



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 AM UTC

PDB ID : 5AFF / pdb_00005aff
Title : Symportin 1 chaperones 5S RNP assembly during ribosome biogenesis by occupying an essential rRNA binding site
Authors : Calvino, F.R.; Kharde, S.; Wild, K.; Bange, G.; Sinning, I.
Deposited on : 2015-01-21
Resolution : 3.40 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

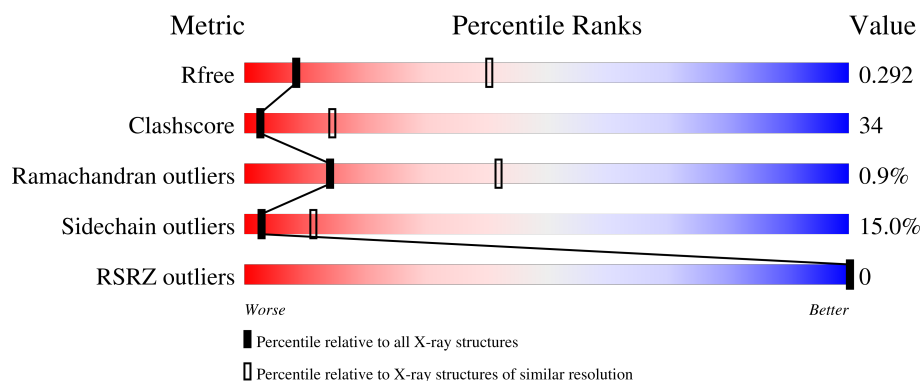
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	654	
2	B	48	
3	C	173	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5606 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 SYMPORTIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4414	2800	756	845	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP G0S5S6

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	0	0	0
			245	161	45	39			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	expression tag	UNP G0SEG2
B	-5	HIS	-	expression tag	UNP G0SEG2
B	-4	HIS	-	expression tag	UNP G0SEG2
B	-3	HIS	-	expression tag	UNP G0SEG2
B	-2	HIS	-	expression tag	UNP G0SEG2
B	-1	HIS	-	expression tag	UNP G0SEG2
B	0	HIS	-	expression tag	UNP G0SEG2

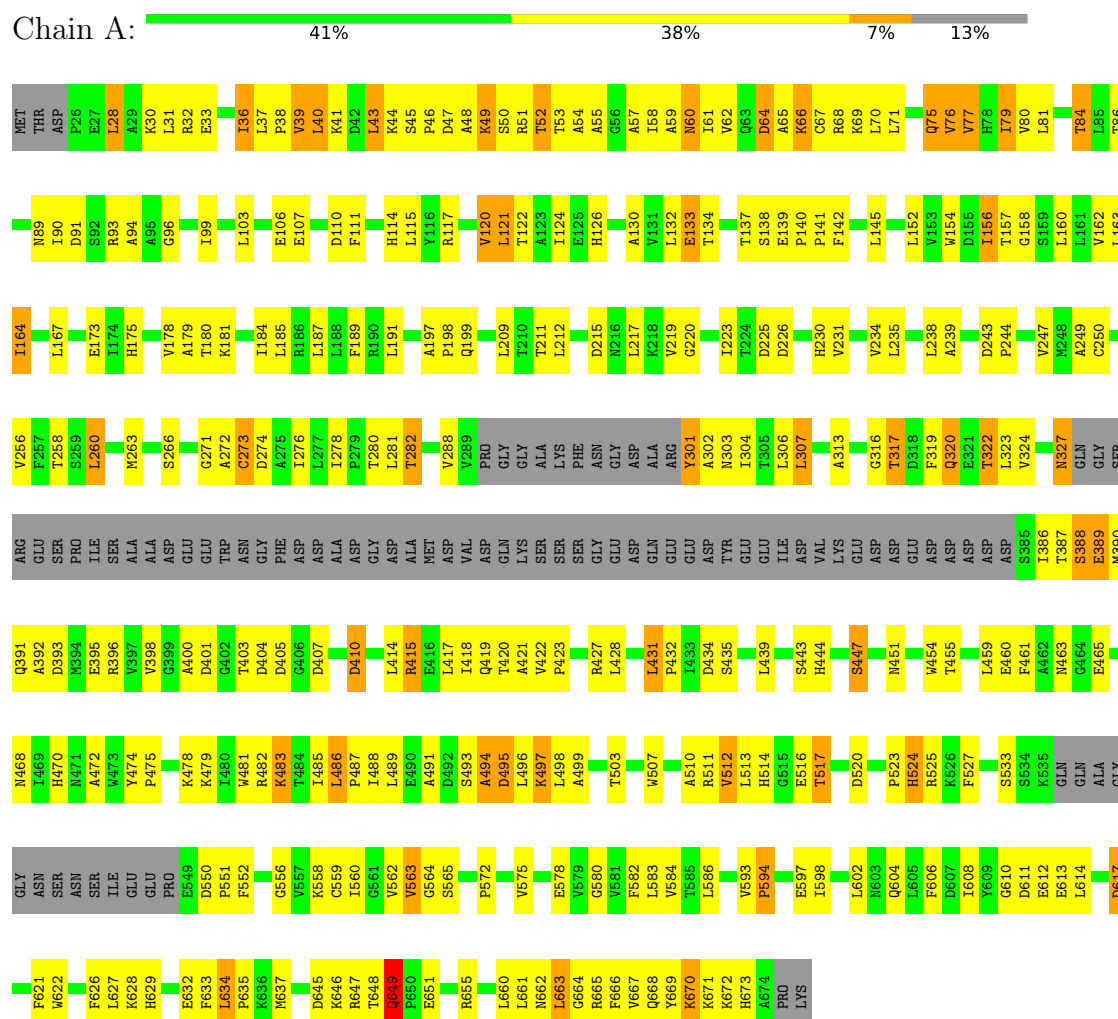
- Molecule 3 is a protein called RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	117	Total	C	N	O	S	0	0	0
			947	601	169	173	4			

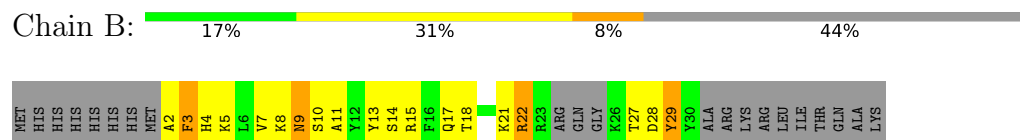
3 Residue-property plots

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.

