



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2021 – 06:02 PM EST

PDB ID : 7LMM
Title : Crystal structure of bovine DNMT1 BAH1 domain in complex with H4K20me2
Authors : Ren, W.; Song, J.
Deposited on : 2021-02-05
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.17
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) : 2.17

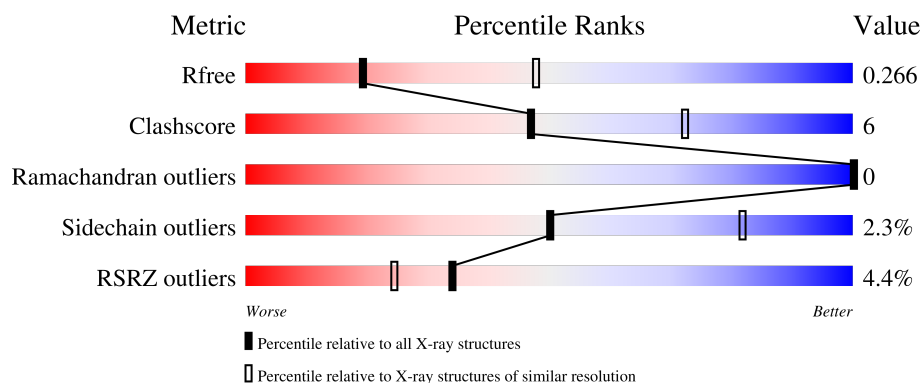
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	158	
1	B	158	
1	C	158	
1	D	158	
2	F	13	

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Mol	Chain	Length	Quality of chain
2	G	13	<div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div><div>8%62%8%8%23%</div></div>
2	H	13	<div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div><div>46%54%15%31%</div></div>
2	I	13	<div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div><div>8%46%23%31%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5206 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 DNA (cytosine-5)-methyltransferase 1, DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1220	779	193	240	8			
1	B	157	Total	C	N	O	S	0	0	0
			1218	778	191	241	8			
1	C	157	Total	C	N	O	S	0	0	0
			1216	774	194	240	8			
1	D	157	Total	C	N	O	S	0	0	0
			1208	770	190	240	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	724	SER	-	expression tag	UNP Q24K09
A	838	GLY	-	linker	UNP Q24K09
A	839	ALA	-	linker	UNP Q24K09
A	840	GLY	-	linker	UNP Q24K09
A	841	SER	-	linker	UNP Q24K09
A	842	ALA	-	linker	UNP Q24K09
B	724	SER	-	expression tag	UNP Q24K09
B	838	GLY	-	linker	UNP Q24K09
B	839	ALA	-	linker	UNP Q24K09
B	840	GLY	-	linker	UNP Q24K09
B	841	SER	-	linker	UNP Q24K09
B	842	ALA	-	linker	UNP Q24K09
C	724	SER	-	expression tag	UNP Q24K09
C	838	GLY	-	linker	UNP Q24K09
C	839	ALA	-	linker	UNP Q24K09
C	840	GLY	-	linker	UNP Q24K09
C	841	SER	-	linker	UNP Q24K09
C	842	ALA	-	linker	UNP Q24K09
D	724	SER	-	expression tag	UNP Q24K09
D	838	GLY	-	linker	UNP Q24K09

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Chain	Residue	Modelled	Actual	Comment	Reference
D	839	ALA	-	linker	UNP Q24K09
D	840	GLY	-	linker	UNP Q24K09
D	841	SER	-	linker	UNP Q24K09
D	842	ALA	-	linker	UNP Q24K09

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	8	Total	C	N	O	0	0	0
			71	44	17	10			
2	G	10	Total	C	N	O	0	0	0
			81	50	19	12			
2	I	9	Total	C	N	O	0	0	0
			76	47	19	10			
2	H	9	Total	C	N	O	0	0	0
			76	47	18	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	26	TYR	ILE	conflict	UNP P62805
G	26	TYR	ILE	conflict	UNP P62805
I	26	TYR	ILE	conflict	UNP P62805
H	26	TYR	ILE	conflict	UNP P62805

