



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 2PXJ / pdb_00002pxj
Title : The complex structure of JMJD2A and monomethylated H3K36 peptide
Authors : Chen, Z.; Zang, J.; Kappler, J.; Hong, X.; Crawford, F.; Zhang, G.
Deposited on : 2007-05-14
Resolution : 2.00 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

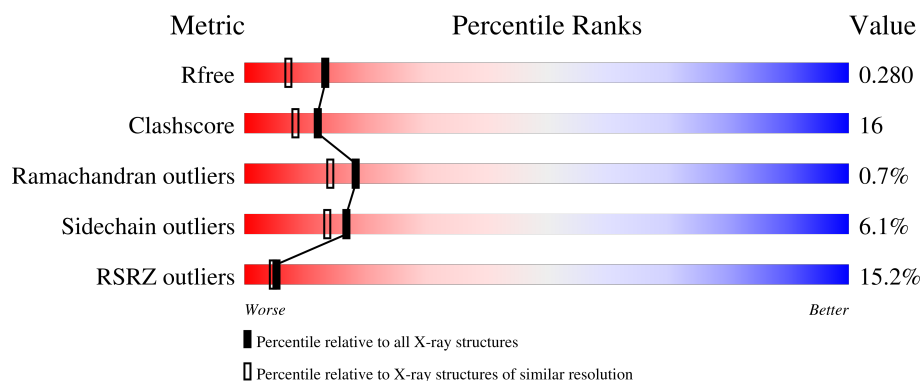
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	347	 14% 68% 28% .
1	B	347	 14% 67% 25% . .
2	I	22	 9% 9% 5% 77%
2	J	22	 14% 9% 5% 73%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5875 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	347	Total	C	N	O	S	0	0	0
			2849	1838	480	516	15			
1	B	337	Total	C	N	O	S	0	0	0
			2776	1796	469	496	15			

- Molecule 2 is a protein called monomethylated Histone H3K36 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	5	Total	C	N	O	0	0	0
			34	22	7	5			
2	J	6	Total	C	N	O	0	0	0
			41	26	8	7			

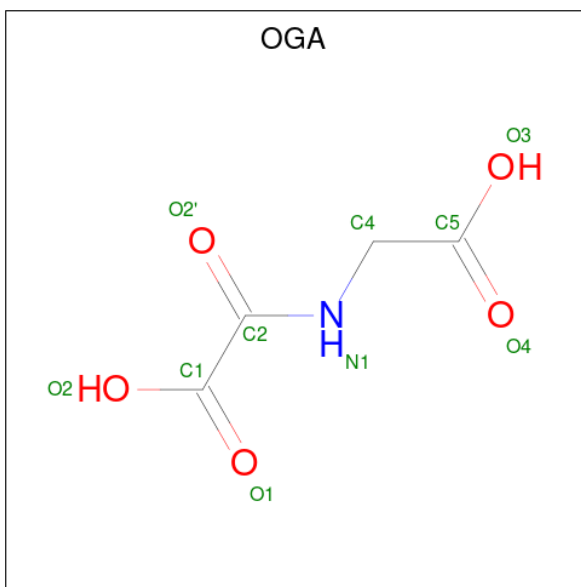
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



