:A:569:GLN:HA	2.54	0.42
1:A:583:THR:HG21	1:C:228:GLN:O	2.19	0.42
1:A:743:ILE:HG22	1:A:747:ASN:ND2	2.35	0.42
1:B:355:MET:HE2	1:B:413:VAL:HG21	2.01	0.42
1:B:452:VAL:CG1	1:B:453:PHE:N	2.81	0.42
1:C:350:LEU:HD13	1:C:981:LEU:HD22	2.00	0.42
1:C:478:MET:O	1:C:481:SER:N	2.52	0.42
1:B:374:VAL:O	1:B:378:GLY:N	2.51	0.42
1:B:382:VAL:O	1:B:385:ALA:HB3	2.19	0.42
1:C:327:TYR:CD2	1:C:327:TYR:O	2.72	0.42
1:C:421:ALA:O	1:C:422:GLU:C	2.62	0.42
1:B:11:PHE:CD1	1:B:15:ILE:HD11	2.54	0.42
1:B:185:ARG:NH1	1:B:272:GLY:O	2.43	0.42
1:B:333:VAL:O	1:B:337:ILE:HD12	2.19	0.42
1:B:599:LEU:HD12	1:B:599:LEU:C	2.45	0.42
1:A:887:ALA:HB1	1:C:11:PHE:HD2	1.84	0.42
1:B:578:LEU:HD13	1:B:587:THR:HG23	2.01	0.42
1:B:731:ILE:HG12	1:B:731:ILE:O	2.18	0.42
1:C:36:PRO:HD3	1:C:391:ASN:ND2	2.34	0.42
1:C:904:LEU:O	1:C:1010:THR:O	2.36	0.42
1:C:952:LYS:C	1:C:954:GLY:N	2.78	0.42
1:B:903:PRO:HA	1:B:906:VAL:HG22	2.01	0.42
1:C:326:PRO:CB	1:C:610:PHE:HB2	2.50	0.42
1:C:357:LEU:HD21	1:C:516:PHE:CZ	2.55	0.42
1:C:572:PHE:CZ	1:C:629:VAL:HG11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:LEU:HA	1:C:881:VAL:CG2	2.49	0.42
1:A:68:ASN:O	1:A:110:LYS:HB3	2.20	0.42
1:A:456:MET:HE2	1:A:467:TYR:HD1	1.84	0.42
1:A:583:THR:HG22	1:A:586:ARG:CD	2.49	0.42
1:B:454:VAL:CB	1:B:455:PRO:CD	2.97	0.42
1:C:160:ALA:HA	1:C:767:ARG:NH2	2.35	0.42
1:C:422:GLU:O	1:C:502:LYS:O	2.38	0.42
1:A:130:GLU:OE2	1:A:174:ASP:OD2	2.37	0.42
1:C:453:PHE:O	1:C:454:VAL:HG23	2.20	0.42
1:B:785:ASP:O	1:B:786:ILE:C	2.63	0.42
1:B:841:MET:O	1:B:842:GLU:C	2.62	0.42
1:B:903:PRO:O	1:B:905:GLY:N	2.53	0.42
1:B:906:VAL:O	1:B:910:LEU:HD13	2.20	0.42
1:A:213:GLN:HB2	1:A:239:ARG:HG2	2.01	0.42
1:A:410:ILE:HD13	1:A:974:MET:HB2	2.01	0.42
1:A:926:VAL:C	1:A:928:LEU:H	2.28	0.42
1:B:27:ILE:CG2	1:B:380:PHE:HD2	2.33	0.42
1:B:45:ILE:HG12	1:B:129:VAL:HG22	2.02	0.42
1:B:216:ALA:HB1	1:B:234:ILE:O	2.19	0.42
1:C:409:ALA:HA	1:C:489:THR:HG21	2.02	0.42
1:C:928:LEU:O	1:C:931:THR:N	2.53	0.42
1:A:641:GLU:N	1:A:641:GLU:OE1	2.52	0.41
1:C:300:LEU:CD1	1:C:333:VAL:HG11	2.50	0.41
1:A:372:VAL:HB	1:A:373:PRO:CD	2.49	0.41
1:B:367:ILE:HB	1:B:368:PRO:CD	2.50	0.41
1:B:445:ILE:CG2	1:B:449:LEU:CG	2.91	0.41
1:C:36:PRO:HG2	1:C:469:GLN:HE22	1.84	0.41
1:C:474:ILE:O	1:C:477:ALA:N	2.53	0.41
1:C:940:ILE:O	1:C:944:GLU:CA	2.68	0.41
1:B:595:THR:HG22	1:B:609:VAL:CG2	2.50	0.41
1:C:34:GLN:OE1	1:C:35:TYR:CE1	2.73	0.41
1:C:425:LEU:CB	1:C:426:PRO:CD	2.97	0.41
1:A:144:ASN:HB2	1:A:154:ILE:HD11	2.03	0.41
1:B:882:PHE:HB2	1:B:899:MET:HE1	2.01	0.41
1:B:976:SER:OG	1:B:1012:THR:HG21	2.21	0.41
1:A:410:ILE:HD13	1:A:974:MET:HB3	2.03	0.41
1:A:578:LEU:HD11	1:A:590:VAL:HG21	2.03	0.41
