



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N9P
Title : ceKDM7A from C.elegans, complex with H3K4me3K27me2 peptide and NOG
Authors : Yang, Y.; Hu, L.; Wang, P.; Hou, H.; Chen, C.D.; Xu, Y.
Deposited on : 2010-05-31
Resolution : 2.39 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

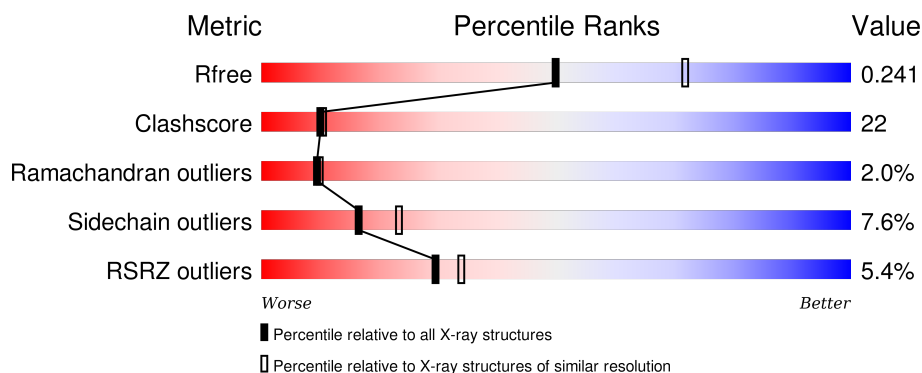
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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 ≥ 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>5%</div> <div>55%</div> <div>33%</div> <div>8%</div> </div>
2	B	32	<div> <div>3%</div> <div>16%</div> <div>81%</div> </div>
2	C	32	<div> <div>3%</div> <div>9%</div> <div>22%</div> <div>69%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4273 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
			70	43	15	12			

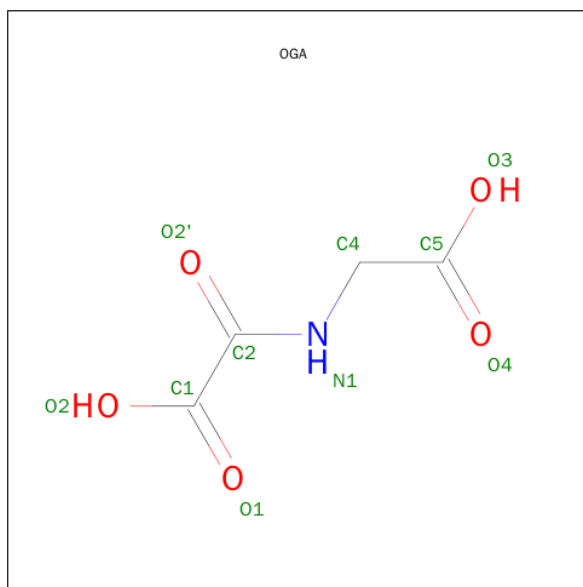
- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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: C₄H₅NO₅).



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	125	Total	O	0	0
			125	125		
6	C	7	Total	O	0	0
			7	7		

ALA	ARG	THR	VAL	GLN	THR	ALA	ARG	LYS	SER	THR	GLY	GLY	LYS	ALA	PRO	ARG	LYS	GLN	LEU	ALA	THR	K23	K27	S28	A29	P30	A31	S32
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.11Å 86.37Å 62.74Å 90.00° 113.18° 90.00°	Depositor
Resolution (Å)	31.48 – 2.39 46.55 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.1 (31.48-2.39) 99.2 (46.55-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.200 , 0.242 0.199 , 0.241	Depositor DCC
R_{free} test set	1199 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.8	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23317 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4273	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/4111	0.56	1/5550 (0.0%)
2	B	0.34	0/38	0.54	0/50
2	C	0.36	0/59	0.71	0/78
All	All	0.39	0/4208	0.57	1/5678 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	CYS	CB-CA-C	-6.58	97.25	110.40

There are no chirality outliers.

