



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:59 AM UTC

PDB ID : 8FVY / pdb_00008fvy
EMDB ID : EMD-29495
Title : 40S subunit of the Giardia lamblia 80S ribosome
Authors : Eiler, D.R.; Wimberly, B.T.; Bilodeau, D.Y.; Rissland, O.S.; Kieft, J.S.
Deposited on : 2023-01-20
Resolution : 2.94 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:

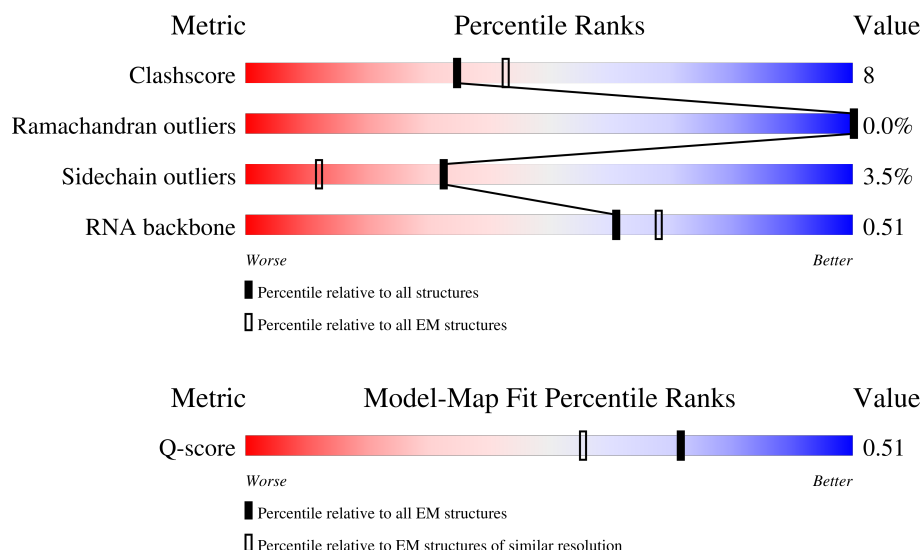
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



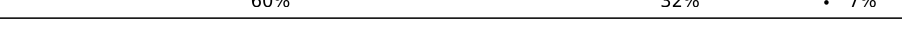
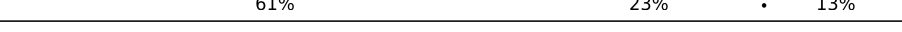
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	1451	
2	A	245	
3	B	248	

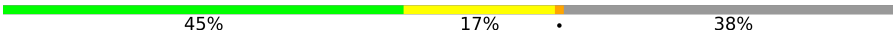
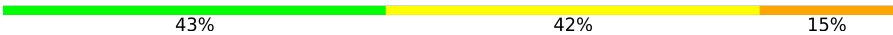
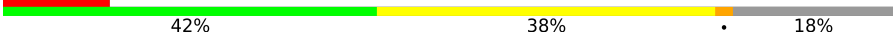
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Mol	Chain	Length	Quality of chain
4	C	242	
5	D	217	
6	E	268	
7	F	190	
8	G	248	
9	H	201	
10	I	174	
11	J	189	
12	K	134	
13	L	199	
14	N	154	
15	O	145	
16	P	145	
17	Q	158	
18	R	137	
19	S	154	
20	T	158	
21	U	126	
22	V	89	
23	W	130	
24	X	143	
25	Y	132	
26	Z	88	
27	a	109	
28	b	124	

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Mol	Chain	Length	Quality of chain
29	c	64	 59% 33% 6%
30	d	137	 45% 17% 38%
31	f	137	 15% 9% 74%
32	g	74	 43% 42% 15%
33	M	125	 12% 42% 38% 18%
34	e	69	 61% 14% 25%

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 119930 atoms, of which 52077 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 rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	2	1441	Total	C	H	N	O	P	0	0
			46630	13746	15711	5742	9991	1440		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	932	C	U	conflict	GB 2333213660

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	199	Total	C	H	N	O	S	0	0
			3230	1030	1632	279	281	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	224	Total	C	H	N	O	S	0	0
			3657	1144	1847	335	318	13		

- Molecule 4 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	209	Total	C	H	N	O	S	0	0
			3267	1028	1651	292	292	4		

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	209	Total	C	H	N	O	S	0	0
			3354	1044	1698	305	291	16		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	258	Total	C	H	N	O	S	0	0
			4212	1323	2144	378	354	13		

- Molecule 7 is a protein called SSU ribosomal protein S7P (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	190	Total	C	H	N	O	S	0	0
			2958	914	1487	279	268	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	216	Total	C	H	N	O	S	0	0
			3532	1081	1814	328	298	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	165	Total	C	H	N	O	S	0	0
			2689	848	1367	227	241	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	167	Total	C	H	N	O	S	0	0
			2659	820	1349	251	236	3		

- Molecule 11 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	164	Total	C	H	N	O	S	0	0
			2733	834	1400	260	233	6		

- Molecule 12 is a protein called Ribosomal protein S10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	105	Total	C	H	N	O	S	0	0
			1700	556	841	144	156	3		

- Molecule 13 is a protein called SSU ribosomal protein S17P.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	170	Total	C	H	N	O	S	0	0
			2826	885	1427	275	232	7		

- Molecule 14 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	153	Total	C	H	N	O	S	0	0
			2532	780	1304	237	206	5		

- Molecule 15 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	139	Total	C	H	N	O	S	0	0
			2113	645	1058	210	196	4		

- Molecule 16 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	108	Total	C	H	N	O	S	0	0
			1825	564	942	172	139	8		

- Molecule 17 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	158	Total	C	H	N	O	S	0	0
			2537	768	1302	244	219	4		

- Molecule 18 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	81	Total	C	H	N	O	S	0	0
			1350	405	699	130	114	2		

- Molecule 19 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	143	Total	C	H	N	O	S	0	0
			2294	701	1156	228	202	7		

- Molecule 20 is a protein called SSU ribosomal protein S19E (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	137	Total	C	H	N	O	S	0	0
			2163	683	1089	203	185	3		

- Molecule 21 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	103	Total	C	H	N	O	S	0	0
			1668	522	849	148	144	5		

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	81	Total	C	H	N	O	S	0	0
			1214	377	607	112	112	6		

- Molecule 23 is a protein called SSU ribosomal protein S8P (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	129	Total	C	H	N	O	S	0	0
			2104	659	1074	192	176	3		

- Molecule 24 is a protein called SSU ribosomal protein S12P.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	143	Total	C	H	N	O	S	0	0
			2310	703	1195	223	185	4		

- Molecule 25 is a protein called Ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	122	Total	C	H	N	O	S	0	0
			1988	613	1019	181	168	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	73	Total	C	H	N	O	S	0	0
			1183	366	605	104	102	6		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	96	Total	C	H	N	O	S	0	0
			1575	480	795	161	132	7		

- Molecule 28 is a protein called Ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	70	Total	C	H	N	O	S	0	0
			1078	349	532	92	101	4		

- Molecule 29 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	c	60	Total	C	H	N	O	S	0	0
			957	293	483	91	88	2		

- Molecule 30 is a protein called Ribosomal protein S29A.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d	85	Total	C	H	N	O	S	0	0
			1336	425	654	129	121	7		

- Molecule 31 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	f	35	Total	C	H	N	O	S	0	0
			535	165	265	53	48	4		

- Molecule 32 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	g	74	Total	C	H	N	O	P	0	0
			2314	701	745	274	521	73		

- Molecule 33 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	M	103	Total	C	H	N	O	S	0	0
			1679	532	843	148	148	8		

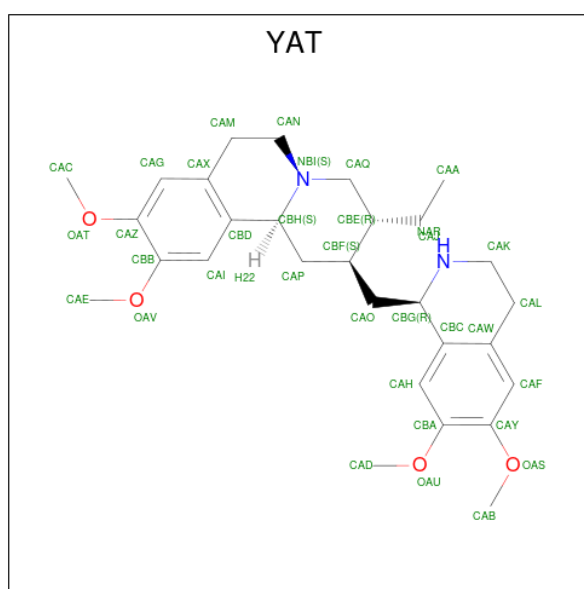
- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	52	Total	C	H	N	O	0	0
			886	269	453	93	71		

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	2	23	Total	Mg	0
			23	23	

- Molecule 36 is emetine (CCD ID: YAT) (formula: C₂₉H₄₀N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
36	2	1	Total	C	H	N	O	0
			75	29	40	2	4	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	2	591	Total	O	0
			591	591	

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Mol	Chain	Residues	Atoms		AltConf
38	B	1	Total 1	O 1	0
38	C	6	Total 6	O 6	0
38	D	6	Total 6	O 6	0
38	E	10	Total 10	O 10	0
38	F	12	Total 12	O 12	0
38	G	2	Total 2	O 2	0
38	H	1	Total 1	O 1	0
38	I	10	Total 10	O 10	0
38	K	7	Total 7	O 7	0
38	L	4	Total 4	O 4	0
38	N	9	Total 9	O 9	0
38	O	3	Total 3	O 3	0
38	P	2	Total 2	O 2	0
38	Q	12	Total 12	O 12	0
38	R	2	Total 2	O 2	0
38	S	10	Total 10	O 10	0
38	T	10	Total 10	O 10	0
38	U	6	Total 6	O 6	0
38	W	4	Total 4	O 4	0
38	X	5	Total 5	O 5	0
38	Z	6	Total 6	O 6	0

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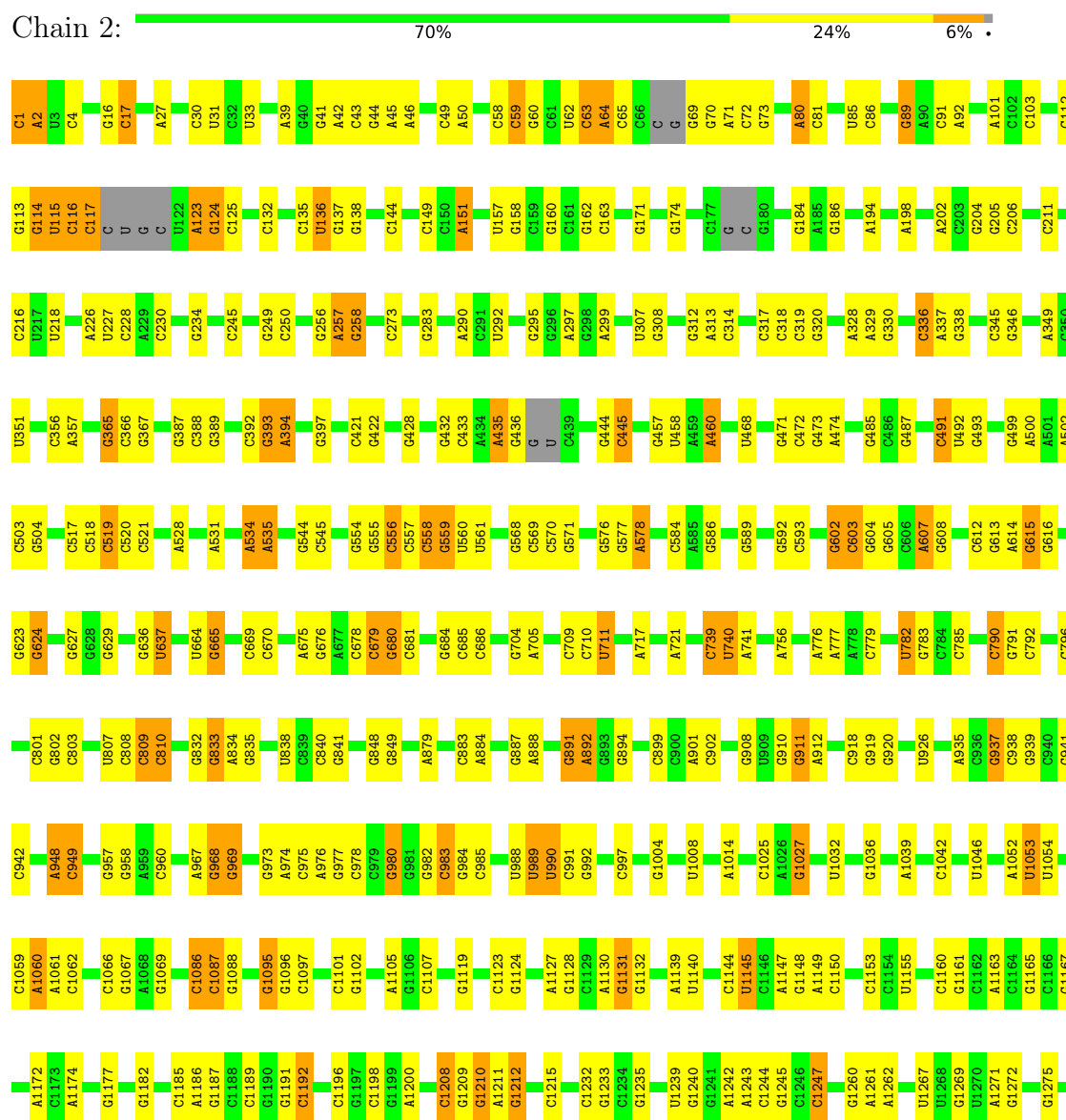
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Mol	Chain	Residues	Atoms		AltConf
38	a	6	Total 6	O 6	0
38	b	1	Total 1	O 1	0
38	d	6	Total 6	O 6	0
38	f	1	Total 1	O 1	0
38	g	2	Total 2	O 2	0
38	M	7	Total 7	O 7	0
38	e	1	Total 1	O 1	0

