



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 08:17 am BST

PDB ID : 9ROV / pdb_00009rov
EMDB ID : EMD-54131
Title : Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15 and RBFA (Inward conformation) (State M2)
Authors : Khawaja, A.; Singh, V.; Shiriaev, D.I.; Rorbach, J.
Deposited on : 2025-06-23
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

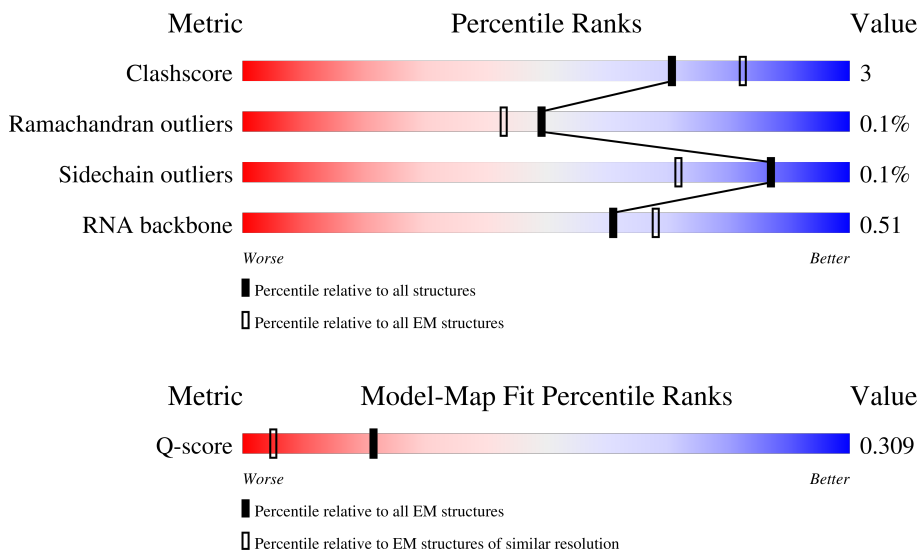
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.





















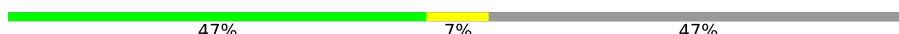






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	218	
2	1	323	
3	3	199	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	296	
5	C	167	
6	E	125	
7	F	242	
8	H	201	
9	I	194	
10	J	138	
11	K	128	
12	L	257	
13	M	137	
14	N	130	
15	O	258	
16	P	142	
17	Q	87	
18	R	360	
19	S	190	
20	T	173	
21	U	205	
22	W	187	
23	X	398	
24	Y	395	
25	Z	106	
26	D	430	
27	G	396	
28	V	414	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	4	689	
30	b	407	
31	A	954	
32	a	343	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	FES	T	201	-	-	X	-
9	5F0	I	184	-	-	X	-

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 127605 atoms, of which 59085 are hydrogens and 0 are deuteriums.

In the tables below, 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 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	0	215	Total	C	H	N	O	S	0	0
			3583	1130	1796	339	313	5		

- Molecule 2 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	1	255	Total	C	H	N	O	S	0	0
			4163	1311	2099	355	388	10		

- Molecule 3 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	3	70	Total	C	H	N	O	S	0	0
			1324	401	699	134	89	1		

- Molecule 4 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	B	225	Total	C	H	N	O	S	0	0
			3643	1164	1815	331	323	10		

- Molecule 5 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	C	132	Total	C	H	N	O	S	0	0
			2171	699	1088	195	185	4		

- Molecule 6 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	E	115	Total	C	H	N	O	S	0	0
			1839	574	929	165	167	4		

- Molecule 7 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	F	205	3421	1076	1736	304	294	11	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	139	2317	739	1173	193	209	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	137	2080	642	1060	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	108	1723	521	884	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	101	1748	537	886	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	L	174	2994	925	1541	270	251	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	M	119	1908	594	966	185	157	6	0	0

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	N	110	1796	562	928	156	147	3	0	0

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	O	194	3164	1019	1565	295	278	7	0	0

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	P	97	1589	501	808	134	138	8	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	Q	87	1502	460	758	150	126	8	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	R	295	4837	1533	2428	413	455	8	0	0

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	S	135	2226	716	1115	198	196	1	0	0

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	T	168	2764	877	1393	239	244	11	0	0

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	U	176	2987	916	1499	301	267	4	0	0

- Molecule 22 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	W	100	1591	498	802	141	146	4	0	0

- Molecule 23 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	X	352	5693	1822	2844	499	517	11	0	0

- Molecule 24 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	Y	121	1993	662	970	168	191	2	0	0

- Molecule 25 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	Z	88	1495	476	750	133	132	4	0	0

- Molecule 26 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	D	308	4967	1549	2505	465	436	12	0	0

- Molecule 27 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	G	313	5138	1637	2562	456	469	14	0	0

- Molecule 28 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	V	362	5930	1904	2961	495	558	12	0	0

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	4	579	9393	3010	4696	794	865	28	0	0

- Molecule 30 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	b	296	4680	1464	2367	410	426	13	0	0

- Molecule 31 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
31	A	949	30392	9040	10236	3633	6534	949	0	0

- Molecule 32 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	a	145	2339	729	1178	206	220	6	0	0

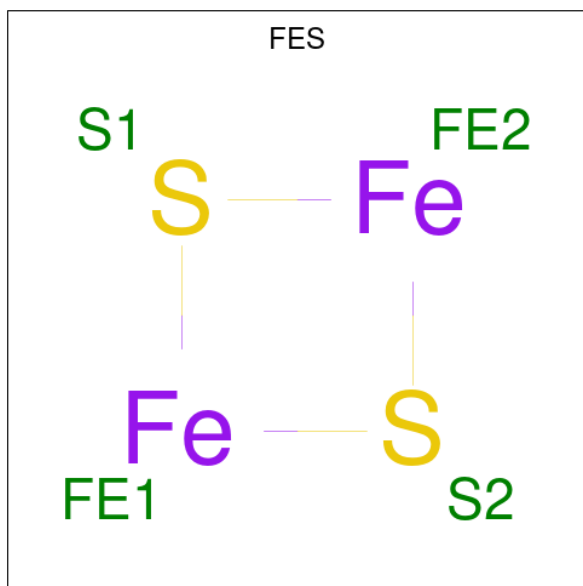
- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
33	F	1	Total K 1 1	0
33	A	6	Total K 6 6	0

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

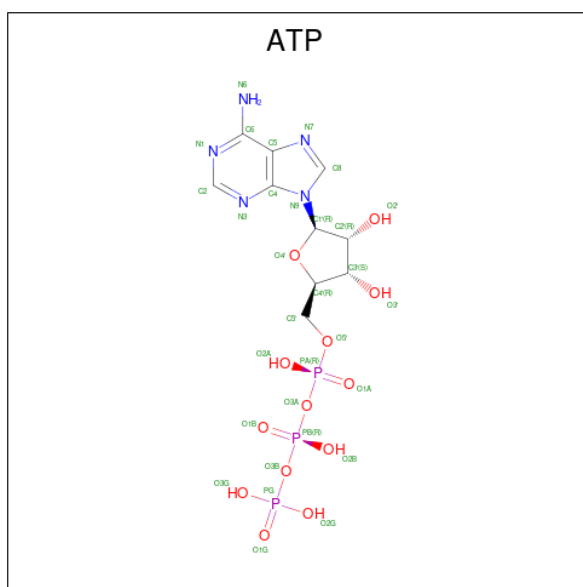
Mol	Chain	Residues	Atoms	AltConf
34	O	1	Total Zn 1 1	0

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



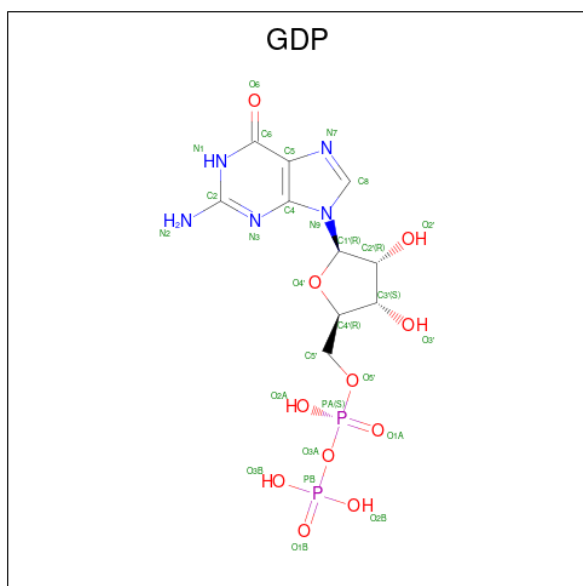
Mol	Chain	Residues	Atoms	AltConf
35	P	1	Total Fe S 4 2 2	0
35	T	1	Total Fe S 4 2 2	0

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



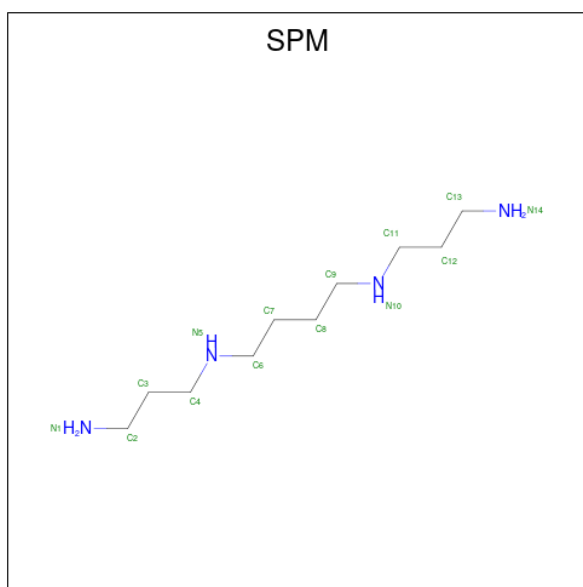
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
36	X	1	43	10	12	5	13	3	0

- Molecule 37 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
37	X	1	38	10	10	5	11	2	0

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).



Mol	Chain	Residues	Atoms		AltConf
40	A	1	Total	C N	0
			14	10 4	

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	K	1	Total	O	0
			1	1	
41	T	1	Total	O	0
			1	1	
41	G	1	Total	O	0
			1	1	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9007	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.053	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	495.0, 495.0, 495.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

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: 5F0, FES, K, ATP, NAD, GDP, SPM, ZN, 5MU, MA6, MG, ACE

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	0	0.09	0/1834	0.23	0/2484
2	1	0.10	0/2109	0.23	0/2854
3	3	0.08	0/636	0.22	0/839
4	B	0.09	0/1871	0.21	0/2531
5	C	0.09	0/1113	0.22	0/1505
6	E	0.10	0/926	0.24	0/1252
7	F	0.32	0/1723	0.49	0/2313
8	H	0.09	0/1170	0.21	0/1587
9	I	0.09	0/1030	0.26	0/1386
10	J	0.62	3/855 (0.4%)	1.07	13/1148 (1.1%)
11	K	0.09	0/880	0.21	0/1182
12	L	0.09	0/1477	0.20	0/1974
13	M	0.10	0/963	0.22	0/1295
14	N	0.09	0/886	0.19	0/1199
15	O	0.24	0/1655	0.36	0/2254
16	P	0.10	0/798	0.23	0/1070
17	Q	0.10	0/754	0.25	0/1003
18	R	0.09	0/2456	0.20	0/3317
19	S	0.09	0/1138	0.19	0/1533
20	T	0.10	0/1402	0.22	0/1883
21	U	0.09	0/1510	0.19	0/2025
22	W	0.08	0/801	0.19	0/1079
23	X	0.09	0/2921	0.22	0/3954
24	Y	0.09	0/1054	0.21	0/1421
25	Z	0.09	0/762	0.20	0/1019
26	D	0.11	0/2511	0.23	0/3365
27	G	0.23	0/2631	0.33	0/3527
28	V	0.08	0/3030	0.21	0/4093
29	4	0.17	0/4803	0.27	0/6496
30	b	0.42	0/2353	0.58	0/3171
31	A	0.10	0/22466	0.19	2/34970 (0.0%)
32	a	0.23	0/1175	0.40	1/1580 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.16	3/71693 (0.0%)	0.28	16/101309 (0.0%)

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
7	F	0	2
9	I	0	2
27	G	0	1
29	4	0	1
30	b	0	5
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	77	ASN	C-N	-8.60	1.22	1.33
10	J	68	ARG	C-N	-8.36	1.17	1.33
10	J	60	GLY	C-N	8.08	1.44	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	84	ARG	O-C-N	16.84	142.42	123.22
10	J	77	ASN	O-C-N	-10.52	111.07	123.27
10	J	84	ARG	CA-C-N	-9.92	100.22	121.45
10	J	84	ARG	C-N-CA	-9.92	100.22	121.45
10	J	68	ARG	O-C-N	8.44	134.51	122.94
10	J	94	PHE	N-CA-CB	7.73	123.56	110.49
10	J	60	GLY	O-C-N	6.90	129.81	123.73
10	J	60	GLY	CA-C-N	-6.36	114.61	123.13
10	J	60	GLY	C-N-CA	-6.36	114.61	123.13
10	J	77	ASN	CA-C-N	6.34	131.94	122.99
10	J	77	ASN	C-N-CA	6.34	131.94	122.99
10	J	97	GLY	CA-C-O	-6.03	117.76	122.52
31	A	1379	A	C5'-C4'-C3'	5.39	124.09	116.00
31	A	1379	A	C5'-C4'-O4'	5.20	117.60	109.80
32	a	47	LYS	N-CA-C	-5.13	106.99	113.20
10	J	63	LEU	N-CA-C	-5.11	104.21	110.65

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	4	350	ARG	Sidechain
7	F	52	ARG	Sidechain
7	F	66	ARG	Sidechain
27	G	365	ARG	Sidechain
9	I	184	5F0	Peptide,Mainchain
30	b	187	ARG	Sidechain
30	b	270	ARG	Sidechain
30	b	276	ARG	Sidechain
30	b	395	ARG	Sidechain
30	b	397	ARG	Sidechain

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	0	1787	1796	1796	8	0
2	1	2064	2099	2098	17	0
3	3	625	699	699	3	0
4	B	1828	1815	1815	6	0
5	C	1083	1088	1088	4	0
6	E	910	929	929	7	0
7	F	1685	1736	1736	12	0
8	H	1144	1173	1172	11	0
9	I	1020	1060	1053	51	0
10	J	839	884	884	29	0
11	K	862	886	885	6	0
12	L	1453	1541	1540	6	0
13	M	942	966	966	5	0
14	N	868	928	928	5	0
15	O	1599	1565	1565	8	0
16	P	781	808	807	3	0
17	Q	744	758	758	25	0
18	R	2409	2428	2428	9	0
19	S	1111	1115	1115	11	0
20	T	1371	1393	1395	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	1488	1499	1499	6	0
22	W	789	802	802	7	0
23	X	2849	2844	2844	7	0
24	Y	1023	970	970	3	0
25	Z	745	750	750	1	0
26	D	2462	2505	2502	18	0
27	G	2576	2562	2560	15	0
28	V	2969	2961	2961	11	0
29	4	4697	4696	4695	20	0
30	b	2313	2367	2366	44	0
31	A	20156	10236	10250	120	0
32	a	1161	1178	1176	35	0
33	A	6	0	0	0	0
33	F	1	0	0	0	0
34	O	1	0	0	0	0
35	P	4	0	0	1	0
35	T	4	0	0	2	0
36	X	31	12	12	0	0
37	X	28	10	12	0	0
38	A	30	0	0	0	0
38	G	1	0	0	0	0
39	A	44	26	26	0	0
40	A	14	0	26	1	0
41	G	1	0	0	1	0
41	K	1	0	0	0	0
41	T	1	0	0	1	0
All	All	68520	59085	59108	423	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 3.

