



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:52 am GMT

PDB ID : 4QXC  
Title : Crystal structure of histone demethylase KDM2A-H3K36ME2 with NOG  
Authors : Cheng, Z.J.; Patel, D.J.  
Deposited on : 2014-07-19  
Resolution : 1.75 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

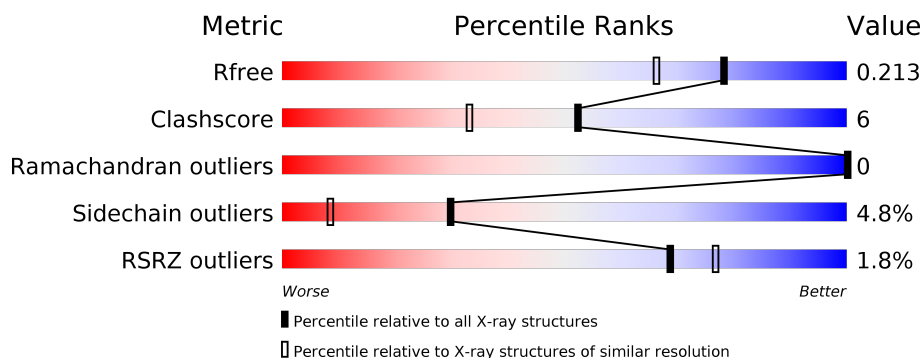
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (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. 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	329	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>
1	C	329	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>•</div> </div>
2	B	68	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
2	D	68	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>
3	E	15	<div> <div>73%</div> <div>7%</div> <div>7%</div> <div>13%</div> </div>
3	F	15	<div> <div>7%</div> <div>53%</div> <div>7%</div> <div>40%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7200 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 Lysine-specific demethylase 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	1	0
			2748	1761	458	508	21			
1	C	329	Total	C	N	O	S	0	2	0
			2757	1766	462	508	21			

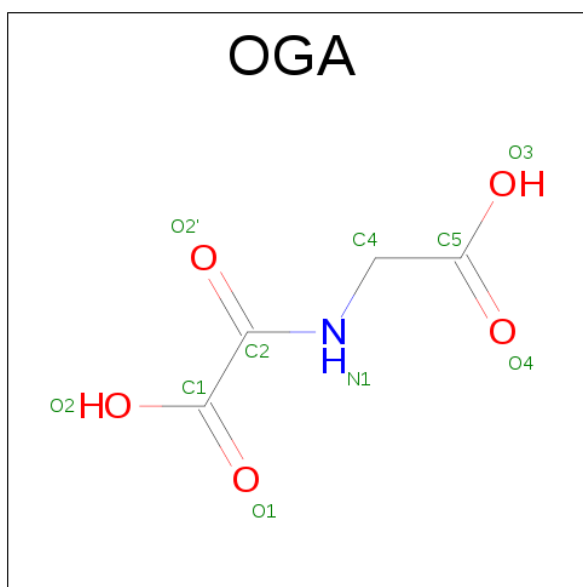
- Molecule 2 is a protein called Lysine-specific demethylase 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	68	Total	C	N	O	S	0	0	0
			528	341	85	100	2			
2	D	68	Total	C	N	O	S	0	2	0
			536	346	85	102	3			

- Molecule 3 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	0	0	0
			99	64	20	15			
3	F	9	Total	C	N	O	0	0	0
			64	41	13	10			

- Molecule 4 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
4	A	1	Total	C	N	O	0	0
			10	4	1	5		
4	C	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ni	0	0
			1	1		
5	C	1	Total	Ni	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total	O	0	0
			208	208		
6	B	42	Total	O	0	0
			42	42		
6	C	162	Total	O	0	0
			162	162		
6	D	22	Total	O	0	0
			22	22		
6	E	8	Total	O	0	0
			8	8		

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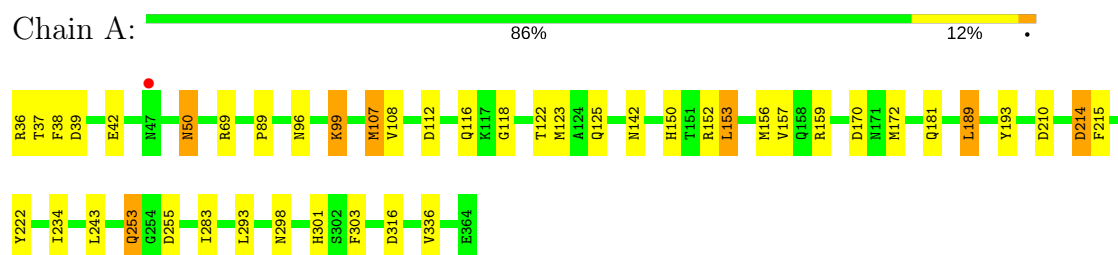
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	4	Total	O	0	0
			4	4		

