Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 03:55 PM EDT

PDB ID	:	2Q8E
Title	:	Specificity and Mechanism of JMJD2A, a Trimethyllysine-Specific Histone Demethylase
Authors	:	Couture, J.-F.; Collazo, E.; Ortiz-Tello, P.; Brunzelle, J.S.; Trievel, R.C.
Deposited on	:	2007-06-10
Resolution	:	2.05 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 ⓘ 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 ⓘ) were used in the production of this report:

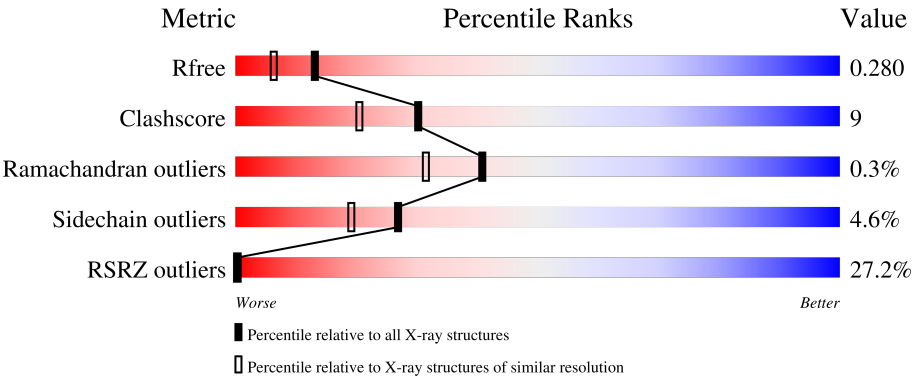
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	352	24% 82% 15%
1	B	352	28% 73% 22%
2	F	16	12% 19% 6% 75%
2	G	16	19% 12% 19% 12% 56%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5928 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 JmjC domain-containing histone demethylation protein 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	3	0
			2790	1803	462	510	15			
1	B	337	Total	C	N	O	S	0	3	0
			2751	1781	463	492	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP O75164
A	0	SER	-	cloning artifact	UNP O75164
B	-1	GLY	-	cloning artifact	UNP O75164
B	0	SER	-	cloning artifact	UNP O75164

- Molecule 2 is a protein called histone 3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	4	Total	C	N	O	0	0	0
			25	16	5	4			
2	G	7	Total	C	N	O	0	0	0
			48	32	9	7			

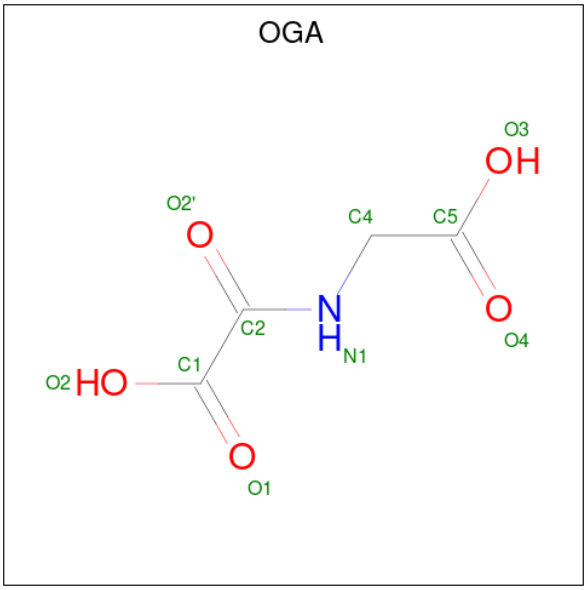
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



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

- Molecule 6 is water.

