



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 2P5B / pdb_00002p5b
Title : The complex structure of JMJD2A and trimethylated H3K36 peptide
Authors : Zhang, G.; Chen, Z.; Zang, J.; Hong, X.; Shi, Y.
Deposited on : 2007-03-14
Resolution : 1.99 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

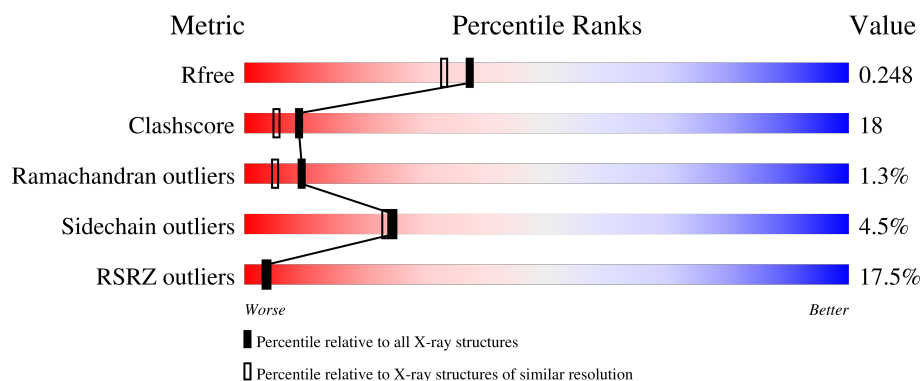
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	352	 13% 67% 28% . .
1	B	352	 14% 66% 27% . .
2	I	22	 73% 32% 41% 5% 23%
2	J	22	 59% 32% 23% 9% 36%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6164 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
			2848	1838	480	515	15			
1	B	337	Total	C	N	O	S	0	0	0
			2776	1796	469	496	15			

There are 6 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
A	1	MET	-	cloning artifact	UNP O75164
B	-1	GLY	-	cloning artifact	UNP O75164
B	0	SER	-	cloning artifact	UNP O75164
B	1	MET	-	cloning artifact	UNP O75164

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	0	0	0
			128	82	27	19			
2	J	14	Total	C	N	O	0	0	0
			98	62	21	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	10	M3L	LYS	modified residue	UNP P84239
I	21	LEU	-	cloning artifact	UNP P84239
J	10	M3L	LYS	modified residue	UNP P84239
J	21	LEU	-	cloning artifact	UNP P84239

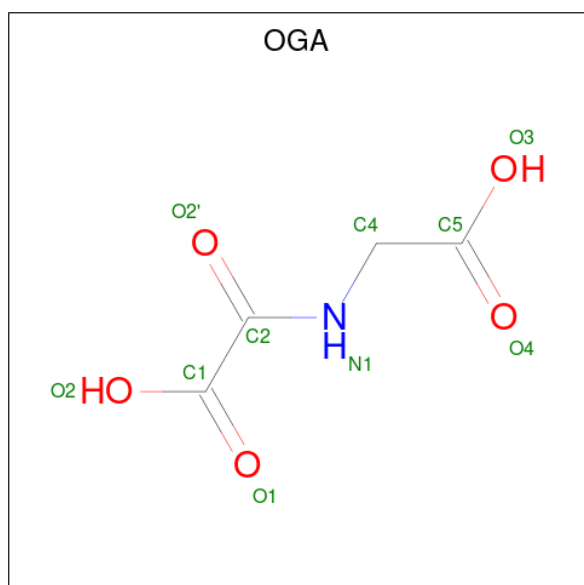
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0

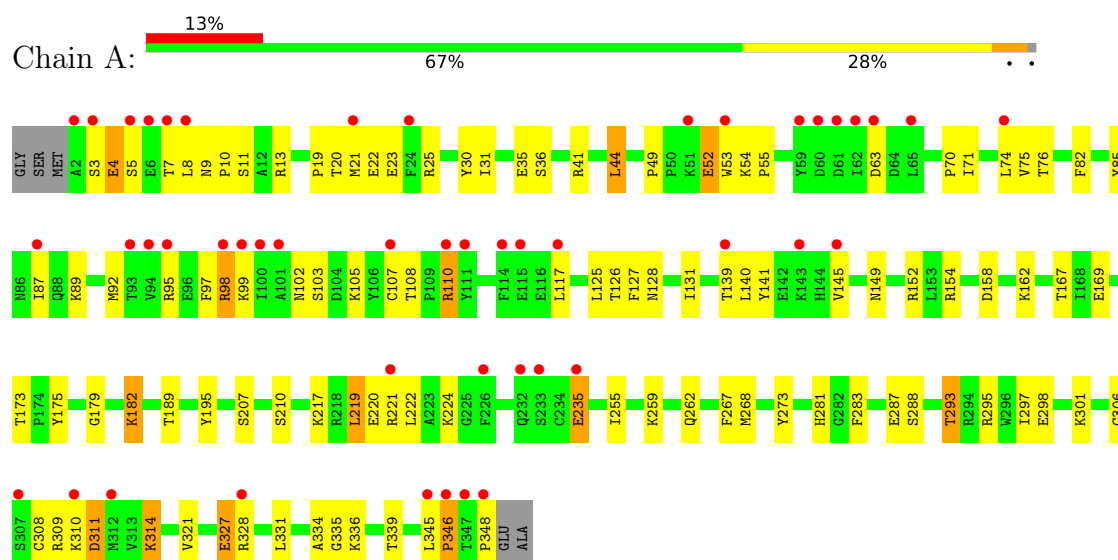
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	139	Total O 139 139	0	0
7	B	140	Total O 140 140	0	0
7	I	4	Total O 4 4	0	0
7	J	1	Total O 1 1	0	0

