Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 04:25 pm BST

PDB ID	:	8S6O
Title	:	Structure of MLLE3 in complex with PAMPL2
Authors	:	Devan, S.; Shanmugasundaram, S.; Muentjes, K.; Smits, S.H.; Altegoer, F.; Feldbruegge, M.
Deposited on	:	2024-02-28
Resolution	:	2.40 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*
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:

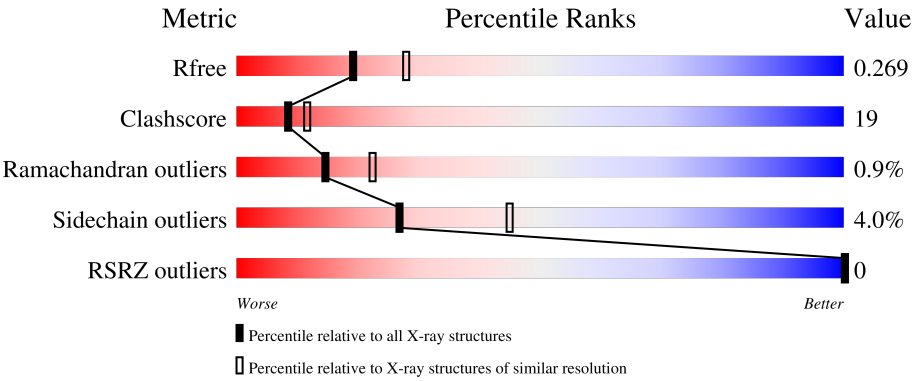
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 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	A	133	58% 22% 5% • 14%
1	C	133	61% 22% • • 14%
1	D	133	59% 20% 7% 14%
1	F	133	59% 22% • • 14%
1	I	133	65% 17% • 14%