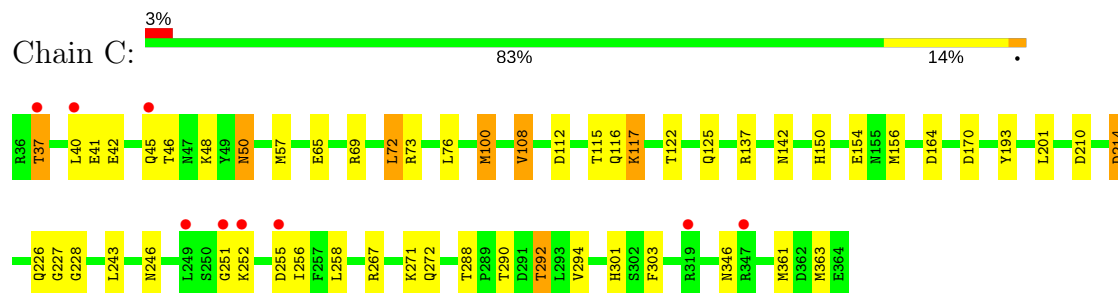
### 3 Residue-property plots [i](#)

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.

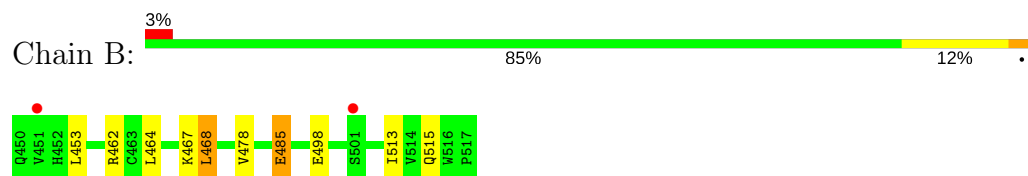
#### • Molecule 1: Lysine-specific demethylase 2A



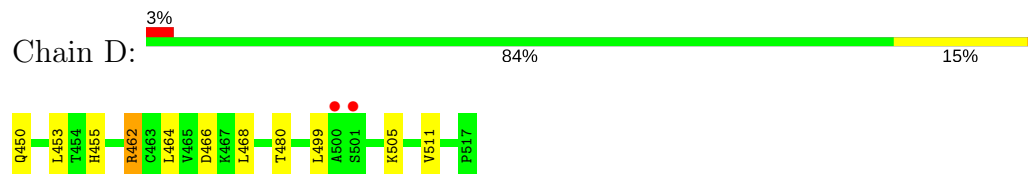
#### • Molecule 1: Lysine-specific demethylase 2A



#### • Molecule 2: Lysine-specific demethylase 2A

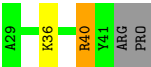


#### • Molecule 2: Lysine-specific demethylase 2A

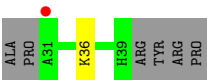


#### • Molecule 3: Histone H3.2





● Molecule 3: Histone H3.2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.60Å 86.71Å 170.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.49 – 1.75 42.74 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (85.49-1.75) 99.0 (42.74-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.175 , 0.204 0.186 , 0.213	Depositor DCC
$R_{free}$ test set	4086 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.26 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.1376e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NI, MLY, OGA

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	0.97	1/2827 (0.0%)	0.97	9/3828 (0.2%)
1	C	0.91	0/2836	1.01	14/3839 (0.4%)
2	B	0.90	0/538	1.11	2/733 (0.3%)
2	D	0.83	0/552	0.88	0/752
3	E	1.05	0/91	1.09	0/123
3	F	0.87	0/54	0.60	0/72
All	All	0.93	1/6898 (0.0%)	0.99	25/9347 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	TYR	CB-CG	-5.25	1.43	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	MET	CG-SD-CE	-13.33	78.86	100.20
1	C	137	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	C	361	MET	CA-CB-CG	-8.29	99.21	113.30
1	C	112	ASP	CB-CG-OD1	7.35	124.92	118.30
1	A	107	MET	CG-SD-CE	-7.12	88.81	100.20
1	C	170	ASP	CB-CG-OD1	6.69	124.32	118.30
2	B	468	LEU	CB-CG-CD1	6.37	121.83	111.00
1	A	214	ASP	CB-CG-OD2	6.33	123.99	118.30
1	A	316[A]	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	316[B]	ASP	CB-CG-OD1	6.17	123.85	118.30
1	C	72	LEU	CB-CG-CD1	6.15	121.45	111.00
1	A	153	LEU	CB-CG-CD2	5.98	121.16	111.00
1	A	112	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	222	TYR	N-CA-CB	-5.63	100.46	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316[A]	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	316[B]	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	C	137	ARG	NE-CZ-NH2	-5.49	117.56	120.30
2	B	462	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	C	164	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	214	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	108	VAL	CB-CA-C	-5.22	101.47	111.40
1	C	156	MET	CG-SD-CE	-5.11	92.03	100.20
1	C	267	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	73	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	C	112	ASP	CB-CG-OD2	-5.02	113.78	118.30