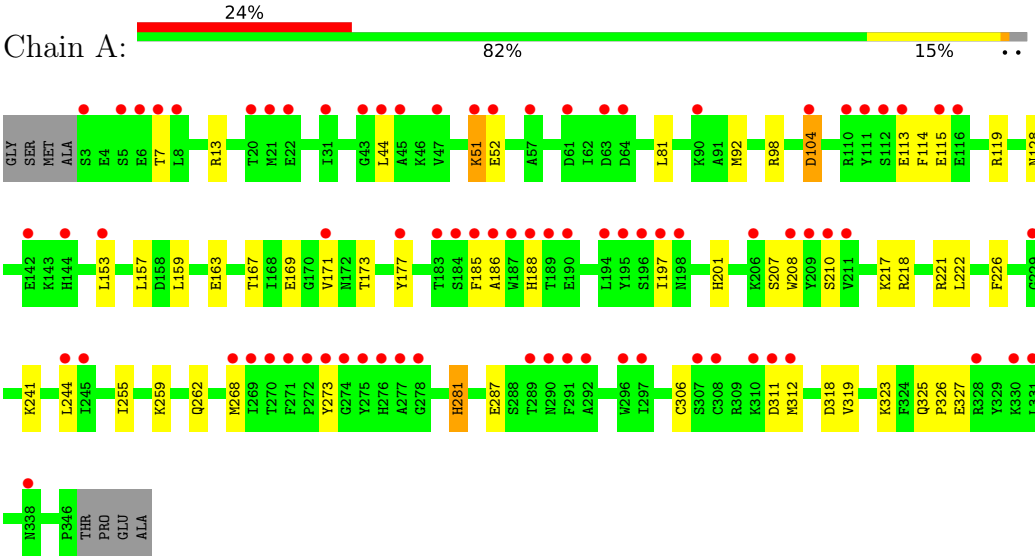
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	156	Total O 156 156	0	0
6	B	130	Total O 130 130	0	0
6	F	1	Total O 1 1	0	0
6	G	3	Total O 3 3	0	0

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.

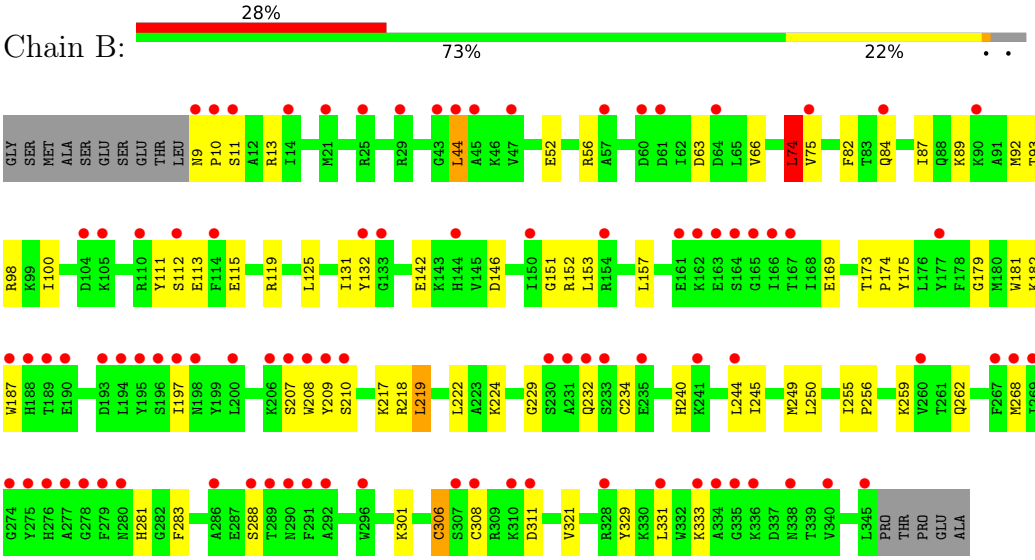
• Molecule 1: JmjC domain-containing histone demethylation protein 3A

Chain A:



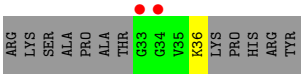
• Molecule 1: JmjC domain-containing histone demethylation protein 3A

Chain B:



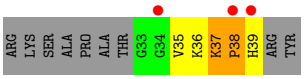
• Molecule 2: histone 3 peptide

Chain F:



