



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 01:50 am GMT

PDB ID : 6ZV6
EMDB ID : EMD-11441
Title : Human RIO1(kd)-StHA late pre-40S particle, structural state B (post 18S rRNA cleavage)
Authors : Plassart, L.; Shayan, R.; Plisson-Chastang, C.
Deposited on : 2020-07-24
Resolution : 2.90 Å(reported)
Based on initial model : 6EK0

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:

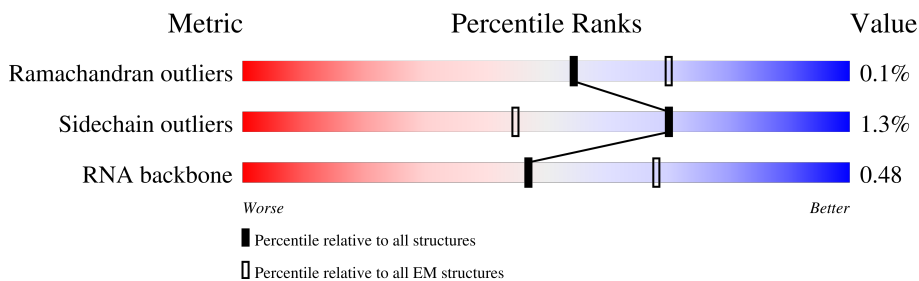
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 2.90 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.



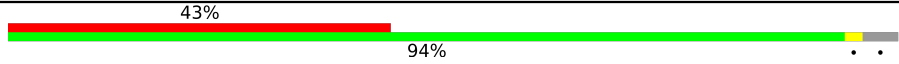
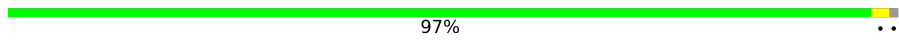
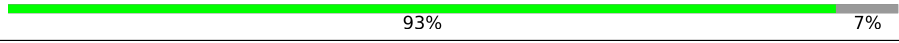

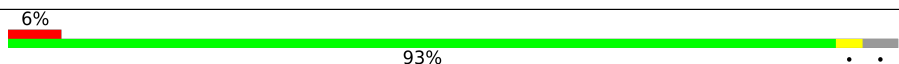
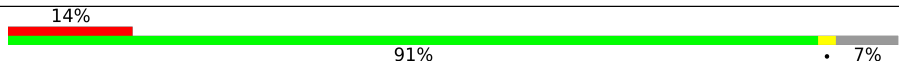
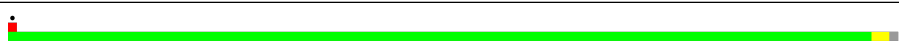
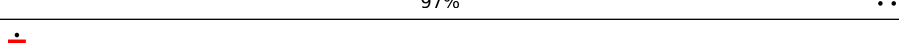


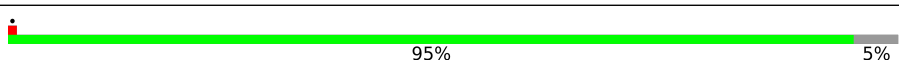
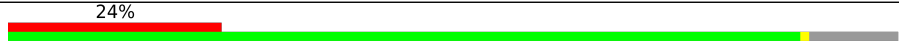
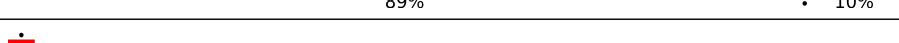
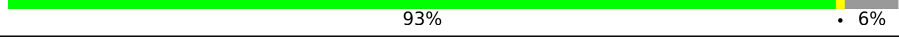



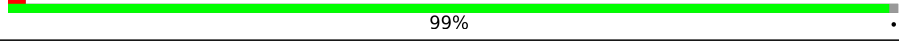
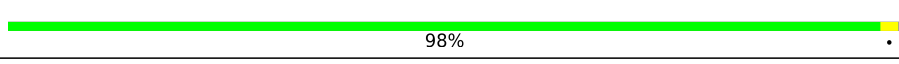
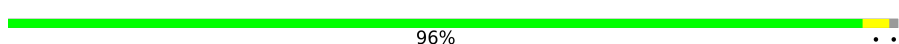
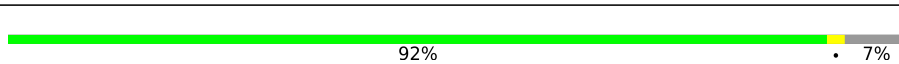

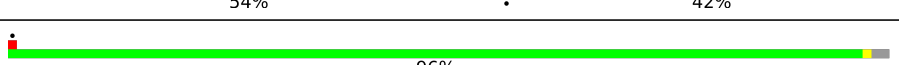
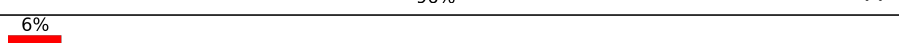

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	2	1869	
2	A	295	
3	B	264	
4	C	293	
5	D	243	
6	E	263	
7	F	204	
8	G	249	

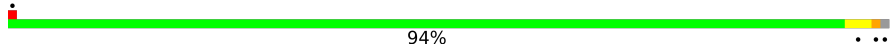

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Mol	Chain	Length	Quality of chain
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	a	115	
22	U	119	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	Z	125	
28	b	84	
29	c	69	
30	d	56	
31	e	59	
32	f	156	
33	g	317	

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Mol	Chain	Length	Quality of chain
34	T	145	 94%
35	h	568	 21% 39% 61%

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 76226 atoms, of which 0 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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1683	35903	16038	6448	11742	1675	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	216	1705	1083	299	315	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	213	1729	1098	309	308	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	218	1690	1094	289	297	10	0	0

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	225	1752	1117	315	313	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	262	2076	1324	386	358	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	189	1495	934	284	270	7	0	0

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	230	1862	1164	371	320	7	0	0

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	186	1501	957	276	267	1	0	0

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	205	1682	1056	331	290	5	0	0

- Molecule 11 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	180	1499	955	300	242	2	0	0

- Molecule 12 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	95	800	522	142	131	5	0	0

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	151	1229	782	230	211	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	123	Total	C	N	O	S	0	0
			954	598	169	178	9		

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 18 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 19 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	122	Total	C	N	O	S	0	0
			992	622	184	183	3		

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 21 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	102	Total	C	N	O	S	1	0
			829	517	174	133	5		

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 24 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 27 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 28 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 29 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 30 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 31 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	56	Total	C	N	O	S	0	0
			442	273	96	72	1		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	63	Total	C	N	O	S	0	0
			510	320	97	86	7		

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 34 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 35 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
35	h	222	1775	1114	315	329	1	16	0	0

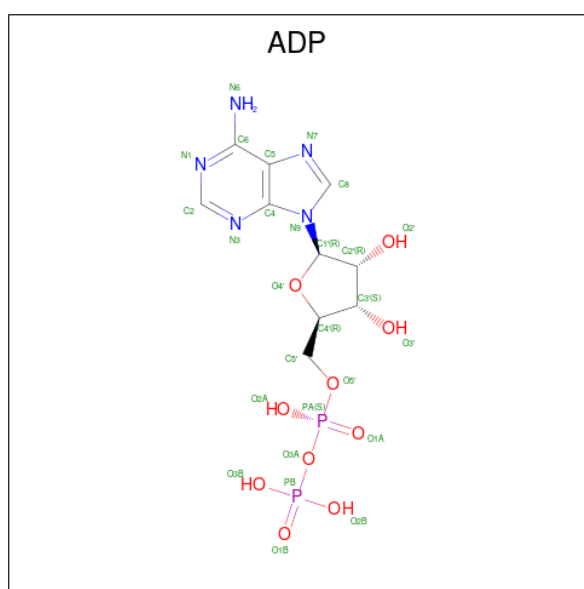
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	2	Total	Mg	0
			2	2	
36	h	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	a	1	Total	Zn	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	h	1	27	10	5	10	2	0

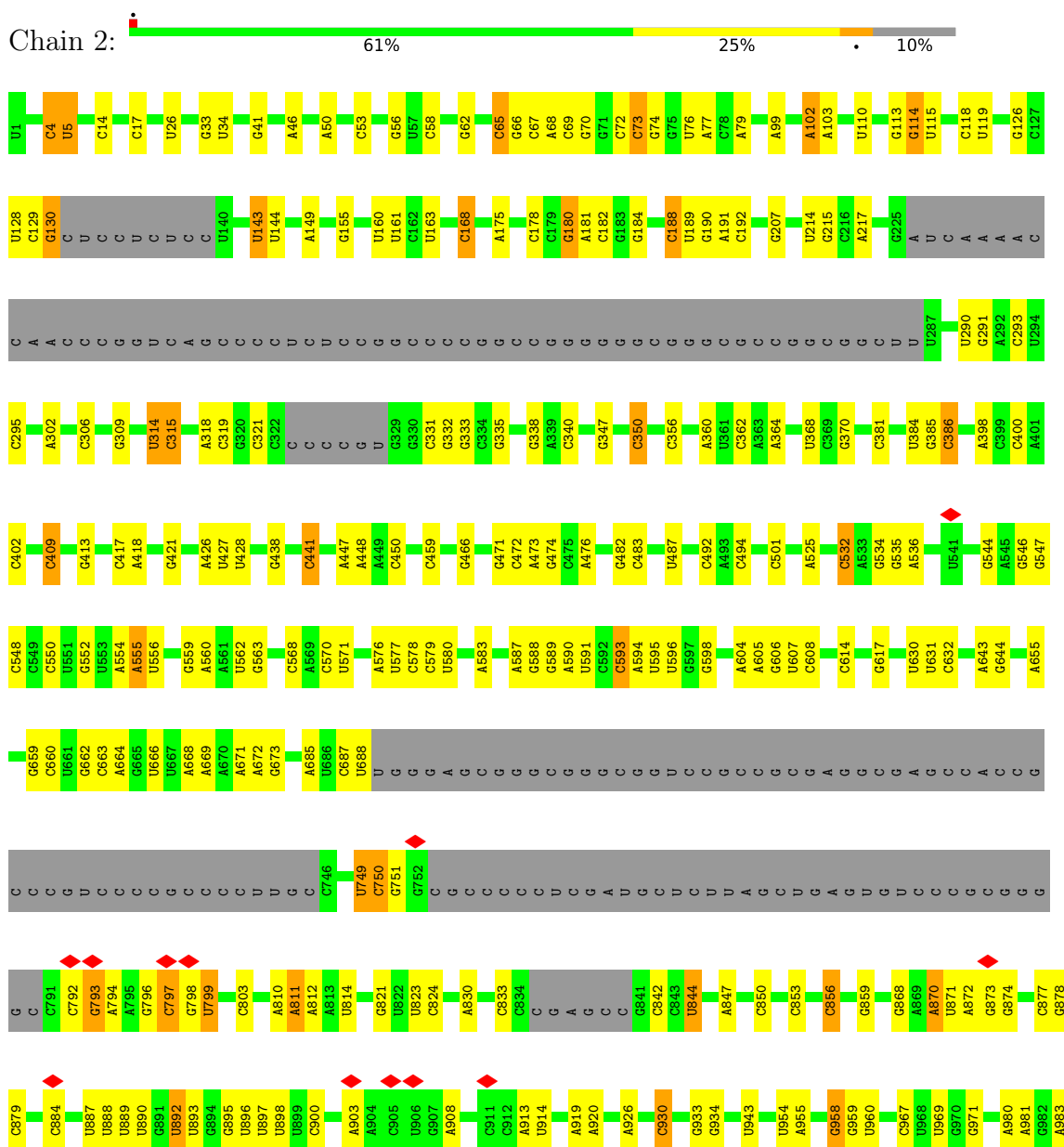
- Molecule 39 is water.

