



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 08:18 am BST

PDB ID : 9RPF / pdb_00009rpf
EMDB ID : EMD-54163
Title : Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15 and mS37 (State M4)
Authors : Khawaja, A.; Singh, V.; Shiriaev, D.I.; Rorbach, J.
Deposited on : 2025-06-24
Resolution : 4.60 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:

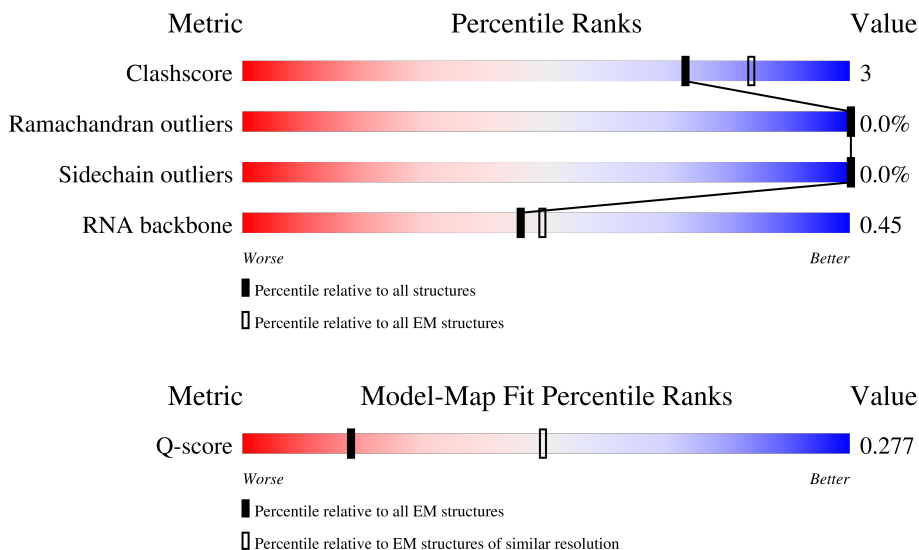
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.60 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	2407 (4.10 - 5.10)

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	2	118	

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Mol	Chain	Length	Quality of chain
4	3	199	
5	B	296	
6	C	167	
7	D	430	
8	E	125	
9	F	242	
10	H	201	
11	I	194	
12	J	138	
13	K	128	
14	L	257	
15	M	137	
16	N	130	
17	O	258	
18	P	142	
19	Q	87	
20	R	360	
21	S	190	
22	T	173	
23	U	205	
24	W	187	
25	X	398	
26	Y	395	
27	Z	106	
28	A	955	

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Mol	Chain	Length	Quality of chain
29	G	396	73% 9% 18%
30	V	414	81% 6% 13%
31	4	689	18% 78% 8% 15%
32	b	407	37% 54% 18% 29%

2 Entry composition i

There are 40 unique types of molecules in this entry. The entry contains 128691 atoms, of which 59624 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	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

- Molecule 3 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	2	118	Total	C	H	N	O	S	0	0
			1903	579	968	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 4 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	3	70	Total	C	H	N	O	S	0	0
			1324	401	699	134	89	1		

- Molecule 5 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 6 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 7 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	D	343	5533	1713	2802	518	487	13	0	0

- Molecule 8 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	E	122	1973	614	1001	177	177	4	0	0

- Molecule 9 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	F	208	3494	1104	1769	312	298	11	0	0

- Molecule 10 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	H	140	2335	745	1183	194	210	3	0	0

- Molecule 11 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	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 12 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 13 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	K	101	1747	537	885	179	141	5	0	0

- Molecule 14 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	L	174	2993	925	1540	270	251	7	0	0

- Molecule 15 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	M	119	1907	594	965	185	157	6	0	0

- Molecule 16 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 17 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 18 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	P	97	1588	501	807	134	138	8	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	Q	87	1501	460	757	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 20 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 21 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 22 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 23 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 24 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	W	100	1589	498	800	141	146	4	0	0

- Molecule 25 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 26 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	Y	122	2004	665	975	169	193	2	0	0

- Molecule 27 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	Z	86	1464	468	734	128	130	4	0	0

- Molecule 28 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
28	A	955	30584	9098	10302	3652	6577	955	0	0

- Molecule 29 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	G	324	5304	1684	2650	473	483	14	0	0

- Molecule 30 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	V	362	5931	1904	2962	495	558	12	0	0

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	4	588	9534	3053	4766	808	879	28	0	0

- Molecule 32 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	b	290	4599	1440	2327	406	415	11	0	0

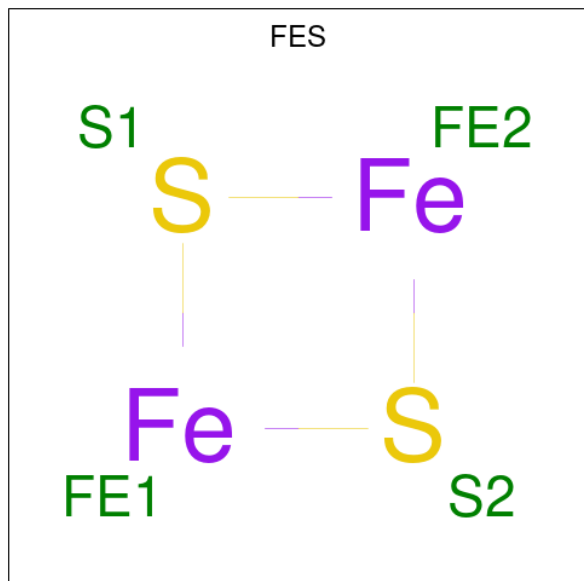
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	3	1	Total	Mg	0
			1	1	
33	B	1	Total	Mg	0
			1	1	
33	A	44	Total	Mg	0
			44	44	

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

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

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

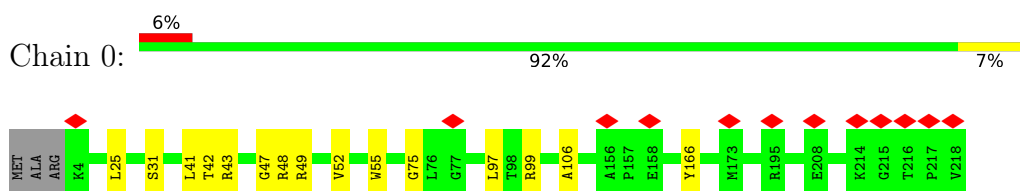


Mol	Chain	Residues	Atoms			AltConf
35	P	1	Total	Fe	S	0
			4	2	2	
35	T	1	Total	Fe	S	0
			4	2	2	

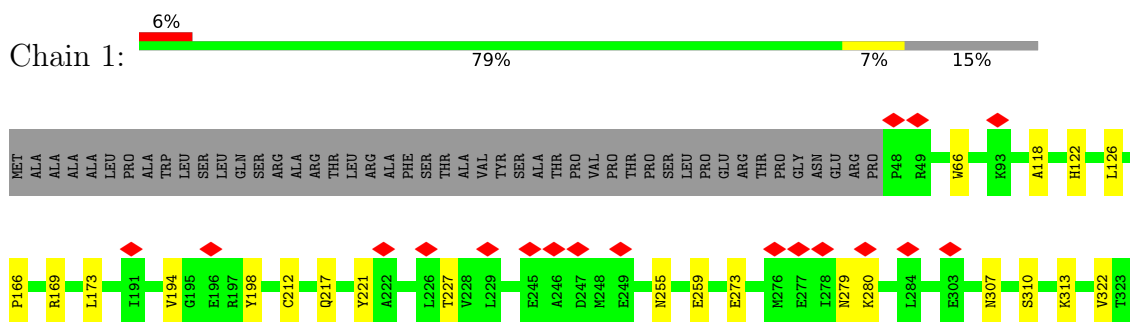
3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

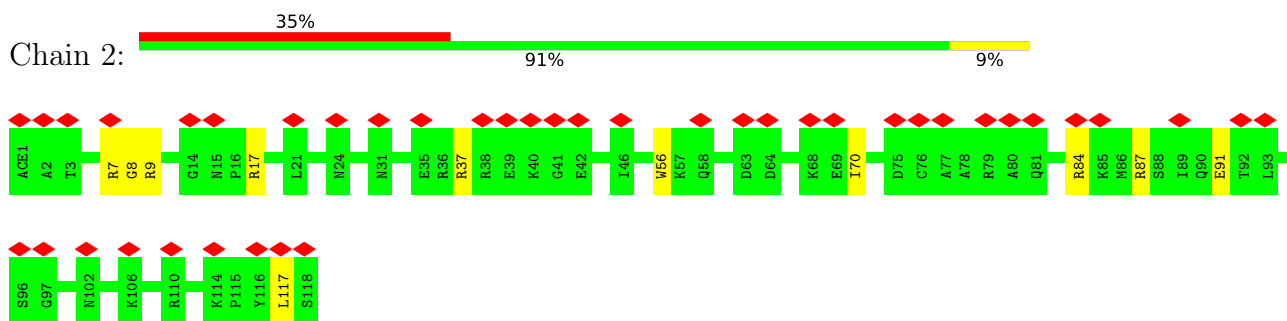
- Molecule 1: 28S ribosomal protein S34, mitochondrial



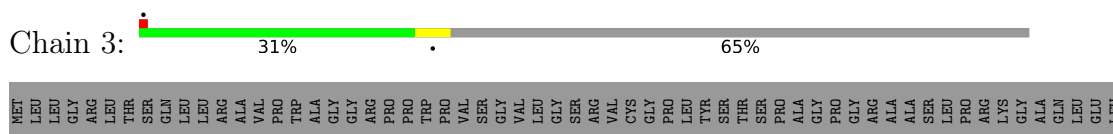
- Molecule 2: 28S ribosomal protein S35, mitochondrial

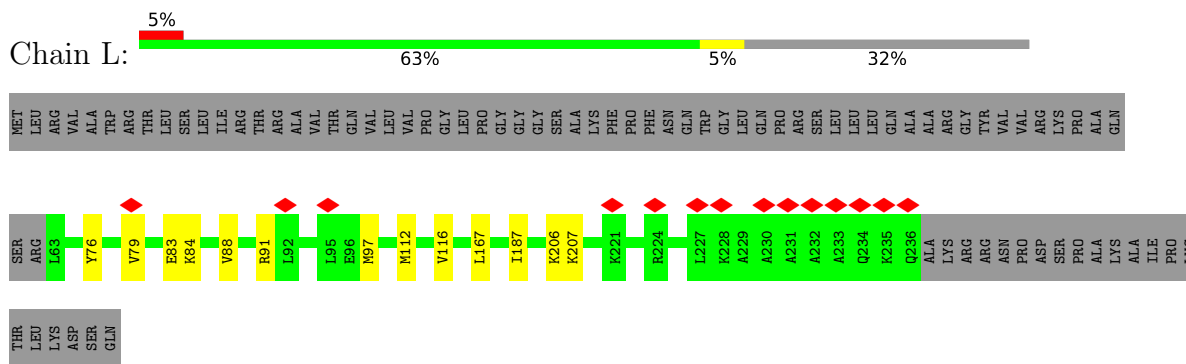


- Molecule 3: Small ribosomal subunit protein mS37

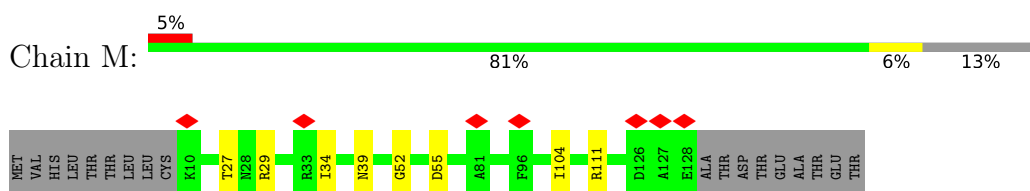


- Molecule 4: Aurora kinase A-interacting protein

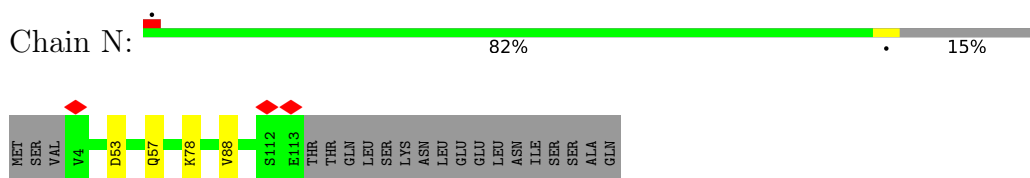




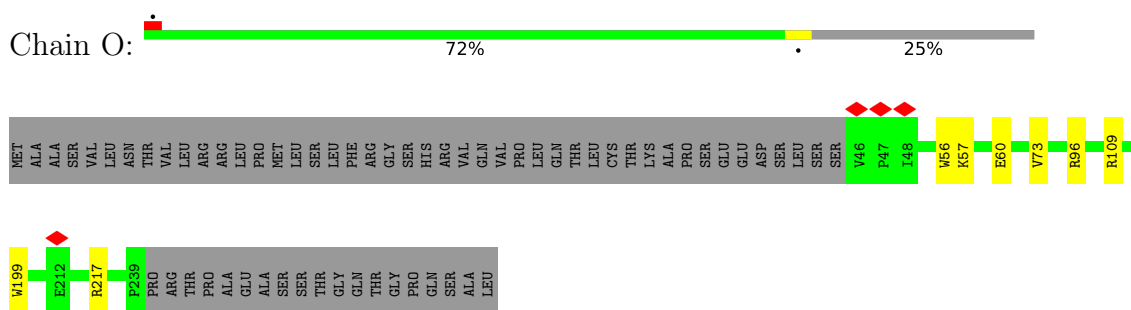
• Molecule 15: 28S ribosomal protein S16, mitochondrial



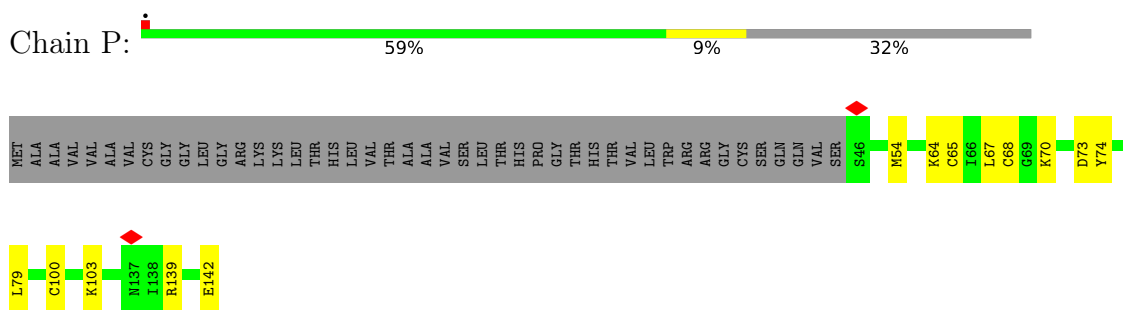
• Molecule 16: 28S ribosomal protein S17, mitochondrial



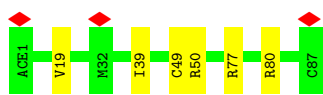
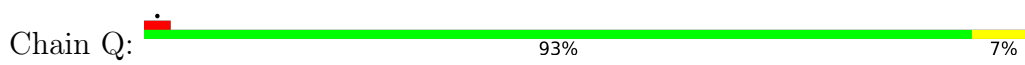
• Molecule 17: 28S ribosomal protein S18b, mitochondrial



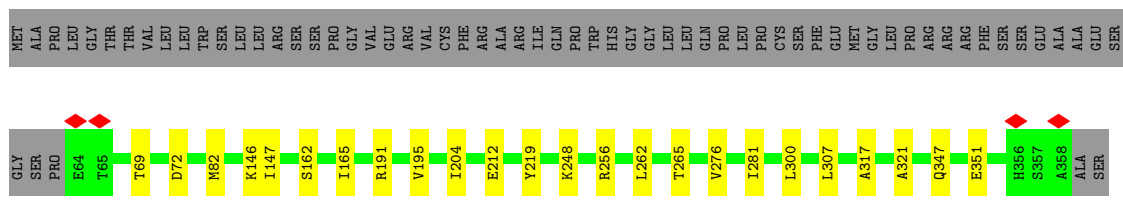
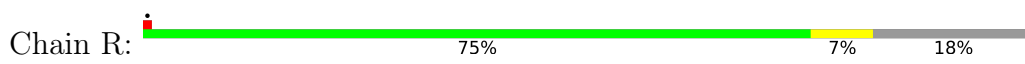
• Molecule 18: 28S ribosomal protein S18c, mitochondrial