3 Residue-property plots

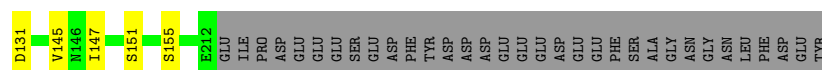
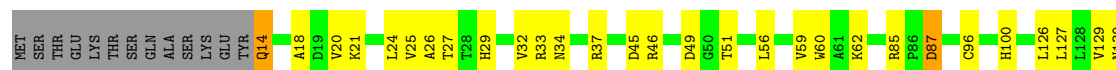
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

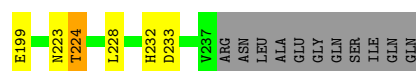
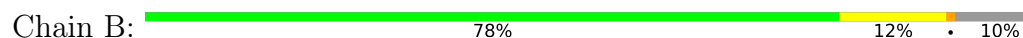




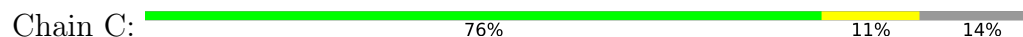
• Molecule 2: 40S ribosomal protein SA



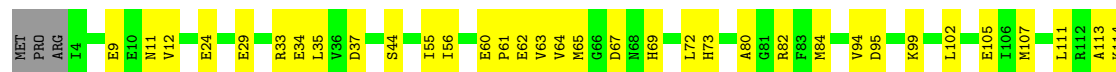
• Molecule 3: 40S ribosomal protein S3a



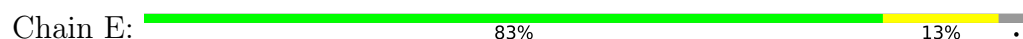
• Molecule 4: Ribosomal protein S2

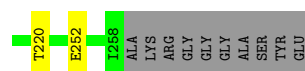


• Molecule 5: Ribosomal protein S3



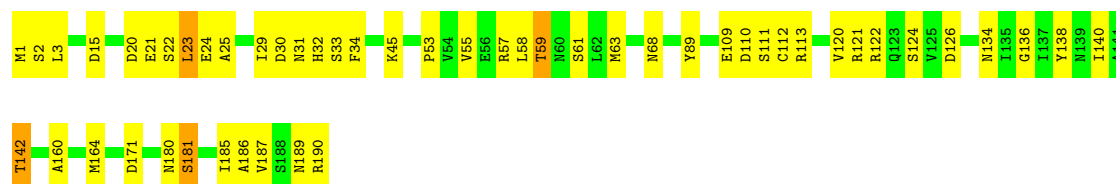
• Molecule 6: 40S ribosomal protein S4





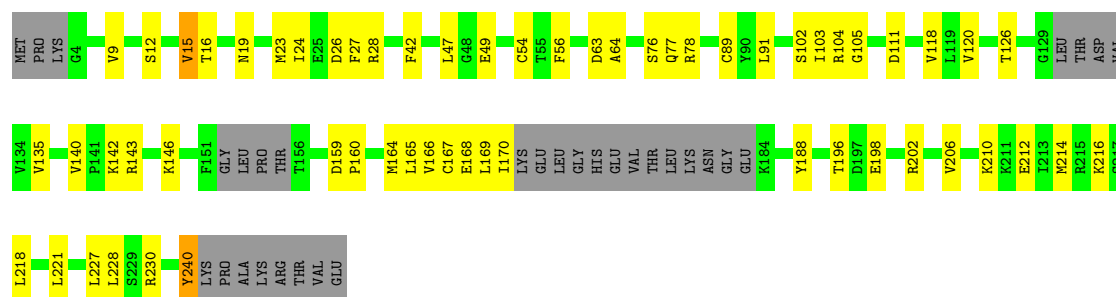
• Molecule 7: SSU ribosomal protein S7P (Fragment)

Chain F: 73% 25%



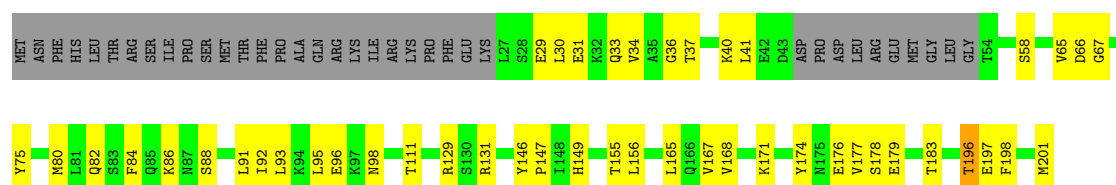
• Molecule 8: 40S ribosomal protein S6

Chain G: 63% 23% 13%



• Molecule 9: 40S ribosomal protein S7

Chain H: 59% 23% 18%



• Molecule 10: 40S ribosomal protein S8

Chain I: 82% 14%



• Molecule 11: Ribosomal protein S9

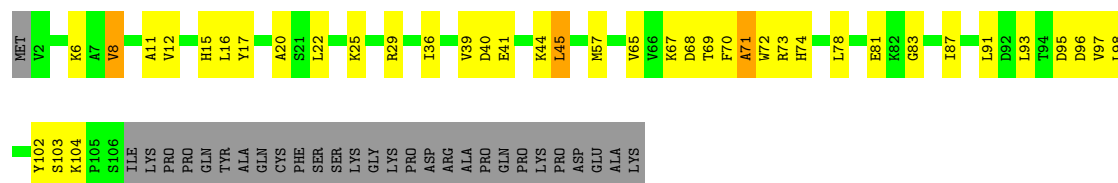
Chain J: 73% 13% 13%



ALA
ALA
ALA
ARG
ARG
GLN
SER
SER
GLY
ASP
ASN
GLU

• Molecule 12: Ribosomal protein S10B

Chain K: 49% 28% • 22%



• Molecule 13: SSU ribosomal protein S17P

Chain L: 76% 10% 15%



• Molecule 14: Ribosomal protein S13

Chain N: 82% 17% ..



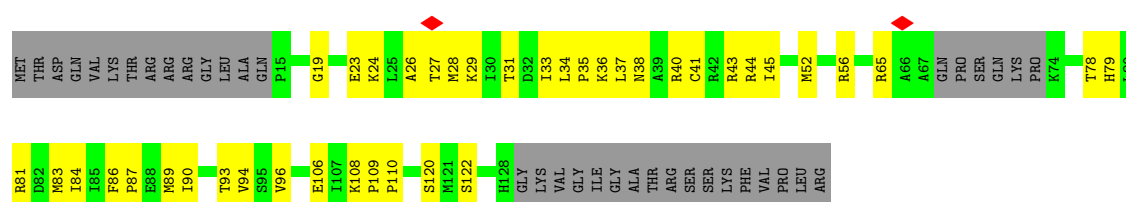
• Molecule 15: Ribosomal protein S14

Chain O: 74% 20% • •



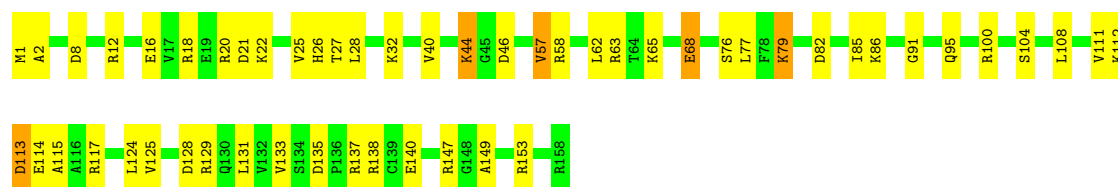
• Molecule 16: Ribosomal protein S15

Chain P: 47% 28% 26%



• Molecule 17: Ribosomal protein S16

Chain Q: 



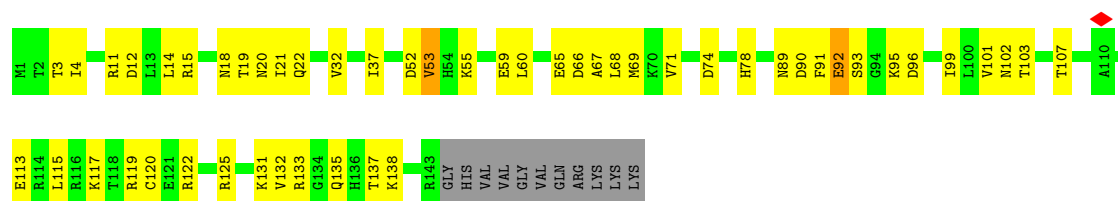
• Molecule 18: Ribosomal protein S17

Chain R: 



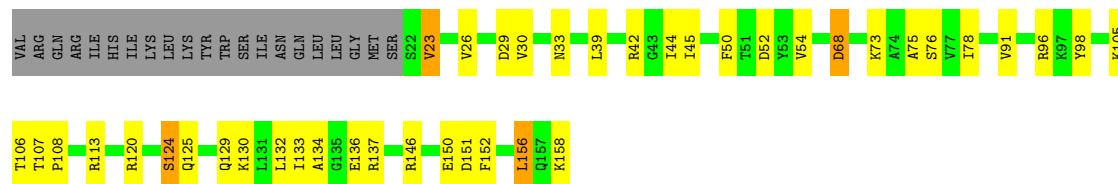
• Molecule 19: Ribosomal protein S18

Chain S: 



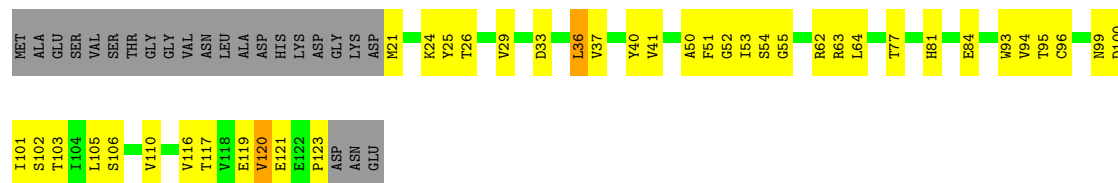
• Molecule 20: SSU ribosomal protein S19E (Fragment)

Chain T: 



• Molecule 21: Ribosomal protein S20

Chain U: 



• Molecule 22: 40S ribosomal protein S21

Chain V:  74% 16% 9%



- Molecule 23: SSU ribosomal protein S8P (Fragment)

Chain W:  87% 12% .



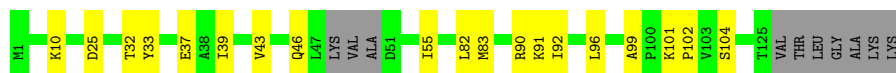
- Molecule 24: SSU ribosomal protein S12P

Chain X:  81% 18% .



