



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:37 AM UTC

PDB ID : 4YHP / pdb_00004yhp
Title : Crystal structure of 309M3-B Fab in complex with H3K9me3 peptide
Authors : Hattori, T.; Dementieva, I.S.; Montano, S.P.; Koide, S.
Deposited on : 2015-02-27
Resolution : 2.53 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

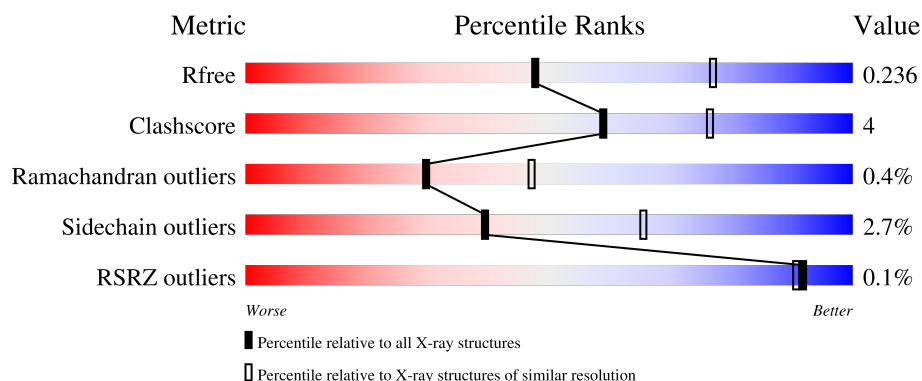
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	P	16	50% 19% 31%
1	Q	16	56% 6% 6% 31%
2	A	229	84% 12% .
2	C	229	86% 8% . .
2	E	229	84% 12% .

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Mol	Chain	Length	Quality of chain
2	H	229	 86% 8% 5%
3	B	215	 82% 14% ..
3	D	215	 89% 10% .
3	F	215	 85% 13% ..
3	L	215	 89% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13773 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 H3K9me3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	P	11	Total	C	N	O	0	0	0
			89	53	20	16			
1	Q	11	Total	C	N	O	0	0	0
			89	53	20	16			

- Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	219	Total	C	N	O	S	0	0	0
			1666	1058	284	318	6			
2	C	219	Total	C	N	O	S	0	0	0
			1666	1058	284	318	6			
2	E	219	Total	C	N	O	S	0	0	0
			1661	1054	283	318	6			
2	H	218	Total	C	N	O	S	0	0	0
			1660	1055	283	316	6			

- Molecule 3 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	212	Total	C	N	O	S	0	0	0
			1614	1005	275	330	4			
3	D	213	Total	C	N	O	S	0	0	0
			1620	1008	276	332	4			
3	L	213	Total	C	N	O	S	0	0	0
			1620	1008	276	332	4			
3	F	211	Total	C	N	O	S	0	0	0
			1602	996	274	328	4			

- Molecule 4 is water.

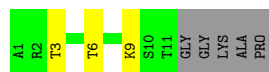
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	9	Total 9	O 9	0	0
4	A	49	Total 49	O 49	0	0
4	B	52	Total 52	O 52	0	0
4	Q	5	Total 5	O 5	0	0
4	C	67	Total 67	O 67	0	0
4	D	59	Total 59	O 59	0	0
4	E	63	Total 63	O 63	0	0
4	H	58	Total 58	O 58	0	0
4	L	59	Total 59	O 59	0	0
4	F	65	Total 65	O 65	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

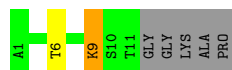
- Molecule 1: H3K9me3 peptide

Chain P: 



