



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 08:56 AM BST

PDB ID : 6PPN
Title : Structure of *S. pombe* Lsm2-8 with unprocessed U6 snRNA
Authors : Montemayor, E.J.; Butcher, S.E.
Deposited on : 2019-07-08
Resolution : 1.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2.13.1
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)	:	2.13.1

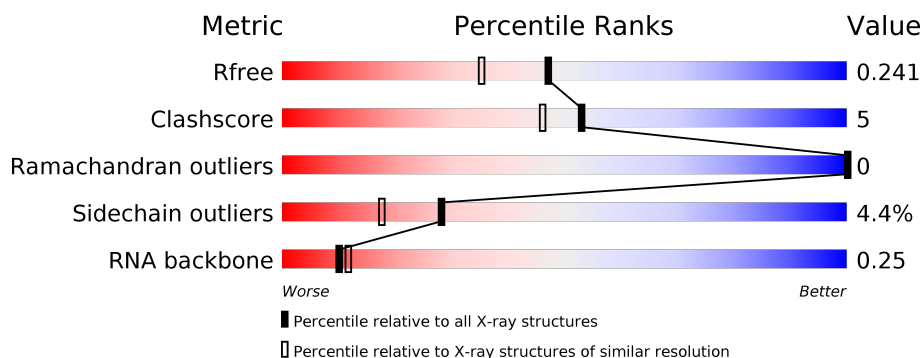
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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.










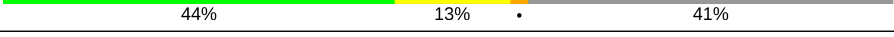
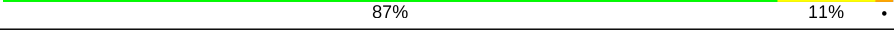

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RNA backbone	3102	1010 (2.44-1.40)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	6	50% 33% 17%
1	I	6	67% 17% 17%
2	B	96	90% 7% ..
2	J	96	82% 8% • 7%
3	C	95	72% 7% 21%
3	K	95	68% 9% • 21%

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Mol	Chain	Length	Quality of chain
4	D	129	
4	L	129	
5	E	80	
5	M	80	
6	F	77	
6	N	77	
7	G	119	
7	O	119	
8	H	94	
8	P	94	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8877 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 RNA chain called Mimic of unprocessed U6 snRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	5	Total	C	N	O	P	0	0	0
			84	36	8	35	5			
1	I	5	Total	C	N	O	P	0	0	0
			84	36	8	35	5			

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	S	0	0	0
			739	474	123	137	5			
2	J	89	Total	C	N	O	S	0	0	0
			711	458	118	130	5			

- Molecule 3 is a protein called Probable U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	75	Total	C	N	O	S	0	0	0
			605	389	104	110	2			
3	K	75	Total	C	N	O	S	0	0	0
			605	389	104	110	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q9Y7M4
C	0	SER	-	expression tag	UNP Q9Y7M4
K	-1	GLY	-	expression tag	UNP Q9Y7M4
K	0	SER	-	expression tag	UNP Q9Y7M4

- Molecule 4 is a protein called Probable U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	88	Total	C	N	O	S	0	0	0
			702	441	127	129	5			
4	L	88	Total	C	N	O	S	0	0	0
			685	432	121	127	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	122	TRP	-	expression tag	UNP O14352
D	123	SER	-	expression tag	UNP O14352
D	124	HIS	-	expression tag	UNP O14352
D	125	PRO	-	expression tag	UNP O14352
D	126	GLN	-	expression tag	UNP O14352
D	127	PHE	-	expression tag	UNP O14352
D	128	GLU	-	expression tag	UNP O14352
D	129	LYS	-	expression tag	UNP O14352
L	122	TRP	-	expression tag	UNP O14352
L	123	SER	-	expression tag	UNP O14352
L	124	HIS	-	expression tag	UNP O14352
L	125	PRO	-	expression tag	UNP O14352
L	126	GLN	-	expression tag	UNP O14352
L	127	PHE	-	expression tag	UNP O14352
L	128	GLU	-	expression tag	UNP O14352
L	129	LYS	-	expression tag	UNP O14352