There are no planarity outliers.

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	4007	0	3870	174	0
2	B	51	0	60	1	0
2	C	70	0	78	11	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	10	0	4	2	0
6	A	125	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	7	0	0	0	0
All	All	4273	0	4012	179	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 22.

All (179) 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	1.25	1.16
1:A:240:GLN:HB3	1:A:253:PHE:CD1	1.88	1.07
1:A:240:GLN:HB3	1:A:253:PHE:HD1	1.20	1.04
1:A:305:GLU:OE2	1:A:536:THR:HG21	1.62	0.99
1:A:441:ARG:HH11	1:A:441:ARG:HG3	1.27	0.97
1:A:676:ALA:HB1	1:A:677:ILE:HA	1.46	0.96
1:A:241:TRP:HB2	2:B:4:M3L:HG3	1.49	0.95
1:A:384:SER:HB3	1:A:404:ASP:HB2	1.55	0.89
1:A:319:GLU:HG3	1:A:515:TYR:OH	1.73	0.88
1:A:198:CYS:SG	1:A:199:GLY:HA3	2.14	0.87
1:A:648:ASN:HD22	1:A:648:ASN:H	1.21	0.86
1:A:591:GLN:OE1	6:A:712:HOH:O	1.92	0.85
1:A:571:THR:HB	6:A:114:HOH:O	1.76	0.84
1:A:405:THR:HA	1:A:408:LYS:HE2	1.62	0.81
1:A:275:VAL:HA	1:A:278:THR:HG22	1.66	0.77
1:A:648:ASN:HD22	1:A:648:ASN:N	1.83	0.77
1:A:269:PHE:CA	1:A:270:PHE:HB2	2.12	0.74
1:A:201:CYS:O	1:A:203:LYS:HG3	1.88	0.73
1:A:376:GLU:O	1:A:380:LYS:HD3	1.87	0.73
1:A:430:ASN:ND2	1:A:433:MET:H	1.89	0.71
1:A:322:VAL:HG22	1:A:550:ARG:HB2	1.72	0.71
1:A:365:ASN:O	6:A:19:HOH:O	2.09	0.70
1:A:426:GLU:OE1	1:A:478:LYS:HE3	1.92	0.70
1:A:361:MET:HG2	6:A:24:HOH:O	1.92	0.70
1:A:581:ASN:OD1	2:C:27:MLY:HH23	1.93	0.69
1:A:608:GLU:OE1	6:A:124:HOH:O	2.10	0.68
1:A:430:ASN:HD22	1:A:433:MET:H	1.39	0.67
1:A:274:CYS:HA	1:A:277:HIS:CE1	2.30	0.66
1:A:507:ILE:HG13	1:A:553:ILE:HG22	1.77	0.66
1:A:589:GLU:HG3	6:A:106:HOH:O	1.96	0.66
1:A:665:ASP:OD2	1:A:669:ARG:HD2	1.94	0.66
1:A:298:ASN:H	1:A:298:ASN:HD22	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLU:CD	1:A:673:GLU:H	1.99	0.66
1:A:681:ASP:O	1:A:685:LYS:HG3	1.97	0.64
1:A:240:GLN:CB	1:A:253:PHE:HD1	2.04	0.64
1:A:488:ALA:HB3	6:A:107:HOH:O	1.96	0.64
1:A:269:PHE:HA	1:A:270:PHE:CB	2.15	0.64
1:A:198:CYS:O	1:A:202:GLY:HA2	1.98	0.63
1:A:262:GLU:HA	1:A:265:LEU:HD12	1.80	0.63
