



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:55 am BST

PDB ID : 3N9Q  
Title : ceKDM7A from C.elegans, complex with H3K4me3 peptide, H3K27me2 peptide and NOG  
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Deposited on : 2010-05-31  
Resolution : 2.30 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

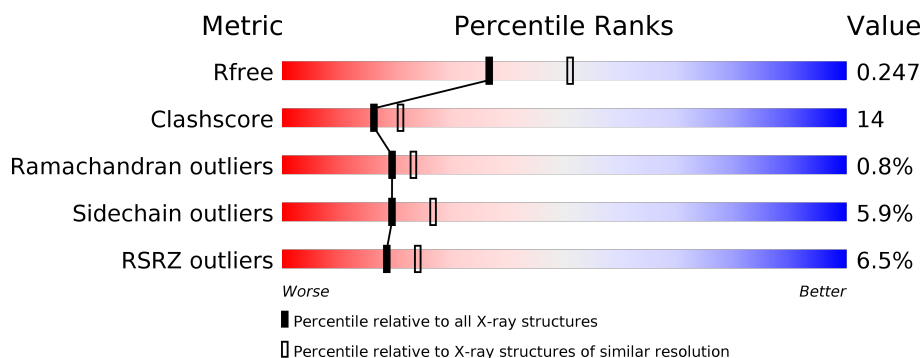
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	528	<div> <div>6%</div> <div>67%</div> <div>22%</div> <div>8%</div> </div>
2	B	15	<div> <div>7%</div> <div>20%</div> <div>20%</div> <div>60%</div> </div>
3	C	17	<div> <div>6%</div> <div>29%</div> <div>18%</div> <div>53%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4261 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3985	2547	668	743	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLU	-	EXPRESSION TAG	UNP Q9GYI0
A	185	PHE	-	EXPRESSION TAG	UNP Q9GYI0
A	186	HIS	-	EXPRESSION TAG	UNP Q9GYI0
A	187	MET	-	EXPRESSION TAG	UNP Q9GYI0

- Molecule 2 is a protein called Histone H3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			51	31	11	9			

- Molecule 3 is a protein called Histone H3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			59	37	13	9			

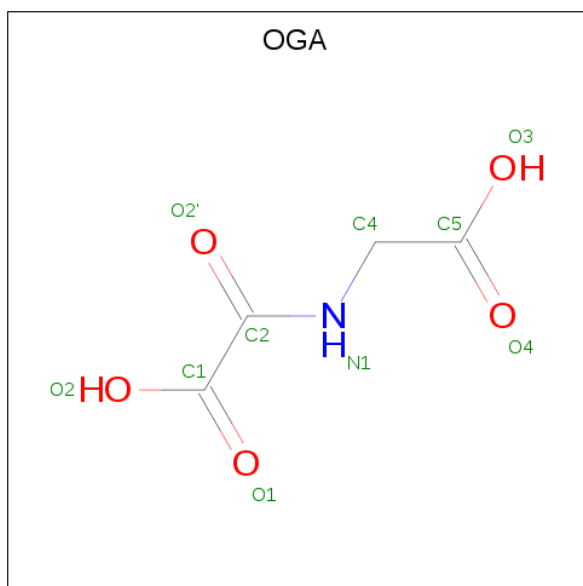
- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		

- 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		

- Molecule 6 is N-OXALYLGLYCINE (three-letter code: OGA) (formula:  $C_4H_5NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	148	Total	O	0	0
			148	148		
7	B	1	Total	O	0	0
			1	1		
7	C	4	Total	O	0	0
			4	4		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.14Å 87.48Å 102.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.25 – 2.30 40.25 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.25-2.30) 99.1 (40.25-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.207 , 0.255 0.200 , 0.247	Depositor DCC
$R_{free}$ test set	1427 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: OGA, ZN, M3L, FE2, 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	0.37	0/4088	0.53	0/5518
2	B	0.27	0/38	0.50	0/50
3	C	0.37	0/48	0.53	0/63
All	All	0.37	0/4174	0.53	0/5631

There are no bond length outliers.

