



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N9N  
Title : ceKDM7A from C.elegans, complex with H3K4me3K9me2 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

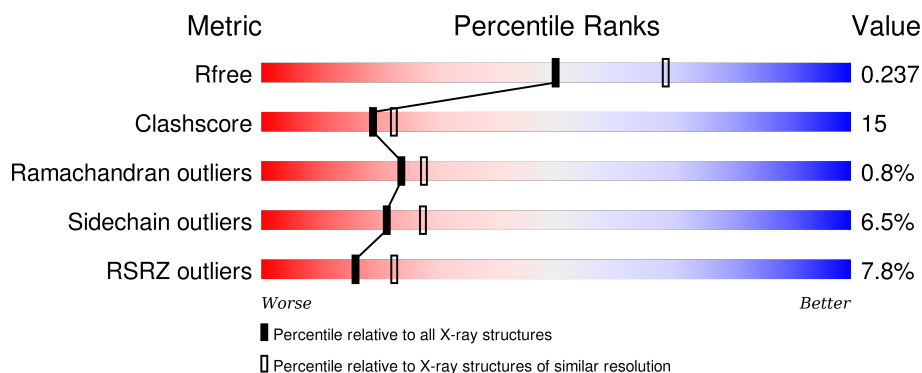
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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>7%</div> <div>66%</div> <div>24%</div> <div>8%</div> </div>
2	B	32	<div> <div>6%</div> <div>9%</div> <div>9%</div> <div>81%</div> </div>
2	C	32	<div> <div>3%</div> <div>6%</div> <div>19%</div> <div>6%</div> <div>69%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4434 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	487	Total	C	N	O	S	0	0	0
			4007	2560	673	747	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			
2	C	10	Total	C	N	O	0	0	0
			73	43	16	14			

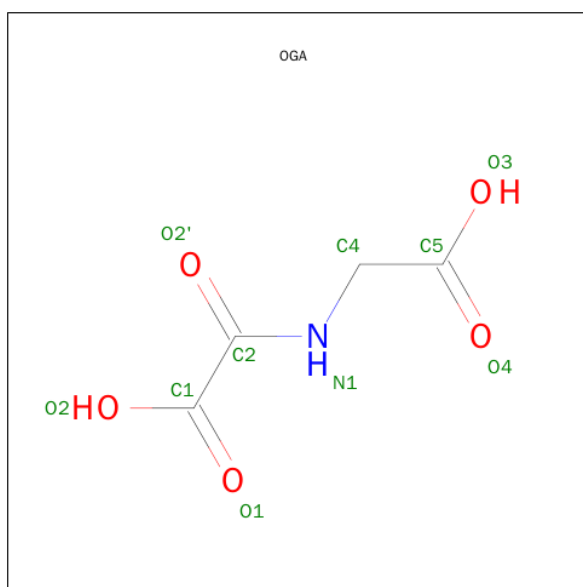
- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C<sub>4</sub>H<sub>5</sub>NO<sub>5</sub>).



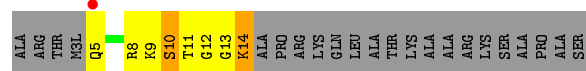
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	283	Total	O	0	0
			283	283		
6	C	7	Total	O	0	0
			7	7		



- Molecule 1: Putative uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.40 Å 85.54 Å 102.55 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.48 – 2.30 39.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (39.48-2.30) 99.9 (39.48-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.189 , 0.240 0.192 , 0.237	Depositor DCC
$R_{free}$ test set	1376 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27412 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.29	0/4111	0.48	0/5550
2	B	0.24	0/38	0.47	0/50
2	C	0.30	0/61	0.69	0/79
All	All	0.29	0/4210	0.48	0/5679

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	4007	0	3870	120	0
2	B	51	0	60	3	0
2	C	73	0	79	15	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	10	0	4	2	0
6	A	283	0	0	7	0
6	C	7	0	0	0	0
All	All	4434	0	4013	125	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 15.

