



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:42 pm BST

PDB ID : 1N0G
Title : Crystal Structure of A Cell Division and Cell Wall Biosynthesis Protein UPF0040 from *Mycoplasma pneumoniae*: Indication of A Novel Fold with A Possible New Conserved Sequence Motif
Authors : Chen, S.; Jancarik, J.; Yokota, H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2002-10-13
Resolution : 2.80 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 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

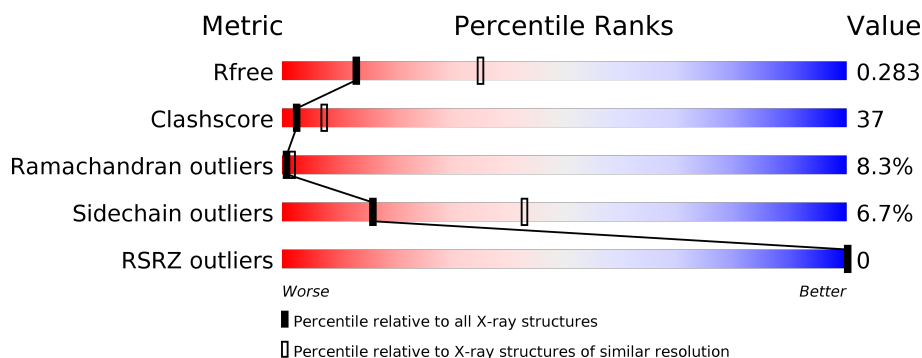
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 ≥ 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	166	
1	B	166	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2383 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 Protein mraZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1153	739	197	214	3			
1	B	141	Total	C	N	O	S	0	0	0
			1153	739	197	214	3			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P75467
A	2	GLY	-	EXPRESSION TAG	UNP P75467
A	3	SER	-	EXPRESSION TAG	UNP P75467
A	4	SER	-	EXPRESSION TAG	UNP P75467
A	5	HIS	-	EXPRESSION TAG	UNP P75467
A	6	HIS	-	EXPRESSION TAG	UNP P75467
A	7	HIS	-	EXPRESSION TAG	UNP P75467
A	8	HIS	-	EXPRESSION TAG	UNP P75467
A	9	HIS	-	EXPRESSION TAG	UNP P75467
A	10	HIS	-	EXPRESSION TAG	UNP P75467
A	11	ASP	-	EXPRESSION TAG	UNP P75467
A	12	TYR	-	EXPRESSION TAG	UNP P75467
A	13	ASP	-	EXPRESSION TAG	UNP P75467
A	14	ILE	-	EXPRESSION TAG	UNP P75467
A	15	PRO	-	EXPRESSION TAG	UNP P75467
A	16	THR	-	EXPRESSION TAG	UNP P75467
A	17	THR	-	EXPRESSION TAG	UNP P75467
A	18	GLU	-	EXPRESSION TAG	UNP P75467
A	19	ASN	-	EXPRESSION TAG	UNP P75467
A	20	LEU	-	EXPRESSION TAG	UNP P75467
A	21	TYR	-	EXPRESSION TAG	UNP P75467
A	22	PHE	-	EXPRESSION TAG	UNP P75467
A	23	GLN	-	EXPRESSION TAG	UNP P75467
A	24	GLY	-	EXPRESSION TAG	UNP P75467
A	25	HIS	-	EXPRESSION TAG	UNP P75467