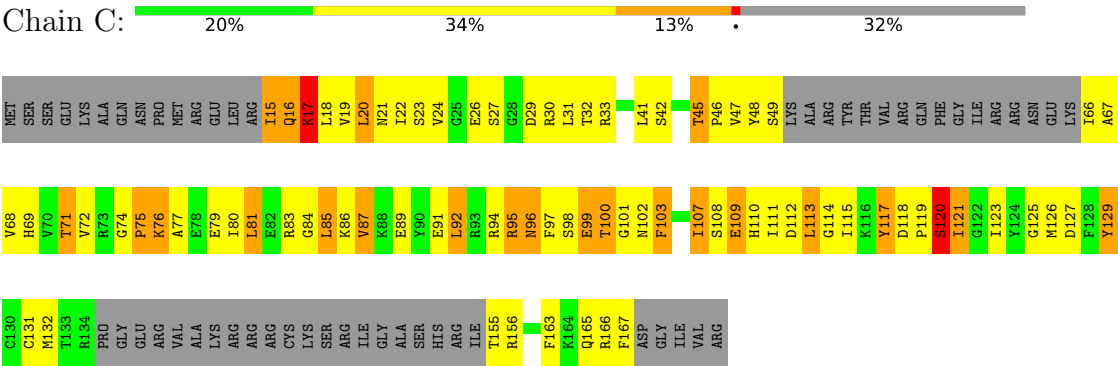
• Molecule 1: SYMPORTIN 1



• Molecule 2: RIBOSOMAL PROTEIN L5



● Molecule 3: RIBOSOMAL PROTEIN L11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.09Å 105.96Å 147.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 3.40 49.26 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.26-3.40) 99.8 (49.26-3.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.236 , 0.300 0.234 , 0.292	Depositor DCC
R_{free} test set	665 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	113.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 138.3	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	0.94	EDS
Total number of atoms	5606	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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	0.36	0/4487	0.92	15/6101 (0.2%)
2	B	0.57	0/251	1.00	0/331
3	C	0.73	0/962	1.62	23/1288 (1.8%)
All	All	0.45	0/5700	1.07	38/7720 (0.5%)