• Molecule 2: histone 3 peptide

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.29Å 148.96Å 56.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.05 29.97 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.97-2.05) 99.6 (29.97-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.260 0.254 , 0.280	Depositor DCC
R_{free} test set	2753 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5928	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OGA, ZN, NI, M3L

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	0.75	0/2890	0.74	0/3919
1	B	0.72	1/2851 (0.0%)	0.75	2/3866 (0.1%)
2	F	0.98	0/12	0.62	0/14
2	G	0.84	0/36	0.81	0/47
All	All	0.73	1/5789 (0.0%)	0.74	2/7846 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	CYS	CB-SG	5.17	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	74	LEU	CA-CB-CG	-6.06	101.37	115.30
1	B	219	LEU	CA-CB-CG	5.41	127.74	115.30

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	2790	0	2672	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2751	0	2640	55	0
2	F	25	0	26	2	0
2	G	48	0	55	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	1	0
5	A	10	0	3	1	0
5	B	10	0	3	1	0
6	A	156	0	0	5	0
6	B	130	0	0	3	0
6	F	1	0	0	0	0
6	G	3	0	0	1	0
All	All	5928	0	5399	101	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 9.

All (101) 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:B:9:ASN:HB3	1:B:10:PRO:HD3	1.43	1.00
1:B:306:CYS:HG	4:B:506:ZN:ZN	0.73	0.97
1:A:306:CYS:HG	4:A:505:ZN:ZN	0.59	0.89
1:A:139:THR:HG21	6:A:539:HOH:O	1.75	0.86
1:B:111:TYR:OH	6:B:596:HOH:O	1.93	0.84
1:B:244:LEU:O	1:B:245:ILE:HD13	1.81	0.81
1:A:139:THR:CG2	1:A:287:GLU:OE1	2.32	0.78
1:B:222:LEU:HD22	1:B:255:ILE:CD1	2.12	0.77
1:A:163:GLU:HG3	1:A:319:VAL:HG21	1.66	0.75
1:A:139:THR:HG23	1:A:287:GLU:OE1	1.87	0.73
2:G:38:PRO:HB2	2:G:39:HIS:HA	1.68	0.73
1:A:222:LEU:HD22	1:A:255:ILE:CD1	2.19	0.73
1:B:9:ASN:HB3	1:B:10:PRO:CD	2.17	0.71
1:B:9:ASN:CB	1:B:10:PRO:HD3	2.20	0.71
1:A:98:ARG:NH2	6:A:633:HOH:O	2.23	0.70
1:B:222:LEU:HD22	1:B:255:ILE:HD13	1.72	0.70
1:B:66:VAL:O	6:B:579:HOH:O	2.09	0.69
1:A:218:ARG:HD2	6:A:582:HOH:O	1.95	0.67
1:A:104:ASP:N	1:A:104:ASP:OD1	2.29	0.66
1:B:217:LYS:HD2	1:B:273:TYR:OH	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:HG22	1:A:287:GLU:OE1	1.99	0.63
1:B:75:VAL:HG11	1:B:125:LEU:HG	1.81	0.63
1:B:10:PRO:HA	1:B:13:ARG:HG3	1.80	0.61
1:B:207:SER:OG	1:B:281:HIS:HE1	1.84	0.61
1:A:186:ALA:HA	1:A:244:LEU:HD23	1.82	0.61
1:A:44:LEU:HD12	1:A:210[B]:SER:HB3	1.83	0.60
1:B:151:GLY:HA2	1:B:174:PRO:HG3	1.84	0.60
2:G:38:PRO:CB	2:G:39:HIS:HA	2.34	0.58
1:B:222:LEU:HD22	1:B:255:ILE:HD11	1.85	0.57
1:A:44:LEU:HD12	1:A:210[A]:SER:HB2	1.85	0.56
1:B:175:TYR:CE1	2:G:36:M3L:O	2.59	0.56
1:A:221:ARG:HH11	1:B:13:ARG:NH2	2.03	0.56
2:G:36:M3L:O	2:G:37:LYS:HB2	2.04	0.56
1:A:323:LYS:HE3	6:A:657:HOH:O	2.05	0.56
1:A:13:ARG:HG2	1:A:13:ARG:HH11	1.71	0.55
1:B:63:ASP:OD1	1:B:98:ARG:NH2	2.40	0.55
1:B:93:THR:OG1	1:B:96:GLU:HG3	2.05	0.55
1:B:56:ARG:HA	1:B:142:GLU:HG3	1.90	0.54
1:B:234:CYS:SG	1:B:306:CYS:SG	3.06	0.54