There are no bond angle outliers.

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	A	3985	0	3845	114	0
2	B	51	0	60	5	0
3	C	59	0	68	6	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	10	0	4	2	0
7	A	148	0	0	2	0
7	B	1	0	0	0	0
7	C	4	0	0	1	0
All	All	4261	0	3977	116	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 14.

All (116) 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:200:GLY:HA3	1:A:201:CYS:HB3	1.07	1.05
1:A:648:ASN:HD22	1:A:648:ASN:H	1.08	0.99
1:A:200:GLY:HA3	1:A:201:CYS:CB	1.96	0.96
1:A:260:GLN:HE21	1:A:400:SER:H	1.04	0.94
1:A:200:GLY:CA	1:A:201:CYS:HB3	2.00	0.87
1:A:260:GLN:NE2	1:A:400:SER:H	1.75	0.83
1:A:648:ASN:HD22	1:A:648:ASN:N	1.76	0.82
1:A:322:VAL:HG22	1:A:550:ARG:HB2	1.61	0.81
1:A:581:ASN:OD1	3:C:27:MLY:HH12	1.83	0.79
1:A:648:ASN:ND2	1:A:648:ASN:H	1.85	0.73
1:A:275:VAL:HA	1:A:278:THR:HG22	1.71	0.72
1:A:694:ILE:O	1:A:698:THR:HG23	1.89	0.72
1:A:319:GLU:OE1	1:A:550:ARG:HD2	1.88	0.71
1:A:305:GLU:HG2	1:A:536:THR:HG23	1.73	0.68
1:A:412:ASP:OD2	1:A:415:ASN:HB3	1.95	0.67
1:A:430:ASN:HD22	1:A:433:MET:H	1.38	0.67
1:A:240:GLN:HB3	1:A:253:PHE:CD1	2.30	0.67
1:A:593:ARG:NH2	7:A:46:HOH:O	2.27	0.66
1:A:201:CYS:O	1:A:203:LYS:HG3	1.95	0.65
1:A:305:GLU:HG2	1:A:536:THR:CG2	2.26	0.64
1:A:247:CYS:SG	1:A:249:THR:HG23	2.39	0.63
1:A:298:ASN:H	1:A:298:ASN:HD22	1.46	0.62
1:A:569:VAL:CG1	6:A:4:OGA:H4C2	2.30	0.61
1:A:427:PHE:CD1	1:A:433:MET:HB3	2.35	0.61
1:A:305:GLU:OE2	1:A:536:THR:HG21	2.00	0.61
1:A:274:CYS:HA	1:A:277:HIS:CE1	2.36	0.60
1:A:241:TRP:CG	2:B:4:M3L:HE2	2.36	0.60
1:A:511:GLU:O	1:A:572:PRO:HD2	2.01	0.60
1:A:629:LEU:HD11	1:A:689:SER:OG	2.02	0.60
1:A:198:CYS:O	1:A:202:GLY:HA2	2.02	0.59
1:A:201:CYS:O	1:A:203:LYS:N	2.36	0.58
1:A:430:ASN:ND2	1:A:433:MET:H	2.01	0.58
1:A:424:SER:HB3	3:C:28:SER:O	2.04	0.58
1:A:369:PRO:HG3	1:A:436:ILE:HG22	1.85	0.58
1:A:625:ARG:HD2	1:A:626:ASN:OD1	2.04	0.57
1:A:569:VAL:HG11	6:A:4:OGA:H4C2	1.86	0.57
