Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 05:08 PM EDT

PDB ID	:	4QXB
Title	:	crystal structure of histone demethylase KDM2A-H3K36ME3 with NOG
Authors	:	Cheng, Z.J.; Patel, D.J.
Deposited on	:	2014-07-19
Resolution	:	1.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

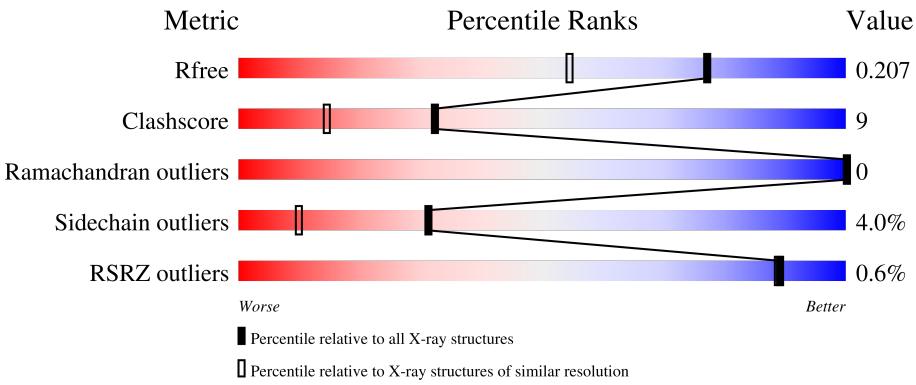
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	84% 14% •
1	C	329	% 79% 17% •
2	B	68	84% 16%
2	D	68	% 85% 10% •
3	E	15	7% 60% 13% 13% 13%

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Mol	Chain	Length	Quality of chain
3	F	15	40% 20% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OGA	C	600	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7585 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
			Total	C	N	O	S			
1	A	329	2757	1766	458	512	21	0	3	0
1	C	329	2749	1761	458	509	21	0	1	0

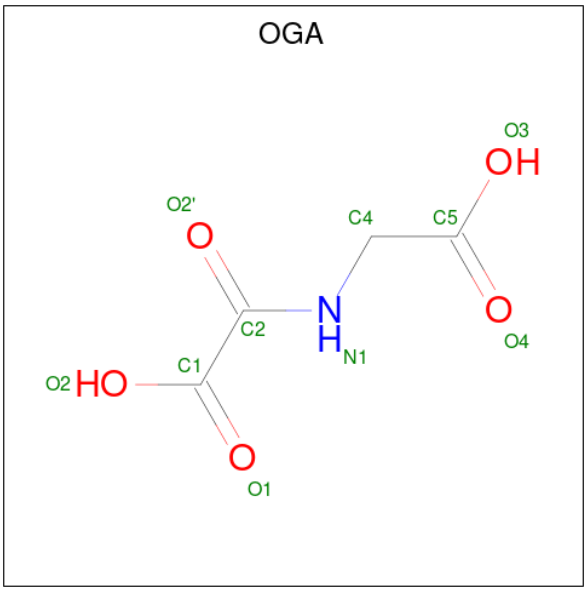
- Molecule 2 is a protein called Lysine-specific demethylase 2A.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	13	100	65	20	15	0	0	0
3	F	9	65	42	13	10	0	0	0

- Molecule 4 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	358	Total O 358 358	0	0
6	B	85	Total O 85 85	0	0
6	C	296	Total O 296 296	0	0
6	D	61	Total O 61 61	0	0
6	E	18	Total O 18 18	0	0

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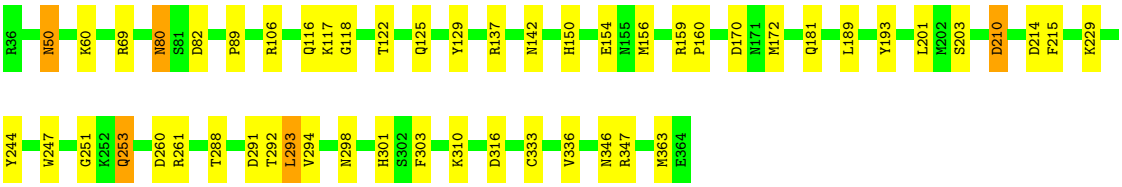
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	F	10	10	10	0	0