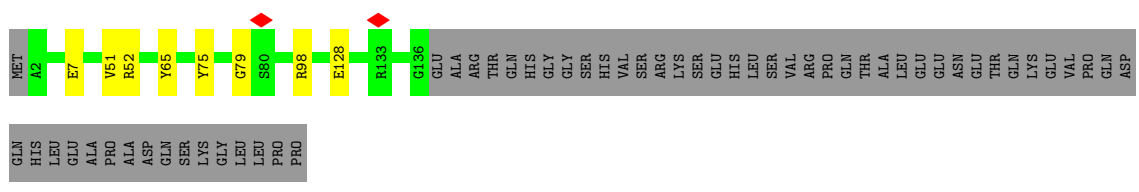
• Molecule 19: Small ribosomal subunit protein bS21m



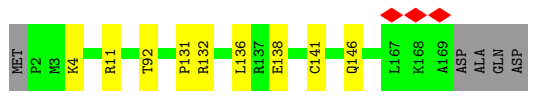
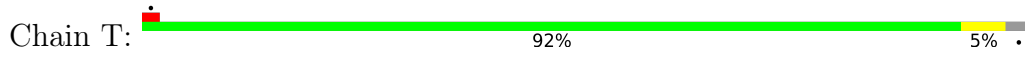
• Molecule 20: 28S ribosomal protein S22, mitochondrial



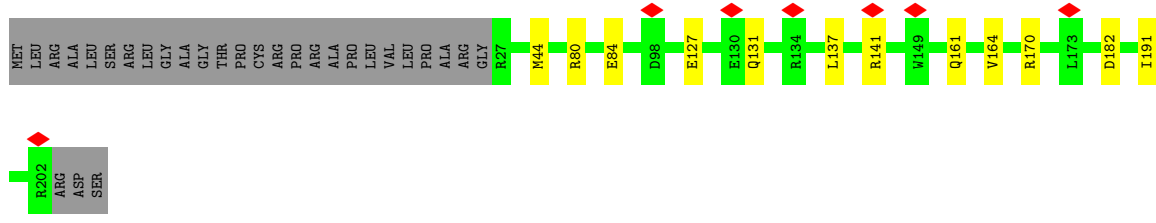
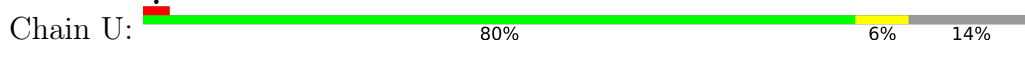
• Molecule 21: 28S ribosomal protein S23, mitochondrial



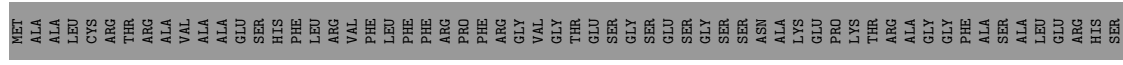
• Molecule 22: 28S ribosomal protein S25, mitochondrial



• Molecule 23: 28S ribosomal protein S26, mitochondrial

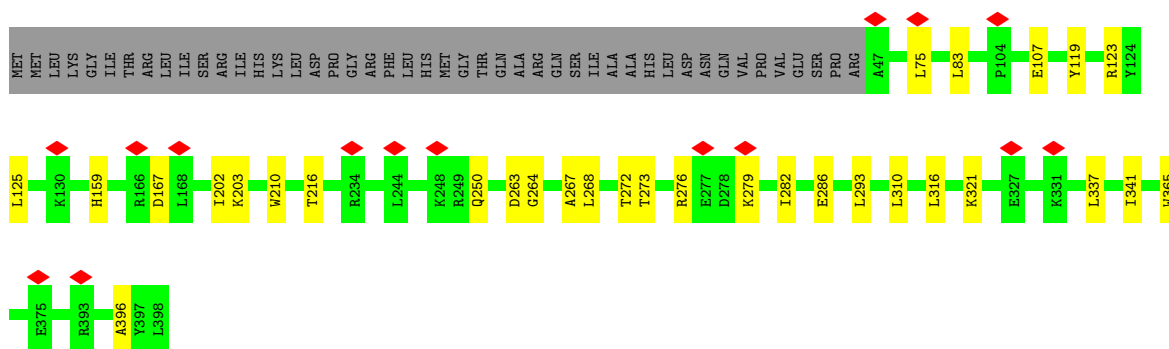
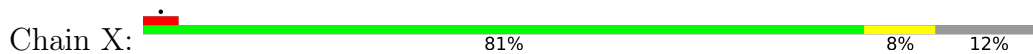


• Molecule 24: 28S ribosomal protein S28, mitochondrial

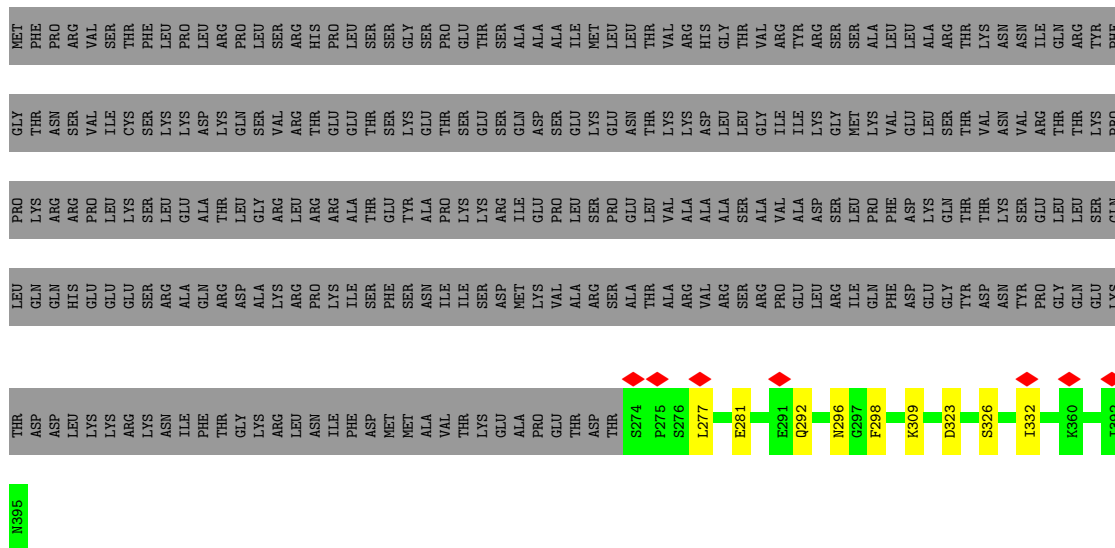




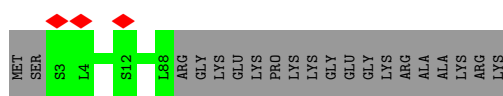
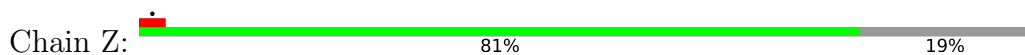
• Molecule 25: 28S ribosomal protein S29, mitochondrial



• Molecule 26: 28S ribosomal protein S31, mitochondrial



• Molecule 27: 28S ribosomal protein S33, mitochondrial



• Molecule 28: 12S mitochondrial rRNA



LEU	GLY	SER	ASP	HIS	GLU	ASN	THR	GLU	VAL	SER	MET	ARG	R370	A371	P372	L373	M374	M375	E376	L377	I378	H379	K380	K381	V382	L383	S384	P385	Q386	D387	Q388	D389	V390	Q391	D392	N393	P394	R395	G396	R397	S398	A399	K400	L401	R402	I405	K406	L407
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3908	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	0.058	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	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: ATP, GDP, MA6, B8T, FES, K, 5MC, 5F0, NAD, MG, ZN, ACE, 5MU

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	0.25	0/2484
2	1	0.08	0/2285	0.24	0/3090
3	2	0.24	0/947	0.39	0/1266
4	3	0.24	0/636	0.41	0/839
5	B	0.08	0/1871	0.23	0/2531
6	C	0.08	0/1113	0.23	0/1505
7	D	0.09	0/2783	0.24	0/3724
8	E	0.08	0/989	0.23	0/1335
9	F	0.08	0/1767	0.23	0/2373
10	H	0.08	0/1178	0.23	0/1598
11	I	0.09	0/1030	0.26	0/1386
12	J	0.87	0/855	0.97	2/1148 (0.2%)
13	K	0.07	0/880	0.22	0/1182
14	L	0.08	0/1477	0.22	0/1974
15	M	0.08	0/963	0.24	0/1295
16	N	0.08	0/886	0.22	0/1199
17	O	0.21	0/1655	0.35	0/2254
18	P	0.09	0/798	0.25	0/1070
19	Q	0.07	0/754	0.22	0/1003
20	R	0.07	0/2456	0.22	0/3317
21	S	0.07	0/1138	0.19	0/1533
22	T	0.08	0/1402	0.24	0/1883
23	U	0.07	0/1510	0.21	0/2025
24	W	0.11	0/801	0.28	0/1079
25	X	0.08	0/2921	0.24	0/3954
26	Y	0.08	0/1060	0.26	0/1430
27	Z	0.08	0/747	0.22	0/1000
28	A	0.10	0/22562	0.23	0/35124
29	G	0.26	0/2710	0.45	2/3635 (0.1%)
30	V	0.22	0/3030	0.40	0/4093
31	4	0.08	0/4877	0.25	0/6598
32	b	0.16	0/2311	0.32	0/3116