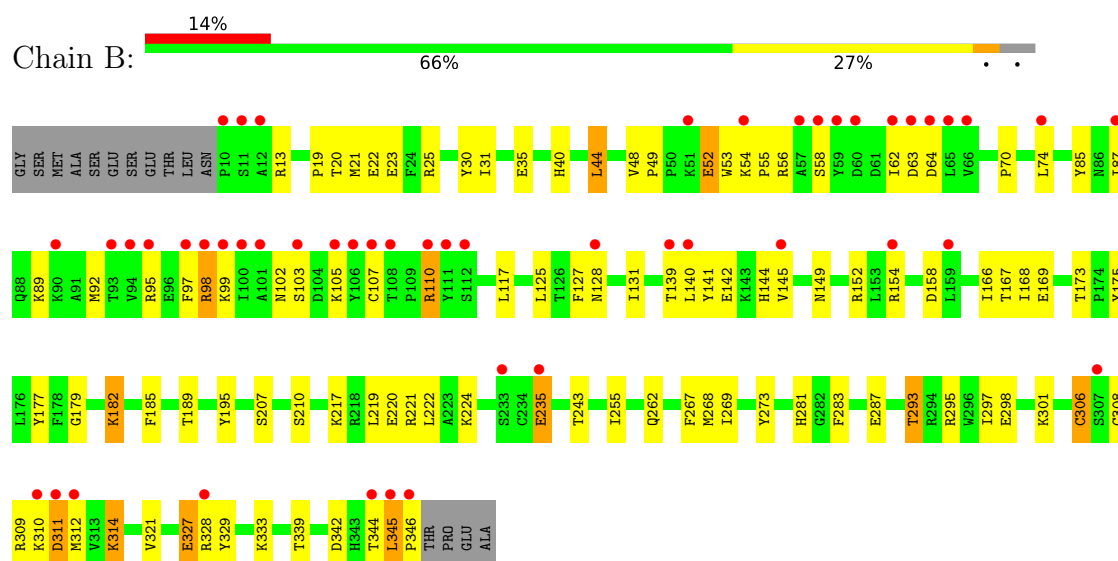
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

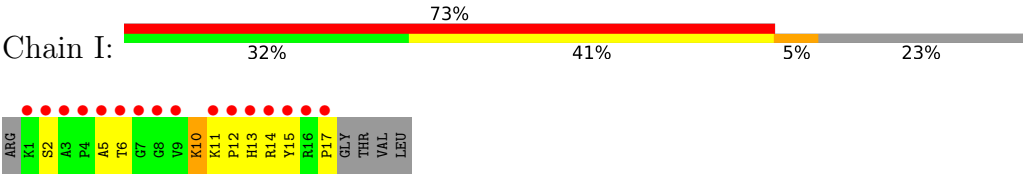
- Molecule 1: JmjC domain-containing histone demethylation protein 3A



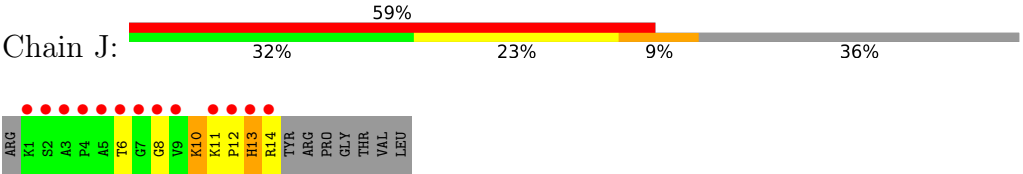
- Molecule 1: JmjC domain-containing histone demethylation protein 3A



