



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:12 pm BST

PDB ID : 2VNF  
Title : MOLECULAR BASIS OF HISTONE H3K4ME3 RECOGNITION BY ING4  
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Deposited on : 2008-02-04  
Resolution : 1.76 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](mailto: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.

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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 : 2.11  
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) : 2.11

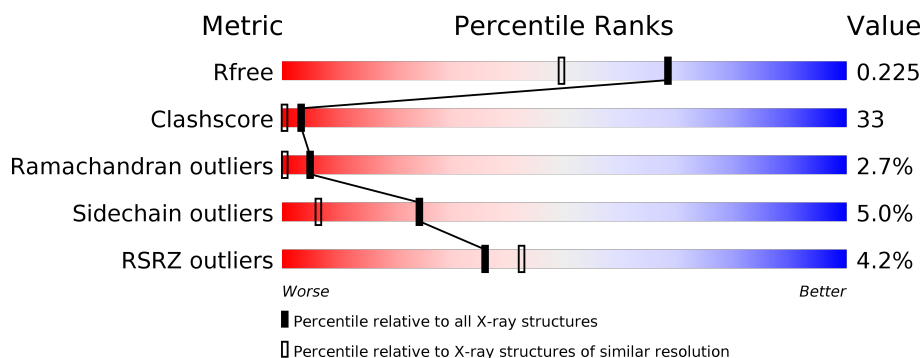
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	60	<div> <div>68%</div> <div>13%</div> <div>•</div> <div>17%</div> </div>
1	C	60	<div>5%</div> <div>63%</div> <div>25%</div> <div>•</div> <div>10%</div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTT	A	1245	-	-	X	-
6	DTU	C	1246	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 1101 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 INHIBITOR OF GROWTH PROTEIN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	50	Total	C	N	O	S	0	0	0
			389	246	64	71	8			
1	C	54	Total	C	N	O	S	0	0	0
			420	265	69	78	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	MET	-	expression tag	UNP Q9UNL4
C	187	MET	-	expression tag	UNP Q9UNL4

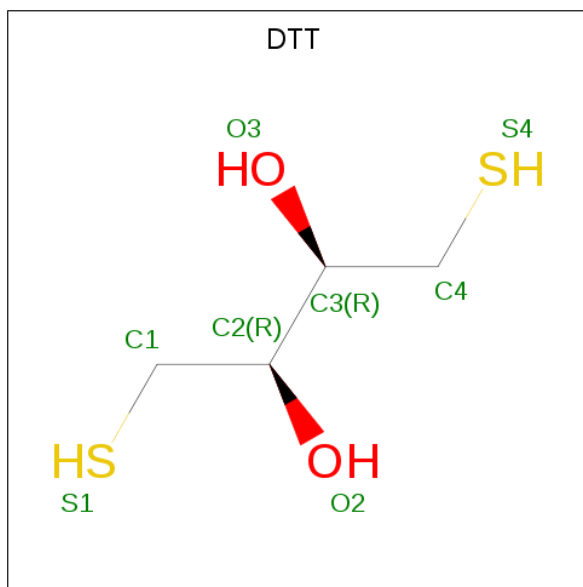
- Molecule 2 is a protein called HISTONE H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			51	31	11	9			
2	D	10	Total	C	N	O	0	1	0
			93	55	23	15			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).

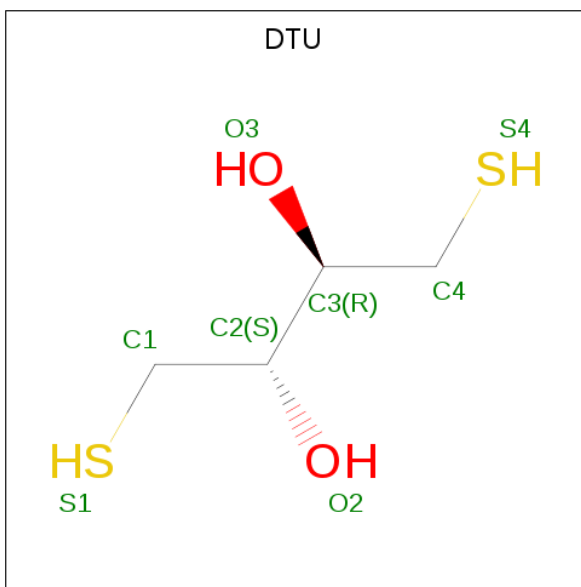


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		

- Molecule 6 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		
7	B	8	Total	O	0	0
			8	8		
7	C	40	Total	O	0	0
			40	40		
7	D	19	Total	O	0	0
			19	19		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