3 Residue-property plots (i)

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

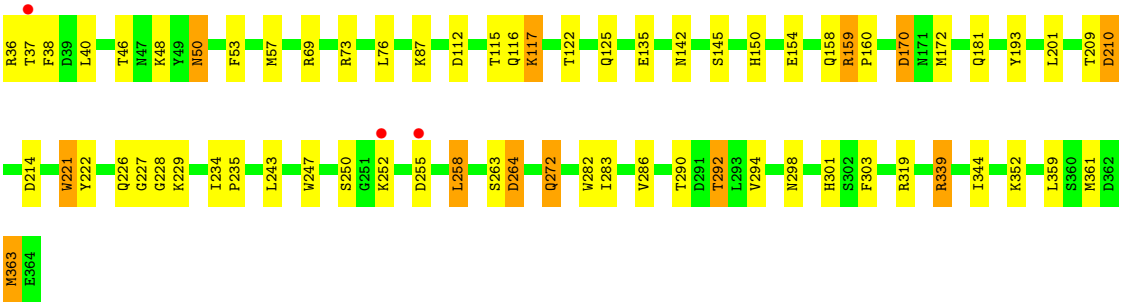
• Molecule 1: Lysine-specific demethylase 2A

Chain A:



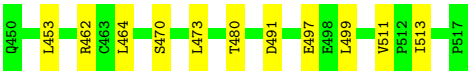
• Molecule 1: Lysine-specific demethylase 2A

Chain C:



• Molecule 2: Lysine-specific demethylase 2A

Chain B:

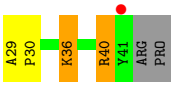


• Molecule 2: Lysine-specific demethylase 2A

Chain D:

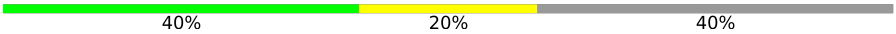
• Molecule 3: Histone H3.2

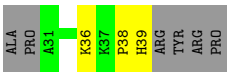
Chain E:



• Molecule 3: Histone H3.2

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.60Å 86.72Å 171.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.55 – 1.60 46.03 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (85.55-1.60) 99.3 (46.03-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0049, PHENIX (phenix.refine: 1.4_162)	Depositor
R, R_{free}	0.169 , 0.207 0.169 , 0.207	Depositor DCC
R_{free} test set	5351 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7585	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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 34.84 % 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 6.4093e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, M3L, NI

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	1.06	0/2842	1.06	8/3847 (0.2%)
1	C	1.05	3/2828 (0.1%)	1.06	10/3828 (0.3%)
2	B	0.97	1/538 (0.2%)	1.04	2/733 (0.3%)
2	D	0.89	0/552	1.00	3/751 (0.4%)
3	E	1.14	0/91	1.17	0/123
3	F	1.03	0/54	0.81	0/72
All	All	1.04	4/6905 (0.1%)	1.05	23/9354 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	470	SER	CB-OG	7.03	1.51	1.42
1	C	282	TRP	CE3-CZ3	5.36	1.47	1.38
1	C	145	SER	CB-OG	-5.16	1.35	1.42
1	C	221	TRP	CE3-CZ3	5.11	1.47	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	511	VAL	CG1-CB-CG2	9.06	125.40	110.90
1	A	363	MET	CG-SD-CE	7.44	112.10	100.20
1	C	73	ARG	NE-CZ-NH1	-7.23	116.68	120.30
1	C	73	ARG	NE-CZ-NH2	7.12	123.86	120.30
2	D	476	LYS	CD-CE-NZ	6.99	127.78	111.70
2	D	468	LEU	CB-CG-CD1	6.94	122.80	111.00
1	C	258	LEU	CB-CG-CD2	6.88	122.69	111.00
1	C	339	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	210	ASP	CB-CG-OD1	6.33	123.99	118.30
1	C	361	MET	CA-CB-CG	-6.19	102.77	113.30
1	C	159	ARG	NE-CZ-NH2	-5.85	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	310	LYS	CD-CE-NZ	5.75	124.91	111.70
2	B	462	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	291	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	316[A]	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	316[B]	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	293	LEU	CA-CB-CG	5.23	127.33	115.30
2	D	495	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	C	170[A]	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	170[B]	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	244	TYR	CD1-CE1-CZ	-5.05	115.25	119.80
1	C	210	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	C	69	ARG	NE-CZ-NH2	5.02	122.81	120.30