1:B:837:THR:HG22	1:B:841:MET:HE3	2.02	0.41
1:C:425:LEU:CD1	1:C:426:PRO:O	2.67	0.41
1:C:877:SER:O	1:C:880:VAL:HG12	2.21	0.41
1:A:697:GLN:O	1:A:698:ALA:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:PHE:CD2	1:B:644:VAL:HG23	2.56	0.41
1:C:576:VAL:HG22	1:C:663:VAL:HG22	2.02	0.41
1:C:659:LYS:O	1:C:660:ASP:C	2.62	0.41
1:A:918:LEU:HD21	1:A:999:ALA:CB	2.51	0.41
1:B:819:TYR:O	1:B:820:ASN:C	2.64	0.41
1:C:74:ASN:O	1:C:95:GLU:N	2.52	0.41
1:C:819:TYR:N	1:C:821:GLY:O	2.53	0.41
1:C:902:VAL:HB	1:C:903:PRO:HD3	2.02	0.41
1:C:949:LEU:HD23	1:C:953:GLU:HB3	2.02	0.41
1:A:371:ALA:O	1:A:374:VAL:HG22	2.21	0.41
1:B:20:MET:CA	1:B:377:LEU:HD21	2.51	0.41
1:B:27:ILE:HG22	1:B:380:PHE:CD2	2.55	0.41
1:C:129:VAL:O	1:C:129:VAL:CG1	2.68	0.41
1:A:15:ILE:HA	1:A:18:ILE:HG22	2.03	0.41
1:A:649:MET:O	1:A:650:ARG:C	2.62	0.41
1:B:317:PHE:CG	1:B:321:LEU:HD23	2.56	0.41
1:B:379:THR:OG1	1:B:398:MET:CE	2.57	0.41
1:B:478:MET:O	1:B:479:ALA:C	2.63	0.41
1:B:987:VAL:HG11	1:B:1005:MET:HG3	2.02	0.41
1:C:13:TRP:HA	1:C:13:TRP:HE3	1.83	0.41
1:C:409:ALA:O	1:C:413:VAL:HB	2.20	0.41
1:C:412:VAL:O	1:C:412:VAL:HG12	2.21	0.41
1:C:724:THR:OG1	1:C:725:PRO:N	2.53	0.41
1:C:937:LYS:CD	1:C:938:ASN:HD22	2.33	0.41
1:A:726:GLN:NE2	1:C:235:ILE:CD1	2.84	0.41
1:A:916:ARG:O	1:A:916:ARG:HG3	2.19	0.41
1:B:5:PHE:CE2	1:B:487:ILE:HD12	2.55	0.41
1:B:164:ASP:O	1:B:165:ALA:HB2	2.21	0.41
1:B:609:VAL:HG13	1:B:609:VAL:O	2.21	0.41
1:B:868:SER:HA	1:B:869:GLY:HA3	1.88	0.41
1:C:464:GLY:O	1:C:468:ARG:HG3	2.20	0.41
1:B:445:ILE:O	1:B:449:LEU:CB	2.61	0.40
1:C:40:PRO:HD2	1:C:674:LEU:HD11	2.03	0.40
1:C:613:ASN:C	1:C:613:ASN:ND2	2.76	0.40
1:C:882:PHE:O	1:C:885:LEU:CD1	2.69	0.40
1:B:240:LEU:CD2	1:B:249:ILE:HD11	2.52	0.40
1:C:284:GLN:HE21	1:C:284:GLN:HB3	1.61	0.40
1:C:952:LYS:HE3	1:C:952:LYS:CA	2.47	0.40
1:A:456:MET:HA	1:A:459:PHE:CD2	2.57	0.40
1:A:617:PHE:O	1:A:618:ALA:HB2	2.21	0.40
1:A:968:ARG:HG2	1:A:971:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:VAL:HG12	1:B:325:TYR:H	1.87	0.40
1:C:76:MET:SD	1:C:95:GLU:HA	2.61	0.40
1:C:878:LEU:O	1:C:881:VAL:N	2.46	0.40
1:A:449:LEU:HB2	1:A:478:MET:HE1	2.02	0.40
1:A:728:LYS:HA	1:C:235:ILE:O	2.22	0.40
1:A:898:VAL:HG11	1:A:940:ILE:HA	2.04	0.40
1:B:177:LEU:C	1:B:177:LEU:HD12	2.46	0.40
1:B:388:PHE:CE2	1:B:472:ILE:HG21	2.55	0.40
1:C:555:LEU:O	1:C:559:LEU:N	2.55	0.40
1:C:677:ALA:HB1	1:C:717:ARG:HH21	1.87	0.40
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.47	0.40
1:C:382:VAL:HG12	1:C:472:ILE:HD11	2.03	0.40
1:C:470:PHE:HA	1:C:473:THR:HG22	2.02	0.40
1:C:901:VAL:HG12	1:C:935:SER:HB3	2.03	0.40
1:C:983:VAL:HG12	1:C:983:VAL:O	2.22	0.40