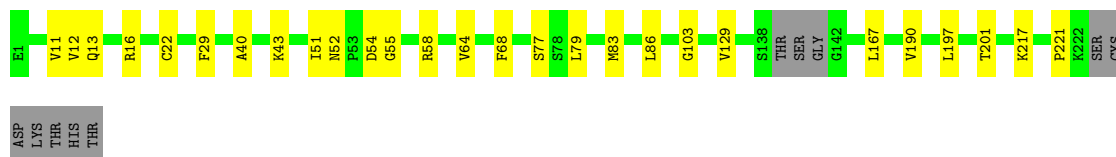
- Molecule 1: H3K9me3 peptide

Chain Q: 



- Molecule 2: Fab Heavy Chain

Chain A: 



- Molecule 2: Fab Heavy Chain

Chain C: 



- Molecule 2: Fab Heavy Chain

Chain E: 



LYS
THR
HIS
THR

• Molecule 2: Fab Heavy Chain

Chain H:  86% 8% 5%

E1 V2 C22 R30 N52 P53 L79 M83 L86 P131 K137 SER THR SER SER GLY G142 K151 F154 P155 S169 S195 S196 T199 N205 D216 K217 K222 SER CYS ASP LYS THR HIS THR

• Molecule 3: Fab Light Chain

Chain B:  82% 14% ..

SER Y2 V3 L4 C22 W34 R38 R53 E59 R60 F61 A70 G80 C87 D92 G100 T106 S124 Q125 S128 G129 Y141 P142 R143 E144 Q148 W149 K150 M153 A154 L155 V164 L176 S183 K184 A185 D186 Y187 E188 K189 H190 K191 V192 R212 G213 GLU CYS

• Molecule 3: Fab Light Chain

Chain D:  89% 10% .

S1 C22 W34 D49 R53 F61 D84 W90 K104 Q125 S128 R143 E144 A145 K146 K150 E188 K189 H190 E196 V197 T198 L202 V206 S209 R212 G213 GLU CYS

• Molecule 3: Fab Light Chain

Chain L:  89% 10% .

S1 T21 C22 W34 R38 Q41 E59 L72 R76 I94 S116 Q125 N138 M139 E144 A145 K146 K150 V164 H190 E196 V197 T198 R212 G213 GLU CYS

• Molecule 3: Fab Light Chain

Chain F:  85% 13% ..

SER TYR V3 P7 P8 R38 R53 F61 E78 A79 G80 D92 Y97 P121 Q125 L126 K127 S128 V133 M138 E144 A145 K146 V147 Q148 W149 K150 V151 A154 L155 S163 D186 Y187 T198 K208 R212 G213 GLU CYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.77Å 159.88Å 128.76Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	31.38 – 2.53 31.38 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (31.38-2.53) 99.7 (31.38-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.211 , 0.250 0.199 , 0.236	Depositor DCC
R_{free} test set	5607 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 15.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l 0.012 for -k,-h,-l 0.478 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13773	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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 ⓘ

5.1 Standard geometry ⓘ

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	P	0.27	0/76	0.69	0/100
1	Q	0.27	0/76	0.64	0/100
2	A	0.32	0/1709	0.74	1/2327 (0.0%)
2	C	0.33	0/1709	0.76	0/2327
2	E	0.31	0/1704	0.72	0/2321
2	H	0.31	0/1703	0.74	0/2319
3	B	0.32	0/1648	0.74	0/2250
3	D	0.32	0/1654	0.73	0/2258
3	F	0.31	0/1635	0.75	1/2232 (0.0%)
3	L	0.33	0/1654	0.74	0/2258
All	All	0.32	0/13568	0.74	2/18492 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	103	GLY	N-CA-C	-5.02	108.72	114.69
3	F	138	ASN	N-CA-C	5.01	116.69	108.52

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	P	89	0	104	0	0
1	Q	89	0	104	2	0
2	A	1666	0	1631	13	0
2	C	1666	0	1631	12	0
2	E	1661	0	1621	14	0
2	H	1660	0	1626	9	0
3	B	1614	0	1546	22	0
3	D	1620	0	1554	15	0
3	F	1602	0	1537	18	0
3	L	1620	0	1554	13	0
4	A	49	0	0	0	0
4	B	52	0	0	0	0
4	C	67	0	0	1	0
4	D	59	0	0	1	0
4	E	63	0	0	2	0
4	F	65	0	0	0	0
4	H	58	0	0	0	0
4	L	59	0	0	1	0
4	P	9	0	0	0	0
4	Q	5	0	0	0	0
All	All	13773	0	12908	114	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 4.

