Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 08:32 PM JST

PDB ID	:	7BQZ
Title	:	Crystal Structure of Spindlin1 bound to H3(K4me3-K9me3) peptide
Authors	:	Zhao, F.; Li, H.
Deposited on	:	2020-03-26
Resolution	:	3.10 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 (i) 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 (1)) were used in the production of this report:

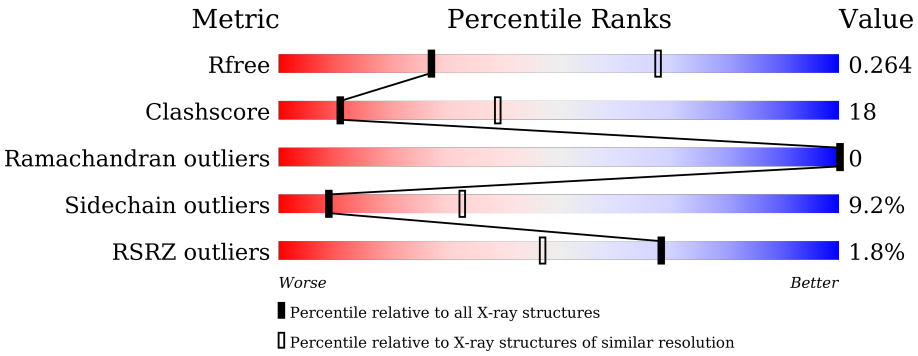
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	220	3% 68% 25%
1	C	220	68% 24% 5%
1	E	220	3% 63% 25% 5% 7%
1	G	220	68% 20% 7%
2	B	15	33% 47% 7% 13%
2	D	15	13% 53% 33%

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Mol	Chain	Length	Quality of chain
2	F	15	27% 40% 33%
2	H	15	20% 47% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	M3L	B	4	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7064 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 Spindlin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1725	1096	286	334	9			
1	C	208	Total	C	N	O	S	0	0	0
			1677	1068	280	320	9			
1	E	204	Total	C	N	O	S	0	0	0
			1649	1053	274	313	9			
1	G	205	Total	C	N	O	S	0	0	0
			1658	1058	277	314	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	-	expression tag	UNP Q9Y657
A	44	SER	-	expression tag	UNP Q9Y657
C	43	GLY	-	expression tag	UNP Q9Y657
C	44	SER	-	expression tag	UNP Q9Y657
E	43	GLY	-	expression tag	UNP Q9Y657
E	44	SER	-	expression tag	UNP Q9Y657
G	43	GLY	-	expression tag	UNP Q9Y657
G	44	SER	-	expression tag	UNP Q9Y657

- Molecule 2 is a protein called H3(K4me3-K9me3) peptide.

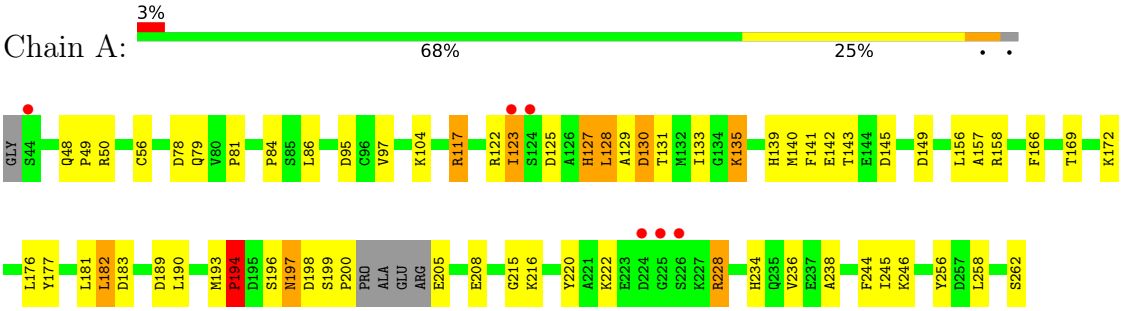
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			100	60	22	18			
2	D	10	Total	C	N	O	0	0	0
			85	52	19	14			
2	F	10	Total	C	N	O	0	0	0
			85	52	19	14			
2	H	10	Total	C	N	O	0	0	0
			85	52	19	14			

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.

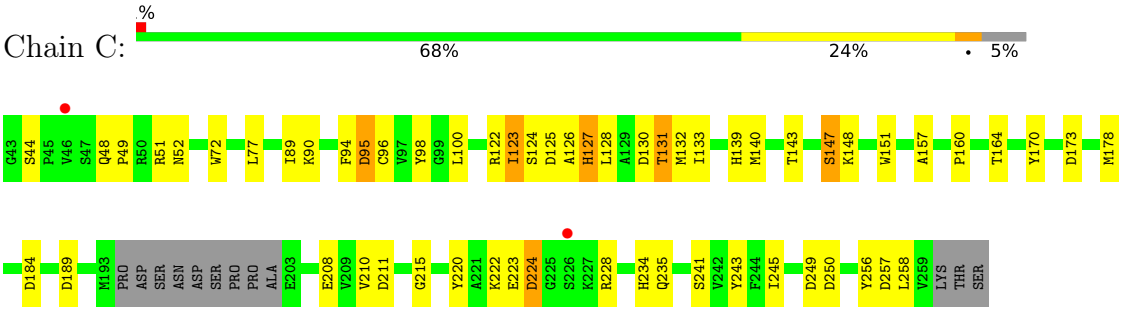
• Molecule 1: Spindlin-1

Chain A:



