



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:57 PM UTC

PDB ID : 2QQS / pdb_00002qqs
Title : JMJD2A tandem tudor domains in complex with a trimethylated histone H4-K20 peptide
Authors : Lee, J.; Botuyan, M.V.; Mer, G.
Deposited on : 2007-07-26
Resolution : 2.82 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

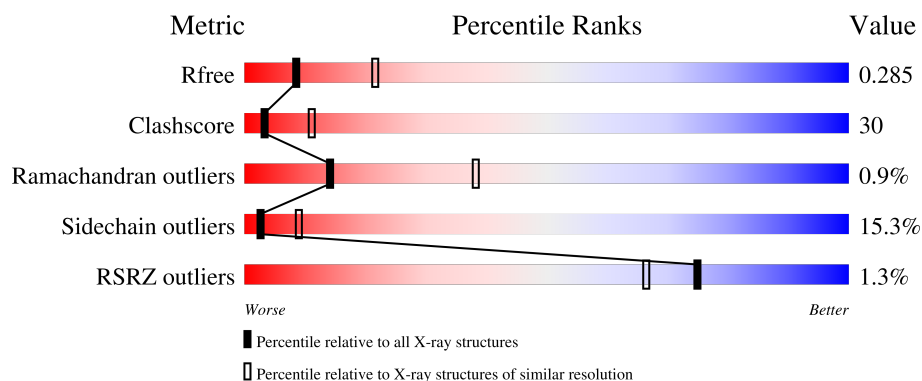
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	118	10% 47% 35% 10% 8%
1	B	118	56% 33% 8%
2	C	10	10% 10% 20% 20% 50%
2	D	10	10% 50% 20% 30%

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	C	20	X	-	-	-
2	M3L	D	20	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1929 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 JmjC domain-containing histone demethylation protein 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			876	554	144	175	3			
1	B	108	Total	C	N	O	S	0	0	0
			869	552	142	172	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	894	GLY	-	expression tag	UNP O75164
A	895	HIS	-	expression tag	UNP O75164
A	896	MET	-	expression tag	UNP O75164
B	894	GLY	-	expression tag	UNP O75164
B	895	HIS	-	expression tag	UNP O75164
B	896	MET	-	expression tag	UNP O75164

- Molecule 2 is a protein called METHYLATED HISTONE H4 PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			51	32	14	5			
2	D	7	Total	C	N	O	0	0	0
			70	44	19	7			

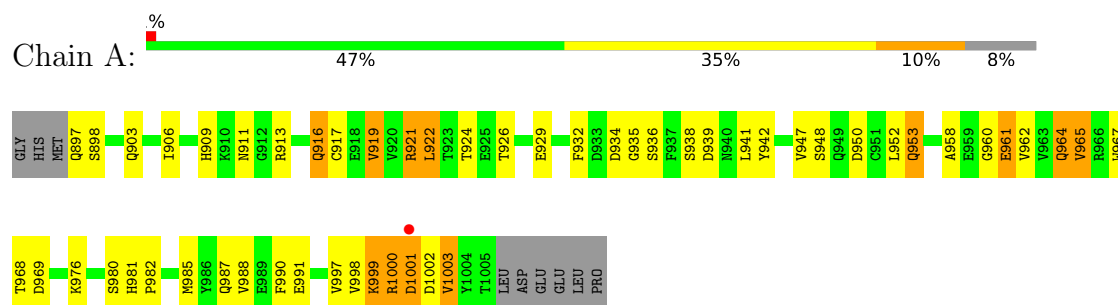
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	30	Total	O	0	0
			30	30		
3	C	1	Total	O	0	0
			1	1		

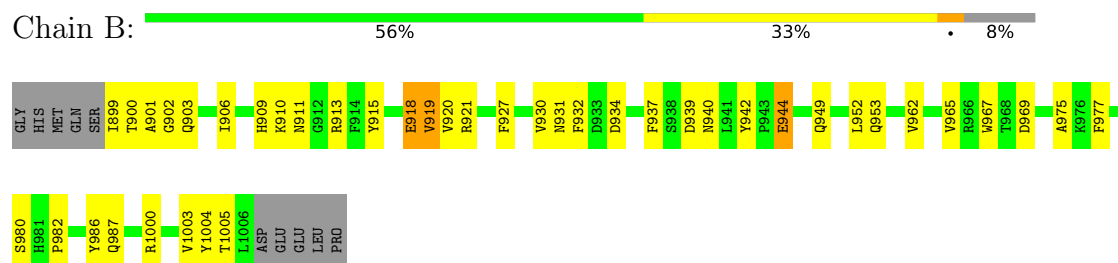
3 Residue-property plots [i](#)

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.