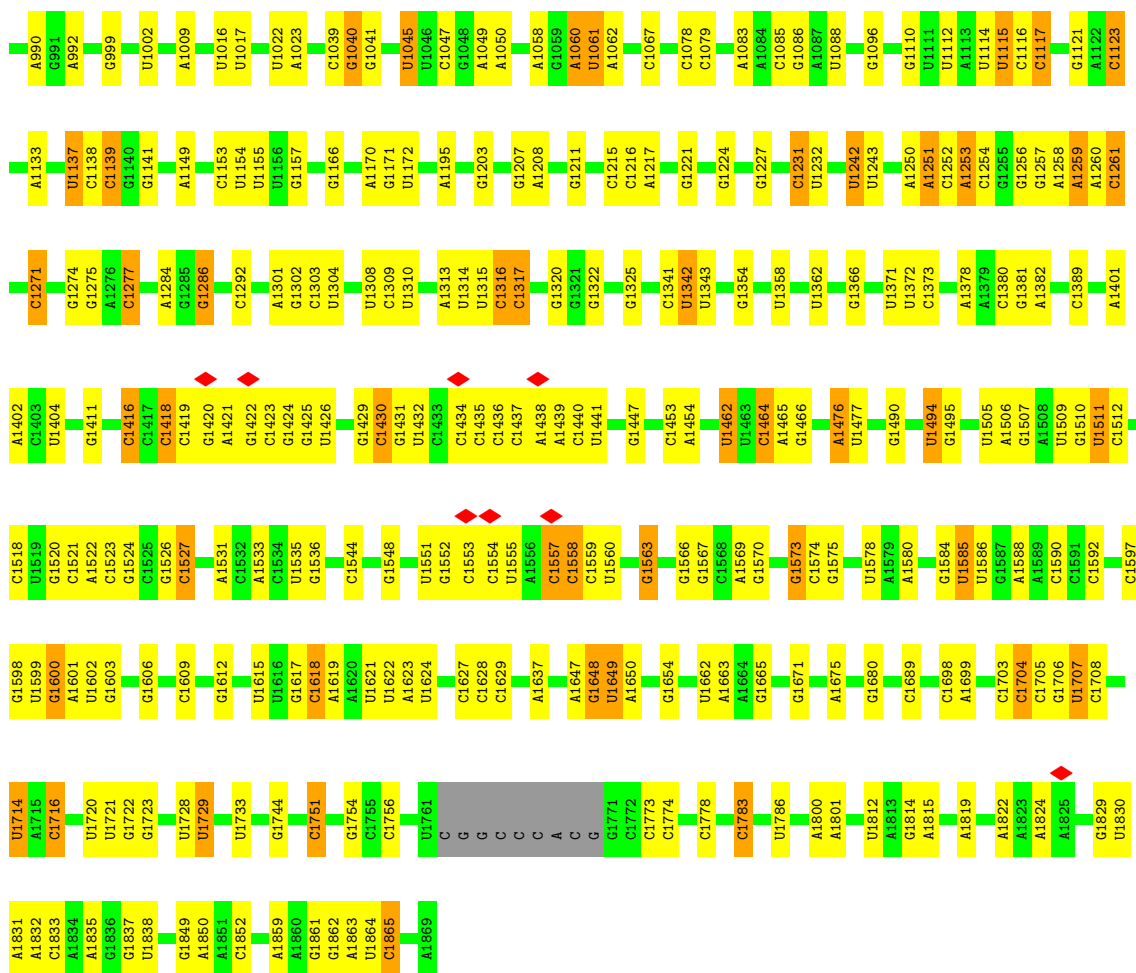
Mol	Chain	Residues	Atoms		AltConf
39	h	3	Total	O	0
			3	3	

3 Residue-property plots

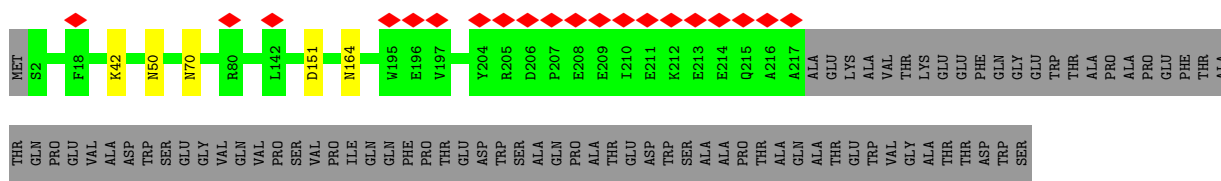
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S ribosomal RNA

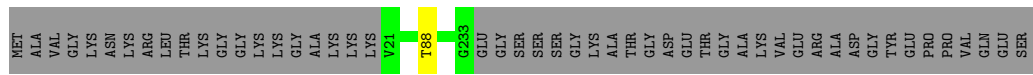
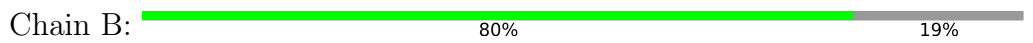




• Molecule 2: 40S ribosomal protein SA

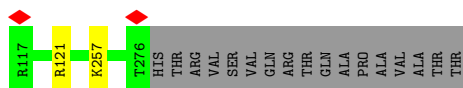
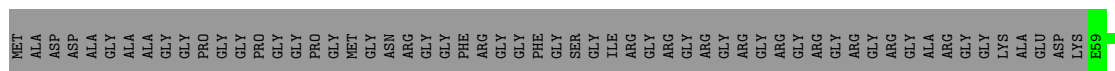


• Molecule 3: 40S ribosomal protein S3a

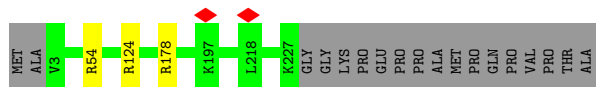
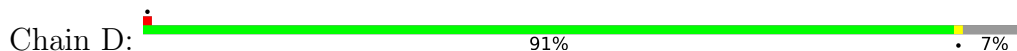


• Molecule 4: 40S ribosomal protein S2

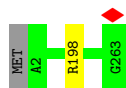




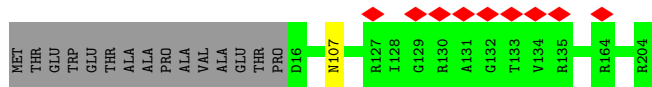
• Molecule 5: 40S ribosomal protein S3



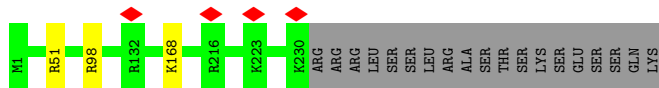
• Molecule 6: 40S ribosomal protein S4, X isoform



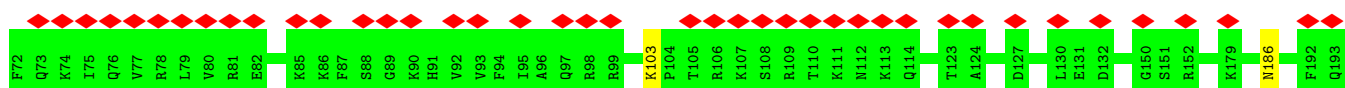
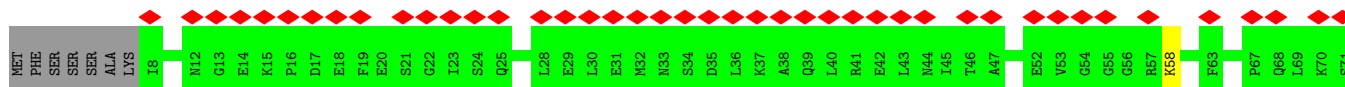
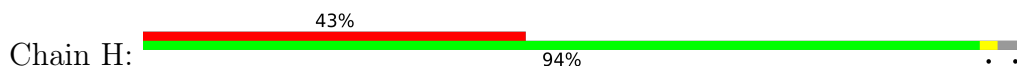
• Molecule 7: 40S ribosomal protein S5



• Molecule 8: 40S ribosomal protein S6



• Molecule 9: 40S ribosomal protein S7



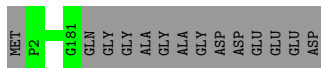
- Molecule 10: 40S ribosomal protein S8

Chain I:  97%



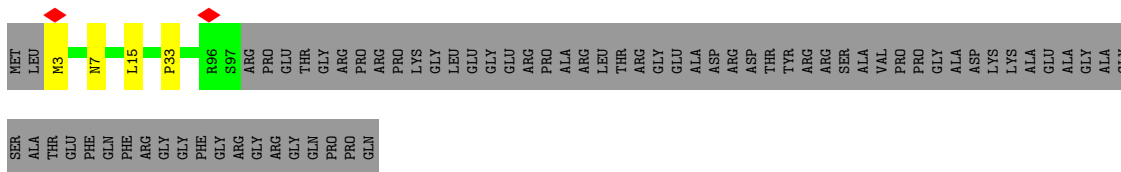
- Molecule 11: 40S ribosomal protein S9

Chain J:  93%



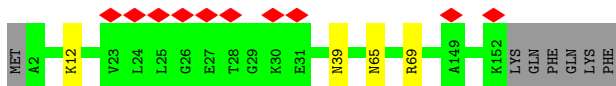
- Molecule 12: 40S ribosomal protein S10

Chain K:  55%



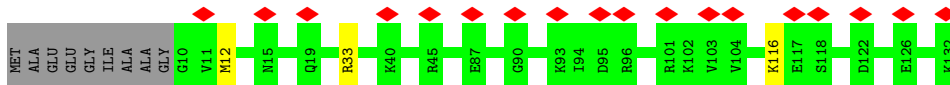
- Molecule 13: 40S ribosomal protein S11

Chain L:  6%



- Molecule 14: 40S ribosomal protein S12

Chain M:  14%




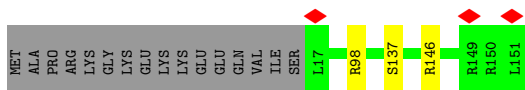
- Molecule 15: 40S ribosomal protein S13

Chain N:  97%

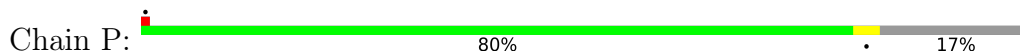


- Molecule 16: 40S ribosomal protein S14

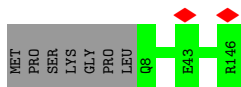
Chain O:  87%



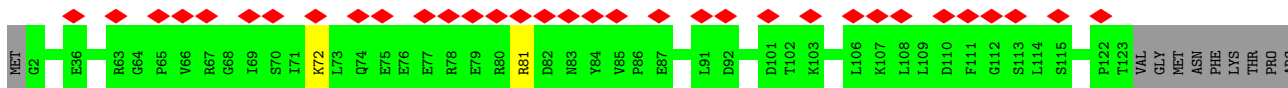
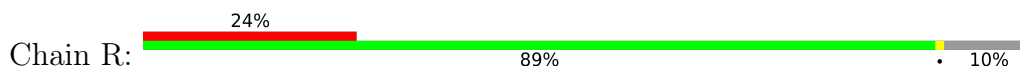
• Molecule 17: 40S ribosomal protein S15



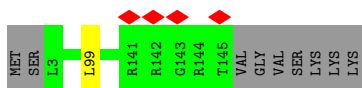
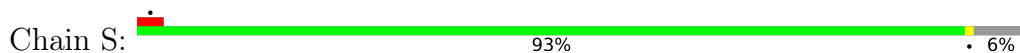
• Molecule 18: 40S ribosomal protein S16



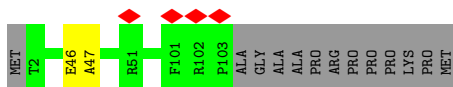
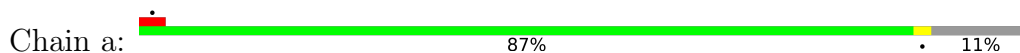
• Molecule 19: 40S ribosomal protein S17



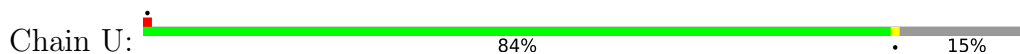
• Molecule 20: 40S ribosomal protein S18

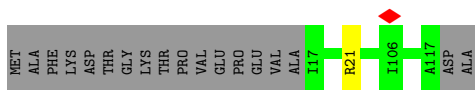


• Molecule 21: 40S ribosomal protein S26

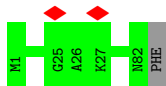


• Molecule 22: 40S ribosomal protein S20

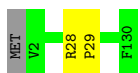




• Molecule 23: 40S ribosomal protein S21



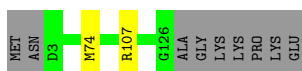
• Molecule 24: 40S ribosomal protein S15a



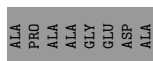
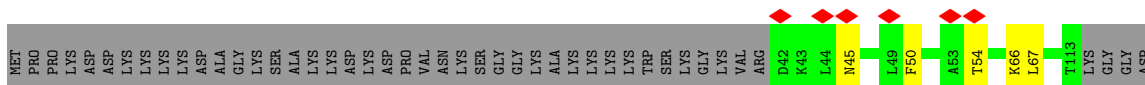
• Molecule 25: 40S ribosomal protein S23



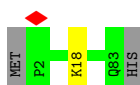
• Molecule 26: 40S ribosomal protein S24



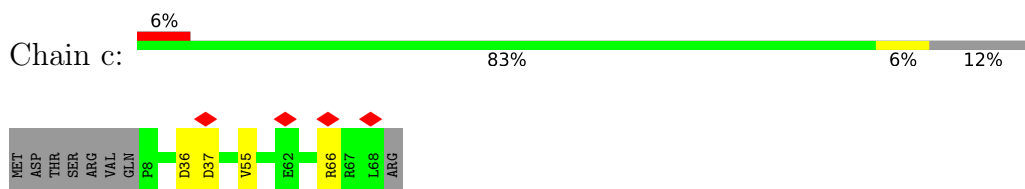
• Molecule 27: 40S ribosomal protein S25



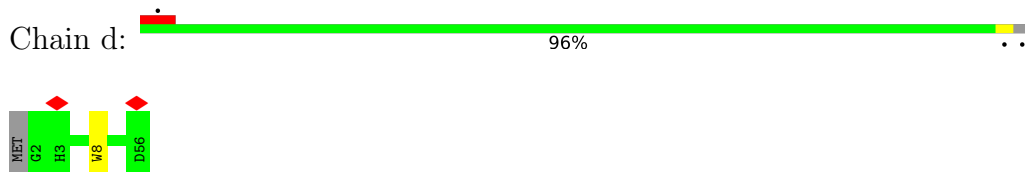
• Molecule 28: 40S ribosomal protein S27



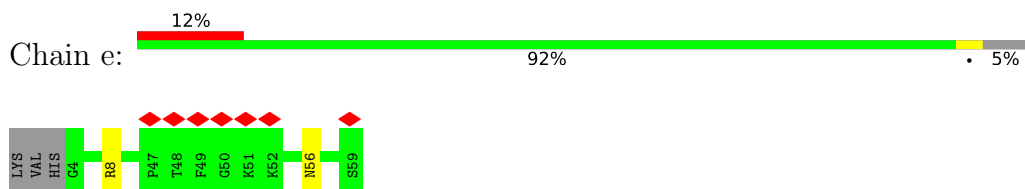
- Molecule 29: 40S ribosomal protein S28