All (125) 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:269:PHE:HA	1:A:270:PHE:HB2	1.22	1.14
1:A:441:ARG:HH11	1:A:441:ARG:HG3	1.16	1.08
1:A:198:CYS:SG	1:A:199:GLY:HA3	2.12	0.90
1:A:648:ASN:HD22	1:A:648:ASN:H	1.22	0.88
1:A:614:PRO:HB3	2:C:13:GLY:HA3	1.56	0.87
1:A:287:VAL:HG13	1:A:300:LYS:HE3	1.56	0.86
1:A:430:ASN:HD22	1:A:433:MET:H	1.26	0.83
1:A:269:PHE:CA	1:A:270:PHE:HB2	2.09	0.81
1:A:430:ASN:ND2	1:A:433:MET:H	1.78	0.81
1:A:441:ARG:NH1	1:A:441:ARG:HG3	1.96	0.80
1:A:676:ALA:HB1	1:A:677:ILE:HA	1.64	0.80
1:A:581:ASN:OD1	2:C:9:MLY:HH12	1.82	0.80
1:A:657:LYS:HD2	1:A:694:ILE:HD12	1.63	0.79
1:A:497:ASP:OD1	2:C:9:MLY:HH13	1.85	0.76
1:A:648:ASN:HD22	1:A:648:ASN:N	1.83	0.75
1:A:269:PHE:HA	1:A:270:PHE:CB	2.11	0.74
1:A:319:GLU:O	1:A:322:VAL:HG12	1.88	0.73
6:A:821:HOH:O	2:C:8:ARG:HG2	1.90	0.71
1:A:200:GLY:HA3	1:A:202:GLY:H	1.55	0.71
1:A:657:LYS:HD2	1:A:694:ILE:CD1	2.22	0.70
1:A:625:ARG:HD2	1:A:626:ASN:OD1	1.91	0.69
1:A:665:ASP:O	1:A:669:ARG:HG3	1.92	0.69
1:A:694:ILE:O	1:A:698:THR:HG23	1.93	0.69
1:A:285:LYS:N	1:A:285:LYS:HD2	2.09	0.68
1:A:322:VAL:HG13	1:A:550:ARG:HB2	1.74	0.68
1:A:459:ALA:O	1:A:463:LYS:HG3	1.94	0.67
1:A:197:ARG:HG2	1:A:198:CYS:O	1.93	0.67
1:A:589:GLU:HG2	1:A:655:ILE:HD13	1.76	0.67
1:A:292:TYR:OH	1:A:306:VAL:O	2.08	0.66
1:A:238:ASP:HB3	1:A:240:GLN:HG3	1.78	0.65
1:A:253:PHE:HD2	1:A:263:TYR:CE1	2.13	0.65
1:A:319:GLU:OE1	1:A:550:ARG:HD2	1.97	0.64
1:A:237:ASN:ND2	1:A:254:LEU:H	1.96	0.63
1:A:589:GLU:HG3	6:A:801:HOH:O	1.98	0.63
1:A:593:ARG:NH2	6:A:78:HOH:O	2.32	0.62
1:A:507:ILE:HG13	1:A:553:ILE:HG22	1.81	0.61
1:A:198:CYS:O	1:A:202:GLY:HA2	1.99	0.61
1:A:379:VAL:HG11	1:A:407:ARG:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG13	1:A:550:ARG:HD3	1.80	0.61
1:A:305:GLU:OE2	1:A:536:THR:HG21	2.01	0.60
1:A:266:TYR:HA	1:A:283:ARG:HA	1.83	0.59
1:A:203:LYS:HG3	6:A:816:HOH:O	2.02	0.58
1:A:396:GLN:O	2:C:5:GLN:HB3	2.04	0.57