There are no symmetry-related clashes.

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	1039/1050 (99%)	877 (84%)	116 (11%)	46 (4%)	2	12
1	B	1028/1050 (98%)	825 (80%)	148 (14%)	55 (5%)	1	9
1	C	1028/1050 (98%)	791 (77%)	155 (15%)	82 (8%)	1	3
All	All	3095/3150 (98%)	2493 (80%)	419 (14%)	183 (6%)	1	7

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	SER
1	A	366	LEU

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Mol	Chain	Res	Type
1	A	464	GLY
1	A	543	VAL
1	A	582	ALA
1	A	677	ALA
1	A	865	GLN
1	A	909	ALA
1	A	1033	LYS
1	B	68	ASN
1	B	165	ALA
1	B	181	GLN
1	B	215	ALA
1	B	337	ILE
1	B	362	PHE
1	B	633	ASP
1	B	636	ASP
1	B	644	VAL
1	B	659	LYS
1	B	861	GLY
1	B	863	SER
1	B	890	GLU
1	B	988	ILE
1	B	989	SER
1	C	7	ASP
1	C	9	PRO
1	C	10	ILE
1	C	62	THR
1	C	82	SER
1	C	83	ASP
1	C	124	GLN
1	C	125	GLN
1	C	401	ALA
1	C	422	GLU
1	C	425	LEU
1	C	431	THR
1	C	432	ARG
1	C	644	VAL
1	C	689	GLY
1	C	693	GLU
1	C	723	ASP
1	C	853	THR
1	C	859	TRP
1	C	870	ALA

