Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 07:35 pm GMT

PDB ID	:	6ZLW
EMDB ID	:	EMD-11276
Title	:	SARS-CoV-2 Nsp1 bound to the human 40S ribosomal subunit
Authors	:	Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2020-07-01
Resolution	:	2.60 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:

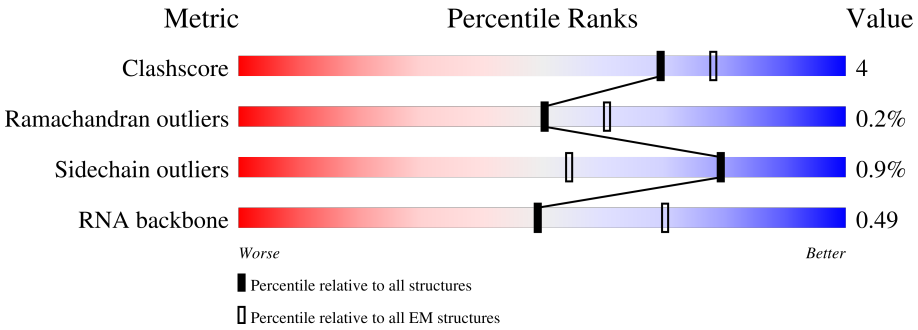
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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.



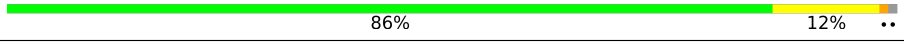
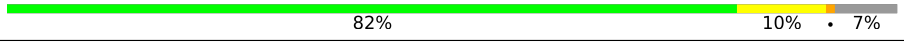
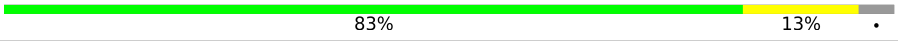
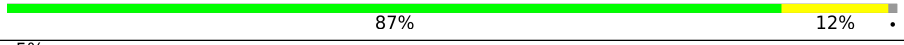
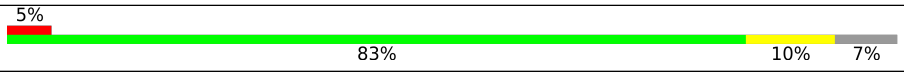
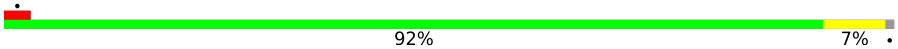
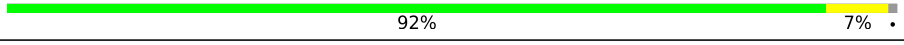
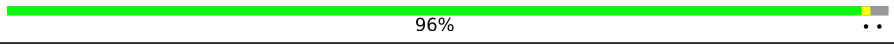
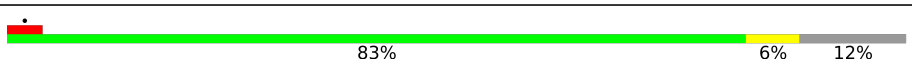
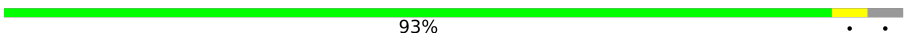
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	B	295	61% 8% 30%
2	C	264	70% 11% 19%
3	D	293	66% 9% 26%
4	E	263	86% 13%
5	F	243	81% 10% 7%
6	G	249	81% 12% 8%
7	H	194	81% 14%

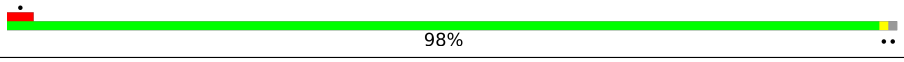
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	208	
9	J	194	
10	K	204	
11	L	158	
12	M	165	
13	N	151	
14	O	132	
15	P	151	
16	Q	145	
17	R	146	
18	S	135	
19	T	152	
20	U	145	
21	V	119	
22	W	130	
23	X	143	
24	Y	133	
25	Z	83	
26	a	125	
27	b	84	
28	c	115	
29	d	69	
30	e	59	
31	f	56	
32	g	156	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	h	25	
34	j	317	
35	2	1868	
36	i	180	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 74568 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 protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	206	1624	1035	287	294	8	0	0

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	218	1682	1090	289	293	10	0	0

- Molecule 4 is a protein called 40S ribosomal protein S4, X isoform.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	225	1748	1115	315	311	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S6.

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

- Molecule 7 is a protein called 40S ribosomal protein S7.

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

- Molecule 8 is a protein called 40S ribosomal protein S8.

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

- Molecule 9 is a protein called 40S ribosomal protein S9.

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

- Molecule 10 is a protein called 40S ribosomal protein S5.

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

- Molecule 11 is a protein called 40S ribosomal protein S11.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 13 is a protein called 40S ribosomal protein S13.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	135	Total	C	N	O	S	0	0
			1006	616	198	186	6		

- Molecule 16 is a protein called 40S ribosomal protein S15.

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

- Molecule 17 is a protein called 40S ribosomal protein S16.

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

- Molecule 18 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 19 is a protein called 40S ribosomal protein S18.

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

- Molecule 20 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 21 is a protein called 40S ribosomal protein S20.

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

- Molecule 22 is a protein called 40S ribosomal protein S15a.

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

- Molecule 23 is a protein called 40S ribosomal protein S23.

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

- Molecule 24 is a protein called 40S ribosomal protein S24.

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

- Molecule 25 is a protein called 40S ribosomal protein S21.

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

- Molecule 26 is a protein called 40S ribosomal protein S25.

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

- Molecule 27 is a protein called 40S ribosomal protein S27.

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

- Molecule 28 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

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

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

- Molecule 30 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	52	Total	C	N	O	S	0	0
			403	246	89	67	1		

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	54	Total	C	N	O	S	0	0
			455	284	93	73	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	72	Total	C	N	O	S	0	0
			591	372	114	98	7		

- Molecule 33 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	22	Total	C	N	O	S	0	0
			213	130	57	23	3		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 35 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	1665	Total	C	N	O	P	0	0
			35552	15869	6385	11633	1665		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1772	C	G	conflict	GB 337376

- Molecule 36 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	33	Total	C	N	O	S	0	0
			261	159	47	54	1		

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

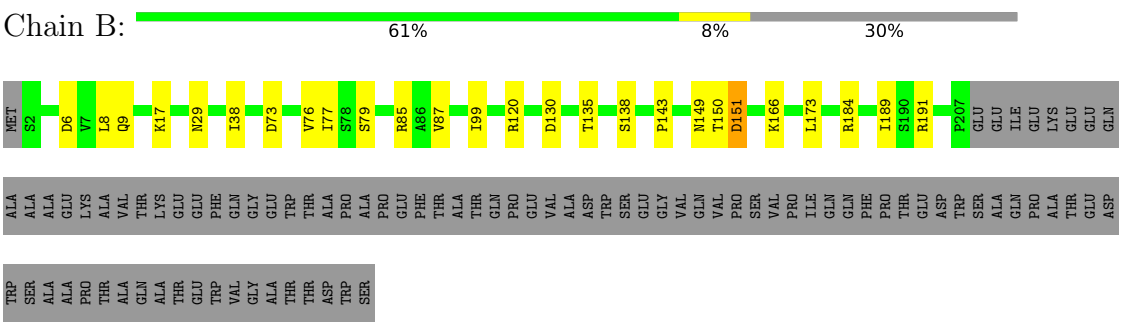
Mol	Chain	Residues	Atoms		AltConf
37	c	1	Total	Zn	0
			1	1	
37	f	1	Total	Zn	0
			1	1	
37	g	1	Total	Zn	0
			1	1	

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.

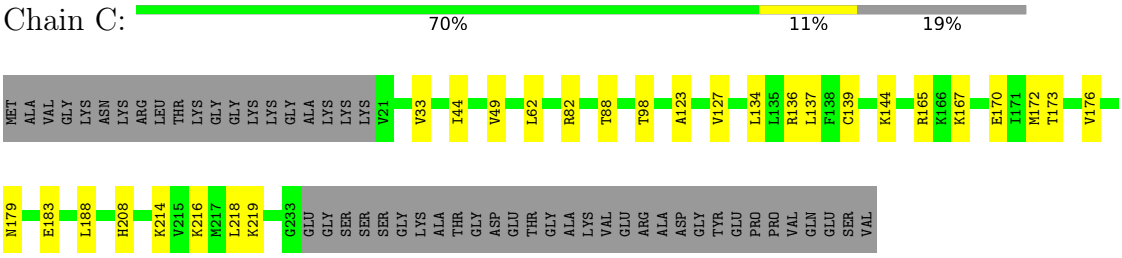
• Molecule 1: 40S ribosomal protein SA

Chain B:



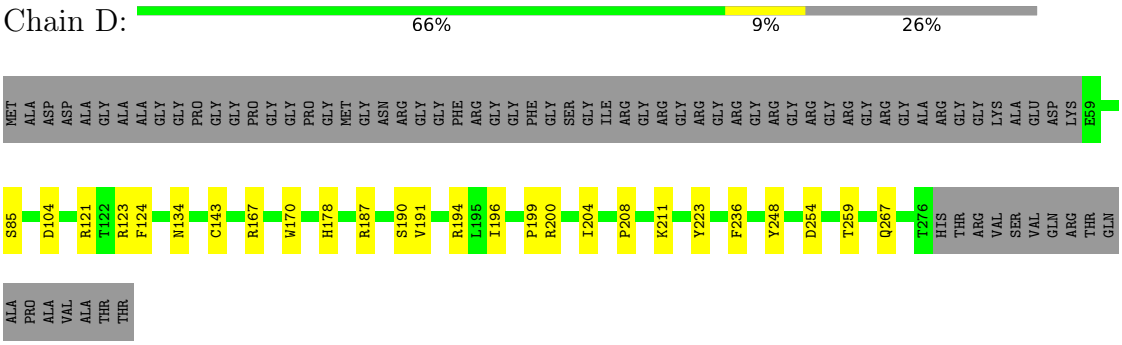
• Molecule 2: 40S ribosomal protein S3a

Chain C:



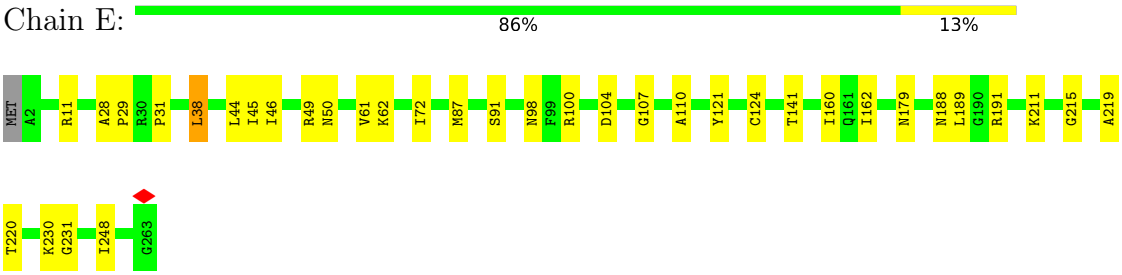
• Molecule 3: 40S ribosomal protein S2

Chain D:



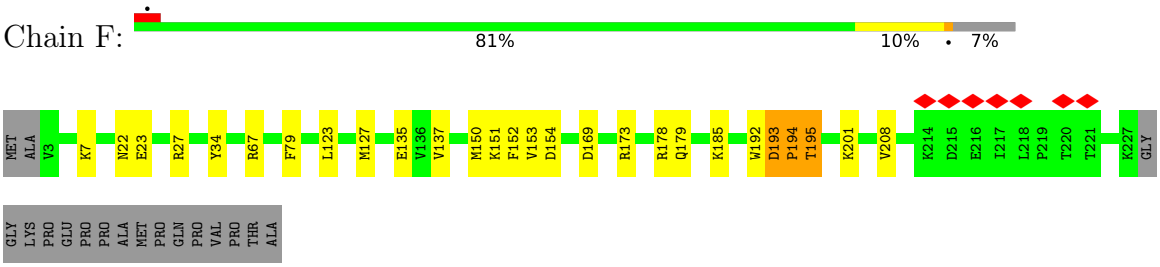
• Molecule 4: 40S ribosomal protein S4, X isoform

Chain E:



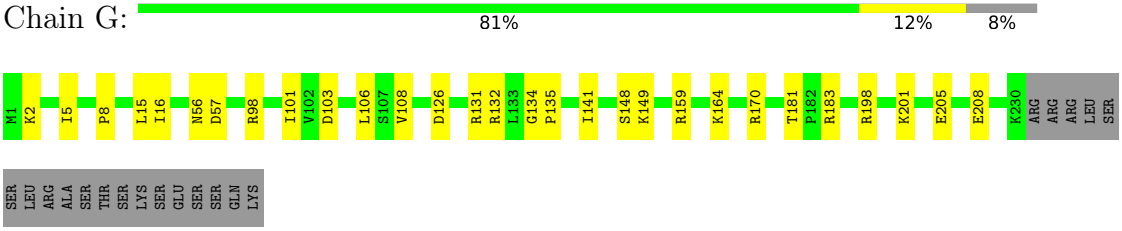
• Molecule 5: 40S ribosomal protein S3

Chain F:



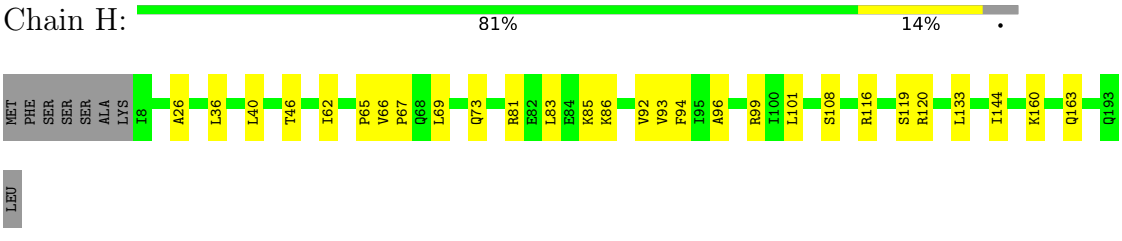
• Molecule 6: 40S ribosomal protein S6

Chain G:



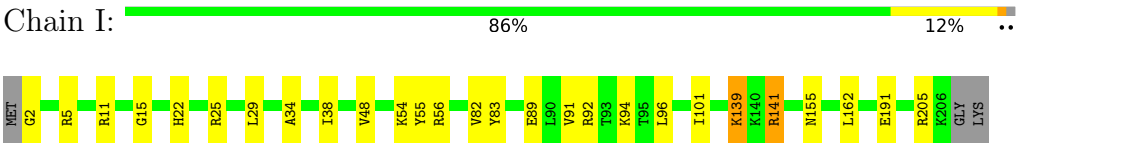
• Molecule 7: 40S ribosomal protein S7

Chain H:



• Molecule 8: 40S ribosomal protein S8

Chain I:

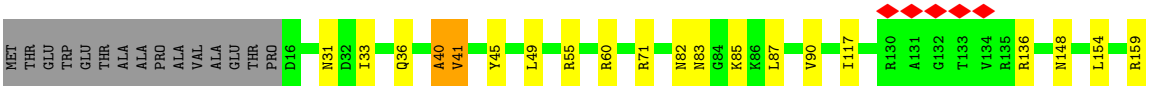


• Molecule 9: 40S ribosomal protein S9

Chain J:

• Molecule 10: 40S ribosomal protein S5

Chain K:

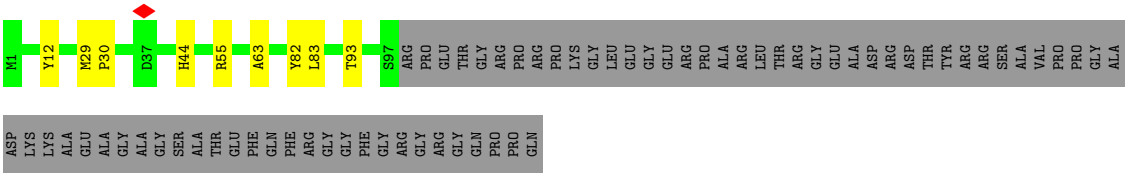


• Molecule 11: 40S ribosomal protein S11

Chain L:

• Molecule 12: 40S ribosomal protein S10

Chain M:

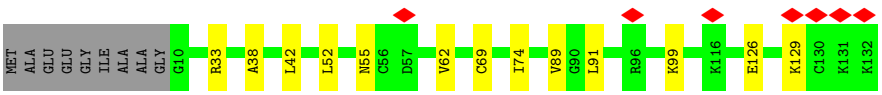


• Molecule 13: 40S ribosomal protein S13

Chain N:

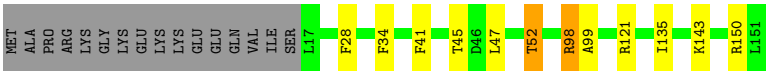
• Molecule 14: 40S ribosomal protein S12

Chain O:



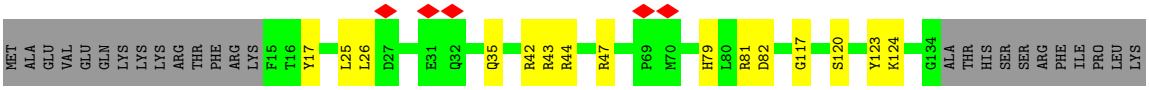
• Molecule 15: 40S ribosomal protein S14

Chain P:



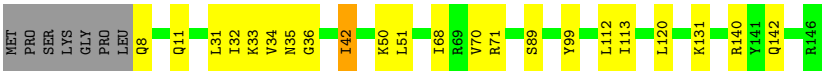
• Molecule 16: 40S ribosomal protein S15

Chain Q:



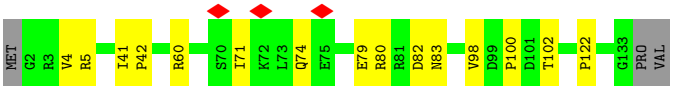
• Molecule 17: 40S ribosomal protein S16

Chain R:



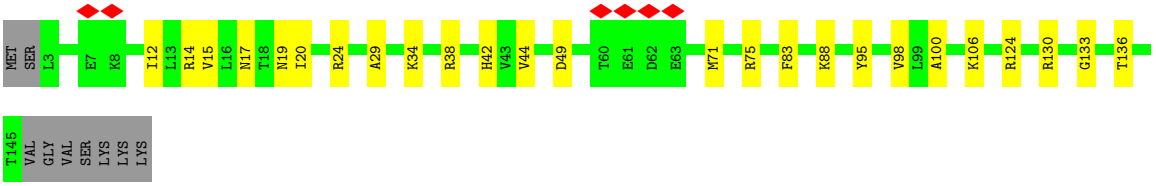
• Molecule 18: 40S ribosomal protein S17

Chain S:



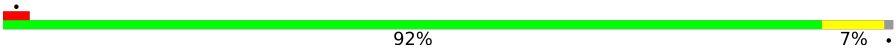
• Molecule 19: 40S ribosomal protein S18

Chain T:



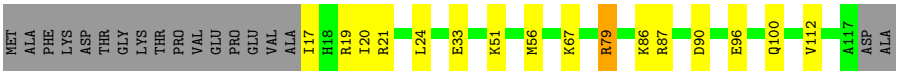
• Molecule 20: 40S ribosomal protein S19

Chain U:



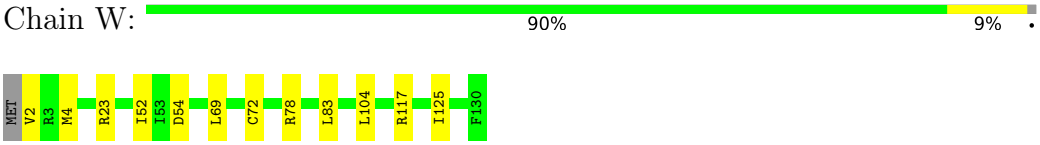
• Molecule 21: 40S ribosomal protein S20

Chain V:



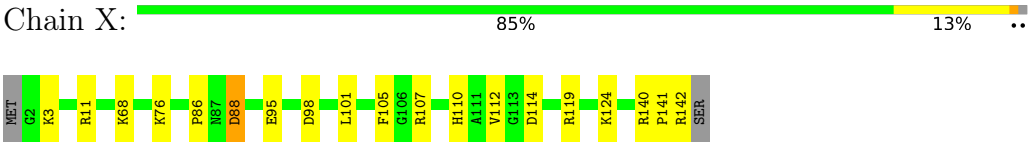
• Molecule 22: 40S ribosomal protein S15a

Chain W:



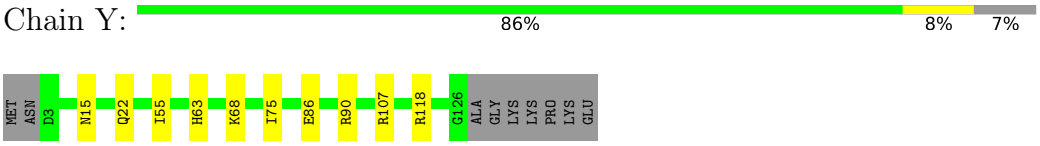
• Molecule 23: 40S ribosomal protein S23

Chain X:



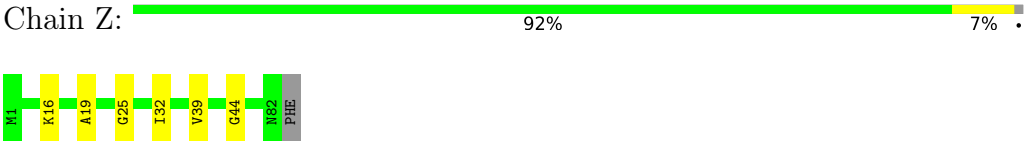
• Molecule 24: 40S ribosomal protein S24

Chain Y:



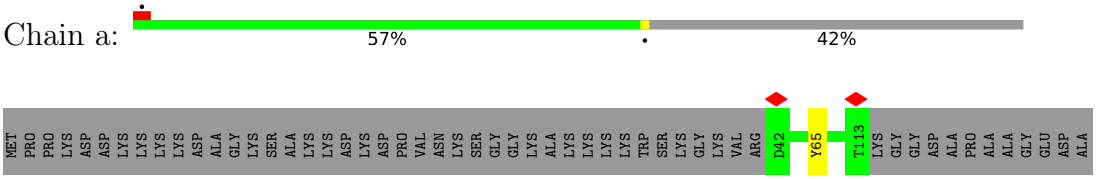
• Molecule 25: 40S ribosomal protein S21

Chain Z:



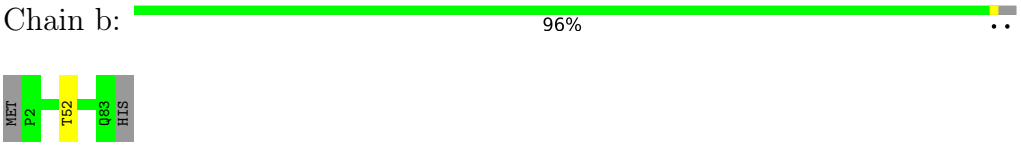
• Molecule 26: 40S ribosomal protein S25

Chain a:



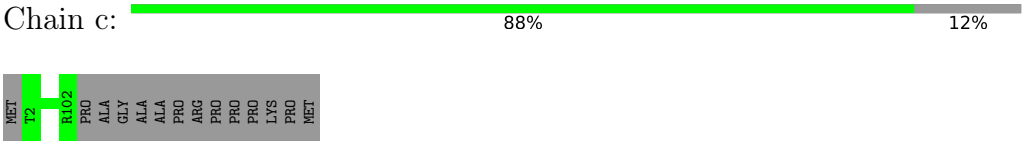
• Molecule 27: 40S ribosomal protein S27

Chain b:



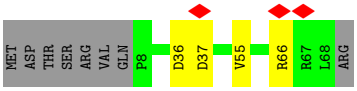
• Molecule 28: 40S ribosomal protein S26

Chain c:



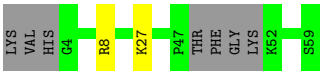
• Molecule 29: 40S ribosomal protein S28

Chain d:



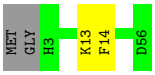
• Molecule 30: 40S ribosomal protein S30

Chain e:



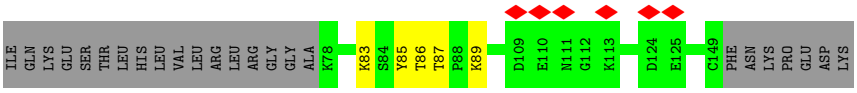
• Molecule 31: 40S ribosomal protein S29

Chain f:



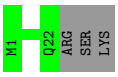
• Molecule 32: Ubiquitin-40S ribosomal protein S27a

Chain g:



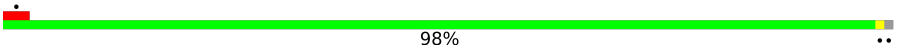
• Molecule 33: 60S ribosomal protein L41

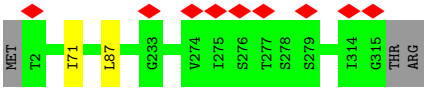
Chain h:



• Molecule 34: Receptor of activated protein C kinase 1

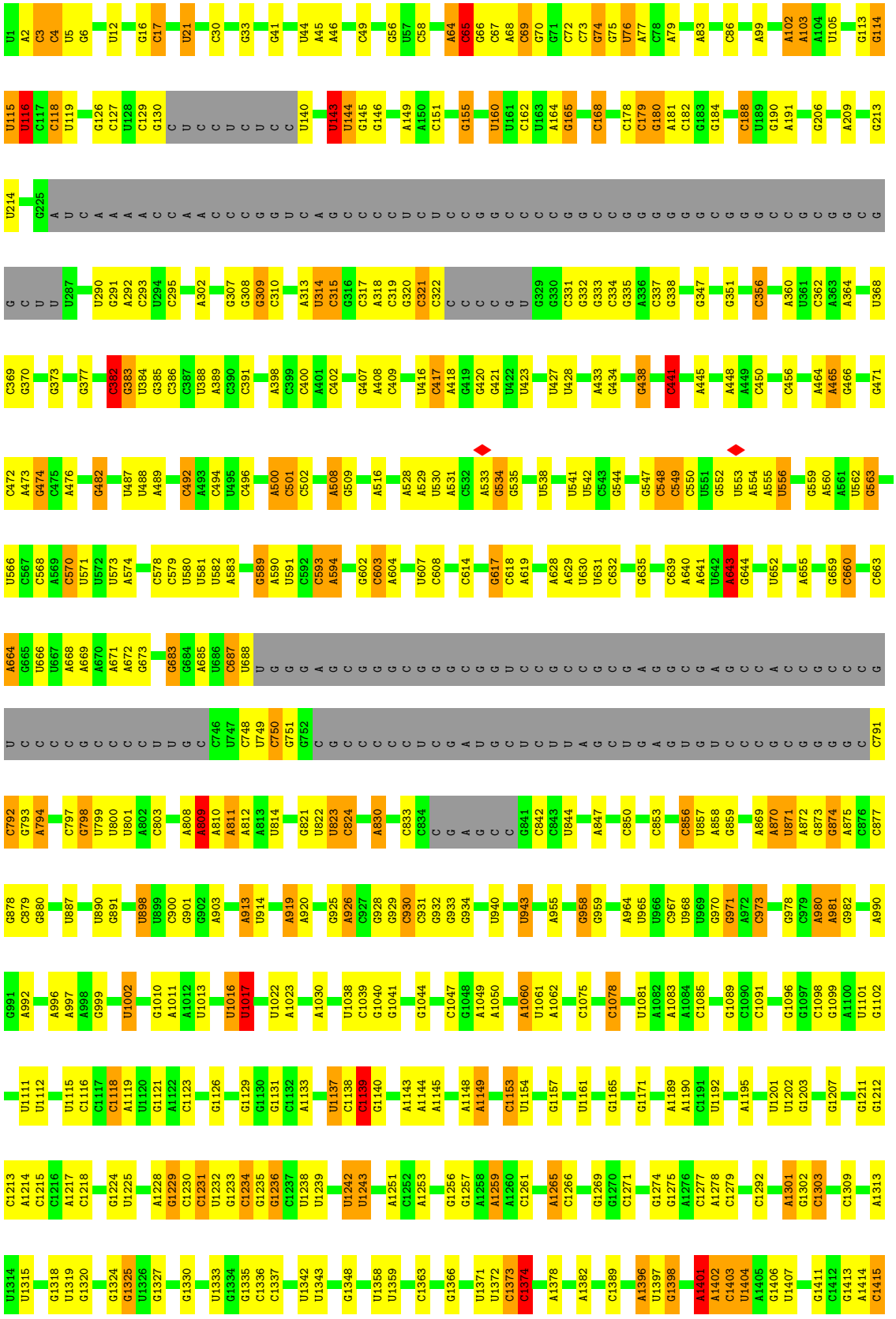
Chain j:

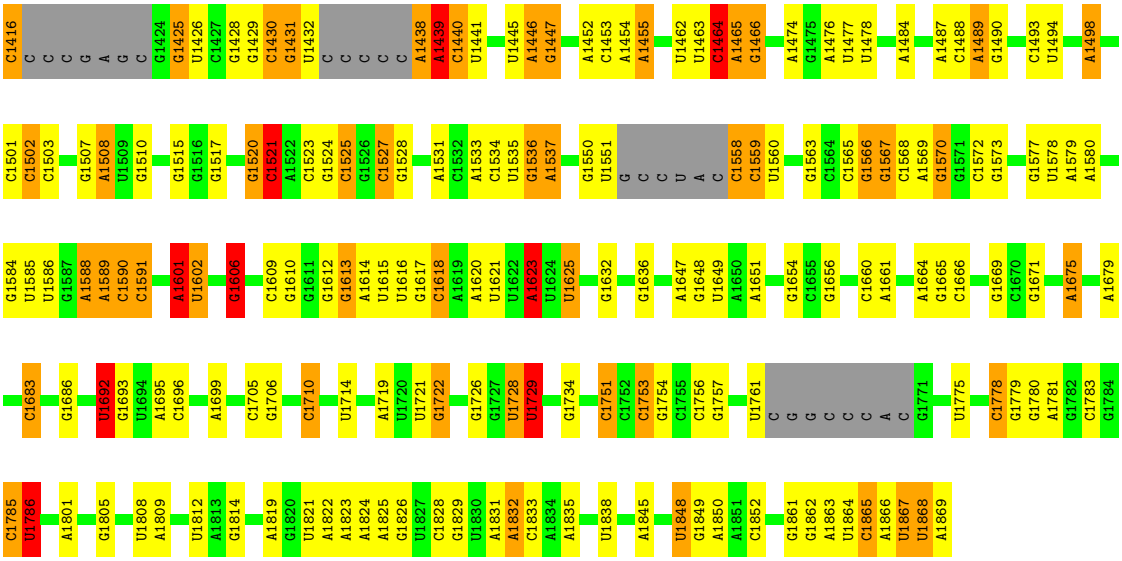




• Molecule 35: 18S ribosomal RNA

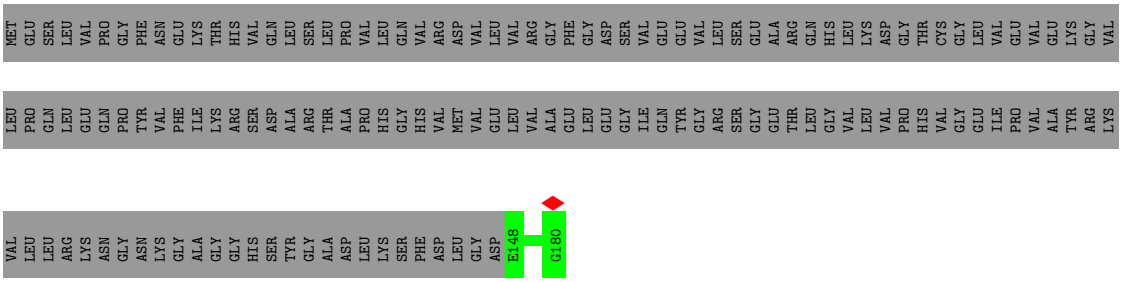
Chain 2:





• Molecule 36: Non-structural protein 1

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173060	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 ($e^-/Å^2$)	44.8	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	43.872	Depositor
Minimum map value	-25.766	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.716	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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

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	B	0.36	0/1661	0.57	0/2259
2	C	0.32	0/1756	0.55	0/2350
3	D	0.39	0/1718	0.56	0/2322
4	E	0.38	0/2118	0.62	1/2849 (0.0%)
5	F	0.44	0/1776	0.57	0/2392
6	G	0.33	0/1885	0.54	0/2510
7	H	0.30	0/1524	0.58	0/2042
8	I	0.39	0/1711	0.60	1/2282 (0.0%)
9	J	0.39	0/1524	0.62	1/2035 (0.0%)
10	K	0.44	0/1516	0.63	0/2037
11	L	0.46	1/1250 (0.1%)	0.60	0/1673
12	M	0.48	0/840	0.58	0/1133
13	N	0.35	0/1226	0.54	0/1649
14	O	0.31	0/963	0.61	0/1291
15	P	0.37	0/1019	0.57	0/1367
16	Q	0.47	0/1003	0.63	0/1341
17	R	0.52	0/1126	0.68	1/1506 (0.1%)
18	S	0.38	0/1080	0.58	0/1449
19	T	0.47	0/1202	0.68	1/1610 (0.1%)
20	U	0.54	0/1142	0.66	0/1530
21	V	0.39	0/813	0.58	0/1092
22	W	0.39	0/1051	0.59	0/1406
23	X	0.42	0/1116	0.62	0/1490
24	Y	0.37	0/1031	0.58	0/1370
25	Z	0.37	0/631	0.55	0/844
26	a	0.45	0/580	0.66	0/780
27	b	0.39	0/653	0.63	0/876
28	c	0.39	0/828	0.54	0/1109
29	d	0.47	0/481	0.77	2/643 (0.3%)
30	e	0.37	0/406	0.61	0/534
31	f	0.53	0/466	0.68	0/618
32	g	0.37	0/602	0.62	0/795

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	h	0.28	0/214	0.52	0/272
34	j	0.42	0/2497	0.61	1/3399 (0.0%)
35	2	0.90	2/39754 (0.0%)	1.27	398/61950 (0.6%)
36	i	0.33	0/266	0.54	0/358
All	All	0.70	3/79429 (0.0%)	1.01	406/115163 (0.4%)

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
5	F	0	2
10	K	0	2
12	M	0	1
17	R	0	1
18	S	0	1
20	U	0	1
22	W	0	1
23	X	0	1
24	Y	0	1
27	b	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	131	CYS	CB-SG	-5.66	1.72	1.81
35	2	1229	G	C8-N7	-5.24	1.27	1.30
35	2	1229	G	N7-C5	-5.01	1.36	1.39

