



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:29 AM UTC

PDB ID : 2Q8C / pdb_00002q8c
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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

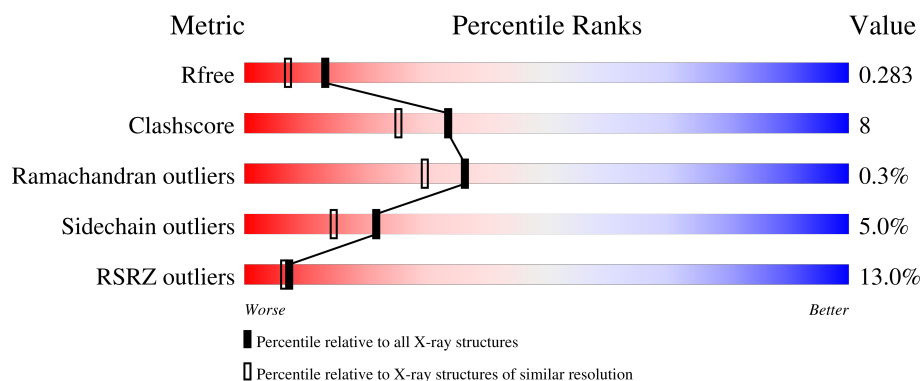
1 Overall quality at a glance

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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 $\leq 5\%$. 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	10% 83% 13% • •
1	B	352	13% 77% 17% • 5%
2	F	15	13% 20% 7% 73%
2	G	15	47% 20% 33% 47%

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			

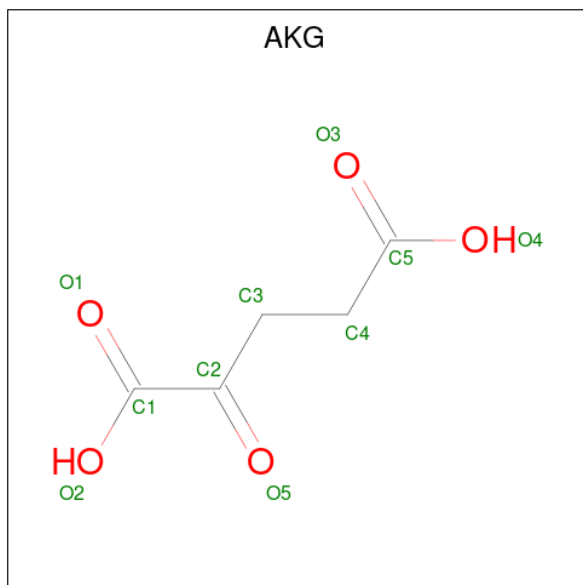
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



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		

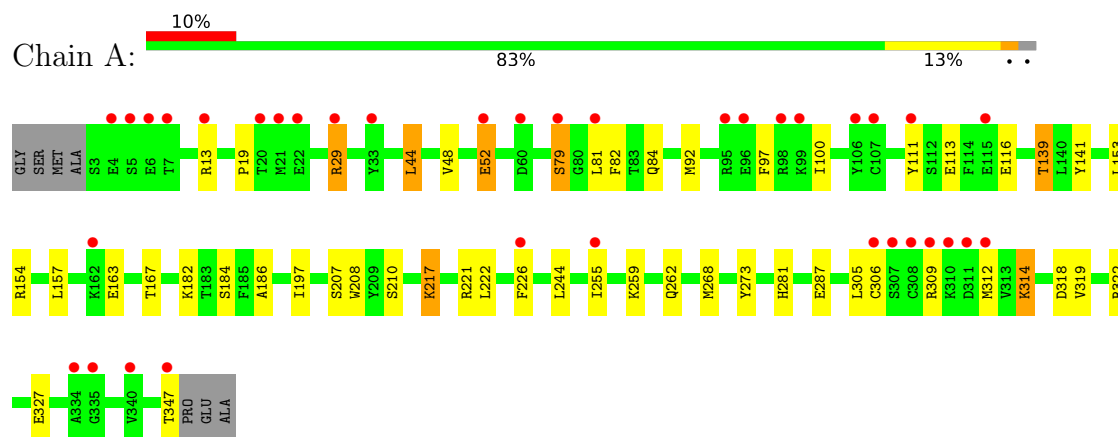
- Molecule 6 is water.