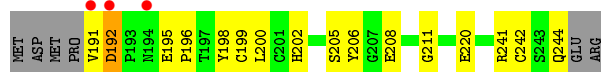
#### • Molecule 1: INHIBITOR OF GROWTH PROTEIN 4

Chain A: 



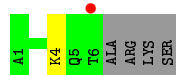
#### • Molecule 1: INHIBITOR OF GROWTH PROTEIN 4

Chain C: 

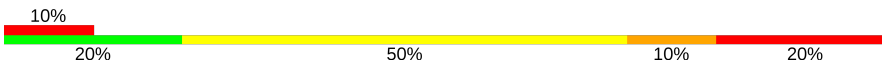


#### • Molecule 2: HISTONE H3

Chain B: 



#### • Molecule 2: HISTONE H3

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.52Å 68.52Å 28.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.51 – 1.76 22.84 – 1.76	Depositor EDS
% Data completeness (in resolution range)	96.9 (68.51-1.76) 97.0 (22.84-1.76)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.156 , 0.227 0.159 , 0.225	Depositor DCC
$R_{free}$ test set	635 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, ZN, M3L, DTU, DTT

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	0.62	0/402	0.73	0/545
1	C	0.52	0/435	0.69	0/593
2	B	0.51	0/38	0.79	0/50
2	D	0.57	0/80	1.36	0/104
All	All	0.57	0/955	0.79	0/1292

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	1
1	C	0	1
2	D	0	4
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	SER	Peptide
1	C	191	VAL	Peptide
2	D	7	ALA	Peptide
2	D	8[B]	ARG	Peptide
2	D	9	LYS	Peptide

## 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	A	389	0	340	20	0
1	C	420	0	366	20	0
2	B	51	0	60	1	0
2	D	93	0	108	25	0
3	A	1	0	0	0	0
4	A	8	0	9	14	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	C	8	0	10	8	0
7	A	60	0	0	6	0
7	B	8	0	0	0	0
7	C	40	0	0	4	0
7	D	19	0	0	5	0
All	All	1101	0	893	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 33.

