



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:35 PM UTC

PDB ID : 4GMN / pdb_00004gmn
Title : Structural basis of Rpl5 recognition by Syo1
Authors : Bange, G.; Sinning, I.
Deposited on : 2012-08-16
Resolution : 2.95 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

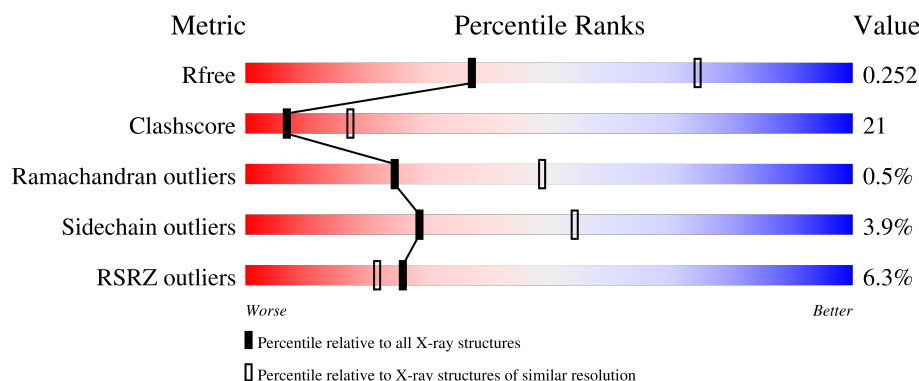
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	B	49	 6% 24% 14% 61%
2	A	676	 5% 52% 25% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4451 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 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	B	19	Total	C	N	O	0	0	0
			166	111	29	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	42	GLY	ASN	conflict	UNP G0SEG2
B	43	SER	LYS	conflict	UNP G0SEG2
B	44	HIS	TYR	conflict	UNP G0SEG2
B	45	HIS	ASN	conflict	UNP G0SEG2
B	46	HIS	-	expression tag	UNP G0SEG2
B	47	HIS	-	expression tag	UNP G0SEG2
B	48	HIS	-	expression tag	UNP G0SEG2
B	49	HIS	-	expression tag	UNP G0SEG2

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	551	Total	C	N	O	S	0	0	0
			4285	2724	738	812	11			

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.62Å 104.23Å 182.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.24 – 2.95 45.24 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.24-2.95) 97.8 (45.24-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.203 , 0.259 0.217 , 0.252	Depositor DCC
R_{free} test set	1606 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4451	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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	B	0.46	0/171	0.72	0/227
2	A	0.59	6/4360 (0.1%)	1.02	23/5931 (0.4%)
All	All	0.58	6/4531 (0.1%)	1.01	23/6158 (0.4%)

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
2	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	266	SER	C-N	5.78	1.41	1.33
2	A	431	LEU	C-N	5.77	1.41	1.33
2	A	197	ALA	C-N	5.48	1.41	1.33
2	A	432	PRO	N-CD	5.39	1.55	1.47
2	A	198	PRO	N-CD	5.18	1.55	1.47
2	A	267	PRO	N-CD	5.04	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	140	PRO	N-CA-C	8.87	121.52	110.70
2	A	661	LEU	N-CA-C	-8.51	101.59	111.03
2	A	74	GLU	N-CA-C	-7.88	99.39	110.50
2	A	140	PRO	CA-C-N	6.96	143.69	127.00
2	A	140	PRO	C-N-CA	6.96	143.69	127.00
2	A	303	ASN	N-CA-C	6.95	118.64	111.14
2	A	140	PRO	C-N-CD	-6.73	105.78	120.60
2	A	431	LEU	CA-C-N	-6.59	113.19	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	431	LEU	C-N-CA	-6.59	113.19	119.85
2	A	197	ALA	CA-C-N	-6.58	113.01	119.78
2	A	197	ALA	C-N-CA	-6.58	113.01	119.78
2	A	266	SER	CA-C-N	-6.49	113.30	119.85
2	A	266	SER	C-N-CA	-6.49	113.30	119.85
2	A	550	ASP	CA-C-N	6.48	126.71	119.32
2	A	550	ASP	C-N-CA	6.48	126.71	119.32
2	A	304	ILE	N-CA-C	5.94	116.72	110.72
2	A	408	LEU	N-CA-C	-5.84	103.55	111.55
2	A	671	LYS	N-CA-C	-5.80	98.45	110.80
2	A	301	TYR	N-CA-C	5.76	117.24	111.07
2	A	659	ALA	N-CA-C	5.72	117.52	111.28
2	A	671	LYS	N-CA-CB	5.71	120.14	110.49
2	A	514	HIS	N-CA-C	5.59	119.29	111.74
2	A	430	ASN	N-CA-C	5.10	116.53	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	140	PRO	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	B	166	0	164	10	0
2	A	4285	0	4365	189	2
All	All	4451	0	4529	192	2