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

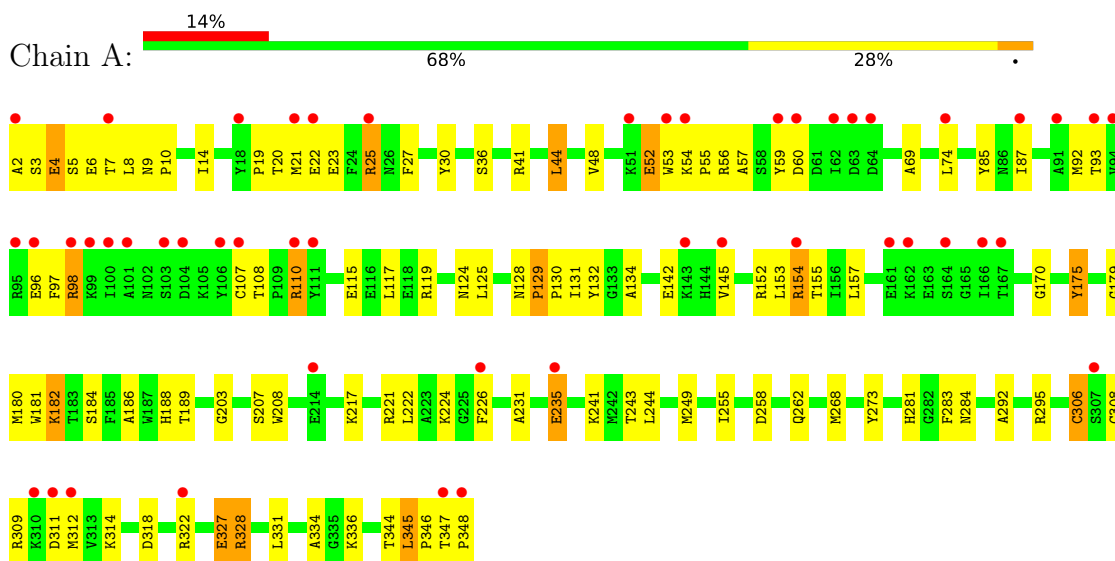
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total	O	0	0
			76	76		
6	B	74	Total	O	0	0
			74	74		
6	J	1	Total	O	0	0
			1	1		

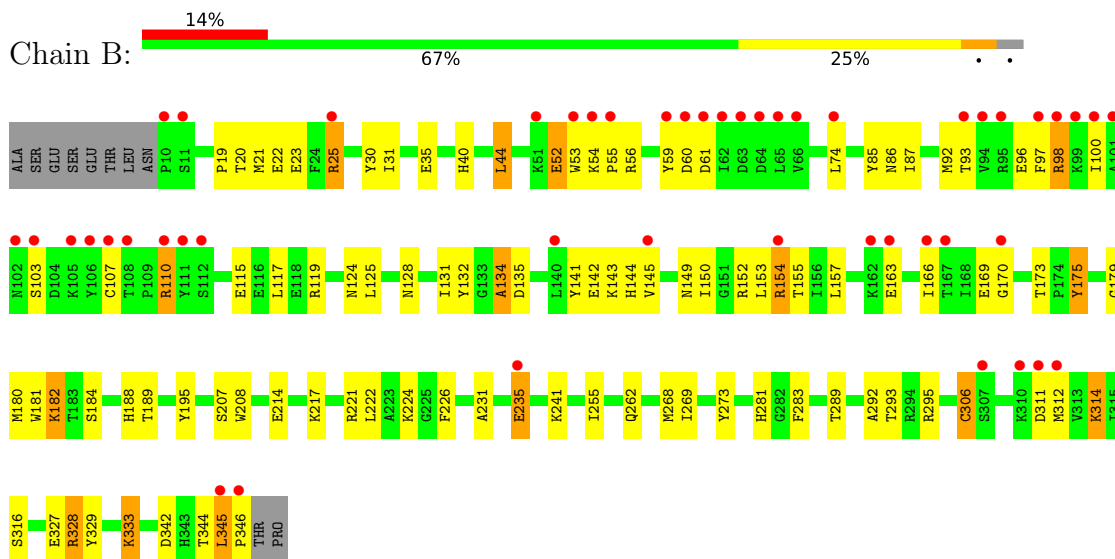
3 Residue-property plots

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.

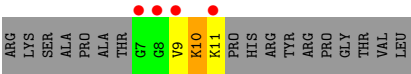
- Molecule 1: JmjC domain-containing histone demethylation protein 3A



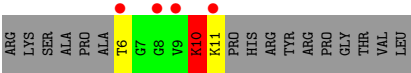
- Molecule 1: JmjC domain-containing histone demethylation protein 3A



- Molecule 2: monomethylated Histone H3K36 peptide



● Molecule 2: monomethylated Histone H3K36 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.86Å 150.17Å 57.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.56 – 2.00 45.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.7 (45.56-2.00) 90.7 (45.56-2.00)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.256 , 0.276 0.259 , 0.280	Depositor DCC
R_{free} test set	2356 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% 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: FE2, MLZ, OGA, ZN