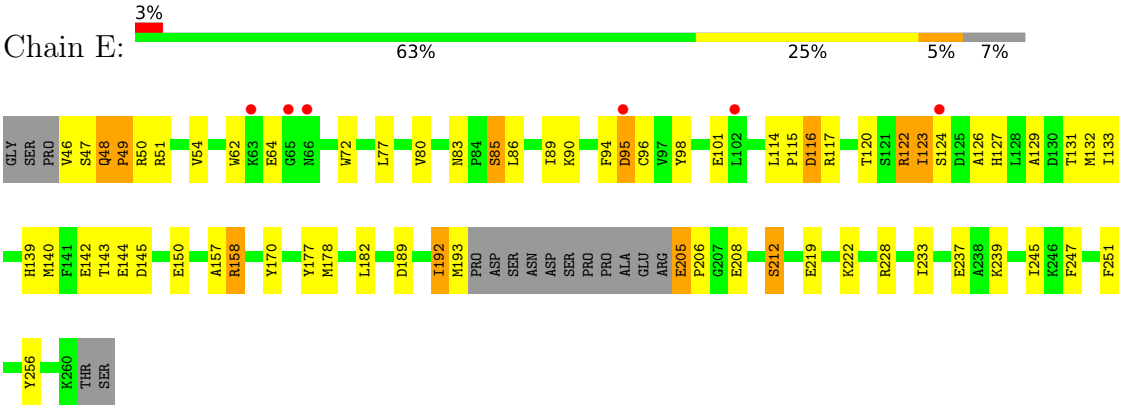
• Molecule 1: Spindlin-1

Chain C:



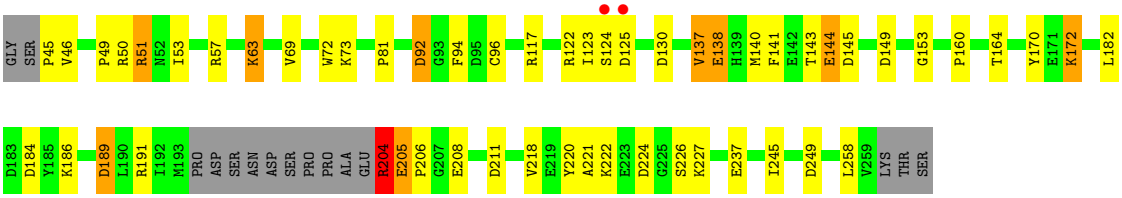
• Molecule 1: Spindlin-1

Chain E:



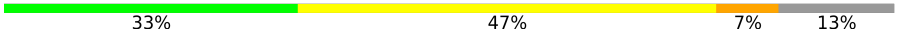
• Molecule 1: Spindlin-1

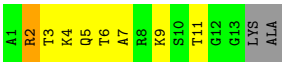
Chain G:



• Molecule 2: H3(K4me3-K9me3) peptide

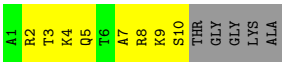
Chain B:





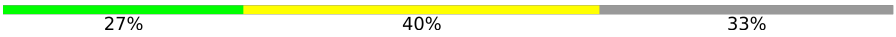
• Molecule 2: H3(K4me3-K9me3) peptide

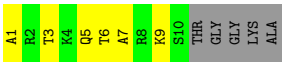
Chain D:



• Molecule 2: H3(K4me3-K9me3) peptide

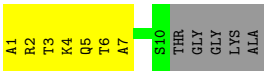
Chain F:





• Molecule 2: H3(K4me3-K9me3) peptide

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.52Å 142.68Å 132.29Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	48.39 – 3.10 48.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.39-3.10) 97.9 (48.39-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.224 , 0.264 0.238 , 0.264	Depositor DCC
R_{free} test set	1330 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.8	Xtriage
Anisotropy	0.873	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7064	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M3L

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	0.57	2/1766 (0.1%)	0.71	1/2395 (0.0%)
1	C	0.47	0/1716	0.69	1/2324 (0.0%)
1	E	0.66	3/1687 (0.2%)	0.77	4/2284 (0.2%)
1	G	0.50	0/1697	0.69	0/2298
2	B	0.70	0/75	0.83	0/99
2	D	0.58	0/60	0.88	0/79
2	F	0.83	0/60	1.09	0/79
2	H	0.57	0/60	0.65	0/79
All	All	0.56	5/7121 (0.1%)	0.72	6/9637 (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
1	G	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	49	PRO	N-CA	13.34	1.70	1.47
1	A	194	PRO	N-CA	12.86	1.69	1.47
1	E	83	ASN	C-N	8.41	1.50	1.34
1	E	48	GLN	C-N	5.73	1.45	1.34
1	A	193	MET	C-N	5.71	1.45	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	49	PRO	CA-N-CD	-8.19	100.03	111.50
1	A	194	PRO	CA-N-CD	-6.73	102.07	111.50
1	E	193	MET	N-CA-C	-6.58	93.23	111.00
1	C	127	HIS	N-CA-C	-5.50	96.16	111.00
1	E	193	MET	CB-CA-C	5.10	120.59	110.40
1	E	192	ILE	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	204	ARG	Peptide

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	1725	0	1670	87	0
1	C	1677	0	1629	52	0
1	E	1649	0	1608	75	1
1	G	1658	0	1616	55	1
2	B	100	0	116	19	0
2	D	85	0	103	11	0
2	F	85	0	103	14	0
2	H	85	0	103	14	0
All	All	7064	0	6948	253	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 18.