- Molecule 2: Histone H3



● Molecule 2: Histone H3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.92Å 150.84Å 57.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.34 – 1.99 47.34 – 1.99	Depositor EDS
% Data completeness (in resolution range)	81.0 (47.34-1.99) 81.1 (47.34-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.263 0.226 , 0.248	Depositor DCC
R_{free} test set	1557 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.4	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	0.94	EDS
Total number of atoms	6164	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.95% 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: OXY, FE2, OGA, ZN, M3L

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/2934	0.88	1/3972 (0.0%)
1	B	0.39	0/2861	0.86	1/3870 (0.0%)
2	I	0.40	0/120	0.82	0/163
2	J	0.42	0/88	1.04	0/119
All	All	0.40	0/6003	0.87	2/8124 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	THR	N-CA-C	-6.19	101.03	110.14
1	B	189	THR	N-CA-C	-5.93	101.42	110.14

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	2848	0	2774	102	0
1	B	2776	0	2710	106	0
2	I	128	0	133	13	0
2	J	98	0	104	7	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
6	A	4	0	0	1	0
6	B	2	0	0	1	0
7	A	139	0	0	9	0
7	B	140	0	0	7	0
7	I	4	0	0	1	0
7	J	1	0	0	0	0
All	All	6164	0	5727	213	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 18.