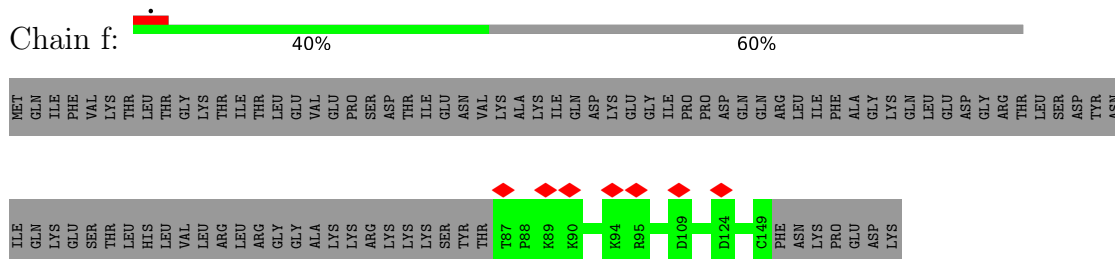
- Molecule 30: 40S ribosomal protein S29



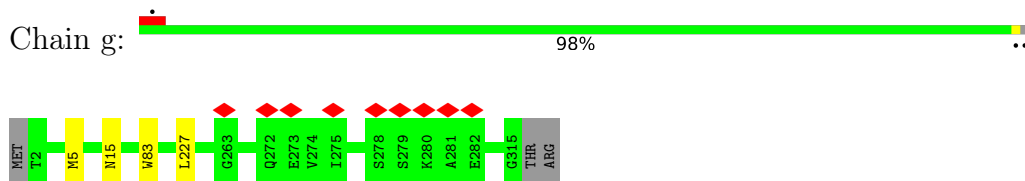
- Molecule 31: 40S ribosomal protein S30



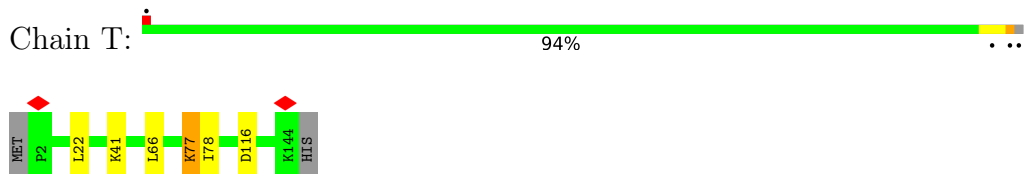
- Molecule 32: Ubiquitin-40S ribosomal protein S27a



- Molecule 33: Receptor of activated protein C kinase 1



- Molecule 34: 40S ribosomal protein S19



- Molecule 35: Serine/threonine-protein kinase RIO1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	276012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0045	Depositor
Map size (\AA)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 6MZ, PHD, ADP, UR3

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	2	0.80	0/40100	1.19	356/62500 (0.6%)
2	A	0.32	0/1742	0.59	1/2367 (0.0%)
3	B	0.41	0/1756	0.58	0/2350
4	C	0.38	0/1726	0.54	0/2332
5	D	0.37	0/1780	0.55	0/2397
6	E	0.43	0/2118	0.57	0/2849
7	F	0.43	0/1516	0.58	0/2037
8	G	0.38	0/1885	0.56	0/2510
9	H	0.28	0/1524	0.50	0/2042
10	I	0.41	0/1711	0.56	0/2282
11	J	0.44	0/1524	0.57	0/2035
12	K	0.42	0/824	0.60	1/1112 (0.1%)
13	L	0.47	0/1250	0.58	0/1673
14	M	0.32	0/964	0.57	0/1291
15	N	0.36	0/1226	0.53	0/1649
16	O	0.39	0/1023	0.62	0/1372
17	P	0.50	0/1003	0.60	0/1341
18	Q	0.47	0/1126	0.64	0/1506
19	R	0.31	0/1004	0.49	0/1348
20	S	0.44	0/1202	0.61	0/1610
21	a	0.42	0/847	0.62	1/1135 (0.1%)
22	U	0.39	0/813	0.59	0/1092
23	V	0.33	0/631	0.53	0/844
24	W	0.44	0/1051	0.60	0/1406
25	X	0.46	0/1116	0.60	0/1490
26	Y	0.42	0/1031	0.56	0/1370
27	Z	0.40	0/580	0.69	0/780
28	b	0.35	0/653	0.51	0/876
29	c	0.36	0/481	0.74	2/643 (0.3%)
30	d	0.47	0/470	0.59	0/623
31	e	0.38	0/447	0.53	0/587
32	f	0.32	0/520	0.51	0/690

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.37	0/2497	0.61	0/3399
34	T	0.47	0/1131	0.80	1/1515 (0.1%)
35	h	0.28	0/1794	0.55	0/2415
All	All	0.63	0/81066	0.95	362/117468 (0.3%)

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
12	K	0	2
14	M	0	2
16	O	0	1
20	S	0	1
24	W	0	1
27	Z	0	3
34	T	0	3
All	All	0	13

There are no bond length outliers.