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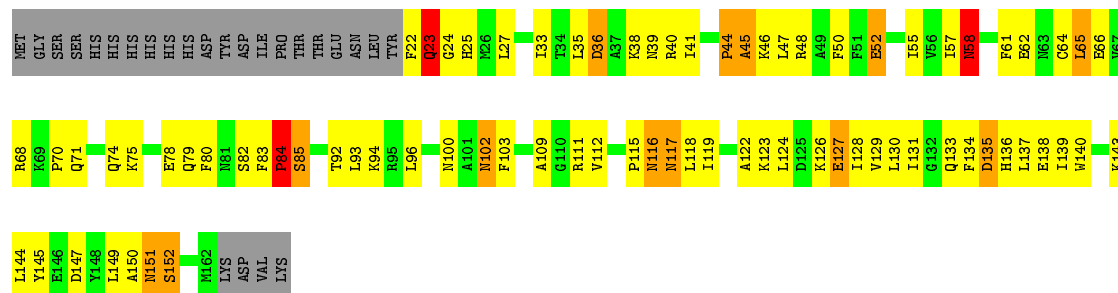
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP P75467
B	2	GLY	-	EXPRESSION TAG	UNP P75467
B	3	SER	-	EXPRESSION TAG	UNP P75467
B	4	SER	-	EXPRESSION TAG	UNP P75467
B	5	HIS	-	EXPRESSION TAG	UNP P75467
B	6	HIS	-	EXPRESSION TAG	UNP P75467
B	7	HIS	-	EXPRESSION TAG	UNP P75467
B	8	HIS	-	EXPRESSION TAG	UNP P75467
B	9	HIS	-	EXPRESSION TAG	UNP P75467
B	10	HIS	-	EXPRESSION TAG	UNP P75467
B	11	ASP	-	EXPRESSION TAG	UNP P75467
B	12	TYR	-	EXPRESSION TAG	UNP P75467
B	13	ASP	-	EXPRESSION TAG	UNP P75467
B	14	ILE	-	EXPRESSION TAG	UNP P75467
B	15	PRO	-	EXPRESSION TAG	UNP P75467
B	16	THR	-	EXPRESSION TAG	UNP P75467
B	17	THR	-	EXPRESSION TAG	UNP P75467
B	18	GLU	-	EXPRESSION TAG	UNP P75467
B	19	ASN	-	EXPRESSION TAG	UNP P75467
B	20	LEU	-	EXPRESSION TAG	UNP P75467
B	21	TYR	-	EXPRESSION TAG	UNP P75467
B	22	PHE	-	EXPRESSION TAG	UNP P75467
B	23	GLN	-	EXPRESSION TAG	UNP P75467
B	24	GLY	-	EXPRESSION TAG	UNP P75467
B	25	HIS	-	EXPRESSION TAG	UNP P75467

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	44	Total O 44 44	0	0
2	B	33	Total O 33 33	0	0

- Molecule 1: Protein mraZ



L144	F68	Met
Y145	K69	Gly
E146	P70	Ser
D147	Q71	Ser
Y148		His
L149	Q74	His
A150	K75	His
M151	Y76	His
S152	F77	His
E153	E78	His
	Q79	Asp
V158	F80	Tyr
	M81	Asp
M162	S82	Ile
Lys	F83	Pro
E165	K84	Thr
Val	S85	Thr
Lys	I86	Glu
	I87	Asn
	F88	Leu
	A89	Tyr
	M100	
	A101	
	M102	
	F103	
	A109	
	R110	
	V112	
	L113	
	M114	
	P115	
	N116	
	M117	
	L118	
	I119	
	A122	
	K123	
	L124	
	D125	
	K126	
	E127	
	I128	
	V129	
	L130	
	I131	
	G132	
	Q133	
	F134	
	D135	
	H136	
	L137	
	E138	
	I139	
	W140	
	Y142	