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Mol	Chain	Res	Type
1	C	917	GLY
1	C	922	VAL
1	C	936	ALA
1	C	953	GLU
1	A	161	ASN
1	A	318	PRO
1	A	420	MET
1	A	435	MET
1	A	439	GLN
1	A	503	GLY
1	A	508	GLY
1	A	616	GLY
1	A	618	ALA
1	A	670	ALA
1	A	994	SER
1	A	1018	PHE
1	A	1034	ASN
1	A	1035	GLU
1	B	34	GLN
1	B	209	ALA
1	B	237	GLN
1	B	319	SER
1	B	359	LEU
1	B	364	ALA
1	B	388	PHE
1	B	432	ARG
1	B	440	GLY
1	B	455	PRO
1	B	456	MET
1	B	778	LYS
1	B	802	SER
1	B	867	ARG
1	C	51	GLY
1	C	61	VAL
1	C	296	GLY
1	C	298	ASN
1	C	299	ALA
1	C	356	TYR
1	C	362	PHE
1	C	400	LEU
1	C	409	ALA
1	C	428	LYS

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Mol	Chain	Res	Type
1	C	437	GLN
1	C	471	SER
1	C	510	LYS
1	C	511	GLY
1	C	640	GLU
1	C	656	SER
1	C	687	GLN
1	C	701	GLN
1	C	722	GLU
1	C	778	LYS
1	C	855	VAL
1	C	861	GLY
1	C	887	ALA
1	C	952	LYS
1	C	957	LEU
1	C	1029	ARG
1	A	21	LEU
1	A	250	LEU
1	A	490	PRO
1	A	533	GLY
1	A	645	GLU
1	A	669	PRO
1	A	795	ASP
1	A	867	ARG
1	A	950	MET
1	B	135	SER
1	B	243	THR
1	B	320	GLY
1	B	367	ILE
1	B	657	GLN
1	B	661	ALA
1	B	678	THR
1	B	795	ASP
1	B	814	PRO
1	B	866	GLU
1	B	959	GLU
1	C	53	ASP
1	C	81	ASN
1	C	106	GLN
1	C	423	GLU
1	C	427	PRO
1	C	454	VAL

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Mol	Chain	Res	Type
1	C	618	ALA
1	C	896	PHE
1	A	35	TYR
1	A	459	PHE
1	A	507	GLU
1	A	538	THR
1	B	36	PRO
1	B	380	PHE
1	B	439	GLN
1	B	800	PRO
1	B	820	ASN
1	C	73	ASP
1	C	390	ILE
1	C	501	ALA
1	C	871	PRO
1	C	875	ALA
1	C	913	ALA
1	C	915	PHE
1	C	955	LYS
1	A	358	PHE
1	A	418	ARG
1	A	509	LYS
1	B	54	ALA
1	B	431	THR
1	B	510	LYS
1	B	895	PRO
1	C	22	ALA
1	C	683	GLU
1	C	692	HIS
1	C	852	PRO
1	C	939	ALA
1	A	929	LEU
1	A	1037	ILE
1	B	402	ILE
1	B	442	LEU
1	B	454	VAL
1	B	539	GLY
1	B	676	THR
1	B	949	LEU
1	C	76	MET
1	C	285	PRO
1	C	387	GLY

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Mol	Chain	Res	Type
1	C	825	MET
1	C	929	LEU
1	C	942	ILE
1	A	368	PRO
1	A	954	GLY
1	C	685	ILE
1	C	823	PRO
1	A	419	VAL
1	C	129	VAL
1	C	822	LEU
1	A	870	ALA
1	C	932	ILE
1	A	14	VAL