All (114) 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)
3:D:188:GLU:HA	3:D:212:ARG:HH22	1.48	0.79
3:B:187:TYR:O	3:B:212:ARG:NH2	2.16	0.78
3:F:38:ARG:NH1	3:F:80:GLY:O	2.18	0.76
3:B:190:HIS:O	3:B:212:ARG:NH2	2.20	0.75
3:B:38:ARG:NH1	3:B:80:GLY:O	2.20	0.74
3:D:144:GLU:OE2	3:D:144:GLU:CG	2.38	0.72
3:B:144:GLU:CG	3:B:144:GLU:OE2	2.38	0.71
3:D:144:GLU:CG	3:D:144:GLU:OE1	2.38	0.71
3:F:144:GLU:CG	3:F:144:GLU:OE2	2.38	0.71
3:L:144:GLU:OE2	3:L:144:GLU:CG	2.38	0.71
3:B:144:GLU:CG	3:B:144:GLU:OE1	2.39	0.71
3:L:144:GLU:CG	3:L:144:GLU:OE1	2.39	0.70
3:F:144:GLU:CG	3:F:144:GLU:OE1	2.39	0.70
2:A:52:ASN:HD21	2:A:54:ASP:HB2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:134:PRO:HG3	2:E:146:LEU:HB3	1.76	0.65
3:B:184:LYS:NZ	3:B:188:GLU:OE2	2.30	0.65
3:D:209:SER:O	4:D:301:HOH:O	2.15	0.64
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.82	0.62
2:C:83:MET:HB3	2:C:86:LEU:HD21	1.82	0.62
2:E:58:ARG:NH2	4:E:301:HOH:O	2.33	0.61
3:B:144:GLU:OE2	3:B:144:GLU:OE1	2.19	0.60
2:C:196:SER:O	2:C:198:GLY:N	2.35	0.60
3:L:144:GLU:OE2	3:L:144:GLU:OE1	2.20	0.60
3:F:144:GLU:OE2	3:F:144:GLU:OE1	2.19	0.60
3:D:144:GLU:OE2	3:D:144:GLU:OE1	2.19	0.59
2:C:104:LEU:HD23	3:D:49:ASP:HB3	1.85	0.59
3:D:53:ARG:NH1	3:D:61:PHE:O	2.36	0.58
2:A:22:CYS:HB3	2:A:79:LEU:HB3	1.86	0.57
3:B:183:SER:OG	3:B:186:ASP:OD1	2.22	0.57
2:E:125:LYS:NZ	4:E:302:HOH:O	2.36	0.57
3:F:183:SER:OG	3:F:186:ASP:OD1	2.22	0.57
3:L:138:ASN:OD1	3:L:139:ASN:ND2	2.37	0.56
3:F:125:GLN:O	3:F:128:SER:OG	2.22	0.56
3:L:150:LYS:NZ	3:L:196:GLU:OE2	2.31	0.56
2:A:51:ILE:HD11	2:A:55:GLY:HA2	1.88	0.55
2:C:30:ARG:NH2	4:C:303:HOH:O	2.40	0.55
3:D:150:LYS:NZ	3:D:196:GLU:OE2	2.31	0.54
3:F:92:ASP:N	3:F:92:ASP:OD1	2.41	0.53
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.91	0.53
2:E:52:ASN:ND2	2:E:54:ASP:OD1	2.39	0.52
1:Q:9:M3L:HE3	3:D:90:TRP:CE2	2.45	0.51
3:B:92:ASP:N	3:B:92:ASP:OD1	2.44	0.51
2:H:1:GLU:OE2	2:H:2:VAL:N	2.43	0.51
3:F:146:LYS:HB3	3:F:198:THR:HB	1.93	0.50
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.92	0.50
3:B:53:ARG:NH2	3:B:59:GLU:HG2	2.27	0.50
2:C:135:SER:OG	2:C:137:LYS:NZ	2.35	0.49
2:C:199:THR:OG1	2:C:200:GLN:N	2.44	0.49
2:E:64:VAL:HB	2:E:68:PHE:CG	2.47	0.49
2:H:205:ASN:ND2	2:H:216:ASP:OD1	2.38	0.49