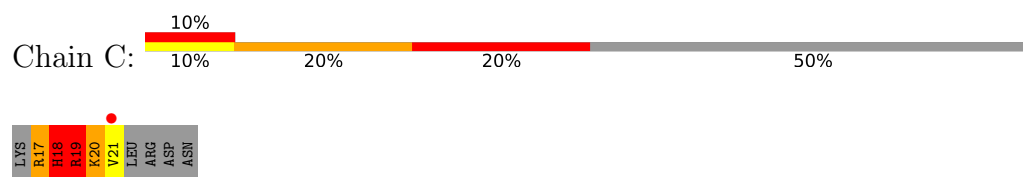
- Molecule 1: JmjC domain-containing histone demethylation protein 3A



- Molecule 1: JmjC domain-containing histone demethylation protein 3A



- Molecule 2: METHYLATED HISTONE H4 PEPTIDE



- Molecule 2: METHYLATED HISTONE H4 PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.97Å 27.69Å 82.42Å 90.00° 90.77° 90.00°	Depositor
Resolution (Å)	25.97 – 2.82 25.97 – 2.82	Depositor EDS
% Data completeness (in resolution range)	85.6 (25.97-2.82) 85.9 (25.97-2.82)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.236 , 0.283 0.233 , 0.285	Depositor DCC
R_{free} test set	237 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	1929	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.21% 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	A	0.77	0/896	0.98	2/1215 (0.2%)
1	B	0.76	0/889	0.99	1/1206 (0.1%)
2	C	1.61	1/39 (2.6%)	2.03	3/50 (6.0%)
2	D	1.03	0/58	1.19	0/75
All	All	0.80	1/1882 (0.1%)	1.02	6/2546 (0.2%)