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	847/856 (99%)	739 (87%)	108 (13%)	4	19
1	B	836/856 (98%)	724 (87%)	112 (13%)	4	18
1	C	836/856 (98%)	702 (84%)	134 (16%)	2	12
All	All	2519/2568 (98%)	2165 (86%)	354 (14%)	3	16

All (354) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	ILE
1	A	18	ILE
1	A	27	ILE
1	A	32	VAL
1	A	46	SER
1	A	50	PRO
1	A	72	ILE
1	A	78	MET

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Mol	Chain	Res	Type
1	A	79	SER
1	A	87	THR
1	A	88	VAL
1	A	96	SER
1	A	107	VAL
1	A	129	VAL
1	A	132	SER
1	A	135	SER
1	A	138	MET
1	A	150	THR
1	A	155	SER
1	A	169	THR
1	A	197	GLN
1	A	230	LEU
1	A	231	ASN
1	A	234	ILE
1	A	242	SER
1	A	243	THR
1	A	249	ILE
1	A	253	VAL
1	A	258	SER
1	A	262	LEU
1	A	323	ILE
1	A	337	ILE
1	A	341	VAL
1	A	343	THR
1	A	348	ILE
1	A	349	ILE
1	A	351	VAL
1	A	355	MET
1	A	366	LEU
1	A	369	THR
1	A	375	VAL
1	A	382	VAL
1	A	392	THR
1	A	406	VAL
1	A	411	VAL
1	A	413	VAL
1	A	422	GLU
1	A	435	MET
1	A	452	VAL
1	A	473	THR

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Mol	Chain	Res	Type
1	A	474	ILE
1	A	475	VAL
1	A	480	LEU
1	A	489	THR
1	A	498	LYS
1	A	510	LYS
1	A	512	PHE
1	A	518	ARG
1	A	535	LEU
1	A	547	ILE
1	A	550	VAL
1	A	552	MET
1	A	587	THR
1	A	595	THR
1	A	603	LYS
1	A	606	VAL
1	A	617	PHE
1	A	626	ILE
1	A	630	SER
1	A	640	GLU
1	A	648	THR
1	A	659	LYS
1	A	662	MET
1	A	721	LEU
1	A	724	THR
1	A	737	GLN
1	A	741	VAL
1	A	778	LYS
1	A	795	ASP
1	A	801	PHE
1	A	802	SER
1	A	806	SER
1	A	808	ARG
1	A	822	LEU
1	A	825	MET
1	A	842	GLU
1	A	844	MET
1	A	847	LEU
1	A	849	SER
1	A	853	THR
1	A	858	ASP
1	A	866	GLU

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Mol	Chain	Res	Type
1	A	897	SER
1	A	910	LEU
1	A	911	LEU
1	A	916	ARG
1	A	918	LEU
1	A	934	LEU
1	A	942	ILE
1	A	966	ARG
1	A	968	ARG
1	A	977	LEU
1	A	990	THR
1	A	1010	THR
1	A	1027	ARG
1	A	1034	ASN
1	A	1038	GLU
1	B	1	MET
1	B	25	LEU
1	B	34	GLN
1	B	56	THR
1	B	57	VAL
1	B	70	ASN
1	B	72	ILE
1	B	75	LEU
1	B	78	MET
1	B	82	SER
1	B	83	ASP
1	B	91	THR
1	B	108	GLN
1	B	130	GLU
1	B	134	SER
1	B	140	VAL
1	B	177	LEU
1	B	185	ARG
1	B	193	LEU
1	B	214	VAL
1	B	233	SER
1	B	234	ILE
1	B	237	GLN
1	B	241	THR
1	B	244	GLU
1	B	267	LYS
1	B	277	ILE

