



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

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
<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

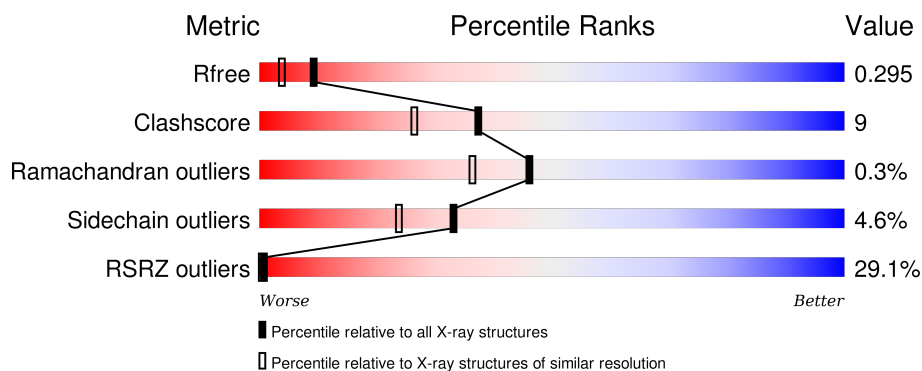
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 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	352	<div> <div>26%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	B	352	<div> <div>30%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>
2	F	16	<div> <div>13%</div> <div>19%</div> <div>6%</div> <div>75%</div> </div>
2	G	16	<div> <div>19%</div> <div>13%</div> <div>19%</div> <div>13%</div> <div>56%</div> </div>

2 Entry composition

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			

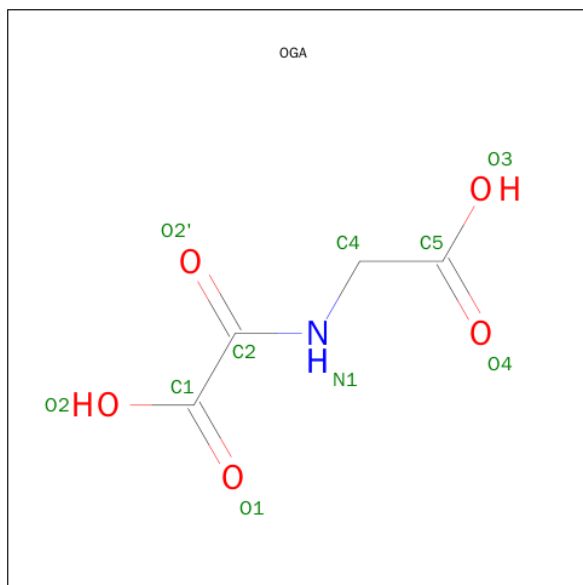
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

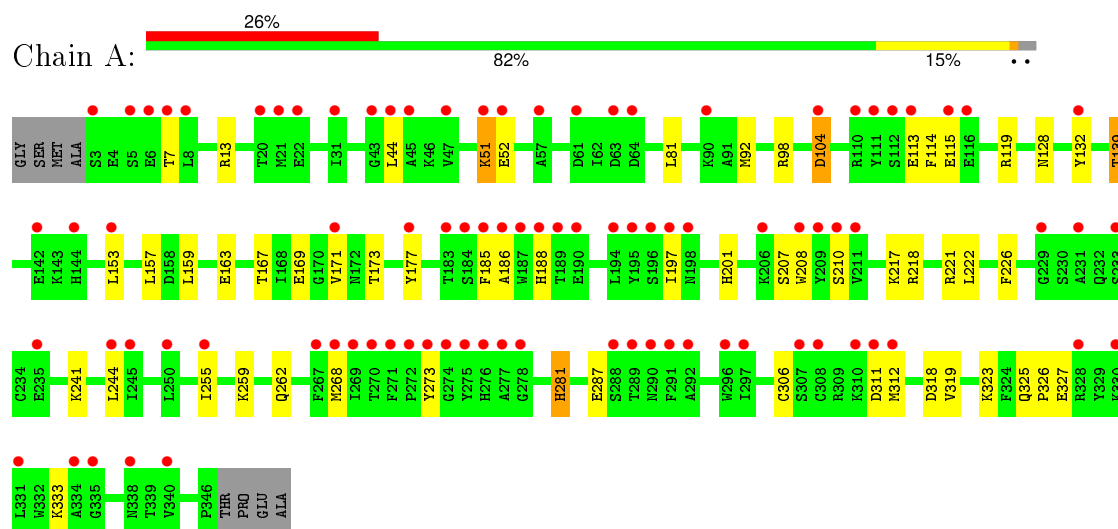
- Molecule 6 is water.