2:E:167:LEU:HD21	2:E:190:VAL:HG21	1.95	0.48
2:H:131:PRO:HD3	2:H:217:LYS:HZ1	1.79	0.48
2:A:167:LEU:HD21	2:A:190:VAL:HG21	1.96	0.48
3:D:84:ASP:OD1	3:D:104:LYS:HE3	2.14	0.48
3:F:186:ASP:OD1	3:F:186:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:PRO:HD3	2:H:217:LYS:NZ	2.29	0.47
3:L:125:GLN:NE2	4:L:304:HOH:O	2.45	0.47
3:B:164:VAL:HG22	3:B:176:LEU:HD12	1.97	0.46
3:B:186:ASP:OD1	3:B:186:ASP:N	2.46	0.46
3:D:125:GLN:O	3:D:128:SER:OG	2.31	0.46
2:A:129:VAL:HG12	2:A:217:LYS:HD2	1.96	0.46
3:B:22:CYS:HB3	3:B:70:ALA:HB3	1.98	0.46
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.97	0.46
3:D:190:HIS:NE2	3:L:59:GLU:OE2	2.48	0.46
3:F:121:PRO:HD3	3:F:133:VAL:HG22	1.97	0.46
2:A:64:VAL:HB	2:A:68:PHE:CG	2.51	0.46
3:L:22:CYS:HB2	3:L:34:TRP:CH2	2.52	0.45
3:B:53:ARG:HD3	3:B:61:PHE:O	2.16	0.45
2:E:29:PHE:CD2	2:E:77:SER:HA	2.52	0.45
2:A:13:GLN:OE1	2:A:16:ARG:NH1	2.50	0.45
3:F:187:TYR:CZ	3:F:212:ARG:HG3	2.52	0.44
3:F:53:ARG:HD3	3:F:61:PHE:O	2.17	0.44
3:B:150:LYS:HE2	3:B:155:LEU:HD12	1.98	0.44
2:A:12:VAL:HG11	2:A:86:LEU:HD13	1.99	0.44
3:F:150:LYS:HD3	3:F:155:LEU:HD23	2.00	0.44
3:B:125:GLN:O	3:B:128:SER:OG	2.32	0.43
3:L:190:HIS:O	3:L:212:ARG:HD3	2.18	0.43
3:L:34:TRP:CD2	3:L:72:LEU:HB2	2.54	0.43
3:F:126:LEU:C	3:F:128:SER:H	2.25	0.43
2:C:30:ARG:O	2:C:53:PRO:HB3	2.19	0.43
2:C:131:PRO:HD3	2:C:217:LYS:HE2	2.01	0.43
3:D:22:CYS:HB2	3:D:34:TRP:CH2	2.53	0.43
3:B:34:TRP:CZ3	3:B:87:CYS:HB3	2.54	0.43
3:B:153:ASN:O	3:B:153:ASN:ND2	2.43	0.43
3:F:212:ARG:HH11	3:F:212:ARG:HB3	1.84	0.43
3:L:38:ARG:HB2	3:L:41:GLN:HG3	1.99	0.43
2:C:196:SER:HA	2:C:199:THR:HG23	2.00	0.42
3:B:22:CYS:HB2	3:B:34:TRP:CH2	2.54	0.42
2:A:29:PHE:CD2	2:A:77:SER:HA	2.54	0.42
3:F:7:PRO:HA	3:F:8:PRO:HD3	1.89	0.42
1:Q:9:M3L:HM12	1:Q:9:M3L:HD3	1.83	0.42
3:B:4:LEU:HB2	3:B:100:GLY:HA2	2.01	0.42
2:C:200:GLN:OE1	2:C:201:THR:N	2.52	0.42
2:E:83:MET:HE1	2:E:94:TYR:CZ	2.55	0.42
2:E:12:VAL:HG21	2:E:86:LEU:HD12	2.00	0.41
2:E:51:ILE:HD11	2:E:55:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:52:ASN:ND2	2:A:54:ASP:H	2.18	0.41
2:E:133:ALA:HA	2:E:134:PRO:HD3	1.90	0.41
3:F:155:LEU:HD23	3:F:155:LEU:HA	1.68	0.41
2:A:40:ALA:HB3	2:A:43:LYS:HB2	2.03	0.41
2:A:83:MET:HB3	2:A:86:LEU:HD21	2.02	0.41
2:E:99:GLU:OE2	3:F:97:TYR:OH	2.30	0.41
2:H:154:PHE:HA	2:H:155:PRO:HA	1.87	0.41