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	2757	0	2652	43	0
1	C	2749	0	2643	59	1
2	B	528	0	546	7	0
2	D	536	0	558	9	0
3	E	100	0	106	6	0
3	F	65	0	72	6	0
4	A	10	0	3	0	0
4	C	10	0	3	4	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	358	0	0	8	0
6	B	85	0	0	1	0
6	C	296	0	0	6	0
6	D	61	0	0	3	0
6	E	18	0	0	0	0
6	F	10	0	0	1	0
All	All	7585	0	6583	117	1

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 9.

All (117) 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)
2:D:450:GLN:HE21	2:D:450:GLN:N	1.61	0.98
1:C:135:GLU:HB3	6:C:969:HOH:O	1.77	0.84
1:C:37:THR:HB	1:C:255:ASP:HA	1.59	0.83
1:A:229:LYS:HE2	1:A:292:THR:HG21	1.62	0.79
1:A:347:ARG:HD2	2:B:491:ASP:OD2	1.83	0.78
1:A:118:GLY:H	3:E:40:ARG:HH21	1.34	0.75
2:D:466:ASP:OD2	6:D:660:HOH:O	2.08	0.71
1:C:57:MET:HE3	1:C:76:LEU:HD22	1.72	0.70
1:C:286:VAL:HG11	4:C:600:OGA:C5	2.22	0.69
1:C:298:ASN:HD21	3:F:36:M3L:HE2	1.58	0.68
1:C:301:HIS:HD2	1:C:303:PHE:H	1.40	0.68
1:C:122:THR:H	1:C:125:GLN:HE21	1.41	0.67
1:C:286:VAL:HG11	4:C:600:OGA:H4C2	1.76	0.67
1:A:301:HIS:HD2	1:A:303:PHE:H	1.43	0.66
1:C:250:SER:HB3	1:C:252:LYS:H	1.59	0.66
1:C:116:GLN:NE2	1:C:210:ASP:H	1.94	0.65
1:A:69:ARG:HH12	1:C:50:ASN:HD21	1.44	0.65
6:A:1044:HOH:O	1:C:264:ASP:CG	2.36	0.63
1:C:247:TRP:O	1:C:250:SER:HB2	1.98	0.63
1:C:209:THR:HB	1:C:286:VAL:HG12	1.79	0.63
1:C:209:THR:HB	1:C:286:VAL:CG1	2.29	0.62
1:A:137:ARG:NH2	6:A:902:HOH:O	2.26	0.62
1:C:154:GLU:HG2	6:C:819:HOH:O	1.99	0.62
2:D:450:GLN:N	2:D:450:GLN:NE2	2.42	0.62
1:C:301:HIS:CD2	1:C:303:PHE:H	2.17	0.62
3:F:39:HIS:HD2	6:F:109:HOH:O	1.82	0.62
1:C:286:VAL:HG11	4:C:600:OGA:C4	2.29	0.61
1:A:288:THR:CG2	1:A:292:THR:HG22	2.31	0.61
1:C:150:HIS:HE1	1:C:193:TYR:OH	1.83	0.60
1:A:69:ARG:NH2	6:A:1044:HOH:O	2.25	0.60
1:C:227:GLY:HA3	1:C:292:THR:HB	1.82	0.59
1:A:150:HIS:HD2	6:A:800:HOH:O	1.84	0.59