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.15	0/72226	0.28	4/102043 (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
3	2	0	1
11	I	0	1
12	J	0	4
17	O	0	1
30	V	0	1
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	64	CYS	N-CA-C	6.42	118.27	108.52
12	J	64	CYS	N-CA-CB	-6.16	101.44	111.24
29	G	239	GLU	N-CA-C	-5.26	105.22	111.69
29	G	198	ARG	N-CA-CB	-5.02	104.32	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	37	ARG	Sidechain
11	I	184	5F0	Mainchain
12	J	127	ARG	Sidechain
12	J	68	ARG	Sidechain
12	J	82	ARG	Sidechain
12	J	89	ARG	Sidechain
17	O	96	ARG	Sidechain
30	V	43	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	10	0
2	1	2238	2269	2269	18	0
3	2	935	968	969	8	0
4	3	625	699	699	5	0
5	B	1828	1815	1815	5	0
6	C	1083	1088	1088	3	0
7	D	2731	2802	2802	18	0
8	E	972	1001	1000	9	0
9	F	1725	1769	1769	15	0
10	H	1152	1183	1183	6	0
11	I	1020	1060	1052	10	0
12	J	839	884	886	43	0
13	K	862	885	885	8	0
14	L	1453	1540	1540	10	0
15	M	942	965	966	7	0
16	N	868	928	928	3	0
17	O	1599	1565	1565	5	0
18	P	781	807	806	10	0
19	Q	744	757	758	7	0
20	R	2409	2428	2428	15	0
21	S	1111	1115	1115	7	0
22	T	1371	1393	1394	7	0
23	U	1488	1499	1499	8	0
24	W	789	800	800	5	0
25	X	2849	2844	2844	22	0
26	Y	1029	975	974	11	0
27	Z	730	734	734	0	0
28	A	20282	10302	10300	82	0
29	G	2654	2650	2649	35	0
30	V	2969	2962	2961	15	0
31	4	4768	4766	4766	36	0
32	b	2272	2327	2325	54	0
33	3	1	0	0	0	0
33	A	44	0	0	0	0
33	B	1	0	0	0	0
34	O	1	0	0	0	0
35	P	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	T	4	0	0	0	0
36	X	31	12	12	0	0
37	X	28	10	12	0	0
38	A	44	26	26	0	0
39	A	3	0	0	0	0
40	T	1	0	0	0	0
All	All	69067	59624	59615	414	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 (414) 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)
12:J:80:CYS:SG	12:J:94:PHE:HA	1.18	1.69
12:J:80:CYS:SG	12:J:94:PHE:CA	2.04	1.42
12:J:64:CYS:SG	12:J:82:ARG:O	2.14	1.05
29:G:200:LEU:HD23	29:G:201:ILE:O	1.58	1.03
29:G:200:LEU:CD2	29:G:201:ILE:O	2.08	1.01
29:G:200:LEU:HD23	29:G:201:ILE:N	1.75	0.98
12:J:93:CYS:SG	12:J:125:VAL:HG21	2.04	0.97
11:I:94:ASN:ND2	28:A:989:U:OP1	2.03	0.91
12:J:93:CYS:SG	12:J:125:VAL:CG2	2.58	0.91
32:b:75:VAL:HG11	32:b:399:ALA:HB3	1.55	0.89
3:2:7:ARG:O	3:2:9:ARG:NH1	2.07	0.87
32:b:106:ILE:HD11	32:b:167:LEU:HD23	1.55	0.87
2:1:273:GLU:OE2	25:X:119:TYR:OH	1.92	0.87
12:J:64:CYS:HB3	12:J:81:CYS:HB2	1.62	0.81
29:G:62:PRO:O	29:G:65:LYS:NZ	2.14	0.80
29:G:200:LEU:HD23	29:G:201:ILE:H	1.47	0.79
3:2:9:ARG:NH2	28:A:1021:U:OP2	2.18	0.77
9:F:48:LYS:NZ	29:G:318:HIS:O	2.16	0.76
32:b:326:ASP:OD1	32:b:327:ARG:N	2.17	0.76
32:b:92:PHE:CD1	32:b:113:ILE:HD11	2.20	0.76
28:A:1583:MA6:H93	28:A:1584:MA6:H92	1.69	0.75
12:J:64:CYS:SG	12:J:82:ARG:HB3	2.27	0.74
29:G:200:LEU:HD23	29:G:201:ILE:C	2.11	0.74
31:4:200:ASP:OD2	31:4:243:ASN:N	2.21	0.73
12:J:80:CYS:SG	12:J:95:ILE:N	2.60	0.73
12:J:63:LEU:C	12:J:64:CYS:SG	2.72	0.72
20:R:347:GLN:NE2	20:R:351:GLU:OE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:132:ARG:NH1	22:T:136:LEU:O	2.22	0.72
12:J:80:CYS:SG	12:J:94:PHE:C	2.72	0.71
29:G:200:LEU:HD21	29:G:201:ILE:O	1.90	0.71
32:b:266:ALA:HB1	32:b:280:ILE:HD12	1.73	0.71
9:F:50:TYR:O	9:F:66:ARG:NH2	2.25	0.70
12:J:80:CYS:SG	12:J:94:PHE:N	2.66	0.68
32:b:94:ASP:OD2	32:b:103:THR:OG1	2.13	0.67
32:b:216:GLN:HB3	32:b:240:VAL:HG21	1.76	0.67
28:A:1307:G:O2'	29:G:120:ARG:NH2	2.26	0.66
20:R:212:GLU:OE1	20:R:248:LYS:NZ	2.22	0.66
17:O:73:VAL:O	17:O:109:ARG:NH2	2.28	0.66
29:G:199:TRP:HA	29:G:245:ARG:HD2	1.79	0.64
13:K:60:ASN:OD1	13:K:68:GLN:NE2	2.30	0.64
2:1:227:THR:HA	10:H:184:ILE:HD11	1.80	0.64
30:V:375:TYR:CE2	30:V:379:LEU:HD11	2.33	0.63
28:A:1454:G:OP2	29:G:377:ARG:NH1	2.31	0.62
30:V:270:PRO:O	30:V:346:LYS:NZ	2.31	0.62
10:H:126:ILE:O	28:A:1226:C:O2'	2.18	0.62
28:A:1561:C:OP1	32:b:270:ARG:NE	2.32	0.62
28:A:1081:U:O2'	28:A:1082:A:O4'	2.15	0.61
7:D:363:ALA:O	7:D:367:GLY:N	2.33	0.61
11:I:71:SER:O	11:I:74:ARG:NH1	2.33	0.61
3:2:56:TRP:HE1	3:2:70:ILE:HD11	1.65	0.61
28:A:1199:G:N1	28:A:1422:G:OP2	2.34	0.61
29:G:200:LEU:HD21	29:G:205:LEU:N	2.16	0.61
3:2:8:GLY:O	3:2:17:ARG:NH2	2.34	0.60
28:A:1583:MA6:C9	28:A:1584:MA6:H92	2.30	0.60
29:G:150:LEU:O	29:G:153:THR:OG1	2.18	0.60
29:G:200:LEU:CD2	29:G:201:ILE:H	2.14	0.60
28:A:1539:C:H3'	28:A:1540:A:H5'	1.83	0.60
28:A:702:C:OP1	28:A:848:U:O2'	2.17	0.60
7:D:234:LYS:NZ	28:A:1322:C:N3	2.50	0.60
12:J:93:CYS:SG	12:J:93:CYS:O	2.59	0.59
11:I:184:5F0:CXT	28:A:1013:A:O2'	2.51	0.59
31:4:259:TYR:HB2	31:4:282:LEU:HD13	1.82	0.59
14:L:83:GLU:OE1	14:L:83:GLU:N	2.36	0.58
14:L:207:LYS:HD3	28:A:763:C:H42	1.68	0.58
26:Y:277:LEU:HD21	31:4:198:TYR:CE2	2.39	0.58
7:D:232:THR:N	7:D:236:GLY:O	2.36	0.57
12:J:64:CYS:CB	12:J:81:CYS:HB2	2.34	0.57
8:E:35:ILE:HD11	14:L:91:ARG:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:27:THR:OG1	28:A:685:A:OP1	2.22	0.57
29:G:155:LYS:NZ	29:G:217:ASP:OD2	2.21	0.57
7:D:421:VAL:HG13	28:A:929:A:O4'	2.05	0.57
5:B:100:ARG:NH2	28:A:1116:A:O5'	2.37	0.56
7:D:320:ILE:O	7:D:324:CYS:N	2.28	0.56
25:X:279:LYS:NZ	28:A:1412:G:OP1	2.36	0.56
26:Y:309:LYS:HE3	31:4:140:LEU:HD11	1.87	0.56
28:A:1289:G:O2'	28:A:1297:G:OP2	2.17	0.56
31:4:282:LEU:HD12	31:4:287:LEU:HB2	1.87	0.56
28:A:1075:A:C8	28:A:1076:5MU:H72	2.40	0.56
32:b:127:LEU:HD13	32:b:175:MET:HG3	1.88	0.56
26:Y:277:LEU:HD23	31:4:197:TYR:HB3	1.87	0.56
13:K:58:ARG:NE	13:K:72:ASP:OD1	2.38	0.56
1:0:41:LEU:HD13	1:0:55:TRP:CG	2.40	0.56
26:Y:292:GLN:OE1	31:4:454:ARG:NH2	2.38	0.56
30:V:184:TYR:HB2	30:V:360:VAL:HG21	1.88	0.56
12:J:66:PHE:CE2	12:J:81:CYS:HA	2.41	0.55
32:b:75:VAL:HG12	32:b:76:MET:HG3	1.89	0.55
1:0:48:ARG:NH2	28:A:701:G:O6	2.39	0.55
29:G:200:LEU:CD2	29:G:201:ILE:N	2.60	0.55
32:b:118:LEU:CD2	32:b:149:ALA:HB2	2.36	0.55
8:E:33:GLY:O	14:L:97:MET:HE1	2.07	0.55
9:F:125:LYS:O	9:F:129:ALA:HB2	2.07	0.55
19:Q:49:CYS:SG	19:Q:50:ARG:NH1	2.80	0.55
7:D:320:ILE:HG22	7:D:324:CYS:SG	2.47	0.55
13:K:81:ASP:OD1	13:K:86:ARG:NH1	2.38	0.54
28:A:1081:U:H4'	28:A:1082:A:OP1	2.06	0.54
32:b:75:VAL:CG1	32:b:399:ALA:HB3	2.35	0.54
31:4:305:ILE:O	31:4:312:LYS:NZ	2.41	0.54
12:J:63:LEU:O	12:J:64:CYS:SG	2.66	0.54
18:P:65:CYS:N	18:P:68:CYS:SG	2.80	0.54
11:I:151:VAL:HG11	11:I:158:ARG:HG3	1.89	0.54
12:J:64:CYS:CB	12:J:82:ARG:H	2.21	0.54
12:J:81:CYS:SG	12:J:82:ARG:N	2.81	0.54
12:J:93:CYS:HG	12:J:125:VAL:HG21	1.71	0.54
28:A:1401:G:N2	28:A:1404:A:OP2	2.40	0.53
29:G:210:VAL:HG12	29:G:210:VAL:O	2.06	0.53
18:P:100:CYS:HB3	35:P:201:FES:S2	2.48	0.53
23:U:161:GLN:O	23:U:164:VAL:HG12	2.06	0.53
32:b:206:THR:O	32:b:210:VAL:N	2.37	0.53
2:1:322:VAL:HG21	25:X:341:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:G:320:VAL:HG23	29:G:322:ARG:HG2	1.89	0.53
20:R:276:VAL:HG11	20:R:307:LEU:HD12	1.90	0.53
8:E:3:ARG:HB3	8:E:99:THR:HG21	1.90	0.53
28:A:1152:A:OP2	28:A:1153:C:N4	2.29	0.53
29:G:169:LEU:HD23	29:G:172:LEU:HD12	1.90	0.53
31:4:239:ARG:O	31:4:242:ASN:ND2	2.41	0.53
7:D:317:HIS:O	7:D:321:ILE:N	2.39	0.53
6:C:124:LEU:O	6:C:132:TYR:OH	2.20	0.52
11:I:179:THR:HG21	19:Q:39:ILE:HD13	1.91	0.52
12:J:85:LEU:HD22	12:J:110:VAL:HG21	1.91	0.52
9:F:170:VAL:HG23	9:F:236:LEU:O	2.10	0.52
28:A:1053:A:N1	28:A:1100:C:O2'	2.43	0.52
12:J:70:PRO:HB3	12:J:117:ASP:HB3	1.91	0.52
25:X:202:ILE:HG23	25:X:250:GLN:OE1	2.10	0.52
1:0:43:ARG:O	1:0:47:GLY:N	2.38	0.52
25:X:321:LYS:NZ	29:G:298:ILE:HG21	2.25	0.52
17:O:56:TRP:O	17:O:60:GLU:OE1	2.29	0.51
29:G:229:LEU:HD11	29:G:241:VAL:HG11	1.91	0.51
28:A:812:A:O2'	28:A:814:A:N1	2.42	0.51
20:R:219:TYR:O	20:R:256:ARG:NH2	2.44	0.51
20:R:317:ALA:O	20:R:321:ALA:N	2.44	0.51
12:J:64:CYS:HB2	12:J:81:CYS:SG	2.51	0.51
17:O:57:LYS:HA	17:O:60:GLU:OE2	2.11	0.51
23:U:80:ARG:O	23:U:84:GLU:N	2.43	0.51
28:A:1583:MA6:OP2	28:A:1583:MA6:H8	2.11	0.51
12:J:81:CYS:SG	12:J:93:CYS:HB3	2.51	0.51
31:4:161:ILE:HA	31:4:194:LEU:HD22	1.93	0.51
2:1:307:ASN:O	2:1:310:SER:OG	2.23	0.50
25:X:273:THR:HG23	25:X:316:LEU:HD13	1.92	0.50
25:X:263:ASP:OD1	25:X:264:GLY:N	2.45	0.50
1:0:52:VAL:HG11	23:U:44:MET:HE1	1.93	0.50
11:I:94:ASN:OD1	11:I:95:THR:N	2.45	0.50
17:O:217:ARG:NH1	30:V:318:ASP:OD2	2.45	0.50
18:P:67:LEU:HD21	18:P:79:LEU:HD11	1.93	0.50
21:S:7:GLU:OE1	21:S:7:GLU:N	2.45	0.50
26:Y:281:GLU:OE2	31:4:164:ARG:NH1	2.40	0.50
14:L:112:MET:O	14:L:116:VAL:HG22	2.12	0.50
26:Y:393:GLN:CD	26:Y:393:GLN:O	2.54	0.50
7:D:320:ILE:CG1	7:D:345:LEU:HD21	2.42	0.50
30:V:46:GLU:HG3	30:V:74:ARG:HG2	1.93	0.49
31:4:349:ALA:HB3	31:4:378:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:122:HIS:HB3	31:4:74:LEU:HD22	1.95	0.49
32:b:80:VAL:CG2	32:b:319:LEU:HD11	2.42	0.49
31:4:470:GLN:NE2	31:4:472:ASP:OD2	2.45	0.49
8:E:35:ILE:HD13	14:L:88:VAL:HG13	1.95	0.49
9:F:106:LEU:O	9:F:110:LEU:HD23	2.12	0.49
12:J:92:VAL:HG11	12:J:121:VAL:HG22	1.94	0.49
18:P:70:LYS:O	18:P:103:LYS:NZ	2.45	0.49
32:b:95:MET:SD	32:b:168:MET:HE3	2.53	0.49
10:H:57:ASP:OD2	31:4:441:THR:HG22	2.13	0.49
20:R:69:THR:OG1	20:R:72:ASP:OD1	2.31	0.49
2:1:166:PRO:O	2:1:169:ARG:NH1	2.45	0.49
28:A:899:G:O2'	28:A:907:A:N1	2.45	0.49
32:b:254:LEU:HG	32:b:285:PHE:CE1	2.48	0.49
32:b:324:LEU:HD12	32:b:324:LEU:H	1.78	0.49
2:1:126:LEU:HD11	31:4:74:LEU:HD21	1.94	0.48
4:3:174:ARG:HA	4:3:177:TRP:CZ2	2.48	0.48
32:b:94:ASP:N	32:b:116:TYR:O	2.45	0.48
20:R:276:VAL:HG22	20:R:281:ILE:HG21	1.95	0.48
31:4:493:MET:HA	31:4:493:MET:HE2	1.94	0.48
32:b:326:ASP:OD1	32:b:326:ASP:C	2.56	0.48
12:J:95:ILE:HG12	12:J:102:LEU:HD12	1.95	0.48
2:1:217:GLN:NE2	26:Y:326:SER:O	2.41	0.48
32:b:214:LEU:O	32:b:243:ARG:NH2	2.40	0.48
18:P:139:ARG:NH2	18:P:142:GLU:OE1	2.47	0.48
18:P:73:ASP:OD1	18:P:74:TYR:N	2.45	0.48
32:b:240:VAL:HG22	32:b:243:ARG:CZ	2.44	0.48
28:A:1537:C:HI1'	28:A:1538:G:OP2	2.14	0.47
30:V:375:TYR:CZ	30:V:379:LEU:HD11	2.49	0.47
32:b:80:VAL:HG22	32:b:319:LEU:HD11	1.95	0.47
2:1:255:ASN:N	2:1:259:GLU:OE1	2.41	0.47
15:M:29:ARG:NE	22:T:141:CYS:SG	2.87	0.47
28:A:1503:G:H2'	28:A:1504:U:O4'	2.14	0.47
26:Y:296:ASN:OD1	26:Y:298:PHE:N	2.47	0.47
31:4:195:LEU:HD11	31:4:247:ILE:HD12	1.97	0.47
7:D:320:ILE:HG12	7:D:345:LEU:HD21	1.95	0.47
7:D:345:LEU:HD23	7:D:345:LEU:C	2.40	0.47
13:K:102:ARG:HD2	28:A:1443:U:OP2	2.15	0.47
12:J:78:ARG:NH2	12:J:117:ASP:OD2	2.48	0.47
28:A:905:A:O2'	28:A:907:A:OP1	2.33	0.47
32:b:106:ILE:HD11	32:b:167:LEU:CD2	2.35	0.47
32:b:299:LEU:HD23	32:b:328:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:381:LYS:O	32:b:382:VAL:HG22	2.15	0.47
25:X:272:THR:OG1	25:X:282:ILE:O	2.32	0.47
1:0:99:ARG:HG3	28:A:1526:U:O2'	2.15	0.47
21:S:98:ARG:NH2	21:S:128:GLU:OE1	2.47	0.47
9:F:129:ALA:HB1	9:F:133:GLU:HB2	1.97	0.47
28:A:1550:A:HO2'	28:A:1551:G:P	2.37	0.46
30:V:123:ASP:OD1	30:V:123:ASP:N	2.48	0.46
31:4:145:PHE:O	31:4:163:LEU:HD13	2.14	0.46
12:J:80:CYS:SG	12:J:93:CYS:O	2.74	0.46
31:4:279:TYR:HB2	31:4:297:LEU:HD21	1.98	0.46
32:b:374:MET:O	32:b:374:MET:HG2	2.15	0.46
2:1:279:ASN:OD1	2:1:280:LYS:N	2.45	0.46
12:J:80:CYS:SG	12:J:93:CYS:C	2.98	0.46
13:K:28:HIS:N	28:A:1248:C:O2	2.49	0.46
20:R:276:VAL:CG1	20:R:307:LEU:HD12	2.45	0.46
29:G:200:LEU:HD23	29:G:201:ILE:CA	2.42	0.46
6:C:157:THR:OG1	31:4:92:ASP:OD1	2.31	0.46
28:A:1550:A:O2'	28:A:1551:G:P	2.73	0.46
29:G:201:ILE:HG23	29:G:204:GLU:H	1.80	0.46
10:H:89:ASP:OD1	10:H:141:ARG:NH1	2.46	0.46
32:b:97:PHE:CD2	32:b:117:ALA:HB1	2.50	0.46
32:b:118:LEU:HD11	32:b:144:GLY:CA	2.46	0.46
32:b:195:ARG:HA	32:b:207:ALA:HB2	1.97	0.46
7:D:245:VAL:HG22	7:D:271:ALA:HB1	1.98	0.46
28:A:1283:A:H3'	28:A:1284:U:H5''	1.98	0.46
28:A:1081:U:H1'	28:A:1082:A:O5'	2.15	0.46
32:b:313:GLY:HA2	32:b:405:ILE:HG23	1.98	0.46
15:M:55:ASP:OD2	22:T:146:GLN:NE2	2.46	0.45
28:A:1582:G:H3'	28:A:1583:MA6:H8	1.97	0.45
16:N:53:ASP:OD2	16:N:57:GLN:N	2.50	0.45
20:R:195:VAL:HG22	20:R:204:ILE:HD13	1.98	0.45
4:3:131:LEU:HD21	28:A:1478:A:C2	2.51	0.45
30:V:34:TYR:HA	30:V:372:ILE:HD11	1.98	0.45
13:K:36:ARG:NH1	28:A:1235:U:OP1	2.49	0.45
29:G:198:ARG:N	29:G:246:ARG:O	2.50	0.45
23:U:127:GLU:O	23:U:131:GLN:N	2.48	0.45
12:J:83:VAL:HG13	12:J:93:CYS:HB2	1.99	0.45
28:A:1508:C:H4'	28:A:1509:U:OP1	2.16	0.45
19:Q:77:ARG:O	19:Q:80:ARG:NH1	2.49	0.45
28:A:940:A:H5'	28:A:941:G:OP2	2.16	0.45
1:0:75:GLY:O	1:0:97:LEU:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:87:ARG:O	3:2:91:GLU:N	2.49	0.45
9:F:46:ILE:HG23	29:G:315:PHE:CZ	2.51	0.45
19:Q:80:ARG:NH2	24:W:164:GLU:OE1	2.50	0.45
9:F:119:LYS:NZ	25:X:365:TRP:O	2.45	0.45
14:L:206:LYS:NZ	28:A:762:G:OP1	2.40	0.45
25:X:125:LEU:HD21	25:X:310:LEU:HD21	1.98	0.45
20:R:262:LEU:O	20:R:265:THR:OG1	2.27	0.45
18:P:65:CYS:SG	18:P:100:CYS:N	2.90	0.44
28:A:1386:U:H3'	28:A:1387:A:H5''	1.99	0.44
31:4:58:VAL:HG23	31:4:58:VAL:O	2.17	0.44
16:N:78:LYS:NZ	28:A:750:G:OP1	2.50	0.44
18:P:64:LYS:HB3	18:P:68:CYS:SG	2.57	0.44
31:4:372:TYR:CE2	31:4:400:LEU:HD21	2.52	0.44
2:1:118:ALA:O	2:1:122:HIS:N	2.44	0.44
8:E:109:VAL:HG23	8:E:109:VAL:O	2.17	0.44
12:J:64:CYS:HB3	12:J:82:ARG:H	1.81	0.44
25:X:75:LEU:HD11	25:X:83:LEU:HD11	2.00	0.44
32:b:135:TYR:HB2	32:b:139:ILE:HG22	1.99	0.44
1:O:166:TYR:O	17:O:199:TRP:NE1	2.42	0.44
2:1:221:TYR:CD1	26:Y:332:ILE:HD13	2.52	0.44
11:I:184:5F0:CXT	28:A:1013:A:HO2'	2.30	0.44
12:J:79:LYS:O	12:J:80:CYS:SG	2.75	0.44
13:K:90:ARG:NH2	28:A:1235:U:O3'	2.50	0.44
15:M:104:ILE:HG23	20:R:147:ILE:HG12	1.99	0.44
7:D:372:GLU:OE1	7:D:374:ARG:NE	2.50	0.44
22:T:131:PRO:HA	22:T:138:GLU:OE2	2.17	0.44
25:X:203:LYS:O	25:X:250:GLN:NE2	2.49	0.44
32:b:86:PRO:CB	32:b:113:ILE:HD12	2.48	0.44
7:D:134:GLU:OE1	7:D:160:ARG:NH2	2.50	0.44
28:A:825:U:O2'	28:A:827:A:N7	2.44	0.44
31:4:508:VAL:HG12	31:4:508:VAL:O	2.17	0.44
4:3:173:LEU:O	4:3:177:TRP:CE3	2.70	0.44
8:E:15:ARG:NH1	23:U:182:ASP:OD1	2.50	0.44
15:M:111:ARG:NH2	20:R:146:LYS:O	2.51	0.44
31:4:369:LEU:HD21	31:4:405:PHE:CE2	2.53	0.44
12:J:80:CYS:HA	12:J:95:ILE:HD12	2.00	0.44
25:X:268:LEU:HD21	25:X:293:LEU:HD23	1.99	0.44
28:A:854:U:O4	28:A:855:A:N6	2.51	0.44
28:A:1057:G:H4'	28:A:1578:A:H4'	1.99	0.44
32:b:119:ASP:O	32:b:144:GLY:N	2.50	0.44
7:D:316:CYS:SG	7:D:321:ILE:HA	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:82:MET:HE1	20:R:300:LEU:HA	2.00	0.44
30:V:266:VAL:HG21	30:V:275:LEU:HG	2.00	0.44
31:4:236:VAL:HG12	31:4:238:TRP:H	1.83	0.44
2:1:66:TRP:CE3	29:G:91:MET:HE2	2.53	0.43
12:J:84:ARG:HA	12:J:90:GLU:HA	2.00	0.43
19:Q:80:ARG:O	28:A:1293:C:N4	2.50	0.43
25:X:321:LYS:HZ1	29:G:298:ILE:HG21	1.83	0.43
30:V:356:THR:O	30:V:360:VAL:HG23	2.18	0.43
2:1:212:CYS:SG	26:Y:332:ILE:HD11	2.59	0.43
28:A:1581:G:N1	28:A:1584:MA6:OP2	2.50	0.43
31:4:367:PRO:HB3	31:4:371:THR:HG21	2.00	0.43
8:E:120:THR:HG21	21:S:51:VAL:HG21	2.00	0.43
14:L:76:TYR:O	14:L:79:VAL:HG22	2.18	0.43
15:M:34:ILE:N	15:M:52:GLY:O	2.51	0.43
28:A:1511:C:O2	28:A:1538:G:C6	2.71	0.43
31:4:267:VAL:HG22	31:4:300:ALA:HB2	2.01	0.43
2:1:173:LEU:HD23	2:1:173:LEU:C	2.44	0.43
28:A:1598:G:HO2'	28:A:1599:A:P	2.40	0.43
1:0:25:LEU:HD11	28:A:1531:C:H2'	1.99	0.43
23:U:137:LEU:O	23:U:141:ARG:N	2.44	0.43
28:A:1116:A:H5'	28:A:1117:A:OP2	2.18	0.43
28:A:1557:A:H2'	28:A:1558:A:C8	2.53	0.43
1:0:31:SER:OG	1:0:106:ALA:HB2	2.17	0.43
22:T:132:ARG:N	22:T:138:GLU:OE2	2.52	0.43
29:G:200:LEU:HD22	29:G:205:LEU:HB2	2.01	0.43
8:E:24:ARG:NH1	8:E:85:ASP:OD1	2.52	0.43
2:1:313:LYS:NZ	25:X:107:GLU:OE2	2.43	0.43
4:3:193:LYS:HB3	4:3:196:LEU:HB2	1.99	0.43
24:W:113:TYR:CE2	24:W:123:VAL:HG22	2.54	0.43
28:A:906:C:H42	29:G:51:HIS:CD2	2.36	0.43
5:B:239:ASN:OD1	24:W:119:LYS:NZ	2.50	0.43
10:H:84:ASP:OD1	10:H:85:LYS:N	2.52	0.43
11:I:166:ILE:HD11	19:Q:19:VAL:HG21	2.00	0.43
13:K:60:ASN:O	13:K:68:GLN:NE2	2.45	0.43
29:G:320:VAL:O	29:G:321:ASP:OD1	2.37	0.43
1:0:42:THR:HG22	1:0:49:ARG:HG2	2.01	0.42
3:2:84:ARG:NH2	28:A:1464:G:OP1	2.52	0.42
3:2:117:LEU:HD11	21:S:51:VAL:HG23	2.00	0.42
16:N:88:VAL:O	16:N:88:VAL:HG13	2.19	0.42
32:b:75:VAL:O	32:b:319:LEU:HD21	2.19	0.42
31:4:481:LEU:O	31:4:485:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:102:HIS:CE1	32:b:319:LEU:HD22	2.54	0.42
32:b:281:ALA:HB1	32:b:285:PHE:CZ	2.54	0.42
5:B:239:ASN:ND2	5:B:242:SER:OG	2.52	0.42
25:X:276:ARG:NH2	25:X:286:GLU:OE1	2.52	0.42
28:A:1522:U:O2'	30:V:65:LEU:HD22	2.20	0.42
29:G:198:ARG:HB3	29:G:246:ARG:HB2	2.01	0.42
31:4:346:HIS:HA	31:4:378:LEU:HD12	2.00	0.42
12:J:80:CYS:O	12:J:81:CYS:HB3	2.19	0.42
25:X:210:TRP:NE1	25:X:216:THR:OG1	2.40	0.42
25:X:365:TRP:O	25:X:365:TRP:CG	2.73	0.42
12:J:93:CYS:HG	12:J:125:VAL:CG2	2.27	0.42
30:V:208:LEU:HD13	30:V:226:TYR:HD2	1.83	0.42
31:4:170:VAL:HG13	31:4:246:ARG:NH2	2.35	0.42
31:4:369:LEU:HD22	31:4:415:PHE:CD2	2.55	0.42
32:b:214:LEU:O	32:b:243:ARG:NH1	2.51	0.42
32:b:270:ARG:CZ	32:b:280:ILE:HG13	2.50	0.42
2:1:217:GLN:NE2	26:Y:323:ASP:OD2	2.51	0.42
12:J:67:THR:HG22	12:J:79:LYS:HA	2.02	0.42
12:J:82:ARG:CG	12:J:90:GLU:HG2	2.50	0.42
25:X:167:ASP:OD1	25:X:167:ASP:N	2.53	0.42
28:A:1225:C:H1'	28:A:1226:C:OP2	2.20	0.42
9:F:116:GLU:CD	25:X:396:ALA:HB1	2.45	0.42
31:4:279:TYR:CB	31:4:297:LEU:HD21	2.49	0.42
32:b:227:GLY:HA3	32:b:287:ALA:HB2	2.02	0.42
7:D:114:ARG:O	28:A:1326:A:N6	2.53	0.42
11:I:81:GLU:OE1	11:I:81:GLU:N	2.46	0.42
25:X:159:HIS:ND1	25:X:267:ALA:HB2	2.34	0.42
28:A:1558:A:H2'	28:A:1559:G:O4'	2.20	0.42
28:A:1562:G:H1'	28:A:1583:MA6:H2	2.02	0.42
31:4:413:ASP:N	31:4:413:ASP:OD1	2.52	0.42
32:b:273:LEU:HB2	32:b:397:ARG:HE	1.85	0.42
3:2:9:ARG:NH2	28:A:1021:U:P	2.93	0.42
9:F:162:LEU:HD11	28:A:1466:C:H1'	2.02	0.42
12:J:42:PRO:CD	28:A:931:C:C6	3.02	0.42
12:J:93:CYS:SG	12:J:125:VAL:HG23	2.53	0.42
24:W:129:VAL:HG23	24:W:130:ASP:N	2.34	0.42
28:A:1598:G:O2'	28:A:1599:A:OP1	2.33	0.42
30:V:179:GLN:OE1	30:V:215:GLN:NE2	2.52	0.42
8:E:31:ASP:OD1	23:U:170:ARG:NH2	2.53	0.41
30:V:75:LEU:C	30:V:75:LEU:HD23	2.45	0.41
32:b:224:ARG:NH2	32:b:230:LYS:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:333:LEU:HD13	32:b:377:LEU:HD21	2.02	0.41
12:J:93:CYS:O	12:J:94:PHE:C	2.62	0.41
15:M:39:ASN:ND2	28:A:841:A:OP1	2.46	0.41
29:G:143:ASP:OD1	29:G:144:GLY:N	2.53	0.41
30:V:116:CYS:HA	30:V:121:ALA:HB3	2.01	0.41
32:b:86:PRO:HB3	32:b:113:ILE:HD12	2.02	0.41
32:b:120:ARG:NH1	32:b:293:ASN:O	2.53	0.41
5:B:89:VAL:O	5:B:89:VAL:HG12	2.21	0.41
7:D:232:THR:OG1	7:D:236:GLY:N	2.54	0.41
9:F:46:ILE:O	9:F:46:ILE:HG22	2.19	0.41
9:F:159:VAL:O	9:F:170:VAL:HG12	2.21	0.41
28:A:1415:G:H5'	28:A:1416:A:OP1	2.20	0.41
28:A:1539:C:H3'	28:A:1540:A:C5'	2.49	0.41
32:b:280:ILE:HG23	32:b:281:ALA:N	2.35	0.41
5:B:177:THR:OG1	28:A:1296:A:N6	2.44	0.41
19:Q:80:ARG:NE	24:W:123:VAL:HG11	2.35	0.41
29:G:197:SER:HB2	29:G:245:ARG:NH2	2.35	0.41
29:G:217:ASP:OD1	29:G:217:ASP:C	2.63	0.41
32:b:229:GLU:OE2	32:b:270:ARG:NH1	2.53	0.41
32:b:317:VAL:HG13	32:b:401:LEU:HG	2.02	0.41
9:F:88:ASP:OD2	9:F:146:HIS:NE2	2.50	0.41
12:J:66:PHE:CD2	12:J:81:CYS:HA	2.54	0.41
32:b:107:LEU:HD13	32:b:135:TYR:CE2	2.54	0.41
20:R:191:ARG:HG3	20:R:204:ILE:HG23	2.03	0.41
22:T:4:LYS:O	22:T:11:ARG:NH1	2.54	0.41
22:T:92:THR:HG22	22:T:92:THR:O	2.21	0.41
28:A:1550:A:O2'	28:A:1551:G:OP1	2.36	0.41
18:P:54:MET:HE1	21:S:65:TYR:O	2.21	0.41
21:S:52:ARG:NH1	28:A:1116:A:OP2	2.54	0.41
28:A:1415:G:OP2	28:A:1415:G:N2	2.43	0.41
32:b:288:LEU:O	32:b:292:VAL:HG23	2.20	0.41
10:H:184:ILE:O	10:H:184:ILE:HG22	2.20	0.41
11:I:187:ARG:O	28:A:1066:C:O2'	2.38	0.41
12:J:66:PHE:CZ	12:J:81:CYS:HA	2.56	0.41
21:S:75:TYR:O	21:S:79:GLY:N	2.54	0.41
31:4:324:VAL:O	31:4:324:VAL:HG12	2.20	0.41
32:b:128:ALA:O	32:b:132:SER:N	2.53	0.41
4:3:165:LYS:HG2	4:3:195:TYR:CE2	2.56	0.41
32:b:92:PHE:CG	32:b:113:ILE:HD11	2.54	0.41
7:D:314:LEU:HD21	7:D:329:ILE:O	2.21	0.40
20:R:162:SER:HB2	20:R:165:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:1247:G:H4'	28:A:1248:C:OP2	2.21	0.40
31:4:306:ASN:OD1	31:4:344:ARG:NH2	2.49	0.40
9:F:161:ILE:HG23	9:F:161:ILE:O	2.21	0.40
12:J:99:GLY:O	12:J:127:ARG:NH2	2.46	0.40
14:L:83:GLU:HG2	14:L:84:LYS:N	2.36	0.40
18:P:67:LEU:HD23	23:U:191:ILE:HD12	2.02	0.40
25:X:123:ARG:NH2	25:X:337:LEU:O	2.55	0.40
32:b:259:ALA:HA	32:b:280:ILE:HG21	2.03	0.40
2:1:194:VAL:HG21	2:1:198:TYR:HB2	2.04	0.40
7:D:263:ASP:OD1	7:D:264:ARG:N	2.54	0.40
28:A:1078:A:O2'	32:b:228:GLU:OE2	2.35	0.40
28:A:1431:G:O2'	28:A:1432:U:OP2	2.38	0.40
6:C:36:LYS:NZ	28:A:1322:C:OP2	2.55	0.40
9:F:201:MET:N	9:F:202:PRO:CD	2.84	0.40
12:J:55:ARG:HD3	12:J:58:LEU:HD21	2.04	0.40
14:L:167:LEU:HD11	14:L:187:ILE:HD12	2.03	0.40
29:G:263:ASP:OD1	29:G:267:MET:N	2.55	0.40
32:b:77:VAL:HG21	32:b:105:ALA:CB	2.51	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%)	210 (99%)	3 (1%)	0	100	100
2	1	274/323 (85%)	263 (96%)	11 (4%)	0	100	100
3	2	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
4	3	68/199 (34%)	68 (100%)	0	0	100	100
5	B	223/296 (75%)	215 (96%)	8 (4%)	0	100	100
6	C	130/167 (78%)	126 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	D	341/430 (79%)	328 (96%)	13 (4%)	0	100	100
8	E	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
9	F	206/242 (85%)	201 (98%)	5 (2%)	0	100	100
10	H	138/201 (69%)	136 (99%)	2 (1%)	0	100	100
11	I	134/194 (69%)	123 (92%)	10 (8%)	1 (1%)	18	55
12	J	106/138 (77%)	95 (90%)	10 (9%)	1 (1%)	14	49
13	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
14	L	172/257 (67%)	168 (98%)	4 (2%)	0	100	100
15	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
16	N	108/130 (83%)	103 (95%)	5 (5%)	0	100	100
17	O	192/258 (74%)	185 (96%)	7 (4%)	0	100	100
18	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
19	Q	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
20	R	293/360 (81%)	288 (98%)	5 (2%)	0	100	100
21	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
22	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
23	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
24	W	98/187 (52%)	94 (96%)	4 (4%)	0	100	100
25	X	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
26	Y	120/395 (30%)	119 (99%)	1 (1%)	0	100	100
27	Z	84/106 (79%)	82 (98%)	2 (2%)	0	100	100
29	G	320/396 (81%)	300 (94%)	20 (6%)	0	100	100
30	V	358/414 (86%)	353 (99%)	5 (1%)	0	100	100
31	4	584/689 (85%)	570 (98%)	14 (2%)	0	100	100
32	b	282/407 (69%)	271 (96%)	11 (4%)	0	100	100
All	All	5899/7710 (76%)	5735 (97%)	162 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	J	81	CYS
11	I	185	GLY