- Molecule 25: Ribosomal protein S24

Chain Y:  78% 14% 8%



- Molecule 26: 40S ribosomal protein S25

Chain Z:  53% 28% 17%

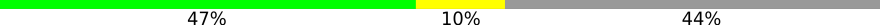


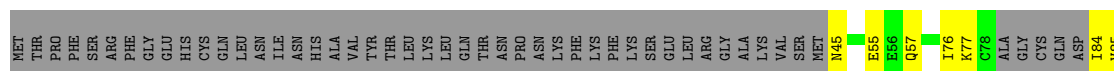
- Molecule 27: 40S ribosomal protein S26

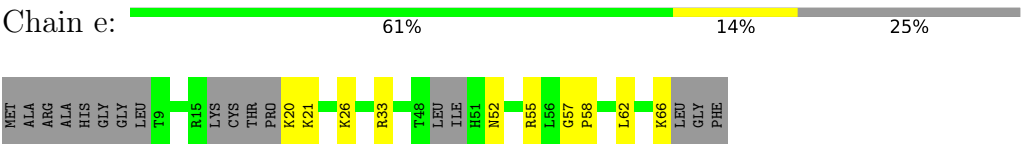
Chain a:  76% 11% 12%



- Molecule 28: Ribosomal protein S27

Chain b:  47% 10% 44%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	289618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72.26	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.990	Depositor
Minimum map value	-1.460	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.152	Depositor
Recommended contour level	0.0895	Depositor
Map size ($\text{\AA}$)	369.495, 369.495, 369.495	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8211, 0.8211, 0.8211	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, YAT, 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	2	0.25	0/34573	0.32	0/53952
2	A	0.21	0/1633	0.32	0/2219
3	B	0.25	0/1845	0.34	0/2488
4	C	0.25	0/1649	0.31	0/2225
5	D	0.56	0/1682	0.47	0/2259
6	E	0.22	0/2114	0.33	0/2852
7	F	0.65	0/1494	0.49	0/2010
8	G	0.19	0/1739	0.34	0/2317
9	H	0.21	0/1345	0.36	0/1815
10	I	0.26	0/1330	0.35	0/1784
11	J	0.20	0/1351	0.31	0/1807
12	K	0.63	0/884	0.52	0/1204
13	L	0.27	0/1429	0.32	0/1912
14	N	0.26	0/1252	0.35	0/1681
15	O	0.25	0/1070	0.35	0/1436
16	P	0.54	0/898	0.49	0/1198
17	Q	0.62	0/1247	0.49	0/1666
18	R	0.48	0/657	0.53	0/877
19	S	0.60	0/1154	0.48	0/1549
20	T	0.67	0/1098	0.49	0/1476
21	U	0.57	0/835	0.46	0/1128
22	V	0.22	0/615	0.32	0/825
23	W	0.27	0/1047	0.37	0/1412
24	X	0.24	0/1130	0.37	0/1512
25	Y	0.17	0/983	0.34	0/1314
26	Z	0.64	0/584	0.56	0/779
27	a	0.28	0/792	0.31	0/1065
28	b	0.24	0/558	0.33	0/757
29	c	0.52	0/477	0.48	0/638
30	d	0.48	0/696	0.45	0/932
31	f	0.32	0/273	0.55	0/362
32	g	0.12	0/1751	0.23	0/2727

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	M	0.37	0/848	0.53	0/1132
34	e	0.21	0/438	0.35	0/578
All	All	0.33	0/71471	0.36	0/103888

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
17	Q	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	Q	57	VAL	Peptide

5.2 Too-close contacts ⓘ

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	2	30919	15711	15718	217	0
2	A	1598	1632	1637	19	0
3	B	1810	1847	1855	20	0
4	C	1616	1651	1658	23	0
5	D	1656	1698	1702	44	0
6	E	2068	2144	2155	21	0
7	F	1471	1487	1500	46	0
8	G	1718	1814	1819	39	0
9	H	1322	1367	1374	38	0
10	I	1310	1349	1360	13	0
11	J	1333	1400	1412	17	0
12	K	859	841	845	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	1399	1427	1432	12	0
14	N	1228	1304	1308	22	0
15	O	1055	1058	1068	23	0
16	P	883	942	955	28	0
17	Q	1235	1302	1315	38	0
18	R	651	699	704	39	0
19	S	1138	1156	1169	29	0
20	T	1074	1089	1101	32	0
21	U	819	849	855	37	0
22	V	607	607	612	9	0
23	W	1030	1074	1082	10	0
24	X	1115	1195	1208	21	0
25	Y	969	1019	1025	14	0
26	Z	578	605	617	27	0
27	a	780	795	808	8	0
28	b	546	532	545	8	0
29	c	474	483	503	15	0
30	d	682	654	659	19	0
31	f	270	265	265	9	0
32	g	1569	745	798	38	0
33	M	836	843	849	48	0
34	e	433	453	463	10	0
35	2	23	0	0	0	0
36	2	35	40	0	1	0
37	a	1	0	0	0	0
38	2	591	0	0	30	0
38	B	1	0	0	0	0
38	C	6	0	0	2	0
38	D	6	0	0	0	0
38	E	10	0	0	0	0
38	F	12	0	0	0	0
38	G	2	0	0	0	0
38	H	1	0	0	0	0
38	I	10	0	0	1	0
38	K	7	0	0	1	0
38	L	4	0	0	0	0
38	M	7	0	0	0	0
38	N	9	0	0	0	0
38	O	3	0	0	0	0
38	P	2	0	0	1	0
38	Q	12	0	0	0	0
38	R	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	S	10	0	0	0	0
38	T	10	0	0	2	0
38	U	6	0	0	0	0
38	W	4	0	0	1	0
38	X	5	0	0	1	0
38	Z	6	0	0	1	0
38	a	6	0	0	1	0
38	b	1	0	0	0	0
38	d	6	0	0	0	0
38	e	1	0	0	0	0
38	f	1	0	0	0	0
38	g	2	0	0	0	0
All	All	67853	52077	52376	937	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 8.