1:A:114:PHE:HE2	1:A:207:SER:HG	1.55	0.53
1:B:175:TYR:HE1	2:G:36:M3L:O	1.90	0.53
1:B:63:ASP:CG	1:B:98:ARG:HH22	2.12	0.53
1:A:115:GLU:HG2	1:A:119:ARG:HH12	1.73	0.53
2:G:35:VAL:HG12	6:G:189:HOH:O	2.09	0.52
1:A:222:LEU:HD22	1:A:255:ILE:HD11	1.90	0.52
1:B:229:GLY:O	1:B:232:GLN:HG2	2.09	0.52
1:A:207:SER:OG	1:A:281:HIS:HE1	1.93	0.51
1:B:74:LEU:HD13	1:B:87:ILE:HD12	1.93	0.50
1:A:81:LEU:HD21	1:A:226:PHE:CD1	2.48	0.49
1:A:115:GLU:HG2	1:A:119:ARG:NH1	2.27	0.49
1:A:159:LEU:HD11	1:A:323:LYS:HD2	1.95	0.48
1:A:177:TYR:OH	2:F:36:M3L:HM33	2.13	0.48
1:A:153:LEU:HD11	1:A:197:ILE:HG21	1.96	0.48
1:B:92:MET:HE1	1:B:100:ILE:HD12	1.96	0.48
1:A:222:LEU:HD22	1:A:255:ILE:HD12	1.95	0.48
1:A:208:TRP:HE1	1:A:262:GLN:NE2	2.12	0.47
1:B:301:LYS:HD3	1:B:321:VAL:HG22	1.94	0.47
1:B:288:SER:OG	2:G:36:M3L:HM31	2.15	0.46
1:A:259:LYS:HB3	6:A:521:HOH:O	2.14	0.46
1:A:188:HIS:CD2	1:A:241:LYS:HE2	2.52	0.45
1:B:84:GLN:NE2	1:B:184:SER:OG	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:HIS:NE2	1:B:306:CYS:SG	2.90	0.45
1:A:208:TRP:HE1	1:A:262:GLN:HE21	1.64	0.45
1:B:9:ASN:N	1:B:11:SER:HG	2.15	0.45
1:A:185:PHE:CG	5:A:503:OGA:H4C2	2.51	0.45
1:B:44:LEU:HD12	1:B:210:SER:HB2	1.98	0.45
1:B:187:TRP:CZ2	1:B:250:LEU:HD11	2.52	0.45
1:B:208:TRP:HE1	1:B:262:GLN:NE2	2.14	0.45
1:B:175:TYR:OH	2:G:36:M3L:O	2.27	0.44
1:A:44:LEU:HD22	1:A:268:MET:HE3	1.98	0.44
1:B:146:ASP:OD1	1:B:152:ARG:NH2	2.51	0.43
1:B:306:CYS:SG	1:B:308:CYS:SG	3.16	0.43
1:B:89:LYS:HG3	1:B:131:ILE:HD12	2.00	0.43
1:B:92:MET:CE	1:B:100:ILE:HD12	2.48	0.43
1:B:153:LEU:HD11	1:B:197:ILE:HG21	2.00	0.43
1:B:186:ALA:HA	1:B:244:LEU:HD23	2.00	0.43
1:B:209:TYR:HE2	1:B:259:LYS:HE2	1.83	0.43
1:A:171:VAL:HG23	2:F:36:M3L:HB3	2.01	0.43
1:B:82:PHE:HB2	1:B:244:LEU:HB2	2.00	0.43
1:B:74:LEU:HD13	1:B:87:ILE:CD1	2.48	0.43
1:B:179:GLY:O	1:B:283:PHE:HA	2.19	0.43
1:B:185:PHE:CG	5:B:504:OGA:H4C2	2.53	0.43
1:A:201:HIS:HE2	1:A:287:GLU:HB2	1.85	0.42
1:B:329:TYR:CE2	1:B:333:LYS:HD2	2.54	0.42
1:B:181:TRP:O	1:B:182:LYS:HB3	2.20	0.42
2:G:36:M3L:HD2	2:G:36:M3L:HM23	1.85	0.42
1:B:224:LYS:CB	1:B:224:LYS:NZ	2.83	0.42
1:B:44:LEU:HD22	1:B:268:MET:HE3	2.02	0.42
1:B:115:GLU:O	1:B:119:ARG:HG3	2.20	0.41
1:B:169:GLU:HA	1:B:173:THR:OG1	2.20	0.41
1:A:13:ARG:HG2	1:A:13:ARG:NH1	2.35	0.41
1:A:44:LEU:HD11	1:A:208:TRP:HB3	2.02	0.41
1:A:92:MET:HE3	1:A:92:MET:HB2	1.69	0.41
1:B:281:HIS:HD2	6:B:596:HOH:O	2.04	0.41
1:A:217:LYS:HD2	1:A:273:TYR:OH	2.20	0.41
1:A:169:GLU:HA	1:A:173:THR:OG1	2.20	0.41
1:A:325:GLN:N	1:A:326:PRO:CD	2.84	0.41
1:A:218:ARG:HD2	1:A:218:ARG:HH11	1.78	0.40
1:B:208:TRP:HE1	1:B:262:GLN:HE21	1.68	0.40
1:B:218:ARG:HH11	1:B:256:PRO:HD3	1.87	0.40
1:A:51:LYS:H	1:A:51:LYS:HD3	1.87	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	345/352 (98%)	337 (98%)	8 (2%)	0	100 100
1	B	338/352 (96%)	335 (99%)	3 (1%)	0	100 100
2	F	2/16 (12%)	2 (100%)	0	0	100 100
2	G	4/16 (25%)	2 (50%)	0	2 (50%)	0 0
All	All	689/736 (94%)	676 (98%)	11 (2%)	2 (0%)	41 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	38	PRO
2	G	37	LYS