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	501	C	N1-C2-O2	14.95	127.87	118.90
35	2	501	C	C2-N1-C1'	14.19	134.41	118.80
35	2	501	C	N3-C2-O2	-12.69	113.02	121.90
35	2	1618	C	N3-C2-O2	-12.13	113.41	121.90
35	2	356	C	N1-C2-O2	11.77	125.96	118.90
35	2	293	C	N1-C2-O2	11.33	125.70	118.90
35	2	1618	C	N1-C2-O2	11.26	125.66	118.90
35	2	369	C	N1-C2-O2	11.08	125.55	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	1868	U	N3-C2-O2	-10.72	114.70	122.20
35	2	1868	U	N1-C2-O2	10.63	130.24	122.80
35	2	356	C	C2-N1-C1'	10.47	130.32	118.80
35	2	501	C	C6-N1-C1'	-10.47	108.24	120.80
35	2	293	C	N3-C2-O2	-10.28	114.71	121.90
35	2	1453	C	N1-C2-O2	10.16	125.00	118.90
35	2	1139	C	N3-C2-O2	-9.97	114.92	121.90
35	2	1751	C	N1-C2-O2	9.80	124.78	118.90
35	2	1618	C	C6-N1-C2	-9.79	116.38	120.30
35	2	427	U	N3-C2-O2	-9.79	115.35	122.20
35	2	293	C	C2-N1-C1'	9.61	129.37	118.80
35	2	1751	C	C2-N1-C1'	9.56	129.32	118.80
35	2	853	C	C2-N1-C1'	9.45	129.19	118.80
35	2	293	C	C6-N1-C2	-9.41	116.54	120.30
35	2	1016	U	N3-C2-O2	-9.35	115.66	122.20
35	2	1016	U	N1-C2-O2	9.29	129.30	122.80
35	2	369	C	C6-N1-C2	-9.21	116.61	120.30
35	2	1139	C	C6-N1-C2	-9.21	116.62	120.30
35	2	356	C	N3-C2-O2	-9.18	115.47	121.90
35	2	369	C	N3-C2-O2	-9.18	115.47	121.90
35	2	314	U	N3-C2-O2	-9.17	115.78	122.20
35	2	1590	C	C6-N1-C2	-9.13	116.65	120.30
29	d	37	ASP	CB-CG-OD1	9.13	126.52	118.30
35	2	65	C	C6-N1-C2	-8.96	116.72	120.30
35	2	1373	C	C6-N1-C2	-8.93	116.73	120.30
35	2	549	C	C2-N1-C1'	8.88	128.57	118.80
35	2	1453	C	C2-N1-C1'	8.84	128.52	118.80
35	2	369	C	C2-N1-C1'	8.82	128.50	118.80
35	2	1389	C	N1-C2-O2	8.77	124.16	118.90
35	2	630	U	N1-C2-O2	8.76	128.93	122.80
35	2	853	C	N1-C2-O2	8.73	124.14	118.90
35	2	1551	U	N3-C2-O2	-8.72	116.09	122.20
35	2	1271	C	N1-C2-O2	8.61	124.07	118.90
35	2	853	C	N3-C2-O2	-8.47	115.97	121.90
35	2	844	U	N3-C2-O2	-8.47	116.27	122.20
35	2	1521	C	N3-C2-O2	-8.45	115.99	121.90
35	2	427	U	N1-C2-O2	8.39	128.67	122.80
35	2	179	C	N1-C2-O2	8.34	123.90	118.90
35	2	1022	U	C2-N1-C1'	8.29	127.65	117.70
35	2	1060	A	O4'-C1'-N9	8.27	114.81	108.20
35	2	1848	U	N3-C2-O2	-8.23	116.44	122.20
35	2	1848	U	N1-C2-O2	8.22	128.55	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	630	U	C2-N1-C1'	8.15	127.48	117.70
35	2	1520	G	C4-N9-C1'	8.14	137.08	126.50
35	2	659	G	C4-N9-C1'	8.10	137.03	126.50
35	2	856	C	C6-N1-C2	-8.10	117.06	120.30
35	2	1016	U	C2-N1-C1'	8.07	127.38	117.70
35	2	823	U	N3-C2-O2	-8.02	116.59	122.20
35	2	1551	U	C2-N1-C1'	7.99	127.29	117.70
35	2	1118	C	N1-C2-O2	7.96	123.67	118.90
35	2	1606	G	O4'-C1'-N9	7.93	114.55	108.20
35	2	1618	C	C2-N1-C1'	7.92	127.51	118.80
35	2	1521	C	N1-C2-O2	7.87	123.62	118.90
35	2	1243	U	N3-C2-O2	-7.79	116.75	122.20
35	2	630	U	N3-C2-O2	-7.78	116.76	122.20
35	2	1848	U	C2-N1-C1'	7.75	127.01	117.70
35	2	1231	C	C6-N1-C2	-7.72	117.21	120.30
35	2	1139	C	N1-C2-O2	7.71	123.53	118.90
35	2	402	C	C5-C6-N1	7.70	124.85	121.00
35	2	1266	C	C6-N1-C2	-7.69	117.22	120.30
35	2	356	C	C6-N1-C1'	-7.67	111.60	120.80
35	2	1022	U	N1-C2-O2	7.61	128.12	122.80
35	2	809	A	O4'-C1'-N9	7.57	114.26	108.20
35	2	1139	C	C2-N1-C1'	7.57	127.12	118.80
35	2	1453	C	N3-C2-O2	-7.56	116.61	121.90
35	2	369	C	C5-C6-N1	7.52	124.76	121.00
35	2	179	C	C2-N1-C1'	7.49	127.04	118.80
35	2	1389	C	N3-C2-O2	-7.48	116.66	121.90
35	2	427	U	C2-N1-C1'	7.42	126.61	117.70
35	2	1520	G	C8-N9-C1'	-7.42	117.35	127.00
35	2	1521	C	C2-N1-C1'	7.42	126.97	118.80
35	2	1527	C	N3-C2-O2	-7.41	116.72	121.90
35	2	501	C	C6-N1-C2	-7.39	117.34	120.30
35	2	1333	U	N3-C2-O2	-7.38	117.03	122.20
35	2	1242	U	N1-C2-O2	7.38	127.97	122.80
35	2	659	G	C8-N9-C1'	-7.37	117.42	127.00
35	2	1218	C	C6-N1-C2	-7.35	117.36	120.30
35	2	1527	C	N1-C2-O2	7.35	123.31	118.90
35	2	1271	C	N3-C2-O2	-7.33	116.77	121.90
35	2	1567	G	O4'-C1'-N9	7.33	114.06	108.20
35	2	1022	U	N3-C2-O2	-7.30	117.09	122.20
35	2	1403	C	P-O3'-C3'	7.27	128.43	119.70
35	2	188	C	C2-N1-C1'	7.25	126.78	118.80
35	2	1333	U	N1-C2-O2	7.25	127.88	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	1868	U	C2-N1-C1'	7.24	126.38	117.70
35	2	973	C	N1-C2-O2	7.23	123.24	118.90
35	2	547	G	C4-N9-C1'	7.21	135.87	126.50
35	2	1430	C	C6-N1-C2	-7.19	117.42	120.30
35	2	1111	U	C2-N1-C1'	7.18	126.32	117.70
35	2	1751	C	N3-C2-O2	-7.18	116.87	121.90
35	2	632	C	C2-N1-C1'	7.16	126.68	118.80
35	2	1336	C	N1-C2-O2	7.16	123.20	118.90
35	2	402	C	C6-N1-C2	-7.16	117.44	120.30
35	2	494	C	N1-C2-O2	7.12	123.17	118.90
35	2	1551	U	N1-C2-O2	7.11	127.78	122.80
35	2	1218	C	C5-C6-N1	7.10	124.55	121.00
35	2	547	G	N3-C4-C5	-7.09	125.05	128.60
19	T	49	ASP	CB-CG-OD1	7.02	124.62	118.30
35	2	856	C	C2-N1-C1'	7.00	126.50	118.80
35	2	1231	C	N3-C2-O2	-6.98	117.01	121.90
35	2	179	C	N3-C2-O2	-6.98	117.02	121.90
35	2	593	C	N1-C2-O2	6.96	123.08	118.90
35	2	314	U	N1-C2-O2	6.95	127.67	122.80
35	2	547	G	N3-C4-N9	6.93	130.16	126.00
35	2	570	C	N1-C2-O2	6.90	123.04	118.90
35	2	65	C	C5-C6-N1	6.86	124.43	121.00
35	2	179	C	C6-N1-C2	-6.81	117.57	120.30
35	2	4	C	C6-N1-C2	-6.79	117.58	120.30
35	2	102	A	P-O3'-C3'	6.79	127.84	119.70
35	2	1751	C	C6-N1-C1'	-6.78	112.67	120.80
35	2	1243	U	N1-C2-O2	6.77	127.54	122.80
35	2	1259	A	C2-N3-C4	6.75	113.97	110.60
4	E	38	LEU	CA-CB-CG	6.75	130.82	115.30
35	2	1589	A	N7-C8-N9	6.73	117.17	113.80
35	2	1692	U	C5-C6-N1	6.71	126.05	122.70
35	2	1692	U	N3-C2-O2	-6.70	117.51	122.20
35	2	1567	G	C4-C5-N7	6.68	113.47	110.80
35	2	823	U	N1-C2-O2	6.67	127.47	122.80
35	2	1336	C	N3-C2-O2	-6.61	117.27	121.90
35	2	570	C	N3-C2-O2	-6.60	117.28	121.90
35	2	1502	C	C6-N1-C2	-6.59	117.66	120.30
35	2	1867	U	N3-C2-O2	-6.58	117.60	122.20
35	2	1623	A	O4'-C1'-N9	6.57	113.46	108.20
35	2	1728	U	C2-N1-C1'	6.57	125.58	117.70
35	2	1590	C	N3-C2-O2	-6.54	117.33	121.90
35	2	1415	C	C6-N1-C2	-6.51	117.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	119	U	N3-C2-O2	-6.50	117.65	122.20
35	2	1389	C	C2-N1-C1'	6.49	125.94	118.80
35	2	417	C	P-O3'-C3'	6.49	127.48	119.70
35	2	1111	U	N1-C2-O2	6.49	127.34	122.80
35	2	549	C	C6-N1-C1'	-6.48	113.02	120.80
35	2	70	G	N3-C2-N2	-6.47	115.37	119.90
35	2	1521	C	C6-N1-C2	-6.46	117.72	120.30
35	2	1111	U	N3-C2-O2	-6.46	117.68	122.20
35	2	321	C	C5-C6-N1	6.45	124.23	121.00
35	2	664	A	C2-N3-C4	6.45	113.82	110.60
35	2	853	C	C6-N1-C1'	-6.44	113.07	120.80
35	2	494	C	C6-N1-C2	-6.43	117.73	120.30
35	2	1234	C	C5-C6-N1	6.43	124.21	121.00
35	2	871	U	O5'-P-OP2	6.42	118.41	110.70
35	2	853	C	C6-N1-C2	-6.42	117.73	120.30
35	2	1118	C	N3-C2-O2	-6.42	117.41	121.90
35	2	143	U	P-O3'-C3'	6.41	127.39	119.70
35	2	750	C	C6-N1-C2	-6.41	117.74	120.30
35	2	1265	A	C5-N7-C8	-6.41	100.70	103.90
35	2	494	C	N3-C2-O2	-6.40	117.42	121.90
35	2	1601	A	P-O3'-C3'	6.40	127.38	119.70
35	2	1567	G	C6-C5-N7	-6.39	126.56	130.40
35	2	973	C	N3-C2-O2	-6.39	117.43	121.90
35	2	1416	C	C6-N1-C2	-6.39	117.75	120.30
35	2	1265	A	N7-C8-N9	6.38	116.99	113.80
35	2	1590	C	N1-C2-O2	6.37	122.72	118.90
35	2	1389	C	C6-N1-C2	-6.36	117.76	120.30
35	2	1696	C	C6-N1-C2	-6.36	117.76	120.30
35	2	1590	C	C5-C6-N1	6.35	124.18	121.00
35	2	1692	U	N1-C2-O2	6.34	127.24	122.80
35	2	1692	U	C6-N1-C2	-6.30	117.22	121.00
35	2	1867	U	N1-C2-O2	6.29	127.20	122.80
35	2	188	C	C5-C6-N1	6.28	124.14	121.00
35	2	1525	C	C5-C6-N1	6.27	124.13	121.00
35	2	1751	C	C5-C6-N1	6.26	124.13	121.00
35	2	824	C	N3-C2-O2	-6.24	117.53	121.90
35	2	1118	C	C2-N1-C1'	6.23	125.65	118.80
35	2	824	C	N1-C2-O2	6.22	122.63	118.90
35	2	1261	C	C6-N1-C2	-6.21	117.82	120.30
35	2	118	C	N1-C2-O2	6.18	122.61	118.90
35	2	1343	U	N3-C2-O2	-6.17	117.88	122.20
35	2	114	G	P-O3'-C3'	6.16	127.10	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	1453	C	C6-N1-C1'	-6.15	113.42	120.80
35	2	823	U	C2-N1-C1'	6.14	125.07	117.70
35	2	1301	A	C8-N9-C4	-6.14	103.34	105.80
35	2	1558	C	P-O3'-C3'	6.14	127.07	119.70
35	2	1568	C	O5'-P-OP1	-6.14	100.18	105.70
35	2	1666	C	C6-N1-C2	-6.13	117.85	120.30
35	2	1446	A	O4'-C1'-N9	6.12	113.10	108.20
35	2	1751	C	C6-N1-C2	-6.12	117.85	120.30
35	2	1696	C	C2-N1-C1'	6.12	125.53	118.80
35	2	293	C	C5-C6-N1	6.11	124.06	121.00
35	2	119	U	N1-C2-O2	6.11	127.07	122.80
17	R	51	LEU	CB-CG-CD2	-6.09	100.65	111.00
35	2	1525	C	C2-N1-C1'	6.09	125.50	118.80
35	2	1778	C	C2-N1-C1'	6.09	125.50	118.80
35	2	1416	C	C5-C6-N1	6.07	124.03	121.00
35	2	1523	C	C6-N1-C2	-6.07	117.87	120.30
35	2	750	C	P-O3'-C3'	6.06	126.97	119.70
35	2	856	C	C5-C6-N1	6.04	124.02	121.00
35	2	1501	C	C5-C6-N1	6.03	124.02	121.00
35	2	1591	C	N1-C2-O2	6.03	122.52	118.90
35	2	1231	C	N1-C2-O2	6.01	122.51	118.90
35	2	547	G	C8-N9-C1'	-6.01	119.19	127.00
35	2	441	C	C2-N1-C1'	6.00	125.41	118.80
35	2	1453	C	C5-C6-N1	6.00	124.00	121.00
35	2	549	C	N1-C2-O2	6.00	122.50	118.90
35	2	1218	C	C2-N1-C1'	5.99	125.39	118.80
35	2	1415	C	P-O3'-C3'	5.98	126.88	119.70
35	2	315	C	C6-N1-C2	-5.96	117.91	120.30
35	2	548	C	N1-C2-O2	5.96	122.48	118.90
35	2	321	C	C6-N1-C2	-5.94	117.92	120.30
35	2	830	A	N9-C4-C5	-5.94	103.42	105.80
35	2	549	C	C5-C6-N1	5.94	123.97	121.00
35	2	534	G	C4-N9-C1'	5.93	134.21	126.50
35	2	1558	C	OP1-P-O3'	5.93	118.24	105.20
35	2	1501	C	C2-N1-C1'	5.92	125.31	118.80
35	2	1396	A	O4'-C1'-N9	5.91	112.93	108.20
35	2	12	U	N3-C2-O2	-5.91	118.06	122.20
35	2	1438	A	P-O3'-C3'	5.91	126.79	119.70
35	2	168	C	N1-C2-O2	5.89	122.44	118.90
35	2	465	A	P-O3'-C3'	5.88	126.76	119.70
35	2	898	U	N1-C2-O2	5.87	126.91	122.80
35	2	1234	C	C6-N1-C2	-5.84	117.96	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	811	A	P-O3'-C3'	5.83	126.70	119.70
35	2	70	G	N3-C4-N9	-5.83	122.50	126.00
35	2	1017	U	N3-C2-O2	-5.83	118.12	122.20
35	2	1567	G	C5-N7-C8	-5.82	101.39	104.30
35	2	1137	U	P-O3'-C3'	5.82	126.68	119.70
35	2	958	G	C4-N9-C1'	5.82	134.06	126.50
35	2	1868	U	P-O3'-C3'	5.81	126.67	119.70
35	2	578	C	N1-C2-O2	5.81	122.39	118.90
35	2	441	C	C5-C6-N1	5.81	123.90	121.00
35	2	1112	U	N1-C2-O2	5.80	126.86	122.80
35	2	118	C	N3-C2-O2	-5.80	117.84	121.90
35	2	1271	C	C6-N1-C2	-5.80	117.98	120.30
35	2	1242	U	C2-N1-C1'	5.79	124.65	117.70
35	2	1430	C	C5-C6-N1	5.79	123.89	121.00
35	2	814	U	N3-C2-O2	-5.79	118.15	122.20
35	2	1567	G	C4-N9-C1'	5.78	134.01	126.50
35	2	1502	C	P-O3'-C3'	5.77	126.63	119.70
35	2	593	C	C2-N1-C1'	5.77	125.15	118.80
35	2	930	C	N1-C2-O2	5.77	122.36	118.90
35	2	792	C	N1-C2-O2	5.76	122.36	118.90
35	2	1373	C	P-O3'-C3'	5.75	126.60	119.70
35	2	188	C	C6-N1-C2	-5.74	118.00	120.30
35	2	750	C	C5-C6-N1	5.72	123.86	121.00
35	2	1112	U	N3-C2-O2	-5.71	118.20	122.20
35	2	842	C	C2-N1-C1'	5.71	125.08	118.80
35	2	1265	A	C8-N9-C4	-5.71	103.52	105.80
35	2	801	U	C2-N1-C1'	5.70	124.54	117.70
35	2	1625	U	C2-N1-C1'	5.70	124.54	117.70
35	2	1137	U	C2'-C3'-O3'	5.70	122.82	113.70
35	2	438	G	C2-N3-C4	5.68	114.74	111.90
35	2	1431	G	P-O3'-C3'	5.68	126.52	119.70
35	2	1325	G	C8-N9-C4	-5.68	104.13	106.40
35	2	1609	C	C6-N1-C2	-5.68	118.03	120.30
35	2	1374	C	C6-N1-C2	-5.67	118.03	120.30
35	2	1559	C	C6-N1-C2	-5.66	118.03	120.30
35	2	618	C	O5'-P-OP1	-5.66	100.61	105.70
35	2	1022	U	C6-N1-C1'	-5.66	113.27	121.20
35	2	958	G	O4'-C1'-N9	5.66	112.73	108.20
35	2	1238	U	N1-C2-O2	5.66	126.76	122.80
35	2	579	C	N1-C2-O2	5.65	122.29	118.90
35	2	926	A	C6-C5-N7	-5.65	128.34	132.30
35	2	391	C	C6-N1-C2	-5.64	118.04	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	441	C	C6-N1-C2	-5.64	118.05	120.30
35	2	750	C	C2-N1-C1'	5.64	125.00	118.80
35	2	1453	C	C6-N1-C2	-5.64	118.04	120.30
35	2	632	C	C6-N1-C2	-5.64	118.05	120.30
35	2	1303	C	N1-C2-O2	5.64	122.28	118.90
35	2	1238	U	N3-C2-O2	-5.63	118.25	122.20
35	2	530	U	C2-N1-C1'	5.63	124.46	117.70
9	J	137	VAL	C-N-CA	5.63	135.78	121.70
35	2	4	C	C2-N1-C1'	5.63	124.99	118.80
35	2	1118	C	C6-N1-C2	-5.63	118.05	120.30
35	2	382	C	P-O3'-C3'	5.62	126.45	119.70
35	2	926	A	N7-C8-N9	5.62	116.61	113.80
35	2	1591	C	C6-N1-C2	-5.62	118.05	120.30
35	2	1242	U	N3-C2-O2	-5.62	118.27	122.20
35	2	334	C	C2-N1-C1'	5.62	124.98	118.80
35	2	293	C	C6-N1-C1'	-5.61	114.07	120.80
35	2	930	C	N3-C2-O2	-5.60	117.98	121.90
35	2	1081	U	N3-C2-O2	-5.60	118.28	122.20
35	2	356	C	C6-N1-C2	-5.59	118.06	120.30
35	2	1266	C	C5-C6-N1	5.59	123.80	121.00
35	2	659	G	N3-C4-N9	5.59	129.35	126.00
35	2	973	C	C6-N1-C2	-5.58	118.07	120.30
35	2	1149	A	C2-N3-C4	5.57	113.39	110.60
35	2	179	C	C5-C6-N1	5.57	123.78	121.00
35	2	1618	C	C5-C4-N4	5.57	124.10	120.20
35	2	1525	C	C6-N1-C2	-5.56	118.08	120.30
35	2	102	A	OP2-P-O3'	5.56	117.43	105.20
35	2	850	C	N1-C2-O2	5.54	122.22	118.90
35	2	844	U	N1-C2-N3	5.54	118.22	114.90
35	2	168	C	N3-C2-O2	-5.54	118.03	121.90
35	2	1303	C	N3-C2-O2	-5.53	118.03	121.90
35	2	791	C	N1-C2-O2	5.52	122.21	118.90
35	2	898	U	N3-C2-O2	-5.52	118.34	122.20
35	2	1729	U	N1-C2-O2	5.51	126.66	122.80
35	2	1464	C	P-O3'-C3'	5.51	126.31	119.70
35	2	1261	C	N3-C2-O2	-5.51	118.05	121.90
35	2	151	C	C2-N1-C1'	5.47	124.82	118.80
35	2	1401	A	O4'-C1'-N9	5.47	112.58	108.20
35	2	105	U	N3-C2-O2	-5.46	118.38	122.20
35	2	877	C	C2-N1-C1'	5.45	124.80	118.80
35	2	1865	C	N3-C2-O2	-5.45	118.09	121.90
35	2	168	C	C6-N1-C2	-5.44	118.12	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	1038	U	N3-C2-O2	-5.44	118.39	122.20
35	2	1374	C	C5-C6-N1	5.44	123.72	121.00
35	2	116	U	C5-C6-N1	5.44	125.42	122.70
35	2	1527	C	C6-N1-C2	-5.43	118.13	120.30
35	2	530	U	N1-C2-O2	5.43	126.60	122.80
35	2	824	C	C6-N1-C2	-5.42	118.13	120.30
35	2	1397	U	C5-C4-O4	-5.41	122.65	125.90
35	2	151	C	N1-C2-O2	5.41	122.14	118.90
35	2	1161	U	N3-C2-O2	-5.38	118.43	122.20
35	2	1315	U	N1-C2-O2	5.38	126.57	122.80
35	2	1363	C	C6-N1-C2	-5.38	118.15	120.30
35	2	1336	C	C6-N1-C2	-5.38	118.15	120.30
35	2	803	C	C2-N1-C1'	5.38	124.71	118.80
35	2	1786	U	C5-C6-N1	5.37	125.39	122.70
35	2	21	U	N3-C2-O2	-5.37	118.44	122.20
35	2	1852	C	C2-N1-C1'	5.37	124.71	118.80
35	2	1567	G	N7-C8-N9	5.36	115.78	113.10
35	2	578	C	N3-C2-O2	-5.34	118.16	121.90
35	2	1439	A	O4'-C1'-N9	5.34	112.47	108.20
35	2	593	C	N3-C2-O2	-5.34	118.16	121.90
35	2	1590	C	C2-N1-C1'	5.33	124.66	118.80
35	2	853	C	O4'-C1'-N1	5.33	112.46	108.20
35	2	630	U	C6-N1-C1'	-5.32	113.75	121.20
35	2	1501	C	C6-N1-C2	-5.32	118.17	120.30
35	2	1649	U	C2-N1-C1'	5.32	124.08	117.70
35	2	1123	C	C6-N1-C2	-5.31	118.18	120.30
35	2	474	G	C4-N9-C1'	5.31	133.40	126.50
35	2	579	C	N3-C2-O2	-5.30	118.19	121.90
35	2	1828	C	C6-N1-C2	-5.30	118.18	120.30
35	2	1078	C	C6-N1-C2	-5.30	118.18	120.30
35	2	856	C	N1-C2-O2	5.30	122.08	118.90
35	2	589	G	C4-N9-C1'	5.30	133.39	126.50
35	2	549	C	C6-N1-C2	-5.29	118.18	120.30
35	2	314	U	P-O3'-C3'	5.29	126.05	119.70
35	2	1201	U	N1-C2-O2	5.29	126.50	122.80
35	2	1259	A	C4-N9-C1'	5.29	135.82	126.30
35	2	337	C	C2-N1-C1'	5.29	124.62	118.80
35	2	140	U	N3-C2-O2	-5.29	118.50	122.20
35	2	560	A	N7-C8-N9	5.28	116.44	113.80
34	j	87	LEU	CA-CB-CG	5.28	127.44	115.30
35	2	1374	C	C2-N1-C1'	5.28	124.61	118.80
35	2	1602	U	O5'-P-OP1	-5.28	100.95	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	1359	U	N3-C2-O2	-5.28	118.50	122.20
35	2	151	C	C6-N1-C2	-5.27	118.19	120.30
35	2	580	U	N3-C2-O2	-5.26	118.52	122.20
35	2	1416	C	C2-N1-C1'	5.26	124.59	118.80
35	2	143	U	OP2-P-O3'	5.26	116.77	105.20
35	2	809	A	C8-N9-C4	-5.25	103.70	105.80
35	2	1425	G	P-O3'-C3'	5.25	126.00	119.70
35	2	1558	C	N1-C2-O2	5.25	122.05	118.90
35	2	105	U	N1-C2-O2	5.24	126.47	122.80
35	2	1520	G	N3-C4-N9	5.24	129.14	126.00
35	2	1591	C	C5-C6-N1	5.24	123.62	121.00
8	I	29	LEU	CA-CB-CG	5.23	127.34	115.30
35	2	632	C	C5-C6-N1	5.23	123.62	121.00
35	2	1710	C	N1-C2-O2	5.23	122.04	118.90
35	2	687	C	N1-C2-O2	5.23	122.04	118.90
35	2	643	A	P-O3'-C3'	5.22	125.96	119.70
35	2	423	U	N3-C2-O2	-5.21	118.55	122.20
35	2	180	G	P-O3'-C3'	5.21	125.95	119.70
35	2	86	C	C6-N1-C2	-5.21	118.22	120.30
35	2	666	U	N1-C2-O2	5.18	126.43	122.80
35	2	1269	G	O5'-P-OP2	-5.17	101.05	105.70
35	2	898	U	C2-N1-C1'	5.17	123.90	117.70
35	2	1753	C	C2-N1-C1'	5.16	124.48	118.80
29	d	36	ASP	C-N-CA	5.16	134.59	121.70
35	2	165	G	C4-N9-C1'	5.15	133.20	126.50
35	2	566	U	N3-C2-O2	-5.15	118.60	122.20
35	2	556	U	C5-C6-N1	5.15	125.27	122.70
35	2	508	A	N1-C6-N6	-5.14	115.51	118.60
35	2	792	C	C2-N1-C1'	5.14	124.46	118.80
35	2	534	G	C8-N9-C1'	-5.14	120.32	127.00
35	2	1165	G	O4'-C1'-N9	5.13	112.31	108.20
35	2	870	A	P-O3'-C3'	5.12	125.84	119.70
35	2	1660	C	C6-N1-C2	-5.12	118.25	120.30
35	2	750	C	N1-C2-O2	5.10	121.96	118.90
35	2	850	C	N3-C2-O2	-5.10	118.33	121.90
35	2	830	A	N3-C4-N9	5.10	131.48	127.40
35	2	1832	A	C2'-C3'-O3'	5.09	121.85	113.70
35	2	1729	U	N3-C2-O2	-5.08	118.64	122.20
35	2	814	U	N1-C2-O2	5.08	126.35	122.80
35	2	30	C	C6-N1-C2	-5.07	118.27	120.30
35	2	534	G	P-O3'-C3'	5.07	125.78	119.70
35	2	331	C	C2-N1-C1'	5.07	124.38	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	850	C	C6-N1-C2	-5.07	118.27	120.30
35	2	824	C	C2-N1-C1'	5.07	124.37	118.80
35	2	571	U	N3-C2-O2	-5.06	118.66	122.20
35	2	1753	C	C6-N1-C2	-5.06	118.28	120.30
35	2	1319	U	N1-C2-O2	5.06	126.34	122.80
35	2	1292	C	N1-C2-O2	5.05	121.93	118.90
35	2	474	G	C8-N9-C1'	-5.05	120.44	127.00
35	2	4	C	C5-C6-N1	5.05	123.52	121.00
35	2	1756	C	N1-C2-O2	5.04	121.93	118.90
35	2	456	C	C5-C6-N1	5.03	123.52	121.00
35	2	687	C	N3-C2-O2	-5.03	118.38	121.90
35	2	1728	U	N1-C2-O2	5.03	126.32	122.80
35	2	660	C	C6-N1-C2	-5.03	118.29	120.30
35	2	687	C	C2-N1-C1'	5.01	124.31	118.80
35	2	973	C	C2-N1-C1'	5.01	124.31	118.80
35	2	1153	C	N1-C2-O2	5.01	121.91	118.90
35	2	1618	C	O4'-C1'-N1	5.01	112.21	108.20
35	2	1683	C	N1-C2-O2	5.01	121.91	118.90
35	2	70	G	N1-C2-N2	5.01	120.71	116.20
35	2	666	U	C2-N1-C1'	5.00	123.71	117.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	194	PRO	Peptide
5	F	195	THR	Peptide
10	K	165	ASN	Peptide
10	K	40	ALA	Peptide
12	M	63	ALA	Peptide
17	R	42	ILE	Peptide
18	S	42	PRO	Peptide
20	U	36	THR	Peptide
22	W	54	ASP	Peptide
23	X	112	VAL	Peptide
24	Y	118	ARG	Peptide
27	b	52	THR	Peptide