All (937) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:554:G:N2	1:2:558:C:O2	1.89	1.05
29:c:8:ARG:NH1	29:c:30:MET:SD	2.35	0.99
1:2:257:A:O2'	1:2:258:G:O4'	1.82	0.98
1:2:297:A:OP2	6:E:1:MET:N	1.97	0.98
1:2:184:G:O2'	13:L:82:GLY:O	1.82	0.95
15:O:102:TYR:OH	15:O:125:ASP:OD1	1.84	0.95
7:F:110:ASP:OD1	7:F:111:SER:N	2.00	0.93
1:2:975:C:OP1	30:d:46:ARG:N	2.04	0.91
30:d:103:ARG:NH1	30:d:117:LEU:O	2.03	0.91
12:K:68:ASP:OD1	12:K:69:THR:N	2.04	0.91
12:K:22:LEU:HD23	12:K:57:MET:HE3	1.52	0.90
4:C:220:THR:OG1	4:C:222:ASP:OD1	1.90	0.88
32:g:21:U:O4	32:g:44:G:N1	2.05	0.87
1:2:1233:G:OP2	19:S:133:ARG:NH1	2.08	0.87
20:T:33:ASN:OD1	38:T:201:HOH:O	1.92	0.86
20:T:151:ASP:OD1	20:T:152:PHE:N	2.08	0.86
7:F:1:MET:SD	7:F:2:SER:OG	2.34	0.85
1:2:558:C:O2'	1:2:559:G:OP1	1.92	0.85
5:D:11:ASN:OD1	21:U:62:ARG:NH2	2.08	0.85
9:H:82:GLN:O	9:H:86:LYS:NZ	2.08	0.85
1:2:205:G:O6	8:G:210:LYS:NZ	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:56:U:O2	32:g:58:G:O2'	1.94	0.85
16:P:65:ARG:NH1	38:P:201:HOH:O	2.09	0.84
1:2:1242:A:O3'	16:P:44:ARG:NH1	2.10	0.84
8:G:63:ASP:OD1	8:G:64:ALA:N	2.10	0.84
8:G:23:MET:HE3	8:G:24:ILE:H	1.42	0.84
5:D:107:MET:HA	5:D:107:MET:HE2	1.60	0.84
1:2:393:G:O2'	1:2:394:A:O4'	1.96	0.83
1:2:1191:G:O2'	1:2:1192:C:OP2	1.96	0.83
1:2:336:C:O2'	1:2:338:G:OP1	1.97	0.83
6:E:141:THR:OG1	6:E:143:ASP:OD1	1.96	0.83
28:b:76:ILE:O	28:b:84:ILE:N	2.11	0.83
26:Z:83:ASN:O	26:Z:86:LYS:NZ	2.11	0.82
1:2:85:U:O4	38:2:1602:HOH:O	1.96	0.82
1:2:709:C:O2'	1:2:711:U:OP1	1.98	0.82
7:F:1:MET:SD	7:F:2:SER:N	2.53	0.81
1:2:1102:G:N2	1:2:1105:A:OP2	2.12	0.81
1:2:841:G:OP1	38:2:1601:HOH:O	1.96	0.81
1:2:113:G:O2'	1:2:114:G:OP1	1.99	0.81
1:2:393:G:O2'	1:2:394:A:O5'	1.99	0.81
1:2:739:C:O2'	1:2:740:U:OP2	1.99	0.81
1:2:1215:C:O2	17:Q:58:ARG:NH2	2.13	0.81
1:2:299:A:N7	38:2:1619:HOH:O	2.14	0.81
1:2:977:G:OP1	38:2:1605:HOH:O	1.99	0.81
1:2:1198:C:O2	38:2:1604:HOH:O	1.99	0.80
1:2:1365:G:OP2	38:2:1606:HOH:O	2.00	0.80
1:2:103:C:O2'	1:2:245:C:O2	1.99	0.79
29:c:31:THR:OG1	29:c:33:GLU:OE1	2.00	0.79
1:2:30:C:OP1	24:X:138:ARG:NH1	2.15	0.79
1:2:218:U:O2	13:L:112:ARG:NH1	2.14	0.79
1:2:1239:U:O4	16:P:40:ARG:NH2	2.16	0.78
4:C:89:ARG:O	38:C:301:HOH:O	2.01	0.78
12:K:16:LEU:O	12:K:20:ALA:N	2.17	0.78
32:g:2:G:H1	32:g:69:U:H3	1.31	0.78
32:g:12:G:O6	32:g:22:A:N1	2.17	0.78
32:g:29:G:H1	32:g:38:A:H2	1.30	0.78
2:A:20:VAL:O	2:A:24:LEU:HD12	1.84	0.77
22:V:49:LYS:NZ	22:V:50:GLY:O	2.16	0.77
1:2:1421:U:OP1	38:2:1607:HOH:O	2.02	0.77
32:g:29:G:O6	32:g:38:A:N1	2.17	0.77
1:2:1322:C:N4	38:2:1626:HOH:O	2.17	0.77
7:F:21:GLU:N	7:F:21:GLU:OE1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:34:ILE:HD11	26:Z:45:ILE:HD12	1.66	0.77
28:b:103:GLN:OE1	28:b:105:SER:OG	2.00	0.77
1:2:1209:G:OP2	1:2:1209:G:N2	2.18	0.76
17:Q:135:ASP:OD2	17:Q:137:ARG:NH1	2.19	0.76
15:O:76:ILE:O	15:O:80:THR:OG1	2.02	0.76
21:U:116:VAL:O	21:U:117:THR:OG1	2.02	0.76
19:S:90:ASP:OD1	19:S:91:PHE:N	2.19	0.75
1:2:136:U:O4'	8:G:19:ASN:ND2	2.20	0.75
33:M:14:PHE:CD2	33:M:80:LEU:HD21	2.21	0.75
18:R:13:ALA:O	18:R:17:VAL:HG23	1.86	0.75
12:K:11:ALA:HB1	12:K:36:ILE:HD11	1.68	0.75
21:U:100:ASP:N	21:U:103:THR:OG1	2.20	0.74
5:D:9:GLU:OE1	5:D:9:GLU:N	2.20	0.74
32:g:50:G:H1	32:g:60:U:H3	0.78	0.74
30:d:61:HIS:CE1	30:d:63:SER:HG	2.04	0.74
8:G:167:CYS:SG	8:G:168:GLU:N	2.61	0.74
23:W:12:LYS:NZ	38:W:201:HOH:O	2.19	0.74
1:2:487:G:OP2	38:2:1609:HOH:O	2.06	0.73
19:S:11:ARG:NH2	19:S:60:LEU:O	2.21	0.73
1:2:63:C:OP1	8:G:142:LYS:NZ	2.20	0.73
1:2:776:A:OP2	38:2:1610:HOH:O	2.07	0.73
34:e:20:LYS:NZ	34:e:21:LYS:O	2.20	0.73
1:2:637:U:N3	15:O:132:ASP:OD2	2.22	0.73
24:X:24:ASP:N	24:X:24:ASP:OD1	2.18	0.72
1:2:151:A:OP2	8:G:146:LYS:NZ	2.22	0.72
24:X:77:ASN:O	24:X:78:SER:OG	2.07	0.72
14:N:38:CYS:SG	14:N:42:LYS:NZ	2.62	0.72
17:Q:46:ASP:N	17:Q:82:ASP:OD1	2.23	0.72
8:G:104:ARG:NE	8:G:111:ASP:OD2	2.22	0.71
1:2:835:G:OP2	38:2:1611:HOH:O	2.08	0.71
18:R:54:ALA:O	18:R:58:THR:HG23	1.89	0.71
1:2:741:A:OP2	38:2:1613:HOH:O	2.09	0.71
1:2:1027:G:N7	1:2:1053:U:O2'	2.19	0.71
18:R:75:ARG:O	18:R:75:ARG:NE	2.23	0.71
17:Q:25:VAL:O	17:Q:26:HIS:ND1	2.23	0.71
1:2:72:C:O2	1:2:132:C:O2'	2.07	0.71
1:2:670:C:O2	15:O:44:ARG:NH1	2.24	0.70
1:2:1211:A:O2'	1:2:1212:G:OP2	2.07	0.70
1:2:990:U:O2'	1:2:991:C:OP2	2.08	0.70
2:A:45:ASP:OD1	2:A:46:ARG:N	2.24	0.70
22:V:74:SER:O	22:V:78:LEU:HD22	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1086:C:O2'	1:2:1087:C:OP2	2.09	0.70
32:g:1:G:O2'	32:g:2:G:OP1	2.09	0.70
1:2:911:G:O6	1:2:1172:A:N1	2.24	0.70
1:2:1240:G:O6	16:P:43:ARG:NH1	2.25	0.70
10:I:158:ILE:O	38:I:201:HOH:O	2.09	0.69
32:g:50:G:N2	32:g:60:U:O2	2.17	0.69
1:2:491:C:OP1	38:2:1614:HOH:O	2.09	0.69
1:2:1132:G:OP2	38:2:1615:HOH:O	2.10	0.69
18:R:53:VAL:O	18:R:57:VAL:HG23	1.92	0.69
19:S:68:LEU:O	19:S:71:VAL:HG12	1.92	0.69
20:T:156:LEU:HD12	20:T:156:LEU:O	1.92	0.69
1:2:1:C:O2'	1:2:2:A:OP1	2.08	0.69
17:Q:77:LEU:HD12	17:Q:77:LEU:H	1.58	0.69
15:O:40:ASP:OD2	15:O:42:SER:OG	2.06	0.69
29:c:60:ALA:O	29:c:61:ARG:HB2	1.92	0.69
17:Q:128:ASP:OD1	17:Q:129:ARG:N	2.26	0.69
1:2:937:G:HO2'	1:2:1287:C:HO2'	1.41	0.68
1:2:1262:A:OP1	32:g:33:C:O2'	2.07	0.68
7:F:112:CYS:SG	7:F:113:ARG:N	2.66	0.68
12:K:72:TRP:O	38:K:201:HOH:O	2.11	0.68
5:D:178:THR:O	5:D:179:ARG:NE	2.27	0.68
33:M:51:LYS:O	33:M:54:ALA:N	2.24	0.68
8:G:26:ASP:OD1	8:G:28:ARG:N	2.26	0.68
5:D:69:HIS:O	5:D:73:HIS:ND1	2.26	0.68
32:g:56:U:O2'	32:g:58:G:OP2	2.11	0.68
8:G:26:ASP:OD1	8:G:27:PHE:N	2.27	0.67
7:F:190:ARG:HD3	15:O:66:TYR:OH	1.94	0.67
1:2:89:G:O6	38:2:1612:HOH:O	2.08	0.67
1:2:910:G:N1	1:2:1260:G:OP2	2.28	0.67
20:T:29:ASP:O	20:T:33:ASN:ND2	2.27	0.67
16:P:86:PHE:H	16:P:89:MET:HE3	1.60	0.67
7:F:187:VAL:HG22	7:F:190:ARG:CZ	2.25	0.67
1:2:1036:G:N2	1:2:1039:A:OP2	2.24	0.66
5:D:99:LYS:HB3	5:D:102:LEU:HD23	1.77	0.66
1:2:1131:G:OP2	38:2:1617:HOH:O	2.13	0.66
1:2:937:G:O2'	1:2:1287:C:O2'	2.09	0.66
33:M:13:THR:O	33:M:16:ARG:NH1	2.29	0.66
32:g:3:G:H22	32:g:68:U:H3	1.43	0.66
1:2:295:G:O6	38:2:1616:HOH:O	2.11	0.66
1:2:949:C:OP2	38:2:1618:HOH:O	2.13	0.66
6:E:104:ASP:OD1	6:E:108:ARG:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:55:ILE:C	5:D:56:ILE:HD13	2.21	0.65
21:U:106:SER:O	21:U:110:VAL:HG23	1.96	0.65
21:U:24:LYS:HA	21:U:96:CYS:HA	1.78	0.65
18:R:61:MET:O	18:R:65:VAL:HG23	1.96	0.65
1:2:607:A:N7	9:H:111:THR:HG22	2.11	0.64
8:G:169:LEU:HD23	8:G:170:ILE:N	2.12	0.64
17:Q:68:GLU:OE2	17:Q:100:ARG:NH1	2.31	0.64
7:F:126:ASP:OD2	29:c:53:LEU:HD23	1.96	0.64
21:U:95:THR:OG1	21:U:96:CYS:N	2.24	0.64
24:X:1:MET:N	38:X:201:HOH:O	2.28	0.64
21:U:26:THR:HG22	21:U:93:TRP:HB2	1.79	0.64
21:U:40:TYR:OH	21:U:119:GLU:OE2	2.12	0.64
1:2:1281:C:O2	38:2:1621:HOH:O	2.15	0.64
1:2:669:C:OP2	38:2:1620:HOH:O	2.14	0.64
1:2:977:G:N1	1:2:988:U:O4	2.31	0.64
1:2:980:G:N2	1:2:983:C:OP2	2.29	0.64
1:2:1240:G:N1	1:2:1243:A:OP2	2.30	0.64
19:S:74:ASP:O	19:S:78:HIS:ND1	2.30	0.64
9:H:168:VAL:HG13	9:H:201:MET:HB3	1.78	0.63
14:N:86:GLU:N	14:N:86:GLU:OE1	2.29	0.63
21:U:53:ILE:HG22	21:U:54:SER:N	2.13	0.63
1:2:615:G:OP1	14:N:13:ARG:NH1	2.31	0.63
12:K:93:LEU:HD12	12:K:97:VAL:HG21	1.81	0.63
19:S:66:ASP:OD1	19:S:67:ALA:N	2.32	0.63
1:2:211:C:O2	6:E:33:ASN:ND2	2.32	0.63
7:F:1:MET:SD	7:F:3:LEU:N	2.69	0.62
9:H:168:VAL:CG1	9:H:201:MET:HB3	2.29	0.62
1:2:80:A:OP1	38:2:1623:HOH:O	2.16	0.62
11:J:65:ASP:OD1	11:J:67:ASN:N	2.31	0.62
26:Z:86:LYS:HD3	38:Z:104:HOH:O	2.00	0.62
1:2:64:A:N6	1:2:69:G:OP2	2.26	0.62
1:2:1239:U:OP2	16:P:43:ARG:NH2	2.32	0.62