All (362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	C2-N1-C1'	14.46	134.71	118.80
1	2	501	C	N1-C2-O2	14.32	127.49	118.90
1	2	1557	C	N1-C2-O2	14.28	127.47	118.90
1	2	293	C	N1-C2-O2	12.34	126.30	118.90
1	2	356	C	N1-C2-O2	12.31	126.28	118.90
1	2	356	C	C2-N1-C1'	11.59	131.55	118.80
1	2	799	U	C2-N1-C1'	10.99	130.89	117.70
1	2	501	C	N3-C2-O2	-10.98	114.21	121.90
1	2	799	U	N1-C2-O2	10.96	130.47	122.80
1	2	1115	U	C2-N1-C1'	10.95	130.84	117.70
1	2	1751	C	N1-C2-O2	10.95	125.47	118.90
1	2	1115	U	N1-C2-O2	10.94	130.46	122.80
1	2	501	C	C6-N1-C1'	-10.83	107.80	120.80
1	2	799	U	N3-C2-O2	-10.77	114.66	122.20
1	2	1416	C	C6-N1-C2	-10.59	116.06	120.30
1	2	1115	U	N3-C2-O2	-10.37	114.94	122.20
1	2	1557	C	N3-C2-O2	-10.27	114.71	121.90
1	2	293	C	C2-N1-C1'	10.27	130.10	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1453	C	C2-N1-C1'	10.27	130.10	118.80
1	2	1453	C	N1-C2-O2	9.99	124.89	118.90
1	2	1117	C	N1-C2-O2	9.84	124.80	118.90
2	A	151	ASP	CB-CG-OD1	9.77	127.09	118.30
1	2	1016	U	N3-C2-O2	-9.74	115.38	122.20
1	2	293	C	N3-C2-O2	-9.71	115.10	121.90
1	2	1016	U	N1-C2-O2	9.41	129.39	122.80
1	2	853	C	N1-C2-O2	9.31	124.48	118.90
1	2	1751	C	C2-N1-C1'	9.29	129.02	118.80
1	2	853	C	C2-N1-C1'	9.24	128.97	118.80
1	2	1315	U	N1-C2-O2	9.22	129.25	122.80
1	2	356	C	N3-C2-O2	-9.18	115.47	121.90
1	2	1520	G	C4-N9-C1'	9.16	138.41	126.50
1	2	1139	C	C2-N1-C1'	9.12	128.84	118.80
1	2	1139	C	N1-C2-O2	9.09	124.36	118.90
1	2	853	C	N3-C2-O2	-9.04	115.58	121.90
1	2	1751	C	N3-C2-O2	-8.94	115.64	121.90
1	2	1016	U	C2-N1-C1'	8.89	128.37	117.70
1	2	1624	U	N3-C2-O2	-8.81	116.03	122.20
1	2	356	C	C6-N1-C1'	-8.71	110.34	120.80
1	2	1315	U	N3-C2-O2	-8.70	116.11	122.20
29	c	37	ASP	CB-CG-OD1	8.69	126.12	118.30
1	2	1261	C	N3-C2-O2	-8.61	115.87	121.90
1	2	1618	C	N1-C2-O2	8.61	124.06	118.90
1	2	823	U	N3-C2-O2	-8.59	116.19	122.20
1	2	1139	C	N3-C2-O2	-8.49	115.95	121.90
1	2	1557	C	C6-N1-C2	-8.48	116.91	120.30
1	2	1416	C	N1-C2-O2	8.44	123.97	118.90
1	2	427	U	N3-C2-O2	-8.38	116.33	122.20
1	2	73	C	N1-C2-O2	8.32	123.89	118.90
1	2	1716	C	C2-N1-C1'	8.30	127.93	118.80
1	2	76	U	N1-C2-O2	8.24	128.56	122.80
1	2	1315	U	C2-N1-C1'	8.22	127.56	117.70
1	2	1520	G	C8-N9-C1'	-8.21	116.33	127.00
1	2	1117	C	N3-C2-O2	-8.19	116.17	121.90
1	2	532	C	C2-N1-C1'	8.14	127.75	118.80
1	2	1557	C	C5-C6-N1	8.13	125.07	121.00
1	2	427	U	N1-C2-O2	8.07	128.45	122.80
1	2	76	U	N3-C2-O2	-8.06	116.56	122.20
1	2	1292	C	N1-C2-O2	8.00	123.70	118.90
1	2	1416	C	N3-C2-O2	-7.97	116.32	121.90
1	2	1624	U	N1-C2-O2	7.92	128.35	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	441	C	C2-N1-C1'	7.91	127.50	118.80
1	2	427	U	C2-N1-C1'	7.85	127.12	117.70
1	2	1453	C	C6-N1-C1'	-7.85	111.38	120.80
1	2	1624	U	C2-N1-C1'	7.83	127.10	117.70
1	2	321	C	N1-C2-O2	7.80	123.58	118.90
1	2	76	U	C2-N1-C1'	7.76	127.02	117.70
1	2	1416	C	C5-C6-N1	7.75	124.88	121.00
1	2	1117	C	C2-N1-C1'	7.74	127.31	118.80
34	T	22	LEU	CA-CB-CG	7.73	133.08	115.30
1	2	1115	U	C5-C6-N1	7.69	126.54	122.70
1	2	630	U	C2-N1-C1'	7.65	126.89	117.70
1	2	1662	U	N1-C2-O2	7.64	128.15	122.80
1	2	1592	C	N3-C2-O2	-7.62	116.57	121.90
1	2	65	C	C6-N1-C2	-7.61	117.26	120.30
1	2	1662	U	N3-C2-O2	-7.60	116.88	122.20
1	2	1261	C	N1-C2-O2	7.50	123.40	118.90
1	2	417	C	N1-C2-O2	7.48	123.39	118.90
1	2	73	C	N3-C2-O2	-7.46	116.68	121.90
1	2	630	U	N1-C2-O2	7.46	128.02	122.80
1	2	1123	C	N1-C2-O2	7.45	123.37	118.90
1	2	293	C	C6-N1-C1'	-7.42	111.89	120.80
1	2	1751	C	C6-N1-C2	-7.27	117.39	120.30
1	2	1662	U	C2-N1-C1'	7.25	126.41	117.70
1	2	409	C	C6-N1-C2	-7.21	117.42	120.30
1	2	814	U	N3-C2-O2	-7.20	117.16	122.20
1	2	178	C	N1-C2-O2	7.19	123.22	118.90
1	2	1520	G	N3-C4-N9	7.17	130.30	126.00
1	2	1592	C	N1-C2-O2	7.13	123.17	118.90
1	2	1061	U	N1-C2-O2	7.09	127.76	122.80
1	2	1629	C	C5-C6-N1	7.06	124.53	121.00
1	2	119	U	N3-C2-O2	-7.04	117.27	122.20
1	2	1061	U	C2-N1-C1'	7.04	126.15	117.70
1	2	501	C	C6-N1-C2	-7.03	117.49	120.30
1	2	130	G	C4-N9-C1'	7.03	135.64	126.50
1	2	1310	U	N1-C2-O2	7.00	127.70	122.80
1	2	799	U	C6-N1-C1'	-6.97	111.44	121.20
1	2	1649	U	C5-C6-N1	6.97	126.18	122.70
1	2	1430	C	P-O3'-C3'	6.95	128.04	119.70
1	2	119	U	N1-C2-O2	6.95	127.66	122.80
1	2	630	U	N3-C2-O2	-6.95	117.34	122.20
1	2	1558	C	C2-N1-C1'	6.93	126.43	118.80
1	2	1520	G	C6-C5-N7	-6.92	126.25	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1756	C	C2-N1-C1'	6.89	126.38	118.80
1	2	1774	C	N3-C2-O2	-6.88	117.08	121.90
1	2	1618	C	N3-C2-O2	-6.88	117.09	121.90
1	2	314	U	N3-C2-O2	-6.87	117.39	122.20
1	2	1462	U	C2-N1-C1'	6.85	125.92	117.70
1	2	1453	C	N3-C2-O2	-6.84	117.11	121.90
1	2	1060	A	P-O3'-C3'	6.82	127.89	119.70
1	2	792	C	C5-C6-N1	6.79	124.39	121.00
1	2	130	G	N3-C4-N9	6.78	130.07	126.00
1	2	1115	U	C6-N1-C1'	-6.72	111.79	121.20
1	2	188	C	C2-N1-C1'	6.71	126.17	118.80
1	2	1139	C	C6-N1-C2	-6.67	117.63	120.30
1	2	76	U	C5-C6-N1	6.65	126.03	122.70
1	2	1271	C	N1-C2-O2	6.64	122.89	118.90
1	2	1464	C	P-O3'-C3'	6.64	127.67	119.70
1	2	417	C	C2-N1-C1'	6.64	126.10	118.80
1	2	1865	C	C6-N1-C2	-6.63	117.65	120.30
1	2	593	C	N1-C2-O2	6.62	122.87	118.90
1	2	1316	C	P-O3'-C3'	6.61	127.63	119.70
1	2	1292	C	N3-C2-O2	-6.59	117.29	121.90
1	2	168	C	N1-C2-O2	6.59	122.85	118.90
1	2	1703	C	C6-N1-C2	-6.59	117.67	120.30
1	2	1649	U	C6-N1-C2	-6.57	117.06	121.00
1	2	814	U	N1-C2-O2	6.51	127.35	122.80
1	2	853	C	C6-N1-C2	-6.50	117.70	120.30
1	2	1123	C	N3-C2-O2	-6.50	117.35	121.90
1	2	1618	C	C2-N1-C1'	6.49	125.94	118.80
1	2	1689	C	C2-N1-C1'	6.48	125.93	118.80
1	2	1558	C	C6-N1-C2	-6.43	117.73	120.30
1	2	1592	C	C2-N1-C1'	6.43	125.87	118.80
1	2	532	C	N1-C2-O2	6.42	122.75	118.90
1	2	441	C	C6-N1-C2	-6.42	117.73	120.30
1	2	1123	C	C2-N1-C1'	6.42	125.86	118.80
1	2	1314	U	C2-N1-C1'	6.41	125.39	117.70
1	2	178	C	N3-C2-O2	-6.40	117.42	121.90
1	2	1061	U	N3-C2-O2	-6.38	117.74	122.20
1	2	1117	C	C6-N1-C2	-6.37	117.75	120.30
1	2	1261	C	C6-N1-C2	-6.35	117.76	120.30
1	2	1629	C	C2-N1-C1'	6.34	125.78	118.80
1	2	749	U	C2-N1-C1'	6.34	125.31	117.70
1	2	1649	U	N3-C2-O2	-6.32	117.78	122.20
1	2	321	C	C2-N1-C1'	6.31	125.74	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	823	U	C2-N1-C1'	6.30	125.26	117.70
1	2	1310	U	C2-N1-C1'	6.28	125.23	117.70
1	2	1778	C	N1-C2-O2	6.27	122.66	118.90
1	2	130	G	N3-C4-C5	-6.26	125.47	128.60
1	2	321	C	N3-C2-O2	-6.26	117.52	121.90
1	2	1310	U	N3-C2-O2	-6.25	117.82	122.20
1	2	659	G	C4-N9-C1'	6.24	134.61	126.50
1	2	1494	U	P-O3'-C3'	6.24	127.18	119.70
1	2	853	C	C6-N1-C1'	-6.23	113.33	120.80
1	2	1389	C	C2-N1-C1'	6.22	125.64	118.80
1	2	168	C	N3-C2-O2	-6.18	117.57	121.90
1	2	1253	A	P-O3'-C3'	6.17	127.10	119.70
1	2	1707	U	N1-C2-O2	6.17	127.12	122.80
1	2	130	G	C8-N9-C1'	-6.16	118.99	127.00
1	2	386	C	N1-C2-O2	6.16	122.59	118.90
1	2	749	U	C5-C6-N1	6.15	125.78	122.70
1	2	579	C	N1-C2-O2	6.15	122.59	118.90
1	2	143	U	P-O3'-C3'	6.15	127.08	119.70
1	2	441	C	C5-C6-N1	6.14	124.07	121.00
1	2	1419	C	C6-N1-C2	-6.14	117.84	120.30
1	2	792	C	C6-N1-C2	-6.14	117.84	120.30
1	2	1259	A	C2-N3-C4	6.13	113.67	110.60
1	2	577	U	N3-C2-O2	-6.13	117.91	122.20
1	2	501	C	C5-C6-N1	6.12	124.06	121.00
1	2	1778	C	N3-C2-O2	-6.12	117.62	121.90
1	2	114	G	P-O3'-C3'	6.11	127.03	119.70
1	2	1139	C	C6-N1-C1'	-6.11	113.47	120.80
1	2	5	U	N3-C2-O2	-6.08	117.95	122.20
1	2	1115	U	C6-N1-C2	-6.06	117.36	121.00
1	2	1153	C	N1-C2-O2	6.06	122.53	118.90
1	2	1751	C	C6-N1-C1'	-6.05	113.54	120.80
1	2	1557	C	C2-N3-C4	6.05	122.92	119.90
1	2	870	A	P-O3'-C3'	6.02	126.92	119.70
1	2	1453	C	C5-C6-N1	5.99	123.99	121.00
1	2	1648	G	P-O3'-C3'	5.98	126.87	119.70
1	2	570	C	N1-C2-O2	5.96	122.48	118.90
1	2	1751	C	C5-C6-N1	5.93	123.97	121.00
1	2	1112	U	N1-C2-O2	5.92	126.95	122.80
1	2	1304	U	N1-C2-O2	5.92	126.95	122.80
1	2	1418	C	C2-N1-C1'	5.91	125.30	118.80
1	2	532	C	C6-N1-C2	-5.90	117.94	120.30
1	2	750	C	C5-C6-N1	5.89	123.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	73	C	C6-N1-C2	-5.89	117.94	120.30
1	2	350	C	N1-C2-O2	5.89	122.44	118.90
1	2	887	U	C2-N1-C1'	5.89	124.76	117.70
1	2	1716	C	C6-N1-C1'	-5.88	113.75	120.80
1	2	1342	U	P-O3'-C3'	5.87	126.74	119.70
1	2	1716	C	C5-C6-N1	5.85	123.92	121.00
1	2	799	U	C5-C6-N1	5.84	125.62	122.70
1	2	1418	C	N1-C2-O2	5.83	122.40	118.90
1	2	70	G	N3-C4-N9	-5.82	122.51	126.00
1	2	409	C	C5-C6-N1	5.82	123.91	121.00
1	2	1123	C	C6-N1-C2	-5.82	117.97	120.30
1	2	1615	U	N1-C2-O2	5.82	126.87	122.80
21	a	46	GLU	CA-CB-CG	5.80	126.17	113.40
1	2	76	U	C6-N1-C2	-5.80	117.52	121.00
1	2	570	C	N3-C2-O2	-5.80	117.84	121.90
1	2	1865	C	C2-N1-C1'	5.80	125.18	118.80
1	2	1585	U	C2-N1-C1'	5.79	124.65	117.70
1	2	580	U	N1-C2-O2	5.78	126.84	122.80
1	2	532	C	C5-C6-N1	5.78	123.89	121.00
1	2	1039	C	C2-N1-C1'	5.77	125.15	118.80
1	2	750	C	N1-C2-O2	5.77	122.36	118.90
1	2	803	C	C2-N1-C1'	5.77	125.15	118.80
1	2	402	C	C5-C6-N1	5.77	123.89	121.00
1	2	1716	C	N1-C2-O2	5.76	122.36	118.90
1	2	178	C	C2-N1-C1'	5.76	125.14	118.80
1	2	930	C	C6-N1-C2	-5.76	118.00	120.30
1	2	823	U	N1-C2-O2	5.75	126.83	122.80
1	2	1704	C	N1-C2-O2	5.75	122.35	118.90
1	2	34	U	N3-C2-O2	-5.75	118.18	122.20
1	2	1304	U	N3-C2-O2	-5.73	118.19	122.20
1	2	293	C	C6-N1-C2	-5.72	118.01	120.30
1	2	102	A	P-O3'-C3'	5.72	126.56	119.70
1	2	930	C	N1-C2-O2	5.72	122.33	118.90
1	2	580	U	N3-C2-O2	-5.71	118.20	122.20
1	2	1783	C	N1-C2-O2	5.71	122.32	118.90
1	2	850	C	N1-C2-O2	5.70	122.32	118.90
1	2	824	C	N1-C2-O2	5.69	122.31	118.90
1	2	1728	U	N1-C2-O2	5.69	126.78	122.80
1	2	1045	U	N1-C2-O2	5.67	126.77	122.80
1	2	1649	U	P-O3'-C3'	5.67	126.50	119.70
1	2	578	C	N1-C2-O2	5.66	122.30	118.90
1	2	356	C	C6-N1-C2	-5.66	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	65	C	C5-C6-N1	5.66	123.83	121.00
1	2	1040	G	N3-C4-N9	5.65	129.39	126.00
1	2	1251	A	P-O3'-C3'	5.65	126.48	119.70
1	2	1277	C	C2-N1-C1'	5.65	125.01	118.80
1	2	53	C	C6-N1-C2	-5.63	118.05	120.30
1	2	1557	C	C4-C5-C6	-5.63	114.58	117.40
1	2	1714	U	C5-C6-N1	5.62	125.51	122.70
1	2	1728	U	N3-C2-O2	-5.61	118.27	122.20
1	2	1615	U	N3-C2-O2	-5.60	118.28	122.20
1	2	1389	C	C6-N1-C2	-5.58	118.07	120.30
1	2	1573	G	P-O3'-C3'	5.58	126.39	119.70
1	2	571	U	N3-C2-O2	-5.56	118.31	122.20
1	2	1242	U	C2-N1-C1'	5.56	124.37	117.70
1	2	799	U	C6-N1-C2	-5.56	117.66	121.00
1	2	532	C	C6-N1-C1'	-5.55	114.14	120.80
1	2	1629	C	C6-N1-C2	-5.55	118.08	120.30
1	2	356	C	C5-C6-N1	5.55	123.77	121.00
1	2	793	G	P-O3'-C3'	5.54	126.35	119.70
1	2	1304	U	C2-N1-C1'	5.54	124.35	117.70
1	2	70	G	N3-C2-N2	-5.52	116.04	119.90
1	2	314	U	P-O3'-C3'	5.52	126.32	119.70
1	2	178	C	C6-N1-C2	-5.52	118.09	120.30
1	2	1286	G	N3-C4-N9	5.51	129.31	126.00
1	2	1600	G	C4-N9-C1'	5.51	133.67	126.50
1	2	1153	C	N3-C2-O2	-5.51	118.04	121.90
1	2	190	G	O4'-C1'-N9	5.50	112.60	108.20
1	2	1137	U	P-O3'-C3'	5.50	126.30	119.70
1	2	1418	C	C6-N1-C2	-5.49	118.11	120.30
1	2	1476	A	P-O3'-C3'	5.49	126.29	119.70
1	2	1729	U	N1-C2-O2	5.48	126.64	122.80
1	2	892	U	C2-N1-C1'	5.47	124.26	117.70
1	2	1597	C	N1-C2-O2	5.47	122.18	118.90
1	2	1045	U	N3-C2-O2	-5.47	118.37	122.20
1	2	1558	C	C5-C6-N1	5.46	123.73	121.00
1	2	577	U	N1-C2-O2	5.46	126.62	122.80
1	2	417	C	C5-C6-N1	5.45	123.72	121.00
1	2	180	G	P-O3'-C3'	5.45	126.23	119.70
1	2	1520	G	C4-C5-N7	5.44	112.97	110.80
1	2	368	U	N3-C2-O2	-5.43	118.40	122.20
1	2	1563	G	C4-N9-C1'	5.42	133.55	126.50
1	2	1172	U	N1-C2-O2	5.42	126.59	122.80
1	2	441	C	N1-C2-O2	5.42	122.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1689	C	N1-C2-O2	5.41	122.15	118.90
1	2	368	U	C2-N1-C1'	5.41	124.19	117.70
1	2	1708	C	N1-C2-O2	5.40	122.14	118.90
1	2	1708	C	N3-C2-O2	-5.40	118.12	121.90
12	K	15	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	2	593	C	N3-C2-O2	-5.37	118.14	121.90
1	2	1259	A	C4-N9-C1'	5.37	135.97	126.30
1	2	811	A	P-O3'-C3'	5.36	126.13	119.70
1	2	402	C	C6-N1-C2	-5.36	118.16	120.30
1	2	1527	C	N1-C2-O2	5.35	122.11	118.90
1	2	315	C	C2-N1-C1'	5.34	124.68	118.80
1	2	1172	U	N3-C2-O2	-5.34	118.46	122.20
1	2	844	U	N3-C2-O2	-5.34	118.46	122.20
1	2	1520	G	N3-C4-C5	-5.34	125.93	128.60
1	2	459	C	C2-N1-C1'	5.34	124.67	118.80
1	2	1315	U	C6-N1-C1'	-5.32	113.75	121.20
1	2	856	C	C6-N1-C2	-5.32	118.17	120.30
1	2	1016	U	C6-N1-C1'	-5.31	113.76	121.20
1	2	632	C	C2-N1-C1'	5.31	124.64	118.80
1	2	1600	G	N3-C4-C5	-5.31	125.94	128.60
1	2	1618	C	C6-N1-C2	-5.28	118.19	120.30
1	2	1704	C	C2-N1-C1'	5.28	124.61	118.80
1	2	887	U	N1-C2-O2	5.28	126.50	122.80
1	2	350	C	N3-C2-O2	-5.28	118.20	121.90
1	2	659	G	C8-N9-C1'	-5.28	120.14	127.00
1	2	1733	U	N3-C2-O2	-5.28	118.51	122.20
1	2	1261	C	C2-N1-C1'	5.27	124.60	118.80
1	2	1603	G	N1-C6-O6	5.27	123.06	119.90
1	2	750	C	C6-N1-C2	-5.25	118.20	120.30
1	2	824	C	N3-C2-O2	-5.25	118.23	121.90
1	2	417	C	N3-C2-O2	-5.25	118.23	121.90
1	2	494	C	N1-C2-O2	5.24	122.05	118.90
1	2	1016	U	C6-N1-C2	-5.24	117.86	121.00
1	2	1058	A	O4'-C1'-N9	5.23	112.38	108.20
1	2	1511	U	P-O3'-C3'	5.22	125.97	119.70
1	2	4	C	C2-N1-C1'	5.22	124.54	118.80
1	2	1462	U	N1-C2-O2	5.22	126.46	122.80
1	2	1016	U	C5-C6-N1	5.22	125.31	122.70
1	2	494	C	C6-N1-C2	-5.21	118.22	120.30
1	2	1756	C	C6-N1-C2	-5.21	118.22	120.30
1	2	1271	C	N3-C2-O2	-5.21	118.25	121.90
1	2	1585	U	N3-C2-O2	-5.21	118.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	427	U	C6-N1-C1'	-5.20	113.92	121.20
1	2	1600	G	N3-C4-N9	5.20	129.12	126.00
1	2	1716	C	C6-N1-C2	-5.20	118.22	120.30
1	2	666	U	C2-N1-C1'	5.19	123.92	117.70
1	2	578	C	N3-C2-O2	-5.19	118.27	121.90
1	2	1362	U	N3-C2-O2	-5.18	118.57	122.20
1	2	441	C	C6-N1-C1'	-5.18	114.58	120.80
1	2	340	C	N1-C2-O2	5.17	122.00	118.90
1	2	1047	C	C6-N1-C2	-5.17	118.23	120.30
1	2	814	U	C2-N1-C1'	5.17	123.90	117.70
1	2	1585	U	N1-C2-O2	5.16	126.41	122.80
1	2	1865	C	N3-C2-O2	-5.16	118.29	121.90
1	2	1411	G	N3-C4-N9	5.16	129.09	126.00
1	2	630	U	C6-N1-C1'	-5.15	113.99	121.20
1	2	749	U	N1-C2-O2	5.15	126.41	122.80
1	2	1648	G	OP2-P-O3'	5.14	116.51	105.20
1	2	494	C	N3-C2-O2	-5.13	118.31	121.90
1	2	1416	C	C2-N1-C1'	5.12	124.44	118.80
1	2	1689	C	C6-N1-C2	-5.12	118.25	120.30
1	2	118	C	N1-C2-O2	5.12	121.97	118.90
1	2	750	C	P-O3'-C3'	5.12	125.85	119.70
1	2	1662	U	C6-N1-C1'	-5.12	114.04	121.20
1	2	823	U	C6-N1-C2	-5.12	117.93	121.00
1	2	555	A	OP2-P-O3'	5.11	116.45	105.20
1	2	958	G	P-O3'-C3'	5.11	125.83	119.70
1	2	930	C	C2-N1-C1'	5.11	124.42	118.80
1	2	555	A	P-O3'-C3'	5.11	125.83	119.70
1	2	1314	U	C6-N1-C1'	-5.11	114.05	121.20
1	2	168	C	C6-N1-C2	-5.10	118.26	120.30
1	2	842	C	C6-N1-C2	-5.10	118.26	120.30
1	2	189	U	C2-N1-C1'	5.09	123.81	117.70
1	2	1389	C	N1-C2-O2	5.09	121.95	118.90
1	2	1242	U	N1-C2-O2	5.09	126.36	122.80
1	2	1317	C	C5-C6-N1	5.08	123.54	121.00
1	2	1649	U	N1-C2-O2	5.08	126.36	122.80
1	2	331	C	N1-C2-O2	5.08	121.95	118.90
1	2	1494	U	OP2-P-O3'	5.08	116.38	105.20
1	2	797	C	C2-N1-C1'	5.08	124.39	118.80
1	2	1292	C	C2-N1-C1'	5.05	124.36	118.80
29	c	36	ASP	C-N-CA	5.05	134.33	121.70
1	2	1597	C	N3-C2-O2	-5.05	118.37	121.90
1	2	1705	C	N1-C2-O2	5.04	121.93	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1231	C	C6-N1-C2	-5.04	118.28	120.30
1	2	1703	C	N3-C2-O2	-5.04	118.37	121.90
1	2	1117	C	C6-N1-C1'	-5.04	114.76	120.80
1	2	293	C	C5-C6-N1	5.03	123.52	121.00
1	2	1022	U	C2-N1-C1'	5.03	123.74	117.70
1	2	188	C	C6-N1-C2	-5.02	118.29	120.30
1	2	118	C	C6-N1-C2	-5.01	118.30	120.30
1	2	189	U	N1-C2-O2	5.01	126.30	122.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	K	3	MET	Peptide
12	K	33	PRO	Peptide
14	M	116	LYS	Peptide
14	M	12	MET	Peptide
16	O	137	SER	Peptide
20	S	99	LEU	Peptide
34	T	116	ASP	Peptide
34	T	41	LYS	Peptide
34	T	77	LYS	Peptide
24	W	28	ARG	Peptide
27	Z	54	THR	Peptide
27	Z	66	LYS	Peptide
27	Z	67	LEU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
2	A	214/295 (72%)	203 (95%)	11 (5%)	0	100	100
3	B	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
4	C	216/293 (74%)	207 (96%)	9 (4%)	0	100	100
5	D	223/243 (92%)	213 (96%)	10 (4%)	0	100	100
6	E	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
7	F	187/204 (92%)	173 (92%)	14 (8%)	0	100	100
8	G	228/249 (92%)	218 (96%)	10 (4%)	0	100	100
9	H	184/194 (95%)	177 (96%)	7 (4%)	0	100	100
10	I	203/208 (98%)	192 (95%)	11 (5%)	0	100	100
11	J	178/194 (92%)	170 (96%)	8 (4%)	0	100	100
12	K	93/165 (56%)	87 (94%)	6 (6%)	0	100	100
13	L	149/158 (94%)	144 (97%)	5 (3%)	0	100	100
14	M	121/132 (92%)	116 (96%)	5 (4%)	0	100	100
15	N	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
16	O	133/151 (88%)	123 (92%)	10 (8%)	0	100	100
17	P	118/145 (81%)	114 (97%)	4 (3%)	0	100	100
18	Q	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
19	R	120/135 (89%)	113 (94%)	7 (6%)	0	100	100
20	S	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
21	a	101/115 (88%)	90 (89%)	10 (10%)	1 (1%)	15	45
22	U	99/119 (83%)	92 (93%)	7 (7%)	0	100	100
23	V	80/83 (96%)	80 (100%)	0	0	100	100
24	W	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	19	51
25	X	139/143 (97%)	134 (96%)	3 (2%)	2 (1%)	11	36
26	Y	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
27	Z	70/125 (56%)	61 (87%)	9 (13%)	0	100	100
28	b	80/84 (95%)	70 (88%)	10 (12%)	0	100	100
29	c	59/69 (86%)	56 (95%)	3 (5%)	0	100	100
30	d	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
31	e	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
32	f	61/156 (39%)	54 (88%)	7 (12%)	0	100	100
33	g	312/317 (98%)	277 (89%)	35 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	T	141/145 (97%)	125 (89%)	14 (10%)	2 (1%)	11	36
35	h	217/568 (38%)	195 (90%)	22 (10%)	0	100	100
All	All	4978/6044 (82%)	4685 (94%)	287 (6%)	6 (0%)	54	82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	W	29	PRO
34	T	78	ILE
34	T	77	LYS
25	X	87	ASN
21	a	47	ALA
25	X	86	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	
2	A	180/243 (74%)	176 (98%)	4 (2%)	52	81
3	B	194/231 (84%)	193 (100%)	1 (0%)	88	96
4	C	184/225 (82%)	182 (99%)	2 (1%)	73	92
5	D	189/202 (94%)	186 (98%)	3 (2%)	62	86
6	E	224/225 (100%)	223 (100%)	1 (0%)	91	97
7	F	159/170 (94%)	158 (99%)	1 (1%)	86	96
8	G	200/218 (92%)	197 (98%)	3 (2%)	65	87
9	H	167/174 (96%)	164 (98%)	3 (2%)	59	85
10	I	178/180 (99%)	174 (98%)	4 (2%)	52	81
11	J	160/168 (95%)	160 (100%)	0	100	100
12	K	86/136 (63%)	85 (99%)	1 (1%)	71	91
13	L	135/142 (95%)	131 (97%)	4 (3%)	41	75
14	M	104/108 (96%)	103 (99%)	1 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	N	130/131 (99%)	127 (98%)	3 (2%)	50	80
16	O	105/119 (88%)	103 (98%)	2 (2%)	57	84
17	P	107/130 (82%)	103 (96%)	4 (4%)	34	68
18	Q	115/121 (95%)	115 (100%)	0	100	100
19	R	111/122 (91%)	109 (98%)	2 (2%)	59	85
20	S	124/132 (94%)	124 (100%)	0	100	100
21	a	90/98 (92%)	90 (100%)	0	100	100
22	U	93/107 (87%)	92 (99%)	1 (1%)	73	92
23	V	66/67 (98%)	66 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	113/115 (98%)	111 (98%)	2 (2%)	59	85
26	Y	108/115 (94%)	106 (98%)	2 (2%)	57	84
27	Z	64/103 (62%)	62 (97%)	2 (3%)	40	74
28	b	74/76 (97%)	73 (99%)	1 (1%)	67	89
29	c	54/62 (87%)	52 (96%)	2 (4%)	34	68
30	d	48/49 (98%)	47 (98%)	1 (2%)	53	81
31	e	45/48 (94%)	43 (96%)	2 (4%)	28	61
32	f	56/140 (40%)	56 (100%)	0	100	100
33	g	272/275 (99%)	268 (98%)	4 (2%)	65	87
34	T	113/115 (98%)	112 (99%)	1 (1%)	78	93
35	h	191/511 (37%)	190 (100%)	1 (0%)	88	96
All	All	4351/5171 (84%)	4293 (99%)	58 (1%)	70	90

