



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:01 am BST

PDB ID : 5AFF  
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](mailto: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.

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

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

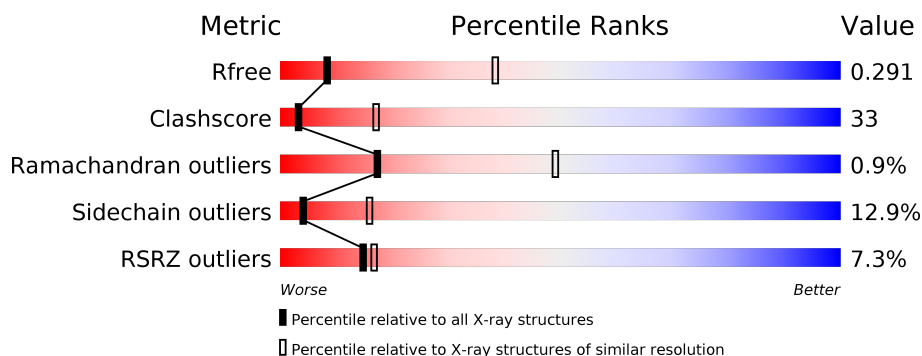
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>4%</div> <div>42%</div> <div>39%</div> <div>6%</div> <div>13%</div> </div>
2	B	48	<div> <div>23%</div> <div>23%</div> <div>10%</div> <div>44%</div> </div>
3	C	173	<div> <div>17%</div> <div>25%</div> <div>34%</div> <div>9%</div> <div>32%</div> </div>

## 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			

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

Chain A:

Position	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20																																			
Met	THR	ASP	P26	E27	L28	A29	K30	R31	L32	R33	E33	T36	L37	P38	V39	L40	K41	D42	L43	K44	S45	P46	D47	A48	K49	L50	R51	T52	T53	A54	G56	A57	I58	A59	N60	I61	V62	Q63	D64	A65	K66	C67	R68	K69	L70	L71	Q75	V76	V77	H78	I79	L81	T84	I85	T86

Chain B:  23% 23% 10% 44%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.236 , 0.300 0.234 , 0.291	Depositor DCC
$R_{free}$ test set	665 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	113.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 115.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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	0.27	0/4487	0.54	1/6101 (0.0%)
2	B	0.53	0/251	0.69	0/331
3	C	0.57	0/962	1.10	4/1288 (0.3%)
All	All	0.35	0/5700	0.67	5/7720 (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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	LEU	CA-CB-CG	-7.02	99.16	115.30
3	C	108	SER	N-CA-C	5.92	126.98	111.00
1	A	666	PHE	CB-CG-CD1	-5.29	117.09	120.80
3	C	95	ARG	CB-CA-C	-5.09	100.22	110.40
3	C	114	GLY	N-CA-C	5.07	125.77	113.10

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	299	1
2	B	245	0	244	24	0
3	C	947	0	953	88	0
All	All	5606	0	5685	372	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 33.