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	B	1624	0	1634	16	0
2	C	1729	0	1803	15	0
3	D	1682	0	1769	19	0
4	E	2076	0	2177	22	0
5	F	1748	0	1844	20	0
6	G	1862	0	2018	21	0
7	H	1501	0	1593	18	0
8	I	1682	0	1769	17	0
9	J	1499	0	1618	17	0
10	K	1495	0	1549	15	0
11	L	1229	0	1302	13	0
12	M	816	0	841	5	0
13	N	1202	0	1289	12	0
14	O	953	0	990	7	0
15	P	1006	0	1030	6	0
16	Q	984	0	1028	10	0
17	R	1109	0	1174	13	0
18	S	1066	0	1116	9	0
19	T	1184	0	1244	14	0
20	U	1122	0	1153	6	0
21	V	803	0	873	11	0
22	W	1034	0	1080	7	0
23	X	1098	0	1167	12	0
24	Y	1014	0	1082	5	0
25	Z	625	0	628	6	0
26	a	574	0	627	0	0
27	b	640	0	665	0	0
28	c	814	0	864	0	0
29	d	479	0	507	0	0
30	e	403	0	432	0	0
31	f	455	0	446	0	0
32	g	591	0	622	0	0
33	h	213	0	258	0	0
34	j	2440	0	2396	0	0
35	2	35552	0	17949	160	0
36	i	261	0	229	0	0
37	c	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	f	1	0	0	0	0
37	g	1	0	0	0	0
All	All	74568	0	58766	387	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 4.