- Molecule 5 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	68	Total	C	N	O	S	0	0	0
			518	333	82	97	6			
5	M	68	Total	C	N	O	S	0	0	0
			514	330	81	97	6			

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	68	Total	C	N	O	S	0	0	0
			505	324	84	95	2			
6	N	68	Total	C	N	O	S	0	0	0
			499	321	81	95	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP Q9UUI1
F	0	SER	-	expression tag	UNP Q9UUI1
N	-1	GLY	-	expression tag	UNP Q9UUI1
N	0	SER	-	expression tag	UNP Q9UUI1

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			572	365	98	107	2			
7	O	70	Total	C	N	O	S	0	0	0
			534	339	92	101	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	114	HIS	-	expression tag	UNP O74499
G	115	HIS	-	expression tag	UNP O74499
G	116	HIS	-	expression tag	UNP O74499
G	117	HIS	-	expression tag	UNP O74499
G	118	HIS	-	expression tag	UNP O74499
G	119	HIS	-	expression tag	UNP O74499
O	114	HIS	-	expression tag	UNP O74499
O	115	HIS	-	expression tag	UNP O74499
O	116	HIS	-	expression tag	UNP O74499
O	117	HIS	-	expression tag	UNP O74499
O	118	HIS	-	expression tag	UNP O74499
O	119	HIS	-	expression tag	UNP O74499

- Molecule 8 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	94	Total	C	N	O	S	0	0	0
			713	450	121	138	4			
8	P	94	Total	C	N	O	S	0	0	0
			713	450	121	138	4			

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	24	Total 24	O 24	0	0
9	C	11	Total 11	O 11	0	0
9	D	5	Total 5	O 5	0	0
9	E	1	Total 1	O 1	0	0
9	F	6	Total 6	O 6	0	0
9	G	3	Total 3	O 3	0	0
9	H	12	Total 12	O 12	0	0
9	I	2	Total 2	O 2	0	0
9	J	21	Total 21	O 21	0	0
9	K	7	Total 7	O 7	0	0

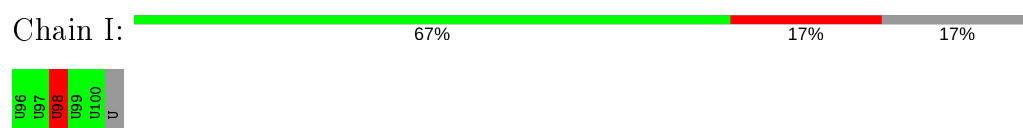
3 Residue-property plots [i](#)

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. 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. 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.

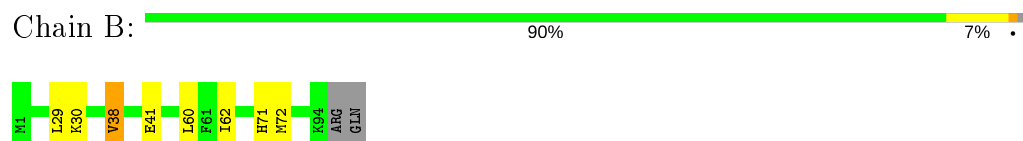
- Molecule 1: Mimic of unprocessed U6 snRNA



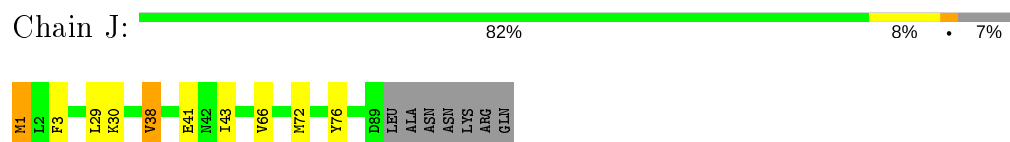
- Molecule 1: Mimic of unprocessed U6 snRNA