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	2748	0	2643	29	0
1	C	2757	0	2656	37	0
2	B	528	0	546	8	0
2	D	536	0	555	8	0
3	E	99	0	103	4	0
3	F	64	0	69	3	0
4	A	10	0	3	0	0
4	C	10	0	3	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	208	0	0	10	0
6	B	42	0	0	4	0
6	C	162	0	0	8	0
6	D	22	0	0	1	0
6	E	8	0	0	1	0
6	F	4	0	0	0	0
All	All	7200	0	6578	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (84) 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:298:ASN:HD21	3:E:36:MLY:HH12	1.33	0.93
1:C:246:ASN:HB3	6:C:816:HOH:O	1.73	0.87
1:C:115:THR:OG1	1:C:117:LYS:HG3	1.77	0.83
1:A:37:THR:HG22	1:A:255:ASP:HA	1.63	0.80
1:C:252:LYS:O	1:C:255:ASP:HB2	1.82	0.79
2:B:467:LYS:HE2	6:B:620:HOH:O	1.84	0.78
1:A:156:MET:CE	6:A:840:HOH:O	2.33	0.77
1:A:37:THR:HG23	6:A:772:HOH:O	1.83	0.76
6:A:852:HOH:O	2:D:505:LYS:HG2	1.87	0.75
1:A:298:ASN:ND2	3:E:36:MLY:HH12	2.05	0.70
2:B:478:VAL:HG21	2:B:485:GLU:HG2	1.74	0.70
1:C:115:THR:OG1	1:C:117:LYS:CG	2.41	0.69
1:A:37:THR:HG21	6:A:857:HOH:O	1.93	0.68
1:A:108:VAL:HG21	1:A:123:MET:SD	2.35	0.66
6:C:860:HOH:O	2:D:480:THR:HG21	1.98	0.63
1:A:301:HIS:HD2	1:A:303:PHE:H	1.48	0.62
1:C:271:LYS:HD3	6:C:857:HOH:O	1.99	0.61
1:C:37:THR:HB	1:C:255:ASP:OD1	2.01	0.60
1:C:46:THR:OG1	1:C:48:LYS:HG2	2.02	0.60
1:A:39:ASP:HB3	1:A:42:GLU:HG2	1.84	0.60
6:A:852:HOH:O	2:D:505:LYS:CG	2.47	0.60
1:C:150:HIS:HD2	6:C:798:HOH:O	1.86	0.59
1:C:150:HIS:HE1	1:C:193:TYR:OH	1.84	0.59
6:A:821:HOH:O	1:C:69[B]:ARG:HD2	2.02	0.59
1:C:122:THR:H	1:C:125:GLN:HE21	1.49	0.58
1:C:301:HIS:HD2	1:C:303:PHE:H	1.51	0.58
1:A:150:HIS:HE1	1:A:193:TYR:OH	1.87	0.57
1:C:65:GLU:OE1	1:C:69[A]:ARG:NH1	2.37	0.57
1:A:118:GLY:H	3:E:40:ARG:HH21	1.53	0.57
4:C:600:OGA:C1	3:F:36:MLY:HH13	2.35	0.57
3:E:40:ARG:HD2	3:E:40:ARG:H	1.71	0.56
1:A:150:HIS:HD2	6:A:808:HOH:O	1.88	0.56
4:C:600:OGA:O2	3:F:36:MLY:HH13	2.06	0.56
1:A:253:GLN:H	1:A:253:GLN:HE21	1.54	0.55
1:C:226:GLN:O	1:C:292:THR:HB	2.06	0.55
1:A:301:HIS:CD2	1:A:303:PHE:H	2.25	0.55