4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	101.44Å 101.44Å 38.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.22 – 2.80 38.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.22-2.80) 99.5 (38.19-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.283 0.229 , 0.283	Depositor DCC
R_{free} test set	475 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2383	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/1175	0.69	1/1584 (0.1%)
1	B	0.43	0/1175	0.70	1/1584 (0.1%)
All	All	0.43	0/2350	0.70	2/3168 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	102	ASN	N-CA-C	5.05	124.63	111.00
1	B	102	ASN	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1153	0	1148	86	0
1	B	1153	0	1148	90	0
2	A	44	0	0	8	0
2	B	33	0	0	5	0
All	All	2383	0	2296	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (169) 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:206:HOH:O	1:B:135:ASP:HB2	1.75	0.87
1:A:35:LEU:HD11	1:A:39:ASN:HD22	1.40	0.84
1:A:109:ALA:HB3	1:A:111:ARG:HH11	1.42	0.84
1:B:109:ALA:HB3	1:B:111:ARG:HH11	1.42	0.84
1:A:126:LYS:O	1:A:127:GLU:HB2	1.75	0.84
1:B:126:LYS:O	1:B:127:GLU:HB2	1.77	0.83
1:B:35:LEU:HD11	1:B:39:ASN:HD22	1.41	0.83
1:B:71:GLN:O	1:B:74:GLN:HB3	1.80	0.82
1:A:71:GLN:O	1:A:74:GLN:HB3	1.80	0.80
1:A:109:ALA:HB3	1:A:111:ARG:HD3	1.64	0.80
1:B:109:ALA:HB3	1:B:111:ARG:HD3	1.64	0.79
1:A:84:PRO:O	1:A:85:SER:HB2	1.85	0.77
1:B:84:PRO:O	1:B:85:SER:HB2	1.85	0.75
1:A:102:ASN:O	1:A:103:PHE:HB2	1.87	0.74
1:B:102:ASN:O	1:B:103:PHE:HB2	1.87	0.74
1:A:23:GLN:NE2	2:A:167:HOH:O	2.22	0.72
1:B:22:PHE:N	1:B:23:GLN:NE2	2.39	0.71
1:A:40:ARG:NH1	1:A:111:ARG:HH21	1.88	0.71
1:B:57:ILE:O	1:B:66:GLU:O	2.08	0.70
1:A:22:PHE:N	1:A:23:GLN:NE2	2.40	0.70
1:B:35:LEU:HD11	1:B:39:ASN:ND2	2.07	0.69
1:A:117:ASN:HD22	1:A:117:ASN:H	1.40	0.69
1:B:116:ASN:HB3	2:B:171:HOH:O	1.92	0.68
1:A:35:LEU:HD11	1:A:39:ASN:ND2	2.07	0.68
1:B:117:ASN:HD22	1:B:117:ASN:H	1.42	0.68
1:B:40:ARG:NH1	1:B:111:ARG:HH21	1.92	0.68
1:A:57:ILE:O	1:A:66:GLU:O	2.11	0.67
1:B:44:PRO:HD2	1:B:47:LEU:HD22	1.76	0.67
1:A:44:PRO:HD2	1:A:47:LEU:HD22	1.77	0.66
1:A:22:PHE:N	1:A:23:GLN:HE22	1.93	0.66
1:B:22:PHE:N	1:B:23:GLN:HE21	1.92	0.66
1:B:79:GLN:O	1:B:82:SER:HB3	1.96	0.65
1:A:38:LYS:HD2	1:A:40:ARG:CZ	2.27	0.65
1:A:65:LEU:HD13	1:A:122:ALA:HB2	1.78	0.65
1:B:38:LYS:HD2	1:B:40:ARG:CZ	2.27	0.65
1:B:65:LEU:HD13	1:B:122:ALA:HB2	1.78	0.64
1:A:79:GLN:O	1:A:82:SER:HB3	1.96	0.64
1:A:109:ALA:CB	1:A:111:ARG:HH11	2.11	0.62
1:B:109:ALA:CB	1:B:111:ARG:HH11	2.11	0.62
1:A:102:ASN:HA	2:A:181:HOH:O	1.98	0.62
1:A:64:CYS:O	1:A:139:ILE:O	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ALA:HB3	1:A:111:ARG:CD	2.30	0.62
1:A:96:LEU:O	1:A:100:ASN:ND2	2.33	0.62
1:B:96:LEU:O	1:B:100:ASN:ND2	2.31	0.61
1:B:64:CYS:O	1:B:139:ILE:O	2.18	0.61