All (423) 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)
9:I:185:GLY:N	31:A:1013:A:N3	2.00	1.10
9:I:185:GLY:O	31:A:1013:A:H1'	1.54	1.04
9:I:191:ALA:HB2	32:a:171:GLN:HG2	1.41	1.03
20:T:141:CYS:SG	35:T:201:FES:S2	2.58	1.01
10:J:80:CYS:SG	10:J:93:CYS:HB2	2.03	0.99
9:I:184:5F0:O	31:A:976:A:C2	2.19	0.95
10:J:80:CYS:HG	10:J:93:CYS:HB2	1.31	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:80:CYS:SG	10:J:81:CYS:N	2.35	0.91
9:I:187:ARG:NH2	17:Q:45:TYR:CE2	2.43	0.86
9:I:191:ALA:HB2	32:a:171:GLN:CG	2.07	0.85
9:I:189:ARG:O	17:Q:45:TYR:N	2.12	0.83
9:I:187:ARG:CZ	17:Q:45:TYR:CZ	2.62	0.81
9:I:185:GLY:N	31:A:1013:A:C2	2.47	0.79
9:I:89:LYS:NZ	31:A:1004:G:OP1	2.17	0.77
10:J:117:ASP:OD2	31:A:894:C:N4	2.17	0.76
31:A:1175:G:O6	31:A:1479:C:N4	2.19	0.76
9:I:94:ASN:ND2	31:A:989:U:OP1	2.20	0.75
4:B:72:PHE:O	4:B:263:LYS:NZ	2.20	0.75
9:I:184:5F0:O	31:A:976:A:H2	1.68	0.74
10:J:80:CYS:SG	10:J:93:CYS:C	2.71	0.73
9:I:191:ALA:CB	32:a:171:GLN:CG	2.66	0.73
10:J:80:CYS:SG	10:J:93:CYS:CB	2.76	0.73
1:0:23:GLU:OE1	1:0:24:GLN:NE2	2.23	0.72
10:J:80:CYS:HG	10:J:81:CYS:N	1.85	0.72
1:0:99:ARG:NH2	31:A:1527:A:O3'	2.23	0.71
9:I:187:ARG:NE	17:Q:45:TYR:CE1	2.59	0.71
26:D:320:ILE:HG22	26:D:324:CYS:SG	2.31	0.71
9:I:184:5F0:CXT	9:I:186:CYS:O	2.39	0.70
11:K:51:ARG:NH2	31:A:1402:A:OP1	2.25	0.70
12:L:83:GLU:N	12:L:83:GLU:OE1	2.25	0.69
9:I:191:ALA:CB	32:a:171:GLN:HG2	2.21	0.69
27:G:276:ARG:NH1	41:G:2001:HOH:O	2.25	0.69
31:A:843:G:N2	31:A:846:A:OP2	2.24	0.69
10:J:80:CYS:SG	10:J:93:CYS:CA	2.80	0.69
18:R:242:TYR:O	18:R:246:HIS:ND1	2.26	0.68
19:S:42:ARG:NH2	19:S:47:GLN:OE1	2.26	0.68
18:R:208:ILE:O	18:R:214:ASN:ND2	2.27	0.68
29:4:193:ASP:OD1	29:4:261:THR:OG1	2.09	0.68
9:I:187:ARG:CZ	17:Q:45:TYR:CE2	2.78	0.67
7:F:119:LYS:NZ	23:X:398:LEU:OXT	2.21	0.67
31:A:1290:C:O2'	31:A:1291:U:O5'	2.12	0.67
29:4:239:ARG:O	29:4:242:ASN:ND2	2.29	0.66
32:a:298:GLY:O	32:a:301:VAL:HG22	1.94	0.66
9:I:187:ARG:HG3	17:Q:45:TYR:CD1	2.31	0.66
9:I:187:ARG:NE	17:Q:45:TYR:CD1	2.64	0.65
19:S:21:ARG:NH1	26:D:281:TYR:OH	2.28	0.65
15:O:233:GLU:N	15:O:233:GLU:OE1	2.30	0.65
11:K:40:ARG:NH1	11:K:81:ASP:OD1	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1407:U:HO2'	31:A:1446:A:HO2'	1.45	0.65
3:3:128:LYS:NZ	31:A:1107:U:O4	2.29	0.65
30:b:94:ASP:OD1	30:b:95:MET:N	2.31	0.64
10:J:80:CYS:SG	10:J:93:CYS:N	2.71	0.64
19:S:61:GLN:N	19:S:61:GLN:OE1	2.30	0.64
3:3:148:LYS:O	3:3:151:ARG:NH1	2.31	0.64
11:K:36:ARG:NH1	31:A:1237:A:OP1	2.31	0.63
29:4:550:ASP:OD1	29:4:588:ARG:NH2	2.31	0.63
8:H:64:THR:HG1	29:4:64:THR:HG1	1.45	0.63
19:S:27:GLU:OE2	19:S:28:LYS:N	2.31	0.63
28:V:97:HIS:O	28:V:97:HIS:ND1	2.31	0.63
1:0:101:ARG:NE	31:A:1527:A:O2'	2.32	0.62
2:1:64:GLN:N	2:1:64:GLN:OE1	2.33	0.62
4:B:180:ARG:NH1	4:B:185:PRO:O	2.33	0.62
18:R:317:ALA:O	18:R:321:ALA:N	2.32	0.62
30:b:96:THR:OG1	30:b:170:LEU:HD23	2.00	0.61
32:a:187:ASN:O	32:a:191:ALA:N	2.34	0.61
9:I:190:LYS:HG2	31:A:1068:A:OP1	2.00	0.61
32:a:190:LEU:HA	32:a:193:LEU:HD23	1.81	0.61
20:T:126:PRO:O	41:T:301:HOH:O	2.16	0.61
6:E:115:GLU:HB3	32:a:48:PHE:CE2	2.36	0.61
27:G:388:ARG:NH1	31:A:1430:A:O5'	2.35	0.60
15:O:105:CYS:SG	15:O:143:CYS:N	2.74	0.60
7:F:79:ALA:O	27:G:312:GLN:NE2	2.35	0.60
9:I:146:HIS:ND1	9:I:171:GLU:OE1	2.33	0.60
7:F:166:ARG:NH2	30:b:339:THR:OG1	2.35	0.60
27:G:136:ARG:O	27:G:139:GLN:NE2	2.35	0.60
10:J:98:GLU:N	10:J:98:GLU:OE1	2.35	0.60
31:A:1125:A:P	32:a:46:LYS:HE2	2.42	0.60
31:A:1175:G:N2	31:A:1481:C:O2'	2.34	0.60
8:H:127:TYR:OH	31:A:1327:G:N2	2.35	0.59
10:J:62:VAL:HG22	10:J:83:VAL:HG12	1.85	0.59
10:J:80:CYS:HB2	10:J:94:PHE:HA	1.84	0.59
11:K:88:ARG:NH2	31:A:1231:A:OP1	2.34	0.59
9:I:73:LEU:O	9:I:79:LYS:NZ	2.35	0.59
17:Q:2:ALA:N	31:A:977:A:OP2	2.36	0.59
2:1:166:PRO:O	2:1:169:ARG:NH1	2.35	0.59
32:a:143:THR:HG22	32:a:144:LEU:H	1.67	0.59
18:R:260:ASP:OD1	18:R:263:ARG:NH2	2.36	0.58
31:A:947:U:P	31:A:1045:G:O6	2.61	0.58
10:J:80:CYS:HG	10:J:81:CYS:H	1.43	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:249:GLU:OE1	2:1:249:GLU:N	2.33	0.58
31:A:905:A:O2'	31:A:907:A:OP1	2.21	0.57
29:4:543:GLU:OE1	29:4:543:GLU:N	2.35	0.57
7:F:168:TYR:O	7:F:170:VAL:HG13	2.02	0.57
21:U:80:ARG:O	21:U:84:GLU:N	2.38	0.57
26:D:317:HIS:O	26:D:321:ILE:N	2.34	0.57
2:1:87:MET:HE1	2:1:108:ILE:HD12	1.85	0.57
10:J:64:CYS:O	10:J:65:THR:HG23	2.05	0.57
30:b:86:PRO:HB2	30:b:113:ILE:HD11	1.87	0.57
20:T:11:ARG:NH2	31:A:932:C:N3	2.52	0.56
31:A:1583:MA6:H93	31:A:1584:MA6:C2	2.34	0.56
32:a:193:LEU:HD12	32:a:197:LEU:CB	2.34	0.56
31:A:1124:A:O3'	32:a:46:LYS:CE	2.53	0.56
19:S:7:GLU:N	19:S:7:GLU:OE1	2.37	0.56
24:Y:360:LYS:NZ	25:Z:21:GLU:OE1	2.28	0.56
26:D:320:ILE:O	26:D:324:CYS:N	2.24	0.56
26:D:375:GLU:N	26:D:375:GLU:OE1	2.35	0.56
32:a:135:ALA:O	32:a:137:ARG:NH1	2.39	0.56
31:A:1583:MA6:H93	31:A:1584:MA6:N1	2.20	0.56
9:I:192:ARG:CD	17:Q:44:TYR:OH	2.53	0.55
31:A:1106:C:O2'	31:A:1108:C:OP2	2.23	0.55
30:b:97:PHE:CD2	30:b:128:ALA:HB2	2.41	0.55
9:I:98:GLN:HE22	31:A:1004:G:H21	1.54	0.55
31:A:769:G:N2	31:A:772:A:OP2	2.39	0.55
2:1:269:MET:HE2	2:1:320:LEU:CD1	2.36	0.55
22:W:112:LEU:N	22:W:124:CYS:O	2.39	0.54
28:V:397:ARG:NH1	31:A:1523:A:O5'	2.40	0.54
2:1:53:LEU:HD13	29:4:518:GLU:OE2	2.07	0.54
4:B:243:PRO:O	4:B:247:HIS:ND1	2.40	0.54
9:I:191:ALA:HB1	32:a:171:GLN:HB3	1.90	0.54
30:b:91:ILE:HD13	30:b:116:TYR:CE2	2.42	0.54
24:Y:339:GLU:OE1	24:Y:339:GLU:N	2.34	0.54
31:A:917:C:O2'	31:A:921:U:OP1	2.25	0.54
4:B:165:TYR:OH	27:G:146:PRO:O	2.24	0.54
7:F:156:ILE:HD12	7:F:230:ALA:HB3	1.89	0.54
9:I:187:ARG:CD	17:Q:45:TYR:CE1	2.90	0.54
7:F:136:THR:HG22	7:F:136:THR:O	2.08	0.54
9:I:153:GLY:O	9:I:158:ARG:NH1	2.39	0.54
31:A:1124:A:H4'	32:a:46:LYS:NZ	2.22	0.53
31:A:1558:A:H1'	31:A:1559:G:OP1	2.08	0.53
7:F:155:MET:O	32:a:196:LEU:HD11	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:948:U:OP2	31:A:1045:G:N2	2.41	0.53
9:I:187:ARG:NH2	17:Q:45:TYR:CD2	2.77	0.53
10:J:48:LYS:NZ	31:A:1162:A:OP1	2.36	0.53
15:O:73:VAL:O	15:O:109:ARG:NH2	2.41	0.53
10:J:60:GLY:HA2	10:J:84:ARG:O	2.08	0.53
4:B:239:ASN:OD1	22:W:119:LYS:NZ	2.42	0.53
9:I:183:HIS:CD2	31:A:976:A:H1'	2.44	0.53
31:A:1293:C:O2'	31:A:1294:A:OP1	2.24	0.53
30:b:166:VAL:CG2	30:b:310:LEU:HD13	2.38	0.53
18:R:73:GLU:N	18:R:73:GLU:OE1	2.40	0.52
30:b:158:VAL:HG13	30:b:158:VAL:O	2.09	0.52
31:A:942:A:N6	31:A:1047:A:OP2	2.36	0.52
30:b:338:MET:N	30:b:338:MET:SD	2.82	0.52
17:Q:24:ARG:NH2	32:a:118:TYR:O	2.42	0.52
29:4:200:ASP:O	29:4:239:ARG:NH2	2.42	0.52
31:A:1489:G:O2'	31:A:1490:U:O4'	2.22	0.52
2:1:269:MET:HE2	2:1:320:LEU:HD13	1.91	0.52
28:V:151:PHE:O	28:V:155:GLU:N	2.43	0.52
15:O:211:ARG:O	15:O:214:SER:OG	2.21	0.52
29:4:131:ASP:OD2	29:4:136:HIS:ND1	2.40	0.52
31:A:899:G:O2'	31:A:907:A:N1	2.39	0.51
2:1:150:GLU:OE1	2:1:174:ARG:NH2	2.43	0.51
9:I:183:HIS:C	9:I:184:5F0:O	2.54	0.51
23:X:203:LYS:O	23:X:250:GLN:NE2	2.43	0.51
19:S:62:ASP:OD2	19:S:64:TRP:NE1	2.41	0.51
28:V:405:GLN:N	28:V:405:GLN:OE1	2.43	0.51
31:A:1464:G:H21	31:A:1466:C:H41	1.58	0.51
28:V:132:LYS:O	28:V:136:GLY:N	2.39	0.51
10:J:81:CYS:SG	10:J:93:CYS:HB2	2.51	0.51
31:A:1124:A:N6	31:A:1127:A:OP1	2.44	0.51
6:E:85:ASP:OD1	6:E:87:ASP:N	2.41	0.51
30:b:310:LEU:HD12	30:b:311:ARG:H	1.76	0.51
14:N:73:ARG:NH2	31:A:769:G:OP2	2.44	0.51
32:a:193:LEU:HD12	32:a:197:LEU:HB3	1.92	0.51
9:I:133:ILE:HD13	9:I:164:GLY:O	2.11	0.50
26:D:400:GLU:OE1	26:D:400:GLU:N	2.38	0.50
9:I:82:GLU:OE1	9:I:82:GLU:N	2.44	0.50
31:A:700:A:N1	31:A:709:G:O2'	2.39	0.50
31:A:1124:A:H4'	32:a:46:LYS:HZ1	1.75	0.50
9:I:187:ARG:HG3	17:Q:45:TYR:HD1	1.76	0.50
2:1:87:MET:HE3	2:1:105:LEU:HD23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1191:C:H1'	31:A:1466:C:H42	1.77	0.50
9:I:182:PRO:HB3	31:A:977:A:H1'	1.93	0.50
27:G:320:VAL:HG23	27:G:322:ARG:HG2	1.94	0.50
29:4:237:THR:O	29:4:237:THR:HG22	2.11	0.50
30:b:96:THR:HG23	30:b:170:LEU:CD2	2.41	0.50
31:A:946:U:OP2	40:A:1702:SPM:N10	2.45	0.50
9:I:89:LYS:HD2	31:A:1004:G:H5''	1.94	0.50
9:I:188:PRO:O	17:Q:45:TYR:HB2	2.12	0.50
12:L:76:TYR:O	12:L:79:VAL:HG12	2.12	0.50
9:I:192:ARG:HD3	17:Q:44:TYR:OH	2.12	0.49
15:O:62:GLU:OE1	15:O:62:GLU:N	2.39	0.49
32:a:130:THR:OG1	32:a:137:ARG:NH2	2.40	0.49
31:A:657:G:O4'	31:A:1480:A:O2'	2.22	0.49
31:A:1044:U:OP1	31:A:1110:A:O2'	2.30	0.49
31:A:1598:G:O2'	31:A:1599:A:O4'	2.24	0.49
28:V:67:VAL:O	28:V:100:ASN:ND2	2.45	0.49
30:b:174:SER:O	30:b:178:ASP:N	2.44	0.49
20:T:132:ARG:NH1	20:T:135:CYS:O	2.46	0.49
10:J:74:ASN:ND2	10:J:117:ASP:OD1	2.45	0.49
19:S:115:GLU:OE1	19:S:115:GLU:N	2.41	0.49
29:4:600:ARG:NH2	29:4:636:ALA:O	2.45	0.49
30:b:204:MET:HE3	30:b:205:PRO:O	2.12	0.49
2:1:86:ARG:NH1	2:1:96:PRO:O	2.45	0.49
22:W:97:ASP:N	22:W:144:LEU:O	2.45	0.49
30:b:170:LEU:HD12	30:b:170:LEU:C	2.38	0.49
30:b:258:VAL:HG11	30:b:281:ALA:HA	1.95	0.49
31:A:1098:C:OP1	31:A:1151:C:N4	2.46	0.49
32:a:143:THR:HG22	32:a:144:LEU:N	2.26	0.49
10:J:60:GLY:CA	10:J:84:ARG:O	2.61	0.49
31:A:1389:G:OP2	31:A:1389:G:N2	2.41	0.49
23:X:64:GLU:OE1	23:X:65:GLY:N	2.45	0.49
5:C:39:ALA:O	5:C:41:ARG:NH1	2.45	0.48
14:N:93:ASP:O	14:N:97:GLY:N	2.42	0.48
17:Q:20:GLU:N	17:Q:20:GLU:OE1	2.46	0.48
27:G:301:GLN:N	27:G:301:GLN:OE1	2.46	0.48
31:A:1053:A:N1	31:A:1100:C:O2'	2.42	0.48
5:C:126:GLN:OE1	5:C:126:GLN:N	2.39	0.48
22:W:146:ASP:OD1	22:W:147:LEU:N	2.44	0.48
12:L:207:LYS:CD	31:A:763:C:H42	2.26	0.48
15:O:156:LYS:O	15:O:160:HIS:ND1	2.42	0.48
30:b:159:GLN:N	30:b:160:PRO:CD	2.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1243:U:H3	31:A:1346:A:H61	1.59	0.48
2:1:255:ASN:N	2:1:259:GLU:OE1	2.37	0.48
10:J:62:VAL:HG22	10:J:83:VAL:CG1	2.44	0.48
31:A:1492:A:H3'	31:A:1493:C:H5''	1.94	0.48
32:a:193:LEU:HD12	32:a:197:LEU:HB2	1.94	0.48
29:4:297:LEU:O	29:4:301:THR:N	2.47	0.48
29:4:655:ILE:O	29:4:659:GLN:N	2.46	0.48
30:b:381:LYS:HG2	30:b:383:LEU:HD13	1.96	0.48
31:A:1386:U:H3'	31:A:1387:A:C5'	2.43	0.48
20:T:139:CYS:SG	20:T:140:ILE:N	2.86	0.48
26:D:184:LYS:O	26:D:185:MET:C	2.57	0.48
29:4:372:TYR:HA	29:4:375:ILE:HB	1.96	0.48
30:b:91:ILE:HD12	30:b:162:THR:HB	1.96	0.48
30:b:266:ALA:HB1	30:b:280:ILE:HD12	1.96	0.48
31:A:760:A:N1	31:A:780:C:O2'	2.40	0.48
9:I:192:ARG:HD2	17:Q:44:TYR:OH	2.14	0.47
9:I:187:ARG:CZ	17:Q:45:TYR:CE1	2.98	0.47
30:b:84:LEU:O	30:b:85:SER:C	2.57	0.47
10:J:116:GLN:NE2	31:A:897:C:OP2	2.43	0.47
31:A:1290:C:O2'	31:A:1291:U:O4'	2.33	0.47
31:A:1505:A:O2'	31:A:1506:U:O5'	2.31	0.47
10:J:103:GLN:N	10:J:103:GLN:OE1	2.48	0.47
13:M:94:ALA:O	18:R:181:LEU:HD21	2.14	0.47
27:G:196:GLY:HA2	27:G:250:LEU:HD13	1.95	0.47
31:A:1185:C:N4	31:A:1186:A:N7	2.63	0.47
1:0:186:THR:O	1:0:186:THR:HG22	2.15	0.47
31:A:1505:A:HO2'	31:A:1506:U:P	2.37	0.47
2:1:265:THR:HG22	2:1:269:MET:HE3	1.97	0.47
9:I:191:ALA:HB1	32:a:171:GLN:CG	2.44	0.47
13:M:55:ASP:OD2	20:T:146:GLN:NE2	2.48	0.47
23:X:252:SER:O	23:X:302:HIS:NE2	2.48	0.47
8:H:52:VAL:HG11	29:4:477:TRP:HE1	1.79	0.46
14:N:6:SER:OG	14:N:69:LEU:O	2.28	0.46
12:L:82:ILE:O	12:L:85:VAL:HG22	2.15	0.46
28:V:137:ILE:HG22	28:V:139:PRO:HD3	1.97	0.46
31:A:752:C:O2'	31:A:793:C:N4	2.48	0.46
31:A:1124:A:O3'	32:a:46:LYS:HE2	2.14	0.46
31:A:1293:C:H4'	31:A:1294:A:OP2	2.14	0.46
10:J:63:LEU:HA	10:J:104:GLU:HG3	1.97	0.46
18:R:182:ARG:NH1	18:R:183:LYS:O	2.49	0.46
29:4:641:ILE:O	29:4:645:LEU:N	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:176:ASP:OD1	7:F:177:ARG:N	2.49	0.46
30:b:262:PHE:HB3	30:b:263:PRO:HD2	1.97	0.46
26:D:314:LEU:HD22	26:D:324:CYS:HB3	1.98	0.46
28:V:202:ARG:NE	28:V:247:MET:SD	2.89	0.46
28:V:382:TRP:O	28:V:386:LEU:N	2.48	0.46
30:b:115:LEU:N	30:b:138:GLN:O	2.44	0.46
30:b:378:ILE:HG22	30:b:378:ILE:O	2.16	0.46
27:G:315:PHE:HB3	27:G:316:PRO:HD3	1.98	0.46
20:T:155:LEU:O	20:T:160:ARG:NH1	2.49	0.46
26:D:91:THR:HG23	26:D:92:LYS:N	2.32	0.46
31:A:1289:G:H5'	31:A:1290:C:OP1	2.16	0.46
31:A:1370:U:O4	31:A:1382:A:N6	2.39	0.46
9:I:89:LYS:CD	31:A:1004:G:H5''	2.46	0.45
30:b:220:ALA:O	30:b:224:ARG:N	2.49	0.45
30:b:239:ILE:HD12	30:b:254:LEU:HD11	1.97	0.45
31:A:957:C:C6	31:A:958:C:H2'	2.51	0.45
31:A:1464:G:H21	31:A:1466:C:N4	2.14	0.45
10:J:106:GLN:N	10:J:106:GLN:OE1	2.49	0.45
31:A:1106:C:O2	31:A:1125:A:N6	2.49	0.45
31:A:1316:U:H2'	31:A:1317:A:O4'	2.16	0.45
32:a:198:ALA:O	32:a:199:VAL:C	2.58	0.45
9:I:179:THR:O	9:I:181:ILE:HD12	2.16	0.45
26:D:285:TYR:N	26:D:289:THR:O	2.48	0.45
8:H:137:ARG:NH2	31:A:1309:A:O2'	2.49	0.45
10:J:31:ALA:O	20:T:4:LYS:NZ	2.49	0.45
17:Q:26:LEU:O	17:Q:29:ILE:HG22	2.17	0.45
27:G:305:PRO:O	27:G:310:ARG:NH1	2.48	0.45
27:G:237:GLU:OE1	27:G:237:GLU:N	2.50	0.45
28:V:123:ASP:OD1	28:V:123:ASP:N	2.50	0.45
16:P:140:TYR:CD1	17:Q:29:ILE:HD12	2.52	0.45
26:D:231:MET:HE1	31:A:1480:A:N3	2.32	0.45
29:4:371:THR:HG22	29:4:375:ILE:HD12	1.99	0.45
8:H:71:ILE:O	8:H:150:GLY:N	2.50	0.45
9:I:180:PRO:HB2	31:A:977:A:O3'	2.16	0.45
23:X:129:GLU:O	23:X:134:LYS:NZ	2.42	0.45
26:D:95:ALA:HB3	26:D:99:TRP:CZ2	2.51	0.45
30:b:128:ALA:HB1	30:b:141:ALA:HB2	1.97	0.45
31:A:812:A:O2'	31:A:814:A:N1	2.49	0.45
8:H:126:ILE:O	31:A:1226:C:O2'	2.35	0.45
9:I:187:ARG:HD2	17:Q:45:TYR:CE1	2.52	0.45
13:M:114:ARG:O	13:M:118:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:80:ARG:NH1	29:4:480:ASP:O	2.50	0.45
17:Q:3:LYS:N	31:A:976:A:OP1	2.50	0.44
13:M:24:GLY:N	13:M:31:PHE:O	2.50	0.44
20:T:42:GLU:OE1	20:T:45:ARG:NH2	2.44	0.44
26:D:340:ILE:HG23	26:D:340:ILE:O	2.17	0.44
1:0:43:ARG:O	1:0:47:GLY:N	2.45	0.44
30:b:128:ALA:HB1	30:b:141:ALA:CB	2.47	0.44
31:A:1272:A:N1	31:A:1303:G:O2'	2.43	0.44
32:a:142:THR:HG22	32:a:143:THR:N	2.33	0.44
31:A:1272:A:N6	31:A:1320:G:O2'	2.50	0.44
32:a:130:THR:OG1	32:a:137:ARG:NH1	2.50	0.44
16:P:103:LYS:HB2	35:P:201:FES:S1	2.58	0.44
19:S:62:ASP:N	19:S:62:ASP:OD1	2.51	0.44
31:A:1081:U:H2'	31:A:1082:A:O4'	2.18	0.44
6:E:105:CYS:HB3	16:P:68:CYS:SG	2.57	0.44
20:T:52:ILE:N	20:T:53:PRO:CD	2.81	0.44
27:G:289:GLY:N	27:G:325:LYS:O	2.50	0.44
31:A:1108:C:H42	31:A:1125:A:H2'	1.82	0.44
2:1:100:GLU:OE1	2:1:100:GLU:N	2.49	0.44
7:F:88:ASP:OD2	7:F:146:HIS:NE2	2.50	0.44
18:R:162:SER:HB3	18:R:165:ILE:HD12	1.99	0.44
14:N:24:LYS:NZ	14:N:54:ALA:O	2.49	0.43
8:H:52:VAL:HG12	8:H:52:VAL:O	2.18	0.43
30:b:273:LEU:HB2	30:b:397:ARG:HD3	2.00	0.43
21:U:64:ARG:NH2	31:A:845:A:OP1	2.47	0.43
31:A:1506:U:O2'	31:A:1507:A:OP2	2.28	0.43
6:E:75:VAL:HG21	31:A:1034:U:O2'	2.18	0.43
9:I:120:ALA:HB2	31:A:995:A:OP2	2.18	0.43
21:U:161:GLN:O	21:U:164:VAL:HG12	2.19	0.43
30:b:114:VAL:O	30:b:115:LEU:HD23	2.18	0.43
31:A:1227:G:O5'	31:A:1228:A:H2'	2.19	0.43
6:E:115:GLU:O	6:E:116:LYS:C	2.61	0.43
24:Y:296:ASN:OD1	24:Y:298:PHE:N	2.50	0.43
31:A:1125:A:P	32:a:46:LYS:CE	3.06	0.43
10:J:81:CYS:SG	10:J:93:CYS:CB	3.07	0.43
21:U:42:VAL:HG13	21:U:42:VAL:O	2.19	0.43
30:b:204:MET:HE2	30:b:292:VAL:O	2.19	0.43
31:A:806:C:OP2	31:A:807:A:N6	2.36	0.43
23:X:123:ARG:NH2	23:X:337:LEU:O	2.52	0.43
30:b:235:ILE:HD11	30:b:258:VAL:HG13	2.00	0.43
31:A:958:C:O2'	31:A:959:C:OP2	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:52:THR:HG22	5:C:53:TYR:N	2.34	0.43
26:D:290:ILE:HD12	26:D:292:HIS:O	2.19	0.43
30:b:396:GLY:HA2	30:b:399:ALA:HB2	2.01	0.43
14:N:88:VAL:O	14:N:88:VAL:HG13	2.19	0.42
31:A:1488:C:O2'	31:A:1489:G:O4'	2.37	0.42
8:H:123:SER:OG	31:A:1265:C:O2'	2.35	0.42
23:X:174:ASN:OD1	23:X:175:LYS:N	2.52	0.42
32:a:194:ASP:O	32:a:198:ALA:HB3	2.19	0.42
7:F:156:ILE:HG22	32:a:196:LEU:HD23	2.00	0.42
9:I:191:ALA:CB	32:a:171:GLN:HG3	2.48	0.42
29:4:542:PRO:O	29:4:546:VAL:N	2.43	0.42
22:W:129:VAL:HG23	22:W:130:ASP:N	2.34	0.42
30:b:106:ILE:HG22	30:b:113:ILE:HD13	2.02	0.42
5:C:103:CYS:O	5:C:124:LEU:N	2.46	0.42
11:K:31:ASP:N	11:K:31:ASP:OD1	2.52	0.42
21:U:166:ASN:O	21:U:176:ARG:NH1	2.39	0.42
2:1:57:THR:HA	2:1:60:MET:HE3	2.02	0.42
6:E:3:ARG:NH2	6:E:67:ASP:OD2	2.46	0.42
15:O:238:MET:SD	15:O:238:MET:N	2.92	0.42
22:W:92:MET:O	22:W:98:LYS:NZ	2.52	0.42
31:A:955:A:OP2	31:A:956:C:N4	2.44	0.42
4:B:89:VAL:O	4:B:89:VAL:HG12	2.19	0.42
2:1:129:PHE:CB	8:H:155:VAL:HG21	2.50	0.42
9:I:88:ILE:HD12	9:I:149:VAL:HG13	2.01	0.42
19:S:83:ARG:NH1	19:S:93:LYS:O	2.53	0.42
27:G:196:GLY:O	27:G:248:VAL:N	2.52	0.42
30:b:192:LEU:HB2	30:b:208:ALA:HB2	2.02	0.42
31:A:1080:A:H2'	31:A:1081:U:C5'	2.49	0.42
26:D:178:GLU:O	26:D:182:LYS:N	2.48	0.42
28:V:40:TRP:O	28:V:43:ARG:NH1	2.53	0.42
30:b:166:VAL:HG23	30:b:310:LEU:HD13	2.00	0.42
31:A:1271:C:N4	31:A:1320:G:O2'	2.53	0.42
31:A:1398:U:H3	31:A:1408:A:H61	1.67	0.42
2:1:91:VAL:O	2:1:94:GLY:N	2.53	0.41
3:3:130:VAL:HG13	3:3:133:ILE:HB	2.02	0.41
6:E:27:GLU:OE1	21:U:170:ARG:NH1	2.53	0.41
19:S:50:ARG:NH2	31:A:1119:U:O5'	2.51	0.41
30:b:239:ILE:HG23	30:b:254:LEU:HD11	2.01	0.41
31:A:1488:C:H2'	31:A:1489:G:C8	2.55	0.41
32:a:90:HIS:O	32:a:94:ARG:N	2.53	0.41
1:0:83:LYS:N	1:0:138:ASP:OD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:46:GLU:N	11:K:46:GLU:OE1	2.52	0.41
15:O:97:ARG:HH12	31:A:870:C:H3'	1.85	0.41
26:D:245:VAL:HG22	26:D:271:ALA:HB1	2.01	0.41
31:A:1391:U:H3'	31:A:1392:A:C5'	2.50	0.41
32:a:297:SER:O	32:a:301:VAL:HG13	2.20	0.41
1:O:57:ASP:OD2	31:A:704:U:N3	2.45	0.41
9:I:154:LEU:HD12	17:Q:39:ILE:HG21	2.02	0.41
19:S:117:LEU:O	19:S:121:THR:OG1	2.34	0.41
26:D:355:ARG:NE	31:A:1118:A:N7	2.68	0.41
30:b:84:LEU:HD12	30:b:168:MET:HE2	2.02	0.41
31:A:1478:A:N3	31:A:1478:A:H2'	2.35	0.41
9:I:194:LEU:HD12	31:A:1083:C:O2'	2.21	0.41
12:L:201:ARG:NH2	31:A:1151:C:OP1	2.51	0.41
13:M:94:ALA:HB2	18:R:158:PHE:CD1	2.56	0.41
20:T:149:CYS:HB2	35:T:201:FES:S2	2.60	0.41
22:W:132:GLU:O	22:W:135:GLN:NE2	2.50	0.41
26:D:95:ALA:HB1	26:D:98:LEU:HD13	2.03	0.41
30:b:98:GLY:O	30:b:99:SER:C	2.63	0.41
31:A:1560:U:C4	31:A:1561:C:C4	3.08	0.41
7:F:161:ILE:HG21	7:F:167:PHE:HB3	2.03	0.41
12:L:86:ASP:OD1	12:L:87:ASP:N	2.54	0.41
17:Q:46:GLU:OE1	17:Q:51:ARG:HG2	2.21	0.41
27:G:389:ARG:HD2	31:A:1434:A:OP2	2.21	0.41
29:4:655:ILE:HG22	29:4:656:ASN:N	2.36	0.41
30:b:331:ARG:HG2	30:b:336:ILE:HA	2.03	0.41
31:A:764:A:O2'	31:A:765:C:OP2	2.37	0.41
1:O:110:ASP:OD1	1:O:110:ASP:N	2.52	0.41
30:b:214:LEU:O	30:b:243:ARG:NH2	2.53	0.41
30:b:328:ILE:O	30:b:332:PHE:N	2.54	0.41
9:I:191:ALA:HA	17:Q:44:TYR:HB3	2.02	0.41
10:J:92:VAL:HG11	10:J:121:VAL:HG22	2.02	0.41
10:J:99:GLY:O	10:J:127:ARG:NH2	2.47	0.41
30:b:205:PRO:HD3	32:a:252:LYS:HD2	2.02	0.41
32:a:176:VAL:O	32:a:176:VAL:HG13	2.21	0.40
7:F:174:LEU:O	7:F:179:ARG:NH2	2.46	0.40
8:H:184:ILE:O	8:H:184:ILE:HG22	2.20	0.40
29:4:66:ASP:OD1	29:4:69:ALA:HB2	2.20	0.40
20:T:52:ILE:CG1	20:T:53:PRO:HD3	2.52	0.40
30:b:106:ILE:HG21	30:b:115:LEU:HD21	2.02	0.40
31:A:1431:G:O2'	31:A:1457:G:O6	2.30	0.40
2:1:131:THR:OG1	8:H:149:THR:OG1	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:96:GLN:OE1	31:A:1003:A:O2'	2.38	0.40
30:b:330:LYS:NZ	30:b:331:ARG:HE	2.19	0.40
31:A:1584:MA6:OP2	31:A:1584:MA6:H8	2.22	0.40
10:J:80:CYS:SG	10:J:94:PHE:N	2.94	0.40
27:G:377:ARG:NH1	31:A:1454:G:OP2	2.52	0.40
31:A:1569:G:O2'	31:A:1570:G:OP2	2.33	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 PDB entries followed by that with respect to all EM entries.