1:A:36:ARG:HD2	1:A:38:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:453:LEU:HD12	2:D:499:LEU:HD13	1.91	0.52
1:A:156:MET:HE3	6:A:840:HOH:O	2.05	0.52
1:C:50:ASN:HD22	1:C:50:ASN:H	1.57	0.52
1:C:271:LYS:CD	6:C:857:HOH:O	2.58	0.52
1:A:96:ASN:HA	1:A:99:LYS:HG2	1.92	0.52
6:A:855:HOH:O	2:D:455:HIS:HE1	1.93	0.51
1:A:69:ARG:HH12	1:C:50:ASN:HD21	1.58	0.51
2:B:515:GLN:HG2	6:B:613:HOH:O	2.09	0.51
1:C:301:HIS:CD2	1:C:303:PHE:H	2.29	0.51
2:D:455:HIS:HD2	6:D:613:HOH:O	1.94	0.51
1:C:251:GLY:CA	6:C:811:HOH:O	2.59	0.51
1:C:228:GLY:O	1:C:292:THR:HG21	2.11	0.50
2:D:462:ARG:NH2	2:D:466:ASP:OD1	2.44	0.50
1:C:116:GLN:NE2	1:C:210:ASP:H	2.09	0.49
1:C:227:GLY:HA3	1:C:292:THR:HB	1.92	0.49
1:A:122:THR:H	1:A:125:GLN:HE21	1.58	0.49
1:A:172:MET:HG3	1:A:336:VAL:HG22	1.94	0.49
6:C:860:HOH:O	2:D:480:THR:CG2	2.59	0.49
1:C:228:GLY:H	1:C:292:THR:HG21	1.76	0.48
1:C:252:LYS:HB2	1:C:256:ILE:HD12	1.95	0.48
1:A:150:HIS:CE1	1:A:181:GLN:HG2	2.48	0.48
1:A:152:ARG:HD2	6:A:899:HOH:O	2.12	0.48
2:B:478:VAL:CG2	2:B:485:GLU:HG2	2.41	0.48
1:A:234:ILE:HB	1:A:283:ILE:HB	1.96	0.48
1:A:89:PRO:HD3	1:A:157:VAL:HG22	1.94	0.48
1:A:189:LEU:HD23	6:E:106:HOH:O	2.14	0.47
1:C:201:LEU:HD11	3:F:36:MLY:HH22	1.96	0.47
2:B:453:LEU:CD2	2:B:513:ILE:HG13	2.44	0.47
1:C:37:THR:CB	1:C:255:ASP:OD1	2.63	0.47
1:A:159:ARG:NH2	1:A:170:ASP:OD2	2.45	0.46
2:B:478:VAL:HG11	2:B:485:GLU:HG3	1.97	0.46
1:C:37:THR:HB	1:C:255:ASP:HA	1.97	0.46
1:C:290:THR:O	1:C:292:THR:CG2	2.64	0.46
1:C:150:HIS:CE1	1:C:193:TYR:OH	2.69	0.45
1:C:154:GLU:OE2	6:C:801:HOH:O	2.21	0.44
1:A:116:GLN:NE2	1:A:210:ASP:H	2.16	0.43
1:C:41:GLU:OE1	1:C:45:GLN:NE2	2.50	0.43
1:C:201:LEU:HB2	1:C:294:VAL:HB	2.01	0.43
1:A:108:VAL:CG2	1:A:123:MET:HG2	2.49	0.43
1:C:288:THR:HG22	1:C:290:THR:O	2.18	0.43
1:C:228:GLY:H	1:C:292:THR:CG2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:MET:HB2	1:C:57:MET:HE3	1.86	0.42
1:C:41:GLU:O	1:C:45:GLN:HG3	2.19	0.42
2:B:498:GLU:HG3	6:B:634:HOH:O	2.20	0.42
1:C:57:MET:HE3	1:C:76:LEU:HD22	2.02	0.42
2:B:467:LYS:CE	6:B:620:HOH:O	2.55	0.41
1:A:50:ASN:H	1:A:50:ASN:HD22	1.69	0.41