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

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	108	SER	N-CA-C	10.96	126.98	113.17
3	C	95	ARG	N-CA-C	10.20	123.65	111.82
3	C	129	TYR	N-CA-C	9.17	123.48	108.26
3	C	120	SER	N-CA-C	-8.61	102.33	112.92
3	C	45	THR	CA-C-N	8.18	128.62	120.52
3	C	45	THR	C-N-CA	8.18	128.62	120.52
3	C	117	TYR	N-CA-C	7.60	120.91	108.52
3	C	94	ARG	N-CA-C	7.44	120.44	111.82
3	C	119	PRO	CA-C-N	-7.28	111.00	122.65
3	C	119	PRO	C-N-CA	-7.28	111.00	122.65
3	C	114	GLY	N-CA-C	7.27	125.77	115.30
1	A	649	GLN	CA-C-N	7.20	127.04	119.05
1	A	649	GLN	C-N-CA	7.20	127.04	119.05
1	A	495	ASP	N-CA-C	6.90	119.47	110.43
1	A	388	SER	CB-CA-C	-6.84	108.69	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	LEU	CA-C-N	6.65	126.67	119.89
1	A	431	LEU	C-N-CA	6.65	126.67	119.89
3	C	21	ASN	N-CA-C	6.30	119.84	108.69
3	C	165	GLN	N-CA-C	6.26	117.77	111.07
3	C	17	LYS	N-CA-C	6.07	119.43	109.72
1	A	494	ALA	CB-CA-C	-5.98	109.69	116.63
3	C	110	HIS	N-CA-C	-5.90	106.43	113.21
3	C	92	LEU	N-CA-C	5.84	118.99	110.17
3	C	99	GLU	N-CA-C	-5.81	105.29	112.38
1	A	388	SER	N-CA-C	5.47	117.32	108.08
3	C	95	ARG	CB-CA-C	-5.44	100.22	110.67
1	A	36	ILE	N-CA-C	5.44	116.51	111.45
3	C	18	LEU	N-CA-C	-5.34	100.47	109.07
1	A	52	THR	N-CA-C	-5.33	105.47	111.28
3	C	45	THR	N-CA-C	-5.31	102.96	109.65
1	A	517	THR	CA-C-N	5.25	126.40	119.84
1	A	517	THR	C-N-CA	5.25	126.40	119.84
3	C	103	PHE	N-CA-C	5.25	116.82	108.79
3	C	121	ILE	CA-C-N	-5.14	112.55	121.39
3	C	121	ILE	C-N-CA	-5.14	112.55	121.39
1	A	594	PRO	CA-C-N	5.05	124.65	119.05
1	A	594	PRO	C-N-CA	5.05	124.65	119.05
1	A	463	ASN	CB-CA-C	-5.02	110.81	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4414	0	4488	308	1
2	B	245	0	244	25	0
3	C	947	0	953	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5606	0	5685	383	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:VAL:HG12	2:B:8:LYS:HG3	1.18	1.10
3:C:24:VAL:HG11	3:C:30:ARG:HG2	1.35	1.07
3:C:29:ASP:OD2	3:C:33:ARG:NH2	1.88	1.06
1:A:670:LYS:HA	1:A:670:LYS:HE2	1.40	1.00
1:A:47:ASP:HB2	1:A:50:SER:HB3	1.48	0.95
3:C:47:VAL:HG11	3:C:69:HIS:CE1	2.00	0.95
1:A:386:ILE:HD13	3:C:71:THR:HG21	1.50	0.94
1:A:51:ARG:HA	1:A:54:ALA:HB3	1.49	0.92
1:A:403:THR:CG2	3:C:125:GLY:HA3	2.00	0.92
1:A:403:THR:HG21	3:C:125:GLY:HA3	1.53	0.91
1:A:55:ALA:HA	1:A:58:ILE:HG13	1.53	0.90
1:A:303:ASN:HA	1:A:306:LEU:CD1	2.02	0.88
1:A:393:ASP:O	1:A:396:ARG:N	2.07	0.87
1:A:303:ASN:HA	1:A:306:LEU:HD12	1.56	0.87
1:A:431:LEU:HB2	1:A:432:PRO:HD2	1.54	0.87
1:A:482:ARG:HA	1:A:486:LEU:HD22	1.57	0.86
1:A:386:ILE:CD1	3:C:71:THR:HG21	2.06	0.86
1:A:282:THR:HG21	1:A:420:THR:HG22	1.58	0.86
3:C:16:GLN:OE1	3:C:17:LYS:NZ	2.08	0.85
1:A:32:ARG:HD2	1:A:70:LEU:HD11	1.58	0.85
1:A:220:GLY:HA3	1:A:260:LEU:HD21	1.59	0.84
1:A:247:VAL:HG12	1:A:307:LEU:HD23	1.58	0.83
1:A:401:ASP:OD2	1:A:472:ALA:HA	1.78	0.83
1:A:32:ARG:CD	1:A:70:LEU:HD11	2.08	0.83
1:A:68:ARG:NH1	1:A:106:GLU:HB3	1.95	0.82
1:A:64:ASP:OD1	1:A:64:ASP:N	2.11	0.81
1:A:211:THR:OG1	2:B:22:ARG:NH1	2.14	0.81
3:C:118:ASP:HB3	3:C:121:ILE:HD13	1.62	0.80
1:A:273:CYS:SG	1:A:274:ASP:N	2.54	0.79
1:A:672:LYS:HD3	1:A:673:HIS:HE2	1.48	0.79
1:A:482:ARG:HA	1:A:486:LEU:CD2	2.13	0.78
1:A:403:THR:HG21	3:C:125:GLY:CA	2.14	0.78
1:A:404:ASP:OD2	3:C:23:SER:N	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:VAL:HG13	3:C:76:LYS:HE3	1.64	0.78
1:A:59:ALA:HA	1:A:62:VAL:HG12	1.66	0.78
1:A:395:GLU:O	1:A:398:VAL:HG12	1.83	0.77
1:A:583:LEU:HA	1:A:586:LEU:HD12	1.66	0.76
2:B:7:VAL:CG1	2:B:8:LYS:HG3	2.10	0.76
1:A:219:VAL:O	1:A:223:ILE:HG13	1.84	0.76
1:A:486:LEU:HB2	1:A:487:PRO:HD3	1.66	0.76
1:A:606:PHE:HZ	1:A:663:LEU:HB2	1.51	0.76
1:A:670:LYS:HA	1:A:670:LYS:CE	2.14	0.75