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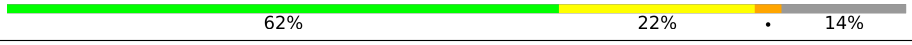
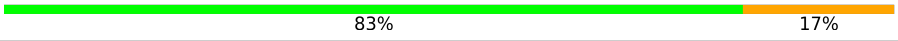
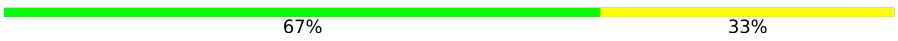
Mol	Chain	Length	Quality of chain
1	K	133	
1	M	133	
1	O	133	
2	B	6	
2	E	6	
2	G	6	
2	H	6	
2	J	6	
2	L	6	
2	N	6	
2	P	6	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15073 atoms, of which 7616 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 RNA-binding protein RRM4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	115	Total	C	H	N	O	S	0	0	0
			1781	551	908	156	165	1			
1	A	115	Total	C	H	N	O	S	0	0	0
			1781	551	908	156	165	1			
1	C	115	Total	C	H	N	O	S	0	0	0
			1781	551	908	156	165	1			
1	F	115	Total	C	H	N	O	S	0	0	0
			1781	551	908	156	165	1			
1	I	115	Total	C	H	N	O	S	0	0	0
			1781	551	908	156	165	1			
1	K	115	Total	C	H	N	O	S	0	0	0
			1781	551	908	156	165	1			
1	M	115	Total	C	H	N	O	S	0	0	0
			1781	551	908	156	165	1			
1	O	115	Total	C	H	N	O	S	0	0	0
			1781	551	908	156	165	1			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	3	HIS	-	expression tag	UNP A0A0D1DWZ5
D	118	VAL	-	expression tag	UNP A0A0D1DWZ5
D	119	LYS	-	expression tag	UNP A0A0D1DWZ5
D	120	GLY	-	expression tag	UNP A0A0D1DWZ5
D	121	ALA	-	expression tag	UNP A0A0D1DWZ5
D	122	PRO	-	expression tag	UNP A0A0D1DWZ5
D	123	LYS	-	expression tag	UNP A0A0D1DWZ5
D	124	LEU	-	expression tag	UNP A0A0D1DWZ5
D	125	THR	-	expression tag	UNP A0A0D1DWZ5
D	126	ILE	-	expression tag	UNP A0A0D1DWZ5
D	127	HIS	-	expression tag	UNP A0A0D1DWZ5
D	128	LEU	-	expression tag	UNP A0A0D1DWZ5
D	129	LEU	-	expression tag	UNP A0A0D1DWZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	130	ASP	-	expression tag	UNP A0A0D1DWZ5
D	131	SER	-	expression tag	UNP A0A0D1DWZ5
D	132	GLU	-	expression tag	UNP A0A0D1DWZ5
D	133	ASP	-	expression tag	UNP A0A0D1DWZ5
D	134	LEU	-	expression tag	UNP A0A0D1DWZ5
D	135	ARG	-	expression tag	UNP A0A0D1DWZ5
A	3	HIS	-	expression tag	UNP A0A0D1DWZ5
A	118	VAL	-	expression tag	UNP A0A0D1DWZ5
A	119	LYS	-	expression tag	UNP A0A0D1DWZ5
A	120	GLY	-	expression tag	UNP A0A0D1DWZ5
A	121	ALA	-	expression tag	UNP A0A0D1DWZ5
A	122	PRO	-	expression tag	UNP A0A0D1DWZ5
A	123	LYS	-	expression tag	UNP A0A0D1DWZ5
A	124	LEU	-	expression tag	UNP A0A0D1DWZ5
A	125	THR	-	expression tag	UNP A0A0D1DWZ5
A	126	ILE	-	expression tag	UNP A0A0D1DWZ5
A	127	HIS	-	expression tag	UNP A0A0D1DWZ5
A	128	LEU	-	expression tag	UNP A0A0D1DWZ5
A	129	LEU	-	expression tag	UNP A0A0D1DWZ5
A	130	ASP	-	expression tag	UNP A0A0D1DWZ5
A	131	SER	-	expression tag	UNP A0A0D1DWZ5
A	132	GLU	-	expression tag	UNP A0A0D1DWZ5
A	133	ASP	-	expression tag	UNP A0A0D1DWZ5
A	134	LEU	-	expression tag	UNP A0A0D1DWZ5
A	135	ARG	-	expression tag	UNP A0A0D1DWZ5
C	3	HIS	-	expression tag	UNP A0A0D1DWZ5
C	118	VAL	-	expression tag	UNP A0A0D1DWZ5
C	119	LYS	-	expression tag	UNP A0A0D1DWZ5
C	120	GLY	-	expression tag	UNP A0A0D1DWZ5
C	121	ALA	-	expression tag	UNP A0A0D1DWZ5
C	122	PRO	-	expression tag	UNP A0A0D1DWZ5
C	123	LYS	-	expression tag	UNP A0A0D1DWZ5
C	124	LEU	-	expression tag	UNP A0A0D1DWZ5
C	125	THR	-	expression tag	UNP A0A0D1DWZ5
C	126	ILE	-	expression tag	UNP A0A0D1DWZ5
C	127	HIS	-	expression tag	UNP A0A0D1DWZ5
C	128	LEU	-	expression tag	UNP A0A0D1DWZ5
C	129	LEU	-	expression tag	UNP A0A0D1DWZ5
C	130	ASP	-	expression tag	UNP A0A0D1DWZ5
C	131	SER	-	expression tag	UNP A0A0D1DWZ5
C	132	GLU	-	expression tag	UNP A0A0D1DWZ5
C	133	ASP	-	expression tag	UNP A0A0D1DWZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	134	LEU	-	expression tag	UNP A0A0D1DWZ5
C	135	ARG	-	expression tag	UNP A0A0D1DWZ5
F	3	HIS	-	expression tag	UNP A0A0D1DWZ5
F	118	VAL	-	expression tag	UNP A0A0D1DWZ5
F	119	LYS	-	expression tag	UNP A0A0D1DWZ5
F	120	GLY	-	expression tag	UNP A0A0D1DWZ5
F	121	ALA	-	expression tag	UNP A0A0D1DWZ5
F	122	PRO	-	expression tag	UNP A0A0D1DWZ5
F	123	LYS	-	expression tag	UNP A0A0D1DWZ5
F	124	LEU	-	expression tag	UNP A0A0D1DWZ5
F	125	THR	-	expression tag	UNP A0A0D1DWZ5
F	126	ILE	-	expression tag	UNP A0A0D1DWZ5
F	127	HIS	-	expression tag	UNP A0A0D1DWZ5
F	128	LEU	-	expression tag	UNP A0A0D1DWZ5
F	129	LEU	-	expression tag	UNP A0A0D1DWZ5
F	130	ASP	-	expression tag	UNP A0A0D1DWZ5
F	131	SER	-	expression tag	UNP A0A0D1DWZ5
F	132	GLU	-	expression tag	UNP A0A0D1DWZ5
F	133	ASP	-	expression tag	UNP A0A0D1DWZ5
F	134	LEU	-	expression tag	UNP A0A0D1DWZ5
F	135	ARG	-	expression tag	UNP A0A0D1DWZ5
I	3	HIS	-	expression tag	UNP A0A0D1DWZ5
I	118	VAL	-	expression tag	UNP A0A0D1DWZ5
I	119	LYS	-	expression tag	UNP A0A0D1DWZ5
I	120	GLY	-	expression tag	UNP A0A0D1DWZ5
I	121	ALA	-	expression tag	UNP A0A0D1DWZ5
I	122	PRO	-	expression tag	UNP A0A0D1DWZ5
I	123	LYS	-	expression tag	UNP A0A0D1DWZ5
I	124	LEU	-	expression tag	UNP A0A0D1DWZ5
I	125	THR	-	expression tag	UNP A0A0D1DWZ5
I	126	ILE	-	expression tag	UNP A0A0D1DWZ5
I	127	HIS	-	expression tag	UNP A0A0D1DWZ5
I	128	LEU	-	expression tag	UNP A0A0D1DWZ5
I	129	LEU	-	expression tag	UNP A0A0D1DWZ5
I	130	ASP	-	expression tag	UNP A0A0D1DWZ5
I	131	SER	-	expression tag	UNP A0A0D1DWZ5
I	132	GLU	-	expression tag	UNP A0A0D1DWZ5
I	133	ASP	-	expression tag	UNP A0A0D1DWZ5
I	134	LEU	-	expression tag	UNP A0A0D1DWZ5
I	135	ARG	-	expression tag	UNP A0A0D1DWZ5
K	3	HIS	-	expression tag	UNP A0A0D1DWZ5
K	118	VAL	-	expression tag	UNP A0A0D1DWZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	119	LYS	-	expression tag	UNP A0A0D1DWZ5
K	120	GLY	-	expression tag	UNP A0A0D1DWZ5
K	121	ALA	-	expression tag	UNP A0A0D1DWZ5
K	122	PRO	-	expression tag	UNP A0A0D1DWZ5
K	123	LYS	-	expression tag	UNP A0A0D1DWZ5
K	124	LEU	-	expression tag	UNP A0A0D1DWZ5
K	125	THR	-	expression tag	UNP A0A0D1DWZ5
K	126	ILE	-	expression tag	UNP A0A0D1DWZ5
K	127	HIS	-	expression tag	UNP A0A0D1DWZ5
K	128	LEU	-	expression tag	UNP A0A0D1DWZ5
K	129	LEU	-	expression tag	UNP A0A0D1DWZ5
K	130	ASP	-	expression tag	UNP A0A0D1DWZ5
K	131	SER	-	expression tag	UNP A0A0D1DWZ5
K	132	GLU	-	expression tag	UNP A0A0D1DWZ5
K	133	ASP	-	expression tag	UNP A0A0D1DWZ5
K	134	LEU	-	expression tag	UNP A0A0D1DWZ5
K	135	ARG	-	expression tag	UNP A0A0D1DWZ5
M	3	HIS	-	expression tag	UNP A0A0D1DWZ5
M	118	VAL	-	expression tag	UNP A0A0D1DWZ5
M	119	LYS	-	expression tag	UNP A0A0D1DWZ5
M	120	GLY	-	expression tag	UNP A0A0D1DWZ5
M	121	ALA	-	expression tag	UNP A0A0D1DWZ5
M	122	PRO	-	expression tag	UNP A0A0D1DWZ5
M	123	LYS	-	expression tag	UNP A0A0D1DWZ5
M	124	LEU	-	expression tag	UNP A0A0D1DWZ5
M	125	THR	-	expression tag	UNP A0A0D1DWZ5
M	126	ILE	-	expression tag	UNP A0A0D1DWZ5
M	127	HIS	-	expression tag	UNP A0A0D1DWZ5
M	128	LEU	-	expression tag	UNP A0A0D1DWZ5
M	129	LEU	-	expression tag	UNP A0A0D1DWZ5
M	130	ASP	-	expression tag	UNP A0A0D1DWZ5
M	131	SER	-	expression tag	UNP A0A0D1DWZ5
M	132	GLU	-	expression tag	UNP A0A0D1DWZ5
M	133	ASP	-	expression tag	UNP A0A0D1DWZ5
M	134	LEU	-	expression tag	UNP A0A0D1DWZ5
M	135	ARG	-	expression tag	UNP A0A0D1DWZ5
O	3	HIS	-	expression tag	UNP A0A0D1DWZ5
O	118	VAL	-	expression tag	UNP A0A0D1DWZ5
O	119	LYS	-	expression tag	UNP A0A0D1DWZ5
O	120	GLY	-	expression tag	UNP A0A0D1DWZ5
O	121	ALA	-	expression tag	UNP A0A0D1DWZ5
O	122	PRO	-	expression tag	UNP A0A0D1DWZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
O	123	LYS	-	expression tag	UNP A0A0D1DWZ5
O	124	LEU	-	expression tag	UNP A0A0D1DWZ5
O	125	THR	-	expression tag	UNP A0A0D1DWZ5
O	126	ILE	-	expression tag	UNP A0A0D1DWZ5
O	127	HIS	-	expression tag	UNP A0A0D1DWZ5
O	128	LEU	-	expression tag	UNP A0A0D1DWZ5
O	129	LEU	-	expression tag	UNP A0A0D1DWZ5
O	130	ASP	-	expression tag	UNP A0A0D1DWZ5
O	131	SER	-	expression tag	UNP A0A0D1DWZ5
O	132	GLU	-	expression tag	UNP A0A0D1DWZ5
O	133	ASP	-	expression tag	UNP A0A0D1DWZ5
O	134	LEU	-	expression tag	UNP A0A0D1DWZ5
O	135	ARG	-	expression tag	UNP A0A0D1DWZ5

- Molecule 2 is a protein called PAMPL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	B	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	E	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	G	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	J	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	L	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	N	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	P	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	5	Total	O	0	0
			5	5		
3	A	4	Total	O	0	0
			4	4		
3	C	4	Total	O	0	0
			4	4		

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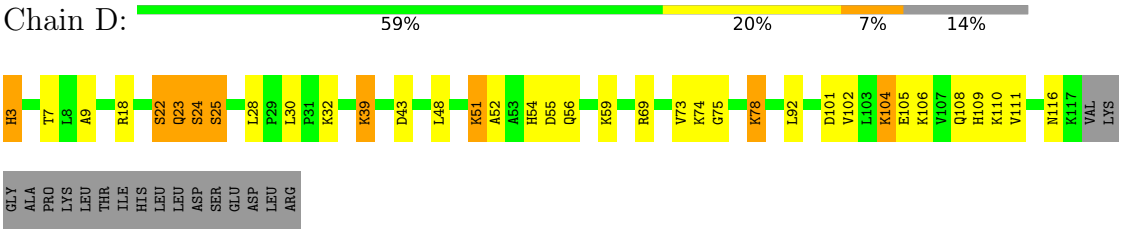
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	4	Total O 4 4	0	0
3	G	1	Total O 1 1	0	0
3	I	6	Total O 6 6	0	0
3	J	1	Total O 1 1	0	0
3	K	5	Total O 5 5	0	0
3	M	2	Total O 2 2	0	0
3	P	1	Total O 1 1	0	0

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 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.