1:A:441:ARG:HH11	1:A:441:ARG:CG	2.01	0.57
1:A:643:ARG:HD2	1:A:701:GLN:CD	2.25	0.57
1:A:648:ASN:ND2	1:A:648:ASN:H	1.98	0.57
1:A:648:ASN:ND2	1:A:648:ASN:N	2.54	0.56
1:A:285:LYS:HD2	1:A:285:LYS:H	1.70	0.56
1:A:563:ALA:H	1:A:587:ASN:ND2	2.03	0.56
2:C:11:THR:OG1	2:C:12:GLY:N	2.38	0.56
1:A:253:PHE:HD2	1:A:263:TYR:CZ	2.24	0.56
1:A:638:GLU:O	1:A:639:GLY:C	2.44	0.56
1:A:200:GLY:CA	1:A:201:CYS:HB3	2.37	0.55
1:A:201:CYS:HB2	1:A:255:CYS:SG	2.46	0.55
1:A:361:MET:HG2	6:A:39:HOH:O	2.07	0.55
1:A:369:PRO:HG3	1:A:436:ILE:HG22	1.89	0.54
1:A:431:ASN:HA	1:A:434:LYS:HE3	1.90	0.54
1:A:237:ASN:HD22	1:A:254:LEU:H	1.55	0.54
1:A:315:PHE:O	1:A:319:GLU:HB2	2.09	0.53
1:A:206:HIS:CE1	1:A:207:GLU:HG2	2.44	0.53
1:A:641:ASP:O	1:A:644:GLU:HG2	2.09	0.52
1:A:200:GLY:HA2	1:A:201:CYS:HB3	1.91	0.52
1:A:641:ASP:OD1	1:A:643:ARG:HD3	2.10	0.52
1:A:479:VAL:HG12	2:C:11:THR:HG21	1.91	0.51
1:A:645:GLN:O	1:A:646:GLU:HG3	2.11	0.51
1:A:287:VAL:CG1	1:A:300:LYS:HE3	2.34	0.51
1:A:377:ASP:OD1	1:A:377:ASP:N	2.44	0.51
1:A:239:PHE:HE1	6:A:800:HOH:O	1.93	0.50
1:A:614:PRO:HG3	2:C:11:THR:OG1	2.12	0.50
1:A:664:MET:HA	1:A:664:MET:CE	2.42	0.50
1:A:614:PRO:HB3	2:C:13:GLY:CA	2.37	0.49
1:A:676:ALA:CB	1:A:677:ILE:HA	2.31	0.49
1:A:676:ALA:HB1	1:A:677:ILE:CA	2.38	0.49
1:A:531:GLU:HG2	1:A:601:ILE:HD13	1.93	0.49
1:A:335:ASP:HA	1:A:360:ASP:O	2.13	0.48
1:A:244:CYS:HA	1:A:269:PHE:O	2.13	0.48
1:A:283:ARG:HH22	1:A:418:LEU:HD22	1.79	0.48
1:A:237:ASN:HB2	1:A:254:LEU:HD12	1.95	0.48
1:A:484:LEU:HD12	1:A:484:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ILE:N	1:A:553:ILE:HD12	2.29	0.47
1:A:619:LEU:C	1:A:619:LEU:HD23	2.35	0.47
1:A:239:PHE:O	2:B:5:GLN:HA	2.14	0.47
1:A:569:VAL:CG1	5:A:4:OGA:H4C2	2.45	0.46
1:A:474:ASP:O	2:C:14:LYS:HB3	2.15	0.46
1:A:494:PHE:CD1	1:A:540:PHE:HB3	2.51	0.46
1:A:478:LYS:HB3	1:A:478:LYS:HE2	1.65	0.46
1:A:199:GLY:N	1:A:200:GLY:HA3	2.31	0.45
1:A:569:VAL:HG13	5:A:4:OGA:H4C2	1.98	0.45