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	0.48	0/2935	0.93	6/3972 (0.2%)
1	B	0.48	0/2861	0.93	5/3870 (0.1%)
2	I	1.07	0/22	0.84	0/25
2	J	0.79	0/29	0.74	0/35
All	All	0.49	0/5847	0.93	11/7902 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	THR	N-CA-C	-7.07	99.75	110.14
1	B	25	ARG	N-CA-C	6.15	117.98	111.28
1	B	189	THR	N-CA-C	-5.77	101.19	110.14
1	A	124	ASN	N-CA-C	5.72	120.26	112.88
1	A	25	ARG	N-CA-C	5.67	117.46	111.28
1	B	124	ASN	N-CA-C	5.35	119.78	112.88
1	B	134	ALA	N-CA-C	5.23	118.20	110.46
1	A	243	THR	N-CA-C	5.17	117.15	108.73
1	B	184	SER	N-CA-C	5.07	116.90	109.24
1	A	184	SER	N-CA-C	5.07	116.77	109.07
1	A	27	PHE	N-CA-C	5.06	117.19	111.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	10	MLZ	Mainchain

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	2849	0	2774	88	0
1	B	2776	0	2710	91	0
2	I	34	0	41	6	0
2	J	41	0	48	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	3	0	0
5	B	10	0	3	0	0
6	A	76	0	0	1	0
6	B	74	0	0	3	0
6	J	1	0	0	0	0
All	All	5875	0	5579	176	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 16.