All (213) 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:139:THR:HG22	1:B:141:TYR:H	1.23	0.99
1:A:139:THR:HG22	1:A:141:TYR:H	1.29	0.95
1:B:40:HIS:NE2	1:B:346:PRO:HG2	1.89	0.88
1:A:75:VAL:HG12	7:A:515:HOH:O	1.78	0.82
1:A:139:THR:HG23	1:A:287:GLU:OE1	1.79	0.81
1:B:139:THR:HG23	1:B:287:GLU:OE1	1.82	0.80
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.48	0.78
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.51	0.74
1:B:342:ASP:HB3	1:B:345:LEU:HG	1.69	0.74
1:B:139:THR:HG21	7:B:594:HOH:O	1.88	0.73
1:A:25:ARG:HB2	1:A:25:ARG:NH1	2.04	0.73
1:A:126:THR:HG22	7:A:515:HOH:O	1.90	0.71
1:B:154:ARG:HD2	7:B:588:HOH:O	1.91	0.70
1:A:19:PRO:HB3	1:A:30:TYR:CZ	2.26	0.70
1:A:217:LYS:HD2	1:A:273:TYR:OH	1.92	0.70
1:B:25:ARG:NH1	1:B:25:ARG:HB2	2.06	0.70
1:B:110:ARG:H	1:B:110:ARG:NE	1.91	0.69
1:A:4:GLU:HA	1:A:7:THR:HB	1.77	0.67
1:A:110:ARG:H	1:A:110:ARG:NE	1.92	0.67
1:A:3:SER:C	1:A:5:SER:H	2.03	0.67
1:B:40:HIS:HE2	1:B:346:PRO:HG2	1.61	0.66
1:A:154:ARG:HD2	7:A:596:HOH:O	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PRO:HB3	1:B:30:TYR:CZ	2.30	0.66
1:A:314:LYS:O	2:I:6:THR:HA	1.95	0.66
1:B:128:ASN:HB2	7:B:596:HOH:O	1.94	0.65
1:A:3:SER:O	1:A:4:GLU:HG2	1.97	0.63
1:A:71:ILE:HD13	2:I:14:ARG:NH1	2.13	0.63
1:A:235:GLU:N	1:A:235:GLU:OE1	2.32	0.63
1:B:74:LEU:HD22	1:B:87:ILE:HD11	1.79	0.63
1:B:295:ARG:HD2	1:B:346:PRO:HG3	1.79	0.63
1:A:345:LEU:HD23	1:A:346:PRO:N	2.14	0.63
1:B:217:LYS:HD2	1:B:273:TYR:OH	1.99	0.63
1:A:74:LEU:HD22	1:A:87:ILE:HD11	1.80	0.62
1:A:105:LYS:HE3	1:A:128:ASN:HD21	1.64	0.62
1:A:310:LYS:O	1:A:311:ASP:HB2	1.98	0.61
2:I:13:HIS:O	2:I:14:ARG:HD3	1.99	0.61
1:A:98:ARG:HG2	1:A:98:ARG:HH11	1.65	0.61
1:A:195:TYR:CE1	1:A:293:THR:HB	2.36	0.61
1:A:4:GLU:O	1:A:8:LEU:HG	2.01	0.61
1:B:98:ARG:HG2	1:B:98:ARG:HH11	1.64	0.61
1:B:92:MET:HE2	1:B:97:PHE:N	2.15	0.60
1:B:127:PHE:O	1:B:182:LYS:NZ	2.34	0.60
1:B:20:THR:OG1	1:B:23:GLU:HG3	2.01	0.60
1:B:195:TYR:CE1	1:B:293:THR:HB	2.36	0.60
1:B:310:LYS:O	1:B:311:ASP:HB2	2.01	0.60
1:B:220:GLU:O	1:B:224:LYS:HD3	2.01	0.59
1:A:20:THR:OG1	1:A:23:GLU:HG3	2.01	0.59
1:A:25:ARG:HB2	1:A:25:ARG:HH11	1.67	0.59
1:B:235:GLU:OE1	1:B:235:GLU:N	2.35	0.59
1:A:44:LEU:HD22	1:A:268:MET:HE3	1.83	0.59
1:A:127:PHE:O	1:A:182:LYS:NZ	2.35	0.59
1:B:70:PRO:HG2	1:B:89:LYS:HB2	1.83	0.59
1:A:222:LEU:HD22	1:A:255:ILE:HD12	1.84	0.58
1:A:92:MET:HE2	1:A:97:PHE:N	2.19	0.58
1:B:44:LEU:HD22	1:B:268:MET:HE3	1.85	0.58
1:B:139:THR:HG22	1:B:140:LEU:N	2.18	0.58
1:A:293:THR:CG2	1:A:295:ARG:H	2.15	0.58
6:B:503:OXY:O2	2:J:10:M3L:HM22	2.03	0.58
1:B:222:LEU:HD22	1:B:255:ILE:HD12	1.83	0.58
1:B:25:ARG:HB2	1:B:25:ARG:HH11	1.67	0.58
1:B:169:GLU:HA	1:B:173:THR:OG1	2.02	0.58
1:A:8:LEU:HD13	1:A:36:SER:O	2.03	0.58
1:A:293:THR:HG22	1:A:295:ARG:H	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HG3	1:B:102:ASN:ND2	2.19	0.58
1:B:103:SER:O	1:B:107:CYS:HB2	2.04	0.58
1:A:9:ASN:N	1:A:10:PRO:HD3	2.20	0.57
1:B:293:THR:HG22	1:B:295:ARG:H	1.69	0.57
1:B:328:ARG:NH2	1:B:339:THR:OG1	2.37	0.57
1:A:298:GLU:OE2	1:A:301:LYS:HE2	2.04	0.57
1:A:98:ARG:HG3	1:A:102:ASN:ND2	2.18	0.57
1:B:105:LYS:HE3	1:B:128:ASN:HD21	1.69	0.57
1:A:217:LYS:O	1:A:221:ARG:HG3	2.03	0.57
1:A:70:PRO:HG2	1:A:89:LYS:HB2	1.87	0.57