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		

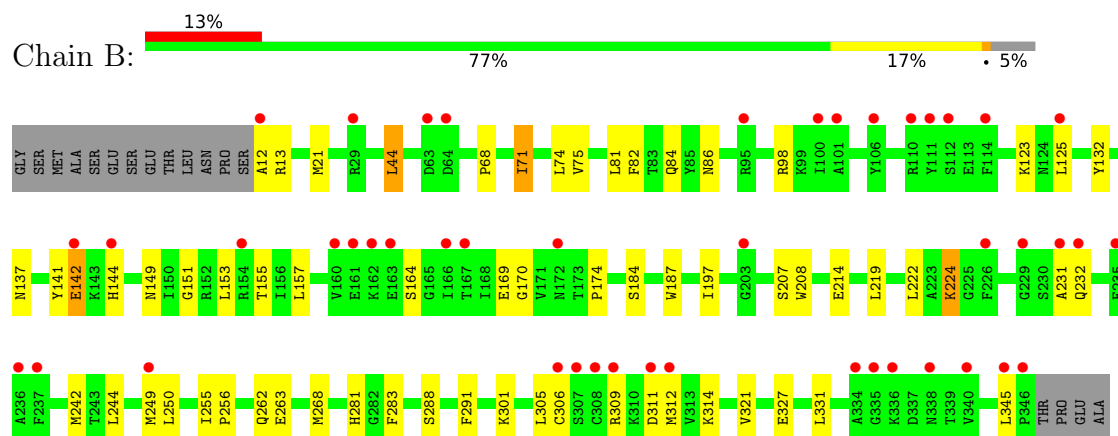
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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



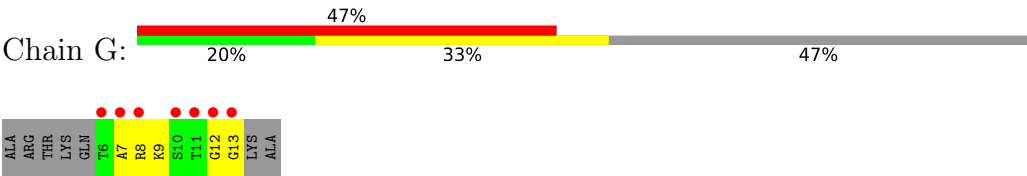
- Molecule 1: JmjC domain-containing histone demethylation protein 3A



- 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	100.89Å 149.12Å 57.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.90 – 2.05 28.90 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.90-2.05) 98.9 (28.90-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.236 0.261 , 0.283	Depositor DCC
R_{free} test set	2762 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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, 0.333 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: ZN, M3L, AKG, 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	0.68	0/2884	0.83	0/3911
1	B	0.65	0/2842	0.83	0/3853
2	F	0.60	0/21	0.43	0/26
2	G	0.64	0/50	0.87	0/62
All	All	0.66	0/5797	0.83	0/7852

There are no bond length outliers.

There are no bond angle outliers.

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	42	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
4	A	1	0	0	1	0
4	B	1	0	0	1	0
5	A	10	0	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	83	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 (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:HE1	1:A:100:ILE:HD12	1.39	1.02
1:B:249:MET:HE3	6:B:554:HOH:O	1.59	1.01
1:A:306:CYS:HG	4:A:505:ZN:ZN	0.75	1.01
1:A:139:THR:HG23	1:A:287:GLU:OE1	1.73	0.88
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: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:222:LEU:HD22	1:A:255:ILE:HD11	1.69	0.73
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:A:44:LEU:HD22	1:A:268:MET:HE3	1.75	0.69
1:A:92:MET:CE	1:A:100:ILE:HD12	2.19	0.69
1:B:306:CYS:HG	4:B:506:ZN:ZN	1.07	0.69
1:B:214:GLU:HG3	6:B:512:HOH:O	1.94	0.67
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:B:44:LEU:HD22	1:B:268:MET:HE3	1.80	0.62
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:A:92:MET:HE2	1:A:97:PHE:HA	1.82	0.61
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:A:92:MET:HE1	1:A:100:ILE:CD1	2.26	0.57
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:O	1:A:79:SER:OG	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

Continued on next page...