1:A:432:GLU:OE1	6:A:66:HOH:O	2.14	0.63
1:A:369:PRO:HG3	1:A:436:ILE:HG22	1.79	0.63
1:A:593:ARG:NH2	6:A:38:HOH:O	2.31	0.63
1:A:197:ARG:HG2	1:A:198:CYS:O	1.98	0.63
1:A:602:ARG:HD3	6:A:104:HOH:O	1.98	0.62
1:A:589:GLU:HG2	1:A:655:ILE:HD13	1.81	0.62
1:A:648:ASN:ND2	1:A:648:ASN:N	2.47	0.62
1:A:201:CYS:O	1:A:203:LYS:N	2.34	0.61
1:A:495:HIS:HA	1:A:527:TYR:OH	2.00	0.61
1:A:511:GLU:O	1:A:572:PRO:HD2	2.00	0.61
1:A:200:GLY:CA	1:A:201:CYS:HB3	2.30	0.61
1:A:373:PHE:HZ	1:A:433:MET:HE1	1.65	0.61
1:A:240:GLN:HB3	1:A:253:PHE:CE1	2.33	0.61
1:A:623:TYR:OH	6:A:10:HOH:O	1.87	0.61
1:A:686:ILE:O	1:A:690:VAL:HG23	2.02	0.60
1:A:447:SER:O	6:A:11:HOH:O	2.16	0.59
1:A:350:ASP:O	6:A:102:HOH:O	2.17	0.59
1:A:292:TYR:CD1	2:C:23:LYS:HD2	2.38	0.58
1:A:266:TYR:HA	1:A:283:ARG:HA	1.84	0.58
2:C:30:PRO:C	2:C:32:SER:HA	2.24	0.58
1:A:607:SER:HB3	6:A:104:HOH:O	2.02	0.58
2:C:30:PRO:O	2:C:32:SER:HA	2.04	0.58
1:A:319:GLU:OE1	1:A:550:ARG:HD2	2.03	0.57
1:A:287:VAL:HG11	1:A:297:PRO:HA	1.85	0.57
1:A:366:MET:HA	6:A:19:HOH:O	2.03	0.57
1:A:292:TYR:OH	1:A:306:VAL:O	2.12	0.57
1:A:461:TYR:CE2	1:A:465:LEU:HD11	2.40	0.56
1:A:319:GLU:OE1	1:A:550:ARG:NH1	2.30	0.56
1:A:441:ARG:NH1	1:A:441:ARG:HG3	2.05	0.56
1:A:417:PRO:HD2	6:A:54:HOH:O	2.04	0.55
1:A:639:GLY:N	1:A:640:SER:HB2	2.21	0.55
1:A:201:CYS:SG	1:A:201:CYS:O	2.64	0.55
1:A:274:CYS:HA	1:A:277:HIS:NE2	2.22	0.55
1:A:624:MET:O	1:A:629:LEU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:HB2	1:A:273:LYS:NZ	2.21	0.55
1:A:395:ASN:HD22	1:A:397:SER:HB2	1.72	0.55
1:A:467:ARG:NH1	1:A:469:GLU:OE1	2.41	0.54
1:A:624:MET:CE	1:A:628:LEU:HB3	2.37	0.53
1:A:200:GLY:HA2	1:A:201:CYS:HB3	1.89	0.53
1:A:467:ARG:C	1:A:469:GLU:H	2.12	0.53
1:A:641:ASP:OD1	1:A:643:ARG:HD3	2.08	0.53
1:A:268:LYS:HB2	1:A:282:ILE:HB	1.91	0.53
1:A:461:TYR:HE2	1:A:465:LEU:HD11	1.73	0.53
1:A:404:ASP:O	1:A:408:LYS:HG3	2.09	0.52
1:A:497:ASP:OD1	2:C:27:MLY:HH11	2.09	0.52
1:A:694:ILE:O	1:A:698:THR:HG23	2.10	0.52
1:A:253:PHE:CD2	1:A:263:TYR:CE1	2.98	0.51
2:C:31:ALA:N	2:C:32:SER:HA	2.23	0.51
1:A:244:CYS:O	1:A:248:GLN:HA	2.11	0.51
1:A:359:LYS:HG2	1:A:557:GLN:NE2	2.26	0.51