1:A:479:LYS:NZ	3:C:109:GLU:HG3	2.02	0.75
1:A:427:ARG:HD2	3:C:117:TYR:CE2	2.22	0.75
1:A:43:LEU:HD12	1:A:58:ILE:CD1	2.17	0.74
1:A:65:ALA:O	1:A:68:ARG:HG2	1.87	0.74
3:C:15:ILE:N	3:C:131:CYS:O	2.22	0.73
1:A:55:ALA:HA	1:A:58:ILE:CG1	2.19	0.72
1:A:403:THR:HG1	3:C:107:ILE:C	1.96	0.72
3:C:99:GLU:HG3	3:C:156:ARG:NH2	2.04	0.72
3:C:48:TYR:CE1	3:C:68:VAL:HG12	2.24	0.72
1:A:651:GLU:OE2	2:B:15:ARG:NH2	2.23	0.71
1:A:45:SER:C	1:A:47:ASP:H	1.99	0.71
3:C:47:VAL:HG12	3:C:69:HIS:O	1.91	0.71
1:A:247:VAL:CG1	1:A:307:LEU:HD23	2.20	0.71
1:A:427:ARG:HD2	3:C:117:TYR:HE2	1.53	0.71
1:A:671:LYS:HG2	1:A:672:LYS:N	2.05	0.70
1:A:278:ILE:O	1:A:282:THR:OG1	2.09	0.70
1:A:410:ASP:OD1	1:A:410:ASP:N	2.22	0.70
1:A:55:ALA:CA	1:A:58:ILE:HG13	2.21	0.70
1:A:666:PHE:CZ	2:B:2:ALA:HB1	2.26	0.70
3:C:24:VAL:CG1	3:C:30:ARG:HG2	2.18	0.70
1:A:403:THR:OG1	3:C:107:ILE:O	2.09	0.69
1:A:662:ASN:O	1:A:666:PHE:HB2	1.91	0.69
1:A:57:ALA:C	1:A:61:ILE:HD12	2.18	0.69
1:A:48:ALA:O	1:A:52:THR:HG23	1.93	0.69
1:A:649:GLN:OE1	1:A:649:GLN:N	2.26	0.69
1:A:47:ASP:CB	1:A:50:SER:HB3	2.21	0.69
3:C:92:LEU:HD12	3:C:92:LEU:N	2.07	0.69
3:C:98:SER:O	3:C:156:ARG:HG2	1.93	0.68
1:A:60:ASN:ND2	1:A:60:ASN:H	1.91	0.68
1:A:115:LEU:HB3	1:A:120:VAL:HG11	1.75	0.67
3:C:83:ARG:HD2	3:C:113:LEU:O	1.93	0.67
3:C:118:ASP:HB3	3:C:121:ILE:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:O	1:A:191:LEU:HD12	1.93	0.67
1:A:451:ASN:O	2:B:17:GLN:NE2	2.27	0.67
1:A:461:PHE:CD1	1:A:470:HIS:HB2	2.29	0.67
1:A:110:ASP:OD1	1:A:111:PHE:N	2.29	0.66
3:C:118:ASP:CB	3:C:121:ILE:HD13	2.24	0.66
1:A:43:LEU:HB2	1:A:58:ILE:HD11	1.78	0.65
2:B:28:ASP:O	2:B:29:TYR:HB2	1.95	0.65
3:C:97:PHE:HA	3:C:102:ASN:O	1.97	0.65
1:A:181:LYS:HB2	1:A:184:ILE:HD12	1.78	0.64
1:A:317:THR:O	1:A:320:GLN:HB3	1.96	0.64
1:A:76:VAL:O	1:A:80:VAL:HG23	1.97	0.64
1:A:388:SER:OG	1:A:389:GLU:N	2.28	0.64
1:A:28:LEU:O	1:A:32:ARG:HG3	1.97	0.64
1:A:96:GLY:HA2	1:A:99:ILE:HD12	1.79	0.64
3:C:48:TYR:CD1	3:C:68:VAL:HG12	2.32	0.64
1:A:661:LEU:HD21	1:A:665:ARG:CZ	2.28	0.64
1:A:666:PHE:CZ	2:B:3:PHE:O	2.51	0.64
1:A:32:ARG:NH2	1:A:66:LYS:HG2	2.13	0.64
2:B:9:ASN:N	2:B:9:ASN:OD1	2.30	0.63
1:A:64:ASP:HB2	1:A:67:CYS:SG	2.38	0.63
1:A:486:LEU:O	1:A:489:LEU:N	2.30	0.63
1:A:661:LEU:HD11	1:A:665:ARG:HE	1.63	0.63
1:A:386:ILE:CD1	3:C:71:THR:CG2	2.76	0.63
1:A:57:ALA:O	1:A:60:ASN:ND2	2.27	0.63
1:A:491:ALA:HB1	1:A:493:SER:HB3	1.80	0.63
1:A:455:THR:OG1	2:B:17:GLN:NE2	2.32	0.62
1:A:230:HIS:O	1:A:234:VAL:HG23	2.00	0.62
1:A:666:PHE:HZ	2:B:3:PHE:H	1.46	0.62
1:A:133:GLU:O	1:A:137:THR:HB	1.99	0.62
1:A:495:ASP:OD1	1:A:496:LEU:N	2.33	0.62
3:C:85:LEU:HD11	3:C:163:PHE:HE1	1.63	0.62
1:A:57:ALA:O	1:A:61:ILE:HD12	2.00	0.61
1:A:672:LYS:HD3	1:A:673:HIS:NE2	2.14	0.61
1:A:36:ILE:C	1:A:38:PRO:HD2	2.25	0.61
1:A:661:LEU:HD21	1:A:665:ARG:NH2	2.16	0.61
1:A:163:LEU:O	1:A:167:LEU:HD12	2.01	0.61
1:A:55:ALA:HA	1:A:58:ILE:CD1	2.30	0.61
1:A:497:LYS:HB2	1:A:497:LYS:HZ3	1.66	0.61
1:A:313:ALA:HB1	1:A:451:ASN:ND2	2.15	0.61
1:A:404:ASP:CG	3:C:23:SER:H	2.09	0.61
1:A:479:LYS:HZ2	3:C:109:GLU:HG3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ARG:CD	3:C:117:TYR:CE2	2.85	0.60
1:A:139:GLU:HB2	1:A:140:PRO:HD3	1.84	0.60
1:A:617:ASP:O	1:A:621:PHE:HB3	2.01	0.60
1:A:59:ALA:O	1:A:62:VAL:HG12	2.00	0.60
3:C:99:GLU:HG3	3:C:156:ARG:CZ	2.31	0.60
3:C:41:LEU:HD13	3:C:41:LEU:O	2.02	0.60
1:A:611:ASP:HB3	1:A:614:LEU:HG	1.83	0.59
1:A:124:ILE:HG23	1:A:160:LEU:HD22	1.85	0.59
1:A:134:THR:HG22	1:A:142:PHE:HD1	1.68	0.59
1:A:220:GLY:CA	1:A:260:LEU:HD21	2.30	0.59
1:A:486:LEU:HB2	1:A:487:PRO:CD	2.32	0.58
1:A:320:GLN:O	1:A:324:VAL:HG23	2.03	0.58
3:C:98:SER:O	3:C:101:GLY:N	2.30	0.58
1:A:43:LEU:HD12	1:A:58:ILE:HD13	1.83	0.58