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Mol	Chain	Res	Type
1	B	293	LEU
1	B	309	GLU
1	B	330	THR
1	B	337	ILE
1	B	345	VAL
1	B	349	ILE
1	B	354	VAL
1	B	356	TYR
1	B	361	ASN
1	B	362	PHE
1	B	369	THR
1	B	370	ILE
1	B	372	VAL
1	B	374	VAL
1	B	377	LEU
1	B	383	LEU
1	B	393	LEU
1	B	404	LEU
1	B	405	LEU
1	B	423	GLU
1	B	478	MET
1	B	480	LEU
1	B	484	VAL
1	B	486	LEU
1	B	495	THR
1	B	500	ILE
1	B	519	MET
1	B	524	THR
1	B	526	HIS
1	B	529	ASP
1	B	535	LEU
1	B	548	ILE
1	B	556	PHE
1	B	558	ARG
1	B	564	LEU
1	B	586	ARG
1	B	588	GLN
1	B	599	LEU
1	B	604	ASN
1	B	608	SER
1	B	626	ILE
1	B	630	SER

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Mol	Chain	Res	Type
1	B	652	THR
1	B	666	PHE
1	B	674	LEU
1	B	693	GLU
1	B	708	LYS
1	B	713	LEU
1	B	714	THR
1	B	726	GLN
1	B	729	ILE
1	B	730	ASP
1	B	731	ILE
1	B	739	LEU
1	B	773	VAL
1	B	791	VAL
1	B	797	GLN
1	B	825	MET
1	B	828	LEU
1	B	843	LEU
1	B	846	GLN
1	B	858	ASP
1	B	862	MET
1	B	865	GLN
1	B	867	ARG
1	B	877	SER
1	B	878	LEU
1	B	879	ILE
1	B	883	LEU
1	B	891	SER
1	B	893	SER
1	B	899	MET
1	B	900	LEU
1	B	907	ILE
1	B	914	THR
1	B	915	PHE
1	B	918	LEU
1	B	919	THR
1	B	963	ASP
1	B	968	ARG
1	B	969	LEU
1	B	987	VAL
1	B	988	ILE
1	B	990	THR

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Mol	Chain	Res	Type
1	B	1000	VAL
1	C	13	TRP
1	C	18	ILE
1	C	29	LYS
1	C	30	LEU
1	C	32	VAL
1	C	38	ILE
1	C	41	PRO
1	C	43	VAL
1	C	58	GLN
1	C	61	VAL
1	C	77	TYR
1	C	79	SER
1	C	80	SER
1	C	84	SER
1	C	91	THR
1	C	93	THR
1	C	102	ILE
1	C	122	VAL
1	C	125	GLN
1	C	129	VAL
1	C	145	THR
1	C	158	VAL
1	C	172	VAL
1	C	177	LEU
1	C	185	ARG
1	C	197	GLN
1	C	237	GLN
1	C	239	ARG
1	C	241	THR
1	C	242	SER
1	C	252	LYS
1	C	254	ASN
1	C	268	ILE
1	C	285	PRO
1	C	300	LEU
1	C	301	ASP
1	C	302	THR
1	C	310	LEU
1	C	314	GLU
1	C	329	THR
1	C	337	ILE

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Mol	Chain	Res	Type
1	C	348	ILE
1	C	349	ILE
1	C	357	LEU
1	C	363	ARG
1	C	389	SER
1	C	394	THR
1	C	395	MET
1	C	399	VAL
1	C	404	LEU
1	C	408	ASP
1	C	413	VAL
1	C	414	GLU
1	C	417	GLU
1	C	419	VAL
1	C	422	GLU
1	C	423	GLU
1	C	425	LEU
1	C	435	MET
1	C	454	VAL
1	C	456	MET
1	C	463	THR
1	C	469	GLN
1	C	471	SER
1	C	483	LEU
1	C	487	ILE
1	C	495	THR
1	C	504	ASP
1	C	517	ASN
1	C	544	LEU
1	C	546	LEU
1	C	549	VAL
1	C	550	VAL
1	C	552	MET
1	C	583	THR
1	C	587	THR
1	C	591	LEU
1	C	604	ASN
1	C	613	ASN
1	C	620	ARG
1	C	622	GLN
1	C	624	THR
1	C	626	ILE