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
2	1	254/291 (87%)	254 (100%)	0	100	100
3	2	100/100 (100%)	100 (100%)	0	100	100
4	3	65/166 (39%)	65 (100%)	0	100	100
5	B	198/249 (80%)	198 (100%)	0	100	100
6	C	115/143 (80%)	115 (100%)	0	100	100
7	D	286/357 (80%)	286 (100%)	0	100	100
8	E	104/107 (97%)	104 (100%)	0	100	100
9	F	185/209 (88%)	185 (100%)	0	100	100
10	H	130/180 (72%)	130 (100%)	0	100	100
11	I	104/146 (71%)	104 (100%)	0	100	100
12	J	93/118 (79%)	92 (99%)	1 (1%)	65	74
13	K	91/113 (80%)	91 (100%)	0	100	100
14	L	158/226 (70%)	158 (100%)	0	100	100
15	M	97/113 (86%)	97 (100%)	0	100	100
16	N	96/115 (84%)	96 (100%)	0	100	100
17	O	175/230 (76%)	175 (100%)	0	100	100
18	P	88/123 (72%)	88 (100%)	0	100	100
19	Q	78/78 (100%)	78 (100%)	0	100	100
20	R	264/318 (83%)	264 (100%)	0	100	100
21	S	116/164 (71%)	116 (100%)	0	100	100
22	T	153/157 (98%)	153 (100%)	0	100	100
23	U	152/174 (87%)	152 (100%)	0	100	100
24	W	87/158 (55%)	87 (100%)	0	100	100
25	X	311/351 (89%)	311 (100%)	0	100	100
26	Y	113/357 (32%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	Z	80/95 (84%)	80 (100%)	0	100	100
29	G	282/342 (82%)	282 (100%)	0	100	100
30	V	325/364 (89%)	324 (100%)	1 (0%)	86	84
31	4	526/609 (86%)	526 (100%)	0	100	100
32	b	244/350 (70%)	244 (100%)	0	100	100
All	All	5258/6693 (79%)	5256 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	108	VAL
30	V	38	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	133	HIS
1	0	145	HIS
3	2	15	ASN
7	D	415	GLN
8	E	54	HIS
8	E	81	HIS
10	H	133	GLN
12	J	37	HIS
14	L	162	GLN
14	L	218	GLN
15	M	16	HIS
16	N	52	HIS
17	O	130	HIS
17	O	169	GLN
18	P	95	HIS
20	R	167	HIS
20	R	246	HIS
20	R	278	ASN
20	R	299	ASN
21	S	66	HIS
24	W	106	HIS
25	X	69	ASN
25	X	140	HIS