All (176) 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:328:ARG:HH11	1:A:328:ARG:HG2	1.15	1.08
1:B:328:ARG:HH11	1:B:328:ARG:HG2	1.12	1.07
1:B:328:ARG:HG2	1:B:328:ARG:NH1	1.88	0.82
1:B:40:HIS:CD2	1:B:346:PRO:HG2	2.20	0.77
6:A:5044:HOH:O	2:I:9:VAL:HG12	1.85	0.77
1:A:217:LYS:HD2	1:A:273:TYR:OH	1.85	0.75
1:B:217:LYS:HD2	1:B:273:TYR:OH	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD22	1:B:255:ILE:HD12	1.68	0.74
1:A:222:LEU:HD22	1:A:255:ILE:HD12	1.70	0.73
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.01	0.72
1:A:69:ALA:HB3	2:I:11:LYS:HZ1	1.55	0.71
1:A:19:PRO:HB3	1:A:30:TYR:CZ	2.25	0.71
1:B:166:ILE:HD13	2:J:6:THR:O	1.90	0.71
1:A:235:GLU:N	1:A:235:GLU:OE1	2.24	0.70
1:A:110:ARG:NE	1:A:110:ARG:H	1.88	0.70
1:B:328:ARG:HH11	1:B:328:ARG:CG	1.98	0.70
1:B:19:PRO:HB3	1:B:30:TYR:CZ	2.27	0.69
1:B:295:ARG:HD2	1:B:346:PRO:HG3	1.74	0.69
1:B:135:ASP:HB2	2:J:11:LYS:HE2	1.75	0.69
1:A:328:ARG:HG2	1:A:328:ARG:NH1	1.92	0.68
1:B:110:ARG:NE	1:B:110:ARG:H	1.92	0.68
1:A:346:PRO:O	1:A:348:PRO:HD3	1.94	0.67
1:A:2:ALA:HA	1:A:6:GLU:HB2	1.77	0.67
1:A:175:TYR:HE1	2:I:10:MLZ:HB3	1.60	0.67
1:A:181:TRP:CE2	1:A:182:LYS:HG3	2.30	0.66
1:B:314:LYS:O	2:J:6:THR:HA	1.96	0.65
1:B:74:LEU:HD22	1:B:87:ILE:HD11	1.79	0.65
1:A:69:ALA:HB3	2:I:11:LYS:NZ	2.13	0.64
1:B:342:ASP:OD2	1:B:345:LEU:HG	1.97	0.63
1:A:175:TYR:CE1	2:I:10:MLZ:HB3	2.33	0.63
1:B:40:HIS:CE1	1:B:346:PRO:HB2	2.33	0.63
1:B:181:TRP:CE2	1:B:182:LYS:HG3	2.34	0.63
1:A:85:TYR:CG	1:B:74:LEU:HD21	2.34	0.63
1:A:56:ARG:HD2	1:A:59:TYR:CE2	2.34	0.62
1:B:235:GLU:N	1:B:235:GLU:OE1	2.32	0.62
1:B:222:LEU:HD22	1:B:255:ILE:CD1	2.30	0.61
1:B:175:TYR:CE1	2:J:10:MLZ:HB3	2.36	0.60
1:A:110:ARG:O	1:A:110:ARG:HD2	2.00	0.60
1:A:44:LEU:HD22	1:A:268:MET:HE3	1.84	0.60
1:A:115:GLU:HG2	1:A:119:ARG:HH12	1.65	0.60
1:A:74:LEU:HD22	1:A:87:ILE:HD11	1.84	0.59
1:A:188:HIS:CD2	1:A:241:LYS:HE2	2.37	0.59
1:A:222:LEU:HD22	1:A:255:ILE:CD1	2.32	0.59
1:B:53:TRP:O	1:B:54:LYS:HD3	2.02	0.59
1:B:56:ARG:HD2	1:B:59:TYR:CE2	2.38	0.59
1:B:92:MET:HE2	1:B:97:PHE:CA	2.32	0.59
1:B:142:GLU:OE1	1:B:144:HIS:HE1	1.84	0.59
1:B:329:TYR:CE2	1:B:333:LYS:HD3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASN:N	1:A:10:PRO:HD3	2.20	0.57
1:B:40:HIS:NE2	1:B:346:PRO:HG2	2.20	0.56
1:A:85:TYR:CB	1:B:74:LEU:HD21	2.35	0.56
1:A:22:GLU:OE2	1:A:25:ARG:NH1	2.38	0.56
1:B:20:THR:OG1	1:B:23:GLU:HG3	2.06	0.56
1:B:208:TRP:HE1	1:B:262:GLN:HE21	1.53	0.56
1:A:345:LEU:HD23	1:A:346:PRO:CD	2.35	0.56
1:B:44:LEU:HD22	1:B:268:MET:HE3	1.88	0.56
1:B:115:GLU:HG2	1:B:119:ARG:HH12	1.70	0.56
1:A:55:PRO:HA	1:A:145:VAL:HG21	1.88	0.55
1:A:92:MET:HE2	1:A:97:PHE:CA	2.37	0.55
1:B:103:SER:O	1:B:107:CYS:HB2	2.07	0.55