2:A:197:LEU:HA	2:A:197:LEU:HD23	1.76	0.41
3:L:94:ILE:H	3:L:94:ILE:HG13	1.78	0.41
3:B:129:GLY:HA2	3:B:184:LYS:HB2	2.03	0.41
3:B:141:TYR:CG	3:B:142:PRO:HA	2.56	0.41
2:E:81:LEU:HD12	2:E:81:LEU:HA	1.92	0.41
2:H:196:SER:HA	2:H:199:THR:HG23	2.03	0.41
2:C:52:ASN:HB3	2:C:57:THR:HB	2.03	0.40
2:H:30:ARG:O	2:H:53:PRO:HB3	2.21	0.40
3:L:146:LYS:HB3	3:L:198:THR:HB	2.03	0.40
3:D:146:LYS:HB3	3:D:198:THR:HB	2.03	0.40
3:D:202:LEU:HD13	3:D:206:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	8/16 (50%)	7 (88%)	1 (12%)	0	100	100
1	Q	8/16 (50%)	7 (88%)	1 (12%)	0	100	100
2	A	215/229 (94%)	211 (98%)	3 (1%)	1 (0%)	24	41
2	C	215/229 (94%)	210 (98%)	3 (1%)	2 (1%)	14	26
2	E	215/229 (94%)	210 (98%)	4 (2%)	1 (0%)	24	41
2	H	214/229 (93%)	208 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	210/215 (98%)	201 (96%)	8 (4%)	1 (0%)	24	41
3	D	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
3	F	209/215 (97%)	196 (94%)	11 (5%)	2 (1%)	12	23
3	L	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
All	All	1716/1808 (95%)	1653 (96%)	56 (3%)	7 (0%)	30	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	196	SER
3	B	212	ARG
2	C	197	LEU
3	F	154	ALA
3	F	212	ARG
2	E	135	SER
2	A	221	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	8/10 (80%)	6 (75%)	2 (25%)	0	1
1	Q	8/10 (80%)	7 (88%)	1 (12%)	4	8
2	A	184/193 (95%)	181 (98%)	3 (2%)	55	78
2	C	184/193 (95%)	177 (96%)	7 (4%)	29	53
2	E	183/193 (95%)	180 (98%)	3 (2%)	55	78
2	H	183/193 (95%)	178 (97%)	5 (3%)	39	65
3	B	182/186 (98%)	174 (96%)	8 (4%)	25	47
3	D	183/186 (98%)	182 (100%)	1 (0%)	81	91
3	F	181/186 (97%)	175 (97%)	6 (3%)	33	58
3	L	183/186 (98%)	179 (98%)	4 (2%)	45	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1479/1536 (96%)	1439 (97%)	40 (3%)	39 65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	3	THR
1	P	6	THR
2	A	11	VAL
2	A	58	ARG
2	A	201	THR
3	B	2	TYR
3	B	106	THR
3	B	124	SER
3	B	148	GLN
3	B	153	ASN
3	B	155	LEU
3	B	186	ASP
3	B	192	VAL
1	Q	6	THR
2	C	52	ASN
2	C	137	LYS
2	C	143	THR
2	C	185	SER
2	C	195	SER
2	C	199	THR
2	C	222	LYS
3	D	143	ARG
2	E	11	VAL
2	E	104	LEU
2	E	201	THR
2	H	52	ASN
2	H	151	LYS
2	H	169	SER
2	H	195	SER
2	H	199	THR
3	L	21	THR
3	L	76	ARG
3	L	115	SER
3	L	164	VAL
3	F	78	GLU
3	F	147	VAL
3	F	148	GLN