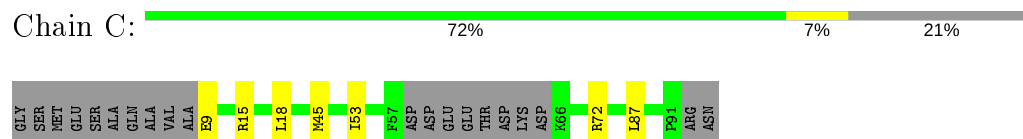
- Molecule 2: U6 snRNA-associated Sm-like protein LSm2



- Molecule 2: U6 snRNA-associated Sm-like protein LSm2



- Molecule 3: Probable U6 snRNA-associated Sm-like protein LSm3



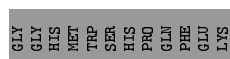
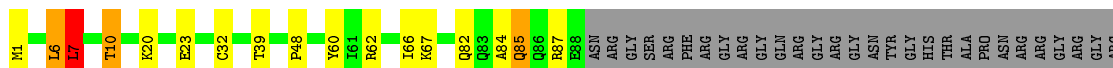
- Molecule 3: Probable U6 snRNA-associated Sm-like protein LSm3





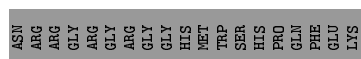
- Molecule 4: Probable U6 snRNA-associated Sm-like protein LSm4

Chain D: 55% 10% 32%



- Molecule 4: Probable U6 snRNA-associated Sm-like protein LSm4

Chain L: 53% 14% 32%



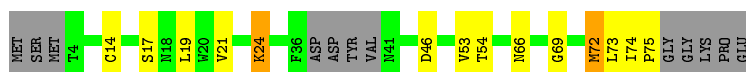
- Molecule 5: U6 snRNA-associated Sm-like protein LSm5