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		

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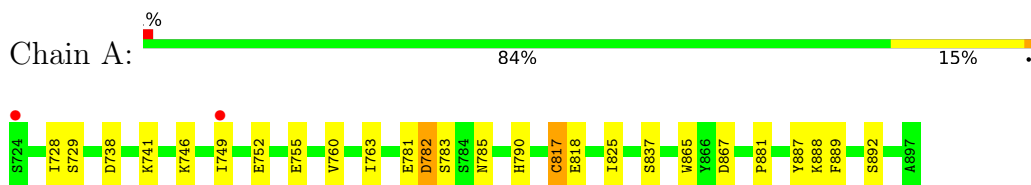
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	9	Total 9	O 9	0	0
4	C	4	Total 4	O 4	0	0
4	D	3	Total 3	O 3	0	0
4	F	1	Total 1	O 1	0	0
4	G	2	Total 2	O 2	0	0
4	I	1	Total 1	O 1	0	0

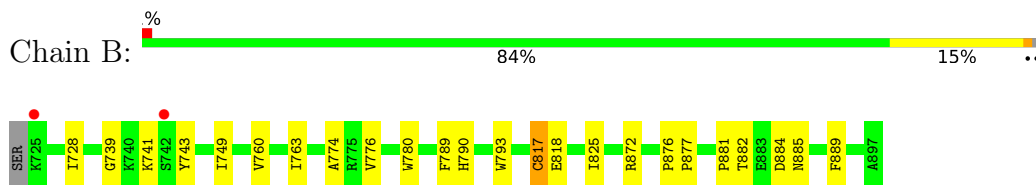
3 Residue-property plots

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.

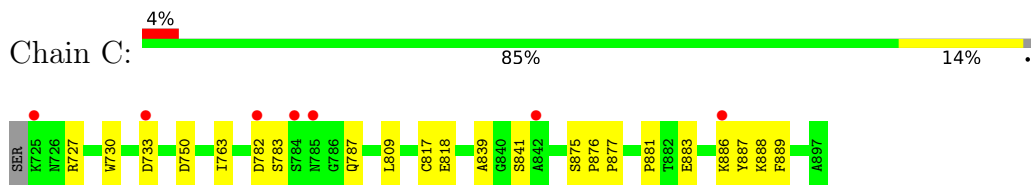
- Molecule 1: DNA (cytosine-5)-methyltransferase 1, DNA (cytosine-5)-methyltransferase 1



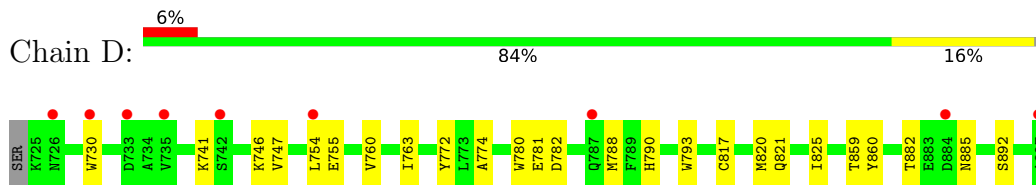
- Molecule 1: DNA (cytosine-5)-methyltransferase 1, DNA (cytosine-5)-methyltransferase 1



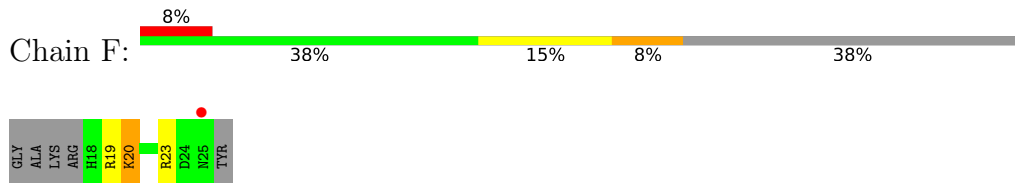
- Molecule 1: DNA (cytosine-5)-methyltransferase 1, DNA (cytosine-5)-methyltransferase 1



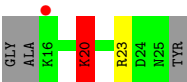
- Molecule 1: DNA (cytosine-5)-methyltransferase 1, DNA (cytosine-5)-methyltransferase 1