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 21.

All (192) 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:A:432:PRO:CA	2:A:433:ILE:HG22	1.15	1.58
2:A:432:PRO:HA	2:A:433:ILE:CG2	1.23	1.57
2:A:244:PRO:HB3	2:A:300:ARG:NH2	1.80	0.96
2:A:65:ALA:O	2:A:66:LYS:HG2	1.67	0.93
2:A:78:HIS:O	2:A:82:THR:HG22	1.69	0.92
2:A:432:PRO:CB	2:A:433:ILE:HG22	2.03	0.89
2:A:432:PRO:CA	2:A:433:ILE:CG2	2.03	0.88
2:A:244:PRO:HB3	2:A:300:ARG:HH21	1.38	0.88
2:A:432:PRO:CB	2:A:433:ILE:CG2	2.50	0.88
2:A:285:LEU:HD22	2:A:428:LEU:CD1	2.04	0.87
2:A:432:PRO:HA	2:A:433:ILE:CB	2.06	0.84
2:A:507:TRP:O	2:A:511:ARG:HG3	1.75	0.84
1:B:18:THR:H	2:A:451:ASN:HD21	1.29	0.81
2:A:672:LYS:C	2:A:673:HIS:HD2	1.88	0.81
2:A:285:LEU:HD22	2:A:428:LEU:HD11	1.65	0.78
2:A:174:ILE:O	2:A:178:VAL:HG23	1.85	0.77
1:B:12:TYR:CE2	2:A:655:ARG:HD3	2.19	0.77
2:A:65:ALA:O	2:A:66:LYS:CG	2.32	0.77
2:A:417:LEU:O	2:A:422:VAL:HG23	1.85	0.76
1:B:17:GLN:HE22	2:A:451:ASN:HB3	1.50	0.76
2:A:432:PRO:CB	2:A:433:ILE:HG23	2.17	0.74
2:A:133:GLU:O	2:A:137:THR:HB	1.88	0.73
2:A:285:LEU:HD22	2:A:428:LEU:HD12	1.71	0.72
2:A:493:SER:HB2	2:A:494:ALA:HB2	1.72	0.71
2:A:101:LYS:HD3	2:A:159:SER:HA	1.72	0.70
2:A:262:TRP:CD2	2:A:268:GLY:HA3	2.26	0.69
2:A:51:ARG:HG3	2:A:52:THR:H	1.57	0.69
2:A:672:LYS:C	2:A:673:HIS:CD2	2.70	0.68
2:A:238:LEU:HD23	2:A:249:ALA:HB2	1.76	0.67
2:A:300:ARG:O	2:A:304:ILE:N	2.22	0.66
2:A:217:LEU:HD12	2:A:260:LEU:HD23	1.77	0.66
2:A:519:THR:HG23	2:A:519:THR:O	1.95	0.66
2:A:51:ARG:HG3	2:A:52:THR:N	2.12	0.65
2:A:139:GLU:HB2	2:A:140:PRO:HD3	1.78	0.65
2:A:108:GLU:HA	2:A:108:GLU:OE1	1.97	0.65
2:A:221:GLN:O	2:A:225:ASP:HB2	1.97	0.64
2:A:268:GLY:O	2:A:269:LYS:C	2.40	0.64
2:A:434:ASP:OD2	2:A:435:SER:N	2.31	0.64
2:A:436:ASP:O	2:A:439:LEU:HB3	1.98	0.64
2:A:647:ARG:HG3	2:A:648:THR:HG23	1.81	0.63
2:A:524:HIS:HE1	2:A:578:GLU:OE1	1.82	0.63
2:A:649:GLN:NE2	2:A:649:GLN:H	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:131:VAL:HG12	2:A:135:LEU:CD1	2.29	0.63
2:A:432:PRO:HB3	2:A:433:ILE:HG23	1.81	0.62
2:A:139:GLU:CB	2:A:140:PRO:HD3	2.29	0.62