1:A:330:VAL:HB	1:A:355:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ARG:HD3	1:A:612:TYR:CE1	2.40	0.56
1:A:426:GLU:HG3	1:A:478:LYS:O	2.05	0.56
1:A:237:ASN:HB2	1:A:254:LEU:HG	1.86	0.56
1:A:638:GLU:O	1:A:639:GLY:C	2.45	0.55
1:A:201:CYS:SG	1:A:201:CYS:O	2.64	0.55
1:A:237:ASN:CB	1:A:254:LEU:HG	2.37	0.55
1:A:253:PHE:CD2	1:A:263:TYR:CE1	2.95	0.55
1:A:198:CYS:C	1:A:200:GLY:H	2.11	0.55
1:A:240:GLN:HB3	1:A:253:PHE:HD1	1.70	0.55
1:A:465:LEU:HD23	1:A:470:TYR:HB2	1.88	0.55
1:A:369:PRO:HG3	1:A:436:ILE:CG2	2.37	0.54
1:A:610:LYS:NZ	3:C:23:LYS:HD3	2.22	0.54
1:A:608:GLU:OE1	3:C:23:LYS:HG2	2.08	0.53
1:A:507:ILE:N	1:A:507:ILE:HD13	2.24	0.53
1:A:270:PHE:HB3	1:A:278:THR:HG21	1.92	0.52
1:A:657:LYS:HD2	1:A:694:ILE:CD1	2.40	0.52
1:A:605:ILE:HD12	1:A:605:ILE:C	2.29	0.52
1:A:271:CYS:O	1:A:275:VAL:HG23	2.10	0.52
1:A:292:TYR:OH	1:A:306:VAL:O	2.15	0.51
1:A:241:TRP:HB2	2:B:4:M3L:HG3	1.92	0.51
1:A:563:ALA:H	1:A:587:ASN:ND2	2.08	0.51
1:A:648:ASN:ND2	1:A:648:ASN:N	2.48	0.51
1:A:619:LEU:HD23	1:A:619:LEU:C	2.31	0.50
1:A:238:ASP:CG	1:A:239:PHE:H	2.13	0.50
1:A:588:LEU:HD12	7:A:82:HOH:O	2.11	0.50
1:A:639:GLY:N	1:A:640:SER:HB2	2.25	0.50
1:A:379:VAL:HG11	1:A:407:ARG:HD3	1.93	0.49
1:A:240:GLN:HB3	1:A:253:PHE:CE1	2.46	0.49
1:A:325:PRO:CB	1:A:330:VAL:HG13	2.43	0.49
1:A:641:ASP:HB3	1:A:644:GLU:HG2	1.94	0.49
1:A:596:HIS:HE1	1:A:659:GLU:OE1	1.95	0.49
1:A:240:GLN:CB	1:A:253:PHE:HD1	2.25	0.49
1:A:253:PHE:CD2	1:A:263:TYR:CZ	3.02	0.48
1:A:287:VAL:HG13	1:A:300:LYS:HE2	1.96	0.48
1:A:375:LEU:O	1:A:379:VAL:HG12	2.13	0.48
1:A:253:PHE:HB3	1:A:263:TYR:OH	2.14	0.48
1:A:319:GLU:CG	1:A:515:TYR:OH	2.63	0.47
1:A:201:CYS:O	1:A:202:GLY:C	2.53	0.47
1:A:553:ILE:N	1:A:553:ILE:HD12	2.31	0.46
1:A:635:ALA:O	1:A:640:SER:HB3	2.16	0.46
1:A:319:GLU:O	1:A:322:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:LEU:HD22	1:A:682:ASP:HB2	1.98	0.46
1:A:657:LYS:HD2	1:A:694:ILE:HD12	1.98	0.46
1:A:456:VAL:HG13	1:A:457:SER:N	2.31	0.45
1:A:241:TRP:CD2	2:B:4:M3L:HE2	2.52	0.45