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	A	0	3
2	C	1	1
2	D	1	0
All	All	2	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	20	M3L	C-N	8.59	1.45	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	20	M3L	CA-C-N	7.58	135.35	121.70
2	C	20	M3L	C-N-CA	7.58	135.35	121.70
1	B	920	VAL	N-CA-C	-7.20	104.83	111.67
2	C	20	M3L	O-C-N	5.72	132.15	123.00
1	A	942	TYR	CA-C-N	5.49	125.84	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	942	TYR	C-N-CA	5.49	125.84	119.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	20	M3L	CA
2	D	20	M3L	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1000	ARG	Peptide
1	A	1001	ASP	Peptide
1	A	999	LYS	Peptide
2	C	18	HIS	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	876	0	821	56	0
1	B	869	0	819	39	0
2	C	51	0	59	27	0
2	D	70	0	84	13	0
3	A	32	0	0	3	0
3	B	30	0	0	3	0
3	C	1	0	0	0	0
All	All	1929	0	1783	111	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 30.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:LEU:HB3	2:D:23:ARG:C	1.61	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:ARG:HB2	1:A:1002:ASP:N	1.70	1.07
1:A:961:GLU:OE1	2:C:18:HIS:ND1	1.96	0.98
2:C:18:HIS:CA	2:C:19:ARG:HB2	1.95	0.96
1:B:942:TYR:HB3	1:B:944:GLU:OE2	1.70	0.91
1:B:939:ASP:OD1	2:C:21:VAL:HG22	1.71	0.90
2:C:19:ARG:HG2	2:C:19:ARG:HH11	1.37	0.89
2:D:22:LEU:CB	2:D:23:ARG:C	2.48	0.86
2:C:18:HIS:N	2:C:19:ARG:HB2	1.91	0.84
1:A:1000:ARG:CB	1:A:1001:ASP:C	2.52	0.83
1:A:1000:ARG:CB	1:A:1002:ASP:N	2.43	0.82
1:B:967:TRP:CZ2	2:C:20:M3L:HM23	2.15	0.81
1:A:1000:ARG:HB2	1:A:1002:ASP:H	1.46	0.80
2:C:19:ARG:HH11	2:C:19:ARG:CG	1.95	0.80
1:A:935:GLY:O	2:D:17:ARG:HG2	1.84	0.78
1:A:1000:ARG:HB2	1:A:1001:ASP:C	2.08	0.77
1:B:937:PHE:CZ	2:C:21:VAL:HG23	2.20	0.77
1:B:967:TRP:HZ2	2:C:20:M3L:HM23	1.51	0.73
2:C:18:HIS:HA	2:C:19:ARG:HB2	1.72	0.71
1:B:931:ASN:O	1:B:975:ALA:HB1	1.92	0.70
1:B:937:PHE:CZ	2:C:21:VAL:CG2	2.77	0.68
1:A:1000:ARG:HB3	1:A:1001:ASP:C	2.19	0.68
1:A:1001:ASP:H	1:A:1003:VAL:HG23	1.58	0.68
1:A:1000:ARG:CB	1:A:1002:ASP:H	2.06	0.67
1:A:1001:ASP:H	1:A:1003:VAL:CG2	2.07	0.66
2:C:17:ARG:N	2:C:19:ARG:HG3	2.12	0.65
2:C:18:HIS:H	2:C:19:ARG:HB2	1.60	0.65
1:A:1000:ARG:N	1:A:1002:ASP:H	1.92	0.65
1:A:991:GLU:HG2	3:A:48:HOH:O	1.96	0.64
2:C:19:ARG:HG2	2:C:19:ARG:NH1	2.10	0.64
1:B:909:HIS:HD2	1:B:911:ASN:H	1.44	0.64
1:B:1000:ARG:NH1	3:B:19:HOH:O	2.25	0.63
1:B:909:HIS:CD2	1:B:911:ASN:H	2.18	0.62
1:A:967:TRP:NE1	2:D:22:LEU:O	2.33	0.62
1:A:962:VAL:HG23	3:B:51:HOH:O	2.00	0.61
1:B:980:SER:O	1:B:982:PRO:HD3	2.00	0.61
1:A:921:ARG:HB3	1:A:987:GLN:HE21	1.65	0.61
1:A:929:GLU:HA	1:A:938:SER:O	2.02	0.60
1:B:986:TYR:HE1	1:B:1000:ARG:CA	2.15	0.60
1:B:986:TYR:HE1	1:B:1000:ARG:HA	1.68	0.59
1:B:986:TYR:CE1	1:B:1000:ARG:HA	2.37	0.59
1:A:1000:ARG:CA	1:A:1002:ASP:H	2.15	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:ARG:NH1	1:A:1001:ASP:O	2.36	0.58
1:A:917:CYS:HB3	1:A:988:VAL:HB	1.86	0.57
1:A:950:ASP:CG	1:A:953:GLN:HB3	2.29	0.57
1:A:980:SER:O	1:A:982:PRO:HD3	2.05	0.57
1:A:958:ALA:HB2	2:C:19:ARG:H	1.69	0.57
1:A:929:GLU:OE2	1:A:981:HIS:HE1	1.88	0.56
1:B:939:ASP:CG	2:C:21:VAL:CG2	2.78	0.56
1:A:961:GLU:OE1	2:C:18:HIS:CE1	2.57	0.55