5:D:208:ILE:HD12	18:R:12:ALA:HB2	1.82	0.62
34:e:62:LEU:O	34:e:66:LYS:HG3	2.00	0.61
1:2:43:C:OP2	1:2:349:A:N6	2.32	0.61
2:A:14:GLN:O	2:A:60:TRP:NE1	2.33	0.61
1:2:785:C:HO2'	23:W:2:VAL:N	1.98	0.61
33:M:34:LEU:CD1	33:M:60:LEU:HD11	2.30	0.61
18:R:4:VAL:HG13	18:R:4:VAL:O	2.00	0.61
24:X:71:ARG:NH1	24:X:82:THR:OG1	2.34	0.61
26:Z:24:GLU:O	26:Z:28:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:43:ILE:O	18:R:43:ILE:HG23	2.00	0.61
19:S:113:GLU:OE2	19:S:117:LYS:NZ	2.28	0.61
25:Y:82:LEU:HD23	25:Y:82:LEU:O	1.99	0.61
27:a:83:CYS:O	27:a:87:SER:OG	2.18	0.61
18:R:15:LYS:HE3	18:R:15:LYS:HA	1.83	0.61
21:U:99:ASN:CG	21:U:103:THR:HG1	2.09	0.61
24:X:105:PHE:HB3	24:X:112:VAL:HG21	1.81	0.61
30:d:75:ASN:OD1	30:d:76:LEU:N	2.34	0.61
1:2:162:G:OP1	8:G:240:TYR:HB3	2.01	0.61
8:G:198:GLU:N	8:G:198:GLU:OE1	2.34	0.61
17:Q:18:ARG:O	17:Q:22:LYS:NZ	2.33	0.61
32:g:1:G:HO2'	32:g:2:G:P	2.24	0.61
1:2:485:G:OP2	38:2:1624:HOH:O	2.16	0.60
1:2:615:G:OP2	14:N:13:ARG:NH2	2.33	0.60
7:F:45:LYS:HE2	7:F:45:LYS:HA	1.82	0.60
8:G:23:MET:C	8:G:24:ILE:HD12	2.26	0.60
31:f:100:ILE:N	31:f:103:ASP:OD2	2.34	0.60
5:D:210:ILE:HG22	5:D:211:GLY:H	1.66	0.60
7:F:55:VAL:O	7:F:59:THR:HG23	2.00	0.60
7:F:15:ASP:OD1	7:F:15:ASP:N	2.34	0.60
1:2:1095:G:N7	18:R:3:LYS:NZ	2.49	0.60
1:2:1032:U:OP2	38:2:1622:HOH:O	2.15	0.60
1:2:30:C:OP1	24:X:138:ARG:NH2	2.35	0.60
5:D:208:ILE:CD1	18:R:12:ALA:HB2	2.32	0.60
19:S:14:LEU:O	19:S:21:ILE:N	2.30	0.60
18:R:15:LYS:HA	18:R:18:GLU:OE2	2.02	0.59
20:T:29:ASP:OD1	20:T:30:VAL:HG13	2.03	0.59
31:f:124:HIS:ND1	31:f:125:ALA:O	2.35	0.59
32:g:2:G:H22	32:g:69:U:H3	1.49	0.59
4:C:231:HIS:ND1	4:C:231:HIS:O	2.35	0.59
33:M:60:LEU:HD12	33:M:60:LEU:O	2.03	0.59
33:M:30:VAL:HG23	33:M:103:VAL:CG2	2.32	0.59
1:2:528:A:OP2	38:2:1627:HOH:O	2.17	0.59
5:D:29:GLU:OE2	5:D:33:ARG:NE	2.35	0.59
16:P:23:GLU:OE1	16:P:24:LYS:N	2.36	0.59
27:a:37:ARG:NH2	38:a:1101:HOH:O	2.34	0.59
7:F:171:ASP:OD2	7:F:180:ASN:ND2	2.35	0.59
6:E:86:PHE:CE2	6:E:87:MET:HE2	2.38	0.59
7:F:32:HIS:O	7:F:33:SER:OG	2.13	0.59
10:I:78:SER:OG	10:I:160:GLU:OE2	2.12	0.59
19:S:125:ARG:NH1	19:S:131:LYS:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:130:LYS:HA	20:T:130:LYS:HE2	1.84	0.58
1:2:346:G:N2	1:2:349:A:OP2	2.36	0.58
1:2:989:U:O2'	1:2:990:U:OP1	2.21	0.58
21:U:53:ILE:HG22	21:U:54:SER:H	1.68	0.58
1:2:982:G:O2'	1:2:983:C:H5'	2.04	0.58
31:f:101:LYS:N	31:f:103:ASP:OD2	2.34	0.58
16:P:19:GLY:N	19:S:92:GLU:O	2.37	0.58
32:g:50:G:O6	32:g:60:U:O4	2.20	0.58
5:D:9:GLU:O	5:D:12:VAL:HG22	2.04	0.58
10:I:135:ILE:HD13	10:I:140:ILE:HD11	1.85	0.58
1:2:558:C:HO2'	1:2:559:G:P	2.23	0.58
15:O:144:ARG:O	15:O:145:LEU:HB2	2.04	0.58
19:S:14:LEU:N	19:S:21:ILE:O	2.33	0.58
8:G:15:VAL:HG13	8:G:16:THR:HG23	1.85	0.58
18:R:71:GLY:C	18:R:72:ILE:HD12	2.29	0.58
18:R:81:ARG:NH1	18:R:82:GLU:OE2	2.36	0.58
5:D:210:ILE:HG22	5:D:211:GLY:N	2.18	0.58
7:F:138:TYR:O	7:F:142:THR:OG1	2.19	0.58
1:2:1059:C:N4	1:2:1062:C:OP1	2.37	0.57
1:2:1267:U:O2	1:2:1299:G:N1	2.37	0.57
13:L:31:ARG:HD3	13:L:31:ARG:H	1.67	0.57
25:Y:83:MET:SD	25:Y:91:LYS:NZ	2.74	0.57
8:G:77:GLN:NE2	8:G:78:ARG:O	2.37	0.57
5:D:84:MET:HE1	30:d:73:ASN:OD1	2.04	0.57
1:2:704:G:H2'	1:2:705:A:C8	2.39	0.57
1:2:792:C:OP2	2:A:37:ARG:NH2	2.37	0.57
5:D:114:LYS:HB3	5:D:119:MET:HE3	1.85	0.57
3:B:196:LYS:O	3:B:199:GLU:OE1	2.23	0.57
25:Y:55:ILE:HD12	25:Y:55:ILE:O	2.04	0.57
1:2:290:A:OP1	38:2:1625:HOH:O	2.16	0.57
5:D:105:GLU:OE1	5:D:105:GLU:HA	2.03	0.57
26:Z:34:ILE:HD11	26:Z:45:ILE:CD1	2.33	0.57
1:2:517:C:O2	9:H:129:ARG:NH2	2.30	0.57
36:2:1524:YAT:NAR	15:O:145:LEU:O	2.38	0.57
9:H:98:ASN:C	9:H:98:ASN:HD22	2.13	0.57
34:e:62:LEU:C	34:e:66:LYS:HE3	2.30	0.57
1:2:602:G:H2'	1:2:603:C:O4'	2.05	0.56
1:2:1153:C:O2'	30:d:92:PHE:O	2.15	0.56
8:G:104:ARG:NH1	8:G:105:GLY:O	2.38	0.56
9:H:179:GLU:N	9:H:179:GLU:OE1	2.34	0.56
1:2:975:C:C2	1:2:976:A:C8	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:89:ARG:NH1	38:C:301:HOH:O	2.32	0.56
1:2:1042:C:O2'	1:2:1061:A:OP2	2.24	0.56
1:2:30:C:OP1	24:X:138:ARG:CZ	2.54	0.56
6:E:170:ASP:OD1	6:E:170:ASP:N	2.39	0.56
5:D:82:ARG:O	5:D:82:ARG:NH1	2.38	0.56
18:R:72:ILE:HD12	18:R:72:ILE:N	2.21	0.56
22:V:85:LEU:HD23	22:V:85:LEU:H	1.70	0.56
26:Z:41:THR:HG22	26:Z:42:HIS:N	2.21	0.56
18:R:59:THR:O	18:R:62:ASN:OD1	2.23	0.56
30:d:87:MET:SD	30:d:88:ARG:N	2.78	0.55
17:Q:111:VAL:O	17:Q:117:ARG:NH1	2.37	0.55
20:T:156:LEU:HD12	20:T:156:LEU:C	2.32	0.55
14:N:35:GLU:N	14:N:35:GLU:OE1	2.39	0.55
21:U:21:MET:N	21:U:100:ASP:OD2	2.40	0.55
30:d:76:LEU:O	30:d:77:ALA:HB2	2.06	0.55
1:2:292:U:H4'	11:J:2:PRO:HG3	1.89	0.55
32:g:27:G:O2'	32:g:28:C:O4'	2.21	0.55
1:2:1182:G:OP1	20:T:73:LYS:NZ	2.39	0.55
19:S:115:LEU:HD22	19:S:120:CYS:SG	2.47	0.55
5:D:80:ALA:O	5:D:84:MET:N	2.39	0.54
8:G:196:THR:OG1	8:G:198:GLU:OE1	2.24	0.54
12:K:91:LEU:HB2	12:K:93:LEU:HD23	1.88	0.54
25:Y:37:GLU:OE2	25:Y:37:GLU:HA	2.07	0.54
26:Z:27:MET:SD	26:Z:27:MET:N	2.77	0.54
12:K:96:ASP:OD1	12:K:97:VAL:N	2.40	0.54
20:T:136:GLU:OE1	20:T:136:GLU:N	2.34	0.54
33:M:52:GLN:O	33:M:56:ILE:HB	2.08	0.54
33:M:77:LEU:O	33:M:81:THR:HG23	2.07	0.54
1:2:428:G:O2'	1:2:435:A:N1	2.36	0.54
3:B:195:ALA:O	3:B:198:THR:HG22	2.08	0.54
8:G:23:MET:HE3	8:G:24:ILE:N	2.19	0.54
1:2:86:C:OP2	1:2:290:A:O2'	2.25	0.54
1:2:345:C:H2'	1:2:346:G:O4'	2.07	0.54
1:2:1153:C:OP1	12:K:29:ARG:NH2	2.41	0.54
4:C:36:LEU:HD23	4:C:41:LYS:HD3	1.89	0.54
12:K:96:ASP:OD1	12:K:96:ASP:C	2.51	0.54
19:S:89:ASN:N	19:S:96:ASP:OD1	2.37	0.54
19:S:52:ASP:OD1	19:S:53:VAL:N	2.40	0.53
21:U:50:ALA:O	21:U:52:GLY:N	2.40	0.53
33:M:73:THR:O	33:M:76:THR:HG22	2.08	0.53
9:H:171:LYS:NZ	9:H:201:MET:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:25:LYS:NZ	12:K:74:HIS:CD2	2.77	0.53
21:U:25:TYR:HA	21:U:123:PRO:HA	1.90	0.53
7:F:109:GLU:OE1	7:F:124:SER:OG	2.21	0.53
9:H:29:GLU:OE1	9:H:30:LEU:HD12	2.09	0.53
20:T:68:ASP:OD1	20:T:68:ASP:N	2.39	0.53
29:c:6:ASN:OD1	29:c:6:ASN:N	2.41	0.53
1:2:636:G:H2'	1:2:637:U:C6	2.43	0.53
9:H:196:THR:OG1	9:H:197:GLU:N	2.41	0.53
29:c:22:ILE:N	29:c:22:ILE:HD12	2.23	0.53
32:g:3:G:H1	32:g:68:U:H3	1.55	0.53
5:D:24:GLU:OE1	30:d:130:LYS:NZ	2.41	0.53
8:G:42:PHE:N	8:G:56:PHE:O	2.40	0.53
10:I:81:ILE:HD13	10:I:122:LEU:HD21	1.89	0.53
13:L:41:LYS:HA	13:L:41:LYS:HE2	1.91	0.53
16:P:38:ASN:C	16:P:38:ASN:OD1	2.52	0.53
21:U:105:LEU:HD13	21:U:105:LEU:C	2.34	0.53
25:Y:83:MET:HE1	25:Y:96:LEU:HD12	1.90	0.53
7:F:3:LEU:O	7:F:3:LEU:HG	2.09	0.53
1:2:151:A:OP1	8:G:142:LYS:N	2.37	0.52
3:B:224:THR:O	3:B:224:THR:OG1	2.20	0.52
9:H:31:GLU:OE1	9:H:31:GLU:N	2.39	0.52
18:R:55:GLY:O	18:R:59:THR:HG23	2.09	0.52
29:c:46:ARG:N	29:c:49:ASP:OD2	2.41	0.52
32:g:1:G:O2'	32:g:2:G:P	2.66	0.52
1:2:710:C:O2'	14:N:62:GLN:OE1	2.27	0.52
1:2:1448:C:OP2	27:a:14:ARG:NH1	2.42	0.52
2:A:96:CYS:O	2:A:100:HIS:N	2.42	0.52
9:H:58:SER:OG	9:H:75:TYR:O	2.19	0.52
9:H:84:PHE:O	9:H:88:SER:HB3	2.09	0.52
25:Y:92:ILE:HD12	25:Y:99:ALA:HB2	1.92	0.52
2:A:145:VAL:HG23	2:A:147:ILE:HD12	1.90	0.52
3:B:98:THR:O	3:B:232:HIS:NE2	2.40	0.52
8:G:15:VAL:CG1	8:G:16:THR:HG23	2.39	0.52
22:V:86:MET:O	22:V:87:GLU:HG3	2.10	0.52
26:Z:33:PHE:CD1	26:Z:33:PHE:C	2.87	0.52
29:c:3:GLU:OE1	29:c:3:GLU:HA	2.09	0.52
2:A:62:LYS:NZ	22:V:77:MET:HE3	2.25	0.52
3:B:60:ASN:O	3:B:88:THR:OG1	2.12	0.52
33:M:75:ARG:O	33:M:75:ARG:NH1	2.42	0.52
6:E:95:VAL:HG12	6:E:95:VAL:O	2.09	0.52
14:N:148:ALA:O	14:N:152:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:33:LEU:HD12	4:C:60:ILE:HD13	1.92	0.52
4:C:88:GLN:OE1	4:C:88:GLN:N	2.43	0.52
10:I:125:ASP:OD1	10:I:126:THR:N	2.43	0.52