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	42	LYS
2	A	50	ASN
2	A	70	ASN
2	A	164	ASN
3	B	88	THR
4	C	121	ARG
4	C	257	LYS
5	D	54	ARG
5	D	124	ARG

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Mol	Chain	Res	Type
5	D	178	ARG
6	E	198	ARG
7	F	107	ASN
8	G	51	ARG
8	G	98	ARG
8	G	168	LYS
9	H	58	LYS
9	H	103	LYS
9	H	186	ASN
10	I	47	ARG
10	I	84	ASN
10	I	110	ARG
10	I	140	LYS
12	K	7	ASN
13	L	12	LYS
13	L	39	ASN
13	L	65	ASN
13	L	69	ARG
14	M	33	ARG
15	N	27	LYS
15	N	39	LYS
15	N	121	ARG
16	O	98	ARG
16	O	146	ARG
17	P	37	TYR
17	P	61	ARG
17	P	111	MET
17	P	127	LYS
19	R	72	LYS
19	R	81	ARG
22	U	21	ARG
25	X	105	PHE
25	X	142	ARG
26	Y	74	MET
26	Y	107	ARG
27	Z	45	ASN
27	Z	50	PHE
28	b	18	LYS
29	c	55	VAL
29	c	66	ARG
30	d	8	TRP
31	e	8	ARG

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Mol	Chain	Res	Type
31	e	56	ASN
33	g	5	MET
33	g	15	ASN
33	g	83	TRP
33	g	227	LEU
34	T	66	LEU
35	h	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	50	ASN
2	A	70	ASN
2	A	113	GLN
2	A	164	ASN
3	B	40	ASN
3	B	186	ASN
3	B	232	HIS
4	C	272	HIS
5	D	145	GLN
6	E	8	HIS
6	E	188	ASN
6	E	201	HIS
7	F	107	ASN
7	F	110	GLN
7	F	114	ASN
7	F	137	GLN
8	G	59	GLN
8	G	81	HIS
9	H	73	GLN
9	H	186	ASN
10	I	84	ASN
10	I	181	GLN
11	J	132	GLN
11	J	140	GLN
12	K	7	ASN
13	L	11	GLN
13	L	39	ASN
13	L	65	ASN
13	L	83	GLN
14	M	72	HIS
15	N	105	ASN

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Mol	Chain	Res	Type
17	P	103	ASN
18	Q	48	GLN
20	S	134	GLN
22	U	81	GLN
25	X	20	GLN
27	Z	45	ASN
27	Z	103	HIS
29	c	29	GLN
30	d	3	HIS
30	d	26	ASN
30	d	45	GLN
31	e	44	ASN
31	e	56	ASN
32	f	139	HIS
33	g	15	ASN
33	g	76	GLN
33	g	133	ASN
33	g	272	GLN
34	T	63	HIS
35	h	193	ASN
35	h	196	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1674/1869 (89%)	444 (26%)	36 (2%)

All (444) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	C
1	2	5	U
1	2	14	C
1	2	17	C
1	2	26	U
1	2	33	G
1	2	41	G
1	2	46	A
1	2	50	A
1	2	56	G
1	2	58	C

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Mol	Chain	Res	Type
1	2	62	G
1	2	65	C
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	72	C
1	2	73	C
1	2	74	G
1	2	77	A
1	2	79	A
1	2	99	A
1	2	103	A
1	2	110	U
1	2	113	G
1	2	115	U
1	2	126	G
1	2	128	U
1	2	129	C
1	2	130	G
1	2	143	U
1	2	144	U
1	2	149	A
1	2	155	G
1	2	160	U
1	2	161	U
1	2	163	U
1	2	168	C
1	2	175	A
1	2	181	A
1	2	182	C
1	2	184	G
1	2	188	C
1	2	191	A
1	2	192	C
1	2	207	G
1	2	214	U
1	2	215	G
1	2	217	A
1	2	290	U
1	2	291	G
1	2	295	C

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Mol	Chain	Res	Type
1	2	302	A
1	2	306	C
1	2	309	G
1	2	315	C
1	2	318	A
1	2	319	C
1	2	332	G
1	2	333	G
1	2	335	G
1	2	338	G
1	2	347	G
1	2	350	C
1	2	360	A
1	2	362	C
1	2	364	A
1	2	370	G
1	2	381	C
1	2	384	U
1	2	385	G
1	2	386	C
1	2	398	A
1	2	400	C
1	2	409	C
1	2	413	G
1	2	418	A
1	2	421	G
1	2	426	A
1	2	428	U
1	2	438	G
1	2	441	C
1	2	447	A
1	2	448	A
1	2	450	C
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	483	C
1	2	487	U