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:202:HIS:HE1	4:A:1245:DTT:C1	1.07	1.60
1:A:202:HIS:CE1	4:A:1245:DTT:H12	1.03	1.56
1:C:202:HIS:HE1	6:C:1246:DTU:S4	1.31	1.52
1:A:202:HIS:NE2	4:A:1245:DTT:H41	1.24	1.43
1:C:202:HIS:CE1	6:C:1246:DTU:S4	2.11	1.43
1:A:202:HIS:CE1	4:A:1245:DTT:C1	1.85	1.38
1:A:240:PRO:N	7:A:2054:HOH:O	1.57	1.29
1:A:202:HIS:NE2	4:A:1245:DTT:C4	1.99	1.25
1:A:202:HIS:HE1	4:A:1245:DTT:C2	1.47	1.25
1:A:225:ALA:O	7:A:2041:HOH:O	1.57	1.23
1:A:202:HIS:ND1	4:A:1245:DTT:H12	1.53	1.22
1:A:202:HIS:CE1	4:A:1245:DTT:H41	1.78	1.17
1:C:202:HIS:NE2	6:C:1246:DTU:O2	1.85	1.08
2:D:8[A]:ARG:HH21	2:D:8[A]:ARG:HG3	1.17	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8[B]:ARG:O	2:D:10:SER:HA	1.64	0.97
1:C:202:HIS:NE2	6:C:1246:DTU:C2	2.33	0.91
1:A:202:HIS:CE1	4:A:1245:DTT:C4	2.51	0.89
4:A:1245:DTT:C2	7:A:2061:HOH:O	2.22	0.87
2:D:8[A]:ARG:NH2	2:D:8[A]:ARG:HG3	1.80	0.87
6:C:1246:DTU:S4	7:C:2039:HOH:O	2.33	0.85
1:C:242:CYS:O	7:C:2036:HOH:O	1.95	0.84
1:A:202:HIS:CE1	4:A:1245:DTT:C2	2.34	0.84
1:C:208:GLU:HG2	2:D:5:GLN:NE2	1.93	0.82
2:D:8[B]:ARG:NH2	7:D:2017:HOH:O	1.89	0.80
1:A:202:HIS:CE1	4:A:1245:DTT:C3	2.66	0.79
1:A:225:ALA:C	7:A:2041:HOH:O	2.07	0.77
2:D:8[A]:ARG:CG	2:D:8[A]:ARG:HH21	1.97	0.77
1:C:202:HIS:NE2	6:C:1246:DTU:H2	2.02	0.73
1:A:244:GLN:OE1	7:A:2060:HOH:O	2.10	0.69
1:C:202:HIS:CE1	6:C:1246:DTU:O2	2.42	0.67
1:C:202:HIS:CE1	6:C:1246:DTU:C4	2.84	0.61
4:A:1245:DTT:S4	4:A:1245:DTT:O2	2.59	0.60
1:A:202:HIS:NE2	4:A:1245:DTT:H42	2.09	0.59
1:C:208:GLU:CG	2:D:5:GLN:NE2	2.67	0.57
1:A:195:GLU:HB2	7:D:2019:HOH:O	2.04	0.56
2:D:6:THR:CG2	2:D:10:SER:HB3	2.36	0.55
1:C:205:SER:HB2	2:D:10:SER:OG	2.08	0.54
1:C:192:ASP:HB3	7:C:2002:HOH:O	2.06	0.53
2:D:9:LYS:HG3	2:D:9:LYS:O	2.07	0.53
1:C:244:GLN:CD	7:C:2038:HOH:O	2.48	0.52
2:D:7:ALA:O	2:D:8[B]:ARG:HB2	2.10	0.52
1:A:195:GLU:OE2	1:A:196:PRO:HD2	2.09	0.52
2:D:8[B]:ARG:O	2:D:10:SER:CA	2.50	0.51
2:D:8[B]:ARG:N	7:D:2012:HOH:O	2.36	0.50
2:D:6:THR:HG22	2:D:8[B]:ARG:HA	1.92	0.50
1:A:225:ALA:HB1	7:A:2041:HOH:O	2.13	0.48
1:C:195:GLU:HG3	1:C:196:PRO:HD2	1.94	0.48
2:D:6:THR:HG21	2:D:8[A]:ARG:O	2.14	0.48
1:C:198:TYR:CZ	2:D:4:M3L:HM31	2.49	0.48
2:D:7:ALA:O	2:D:8[A]:ARG:HB2	2.14	0.48
1:C:195:GLU:OE2	2:D:10:SER:C	2.54	0.46
2:D:9:LYS:HE2	7:D:2016:HOH:O	2.14	0.46
1:C:211:GLY:HA2	1:C:220:GLU:O	2.17	0.45
2:D:7:ALA:O	2:D:8[A]:ARG:CB	2.65	0.45
1:A:221:TRP:CE2	2:B:4:M3L:HM22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:LYS:HB2	2:D:9:LYS:HE2	1.30	0.43
2:D:6:THR:CG2	2:D:8[A]:ARG:O	2.67	0.42
1:C:208:GLU:HG2	2:D:5:GLN:CD	2.40	0.42
1:C:199:CYS:SG	1:C:200:LEU:N	2.92	0.42
1:C:206:TYR:HA	2:D:8[A]:ARG:O	2.20	0.41
2:D:2:ARG:NE	7:D:2002:HOH:O	2.22	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	48/60 (80%)	45 (94%)	3 (6%)	0	100	100
1	C	52/60 (87%)	47 (90%)	4 (8%)	1 (2%)	8	1
2	B	3/10 (30%)	3 (100%)	0	0	100	100
2	D	8/10 (80%)	5 (62%)	0	3 (38%)	0	0
All	All	111/140 (79%)	100 (90%)	7 (6%)	4 (4%)	5	0