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	0	213/218 (98%)	207 (97%)	6 (3%)	0	100	100
2	1	251/323 (78%)	246 (98%)	5 (2%)	0	100	100
3	3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
4	B	223/296 (75%)	219 (98%)	4 (2%)	0	100	100
5	C	130/167 (78%)	122 (94%)	8 (6%)	0	100	100
6	E	113/125 (90%)	111 (98%)	1 (1%)	1 (1%)	14	44
7	F	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
8	H	137/201 (68%)	134 (98%)	3 (2%)	0	100	100
9	I	134/194 (69%)	130 (97%)	4 (3%)	0	100	100
10	J	106/138 (77%)	94 (89%)	11 (10%)	1 (1%)	14	44
11	K	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
12	L	172/257 (67%)	166 (96%)	6 (4%)	0	100	100
13	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
14	N	108/130 (83%)	104 (96%)	4 (4%)	0	100	100
15	O	192/258 (74%)	185 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
17	Q	85/87 (98%)	82 (96%)	2 (2%)	1 (1%)	10	37
18	R	293/360 (81%)	283 (97%)	10 (3%)	0	100	100
19	S	133/190 (70%)	127 (96%)	6 (4%)	0	100	100
20	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
21	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
22	W	98/187 (52%)	94 (96%)	4 (4%)	0	100	100
23	X	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
24	Y	119/395 (30%)	119 (100%)	0	0	100	100
25	Z	86/106 (81%)	84 (98%)	2 (2%)	0	100	100
26	D	300/430 (70%)	289 (96%)	11 (4%)	0	100	100
27	G	309/396 (78%)	300 (97%)	9 (3%)	0	100	100
28	V	358/414 (86%)	350 (98%)	8 (2%)	0	100	100
29	4	573/689 (83%)	566 (99%)	7 (1%)	0	100	100
30	b	290/407 (71%)	263 (91%)	27 (9%)	0	100	100
32	a	137/343 (40%)	128 (93%)	9 (7%)	0	100	100
All	All	5832/7935 (74%)	5660 (97%)	169 (3%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	94	PHE
17	Q	2	ALA
6	E	112	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 PDB entries followed by that with respect to all EM entries.