1:A:643:ARG:HD2	1:A:701:GLN:NE2	2.25	0.51
1:A:625:ARG:HD2	1:A:626:ASN:OD1	2.11	0.51
1:A:376:GLU:OE2	1:A:411:ARG:HD3	2.11	0.50
1:A:430:ASN:HD22	1:A:433:MET:N	2.08	0.50
1:A:247:CYS:HB3	1:A:274:CYS:SG	2.51	0.49
1:A:623:TYR:HD1	1:A:628:LEU:HD22	1.77	0.49
1:A:488:ALA:O	6:A:107:HOH:O	2.20	0.49
1:A:424:SER:HB3	2:C:28:SER:O	2.13	0.49
1:A:273:LYS:HE3	1:A:273:LYS:N	2.28	0.48
1:A:395:ASN:ND2	1:A:397:SER:HB2	2.27	0.48
1:A:441:ARG:HH11	1:A:441:ARG:CG	2.11	0.48
1:A:298:ASN:HD22	1:A:298:ASN:N	2.11	0.48
1:A:252:HIS:HB2	1:A:255:CYS:SG	2.54	0.48
1:A:200:GLY:HA3	1:A:202:GLY:H	1.78	0.48
1:A:352:TRP:NE1	1:A:562:PRO:HG3	2.29	0.48
1:A:697:GLN:O	1:A:701:GLN:HG3	2.14	0.48
1:A:487:MET:C	6:A:114:HOH:O	2.52	0.47
1:A:503:VAL:HG13	2:C:27:MLY:HH21	1.96	0.47
1:A:519:PRO:HB3	1:A:564:GLY:HA3	1.97	0.47
1:A:536:THR:HG23	1:A:536:THR:O	2.14	0.47
1:A:639:GLY:CA	1:A:640:SER:HB2	2.45	0.47
1:A:198:CYS:SG	1:A:200:GLY:HA2	2.54	0.47
1:A:427:PHE:CD1	1:A:433:MET:HB3	2.50	0.47
1:A:237:ASN:O	1:A:240:GLN:HB2	2.15	0.47
1:A:650:TRP:CZ3	1:A:697:GLN:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:HB3	1:A:263:TYR:OH	2.14	0.47
1:A:664:MET:HG3	1:A:687:MET:HG3	1.97	0.46
1:A:253:PHE:CD2	1:A:263:TYR:CZ	3.04	0.46
1:A:613:PHE:HA	1:A:614:PRO:HD3	1.80	0.46
1:A:337:TYR:HE2	1:A:362:ASP:OD2	1.99	0.46
1:A:335:ASP:HA	1:A:360:ASP:O	2.16	0.46
1:A:569:VAL:HG13	5:A:4:OGA:H4C2	1.98	0.46
1:A:206:HIS:O	1:A:207:GLU:C	2.54	0.46
1:A:238:ASP:OD2	1:A:239:PHE:N	2.48	0.46
1:A:298:ASN:N	1:A:298:ASN:ND2	2.64	0.46
1:A:512:LYS:HD3	1:A:571:THR:HG23	1.98	0.46
6:A:5:HOH:O	2:C:27:MLY:HH13	2.15	0.46
1:A:506:HIS:O	1:A:577:VAL:HG13	2.16	0.45
1:A:648:ASN:ND2	1:A:648:ASN:H	1.97	0.45
1:A:309:LYS:O	1:A:313:GLU:HB2	2.16	0.45
1:A:563:ALA:H	1:A:587:ASN:ND2	2.15	0.45
1:A:505:TYR:OH	1:A:512:LYS:HE3	2.16	0.45
1:A:478:LYS:HE2	1:A:478:LYS:HB3	1.71	0.45
1:A:624:MET:HE1	1:A:628:LEU:HB3	1.99	0.45
1:A:200:GLY:CA	1:A:201:CYS:CB	2.94	0.45
1:A:571:THR:CG2	6:A:114:HOH:O	2.65	0.44
1:A:541:GLY:HA2	1:A:548:VAL:HG21	2.00	0.44
1:A:305:GLU:OE2	1:A:536:THR:CG2	2.51	0.44
1:A:487:MET:O	6:A:114:HOH:O	2.21	0.44