All (372) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:48:ALA:O	1:A:52:THR:HG23	1.93	0.69
1:A:649:GLN:N	1:A:649:GLN:OE1	2.26	0.69
1:A:47:ASP:CB	1:A:50:SER:HB3	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:403:THR:HG1	3:C:107:ILE:C	1.95	0.68
1:A:60:ASN:H	1:A:60:ASN:ND2	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
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:45:SER:C	1:A:47:ASP:H	1.99	0.66
2:B:28:ASP:O	2:B:29:TYR:HB2	1.95	0.66
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:479:LYS:HZ2	3:C:109:GLU:HG3	1.60	0.65
1:A:43:LEU:HB2	1:A:58:ILE:HD11	1.78	0.65
3:C:97:PHE:HA	3:C:102:ASN:O	1.97	0.65
1:A:57:ALA:C	1:A:61:ILE:HD12	2.18	0.64
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:388:SER:OG	1:A:389:GLU:N	2.28	0.64
1:A:76:VAL:O	1:A:80:VAL:HG23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:313:ALA:HB1	1:A:451:ASN:ND2	2.15	0.61
1:A:497:LYS:HB2	1:A:497:LYS:HZ3	1.66	0.61
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:415:ARG:O	1:A:419:GLN:HB2	2.03	0.58
1:A:43:LEU:HD12	1:A:58:ILE:HD13	1.83	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:386:ILE:HD13	3:C:71:THR:CG2	2.30	0.58
1:A:54:ALA:O	1:A:58:ILE:HG13	2.04	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:36:ILE:C	1:A:38:PRO:HD2	2.25	0.56
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
1:A:404:ASP:CG	3:C:23:SER:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:LEU:HD11	1:A:665:ARG:NE	2.21	0.56
1:A:604:GLN:O	1:A:608:ILE:HG13	2.06	0.56
1:A:427:ARG:CD	3:C:117:TYR:HE2	2.18	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
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:115:ILE:N	3:C:115:ILE:HD12	2.22	0.54
3:C:99:GLU:CG	3:C:156:ARG:CZ	2.85	0.54
3:C:15:ILE:HD12	3:C:132:MET:HE3	1.90	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:HD22	3:C:41:LEU:O	2.08	0.53
1:A:89:ASN:OD1	1:A:91:ASP:HB2	2.07	0.53
1:A:427:ARG:NH2	1:A:428:LEU:HD21	2.24	0.53
3:C:115:ILE:H	3:C:115:ILE:HD12	1.73	0.53
1:A:158:GLY:O	1:A:162:VAL:HG23	2.08	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
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:594:PRO:HD2	1:A:597:GLU:OE1	2.08	0.53
3:C:109:GLU:C	3:C:111:ILE:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:O	1:A:663:LEU:HD12	2.12	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:479:LYS:O	1:A:483:LYS:HB2	2.13	0.48
1:A:663:LEU:C	1:A:663:LEU:HD12	2.33	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:395:GLU:C	1:A:398:VAL:HG12	2.34	0.48
1:A:62:VAL:O	1:A:62:VAL:HG22	2.13	0.48
1:A:189:PHE:CD1	1:A:231:VAL:HG11	2.49	0.48
1:A:44:LYS:O	1:A:46:PRO:HD3	2.13	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:403:THR:HG21	3:C:125:GLY:C	2.34	0.48
3:C:41:LEU:C	3:C:41:LEU:HD13	2.34	0.48
1:A:551:PRO:HB2	1:A:552:PHE:CD1	2.49	0.47
1:A:76:VAL:HG13	1:A:77:VAL:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:SER:C	1:A:47:ASP:N	2.67	0.47
1:A:610:GLY:O	2:B:2:ALA:HB2	2.15	0.47
3:C:75:PRO:O	3:C:79:GLU:HG3	2.14	0.47
1:A:621:PHE:HE2	1:A:622:TRP:CH2	2.32	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: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
1:A:49:LYS:HA	1:A:52:THR:HG23	1.97	0.46
3:C:45:THR:HA	3:C:46:PRO:HD3	1.56	0.46
1:A:454:TRP:CH2	1:A:511:ARG:HD2	2.50	0.46
1:A:496:LEU:O	1:A:499:ALA:HB3	2.14	0.46
1:A:51:ARG:O	1:A:55:ALA:HB3	2.16	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: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:98:SER:C	3:C:156:ARG:HE	2.19	0.45
3:C:166:ARG:O	3:C:167:PHE:CB	2.64	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:90:ILE:HB	1:A:93:ARG:HH21	1.82	0.45
1:A:392:ALA:O	1:A:395:GLU:HB2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:SER:OG	1:A:266:SER:O	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:115:LEU:C	1:A:120:VAL:HG12	2.38	0.44
1:A:138:SER:HA	1:A:141:PRO:HB3	1.99	0.44
1:A:94:ALA:HA	1:A:156:ILE:HG13	1.99	0.44
1:A:454:TRP:CZ3	2:B:13:TYR:HB3	2.52	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
1:A:32:ARG:HB3	1:A:70:LEU:CD1	2.48	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:102:ASN:HB2	3:C:129:TYR:OH	2.17	0.44
3:C:77:ALA:O	3:C:81:LEU:HB2	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:197:ALA:HB1	1:A:198:PRO:CD	2.48	0.44
1:A:49:LYS:HB2	1:A:49:LYS:HE3	1.79	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:138:SER:C	1:A:141:PRO:HB3	2.38	0.44
1:A:414:LEU:HD12	1:A:414:LEU:O	2.17	0.44
1:A:154:TRP:CE3	1:A:154:TRP:HA	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:563:VAL:CG1	1:A:564:GLY:N	2.81	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:59:ALA:C	1:A:62:VAL:HG12	2.39	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:614:LEU:O	1:A:617:ASP:HB3	2.18	0.43
1:A:76:VAL:HG13	1:A:77:VAL:N	2.33	0.43
1:A:154:TRP:HE3	1:A:154:TRP:HA	1.83	0.43
3:C:22:ILE:O	3:C:68:VAL:N	2.52	0.43
1:A:142:PHE:HA	1:A:145:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HA	1:A:61:ILE:HD12	2.00	0.43
1:A:629:HIS:O	1:A:632:GLU:HB2	2.18	0.43
1:A:610:GLY:O	2:B:2:ALA:CB	2.67	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:389:GLU:HA	1:A:392:ALA:CB	2.50	0.42
1:A:313:ALA:HB1	1:A:451:ASN:HD22	1.81	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:439:LEU:C	1:A:439:LEU:HD13	2.40	0.42
1:A:556:GLY:O	1:A:560:ILE:HG13	2.20	0.41
1:A:68:ARG:CG	1:A:69:LYS:N	2.83	0.41
1:A:121:LEU:HD11	1:A:178:VAL:HG22	2.01	0.41
1:A:460:GLU:HB3	1:A:465:GLU:HG2	2.01	0.41
1:A:459:LEU:HB2	1:A:461:PHE:CE2	2.56	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:HA	1:A:121:LEU:HD12	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:132:LEU:HD13	1:A:187:LEU:HD13	2.03	0.41
1:A:36:ILE:O	1:A:39:VAL:HG23	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:669:TYR:CD1	1:A:669:TYR:C	2.94	0.40
1:A:68:ARG:HA	1:A:71:LEU:HD12	2.02	0.40
3:C:101:GLY:HA3	3:C:155:THR:C	2.42	0.40
1:A:130:ALA:HA	1:A:133:GLU:HG3	2.04	0.40
1:A:178:VAL:C	1:A:180:THR:H	2.25	0.40
3:C:117:TYR:C	3:C:117:TYR:CD1	2.94	0.40
3:C:99:GLU:HA	3:C:156:ARG:CG	2.51	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