1:B:175:TYR:HE1	2:J:10:MLZ:HB3	1.70	0.55
1:A:334:ALA:O	1:A:336:LYS:HG3	2.07	0.55
1:A:331:LEU:CD1	1:A:336:LYS:HB2	2.36	0.54
1:B:152:ARG:O	1:B:154:ARG:HD2	2.06	0.54
1:B:295:ARG:HD2	1:B:346:PRO:CG	2.38	0.54
1:B:22:GLU:OE2	1:B:25:ARG:NH1	2.40	0.54
1:A:20:THR:OG1	1:A:23:GLU:HG3	2.08	0.53
1:A:328:ARG:CG	1:A:328:ARG:NH1	2.64	0.53
1:A:56:ARG:HD2	1:A:59:TYR:CD2	2.43	0.53
1:A:152:ARG:O	1:A:154:ARG:HD2	2.07	0.53
1:A:208:TRP:HE1	1:A:262:GLN:HE21	1.55	0.53
1:B:306:CYS:SG	1:B:312:MET:HG3	2.49	0.53
1:A:224:LYS:HG3	1:A:231:ALA:HB1	1.91	0.53
1:A:318:ASP:OD1	1:A:322:ARG:NH2	2.41	0.52
1:B:110:ARG:O	1:B:110:ARG:HD2	2.08	0.52
1:A:98:ARG:HH11	1:A:98:ARG:HG2	1.75	0.52
1:A:224:LYS:HG3	1:A:231:ALA:CB	2.39	0.52
1:A:331:LEU:HD12	1:A:336:LYS:HB2	1.92	0.51
1:A:2:ALA:N	1:A:6:GLU:OE2	2.43	0.51
1:B:188:HIS:CD2	1:B:241:LYS:HE2	2.46	0.51
1:A:93:THR:HG23	1:A:96:GLU:OE1	2.11	0.51
1:A:74:LEU:HD21	1:B:85:TYR:CG	2.46	0.50
1:A:132:TYR:CD2	1:A:134:ALA:HB2	2.46	0.50
1:B:328:ARG:NH1	1:B:328:ARG:CG	2.62	0.50
1:A:85:TYR:HB2	1:B:74:LEU:HD21	1.92	0.50
1:B:40:HIS:NE2	1:B:346:PRO:HB2	2.25	0.50
1:B:92:MET:HE2	1:B:97:PHE:N	2.26	0.50
1:B:55:PRO:HA	1:B:145:VAL:HG21	1.93	0.50
1:B:224:LYS:HG3	1:B:231:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:HE2	1:A:97:PHE:HA	1.94	0.50
1:B:217:LYS:O	1:B:221:ARG:HG3	2.12	0.49
1:B:208:TRP:HE1	1:B:262:GLN:NE2	2.09	0.49
1:A:41:ARG:NE	1:A:344:THR:HG22	2.28	0.49
1:A:170:GLY:O	2:I:10:MLZ:HE2	2.13	0.49
1:B:56:ARG:HD2	1:B:59:TYR:CD2	2.49	0.48
1:B:224:LYS:HG3	1:B:231:ALA:CB	2.43	0.48
1:B:153:LEU:O	1:B:154:ARG:HD3	2.14	0.48
1:A:3:SER:C	1:A:5:SER:H	2.20	0.47
1:A:7:THR:HG22	1:A:7:THR:O	2.14	0.47
1:A:208:TRP:HE1	1:A:262:GLN:NE2	2.12	0.47
1:A:217:LYS:O	1:A:221:ARG:HG3	2.14	0.47
1:A:8:LEU:HD13	1:A:36:SER:O	2.14	0.47
1:B:155:THR:HB	1:B:292:ALA:O	2.14	0.47
1:A:155:THR:HB	1:A:292:ALA:O	2.15	0.47
1:B:93:THR:HG23	1:B:96:GLU:OE1	2.14	0.47
1:A:53:TRP:CZ3	1:A:55:PRO:HD3	2.50	0.47
1:B:222:LEU:HG	1:B:226:PHE:CE1	2.50	0.47
1:A:181:TRP:NE1	1:A:182:LYS:HG3	2.29	0.47
1:A:56:ARG:HA	1:A:142:GLU:OE2	2.15	0.47
1:B:131:ILE:O	1:B:180:MET:HE3	2.15	0.47
1:B:295:ARG:CD	1:B:346:PRO:HG3	2.45	0.46
1:A:306:CYS:SG	1:A:312:MET:HG3	2.56	0.46
1:A:14:ILE:HG13	1:A:258:ASP:HB3	1.97	0.46
1:B:92:MET:HE2	1:B:97:PHE:HA	1.97	0.46
1:B:86:ASN:ND2	6:B:6026:HOH:O	2.48	0.46
1:B:163:GLU:O	1:B:163:GLU:HG3	2.15	0.46
1:B:179:GLY:O	1:B:283:PHE:HA	2.15	0.46
6:B:6050:HOH:O	2:J:10:MLZ:HE3	2.16	0.45
1:A:4:GLU:O	1:A:4:GLU:HG3	2.16	0.45
1:B:98:ARG:HH11	1:B:98:ARG:HG2	1.81	0.44
1:A:153:LEU:O	1:A:154:ARG:HD3	2.17	0.44
1:A:295:ARG:HB2	1:A:347:THR:OG1	2.17	0.44
1:B:135:ASP:HB2	2:J:11:LYS:CE	2.43	0.44