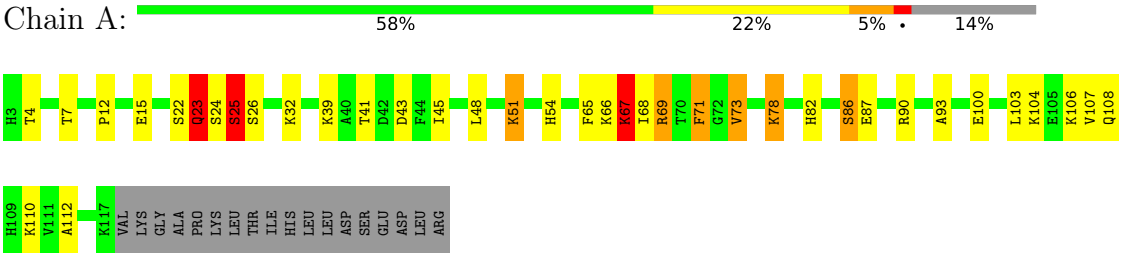
• Molecule 1: RNA-binding protein RRM4

Chain D:



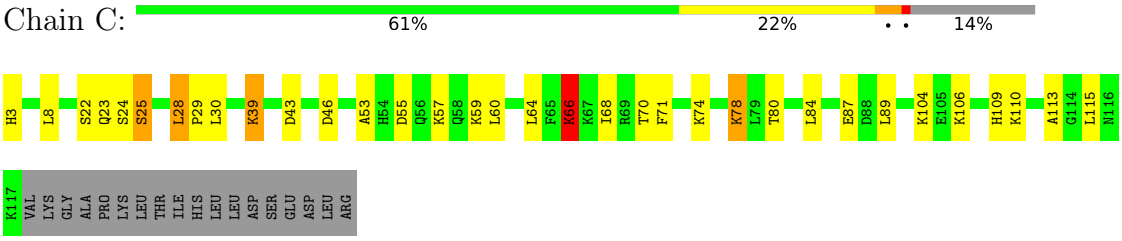
• Molecule 1: RNA-binding protein RRM4

Chain A:



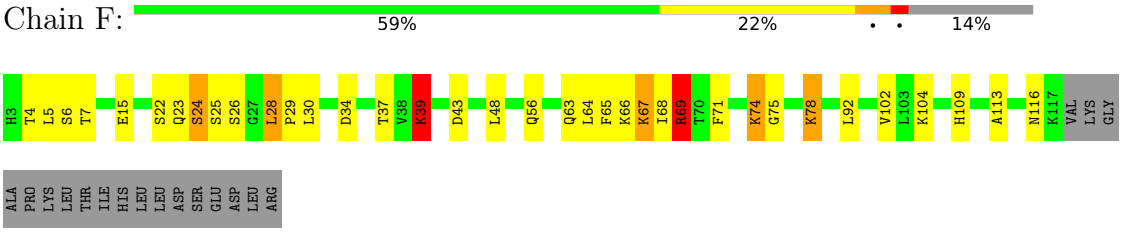
• Molecule 1: RNA-binding protein RRM4

Chain C:



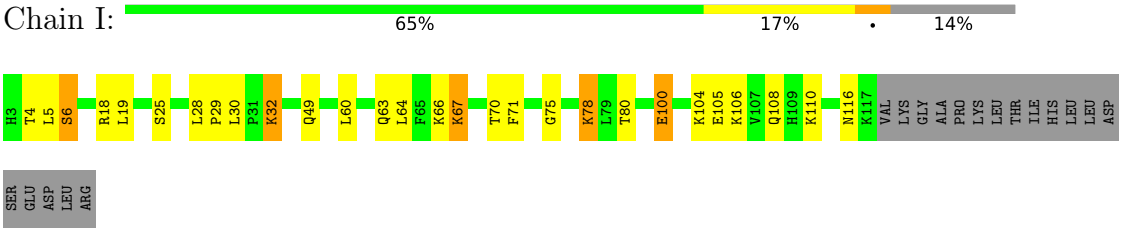
• Molecule 1: RNA-binding protein RRM4

Chain F:



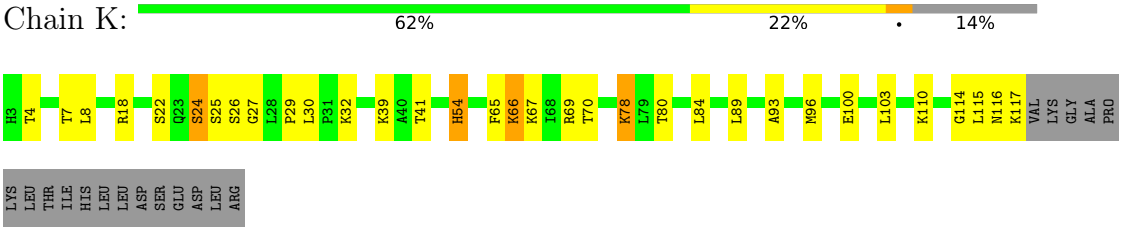
• Molecule 1: RNA-binding protein RRM4

Chain I:



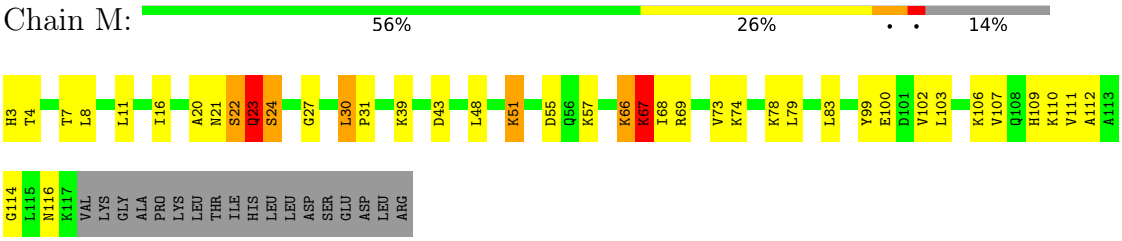
• Molecule 1: RNA-binding protein RRM4

Chain K:



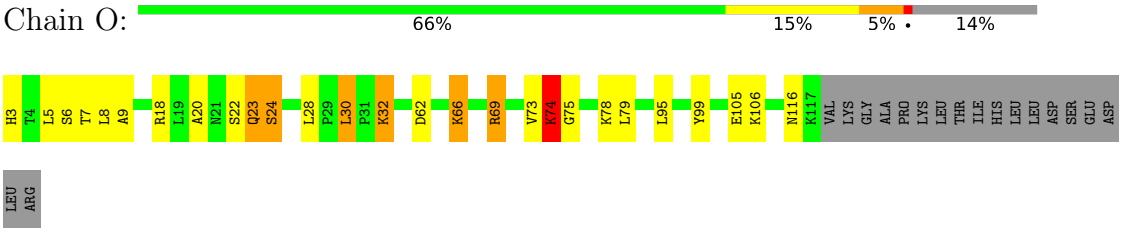
• Molecule 1: RNA-binding protein RRM4

Chain M:



• Molecule 1: RNA-binding protein RRM4

Chain O:



• Molecule 2: PAMPL2

Chain H:

• Molecule 2: PAMPL2

Chain B:

• Molecule 2: PAMPL2

Chain E:

• Molecule 2: PAMPL2

Chain G:

• Molecule 2: PAMPL2

Chain J:

• Molecule 2: PAMPL2

Chain L:

• Molecule 2: PAMPL2

Chain N:

• Molecule 2: PAMPL2

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	82.88Å 74.63Å 168.51Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	56.17 – 2.40 56.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (56.17-2.40) 81.2 (56.17-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-0.21 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.240 , 0.276 0.230 , 0.269	Depositor DCC
R_{free} test set	32173 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.318 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15073	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	A	1.26	9/886 (1.0%)	1.13	8/1195 (0.7%)
1	C	1.03	8/886 (0.9%)	1.09	10/1195 (0.8%)
1	D	1.11	7/886 (0.8%)	1.01	4/1195 (0.3%)
1	F	0.96	5/886 (0.6%)	1.26	8/1195 (0.7%)
1	I	0.96	3/886 (0.3%)	0.99	4/1195 (0.3%)
1	K	1.01	8/886 (0.9%)	1.11	8/1195 (0.7%)
1	M	0.97	6/886 (0.7%)	1.34	15/1195 (1.3%)
1	O	1.12	5/886 (0.6%)	1.44	14/1195 (1.2%)
2	B	1.11	0/57	1.45	1/77 (1.3%)
2	E	1.69	2/57 (3.5%)	1.24	0/77
2	G	1.29	0/57	1.14	0/77
2	H	2.11	3/57 (5.3%)	1.23	0/77
2	J	0.87	0/57	1.43	1/77 (1.3%)
2	L	1.12	0/57	1.44	0/77
2	N	2.11	2/57 (3.5%)	1.87	4/77 (5.2%)
2	P	0.90	0/57	0.91	0/77
All	All	1.09	58/7544 (0.8%)	1.19	77/10176 (0.8%)