25:Y:25:ASP:OD1	25:Y:25:ASP:N	2.40	0.52
23:W:28:ARG:HB2	23:W:29:PRO:HD3	1.91	0.52
1:2:974:A:N6	38:2:1679:HOH:O	2.43	0.52
9:H:176:GLU:CD	9:H:176:GLU:H	2.18	0.52
26:Z:24:GLU:HA	26:Z:24:GLU:OE2	2.10	0.52
19:S:101:VAL:O	19:S:103:THR:N	2.40	0.51
24:X:139:GLU:HG3	24:X:141:ARG:HE	1.76	0.51
33:M:14:PHE:CE2	33:M:80:LEU:HD21	2.46	0.51
9:H:111:THR:HG23	9:H:131:ARG:HD2	1.91	0.51
21:U:84:GLU:OE2	30:d:136:LEU:HD11	2.10	0.51
11:J:115:ILE:HD11	11:J:127:ALA:HB1	1.93	0.51
17:Q:85:ILE:HG22	17:Q:86:LYS:N	2.25	0.51
33:M:41:ILE:HD11	33:M:69:CYS:SG	2.51	0.51
2:A:32:VAL:HG12	2:A:33:ARG:N	2.25	0.51
4:C:147:THR:OG1	4:C:189:ASP:O	2.18	0.51
18:R:39:ARG:O	18:R:39:ARG:NH1	2.43	0.51
7:F:30:ASP:OD1	7:F:31:ASN:N	2.44	0.51
21:U:54:SER:HA	21:U:94:VAL:HB	1.93	0.51
3:B:120:CYS:SG	3:B:140:ILE:HD11	2.51	0.51
20:T:151:ASP:OD1	20:T:151:ASP:C	2.54	0.51
26:Z:53:VAL:O	26:Z:56:ALA:HB3	2.10	0.51
33:M:11:LYS:CD	33:M:11:LYS:H	2.24	0.51
1:2:607:A:C8	9:H:111:THR:HG22	2.46	0.51
1:2:810:C:OP1	2:A:46:ARG:NH1	2.43	0.51
1:2:989:U:HO2'	1:2:990:U:P	2.33	0.51
1:2:1300:C:N4	7:F:45:LYS:O	2.44	0.51
17:Q:124:LEU:HD21	17:Q:131:LEU:HD13	1.91	0.51
5:D:44:SER:OG	5:D:55:ILE:HD13	2.11	0.51
30:d:47:ASN:OD1	30:d:48:LEU:N	2.43	0.51
33:M:80:LEU:C	33:M:80:LEU:HD23	2.35	0.51
1:2:113:G:H3'	1:2:114:G:H5''	1.93	0.51
1:2:612:C:H2'	1:2:613:G:O4'	2.10	0.51
9:H:66:ASP:OD1	9:H:67:GLY:N	2.44	0.51
32:g:3:G:N2	32:g:68:U:H3	2.09	0.51
10:I:114:ASP:C	10:I:114:ASP:OD1	2.54	0.50
11:J:110:ARG:O	11:J:114:VAL:HG13	2.11	0.50
18:R:24:LEU:HB3	18:R:61:MET:HE1	1.93	0.50
5:D:149:ARG:NH2	5:D:152:ARG:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:20:ASP:HB3	7:F:23:LEU:HD11	1.92	0.50
17:Q:112:LYS:HE2	17:Q:112:LYS:H	1.76	0.50
33:M:12:GLU:HA	33:M:15:LYS:HE2	1.93	0.50
33:M:30:VAL:HG23	33:M:103:VAL:HG23	1.92	0.50
33:M:59:CYS:O	33:M:63:GLU:HB3	2.12	0.50
1:2:472:C:H2'	1:2:473:G:O4'	2.12	0.50
17:Q:32:LYS:O	17:Q:138:ARG:NH1	2.44	0.50
7:F:24:GLU:OE1	7:F:25:ALA:N	2.45	0.50
17:Q:25:VAL:HG12	17:Q:26:HIS:N	2.27	0.50
6:E:252:GLU:OE2	6:E:252:GLU:HA	2.11	0.50
16:P:81:ARG:NH1	16:P:120:SER:OG	2.45	0.50
33:M:30:VAL:HG23	33:M:103:VAL:HG21	1.93	0.50
5:D:205:PRO:O	5:D:206:ASP:OD1	2.30	0.50
6:E:59:ALA:O	6:E:62:SER:OG	2.20	0.50
23:W:49:ASP:OD1	23:W:64:ASN:ND2	2.45	0.50
8:G:9:VAL:HG23	8:G:24:ILE:HD13	1.93	0.50
26:Z:24:GLU:HA	26:Z:27:MET:SD	2.52	0.50
12:K:95:ASP:O	12:K:96:ASP:CG	2.54	0.49
24:X:88:ASP:OD1	24:X:89:GLY:N	2.45	0.49
25:Y:39:ILE:O	25:Y:43:VAL:HG23	2.11	0.49
12:K:25:LYS:HZ1	12:K:74:HIS:CD2	2.31	0.49
17:Q:76:SER:O	17:Q:79:LYS:NZ	2.41	0.49
5:D:62:GLU:OE1	5:D:63:VAL:HG23	2.12	0.49
9:H:31:GLU:HA	9:H:34:VAL:HG22	1.93	0.49
12:K:71:ALA:O	12:K:73:ARG:N	2.43	0.49
15:O:130:PRO:HB2	15:O:132:ASP:O	2.12	0.49
33:M:51:LYS:O	33:M:55:ASP:N	2.40	0.49
33:M:102:CYS:SG	33:M:103:VAL:N	2.85	0.49
1:2:31:U:OP1	24:X:137:LYS:NZ	2.35	0.49
1:2:445:C:O2'	1:2:457:G:N2	2.45	0.49
4:C:129:ASN:OD1	4:C:129:ASN:O	2.31	0.49
5:D:65:MET:O	5:D:69:HIS:HA	2.12	0.49
23:W:81:ILE:HG22	23:W:82:PRO:O	2.12	0.49
28:b:77:LYS:HD3	28:b:119:GLU:OE1	2.12	0.49
16:P:86:PHE:N	16:P:89:MET:HE3	2.27	0.49
17:Q:135:ASP:OD1	17:Q:137:ARG:HG2	2.12	0.49
1:2:894:G:N7	38:2:1649:HOH:O	2.34	0.49
5:D:34:GLU:HG3	5:D:35:LEU:HD23	1.93	0.49
17:Q:27:THR:HG22	17:Q:28:LEU:N	2.27	0.49
21:U:55:GLY:N	21:U:94:VAL:HG21	2.27	0.49
26:Z:24:GLU:C	26:Z:28:ASN:ND2	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:59:ALA:O	6:E:63:MET:HG3	2.12	0.49
34:e:52:ASN:O	34:e:55:ARG:NH1	2.44	0.49
4:C:37:VAL:HG22	4:C:42:ILE:HD11	1.95	0.49
3:B:32:ALA:O	3:B:39:ARG:NH2	2.45	0.49
3:B:233:ASP:C	3:B:233:ASP:OD1	2.55	0.49
12:K:98:LEU:HD13	12:K:102:TYR:CD2	2.48	0.49
24:X:21:ARG:HD3	24:X:27:TYR:CZ	2.48	0.49
30:d:61:HIS:O	30:d:63:SER:N	2.46	0.48
1:2:1096:G:C2	1:2:1097:C:C6	3.01	0.48
4:C:59:GLU:OE1	4:C:59:GLU:N	2.40	0.48
14:N:114:ARG:O	14:N:118:VAL:HG23	2.13	0.48
18:R:32:ASN:OD1	18:R:58:THR:HG22	2.14	0.48
1:2:1239:U:H2'	1:2:1240:G:O4'	2.13	0.48
1:2:782:U:O2'	38:2:1628:HOH:O	2.20	0.48
21:U:55:GLY:H	21:U:94:VAL:HG21	1.79	0.48
1:2:739:C:O2'	1:2:740:U:H6	1.95	0.48
1:2:975:C:O2	31:f:126:ASP:CG	2.57	0.48
2:A:129:VAL:HG12	2:A:130:ASN:N	2.28	0.48
14:N:31:GLU:O	14:N:34:CYS:N	2.46	0.48
32:g:57:C:H2'	32:g:57:C:O2	2.13	0.48
33:M:51:LYS:O	33:M:52:GLN:C	2.56	0.48
1:2:157:U:H2'	1:2:158:G:O4'	2.14	0.48
1:2:664:U:O2'	1:2:665:G:OP1	2.28	0.48
1:2:1200:A:HO2'	1:2:1247:C:HO2'	1.61	0.48
3:B:55:ALA:HA	3:B:58:VAL:HG22	1.95	0.48
9:H:30:LEU:O	9:H:34:VAL:HG13	2.12	0.48
26:Z:86:LYS:HD2	26:Z:86:LYS:N	2.29	0.48
29:c:10:ILE:HD12	29:c:10:ILE:C	2.38	0.48
30:d:136:LEU:O	30:d:137:HIS:HB3	2.13	0.48
32:g:29:G:C6	32:g:38:A:N1	2.81	0.48
8:G:202:ARG:O	8:G:206:VAL:HG23	2.13	0.48
21:U:36:LEU:HD22	21:U:36:LEU:H	1.78	0.48
26:Z:41:THR:HG22	26:Z:42:HIS:H	1.79	0.48
7:F:29:ILE:HA	7:F:32:HIS:NE2	2.28	0.48
7:F:57:ARG:NH2	7:F:134:ASN:OD1	2.42	0.48
8:G:227:LEU:O	8:G:228:LEU:HB2	2.14	0.48
8:G:230:ARG:H	8:G:230:ARG:HD3	1.79	0.48
1:2:115:U:H1'	1:2:116:C:OP2	2.13	0.47
21:U:105:LEU:O	21:U:106:SER:C	2.57	0.47
33:M:22:GLY:O	33:M:24:VAL:HG23	2.14	0.47
1:2:365:G:N2	6:E:67:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:388:C:O4'	1:2:388:C:O2	2.32	0.47
1:2:636:G:N2	15:O:132:ASP:OD2	2.47	0.47
14:N:31:GLU:O	14:N:35:GLU:OE1	2.32	0.47
25:Y:32:THR:OG1	25:Y:33:TYR:N	2.46	0.47
4:C:33:LEU:HD13	4:C:33:LEU:O	2.14	0.47
6:E:43:PRO:HD2	6:E:46:LEU:HD12	1.96	0.47
9:H:174:TYR:O	9:H:178:SER:N	2.47	0.47
18:R:58:THR:O	18:R:62:ASN:OD1	2.31	0.47
21:U:25:TYR:HD1	21:U:123:PRO:HA	1.79	0.47
21:U:81:HIS:CE1	30:d:135:LYS:HE2	2.49	0.47
1:2:114:G:O2'	1:2:163:C:OP1	2.28	0.47
5:D:125:ALA:O	5:D:129:ILE:HG13	2.14	0.47
11:J:43:GLU:OE1	11:J:43:GLU:N	2.42	0.47
14:N:31:GLU:OE2	14:N:31:GLU:HA	2.15	0.47
20:T:23:VAL:O	20:T:26:VAL:HG12	2.14	0.47
1:2:918:C:H41	19:S:138:LYS:NZ	2.12	0.47
10:I:128:ASP:OD2	10:I:131:ILE:HG12	2.15	0.47
34:e:33:ARG:NH1	34:e:33:ARG:HB2	2.29	0.47
1:2:16:G:H2'	1:2:17:C:C6	2.49	0.47
1:2:468:U:OP1	34:e:26:LYS:NZ	2.24	0.47
1:2:1245:G:O6	16:P:40:ARG:NH1	2.43	0.47
21:U:37:VAL:O	21:U:41:VAL:HG23	2.13	0.47
24:X:40:PRO:O	24:X:77:ASN:ND2	2.48	0.47
1:2:555:G:H2'	1:2:556:C:O4'	2.14	0.47
1:2:1192:C:O2	20:T:137:ARG:NH2	2.48	0.47
7:F:186:ALA:O	7:F:189:ASN:N	2.39	0.47
12:K:39:VAL:HG23	12:K:44:LYS:O	2.15	0.47
15:O:10:GLU:CD	15:O:10:GLU:H	2.23	0.47
17:Q:91:GLY:O	17:Q:95:GLN:HG3	2.14	0.47
19:S:65:GLU:OE2	19:S:69:MET:HE2	2.15	0.47
19:S:99:ILE:HB	19:S:103:THR:OG1	2.15	0.47
23:W:81:ILE:HD12	23:W:81:ILE:N	2.30	0.47
33:M:55:ASP:HA	33:M:58:GLU:HG2	1.96	0.47
1:2:623:G:H2'	1:2:624:G:C8	2.50	0.47
3:B:195:ALA:O	3:B:199:GLU:HG3	2.15	0.47
4:C:146:HIS:ND1	4:C:189:ASP:OD2	2.45	0.47
7:F:58:LEU:O	7:F:61:SER:OG	2.31	0.47
26:Z:41:THR:O	26:Z:45:ILE:HG22	2.15	0.47
30:d:59:ARG:HG2	30:d:60:VAL:N	2.29	0.47
34:e:62:LEU:O	34:e:66:LYS:HE3	2.14	0.47
1:2:840:C:C2'	1:2:841:G:OP1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:124:SER:HB3	7:F:190:ARG:HA	1.97	0.47
7:F:126:ASP:O	29:c:42:ILE:HG22	2.15	0.47
12:K:40:ASP:O	12:K:41:GLU:HB3	2.15	0.47
15:O:66:TYR:O	15:O:70:GLN:HG3	2.15	0.47
18:R:39:ARG:NE	18:R:43:ILE:HD13	2.29	0.47
26:Z:24:GLU:HG3	26:Z:28:ASN:HD22	1.79	0.47
32:g:5:A:H2'	32:g:6:A:C8	2.49	0.47
33:M:45:ALA:O	33:M:70:LYS:HE2	2.15	0.47
1:2:887:G:H2'	1:2:888:A:C8	2.50	0.47
4:C:168:ARG:O	11:J:55:ARG:NH2	2.44	0.47
17:Q:16:GLU:OE2	17:Q:16:GLU:HA	2.14	0.47
33:M:26:GLY:O	33:M:30:VAL:HG12	2.15	0.47
1:2:116:C:H2'	1:2:117:C:O4'	2.15	0.46
1:2:518:C:C3'	1:2:519:C:H5''	2.43	0.46