1:A:139:THR:HG21	7:A:592:HOH:O	2.04	0.57
1:B:293:THR:HG22	1:B:295:ARG:N	2.19	0.56
1:A:105:LYS:HE3	1:A:128:ASN:ND2	2.21	0.56
1:B:207:SER:OG	1:B:281:HIS:HE1	1.88	0.56
1:B:217:LYS:O	1:B:221:ARG:HG3	2.05	0.56
1:A:334:ALA:O	1:A:336:LYS:HG3	2.05	0.56
1:A:85:TYR:CG	1:B:74:LEU:HD21	2.41	0.56
1:A:293:THR:HG22	1:A:295:ARG:N	2.21	0.56
1:A:345:LEU:HD21	1:A:348:PRO:HD3	1.88	0.56
1:A:293:THR:HG23	7:A:628:HOH:O	2.05	0.55
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.22	0.55
1:B:40:HIS:CD2	1:B:346:PRO:HG2	2.40	0.55
1:B:293:THR:CG2	1:B:295:ARG:H	2.19	0.55
1:A:220:GLU:O	1:A:224:LYS:HD3	2.08	0.54
1:A:110:ARG:HD2	1:A:110:ARG:O	2.06	0.54
1:B:222:LEU:HD22	1:B:255:ILE:CD1	2.35	0.54
1:B:345:LEU:O	1:B:346:PRO:C	2.51	0.54
1:B:301:LYS:HD3	1:B:321:VAL:HG22	1.90	0.54
1:A:71:ILE:HD13	2:I:14:ARG:HH12	1.72	0.53
1:B:110:ARG:HD2	1:B:110:ARG:O	2.07	0.53
1:A:301:LYS:HD3	1:A:321:VAL:HG22	1.91	0.53
1:B:235:GLU:HG2	7:B:610:HOH:O	2.08	0.53
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.19	0.53
1:A:85:TYR:CB	1:B:74:LEU:HD21	2.39	0.53
1:A:222:LEU:HD22	1:A:255:ILE:CD1	2.38	0.52
1:B:139:THR:HG22	1:B:141:TYR:N	2.08	0.52
1:A:3:SER:O	1:A:5:SER:N	2.39	0.52
1:A:288:SER:OG	2:I:10:M3L:HM21	2.09	0.52
6:A:502:OXY:O2	2:I:10:M3L:HM22	2.10	0.52
1:B:179:GLY:O	1:B:283:PHE:HA	2.10	0.51
1:A:207:SER:OG	1:A:281:HIS:HE1	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HA	1:A:173:THR:OG1	2.10	0.51
1:A:139:THR:HG22	1:A:140:LEU:N	2.25	0.51
1:A:131:ILE:HD12	1:A:131:ILE:N	2.26	0.50
1:A:179:GLY:O	1:A:283:PHE:HA	2.11	0.50
1:B:105:LYS:HE3	1:B:128:ASN:ND2	2.26	0.50
1:A:82:PHE:HD2	7:A:515:HOH:O	1.93	0.50
1:B:21:MET:HE2	1:B:52:GLU:OE1	2.11	0.50
1:A:297:ILE:O	1:A:301:LYS:HG3	2.12	0.50
1:A:85:TYR:HB2	1:B:74:LEU:HD21	1.94	0.49
1:A:103:SER:O	1:A:107:CYS:HB2	2.12	0.49
1:A:8:LEU:O	1:A:41:ARG:NH1	2.46	0.49
1:A:259:LYS:HB2	7:A:549:HOH:O	2.12	0.49
2:J:13:HIS:O	2:J:14:ARG:HD2	2.13	0.49
1:B:131:ILE:N	1:B:131:ILE:HD12	2.27	0.49
1:B:297:ILE:O	1:B:301:LYS:HG3	2.13	0.49
1:B:298:GLU:OE2	1:B:301:LYS:HE2	2.13	0.49
1:B:342:ASP:CB	1:B:345:LEU:HG	2.42	0.48
1:A:76:THR:C	7:A:515:HOH:O	2.56	0.48
1:A:110:ARG:H	1:A:110:ARG:CD	2.27	0.48
1:B:166:ILE:HD13	2:J:6:THR:O	2.14	0.48
1:B:110:ARG:H	1:B:110:ARG:CD	2.27	0.47
1:A:31:ILE:O	1:A:35:GLU:HG3	2.14	0.47
1:B:295:ARG:HD2	1:B:346:PRO:CG	2.44	0.47
1:A:314:LYS:HD2	2:I:5:ALA:O	2.14	0.47
1:A:74:LEU:HD21	1:B:85:TYR:CG	2.50	0.47
1:A:55:PRO:HA	1:A:145:VAL:HG21	1.97	0.47
1:B:31:ILE:O	1:B:35:GLU:HG3	2.15	0.47
1:B:98:ARG:HG3	1:B:102:ASN:HD22	1.78	0.47
1:B:314:LYS:O	2:J:6:THR:HA	2.14	0.47
1:B:342:ASP:OD1	1:B:344:THR:HB	2.14	0.47
1:A:21:MET:HE2	1:A:52:GLU:OE1	2.15	0.47
1:A:98:ARG:HG3	1:A:102:ASN:HD22	1.79	0.47
2:I:14:ARG:HB2	7:I:256:HOH:O	2.14	0.47
1:A:328:ARG:NH2	1:A:339:THR:OG1	2.45	0.46
1:B:95:ARG:O	1:B:99:LYS:HG2	2.16	0.46
1:B:243:THR:HG22	7:B:504:HOH:O	2.15	0.46
1:A:19:PRO:HB3	1:A:30:TYR:CE1	2.50	0.46
1:A:44:LEU:HD12	1:A:210:SER:HB2	1.97	0.46
1:A:308:CYS:SG	1:A:309:ARG:HG3	2.55	0.46
1:B:55:PRO:HA	1:B:145:VAL:HG21	1.98	0.46
1:A:74:LEU:HD22	1:A:87:ILE:CD1	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HG2	1:B:98:ARG:NH1	2.32	0.45
2:I:11:LYS:HG3	2:I:14:ARG:NH2	2.32	0.45