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Mol	Chain	Res	Type
3	F	151	VAL
3	F	186	ASP
3	F	208	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	36	GLN
2	C	82	GLN
2	C	84	ASN
2	E	101	HIS
2	H	82	GLN
2	H	172	HIS
2	H	200	GLN
2	H	207	ASN
3	L	26	ASN
3	L	36	GLN
3	L	138	ASN
3	L	139	ASN
3	L	161	GLN
3	F	36	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
1	M3L	Q	9	1	10,11,12	1.72	3 (30%)	9,14,16	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M3L	P	9	1	10,11,12	1.64	3 (30%)	9,14,16	0.71	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
1	M3L	Q	9	1	-	4/9/10/12	-
1	M3L	P	9	1	-	2/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	9	M3L	CB-CA	3.03	1.58	1.53
1	Q	9	M3L	CM3-NZ	-3.01	1.41	1.50
1	P	9	M3L	CM3-NZ	-2.85	1.41	1.50
1	P	9	M3L	CB-CA	2.66	1.57	1.53
1	P	9	M3L	CM1-NZ	-2.14	1.43	1.50
1	Q	9	M3L	CM1-NZ	-2.01	1.44	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Q	9	M3L	C-CA-CB-CG
1	Q	9	M3L	CG-CD-CE-NZ
1	P	9	M3L	CE-CD-CG-CB
1	Q	9	M3L	N-CA-CB-CG
1	Q	9	M3L	CA-CB-CG-CD
1	P	9	M3L	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Q	9	M3L	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	10/16 (62%)	-1.35	0 100 100	27, 39, 56, 72	0
1	Q	10/16 (62%)	-1.44	0 100 100	28, 39, 52, 80	0
2	A	219/229 (95%)	-1.48	0 100 100	22, 37, 60, 109	0
2	C	219/229 (95%)	-1.52	0 100 100	24, 34, 69, 91	0
2	E	219/229 (95%)	-1.49	1 (0%) 87 85	23, 36, 61, 92	0
2	H	218/229 (95%)	-1.52	0 100 100	23, 34, 68, 92	0
3	B	212/215 (98%)	-1.44	0 100 100	22, 36, 75, 87	0
3	D	213/215 (99%)	-1.48	0 100 100	25, 41, 58, 73	0
3	F	211/215 (98%)	-1.47	0 100 100	21, 36, 76, 88	0
3	L	213/215 (99%)	-1.47	0 100 100	23, 41, 60, 79	0
All	All	1744/1808 (96%)	-1.48	1 (0%) 92 91	21, 37, 68, 109	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	141	GLY	2.6

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, 95th 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
1	M3L	P	9	12/13	0.99	0.04	21,34,46,46	0
1	M3L	Q	9	12/13	0.99	0.04	20,37,43,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.