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Mol	Chain	Res	Type
1	2	492	C
1	2	525	A
1	2	532	C
1	2	534	G
1	2	535	G
1	2	536	A
1	2	544	G
1	2	546	G
1	2	547	G
1	2	548	C
1	2	550	C
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	562	U
1	2	563	G
1	2	568	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	594	A
1	2	595	U
1	2	596	U
1	2	598	G
1	2	604	A
1	2	605	A
1	2	606	G
1	2	607	U
1	2	608	C
1	2	614	C
1	2	617	G
1	2	631	U
1	2	643	A
1	2	644	G

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Mol	Chain	Res	Type
1	2	655	A
1	2	660	C
1	2	662	G
1	2	663	C
1	2	664	A
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	685	A
1	2	687	C
1	2	688	U
1	2	749	U
1	2	750	C
1	2	751	G
1	2	794	A
1	2	796	G
1	2	797	C
1	2	798	G
1	2	799	U
1	2	810	A
1	2	811	A
1	2	812	A
1	2	821	G
1	2	830	A
1	2	833	C
1	2	844	U
1	2	847	A
1	2	856	C
1	2	859	G
1	2	868	G
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	877	C
1	2	878	G
1	2	879	C
1	2	884	C
1	2	888	U

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Mol	Chain	Res	Type
1	2	889	U
1	2	890	U
1	2	892	U
1	2	893	U
1	2	895	G
1	2	896	U
1	2	897	U
1	2	898	U
1	2	900	C
1	2	903	A
1	2	908	A
1	2	913	A
1	2	914	U
1	2	919	A
1	2	920	A
1	2	926	A
1	2	930	C
1	2	933	G
1	2	934	G
1	2	943	U
1	2	954	U
1	2	955	A
1	2	959	G
1	2	960	U
1	2	967	C
1	2	969	U
1	2	971	G
1	2	981	A
1	2	983	A
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1002	U
1	2	1009	A
1	2	1017	U
1	2	1023	A
1	2	1040	G
1	2	1041	G
1	2	1045	U
1	2	1049	A
1	2	1050	A
1	2	1060	A

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Mol	Chain	Res	Type
1	2	1061	U
1	2	1062	A
1	2	1067	C
1	2	1078	C
1	2	1079	C
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1088	U
1	2	1096	G
1	2	1110	G
1	2	1114	U
1	2	1115	U
1	2	1116	C
1	2	1117	C
1	2	1121	G
1	2	1123	C
1	2	1133	A
1	2	1137	U
1	2	1138	C
1	2	1139	C
1	2	1141	G
1	2	1149	A
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1166	G
1	2	1170	A
1	2	1171	G
1	2	1195	A
1	2	1203	G
1	2	1207	G
1	2	1208	A
1	2	1211	G
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1242	U

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Mol	Chain	Res	Type
1	2	1243	U
1	2	1250	A
1	2	1251	A
1	2	1252	C
1	2	1253	A
1	2	1254	C
1	2	1256	G
1	2	1257	G
1	2	1258	A
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1271	C
1	2	1274	G
1	2	1275	G
1	2	1277	C
1	2	1284	A
1	2	1286	G
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1317	C
1	2	1320	G
1	2	1322	G
1	2	1325	G
1	2	1341	C
1	2	1343	U
1	2	1354	G
1	2	1358	U
1	2	1366	G
1	2	1371	U
1	2	1372	U
1	2	1373	C
1	2	1378	A
1	2	1380	C
1	2	1381	G
1	2	1382	A
1	2	1401	A
1	2	1402	A

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Mol	Chain	Res	Type
1	2	1404	U
1	2	1416	C
1	2	1418	C
1	2	1420	G
1	2	1421	A
1	2	1422	G
1	2	1423	C
1	2	1424	G
1	2	1426	U
1	2	1429	G
1	2	1430	C
1	2	1431	G
1	2	1432	U
1	2	1434	C
1	2	1435	C
1	2	1436	C
1	2	1437	C
1	2	1438	A
1	2	1439	A
1	2	1440	C
1	2	1441	U
1	2	1447	G
1	2	1454	A
1	2	1462	U
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1477	U
1	2	1490	G
1	2	1494	U
1	2	1495	G
1	2	1505	U
1	2	1506	A
1	2	1507	G
1	2	1509	U
1	2	1510	G
1	2	1512	C
1	2	1518	C
1	2	1521	C
1	2	1522	A
1	2	1523	C
1	2	1524	G

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Mol	Chain	Res	Type
1	2	1526	G
1	2	1527	C
1	2	1531	A
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1544	C
1	2	1548	G
1	2	1552	G
1	2	1553	C
1	2	1554	C
1	2	1555	U
1	2	1557	C
1	2	1558	C
1	2	1559	C
1	2	1560	U
1	2	1563	G
1	2	1566	G
1	2	1567	G
1	2	1569	A
1	2	1570	G
1	2	1574	C
1	2	1575	G
1	2	1578	U
1	2	1580	A
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1588	A
1	2	1590	C
1	2	1598	G
1	2	1599	U
1	2	1601	A
1	2	1602	U
1	2	1606	G
1	2	1609	C
1	2	1612	G
1	2	1617	G
1	2	1618	C
1	2	1619	A
1	2	1621	U
1	2	1622	U

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Mol	Chain	Res	Type
1	2	1623	A
1	2	1627	C
1	2	1628	C
1	2	1637	A
1	2	1647	A
1	2	1648	G
1	2	1649	U
1	2	1650	A
1	2	1654	G
1	2	1663	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1680	G
1	2	1698	C
1	2	1699	A
1	2	1704	C
1	2	1706	G
1	2	1707	U
1	2	1714	U
1	2	1716	C
1	2	1720	U
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1729	U
1	2	1744	G
1	2	1751	C
1	2	1754	G
1	2	1773	C
1	2	1783	C
1	2	1786	U
1	2	1800	A
1	2	1801	A
1	2	1812	U
1	2	1814	G
1	2	1815	A
1	2	1819	A
1	2	1822	A
1	2	1824	A
1	2	1829	G
1	2	1831	A

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Mol	Chain	Res	Type
1	2	1833	C
1	2	1835	A
1	2	1837	G
1	2	1838	U
1	2	1849	G
1	2	1850	A
1	2	1852	C
1	2	1859	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	65	C
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	314	U
1	2	332	G
1	2	472	C
1	2	554	A
1	2	555	A
1	2	594	A
1	2	750	C
1	2	793	G
1	2	811	A
1	2	870	A
1	2	958	G
1	2	980	A
1	2	1060	A
1	2	1137	U
1	2	1231	C
1	2	1251	A
1	2	1253	A
1	2	1316	C
1	2	1342	U
1	2	1425	G

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Mol	Chain	Res	Type
1	2	1430	C
1	2	1440	C
1	2	1464	C
1	2	1476	A
1	2	1494	U
1	2	1511	U
1	2	1551	U
1	2	1573	G
1	2	1600	G
1	2	1648	G
1	2	1649	U

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

3 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$
1	6MZ	2	1832	1	18,25,26	2.12	2 (11%)	16,36,39	2.58	3 (18%)
1	UR3	2	1830	1	19,22,23	2.80	6 (31%)	26,32,35	1.48	3 (11%)
35	PHD	h	341	36,35	9,11,12	1.65	1 (11%)	10,15,17	1.59	1 (10%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	2	1832	1	-	2/5/27/28	0/3/3/3
1	UR3	2	1830	1	-	2/7/25/26	0/2/2/2
35	PHD	h	341	36,35	-	1/8/11/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1830	UR3	C2-N1	7.86	1.49	1.38
1	2	1832	6MZ	C6-N6	7.66	1.47	1.35
1	2	1830	UR3	C6-C5	5.78	1.48	1.35
1	2	1830	UR3	C2-N3	4.69	1.48	1.39
35	h	341	PHD	P-OD1	4.07	1.65	1.59
1	2	1830	UR3	C6-N1	3.50	1.46	1.38
1	2	1832	6MZ	C5-C4	-2.75	1.33	1.40
1	2	1830	UR3	C5-C4	2.64	1.50	1.43
1	2	1830	UR3	C4-N3	2.26	1.45	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1832	6MZ	C2-N1-C6	7.16	122.73	116.59
1	2	1832	6MZ	N3-C2-N1	-6.55	118.44	128.68
1	2	1830	UR3	C4-N3-C2	-4.33	120.49	124.56
1	2	1830	UR3	C1'-N1-C2	3.74	123.31	116.99
35	h	341	PHD	OD1-CG-CB	3.33	120.27	111.11
1	2	1832	6MZ	C9-N6-C6	2.45	124.98	122.87
1	2	1830	UR3	C6-N1-C2	-2.44	119.60	121.79

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1830	UR3	O4'-C1'-N1-C2
1	2	1832	6MZ	N1-C6-N6-C9
1	2	1830	UR3	O4'-C1'-N1-C6
1	2	1832	6MZ	C5-C6-N6-C9
35	h	341	PHD	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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
38	ADP	h	601	36	24,29,29	3.17	8 (33%)	29,45,45	3.01	6 (20%)

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
38	ADP	h	601	36	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	h	601	ADP	C3'-C4'	-8.95	1.30	1.53
38	h	601	ADP	O4'-C1'	-7.45	1.30	1.41
38	h	601	ADP	O4'-C4'	7.42	1.61	1.45
38	h	601	ADP	C6-N6	3.08	1.45	1.34
38	h	601	ADP	O2'-C2'	-2.94	1.36	1.43
38	h	601	ADP	C5-C4	-2.78	1.33	1.40
38	h	601	ADP	O3'-C3'	2.77	1.49	1.43
38	h	601	ADP	C2-N3	2.19	1.35	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	h	601	ADP	C5-C6-N6	10.52	136.34	120.35
38	h	601	ADP	N6-C6-N1	-7.28	103.47	118.57
38	h	601	ADP	N3-C2-N1	-5.84	119.55	128.68
38	h	601	ADP	C1'-N9-C4	-5.49	117.00	126.64
38	h	601	ADP	C3'-C2'-C1'	3.29	105.93	100.98
38	h	601	ADP	PA-O3A-PB	-2.85	123.05	132.83

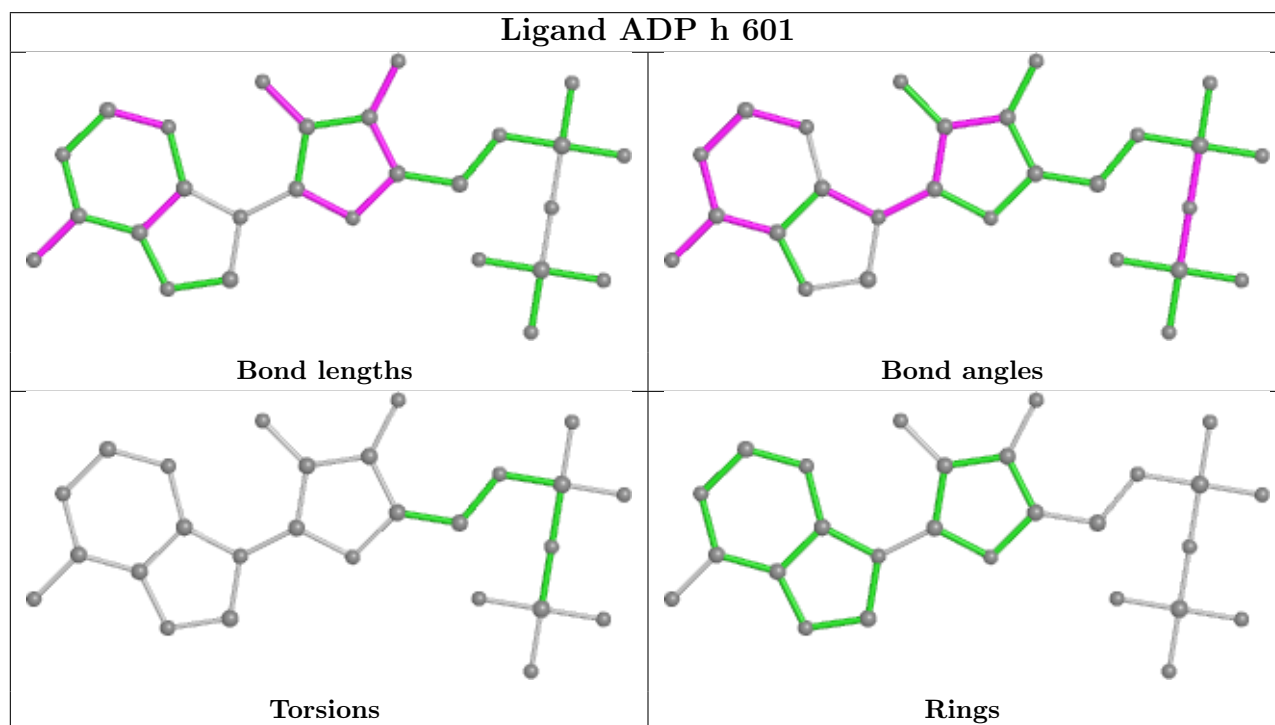
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [\(i\)](#)

There are no chain breaks in this entry.

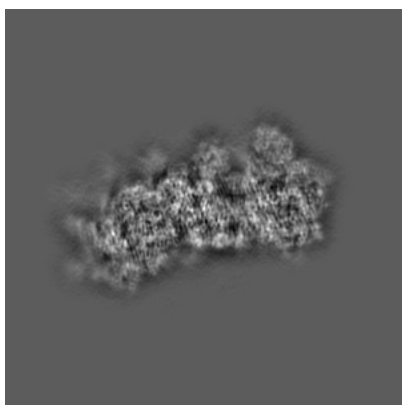
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11441. These allow visual inspection of the internal detail of the map and identification of artifacts.