2:A:207:HOH:O	1:B:23:GLN:HG3	2.00	0.61
1:A:75:LYS:HA	1:A:78:GLU:HG2	1.83	0.61
1:A:84:PRO:O	1:A:85:SER:CB	2.49	0.61
1:B:75:LYS:HA	1:B:78:GLU:HG2	1.83	0.61
1:A:117:ASN:ND2	1:A:117:ASN:H	1.99	0.61
1:A:27:LEU:HD22	1:A:137:LEU:HD13	1.83	0.61
1:B:84:PRO:O	1:B:85:SER:CB	2.49	0.61
1:B:36:ASP:OD2	1:B:40:ARG:HB2	2.01	0.60
1:B:109:ALA:HB3	1:B:111:ARG:CD	2.30	0.60
1:B:55:ILE:HD12	1:B:55:ILE:C	2.22	0.60
1:A:64:CYS:O	1:A:65:LEU:HB2	2.01	0.60
1:B:64:CYS:O	1:B:65:LEU:HB2	2.02	0.59
1:A:36:ASP:OD2	1:A:40:ARG:HB2	2.03	0.59
1:B:57:ILE:HD12	1:B:66:GLU:O	2.03	0.59
1:A:40:ARG:NH1	1:A:111:ARG:NH2	2.50	0.59
1:A:55:ILE:HD12	1:A:55:ILE:C	2.23	0.59
1:B:113:LEU:HB3	2:B:192:HOH:O	2.02	0.59
1:B:117:ASN:ND2	1:B:117:ASN:H	2.01	0.58
1:B:27:LEU:HD22	1:B:137:LEU:HD13	1.85	0.58
1:B:115:PRO:O	1:B:119:ILE:HG12	2.03	0.58
1:A:115:PRO:O	1:A:119:ILE:HG12	2.04	0.57
1:A:35:LEU:HD13	1:A:36:ASP:O	2.05	0.57
1:A:57:ILE:HD12	1:A:66:GLU:O	2.05	0.56
1:B:35:LEU:HD13	1:B:36:ASP:O	2.06	0.56
1:B:40:ARG:NH1	1:B:111:ARG:NH2	2.54	0.55
1:A:23:GLN:NE2	2:A:197:HOH:O	2.35	0.54
1:A:93:LEU:HD12	1:B:162:MET:SD	2.48	0.53
1:A:23:GLN:HB3	2:A:179:HOH:O	2.09	0.53
1:B:140:TRP:HB3	1:B:145:TYR:HB2	1.90	0.53
1:A:35:LEU:HD12	2:A:172:HOH:O	2.09	0.53
1:A:33:ILE:CD1	1:A:41:ILE:HG13	2.39	0.53
1:B:33:ILE:CD1	1:B:41:ILE:HG13	2.39	0.52
1:A:140:TRP:HB3	1:A:145:TYR:HB2	1.90	0.52
1:A:35:LEU:HD11	1:A:39:ASN:HA	1.91	0.52
1:B:44:PRO:HD2	1:B:47:LEU:CD2	2.40	0.52
1:A:44:PRO:HD2	1:A:47:LEU:CD2	2.41	0.51
1:A:143:LYS:HE2	1:A:147:ASP:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HD11	1:A:41:ILE:HG13	1.92	0.51
1:A:25:HIS:HA	1:A:50:PHE:HD1	1.76	0.51
1:B:128:ILE:HG22	1:B:129:VAL:N	2.26	0.50
1:A:27:LEU:HD11	1:A:50:PHE:CE2	2.47	0.50
1:A:45:ALA:HA	1:A:48:ARG:CD	2.42	0.50
1:A:52:GLU:HA	1:A:52:GLU:OE2	2.12	0.50
1:B:23:GLN:HG2	2:B:175:HOH:O	2.12	0.50
1:B:44:PRO:O	1:B:46:LYS:N	2.45	0.50
1:B:33:ILE:HD11	1:B:41:ILE:HG13	1.93	0.49
1:A:128:ILE:HG22	1:A:129:VAL:N	2.26	0.49
1:A:44:PRO:O	1:A:46:LYS:N	2.46	0.49
1:B:35:LEU:HD11	1:B:39:ASN:HA	1.93	0.49
1:B:143:LYS:HE2	1:B:147:ASP:OD1	2.11	0.49
1:B:46:LYS:HG3	1:B:47:LEU:HD13	1.94	0.49
1:B:33:ILE:HD11	1:B:130:LEU:HD11	1.94	0.49
1:A:65:LEU:HD21	1:A:118:LEU:HB3	1.93	0.49
1:B:61:PHE:O	1:B:62:GLU:HB2	2.12	0.49
1:B:45:ALA:HA	1:B:48:ARG:CD	2.43	0.49
1:A:147:ASP:O	1:A:150:ALA:HB3	2.13	0.48
1:A:33:ILE:HD11	1:A:130:LEU:HD11	1.95	0.48
1:B:27:LEU:HD11	1:B:50:PHE:CE2	2.48	0.48
1:B:151:ASN:O	1:B:152:SER:O	2.32	0.48
1:B:26:MET:HG2	1:B:134:PHE:CZ	2.48	0.48
1:A:151:ASN:O	1:A:152:SER:O	2.31	0.48
1:B:52:GLU:HA	1:B:52:GLU:OE2	2.12	0.48
1:B:65:LEU:HD21	1:B:118:LEU:HB3	1.95	0.48
1:A:46:LYS:HG3	1:A:47:LEU:HD13	1.96	0.48
1:A:61:PHE:O	1:A:62:GLU:HB2	2.14	0.47
1:B:116:ASN:O	1:B:119:ILE:HB	2.14	0.47
1:A:128:ILE:HG21	1:A:139:ILE:HG23	1.96	0.47