1:A:415:ARG:O	1:A:419:GLN:HB2	2.03	0.58
1:A:316:GLY:HA2	1:A:319:PHE:CE2	2.38	0.58
1:A:663:LEU:CD1	1:A:667:VAL:HG23	2.34	0.58
1:A:68:ARG:HH12	1:A:106:GLU:HB3	1.68	0.58
3:C:20:LEU:HA	3:C:127:ASP:O	2.04	0.58
1:A:54:ALA:O	1:A:58:ILE:HG13	2.04	0.58
1:A:386:ILE:HD13	3:C:71:THR:CG2	2.30	0.58
1:A:226:ASP:O	1:A:230:HIS:HA	2.04	0.57
1:A:621:PHE:CZ	1:A:627:LEU:HB2	2.39	0.57
1:A:256:VAL:HG12	1:A:260:LEU:HD11	1.86	0.57
3:C:33:ARG:HD3	3:C:120:SER:O	2.05	0.57
1:A:303:ASN:CA	1:A:306:LEU:HD12	2.31	0.57
1:A:507:TRP:O	1:A:511:ARG:HG3	2.05	0.57
1:A:414:LEU:HD11	1:A:418:ILE:HD11	1.86	0.56
1:A:660:LEU:O	1:A:664:GLY:N	2.29	0.56
1:A:668:GLN:O	1:A:671:LYS:HD2	2.05	0.56
1:A:37:LEU:N	1:A:38:PRO:HD2	2.20	0.56
1:A:400:ALA:HB2	3:C:96:ASN:OD1	2.05	0.56
3:C:109:GLU:C	3:C:111:ILE:H	2.12	0.56
1:A:661:LEU:HD11	1:A:665:ARG:NE	2.21	0.56
1:A:427:ARG:CD	3:C:117:TYR:HE2	2.18	0.56
1:A:604:GLN:O	1:A:608:ILE:HG13	2.06	0.56
1:A:580:GLY:O	1:A:584:VAL:HG23	2.06	0.56
3:C:15:ILE:N	3:C:132:MET:HA	2.21	0.56
1:A:51:ARG:O	1:A:55:ALA:N	2.34	0.55
1:A:59:ALA:HA	1:A:62:VAL:CG1	2.35	0.55
1:A:665:ARG:HH12	2:B:5:LYS:HE3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HD3	1:A:70:LEU:HD11	1.86	0.55
1:A:474:TYR:HB3	1:A:475:PRO:HD3	1.87	0.55
1:A:666:PHE:CE2	2:B:2:ALA:HB1	2.41	0.55
1:A:662:ASN:O	1:A:666:PHE:N	2.37	0.55
1:A:59:ALA:CA	1:A:62:VAL:HG12	2.35	0.55
1:A:434:ASP:OD1	1:A:435:SER:N	2.40	0.54
2:B:4:HIS:ND1	2:B:5:LYS:N	2.55	0.54
1:A:386:ILE:HD12	3:C:71:THR:HG21	1.90	0.54
1:A:217:LEU:HD12	1:A:260:LEU:HD23	1.89	0.54
3:C:23:SER:HA	3:C:67:ALA:HA	1.90	0.54
1:A:524:HIS:CE1	1:A:575:VAL:HG13	2.42	0.54
3:C:99:GLU:CG	3:C:156:ARG:CZ	2.85	0.54
3:C:115:ILE:HD12	3:C:115:ILE:N	2.22	0.54
1:A:62:VAL:HG23	1:A:71:LEU:HD13	1.90	0.54
1:A:663:LEU:HD12	1:A:667:VAL:HG23	1.88	0.54
3:C:41:LEU:O	3:C:41:LEU:HD22	2.08	0.53
1:A:89:ASN:OD1	1:A:91:ASP:HB2	2.07	0.53
1:A:663:LEU:HD12	1:A:663:LEU:C	2.33	0.53
1:A:427:ARG:NH2	1:A:428:LEU:HD21	2.24	0.53
3:C:115:ILE:HD12	3:C:115:ILE:H	1.73	0.53
1:A:48:ALA:HA	1:A:51:ARG:HG2	1.89	0.53
1:A:51:ARG:HA	1:A:54:ALA:CB	2.31	0.53
1:A:158:GLY:O	1:A:162:VAL:HG23	2.08	0.53
3:C:76:LYS:O	3:C:80:ILE:HG13	2.08	0.53
1:A:256:VAL:CG1	1:A:260:LEU:HD11	2.39	0.53
1:A:395:GLU:C	1:A:398:VAL:HG12	2.34	0.53
1:A:594:PRO:HD2	1:A:597:GLU:OE1	2.08	0.53
1:A:403:THR:HG21	3:C:125:GLY:C	2.34	0.52
3:C:41:LEU:HD13	3:C:41:LEU:C	2.34	0.52
3:C:166:ARG:O	3:C:167:PHE:CD2	2.63	0.52
1:A:247:VAL:HG12	1:A:307:LEU:CD2	2.34	0.52
1:A:404:ASP:OD2	3:C:23:SER:CB	2.58	0.52
1:A:30:LYS:O	1:A:33:GLU:HG3	2.10	0.52
1:A:485:ILE:O	1:A:489:LEU:HG	2.10	0.52
1:A:491:ALA:HB1	1:A:493:SER:CB	2.40	0.51
3:C:15:ILE:HD12	3:C:132:MET:HE3	1.93	0.51
3:C:47:VAL:HG11	3:C:69:HIS:ND1	2.23	0.51
1:A:481:TRP:O	1:A:485:ILE:HB	2.10	0.51
3:C:48:TYR:CE1	3:C:68:VAL:CG1	2.93	0.51
1:A:239:ALA:HB1	1:A:250:CYS:SG	2.51	0.50
1:A:231:VAL:O	1:A:235:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:TYR:O	1:A:304:ILE:HB	2.12	0.50
1:A:672:LYS:HB3	1:A:673:HIS:HD2	1.76	0.50
1:A:130:ALA:O	1:A:133:GLU:HG3	2.12	0.50
3:C:84:GLY:HA2	3:C:87:VAL:HG23	1.93	0.50
3:C:98:SER:OG	3:C:102:ASN:HB2	2.10	0.50
3:C:98:SER:C	3:C:156:ARG:HE	2.19	0.50
1:A:386:ILE:HD12	3:C:71:THR:CG2	2.42	0.50
3:C:48:TYR:HE1	3:C:68:VAL:CG1	2.24	0.50
1:A:647:ARG:HG3	1:A:648:THR:HG23	1.93	0.50
1:A:525:ARG:NH2	1:A:578:GLU:OE2	2.45	0.49
1:A:115:LEU:C	1:A:120:VAL:HG12	2.38	0.49
1:A:661:LEU:O	1:A:665:ARG:N	2.24	0.49
1:A:443:SER:O	1:A:447:SER:OG	2.29	0.49
1:A:663:LEU:HD12	1:A:663:LEU:O	2.12	0.49
2:B:11:ALA:O	2:B:14:SER:OG	2.26	0.49
2:B:10:SER:O	2:B:14:SER:HB3	2.13	0.49
3:C:42:SER:HB2	3:C:72:VAL:HG21	1.95	0.49
1:A:160:LEU:O	1:A:164:ILE:HG13	2.13	0.49