Chain E: 74% 11% 15%



- Molecule 5: U6 snRNA-associated Sm-like protein LSm5

Chain M: 68% 15% 15%



- Molecule 6: U6 snRNA-associated Sm-like protein LSm6

Chain F: 73% 12% 12%

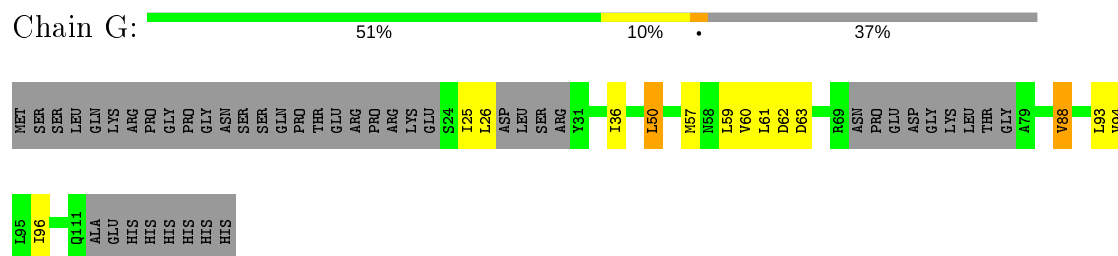


- Molecule 6: U6 snRNA-associated Sm-like protein LSm6

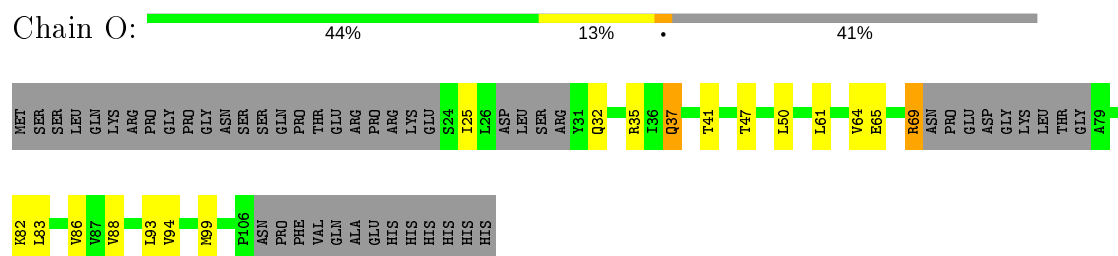
Chain N: 77% 9% 12%



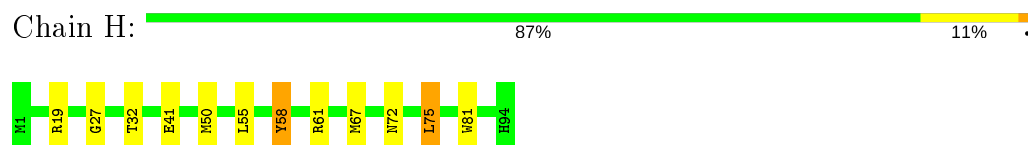
- Molecule 7: U6 snRNA-associated Sm-like protein LSm7



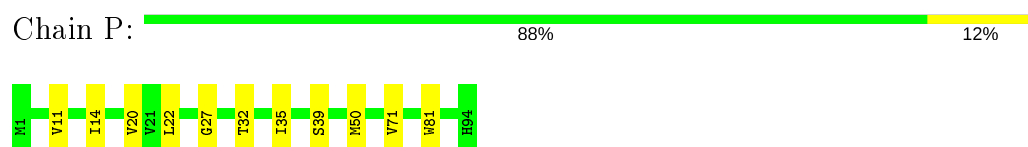
- Molecule 7: U6 snRNA-associated Sm-like protein LSm7



- Molecule 8: U6 snRNA-associated Sm-like protein LSm8



- Molecule 8: U6 snRNA-associated Sm-like protein LSm8



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	70.28Å 135.39Å 168.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.70 – 1.91 71.38 – 1.91	Depositor EDS
% Data completeness (in resolution range)	63.3 (67.70-1.91) 64.0 (71.38-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.216 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8877	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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	0.91	0/91	1.58	3/139 (2.2%)
1	I	0.59	0/91	1.56	2/139 (1.4%)
2	B	0.53	0/750	0.73	0/1014
2	J	0.50	0/722	0.73	0/974
3	C	0.53	0/614	0.75	0/829
3	K	0.46	0/614	0.80	1/829 (0.1%)
4	D	0.49	0/712	0.75	1/962 (0.1%)
4	L	0.32	0/695	0.59	0/942
5	E	0.51	1/524 (0.2%)	0.65	0/707
5	M	0.35	0/520	0.65	0/703
6	F	0.49	1/511 (0.2%)	0.72	1/691 (0.1%)
6	N	0.41	0/505	0.78	1/684 (0.1%)
7	G	0.41	0/576	0.64	0/778
7	O	0.34	0/536	0.61	0/722
8	H	0.50	0/722	0.69	0/979
8	P	0.38	0/722	0.63	0/979
All	All	0.46	2/8905 (0.0%)	0.73	9/12071 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	71	CYS	CB-SG	-7.92	1.68	1.82
6	F	33	CYS	CB-SG	-5.09	1.73	1.81

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	98	U	O4'-C1'-N1	7.18	113.94	108.20
6	N	34	LEU	CA-CB-CG	7.10	131.64	115.30
3	K	87	LEU	CA-CB-CG	6.81	130.96	115.30
1	I	98	U	N1-C2-O2	-5.95	118.63	122.80
1	A	98	U	O4'-C1'-N1	5.61	112.69	108.20

There are no chirality outliers.

There are no planarity outliers.