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	296/308 (96%)	280 (95%)	16 (5%)	22 13
1	B	289/308 (94%)	278 (96%)	11 (4%)	33 26
2	G	3/11 (27%)	3 (100%)	0	100 100
All	All	588/627 (94%)	561 (95%)	27 (5%)	27 19

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	51	LYS
1	A	52	GLU
1	A	104	ASP
1	A	113	GLU
1	A	128	ASN
1	A	132	TYR
1	A	139	THR
1	A	157	LEU
1	A	167	THR
1	A	281	HIS
1	A	311	ASP
1	A	312	MET
1	A	318	ASP
1	A	327	GLU
1	A	333	LYS
1	B	44	LEU
1	B	52	GLU
1	B	74	LEU
1	B	112	SER
1	B	113	GLU
1	B	132	TYR
1	B	157	LEU
1	B	219	LEU
1	B	249	MET
1	B	311	ASP
1	B	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	262	GLN
1	A	281	HIS
1	B	9	ASN
1	B	86	ASN
1	B	232	GLN
1	B	262	GLN
1	B	281	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	$\#\|Z\| > 2$
2	M3L	F	36	2	10,11,12	0.49	0	9,14,16	0.59	0
2	M3L	G	36	2	10,11,12	0.60	0	9,14,16	0.76	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
2	M3L	F	36	2	-	0/9/10/12	-
2	M3L	G	36	2	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	36	M3L	2	0
2	G	36	M3L	6	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
5	OGA	B	504	3	9,9,9	1.22	1 (11%)	10,11,11	1.81	2 (20%)
5	OGA	A	503	3	9,9,9	1.08	0	10,11,11	1.44	1 (10%)