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

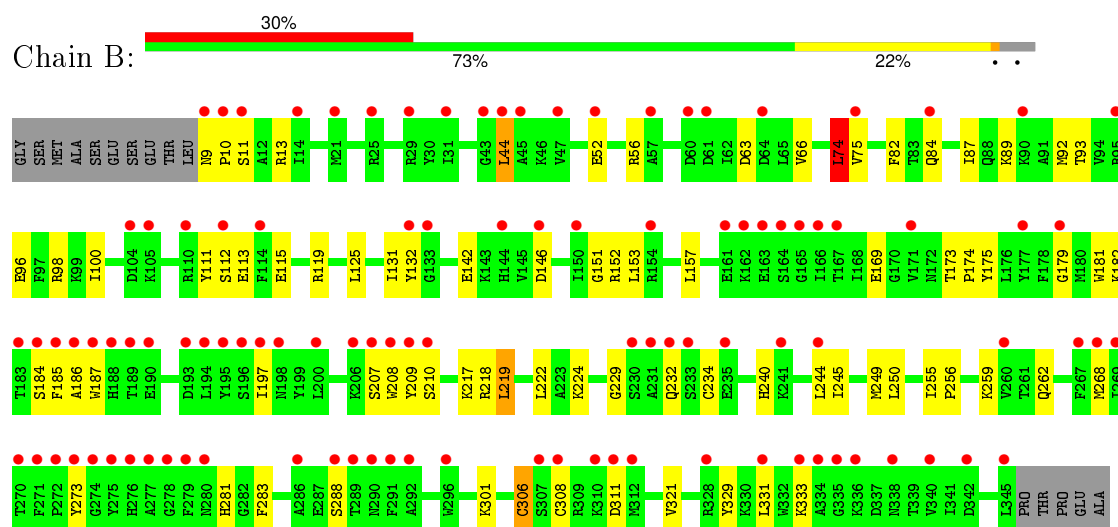
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



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

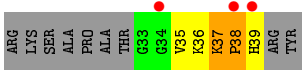
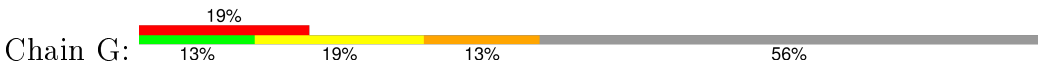


- Molecule 2: histone 3 peptide





● Molecule 2: histone 3 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.29 Å 148.96 Å 56.81 Å 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
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.05 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.260 0.257 , 0.295	Depositor DCC
R_{free} test set	2753 reflections (5.37%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 54030 reflections	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.*

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: NI, ZN, M3L, 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	0.75	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(°)	Ideal(°)
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 [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	2790	0	2672	42	0

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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

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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:234:CYS:SG	1:B:306:CYS:SG	3.06	0.54
1:B:56:ARG:HA	1:B:142:GLU:HG3	1.90	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:B:92:MET:HE1	1:B:100:ILE:HD12	1.96	0.48
1:A:153:LEU:HD11	1:A:197:ILE:HG21	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:B:240:HIS:NE2	1:B:306:CYS:SG	2.90	0.45
1:A:188:HIS:CD2	1:A:241:LYS:HE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLN:NE2	1:B:184:SER:OG	2.48	0.45
1:B:9:ASN:N	1:B:11:SER:HG	2.15	0.45
1:A:208:TRP:HE1	1:A:262:GLN:HE21	1.64	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:306:CYS:SG	1:B:308:CYS:SG	3.16	0.43
1:B:146:ASP:OD1	1:B:152:ARG:NH2	2.51	0.43
1:B:186:ALA:HA	1:B:244:LEU:HD23	2.00	0.43
1:B:92:MET:CE	1:B:100:ILE:HD12	2.48	0.43
1:B:89:LYS:HG3	1:B:131:ILE:HD12	2.00	0.43
1:B:153:LEU:HD11	1:B:197:ILE:HG21	2.00	0.43
1:B:209:TYR:HE2	1:B:259:LYS:HE2	1.83	0.43
1:B:82:PHE:HB2	1:B:244:LEU:HB2	2.00	0.43
1:A:171:VAL:HG23	2:F:36:M3L:HB3	2.01	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:NZ	1:B:224:LYS:CB	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:44:LEU:HD11	1:A:208:TRP:HB3	2.02	0.41
1:A:13:ARG:HG2	1:A:13:ARG:NH1	2.35	0.41
1:A:92:MET:HB2	1:A:92:MET:HE3	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%)	46	36

