Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 01:30 AM EST

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

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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	Percentile Ranks	Value
Rfree		0.252
Clashscore		21
Ramachandran outliers		0.5%
Sidechain outliers		3.1%
RSRZ outliers		4.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
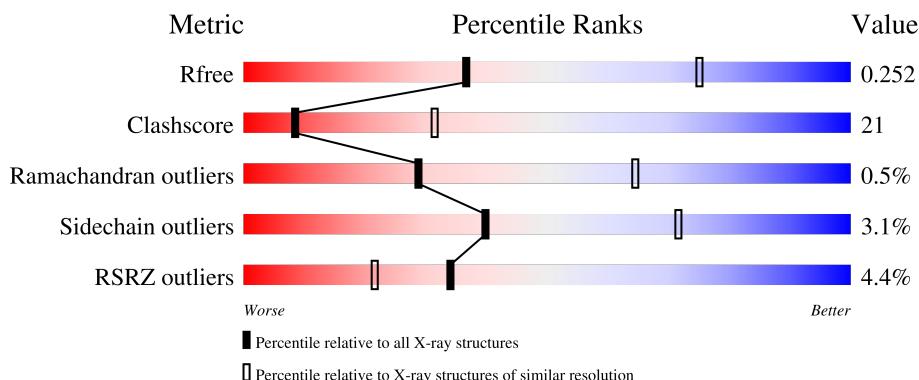
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	2% ■ 24% 14% 61%
2	A	676	4% ■ 52% 27% · 18%
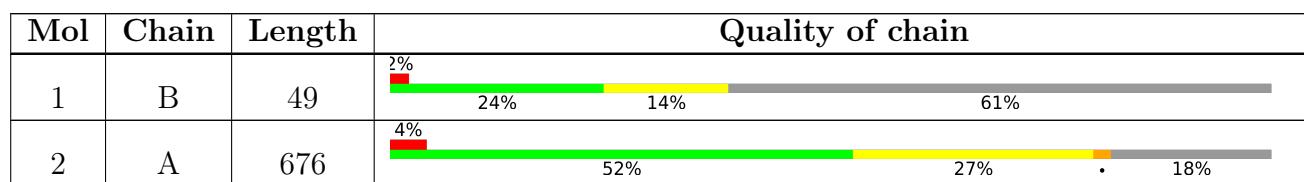
2 Entry composition ⓘ

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 166	C 111	N 29	O 26	0	0	0

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 4285	C 2724	N 738	O 812	S 11	0	0	0

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: 60S ribosomal protein l5-like protein

Chain B:
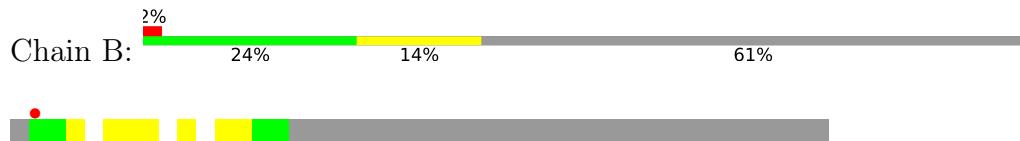
- Molecule 2: Putative uncharacterized protein

Chain A:
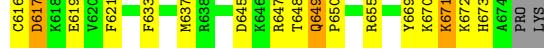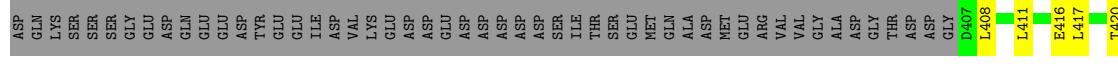
4 Data and refinement statistics ⓘ

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 59.77 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.24-2.95) 97.8 (59.77-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (10.04%)	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 , 40.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.47	0/171	0.46	0/227
2	A	0.44	2/4360 (0.0%)	0.64	6/5931 (0.1%)
All	All	0.45	2/4531 (0.0%)	0.64	6/6158 (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
2	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	432	PRO	N-CD	5.32	1.55	1.47
2	A	198	PRO	N-CD	5.11	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	140	PRO	C-N-CD	-6.73	105.78	120.60
2	A	197	ALA	C-N-CD	5.73	140.44	128.40
2	A	266	SER	C-N-CD	5.73	140.43	128.40
2	A	431	LEU	C-N-CD	5.55	140.06	128.40
2	A	671	LYS	N-CA-CB	5.30	120.14	110.60
2	A	140	PRO	C-N-CA	5.17	143.69	122.00