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	B	504	3	-	0/8/9/9	-
5	OGA	A	503	3	-	0/8/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504	OGA	C4-C5	2.09	1.55	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	504	OGA	O2'-C2-C1	-3.76	116.02	121.32
5	A	503	OGA	O2'-C2-C1	-2.82	117.34	121.32
5	B	504	OGA	O1-C1-C2	-2.38	116.87	122.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	OGA	1	0
5	A	503	OGA	1	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^{th} 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	344/352 (97%)	1.27	84 (24%)	0	0	38, 46, 57, 72	0
1	B	337/352 (95%)	1.50	99 (29%)	0	0	37, 46, 61, 69	2 (0%)
2	F	3/16 (18%)	2.88	2 (66%)	0	0	69, 69, 70, 70	0
2	G	6/16 (37%)	2.39	3 (50%)	0	0	79, 80, 86, 88	0
All	All	690/736 (93%)	1.40	188 (27%)	0	0	37, 46, 60, 88	2 (0%)

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	ILE	7.1
1	B	197	ILE	7.0
1	B	194	LEU	6.7
1	A	197	ILE	6.7
1	B	166	ILE	6.7
1	A	269	ILE	6.5
1	B	196	SER	6.4
1	B	208	TRP	6.4
1	A	195	TYR	6.1
1	A	7	THR	6.1
1	A	196[A]	SER	6.1
1	B	308	CYS	6.1
1	A	291	PHE	5.8
1	A	194	LEU	5.8
1	A	311	ASP	5.8
1	B	270	THR	5.7
1	B	162	LYS	5.6
1	B	185	PHE	5.6
1	B	44	LEU	5.3
1	B	195	TYR	5.2
1	A	270	THR	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	268	MET	5.1
1	B	307	SER	5.1
2	F	34	GLY	5.1
1	B	165	GLY	5.0
1	A	185	PHE	5.0
1	B	45	ALA	5.0
1	A	271	PHE	4.9
1	A	104	ASP	4.9
1	B	271	PHE	4.9
1	A	310	LYS	4.9
1	A	208	TRP	4.8
1	A	187	TRP	4.8
1	A	44	LEU	4.7
1	B	345	LEU	4.7
1	B	291	PHE	4.6
1	B	198	ASN	4.6
1	A	110	ARG	4.6
1	A	338	ASN	4.6
1	B	311	ASP	4.5
2	G	38	PRO	4.5
1	B	276	HIS	4.5
1	B	186	ALA	4.5
1	A	112	SER	4.5
1	B	277	ALA	4.5
1	B	64	ASP	4.4
1	B	187	TRP	4.3
1	B	104	ASP	4.3
1	B	274	GLY	4.3
1	B	278	GLY	4.3
1	A	307	SER	4.3
1	B	334	ALA	4.2
1	B	161	GLU	4.2
1	A	113	GLU	4.2
1	A	45	ALA	4.2
1	A	334	ALA	4.1
1	B	10	PRO	4.1
1	A	277	ALA	4.1
1	B	232	GLN	4.0
1	B	167	THR	3.9
1	A	268	MET	3.9
1	B	177	TYR	3.9
1	B	60	ASP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	5	SER	3.9
1	B	164	SER	3.9
1	B	331	LEU	3.9
1	A	274	GLY	3.9
1	B	310	LYS	3.8
1	A	20	THR	3.8
1	A	272	PRO	3.8
1	A	275	TYR	3.8
1	A	52	GLU	3.7
1	A	312	MET	3.6
1	B	11	SER	3.6
1	B	286	ALA	3.6
1	B	114[A]	PHE	3.6
1	A	57	ALA	3.5
1	B	188	HIS	3.5
1	A	211	VAL	3.5
1	A	43	GLY	3.5
1	A	335	GLY	3.5
1	A	111	TYR	3.4
1	A	31	ILE	3.4