1:A:458:GLY:O	1:A:462:ILE:HG12	2.17	0.45
1:A:668:LEU:N	1:A:668:LEU:HD23	2.32	0.45
1:A:198:CYS:HA	1:A:250:TRP:O	2.18	0.44
1:A:463:LYS:O	1:A:467:ARG:HG3	2.18	0.44
1:A:624:MET:O	1:A:629:LEU:HB2	2.17	0.44
1:A:325:PRO:HB2	1:A:330:VAL:HG13	2.00	0.44
1:A:287:VAL:HG11	1:A:297:PRO:HA	2.00	0.44
1:A:515:TYR:O	1:A:567:HIS:HA	2.18	0.44
1:A:298:ASN:H	1:A:298:ASN:ND2	2.14	0.43
1:A:239:PHE:O	2:B:5:GLN:HA	2.17	0.43
1:A:456:VAL:HG11	1:A:460:GLU:HB3	2.00	0.43
1:A:407:ARG:O	1:A:411:ARG:HG3	2.19	0.43
1:A:514:PHE:HB2	1:A:551:VAL:HG13	2.00	0.43
1:A:484:LEU:HD12	1:A:484:LEU:N	2.34	0.42
1:A:208:ASP:N	1:A:208:ASP:OD1	2.52	0.42
1:A:298:ASN:N	1:A:298:ASN:ND2	2.66	0.42
1:A:296:SER:HA	1:A:297:PRO:HD3	1.89	0.42
1:A:322:VAL:HA	1:A:323:PRO:HD3	1.84	0.42
1:A:678:LEU:HD23	1:A:678:LEU:HA	1.85	0.42
1:A:207:GLU:HG3	1:A:208:ASP:OD1	2.20	0.42
1:A:386:TYR:CE2	1:A:425:LEU:CD1	3.03	0.41
1:A:497:ASP:OD1	3:C:27:MLY:HH13	2.20	0.41
1:A:266:TYR:HA	1:A:283:ARG:HA	2.02	0.41
1:A:570:LEU:O	1:A:572:PRO:HD3	2.20	0.41
1:A:664:MET:CE	1:A:664:MET:HA	2.51	0.41
1:A:664:MET:O	1:A:668:LEU:HG	2.20	0.41
1:A:464:LEU:CD1	1:A:470:TYR:HA	2.51	0.41
3:C:23:LYS:N	7:C:101:HOH:O	2.53	0.41
1:A:467:ARG:O	1:A:468:GLU:HB2	2.20	0.41
1:A:403:LEU:HD12	1:A:403:LEU:HA	1.85	0.41
1:A:456:VAL:CG1	1:A:460:GLU:HB3	2.51	0.41
1:A:328:ASP:O	1:A:354:LYS:HE2	2.21	0.40
1:A:613:PHE:HA	1:A:614:PRO:HD3	1.81	0.40
2:B:2:ARG:H	2:B:2:ARG:HG2	1.67	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	A	478/528 (90%)	450 (94%)	24 (5%)	4 (1%)	19	23
2	B	3/15 (20%)	3 (100%)	0	0	100	100
3	C	5/17 (29%)	4 (80%)	1 (20%)	0	100	100
All	All	486/560 (87%)	457 (94%)	25 (5%)	4 (1%)	19	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	GLY
1	A	639	GLY
1	A	605	ILE
1	A	672	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	A	434/475 (91%)	408 (94%)	26 (6%)	19	26
2	B	4/9 (44%)	4 (100%)	0	100	100
3	C	4/9 (44%)	4 (100%)	0	100	100
All	All	442/493 (90%)	416 (94%)	26 (6%)	19	27