1:A:412:ASP:OD2	1:A:415:ASN:HB3	2.16	0.45
1:A:287:VAL:HG11	1:A:297:PRO:HA	1.98	0.44
1:A:673:GLU:H	1:A:673:GLU:CD	2.20	0.44
1:A:497:ASP:OD1	2:C:9:MLY:CH1	2.60	0.44
1:A:441:ARG:NH1	1:A:441:ARG:CG	2.67	0.44
1:A:240:GLN:HB3	1:A:253:PHE:CD1	2.52	0.44
1:A:559:LEU:HD23	1:A:561:ILE:HD11	1.99	0.44
1:A:238:ASP:CG	1:A:239:PHE:H	2.20	0.44
1:A:561:ILE:HA	1:A:562:PRO:HD3	1.89	0.44
1:A:676:ALA:HB1	1:A:677:ILE:HG12	2.00	0.43
1:A:639:GLY:CA	1:A:640:SER:HB2	2.48	0.43
1:A:241:TRP:CZ2	1:A:252:HIS:NE2	2.86	0.43
1:A:374:ASP:OD2	1:A:376:GLU:HG2	2.19	0.43
1:A:588:LEU:HD21	1:A:656:MET:HB2	2.01	0.43
1:A:602:ARG:HD3	1:A:612:TYR:CE1	2.54	0.42
1:A:198:CYS:O	1:A:202:GLY:CA	2.64	0.42
1:A:465:LEU:HD23	1:A:470:TYR:HB2	2.00	0.42
1:A:679:PRO:HD2	1:A:682:ASP:OD1	2.20	0.42
2:C:13:GLY:HA2	2:C:14:LYS:HA	1.72	0.42
1:A:424:SER:HB3	2:C:10:SER:O	2.19	0.42
2:C:9:MLY:HD3	2:C:9:MLY:HH13	1.78	0.42
1:A:370:LYS:HE2	1:A:370:LYS:HB2	1.86	0.42
1:A:541:GLY:HA2	1:A:548:VAL:HG21	2.02	0.41
1:A:271:CYS:HB2	1:A:272:PRO:HD2	2.02	0.41
1:A:515:TYR:O	1:A:567:HIS:HA	2.20	0.41
1:A:664:MET:HG3	1:A:687:MET:HG3	2.02	0.41
1:A:241:TRP:HB2	2:B:4:M3L:HG2	2.03	0.41
2:C:12:GLY:O	2:C:14:LYS:HA	2.20	0.41
1:A:312:ILE:O	1:A:316:ILE:HG13	2.21	0.41
1:A:322:VAL:CG1	1:A:550:ARG:HB2	2.49	0.41
1:A:206:HIS:ND1	1:A:207:GLU:HG2	2.36	0.41
1:A:676:ALA:HB1	1:A:677:ILE:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:CG1	1:A:550:ARG:HD3	2.46	0.41
1:A:624:MET:O	1:A:629:LEU:HB2	2.21	0.41
1:A:403:LEU:HA	1:A:403:LEU:HD12	1.89	0.41
1:A:244:CYS:O	2:B:2:ARG:NH2	2.55	0.40
1:A:345:LYS:HE2	6:A:807: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	483/528 (92%)	452 (94%)	27 (6%)	4 (1%)	24	27
2	B	3/32 (9%)	3 (100%)	0	0	100	100
2	C	7/32 (22%)	4 (57%)	3 (43%)	0	100	100
All	All	493/592 (83%)	459 (93%)	30 (6%)	4 (1%)	24	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PHE
1	A	639	GLY
1	A	673	GLU
1	A	479	VAL