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	84	0	40	0	0
1	I	84	0	40	1	0
2	B	739	0	747	7	0
2	J	711	0	729	6	0
3	C	605	0	617	5	0
3	K	605	0	617	10	0
4	D	702	0	698	12	0
4	L	685	0	666	13	0
5	E	518	0	529	4	0
5	M	514	0	518	9	0
6	F	505	0	489	9	0
6	N	499	0	478	5	0
7	G	572	0	580	10	0
7	O	534	0	547	13	0
8	H	713	0	690	8	0
8	P	713	0	690	5	0
9	A	2	0	0	0	0
9	B	24	0	0	1	0
9	C	11	0	0	0	0
9	D	5	0	0	0	0
9	E	1	0	0	0	0
9	F	6	0	0	0	0
9	G	3	0	0	0	0
9	H	12	0	0	0	0
9	I	2	0	0	1	0
9	J	21	0	0	2	0
9	K	7	0	0	0	0
All	All	8877	0	8675	95	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 5.

The worst 5 of 95 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)
4:L:10:THR:HG22	4:L:75:VAL:HG11	1.64	0.80
4:L:20:LYS:HA	4:L:67:LYS:HD3	1.64	0.79
4:D:20:LYS:HA	4:D:67:LYS:HD3	1.66	0.76
3:K:12:ASP:OD1	3:K:15:ARG:NH1	2.23	0.72
3:K:9:GLU:HG2	6:N:33:CYS:SG	2.29	0.72

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	
2	B	92/96 (96%)	91 (99%)	1 (1%)	0	100	100
2	J	87/96 (91%)	86 (99%)	1 (1%)	0	100	100
3	C	71/95 (75%)	71 (100%)	0	0	100	100
3	K	71/95 (75%)	71 (100%)	0	0	100	100
4	D	86/129 (67%)	85 (99%)	1 (1%)	0	100	100
4	L	86/129 (67%)	85 (99%)	1 (1%)	0	100	100
5	E	64/80 (80%)	62 (97%)	2 (3%)	0	100	100
5	M	64/80 (80%)	62 (97%)	2 (3%)	0	100	100
6	F	66/77 (86%)	62 (94%)	4 (6%)	0	100	100
6	N	66/77 (86%)	61 (92%)	5 (8%)	0	100	100
7	G	69/119 (58%)	68 (99%)	1 (1%)	0	100	100
7	O	64/119 (54%)	64 (100%)	0	0	100	100
8	H	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
8	P	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
All	All	1070/1380 (78%)	1048 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	B	82/87 (94%)	80 (98%)	2 (2%)	49	41
2	J	80/87 (92%)	75 (94%)	5 (6%)	18	8
3	C	66/83 (80%)	63 (96%)	3 (4%)	27	17
3	K	66/83 (80%)	64 (97%)	2 (3%)	41	31
4	D	75/110 (68%)	71 (95%)	4 (5%)	22	12
4	L	71/110 (64%)	69 (97%)	2 (3%)	43	34
5	E	59/71 (83%)	57 (97%)	2 (3%)	37	27
5	M	58/71 (82%)	54 (93%)	4 (7%)	15	6
6	F	50/66 (76%)	49 (98%)	1 (2%)	55	49
6	N	49/66 (74%)	46 (94%)	3 (6%)	18	8
7	G	61/104 (59%)	58 (95%)	3 (5%)	25	14
7	O	57/104 (55%)	53 (93%)	4 (7%)	15	6
8	H	75/84 (89%)	72 (96%)	3 (4%)	31	21
8	P	75/84 (89%)	72 (96%)	3 (4%)	31	21
All	All	924/1210 (76%)	883 (96%)	41 (4%)	28	18

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	1	MET
2	J	72	MET
7	O	88	VAL
2	J	38	VAL
2	J	43	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	L	64	ASN
7	O	32	GLN
4	L	83	GLN
6	F	55	ASN
5	M	60	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3/6 (50%)	0	0
1	I	3/6 (50%)	0	1 (33%)
All	All	6/12 (50%)	0	1 (16%)

There are no RNA backbone outliers to report.

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	98	U

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 monosaccharides 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.