All (253) 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:E:49:PRO:N	1:E:49:PRO:CA	1.69	1.37
1:A:194:PRO:N	1:A:194:PRO:CA	1.69	1.35
1:A:141:PHE:CE2	2:B:4:M3L:HM12	1.84	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:HG2	1:C:160:PRO:O	1.48	1.13
1:E:48:GLN:HG3	1:E:49:PRO:HD2	1.34	1.10
1:A:141:PHE:HE2	2:B:4:M3L:HM12	1.10	1.10
1:G:73:LYS:O	1:G:92:ASP:OD1	1.69	1.10
1:A:130:ASP:HA	1:A:133:ILE:HG13	1.23	1.08
1:E:95:ASP:OD2	1:E:177:TYR:CD1	2.09	1.06
1:A:228:ARG:HH21	1:A:228:ARG:HG3	1.22	1.02
1:A:123:ILE:HG22	1:A:158:ARG:NH2	1.75	1.00
1:G:57:ARG:NH2	1:G:92:ASP:OD2	1.94	0.99
1:C:241:SER:OG	1:C:257:ASP:OD1	1.79	0.99
1:G:72:TRP:HZ3	1:G:94:PHE:CE2	1.80	0.98
1:G:184:ASP:OD2	2:H:2:ARG:HD2	1.64	0.98
1:A:205:GLU:CG	1:C:160:PRO:O	2.13	0.96
1:A:117:ARG:HG2	1:A:117:ARG:HH11	1.32	0.95
1:A:141:PHE:HE2	2:B:4:M3L:CM1	1.80	0.94
1:A:141:PHE:CE2	2:B:4:M3L:HM33	2.08	0.88
1:A:50:ARG:HH21	1:A:50:ARG:HG3	1.38	0.88
1:A:48:GLN:HG3	1:A:49:PRO:HD2	1.54	0.87
1:A:205:GLU:HB3	1:C:160:PRO:O	1.73	0.87
2:H:2:ARG:HG2	2:H:2:ARG:HH11	1.37	0.87
1:C:122:ARG:HB2	1:G:124:SER:O	1.75	0.86
1:A:130:ASP:CA	1:A:133:ILE:HG13	2.05	0.85
1:A:127:HIS:CE1	1:E:131:THR:CG2	2.60	0.85
1:G:72:TRP:CZ3	1:G:94:PHE:CE2	2.66	0.84
1:C:96:CYS:HB2	2:D:7:ALA:O	1.79	0.83
1:A:205:GLU:CB	1:C:160:PRO:O	2.27	0.83
1:C:228:ARG:NH1	1:C:250:ASP:OD2	2.11	0.83
1:A:127:HIS:CE1	1:E:131:THR:HG22	2.14	0.83
1:A:48:GLN:CG	1:A:49:PRO:HD2	2.09	0.81
1:A:135:LYS:HZ2	1:E:127:HIS:CE1	2.00	0.80
1:C:98:TYR:OH	2:D:9:M3L:HG3	1.82	0.79
1:A:197:ASN:HD22	1:A:197:ASN:H	1.31	0.79
1:A:123:ILE:HG22	1:A:158:ARG:HH21	1.48	0.77
1:G:141:PHE:CE2	2:H:4:M3L:HE3	2.19	0.77
1:E:95:ASP:CG	1:E:177:TYR:CD1	2.58	0.76
1:C:48:GLN:HB2	1:C:49:PRO:HD2	1.68	0.76
1:E:48:GLN:CG	1:E:49:PRO:HD2	2.15	0.76
1:A:123:ILE:CG2	1:A:158:ARG:NH2	2.48	0.75
1:C:224:ASP:N	1:C:224:ASP:OD1	2.18	0.75
1:G:72:TRP:HZ3	1:G:94:PHE:HE2	1.28	0.75
1:A:130:ASP:HA	1:A:133:ILE:CG1	2.10	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:GLU:OE2	1:G:138:GLU:HA	1.88	0.74
1:A:128:LEU:O	1:A:128:LEU:HD22	1.87	0.74
1:G:221:ALA:HA	1:G:227:LYS:HA	1.69	0.73
1:A:127:HIS:CE1	1:E:131:THR:HG21	2.23	0.73
1:G:72:TRP:CZ3	1:G:94:PHE:HE2	2.03	0.73
1:A:123:ILE:N	1:A:123:ILE:HD13	2.03	0.73
2:H:2:ARG:HG2	2:H:2:ARG:NH1	1.99	0.73
1:E:95:ASP:CG	1:E:177:TYR:HD1	1.92	0.72
1:E:95:ASP:OD2	2:F:7:ALA:HB1	1.89	0.72
1:A:141:PHE:CE2	2:B:4:M3L:CM1	2.66	0.70
2:F:3:THR:HG22	2:F:5:GLN:H	1.57	0.69
1:E:157:ALA:CB	1:G:208:GLU:HG2	2.23	0.68
1:A:117:ARG:HG2	1:A:117:ARG:NH1	1.96	0.68
1:E:157:ALA:HB3	1:G:208:GLU:HG2	1.73	0.68
1:A:104:LYS:N	1:A:104:LYS:HD2	2.08	0.68
1:E:94:PHE:CD2	2:F:9:M3L:HG2	2.28	0.68
1:G:205:GLU:HG3	1:G:206:PRO:HD3	1.76	0.67
1:E:205:GLU:N	1:E:206:PRO:CD	2.58	0.67
1:G:63:LYS:HB2	1:G:69:VAL:HG22	1.78	0.66
1:C:124:SER:HB3	1:G:122:ARG:HG3	1.76	0.65
1:A:197:ASN:HD22	1:A:197:ASN:N	1.93	0.65
1:A:123:ILE:HG22	1:A:158:ARG:HH22	1.63	0.64
1:A:135:LYS:NZ	1:E:127:HIS:CE1	2.66	0.63
1:A:141:PHE:HE2	2:B:4:M3L:HM33	1.62	0.63
1:A:50:ARG:HG3	1:A:50:ARG:NH2	2.09	0.63
1:C:125:ASP:HB2	1:G:123:ILE:H	1.61	0.63
1:E:94:PHE:HD2	2:F:9:M3L:HG2	1.63	0.63
1:C:123:ILE:HG22	1:C:164:THR:HA	1.80	0.63
2:D:3:THR:HG22	2:D:5:GLN:H	1.64	0.62
1:E:98:TYR:HD2	1:E:251:PHE:HD2	1.46	0.62
1:A:208:GLU:OE1	1:C:234:HIS:NE2	2.27	0.62
1:G:170:TYR:CD1	2:H:4:M3L:HM21	2.33	0.62
1:A:129:ALA:CB	1:A:166:PHE:HZ	2.13	0.62
1:A:141:PHE:CE2	2:B:4:M3L:CM3	2.83	0.62
1:A:194:PRO:N	1:A:194:PRO:C	2.49	0.62
2:B:2:ARG:CG	2:B:2:ARG:HH11	2.13	0.61
1:A:95:ASP:HB2	2:B:7:ALA:HA	1.82	0.61
1:E:95:ASP:HB3	2:F:7:ALA:HA	1.82	0.61
1:E:123:ILE:HG12	1:E:158:ARG:HH22	1.65	0.61
1:A:228:ARG:HG3	1:A:228:ARG:NH2	2.02	0.61
1:E:77:LEU:HD11	1:E:178:MET:SD	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:GLU:O	1:E:205:GLU:HG3	2.00	0.61
2:D:10:SER:O	2:D:10:SER:OG	2.14	0.60
1:E:46:VAL:HG23	1:E:46:VAL:O	2.01	0.60
1:A:127:HIS:NE2	1:E:192:ILE:HG21	2.17	0.60
1:E:96:CYS:HB2	2:F:7:ALA:O	2.02	0.60
1:E:80:VAL:HG21	1:E:86:LEU:HD23	1.83	0.60
1:E:120:THR:HG23	1:E:120:THR:O	2.02	0.60
1:A:157:ALA:HB1	1:C:208:GLU:HB2	1.84	0.59
2:H:3:THR:HG22	2:H:5:GLN:H	1.66	0.59
1:C:132:MET:O	1:C:132:MET:HG3	2.02	0.59
1:A:128:LEU:HD22	1:A:128:LEU:C	2.21	0.59
1:G:204:ARG:HD2	1:G:204:ARG:O	2.03	0.58
1:A:129:ALA:HB2	1:A:166:PHE:HZ	1.69	0.58
1:C:173:ASP:OD2	2:D:8:ARG:NH2	2.36	0.58
1:E:212:SER:H	1:G:81:PRO:HG3	1.67	0.58
1:E:95:ASP:OD1	1:E:177:TYR:CD1	2.56	0.58
1:A:123:ILE:HD13	1:A:123:ILE:H	1.67	0.58
1:E:140:MET:HB3	1:E:189:ASP:HB3	1.86	0.58
1:A:141:PHE:HE2	2:B:4:M3L:CM3	2.16	0.57
1:C:123:ILE:HD11	1:C:126:ALA:HB3	1.86	0.57
1:G:92:ASP:OD1	1:G:92:ASP:N	2.37	0.57
1:E:72:TRP:CH2	2:F:9:M3L:HG3	2.39	0.57
1:C:139:HIS:ND1	1:C:170:TYR:OH	2.31	0.57
1:E:95:ASP:OD1	1:E:177:TYR:HB3	2.05	0.57
1:E:95:ASP:OD1	1:E:177:TYR:HD1	1.86	0.57
1:G:122:ARG:O	1:G:122:ARG:HG2	2.04	0.56
1:A:228:ARG:HH21	1:A:228:ARG:CG	2.04	0.56
1:C:98:TYR:CZ	2:D:9:M3L:HG3	2.41	0.55
1:E:72:TRP:CH2	1:E:94:PHE:HE2	2.24	0.55
1:G:189:ASP:OD2	2:H:1:ALA:N	2.37	0.55
1:E:95:ASP:OD2	1:E:177:TYR:CE1	2.57	0.55
1:A:197:ASN:H	1:A:197:ASN:ND2	2.01	0.54
1:C:133:ILE:HD12	1:C:157:ALA:HA	1.89	0.54
1:C:184:ASP:OD1	2:D:2:ARG:NH1	2.38	0.54
1:A:127:HIS:CD2	1:E:192:ILE:HG21	2.43	0.54
1:E:72:TRP:HH2	1:E:94:PHE:HE2	1.55	0.54
1:G:94:PHE:HA	2:H:6:THR:O	2.08	0.54
1:A:196:SER:O	1:A:196:SER:OG	2.15	0.54
1:C:151:TRP:CG	2:D:4:M3L:HM32	2.43	0.54
1:A:205:GLU:HG2	1:C:160:PRO:C	2.22	0.54
1:A:129:ALA:HB1	1:A:166:PHE:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:ALA:HB2	1:G:227:LYS:HB3	1.89	0.53