1:C:209:THR:HG23	3:F:38:PRO:HG3	1.84	0.59
1:C:46:THR:OG1	1:C:48:LYS:HG2	2.03	0.58
2:B:497:GLU:HG3	6:B:677:HOH:O	2.03	0.57
6:A:1004:HOH:O	2:B:480:THR:HG21	2.04	0.57
1:A:129:TYR:CE1	1:A:137:ARG:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:HB2	1:A:160:PRO:CD	2.34	0.56
1:A:301:HIS:CD2	1:A:303:PHE:H	2.24	0.56
1:A:116:GLN:NE2	1:A:210:ASP:H	2.03	0.56
1:A:150:HIS:HE1	1:A:193:TYR:OH	1.89	0.56
2:D:455:HIS:HD2	2:D:459:GLU:OE2	1.90	0.55
1:A:89:PRO:HB3	1:A:156:MET:HE2	1.89	0.55
1:C:159:ARG:NH2	1:C:170[B]:ASP:OD1	2.40	0.54
3:E:29:ALA:N	3:E:30:PRO:CD	2.70	0.54
1:A:122:THR:H	1:A:125:GLN:HE21	1.54	0.54
3:E:40:ARG:HD2	3:E:40:ARG:H	1.71	0.54
1:C:228:GLY:H	1:C:292:THR:HG21	1.73	0.53
1:A:80:ASN:HD22	1:A:82:ASP:H	1.56	0.53
1:C:228:GLY:O	1:C:292:THR:HG21	2.09	0.53
1:A:150:HIS:CE1	1:A:181:GLN:HG2	2.44	0.52
1:C:201:LEU:HB2	1:C:294:VAL:HB	1.92	0.52
1:A:229:LYS:HE2	1:A:292:THR:CG2	2.35	0.52
1:A:288:THR:HG23	1:A:292:THR:CG2	2.41	0.51
1:A:288:THR:HG21	1:A:292:THR:HG22	1.93	0.51
1:C:290:THR:O	1:C:292:THR:HG23	2.11	0.50
1:C:228:GLY:H	1:C:292:THR:CG2	2.25	0.50
1:A:172:MET:HG3	1:A:336:VAL:HG22	1.94	0.50
1:C:112:ASP:CG	6:C:759:HOH:O	2.50	0.50
1:A:253:GLN:HE21	1:A:253:GLN:H	1.58	0.49
2:B:453:LEU:CD2	2:B:513:ILE:HG13	2.42	0.49
2:D:459:GLU:OE1	6:D:636:HOH:O	2.20	0.48
1:A:203:SER:HB2	1:A:292:THR:HG23	1.95	0.48
1:A:69:ARG:HH22	1:C:50:ASN:ND2	2.12	0.48
1:A:50:ASN:H	1:A:50:ASN:HD22	1.62	0.47
6:A:836:HOH:O	2:D:455:HIS:HE1	1.96	0.47
1:C:115:THR:OG1	1:C:117:LYS:HG2	2.14	0.47
1:A:247:TRP:CZ2	1:A:253:GLN:HB3	2.50	0.47
1:C:37:THR:HB	1:C:255:ASP:CA	2.37	0.47
1:C:115:THR:HG21	6:C:972:HOH:O	2.14	0.46
1:A:251:GLY:HA2	1:A:253:GLN:NE2	2.30	0.46
1:C:250:SER:HB3	1:C:252:LYS:HB2	1.98	0.46
1:C:150:HIS:CE1	1:C:181:GLN:HG2	2.50	0.46
1:C:226:GLN:O	1:C:292:THR:HB	2.15	0.46
1:A:154:GLU:HG2	6:A:847:HOH:O	2.15	0.46
1:A:80:ASN:HD22	1:A:80:ASN:C	2.19	0.46