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	328/329 (100%)	323 (98%)	5 (2%)	0	100	100
1	C	329/329 (100%)	322 (98%)	7 (2%)	0	100	100
2	B	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
2	D	68/68 (100%)	66 (97%)	2 (3%)	0	100	100
3	E	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
3	F	6/15 (40%)	6 (100%)	0	0	100	100
All	All	807/824 (98%)	791 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	306/305 (100%)	295 (96%)	11 (4%)	40	15
1	C	307/305 (101%)	291 (95%)	16 (5%)	27	7
2	B	61/61 (100%)	58 (95%)	3 (5%)	29	8
2	D	63/61 (103%)	58 (92%)	5 (8%)	14	2
3	E	8/10 (80%)	7 (88%)	1 (12%)	5	0
3	F	5/10 (50%)	5 (100%)	0	100	100
All	All	750/752 (100%)	714 (95%)	36 (5%)	30	8

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	99	LYS
1	A	107	MET
1	A	142	ASN
1	A	153	LEU
1	A	189	LEU
1	A	214	ASP
1	A	215	PHE
1	A	243	LEU
1	A	253	GLN
1	A	293	LEU
2	B	464	LEU
2	B	468	LEU
2	B	485	GLU
1	C	37	THR
1	C	40	LEU
1	C	42	GLU
1	C	50	ASN
1	C	72	LEU
1	C	100	MET
1	C	108	VAL
1	C	117	LYS
1	C	142	ASN
1	C	214	ASP
1	C	243	LEU
1	C	258	LEU
1	C	272	GLN
1	C	292	THR
1	C	346	ASN
1	C	363	MET

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Mol	Chain	Res	Type
2	D	450	GLN
2	D	462	ARG
2	D	464	LEU
2	D	468	LEU
2	D	511	VAL
3	E	40	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	116	GLN
1	A	125	GLN
1	A	142	ASN
1	A	150	HIS
1	A	158	GLN
1	A	253	GLN
1	A	298	ASN
1	A	301	HIS
1	C	50	ASN
1	C	52	ASN
1	C	116	GLN
1	C	125	GLN
1	C	142	ASN
1	C	150	HIS
1	C	298	ASN
1	C	301	HIS
1	C	346	ASN
2	D	455	HIS
3	F	39	HIS

### 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	E	36	3	10,10,11	1.08	1 (10%)	8,11,13	1.39	1 (12%)
3	MLY	F	36	3	10,10,11	0.79	1 (10%)	8,11,13	1.94	3 (37%)

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	E	36	3	-	0/7/9/11	0/0/0/0
3	MLY	F	36	3	-	0/7/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	36	MLY	CA-C	2.04	1.52	1.50
3	E	36	MLY	CA-C	2.87	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	36	MLY	O-C-CA	-3.04	116.63	125.02
3	F	36	MLY	CH1-NZ-CE	2.12	119.08	110.75
3	F	36	MLY	CH2-NZ-CH1	2.71	117.00	109.72
3	F	36	MLY	CH2-NZ-CE	3.33	123.87	110.75

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
3	E	36	MLY	2	0
3	F	36	MLY	3	0



## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
4	OGA	A	600	5	3,9,9	0.72	0	3,11,11	2.85	1 (33%)
4	OGA	C	600	5	3,9,9	0.53	0	3,11,11	2.68	1 (33%)

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
4	OGA	A	600	5	-	0/3/9/9	0/0/0/0
4	OGA	C	600	5	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	600	OGA	C1-C2-N1	4.41	119.71	115.80
4	A	600	OGA	C1-C2-N1	4.50	119.79	115.80

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
4	C	600	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 [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	329/329 (100%)	-0.27	1 (0%) 93 95	12, 19, 35, 54	0
1	C	329/329 (100%)	0.00	9 (2%) 55 62	13, 22, 45, 76	0
2	B	68/68 (100%)	-0.18	2 (2%) 52 59	16, 22, 34, 43	0
2	D	68/68 (100%)	-0.01	2 (2%) 52 59	17, 27, 48, 61	0
3	E	12/15 (80%)	0.19	0 100 100	16, 21, 45, 46	0
3	F	8/15 (53%)	1.24	1 (12%) 4 6	29, 34, 42, 55	0
All	All	814/824 (98%)	-0.11	15 (1%) 69 77	12, 21, 42, 76	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	251	GLY	4.9
1	C	249	LEU	3.4
1	C	252	LYS	3.3
1	C	255	ASP	3.2
3	F	31	ALA	2.9
2	B	451	VAL	2.8
1	C	37	THR	2.8
1	C	319	ARG	2.7
2	D	501	SER	2.5
1	A	47	ASN	2.3
1	C	40	LEU	2.3
2	D	500	ALA	2.3
1	C	347	ARG	2.1
1	C	45	GLN	2.1
2	B	501	SER	2.1

## 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
3	MLY	E	36	11/12	0.96	0.11	-	15,17,27,28	0
3	MLY	F	36	11/12	0.76	0.18	-	29,32,40,44	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(Å <sup>2</sup> )	Q<0.9
4	OGA	C	600	10/10	0.93	0.09	-0.34	26,31,40,44	0
4	OGA	A	600	10/10	0.96	0.06	-1.14	20,23,30,33	0
5	NI	C	601	1/1	0.99	0.05	-	31,31,31,31	0
5	NI	A	601	1/1	1.00	0.03	-	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.