



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID : 2Q8C
Title : Crystal structure of JMJD2A in ternary complex with an histone H3K9me3 peptide and 2-oxoglutarate
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

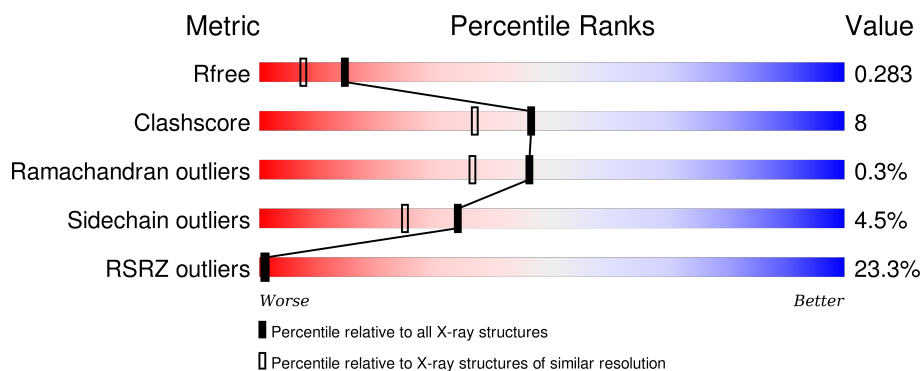
1 Overall quality at a glance

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>21%</div> <div>84%</div> <div>13%</div> <div>• •</div> </div>
1	B	352	<div> <div>23%</div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div>
2	F	15	<div> <div>13%</div> <div>20%</div> <div>7%</div> <div>73%</div> </div>
2	G	15	<div> <div>27%</div> <div>20%</div> <div>33%</div> <div>47%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5851 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	345	Total	C	N	O	S	0	1	0
			2794	1802	468	509	15			
1	B	335	Total	C	N	O	S	0	3	0
			2743	1775	461	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
			34	21	8	5			
2	G	8	Total	C	N	O	0	1	0
			57	32	15	10			

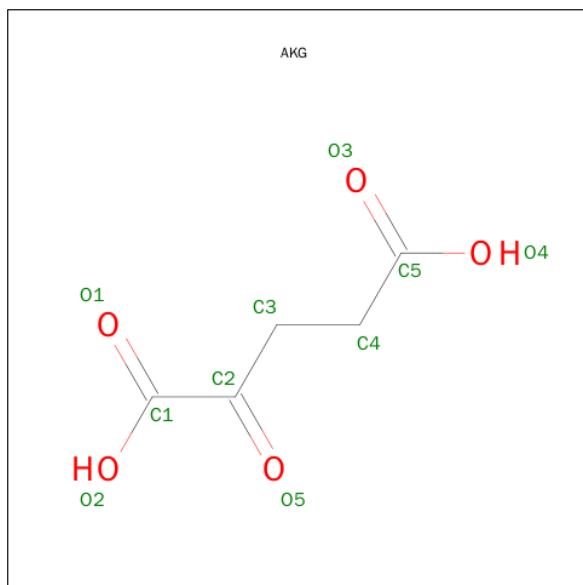
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



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

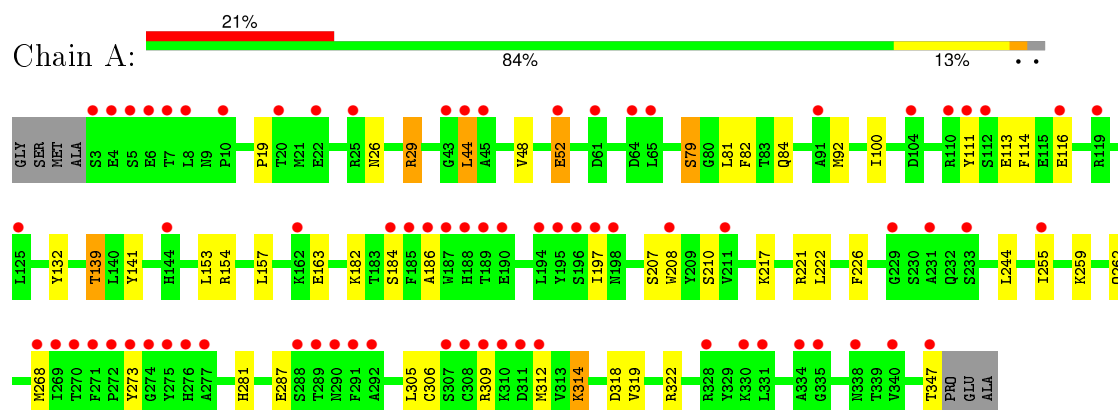
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	104	Total	O	0	0
			104	104		
6	B	94	Total	O	0	0
			94	94		
6	F	1	Total	O	0	0
			1	1		