- Molecule 2: Histone H4



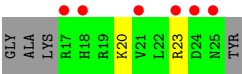
- Molecule 2: Histone H4



• Molecule 2: Histone H4



• Molecule 2: Histone H4



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	70.70Å 80.28Å 130.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 – 2.80 34.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.91-2.80) 99.3 (34.91-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.207 , 0.267 0.206 , 0.266	Depositor DCC
R_{free} test set	1881 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5206	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 4.84% 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: ZN, MLY

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	0.59	1/1253 (0.1%)	0.68	0/1710
1	B	0.44	1/1251 (0.1%)	0.84	2/1706 (0.1%)
1	C	0.45	1/1249 (0.1%)	0.61	0/1705
1	D	0.43	0/1241	0.54	0/1696
2	F	0.31	0/60	0.74	0/79
2	G	0.31	0/70	0.56	0/93
2	H	0.25	0/65	0.43	0/86
2	I	0.35	0/65	0.63	0/86
All	All	0.47	3/5254 (0.1%)	0.67	2/7161 (0.0%)

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
2	F	0	1
2	G	0	1
2	I	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	817	CYS	CB-SG	-8.36	1.68	1.82
1	C	817	CYS	CB-SG	-6.62	1.71	1.82
1	B	817	CYS	CB-SG	-5.02	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	872	ARG	NE-CZ-NH1	-19.71	110.45	120.30
1	B	872	ARG	NE-CZ-NH2	13.06	126.83	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	20	MLY	Mainchain
2	G	20	MLY	Mainchain
2	I	20	MLY	Mainchain

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	1220	0	1115	13	0
1	B	1218	0	1118	14	0
1	C	1216	0	1112	17	0
1	D	1208	0	1094	16	0
2	F	71	0	73	4	0
2	G	81	0	78	2	0
2	H	76	0	75	2	0
2	I	76	0	77	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	0	0	0
4	B	9	0	0	1	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	I	1	0	0	0	0
All	All	5206	0	4742	61	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 6.