1:A:327:GLU:CD	1:A:327:GLU:H	2.26	0.44
1:A:345:LEU:HD23	1:A:346:PRO:HD2	1.99	0.44
1:B:125:LEU:HA	1:B:182:LYS:HD2	1.99	0.44
1:A:85:TYR:HB2	1:B:74:LEU:CD2	2.46	0.44
1:A:110:ARG:H	1:A:110:ARG:CD	2.31	0.44
1:B:195:TYR:CE1	1:B:293:THR:HG23	2.53	0.44
1:A:131:ILE:O	1:A:180:MET:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:CYS:SG	1:A:309:ARG:HG3	2.58	0.43
1:B:207:SER:OG	1:B:281:HIS:HE1	2.01	0.43
1:A:345:LEU:HD22	1:A:346:PRO:O	2.17	0.43
1:B:115:GLU:HG2	1:B:119:ARG:NH1	2.34	0.43
1:B:345:LEU:CB	1:B:346:PRO:CD	2.96	0.43
1:B:214:GLU:HB2	6:B:6075:HOH:O	2.18	0.43
1:A:53:TRP:O	1:A:54:LYS:HD3	2.19	0.43
1:B:31:ILE:O	1:B:35:GLU:HG3	2.17	0.43
1:B:170:GLY:O	2:J:10:MLZ:HE2	2.19	0.43
1:B:295:ARG:NH1	1:B:346:PRO:HG3	2.33	0.43
1:A:179:GLY:O	1:A:283:PHE:HA	2.18	0.43
1:B:295:ARG:CZ	1:B:346:PRO:HG3	2.49	0.42
1:A:19:PRO:HB3	1:A:30:TYR:CE1	2.54	0.42
1:A:19:PRO:HD2	1:A:48:VAL:O	2.19	0.42
1:A:207:SER:OG	1:A:281:HIS:HE1	2.02	0.42
1:B:345:LEU:HB2	1:B:346:PRO:CD	2.48	0.42
1:B:21:MET:HE2	1:B:52:GLU:CD	2.44	0.42
1:B:345:LEU:O	1:B:346:PRO:C	2.61	0.42
1:A:44:LEU:CD2	1:A:268:MET:HE3	2.49	0.42
1:B:169:GLU:HA	1:B:173:THR:OG1	2.19	0.42
1:A:21:MET:HE2	1:A:52:GLU:OE1	2.19	0.42
1:B:132:TYR:CD2	1:B:134:ALA:HB2	2.55	0.42
1:A:115:GLU:HG2	1:A:119:ARG:NH1	2.33	0.41
1:A:186:ALA:HA	1:A:244:LEU:HD23	2.01	0.41
1:B:181:TRP:NE1	1:B:182:LYS:HG3	2.35	0.41
1:B:31:ILE:CD1	1:B:269:ILE:HD13	2.50	0.41
1:A:203:GLY:HA3	1:A:284:ASN:HA	2.01	0.41
1:B:21:MET:HE2	1:B:52:GLU:OE1	2.21	0.41
1:B:44:LEU:CD2	1:B:268:MET:HE3	2.50	0.41
1:B:316:SER:H	2:J:6:THR:HG1	1.64	0.41
1:A:129:PRO:HA	1:A:130:PRO:HD2	1.94	0.41
1:B:150:ILE:HG23	1:B:289:THR:HG22	2.03	0.41
1:B:342:ASP:CG	1:B:345:LEU:HG	2.45	0.41
1:A:57:ALA:N	1:A:142:GLU:OE2	2.54	0.41
1:A:74:LEU:HD13	1:A:87:ILE:HD12	2.02	0.41
1:A:226:PHE:CZ	1:A:249:MET:HE3	2.56	0.41
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.56	0.41
1:B:56:ARG:HA	1:B:142:GLU:OE2	2.21	0.40
1:B:74:LEU:HD13	1:B:87:ILE:HD12	2.02	0.40
1:A:107:CYS:SG	1:A:108:THR:N	2.94	0.40
1:A:125:LEU:HA	1:A:182:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLN:CD	1:A:268:MET:HG2	2.46	0.40
1:A:8:LEU:O	1:A:41:ARG:NH1	2.54	0.40
1:B:96:GLU:O	1:B:100:ILE:HG13	2.22	0.40
1:B:262:GLN:CD	1:B:268:MET:HG2	2.47	0.40
1:B:345:LEU:HB2	1:B:346:PRO:HD2	2.02	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	345/347 (99%)	321 (93%)	22 (6%)	2 (1%)	21	17
1	B	335/347 (96%)	313 (93%)	19 (6%)	3 (1%)	14	9
2	I	2/22 (9%)	2 (100%)	0	0	100	100
2	J	3/22 (14%)	3 (100%)	0	0	100	100
All	All	685/738 (93%)	639 (93%)	41 (6%)	5 (1%)	18	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	ASP
1	B	311	ASP
1	B	143	LYS
1	B	345	LEU
1	A	129	PRO