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	LYS	CD-CE	18.68	1.98	1.51
1	O	74	LYS	CD-CE	14.35	1.87	1.51
1	A	51	LYS	CE-NZ	13.99	1.84	1.49
1	I	32	LYS	CD-CE	13.61	1.85	1.51
1	O	74	LYS	CE-NZ	12.12	1.79	1.49
1	D	78	LYS	CD-CE	11.73	1.80	1.51
1	M	24	SER	CB-OG	11.35	1.57	1.42
1	C	66	LYS	CD-CE	11.29	1.79	1.51
1	D	39	LYS	CE-NZ	11.02	1.76	1.49
2	N	117	GLU	CD-OE2	10.84	1.37	1.25
1	A	67	LYS	CE-NZ	10.45	1.75	1.49
2	H	117	GLU	CD-OE2	10.42	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	66	LYS	CE-NZ	9.31	1.72	1.49
1	C	78	LYS	CD-CE	9.29	1.74	1.51
1	K	78	LYS	CG-CD	8.62	1.81	1.52
1	O	69	ARG	CG-CD	8.43	1.73	1.51
2	E	117	GLU	CB-CG	8.41	1.68	1.52
2	H	117	GLU	CB-CG	8.39	1.68	1.52
1	M	23	GLN	CA-C	8.14	1.74	1.52
1	F	39	LYS	CE-NZ	7.93	1.68	1.49
1	K	24	SER	CB-OG	7.68	1.52	1.42
1	D	51	LYS	CE-NZ	7.66	1.68	1.49
1	D	25	SER	CB-OG	7.65	1.52	1.42
1	A	86	SER	CB-OG	7.48	1.51	1.42
1	C	66	LYS	CE-NZ	7.37	1.67	1.49
1	K	66	LYS	CD-CE	7.26	1.69	1.51
1	A	26	SER	CB-OG	7.15	1.51	1.42
1	C	39	LYS	CG-CD	7.01	1.76	1.52
1	F	78	LYS	CD-CE	7.01	1.68	1.51
2	N	117	GLU	CB-CG	6.94	1.65	1.52
1	K	39	LYS	CE-NZ	6.88	1.66	1.49
1	K	66	LYS	CE-NZ	6.84	1.66	1.49
1	C	39	LYS	CE-NZ	6.83	1.66	1.49
1	A	25	SER	CB-OG	6.58	1.50	1.42
2	E	117	GLU	CG-CD	6.49	1.61	1.51
1	I	71	PHE	CE2-CZ	6.36	1.49	1.37
1	K	26	SER	CB-OG	6.36	1.50	1.42
2	H	117	GLU	CD-OE1	6.25	1.32	1.25
1	C	39	LYS	CD-CE	6.22	1.66	1.51
1	O	5	LEU	CG-CD1	6.06	1.74	1.51
1	F	74	LYS	CD-CE	5.96	1.66	1.51
1	K	39	LYS	CD-CE	5.91	1.66	1.51
1	C	87	GLU	CG-CD	5.88	1.60	1.51
1	A	73	VAL	CB-CG1	5.73	1.64	1.52
1	D	78	LYS	CG-CD	5.70	1.71	1.52
1	O	74	LYS	CG-CD	5.67	1.71	1.52
1	F	69	ARG	CG-CD	5.39	1.65	1.51
1	K	78	LYS	CD-CE	5.38	1.64	1.51
1	M	55	ASP	CG-OD2	5.37	1.37	1.25
1	F	15	GLU	CG-CD	5.35	1.59	1.51
1	M	78	LYS	CD-CE	5.20	1.64	1.51
1	D	104	LYS	CD-CE	5.19	1.64	1.51
1	A	87	GLU	CG-CD	5.16	1.59	1.51
1	M	22	SER	C-N	5.12	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	100	GLU	CG-CD	5.09	1.59	1.51
1	C	78	LYS	CE-NZ	5.08	1.61	1.49
1	A	71	PHE	CE2-CZ	5.06	1.47	1.37
1	D	104	LYS	CG-CD	5.04	1.69	1.52

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	5	LEU	CB-CG-CD2	18.38	142.25	111.00
1	F	69	ARG	NE-CZ-NH1	17.60	129.10	120.30
1	F	69	ARG	NE-CZ-NH2	-17.14	111.73	120.30
1	O	5	LEU	CB-CG-CD1	-15.88	84.00	111.00
1	O	30	LEU	CA-CB-CG	14.69	149.08	115.30
1	M	67	LYS	CD-CE-NZ	-12.73	82.41	111.70
1	M	30	LEU	CB-CG-CD1	11.89	131.21	111.00
1	K	66	LYS	CD-CE-NZ	-11.83	84.49	111.70
1	M	30	LEU	CB-CG-CD2	-11.41	91.61	111.00
1	O	74	LYS	CD-CE-NZ	-11.19	85.97	111.70
1	C	66	LYS	CD-CE-NZ	-10.34	87.93	111.70
1	O	74	LYS	CB-CG-CD	-10.07	85.41	111.60
1	A	67	LYS	CD-CE-NZ	-9.95	88.83	111.70
1	M	30	LEU	CA-CB-CG	9.78	137.80	115.30
1	F	67	LYS	CD-CE-NZ	-9.50	89.84	111.70
1	M	69	ARG	CB-CA-C	-9.27	91.87	110.40
1	I	32	LYS	CG-CD-CE	-9.21	84.26	111.90
1	K	39	LYS	CD-CE-NZ	-9.11	90.74	111.70
2	J	116	ASP	N-CA-C	-8.50	88.05	111.00
1	O	30	LEU	CB-CG-CD2	8.44	125.35	111.00
1	O	30	LEU	CB-CG-CD1	-8.22	97.02	111.00
1	K	39	LYS	CA-CB-CG	7.96	130.92	113.40
1	O	78	LYS	CD-CE-NZ	-7.85	93.65	111.70
1	M	55	ASP	CB-CG-OD1	-7.76	111.32	118.30
1	O	69	ARG	CA-CB-CG	7.69	130.31	113.40
1	D	78	LYS	CG-CD-CE	-7.60	89.10	111.90
1	C	28	LEU	CB-CG-CD1	7.57	123.87	111.00
2	N	117	GLU	CA-CB-CG	7.45	129.80	113.40
1	F	69	ARG	CA-CB-CG	7.29	129.43	113.40
2	N	117	GLU	CG-CD-OE2	7.23	132.77	118.30
1	F	78	LYS	CG-CD-CE	-7.16	90.42	111.90
1	A	51	LYS	CA-CB-CG	-7.10	97.78	113.40
1	C	28	LEU	CA-CB-CG	-7.03	99.14	115.30
1	M	69	ARG	CA-CB-CG	6.79	128.34	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	LYS	CA-CB-CG	6.73	128.20	113.40
1	K	78	LYS	CG-CD-CE	-6.69	91.83	111.90
1	F	69	ARG	CD-NE-CZ	6.66	132.92	123.60
2	N	117	GLU	CG-CD-OE1	-6.64	105.01	118.30
1	C	78	LYS	CG-CD-CE	-6.59	92.11	111.90
1	M	69	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	F	69	ARG	N-CA-CB	-6.53	98.84	110.60
1	D	104	LYS	CA-CB-CG	-6.44	99.24	113.40
1	A	23	GLN	CA-CB-CG	-6.36	99.41	113.40
1	M	78	LYS	CG-CD-CE	-6.21	93.25	111.90
1	M	69	ARG	CD-NE-CZ	6.17	132.24	123.60
1	M	51	LYS	CA-CB-CG	6.14	126.92	113.40
2	N	117	GLU	N-CA-CB	6.14	121.66	110.60
1	K	32	LYS	CG-CD-CE	-6.11	93.57	111.90
1	D	92	LEU	CB-CG-CD1	6.06	121.30	111.00
1	C	46	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	C	28	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	A	67	LYS	CB-CA-C	6.00	122.40	110.40
1	D	32	LYS	CG-CD-CE	5.98	129.83	111.90
1	I	63	GLN	CA-CB-CG	5.96	126.52	113.40
1	A	23	GLN	N-CA-C	5.85	126.80	111.00
1	K	32	LYS	CA-CB-CG	-5.81	100.61	113.40
1	K	54	HIS	N-CA-CB	-5.75	100.24	110.60
1	C	3	HIS	N-CA-C	-5.75	95.47	111.00
1	A	69	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	O	66	LYS	CA-CB-CG	5.63	125.79	113.40
1	M	69	ARG	CG-CD-NE	-5.60	100.05	111.80
1	O	23	GLN	CA-CB-CG	5.44	125.37	113.40
1	O	69	ARG	CG-CD-NE	5.40	123.15	111.80
1	M	23	GLN	N-CA-CB	5.36	120.25	110.60
1	C	66	LYS	CG-CD-CE	-5.35	95.86	111.90
1	O	66	LYS	CB-CG-CD	-5.34	97.71	111.60
1	I	18	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	I	32	LYS	CB-CG-CD	5.32	125.42	111.60
1	M	55	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	28	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	A	69	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	B	116	ASP	CA-C-N	-5.21	105.74	117.20
1	M	69	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	3	HIS	CB-CA-C	5.14	120.68	110.40
1	K	54	HIS	CB-CA-C	5.02	120.45	110.40
1	O	69	ARG	N-CA-CB	-5.02	101.56	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	39	LYS	CG-CD-CE	-5.01	96.88	111.90