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.52	0.45
1:A:95:ARG:O	1:A:99:LYS:HG2	2.16	0.45
1:A:53:TRP:CZ3	1:A:55:PRO:HD3	2.52	0.45
1:A:154:ARG:HA	1:A:158:ASP:OD2	2.17	0.45
1:A:327:GLU:H	1:A:327:GLU:CD	2.25	0.44
1:B:295:ARG:CD	1:B:346:PRO:HG3	2.45	0.44
1:B:13:ARG:HA	7:B:575:HOH:O	2.16	0.44
1:A:92:MET:HE2	1:A:97:PHE:CA	2.47	0.44
1:B:19:PRO:HB3	1:B:30:TYR:CE1	2.53	0.44
1:B:74:LEU:HD22	1:B:87:ILE:CD1	2.44	0.44
1:B:49:PRO:HG3	1:B:267:PHE:CD1	2.53	0.44
1:B:168:ILE:HG23	2:J:8:GLY:O	2.18	0.44
1:A:125:LEU:HA	1:A:182:LYS:HD2	1.99	0.44
1:A:3:SER:C	1:A:5:SER:N	2.70	0.44
1:B:63:ASP:HB3	1:B:95:ARG:NH2	2.33	0.44
2:J:11:LYS:HD3	2:J:14:ARG:HG2	2.00	0.44
1:B:54:LYS:HD3	1:B:54:LYS:HA	1.80	0.43
1:B:142:GLU:OE1	1:B:144:HIS:HE1	2.00	0.43
1:B:182:LYS:HE3	7:B:595:HOH:O	2.19	0.43
1:A:44:LEU:HD22	1:A:268:MET:CE	2.48	0.43
1:B:87:ILE:CG2	2:I:15:TYR:HB3	2.48	0.43
1:B:327:GLU:CD	1:B:327:GLU:H	2.25	0.43
1:B:185:PHE:CG	5:B:402:OGA:H4C2	2.54	0.43
1:B:31:ILE:CD1	1:B:269:ILE:HD13	2.49	0.43
1:B:262:GLN:CD	1:B:268:MET:HG2	2.44	0.43
1:A:262:GLN:CD	1:A:268:MET:HG2	2.44	0.43
1:B:125:LEU:HD23	1:B:125:LEU:N	2.34	0.43
1:B:328:ARG:NH1	1:B:328:ARG:CG	2.80	0.43
1:A:54:LYS:HA	1:A:54:LYS:HD3	1.81	0.43
1:A:11:SER:OG	1:A:13:ARG:HG3	2.19	0.42
1:A:107:CYS:SG	1:A:108:THR:N	2.92	0.42
1:B:56:ARG:HD3	1:B:58:SER:O	2.20	0.42
1:B:44:LEU:HD12	1:B:210:SER:HB2	2.01	0.42
1:A:141:TYR:CE2	1:A:149:ASN:HA	2.54	0.42
1:A:328:ARG:NH1	1:A:328:ARG:CG	2.82	0.42
1:B:53:TRP:CZ3	1:B:55:PRO:HD3	2.55	0.42
1:B:177:TYR:OH	2:J:10:M3L:HM23	2.19	0.42
1:A:331:LEU:HD12	1:A:336:LYS:HB2	2.02	0.42
1:B:329:TYR:CE2	1:B:333:LYS:HD3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:HB3	1:A:95:ARG:NH2	2.35	0.42
1:B:308:CYS:SG	1:B:309:ARG:HG3	2.60	0.42
1:B:344:THR:O	1:B:345:LEU:C	2.63	0.42
1:B:125:LEU:HA	1:B:182:LYS:HD2	2.02	0.42
1:B:125:LEU:HD23	1:B:125:LEU:H	1.84	0.41
1:A:331:LEU:CD1	1:A:336:LYS:HB2	2.50	0.41
1:B:92:MET:HE2	1:B:97:PHE:CA	2.50	0.41
1:A:152:ARG:O	1:A:152:ARG:HG3	2.20	0.41
1:A:335:GLY:HA2	7:A:604:HOH:O	2.19	0.41
1:B:127:PHE:O	1:B:128:ASN:C	2.63	0.41
1:A:125:LEU:H	1:A:125:LEU:HD23	1.85	0.41
1:A:22:GLU:HA	1:A:25:ARG:HH12	1.84	0.41
1:B:62:ILE:C	1:B:64:ASP:N	2.76	0.41
2:I:11:LYS:HG3	2:I:14:ARG:HH21	1.86	0.41
1:B:22:GLU:HA	1:B:25:ARG:HH12	1.86	0.41
1:A:49:PRO:HG3	1:A:267:PHE:CD1	2.55	0.41
2:I:11:LYS:HD3	2:I:14:ARG:HE	1.85	0.41
1:B:19:PRO:HD2	1:B:48:VAL:O	2.21	0.41
1:B:154:ARG:HA	1:B:158:ASP:OD2	2.21	0.41
1:A:219:LEU:HA	1:A:255:ILE:HD13	2.03	0.40
1:B:342:ASP:C	1:B:344:THR:H	2.29	0.40
1:A:87:ILE:CG2	2:I:17:PRO:HD3	2.50	0.40
1:A:162:LYS:HE2	1:A:162:LYS:HB2	1.91	0.40
1:B:152:ARG:O	1:B:152:ARG:HG3	2.22	0.40
1:B:306:CYS:SG	1:B:312:MET:HG3	2.62	0.40
1:B:22:GLU:HA	1:B:25:ARG:NH1	2.35	0.40
1:B:139:THR:CG2	1:B:140:LEU:N	2.84	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	345/352 (98%)	328 (95%)	14 (4%)	3 (1%)	14	9
1	B	335/352 (95%)	318 (95%)	15 (4%)	2 (1%)	21	17
2	I	14/22 (64%)	12 (86%)	0	2 (14%)	0	0
2	J	11/22 (50%)	8 (73%)	1 (9%)	2 (18%)	0	0
All	All	705/748 (94%)	666 (94%)	30 (4%)	9 (1%)	9	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	ASP
1	B	311	ASP
1	B	345	LEU
1	A	346	PRO
2	I	2	SER
2	J	13	HIS
1	A	4	GLU
2	J	12	PRO
2	I	12	PRO