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	305/305 (100%)	287 (94%)	18 (6%)	18	14
1	B	296/305 (97%)	277 (94%)	19 (6%)	16	12
2	I	2/16 (12%)	2 (100%)	0	100	100
2	J	3/16 (19%)	3 (100%)	0	100	100
All	All	606/642 (94%)	569 (94%)	37 (6%)	17	14

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	44	LEU
1	A	52	GLU
1	A	60	ASP
1	A	98	ARG
1	A	110	ARG
1	A	117	LEU
1	A	128	ASN
1	A	154	ARG
1	A	157	LEU
1	A	175	TYR
1	A	182	LYS
1	A	235	GLU
1	A	306	CYS
1	A	314	LYS
1	A	327	GLU
1	A	328	ARG
1	A	345	LEU
1	B	44	LEU
1	B	52	GLU
1	B	60	ASP
1	B	61	ASP
1	B	98	ARG
1	B	110	ARG
1	B	117	LEU
1	B	128	ASN
1	B	154	ARG
1	B	157	LEU

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Mol	Chain	Res	Type
1	B	175	TYR
1	B	182	LYS
1	B	235	GLU
1	B	306	CYS
1	B	314	LYS
1	B	327	GLU
1	B	328	ARG
1	B	333	LYS
1	B	344	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	124	ASN
1	A	128	ASN
1	A	262	GLN
1	A	281	HIS
1	B	37	GLN
1	B	84	GLN
1	B	124	ASN
1	B	128	ASN
1	B	144	HIS
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	MLZ	I	10	2	8,9,10	0.88	0	4,9,11	1.91	1 (25%)
2	MLZ	J	10	2	8,9,10	0.90	0	4,9,11	2.00	1 (25%)

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	MLZ	I	10	2	-	1/7/8/10	-
2	MLZ	J	10	2	-	1/7/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	10	MLZ	CD-CG-CB	-3.38	100.87	113.62
2	I	10	MLZ	CD-CG-CB	-3.29	101.22	113.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	10	MLZ	O-C-CA-CB
2	J	10	MLZ	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	10	MLZ	3	0
2	J	10	MLZ	4	0

5.5 Carbohydrates

There are no oligosaccharides 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	B	6001	4	9,9,9	4.19	5 (55%)	8,11,11	2.78	2 (25%)
5	OGA	A	5001	4	9,9,9	4.21	6 (66%)	8,11,11	2.65	2 (25%)