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	873	908	908	44	2
1	C	873	908	908	37	0
1	D	873	908	908	31	2
1	F	873	908	908	45	1
1	I	873	908	908	23	0
1	K	873	908	908	25	0
1	M	873	908	908	38	0
1	O	873	908	908	34	0
2	B	55	44	45	3	0
2	E	55	44	45	1	0
2	G	55	44	45	2	0
2	H	55	44	45	3	0
2	J	55	44	45	4	0
2	L	55	44	45	4	0
2	N	55	44	45	2	1
2	P	55	44	45	1	0
3	A	4	0	0	1	0
3	C	4	0	0	0	0
3	D	5	0	0	0	0
3	F	4	0	0	2	0
3	G	1	0	0	0	0
3	I	6	0	0	2	0
3	J	1	0	0	0	0
3	K	5	0	0	0	0
3	M	2	0	0	0	0
3	P	1	0	0	1	0
All	All	7457	7616	7624	281	3

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 19.

All (281) 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)
1:C:39:LYS:CD	1:C:39:LYS:CG	1.76	1.60
1:C:78:LYS:CE	1:C:78:LYS:CD	1.74	1.58
1:C:66:LYS:CE	1:C:66:LYS:CD	1.79	1.57
1:K:78:LYS:CD	1:K:78:LYS:CG	1.81	1.56
1:D:78:LYS:CD	1:D:78:LYS:CE	1.80	1.56
1:D:51:LYS:NZ	1:D:51:LYS:CE	1.68	1.54
1:F:39:LYS:NZ	1:F:39:LYS:CE	1.68	1.53
1:O:74:LYS:CE	1:O:74:LYS:CD	1.87	1.53
1:I:32:LYS:CE	1:I:32:LYS:CD	1.85	1.52
1:C:66:LYS:CE	1:C:66:LYS:NZ	1.67	1.50
1:M:66:LYS:CE	1:M:66:LYS:NZ	1.72	1.49
1:A:67:LYS:CE	1:A:67:LYS:NZ	1.75	1.48
1:D:39:LYS:NZ	1:D:39:LYS:CE	1.76	1.46
1:O:74:LYS:CE	1:O:74:LYS:NZ	1.79	1.43
1:A:67:LYS:CE	1:A:67:LYS:CD	1.97	1.40
1:A:51:LYS:NZ	1:A:51:LYS:CE	1.84	1.39
1:A:67:LYS:NZ	1:A:100:GLU:OE1	1.81	1.13
1:A:39:LYS:NZ	1:A:43:ASP:OD2	1.83	1.10
1:F:25:SER:HA	1:F:28:LEU:HD12	1.34	1.05
1:F:39:LYS:HE2	1:F:43:ASP:OD2	1.57	1.05
1:A:65:PHE:HE2	2:B:116:ASP:OD1	1.42	1.03
1:I:32:LYS:CE	1:I:32:LYS:CG	2.37	1.02
1:O:3:HIS:HE1	1:O:8:LEU:N	1.60	0.98
1:C:78:LYS:CE	1:C:78:LYS:CG	2.43	0.97
1:O:3:HIS:HE1	1:O:8:LEU:CA	1.79	0.96
1:F:25:SER:HA	1:F:28:LEU:CD1	1.97	0.95
1:C:66:LYS:CE	1:C:66:LYS:CG	2.48	0.92
1:D:78:LYS:CE	1:D:78:LYS:CG	2.47	0.91
1:A:65:PHE:CE2	2:B:116:ASP:OD1	2.24	0.91
1:K:78:LYS:CG	1:K:78:LYS:CE	2.48	0.91
1:O:20:ALA:HB2	1:O:30:LEU:HD11	1.50	0.91
1:I:32:LYS:CE	1:I:32:LYS:HG3	2.02	0.90
1:I:67:LYS:HZ2	1:I:100:GLU:HG2	1.38	0.87
2:J:119:ILE:O	2:J:119:ILE:HD12	1.73	0.87
1:C:25:SER:HA	1:C:28:LEU:HD12	1.55	0.86
1:D:48:LEU:HB3	1:D:56:GLN:HG2	1.56	0.85
1:I:25:SER:OG	3:I:201:HOH:O	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:3:HIS:CE1	1:O:8:LEU:CA	2.59	0.85
1:A:39:LYS:NZ	1:A:43:ASP:CG	2.29	0.85
1:C:66:LYS:CD	1:C:66:LYS:NZ	2.40	0.84
1:F:25:SER:CA	1:F:28:LEU:HD12	2.06	0.84
1:A:4:THR:CG2	1:A:7:THR:HG23	2.08	0.84
1:A:39:LYS:HZ2	1:A:43:ASP:CG	1.81	0.84
1:C:39:LYS:CG	1:C:39:LYS:CE	2.56	0.83
1:O:3:HIS:CE1	1:O:8:LEU:N	2.46	0.83
1:A:67:LYS:NZ	1:A:100:GLU:CD	2.34	0.80
1:O:20:ALA:CB	1:O:30:LEU:HD11	2.11	0.80
1:O:3:HIS:CE1	1:O:8:LEU:HA	2.18	0.78
1:F:48:LEU:O	1:F:56:GLN:NE2	2.17	0.77
1:F:39:LYS:CE	1:F:43:ASP:OD2	2.31	0.77
1:F:39:LYS:C	1:F:39:LYS:HD3	2.05	0.76
1:M:30:LEU:HB2	1:M:31:PRO:HD2	1.68	0.76
1:M:21:ASN:O	1:M:23:GLN:OE1	2.04	0.75
2:J:116:ASP:C	2:J:116:ASP:OD1	2.23	0.75
1:O:3:HIS:HE1	1:O:8:LEU:HA	1.51	0.74
1:A:67:LYS:HZ3	1:A:100:GLU:CD	1.90	0.74
1:O:74:LYS:CD	1:O:74:LYS:NZ	2.49	0.74
1:C:60:LEU:HD22	1:C:89:LEU:HG	1.69	0.73
1:F:4:THR:HG22	1:F:7:THR:HG23	1.69	0.73
1:M:67:LYS:HE2	1:M:100:GLU:CD	2.10	0.72
2:P:116:ASP:O	3:P:201:HOH:O	2.06	0.72
1:M:67:LYS:CE	1:M:100:GLU:OE1	2.38	0.72
1:C:39:LYS:NZ	1:C:43:ASP:OD2	2.21	0.71
1:D:3:HIS:ND1	1:D:7:THR:OG1	2.22	0.71
1:C:23:GLN:O	1:C:23:GLN:HG3	1.90	0.70
1:I:49:GLN:O	3:I:202:HOH:O	2.09	0.69
1:M:22:SER:O	1:M:24:SER:N	2.24	0.69
1:M:39:LYS:NZ	1:M:43:ASP:OD2	2.25	0.69
1:D:78:LYS:CG	1:D:78:LYS:HE3	2.23	0.69
1:A:39:LYS:NZ	1:A:43:ASP:OD1	2.24	0.68
1:K:67:LYS:NZ	1:K:100:GLU:OE1	2.26	0.68
1:I:32:LYS:HG3	1:I:32:LYS:HE3	1.75	0.68
1:I:67:LYS:HZ2	1:I:100:GLU:CG	2.06	0.67
1:F:39:LYS:NZ	1:F:39:LYS:CD	2.58	0.67
1:C:66:LYS:O	1:C:70:THR:HG23	1.94	0.67
1:K:4:THR:OG1	1:K:7:THR:HG23	1.94	0.66
1:F:39:LYS:HE2	1:F:43:ASP:CG	2.16	0.64
1:A:4:THR:HG23	1:A:7:THR:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:NZ	1:A:67:LYS:CD	2.61	0.64
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.80	0.64
1:O:62:ASP:O	1:O:66:LYS:HD3	1.99	0.63
1:O:30:LEU:HD22	1:O:99:TYR:CD1	2.35	0.62
1:F:68:ILE:O	1:F:71:PHE:HB2	2.00	0.62