1:2:531:A:OP2	6:E:187:ARG:NH2	2.47	0.46
5:D:154:ARG:NH1	5:D:154:ARG:HB3	2.30	0.46
9:H:37:THR:O	9:H:41:LEU:HG	2.15	0.46
9:H:93:LEU:O	9:H:93:LEU:HD12	2.15	0.46
12:K:67:LYS:HE2	12:K:78:LEU:HB2	1.97	0.46
14:N:29:THR:HG22	14:N:32:ASP:OD1	2.15	0.46
21:U:33:ASP:OD2	21:U:36:LEU:HD22	2.16	0.46
33:M:11:LYS:H	33:M:11:LYS:HD3	1.80	0.46
1:2:589:G:N1	1:2:602:G:O6	2.48	0.46
7:F:22:SER:HA	29:c:50:ILE:HB	1.97	0.46
11:J:50:MET:O	11:J:54:ILE:HG12	2.16	0.46
19:S:4:ILE:N	19:S:4:ILE:HD13	2.29	0.46
19:S:22:GLN:OE1	19:S:22:GLN:N	2.49	0.46
21:U:51:PHE:CE1	21:U:103:THR:HB	2.50	0.46
12:K:81:GLU:N	12:K:81:GLU:CD	2.74	0.46
17:Q:44:LYS:HD2	17:Q:44:LYS:C	2.39	0.46
17:Q:76:SER:HA	17:Q:79:LYS:HE3	1.97	0.46
18:R:11:ARG:HG3	18:R:12:ALA:N	2.30	0.46
19:S:119:ARG:HH11	19:S:119:ARG:HG3	1.80	0.46
32:g:2:G:N2	32:g:69:U:H3	2.13	0.46
33:M:20:MET:HE2	33:M:20:MET:N	2.31	0.46
33:M:27:HIS:HB3	33:M:53:TYR:CZ	2.50	0.46
2:A:87:ASP:OD1	2:A:87:ASP:N	2.48	0.46
9:H:65:VAL:HG12	9:H:66:ASP:N	2.31	0.46
9:H:197:GLU:OE1	9:H:198:PHE:N	2.48	0.46
12:K:6:LYS:HE2	12:K:6:LYS:H	1.79	0.46
12:K:15:HIS:HB2	12:K:36:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:32:VAL:HG12	19:S:32:VAL:O	2.16	0.46
1:2:393:G:HO2'	1:2:394:A:C4'	2.23	0.46
7:F:23:LEU:HD12	7:F:23:LEU:C	2.41	0.46
7:F:113:ARG:NE	32:g:32:U:OP2	2.49	0.46
33:M:24:VAL:O	33:M:102:CYS:HA	2.15	0.46
33:M:53:TYR:CD1	33:M:53:TYR:O	2.69	0.46
1:2:30:C:H6	1:2:30:C:O5'	1.98	0.46
1:2:678:C:O2	15:O:132:ASP:CB	2.63	0.46
9:H:36:GLY:O	9:H:40:LYS:HG2	2.16	0.46
9:H:80:MET:O	9:H:84:PHE:CD1	2.68	0.46
12:K:70:PHE:CE2	12:K:73:ARG:HA	2.51	0.46
16:P:24:LYS:HD2	16:P:24:LYS:O	2.15	0.46
1:2:679:C:H4'	1:2:680:G:O5'	2.16	0.46
1:2:796:C:OP1	3:B:151:ARG:NH1	2.48	0.46
13:L:31:ARG:H	13:L:31:ARG:CD	2.29	0.46
1:2:1242:A:H4'	16:P:44:ARG:NH1	2.31	0.46
1:2:1419:G:OP1	1:2:1422:A:H4'	2.16	0.46
3:B:22:TYR:HA	3:B:25:LYS:HG3	1.98	0.46
4:C:51:TYR:CD1	4:C:233:GLN:HG2	2.51	0.46
1:2:1296:G:O2'	1:2:1297:A:P	2.74	0.46
5:D:196:ASN:OD1	5:D:199:ILE:N	2.48	0.46
7:F:63:MET:HB2	7:F:68:ASN:O	2.16	0.46
29:c:33:GLU:CD	29:c:33:GLU:N	2.74	0.46
30:d:122:ARG:HG3	30:d:122:ARG:HH11	1.81	0.46
32:g:11:C:H2'	32:g:12:G:C8	2.51	0.46
32:g:13:C:H2'	32:g:14:A:C8	2.51	0.46
4:C:43:GLU:N	4:C:43:GLU:OE1	2.49	0.45
17:Q:57:VAL:HG23	17:Q:63:ARG:HG2	1.98	0.45
18:R:21:TYR:CD2	18:R:74:LEU:HD11	2.50	0.45
19:S:19:THR:HG22	19:S:20:ASN:N	2.29	0.45
1:2:948:A:N3	1:2:948:A:H2'	2.31	0.45
3:B:125:MET:HE3	3:B:172:LEU:HD23	1.98	0.45
4:C:26:GLU:OE2	4:C:26:GLU:HA	2.16	0.45
7:F:34:PHE:N	7:F:34:PHE:CD1	2.83	0.45
9:H:80:MET:O	9:H:84:PHE:HD1	1.99	0.45
9:H:197:GLU:OE1	9:H:197:GLU:C	2.60	0.45
20:T:120:ARG:O	20:T:124:SER:OG	2.33	0.45
1:2:919:G:C6	1:2:1165:G:O6	2.69	0.45
13:L:110:ARG:HG3	13:L:110:ARG:HH11	1.82	0.45
16:P:41:CYS:O	16:P:45:ILE:HG12	2.16	0.45
18:R:17:VAL:HG22	18:R:57:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:125:GLN:O	20:T:129:GLN:OE1	2.35	0.45
21:U:100:ASP:N	21:U:100:ASP:OD1	2.49	0.45
26:Z:28:ASN:OD1	26:Z:29:GLU:HG2	2.16	0.45
1:2:58:C:HO2'	1:2:59:C:H6	1.58	0.45
1:2:739:C:O2'	1:2:740:U:P	2.74	0.45
2:A:18:ALA:O	2:A:21:LYS:HG3	2.16	0.45
5:D:208:ILE:HD12	18:R:12:ALA:CB	2.47	0.45
13:L:31:ARG:HD3	13:L:31:ARG:N	2.31	0.45
17:Q:125:VAL:HA	17:Q:128:ASP:O	2.17	0.45
18:R:24:LEU:CB	18:R:61:MET:HE1	2.45	0.45
18:R:62:ASN:OD1	18:R:62:ASN:N	2.48	0.45
21:U:63:ARG:HG3	21:U:63:ARG:O	2.16	0.45
1:2:256:G:H2'	1:2:257:A:O4'	2.17	0.45
3:B:88:THR:HG22	3:B:98:THR:HG22	1.97	0.45
5:D:107:MET:HA	5:D:107:MET:CE	2.41	0.45
11:J:33:CYS:O	11:J:37:GLY:N	2.49	0.45
19:S:15:ARG:NH2	19:S:18:ASN:O	2.49	0.45
20:T:39:LEU:HD12	20:T:44:ILE:HD12	1.99	0.45
33:M:34:LEU:HD11	33:M:60:LEU:HD11	1.97	0.45
1:2:387:G:H2'	1:2:388:C:O2	2.17	0.45
1:2:848:G:O2'	1:2:849:G:H5'	2.17	0.45
10:I:22:HIS:ND1	10:I:23:LYS:O	2.34	0.45
1:2:982:G:C2'	1:2:983:C:H5'	2.47	0.45
2:A:34:ASN:O	2:A:155:SER:OG	2.34	0.45
16:P:26:ALA:C	16:P:27:THR:HG23	2.41	0.45
20:T:42:ARG:HA	20:T:42:ARG:NH1	2.32	0.45
31:f:90:VAL:HG12	31:f:91:ARG:N	2.31	0.45
5:D:67:ASP:OD1	5:D:67:ASP:N	2.49	0.45
7:F:181:SER:O	7:F:185:ILE:HG12	2.17	0.45
8:G:165:LEU:O	8:G:165:LEU:HG	2.17	0.45
11:J:129:ASN:HD22	11:J:129:ASN:HA	1.57	0.45
18:R:74:LEU:O	18:R:74:LEU:HG	2.17	0.45
21:U:53:ILE:CG2	21:U:54:SER:N	2.79	0.45
24:X:1:MET:N	24:X:1:MET:HE3	2.32	0.45
33:M:29:GLN:O	33:M:33:TYR:HD1	1.99	0.45
33:M:52:GLN:HA	33:M:56:ILE:HG12	1.99	0.45
1:2:39:A:OP1	11:J:5:SER:OG	2.35	0.45
1:2:432:G:OP2	1:2:433:C:O2'	2.28	0.45
1:2:989:U:O2'	1:2:990:U:P	2.74	0.45
26:Z:33:PHE:CZ	26:Z:48:ARG:HG2	2.52	0.45
27:a:21:LYS:HG3	27:a:24:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:48:U:H3	32:g:62:C:H42	1.63	0.45
33:M:44:LEU:HD12	33:M:45:ALA:H	1.82	0.45
1:2:968:G:O2'	1:2:969:G:OP1	2.29	0.45
1:2:1271:A:H2'	1:2:1272:G:O4'	2.17	0.45
14:N:131:GLN:O	14:N:132:ALA:HB3	2.17	0.45
1:2:891:G:H4'	1:2:892:A:OP2	2.16	0.44
6:E:120:GLY:O	6:E:163:ASN:ND2	2.44	0.44
15:O:106:GLY:O	15:O:110:ILE:HG12	2.17	0.44
15:O:109:ALA:O	15:O:113:LEU:HD12	2.18	0.44
16:P:28:MET:HG2	16:P:29:LYS:N	2.32	0.44
18:R:6:THR:CG2	18:R:7:LYS:N	2.80	0.44
32:g:52:G:H1	32:g:56:U:H5	1.65	0.44
7:F:89:TYR:HD2	7:F:164:MET:HE1	1.83	0.44
12:K:73:ARG:HB2	12:K:73:ARG:CZ	2.47	0.44
1:2:629:G:O2'	14:N:108:ASP:OD1	2.30	0.44
5:D:56:ILE:HD13	5:D:56:ILE:N	2.32	0.44
16:P:106:GLU:OE2	16:P:108:LYS:NZ	2.47	0.44
4:C:37:VAL:HG21	4:C:60:ILE:HG23	1.98	0.44
4:C:223:LEU:O	22:V:23:LYS:NZ	2.47	0.44
18:R:6:THR:HG22	18:R:7:LYS:N	2.32	0.44
18:R:14:ARG:O	18:R:18:GLU:OE1	2.34	0.44
18:R:17:VAL:HG21	18:R:60:LEU:CD2	2.47	0.44
21:U:100:ASP:HB2	21:U:103:THR:HG23	1.99	0.44
5:D:146:GLY:C	5:D:153:ALA:HB1	2.42	0.44
7:F:45:LYS:HE2	7:F:45:LYS:CA	2.47	0.44
1:2:636:G:N2	15:O:132:ASP:HB3	2.33	0.44
3:B:171:THR:HG23	3:B:175:GLU:OE1	2.18	0.44
11:J:93:ASP:OD1	11:J:93:ASP:N	2.50	0.44
19:S:122:ARG:HG2	19:S:132:VAL:HG13	2.00	0.44
23:W:101:HIS:ND1	23:W:112:ASP:OD2	2.50	0.44
34:e:33:ARG:HB2	34:e:33:ARG:CZ	2.47	0.44
2:A:126:LEU:HD13	2:A:127:LEU:N	2.33	0.44
7:F:126:ASP:OD1	7:F:126:ASP:N	2.50	0.44
15:O:77:GLU:OE1	15:O:78:ILE:N	2.50	0.44
17:Q:25:VAL:HB	17:Q:40:VAL:HB	2.00	0.44
20:T:50:PHE:O	20:T:54:VAL:HG13	2.18	0.44
21:U:33:ASP:OD2	21:U:36:LEU:CD2	2.66	0.44
1:2:123:A:H4'	1:2:124:G:O5'	2.17	0.44
1:2:739:C:O2'	1:2:740:U:C6	2.71	0.44
1:2:883:C:H2'	1:2:884:A:O4'	2.17	0.44
2:A:49:ASP:OD1	2:A:51:THR:OG1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:56:ILE:HB	5:D:94:VAL:HG12	1.99	0.44
12:K:25:LYS:NZ	12:K:74:HIS:HD2	2.15	0.44
26:Z:23:ASP:O	26:Z:25:ALA:N	2.51	0.44
1:2:81:C:O2'	6:E:8:HIS:ND1	2.48	0.44
1:2:387:G:H4'	11:J:132:LYS:HE3	1.99	0.44
5:D:113:ALA:O	5:D:117:GLU:HG2	2.18	0.44
7:F:160:ALA:O	7:F:164:MET:SD	2.76	0.44
12:K:69:THR:HG22	12:K:69:THR:O	2.18	0.44
12:K:73:ARG:O	12:K:73:ARG:HG3	2.17	0.44
17:Q:62:LEU:O	17:Q:65:LYS:N	2.51	0.44
1:2:1191:G:O2'	1:2:1192:C:P	2.76	0.43
12:K:103:SER:O	12:K:104:LYS:C	2.60	0.43
16:P:83:MET:HE3	16:P:84:ILE:O	2.18	0.43
18:R:43:ILE:O	18:R:43:ILE:CG2	2.64	0.43
19:S:3:THR:O	26:Z:20:LEU:HD21	2.17	0.43
32:g:57:C:H3'	32:g:58:G:H8	1.83	0.43
1:2:112:C:H2'	1:2:113:G:O4'	2.17	0.43
3:B:159:ARG:O	3:B:163:MET:HG3	2.18	0.43
7:F:1:MET:SD	7:F:3:LEU:HD23	2.58	0.43
24:X:6:GLY:O	24:X:9:THR:OG1	2.27	0.43
24:X:96:ASN:OD1	24:X:97:ASN:N	2.51	0.43
1:2:1210:G:H4'	20:T:96:ARG:HH21	1.83	0.43
1:2:1210:G:C2	17:Q:1:MET:HB2	2.53	0.43
6:E:15:PRO:HB3	6:E:17:HIS:CE1	2.53	0.43
20:T:52:ASP:OD2	38:T:202:HOH:O	2.20	0.43
20:T:113:ARG:HG2	20:T:113:ARG:HH11	1.84	0.43
32:g:56:U:HO2'	32:g:58:G:P	2.38	0.43