2:A:69:LYS:HD2	2:A:69:LYS:N	2.13	0.62
2:A:513:LEU:HD13	2:A:517:THR:HA	1.82	0.62
2:A:430:ASN:HD21	2:A:483:LYS:HE2	1.64	0.61
2:A:244:PRO:HB3	2:A:300:ARG:CZ	2.31	0.61
2:A:112:CYS:HB3	2:A:167:LEU:HD23	1.80	0.61
2:A:495:ASP:HB3	2:A:498:LEU:HB3	1.83	0.60
2:A:566:LEU:HD12	2:A:566:LEU:C	2.26	0.60
2:A:36:ILE:HD12	2:A:61:ILE:HG21	1.84	0.60
2:A:262:TRP:CE3	2:A:268:GLY:HA3	2.37	0.59
2:A:563:VAL:HG13	2:A:579:VAL:HG13	1.84	0.59
2:A:254:HIS:HD2	2:A:274:ASP:OD1	1.86	0.59
2:A:62:VAL:HG21	2:A:103:LEU:HD21	1.85	0.59
2:A:36:ILE:HG21	2:A:71:LEU:HG	1.85	0.58
2:A:146:LEU:HB2	2:A:149:GLN:HB2	1.85	0.58
2:A:432:PRO:HB3	2:A:433:ILE:CG2	2.32	0.58
2:A:268:GLY:O	2:A:272:ALA:N	2.36	0.58
2:A:609:TYR:O	2:A:670:LYS:CE	2.52	0.57
2:A:293:ALA:HB1	2:A:437:GLU:OE1	2.04	0.57
2:A:43:LEU:HD21	2:A:84:THR:OG1	2.05	0.57
2:A:138:SER:HA	2:A:141:PRO:HB3	1.87	0.57
2:A:43:LEU:HD12	2:A:58:ILE:CD1	2.35	0.56
2:A:99:ILE:O	2:A:103:LEU:HG	2.05	0.56
2:A:98:GLU:O	2:A:102:VAL:HG23	2.05	0.56
2:A:670:LYS:O	2:A:673:HIS:N	2.26	0.55
2:A:76:VAL:HG13	2:A:77:VAL:N	2.22	0.55
2:A:617:ASP:O	2:A:621:PHE:HB3	2.06	0.55
2:A:101:LYS:O	2:A:105:GLN:HG3	2.06	0.54
2:A:62:VAL:CG2	2:A:103:LEU:HD21	2.38	0.54
1:B:18:THR:H	2:A:451:ASN:ND2	2.03	0.54
2:A:524:HIS:CE1	2:A:578:GLU:OE1	2.62	0.53
2:A:515:GLY:H	2:A:517:THR:CG2	2.22	0.53
1:B:17:GLN:HE22	2:A:451:ASN:CB	2.19	0.53
2:A:110:ASP:OD2	2:A:111:PHE:N	2.41	0.53
2:A:65:ALA:C	2:A:66:LYS:HG2	2.32	0.52
2:A:60:ASN:O	2:A:63:GLN:HG3	2.10	0.52
2:A:611:ASP:HB3	2:A:614:LEU:HG	1.92	0.52
2:A:139:GLU:HB2	2:A:140:PRO:CD	2.39	0.52
2:A:223:ILE:HG23	2:A:231:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:48:ALA:HA	2:A:51:ARG:HG2	1.92	0.51
2:A:670:LYS:O	2:A:671:LYS:C	2.52	0.51
2:A:670:LYS:C	2:A:672:LYS:N	2.65	0.51
2:A:243:ASP:OD1	2:A:244:PRO:HD2	2.10	0.51
2:A:532:HIS:O	2:A:535:LYS:HB2	2.10	0.51
2:A:244:PRO:CB	2:A:300:ARG:HH21	2.16	0.51
2:A:479:LYS:HE3	2:A:483:LYS:CD	2.41	0.51
2:A:550:ASP:OD1	2:A:550:ASP:C	2.54	0.51
2:A:609:TYR:O	2:A:670:LYS:HE3	2.10	0.51
2:A:106:GLU:HA	2:A:106:GLU:OE1	2.11	0.51
2:A:609:TYR:O	2:A:670:LYS:HE2	2.11	0.50