1:A:398:VAL:HG22	1:A:398:VAL:O	2.12	0.49
1:A:558:LYS:O	1:A:562:VAL:HG12	2.12	0.49
1:A:138:SER:C	1:A:141:PRO:HB3	2.38	0.48
1:A:479:LYS:O	1:A:483:LYS:HB2	2.13	0.48
1:A:479:LYS:HG3	1:A:483:LYS:HG3	1.95	0.48
1:A:634:LEU:N	1:A:635:PRO:HD2	2.29	0.48
3:C:15:ILE:HD12	3:C:132:MET:CE	2.43	0.48
1:A:179:ALA:HB1	1:A:219:VAL:HG23	1.94	0.48
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.66	0.48
3:C:166:ARG:O	3:C:167:PHE:HB2	2.13	0.48
1:A:115:LEU:O	1:A:120:VAL:HG12	2.13	0.48
1:A:59:ALA:C	1:A:62:VAL:HG12	2.39	0.48
1:A:44:LYS:O	1:A:46:PRO:HD3	2.13	0.48
1:A:189:PHE:CD1	1:A:231:VAL:HG11	2.49	0.48
3:C:97:PHE:CD2	3:C:103:PHE:HB3	2.49	0.48
1:A:621:PHE:HZ	1:A:627:LEU:HB2	1.79	0.48
1:A:45:SER:C	1:A:47:ASP:N	2.67	0.47
1:A:76:VAL:HG13	1:A:77:VAL:H	1.79	0.47
1:A:551:PRO:HB2	1:A:552:PHE:CD1	2.49	0.47
1:A:323:LEU:O	1:A:327:ASN:ND2	2.47	0.47
1:A:156:ILE:HG22	1:A:157:THR:N	2.30	0.47
1:A:610:GLY:O	2:B:2:ALA:HB2	2.15	0.47
1:A:62:VAL:O	1:A:62:VAL:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:PHE:HE2	1:A:622:TRP:CH2	2.32	0.47
3:C:75:PRO:O	3:C:79:GLU:HG3	2.14	0.47
1:A:572:PRO:HB2	1:A:575:VAL:HG23	1.97	0.47
1:A:666:PHE:CE1	2:B:3:PHE:O	2.68	0.47
1:A:49:LYS:HA	1:A:52:THR:HG23	1.97	0.46
1:A:134:THR:O	1:A:137:THR:HG22	2.14	0.46
1:A:302:ALA:O	1:A:306:LEU:HD12	2.15	0.46
3:C:45:THR:HA	3:C:46:PRO:HD3	1.56	0.46
1:A:439:LEU:HD13	1:A:439:LEU:C	2.40	0.46
1:A:454:TRP:CH2	1:A:511:ARG:HD2	2.50	0.46
1:A:479:LYS:HZ3	3:C:109:GLU:HG3	1.78	0.46
1:A:51:ARG:O	1:A:55:ALA:HB3	2.16	0.46
1:A:496:LEU:O	1:A:499:ALA:HB3	2.14	0.46
1:A:322:THR:HG22	1:A:323:LEU:HD23	1.97	0.46
3:C:101:GLY:HA3	3:C:155:THR:O	2.14	0.46
1:A:68:ARG:HG3	1:A:69:LYS:N	2.31	0.46
1:A:80:VAL:HA	1:A:84:THR:OG1	2.16	0.46
1:A:258:THR:HA	1:A:263:MET:HE3	1.97	0.46
1:A:271:GLY:O	1:A:273:CYS:N	2.48	0.46
1:A:427:ARG:NH1	3:C:117:TYR:HE2	2.14	0.46
1:A:39:VAL:HG11	1:A:61:ILE:HD13	1.97	0.46
1:A:524:HIS:ND1	1:A:575:VAL:HG13	2.31	0.46
3:C:109:GLU:CB	3:C:112:ASP:OD2	2.64	0.46
1:A:40:LEU:HD23	1:A:44:LYS:HE3	1.98	0.45
1:A:58:ILE:HA	1:A:61:ILE:CD1	2.45	0.45
1:A:115:LEU:HB3	1:A:120:VAL:CG1	2.46	0.45
1:A:621:PHE:HA	1:A:626:PHE:CD2	2.51	0.45
1:A:41:LYS:HA	1:A:44:LYS:HD2	1.99	0.45
1:A:75:GLN:O	1:A:79:ILE:HG13	2.16	0.45
3:C:100:THR:OG1	3:C:102:ASN:ND2	2.49	0.45
3:C:166:ARG:O	3:C:167:PHE:CB	2.64	0.45
1:A:90:ILE:HB	1:A:93:ARG:HH21	1.82	0.45
1:A:130:ALA:HA	1:A:133:GLU:CG	2.47	0.45
1:A:673:HIS:N	1:A:673:HIS:CD2	2.84	0.45
1:A:392:ALA:O	1:A:395:GLU:HB2	2.16	0.45
1:A:669:TYR:CD1	1:A:669:TYR:C	2.94	0.45
3:C:74:GLY:HA3	3:C:75:PRO:HD2	1.83	0.45
1:A:247:VAL:O	1:A:250:CYS:HB2	2.17	0.45
1:A:582:PHE:CE2	1:A:586:LEU:HD11	2.52	0.45
2:B:3:PHE:HD1	2:B:3:PHE:HA	1.54	0.45
1:A:178:VAL:C	1:A:180:THR:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:SER:O	1:A:266:SER:OG	2.29	0.45
1:A:239:ALA:HB2	1:A:249:ALA:CB	2.47	0.45
1:A:645:ASP:OD1	1:A:647:ARG:HG2	2.17	0.45
3:C:47:VAL:HG11	3:C:69:HIS:NE2	2.29	0.45
1:A:223:ILE:HG23	1:A:231:VAL:HG13	1.98	0.45
1:A:649:GLN:N	1:A:649:GLN:CD	2.74	0.45
1:A:94:ALA:HA	1:A:156:ILE:HG13	1.99	0.44
1:A:138:SER:HA	1:A:141:PRO:HB3	1.99	0.44
1:A:454:TRP:CZ3	2:B:13:TYR:HB3	2.52	0.44
1:A:514:HIS:C	1:A:516:GLU:H	2.25	0.44
1:A:32:ARG:HB3	1:A:70:LEU:CD1	2.48	0.44
1:A:163:LEU:C	1:A:167:LEU:HD12	2.43	0.44
1:A:239:ALA:HB2	1:A:249:ALA:HB3	1.98	0.44
1:A:598:ILE:O	1:A:602:LEU:HG	2.17	0.44
3:C:42:SER:HB2	3:C:72:VAL:CG2	2.48	0.44
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.80	0.44
1:A:273:CYS:O	1:A:276:ILE:HG12	2.17	0.44
1:A:672:LYS:CB	1:A:673:HIS:HD2	2.30	0.44
3:C:77:ALA:O	3:C:81:LEU:HB2	2.17	0.44
3:C:101:GLY:HA3	3:C:155:THR:C	2.42	0.44
3:C:102:ASN:HB2	3:C:129:TYR:OH	2.17	0.44
1:A:486:LEU:CB	1:A:487:PRO:HD3	2.42	0.44