1:A:1001:ASP:HA	1:A:1003:VAL:C	2.31	0.55
1:B:939:ASP:CG	2:C:21:VAL:HG22	2.32	0.54
1:B:900:THR:HG22	1:B:903:GLN:HE21	1.73	0.54
2:C:19:ARG:HH11	2:C:19:ARG:CB	2.21	0.53
2:D:18:HIS:CD2	2:D:18:HIS:H	2.28	0.52
1:A:903:GLN:O	1:A:919:VAL:HG23	2.10	0.51
1:B:949:GLN:NE2	3:B:2:HOH:O	2.43	0.51
1:A:922:LEU:HB2	3:A:47:HOH:O	2.12	0.50
1:B:937:PHE:CE2	2:C:21:VAL:HG23	2.47	0.50
1:A:936:SER:HB3	2:D:18:HIS:CE1	2.46	0.49
1:B:939:ASP:OD1	2:C:21:VAL:CG2	2.53	0.49
1:A:948:SER:HB3	1:A:964:GLN:HB2	1.95	0.49
1:B:899:ILE:O	1:B:899:ILE:HG22	2.11	0.48
1:A:1001:ASP:HA	1:A:1003:VAL:O	2.13	0.48
1:B:967:TRP:HB3	1:B:969:ASP:OD1	2.14	0.48
1:A:967:TRP:CG	1:A:968:THR:H	2.32	0.48
2:D:22:LEU:CA	2:D:23:ARG:C	2.87	0.47
1:B:937:PHE:CE2	2:C:21:VAL:CG2	2.97	0.47
1:B:930:VAL:HG12	1:B:977:PHE:HA	1.97	0.47
1:B:939:ASP:CG	2:C:21:VAL:HG21	2.41	0.46
1:B:1003:VAL:C	1:B:1004:TYR:HD1	2.23	0.46
1:B:931:ASN:O	1:B:975:ALA:CB	2.63	0.46
1:A:991:GLU:HG2	1:A:991:GLU:H	1.50	0.45
1:B:921:ARG:HD2	1:B:987:GLN:NE2	2.31	0.45
1:A:999:LYS:O	1:A:1000:ARG:C	2.59	0.45
1:A:969:ASP:HB3	2:D:23:ARG:HH11	1.82	0.45
1:B:903:GLN:O	1:B:918:GLU:HA	2.17	0.45
3:A:42:HOH:O	2:C:17:ARG:NH2	2.50	0.45
1:A:921:ARG:HB3	1:A:987:GLN:NE2	2.32	0.44
1:A:950:ASP:OD1	1:A:953:GLN:HB3	2.17	0.44
1:A:909:HIS:CD2	1:A:911:ASN:H	2.35	0.44
1:A:950:ASP:OD1	1:A:953:GLN:N	2.50	0.44
1:A:1001:ASP:CA	1:A:1003:VAL:H	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:PHE:C	1:A:934:ASP:H	2.25	0.44
1:A:913:ARG:HH11	1:A:913:ARG:HB3	1.82	0.44
1:A:1000:ARG:HB3	1:A:1001:ASP:CA	2.48	0.44
2:D:20:M3L:HM13	2:D:20:M3L:HD2	1.82	0.43
1:A:909:HIS:HD2	1:A:911:ASN:H	1.66	0.43
1:A:947:VAL:HG22	1:A:964:GLN:HB3	2.00	0.43
1:A:1001:ASP:H	1:A:1003:VAL:HG22	1.83	0.43
1:A:916:GLN:HE21	1:A:916:GLN:HB3	1.43	0.43
1:B:932:PHE:C	1:B:934:ASP:H	2.27	0.43
1:A:998:VAL:HG22	1:A:999:LYS:N	2.34	0.43
1:A:936:SER:OG	2:D:20:M3L:HD3	2.19	0.43
1:A:985:MET:HE3	1:A:997:VAL:HG12	2.00	0.43
1:A:939:ASP:OD1	2:D:19:ARG:NH2	2.52	0.42
1:B:967:TRP:HZ2	2:C:20:M3L:CM2	2.28	0.42
1:A:960:GLY:HA3	2:C:21:VAL:HG11	2.01	0.42
1:B:900:THR:OG1	1:B:901:ALA:N	2.53	0.42
1:B:937:PHE:CZ	2:C:21:VAL:HG21	2.53	0.42
1:A:941:LEU:HD11	1:A:965:VAL:HG21	2.02	0.42
1:A:917:CYS:SG	1:A:990:PHE:CE2	3.13	0.41
1:B:913:ARG:HB2	1:B:915:TYR:CE1	2.56	0.41
1:B:986:TYR:HE1	1:B:1000:ARG:HB2	1.85	0.41
1:A:969:ASP:HB3	2:D:23:ARG:HD3	2.03	0.41
1:B:901:ALA:HA	1:B:902:GLY:HA2	1.54	0.41
1:B:927:PHE:CD2	1:B:940:ASN:HA	2.56	0.41
2:D:18:HIS:CD2	2:D:18:HIS:N	2.89	0.40
1:B:902:GLY:HA3	1:B:919:VAL:O	2.22	0.40
1:A:1001:ASP:C	1:A:1003:VAL:N	2.79	0.40
1:B:899:ILE:HG21	1:B:986:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/118 (91%)	96 (90%)	11 (10%)	0	100	100
1	B	106/118 (90%)	98 (92%)	8 (8%)	0	100	100
2	C	2/10 (20%)	0	0	2 (100%)	0	0
2	D	4/10 (40%)	3 (75%)	1 (25%)	0	100	100
All	All	219/256 (86%)	197 (90%)	20 (9%)	2 (1%)	14	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	19	ARG
2	C	18	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/105 (92%)	81 (84%)	16 (16%)	2	7
1	B	96/105 (91%)	86 (90%)	10 (10%)	7	21
2	C	4/9 (44%)	2 (50%)	2 (50%)	0	0
2	D	6/9 (67%)	3 (50%)	3 (50%)	0	0
All	All	203/228 (89%)	172 (85%)	31 (15%)	3	9