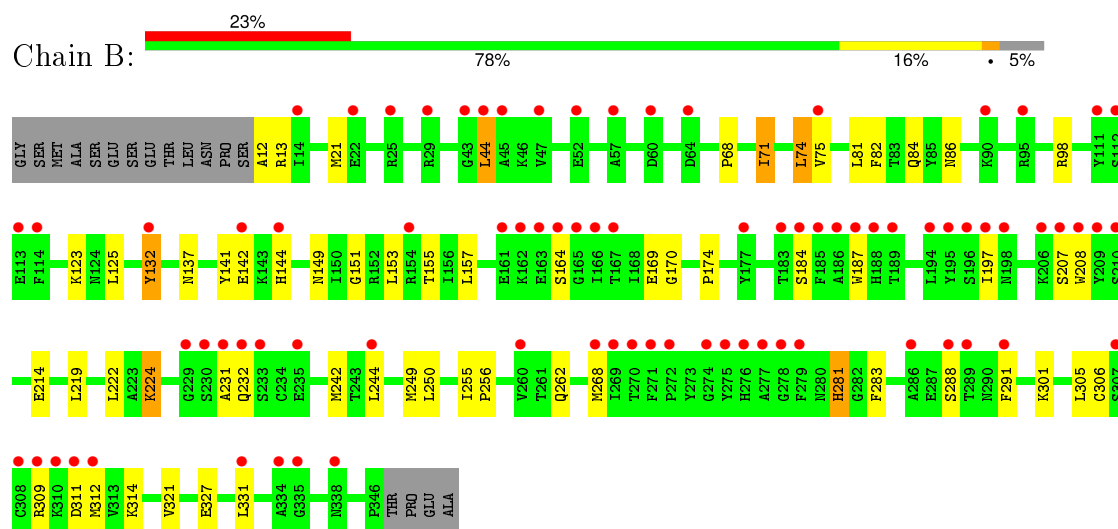
3 Residue-property plots [i](#)

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



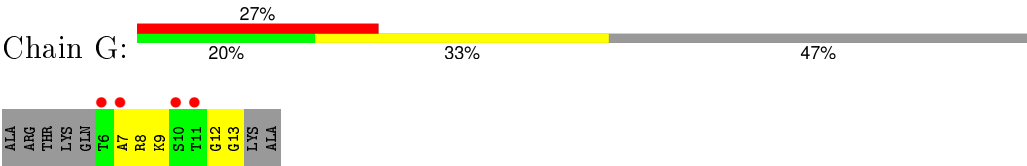
- Molecule 1: JmjC domain-containing histone demethylation protein 3A



- 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	100.89 Å 149.12 Å 57.06 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.90 – 2.05 28.97 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.90-2.05) 99.0 (28.97-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.04 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.236 0.262 , 0.283	Depositor DCC
R_{free} test set	2762 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54535 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5851	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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, AKG

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	0.55	0/2884	0.60	0/3911
1	B	0.54	0/2842	0.61	1/3853 (0.0%)
2	F	0.60	0/21	0.80	0/26
2	G	0.62	0/50	0.76	0/62
All	All	0.55	0/5797	0.61	1/7852 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	LEU	CA-CB-CG	-5.49	102.68	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	2794	0	2674	41	0
1	B	2743	0	2628	41	0
2	F	34	0	41	1	0
2	G	57	0	56	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	1	0
4	B	1	0	0	1	0
5	A	10	0	4	0	0
5	B	10	0	4	1	0
6	A	104	0	0	3	0
6	B	94	0	0	4	0
6	F	1	0	0	1	0
All	All	5851	0	5407	82	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 8.