All (387) 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)
35:2:925:G:H1	35:2:1017:U:H3	1.02	0.90
35:2:1729:U:H3	35:2:1805:G:H1	1.26	0.81
17:R:11:GLN:HE21	17:R:71:ARG:HH12	1.36	0.74
20:U:76:THR:HG22	20:U:94:ARG:HB3	1.73	0.70
19:T:133:GLY:HA3	35:2:1623:A:H5"	1.75	0.69
9:J:172:ARG:NH2	35:2:563:G:N7	2.42	0.68
35:2:64:A:H2	35:2:83:A:H62	1.41	0.67
19:T:75:ARG:HH21	19:T:95:TYR:HB2	1.60	0.67
1:B:120:ARG:HH22	3:D:267:GLN:HG3	1.61	0.66
5:F:150:MET:HE1	5:F:152:PHE:HZ	1.61	0.66
16:Q:35:GLN:O	19:T:88:LYS:NZ	2.29	0.65
35:2:1601:A:H5'	35:2:1636:G:H22	1.61	0.65
35:2:1236:G:H1	35:2:1521:C:H5	1.44	0.65
10:K:41:VAL:HA	10:K:45:TYR:HB2	1.80	0.64
3:D:190:SER:HB3	35:2:1143:A:H5'	1.79	0.64
21:V:33:GLU:OE2	21:V:87:ARG:NH1	2.31	0.63
6:G:181:THR:HG22	6:G:183:ARG:H	1.63	0.63
35:2:928:G:H1	35:2:1013:U:H3	1.46	0.62
7:H:26:ALA:O	7:H:86:LYS:NZ	2.33	0.62
10:K:49:LEU:HD12	17:R:50:LYS:HG2	1.82	0.62
35:2:103:A:OP2	35:2:356:C:N4	2.33	0.62
8:I:82:VAL:O	8:I:205:ARG:NH1	2.33	0.62
6:G:198:ARG:NH1	35:2:126:G:OP1	2.32	0.62
1:B:73:ASP:HB3	1:B:120:ARG:HG2	1.82	0.61
7:H:93:VAL:HG21	7:H:133:LEU:HD12	1.83	0.61
4:E:179:ASN:HD22	4:E:231:GLY:H	1.49	0.61
16:Q:81:ARG:NH2	16:Q:120:SER:O	2.34	0.60
35:2:516:A:N1	35:2:643:A:O2'	2.34	0.60
4:E:211:LYS:HE2	4:E:215:GLY:HA2	1.83	0.60
16:Q:44:ARG:NH1	16:Q:82:ASP:O	2.33	0.60
4:E:100:ARG:NH2	4:E:121:TYR:O	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:161:ALA:O	10:K:165:ASN:ND2	2.35	0.60
5:F:178:ARG:HH21	5:F:179:GLN:HE21	1.49	0.60
23:X:119:ARG:NH2	35:2:1192:U:OP2	2.35	0.59
2:C:82:ARG:NH1	2:C:188:LEU:O	2.34	0.59
18:S:60:ARG:NH1	35:2:1465:A:OP1	2.35	0.59
35:2:1396:A:O2'	35:2:1398:G:N7	2.36	0.59
35:2:940:U:H3	35:2:1002:U:H3	1.50	0.59
22:W:2:VAL:N	35:2:1091:C:HO2'	2.01	0.58
3:D:200:ARG:O	9:J:54:ARG:NH2	2.37	0.58
7:H:99:ARG:H	35:2:913:A:H2	1.51	0.58
15:P:98:ARG:NH1	15:P:99:ALA:O	2.35	0.58
20:U:97:LYS:NZ	35:2:1570:G:N7	2.52	0.58
17:R:31:LEU:HD11	17:R:33:LYS:HE3	1.87	0.57
21:V:96:GLU:O	21:V:100:GLN:NE2	2.37	0.57
1:B:17:LYS:HB3	1:B:173:LEU:HD11	1.85	0.57
10:K:71:ARG:NH2	10:K:148:ASN:OD1	2.36	0.57
3:D:187:ARG:HH21	3:D:190:SER:HA	1.69	0.56
4:E:31:PRO:HG2	4:E:38:LEU:HB2	1.87	0.56
3:D:191:VAL:HG11	3:D:236:PHE:HA	1.88	0.56
21:V:21:ARG:NH2	35:2:1404:U:OP1	2.37	0.56
3:D:104:ASP:N	3:D:104:ASP:OD1	2.39	0.56
9:J:133:ARG:NH2	35:2:581:U:OP1	2.39	0.56
4:E:45:ILE:HG13	4:E:61:VAL:HG21	1.88	0.56
21:V:17:ILE:HG22	21:V:20:ILE:HD11	1.87	0.56
16:Q:123:TYR:OH	19:T:124:ARG:NH1	2.38	0.56
4:E:188:ASN:OD1	4:E:191:ARG:NH2	2.39	0.56
14:O:33:ARG:HD3	14:O:89:VAL:HG11	1.88	0.56
19:T:130:ARG:NH2	35:2:1230:C:OP1	2.39	0.56
6:G:134:GLY:O	35:2:65:C:N4	2.32	0.56
9:J:17:ARG:NH1	35:2:21:U:O2	2.36	0.55
16:Q:124:LYS:HD3	35:2:1239:U:H5"	1.88	0.55
8:I:11:ARG:NH1	8:I:15:GLY:O	2.40	0.55
5:F:67:ARG:NH1	12:M:93:THR:O	2.38	0.55
14:O:52:LEU:HD21	14:O:62:VAL:HG23	1.89	0.55
35:2:1751:C:N4	35:2:1781:A:N1	2.55	0.55
4:E:160:ILE:HD12	4:E:162:ILE:HD11	1.89	0.54
19:T:34:LYS:HB2	19:T:100:ALA:HA	1.89	0.54
1:B:149:ASN:HD22	1:B:166:LYS:HE2	1.71	0.54
7:H:69:LEU:HG	7:H:73:GLN:HE21	1.72	0.54
13:N:63:VAL:HG21	13:N:71:ILE:HD11	1.88	0.54
7:H:108:SER:HB2	35:2:798:G:H4'	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2:164:A:H3'	35:2:165:G:H21	1.73	0.54
35:2:1228:A:H2'	35:2:1229:G:C8	2.42	0.54
35:2:1588:A:H2'	35:2:1589:A:C8	2.43	0.54
35:2:1821:U:H2'	35:2:1822:A:H8	1.72	0.54
6:G:135:PRO:HG2	6:G:141:ILE:HD13	1.89	0.54
11:L:104:LYS:O	23:X:11:ARG:NH2	2.38	0.54
5:F:22:ASN:ND2	5:F:34:TYR:OH	2.41	0.53
5:F:135:GLU:HG3	5:F:153:VAL:HG12	1.89	0.53
2:C:214:LYS:NZ	35:2:943:U:OP1	2.39	0.53
3:D:187:ARG:NH2	35:2:1143:A:OP2	2.41	0.53
8:I:89:GLU:OE2	8:I:92:ARG:NH1	2.41	0.53
10:K:165:ASN:O	10:K:167:LYS:N	2.42	0.53
15:P:143:LYS:HA	35:2:1047:C:H5"	1.91	0.53
3:D:259:THR:HG21	25:Z:16:LYS:H	1.74	0.53
18:S:5:ARG:NH2	35:2:1455:A:OP1	2.41	0.53
35:2:416:U:HO2'	35:2:652:U:HO2'	1.54	0.53
17:R:8:GLN:N	17:R:99:TYR:HH	2.06	0.53
19:T:24:ARG:HB2	19:T:29:ALA:HB2	1.91	0.53
16:Q:81:ARG:HB3	16:Q:117:GLY:HA3	1.91	0.52
8:I:11:ARG:O	11:L:136:LYS:NZ	2.35	0.52
23:X:95:GLU:HG2	23:X:140:ARG:HH12	1.74	0.52
18:S:71:ILE:HB	18:S:74:GLN:H	1.74	0.52
1:B:29:ASN:HB2	1:B:151:ASP:HB3	1.92	0.52
3:D:199:PRO:HG2	9:J:58:ARG:HD2	1.92	0.52
7:H:69:LEU:HD13	7:H:96:ALA:HB2	1.92	0.52
5:F:169:ASP:N	5:F:169:ASP:OD1	2.43	0.52
20:U:13:GLU:OE2	20:U:16:ARG:NH1	2.43	0.52
8:I:155:ASN:O	11:L:21:LYS:NZ	2.42	0.52
6:G:164:LYS:NZ	35:2:69:C:OP2	2.40	0.51
2:C:167:LYS:HA	2:C:170:GLU:HG2	1.92	0.51
11:L:85:THR:HG21	35:2:373:G:H4'	1.91	0.51
20:U:101:ARG:NH2	35:2:1566:G:N7	2.58	0.51
5:F:127:MET:HG3	5:F:154:ASP:OD2	2.10	0.51
7:H:83:LEU:HD23	7:H:92:VAL:HG11	1.91	0.51
21:V:79:ARG:NH1	35:2:1669:G:OP1	2.43	0.51
6:G:5:ILE:HD12	6:G:16:ILE:HD12	1.93	0.51
35:2:900:C:H2'	35:2:901:G:H8	1.74	0.51
16:Q:42:ARG:NH2	35:2:1613:G:OP1	2.37	0.51
5:F:27:ARG:NH2	35:2:1498:A:OP2	2.44	0.51
7:H:144:ILE:HB	22:W:52:ILE:HB	1.93	0.51
15:P:135:ILE:O	35:2:943:U:O2'	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:113:ILE:HG13	17:R:120:LEU:HD12	1.93	0.51
19:T:12:ILE:HD11	19:T:19:ASN:HB3	1.92	0.51
3:D:204:ILE:O	3:D:211:LYS:NZ	2.44	0.50
8:I:139:LYS:HD2	8:I:141:ARG:HD2	1.93	0.50
12:M:55:ARG:HE	35:2:1277:C:H5"	1.76	0.50
35:2:143:U:H4'	35:2:144:U:H5'	1.93	0.50
6:G:148:SER:OG	6:G:149:LYS:N	2.44	0.50
35:2:748:C:H42	35:2:794:A:H61	1.59	0.50
13:N:37:ILE:HG23	13:N:50:ILE:HG21	1.94	0.50
35:2:1719:A:N6	35:2:1814:G:O2'	2.44	0.50
8:I:48:VAL:HG11	8:I:54:LYS:HE3	1.94	0.50
23:X:114:ASP:HB2	35:2:619:A:N1	2.26	0.50
9:J:162:ARG:NH1	35:2:582:U:OP1	2.45	0.50
17:R:89:SER:HB3	17:R:112:LEU:HD13	1.93	0.50
21:V:51:LYS:HB2	21:V:90:ASP:HB2	1.93	0.49
35:2:1324:G:O2'	35:2:1510:G:O2'	2.26	0.49
19:T:136:THR:OG1	35:2:1521:C:OP2	2.20	0.49
1:B:143:PRO:HG3	25:Z:32:ILE:HG23	1.95	0.49
24:Y:63:HIS:HD2	24:Y:68:LYS:HB3	1.76	0.49
8:I:5:ARG:NH2	35:2:384:U:O4	2.37	0.49
19:T:44:VAL:HG11	19:T:71:MET:HG3	1.94	0.49
1:B:85:ARG:NH2	18:S:82:ASP:O	2.45	0.49
35:2:531:A:N1	35:2:552:G:O6	2.46	0.49
35:2:1144:A:H2'	35:2:1145:A:C8	2.47	0.49
8:I:162:LEU:HD11	8:I:191:GLU:HG2	1.95	0.49
21:V:67:LYS:HE3	35:2:1337:C:H5"	1.95	0.49
1:B:191:ARG:NH2	25:Z:44:GLY:O	2.46	0.49
5:F:194:PRO:HA	5:F:201:LYS:HA	1.94	0.49
8:I:34:ALA:HB3	8:I:56:ARG:HD2	1.95	0.49
16:Q:17:TYR:HB3	16:Q:25:LEU:HD11	1.93	0.49
35:2:528:A:H2'	35:2:529:A:C8	2.48	0.49
35:2:640:A:H2'	35:2:641:A:C8	2.48	0.49
35:2:981:A:H2'	35:2:982:G:C8	2.48	0.48
10:K:83:ASN:ND2	35:2:1651:A:O2'	2.37	0.48
23:X:3:LYS:NZ	35:2:663:C:OP2	2.46	0.48
4:E:11:ARG:HA	4:E:28:ALA:HB2	1.95	0.48
35:2:115:U:OP1	35:2:382:C:O2'	2.31	0.48
35:2:382:C:H2'	35:2:383:G:H8	1.79	0.48
35:2:1710:C:H42	35:2:1823:A:H61	1.61	0.48
7:H:36:LEU:HB3	7:H:40:LEU:HD13	1.96	0.48
9:J:44:TRP:HA	9:J:47:LYS:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:159:ARG:NH1	35:2:76:U:OP1	2.39	0.48
10:K:159:ARG:NH1	35:2:1535:U:O4	2.41	0.48
23:X:68:LYS:NZ	35:2:617:G:OP2	2.41	0.48
4:E:46:ILE:HA	4:E:50:ASN:HD22	1.77	0.48
10:K:154:LEU:HD22	10:K:177:LEU:HD12	1.96	0.48
1:B:77:ILE:HG12	1:B:99:ILE:HB	1.95	0.48
7:H:46:THR:HG23	7:H:65:PRO:HD3	1.95	0.48
11:L:48:LYS:HA	11:L:51:ILE:HG12	1.96	0.48
11:L:147:LYS:HB3	11:L:151:THR:HG21	1.96	0.48
24:Y:15:ASN:ND2	24:Y:22:GLN:OE1	2.46	0.48
35:2:928:G:H2'	35:2:929:G:C8	2.49	0.48
1:B:38:ILE:HD11	1:B:150:THR:HG22	1.95	0.48
1:B:184:ARG:HG2	1:B:189:ILE:HG13	1.95	0.48
15:P:34:PHE:HB3	15:P:41:PHE:HB2	1.96	0.48
21:V:24:LEU:HD23	21:V:112:VAL:HG22	1.95	0.48
5:F:137:VAL:HG22	5:F:151:LYS:HG3	1.95	0.47
7:H:101:LEU:O	7:H:116:ARG:NH1	2.47	0.47
13:N:14:SER:HB3	35:2:1016:U:H5"	1.95	0.47
2:C:33:VAL:HG12	2:C:44:ILE:HD12	1.95	0.47
22:W:23:ARG:NH2	25:Z:19:ALA:O	2.47	0.47
23:X:101:LEU:HB3	23:X:124:LYS:HB2	1.95	0.47
35:2:602:G:H5"	35:2:603:C:H2'	1.96	0.47
35:2:1488:C:H3'	35:2:1489:A:H4'	1.97	0.47
3:D:121:ARG:HH12	3:D:123:ARG:HD3	1.80	0.47
5:F:150:MET:CE	5:F:152:PHE:HZ	2.26	0.47
8:I:2:GLY:N	35:2:441:C:OP2	2.48	0.47
19:T:98:VAL:HG11	19:T:106:LYS:HG3	1.97	0.47
35:2:1407:U:H3	35:2:1439:A:H62	1.62	0.47
21:V:87:ARG:NH2	35:2:1447:G:OP1	2.36	0.47
22:W:4:MET:HG3	35:2:683:G:H4'	1.95	0.47
23:X:107:ARG:O	23:X:110:HIS:ND1	2.43	0.47
9:J:113:GLN:OE1	9:J:154:GLN:NE2	2.48	0.47
17:R:131:LYS:HB2	17:R:140:ARG:HH22	1.80	0.47
24:Y:107:ARG:NH2	35:2:492:C:OP2	2.47	0.47
2:C:134:LEU:HB3	2:C:219:LYS:HB2	1.95	0.47
14:O:38:ALA:O	14:O:42:LEU:N	2.47	0.47
6:G:2:LYS:HB2	6:G:108:VAL:HG22	1.96	0.47
8:I:22:HIS:HB3	35:2:433:A:H5"	1.96	0.47
9:J:121:LYS:H	9:J:125:HIS:HD2	1.62	0.47
13:N:107:LYS:NZ	35:2:1075:C:OP1	2.46	0.47
17:R:34:VAL:HB	17:R:42:ILE:HD11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2:874:G:H2'	35:2:875:A:H8	1.80	0.47
4:E:49:ARG:NH2	35:2:496:C:OP1	2.43	0.47
5:F:123:LEU:O	5:F:127:MET:HG2	2.15	0.47
35:2:1692:U:H2'	35:2:1693:G:C8	2.50	0.46
3:D:196:ILE:HB	3:D:223:TYR:HB2	1.97	0.46
35:2:1726:G:H1	35:2:1808:U:H3	1.62	0.46
5:F:208:VAL:HG13	18:S:41:ILE:HG12	1.98	0.46
6:G:57:ASP:HA	6:G:106:LEU:HA	1.96	0.46
18:S:98:VAL:HG13	18:S:102:THR:HB	1.97	0.46
23:X:88:ASP:OD1	23:X:88:ASP:N	2.37	0.46
35:2:1413:G:H2'	35:2:1414:A:H8	1.79	0.46
2:C:136:ARG:HB2	2:C:218:LEU:HD11	1.96	0.46
5:F:195:THR:HG23	5:F:201:LYS:HG3	1.97	0.46
11:L:88:ILE:HD11	11:L:109:MET:HE2	1.97	0.46
1:B:6:ASP:HA	1:B:9:GLN:HG2	1.96	0.46
13:N:91:LEU:HD12	13:N:125:LEU:HD12	1.96	0.46
8:I:91:VAL:O	8:I:94:LYS:NZ	2.41	0.46
35:2:1139:C:H5	35:2:1149:A:H62	1.61	0.46
12:M:12:TYR:HB3	12:M:83:LEU:HD11	1.98	0.46
35:2:1101:U:H2'	35:2:1102:G:C8	2.50	0.46
17:R:140:ARG:HA	17:R:140:ARG:HD3	1.71	0.46
4:E:104:ASP:HB3	4:E:110:ALA:HB2	1.98	0.45
4:E:87:MET:HB3	4:E:87:MET:HE2	1.84	0.45
24:Y:55:ILE:HG12	24:Y:75:ILE:HG12	1.99	0.45
10:K:87:LEU:HA	10:K:90:VAL:HG22	1.98	0.45
2:C:139:CYS:HB2	2:C:172:MET:HE1	1.98	0.45
6:G:2:LYS:HD3	6:G:15:LEU:HD21	1.98	0.45
6:G:56:ASN:HD21	35:2:155:G:H21	1.65	0.45
14:O:126:GLU:HA	14:O:129:LYS:HG2	1.99	0.45
35:2:857:U:H2'	35:2:858:A:C8	2.51	0.45
19:T:15:VAL:HB	19:T:20:ILE:HD12	1.99	0.45
35:2:1550:G:O2'	35:2:1577:G:N2	2.50	0.45
9:J:18:ARG:NH1	35:2:3:C:O2	2.49	0.45
15:P:45:THR:HA	15:P:52:THR:HA	1.98	0.45
35:2:955:A:N1	35:2:968:U:O2'	2.40	0.45
35:2:980:A:H2'	35:2:981:A:C8	2.51	0.45
1:B:79:SER:HB2	1:B:130:ASP:HB3	1.99	0.45
6:G:8:PRO:O	6:G:131:ARG:NH2	2.50	0.45
6:G:126:ASP:OD1	6:G:126:ASP:N	2.49	0.45
22:W:69:LEU:HD21	22:W:72:CYS:HB2	1.99	0.45
22:W:104:LEU:HD12	22:W:125:ILE:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:18:ARG:NH2	35:2:4:C:O2'	2.50	0.45
2:C:88:THR:HA	2:C:98:THR:HA	1.98	0.44
7:H:65:PRO:HB2	7:H:67:PRO:HD2	1.99	0.44
2:C:127:VAL:HG21	2:C:173:THR:HA	1.99	0.44
35:2:1536:G:H2'	35:2:1537:A:C8	2.51	0.44
35:2:1785:C:O2'	35:2:1786:U:O5'	2.34	0.44
5:F:173:ARG:HD3	5:F:173:ARG:HA	1.82	0.44
10:K:82:ASN:HA	10:K:85:LYS:HD2	1.99	0.44
13:N:121:ARG:NH1	35:2:925:G:OP1	2.51	0.44
5:F:185:LYS:HE2	35:2:1335:G:H5'	1.99	0.44
21:V:67:LYS:HB3	35:2:1337:C:H5"	1.99	0.44
8:I:55:TYR:OH	35:2:309:G:OP2	2.33	0.44
10:K:201:LYS:HE3	10:K:204:ARG:HH21	1.83	0.44
17:R:142:GLN:HE22	35:2:1225:U:H1'	1.83	0.44
11:L:4:ILE:HG21	11:L:56:ILE:HD12	2.00	0.44
35:2:1722:G:O6	35:2:1812:U:O2	2.34	0.44
3:D:178:HIS:CD2	3:D:200:ARG:HH21	2.36	0.44
10:K:31:ASN:HB2	10:K:117:ILE:HD13	2.00	0.44
17:R:35:ASN:N	17:R:70:VAL:O	2.46	0.44
1:B:8:LEU:HD11	25:Z:39:VAL:HG21	2.00	0.44
2:C:123:ALA:HB2	2:C:165:ARG:HG3	2.00	0.44
9:J:88:ASP:OD1	9:J:88:ASP:N	2.44	0.44
10:K:201:LYS:HG3	10:K:204:ARG:HE	1.83	0.44
17:R:36:GLY:HA3	20:U:7:LYS:HE2	1.99	0.44
6:G:170:ARG:HH22	35:2:74:G:H22	1.66	0.43
13:N:24:THR:O	13:N:27:LYS:NZ	2.51	0.43
6:G:183:ARG:NH1	35:2:317:C:OP2	2.36	0.43
19:T:38:ARG:O	19:T:42:HIS:ND1	2.45	0.43
35:2:115:U:H2'	35:2:116:U:C6	2.53	0.43
35:2:1374:C:O2'	35:2:1464:C:O2	2.33	0.43
6:G:132:ARG:O	35:2:168:C:O2'	2.36	0.43
35:2:931:C:H2'	35:2:932:G:C8	2.54	0.43
35:2:964:A:H2'	35:2:965:U:H6	1.83	0.43
3:D:124:PHE:O	3:D:143:CYS:HA	2.18	0.43
11:L:51:ILE:HG13	11:L:52:GLU:HG2	2.00	0.43
35:2:145:G:H2'	35:2:146:G:C8	2.54	0.43
35:2:160:U:O2'	35:2:162:C:OP2	2.30	0.43
35:2:1013:U:OP1	35:2:1129:G:O2'	2.35	0.43
35:2:1098:C:H2'	35:2:1099:G:C8	2.53	0.43
2:C:179:ASN:HB3	2:C:183:GLU:HB3	1.99	0.43
9:J:138:ARG:HG2	9:J:156:HIS:CD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:56:MET:HB2	21:V:86:LYS:HB3	2.01	0.43
23:X:141:PRO:O	23:X:142:ARG:NE	2.50	0.43
35:2:996:A:H2'	35:2:997:A:C8	2.54	0.43
3:D:134:ASN:HA	3:D:167:ARG:HH12	1.83	0.43
35:2:1617:G:N1	35:2:1620:A:OP2	2.52	0.43
2:C:137:LEU:HD11	2:C:176:VAL:HG21	2.00	0.43
7:H:81:ARG:O	7:H:85:LYS:NZ	2.46	0.43
35:2:500:A:H5'	35:2:501:C:H5	1.84	0.43
4:E:91:SER:OG	4:E:98:ASN:ND2	2.52	0.43
13:N:64:ARG:NH2	35:2:919:A:OP2	2.52	0.43
2:C:216:LYS:NZ	35:2:943:U:OP2	2.37	0.42
4:E:248:ILE:HD12	4:E:248:ILE:HA	1.87	0.42
35:2:594:A:H61	35:2:643:A:H5"	1.83	0.42
35:2:1401:A:H2'	35:2:1402:A:C8	2.54	0.42
6:G:205:GLU:HA	6:G:208:GLU:HG2	2.01	0.42
18:S:100:PRO:HG2	18:S:122:PRO:HD3	2.01	0.42
35:2:1277:C:H2'	35:2:1278:A:H8	1.84	0.42
35:2:1779:G:H2'	35:2:1780:G:C8	2.54	0.42
8:I:25:ARG:NH2	35:2:434:G:OP2	2.52	0.42
12:M:82:TYR:HD2	12:M:83:LEU:HD12	1.85	0.42
35:2:808:A:O2'	35:2:809:A:O5'	2.36	0.42
1:B:76:VAL:HG12	1:B:87:VAL:HG13	2.00	0.42
4:E:219:ALA:O	35:2:808:A:H5"	2.18	0.42
35:2:488:U:H6	35:2:488:U:H2'	1.70	0.42
35:2:639:C:H2'	35:2:640:A:C8	2.55	0.42
13:N:87:ASP:N	13:N:87:ASP:OD1	2.53	0.42
35:2:1757:G:O6	35:2:1775:U:O2	2.36	0.42
7:H:66:VAL:HB	35:2:913:A:H1'	2.01	0.42
10:K:33:ILE:HA	10:K:36:GLN:HB2	2.00	0.42
16:Q:26:LEU:HD23	16:Q:26:LEU:HA	1.90	0.42
35:2:190:G:O2'	35:2:209:A:N6	2.49	0.42
13:N:54:LEU:HB3	13:N:60:VAL:HB	2.01	0.42
13:N:55:ARG:NH1	13:N:56:ASP:OD1	2.53	0.42
16:Q:43:ARG:O	16:Q:47:ARG:HG2	2.20	0.42
35:2:955:A:N6	35:2:971:G:O2'	2.51	0.42
8:I:38:ILE:HG13	8:I:96:LEU:HD11	2.01	0.42
8:I:83:TYR:HD2	8:I:101:ILE:HD13	1.85	0.42
24:Y:86:GLU:OE2	24:Y:90:ARG:NH1	2.40	0.42
13:N:109:LYS:HD3	13:N:109:LYS:HA	1.88	0.42
23:X:98:ASP:OD2	23:X:140:ARG:NH2	2.52	0.42
35:2:1705:C:H2'	35:2:1706:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:98:ARG:HH22	6:G:103:ASP:HB2	1.84	0.42
35:2:388:U:H2'	35:2:389:A:C8	2.55	0.42
4:E:44:LEU:HD13	4:E:72:ILE:HD11	2.01	0.41
7:H:119:SER:OG	7:H:120:ARG:NH1	2.53	0.41
11:L:121:GLN:HG2	11:L:147:LYS:HZ1	1.85	0.41
35:2:1213:C:H2'	35:2:1214:A:C8	2.55	0.41
4:E:62:LYS:HE2	4:E:62:LYS:HB3	1.81	0.41
5:F:7:LYS:HA	5:F:7:LYS:HD3	1.89	0.41
11:L:4:ILE:HD11	11:L:54:THR:HB	2.03	0.41
14:O:33:ARG:HD2	14:O:91:LEU:HD11	2.02	0.41
14:O:55:ASN:OD1	14:O:55:ASN:N	2.54	0.41
35:2:118:C:H1'	35:2:445:A:C5	2.56	0.41
35:2:500:A:H5'	35:2:501:C:C5	2.55	0.41
35:2:1265:A:O2'	35:2:1327:G:OP2	2.36	0.41
35:2:1753:C:H2'	35:2:1754:G:C8	2.55	0.41
11:L:12:LYS:HE2	11:L:12:LYS:HB3	1.82	0.41
18:S:4:VAL:HG22	35:2:1466:G:H5'	2.03	0.41
22:W:83:LEU:HD11	22:W:117:ARG:HD3	2.02	0.41
35:2:5:U:H2'	35:2:6:G:H8	1.85	0.41
35:2:1508:A:H5"	35:2:1508:A:H8	1.84	0.41
3:D:85:SER:OG	25:Z:25:GLY:O	2.32	0.41
4:E:49:ARG:HH22	35:2:496:C:P	2.43	0.41
4:E:124:CYS:HB3	4:E:141:THR:HB	2.03	0.41
17:R:32:ILE:HG12	17:R:68:ILE:HD12	2.02	0.41
35:2:420:G:O2'	35:2:660:C:N3	2.41	0.41
35:2:1413:G:H2'	35:2:1414:A:C8	2.56	0.41
4:E:29:PRO:HA	35:2:496:C:H5'	2.02	0.41
4:E:179:ASN:HD21	4:E:230:LYS:HD2	1.86	0.41
5:F:193:ASP:HA	5:F:194:PRO:HD2	1.76	0.41
6:G:201:LYS:HB3	6:G:201:LYS:HE3	1.79	0.41
7:H:62:ILE:HD12	7:H:94:PHE:HE1	1.85	0.41
9:J:18:ARG:O	9:J:24:ARG:NH1	2.53	0.41
35:2:1439:A:H2'	35:2:1440:C:O4'	2.20	0.41
3:D:170:TRP:CE2	3:D:199:PRO:HG3	2.55	0.41
4:E:107:GLY:HA2	4:E:189:LEU:HG	2.03	0.41
5:F:195:THR:H	5:F:201:LYS:HG2	1.85	0.41
6:G:98:ARG:NH2	6:G:101:ILE:O	2.50	0.41
14:O:69:CYS:HA	14:O:74:ILE:HB	2.02	0.41
15:P:28:PHE:HB3	15:P:47:LEU:HD21	2.03	0.41
35:2:178:C:H2'	35:2:179:C:H6	1.86	0.41
35:2:562:U:H2'	35:2:563:G:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2:1010:G:H2'	35:2:1011:A:C8	2.56	0.41
35:2:1189:A:H2'	35:2:1190:A:C8	2.55	0.41
35:2:1590:C:H3'	35:2:1591:C:H6	1.84	0.41
35:2:1606:G:N2	35:2:1632:G:H1'	2.35	0.41
35:2:1808:U:H2'	35:2:1809:A:C8	2.56	0.41
2:C:144:LYS:HB2	2:C:208:HIS:HB2	2.03	0.41
5:F:23:GLU:O	5:F:27:ARG:HG3	2.21	0.41
10:K:60:ARG:HD2	35:2:1679:A:H2'	2.02	0.41
19:T:14:ARG:HE	19:T:17:ASN:HA	1.86	0.41
7:H:119:SER:HB2	35:2:913:A:N6	2.36	0.40
9:J:121:LYS:HG2	9:J:125:HIS:CD2	2.56	0.40
20:U:115:LYS:HE3	20:U:115:LYS:HB2	1.93	0.40
23:X:76:LYS:HB3	35:2:482:G:H5'	2.02	0.40
35:2:508:A:H3'	35:2:509:G:H8	1.85	0.40
7:H:160:LYS:HA	7:H:163:GLN:HB3	2.02	0.40
9:J:151:LEU:HD12	9:J:151:LEU:HA	1.95	0.40
35:2:531:A:N1	35:2:552:G:C6	2.89	0.40
35:2:1139:C:H2'	35:2:1140:G:O4'	2.21	0.40
3:D:208:PRO:HD3	9:J:18:ARG:HH12	1.86	0.40
18:S:79:GLU:O	18:S:83:ASN:ND2	2.54	0.40
35:2:16:G:H2'	35:2:17:C:C6	2.56	0.40
35:2:799:U:H2'	35:2:800:U:C6	2.57	0.40
35:2:1648:G:N2	35:2:1675:A:OP2	2.41	0.40
1:B:135:THR:O	1:B:138:SER:OG	2.34	0.40
2:C:49:VAL:HB	2:C:62:LEU:HD13	2.04	0.40
12:M:29:MET:HA	12:M:30:PRO:HD3	1.91	0.40
3:D:194:ARG:HD3	3:D:196:ILE:HD11	2.04	0.40
11:L:33:LEU:HD23	11:L:33:LEU:HA	1.91	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	B	204/295 (69%)	195 (96%)	9 (4%)	0	100	100
2	C	211/264 (80%)	207 (98%)	4 (2%)	0	100	100
3	D	216/293 (74%)	211 (98%)	5 (2%)	0	100	100
4	E	260/263 (99%)	251 (96%)	9 (4%)	0	100	100
5	F	223/243 (92%)	211 (95%)	10 (4%)	2 (1%)	17	35
6	G	228/249 (92%)	221 (97%)	7 (3%)	0	100	100
7	H	184/194 (95%)	179 (97%)	5 (3%)	0	100	100
8	I	203/208 (98%)	200 (98%)	3 (2%)	0	100	100
9	J	178/194 (92%)	170 (96%)	7 (4%)	1 (1%)	25	47
10	K	187/204 (92%)	176 (94%)	8 (4%)	3 (2%)	9	19
11	L	149/158 (94%)	140 (94%)	9 (6%)	0	100	100
12	M	95/165 (58%)	91 (96%)	4 (4%)	0	100	100
13	N	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
14	O	121/132 (92%)	118 (98%)	3 (2%)	0	100	100
15	P	133/151 (88%)	129 (97%)	4 (3%)	0	100	100
16	Q	118/145 (81%)	116 (98%)	2 (2%)	0	100	100
17	R	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
18	S	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
19	T	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
20	U	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
21	V	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
22	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
23	X	139/143 (97%)	135 (97%)	3 (2%)	1 (1%)	22	43
24	Y	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
25	Z	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
26	a	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
27	b	80/84 (95%)	72 (90%)	8 (10%)	0	100	100
28	c	99/115 (86%)	99 (100%)	0	0	100	100
29	d	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
30	e	48/59 (81%)	45 (94%)	2 (4%)	1 (2%)	7	13
31	f	52/56 (93%)	50 (96%)	0	2 (4%)	3	4
32	g	70/156 (45%)	62 (89%)	6 (9%)	2 (3%)	4	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
33	h	20/25 (80%)	20 (100%)	0	0	100 100
34	j	312/317 (98%)	293 (94%)	19 (6%)	0	100 100
36	i	31/180 (17%)	29 (94%)	2 (6%)	0	100 100
All	All	4815/5681 (85%)	4625 (96%)	178 (4%)	12 (0%)	50 71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	K	166	ILE
32	g	89	LYS
9	J	161	LEU
10	K	41	VAL
32	g	83	LYS
5	F	192	TRP
10	K	40	ALA
30	e	27	LYS
31	f	13	LYS
31	f	14	PHE
23	X	86	PRO
5	F	193	ASP