1:B:123:LYS:HB2	1:B:144:LEU:HD11	1.96	0.47
1:B:38:LYS:HB2	1:B:40:ARG:NE	2.29	0.47
1:B:57:ILE:HG12	1:B:118:LEU:HD23	1.97	0.47
1:A:123:LYS:HB2	1:A:144:LEU:HD11	1.96	0.47
1:B:128:ILE:HG21	1:B:139:ILE:HG23	1.97	0.46
1:A:116:ASN:O	1:A:119:ILE:HB	2.15	0.46
1:A:38:LYS:HB2	1:A:40:ARG:NE	2.31	0.46
1:A:94:LYS:HB3	1:B:133:GLN:NE2	2.30	0.46
1:A:57:ILE:HG12	1:A:118:LEU:HD23	1.98	0.46
1:B:147:ASP:O	1:B:150:ALA:HB3	2.15	0.46
1:A:117:ASN:N	1:A:117:ASN:ND2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:CYS:O	1:A:65:LEU:CB	2.61	0.45
1:A:131:ILE:HD11	1:A:138:GLU:OE1	2.17	0.45
1:B:49:ALA:HB2	2:B:197:HOH:O	2.17	0.45
1:A:93:LEU:CD1	1:B:162:MET:HG3	2.47	0.45
1:A:41:ILE:HD12	1:A:41:ILE:HA	1.84	0.44
1:A:133:GLN:O	1:A:135:ASP:N	2.51	0.44
1:A:22:PHE:O	1:A:23:GLN:C	2.54	0.44
1:B:153:GLU:HG3	2:B:174:HOH:O	2.17	0.44
1:B:57:ILE:O	1:B:58:ASN:O	2.35	0.44
1:A:41:ILE:O	1:A:111:ARG:HA	2.18	0.44
1:B:55:ILE:HA	1:B:70:PRO:HD3	2.00	0.44
1:B:41:ILE:O	1:B:111:ARG:HA	2.18	0.44
1:B:36:ASP:CG	1:B:38:LYS:H	2.20	0.44
1:A:80:PHE:HA	1:A:83:PHE:CD2	2.54	0.43
1:B:117:ASN:N	1:B:117:ASN:ND2	2.65	0.43
1:A:80:PHE:C	1:A:82:SER:N	2.69	0.43
1:B:43:LEU:HA	1:B:44:PRO:HD3	1.82	0.43
1:A:57:ILE:O	1:A:58:ASN:O	2.37	0.43
1:A:45:ALA:HA	1:A:48:ARG:HD2	2.01	0.43
1:A:83:PHE:HB3	1:B:162:MET:HE1	2.01	0.43
1:B:131:ILE:HD11	1:B:138:GLU:OE1	2.19	0.43
1:B:133:GLN:O	1:B:135:ASP:N	2.52	0.43
1:B:45:ALA:HA	1:B:48:ARG:HD2	2.01	0.43
1:A:36:ASP:CG	1:A:38:LYS:H	2.22	0.42
1:A:41:ILE:HG22	1:A:112:VAL:HB	2.01	0.42
1:A:93:LEU:HD11	1:B:162:MET:HG3	2.00	0.42
1:A:55:ILE:HA	1:A:70:PRO:HD3	2.01	0.42
1:A:22:PHE:O	1:A:24:GLY:N	2.52	0.42
1:A:92:THR:HB	1:B:158:VAL:HG11	2.02	0.42
1:B:80:PHE:C	1:B:82:SER:N	2.69	0.42
1:B:80:PHE:HA	1:B:83:PHE:CD2	2.54	0.42
1:B:80:PHE:O	1:B:83:PHE:N	2.53	0.42
1:A:68:ARG:HG2	1:A:136:HIS:HB3	2.02	0.41
1:B:64:CYS:O	1:B:65:LEU:CB	2.62	0.41
1:A:22:PHE:N	2:A:167:HOH:O	2.52	0.41
1:A:80:PHE:O	1:A:83:PHE:N	2.54	0.41
1:A:147:ASP:O	1:A:150:ALA:N	2.53	0.41
1:B:22:PHE:HB3	1:B:26:MET:HE2	2.02	0.41
1:B:147:ASP:O	1:B:150:ALA:N	2.54	0.41
1:B:41:ILE:HG22	1:B:112:VAL:HB	2.02	0.41
1:B:77:PHE:HD1	1:B:98:PHE:CZ	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:O	1:B:48:ARG:C	2.60	0.40
1:A:94:LYS:HB3	1:B:133:GLN:HE22	1.84	0.40
1:B:44:PRO:CD	1:B:47:LEU:HD22	2.49	0.40
1:B:68:ARG:HG2	1:B:136:HIS:HB3	2.02	0.40
1:B:41:ILE:HD12	1:B:41:ILE:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	139/166 (84%)	116 (84%)	11 (8%)	12 (9%)	1	1
1	B	139/166 (84%)	116 (84%)	12 (9%)	11 (8%)	1	2
All	All	278/332 (84%)	232 (84%)	23 (8%)	23 (8%)	1	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	84	PRO
1	B	58	ASN
1	B	84	PRO
1	A	85	SER
1	A	151	ASN
1	A	152	SER
1	B	85	SER
1	B	151	ASN
1	B	152	SER
1	A	23	GLN
1	A	127	GLU
1	A	134	PHE