All (82) 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:249:MET:HE3	6:B:554:HOH:O	1.57	1.02
1:A:139:THR:HG23	1:A:287:GLU:OE1	1.73	0.88
1:A:306:CYS:HG	4:A:505:ZN:ZN	0.85	0.86
1:A:139:THR:HG21	6:A:532:HOH:O	1.77	0.85
1:B:81:LEU:HG	1:B:249:MET:SD	2.22	0.79
1:B:306:CYS:HG	4:B:506:ZN:ZN	0.92	0.79
1:B:169:GLU:OE1	2:G:8[A]:ARG:NH1	2.16	0.79
1:A:163:GLU:HG3	1:A:319:VAL:HG21	1.65	0.78
1:A:92:MET:HE1	1:A:100:ILE:HD12	1.67	0.75
1:A:222:LEU:HD22	1:A:255:ILE:HD11	1.69	0.73
1:A:92:MET:CE	1:A:100:ILE:HD12	2.19	0.71
1:A:222:LEU:HD22	1:A:255:ILE:CD1	2.20	0.71
1:A:84:GLN:HE22	1:A:184:SER:HB2	1.57	0.70
1:B:214:GLU:HG3	6:B:512:HOH:O	1.94	0.67
1:A:44:LEU:HD22	1:A:268:MET:HE3	1.78	0.66
1:B:222:LEU:HD22	1:B:255:ILE:CD1	2.25	0.65
1:B:151:GLY:HA2	1:B:174:PRO:HG3	1.80	0.63
1:A:217:LYS:HD2	1:A:273:TYR:OH	2.00	0.62
1:A:222:LEU:HG	1:A:226:PHE:CE1	2.35	0.62
1:B:207:SER:OG	1:B:281:HIS:HE1	1.86	0.59
1:B:84:GLN:HE22	1:B:184:SER:HB2	1.67	0.58
1:B:306:CYS:HB3	1:B:312:MET:HG3	1.85	0.57
1:A:207:SER:OG	1:A:281:HIS:HE1	1.88	0.57
1:A:79:SER:OG	1:A:79:SER:O	2.22	0.56
1:A:139:THR:CG2	1:A:287:GLU:OE1	2.48	0.56
1:A:305:LEU:CD1	1:A:314:LYS:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:HD2	6:A:598:HOH:O	2.06	0.56
1:B:222:LEU:HD22	1:B:255:ILE:HD12	1.88	0.55
1:B:44:LEU:HD22	1:B:268:MET:HE3	1.88	0.53
1:B:242:MET:CG	2:G:13:GLY:HA2	2.38	0.53
1:A:44:LEU:HD22	1:A:268:MET:CE	2.38	0.53
1:B:242:MET:HG2	2:G:13:GLY:HA2	1.90	0.53
1:B:309[B]:ARG:HB3	1:B:312:MET:HG2	1.92	0.52
1:A:82:PHE:HB2	1:A:244:LEU:HB2	1.93	0.50
1:B:301:LYS:HD3	1:B:321:VAL:HG22	1.93	0.50
1:B:305:LEU:CD1	1:B:314:LYS:HG2	2.40	0.50
1:A:305:LEU:HD12	1:A:314:LYS:HG2	1.94	0.49
1:B:12:ALA:N	6:B:582:HOH:O	2.46	0.48
1:B:153:LEU:HD11	1:B:197:ILE:HG21	1.94	0.48
1:B:155:THR:HG21	1:B:291:PHE:HB2	1.94	0.48
1:A:186:ALA:HA	1:A:244:LEU:HD23	1.96	0.48
1:B:132:TYR:OH	5:B:504:AKG:O4	2.26	0.47
1:A:52:GLU:HG3	1:A:52:GLU:H	1.43	0.47
1:A:222:LEU:HD22	1:A:255:ILE:HD12	1.97	0.46