2:A:57:ALA:O	2:A:61:ILE:HG13	2.12	0.50
2:A:141:PRO:HD2	2:A:144:LYS:HB2	1.93	0.50
2:A:487:PRO:O	2:A:490:GLU:HB2	2.12	0.50
2:A:633:PHE:CE2	2:A:637:MET:HB2	2.46	0.50
2:A:448:ALA:O	2:A:452:ILE:HG13	2.11	0.50
2:A:479:LYS:HE3	2:A:483:LYS:HD2	1.94	0.50
2:A:173:GLU:HG3	2:A:174:ILE:N	2.26	0.49
2:A:138:SER:C	2:A:141:PRO:HB3	2.37	0.49
2:A:431:LEU:HD12	2:A:431:LEU:O	2.13	0.49
2:A:139:GLU:CB	2:A:140:PRO:CD	2.91	0.49
2:A:37:LEU:HB3	2:A:38:PRO:HD3	1.94	0.49
1:B:9:ASN:HB3	1:B:12:TYR:CD2	2.48	0.49
2:A:267:PRO:HB2	2:A:271:GLY:HA2	1.95	0.48
2:A:64:ASP:OD1	2:A:67:CYS:HB2	2.12	0.48
2:A:303:ASN:O	2:A:307:LEU:HB3	2.13	0.48
2:A:131:VAL:O	2:A:135:LEU:HG	2.13	0.48
2:A:131:VAL:HG12	2:A:135:LEU:HD11	1.95	0.48
2:A:450:ASN:HD22	2:A:451:ASN:ND2	2.12	0.48
2:A:455:THR:O	2:A:458:CYS:HB2	2.14	0.48
1:B:7:VAL:HG12	1:B:8:LYS:N	2.29	0.47
2:A:217:LEU:CD1	2:A:260:LEU:HD23	2.43	0.47
2:A:36:ILE:HA	2:A:39:VAL:CG2	2.45	0.47
2:A:569:ASP:OD1	2:A:570:PRO:HA	2.14	0.47
2:A:562:VAL:HG13	2:A:563:VAL:N	2.30	0.46
2:A:576:ASN:ND2	2:A:576:ASN:C	2.73	0.46
2:A:515:GLY:H	2:A:517:THR:HG23	1.79	0.46
2:A:300:ARG:O	2:A:304:ILE:HB	2.16	0.46
2:A:285:LEU:HD21	2:A:309:LEU:CD2	2.46	0.46
2:A:573:ILE:HD11	2:A:616:CYS:HA	1.97	0.46
2:A:36:ILE:HA	2:A:39:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:66:LYS:H	2:A:69:LYS:HD3	1.81	0.46
2:A:533:SER:C	2:A:535:LYS:H	2.22	0.46
2:A:138:SER:HA	2:A:141:PRO:CB	2.47	0.45
2:A:43:LEU:HD12	2:A:58:ILE:HD12	1.99	0.45
2:A:265:HIS:HD2	2:A:266:SER:HB2	1.81	0.45
2:A:493:SER:HA	2:A:494:ALA:HA	1.74	0.45
2:A:431:LEU:HD12	2:A:431:LEU:C	2.41	0.45
2:A:244:PRO:CB	2:A:300:ARG:NH2	2.67	0.45
2:A:73:ARG:O	2:A:75:GLN:NE2	2.50	0.45
2:A:138:SER:CA	2:A:141:PRO:HB3	2.47	0.45
2:A:480:ILE:O	2:A:484:THR:HB	2.17	0.45
2:A:72:LEU:HA	2:A:76:VAL:HG12	1.97	0.45
2:A:522:ASN:ND2	2:A:525:ARG:NH1	2.65	0.45
2:A:181:LYS:HB2	2:A:184:ILE:HD12	1.98	0.44
2:A:669:TYR:CE1	2:A:673:HIS:CE1	3.05	0.44
2:A:43:LEU:O	2:A:43:LEU:HD23	2.17	0.44
2:A:300:ARG:O	2:A:304:ILE:CB	2.65	0.44
2:A:513:LEU:HB3	2:A:517:THR:HG22	1.99	0.44
2:A:69:LYS:HD2	2:A:69:LYS:H	1.82	0.44