1:F:74:LYS:CE	1:F:75:GLY:N	2.63	0.61
1:A:67:LYS:HE3	1:A:71:PHE:CE1	2.35	0.61
1:O:9:ALA:HB1	1:O:106:LYS:HB2	1.82	0.61
1:M:30:LEU:HD13	1:M:99:TYR:CE1	2.35	0.61
1:F:39:LYS:CE	1:F:43:ASP:CG	2.69	0.61
1:C:66:LYS:CE	1:C:66:LYS:HG3	2.30	0.61
1:M:67:LYS:HE2	1:M:100:GLU:OE1	2.01	0.61
1:F:74:LYS:HE2	1:F:75:GLY:N	2.16	0.61
1:M:57:LYS:HD2	2:N:120:TYR:CZ	2.36	0.60
1:K:69:ARG:NH2	2:L:116:ASP:OD2	2.34	0.60
1:A:73:VAL:HG13	1:A:104:LYS:NZ	2.16	0.60
1:O:6:SER:HA	1:O:105:GLU:HG2	1.83	0.59
1:I:78:LYS:H	1:I:78:LYS:HD2	1.66	0.59
1:D:78:LYS:HE3	1:D:78:LYS:HG3	1.82	0.59
1:F:30:LEU:CD2	1:F:102:VAL:HG21	2.32	0.59
1:M:4:THR:HG22	1:M:7:THR:OG1	2.03	0.59
1:A:67:LYS:HZ1	1:A:100:GLU:CD	2.06	0.59
1:A:39:LYS:O	1:A:39:LYS:HD3	2.03	0.59
1:C:53:ALA:O	1:C:57:LYS:HG3	2.02	0.59
1:F:39:LYS:HE3	1:F:43:ASP:OD1	2.03	0.58
1:D:39:LYS:HE2	1:D:43:ASP:OD2	2.03	0.58
1:A:104:LYS:O	1:A:108:GLN:HG3	2.03	0.58
1:C:71:PHE:CG	1:C:104:LYS:HD2	2.39	0.58
1:F:74:LYS:HE2	1:F:75:GLY:CA	2.34	0.58
1:M:66:LYS:NZ	1:M:66:LYS:CD	2.65	0.58
1:D:30:LEU:CD2	1:D:102:VAL:HG21	2.34	0.57
1:K:29:PRO:O	1:K:30:LEU:HD23	2.04	0.57
1:A:78:LYS:H	1:A:78:LYS:HD2	1.69	0.57
1:K:29:PRO:C	1:K:30:LEU:HD23	2.25	0.57
1:M:73:VAL:HG11	1:M:111:VAL:HG21	1.86	0.57
1:F:63:GLN:HA	1:F:66:LYS:HE3	1.86	0.57
1:A:112:ALA:HB1	1:C:74:LYS:HD3	1.85	0.56
1:A:67:LYS:CE	1:A:67:LYS:CG	2.83	0.56
1:C:39:LYS:CG	1:C:39:LYS:HZ3	2.17	0.56
1:F:71:PHE:O	1:F:104:LYS:NZ	2.38	0.56
1:C:39:LYS:HZ3	1:C:39:LYS:HG2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:THR:HG23	1:F:7:THR:H	1.70	0.56
1:A:106:LYS:O	1:A:110:LYS:HG2	2.06	0.56
1:A:41:THR:HG23	1:A:93:ALA:HB1	1.87	0.56
1:A:68:ILE:O	1:A:71:PHE:HB2	2.06	0.56
1:C:55:ASP:O	1:C:59:LYS:HG3	2.05	0.56
1:I:67:LYS:NZ	1:I:100:GLU:CD	2.58	0.56
1:M:3:HIS:HB2	1:M:27:GLY:O	2.06	0.56
1:K:116:ASN:OD1	1:K:116:ASN:N	2.39	0.56
1:M:22:SER:O	1:M:22:SER:OG	2.22	0.55
1:A:4:THR:HG22	1:A:7:THR:HG23	1.84	0.55
1:M:22:SER:C	1:M:24:SER:H	2.10	0.55
1:M:20:ALA:HB2	1:M:30:LEU:HD11	1.89	0.54
1:M:4:THR:HG23	1:M:7:THR:H	1.72	0.54
1:M:67:LYS:CE	1:M:100:GLU:CD	2.75	0.54
1:A:71:PHE:CZ	1:A:103:LEU:HD23	2.42	0.54
1:F:30:LEU:HD22	1:F:102:VAL:HG21	1.90	0.54
1:C:78:LYS:CD	1:C:78:LYS:NZ	2.68	0.54
1:F:48:LEU:HB3	1:F:56:GLN:HG2	1.89	0.54
1:M:30:LEU:CD2	1:M:102:VAL:HG21	2.38	0.53
1:I:67:LYS:HZ1	1:I:100:GLU:CD	2.11	0.53
1:I:106:LYS:O	1:I:110:LYS:HG2	2.08	0.53
1:C:39:LYS:CG	1:C:39:LYS:NZ	2.72	0.53
1:I:4:THR:HG22	1:I:5:LEU:H	1.75	0.52
1:A:82:HIS:O	1:A:86:SER:HB3	2.09	0.52
1:F:34:ASP:HB3	3:F:201:HOH:O	2.10	0.52
1:O:75:GLY:HA3	1:O:116:ASN:HB2	1.90	0.52
1:C:23:GLN:O	1:C:25:SER:N	2.42	0.52
1:C:39:LYS:CD	1:C:39:LYS:CB	2.81	0.51
1:I:64:LEU:HD23	1:I:80:THR:HG23	1.90	0.51
1:D:3:HIS:CE1	1:D:7:THR:OG1	2.62	0.51
1:F:39:LYS:HD3	1:F:39:LYS:O	2.10	0.51
1:I:29:PRO:O	1:I:30:LEU:HD23	2.10	0.51
1:I:75:GLY:HA3	1:I:116:ASN:HB2	1.92	0.51
1:F:23:GLN:O	1:F:25:SER:N	2.42	0.51
1:O:9:ALA:HB1	1:O:106:LYS:CA	2.41	0.51
1:I:67:LYS:NZ	1:I:100:GLU:CG	2.73	0.51
1:C:110:LYS:O	1:C:115:LEU:HB2	2.11	0.51
1:F:65:PHE:CG	2:G:118:PHE:HB2	2.46	0.51
1:O:3:HIS:CE1	1:O:8:LEU:CD1	2.94	0.51
1:A:67:LYS:CE	1:A:71:PHE:CE1	2.94	0.50
1:C:29:PRO:O	1:C:30:LEU:HD23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:HIS:HE2	2:H:121:PRO:C	2.15	0.50
1:C:64:LEU:HD23	1:C:80:THR:HG23	1.93	0.50
1:M:57:LYS:HD2	2:N:120:TYR:OH	2.12	0.50
1:C:106:LYS:O	1:C:109:HIS:HB2	2.10	0.50
1:M:48:LEU:O	1:M:51:LYS:HB2	2.12	0.50
1:I:66:LYS:O	1:I:70:THR:HG23	2.12	0.50
1:D:55:ASP:O	1:D:59:LYS:HG2	2.13	0.49
1:O:79:LEU:HD11	1:O:116:ASN:HB3	1.94	0.49
1:F:22:SER:O	1:F:24:SER:N	2.46	0.49
1:O:20:ALA:HA	1:O:28:LEU:HD21	1.95	0.49
1:O:18:ARG:HH11	1:O:18:ARG:HG3	1.77	0.49
1:F:25:SER:HA	1:F:28:LEU:HD13	1.90	0.49
1:K:84:LEU:HD23	1:K:89:LEU:CD2	2.43	0.49
1:D:48:LEU:C	1:D:56:GLN:HE21	2.15	0.48
1:O:73:VAL:HG12	1:O:74:LYS:O	2.13	0.48
1:A:25:SER:HB3	3:A:201:HOH:O	2.12	0.48
1:O:22:SER:C	1:O:24:SER:N	2.67	0.48
1:K:78:LYS:CE	1:K:78:LYS:HG2	2.40	0.48
1:O:3:HIS:HE1	1:O:7:THR:C	2.16	0.48
2:E:118:PHE:O	2:E:119:ILE:HD13	2.14	0.48
1:F:29:PRO:O	1:F:30:LEU:HD23	2.14	0.48
1:M:103:LEU:O	1:M:107:VAL:HG23	2.14	0.48