1:A:495:ASP:OD2	1:A:497:LYS:HD2	2.18	0.44
1:A:49:LYS:HE3	1:A:49:LYS:HB2	1.79	0.44
1:A:197:ALA:HB1	1:A:198:PRO:CD	2.48	0.44
1:A:520:ASP:O	1:A:523:PRO:HD3	2.17	0.44
3:C:19:VAL:HG22	3:C:71:THR:HB	2.00	0.44
1:A:414:LEU:HD12	1:A:414:LEU:O	2.17	0.44
1:A:154:TRP:HA	1:A:154:TRP:CE3	2.52	0.44
1:A:444:HIS:O	1:A:447:SER:N	2.51	0.44
1:A:431:LEU:HB2	1:A:432:PRO:CD	2.39	0.43
1:A:499:ALA:O	1:A:503:THR:OG1	2.24	0.43
1:A:563:VAL:CG1	1:A:564:GLY:N	2.81	0.43
3:C:117:TYR:CD1	3:C:117:TYR:C	2.94	0.43
1:A:468:ASN:OD1	1:A:468:ASN:N	2.51	0.43
3:C:41:LEU:CD1	3:C:80:ILE:HD13	2.48	0.43
1:A:223:ILE:HG23	1:A:231:VAL:CG1	2.48	0.43
1:A:665:ARG:HH12	2:B:5:LYS:CE	2.32	0.43
1:A:43:LEU:O	1:A:51:ARG:HD3	2.18	0.43
1:A:76:VAL:HG13	1:A:77:VAL:N	2.33	0.43
1:A:614:LEU:O	1:A:617:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TRP:HA	1:A:154:TRP:HE3	1.83	0.43
3:C:22:ILE:O	3:C:68:VAL:N	2.52	0.43
1:A:58:ILE:HA	1:A:61:ILE:HD12	2.00	0.43
1:A:142:PHE:HA	1:A:145:LEU:HD12	2.00	0.43
1:A:610:GLY:O	2:B:2:ALA:CB	2.67	0.43
1:A:629:HIS:O	1:A:632:GLU:HB2	2.18	0.43
1:A:388:SER:O	1:A:391:GLN:N	2.52	0.43
1:A:122:THR:HG22	1:A:126:HIS:NE2	2.34	0.43
1:A:223:ILE:CG2	1:A:231:VAL:HG13	2.49	0.42
1:A:417:LEU:O	1:A:421:ALA:HB3	2.19	0.42
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.85	0.42
1:A:512:VAL:HG12	1:A:513:LEU:N	2.34	0.42
1:A:524:HIS:CD2	1:A:524:HIS:N	2.87	0.42
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.82	0.42
1:A:313:ALA:HB1	1:A:451:ASN:HD22	1.81	0.42
1:A:389:GLU:HA	1:A:392:ALA:CB	2.50	0.42
1:A:496:LEU:HD23	1:A:496:LEU:C	2.44	0.42
1:A:593:VAL:HG13	1:A:597:GLU:OE1	2.19	0.42
1:A:628:LYS:O	1:A:632:GLU:HG3	2.20	0.42
1:A:665:ARG:NH1	2:B:5:LYS:CG	2.83	0.42
1:A:560:ILE:HD11	1:A:597:GLU:HB3	2.00	0.42
1:A:486:LEU:CB	1:A:487:PRO:CD	2.94	0.42
1:A:393:ASP:HA	1:A:396:ARG:HG3	2.01	0.42
1:A:489:LEU:HD11	1:A:527:PHE:CZ	2.55	0.42
1:A:606:PHE:CZ	1:A:663:LEU:HB2	2.41	0.42
1:A:316:GLY:HA2	1:A:319:PHE:HE2	1.82	0.42
1:A:68:ARG:CG	1:A:69:LYS:N	2.83	0.41
1:A:556:GLY:O	1:A:560:ILE:HG13	2.20	0.41
1:A:121:LEU:HD11	1:A:178:VAL:HG22	2.01	0.41
1:A:459:LEU:HB2	1:A:461:PHE:CE2	2.56	0.41
1:A:460:GLU:HB3	1:A:465:GLU:HG2	2.01	0.41
1:A:510:ALA:HB1	1:A:565:SER:HB2	2.02	0.41
2:B:7:VAL:HG12	2:B:8:LYS:N	2.35	0.41
1:A:43:LEU:HD12	1:A:58:ILE:HD12	1.97	0.41
1:A:47:ASP:CB	1:A:50:SER:CB	2.96	0.41
1:A:243:ASP:HA	1:A:244:PRO:HD3	1.88	0.41
1:A:278:ILE:HA	1:A:281:LEU:HD12	2.02	0.41
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.76	0.41
1:A:559:CYS:O	1:A:563:VAL:HB	2.21	0.41
1:A:671:LYS:O	1:A:673:HIS:N	2.53	0.41
1:A:36:ILE:O	1:A:39:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD13	1:A:187:LEU:HD13	2.03	0.41
1:A:389:GLU:HA	1:A:392:ALA:HB3	2.03	0.41
1:A:497:LYS:HD3	1:A:498:LEU:H	1.86	0.41
3:C:91:GLU:C	3:C:92:LEU:HD12	2.46	0.41
1:A:51:ARG:O	1:A:55:ALA:CB	2.69	0.41
1:A:175:HIS:CE1	1:A:212:LEU:HA	2.56	0.41
1:A:478:LYS:O	1:A:481:TRP:HB3	2.21	0.41
1:A:662:ASN:OD1	2:B:5:LYS:HB2	2.21	0.41
1:A:323:LEU:HD13	1:A:459:LEU:HD11	2.03	0.41
1:A:612:GLU:HA	1:A:617:ASP:CG	2.46	0.41
1:A:633:PHE:CE2	1:A:637:MET:HB2	2.56	0.41
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.85	0.40
1:A:422:VAL:N	1:A:423:PRO:HD2	2.36	0.40
3:C:92:LEU:N	3:C:92:LEU:CD1	2.77	0.40
1:A:612:GLU:CD	1:A:673:HIS:ND1	2.80	0.40
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.82	0.40
1:A:646:LYS:O	1:A:646:LYS:HG2	2.22	0.40
1:A:68:ARG:HA	1:A:71:LEU:HD12	2.02	0.40
1:A:130:ALA:HA	1:A:133:GLU:HG3	2.04	0.40
3:C:83:ARG:HD2	3:C:83:ARG:HH11	1.67	0.40
3:C:86:LYS:O	3:C:89:GLU:N	2.51	0.40
3:C:99:GLU:HA	3:C:156:ARG:CG	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:HIS:ND1	1:A:225:ASP:OD2[4_445]	2.11	0.09