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Mol	Chain	Res	Type
25	X	148	GLN
25	X	312	GLN
26	Y	303	GLN
27	Z	54	ASN
29	G	176	GLN
29	G	261	GLN
29	G	288	HIS
29	G	318	HIS
30	V	215	GLN
30	V	245	HIS
30	V	396	GLN
31	4	90	GLN
31	4	274	GLN
31	4	346	HIS
31	4	373	HIS
31	4	453	HIS
31	4	545	GLN
32	b	176	GLN
32	b	212	ASN
32	b	393	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	A	954/955 (99%)	208 (21%)	9 (0%)

All (208) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	A	651	A
28	A	659	U
28	A	680	U
28	A	688	A
28	A	689	U
28	A	690	U
28	A	695	A
28	A	704	U
28	A	718	A
28	A	721	U
28	A	722	C
28	A	730	A

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Mol	Chain	Res	Type
28	A	739	C
28	A	753	A
28	A	757	A
28	A	761	A
28	A	766	G
28	A	777	G
28	A	791	G
28	A	793	C
28	A	794	U
28	A	796	G
28	A	801	A
28	A	803	C
28	A	804	C
28	A	808	C
28	A	814	A
28	A	815	C
28	A	826	A
28	A	828	C
28	A	829	C
28	A	830	U
28	A	832	U
28	A	835	C
28	A	859	U
28	A	860	A
28	A	861	U
28	A	868	C
28	A	871	A
28	A	879	U
28	A	881	A
28	A	884	U
28	A	889	G
28	A	890	C
28	A	896	A
28	A	902	G
28	A	903	U
28	A	904	C
28	A	905	A
28	A	907	A
28	A	919	A
28	A	922	C
28	A	929	A
28	A	930	G

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Mol	Chain	Res	Type
28	A	931	C
28	A	932	C
28	A	933	G
28	A	938	A
28	A	939	A
28	A	940	A
28	A	941	G
28	A	942	A
28	A	953	U
28	A	955	A
28	A	956	C
28	A	958	C
28	A	961	U
28	A	962	C
28	A	966	A
28	A	967	A
28	A	988	G
28	A	993	A
28	A	1000	U
28	A	1001	C
28	A	1002	C
28	A	1003	A
28	A	1011	C
28	A	1015	A
28	A	1030	G
28	A	1042	U
28	A	1044	U
28	A	1049	A
28	A	1069	A
28	A	1073	G
28	A	1081	U
28	A	1082	A
28	A	1103	A
28	A	1105	C
28	A	1106	C
28	A	1107	U
28	A	1109	A
28	A	1116	A
28	A	1117	A
28	A	1118	A
28	A	1119	U
28	A	1120	C

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Mol	Chain	Res	Type
28	A	1121	A
28	A	1126	A
28	A	1128	C
28	A	1137	A
28	A	1142	A
28	A	1144	U
28	A	1151	C
28	A	1154	A
28	A	1155	G
28	A	1160	A
28	A	1187	U
28	A	1188	A
28	A	1189	U
28	A	1190	C
28	A	1194	C
28	A	1199	G
28	A	1200	G
28	A	1213	A
28	A	1215	U
28	A	1220	A
28	A	1222	A
28	A	1223	C
28	A	1225	C
28	A	1226	C
28	A	1227	G
28	A	1235	U
28	A	1245	U
28	A	1246	U
28	A	1247	G
28	A	1248	C
28	A	1250	C
28	A	1251	A
28	A	1269	U
28	A	1271	C
28	A	1282	G
28	A	1284	U
28	A	1290	C
28	A	1291	U
28	A	1292	A
28	A	1295	A
28	A	1299	A
28	A	1312	C

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Mol	Chain	Res	Type
28	A	1313	A
28	A	1326	A
28	A	1327	G
28	A	1338	A
28	A	1343	A
28	A	1344	U
28	A	1345	G
28	A	1352	C
28	A	1354	A
28	A	1355	G
28	A	1357	A
28	A	1378	C
28	A	1379	A
28	A	1386	U
28	A	1387	A
28	A	1390	A
28	A	1392	A
28	A	1401	G
28	A	1402	A
28	A	1404	A
28	A	1405	C
28	A	1406	U
28	A	1416	A
28	A	1430	A
28	A	1443	U
28	A	1447	G
28	A	1465	C
28	A	1474	G
28	A	1478	A
28	A	1480	A
28	A	1482	A
28	A	1483	C
28	A	1487	C
28	A	1490	U
28	A	1502	A
28	A	1503	G
28	A	1509	U
28	A	1510	U
28	A	1512	A
28	A	1519	A
28	A	1520	U
28	A	1521	U

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Mol	Chain	Res	Type
28	A	1523	A
28	A	1524	A
28	A	1525	C
28	A	1526	U
28	A	1527	A
28	A	1532	C
28	A	1533	C
28	A	1537	C
28	A	1538	G
28	A	1539	C
28	A	1548	A
28	A	1549	G
28	A	1551	G
28	A	1558	A
28	A	1561	C
28	A	1562	G
28	A	1564	A
28	A	1568	U
28	A	1570	G
28	A	1571	U
28	A	1582	G
28	A	1583	MA6
28	A	1584	MA6
28	A	1585	A
28	A	1594	G
28	A	1595	G
28	A	1599	A
28	A	1602	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	A	1081	U
28	A	1225	C
28	A	1405	C
28	A	1502	A
28	A	1508	C
28	A	1513	A
28	A	1520	U
28	A	1537	C
28	A	1550	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 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
28	B8T	A	1486	28	19,22,23	3.32	8 (42%)	26,31,34	0.84	1 (3%)
28	5MU	A	1076	28	19,22,23	0.40	0	28,32,35	0.49	0
28	MA6	A	1583	28	23,26,27	1.27	3 (13%)	34,38,41	3.27	14 (41%)
28	MA6	A	1584	28	23,26,27	1.28	3 (13%)	34,38,41	3.10	11 (32%)
28	5MC	A	1488	28	18,22,23	0.54	0	26,32,35	0.49	0
11	5F0	I	184	11	8,8,9	0.58	0	7,9,11	1.17	1 (14%)

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
28	B8T	A	1486	28	-	0/7/27/28	0/2/2/2
28	5MU	A	1076	28	-	0/7/25/26	0/2/2/2
28	MA6	A	1583	28	-	3/11/29/30	0/3/3/3
28	MA6	A	1584	28	-	0/11/29/30	0/3/3/3
28	5MC	A	1488	28	-	0/7/25/26	0/2/2/2
11	5F0	I	184	11	-	2/9/9/10	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	1486	B8T	C4-N3	7.63	1.46	1.32
28	A	1486	B8T	C6-C5	5.99	1.49	1.35
28	A	1486	B8T	C2-N3	5.97	1.48	1.36
28	A	1486	B8T	C4-N4	4.85	1.45	1.35
28	A	1486	B8T	C2-N1	4.56	1.49	1.40
28	A	1486	B8T	C5-C4	3.51	1.48	1.40
28	A	1486	B8T	C6-N1	3.50	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	1584	MA6	C6-N6	3.41	1.46	1.36
28	A	1583	MA6	C6-N6	3.39	1.46	1.36
28	A	1486	B8T	O2-C2	-2.99	1.18	1.23
28	A	1584	MA6	C5-C4	-2.56	1.34	1.39
28	A	1583	MA6	C5-C4	-2.53	1.34	1.39
28	A	1583	MA6	C5-N7	-2.32	1.34	1.39
28	A	1584	MA6	C5-N7	-2.29	1.34	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	1583	MA6	N1-C6-N6	-12.64	103.26	117.08
28	A	1584	MA6	N1-C6-N6	-11.87	104.10	117.08
28	A	1583	MA6	C5-C6-N6	6.61	136.82	125.30
28	A	1584	MA6	C5-C6-N6	5.91	135.59	125.30
28	A	1584	MA6	N1-C2-N3	-5.37	120.20	128.60
28	A	1584	MA6	C5-C4-N3	-5.31	119.82	126.75
28	A	1583	MA6	N1-C2-N3	-5.22	120.43	128.60
28	A	1583	MA6	C5-C4-N3	-5.03	120.18	126.75
28	A	1584	MA6	N9-C8-N7	-4.19	108.19	113.91
28	A	1583	MA6	N9-C8-N7	-4.03	108.40	113.91
28	A	1584	MA6	C4-C5-C6	3.64	119.96	115.88
28	A	1583	MA6	C4-C5-C6	3.56	119.86	115.88
28	A	1584	MA6	C2-N3-C4	3.50	120.03	111.75
28	A	1583	MA6	C2-N1-C6	3.46	119.93	111.75
28	A	1584	MA6	C2-N1-C6	3.36	119.69	111.75
28	A	1583	MA6	C2-N3-C4	3.35	119.67	111.75
28	A	1584	MA6	N3-C4-N9	3.27	132.47	127.08
28	A	1583	MA6	O4'-C4'-C5'	3.20	119.92	109.37
28	A	1583	MA6	C5'-C4'-C3'	3.14	126.95	115.18
28	A	1584	MA6	C5-N7-C8	3.06	107.85	103.51
28	A	1583	MA6	C5-N7-C8	3.01	107.79	103.51
11	I	184	5F0	O-C-CB	-2.75	117.40	125.43
28	A	1583	MA6	N3-C4-N9	2.75	131.61	127.08
28	A	1486	B8T	C6-C5-C4	2.50	120.02	116.96
28	A	1583	MA6	C4-C5-N7	-2.19	107.95	110.62
28	A	1584	MA6	C4-N9-C8	2.14	108.04	105.73
28	A	1583	MA6	C5-C4-N9	2.07	108.19	105.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	1583	MA6	O4'-C4'-C5'-O5'
11	I	184	5F0	OD1-C1-CA-CB
28	A	1583	MA6	C4'-C5'-O5'-P
28	A	1583	MA6	C3'-C4'-C5'-O5'
11	I	184	5F0	O-C-CB-CA

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	1076	5MU	1	0
28	A	1583	MA6	5	0
28	A	1584	MA6	3	0
11	I	184	5F0	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 50 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
37	GDP	X	502	-	28,30,30	1.13	3 (10%)	44,47,47	1.83	8 (18%)
35	FES	P	201	18,8	0,4,4	-	-	-	-	-
38	NAD	A	1701	33	45,48,48	0.73	1 (2%)	63,73,73	0.74	2 (3%)
36	ATP	X	501	-	29,33,33	0.29	0	44,52,52	0.67	1 (2%)
35	FES	T	201	22	0,4,4	-	-	-	-	-

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	-	-	4/16/32/32	0/3/3/3
35	FES	P	201	18,8	-	-	0/1/1/1
38	NAD	A	1701	33	-	3/30/62/62	0/5/5/5
36	ATP	X	501	-	-	5/22/38/38	0/3/3/3
35	FES	T	201	22	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	502	GDP	C5-C4	3.06	1.47	1.38
37	X	502	GDP	C6-N1	-2.44	1.34	1.38
38	A	1701	NAD	O4D-C1D	-2.29	1.37	1.41
37	X	502	GDP	C5-N7	-2.18	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	X	502	GDP	C5-C4-N3	-6.17	118.45	128.46
37	X	502	GDP	C2-N3-C4	4.91	121.05	112.30
37	X	502	GDP	N9-C4-N3	4.69	135.36	125.94
37	X	502	GDP	PA-O3A-PB	-3.70	120.12	132.83
37	X	502	GDP	C6-C5-N7	3.19	136.19	130.25
37	X	502	GDP	C4-C5-N7	-2.66	106.52	110.72
38	A	1701	NAD	PN-O3-PA	-2.26	125.06	132.83
37	X	502	GDP	O6-C6-C5	-2.15	120.89	126.60
38	A	1701	NAD	O7N-C7N-N7N	2.04	125.48	122.58
36	X	501	ATP	PB-O3B-PG	2.01	139.72	132.83
37	X	502	GDP	C8-N7-C5	2.00	107.86	104.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	X	501	ATP	C5'-O5'-PA-O2A
36	X	501	ATP	C5'-O5'-PA-O3A
37	X	502	GDP	C5'-O5'-PA-O3A
38	A	1701	NAD	C5B-O5B-PA-O1A
38	A	1701	NAD	C5B-O5B-PA-O3
37	X	502	GDP	O4'-C4'-C5'-O5'
38	A	1701	NAD	C2B-C1B-N9A-C8A

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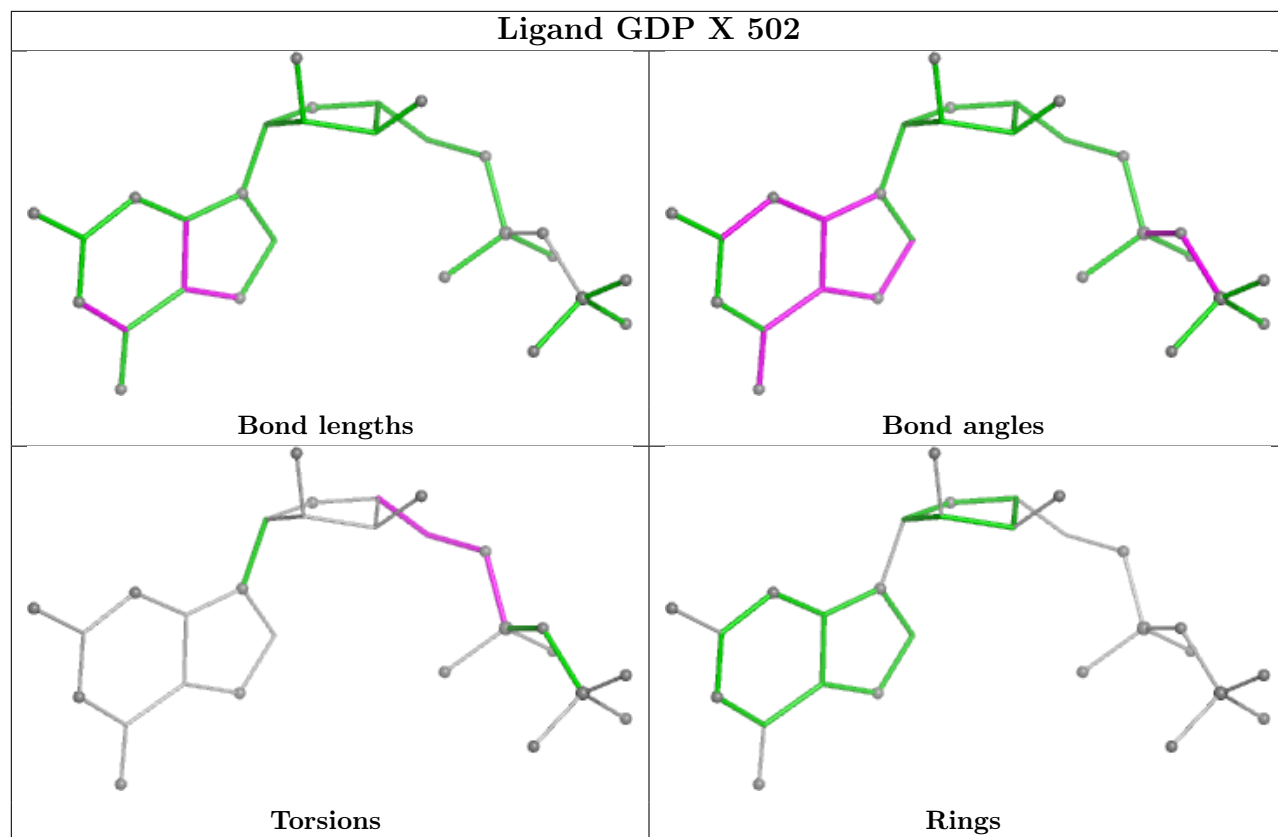
Mol	Chain	Res	Type	Atoms
37	X	502	GDP	C5'-O5'-PA-O1A
36	X	501	ATP	C4'-C5'-O5'-PA
36	X	501	ATP	PB-O3A-PA-O1A
36	X	501	ATP	PB-O3A-PA-O2A
37	X	502	GDP	C4'-C5'-O5'-PA