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	0	188/190 (99%)	188 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	235/291 (81%)	235 (100%)	0	100	100
3	3	65/166 (39%)	65 (100%)	0	100	100
4	B	198/249 (80%)	198 (100%)	0	100	100
5	C	115/143 (80%)	115 (100%)	0	100	100
6	E	97/107 (91%)	97 (100%)	0	100	100
7	F	182/209 (87%)	182 (100%)	0	100	100
8	H	129/180 (72%)	129 (100%)	0	100	100
9	I	104/146 (71%)	104 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	158/226 (70%)	158 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	175/230 (76%)	175 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	Q	78/78 (100%)	78 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	W	87/158 (55%)	87 (100%)	0	100	100
23	X	311/351 (89%)	311 (100%)	0	100	100
24	Y	112/357 (31%)	112 (100%)	0	100	100
25	Z	81/95 (85%)	81 (100%)	0	100	100
26	D	260/357 (73%)	260 (100%)	0	100	100
27	G	272/342 (80%)	271 (100%)	1 (0%)	84	86
28	V	325/364 (89%)	325 (100%)	0	100	100
29	4	518/609 (85%)	518 (100%)	0	100	100
30	b	249/350 (71%)	247 (99%)	2 (1%)	73	81
32	a	127/288 (44%)	127 (100%)	0	100	100
All	All	5216/6881 (76%)	5213 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	G	254	LYS
30	b	269	THR
30	b	384	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	268	GLN
3	3	139	ASN
4	B	148	ASN
4	B	266	GLN
5	C	116	GLN
7	F	151	ASN
7	F	196	HIS
8	H	83	HIS
8	H	122	GLN
9	I	87	HIS
9	I	183	HIS
11	K	68	GLN
13	M	61	HIS
13	M	82	HIS
15	O	98	ASN
15	O	111	HIS
15	O	147	HIS
20	T	146	GLN
21	U	109	ASN
23	X	69	ASN
23	X	148	GLN
23	X	170	GLN
25	Z	63	GLN
26	D	288	HIS
26	D	369	HIS
27	G	82	ASN
27	G	288	HIS
28	V	188	HIS
29	4	470	GLN
29	4	521	HIS
29	4	577	ASN
30	b	102	HIS
30	b	138	GLN
30	b	379	HIS

5.3.3 RNA 

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	A	946/954 (99%)	225 (23%)	6 (0%)

All (225) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	A	650	U
31	A	651	A
31	A	671	U
31	A	680	U
31	A	688	A
31	A	689	U
31	A	695	A
31	A	704	U
31	A	721	U
31	A	730	A
31	A	753	A
31	A	761	A
31	A	763	C
31	A	764	A
31	A	766	G
31	A	773	U
31	A	777	G
31	A	791	G
31	A	794	U
31	A	796	G
31	A	814	A
31	A	815	C
31	A	828	C
31	A	829	C
31	A	830	U
31	A	832	U
31	A	835	C
31	A	860	A
31	A	861	U
31	A	868	C
31	A	871	A
31	A	889	G
31	A	890	C
31	A	893	G
31	A	902	G
31	A	904	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	A	907	A
31	A	908	C
31	A	919	A
31	A	930	G
31	A	931	C
31	A	933	G
31	A	938	A
31	A	939	A
31	A	940	A
31	A	941	G
31	A	954	C
31	A	957	C
31	A	958	C
31	A	961	U
31	A	962	C
31	A	964	C
31	A	967	A
31	A	978	A
31	A	979	C
31	A	993	A
31	A	995	A
31	A	1001	C
31	A	1011	C
31	A	1015	A
31	A	1025	A
31	A	1047	A
31	A	1065	C
31	A	1068	A
31	A	1069	A
31	A	1080	A
31	A	1081	U
31	A	1088	C
31	A	1097	G
31	A	1105	C
31	A	1106	C
31	A	1107	U
31	A	1108	C
31	A	1109	A
31	A	1113	G
31	A	1118	A
31	A	1119	U
31	A	1120	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	A	1121	A
31	A	1126	A
31	A	1128	C
31	A	1137	A
31	A	1151	C
31	A	1154	A
31	A	1160	A
31	A	1167	A
31	A	1175	G
31	A	1176	G
31	A	1177	C
31	A	1178	G
31	A	1181	G
31	A	1184	U
31	A	1185	C
31	A	1186	A
31	A	1188	A
31	A	1189	U
31	A	1190	C
31	A	1193	U
31	A	1200	G
31	A	1201	A
31	A	1215	U
31	A	1222	A
31	A	1223	C
31	A	1225	C
31	A	1226	C
31	A	1229	U
31	A	1236	C
31	A	1238	C
31	A	1244	C
31	A	1245	U
31	A	1246	U
31	A	1247	G
31	A	1248	C
31	A	1251	A
31	A	1255	U
31	A	1259	U
31	A	1269	U
31	A	1273	G
31	A	1278	C
31	A	1285	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	A	1287	A
31	A	1290	C
31	A	1291	U
31	A	1292	A
31	A	1293	C
31	A	1294	A
31	A	1295	A
31	A	1296	A
31	A	1297	G
31	A	1303	G
31	A	1312	C
31	A	1314	C
31	A	1318	A
31	A	1326	A
31	A	1327	G
31	A	1331	A
31	A	1332	A
31	A	1341	C
31	A	1342	C
31	A	1343	A
31	A	1345	G
31	A	1352	C
31	A	1354	A
31	A	1356	A
31	A	1367	A
31	A	1371	U
31	A	1378	C
31	A	1379	A
31	A	1381	A
31	A	1383	A
31	A	1385	C
31	A	1386	U
31	A	1387	A
31	A	1390	A
31	A	1392	A
31	A	1399	A
31	A	1405	C
31	A	1406	U
31	A	1407	U
31	A	1415	G
31	A	1417	A
31	A	1420	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	A	1421	G
31	A	1422	G
31	A	1427	A
31	A	1430	A
31	A	1438	G
31	A	1442	G
31	A	1443	U
31	A	1444	A
31	A	1447	G
31	A	1457	G
31	A	1461	A
31	A	1464	G
31	A	1476	G
31	A	1477	U
31	A	1478	A
31	A	1479	C
31	A	1480	A
31	A	1481	C
31	A	1482	A
31	A	1483	C
31	A	1484	C
31	A	1485	G
31	A	1486	C
31	A	1488	C
31	A	1491	C
31	A	1493	C
31	A	1506	U
31	A	1507	A
31	A	1512	A
31	A	1519	A
31	A	1520	U
31	A	1521	U
31	A	1522	U
31	A	1523	A
31	A	1524	A
31	A	1525	C
31	A	1527	A
31	A	1532	C
31	A	1533	C
31	A	1537	C
31	A	1539	C
31	A	1546	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	A	1547	U
31	A	1548	A
31	A	1557	A
31	A	1558	A
31	A	1559	G
31	A	1560	U
31	A	1562	G
31	A	1563	U
31	A	1564	A
31	A	1565	A
31	A	1567	A
31	A	1568	U
31	A	1569	G
31	A	1570	G
31	A	1571	U
31	A	1572	A
31	A	1584	MA6
31	A	1590	A
31	A	1594	G
31	A	1595	G
31	A	1598	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	A	961	U
31	A	1046	A
31	A	1293	C
31	A	1485	G
31	A	1505	A
31	A	1558	A