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	560/654 (86%)	509 (91%)	49 (9%)	2 (0%)	30	59
2	B	23/48 (48%)	21 (91%)	1 (4%)	1 (4%)	2	13
3	C	111/173 (64%)	97 (87%)	11 (10%)	3 (3%)	4	20
All	All	694/875 (79%)	627 (90%)	61 (9%)	6 (1%)	14	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	ALA
2	B	29	TYR
3	C	87	VAL
3	C	75	PRO
1	A	107	GLU
3	C	16	GLN

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	485/556 (87%)	421 (87%)	64 (13%)	4	16
2	B	25/43 (58%)	19 (76%)	6 (24%)	1	2
3	C	102/150 (68%)	80 (78%)	22 (22%)	1	3
All	All	612/749 (82%)	520 (85%)	92 (15%)	3	11

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	31	LEU
1	A	39	VAL
1	A	40	LEU
1	A	43	LEU
1	A	49	LYS
1	A	53	THR

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Mol	Chain	Res	Type
1	A	60	ASN
1	A	64	ASP
1	A	66	LYS
1	A	75	GLN
1	A	76	VAL
1	A	77	VAL
1	A	79	ILE
1	A	81	LEU
1	A	84	THR
1	A	86	THR
1	A	117	ARG
1	A	120	VAL
1	A	121	LEU
1	A	133	GLU
1	A	152	LEU
1	A	156	ILE
1	A	164	ILE
1	A	173	GLU
1	A	199	GLN
1	A	215	ASP
1	A	238	LEU
1	A	260	LEU
1	A	273	CYS
1	A	280	THR
1	A	282	THR
1	A	288	VAL
1	A	301	TYR
1	A	307	LEU
1	A	317	THR
1	A	320	GLN
1	A	322	THR
1	A	327	ASN
1	A	387	THR
1	A	389	GLU
1	A	390	MET
1	A	405	ASP
1	A	407	ASP
1	A	410	ASP
1	A	415	ARG
1	A	447	SER
1	A	483	LYS
1	A	486	LEU

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Mol	Chain	Res	Type
1	A	488	ILE
1	A	497	LYS
1	A	512	VAL
1	A	517	THR
1	A	524	HIS
1	A	533	SER
1	A	550	ASP
1	A	563	VAL
1	A	613	GLU
1	A	617	ASP
1	A	634	LEU
1	A	649	GLN
1	A	655	ARG
1	A	663	LEU
1	A	670	LYS
2	B	3	PHE
2	B	9	ASN
2	B	18	THR
2	B	21	LYS
2	B	22	ARG
2	B	27	THR
3	C	15	ILE
3	C	17	LYS
3	C	20	LEU
3	C	26	GLU
3	C	27	SER
3	C	31	LEU
3	C	32	THR
3	C	49	SER
3	C	66	ILE
3	C	71	THR
3	C	76	LYS
3	C	81	LEU
3	C	85	LEU
3	C	95	ARG
3	C	96	ASN
3	C	100	THR
3	C	107	ILE
3	C	109	GLU
3	C	113	LEU
3	C	120	SER
3	C	123	ILE

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Mol	Chain	Res	Type
3	C	126	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	105	GLN
1	A	216	ASN
1	A	524	HIS
1	A	589	GLN
1	A	673	HIS
2	B	17	GLN
3	C	102	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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	568/654 (86%)	-0.37	0 100 100	34, 119, 221, 299	0
2	B	27/48 (56%)	-0.12	0 100 100	101, 146, 233, 257	0
3	C	117/173 (67%)	-0.03	0 100 100	109, 196, 282, 392	0
All	All	712/875 (81%)	-0.31	0 100 100	34, 137, 241, 392	0

There are no RSRZ outliers to report.

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.