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Mol	Chain	Res	Type
1	C	641	GLU
1	C	647	ILE
1	C	656	SER
1	C	659	LYS
1	C	685	ILE
1	C	690	LEU
1	C	699	ARG
1	C	701	GLN
1	C	702	LEU
1	C	705	GLU
1	C	729	ILE
1	C	730	ASP
1	C	733	GLN
1	C	737	GLN
1	C	739	LEU
1	C	763	ILE
1	C	768	VAL
1	C	783	PRO
1	C	784	ASP
1	C	786	ILE
1	C	801	PHE
1	C	815	ARG
1	C	825	MET
1	C	828	LEU
1	C	841	MET
1	C	843	LEU
1	C	845	GLU
1	C	849	SER
1	C	853	THR
1	C	863	SER
1	C	881	VAL
1	C	882	PHE
1	C	885	LEU
1	C	888	LEU
1	C	891	SER
1	C	894	ILE
1	C	918	LEU
1	C	930	THR
1	C	937	LYS
1	C	941	LEU
1	C	952	LYS
1	C	953	GLU

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Mol	Chain	Res	Type
1	C	963	ASP
1	C	967	MET
1	C	981	LEU
1	C	987	VAL
1	C	988	ILE
1	C	1014	LEU
1	C	1016	ILE
1	C	1026	VAL
1	C	1029	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	68	ASN
1	A	74	ASN
1	A	109	ASN
1	A	112	GLN
1	A	123	GLN
1	A	144	ASN
1	A	181	GLN
1	A	218	GLN
1	A	229	GLN
1	A	237	GLN
1	A	569	GLN
1	A	726	GLN
1	A	737	GLN
1	A	920	ASN
1	A	925	GLN
1	A	998	ASN
1	B	67	GLN
1	B	74	ASN
1	B	81	ASN
1	B	124	GLN
1	B	151	GLN
1	B	191	ASN
1	B	237	GLN
1	B	338	HIS
1	B	469	GLN
1	B	577	GLN
1	B	588	GLN
1	B	604	ASN