All (61) 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:A:763:ILE:O	2:F:23:ARG:NH1	2.03	0.92
1:C:883:GLU:HA	1:C:886:LYS:HD2	1.56	0.87
1:C:763:ILE:O	2:I:23:ARG:NH2	2.17	0.78
1:D:760:VAL:HG11	1:D:825:ILE:HG12	1.71	0.71
1:C:883:GLU:CA	1:C:886:LYS:HD2	2.24	0.68
1:B:739:GLY:O	4:B:1001:HOH:O	2.14	0.66
1:C:839:ALA:C	1:C:841:SER:H	1.99	0.66
1:A:746:LYS:HG2	1:A:755:GLU:HG2	1.79	0.65
1:C:887:TYR:CE2	1:C:888:LYS:HD3	2.31	0.65
1:B:763:ILE:O	2:G:23:ARG:NH1	2.29	0.65
1:A:790:HIS:NE2	1:A:817:CYS:HB3	2.14	0.61
1:D:859:THR:HG22	1:D:860:TYR:O	2.03	0.59
1:A:818:GLU:HG2	2:F:19:ARG:HD2	1.85	0.58
1:D:747:VAL:HG23	1:D:754:LEU:HB3	1.87	0.57
1:A:782:ASP:HB3	1:A:785:ASN:H	1.70	0.57
1:A:738:ASP:HB2	1:A:741:LYS:H	1.68	0.56
1:A:881:PRO:HB3	1:A:889:PHE:CG	2.44	0.53
1:C:839:ALA:C	1:C:841:SER:N	2.62	0.53
1:D:730:TRP:CZ2	1:D:781:GLU:HB2	2.44	0.53
1:A:760:VAL:HG13	1:A:825:ILE:HG23	1.91	0.52
1:C:887:TYR:CD2	1:C:888:LYS:HG3	2.45	0.52
1:D:780:TRP:CE2	1:D:788:MET:HB2	2.45	0.52
1:B:743:TYR:CD2	1:B:780:TRP:HB3	2.45	0.51
1:B:881:PRO:HB3	1:B:889:PHE:CG	2.46	0.51
1:A:728:ILE:HG12	1:A:749:ILE:HG12	1.93	0.51
1:C:881:PRO:HB3	1:C:889:PHE:CG	2.46	0.50
1:C:883:GLU:CB	1:C:886:LYS:HD2	2.42	0.50
1:B:776:VAL:HG22	1:B:789:PHE:CD2	2.47	0.50
1:D:882:THR:OG1	1:D:885:ASN:N	2.39	0.50
1:D:760:VAL:HG13	1:D:825:ILE:HG23	1.94	0.49
1:D:730:TRP:HZ2	1:D:781:GLU:HB2	1.79	0.48
1:B:818:GLU:OE2	2:G:20:MLY:N	2.45	0.47
1:D:741:LYS:HA	1:D:782:ASP:HA	1.96	0.47
1:A:865:TRP:CZ3	1:A:867:ASP:HB2	2.50	0.47
1:B:760:VAL:HG13	1:B:825:ILE:HG23	1.97	0.47
1:B:882:THR:HB	1:B:885:ASN:H	1.79	0.47
1:B:774:ALA:HB2	1:B:793:TRP:CE3	2.51	0.46
1:B:882:THR:HG22	1:B:884:ASP:H	1.81	0.45
1:A:738:ASP:CB	1:A:741:LYS:H	2.29	0.45
1:C:730:TRP:CZ2	1:C:787:GLN:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:GLU:HG2	2:I:19:ARG:CZ	2.46	0.45
1:D:774:ALA:HB2	1:D:793:TRP:CE3	2.52	0.45
1:A:818:GLU:OE2	2:F:20:MLY:HB2	2.16	0.45
1:D:793:TRP:CZ2	1:D:820:MET:HE1	2.52	0.45
1:C:887:TYR:CZ	1:C:888:LYS:HD3	2.52	0.44
1:C:888:LYS:HE2	1:C:888:LYS:HB2	1.80	0.44
1:C:839:ALA:O	1:C:841:SER:N	2.40	0.44
1:D:763:ILE:O	2:H:23:ARG:NH2	2.46	0.44
1:C:876:PRO:HA	1:C:877:PRO:HD3	1.84	0.44
1:B:876:PRO:HA	1:B:877:PRO:HD3	1.85	0.43
1:B:790:HIS:NE2	1:B:817:CYS:HB3	2.33	0.43
1:B:728:ILE:HG12	1:B:749:ILE:HG23	2.00	0.43
1:D:790:HIS:CE1	1:D:817:CYS:HB3	2.53	0.42
1:B:741:LYS:HB3	1:B:780:TRP:CD1	2.54	0.42
1:A:887:TYR:CZ	1:A:888:LYS:HG2	2.54	0.42
2:F:20:MLY:HH13	2:F:20:MLY:HD3	1.80	0.42
1:D:746:LYS:HG2	1:D:755:GLU:HB3	2.02	0.42
1:D:788:MET:SD	1:D:821:GLN:HG3	2.60	0.41
1:C:809:LEU:HD23	1:C:809:LEU:HA	1.85	0.41
1:D:772:TYR:CE2	2:H:20:MLY:HG3	2.56	0.41
1:C:782:ASP:OD1	1:C:783:SER:N	2.55	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	156/158 (99%)	148 (95%)	8 (5%)	0	100	100
1	B	155/158 (98%)	150 (97%)	5 (3%)	0	100	100
1	C	155/158 (98%)	150 (97%)	5 (3%)	0	100	100
1	D	155/158 (98%)	148 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	5/13 (38%)	5 (100%)	0	0	100	100
2	G	7/13 (54%)	6 (86%)	1 (14%)	0	100	100
2	H	6/13 (46%)	5 (83%)	1 (17%)	0	100	100
2	I	6/13 (46%)	6 (100%)	0	0	100	100
All	All	645/684 (94%)	618 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/137 (92%)	119 (94%)	7 (6%)	21	51
1	B	127/137 (93%)	127 (100%)	0	100	100
1	C	127/137 (93%)	123 (97%)	4 (3%)	40	74
1	D	125/137 (91%)	124 (99%)	1 (1%)	81	94
2	F	6/10 (60%)	6 (100%)	0	100	100
2	G	6/10 (60%)	6 (100%)	0	100	100
2	H	6/10 (60%)	6 (100%)	0	100	100
2	I	6/10 (60%)	6 (100%)	0	100	100
All	All	529/588 (90%)	517 (98%)	12 (2%)	50	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	729	SER
1	A	752	GLU
1	A	781	GLU
1	A	782	ASP
1	A	783	SER
1	A	837	SER