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	6001	4	-	0/8/9/9	-
5	OGA	A	5001	4	-	0/8/9/9	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5001	OGA	C2-N1	10.70	1.51	1.33
5	B	6001	OGA	C2-N1	10.62	1.51	1.33
5	A	5001	OGA	O4-C5	3.91	1.34	1.22
5	B	6001	OGA	O4-C5	3.63	1.34	1.22
5	B	6001	OGA	C2-C1	-3.45	1.50	1.54
5	B	6001	OGA	C4-N1	3.24	1.53	1.45
5	A	5001	OGA	C2-C1	-3.20	1.50	1.54
5	A	5001	OGA	C4-N1	3.05	1.53	1.45
5	B	6001	OGA	O3-C5	-2.33	1.23	1.30
5	A	5001	OGA	O3-C5	-2.26	1.23	1.30
5	A	5001	OGA	O2-C1	2.18	1.36	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	6001	OGA	C4-N1-C2	-6.92	110.61	121.29
5	A	5001	OGA	C4-N1-C2	-6.65	111.03	121.29
5	B	6001	OGA	O3-C5-C4	2.36	121.77	112.81
5	A	5001	OGA	O3-C5-C4	2.02	120.49	112.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	347/347 (100%)	0.88	49 (14%)	6 5	21, 39, 70, 82	0
1	B	337/347 (97%)	0.88	48 (14%)	6 5	21, 39, 70, 82	0
2	I	4/22 (18%)	3.84	4 (100%)	0 0	65, 66, 68, 90	0
2	J	5/22 (22%)	2.82	4 (80%)	0 0	62, 64, 68, 88	0
All	All	693/738 (93%)	0.91	105 (15%)	5 5	21, 39, 70, 90	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ARG	6.0
1	B	62	ILE	5.6
1	A	2	ALA	5.5
2	I	9	VAL	5.4
1	B	10	PRO	4.4
1	B	107	CYS	4.4
2	J	11	LYS	4.1
1	B	106	TYR	4.0
2	J	9	VAL	3.9
2	I	11	LYS	3.9
1	B	346	PRO	3.9
1	A	312	MET	3.9
1	A	235	GLU	3.8
1	B	63	ASP	3.7
1	B	95	ARG	3.6
1	A	62	ILE	3.6
2	I	7	GLY	3.6
1	B	307	SER	3.6
1	A	63	ASP	3.4
1	B	235	GLU	3.4
1	B	54	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	60	ASP	3.3
1	B	65	LEU	3.3
1	A	307	SER	3.2
1	B	110	ARG	3.2
1	B	99	LYS	3.2
1	A	7	THR	3.2
1	A	94	VAL	3.2
1	B	101	ALA	3.1
1	A	99	LYS	3.1
1	B	66	VAL	3.1
1	A	164	SER	3.1
1	B	105	LYS	3.1
1	B	345	LEU	3.1
1	B	74	LEU	3.0
1	B	112	SER	3.0
1	A	347	THR	3.0
1	A	348	PRO	3.0
1	A	59	TYR	2.9
1	B	11	SER	2.9
1	B	93	THR	2.9
1	B	312	MET	2.8
1	A	106	TYR	2.8
1	B	103	SER	2.8
1	A	104	ASP	2.7
1	A	21	MET	2.7
1	A	107	CYS	2.7
1	B	100	ILE	2.7
1	B	61	ASP	2.7
1	B	154	ARG	2.7
1	B	60	ASP	2.7
1	A	98	ARG	2.7
1	A	145	VAL	2.6
1	A	103	SER	2.6
1	B	98	ARG	2.6
1	B	64	ASP	2.6
1	A	310	LYS	2.6
1	A	22	GLU	2.5
1	A	311	ASP	2.5
2	I	8	GLY	2.5
1	A	96	GLU	2.4
1	B	166	ILE	2.4
1	A	226	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	166	ILE	2.4
1	A	51	LYS	2.4
1	A	93	THR	2.4
1	B	170	GLY	2.3
1	A	64	ASP	2.3
1	B	310	LYS	2.3
1	A	74	LEU	2.3
1	A	110	ARG	2.3
1	A	100	ILE	2.3
1	A	111	TYR	2.3
1	B	51	LYS	2.3
1	B	145	VAL	2.3
1	A	143	LYS	2.3
2	J	6	THR	2.2
1	A	25	ARG	2.2
1	A	18	TYR	2.2
1	B	97	PHE	2.2
1	B	25	ARG	2.2
1	A	87	ILE	2.2
2	J	8	GLY	2.2
1	A	91	ALA	2.2
1	A	154	ARG	2.2
1	B	59	TYR	2.2
1	A	162	LYS	2.2
1	B	140	LEU	2.1
1	A	161	GLU	2.1
1	A	214	GLU	2.1
1	A	167	THR	2.1
1	B	162	LYS	2.1
1	B	311	ASP	2.1
1	B	111	TYR	2.1
1	B	55	PRO	2.1
1	B	53	TRP	2.1
1	A	101	ALA	2.1
1	B	102	ASN	2.1
1	B	108	THR	2.1
1	B	167	THR	2.1
1	B	94	VAL	2.1
1	B	163	GLU	2.0
1	A	322	ARG	2.0
1	A	54	LYS	2.0
1	A	53	TRP	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(Å ²)	Q<0.9
2	MLZ	I	10	10/11	0.64	0.23	39,45,61,63	0
2	MLZ	J	10	10/11	0.70	0.21	41,44,59,60	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(Å ²)	Q<0.9
5	OGA	A	5001	10/10	0.68	0.18	39,42,44,46	0
5	OGA	B	6001	10/10	0.79	0.15	37,40,45,45	0
3	ZN	A	1001	1/1	0.94	0.30	90,90,90,90	0
4	FE2	B	4001	1/1	0.97	0.06	33,33,33,33	0
3	ZN	B	2001	1/1	0.99	0.03	29,29,29,29	0
4	FE2	A	3001	1/1	1.00	0.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.