1:O:32:LYS:HA	1:O:32:LYS:CE	2.41	0.48
1:O:20:ALA:CB	1:O:30:LEU:CD1	2.90	0.47
1:I:4:THR:HG22	1:I:5:LEU:N	2.30	0.47
1:M:23:GLN:N	1:M:23:GLN:CD	2.67	0.47
1:D:104:LYS:HE3	1:D:108:GLN:NE2	2.29	0.47
1:D:106:LYS:O	1:D:110:LYS:HG2	2.14	0.47
1:F:74:LYS:CE	1:F:75:GLY:CA	2.93	0.47
1:C:23:GLN:O	1:C:23:GLN:CG	2.61	0.47
1:F:113:ALA:HB2	1:K:54:HIS:HE1	1.80	0.47
1:O:95:LEU:HA	1:O:99:TYR:HB2	1.96	0.47
1:M:30:LEU:HB2	1:M:31:PRO:CD	2.42	0.46
1:D:54:HIS:NE2	2:H:121:PRO:O	2.45	0.46
1:F:74:LYS:HE3	1:F:75:GLY:H	1.80	0.46
1:K:8:LEU:CD2	1:K:30:LEU:HD21	2.45	0.46
1:K:41:THR:CG2	1:K:93:ALA:HB1	2.46	0.46
1:D:73:VAL:HG12	1:D:74:LYS:O	2.16	0.46
1:O:3:HIS:CE1	1:O:8:LEU:CB	2.98	0.46
1:A:23:GLN:HG3	1:A:24:SER:N	2.29	0.45
1:M:22:SER:C	1:M:24:SER:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:9:ALA:HB1	1:O:106:LYS:CB	2.47	0.45
1:C:39:LYS:NZ	1:C:39:LYS:HG2	2.31	0.45
1:C:80:THR:HG22	1:C:84:LEU:CD1	2.47	0.45
1:M:68:ILE:HD11	1:M:83:LEU:HD12	1.98	0.45
1:D:52:ALA:O	1:D:55:ASP:N	2.50	0.45
1:D:25:SER:OG	1:D:28:LEU:HD12	2.17	0.45
1:K:22:SER:C	1:K:24:SER:N	2.70	0.45
1:D:23:GLN:O	1:D:25:SER:N	2.49	0.45
1:I:60:LEU:HD12	1:I:60:LEU:O	2.16	0.45
1:A:48:LEU:HA	1:A:51:LYS:HD2	1.98	0.44
1:A:39:LYS:HZ3	1:A:43:ASP:CG	2.06	0.44
1:K:22:SER:C	1:K:24:SER:H	2.20	0.44
1:K:80:THR:HG22	1:K:84:LEU:CD1	2.47	0.44
1:M:67:LYS:HE3	1:M:100:GLU:OE1	2.16	0.44
1:F:65:PHE:CD2	2:G:118:PHE:HB2	2.53	0.44
1:I:19:LEU:HB3	1:I:28:LEU:HD11	2.00	0.44
1:K:80:THR:HG22	1:K:84:LEU:HD12	1.99	0.44
1:K:25:SER:O	1:K:27:GLY:N	2.48	0.44
1:D:111:VAL:HG22	1:D:116:ASN:ND2	2.32	0.44
1:C:78:LYS:CE	1:C:78:LYS:HG3	2.38	0.44
1:F:74:LYS:HE3	1:F:75:GLY:N	2.33	0.44
1:K:65:PHE:HZ	2:L:116:ASP:HB3	1.81	0.44
1:O:116:ASN:OD1	1:O:116:ASN:N	2.51	0.44
1:C:68:ILE:O	1:C:71:PHE:HB2	2.18	0.43
2:L:116:ASP:OD1	2:L:117:GLU:N	2.51	0.43
1:A:45:ILE:HD11	1:A:93:ALA:HB2	1.99	0.43
1:F:25:SER:C	1:F:28:LEU:HD12	2.38	0.43
1:F:64:LEU:HD22	1:F:92:LEU:HD21	2.00	0.43
1:A:68:ILE:HA	1:A:71:PHE:CD2	2.53	0.43
1:A:73:VAL:HG21	1:A:107:VAL:HG11	1.99	0.43
1:D:18:ARG:NH2	1:A:90:ARG:HD3	2.33	0.43
1:F:22:SER:C	1:F:24:SER:N	2.72	0.43
2:J:116:ASP:OD1	2:J:116:ASP:O	2.36	0.42
1:M:106:LYS:O	1:M:110:LYS:HG2	2.19	0.42
1:F:104:LYS:NZ	1:M:114:GLY:HA3	2.34	0.42
1:D:30:LEU:HD21	1:D:102:VAL:HG21	2.02	0.42
1:D:73:VAL:HG23	1:D:104:LYS:HZ2	1.85	0.42
1:C:8:LEU:HD12	1:C:8:LEU:HA	1.84	0.42
1:F:65:PHE:O	1:F:69:ARG:HB2	2.19	0.42
1:I:104:LYS:HE2	1:I:108:GLN:HE22	1.85	0.42
2:J:119:ILE:O	2:J:119:ILE:CD1	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:LYS:CD	1:K:78:LYS:CB	2.87	0.42
1:M:20:ALA:HB2	1:M:30:LEU:CD1	2.49	0.42
1:O:22:SER:C	1:O:24:SER:H	2.23	0.42
1:D:52:ALA:HB1	1:C:113:ALA:HA	2.02	0.42
1:A:66:LYS:O	1:A:69:ARG:HG3	2.19	0.42
1:F:4:THR:CG2	1:F:7:THR:HG23	2.43	0.42
1:K:110:LYS:O	1:K:115:LEU:HB2	2.18	0.42
1:M:79:LEU:HD11	1:M:116:ASN:HB3	2.02	0.42
1:O:3:HIS:NE2	1:O:8:LEU:HD12	2.35	0.42
1:D:69:ARG:NH1	2:H:116:ASP:CB	2.82	0.41
1:D:74:LYS:HD3	1:D:75:GLY:N	2.35	0.41
1:M:8:LEU:HA	1:M:11:LEU:HD12	2.02	0.41
1:D:22:SER:O	1:D:22:SER:OG	2.23	0.41
1:D:39:LYS:O	1:D:39:LYS:HG3	2.18	0.41
1:A:12:PRO:HD2	1:A:15:GLU:HB2	2.01	0.41
1:F:75:GLY:HA3	1:F:116:ASN:HB2	2.01	0.41
1:F:37:THR:OG1	3:F:201:HOH:O	2.22	0.41
1:A:4:THR:HG22	1:A:7:THR:CG2	2.47	0.41
1:C:80:THR:HG22	1:C:84:LEU:HD12	2.03	0.41
1:F:74:LYS:CE	1:F:75:GLY:H	2.31	0.41
1:M:4:THR:CG2	1:M:7:THR:OG1	2.67	0.41
1:M:8:LEU:O	1:M:16:ILE:HD11	2.20	0.41
1:A:73:VAL:CG1	1:A:104:LYS:NZ	2.82	0.41
1:I:6:SER:HA	1:I:105:GLU:HG2	2.01	0.41
1:K:66:LYS:O	1:K:70:THR:HG23	2.20	0.41
1:M:8:LEU:HA	1:M:8:LEU:HD12	1.92	0.41
1:M:16:ILE:HD13	1:M:102:VAL:HG11	2.02	0.41
1:K:22:SER:O	1:K:24:SER:N	2.53	0.41
1:M:109:HIS:O	1:M:112:ALA:HB3	2.20	0.41
2:L:117:GLU:O	2:L:117:GLU:HG2	2.20	0.41
1:A:22:SER:O	1:A:24:SER:N	2.53	0.41
1:C:22:SER:O	1:C:22:SER:OG	2.37	0.41
1:K:96:MET:HA	1:K:103:LEU:HD22	2.03	0.41
1:O:18:ARG:HG3	1:O:18:ARG:NH1	2.36	0.41
1:D:9:ALA:HB2	1:D:105:GLU:HB3	2.03	0.40
1:A:71:PHE:HZ	1:A:103:LEU:HD23	1.85	0.40
2:B:116:ASP:OD1	2:B:116:ASP:O	2.39	0.40
1:K:114:GLY:HA2	1:K:117:LYS:HD3	2.04	0.40
1:F:39:LYS:HE3	1:F:43:ASP:CG	2.38	0.40