5.4 Non-standard residues in protein, DNA, RNA chains

4 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
31	MA6	A	1583	31	23,26,27	1.28	3 (13%)	34,38,41	3.16	12 (35%)
9	5F0	I	184	9	8,8,9	0.57	0	7,9,11	1.12	1 (14%)
31	MA6	A	1584	31	23,26,27	1.30	3 (13%)	34,38,41	3.18	12 (35%)
31	5MU	A	1076	31	19,22,23	0.41	0	28,32,35	0.52	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
31	MA6	A	1583	31	-	3/11/29/30	0/3/3/3
9	5F0	I	184	9	-	6/9/9/10	-
31	MA6	A	1584	31	-	2/11/29/30	0/3/3/3
31	5MU	A	1076	31	-	0/7/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	1584	MA6	C6-N6	3.36	1.46	1.36
31	A	1583	MA6	C6-N6	3.33	1.46	1.36
31	A	1584	MA6	C5-C4	-2.65	1.34	1.39
31	A	1583	MA6	C5-C4	-2.59	1.34	1.39
31	A	1584	MA6	C5-N7	-2.33	1.34	1.39
31	A	1583	MA6	C5-N7	-2.30	1.34	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1583	MA6	N1-C6-N6	-12.44	103.48	117.08
31	A	1584	MA6	N1-C6-N6	-12.36	103.57	117.08
31	A	1584	MA6	C5-C6-N6	6.29	136.26	125.30
31	A	1583	MA6	C5-C6-N6	6.22	136.13	125.30
31	A	1583	MA6	N1-C2-N3	-5.43	120.10	128.60
31	A	1584	MA6	N1-C2-N3	-5.43	120.11	128.60
31	A	1584	MA6	C5-C4-N3	-5.22	119.94	126.75
31	A	1583	MA6	C5-C4-N3	-5.21	119.95	126.75
31	A	1584	MA6	N9-C8-N7	-4.35	107.96	113.91
31	A	1583	MA6	N9-C8-N7	-4.23	108.12	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1584	MA6	C4-C5-C6	3.62	119.93	115.88
31	A	1583	MA6	C2-N3-C4	3.51	120.04	111.75
31	A	1584	MA6	C2-N3-C4	3.48	119.97	111.75
31	A	1583	MA6	C4-C5-C6	3.45	119.75	115.88
31	A	1584	MA6	C2-N1-C6	3.44	119.88	111.75
31	A	1583	MA6	C2-N1-C6	3.39	119.77	111.75
31	A	1584	MA6	C5-N7-C8	3.16	108.00	103.51
31	A	1584	MA6	N3-C4-N9	3.10	132.20	127.08
31	A	1583	MA6	C5-N7-C8	3.10	107.92	103.51
31	A	1583	MA6	N3-C4-N9	3.05	132.11	127.08
9	I	184	5F0	O-C-CB	-2.57	117.93	125.43
31	A	1584	MA6	C4-N9-C8	2.24	108.16	105.73
31	A	1584	MA6	C4-C5-N7	-2.14	108.01	110.62
31	A	1583	MA6	C4-C5-N7	-2.08	108.08	110.62
31	A	1583	MA6	C4-N9-C8	2.04	107.94	105.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	184	5F0	O1-C1-CA-CB
9	I	184	5F0	OD1-C1-CA-CB
9	I	184	5F0	N-CA-CB-C
31	A	1583	MA6	O4'-C4'-C5'-O5'
31	A	1584	MA6	O4'-C4'-C5'-O5'
31	A	1584	MA6	C3'-C4'-C5'-O5'
31	A	1583	MA6	C3'-C4'-C5'-O5'
9	I	184	5F0	O1-C1-CA-N
9	I	184	5F0	OD1-C1-CA-N
9	I	184	5F0	O-C-CB-CA
31	A	1583	MA6	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	1583	MA6	2	0
9	I	184	5F0	4	0
31	A	1584	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 39 are monoatomic - leaving 6 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
37	GDP	X	502	-	28,30,30	1.14	3 (10%)	44,47,47	1.87	7 (15%)
35	FES	T	201	-	0,4,4	-	-	-	-	-
35	FES	P	201	16,6	0,4,4	-	-	-	-	-
36	ATP	X	501	-	29,33,33	0.50	0	44,52,52	0.81	1 (2%)
40	SPM	A	1702	-	13,13,13	0.34	0	12,12,12	0.97	0
39	NAD	A	1701	38	45,48,48	0.75	1 (2%)	63,73,73	0.71	2 (3%)

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
37	GDP	X	502	-	-	0/16/32/32	0/3/3/3
35	FES	T	201	-	-	-	0/1/1/1
35	FES	P	201	16,6	-	-	0/1/1/1
36	ATP	X	501	-	-	0/22/38/38	0/3/3/3
40	SPM	A	1702	-	-	0/11/11/11	-
39	NAD	A	1701	38	-	6/30/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	502	GDP	C5-C4	3.08	1.47	1.38
37	X	502	GDP	C6-N1	-2.51	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	A	1701	NAD	O4D-C1D	-2.42	1.37	1.41
37	X	502	GDP	C5-N7	-2.22	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	X	502	GDP	C5-C4-N3	-6.38	118.10	128.46
37	X	502	GDP	C2-N3-C4	4.90	121.04	112.30
37	X	502	GDP	N9-C4-N3	4.82	135.63	125.94
37	X	502	GDP	PA-O3A-PB	-3.82	119.72	132.83
36	X	501	ATP	PA-O3A-PB	-3.12	122.13	132.83
37	X	502	GDP	C6-C5-N7	3.00	135.83	130.25
37	X	502	GDP	C4-C5-N7	-2.64	106.54	110.72
37	X	502	GDP	O6-C6-C5	-2.19	120.79	126.60
39	A	1701	NAD	O2A-PA-O1A	2.18	123.02	112.24
39	A	1701	NAD	PN-O3-PA	-2.01	125.93	132.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	A	1701	NAD	C5B-O5B-PA-O3
39	A	1701	NAD	O4B-C4B-C5B-O5B
39	A	1701	NAD	C3B-C4B-C5B-O5B
39	A	1701	NAD	PN-O3-PA-O5B
39	A	1701	NAD	C5B-O5B-PA-O1A
39	A	1701	NAD	PA-O3-PN-O2N

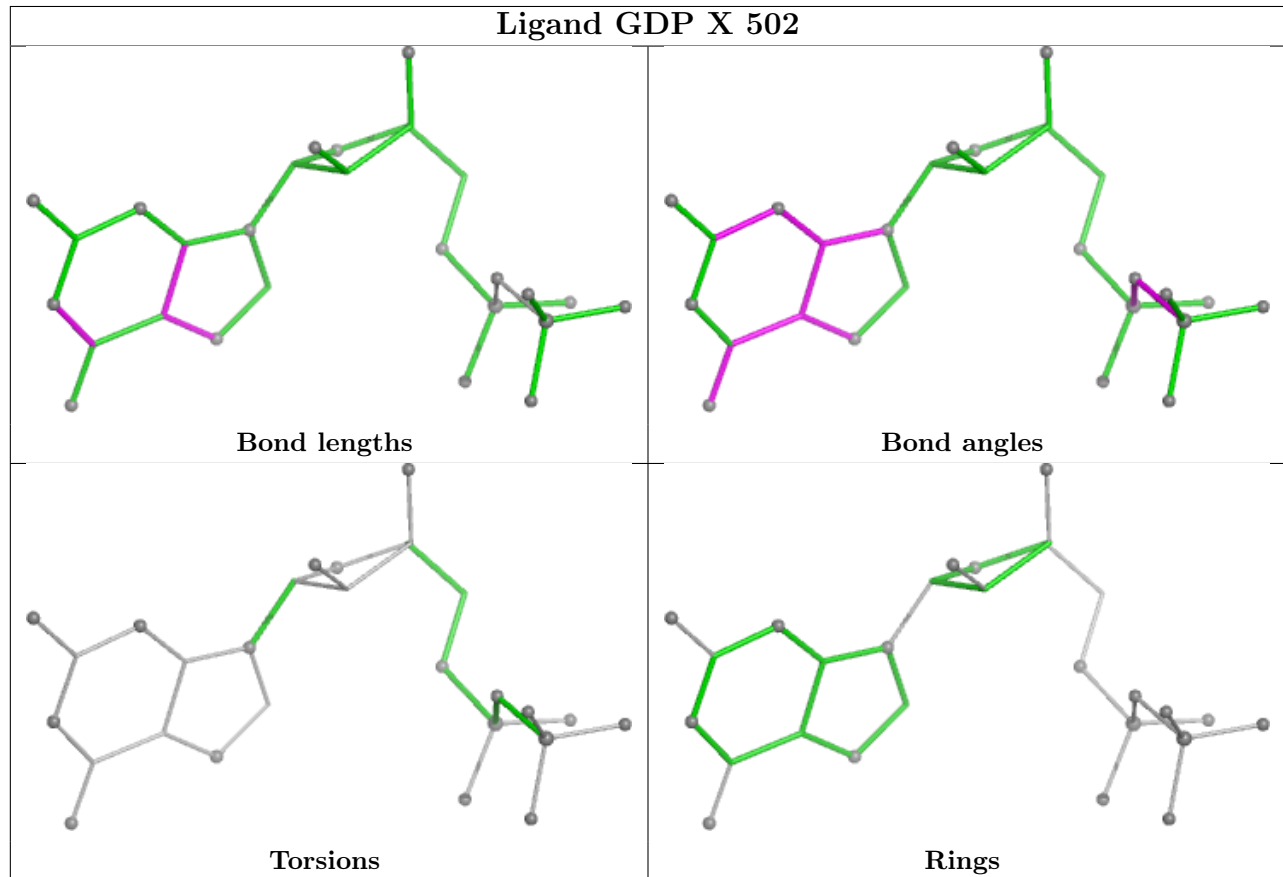
There are no ring outliers.

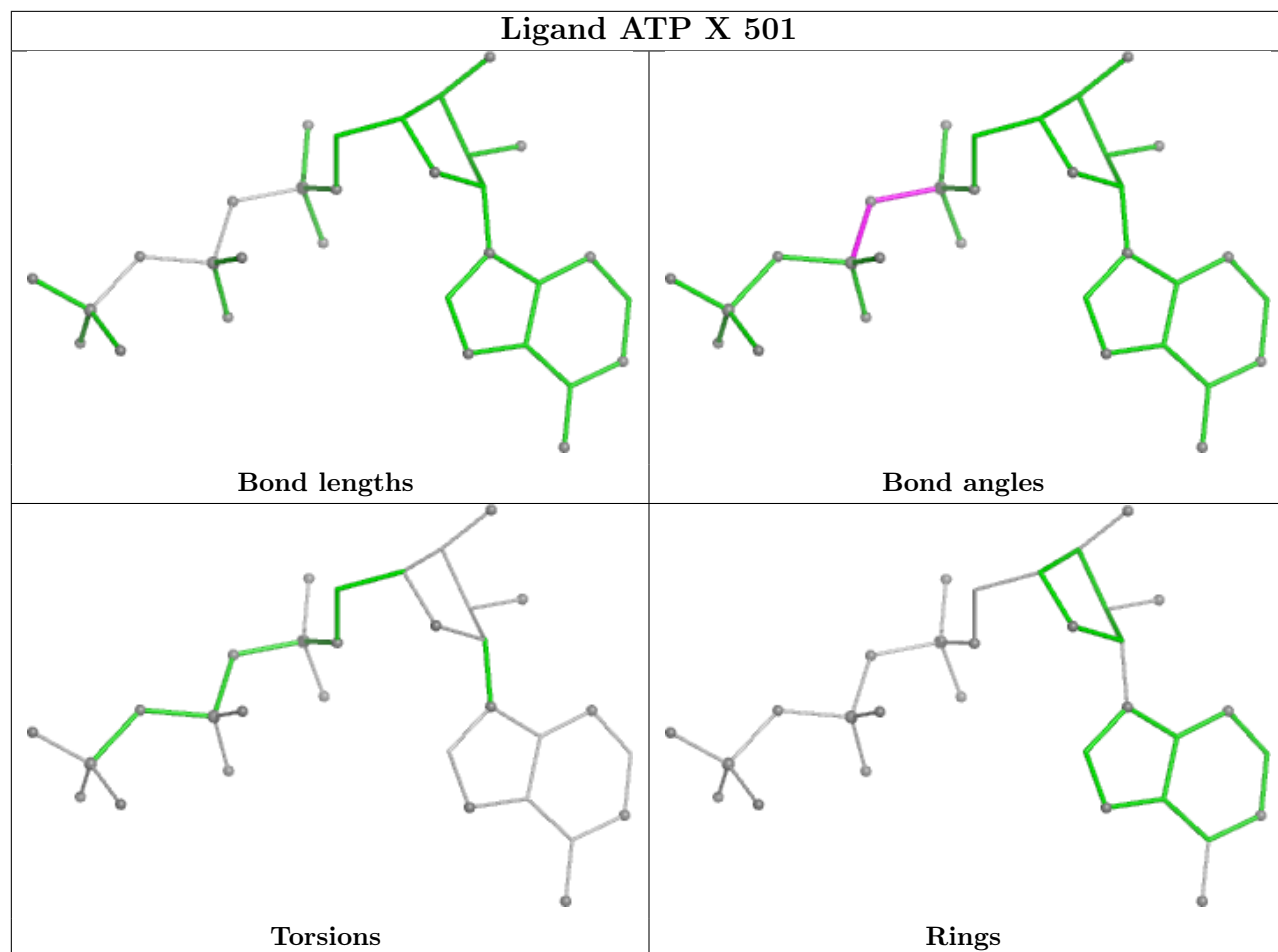
3 monomers are involved in 4 short contacts:

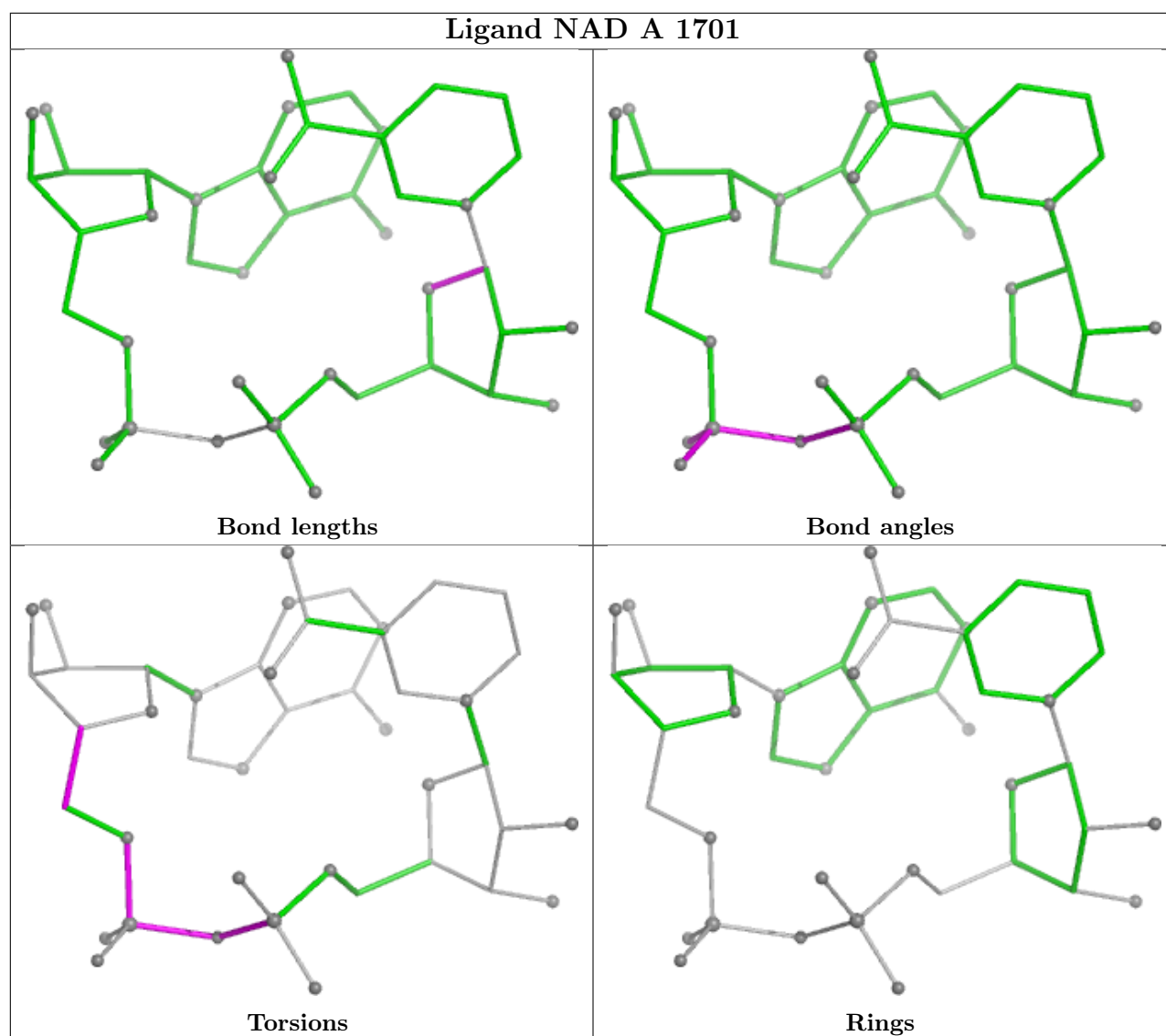
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	T	201	FES	2	0
35	P	201	FES	1	0
40	A	1702	SPM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	68:ARG	C	69:LYS	N	1.17

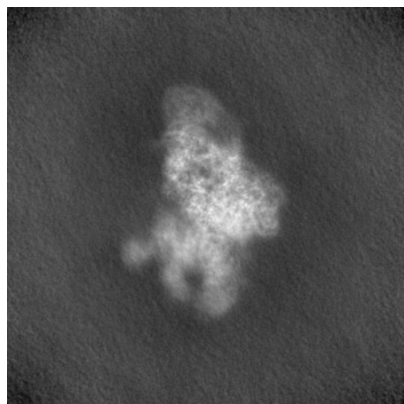
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54131. These allow visual inspection of the internal detail of the map and identification of artifacts.

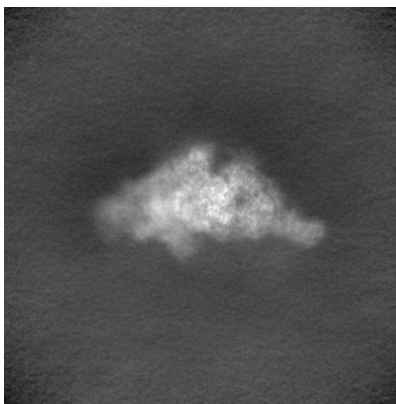
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

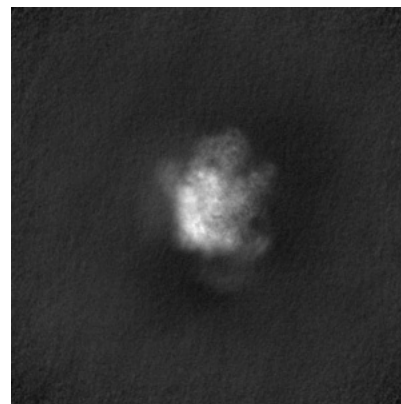
6.1.1 Primary map



X

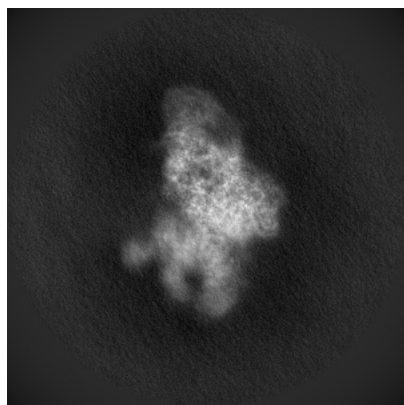


Y

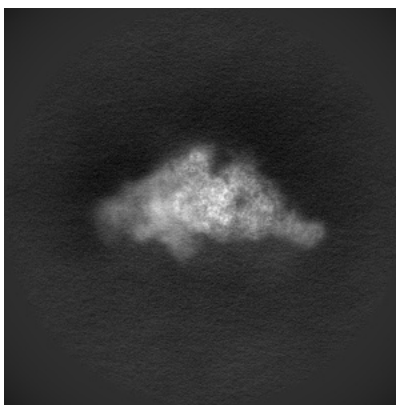


Z

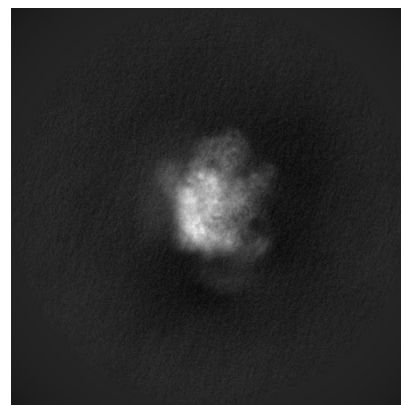
6.1.2 Raw map



X



Y

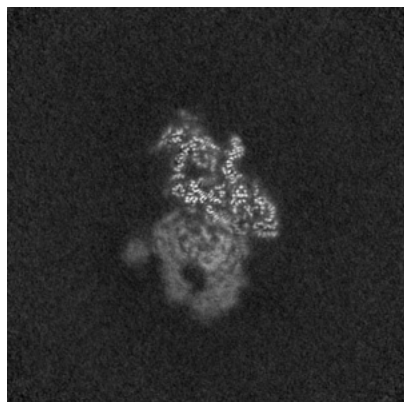


Z

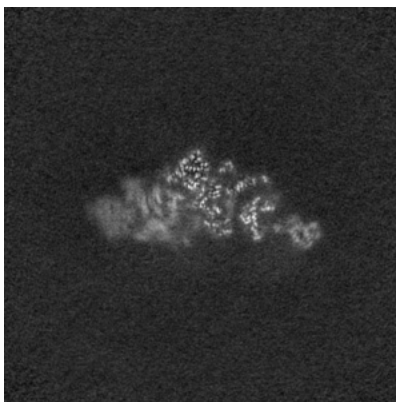
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

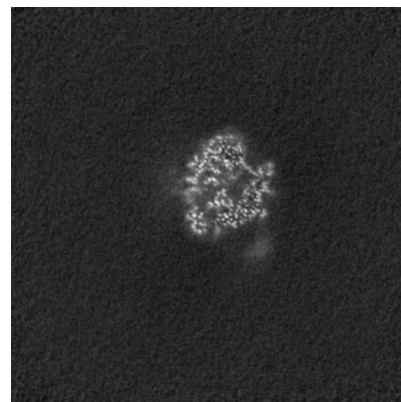
6.2.1 Primary map



X Index: 300

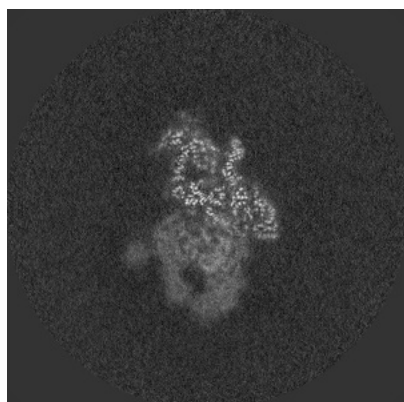


Y Index: 300

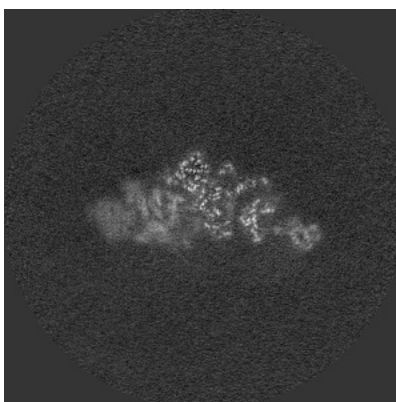


Z Index: 300

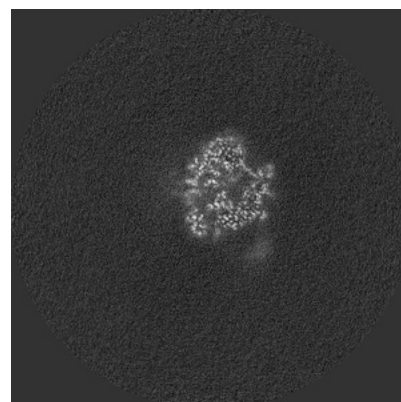
6.2.2 Raw map



X Index: 300



Y Index: 300

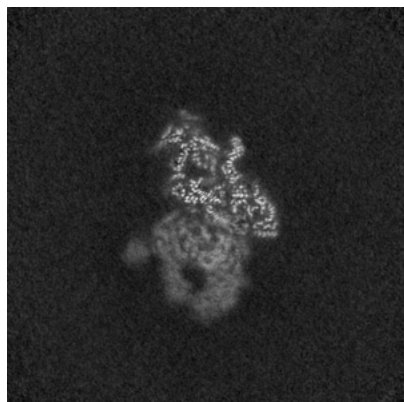


Z Index: 300

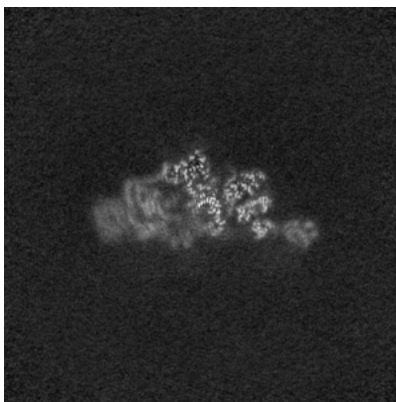
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

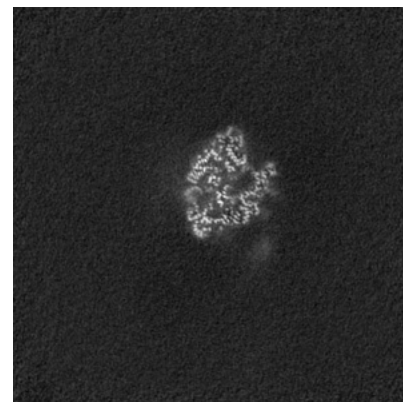
6.3.1 Primary map



X Index: 299

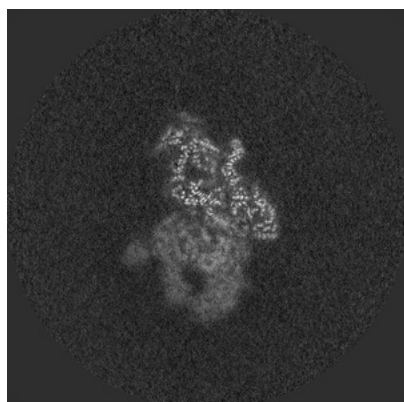


Y Index: 308

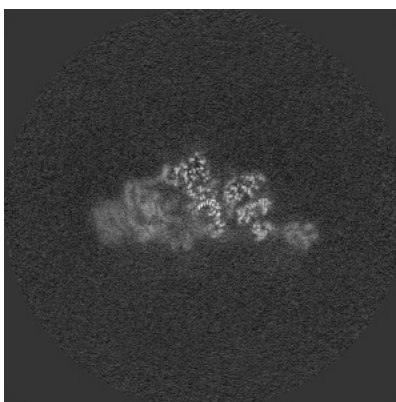


Z Index: 304

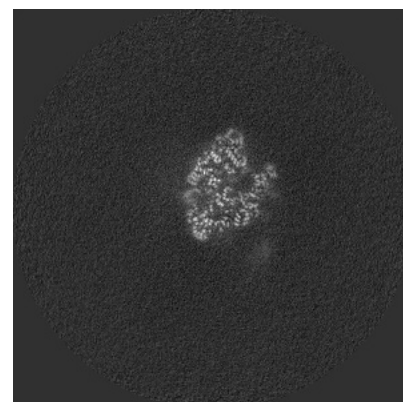
6.3.2 Raw map



X Index: 299



Y Index: 308

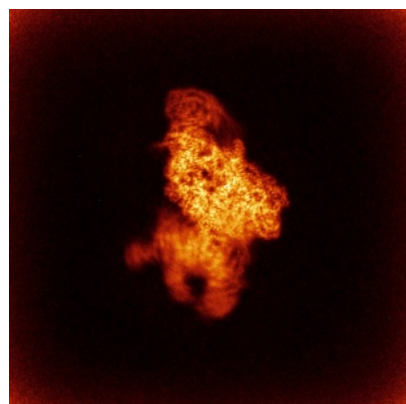


Z Index: 305

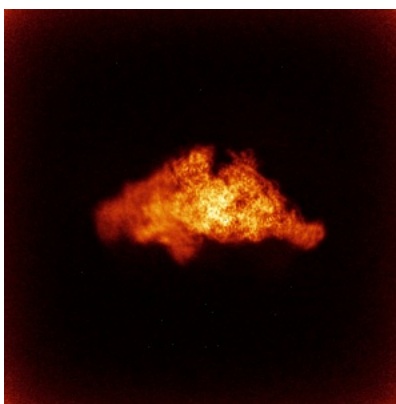
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