1:A:222:LEU:CD2	1:A:255:ILE:CD1	2.93	0.46
1:B:142:GLU:HB2	1:B:144:HIS:CE1	2.50	0.46
1:A:19:PRO:HD2	1:A:48:VAL:O	2.15	0.46
1:A:306:CYS:HB3	1:A:312:MET:HG3	1.98	0.45
1:B:71:ILE:HG21	1:B:86:ASN:HB3	1.96	0.45
1:B:82:PHE:HB2	1:B:244:LEU:HB2	1.99	0.45
1:B:98:ARG:HG3	1:B:283:PHE:CE2	2.51	0.45
1:B:123:LYS:HB2	1:B:123:LYS:HE2	1.80	0.45
1:A:44:LEU:HD12	1:A:210[B]:SER:HB3	1.98	0.44
1:B:75:VAL:HG11	1:B:125:LEU:HG	1.99	0.44
1:B:137:ASN:HD21	2:G:8[A]:ARG:HH12	1.66	0.44
1:B:309[A]:ARG:HB2	1:B:312:MET:HG2	1.99	0.44
1:B:208:TRP:HE1	1:B:262:GLN:NE2	2.16	0.43
1:A:221:ARG:HH11	1:B:13:ARG:CZ	2.31	0.43
1:B:197:ILE:O	1:B:288:SER:HB2	2.19	0.43
1:A:111:TYR:HA	1:A:116:GLU:OE2	2.19	0.43
1:B:170:GLY:O	2:G:9:M3L:HM23	2.19	0.43
1:B:255:ILE:HA	1:B:256:PRO:HD3	1.93	0.43
1:A:139:THR:HG22	1:A:141:TYR:H	1.84	0.42
1:A:222:LEU:CD2	1:A:255:ILE:HD11	2.44	0.42
1:B:68:PRO:HD2	6:B:533:HOH:O	2.19	0.42
1:A:208:TRP:HE1	1:A:262:GLN:NE2	2.18	0.42
1:A:208:TRP:HE1	1:A:262:GLN:HE21	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD11	1:A:197:ILE:HG21	2.01	0.42
1:B:208:TRP:HE1	1:B:262:GLN:HE21	1.68	0.41
1:A:309:ARG:HB2	1:A:312:MET:HG2	2.02	0.41
1:A:318:ASP:OD1	1:A:322:ARG:NH2	2.53	0.41
1:A:92:MET:HE3	1:A:100:ILE:HD12	1.99	0.41
1:B:224:LYS:HG3	1:B:231:ALA:HB2	2.00	0.41
1:A:81:LEU:HD21	1:A:226:PHE:CE1	2.56	0.41
1:A:182:LYS:HE3	6:A:547:HOH:O	2.21	0.41
2:F:7:ALA:O	6:F:95:HOH:O	2.22	0.41
1:A:114:PHE:HE2	1:A:207:SER:HG	1.66	0.40
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.56	0.40
1:A:29:ARG:HH11	1:A:29:ARG:HB3	1.86	0.40
1:B:187:TRP:CZ2	1:B:250:LEU:HD11	2.56	0.40
1:B:224:LYS:HG3	1:B:231:ALA:CB	2.52	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	344/352 (98%)	340 (99%)	4 (1%)	0	100	100
1	B	336/352 (96%)	332 (99%)	4 (1%)	0	100	100
2	F	1/15 (7%)	1 (100%)	0	0	100	100
2	G	6/15 (40%)	3 (50%)	1 (17%)	2 (33%)	0	0
All	All	687/734 (94%)	676 (98%)	9 (1%)	2 (0%)	46	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	7	ALA