1:G:245:ILE:HD11	1:G:258:LEU:HD21	1.90	0.53
1:E:132:MET:HG2	1:E:192:ILE:HD11	1.90	0.53
1:E:212:SER:N	1:G:81:PRO:HG3	2.24	0.53
1:A:127:HIS:CD2	1:E:192:ILE:CG2	2.92	0.53
1:G:172:LYS:HE2	1:G:172:LYS:HA	1.90	0.52
1:G:182:LEU:O	1:G:186:LYS:HG3	2.09	0.52
1:C:148:LYS:O	1:C:148:LYS:HG3	2.10	0.52
1:A:129:ALA:CB	1:A:166:PHE:CZ	2.91	0.52
1:G:184:ASP:OD2	2:H:2:ARG:CD	2.49	0.52
1:A:78:ASP:OD1	1:A:79:GLN:N	2.41	0.52
2:B:2:ARG:HH11	2:B:2:ARG:HG2	1.73	0.52
1:A:79:GLN:NE2	1:A:84:PRO:O	2.37	0.52
1:A:117:ARG:HH11	1:A:117:ARG:CG	2.10	0.52
1:C:140:MET:HB3	1:C:189:ASP:HB3	1.92	0.52
1:G:140:MET:HB3	1:G:189:ASP:HB3	1.93	0.51
1:C:48:GLN:CB	1:C:49:PRO:HD2	2.37	0.51
1:E:205:GLU:N	1:E:206:PRO:HD2	2.26	0.51
1:C:245:ILE:HD12	1:C:256:TYR:HD2	1.77	0.50
2:F:6:THR:O	2:F:6:THR:OG1	2.23	0.50
1:A:139:HIS:HD2	1:A:190:LEU:HD13	1.76	0.50
1:C:235:GLN:HB2	1:C:243:TYR:CE2	2.45	0.50
1:E:212:SER:O	1:G:81:PRO:HG2	2.11	0.50
1:G:138:GLU:HG2	1:G:191:ARG:NH1	2.27	0.50
1:C:52:ASN:OD1	1:C:52:ASN:N	2.43	0.50
1:E:95:ASP:OD1	1:E:177:TYR:CB	2.60	0.49
1:A:197:ASN:N	1:A:197:ASN:ND2	2.60	0.49
1:C:77:LEU:HD11	1:C:90:LYS:HB2	1.94	0.49
1:G:96:CYS:HB2	2:H:7:ALA:O	2.13	0.49
1:E:206:PRO:O	1:E:206:PRO:HG2	2.13	0.49
1:A:234:HIS:HB3	1:A:244:PHE:HB2	1.94	0.49
1:A:141:PHE:CD2	2:B:4:M3L:HM33	2.47	0.49
1:E:98:TYR:CD2	1:E:251:PHE:HD2	2.29	0.49
1:C:210:VAL:HG12	1:C:210:VAL:O	2.12	0.49
1:E:94:PHE:CE2	2:F:9:M3L:HA	2.47	0.49
1:E:116:ASP:N	1:E:116:ASP:OD1	2.47	0.48
1:E:123:ILE:HG21	1:E:126:ALA:HB2	1.94	0.48
1:A:220:TYR:HB2	1:A:228:ARG:HB3	1.95	0.48
1:A:142:GLU:O	1:A:142:GLU:HG3	2.13	0.48
2:H:4:M3L:HM33	2:H:4:M3L:HG2	1.96	0.48
2:B:3:THR:HB	2:B:6:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:PRO:N	1:E:49:PRO:C	2.62	0.48
1:A:199:SER:HB2	1:A:200:PRO:HD2	1.96	0.47
2:B:2:ARG:CG	2:B:2:ARG:NH1	2.73	0.47
1:E:189:ASP:OD2	2:F:1:ALA:HA	2.14	0.47
1:A:140:MET:SD	1:A:149:ASP:O	2.72	0.47
1:A:236:VAL:HG12	1:A:238:ALA:H	1.79	0.47
1:E:122:ARG:HD2	1:E:122:ARG:HA	1.68	0.47
1:A:127:HIS:ND1	1:E:131:THR:HG21	2.30	0.47
1:G:211:ASP:OD1	1:G:211:ASP:N	2.46	0.47
1:A:50:ARG:NH2	1:A:50:ARG:CG	2.73	0.46
1:C:170:TYR:CD2	2:D:4:M3L:HM21	2.50	0.46
1:A:140:MET:HB3	1:A:189:ASP:HB3	1.97	0.46
1:E:245:ILE:HD12	1:E:256:TYR:HD2	1.81	0.46
1:A:127:HIS:NE2	1:E:192:ILE:HD12	2.31	0.46
1:C:72:TRP:HZ3	1:C:94:PHE:HE2	1.62	0.46
1:G:205:GLU:N	1:G:206:PRO:HD2	2.30	0.46
1:C:51:ARG:HE	1:C:51:ARG:HB3	1.57	0.46
1:A:245:ILE:HD12	1:A:256:TYR:HD2	1.80	0.46
1:E:90:LYS:O	1:E:90:LYS:HG3	2.16	0.46
1:G:189:ASP:N	1:G:189:ASP:OD1	2.49	0.46
1:E:114:LEU:HB3	1:E:115:PRO:HD2	1.98	0.46
1:E:139:HIS:ND1	1:E:170:TYR:OH	2.43	0.46
2:B:3:THR:HG22	2:B:5:GLN:H	1.80	0.45
1:E:94:PHE:CD2	2:F:9:M3L:CG	2.99	0.45
2:B:4:M3L:HA	2:B:4:M3L:HD2	1.79	0.45
1:C:94:PHE:CE2	2:D:9:M3L:HA	2.51	0.45
1:C:143:THR:HG22	1:C:147:SER:HB3	1.98	0.45
1:C:220:TYR:O	1:C:228:ARG:N	2.49	0.45
1:A:81:PRO:CD	1:C:210:VAL:HG12	2.47	0.45
1:E:132:MET:HG2	1:E:192:ILE:CD1	2.46	0.45
1:G:205:GLU:HG3	1:G:206:PRO:CD	2.44	0.45
1:A:97:VAL:HG11	1:A:176:LEU:HD23	1.99	0.44
1:E:54:VAL:O	1:E:54:VAL:HG12	2.17	0.44
1:C:127:HIS:O	1:C:127:HIS:CD2	2.70	0.44
1:C:249:ASP:OD1	1:C:249:ASP:N	2.50	0.44
1:E:85:SER:O	1:E:101:GLU:HA	2.17	0.44
2:B:3:THR:HG22	2:B:5:GLN:HB2	1.98	0.44
1:E:129:ALA:O	1:E:133:ILE:HG12	2.16	0.44
1:C:245:ILE:HD11	1:C:258:LEU:HD11	1.98	0.44
1:G:123:ILE:HD12	1:G:123:ILE:HA	1.81	0.44
1:A:245:ILE:HD11	1:A:258:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ILE:HD11	1:E:182:LEU:HD12	1.98	0.44
1:E:228:ARG:HB3	1:E:247:PHE:CE1	2.53	0.44
1:E:157:ALA:CB	1:G:208:GLU:CG	2.96	0.43
1:E:48:GLN:HG3	1:E:49:PRO:CD	2.25	0.43
1:E:80:VAL:HG11	1:E:233:ILE:HB	2.01	0.43
1:G:221:ALA:HB1	1:G:226:SER:O	2.18	0.43
1:A:86:LEU:HD11	1:A:246:LYS:HE3	2.00	0.43
1:E:123:ILE:HD12	1:E:124:SER:H	1.83	0.43
1:C:125:ASP:H	1:G:123:ILE:HG22	1.83	0.43
1:A:208:GLU:O	1:C:160:PRO:HG3	2.19	0.43
1:E:177:TYR:HE1	2:F:7:ALA:O	2.02	0.43
1:E:208:GLU:O	1:G:160:PRO:HG3	2.19	0.43
1:E:144:GLU:H	1:E:144:GLU:HG3	1.54	0.43
1:A:156:LEU:HD21	1:A:169:THR:HG22	2.01	0.43
1:G:144:GLU:H	1:G:144:GLU:HG2	1.34	0.43
1:C:151:TRP:CD2	2:D:4:M3L:HM32	2.54	0.42
1:G:137:VAL:N	1:G:153:GLY:O	2.44	0.42
1:A:48:GLN:HG2	1:A:49:PRO:HD2	1.97	0.42
1:G:141:PHE:HB2	1:G:149:ASP:HB3	2.01	0.42
1:A:127:HIS:ND1	1:A:127:HIS:C	2.72	0.42
1:C:95:ASP:HB3	1:C:178:MET:O	2.20	0.42
1:E:142:GLU:HG3	2:F:1:ALA:CB	2.49	0.42
1:A:129:ALA:HB1	1:A:166:PHE:CE2	2.54	0.42
1:A:205:GLU:N	1:A:205:GLU:OE1	2.52	0.42
1:C:128:LEU:O	1:C:131:THR:HB	2.20	0.42
1:C:89:ILE:HD13	1:C:100:LEU:HD12	2.00	0.42
1:G:205:GLU:N	1:G:206:PRO:CD	2.83	0.42
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.71	0.42
1:G:222:LYS:HD2	1:G:222:LYS:HA	1.93	0.42
1:A:177:TYR:OH	2:B:4:M3L:HM22	2.20	0.42
1:A:172:LYS:HA	1:A:172:LYS:HD3	1.50	0.41
1:C:122:ARG:CB	1:G:125:ASP:HA	2.49	0.41
1:G:117:ARG:HE	1:G:117:ARG:HB2	1.68	0.41
1:A:181:LEU:C	1:A:183:ASP:N	2.74	0.41
1:E:95:ASP:OD2	2:F:7:ALA:CB	2.65	0.41
1:G:184:ASP:OD1	2:H:2:ARG:NE	2.49	0.41
1:C:222:LYS:NZ	1:C:228:ARG:HG3	2.36	0.41
1:E:62:TRP:NE1	1:E:64:GLU:HG3	2.36	0.41
2:B:9:M3L:HM23	2:B:9:M3L:HD2	1.91	0.41
1:E:205:GLU:O	1:E:205:GLU:CG	2.67	0.41
1:G:170:TYR:CE1	2:H:4:M3L:CM2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ARG:HG2	1:G:53:ILE:HG23	2.03	0.40
1:G:222:LYS:O	1:G:222:LYS:NZ	2.53	0.40
1:G:170:TYR:CZ	2:H:4:M3L:HM23	2.56	0.40
1:A:215:GLY:HA3	1:C:215:GLY:HA3	2.03	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)
1:E:117:ARG:NH2	1:E:150:GLU:OE2[1_655]	1.85	0.35
1:G:49:PRO:CB	1:G:220:TYR:CE2[1_455]	2.00	0.20