All (3) 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:D:101:ASP:OD2	1:A:32:LYS:NZ[4_455]	1.82	0.38
1:F:23:GLN:OE1	2:N:117:GLU:OE1[4_456]	1.88	0.32
1:D:101:ASP:OD2	1:A:32:LYS:HZ2[4_455]	1.58	0.02

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	113/133 (85%)	110 (97%)	2 (2%)	1 (1%)	14 22
1	C	113/133 (85%)	109 (96%)	3 (3%)	1 (1%)	14 22
1	D	113/133 (85%)	107 (95%)	4 (4%)	2 (2%)	7 9
1	F	113/133 (85%)	110 (97%)	2 (2%)	1 (1%)	14 22
1	I	113/133 (85%)	111 (98%)	2 (2%)	0	100 100
1	K	113/133 (85%)	109 (96%)	4 (4%)	0	100 100
1	M	113/133 (85%)	108 (96%)	4 (4%)	1 (1%)	14 22
1	O	113/133 (85%)	109 (96%)	2 (2%)	2 (2%)	7 9
2	B	4/6 (67%)	4 (100%)	0	0	100 100
2	E	4/6 (67%)	4 (100%)	0	0	100 100
2	G	4/6 (67%)	4 (100%)	0	0	100 100
2	H	4/6 (67%)	4 (100%)	0	0	100 100
2	J	4/6 (67%)	4 (100%)	0	0	100 100
2	L	4/6 (67%)	4 (100%)	0	0	100 100
2	N	4/6 (67%)	4 (100%)	0	0	100 100
2	P	4/6 (67%)	4 (100%)	0	0	100 100
All	All	936/1112 (84%)	905 (97%)	23 (2%)	8 (1%)	14 22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	F	24	SER
1	M	23	GLN
1	C	24	SER
1	O	24	SER
1	D	24	SER
1	O	23	GLN
1	D	23	GLN

5.3.2 Protein sidechains (i)

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	94/110 (86%)	90 (96%)	4 (4%)	25 42
1	C	94/110 (86%)	92 (98%)	2 (2%)	48 69
1	D	94/110 (86%)	90 (96%)	4 (4%)	25 42
1	F	94/110 (86%)	86 (92%)	8 (8%)	8 14
1	I	94/110 (86%)	91 (97%)	3 (3%)	34 54
1	K	94/110 (86%)	93 (99%)	1 (1%)	70 84
1	M	94/110 (86%)	92 (98%)	2 (2%)	48 69
1	O	94/110 (86%)	91 (97%)	3 (3%)	34 54
2	B	6/6 (100%)	6 (100%)	0	100 100
2	E	6/6 (100%)	6 (100%)	0	100 100
2	G	6/6 (100%)	5 (83%)	1 (17%)	2 2
2	H	6/6 (100%)	5 (83%)	1 (17%)	2 2
2	J	6/6 (100%)	5 (83%)	1 (17%)	2 2
2	L	6/6 (100%)	6 (100%)	0	100 100
2	N	6/6 (100%)	6 (100%)	0	100 100
2	P	6/6 (100%)	4 (67%)	2 (33%)	0 0
All	All	800/928 (86%)	768 (96%)	32 (4%)	27 45

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	HIS
1	D	22	SER
1	D	24	SER
1	D	109	HIS
2	H	116	ASP
1	A	25	SER
1	A	54	HIS
1	A	67	LYS
1	A	78	LYS
1	C	25	SER
1	C	66	LYS
1	F	5	LEU
1	F	6	SER
1	F	26	SER
1	F	39	LYS
1	F	67	LYS
1	F	69	ARG
1	F	78	LYS
1	F	109	HIS
2	G	116	ASP
1	I	6	SER
1	I	67	LYS
1	I	78	LYS
2	J	117	GLU
1	K	18	ARG
1	M	67	LYS
1	M	74	LYS
1	O	32	LYS
1	O	69	ARG
1	O	74	LYS
2	P	116	ASP
2	P	117	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	108	GLN
1	A	23	GLN
1	A	108	GLN
1	F	108	GLN
1	I	97	ASN
1	I	108	GLN
1	K	21	ASN

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Mol	Chain	Res	Type
1	K	54	HIS
1	M	108	GLN
1	O	3	HIS
1	O	23	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 oligosaccharides 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, 95^{th} 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	115/133 (86%)	-0.75	0	100	100	45, 65, 92, 120	0
1	C	115/133 (86%)	-0.76	0	100	100	57, 69, 109, 125	0
1	D	115/133 (86%)	-0.93	0	100	100	48, 63, 94, 124	0
1	F	115/133 (86%)	-0.80	0	100	100	49, 66, 99, 120	0
1	I	115/133 (86%)	-0.80	0	100	100	48, 66, 96, 125	0
1	K	115/133 (86%)	-0.74	0	100	100	55, 69, 104, 126	0
1	M	115/133 (86%)	-0.73	0	100	100	55, 71, 107, 124	0
1	O	115/133 (86%)	-0.81	0	100	100	49, 70, 103, 127	0
2	B	6/6 (100%)	-0.53	0	100	100	74, 82, 95, 96	0
2	E	6/6 (100%)	-0.72	0	100	100	66, 71, 97, 101	0
2	G	6/6 (100%)	-0.75	0	100	100	59, 67, 85, 96	0
2	H	6/6 (100%)	-0.73	0	100	100	68, 75, 89, 94	0
2	J	6/6 (100%)	-0.34	0	100	100	67, 77, 96, 96	0
2	L	6/6 (100%)	-0.79	0	100	100	64, 79, 95, 98	0
2	N	6/6 (100%)	-0.59	0	100	100	73, 77, 102, 107	0
2	P	6/6 (100%)	-0.44	0	100	100	75, 81, 93, 107	0
All	All	968/1112 (87%)	-0.78	0	100	100	45, 68, 103, 127	0

There are no RSRZ outliers to report.

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 (i)

There are no monosaccharides 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.