### 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	436/475 (92%)	409 (94%)	27 (6%)	23	30
2	B	4/20 (20%)	4 (100%)	0	100	100
2	C	6/20 (30%)	4 (67%)	2 (33%)	0	0
All	All	446/515 (87%)	417 (94%)	29 (6%)	21	27

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LYS
1	A	273	LYS
1	A	278	THR
1	A	313	GLU
1	A	320	ASN
1	A	330	VAL
1	A	344	GLU
1	A	355	VAL
1	A	377	ASP
1	A	379	VAL
1	A	388	VAL
1	A	414	LYS
1	A	418	LEU
1	A	433	MET
1	A	441	ARG
1	A	442	PHE
1	A	464	LEU
1	A	497	ASP
1	A	498	PHE
1	A	551	VAL
1	A	569	VAL
1	A	585	LEU
1	A	628	LEU
1	A	629	LEU
1	A	648	ASN
1	A	664	MET
1	A	665	ASP
2	C	10	SER
2	C	14	LYS

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	237	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
1	A	684	ASN
2	C	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	1.79	1 (10%)	12,14,16	2.53	3 (25%)
2	MLY	C	9	2	9,10,11	0.36	0	9,11,13	1.36	1 (11%)

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	-	0/8/10/12	0/0/0/0
2	MLY	C	9	2	-	0/7/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	M3L	CB-CA	-5.08	1.48	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	M3L	CM3-NZ-CM2	-2.98	101.32	108.98
2	B	4	M3L	CM3-NZ-CM1	-2.92	101.46	108.98
2	C	9	MLY	CB-CA-N	2.68	118.13	110.52
2	B	4	M3L	CM2-NZ-CM1	7.01	127.01	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	M3L	1	0
2	C	9	MLY	4	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	$\# Z  > 2$
5	OGA	A	4	3	3,9,9	3.88	1 (33%)	3,11,11	0.94	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
5	OGA	A	4	3	-	0/3/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4	OGA	C2-N1	6.38	1.47	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	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	487/528 (92%)	0.14	36 (7%) 17 25	21, 41, 78, 111	0
2	B	5/32 (15%)	1.77	2 (40%) 0 0	62, 65, 82, 96	0
2	C	9/32 (28%)	0.80	1 (11%) 7 11	40, 47, 62, 68	0
All	All	501/592 (84%)	0.17	39 (7%) 16 22	21, 42, 78, 111	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	VAL	6.5
1	A	703	ALA	5.2
1	A	675	ASN	4.7
1	A	674	LYS	4.6
1	A	272	PRO	4.0
1	A	273	LYS	3.9
1	A	276	PRO	3.9
1	A	253	PHE	3.9
1	A	280	HIS	3.9
1	A	277	HIS	3.8
1	A	239	PHE	3.7
1	A	279	GLY	3.2
1	A	606	ARG	3.1
1	A	204	PHE	2.9
1	A	254	LEU	2.9
2	B	5	GLN	2.9
1	A	200	GLY	2.9
1	A	270	PHE	2.9
1	A	676	ALA	2.8
2	C	5	GLN	2.7
1	A	205	THR	2.7
1	A	192	PRO	2.7
1	A	251	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	206	HIS	2.6
1	A	263	TYR	2.6
1	A	269	PHE	2.5
1	A	207	GLU	2.5
1	A	673	GLU	2.5
1	A	250	TRP	2.4
1	A	492	THR	2.4
2	B	1	ALA	2.3
1	A	202	GLY	2.3
1	A	208	ASP	2.2
1	A	372	GLY	2.2
1	A	203	LYS	2.2
1	A	391	ILE	2.1
1	A	639	GLY	2.0
1	A	568	ALA	2.0
1	A	371	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MLY	C	9	11/12	0.92	0.25	-	31,38,46,62	0
2	M3L	B	4	12/13	0.90	0.25	-	65,72,76,78	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	OGA	A	4	10/10	0.96	0.19	0.11	29,35,39,39	0
4	ZN	A	3	1/1	0.94	0.05	-1.54	72,72,72,72	0
4	ZN	A	2	1/1	0.97	0.05	-2.67	57,57,57,57	0
3	FE2	A	1	1/1	0.99	0.19	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.