2:A:583:LEU:O	2:A:586:LEU:HB2	2.18	0.44
2:A:170:ALA:HB3	2:A:174:ILE:HD12	1.98	0.44
2:A:673:HIS:CD2	2:A:673:HIS:N	2.86	0.44
2:A:482:ARG:O	2:A:487:PRO:HD3	2.18	0.44
2:A:507:TRP:O	2:A:507:TRP:CD1	2.71	0.44
2:A:460:GLU:OE2	2:A:460:GLU:HA	2.17	0.44
2:A:268:GLY:N	2:A:272:ALA:O	2.43	0.43
2:A:519:THR:O	2:A:519:THR:CG2	2.64	0.43
2:A:82:THR:HG23	2:A:83:GLU:HG2	1.99	0.43
2:A:507:TRP:CE3	2:A:558:LYS:HA	2.54	0.43
2:A:70:LEU:HD23	2:A:70:LEU:N	2.34	0.43
2:A:80:VAL:O	2:A:85:LEU:HG	2.18	0.43
2:A:282:THR:HG21	2:A:420:THR:HG22	2.01	0.43
1:B:4:HIS:CE1	2:A:411:LEU:HD11	2.54	0.43
2:A:167:LEU:HB3	2:A:174:ILE:HG21	2.01	0.42
1:B:7:VAL:CG1	1:B:8:LYS:N	2.82	0.42
2:A:513:LEU:CB	2:A:517:THR:HG22	2.49	0.42
2:A:648:THR:O	2:A:648:THR:OG1	2.15	0.42
2:A:301:TYR:OH	2:A:437:GLU:HB3	2.19	0.42
2:A:485:ILE:O	2:A:489:LEU:HB2	2.18	0.42
2:A:672:LYS:HB3	2:A:673:HIS:HD2	1.84	0.42
2:A:278:ILE:HG21	2:A:416:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:450:ASN:HD22	2:A:451:ASN:HD22	1.68	0.42
2:A:533:SER:C	2:A:535:LYS:N	2.77	0.42
2:A:131:VAL:HG12	2:A:135:LEU:HD12	2.00	0.42
2:A:558:LYS:O	2:A:562:VAL:HG12	2.20	0.42
2:A:408:LEU:HD23	2:A:408:LEU:HA	1.85	0.42
2:A:531:TYR:CD1	2:A:531:TYR:C	2.97	0.42
2:A:576:ASN:C	2:A:576:ASN:HD22	2.27	0.41
2:A:70:LEU:O	2:A:74:GLU:HG2	2.20	0.41
2:A:103:LEU:O	2:A:107:GLU:HB2	2.20	0.41
2:A:456:ILE:HG21	2:A:473:TRP:CD1	2.55	0.41
2:A:513:LEU:HD12	2:A:517:THR:HB	2.01	0.41
2:A:647:ARG:C	2:A:648:THR:CG2	2.93	0.41
2:A:433:ILE:H	2:A:438:SER:HB2	1.85	0.41
2:A:672:LYS:HB3	2:A:673:HIS:CD2	2.56	0.41
2:A:615:ALA:O	2:A:619:GLU:HG2	2.20	0.41
2:A:164:ILE:HG23	2:A:178:VAL:HG11	2.02	0.41
2:A:461:PHE:CD1	2:A:470:HIS:HB2	2.56	0.41
2:A:52:THR:HG21	2:A:89:ASN:OD1	2.21	0.41
2:A:569:ASP:HB3	2:A:614:LEU:HD13	2.03	0.41
2:A:672:LYS:O	2:A:673:HIS:HD2	2.02	0.41
2:A:147:LYS:CD	2:A:151:ARG:HH22	2.34	0.40
2:A:76:VAL:O	2:A:80:VAL:HG23	2.22	0.40
2:A:131:VAL:CG1	2:A:135:LEU:HD11	2.52	0.40
1:B:17:GLN:NE2	2:A:317:THR:HA	2.36	0.40
2:A:154:TRP:HA	2:A:154:TRP:CE3	2.57	0.40
2:A:156:ILE:O	2:A:160:LEU:HG	2.21	0.40
2:A:434:ASP:OD2	2:A:435:SER:OG	2.31	0.40