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%)	27	17
1	B	289/308 (94%)	278 (96%)	11 (4%)	40	31
2	G	3/11 (27%)	3 (100%)	0	100	100
All	All	588/627 (94%)	561 (95%)	27 (5%)	33	24

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

Some 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 ⓘ

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	F	36	2	10,11,12	0.47	0	12,14,16	0.72	0
2	M3L	G	36	2	10,11,12	0.65	0	12,14,16	0.84	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	-	0/8/10/12	0/0/0/0
2	M3L	G	36	2	-	0/8/10/12	0/0/0/0

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	503	3	3,9,9	0.20	0	3,11,11	1.23	0
5	OGA	B	504	3	3,9,9	0.33	0	3,11,11	1.37	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	503	3	-	0/3/9/9	0/0/0/0
5	OGA	B	504	3	-	0/3/9/9	0/0/0/0

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	OGA	1	0
5	B	504	OGA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	344/352 (97%)	1.37	90 (26%) 1 0	38, 46, 57, 72	0
1	B	337/352 (95%)	1.60	106 (31%) 1 0	37, 46, 61, 69	2 (0%)
2	F	3/16 (18%)	3.06	2 (66%) 0 0	69, 69, 70, 70	0
2	G	6/16 (37%)	2.52	3 (50%) 0 0	79, 80, 86, 88	0
All	All	690/736 (93%)	1.50	201 (29%) 1 0	37, 46, 60, 88	2 (0%)