Continued from previous page...

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:242:MET:CG	2:G:13:GLY:HA2	2.38	0.53
1:B:242:MET:HG2	2:G:13:GLY:HA2	1.90	0.53
1:A:44:LEU:HD22	1:A:268:MET:CE	2.38	0.52
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:A:52:GLU:H	1:A:52:GLU:HG3	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:HE2	1:B:123:LYS:HB2	1.80	0.45
1:A:92:MET:HE2	1:A:97:PHE:CA	2.47	0.45
1:B:132:TYR:OH	5:B:504:AKG:O4	2.26	0.44
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

Continued on next page...

Continued from previous page...

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: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:29:ARG:HH11	1:A:29:ARG:HB3	1.86	0.40
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.56	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	36	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	7	ALA
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%)	281 (95%)	14 (5%)	23	17
1	B	288/308 (94%)	273 (95%)	15 (5%)	21	14
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%)	560 (95%)	29 (5%)	22	15

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	29	ARG
1	A	44	LEU
1	A	52	GLU
1	A	79	SER
1	A	113	GLU
1	A	139	THR
1	A	157	LEU
1	A	167	THR
1	A	217	LYS
1	A	259	LYS
1	A	314	LYS
1	A	327	GLU
1	A	347	THR
1	B	21	MET
1	B	44	LEU
1	B	71	ILE
1	B	74	LEU
1	B	142	GLU
1	B	157	LEU
1	B	164	SER
1	B	219	LEU
1	B	224	LYS
1	B	232	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	263	GLU
1	B	311	ASP
1	B	327	GLU
1	B	331	LEU
1	B	345	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	84	GLN
1	A	86	ASN
1	A	128	ASN
1	A	262	GLN
1	A	281	HIS
1	B	37	GLN
1	B	84	GLN
1	B	88	GLN
1	B	124	ASN
1	B	137	ASN
1	B	232	GLN
1	B	262	GLN
1	B	281	HIS
1	B	290	ASN
1	B	338	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	0.57	0	9,14,16	0.60	0
2	M3L	G	9	2	10,11,12	0.64	0	9,14,16	0.49	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	-	0/9/10/12	-
2	M3L	G	9	2	-	5/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	9	M3L	O-C-CA-CB
2	G	9	M3L	CD-CE-NZ-CM3
2	G	9	M3L	CD-CE-NZ-CM1
2	G	9	M3L	CD-CE-NZ-CM2
2	G	9	M3L	CE-CD-CG-CB

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 oligosaccharides 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	9,9,9	2.68	3 (33%)	11,11,11	3.06	4 (36%)
5	AKG	B	504	3	9,9,9	2.34	3 (33%)	11,11,11	2.87	3 (27%)

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	-	0/9/9/9	-
5	AKG	B	504	3	-	0/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	AKG	C2-C1	-5.20	1.45	1.53
5	A	503	AKG	C3-C2	5.04	1.56	1.51
5	B	504	AKG	C2-C1	-4.70	1.46	1.53
5	B	504	AKG	C3-C2	3.99	1.55	1.51
5	A	503	AKG	C4-C5	2.35	1.56	1.50
5	B	504	AKG	C4-C5	2.19	1.55	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	AKG	O1-C1-C2	-8.37	111.40	121.81
5	B	504	AKG	O1-C1-C2	-8.00	111.86	121.81
5	A	503	AKG	C3-C2-C1	3.16	121.22	115.86
5	A	503	AKG	O2-C1-C2	2.97	121.81	113.59
5	B	504	AKG	C3-C2-C1	2.89	120.77	115.86
5	B	504	AKG	O2-C1-C2	2.73	121.15	113.59
5	A	503	AKG	C3-C4-C5	-2.64	106.66	113.67