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	305/308 (99%)	291 (95%)	14 (5%)	24	22
1	B	296/308 (96%)	282 (95%)	14 (5%)	23	22
2	I	10/16 (62%)	10 (100%)	0	100	100
2	J	7/16 (44%)	7 (100%)	0	100	100
All	All	618/648 (95%)	590 (96%)	28 (4%)	24	23

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	52	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	98	ARG
1	A	110	ARG
1	A	117	LEU
1	A	167	THR
1	A	175	TYR
1	A	182	LYS
1	A	219	LEU
1	A	235	GLU
1	A	293	THR
1	A	306	CYS
1	A	314	LYS
1	A	327	GLU
1	B	44	LEU
1	B	52	GLU
1	B	98	ARG
1	B	110	ARG
1	B	117	LEU
1	B	167	THR
1	B	175	TYR
1	B	182	LYS
1	B	219	LEU
1	B	235	GLU
1	B	293	THR
1	B	306	CYS
1	B	314	LYS
1	B	327	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	124	ASN
1	A	128	ASN
1	A	144	HIS
1	A	262	GLN
1	A	281	HIS
1	B	37	GLN
1	B	72	GLN
1	B	102	ASN
1	B	124	ASN
1	B	128	ASN
1	B	144	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	262	GLN
1	B	281	HIS
2	I	13	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	I	10	2	10,11,12	0.45	0	9,14,16	1.01	1 (11%)
2	M3L	J	10	2	10,11,12	0.49	0	9,14,16	1.04	1 (11%)