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	THR
1	A	287	VAL
1	A	298	ASN
1	A	320	ASN
1	A	344	GLU
1	A	385	ASP
1	A	418	LEU
1	A	424	SER
1	A	464	LEU
1	A	474	ASP
1	A	498	PHE
1	A	536	THR
1	A	550	ARG
1	A	551	VAL
1	A	569	VAL
1	A	585	LEU
1	A	604	GLU
1	A	606	ARG
1	A	628	LEU
1	A	629	LEU
1	A	648	ASN
1	A	651	THR
1	A	664	MET
1	A	678	LEU
1	A	689	SER
1	A	698	THR

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

Mol	Chain	Res	Type
1	A	260	GLN
1	A	277	HIS
1	A	298	ASN
1	A	320	ASN
1	A	395	ASN
1	A	430	ASN
1	A	522	GLN
1	A	587	ASN
1	A	596	HIS
1	A	648	ASN

### 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	$\# Z  > 2$
3	MLY	C	27	3	9,10,11	2.61	4 (44%)	6,11,13	0.45	0
2	M3L	B	4	2	10,11,12	1.14	1 (10%)	9,14,16	0.59	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
3	MLY	C	27	3	-	4/8/9/11	-
2	M3L	B	4	2	-	0/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	27	MLY	CB-CA	6.04	1.61	1.53
3	C	27	MLY	CE-NZ	2.55	1.55	1.46
3	C	27	MLY	CD-CE	2.20	1.60	1.51
2	B	4	M3L	CM3-NZ	-2.08	1.43	1.50
3	C	27	MLY	CG-CB	2.04	1.60	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	27	MLY	C-CA-CB-CG
3	C	27	MLY	CD-CE-NZ-CH2
3	C	27	MLY	CD-CE-NZ-CH1
3	C	27	MLY	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	27	MLY	2	0
2	B	4	M3L	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	OGA	A	4	4	3,9,9	3.60	2 (66%)	4,11,11	2.03	2 (50%)

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	OGA	A	4	4	-	1/3/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4	OGA	C2-N1	5.83	1.46	1.33
6	A	4	OGA	O2'-C2	-2.21	1.18	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4	OGA	C5-C4-N1	2.91	116.04	110.43
6	A	4	OGA	C1-C2-N1	2.67	118.26	115.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4	OGA	C5-C4-N1-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4	OGA	2	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	484/528 (91%)	0.28	30 (6%) 20 26	30, 49, 78, 102	0
2	B	5/15 (33%)	1.27	1 (20%) 1 1	68, 71, 85, 89	0
3	C	7/17 (41%)	1.22	1 (14%) 2 3	51, 57, 64, 74	0
All	All	496/560 (88%)	0.31	32 (6%) 18 24	30, 49, 78, 102	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	673	GLU	4.6
1	A	236	LYS	4.3
1	A	235	LYS	4.3
1	A	239	PHE	4.2
3	C	30	PRO	4.0
1	A	372	GLY	3.9
1	A	669	ARG	3.8
1	A	677	ILE	3.2
1	A	275	VAL	3.1
1	A	276	PRO	3.0
1	A	277	HIS	2.9
1	A	205	THR	2.9
1	A	668	LEU	2.8
1	A	492	THR	2.8
1	A	704	LYS	2.8
1	A	237	ASN	2.6
1	A	207	GLU	2.6
1	A	569	VAL	2.6
1	A	263	TYR	2.5
2	B	5	GLN	2.5
1	A	703	ALA	2.4
1	A	238	ASP	2.4
1	A	204	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	206	HIS	2.2
1	A	203	LYS	2.1
1	A	200	GLY	2.1
1	A	279	GLY	2.1
1	A	253	PHE	2.1
1	A	208	ASP	2.1
1	A	306	VAL	2.1
1	A	391	ILE	2.0
1	A	568	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
3	MLY	C	27	11/12	0.87	0.23	48,51,57,59	0
2	M3L	B	4	12/13	0.90	0.26	70,73,76,79	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(Å <sup>2</sup> )	Q<0.9
5	ZN	A	2	1/1	0.90	0.11	86,86,86,86	0
5	ZN	A	3	1/1	0.93	0.07	83,83,83,83	0
6	OGA	A	4	10/10	0.94	0.19	44,50,56,57	0
4	FE2	A	1	1/1	0.99	0.20	37,37,37,37	0

## 6.5 Other polymers

There are no such residues in this entry.