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	211/220 (96%)	195 (92%)	16 (8%)	0	100	100
1	C	204/220 (93%)	193 (95%)	11 (5%)	0	100	100
1	E	200/220 (91%)	185 (92%)	15 (8%)	0	100	100
1	G	201/220 (91%)	192 (96%)	9 (4%)	0	100	100
2	B	9/15 (60%)	9 (100%)	0	0	100	100
2	D	6/15 (40%)	6 (100%)	0	0	100	100
2	F	6/15 (40%)	5 (83%)	1 (17%)	0	100	100
2	H	6/15 (40%)	6 (100%)	0	0	100	100
All	All	843/940 (90%)	791 (94%)	52 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	191/194 (98%)	171 (90%)	20 (10%)	7 26
1	C	183/194 (94%)	174 (95%)	9 (5%)	25 57
1	E	180/194 (93%)	162 (90%)	18 (10%)	7 28
1	G	181/194 (93%)	160 (88%)	21 (12%)	5 22
2	B	7/8 (88%)	5 (71%)	2 (29%)	0 1
2	D	6/8 (75%)	6 (100%)	0	100 100
2	F	6/8 (75%)	6 (100%)	0	100 100
2	H	6/8 (75%)	6 (100%)	0	100 100
All	All	760/808 (94%)	690 (91%)	70 (9%)	9 33