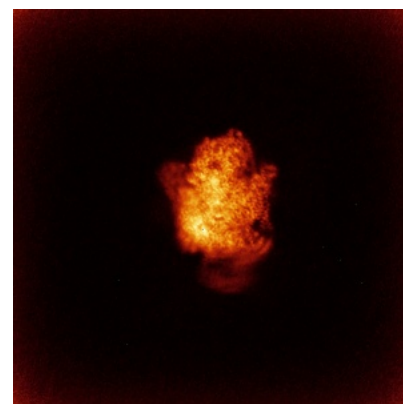
6.4.1 Primary map



X

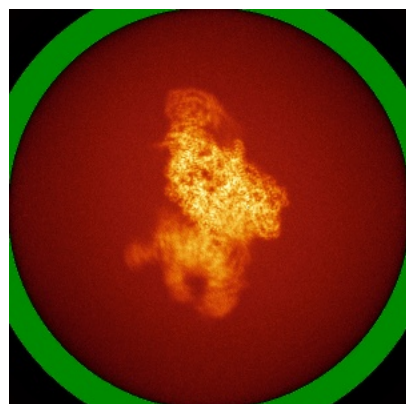


Y

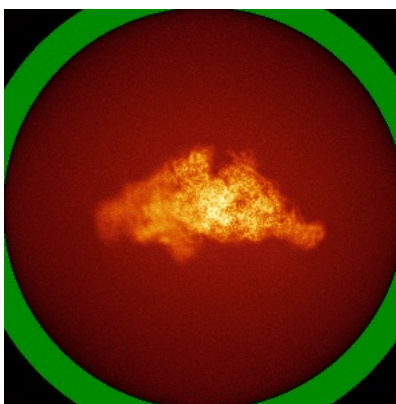


Z

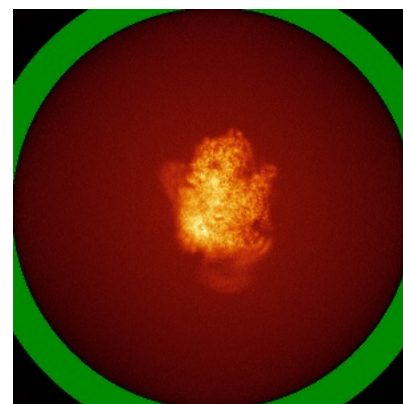
6.4.2 Raw map



X



Y

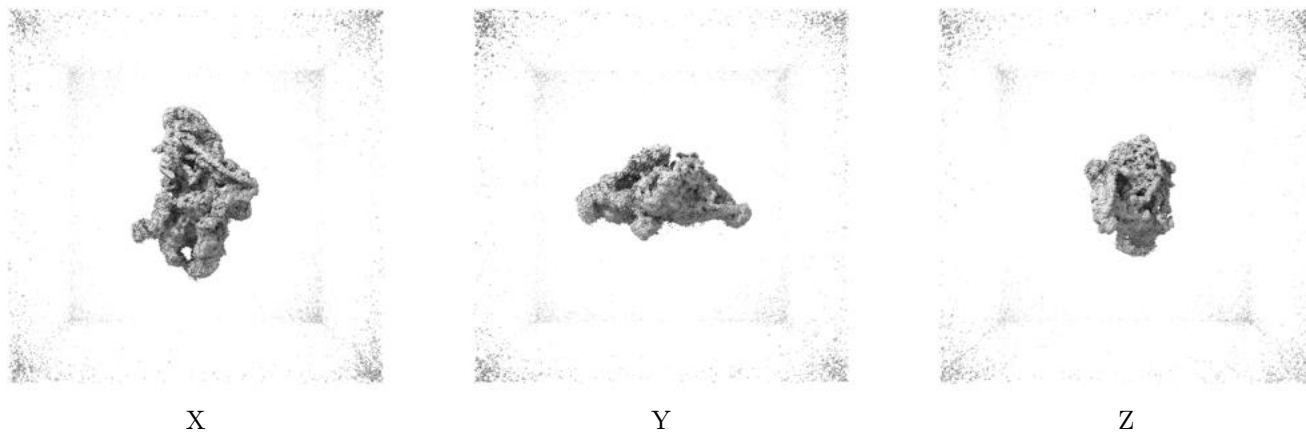


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

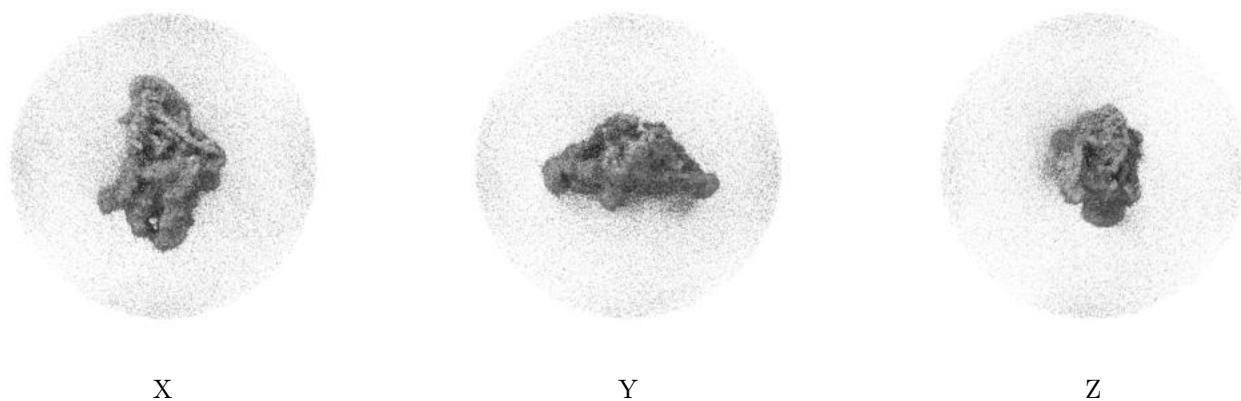
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

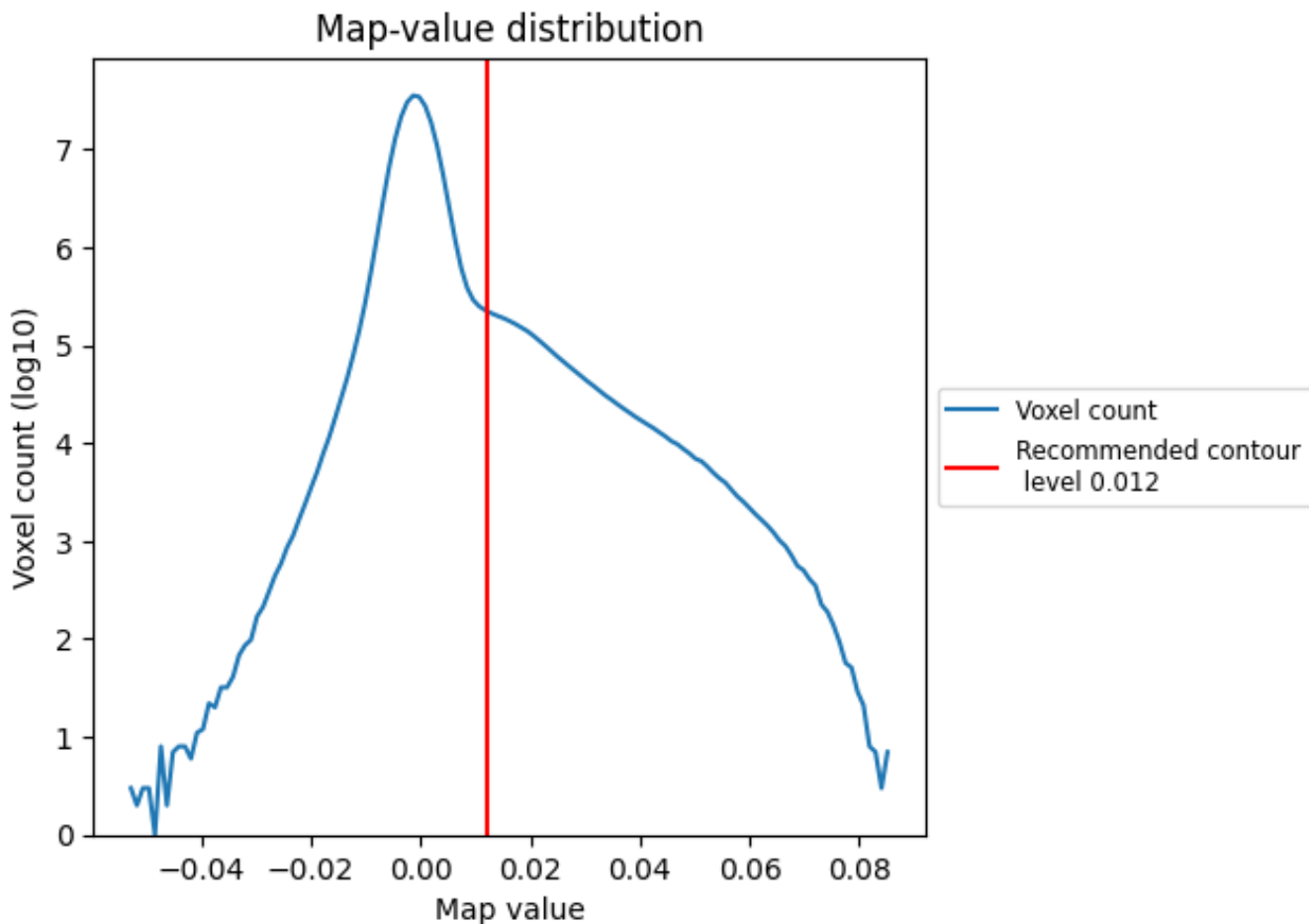
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

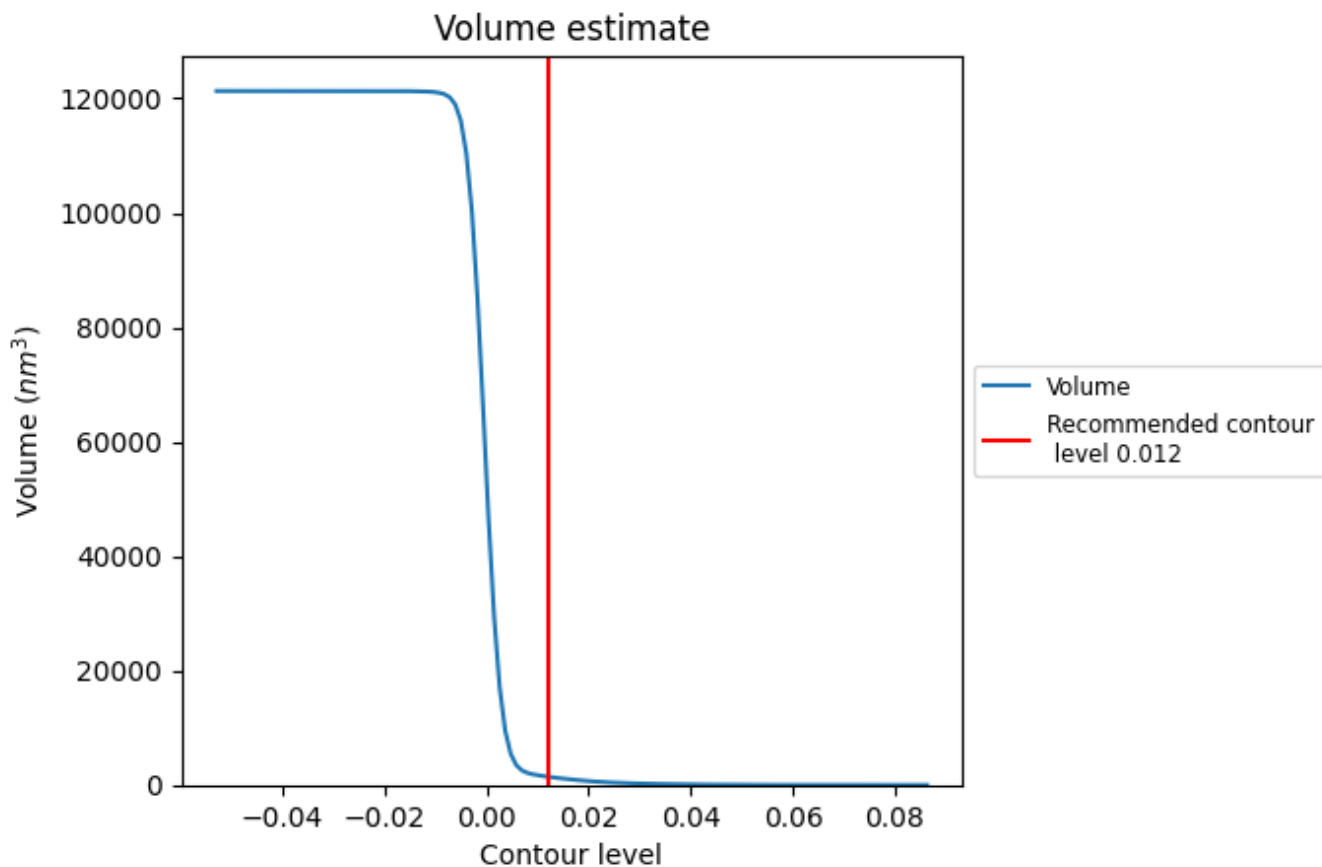
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

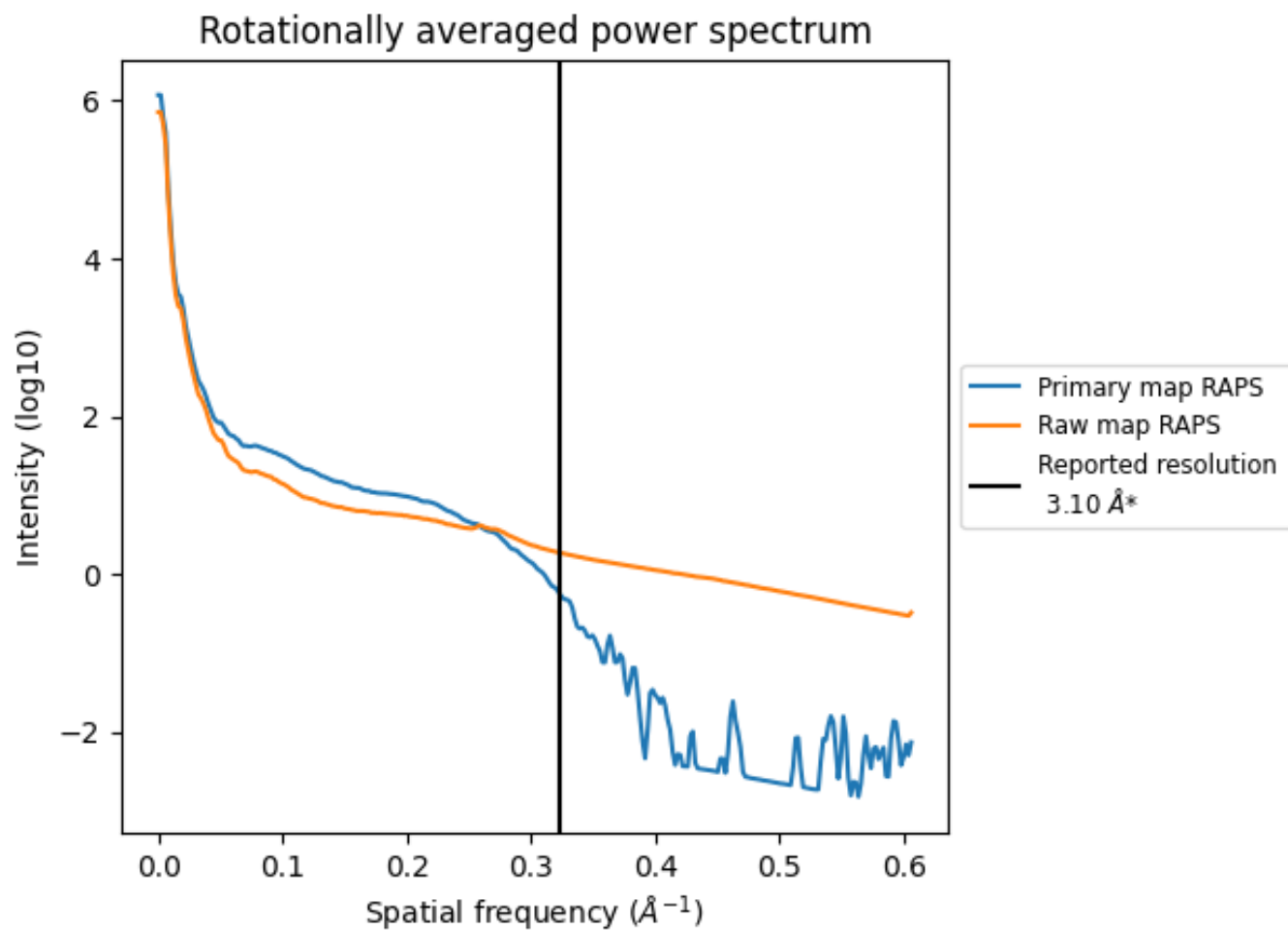
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1439 nm³; this corresponds to an approximate mass of 1300 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