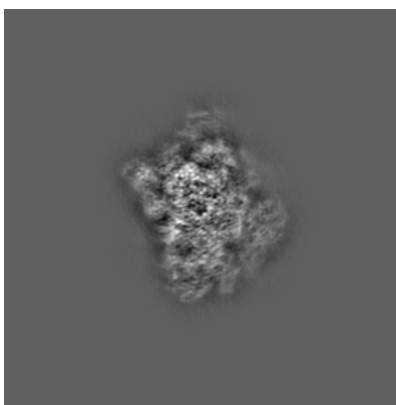
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

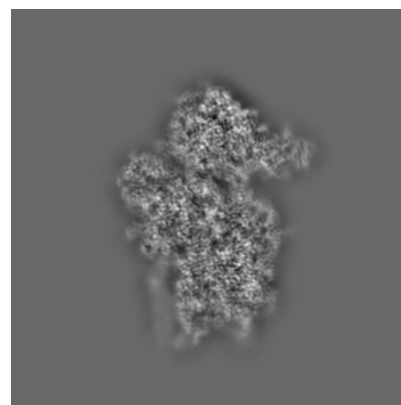
6.1.1 Primary map



X



Y

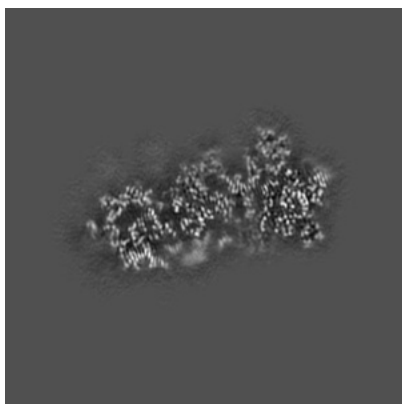


Z

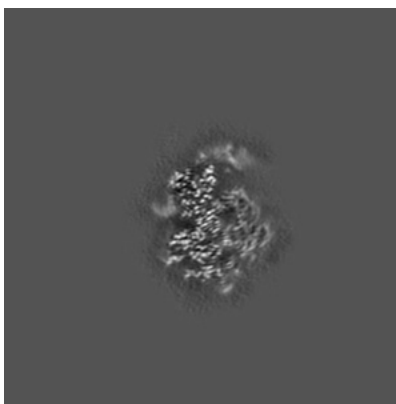
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

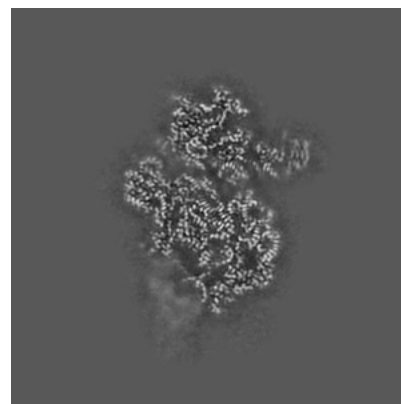
6.2.1 Primary map



X Index: 192



Y Index: 192

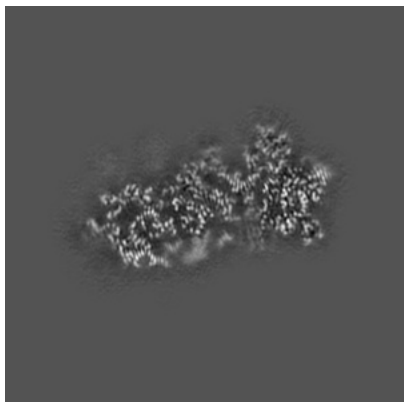


Z Index: 192

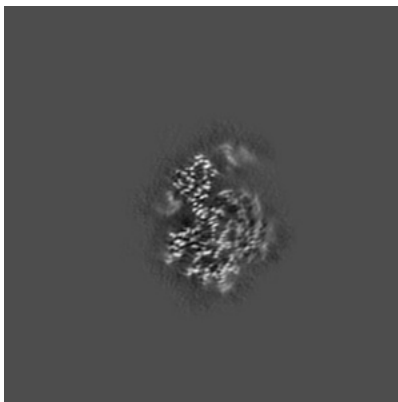
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

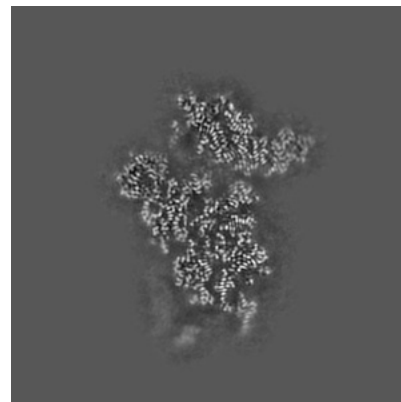
6.3.1 Primary map



X Index: 191



Y Index: 195

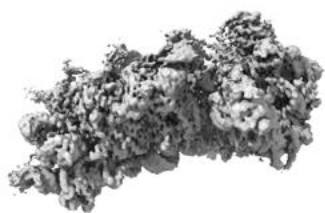


Z Index: 181

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

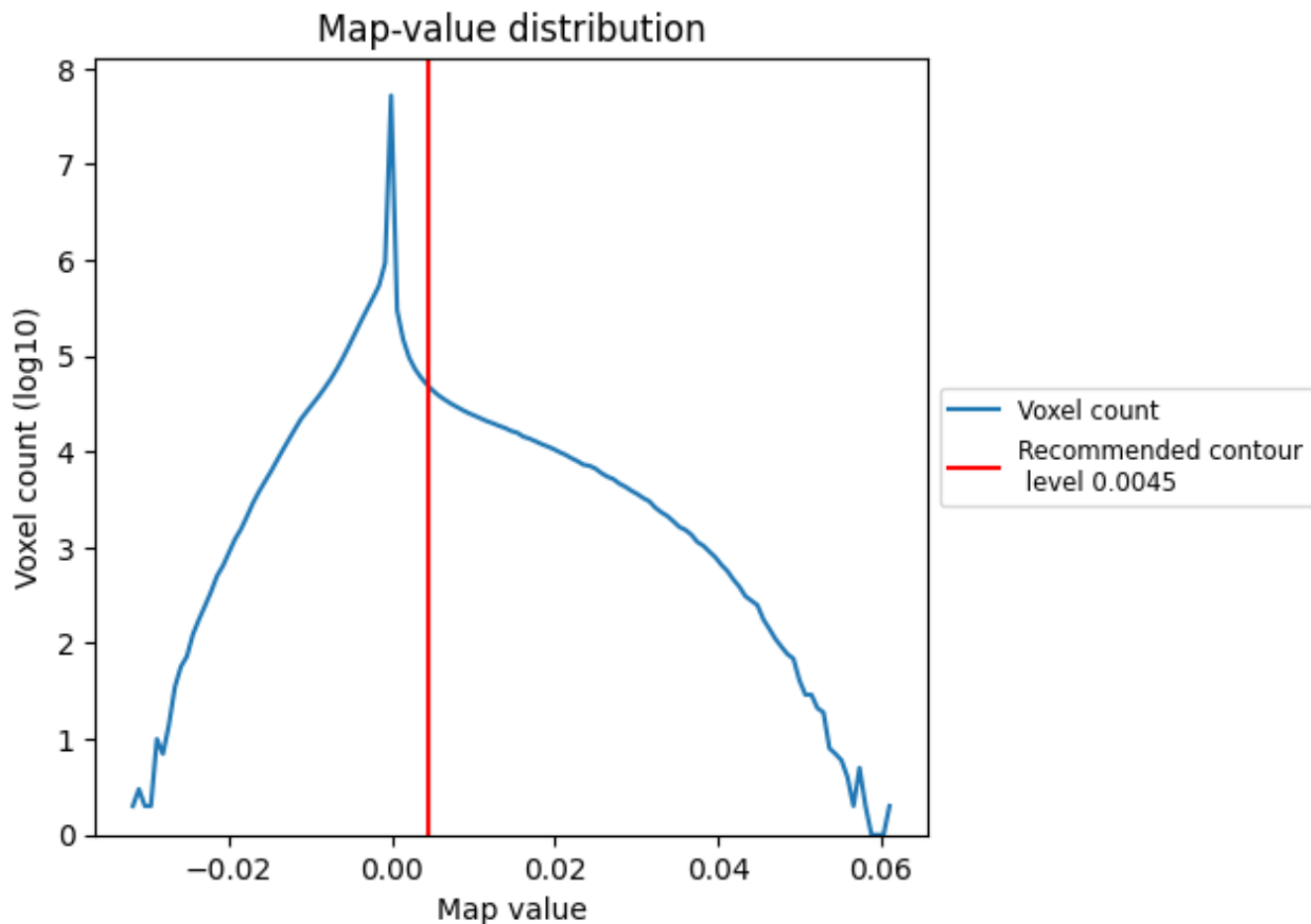
6.5 Mask visualisation

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

7 Map analysis [i](#)

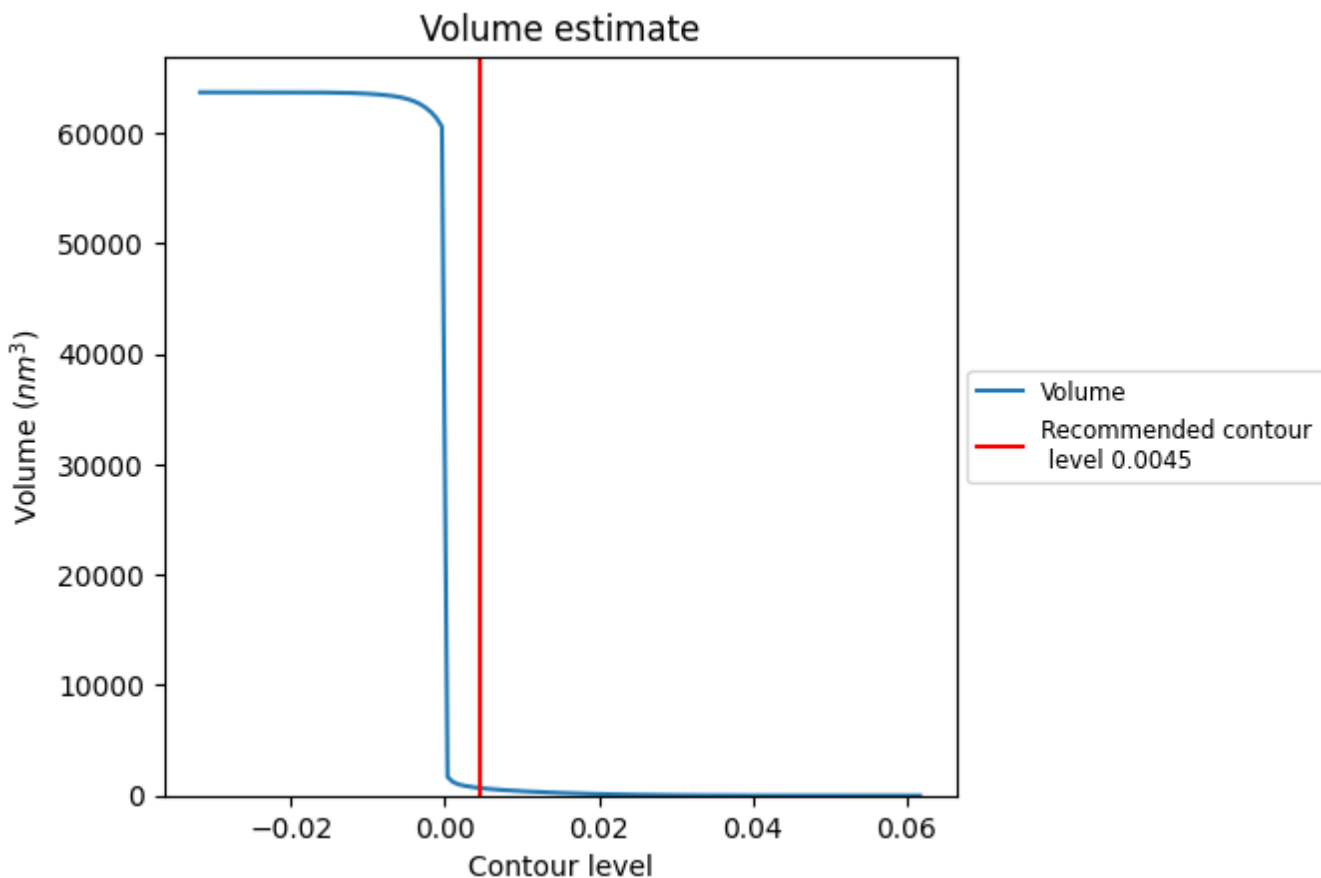
This section contains the results of statistical analysis of the map.

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.