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	I	10	2	-	1/9/10/12	-
2	M3L	J	10	2	-	1/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	10	M3L	CM2-NZ-CM1	-2.21	103.16	108.98
2	J	10	M3L	CM2-NZ-CM1	-2.18	103.25	108.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	10	M3L	CE-CD-CG-CB
2	I	10	M3L	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	10	M3L	2	0
2	J	10	M3L	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
6	OXY	A	502	4	1,1,1	1.11	0	-		
6	OXY	A	501	-	1,1,1	1.09	0	-		
6	OXY	B	503	4	1,1,1	1.07	0	-		
5	OGA	A	401	4	9,9,9	1.41	1 (11%)	8,11,11	1.18	0
5	OGA	B	402	4	9,9,9	1.43	1 (11%)	8,11,11	1.17	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	401	4	-	0/8/9/9	-
5	OGA	B	402	4	-	0/8/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	OGA	C2-C1	-3.47	1.50	1.54
5	A	401	OGA	C2-C1	-3.29	1.50	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	OXY	1	0
6	B	503	OXY	1	0
5	B	402	OGA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	347/352 (98%)	0.87	47 (13%) 7 6	22, 40, 69, 104	0
1	B	337/352 (95%)	0.91	49 (14%) 6 5	23, 41, 70, 79	0
2	I	16/22 (72%)	4.66	16 (100%) 0 0	80, 91, 109, 110	0
2	J	13/22 (59%)	4.10	13 (100%) 0 0	98, 104, 119, 120	0
All	All	713/748 (95%)	1.03	125 (17%) 4 3	22, 42, 78, 120	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	13	HIS	6.9
2	I	5	ALA	6.5
2	J	13	HIS	6.4
2	I	2	SER	6.4
2	I	15	TYR	6.3
1	A	2	ALA	6.1
2	I	17	PRO	5.9
2	I	9	VAL	5.8
2	J	9	VAL	5.8
2	J	3	ALA	5.7
2	I	3	ALA	5.4
1	B	345	LEU	5.1
1	B	106	TYR	5.0
1	B	107	CYS	4.9
1	B	346	PRO	4.6
2	I	4	PRO	4.6
2	J	14	ARG	4.5
2	J	5	ALA	4.5
1	B	139	THR	4.5
1	A	60	ASP	4.4
1	A	346	PRO	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	8	GLY	4.3
2	I	12	PRO	4.3
1	B	62	ILE	4.2
1	A	95	ARG	4.0
1	B	10	PRO	4.0
2	I	8	GLY	3.9
1	A	59	TYR	3.9
1	B	307	SER	3.9
1	A	62	ILE	3.9
1	B	112	SER	3.8
1	A	347	THR	3.7
1	A	107	CYS	3.6
1	A	226	PHE	3.6
1	A	348	PRO	3.5
2	I	6	THR	3.5
1	B	57	ALA	3.5
2	J	12	PRO	3.5
1	A	235	GLU	3.4
2	J	2	SER	3.4
1	A	5	SER	3.3
2	I	14	ARG	3.3
2	J	4	PRO	3.3
1	A	310	LYS	3.3
1	B	99	LYS	3.3
1	B	101	ALA	3.2
2	I	11	LYS	3.2
1	B	100	ILE	3.2
1	B	59	TYR	3.2
2	J	6	THR	3.2
2	I	1	LYS	3.2
2	J	7	GLY	3.2
1	B	110	ARG	3.1
2	J	1	LYS	3.1
1	B	63	ASP	3.0
1	A	51	LYS	3.0
1	B	95	ARG	3.0
1	A	232	GLN	2.9
1	B	64	ASP	2.9
1	B	74	LEU	2.9
1	A	7	THR	2.9
1	B	311	ASP	2.8
1	B	140	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	7	GLY	2.8
1	B	154	ARG	2.8
1	B	235	GLU	2.8
1	B	12	ALA	2.8
1	A	94	VAL	2.8
1	A	111	TYR	2.8
1	A	139	THR	2.8
1	B	108	THR	2.7
1	B	105	LYS	2.7
1	A	53	TRP	2.6
1	A	110	ARG	2.6
1	B	310	LYS	2.6
1	A	65	LEU	2.6
1	A	312	MET	2.6
1	B	111	TYR	2.6
1	B	344	THR	2.6
1	B	159	LEU	2.6
1	A	63	ASP	2.6
1	B	51	LYS	2.6
1	B	54	LYS	2.5
1	A	145	VAL	2.5
1	B	94	VAL	2.5
1	A	61	ASP	2.5
2	J	11	LYS	2.5
1	B	128	ASN	2.5
1	A	221	ARG	2.5
1	A	6	GLU	2.5
1	A	21	MET	2.5
1	B	66	VAL	2.5
1	A	115	GLU	2.4
1	B	98	ARG	2.4
2	I	16	ARG	2.4
1	A	3	SER	2.4
1	B	145	VAL	2.4
1	B	65	LEU	2.4
1	A	307	SER	2.4
1	B	58	SER	2.4
1	A	74	LEU	2.3
1	B	11	SER	2.3
1	A	345	LEU	2.3
1	A	24	PHE	2.3
1	B	312	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	99	LYS	2.3
1	A	233	SER	2.2
1	A	87	ILE	2.2
1	A	328	ARG	2.2
1	B	233	SER	2.2
1	B	97	PHE	2.2
1	A	100	ILE	2.2
1	B	103	SER	2.2
1	A	8	LEU	2.2
1	A	117	LEU	2.2
1	B	90	LYS	2.2
1	A	93	THR	2.1
1	B	60	ASP	2.1
1	A	101	ALA	2.1
1	A	143	LYS	2.1
1	B	328	ARG	2.0
1	A	114	PHE	2.0
1	B	87	ILE	2.0
1	B	93	THR	2.0
1	A	98	ARG	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	M3L	J	10	12/13	0.85	0.27	85,89,98,98	0
2	M3L	I	10	12/13	0.86	0.23	72,75,84,84	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
6	OXY	A	501	2/2	0.81	0.22	34,34,34,39	2
5	OGA	B	402	10/10	0.83	0.14	44,50,56,58	0
5	OGA	A	401	10/10	0.86	0.13	50,53,59,61	0
6	OXY	B	503	2/2	0.87	0.15	41,41,41,41	2
6	OXY	A	502	2/2	0.91	0.14	42,42,42,43	2
4	FE2	B	352	1/1	0.99	0.02	34,34,34,34	0
3	ZN	A	351	1/1	0.99	0.09	26,26,26,26	1
3	ZN	B	351	1/1	1.00	0.03	45,45,45,45	0
4	FE2	A	352	1/1	1.00	0.01	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.