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	8[A]	ARG
2	D	8[B]	ARG
2	D	9	LYS
1	C	192	ASP

### 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	43/55 (78%)	41 (95%)	2 (5%)	26	7
1	C	47/55 (86%)	46 (98%)	1 (2%)	53	31
2	B	4/7 (57%)	4 (100%)	0	100	100
2	D	8/7 (114%)	5 (62%)	3 (38%)	0	0
All	All	102/124 (82%)	96 (94%)	6 (6%)	24	4

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	232	LYS
1	C	241	ARG
2	D	8[A]	ARG
2	D	8[B]	ARG
2	D	9	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	A	244	GLN
1	C	202	HIS
2	D	5	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	$\# Z  > 2$
2	M3L	B	4	2	10,11,12	0.71	0	9,14,16	0.52	0
2	M3L	D	4	2	10,11,12	0.81	0	9,14,16	0.95	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	B	4	2	-	0/9/10/12	-
2	M3L	D	4	2	-	0/9/10/12	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	M3L	1	0
2	D	4	M3L	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
6	DTU	C	1246	-	7,7,7	0.60	0	4,8,8	0.85	0
4	DTT	A	1245	-	7,7,7	1.32	1 (14%)	4,8,8	2.34	1 (25%)

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
6	DTU	C	1246	-	-	6/8/8/8	-
4	DTT	A	1245	-	-	5/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1245	DTT	C3-C2	-2.63	1.46	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	1245	DTT	C2-C1-S1	-4.53	101.29	114.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1246	DTU	C1-C2-C3-O3
6	C	1246	DTU	C1-C2-C3-C4
6	C	1246	DTU	O2-C2-C3-O3
6	C	1246	DTU	O2-C2-C3-C4
6	C	1246	DTU	C2-C3-C4-S4
6	C	1246	DTU	O3-C3-C4-S4
4	A	1245	DTT	C1-C2-C3-C4
4	A	1245	DTT	S1-C1-C2-O2
4	A	1245	DTT	O3-C3-C4-S4
4	A	1245	DTT	O2-C2-C3-C4
4	A	1245	DTT	C2-C3-C4-S4

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1246	DTU	8	0
4	A	1245	DTT	14	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	50/60 (83%)	-0.04	0 <span>100</span> <span>100</span>	16, 23, 41, 53	0
1	C	54/60 (90%)	0.24	3 (5%) <span>24</span> <span>30</span>	20, 33, 57, 66	0
2	B	5/10 (50%)	0.56	1 (20%) <span>1</span> <span>1</span>	23, 26, 39, 43	0
2	D	9/10 (90%)	1.64	1 (11%) <span>5</span> <span>7</span>	23, 31, 50, 60	0
All	All	118/140 (84%)	0.24	5 (4%) <span>36</span> <span>42</span>	16, 28, 53, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	10	SER	9.7
1	C	191	VAL	3.9
2	B	6	THR	3.0
1	C	194	ASN	2.6
1	C	192	ASP	2.5

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	M3L	B	4	12/13	0.96	0.10	25,30,42,44	0
2	M3L	D	4	12/13	0.97	0.17	20,23,25,26	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NA	A	300	1/1	0.78	0.34	61,61,61,61	0
4	DTT	A	1245	8/8	0.91	0.18	8,29,53,62	0
6	DTU	C	1246	8/8	0.92	0.18	34,52,62,76	0
5	ZN	A	1246	1/1	1.00	0.07	18,18,18,18	0
5	ZN	C	1247	1/1	1.00	0.07	25,25,25,25	0
5	ZN	A	1247	1/1	1.00	0.05	21,21,21,21	0
5	ZN	C	1248	1/1	1.00	0.02	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.