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 [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	345/352 (98%)	0.99	36 (10%) 11 11	32, 39, 53, 66	1 (0%)
1	B	335/352 (95%)	1.07	45 (13%) 7 6	26, 39, 58, 63	3 (0%)
2	F	3/15 (20%)	3.08	2 (66%) 0 0	64, 64, 65, 67	0
2	G	7/15 (46%)	4.01	7 (100%) 0 0	44, 69, 72, 74	2 (28%)
All	All	690/734 (94%)	1.07	90 (13%) 7 6	26, 39, 58, 74	6 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	11	THR	6.2
1	A	347	THR	5.3
2	F	7	ALA	5.3
2	G	13	GLY	4.9
2	G	10	SER	4.8
1	B	114[A]	PHE	4.4
1	A	5	SER	4.3
1	B	308	CYS	4.1
1	B	166	ILE	3.9
1	B	232	GLN	3.8
2	G	12	GLY	3.8
1	A	312	MET	3.5
1	A	334	ALA	3.5
1	B	309[A]	ARG	3.5
1	A	6	GLU	3.5
1	B	163	GLU	3.3
1	B	64	ASP	3.2
1	B	95	ARG	3.2
1	B	101	ALA	3.1
1	B	111	TYR	3.1
1	B	335	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	310	LYS	3.0
1	A	311	ASP	3.0
1	B	312	MET	3.0
2	G	8[A]	ARG	3.0
1	B	311	ASP	3.0
2	F	10	SER	2.9
2	G	6	THR	2.9
1	B	307	SER	2.9
1	A	162	LYS	2.9
1	A	255	ILE	2.9
1	B	154	ARG	2.9
1	A	79	SER	2.9
1	B	226	PHE	2.9
1	B	346	PRO	2.8
1	A	306	CYS	2.8
1	A	7	THR	2.8
1	B	249	MET	2.7
1	B	338	ASN	2.7
1	A	95	ARG	2.7
1	A	52	GLU	2.6
1	A	307	SER	2.6
1	A	107	CYS	2.6
1	B	172	ASN	2.6
1	A	111	TYR	2.6
2	G	7	ALA	2.6
1	B	162	LYS	2.6
1	B	336	LYS	2.6
1	A	226	PHE	2.5
1	B	29	ARG	2.5
1	A	29	ARG	2.5
1	B	345	LEU	2.5
1	B	340	VAL	2.4
1	A	22	GLU	2.4
1	B	161	GLU	2.4
1	B	334	ALA	2.4
1	B	100	ILE	2.4
1	A	98	ARG	2.4
1	B	203	GLY	2.4
1	A	60	ASP	2.4
1	B	167	THR	2.4
1	B	12	ALA	2.3
1	A	99	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	GLU	2.3
1	B	142	GLU	2.3
1	B	235	GLU	2.3
1	B	306	CYS	2.3
1	B	63	ASP	2.3
1	B	106	TYR	2.3
1	A	20	THR	2.3
1	A	21	MET	2.3
1	A	115	GLU	2.2
1	B	125	LEU	2.2
1	B	112	SER	2.2
1	A	340	VAL	2.2
1	A	335	GLY	2.2
1	B	231	ALA	2.2
1	B	229	GLY	2.1
1	A	309	ARG	2.1
1	A	106	TYR	2.1
1	B	160	VAL	2.1
1	A	13	ARG	2.1
1	B	110	ARG	2.1
1	A	33	TYR	2.1
1	B	236	ALA	2.1
1	A	4	GLU	2.1
1	A	308	CYS	2.1
1	B	237	PHE	2.0
1	A	81	LEU	2.0
1	B	144	HIS	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, 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($\text{\AA}^2$)	Q<0.9
2	M3L	F	9	12/13	0.85	0.17	48,56,63,63	0
2	M3L	G	9	12/13	0.87	0.17	46,58,67,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	AKG	A	503	10/10	0.76	0.17	36,39,42,43	0
5	AKG	B	504	10/10	0.84	0.14	32,38,40,43	0
4	ZN	A	505	1/1	0.98	0.42	12,12,12,12	0
4	ZN	B	506	1/1	0.98	0.42	12,12,12,12	0
3	NI	A	501	1/1	0.99	0.02	29,29,29,29	0
3	NI	B	502	1/1	1.00	0.02	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.