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Mol	Chain	Res	Type
2	G	12	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/308 (96%)	283 (96%)	12 (4%)	37	28
1	B	288/308 (94%)	274 (95%)	14 (5%)	31	21
2	F	2/9 (22%)	2 (100%)	0	100	100
2	G	4/9 (44%)	4 (100%)	0	100	100
All	All	589/634 (93%)	563 (96%)	26 (4%)	34	26

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	ARG
1	A	44	LEU
1	A	52	GLU
1	A	79	SER
1	A	113	GLU
1	A	132	TYR
1	A	139	THR
1	A	157	LEU
1	A	259	LYS
1	A	314	LYS
1	A	347	THR
1	B	21	MET
1	B	44	LEU
1	B	71	ILE
1	B	74	LEU
1	B	132	TYR
1	B	157	LEU
1	B	164	SER
1	B	219	LEU

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Mol	Chain	Res	Type
1	B	224	LYS
1	B	232	GLN
1	B	281	HIS
1	B	311	ASP
1	B	327	GLU
1	B	331	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	84	GLN
1	A	86	ASN
1	A	262	GLN
1	A	281	HIS
1	B	84	GLN
1	B	232	GLN
1	B	262	GLN
1	B	281	HIS
1	B	290	ASN

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	9	2	10,11,12	0.56	0	12,14,16	0.84	0
2	M3L	G	9	2	10,11,12	0.61	0	12,14,16	0.67	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	9	2	-	0/8/10/12	0/0/0/0
2	M3L	G	9	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	9	M3L	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	AKG	A	503	3	3,9,9	2.15	1 (33%)	4,11,11	1.77	1 (25%)
5	AKG	B	504	3	3,9,9	1.67	1 (33%)	4,11,11	0.94	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	AKG	A	503	3	-	0/3/9/9	0/0/0/0
5	AKG	B	504	3	-	0/3/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504	AKG	C3-C2	2.89	1.55	1.51
5	A	503	AKG	C3-C2	3.64	1.56	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	AKG	C3-C4-C5	-3.32	106.66	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	AKG	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, 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	345/352 (98%)	1.16	74 (21%)  	33, 39, 53, 66	0
1	B	335/352 (95%)	1.30	81 (24%)  	30, 39, 58, 63	0
2	F	3/15 (20%)	2.85	2 (66%)  	64, 64, 65, 67	0
2	G	7/15 (46%)	3.59	4 (57%)  	69, 71, 72, 74	1 (14%)
All	All	690/734 (94%)	1.26	161 (23%)  	30, 39, 58, 74	1 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	6	THR	7.1
1	B	166	ILE	7.1
2	G	11	THR	7.0
1	A	5	SER	6.9
1	A	7	THR	6.4
1	A	197	ILE	6.0
1	B	311	ASP	6.0
1	B	208	TRP	6.0
1	A	3	SER	5.9
1	B	232	GLN	5.9
1	B	269	ILE	5.8
1	B	308	CYS	5.8
1	A	310	LYS	5.7
1	A	196	SER	5.6
1	B	307	SER	5.5
1	A	6	GLU	5.5
1	A	269	ILE	5.5
1	B	270	THR	5.4
1	A	307	SER	5.3
1	A	311	ASP	5.3
1	A	270	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	291	PHE	5.1
1	B	196	SER	5.0
1	B	197	ILE	4.9
1	B	163	GLU	4.8
1	B	185	PHE	4.8
1	A	195	TYR	4.8
1	B	310	LYS	4.7
1	A	194	LEU	4.7
1	A	4	GLU	4.7
1	B	338	ASN	4.7
1	A	334	ALA	4.7
1	B	309[A]	ARG	4.6