2:B:453:LEU:HD22	2:B:513:ILE:HG13	1.98	0.45
1:C:344:ILE:HG21	2:D:495:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLN:HE22	1:C:210:ASP:H	1.61	0.45
1:A:129:TYR:CZ	1:A:137:ARG:HD2	2.52	0.45
1:A:116:GLN:HE22	1:A:210:ASP:H	1.62	0.45
2:B:453:LEU:HG	2:B:499:LEU:HD13	1.99	0.45
1:C:209:THR:CG2	3:F:38:PRO:HG3	2.47	0.45
1:C:290:THR:O	1:C:292:THR:CG2	2.65	0.44
1:A:60:LYS:H	1:A:60:LYS:HG3	1.42	0.44
1:C:222:TYR:CE2	4:C:600:OGA:O1	2.71	0.44
1:C:150:HIS:CE1	1:C:193:TYR:OH	2.68	0.44
1:C:250:SER:C	1:C:252:LYS:H	2.21	0.43
1:C:298:ASN:ND2	3:F:36:M3L:HE2	2.30	0.43
1:C:36:ARG:HD2	1:C:38:PHE:CZ	2.54	0.43
1:A:298:ASN:HD21	3:E:36:M3L:HM32	1.83	0.43
1:A:201:LEU:HB2	1:A:294:VAL:HB	2.00	0.43
1:C:117:LYS:HG2	6:C:972:HOH:O	2.18	0.43
3:E:29:ALA:N	3:E:30:PRO:HD3	2.34	0.43
1:C:222:TYR:OH	1:C:229:LYS:HE3	2.18	0.43
1:A:288:THR:CG2	1:A:292:THR:CG2	2.96	0.42
1:C:234:ILE:HB	1:C:283:ILE:HB	2.01	0.42
1:C:159:ARG:HB2	1:C:160:PRO:CD	2.49	0.42
1:A:203:SER:HB2	1:A:292:THR:CG2	2.50	0.42
1:A:288:THR:HG23	1:A:292:THR:HG21	2.00	0.42
1:C:53:PHE:CE2	1:C:235:PRO:HD3	2.55	0.42
1:A:159:ARG:NH2	1:A:170[B]:ASP:OD2	2.48	0.42
1:A:106:ARG:HD3	6:A:732:HOH:O	2.19	0.42
1:A:333:CYS:HB3	2:B:464:LEU:HD11	2.02	0.42
3:E:40:ARG:H	3:E:40:ARG:CD	2.31	0.41
1:C:272:GLN:O	1:C:272:GLN:HG3	2.14	0.41
1:C:159:ARG:HB3	1:C:221:TRP:CZ2	2.55	0.41
1:C:201:LEU:HD21	3:F:36:M3L:HM11	2.01	0.41
1:A:288:THR:HG23	1:A:292:THR:HG22	2.01	0.41
1:C:112:ASP:OD2	1:C:115:THR:HG23	2.20	0.41
1:C:87:LYS:HB3	1:C:158:GLN:HB2	2.01	0.41
1:C:115:THR:CG2	6:C:972:HOH:O	2.69	0.41
1:C:352:LYS:HD3	1:C:352:LYS:HA	1.72	0.41
1:C:50:ASN:HD22	1:C:50:ASN:H	1.67	0.41
2:D:474:HIS:ND1	6:D:643:HOH:O	2.37	0.41
1:C:172:MET:HA	1:C:339:ARG:HG3	2.03	0.41
1:A:260:ASP:O	2:D:505:LYS:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LYS:NZ	1:C:363:MET:CE[1_655]	2.14	0.06