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	B	172/243 (71%)	171 (99%)	1 (1%)	86 95
2	C	194/231 (84%)	194 (100%)	0	100 100
3	D	182/225 (81%)	180 (99%)	2 (1%)	73 88
4	E	224/225 (100%)	223 (100%)	1 (0%)	91 97
5	F	188/202 (93%)	187 (100%)	1 (0%)	88 96
6	G	200/218 (92%)	200 (100%)	0	100 100
7	H	167/174 (96%)	167 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	I	178/180 (99%)	176 (99%)	2 (1%)	73 88
9	J	160/168 (95%)	158 (99%)	2 (1%)	69 86
10	K	159/170 (94%)	157 (99%)	2 (1%)	69 86
11	L	135/142 (95%)	133 (98%)	2 (2%)	65 83
12	M	88/136 (65%)	87 (99%)	1 (1%)	73 88
13	N	130/131 (99%)	130 (100%)	0	100 100
14	O	104/108 (96%)	103 (99%)	1 (1%)	76 90
15	P	104/119 (87%)	100 (96%)	4 (4%)	33 59
16	Q	107/130 (82%)	106 (99%)	1 (1%)	78 91
17	R	115/121 (95%)	115 (100%)	0	100 100
18	S	118/122 (97%)	117 (99%)	1 (1%)	81 92
19	T	124/132 (94%)	123 (99%)	1 (1%)	81 92
20	U	114/115 (99%)	113 (99%)	1 (1%)	78 91
21	V	93/107 (87%)	91 (98%)	2 (2%)	52 76
22	W	112/113 (99%)	111 (99%)	1 (1%)	78 91
23	X	113/115 (98%)	111 (98%)	2 (2%)	59 80
24	Y	108/115 (94%)	108 (100%)	0	100 100
25	Z	66/67 (98%)	66 (100%)	0	100 100
26	a	64/103 (62%)	63 (98%)	1 (2%)	62 82
27	b	74/76 (97%)	74 (100%)	0	100 100
28	c	88/98 (90%)	88 (100%)	0	100 100
29	d	54/62 (87%)	52 (96%)	2 (4%)	34 60
30	e	40/48 (83%)	39 (98%)	1 (2%)	47 73
31	f	48/49 (98%)	48 (100%)	0	100 100
32	g	65/140 (46%)	62 (95%)	3 (5%)	27 51
33	h	21/24 (88%)	21 (100%)	0	100 100
34	j	272/275 (99%)	271 (100%)	1 (0%)	91 97
36	i	27/151 (18%)	27 (100%)	0	100 100
All	All	4208/4835 (87%)	4172 (99%)	36 (1%)	79 91

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	151	ASP
3	D	248	TYR
3	D	254	ASP
4	E	220	THR
5	F	79	PHE
8	I	139	LYS
8	I	141	ARG
9	J	91	LYS
9	J	156	HIS
10	K	55	ARG
10	K	136	ARG
11	L	30	LYS
11	L	69	ARG
12	M	44	HIS
14	O	99	LYS
15	P	52	THR
15	P	98	ARG
15	P	121	ARG
15	P	150	ARG
16	Q	79	HIS
18	S	80	ARG
19	T	83	PHE
20	U	102	ARG
21	V	19	ARG
21	V	79	ARG
22	W	78	ARG
23	X	88	ASP
23	X	105	PHE
26	a	65	TYR
29	d	55	VAL
29	d	66	ARG
30	e	8	ARG
32	g	85	TYR
32	g	86	THR
32	g	87	THR
34	j	71	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	GLN
2	C	40	ASN
3	D	272	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	8	HIS
4	E	50	ASN
4	E	98	ASN
4	E	179	ASN
5	F	22	ASN
5	F	174	HIS
5	F	179	GLN
6	G	56	ASN
6	G	81	HIS
7	H	73	GLN
7	H	157	HIS
8	I	116	HIS
9	J	125	HIS
9	J	154	GLN
9	J	156	HIS
10	K	31	ASN
10	K	79	HIS
10	K	149	GLN
10	K	203	ASN
11	L	112	HIS
12	M	32	HIS
12	M	44	HIS
13	N	49	GLN
16	Q	79	HIS
17	R	11	GLN
17	R	142	GLN
18	S	83	ASN
19	T	105	ASN
20	U	91	HIS
23	X	46	HIS
24	Y	15	ASN
24	Y	63	HIS
25	Z	47	ASN
26	a	103	HIS
28	c	25	ASN
28	c	72	HIS
34	j	4	GLN
34	j	14	HIS
34	j	64	HIS
34	j	117	ASN
34	j	188	HIS
36	i	158	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	2	1655/1868 (88%)	407 (24%)	41 (2%)