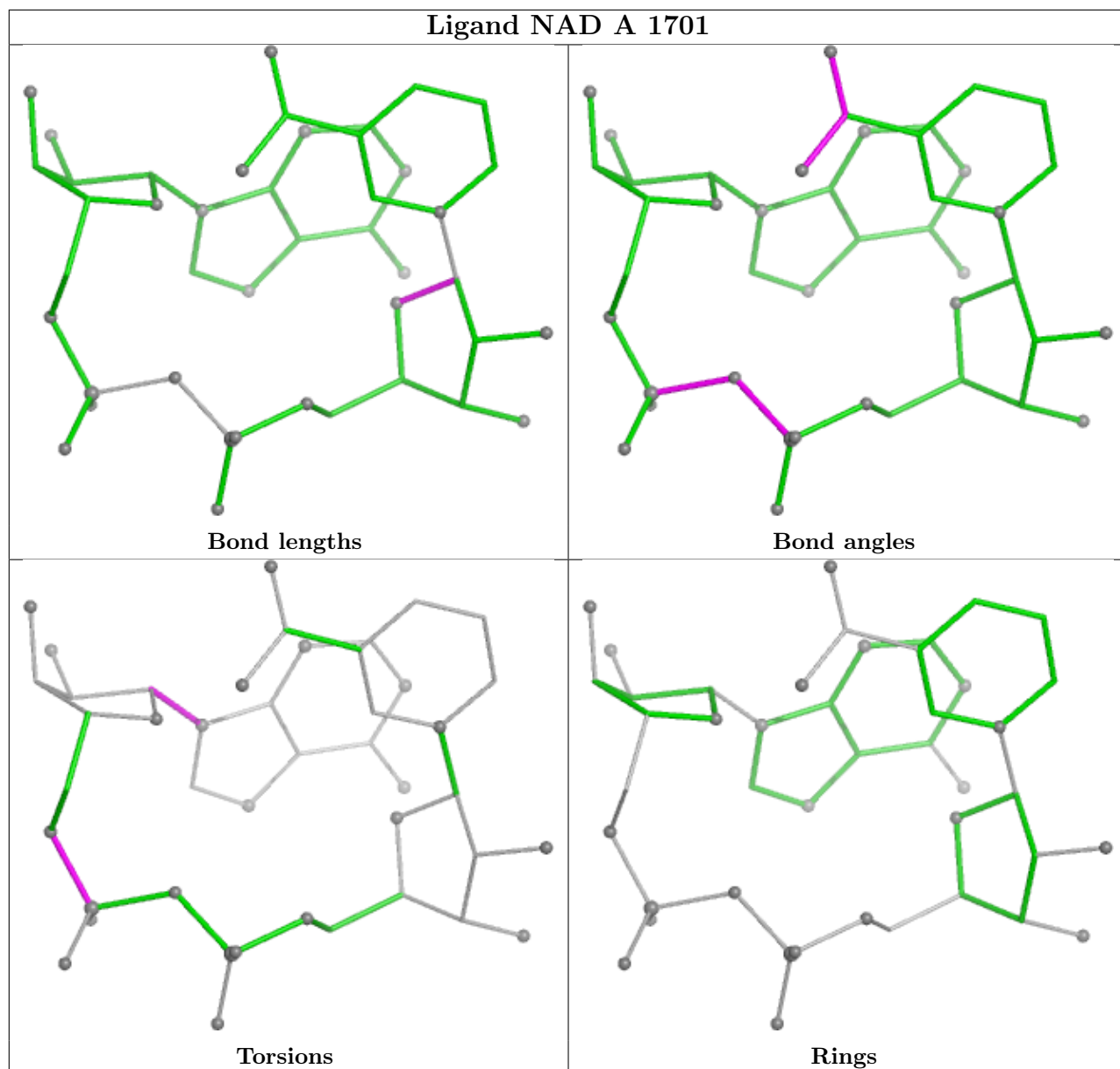
There are no ring outliers.

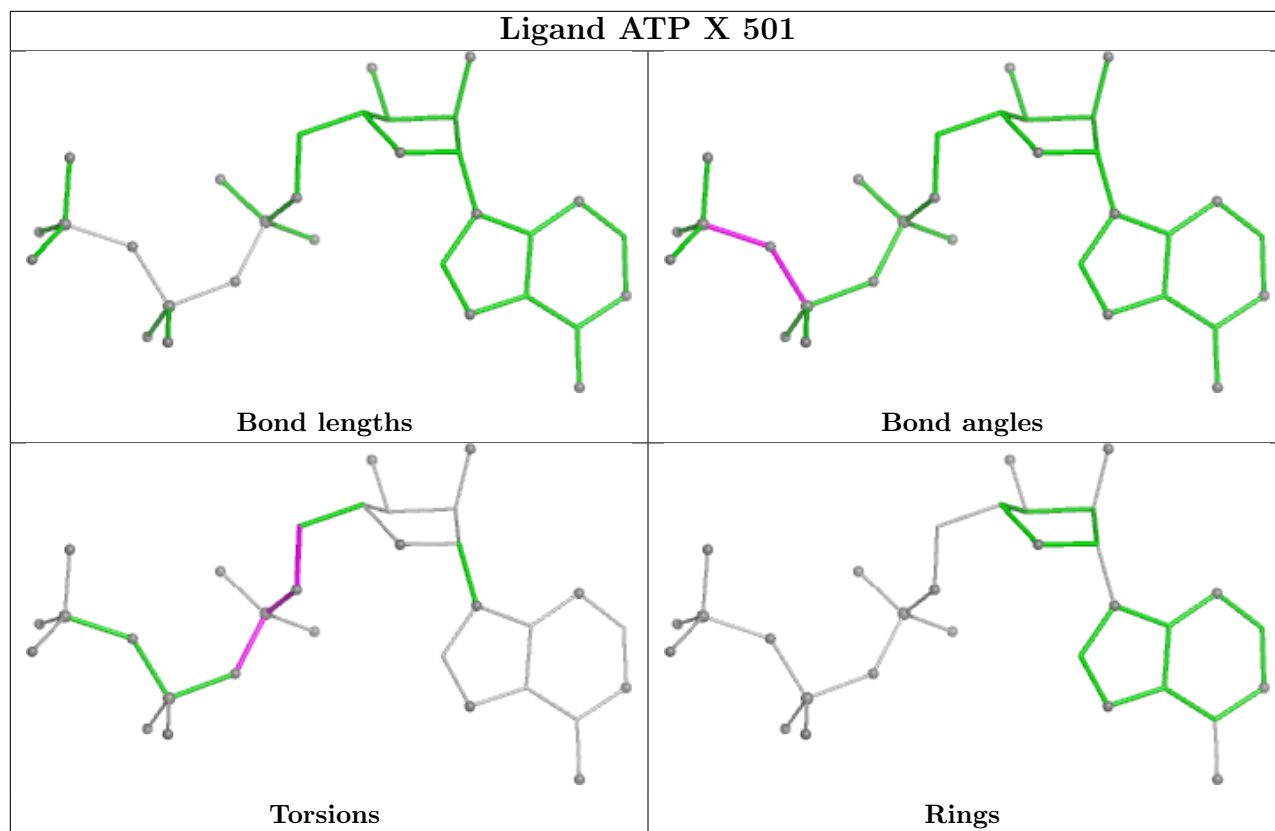
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	P	201	FES	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
28	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1486:B8T	O3'	1487:C	P	3.07

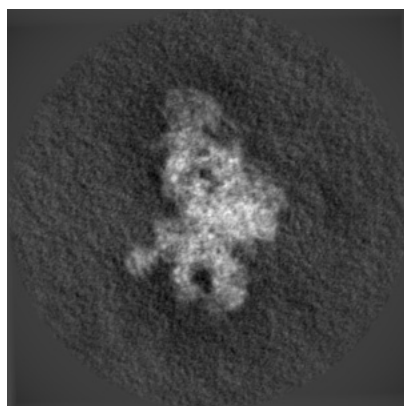
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54163. These allow visual inspection of the internal detail of the map and identification of artifacts.

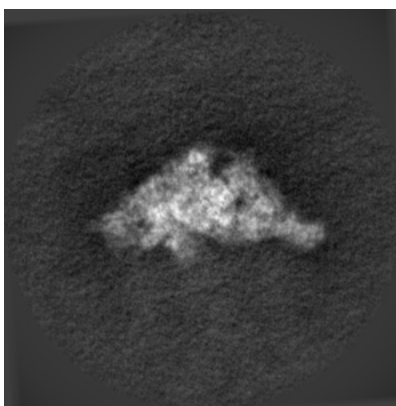
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

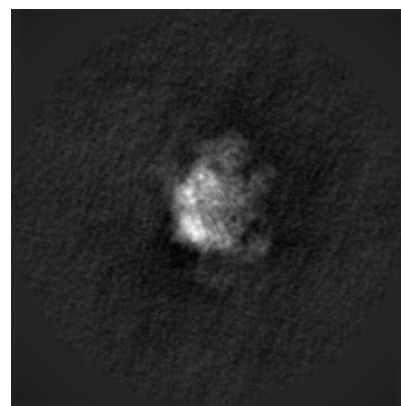
6.1.1 Primary map



X

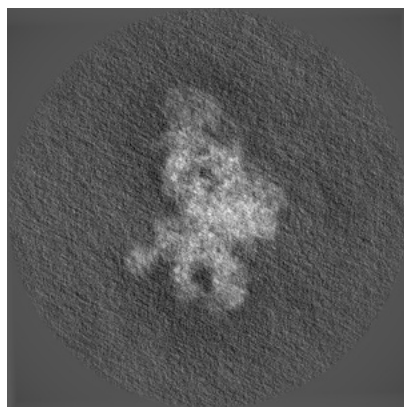


Y

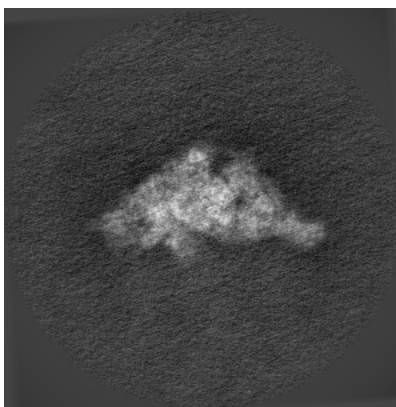


Z

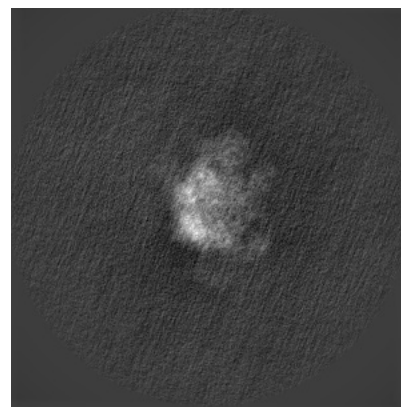
6.1.2 Raw map



X



Y

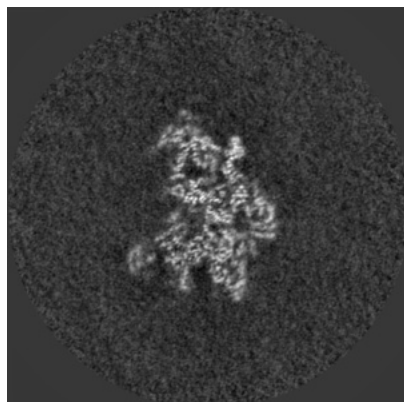


Z

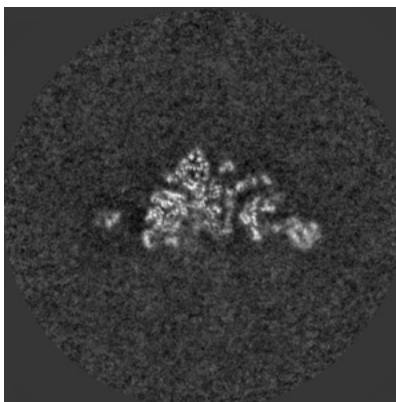
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

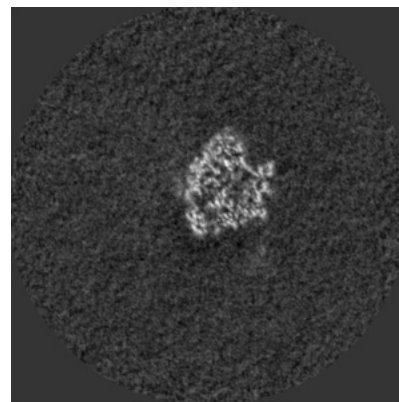
6.2.1 Primary map



X Index: 300

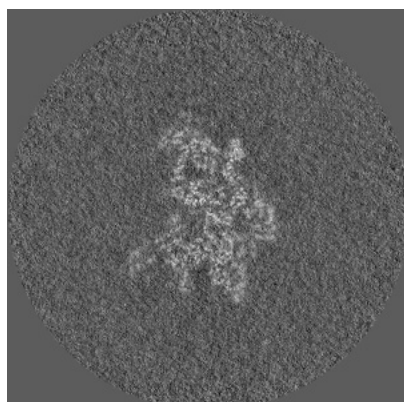


Y Index: 300

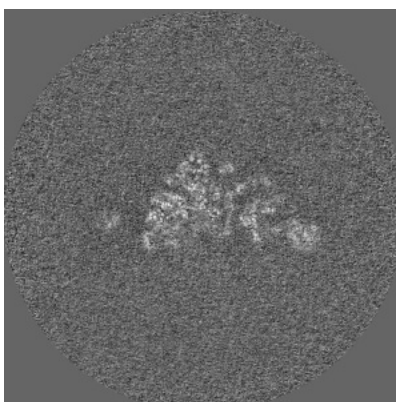


Z Index: 300

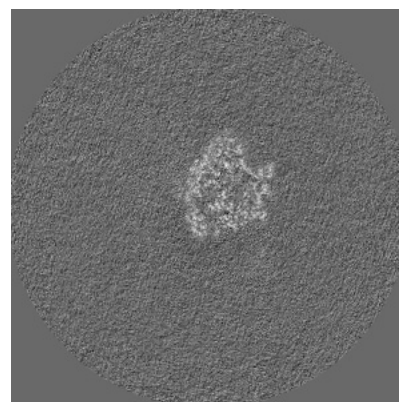
6.2.2 Raw map



X Index: 300



Y Index: 300

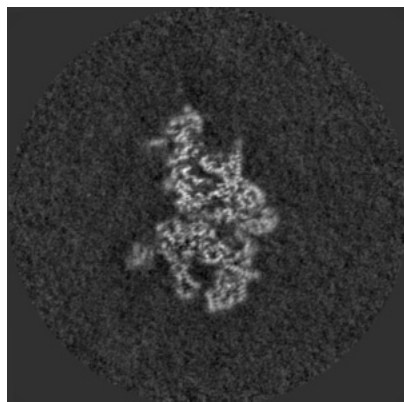


Z Index: 300

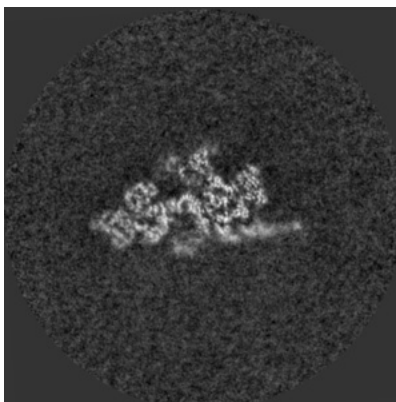
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

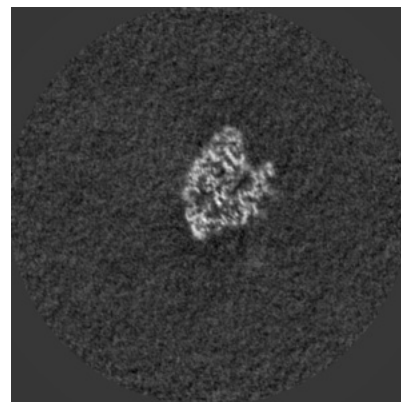
6.3.1 Primary map



X Index: 287

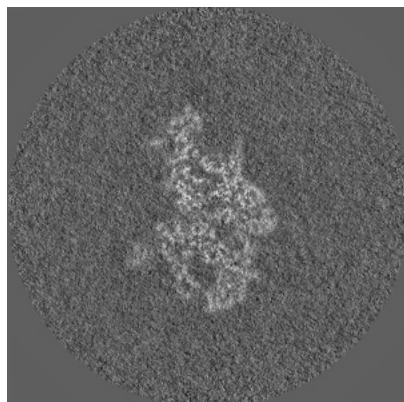


Y Index: 325

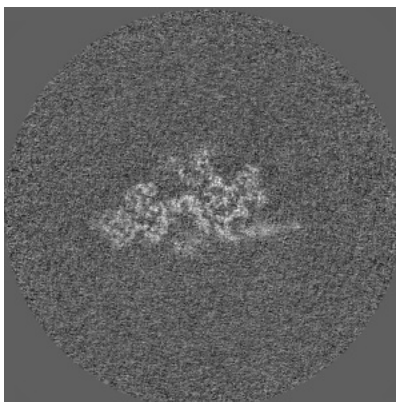


Z Index: 304

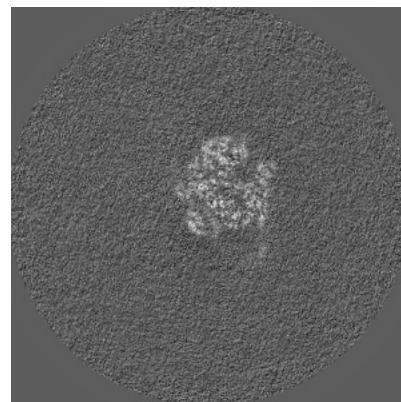
6.3.2 Raw map



X Index: 287



Y Index: 326

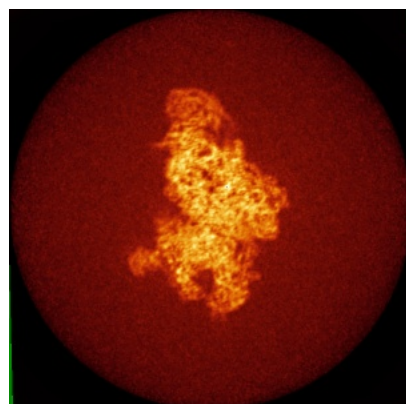


Z Index: 295

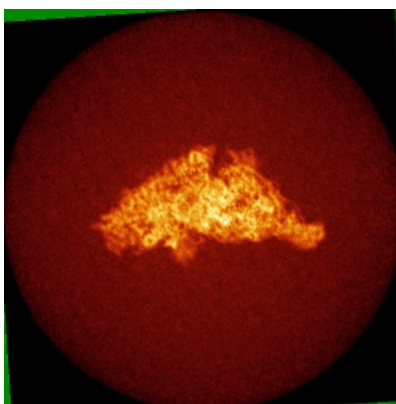
The images above show the largest variance slices of the map in three orthogonal directions.