1	A	308	CYS	3.4
1	B	288	SER	3.3
1	B	189	THR	3.3
1	A	21	MET	3.3
1	A	198	ASN	3.3
1	B	184	SER	3.3
1	A	142	GLU	3.3
1	B	21	MET	3.3
2	G	34	GLY	3.2
1	B	275	TYR	3.2
1	A	144	HIS	3.2
1	B	260	VAL	3.2
1	B	340	VAL	3.2
1	B	57	ALA	3.1
1	A	328	ARG	3.1
1	B	336	LYS	3.1
1	B	272	PRO	3.1
1	A	292	ALA	3.1
1	B	163	GLU	3.1
1	B	289	THR	3.1
1	B	132	TYR	3.1
1	A	51	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	90	LYS	3.0
1	A	22	GLU	3.0
1	B	144	HIS	3.0
1	B	25	ARG	3.0
1	A	177	TYR	3.0
1	B	290	ASN	3.0
1	B	328	ARG	3.0
1	A	273	TYR	2.9
1	A	3	SER	2.9
1	A	184	SER	2.9
1	A	132	TYR	2.9
1	A	6	GLU	2.9
1	B	338	ASN	2.9
1	B	279	PHE	2.9
1	A	276	HIS	2.9
1	B	233	SER	2.9
1	A	189	THR	2.8
1	B	110	ARG	2.8
1	A	278	GLY	2.8
1	A	229	GLY	2.8
1	A	209	TYR	2.8
1	B	14	ILE	2.8
1	A	244	LEU	2.8
1	B	292	ALA	2.7
1	A	64	ASP	2.7
1	B	210	SER	2.7
1	A	186	ALA	2.7
1	B	244	LEU	2.7
1	A	115	GLU	2.7
1	B	183	THR	2.7
1	A	233	SER	2.7
1	B	150	ILE	2.7
1	A	330	LYS	2.7
1	A	8	LEU	2.7
1	A	61	ASP	2.6
1	A	289	THR	2.6
1	B	335	GLY	2.6
1	B	75	VAL	2.6
1	B	84	GLN	2.6
1	B	43	GLY	2.5
1	A	210[A]	SER	2.5
1	B	267	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	9	ASN	2.5
1	B	200	LEU	2.4
1	B	280	ASN	2.4
1	A	206	LYS	2.4
1	A	331	LEU	2.4
1	B	206	LYS	2.4
1	A	116	GLU	2.4
1	A	235	GLU	2.4
1	A	296	TRP	2.4
1	B	241	LYS	2.4
1	B	61	ASP	2.4
1	A	153	LEU	2.3
1	B	29	ARG	2.3
1	B	112	SER	2.3
1	B	190	GLU	2.3
1	B	154	ARG	2.3
1	B	207	SER	2.3
1	A	183	THR	2.3
1	B	296	TRP	2.3
1	A	290	ASN	2.3
1	B	193	ASP	2.2
1	A	245	ILE	2.2
1	A	63	ASP	2.2
1	B	209	TYR	2.2
1	B	230	SER	2.2
1	A	171	VAL	2.2
2	G	39	HIS	2.2
1	A	90	LYS	2.2
1	B	333	LYS	2.1
1	B	105	LYS	2.1
1	B	47	VAL	2.1
2	F	33	GLY	2.1
1	B	235	GLU	2.1
1	A	47	VAL	2.1
1	B	133	GLY	2.1
1	B	95	ARG	2.0
1	A	190	GLU	2.0
1	B	231	ALA	2.0
1	B	273	TYR	2.0
1	A	188	HIS	2.0
1	A	297	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
2	M3L	G	36	12/13	0.62	0.39	58,70,81,81	0
2	M3L	F	36	12/13	0.73	0.27	60,65,69,69	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, 95^{th} 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
5	OGA	A	503	10/10	0.93	0.22	46,53,56,56	0
5	OGA	B	504	10/10	0.95	0.27	40,51,53,54	0
3	NI	B	502	1/1	0.97	0.25	41,41,41,41	0
4	ZN	B	506	1/1	0.97	0.22	17,17,17,17	0
4	ZN	A	505	1/1	0.98	0.24	10,10,10,10	0
3	NI	A	501	1/1	0.99	0.12	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.