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	330/329 (100%)	327 (99%)	3 (1%)	0	100	100
1	C	328/329 (100%)	321 (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%)	10 (100%)	0	0	100	100
3	F	6/15 (40%)	6 (100%)	0	0	100	100
All	All	808/824 (98%)	795 (98%)	13 (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	308/305 (101%)	297 (96%)	11 (4%)	35	12
1	C	306/305 (100%)	292 (95%)	14 (5%)	27	8
2	B	61/61 (100%)	60 (98%)	1 (2%)	62	41
2	D	63/61 (103%)	60 (95%)	3 (5%)	25	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	8/10 (80%)	7 (88%)	1 (12%)	4 0
3	F	5/10 (50%)	5 (100%)	0	100 100
All	All	751/752 (100%)	721 (96%)	30 (4%)	31 10

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	80	ASN
1	A	117	LYS
1	A	142	ASN
1	A	189	LEU
1	A	214	ASP
1	A	215	PHE
1	A	253	GLN
1	A	261	ARG
1	A	293	LEU
1	A	346	ASN
2	B	473	LEU
1	C	40	LEU
1	C	50	ASN
1	C	117	LYS
1	C	142	ASN
1	C	214	ASP
1	C	243	LEU
1	C	258	LEU
1	C	263	SER
1	C	264	ASP
1	C	272	GLN
1	C	292	THR
1	C	319	ARG
1	C	359	LEU
1	C	363	MET
2	D	450	GLN
2	D	468	LEU
2	D	511	VAL
3	E	40	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	80	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	155	ASN
1	C	197	GLN
1	C	239	HIS
1	C	298	ASN
1	C	301	HIS
2	D	455	HIS
3	F	39	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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	M3L	F	36	3	10,11,12	0.66	0	9,14,16	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	M3L	E	36	3	10,11,12	1.26	1 (10%)	9,14,16	1.28	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
3	M3L	F	36	3	-	0/9/10/12	-
3	M3L	E	36	3	-	1/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	36	M3L	CB-CA	3.18	1.57	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	36	M3L	CM2-NZ-CM1	2.33	114.95	108.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	36	M3L	CD-CE-NZ-CM1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	36	M3L	3	0
3	E	36	M3L	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	600	5	9,9,9	1.84	1 (11%)	10,11,11	1.88	4 (40%)
4	OGA	A	600	5	9,9,9	2.17	2 (22%)	10,11,11	1.45	2 (20%)

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	C	600	5	-	0/8/9/9	-
4	OGA	A	600	5	-	0/8/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	OGA	C2-C1	-5.38	1.47	1.54
4	C	600	OGA	C2-C1	-4.68	1.48	1.54
4	A	600	OGA	C4-N1	2.31	1.51	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	600	OGA	O2'-C2-C1	-3.11	116.93	121.32
4	A	600	OGA	O2-C1-C2	2.85	121.54	113.15
4	C	600	OGA	O1-C1-C2	-2.48	116.66	122.18
4	C	600	OGA	O2-C1-C2	2.44	120.34	113.15
4	A	600	OGA	O1-C1-C2	-2.35	116.94	122.18
4	C	600	OGA	O3-C5-C4	2.17	120.27	112.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	600	OGA	4	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, 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	329/329 (100%)	-0.66	0 100 100	11, 17, 33, 53	0
1	C	329/329 (100%)	-0.34	3 (0%) 84 84	12, 21, 43, 59	0
2	B	68/68 (100%)	-0.50	0 100 100	14, 20, 34, 43	0
2	D	68/68 (100%)	-0.27	1 (1%) 73 73	15, 25, 43, 51	0
3	E	12/15 (80%)	0.08	1 (8%) 11 10	15, 18, 41, 45	0
3	F	8/15 (53%)	0.70	0 100 100	24, 28, 34, 42	0
All	All	814/824 (98%)	-0.46	5 (0%) 89 89	11, 20, 39, 59	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	41	TYR	3.7
1	C	37	THR	3.6
1	C	255	ASP	3.4
1	C	252	LYS	2.4
2	D	501	SER	2.2

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, 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	B-factors(Å^2)	Q<0.9
3	M3L	F	36	12/13	0.86	0.12	21,23,27,28	0
3	M3L	E	36	12/13	0.97	0.06	13,14,16,16	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
4	OGA	C	600	10/10	0.94	0.11	23,26,29,30	0
4	OGA	A	600	10/10	0.97	0.06	18,20,20,21	0
5	NI	C	601	1/1	0.99	0.07	27,27,27,27	0
5	NI	A	601	1/1	1.00	0.02	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.