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

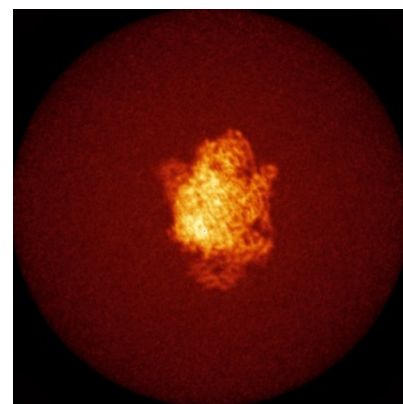
6.4.1 Primary map



X

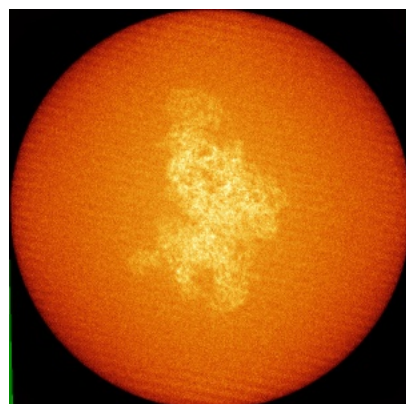


Y

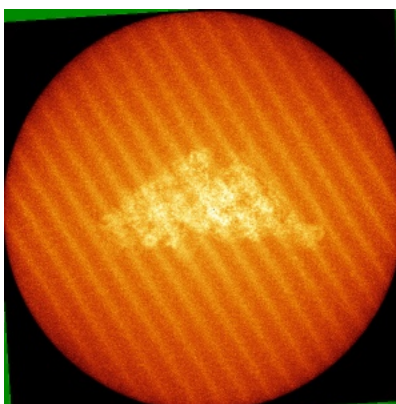


Z

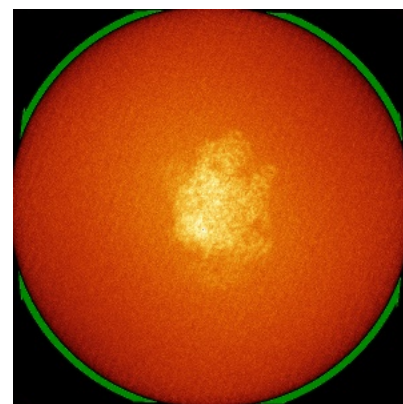
6.4.2 Raw map



X



Y

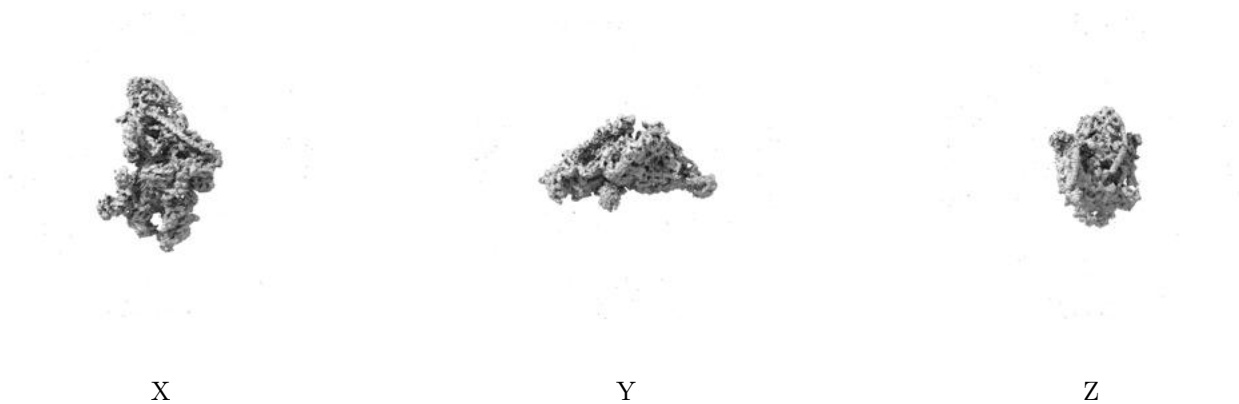


Z

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.

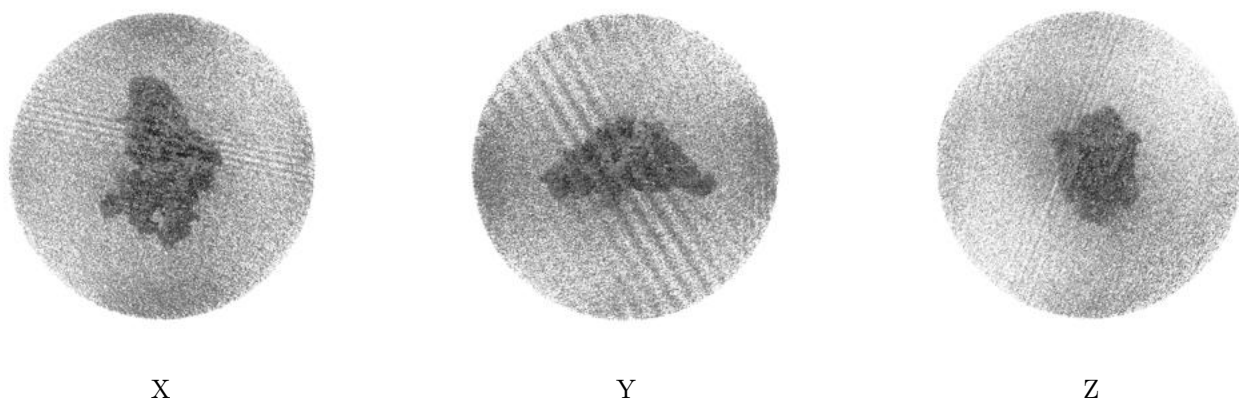
6.5 Orthogonal surface views [i](#)

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.

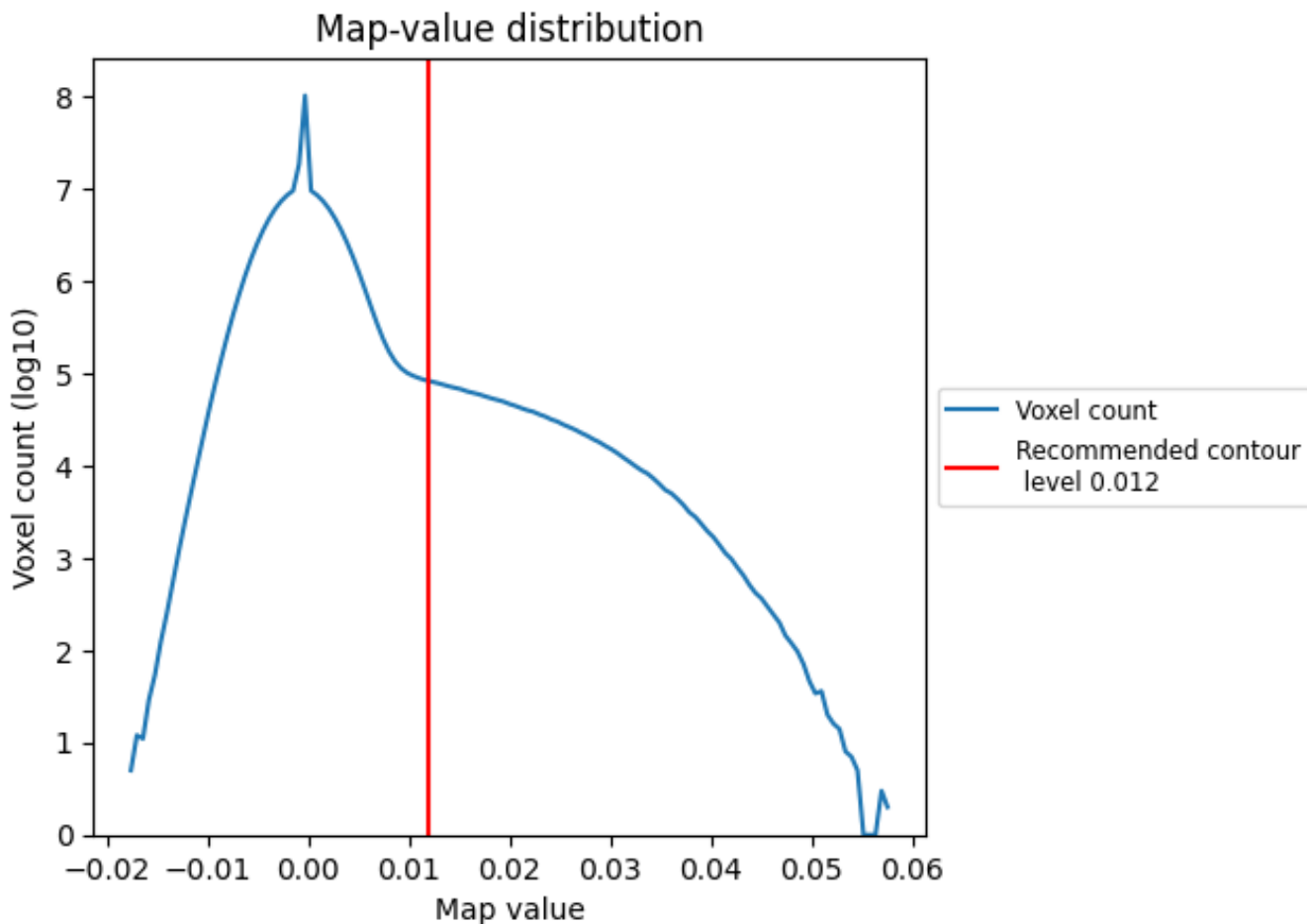
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

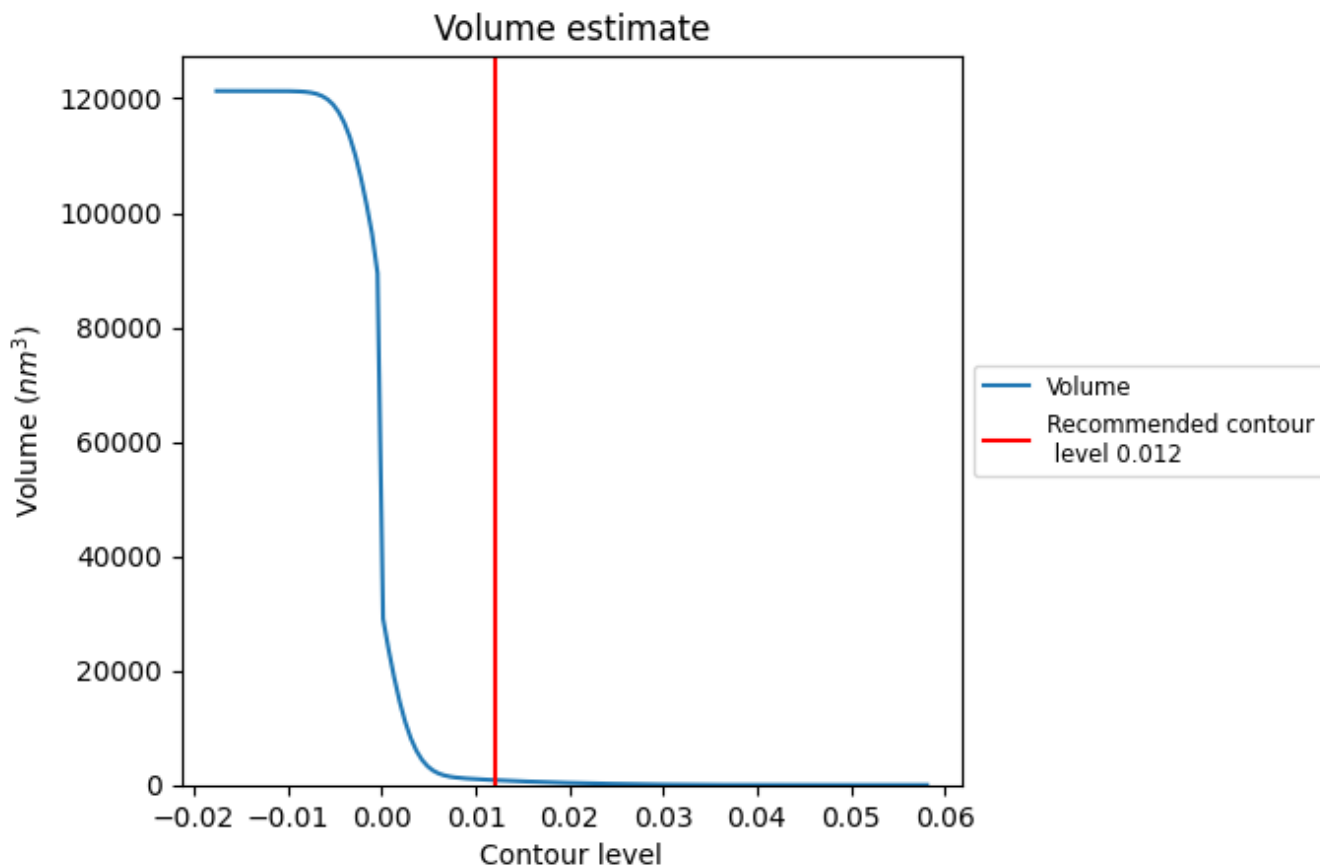
This section contains the results of statistical analysis of the map.

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.