All (407) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	2	2	A
35	2	3	C
35	2	17	C
35	2	33	G
35	2	41	G
35	2	44	U
35	2	45	A
35	2	46	A
35	2	49	C
35	2	56	G
35	2	58	C
35	2	64	A
35	2	65	C
35	2	66	G
35	2	67	C
35	2	68	A
35	2	69	C
35	2	72	C
35	2	73	C
35	2	74	G
35	2	75	G
35	2	76	U
35	2	77	A
35	2	79	A
35	2	99	A
35	2	103	A
35	2	113	G
35	2	114	G
35	2	115	U
35	2	116	U
35	2	127	C
35	2	129	C
35	2	130	G
35	2	143	U
35	2	144	U
35	2	149	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	155	G
35	2	160	U
35	2	181	A
35	2	182	C
35	2	184	G
35	2	188	C
35	2	191	A
35	2	206	G
35	2	213	G
35	2	214	U
35	2	290	U
35	2	291	G
35	2	292	A
35	2	295	C
35	2	302	A
35	2	307	G
35	2	308	G
35	2	309	G
35	2	310	C
35	2	313	A
35	2	315	C
35	2	318	A
35	2	319	C
35	2	320	G
35	2	321	C
35	2	322	C
35	2	332	G
35	2	333	G
35	2	335	G
35	2	338	G
35	2	347	G
35	2	351	G
35	2	360	A
35	2	362	C
35	2	364	A
35	2	368	U
35	2	370	G
35	2	377	G
35	2	383	G
35	2	385	G
35	2	386	C
35	2	398	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	400	C
35	2	407	G
35	2	408	A
35	2	409	C
35	2	418	A
35	2	421	G
35	2	428	U
35	2	438	G
35	2	441	C
35	2	448	A
35	2	450	C
35	2	464	A
35	2	466	G
35	2	471	G
35	2	472	C
35	2	473	A
35	2	474	G
35	2	476	A
35	2	482	G
35	2	487	U
35	2	489	A
35	2	492	C
35	2	500	A
35	2	502	C
35	2	533	A
35	2	534	G
35	2	535	G
35	2	538	U
35	2	541	U
35	2	542	U
35	2	544	G
35	2	548	C
35	2	549	C
35	2	550	C
35	2	553	U
35	2	554	A
35	2	555	A
35	2	556	U
35	2	559	G
35	2	563	G
35	2	568	C
35	2	570	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	573	U
35	2	574	A
35	2	583	A
35	2	589	G
35	2	590	A
35	2	591	U
35	2	593	C
35	2	594	A
35	2	603	C
35	2	604	A
35	2	607	U
35	2	608	C
35	2	614	C
35	2	617	G
35	2	628	A
35	2	629	A
35	2	631	U
35	2	635	G
35	2	643	A
35	2	644	G
35	2	655	A
35	2	664	A
35	2	668	A
35	2	669	A
35	2	671	A
35	2	672	A
35	2	673	G
35	2	683	G
35	2	685	A
35	2	687	C
35	2	688	U
35	2	749	U
35	2	750	C
35	2	751	G
35	2	792	C
35	2	793	G
35	2	794	A
35	2	798	G
35	2	809	A
35	2	810	A
35	2	812	A
35	2	821	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	822	U
35	2	823	U
35	2	824	C
35	2	830	A
35	2	833	C
35	2	847	A
35	2	856	C
35	2	859	G
35	2	869	A
35	2	870	A
35	2	871	U
35	2	872	A
35	2	873	G
35	2	874	G
35	2	878	G
35	2	879	C
35	2	880	G
35	2	887	U
35	2	890	U
35	2	891	G
35	2	898	U
35	2	903	A
35	2	913	A
35	2	914	U
35	2	919	A
35	2	920	A
35	2	926	A
35	2	930	C
35	2	933	G
35	2	934	G
35	2	943	U
35	2	959	G
35	2	967	C
35	2	970	G
35	2	971	G
35	2	973	C
35	2	978	G
35	2	981	A
35	2	990	A
35	2	992	A
35	2	999	G
35	2	1002	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	1017	U
35	2	1023	A
35	2	1030	A
35	2	1039	C
35	2	1040	G
35	2	1041	G
35	2	1044	G
35	2	1049	A
35	2	1050	A
35	2	1060	A
35	2	1061	U
35	2	1062	A
35	2	1078	C
35	2	1083	A
35	2	1085	C
35	2	1089	G
35	2	1096	G
35	2	1115	U
35	2	1116	C
35	2	1118	C
35	2	1119	A
35	2	1121	G
35	2	1126	G
35	2	1131	G
35	2	1133	A
35	2	1138	C
35	2	1139	C
35	2	1148	A
35	2	1153	C
35	2	1154	U
35	2	1157	G
35	2	1171	G
35	2	1195	A
35	2	1202	U
35	2	1203	G
35	2	1207	G
35	2	1211	G
35	2	1212	G
35	2	1215	C
35	2	1217	A
35	2	1224	G
35	2	1232	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	1233	G
35	2	1234	C
35	2	1235	G
35	2	1236	G
35	2	1242	U
35	2	1243	U
35	2	1251	A
35	2	1253	A
35	2	1256	G
35	2	1257	G
35	2	1259	A
35	2	1274	G
35	2	1275	G
35	2	1279	C
35	2	1301	A
35	2	1302	G
35	2	1303	C
35	2	1309	C
35	2	1313	A
35	2	1318	G
35	2	1320	G
35	2	1325	G
35	2	1330	G
35	2	1342	U
35	2	1348	G
35	2	1358	U
35	2	1366	G
35	2	1371	U
35	2	1372	U
35	2	1374	C
35	2	1378	A
35	2	1382	A
35	2	1398	G
35	2	1401	A
35	2	1402	A
35	2	1403	C
35	2	1404	U
35	2	1406	G
35	2	1411	G
35	2	1416	C
35	2	1426	U
35	2	1428	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	1429	G
35	2	1430	C
35	2	1431	G
35	2	1432	U
35	2	1439	A
35	2	1440	C
35	2	1441	U
35	2	1445	U
35	2	1446	A
35	2	1447	G
35	2	1452	A
35	2	1454	A
35	2	1455	A
35	2	1462	U
35	2	1463	U
35	2	1465	A
35	2	1466	G
35	2	1474	A
35	2	1476	A
35	2	1477	U
35	2	1478	U
35	2	1484	A
35	2	1487	A
35	2	1489	A
35	2	1490	G
35	2	1493	C
35	2	1494	U
35	2	1498	A
35	2	1503	C
35	2	1507	G
35	2	1508	A
35	2	1515	G
35	2	1517	G
35	2	1520	G
35	2	1521	C
35	2	1524	G
35	2	1525	C
35	2	1527	C
35	2	1528	G
35	2	1531	A
35	2	1533	A
35	2	1534	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	1536	G
35	2	1537	A
35	2	1559	C
35	2	1560	U
35	2	1563	G
35	2	1566	G
35	2	1567	G
35	2	1569	A
35	2	1570	G
35	2	1572	C
35	2	1573	G
35	2	1578	U
35	2	1579	A
35	2	1580	A
35	2	1584	G
35	2	1585	U
35	2	1586	U
35	2	1588	A
35	2	1601	A
35	2	1602	U
35	2	1606	G
35	2	1610	G
35	2	1612	G
35	2	1613	G
35	2	1614	A
35	2	1615	U
35	2	1616	U
35	2	1618	C
35	2	1621	U
35	2	1623	A
35	2	1625	U
35	2	1647	A
35	2	1654	G
35	2	1656	G
35	2	1661	A
35	2	1664	A
35	2	1665	G
35	2	1671	G
35	2	1675	A
35	2	1683	C
35	2	1686	G
35	2	1692	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	1695	A
35	2	1699	A
35	2	1714	U
35	2	1721	U
35	2	1722	G
35	2	1728	U
35	2	1729	U
35	2	1761	U
35	2	1778	C
35	2	1783	C
35	2	1785	C
35	2	1786	U
35	2	1801	A
35	2	1819	A
35	2	1824	A
35	2	1825	A
35	2	1826	G
35	2	1829	G
35	2	1831	A
35	2	1833	C
35	2	1835	A
35	2	1838	U
35	2	1845	A
35	2	1848	U
35	2	1849	G
35	2	1850	A
35	2	1861	G
35	2	1862	G
35	2	1863	A
35	2	1864	U
35	2	1865	C
35	2	1866	A
35	2	1867	U
35	2	1868	U
35	2	1869	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	2	65	C
35	2	102	A
35	2	114	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2	143	U
35	2	180	G
35	2	291	G
35	2	314	U
35	2	332	G
35	2	382	C
35	2	417	C
35	2	465	A
35	2	643	A
35	2	750	C
35	2	793	G
35	2	797	C
35	2	811	A
35	2	870	A
35	2	958	G
35	2	980	A
35	2	1115	U
35	2	1137	U
35	2	1231	C
35	2	1373	C
35	2	1403	C
35	2	1415	C
35	2	1425	G
35	2	1430	C
35	2	1431	G
35	2	1438	A
35	2	1440	C
35	2	1464	C
35	2	1502	C
35	2	1558	C
35	2	1565	C
35	2	1601	A
35	2	1623	A
35	2	1692	U
35	2	1734	G
35	2	1824	A
35	2	1832	A
35	2	1868	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1550:G	O3'	1551:U	P	4.52

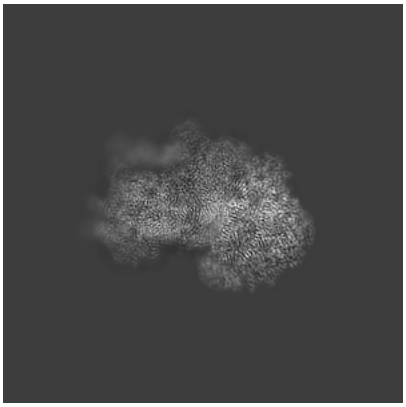
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11276. These allow visual inspection of the internal detail of the map and identification of artifacts.

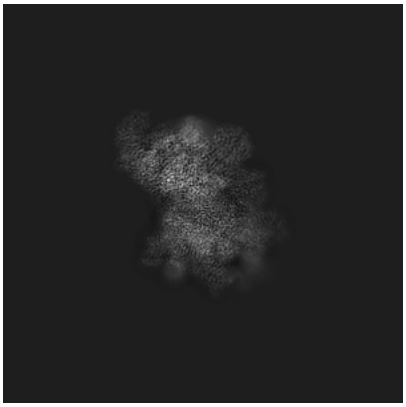
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

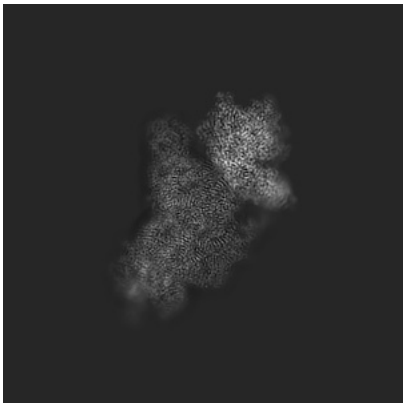
6.1.1 Primary map



X



Y



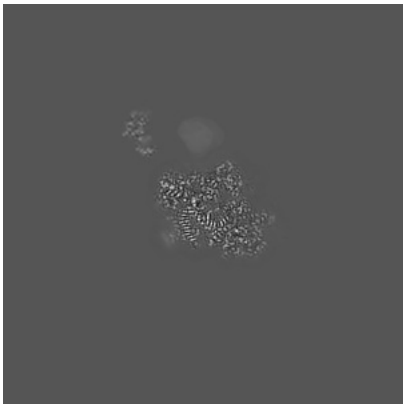
Z

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

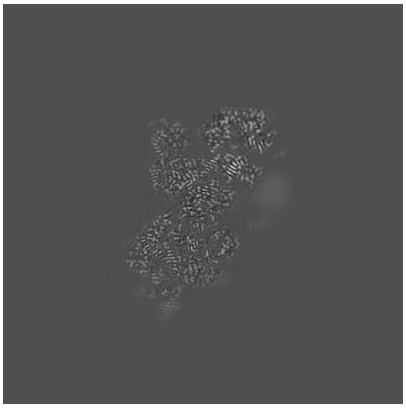
6.2 Central slices

6.2.1 Primary map

X Index: 200



Y Index: 200

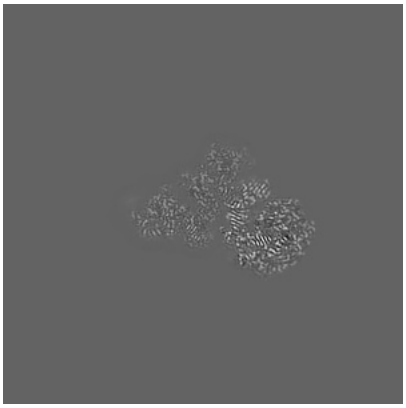


Z Index: 200

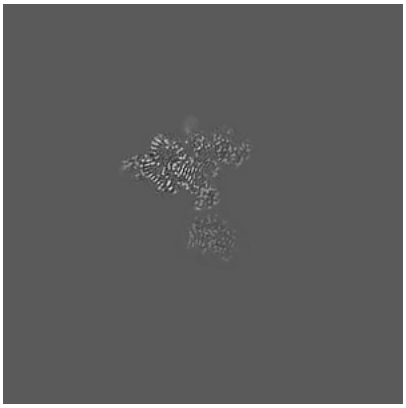
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

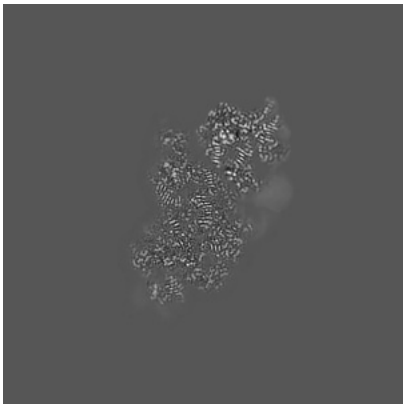
6.3.1 Primary map



X Index: 224



Y Index: 269



Z Index: 191

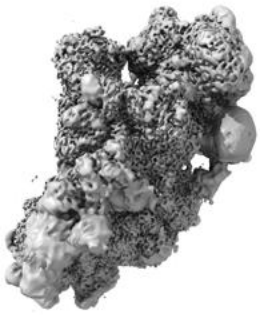
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

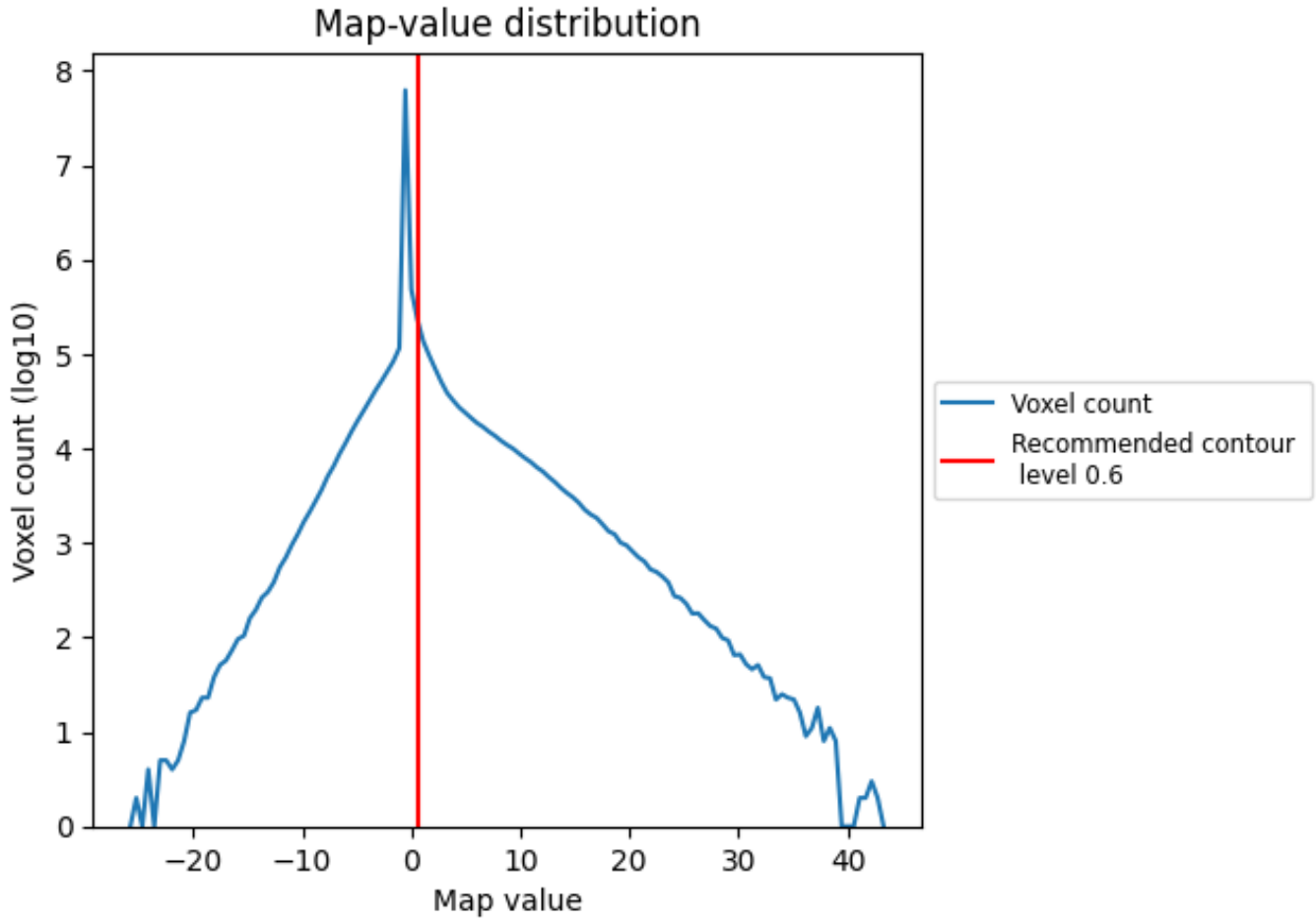
6.5 Mask visualisation (i)