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	184	2
All	All	4451	0	4529	187	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 (187) 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: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:672:LYS:C	2:A:673:HIS:HD2	1.88	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:519:THR:HG23	2:A:519:THR:O	1.95	0.66
2:A:217:LEU:HD12	2:A:260:LEU:HD23	1.77	0.66
2:A:51:ARG:HG3	2:A:52:THR:N	2.12	0.65
2:A:672:LYS:C	2:A:673:HIS:CD2	2.70	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: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
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:36:ILE:HD12	2:A:61:ILE:HG21	1.84	0.60
2:A:268:GLY:O	2:A:269:LYS:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:566:LEU:HD12	2:A:566:LEU:C	2.26	0.55
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:648:THR:O	2:A:648:THR:OG1	2.15	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: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
2:A:48:ALA:HA	2:A:51:ARG:HG2	1.92	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:670:LYS:O	2:A:671:LYS:C	2.52	0.47
2:A:569:ASP:OD1	2:A:570:PRO:HA	2.14	0.47
2:A:65:ALA:C	2:A:66:LYS:HG2	2.32	0.47
2:A:670:LYS:C	2:A:672:LYS:N	2.65	0.47
2:A:550:ASP:OD1	2:A:550:ASP:C	2.54	0.46
2:A:562:VAL:HG13	2:A:563:VAL:N	2.30	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
2:A:66:LYS:H	2:A:69:LYS:HD3	1.81	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: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:138:SER:C	2:A:141:PRO:HB3	2.37	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	2:A:460:GLU:OE2	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: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:576:ASN:ND2	2:A:576:ASN:C	2.73	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
2:A:450:ASN:HD22	2:A:451:ASN:HD22	1.68	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: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: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:533:SER:C	2:A:535:LYS:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	25	60
All	All	562/725 (78%)	527 (94%)	32 (6%)	3 (0%)	29	64

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%)	454 (97%)	15 (3%)	39	71
All	All	486/619 (78%)	471 (97%)	15 (3%)	40	71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	43	LEU
2	A	70	LEU
2	A	92	SER
2	A	180	THR
2	A	199	GLN
2	A	296	ASN
2	A	436	ASP
2	A	517	THR
2	A	553	GLN
2	A	563	VAL
2	A	576	ASN
2	A	613	GLU
2	A	617	ASP
2	A	645	ASP
2	A	649	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
2	A	175	HIS
2	A	254	HIS
2	A	265	HIS
2	A	430	ASN
2	A	451	ASN
2	A	524	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	B	19/49 (38%)	0.35	1 (5%)	26	16	28, 38, 46, 51	0
2	A	551/676 (81%)	0.19	24 (4%)	34	21	25, 40, 76, 138	0
All	All	570/725 (78%)	0.20	25 (4%)	34	21	25, 40, 76, 138	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	295	PHE	8.3
2	A	304	ILE	6.2
2	A	296	ASN	5.6
2	A	293	ALA	5.6
2	A	300	ARG	5.2
2	A	297	GLY	4.7
2	A	494	ALA	4.5
2	A	303	ASN	4.4
2	A	301	TYR	4.2
2	A	299	ALA	3.6
2	A	298	ASP	3.2
2	A	433	ILE	2.8
2	A	290	PRO	2.7
2	A	493	SER	2.6
2	A	292	GLY	2.6
2	A	291	GLY	2.3
2	A	638	ARG	2.2
2	A	60	ASN	2.1
2	A	669	TYR	2.1
2	A	49	LYS	2.1
2	A	54	ALA	2.0
2	A	323	LEU	2.0
1	B	2	ALA	2.0
2	A	170	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	A	289	VAL	2.0

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.