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	CYS
1	A	117	ARG
1	A	122	ARG
1	A	123	ILE
1	A	125	ASP
1	A	127	HIS
1	A	128	LEU
1	A	130	ASP
1	A	131	THR
1	A	135	LYS
1	A	143	THR
1	A	145	ASP
1	A	182	LEU
1	A	194	PRO
1	A	197	ASN
1	A	198	ASP
1	A	216	LYS
1	A	222	LYS
1	A	228	ARG

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Mol	Chain	Res	Type
1	A	262	SER
2	B	2	ARG
2	B	11	THR
1	C	44	SER
1	C	95	ASP
1	C	123	ILE
1	C	130	ASP
1	C	131	THR
1	C	147	SER
1	C	211	ASP
1	C	223	GLU
1	C	224	ASP
1	E	47	SER
1	E	50	ARG
1	E	51	ARG
1	E	85	SER
1	E	89	ILE
1	E	95	ASP
1	E	116	ASP
1	E	122	ARG
1	E	123	ILE
1	E	143	THR
1	E	145	ASP
1	E	158	ARG
1	E	205	GLU
1	E	212	SER
1	E	219	GLU
1	E	222	LYS
1	E	237	GLU
1	E	239	LYS
1	G	45	PRO
1	G	46	VAL
1	G	50	ARG
1	G	51	ARG
1	G	63	LYS
1	G	92	ASP
1	G	130	ASP
1	G	137	VAL
1	G	138	GLU
1	G	143	THR
1	G	144	GLU
1	G	145	ASP