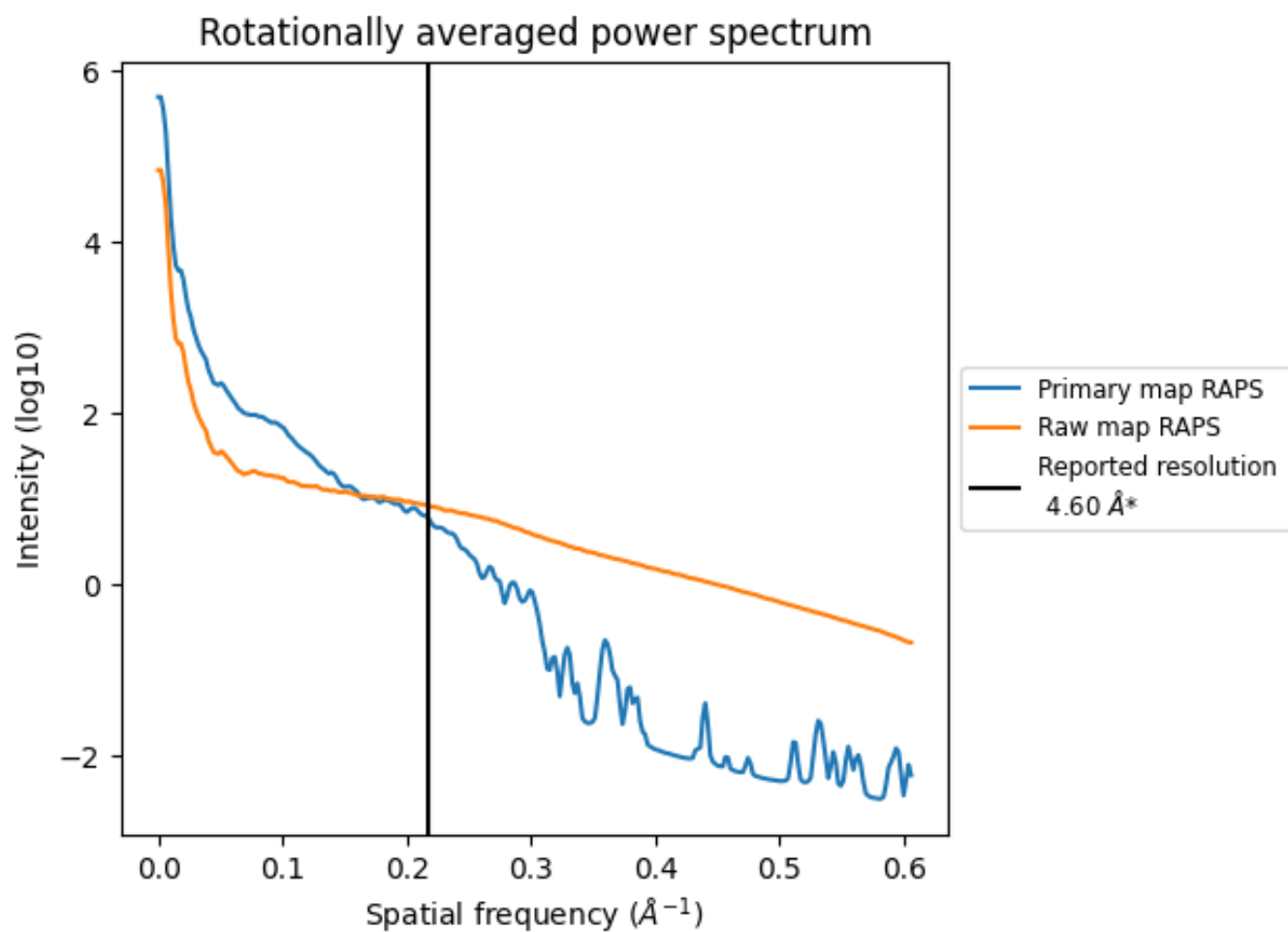
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 850 nm^3 ; this corresponds to an approximate mass of 768 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

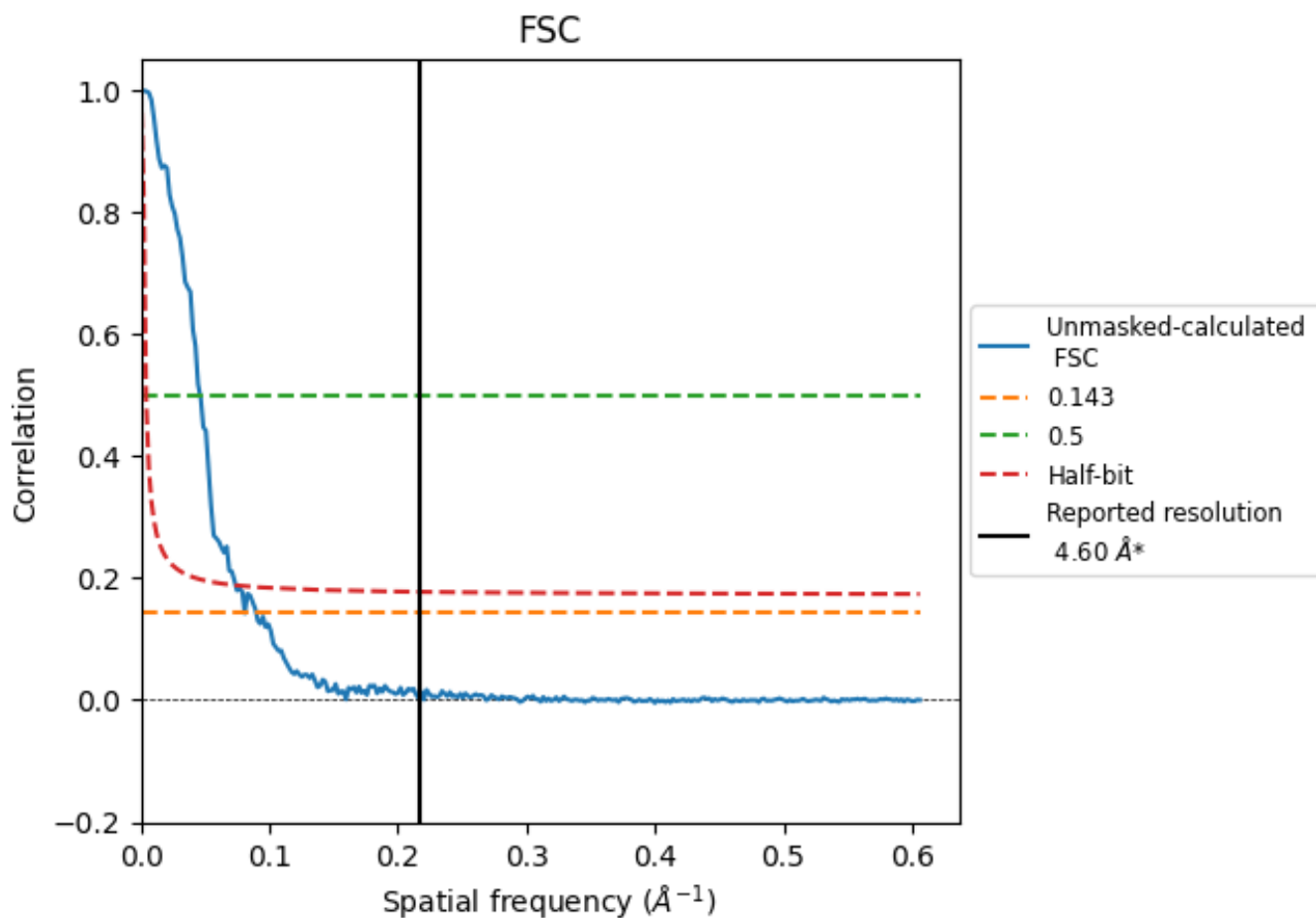


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

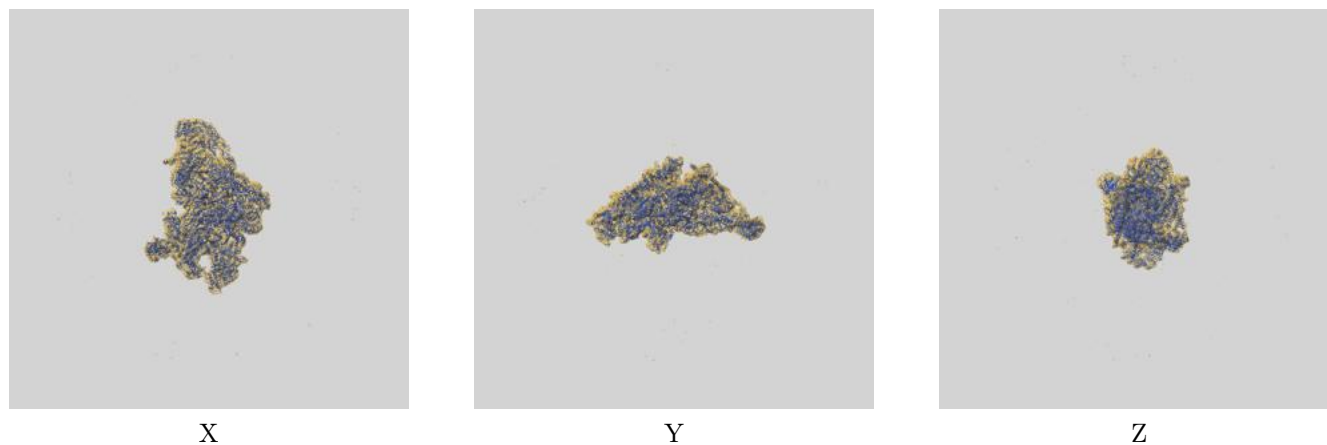
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	12.38	21.79	13.57

*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 12.38 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

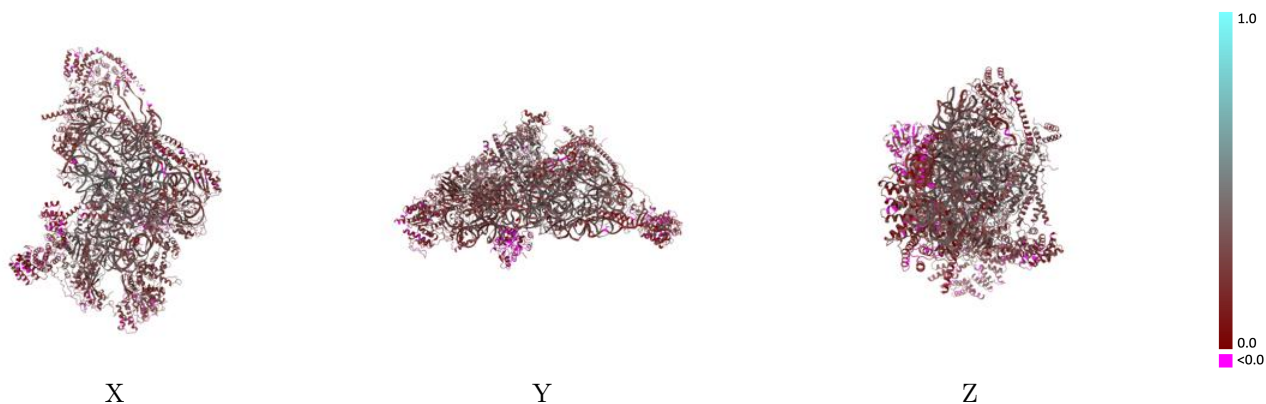
This section contains information regarding the fit between EMDB map EMD-54163 and PDB model 9RPF. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



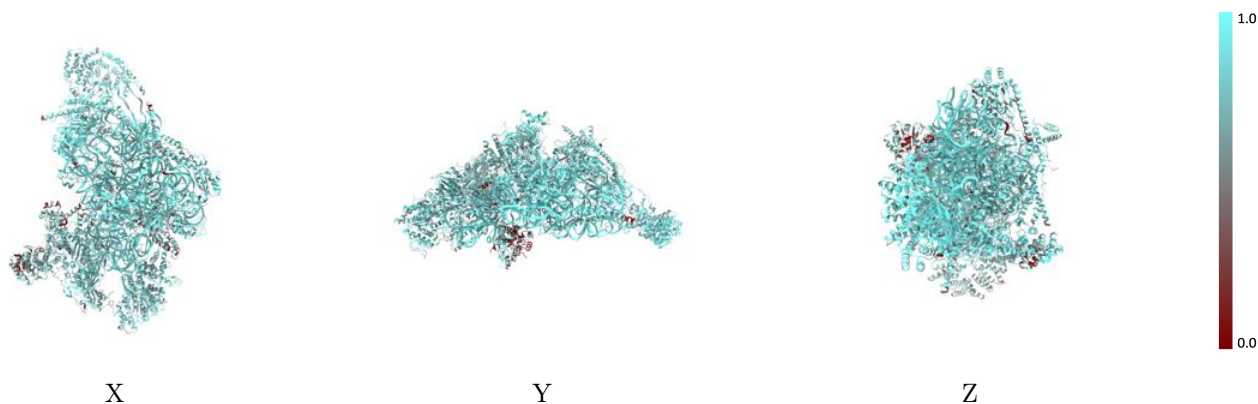
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



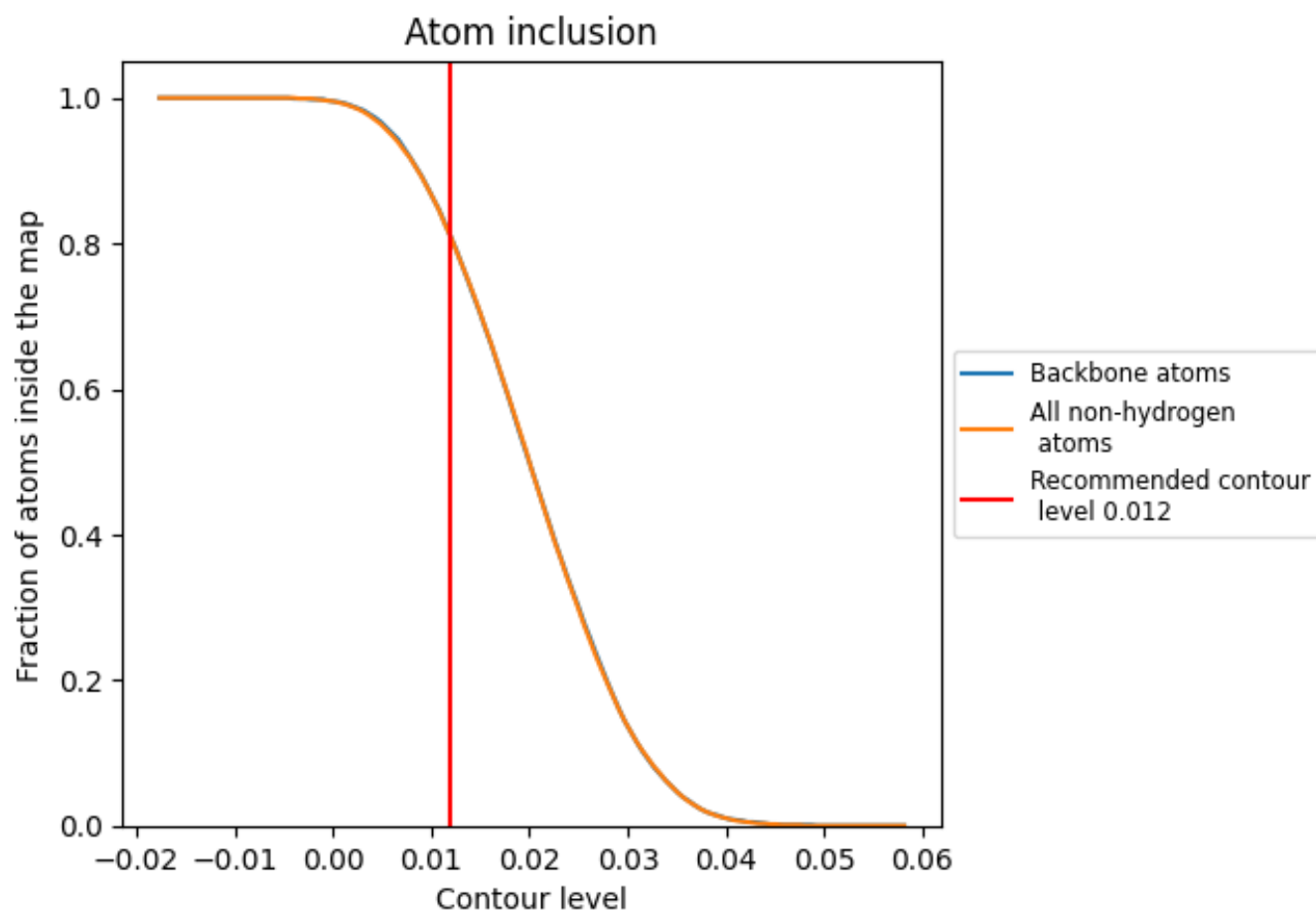
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 81% 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	 0.8090	 0.2770
0	 0.7950	 0.2330
1	 0.7640	 0.2340
2	 0.5320	 0.2330
3	 0.7770	 0.2700
4	 0.6250	 0.1530
A	 0.9510	 0.3420
B	 0.8360	 0.3560
C	 0.7960	 0.3520
D	 0.7690	 0.3390
E	 0.7490	 0.2410
F	 0.7470	 0.2530
G	 0.7770	 0.2690
H	 0.7790	 0.2930
I	 0.8280	 0.2720
J	 0.8260	 0.3590
K	 0.8430	 0.3030
L	 0.7560	 0.2380
M	 0.8300	 0.2910
N	 0.8380	 0.3400
O	 0.8490	 0.3110
P	 0.8090	 0.2990
Q	 0.8020	 0.3130
R	 0.8500	 0.2910
S	 0.8240	 0.3230
T	 0.8310	 0.3430
U	 0.7770	 0.2270
V	 0.8260	 0.1640
W	 0.8550	 0.3490
X	 0.7730	 0.1910
Y	 0.7000	 0.2080
Z	 0.7760	 0.2930
b	 0.4220	 0.0530