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Mol	Chain	Res	Type
1	B	65	LEU
1	B	134	PHE
1	A	45	ALA
1	A	65	LEU
1	B	45	ALA
1	B	127	GLU
1	A	44	PRO
1	A	52	GLU
1	B	44	PRO
1	B	52	GLU

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	126/150 (84%)	117 (93%)	9 (7%)	14	39
1	B	126/150 (84%)	118 (94%)	8 (6%)	18	46
All	All	252/300 (84%)	235 (93%)	17 (7%)	16	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	36	ASP
1	A	58	ASN
1	A	84	PRO
1	A	116	ASN
1	A	117	ASN
1	A	124	LEU
1	A	135	ASP
1	A	149	LEU
1	B	23	GLN
1	B	36	ASP
1	B	58	ASN
1	B	84	PRO

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Mol	Chain	Res	Type
1	B	116	ASN
1	B	117	ASN
1	B	124	LEU
1	B	149	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	25	HIS
1	A	39	ASN
1	A	117	ASN
1	B	23	GLN
1	B	25	HIS
1	B	39	ASN
1	B	117	ASN
1	B	133	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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 [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	141/166 (84%)	-0.28	0 100 100	26, 47, 64, 73	0
1	B	141/166 (84%)	-0.30	0 100 100	27, 47, 65, 73	0
All	All	282/332 (84%)	-0.29	0 100 100	26, 47, 65, 73	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 carbohydrates 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.