1:A:394:TYR:HD2	1:A:418:LEU:HD12	1.81	0.44
1:A:270:PHE:CD1	1:A:281:SER:HA	2.52	0.44
1:A:624:MET:HE3	1:A:628:LEU:HB3	1.99	0.44
1:A:201:CYS:O	1:A:202:GLY:C	2.56	0.44
1:A:208:ASP:OD1	1:A:208:ASP:N	2.48	0.44
1:A:464:LEU:O	1:A:467:ARG:O	2.35	0.44
1:A:404:ASP:OD1	1:A:407:ARG:NH2	2.51	0.43
1:A:452:LEU:C	1:A:454:PRO:HD3	2.39	0.43
1:A:676:ALA:CB	1:A:677:ILE:HA	2.24	0.43
1:A:569:VAL:CG1	5:A:4:OGA:H4C2	2.48	0.43
1:A:484:LEU:HD12	1:A:484:LEU:N	2.33	0.43
1:A:614:PRO:HG3	2:C:29:ALA:O	2.18	0.43
1:A:656:MET:O	1:A:660:MET:HG3	2.19	0.43
1:A:641:ASP:OD1	1:A:643:ARG:CD	2.67	0.42
1:A:237:ASN:O	1:A:238:ASP:HB3	2.20	0.42
1:A:553:ILE:N	1:A:553:ILE:HD12	2.34	0.42
1:A:596:HIS:CE1	1:A:659:GLU:OE2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLU:CD	1:A:673:GLU:N	2.71	0.42
1:A:361:MET:CE	1:A:366:MET:O	2.68	0.42
1:A:271:CYS:HB2	1:A:272:PRO:HD2	2.01	0.42
1:A:296:SER:HA	1:A:297:PRO:HD3	1.75	0.42
1:A:671:GLY:HA2	1:A:672:PRO:HD3	1.76	0.42
1:A:596:HIS:HE1	1:A:659:GLU:OE2	2.02	0.42
1:A:309:LYS:HD2	1:A:394:TYR:CE2	2.55	0.42
1:A:361:MET:HE3	1:A:366:MET:O	2.20	0.41
1:A:283:ARG:NH2	1:A:418:LEU:HD22	2.35	0.41
1:A:468:GLU:O	6:A:88:HOH:O	2.22	0.41
1:A:379:VAL:HG11	1:A:407:ARG:HD3	2.02	0.41
1:A:239:PHE:CD1	1:A:239:PHE:N	2.87	0.41
1:A:288:ALA:O	1:A:294:TRP:HA	2.20	0.41
1:A:691:ARG:O	1:A:695:GLU:HB2	2.20	0.41
1:A:241:TRP:CZ2	1:A:252:HIS:NE2	2.89	0.41
1:A:366:MET:HG3	1:A:438:LYS:O	2.20	0.41
1:A:573:VAL:O	1:A:574:ASP:C	2.60	0.41
1:A:237:ASN:OD1	1:A:254:LEU:HG	2.22	0.40
1:A:539:TRP:CE3	1:A:541:GLY:HA3	2.56	0.40
2:C:27:MLY:HH12	2:C:27:MLY:HD3	1.67	0.40
1:A:464:LEU:HD11	1:A:470:TYR:HA	2.03	0.40
1:A:516:ILE:O	1:A:548:VAL:HA	2.21	0.40
1:A:322:VAL:HG23	1:A:323:PRO:HD2	2.02	0.40
1:A:533:SER:HA	1:A:534:PRO:HD3	1.90	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%)	443 (92%)	30 (6%)	10 (2%)	9 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	450 (91%)	33 (7%)	10 (2%)	9	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PHE
1	A	674	LYS
1	A	202	GLY
1	A	207	GLU
1	A	638	GLU
1	A	639	GLY
1	A	673	GLU
1	A	670	LEU
1	A	479	VAL
1	A	286	VAL