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Mol	Chain	Res	Type
1	G	164	THR
1	G	172	LYS
1	G	189	ASP
1	G	204	ARG
1	G	205	GLU
1	G	218	VAL
1	G	224	ASP
1	G	237	GLU
1	G	249	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	C	127	HIS
1	C	163	ASN
1	E	48	GLN
1	G	252	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	M3L	H	9	2	10,11,12	0.49	0	9,14,16	0.54	0
2	M3L	H	4	2	10,11,12	0.45	0	9,14,16	0.08	0
2	M3L	B	9	2	10,11,12	0.64	0	9,14,16	0.10	0
2	M3L	D	4	2	10,11,12	0.71	0	9,14,16	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	M3L	D	9	2	10,11,12	0.65	0	9,14,16	0.28	0
2	M3L	F	9	2	10,11,12	0.78	0	9,14,16	0.23	0
2	M3L	B	4	2	10,11,12	0.46	0	9,14,16	0.08	0
2	M3L	F	4	2	10,11,12	0.47	0	9,14,16	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	H	9	2	-	5/9/10/12	-
2	M3L	H	4	2	-	8/9/10/12	-
2	M3L	B	9	2	-	2/9/10/12	-
2	M3L	D	4	2	-	0/9/10/12	-
2	M3L	D	9	2	-	1/9/10/12	-
2	M3L	F	9	2	-	3/9/10/12	-
2	M3L	B	4	2	-	5/9/10/12	-
2	M3L	F	4	2	-	5/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	9	M3L	N-CA-CB-CG
2	B	9	M3L	C-CA-CB-CG
2	F	4	M3L	N-CA-CB-CG
2	F	4	M3L	C-CA-CB-CG
2	F	4	M3L	O-C-CA-CB
2	F	9	M3L	C-CA-CB-CG
2	H	4	M3L	N-CA-CB-CG
2	H	4	M3L	C-CA-CB-CG
2	H	9	M3L	N-CA-CB-CG
2	H	9	M3L	C-CA-CB-CG
2	H	4	M3L	CG-CD-CE-NZ
2	B	4	M3L	CA-CB-CG-CD
2	F	4	M3L	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
2	H	9	M3L	CG-CD-CE-NZ
2	F	4	M3L	CG-CD-CE-NZ
2	B	4	M3L	CD-CE-NZ-CM3
2	H	4	M3L	CA-CB-CG-CD
2	B	4	M3L	CD-CE-NZ-CM1
2	B	4	M3L	CD-CE-NZ-CM2
2	B	4	M3L	CE-CD-CG-CB
2	H	4	M3L	CE-CD-CG-CB
2	H	4	M3L	CD-CE-NZ-CM2
2	F	9	M3L	CE-CD-CG-CB
2	H	4	M3L	CD-CE-NZ-CM1
2	H	9	M3L	CE-CD-CG-CB
2	H	4	M3L	CD-CE-NZ-CM3
2	H	9	M3L	CA-CB-CG-CD
2	F	9	M3L	N-CA-CB-CG
2	D	9	M3L	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	4	M3L	5	0
2	B	9	M3L	1	0
2	D	4	M3L	3	0
2	D	9	M3L	3	0
2	F	9	M3L	5	0
2	B	4	M3L	11	0