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Mol	Chain	Res	Type
1	B	605	ASN
1	B	622	GLN
1	B	623	ASN
1	B	642	ASN
1	B	667	ASN
1	B	797	GLN
1	B	820	ASN
1	B	865	GLN
1	B	920	ASN
1	B	997	GLN
1	B	998	ASN
1	C	109	ASN
1	C	210	GLN
1	C	228	GLN
1	C	255	GLN
1	C	284	GLN
1	C	298	ASN
1	C	469	GLN
1	C	613	ASN
1	C	657	GLN
1	C	709	HIS
1	C	719	ASN
1	C	733	GLN
1	C	737	GLN
1	C	744	ASN
1	C	997	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1041/1050 (99%)	0.09	27 (2%)	57	34	21, 70, 147, 190	0
1	B	1030/1050 (98%)	0.38	38 (3%)	45	25	27, 98, 147, 173	0
1	C	1030/1050 (98%)	0.42	66 (6%)	25	13	24, 87, 142, 207	0
All	All	3101/3150 (98%)	0.29	131 (4%)	40	22	21, 86, 147, 207	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	441	ALA	5.4
1	A	499	PRO	5.2
1	A	500	ILE	4.8
1	A	636	ASP	4.8
1	B	957	LEU	4.5
1	A	635	ALA	4.2
1	A	1037	ILE	4.1
1	B	599	LEU	4.1
1	C	6	ILE	4.0
1	A	534	ILE	3.9
1	B	501	ALA	3.8
1	C	55	LYS	3.6
1	C	5	PHE	3.5
1	C	681	ASP	3.5
1	C	854	GLY	3.5
1	A	617	PHE	3.5
1	B	504	ASP	3.4
1	B	421	ALA	3.4
1	C	837	THR	3.3
1	C	855	VAL	3.3
1	C	859	TRP	3.3
1	C	691	GLY	3.3
1	C	958	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	548	ILE	3.3
1	A	501	ALA	3.2
1	C	707	ALA	3.2
1	C	950	MET	3.2
1	B	511	GLY	3.1
1	B	1028	ARG	3.1
1	A	230	LEU	3.0
1	A	544	LEU	3.0
1	C	512	PHE	3.0
1	B	546	LEU	2.9
1	A	866	GLU	2.9
1	A	958	ILE	2.8
1	B	316	PHE	2.8
1	A	541	TYR	2.8
1	C	964	ALA	2.7
1	A	898	VAL	2.7
1	B	548	ILE	2.7
1	A	408	ASP	2.7
1	C	957	LEU	2.7
1	C	515	TRP	2.7
1	C	1021	VAL	2.7
1	B	874	TYR	2.7
1	B	459	PHE	2.7
1	B	890	GLU	2.7
1	A	1014	LEU	2.7
1	C	535	LEU	2.6
1	C	822	LEU	2.6
1	C	427	PRO	2.6
1	B	604	ASN	2.6
1	B	278	ILE	2.6
1	B	956	GLY	2.6
1	C	496	MET	2.5
1	C	823	PRO	2.5
1	B	359	LEU	2.5
1	C	407	ASP	2.5
1	C	417	GLU	2.5
1	B	494	ALA	2.5
1	B	962	LEU	2.5
1	B	497	LEU	2.5
1	C	426	PRO	2.5
1	B	385	ALA	2.4
1	B	870	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	52	ALA	2.4
1	C	999	ALA	2.4
1	B	402	ILE	2.4
1	B	862	MET	2.4
1	B	1008	MET	2.4
1	C	408	ASP	2.4
1	C	536	ARG	2.4
1	C	618	ALA	2.4
1	A	904	LEU	2.4
1	B	350	LEU	2.4
1	A	480	LEU	2.4
1	A	883	LEU	2.4
1	C	352	PHE	2.4
1	C	113	LEU	2.4
1	C	117	LEU	2.4
1	C	548	ILE	2.3
1	C	59	ASP	2.3
1	B	628	PHE	2.3
1	C	429	GLU	2.3
1	B	10	ILE	2.3
1	C	834	GLY	2.3
1	C	969	LEU	2.3
1	A	352	PHE	2.3
1	C	677	ALA	2.3
1	B	918	LEU	2.3
1	B	505	HIS	2.3
1	C	989	SER	2.3
1	C	709	HIS	2.2
1	A	897	SER	2.2
1	C	447	MET	2.2
1	C	415	ASN	2.2
1	C	497	LEU	2.2
1	B	523	SER	2.2
1	C	49	TYR	2.2
1	C	935	SER	2.2
1	C	1016	ILE	2.2
1	A	538	THR	2.1
1	C	853	THR	2.1
1	C	544	LEU	2.1
1	C	941	LEU	2.1
1	A	417	GLU	2.1
1	A	954	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	682	PHE	2.1
1	A	504	ASP	2.1
1	A	529	ASP	2.1
1	B	958	ILE	2.1
1	C	874	TYR	2.1
1	C	339	GLU	2.1
1	B	666	PHE	2.1
1	B	509	LYS	2.1
1	C	949	LEU	2.1
1	C	294	ALA	2.1
1	B	507	GLU	2.1
1	C	883	LEU	2.1
1	C	973	LEU	2.1
1	C	494	ALA	2.1
1	C	831	ALA	2.1
1	B	451	ALA	2.0
1	C	861	GLY	2.0
1	C	499	PRO	2.0
1	C	946	ALA	2.0
1	B	512	PHE	2.0
1	C	503	GLY	2.0
1	C	833	PRO	2.0
1	B	351	VAL	2.0
1	C	419	VAL	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.