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Mol	Chain	Res	Type
1	A	892	SER
1	C	727	ARG
1	C	733	ASP
1	C	750	ASP
1	C	875	SER
1	D	892	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	785	ASN
1	B	785	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	MLY	F	20	2	9,10,11	0.68	0	6,11,13	0.92	0
2	MLY	G	20	2	9,10,11	0.60	0	6,11,13	1.16	1 (16%)
2	MLY	I	20	2	9,10,11	0.62	0	6,11,13	1.15	0
2	MLY	H	20	2	9,10,11	0.61	0	6,11,13	1.00	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	MLY	F	20	2	-	3/8/9/11	-
2	MLY	G	20	2	-	2/8/9/11	-
2	MLY	I	20	2	-	4/8/9/11	-
2	MLY	H	20	2	-	4/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	20	MLY	CH2-NZ-CH1	-2.10	104.30	109.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	20	MLY	N-CA-CB-CG
2	I	20	MLY	C-CA-CB-CG
2	H	20	MLY	N-CA-CB-CG
2	F	20	MLY	CD-CE-NZ-CH2
2	I	20	MLY	CG-CD-CE-NZ
2	F	20	MLY	CD-CE-NZ-CH1
2	I	20	MLY	CE-CD-CG-CB
2	H	20	MLY	CE-CD-CG-CB
2	G	20	MLY	CE-CD-CG-CB
2	G	20	MLY	CD-CE-NZ-CH1
2	H	20	MLY	CG-CD-CE-NZ
2	F	20	MLY	CG-CD-CE-NZ
2	H	20	MLY	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	20	MLY	2	0
2	G	20	MLY	1	0
2	H	20	MLY	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	158/158 (100%)	0.01	2 (1%) 77 72	27, 51, 107, 125	0
1	B	157/158 (99%)	0.13	2 (1%) 77 72	36, 66, 108, 146	0
1	C	157/158 (99%)	0.22	7 (4%) 33 23	35, 61, 123, 147	0
1	D	157/158 (99%)	0.36	9 (5%) 23 15	40, 73, 131, 164	0
2	F	7/13 (53%)	1.08	1 (14%) 2 1	63, 77, 115, 120	0
2	G	9/13 (69%)	0.87	1 (11%) 5 3	59, 79, 114, 128	0
2	H	8/13 (61%)	2.48	6 (75%) 0 0	98, 118, 145, 155	0
2	I	8/13 (61%)	0.68	1 (12%) 3 2	44, 79, 116, 126	0
All	All	661/684 (96%)	0.23	29 (4%) 34 24	27, 65, 118, 164	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	897	ALA	4.1
2	H	18	HIS	4.0
2	H	25	ASN	3.4
1	A	724	SER	3.2
1	C	842	ALA	3.2
2	H	17	ARG	3.1
2	H	24	ASP	3.0
1	B	742	SER	2.8
1	C	784	SER	2.8
2	H	21	VAL	2.7
2	G	16	LYS	2.7
1	D	742	SER	2.6
2	I	17	ARG	2.5
1	C	733	ASP	2.4
1	D	735	VAL	2.3
1	D	884	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	785	ASN	2.3
1	D	726	ASN	2.3
2	H	23	ARG	2.2
1	D	787	GLN	2.2
1	D	733	ASP	2.2
1	C	886	LYS	2.2
1	D	730	TRP	2.1
2	F	25	ASN	2.1
1	B	725	LYS	2.0
1	A	749	ILE	2.0
1	C	782	ASP	2.0
1	D	754	LEU	2.0
1	C	725	LYS	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, 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	MLY	H	20	11/12	0.91	0.23	62,106,116,121	0
2	MLY	G	20	11/12	0.95	0.23	53,58,62,65	0
2	MLY	F	20	11/12	0.95	0.17	47,54,76,80	0
2	MLY	I	20	11/12	0.97	0.20	44,48,53,62	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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
3	ZN	B	901	1/1	0.98	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	D	901	1/1	0.98	0.08	49,49,49,49	0
3	ZN	C	901	1/1	0.99	0.12	47,47,47,47	0
3	ZN	A	901	1/1	0.99	0.13	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.