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%)	34 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	23/48 (48%)	21 (91%)	1 (4%)	1 (4%)	2	17
3	C	111/173 (64%)	97 (87%)	11 (10%)	3 (3%)	5	26
All	All	694/875 (79%)	627 (90%)	61 (9%)	6 (1%)	17	49

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%)	428 (88%)	57 (12%)	5	19
2	B	25/43 (58%)	20 (80%)	5 (20%)	1	3
3	C	102/150 (68%)	85 (83%)	17 (17%)	2	8
All	All	612/749 (82%)	533 (87%)	79 (13%)	4	16

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	31	LEU
1	A	40	LEU
1	A	43	LEU
1	A	49	LYS
1	A	53	THR
1	A	60	ASN
1	A	64	ASP

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Mol	Chain	Res	Type
1	A	66	LYS
1	A	81	LEU
1	A	84	THR
1	A	86	THR
1	A	117	ARG
1	A	121	LEU
1	A	133	GLU
1	A	156	ILE
1	A	164	ILE
1	A	173	GLU
1	A	191	LEU
1	A	193	SER
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	317	THR
1	A	320	GLN
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	427	ARG
1	A	447	SER
1	A	483	LYS
1	A	486	LEU
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

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Mol	Chain	Res	Type
1	A	613	GLU
1	A	617	ASP
1	A	634	LEU
1	A	649	GLN
1	A	663	LEU
1	A	670	LYS
1	A	671	LYS
2	B	3	PHE
2	B	4	HIS
2	B	9	ASN
2	B	21	LYS
2	B	22	ARG
3	C	15	ILE
3	C	17	LYS
3	C	20	LEU
3	C	26	GLU
3	C	27	SER
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	107	ILE
3	C	113	LEU
3	C	120	SER
3	C	123	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
3	C	102	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	568/654 (86%)	0.14	23 (4%) 38 37	34, 119, 221, 299	0
2	B	27/48 (56%)	0.08	0 100 100	101, 146, 233, 257	0
3	C	117/173 (67%)	1.37	29 (24%) 0 0	109, 196, 282, 392	0
All	All	712/875 (81%)	0.34	52 (7%) 15 17	34, 137, 241, 392	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	72	VAL	10.2
3	C	103	PHE	8.4
3	C	18	LEU	6.4
3	C	132	MET	5.9
3	C	167	PHE	5.7
3	C	129	TYR	5.6
1	A	399	GLY	5.0
3	C	97	PHE	4.8
3	C	130	CYS	4.2
1	A	396	ARG	4.1
3	C	94	ARG	4.1
3	C	105	PHE	4.0
3	C	101	GLY	3.9
1	A	593	VAL	3.8
3	C	73	ARG	3.8
3	C	133	THR	3.7
3	C	19	VAL	3.7
3	C	102	ASN	3.6
1	A	142	PHE	3.5
3	C	128	PHE	3.5
1	A	519	THR	3.4
3	C	17	LYS	3.3
3	C	165	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	99	GLU	3.3
3	C	20	LEU	3.3
3	C	104	GLY	3.1
1	A	527	PHE	3.0
1	A	61	ILE	3.0
3	C	161	ARG	3.0
1	A	587	LEU	2.9
3	C	126	MET	2.9
3	C	131	CYS	2.8
1	A	588	ARG	2.8
1	A	583	LEU	2.7
3	C	162	TRP	2.6
1	A	605	LEU	2.6
3	C	16	GLN	2.6
1	A	488	ILE	2.5
1	A	630	LEU	2.5
3	C	84	GLY	2.4
1	A	394	MET	2.3
1	A	393	ASP	2.3
1	A	433	ILE	2.3
1	A	32	ARG	2.2
1	A	563	VAL	2.2
1	A	598	ILE	2.2
1	A	391	GLN	2.2
3	C	25	GLY	2.2
1	A	403	THR	2.1
3	C	41	LEU	2.1
1	A	626	PHE	2.1
1	A	637	MET	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.