All (2) 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)
2:A:107:GLU:OE1	2:A:647:ARG:NH1[8_445]	1.90	0.30
2:A:73:ARG:NH1	2:A:650:PRO:CG[8_445]	2.17	0.03

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	B	17/49 (35%)	16 (94%)	1 (6%)	0	100	100
2	A	545/676 (81%)	511 (94%)	31 (6%)	3 (1%)	21	45
All	All	562/725 (78%)	527 (94%)	32 (6%)	3 (0%)	24	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	433	ILE
2	A	269	LYS
2	A	141	PRO

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	B	17/43 (40%)	17 (100%)	0	100	100
2	A	469/576 (81%)	450 (96%)	19 (4%)	27	53
All	All	486/619 (78%)	467 (96%)	19 (4%)	28	54

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	36	ILE
2	A	40	LEU
2	A	43	LEU

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Mol	Chain	Res	Type
2	A	69	LYS
2	A	70	LEU
2	A	92	SER
2	A	108	GLU
2	A	144	LYS
2	A	180	THR
2	A	296	ASN
2	A	437	GLU
2	A	517	THR
2	A	563	VAL
2	A	576	ASN
2	A	613	GLU
2	A	617	ASP
2	A	649	GLN
2	A	655	ARG
2	A	670	LYS

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

Mol	Chain	Res	Type
1	B	4	HIS
1	B	17	GLN
2	A	150	GLN
2	A	175	HIS
2	A	254	HIS
2	A	261	GLN
2	A	320	GLN
2	A	419	GLN
2	A	430	ASN
2	A	450	ASN
2	A	451	ASN
2	A	466	ASN
2	A	524	HIS
2	A	532	HIS
2	A	576	ASN
2	A	649	GLN
2	A	673	HIS

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 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

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	B	19/49 (38%)	0.26	3 (15%) 5 4	28, 38, 46, 51	0
2	A	551/676 (81%)	0.15	33 (5%) 27 23	25, 40, 76, 138	0
All	All	570/725 (78%)	0.16	36 (6%) 26 22	25, 40, 76, 138	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	304	ILE	7.6
2	A	303	ASN	6.5
2	A	293	ALA	4.6
2	A	494	ALA	4.2
2	A	268	GLY	4.1
2	A	34	ASP	4.1
2	A	674	ALA	4.1
2	A	295	PHE	4.1
2	A	300	ARG	3.8
2	A	292	GLY	3.7
2	A	36	ILE	3.6
2	A	37	LEU	3.6
2	A	433	ILE	3.2
2	A	493	SER	3.0
2	A	297	GLY	3.0
2	A	671	LYS	2.9
2	A	299	ALA	2.8
2	A	301	TYR	2.8
2	A	435	SER	2.6
2	A	302	ALA	2.6
2	A	329	GLY	2.5
2	A	170	ALA	2.5
1	B	10	SER	2.4
2	A	648	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	208	CYS	2.3
2	A	536	GLN	2.3
2	A	436	ASP	2.3
2	A	66	LYS	2.3
2	A	199	GLN	2.2
2	A	227	GLN	2.2
2	A	669	TYR	2.2
2	A	298	ASP	2.1
1	B	8	LYS	2.1
1	B	9	ASN	2.1
2	A	670	LYS	2.1
2	A	672	LYS	2.1

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.