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	ILE	7.5
1	B	197	ILE	7.4
1	A	197	ILE	7.1
1	B	194	LEU	7.1
1	B	166	ILE	7.0
1	A	269	ILE	6.9
1	B	208	TRP	6.7
1	B	196	SER	6.7
1	A	7	THR	6.3
1	A	195	TYR	6.3
1	B	308	CYS	6.3
1	A	196[A]	SER	6.3
1	A	291	PHE	6.1
1	A	194	LEU	6.1
1	B	270	THR	6.0
1	A	311	ASP	6.0
1	B	185	PHE	5.9
1	B	162	LYS	5.8
1	B	44	LEU	5.5
1	B	195	TYR	5.4
1	A	270	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	307	SER	5.3
2	F	34	GLY	5.3
1	B	268	MET	5.3
1	B	165	GLY	5.2
1	A	185	PHE	5.2
1	B	45	ALA	5.2
1	A	271	PHE	5.2
1	B	271	PHE	5.1
1	A	104	ASP	5.1
1	A	208	TRP	5.1
1	A	187	TRP	5.0
1	A	310	LYS	5.0
1	A	44	LEU	4.9
1	B	345	LEU	4.9
1	B	291	PHE	4.9
1	B	198	ASN	4.8
1	B	186	ALA	4.8
1	B	277	ALA	4.8
1	A	338	ASN	4.7
1	B	311	ASP	4.7
1	A	110	ARG	4.7
2	G	38	PRO	4.7
1	A	112	SER	4.7
1	B	276	HIS	4.6
1	B	64	ASP	4.6
1	B	187	TRP	4.6
1	B	274	GLY	4.5
1	B	278	GLY	4.5
1	B	104	ASP	4.5
1	A	307	SER	4.5
1	B	334	ALA	4.4
1	A	45	ALA	4.4
1	A	334	ALA	4.4
1	B	161	GLU	4.3
1	A	277	ALA	4.3
1	B	10	PRO	4.3
1	A	113	GLU	4.3
1	B	232	GLN	4.2
1	B	167	THR	4.1
1	B	164	SER	4.1
1	B	60	ASP	4.1
1	A	274	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	268	MET	4.1
1	B	331	LEU	4.1
1	B	177	TYR	4.0
1	A	5	SER	4.0
1	A	272	PRO	4.0
1	A	20	THR	4.0
1	B	310	LYS	3.9
1	A	275	TYR	3.9
1	A	52	GLU	3.9
1	B	286	ALA	3.8
1	A	312	MET	3.8
1	B	114[A]	PHE	3.8
1	A	57	ALA	3.8
1	A	211	VAL	3.8
1	B	11	SER	3.7
1	A	43	GLY	3.7
1	A	335	GLY	3.6
1	B	188	HIS	3.6
1	A	31	ILE	3.6
1	A	111	TYR	3.6
1	A	308	CYS	3.5
1	B	288	SER	3.5
1	B	189	THR	3.5
1	B	184	SER	3.4
1	A	198	ASN	3.4
2	G	34	GLY	3.4
1	B	21	MET	3.4
1	B	275	TYR	3.4
1	A	21	MET	3.4
1	A	142	GLU	3.4
1	B	260	VAL	3.4
1	B	340	VAL	3.4
1	A	144	HIS	3.3
1	B	57	ALA	3.3
1	A	292	ALA	3.3
1	B	272	PRO	3.2
1	B	289	THR	3.2
1	B	336	LYS	3.2
1	A	328	ARG	3.2
1	B	132	TYR	3.2
1	A	51	LYS	3.2
1	B	163	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	90	LYS	3.2
1	A	22	GLU	3.1
1	B	144	HIS	3.1
1	B	25	ARG	3.1
1	B	290	ASN	3.1
1	A	3	SER	3.1
1	A	177	TYR	3.1
1	A	132	TYR	3.1
1	A	273	TYR	3.1
1	B	328	ARG	3.1
1	B	279	PHE	3.1
1	A	184	SER	3.1
1	B	338	ASN	3.0
1	A	6	GLU	3.0
1	A	189	THR	3.0
1	B	14	ILE	3.0
1	A	276	HIS	3.0
1	B	233	SER	3.0
1	A	278	GLY	3.0
1	A	229	GLY	2.9
1	A	244	LEU	2.9
1	B	110	ARG	2.9
1	A	209	TYR	2.9
1	A	186	ALA	2.9
1	B	292	ALA	2.9
1	B	244	LEU	2.9
1	B	150	ILE	2.9
1	A	64	ASP	2.9
1	B	183	THR	2.8
1	A	8	LEU	2.8
1	B	210	SER	2.8
1	A	233	SER	2.8
1	A	330	LYS	2.8
1	B	75	VAL	2.8
1	A	115	GLU	2.8
1	B	335	GLY	2.7
1	A	61	ASP	2.7
1	A	289	THR	2.7
1	B	43	GLY	2.7
1	B	84	GLN	2.7
1	B	267	PHE	2.6
1	A	210[A]	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	2.6
1	B	9	ASN	2.6
1	B	280	ASN	2.5
1	A	331	LEU	2.5
1	A	206	LYS	2.5
1	A	153	LEU	2.5
1	A	296	TRP	2.5
1	B	206	LYS	2.5
1	B	61	ASP	2.5
1	A	116	GLU	2.5
1	A	235	GLU	2.5
1	B	112	SER	2.5
1	B	29	ARG	2.5
1	B	154	ARG	2.5
1	B	241	LYS	2.5
1	B	190	GLU	2.4
1	B	207	SER	2.4
1	B	296	TRP	2.4
1	A	183	THR	2.4
1	A	245	ILE	2.4
1	A	290	ASN	2.4
1	B	193	ASP	2.3
1	A	171	VAL	2.3
1	A	63	ASP	2.3
1	A	47	VAL	2.3
1	B	47	VAL	2.3
1	B	230	SER	2.3
1	B	209	TYR	2.3
2	G	39	HIS	2.3
2	F	33	GLY	2.2
1	A	90	LYS	2.2
1	B	105	LYS	2.2
1	B	333	LYS	2.2
1	B	235	GLU	2.2
1	A	340	VAL	2.2
1	A	297	ILE	2.2
1	B	133	GLY	2.2
1	B	171	VAL	2.2
1	B	231	ALA	2.2
1	B	95	ARG	2.1
1	A	190	GLU	2.1
1	B	273	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	188	HIS	2.1
1	B	31	ILE	2.1
1	A	250	LEU	2.1
1	A	231	ALA	2.1
1	B	52	GLU	2.1
1	B	312	MET	2.1
1	B	146	ASP	2.1
1	A	255	ILE	2.0
1	B	179	GLY	2.0
1	A	288	SER	2.0
1	A	267	PHE	2.0
1	B	342	ASP	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	M3L	F	36	12/13	0.73	0.28	-	60,65,69,69	0
2	M3L	G	36	12/13	0.62	0.39	-	58,70,81,81	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
4	ZN	A	505	1/1	0.98	0.24	0.65	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	B	506	1/1	0.97	0.22	0.04	17,17,17,17	0
5	OGA	A	503	10/10	0.93	0.22	-1.31	46,53,56,56	0
5	OGA	B	504	10/10	0.95	0.27	-1.50	40,51,53,54	0
3	NI	A	501	1/1	0.99	0.12	-2.94	37,37,37,37	0
3	NI	B	502	1/1	0.97	0.25	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.