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

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	215/220 (97%)	0.13	6 (2%) 53 30	30, 63, 125, 146	0
1	C	208/220 (94%)	0.08	2 (0%) 82 67	30, 66, 108, 130	0
1	E	204/220 (92%)	0.16	6 (2%) 51 28	30, 65, 111, 142	0
1	G	205/220 (93%)	0.07	2 (0%) 82 67	29, 65, 117, 142	0
2	B	11/15 (73%)	0.06	0 100 100	30, 64, 75, 102	0
2	D	8/15 (53%)	0.05	0 100 100	55, 73, 82, 86	0
2	F	8/15 (53%)	-0.21	0 100 100	67, 73, 82, 84	0
2	H	8/15 (53%)	0.28	0 100 100	60, 75, 88, 93	0
All	All	867/940 (92%)	0.11	16 (1%) 68 47	29, 65, 117, 146	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	SER	4.0
1	A	124	SER	3.6
1	E	66	ASN	3.4
1	A	44	SER	3.0
1	G	125	ASP	2.8
1	A	225	GLY	2.6
1	E	65	GLY	2.6
1	A	123	ILE	2.5
1	E	95	ASP	2.4
1	E	63	LYS	2.3
1	E	102	LEU	2.2
1	G	124	SER	2.2
1	E	124	SER	2.1
1	C	46	VAL	2.1
1	C	226	SER	2.1
1	A	224	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	M3L	F	9	12/13	0.88	0.35	60,73,82,85	0
2	M3L	H	4	12/13	0.91	0.29	39,53,69,70	0
2	M3L	D	9	12/13	0.93	0.35	48,70,76,89	0
2	M3L	B	9	12/13	0.94	0.30	53,65,85,87	0
2	M3L	H	9	12/13	0.94	0.29	54,70,84,97	0
2	M3L	F	4	12/13	0.95	0.27	47,58,83,91	0
2	M3L	D	4	12/13	0.96	0.28	38,53,71,72	0
2	M3L	B	4	12/13	0.96	0.30	42,56,70,70	0

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.