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	897	GLN
1	A	898	SER
1	A	906	ILE
1	A	916	GLN
1	A	919	VAL
1	A	921	ARG
1	A	922	LEU
1	A	924	THR
1	A	926	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	952	LEU
1	A	953	GLN
1	A	961	GLU
1	A	964	GLN
1	A	965	VAL
1	A	976	LYS
1	A	1003	VAL
1	B	906	ILE
1	B	910	LYS
1	B	918	GLU
1	B	919	VAL
1	B	944	GLU
1	B	952	LEU
1	B	953	GLN
1	B	962	VAL
1	B	965	VAL
1	B	1005	THR
2	C	17	ARG
2	C	19	ARG
2	D	18	HIS
2	D	21	VAL
2	D	23	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	909	HIS
1	A	916	GLN
1	A	981	HIS
1	A	987	GLN
1	B	903	GLN
1	B	909	HIS
1	B	931	ASN
1	B	949	GLN
1	B	995	GLN
2	D	18	HIS

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
2	M3L	C	20	2	10,11,12	1.04	1 (10%)	9,14,16	0.71	0
2	M3L	D	20	2	10,11,12	0.86	0	9,14,16	0.53	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	C	20	2	1/1/2/3	3/9/10/12	-
2	M3L	D	20	2	1/1/2/3	4/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	20	M3L	O-C	2.66	1.30	1.20

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	20	M3L	CA
2	D	20	M3L	CA

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	20	M3L	CG-CD-CE-NZ
2	D	20	M3L	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	20	M3L	CG-CD-CE-NZ
2	D	20	M3L	CA-CB-CG-CD
2	D	20	M3L	CD-CE-NZ-CM3
2	C	20	M3L	CE-CD-CG-CB
2	C	20	M3L	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	20	M3L	3	0
2	D	20	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	A	109/118 (92%)	-0.07	1 (0%) 81 74	12, 23, 35, 40	0
1	B	108/118 (91%)	-0.13	0 100 100	8, 21, 35, 39	0
2	C	4/10 (40%)	1.68	1 (25%) 2 1	46, 47, 47, 50	0
2	D	6/10 (60%)	0.96	1 (16%) 4 3	38, 41, 43, 44	0
All	All	227/256 (88%)	-0.04	3 (1%) 75 66	8, 22, 38, 50	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	22	LEU	3.2
2	C	21	VAL	2.9
1	A	1001	ASP	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
2	M3L	C	20	12/13	0.75	0.22	46,47,49,49	0
2	M3L	D	20	12/13	0.93	0.13	23,29,39,39	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.