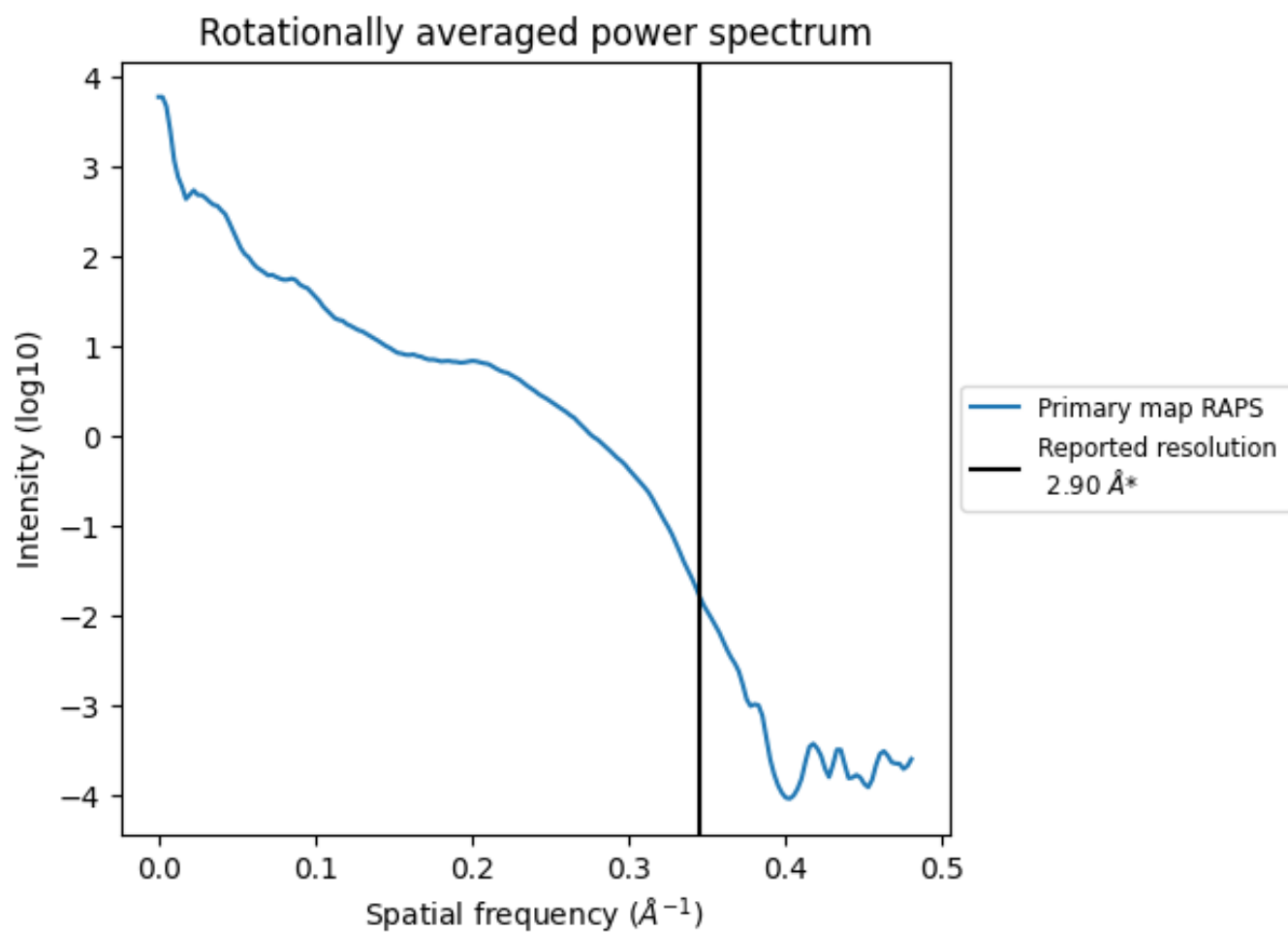
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 689 nm^3 ; this corresponds to an approximate mass of 622 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 0.345 Å⁻¹

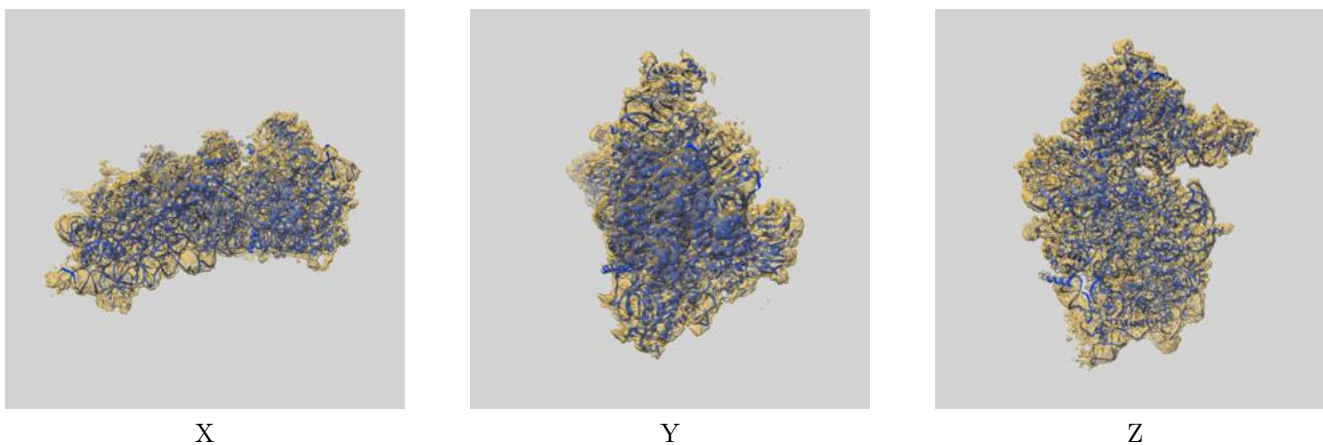
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

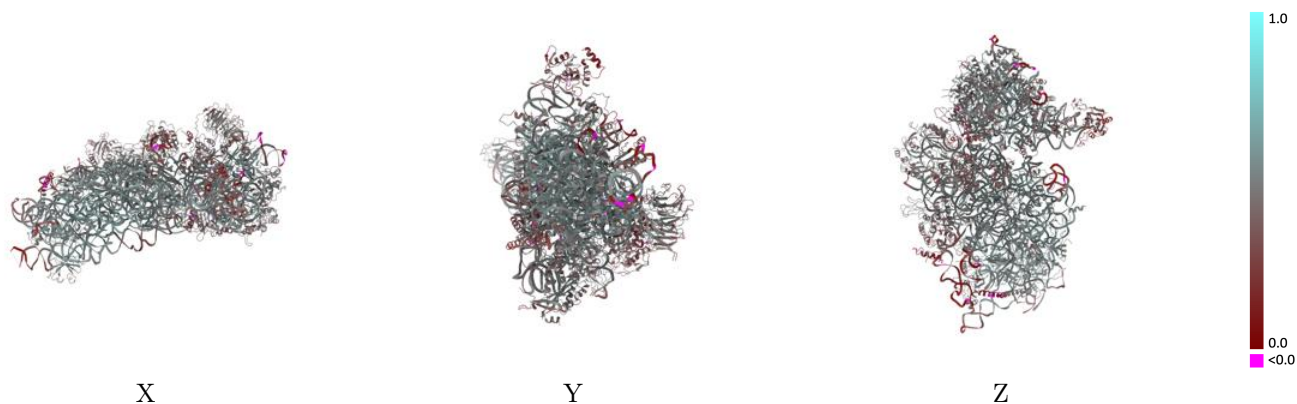
This section contains information regarding the fit between EMDB map EMD-11441 and PDB model 6ZV6. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



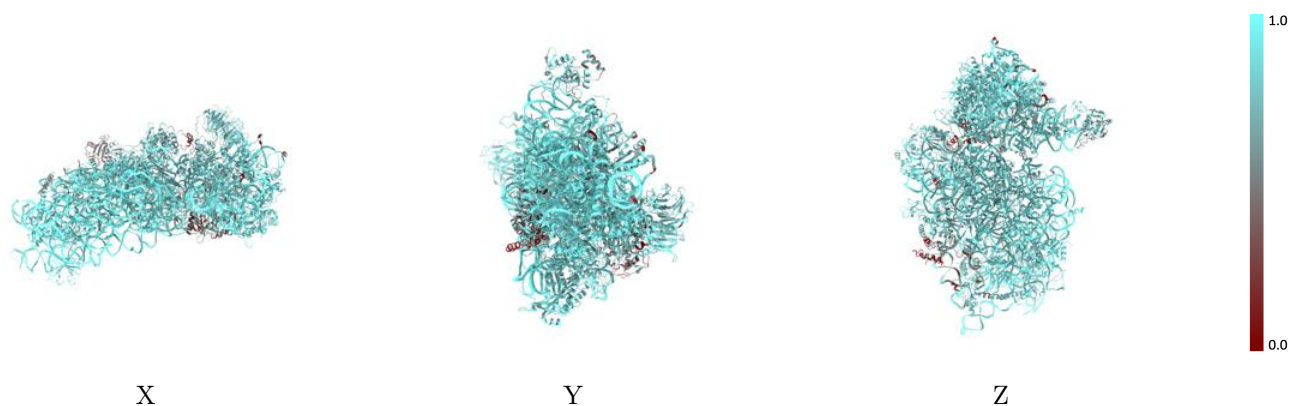
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



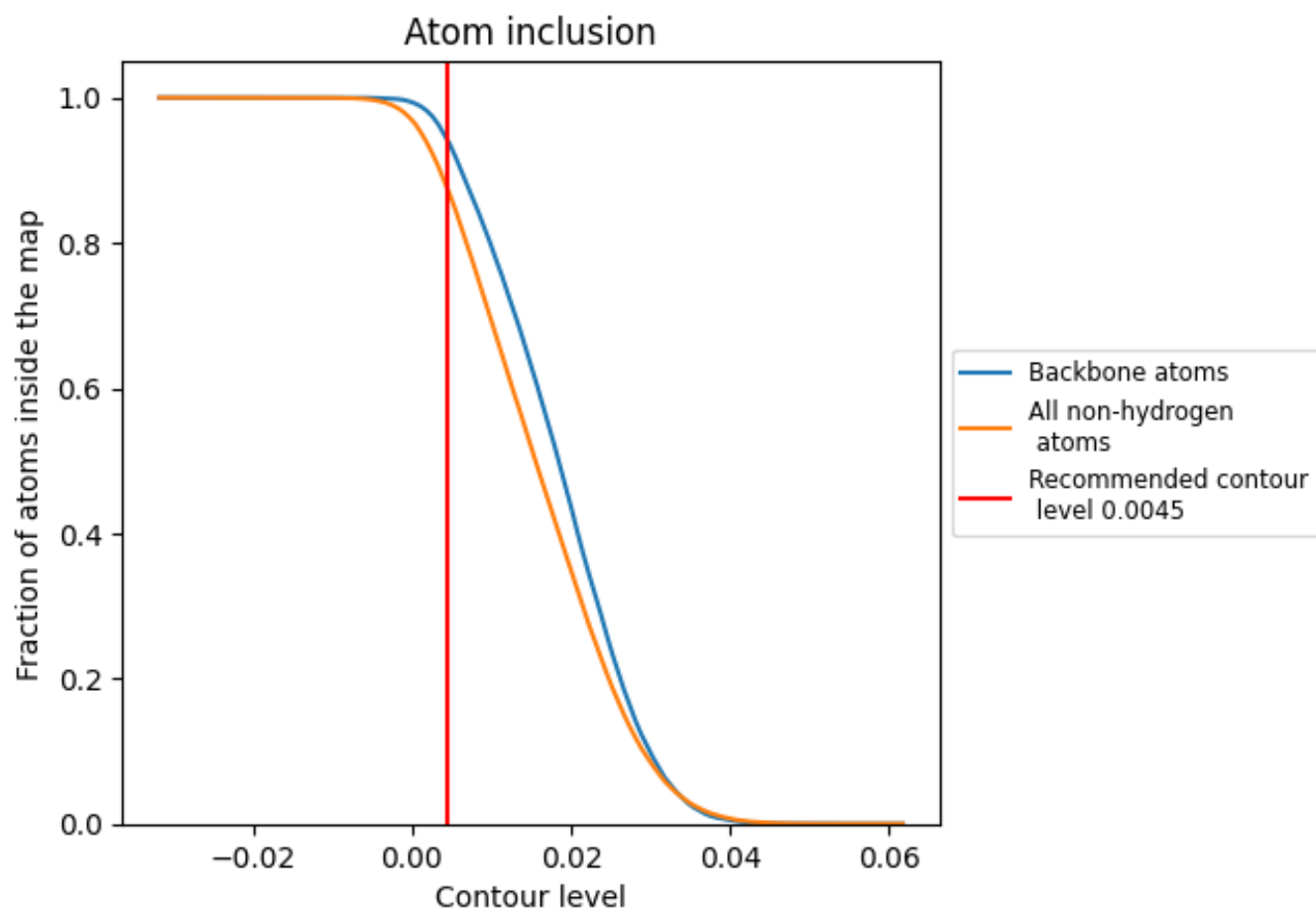
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8736	 0.4680
2	 0.9542	 0.4910
A	 0.7578	 0.3870
B	 0.8735	 0.4580
C	 0.8142	 0.4610
D	 0.7888	 0.4310
E	 0.8973	 0.5250
F	 0.8528	 0.4670
G	 0.8778	 0.4450
H	 0.4457	 0.3160
I	 0.8799	 0.4860
J	 0.8985	 0.5150
K	 0.8705	 0.4510
L	 0.8501	 0.5160
M	 0.6766	 0.2720
N	 0.8619	 0.4580
O	 0.8277	 0.4580
P	 0.8826	 0.4730
Q	 0.8705	 0.5100
R	 0.6110	 0.3660
S	 0.8472	 0.4570
T	 0.8604	 0.4660
U	 0.8043	 0.4370
V	 0.8134	 0.4210
W	 0.8287	 0.5010
X	 0.9113	 0.5440
Y	 0.9228	 0.5140
Z	 0.7986	 0.3950
a	 0.7959	 0.4680
b	 0.8137	 0.4530
c	 0.7852	 0.4170
d	 0.8367	 0.4990
e	 0.7681	 0.4670
f	 0.7238	 0.3230
g	 0.8330	 0.4190
h	 0.3814	 0.3610