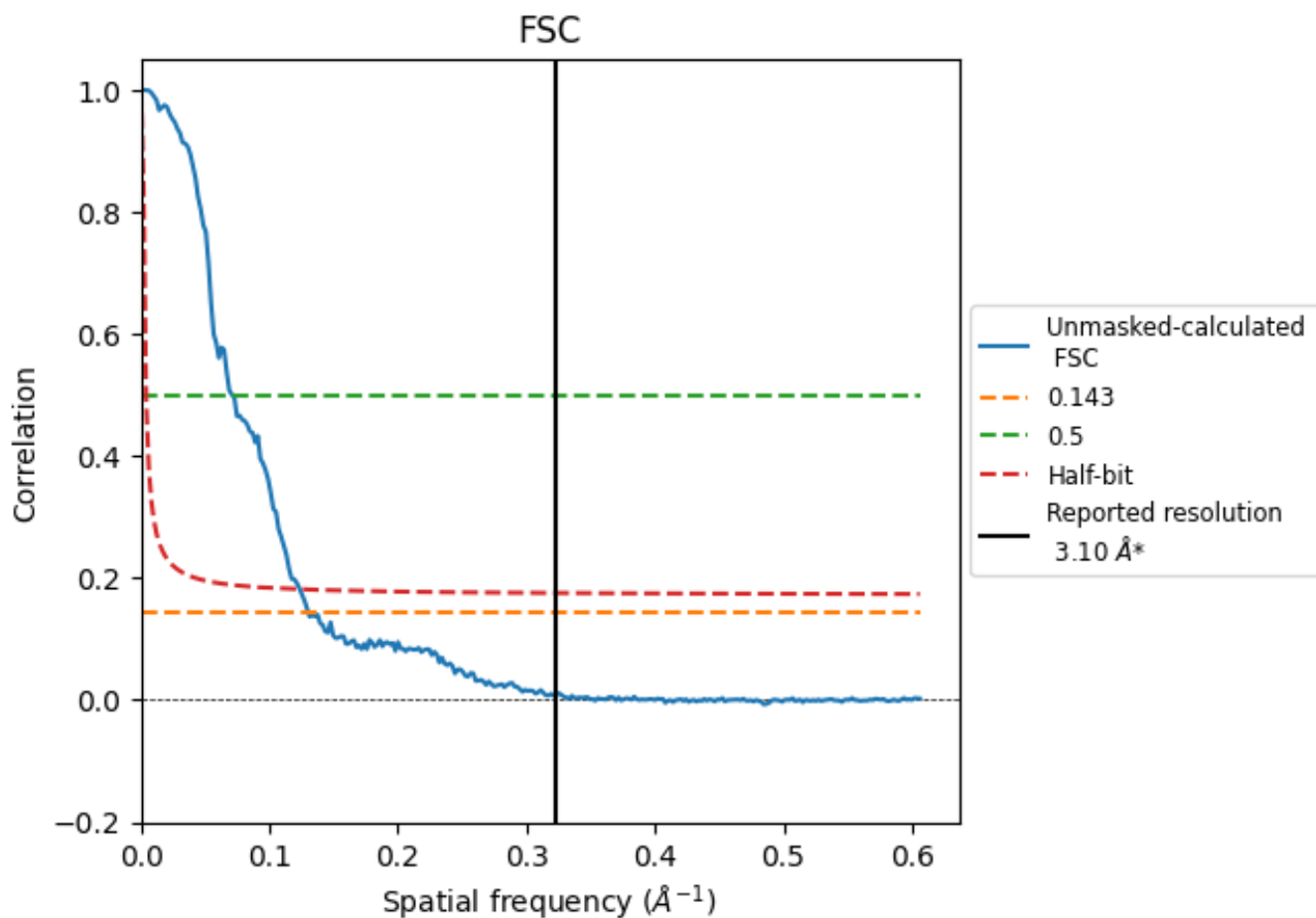


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

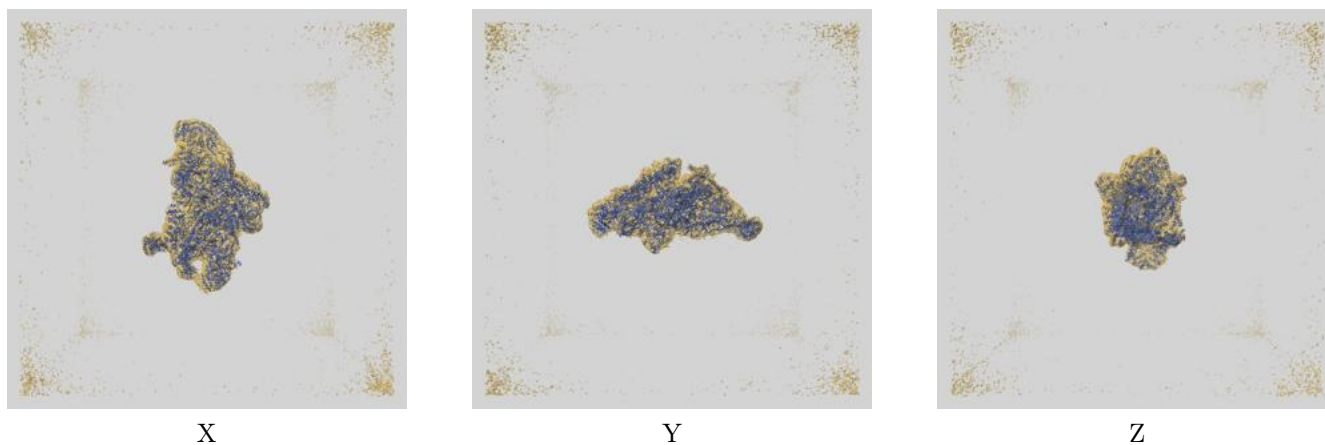
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.67	14.12	8.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.67 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

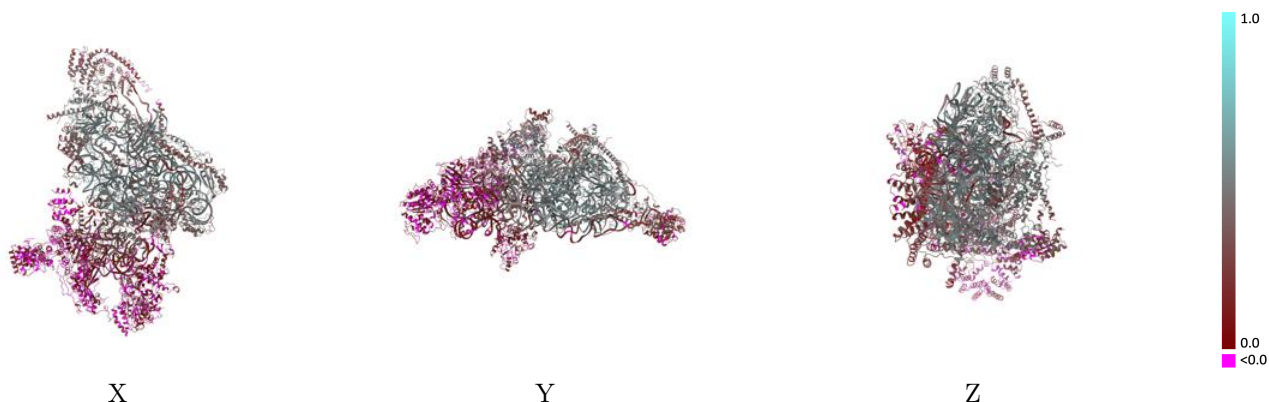
This section contains information regarding the fit between EMDB map EMD-54131 and PDB model 9ROV. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



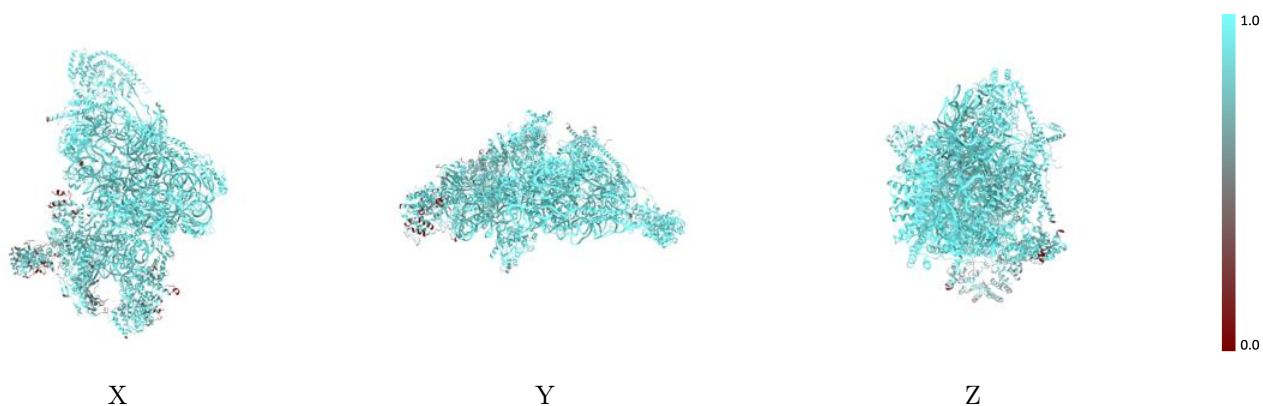
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



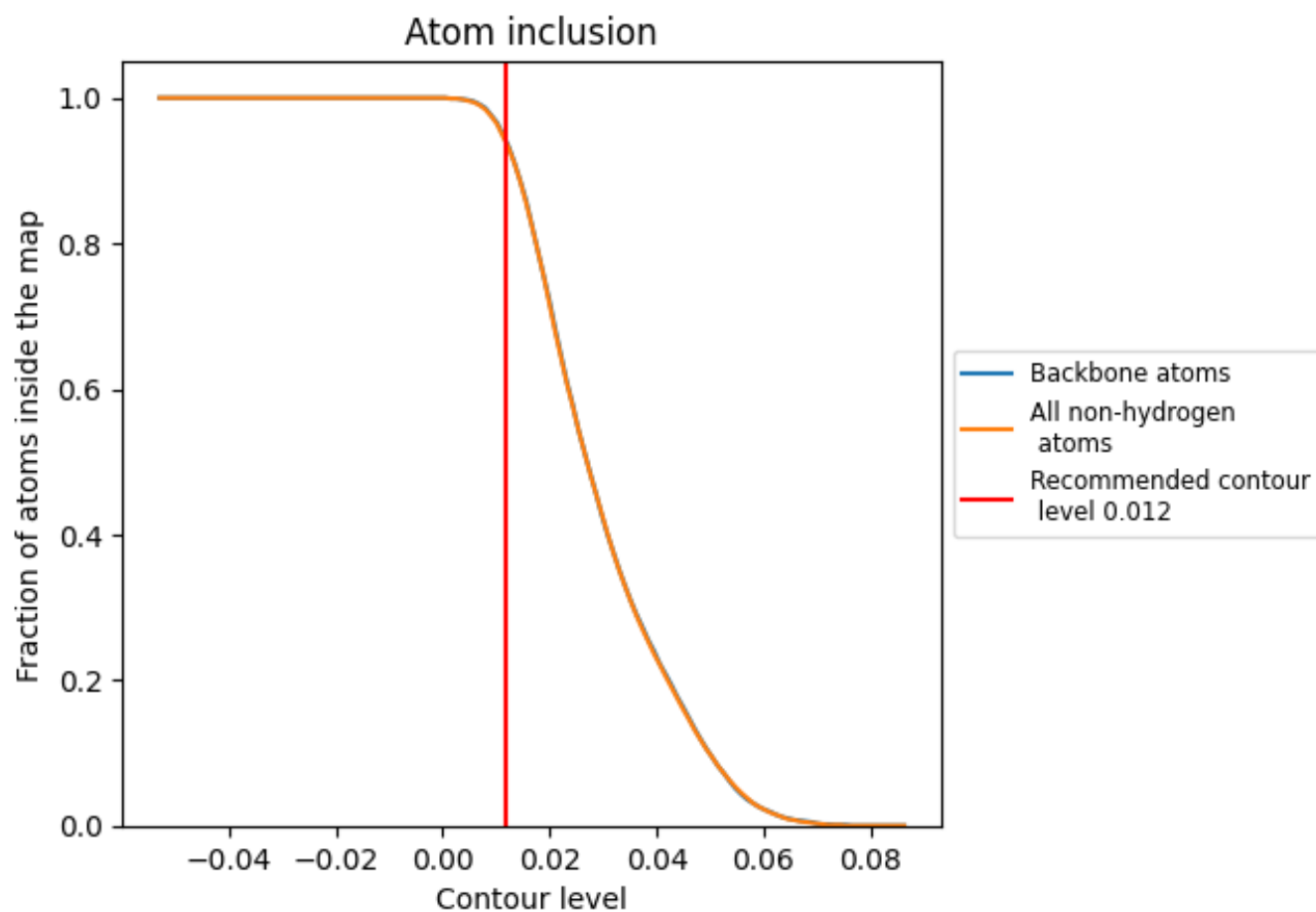
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9370	 0.3090
0	 0.9650	 0.3760
1	 0.8540	 0.0950
3	 0.9660	 0.4330
4	 0.7260	 0.0550
A	 0.9960	 0.3830
B	 0.9710	 0.4700
C	 0.9750	 0.1710
D	 0.9750	 0.4170
E	 0.9720	 0.4390
F	 0.8500	 0.0750
G	 0.9300	 0.1940
H	 0.8680	 0.1030
I	 0.9760	 0.4250
J	 0.9850	 0.4820
K	 0.9620	 0.1510
L	 0.9630	 0.4530
M	 0.9660	 0.4870
N	 0.9710	 0.5020
O	 0.9720	 0.4710
P	 0.9740	 0.4660
Q	 0.9770	 0.4230
R	 0.9380	 0.4380
S	 0.9520	 0.4100
T	 0.9750	 0.4810
U	 0.9470	 0.3980
V	 0.9480	 0.2370
W	 0.9750	 0.4480
X	 0.8270	 0.0550
Y	 0.8360	 0.0580
Z	 0.8840	 0.1570
a	 0.9600	 0.3040
b	 0.9470	 0.1490