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	436/475 (92%)	402 (92%)	34 (8%)	16	22
2	B	4/20 (20%)	4 (100%)	0	100	100
2	C	5/20 (25%)	5 (100%)	0	100	100
All	All	445/515 (86%)	411 (92%)	34 (8%)	16	23

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	208	ASP
1	A	236	LYS
1	A	253	PHE

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Mol	Chain	Res	Type
1	A	273	LYS
1	A	298	ASN
1	A	313	GLU
1	A	319	GLU
1	A	322	VAL
1	A	330	VAL
1	A	355	VAL
1	A	377	ASP
1	A	379	VAL
1	A	400	SER
1	A	402	LYS
1	A	414	LYS
1	A	418	LEU
1	A	434	LYS
1	A	441	ARG
1	A	456	VAL
1	A	474	ASP
1	A	498	PHE
1	A	531	GLU
1	A	536	THR
1	A	551	VAL
1	A	569	VAL
1	A	571	THR
1	A	585	LEU
1	A	604	GLU
1	A	628	LEU
1	A	629	LEU
1	A	648	ASN
1	A	651	THR
1	A	664	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	HIS
1	A	298	ASN
1	A	395	ASN
1	A	430	ASN
1	A	596	HIS
1	A	648	ASN
1	A	701	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	1.15	1 (10%)	12,14,16	0.72	0
2	MLY	C	27	2	9,10,11	2.99	2 (22%)	9,11,13	0.97	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	27	2	-	0/7/9/11	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	M3L	CM3-NZ	-2.03	1.44	1.50
2	C	27	MLY	CE-NZ	2.08	1.54	1.46
2	C	27	MLY	CB-CA	7.86	1.61	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	27	MLY	CB-CA-N	2.27	116.97	110.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	M3L	1	0
2	C	27	MLY	5	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	3.58	2 (66%)	3,11,11	1.40	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4	OGA	O2'-C2	-2.38	1.18	1.23
5	A	4	OGA	C2-N1	5.72	1.46	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, 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	487/528 (92%)	0.36	25 (5%) 32 36	41, 62, 97, 122	0
2	B	5/32 (15%)	1.04	1 (20%) 1 1	85, 88, 95, 96	0
2	C	9/32 (28%)	0.88	1 (11%) 7 8	53, 60, 75, 82	0
All	All	501/592 (84%)	0.38	27 (5%) 29 34	41, 62, 97, 122	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	LYS	4.8
1	A	645	GLN	4.7
1	A	269	PHE	4.5
1	A	265	LEU	4.5
1	A	703	ALA	4.3
1	A	273	LYS	4.2
1	A	276	PRO	3.8
1	A	275	VAL	3.6
1	A	272	PRO	3.5
2	C	23	LYS	3.5
1	A	263	TYR	3.4
1	A	675	ASN	3.2
1	A	253	PHE	3.0
1	A	270	PHE	2.9
1	A	332	ILE	2.9
1	A	236	LYS	2.8
1	A	205	THR	2.7
1	A	282	ILE	2.7
1	A	287	VAL	2.6
1	A	704	LYS	2.6
1	A	250	TRP	2.6
2	B	1	ALA	2.3
1	A	279	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	235	LYS	2.1
1	A	606	ARG	2.1
1	A	441	ARG	2.1
1	A	344	GLU	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	MLY	C	27	11/12	0.93	0.22	-	50,55,60,62	0
2	M3L	B	4	12/13	0.89	0.18	-	79,88,93,93	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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	OGA	A	4	10/10	0.96	0.17	0.56	47,52,61,62	0
4	ZN	A	2	1/1	0.97	0.13	-0.38	78,78,78,78	0
4	ZN	A	3	1/1	0.93	0.05	-0.99	108,108,108,108	0
3	FE2	A	1	1/1	0.99	0.19	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.