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

7 Map analysis

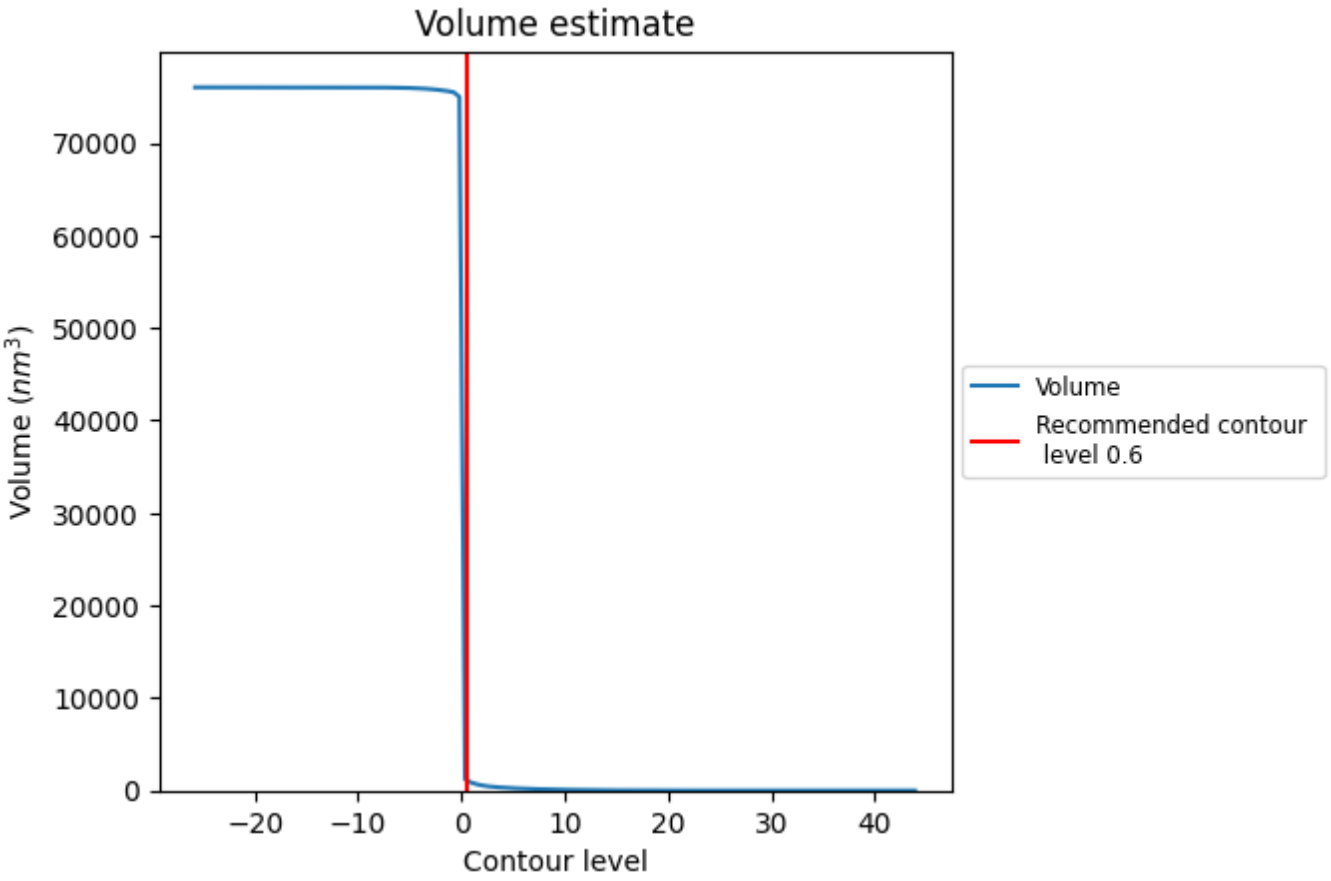
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

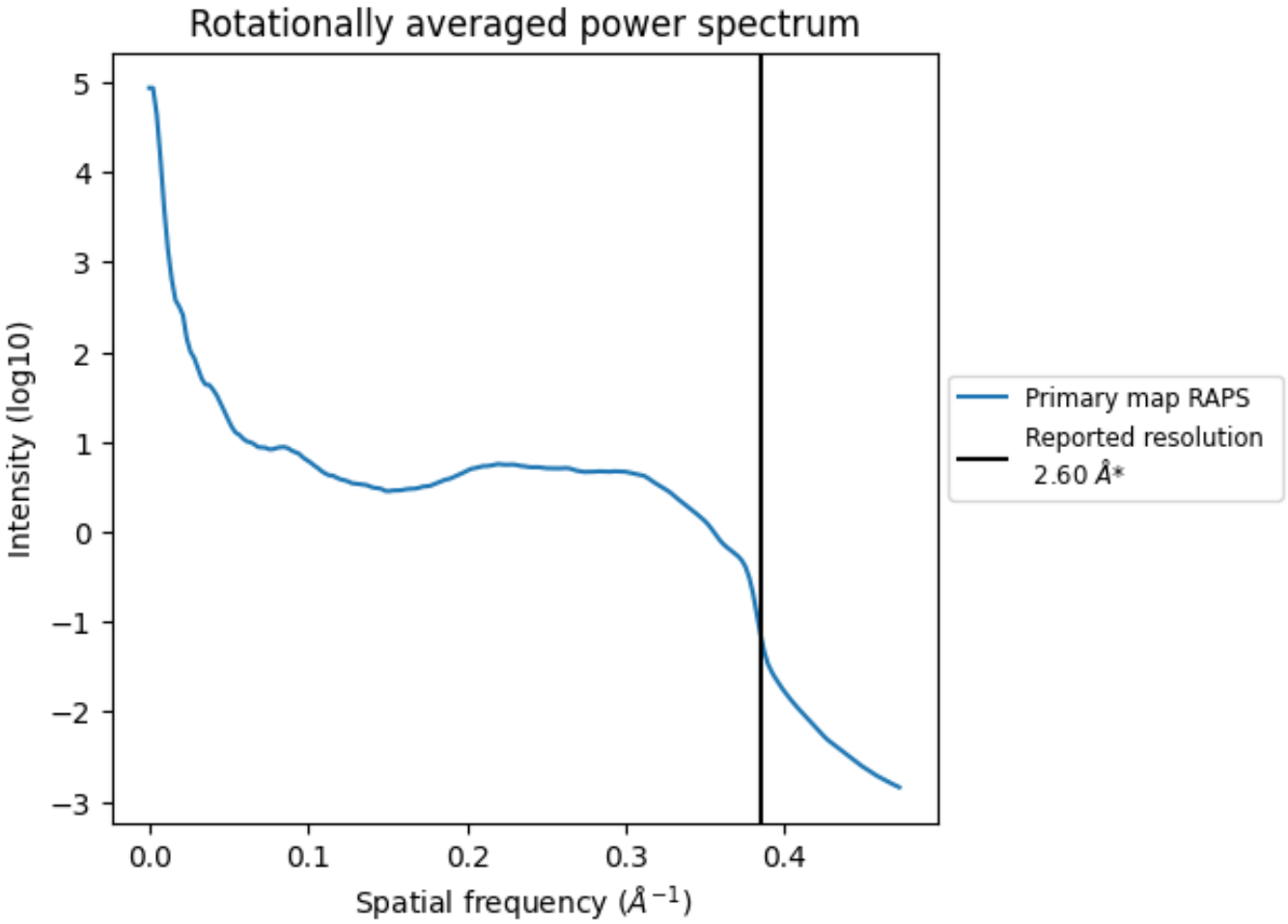
7.2 Volume estimate (i)



The volume at the recommended contour level is 1067 nm^3; this corresponds to an approximate mass of 964 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 0.385 Å^{-1}

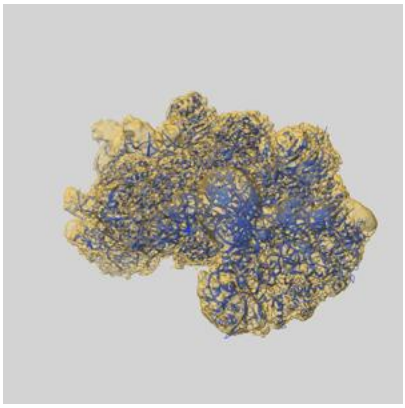
8 Fourier-Shell correlation (i)

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

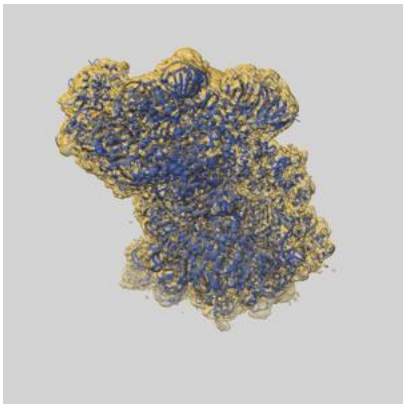
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11276 and PDB model 6ZLW. Per-residue inclusion information can be found in section 3 on page 11.

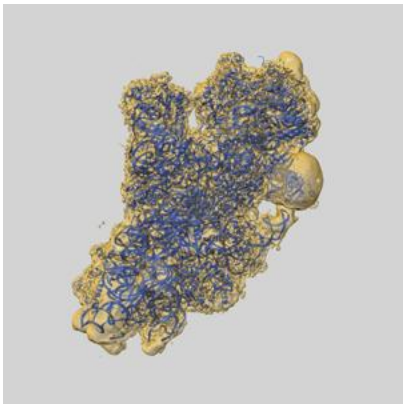
9.1 Map-model overlay



X



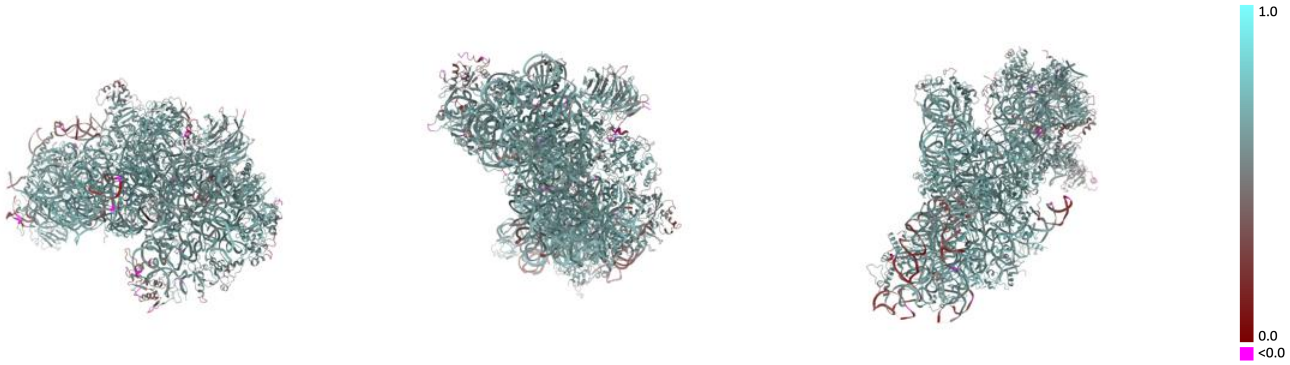
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

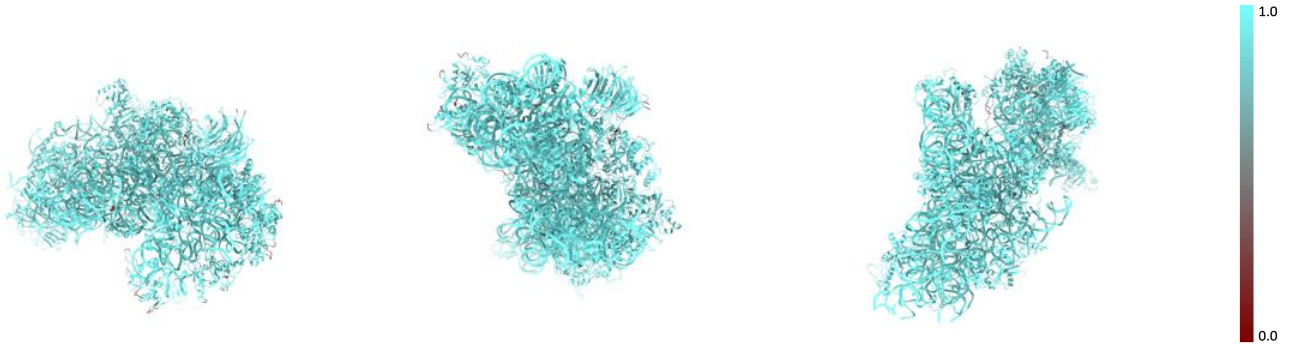
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

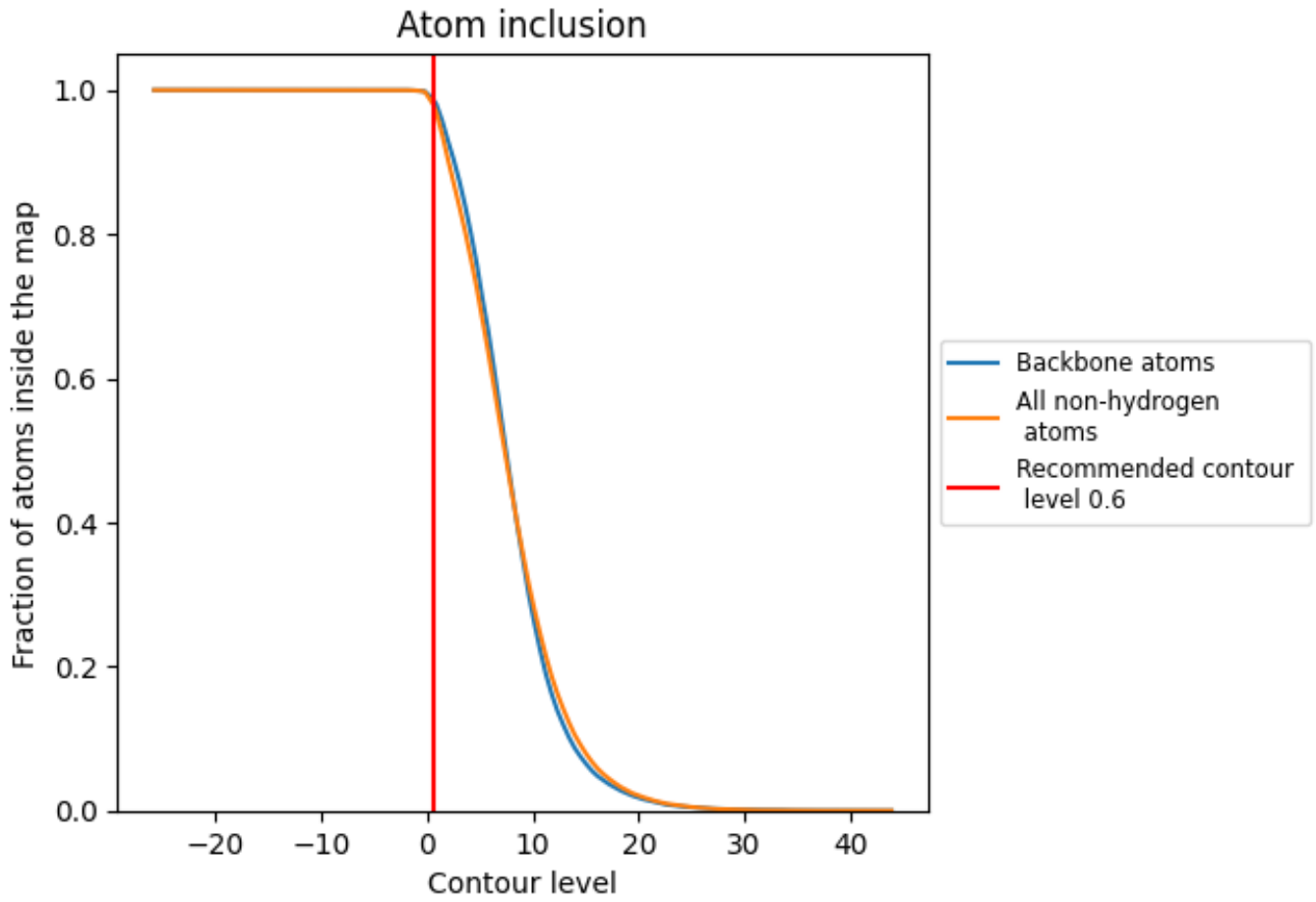
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9796	0.5950
2	0.9936	0.6080
B	0.9817	0.6240
C	0.9747	0.6020
D	0.9903	0.6510
E	0.9877	0.6470
F	0.9548	0.5420
G	0.9856	0.5770
H	0.9443	0.5000
I	0.9827	0.6010
J	0.9882	0.6470
K	0.9484	0.5670
L	0.9774	0.6130
M	0.9749	0.5750
N	0.9906	0.6230
O	0.8850	0.3610
P	0.9744	0.5920
Q	0.9382	0.5510
R	0.9925	0.6260
S	0.9411	0.5180
T	0.9201	0.5390
U	0.9542	0.5930
V	0.9731	0.5370
W	0.9901	0.6580
X	0.9832	0.6420
Y	0.9868	0.6210
Z	0.9771	0.6230
a	0.9234	0.5440
b	0.9729	0.5820
c	0.9706	0.6120
d	0.9046	0.5020
e	0.9768	0.6010
f	0.9817	0.6170
g	0.8957	0.4450
h	0.9897	0.6010

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.9804	0.6280
j	0.9553	0.5480