1	B	277	ALA	4.6
1	B	195	TYR	4.5
1	B	271	PHE	4.5
1	A	271	PHE	4.5
2	F	7	ALA	4.4
1	B	162	LYS	4.4
1	B	194	LEU	4.4
1	B	45	ALA	4.4
1	A	185	PHE	4.3
1	A	331	LEU	4.2
1	B	44	LEU	4.2
1	B	276	HIS	4.1
1	B	268	MET	4.1
1	B	154	ARG	4.1
1	A	111	TYR	4.1
1	B	278	GLY	4.1
1	B	260	VAL	4.0
1	A	335	GLY	4.0
1	A	20	THR	4.0
1	B	274	GLY	3.9
1	A	110	ARG	3.9
1	A	187	TRP	3.9
1	B	331	LEU	3.8
1	A	25	ARG	3.8
1	A	274	GLY	3.8
1	B	291	PHE	3.8
1	B	229	GLY	3.7
1	B	335	GLY	3.7
1	A	208	TRP	3.7
2	G	7	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	184	SER	3.6
1	A	144	HIS	3.6
1	B	161	GLU	3.6
1	B	167	THR	3.6
1	A	309	ARG	3.6
1	B	189	THR	3.6
1	A	44	LEU	3.5
1	B	187	TRP	3.5
1	B	334	ALA	3.5
1	B	165	GLY	3.5
1	B	111	TYR	3.5
1	A	272	PRO	3.5
1	A	308	CYS	3.5
1	A	275	TYR	3.5
1	B	186	ALA	3.4
1	A	276	HIS	3.4
1	B	60	ASP	3.4
1	A	188	HIS	3.3
1	B	312	MET	3.3
1	B	112	SER	3.3
1	A	277	ALA	3.3
1	A	43	GLY	3.3
1	A	347	THR	3.2
1	A	8	LEU	3.2
1	A	22	GLU	3.2
2	G	10	SER	3.2
1	A	312	MET	3.2
1	A	231	ALA	3.1
1	A	45	ALA	3.1
1	A	330	LYS	3.1
1	A	338	ASN	3.1
1	A	52	GLU	3.1
1	A	289	THR	3.0
1	B	188	HIS	3.0
1	B	114[A]	PHE	3.0
1	A	268	MET	3.0
1	B	230	SER	3.0
1	A	292	ALA	3.0
1	A	211	VAL	2.9
1	B	177	TYR	2.9
1	B	183	THR	2.9
1	B	198	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	198	ASN	2.9
1	B	14	ILE	2.9
1	A	162	LYS	2.8
1	B	235	GLU	2.8
1	A	273	TYR	2.8
1	A	189	THR	2.8
1	A	233	SER	2.8
1	B	286	ALA	2.8
1	B	272	PRO	2.7
2	F	10	SER	2.7
1	B	64	ASP	2.7
1	B	279	PHE	2.7
1	A	112	SER	2.7
1	B	275	TYR	2.7
1	A	340	VAL	2.6
1	B	144	HIS	2.6
1	A	290	ASN	2.6
1	B	288	SER	2.5
1	B	75	VAL	2.5
1	A	184	SER	2.5
1	B	231	ALA	2.5
1	B	207	SER	2.5
1	B	47	VAL	2.5
1	B	244	LEU	2.5
1	B	233	SER	2.5
1	A	328	ARG	2.5
1	B	29	ARG	2.5
1	B	95	ARG	2.5
1	A	186	ALA	2.4
1	B	57	ALA	2.4
1	B	25	ARG	2.4
1	B	43	GLY	2.4
1	A	255	ILE	2.4
1	A	64	ASP	2.4
1	A	65	LEU	2.4
1	A	288	SER	2.3
1	A	61	ASP	2.3
1	A	229	GLY	2.3
1	B	52	GLU	2.2
1	B	289	THR	2.2
1	A	125	LEU	2.2
1	B	142	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	206	LYS	2.2
1	B	164	SER	2.2
1	A	91	ALA	2.2
1	B	90	LYS	2.2
1	B	210	SER	2.2
1	B	22	GLU	2.2
1	A	104	ASP	2.1
1	B	132	TYR	2.1
1	A	116	GLU	2.1
1	A	119	ARG	2.1
1	A	190	GLU	2.1
1	B	113	GLU	2.0
1	B	209	TYR	2.0
1	A	10	PRO	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	G	9	12/13	0.83	0.26	-	46,58,67,67	0
2	M3L	F	9	12/13	0.77	0.22	-	48,56,63,63	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(\AA^2)	Q<0.9
4	ZN	A	505	1/1	0.97	0.36	1.24	12,12,12,12	0
4	ZN	B	506	1/1	0.97	0.35	0.45	12,12,12,12	0
5	AKG	A	503	10/10	0.84	0.25	-0.68	36,39,42,43	0
5	AKG	B	504	10/10	0.82	0.25	-1.13	32,38,40,43	0
3	NI	B	502	1/1	0.99	0.16	-	30,30,30,30	0
3	NI	A	501	1/1	0.98	0.11	-	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.