1:2:833:G:O2'	1:2:834:A:H3'	2.19	0.43
4:C:51:TYR:CZ	4:C:233:GLN:HB3	2.52	0.43
6:E:15:PRO:HB3	6:E:17:HIS:HE1	1.84	0.43
6:E:125:ARG:NH2	6:E:157:ASN:OD1	2.51	0.43
17:Q:12:ARG:O	17:Q:20:ARG:HD2	2.19	0.43
25:Y:101:LYS:NZ	25:Y:102:PRO:O	2.51	0.43
1:2:27:A:O2'	24:X:46:MET:HE1	2.18	0.43
11:J:46:ARG:O	11:J:50:MET:HG3	2.18	0.43
14:N:128:TYR:O	14:N:131:GLN:O	2.36	0.43
17:Q:140:GLU:OE1	17:Q:149:ALA:CB	2.67	0.43
22:V:52:MET:HE1	22:V:53:ILE:O	2.19	0.43
26:Z:16:ASP:C	26:Z:16:ASP:OD1	2.62	0.43
1:2:194:A:N7	38:2:1656:HOH:O	2.37	0.43
1:2:471:G:H2'	1:2:472:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1144:C:O2'	1:2:1145:U:O5'	2.36	0.43
8:G:164:MET:HE2	8:G:166:VAL:H	1.84	0.43
9:H:29:GLU:CD	9:H:29:GLU:H	2.26	0.43
9:H:146:TYR:CG	9:H:147:PRO:HD3	2.54	0.43
10:I:10:LYS:O	10:I:18:GLN:OE1	2.36	0.43
14:N:29:THR:HG23	14:N:31:GLU:H	1.83	0.43
19:S:95:LYS:HZ3	19:S:95:LYS:HB2	1.83	0.43
21:U:64:LEU:O	21:U:84:GLU:HA	2.19	0.43
28:b:77:LYS:HD2	28:b:77:LYS:N	2.32	0.43
29:c:59:GLU:OE2	29:c:59:GLU:HA	2.18	0.43
1:2:319:C:H2'	1:2:320:G:H8	1.83	0.43
1:2:577:G:O2'	1:2:578:A:N7	2.45	0.43
3:B:93:ASP:N	3:B:93:ASP:OD1	2.51	0.43
10:I:138:ASP:OD1	10:I:138:ASP:N	2.50	0.43
15:O:111:ARG:O	15:O:115:ARG:HG2	2.18	0.43
1:2:1161:G:N3	1:2:1161:G:H2'	2.34	0.43
1:2:1451:U:O2	1:2:1451:U:O4'	2.37	0.43
10:I:55:ILE:N	10:I:63:LYS:O	2.46	0.43
12:K:17:TYR:HD2	12:K:87:ILE:HG21	1.84	0.43
16:P:33:ILE:O	16:P:33:ILE:HG13	2.18	0.43
18:R:4:VAL:O	18:R:4:VAL:CG1	2.66	0.43
25:Y:90:ARG:HG3	25:Y:90:ARG:HH11	1.84	0.43
26:Z:54:ALA:O	26:Z:58:ARG:HG2	2.19	0.43
33:M:34:LEU:HD12	33:M:35:GLU:N	2.33	0.43
33:M:44:LEU:CG	33:M:45:ALA:H	2.31	0.43
2:A:85:ARG:NH2	2:A:131:ASP:OD2	2.52	0.43
4:C:84:THR:OG1	4:C:87:GLY:O	2.33	0.43
6:E:95:VAL:HB	6:E:97:LYS:HG3	2.01	0.43
16:P:52:MET:HE3	16:P:56:ARG:HD3	2.01	0.43
20:T:133:ILE:HG12	20:T:134:ALA:N	2.33	0.43
26:Z:45:ILE:CG1	26:Z:49:LEU:HD21	2.48	0.43
33:M:86:CYS:HA	33:M:92:LYS:HA	2.01	0.43
1:2:307:U:H2'	1:2:308:G:O4'	2.19	0.43
1:2:675:A:H2'	1:2:676:G:C8	2.54	0.43
1:2:1187:G:OP2	17:Q:2:ALA:O	2.37	0.43
5:D:61:PRO:HA	5:D:64:VAL:HG12	2.00	0.43
7:F:30:ASP:OD1	7:F:30:ASP:C	2.62	0.43
8:G:212:GLU:O	8:G:216:LYS:HG3	2.18	0.43
15:O:38:VAL:HG23	15:O:75:LEU:HD21	2.01	0.43
22:V:48:ASP:OD1	22:V:49:LYS:N	2.52	0.43
29:c:56:SER:OG	29:c:57:GLU:OE1	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:57:GLY:N	34:e:58:PRO:CD	2.82	0.43
8:G:103:ILE:HD12	8:G:103:ILE:O	2.19	0.42
9:H:171:LYS:HZ1	9:H:201:MET:HA	1.82	0.42
16:P:78:THR:OG1	16:P:79:HIS:N	2.51	0.42
16:P:93:THR:HG23	16:P:93:THR:O	2.17	0.42
21:U:26:THR:HA	21:U:93:TRP:HA	2.01	0.42
24:X:77:ASN:C	24:X:78:SER:OG	2.62	0.42
28:b:76:ILE:HD11	28:b:118:VAL:HG21	1.99	0.42
1:2:969:G:C6	33:M:26:GLY:HA3	2.54	0.42
8:G:24:ILE:HD12	8:G:24:ILE:N	2.34	0.42
16:P:34:LEU:N	16:P:35:PRO:HD2	2.33	0.42
17:Q:112:LYS:N	17:Q:112:LYS:CD	2.82	0.42
17:Q:147:ARG:CD	17:Q:147:ARG:N	2.82	0.42
27:a:61:ASP:OD1	27:a:61:ASP:N	2.52	0.42
30:d:67:TRP:H	30:d:67:TRP:CD1	2.36	0.42
30:d:73:ASN:OD1	30:d:75:ASN:ND2	2.51	0.42
1:2:85:U:OP1	38:2:1629:HOH:O	2.21	0.42
1:2:1262:A:OP2	32:g:34:U:OP1	2.36	0.42
12:K:65:VAL:HG13	12:K:83:GLY:HA3	2.00	0.42
17:Q:112:LYS:N	17:Q:112:LYS:HD3	2.33	0.42
17:Q:113:ASP:OD1	17:Q:113:ASP:N	2.52	0.42
14:N:100:LYS:O	14:N:103:GLU:HG3	2.19	0.42
21:U:120:VAL:C	21:U:121:GLU:OE2	2.62	0.42
23:W:57:ARG:O	23:W:57:ARG:HG2	2.19	0.42
24:X:96:ASN:OD1	24:X:97:ASN:ND2	2.52	0.42
28:b:57:GLN:OE1	28:b:57:GLN:HA	2.19	0.42
3:B:233:ASP:OD1	3:B:233:ASP:O	2.37	0.42
7:F:23:LEU:C	7:F:23:LEU:CD1	2.92	0.42
18:R:28:ASP:CG	18:R:31:ASN:HB3	2.45	0.42
20:T:26:VAL:HG21	20:T:156:LEU:HD11	2.00	0.42
20:T:29:ASP:OD1	20:T:30:VAL:N	2.51	0.42
21:U:33:ASP:O	21:U:37:VAL:HG23	2.19	0.42
7:F:136:GLY:O	7:F:140:ILE:HG12	2.20	0.42
8:G:49:GLU:H	8:G:49:GLU:CD	2.28	0.42
10:I:39:ILE:O	10:I:40:VAL:HG22	2.19	0.42
33:M:35:GLU:HA	33:M:64:TYR:CE2	2.55	0.42
33:M:87:LEU:HD23	33:M:93:ILE:HD13	2.00	0.42
1:2:135:C:O2'	8:G:19:ASN:ND2	2.48	0.42
6:E:149:PHE:HZ	8:G:221:LEU:HD23	1.84	0.42
7:F:113:ARG:NH2	32:g:32:U:OP2	2.52	0.42
9:H:30:LEU:HA	9:H:33:GLN:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:93:ILE:HG22	33:M:93:ILE:O	2.19	0.42
13:L:41:LYS:O	13:L:45:GLU:OE1	2.37	0.42
16:P:36:LYS:O	16:P:37:LEU:HD12	2.20	0.42
20:T:146:ARG:O	20:T:150:GLU:HG3	2.20	0.42
21:U:53:ILE:CG2	21:U:54:SER:H	2.32	0.42
32:g:20:U:N3	32:g:46:G:N7	2.68	0.42
1:2:556:C:H41	25:Y:10:LYS:CG	2.32	0.42
1:2:678:C:O2	15:O:132:ASP:HB2	2.19	0.42
1:2:801:C:H42	1:2:809:C:H42	1.67	0.42
3:B:89:GLN:HB2	3:B:228:LEU:HD22	2.02	0.42
12:K:73:ARG:HH11	12:K:73:ARG:HB3	1.85	0.42
14:N:100:LYS:O	14:N:104:ARG:HG3	2.20	0.42
24:X:74:LEU:N	24:X:74:LEU:HD22	2.34	0.42
27:a:97:SER:O	27:a:101:ARG:HG3	2.20	0.42
32:g:34:U:C6	32:g:34:U:OP2	2.73	0.42
33:M:29:GLN:O	33:M:33:TYR:CD1	2.73	0.42
1:2:1208:C:O2'	1:2:1209:G:H5'	2.20	0.42
1:2:1211:A:O2'	1:2:1212:G:C8	2.73	0.42
20:T:136:GLU:HG2	20:T:137:ARG:HG3	2.01	0.42
23:W:55:ASN:O	23:W:56:HIS:HB2	2.20	0.42
28:b:85:VAL:HG22	28:b:86:VAL:N	2.35	0.42
1:2:1060:A:H4'	1:2:1061:A:O5'	2.20	0.41
1:2:1232:C:O2'	1:2:1233:G:H5'	2.20	0.41
8:G:159:ASP:N	8:G:160:PRO:HD2	2.35	0.41
9:H:149:HIS:NE2	14:N:21:ALA:CB	2.83	0.41
13:L:65:ARG:NH1	13:L:74:CYS:O	2.52	0.41
17:Q:114:GLU:CD	17:Q:114:GLU:C	2.88	0.41
20:T:76:SER:OG	20:T:98:TYR:OH	2.32	0.41
1:2:1299:G:O2'	1:2:1300:C:H5'	2.20	0.41
2:A:21:LYS:O	2:A:25:VAL:HG13	2.20	0.41
11:J:39:LYS:HA	34:e:33:ARG:HG2	2.01	0.41
14:N:149:LEU:N	14:N:149:LEU:HD23	2.35	0.41
18:R:75:ARG:NH2	18:R:76:LEU:HA	2.35	0.41
31:f:98:TYR:O	31:f:105:ALA:CB	2.68	0.41
33:M:30:VAL:HG13	33:M:31:PHE:N	2.35	0.41
5:D:60:GLU:O	5:D:60:GLU:HG2	2.19	0.41
5:D:117:GLU:O	5:D:118:ALA:HB3	2.21	0.41
11:J:120:LEU:HD23	11:J:120:LEU:O	2.19	0.41
1:2:151:A:OP1	8:G:143:ARG:HG3	2.20	0.41
1:2:202:A:H2'	1:2:202:A:N3	2.35	0.41
1:2:534:A:H2'	1:2:535:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:174:TYR:N	9:H:176:GLU:OE2	2.53	0.41
12:K:68:ASP:OD1	12:K:70:PHE:N	2.53	0.41
18:R:28:ASP:OD1	18:R:31:ASN:N	2.54	0.41
20:T:75:ALA:O	20:T:78:ILE:HG22	2.20	0.41
26:Z:16:ASP:OD1	26:Z:16:ASP:O	2.38	0.41
27:a:68:ILE:HG22	27:a:69:GLN:N	2.35	0.41
1:2:1211:A:O2'	1:2:1212:G:H8	2.03	0.41
9:H:37:THR:HG21	9:H:95:LEU:CD1	2.51	0.41
9:H:96:GLU:HA	9:H:96:GLU:OE2	2.21	0.41
10:I:64:ARG:HB3	10:I:64:ARG:NH1	2.35	0.41
15:O:69:MET:O	15:O:73:GLN:HG3	2.20	0.41
1:2:492:U:OP2	1:2:493:G:O2'	2.36	0.41
1:2:790:C:H2'	1:2:791:G:O4'	2.21	0.41
1:2:802:G:H2'	1:2:803:C:C6	2.55	0.41
1:2:1127:A:H2'	1:2:1128:G:O4'	2.20	0.41
1:2:1368:G:H2'	1:2:1368:G:N3	2.35	0.41
2:A:56:LEU:HA	2:A:59:VAL:HG12	2.03	0.41
8:G:164:MET:HE2	8:G:166:VAL:N	2.35	0.41
9:H:92:ILE:N	9:H:92:ILE:HD13	2.35	0.41
12:K:8:VAL:O	12:K:12:VAL:HG23	2.20	0.41
16:P:87:PRO:O	16:P:90:ILE:CG1	2.68	0.41
20:T:105:LYS:O	20:T:106:THR:HG22	2.20	0.41
32:g:40:U:H2'	32:g:41:C:C6	2.55	0.41
5:D:124:ALA:O	5:D:128:ILE:HG12	2.21	0.41
7:F:31:ASN:O	7:F:53:PRO:HG3	2.21	0.41
8:G:91:LEU:HD23	8:G:91:LEU:HA	1.95	0.41
15:O:74:ASP:O	15:O:78:ILE:HG13	2.21	0.41
18:R:74:LEU:O	18:R:74:LEU:CG	2.69	0.41
25:Y:90:ARG:HG3	25:Y:90:ARG:NH1	2.35	0.41
26:Z:33:PHE:C	26:Z:33:PHE:HD1	2.29	0.41
28:b:45:ASN:OD1	28:b:45:ASN:N	2.53	0.41
33:M:75:ARG:CZ	33:M:75:ARG:HB3	2.51	0.41
3:B:125:MET:HG2	3:B:126:ASP:N	2.34	0.41
4:C:33:LEU:HD13	4:C:33:LEU:C	2.46	0.41
5:D:115:LEU:HA	5:D:115:LEU:HD23	1.88	0.41
5:D:192:VAL:HG12	5:D:193:ARG:N	2.35	0.41
11:J:113:SER:O	11:J:117:GLU:HG2	2.21	0.41
17:Q:85:ILE:CG2	17:Q:86:LYS:N	2.84	0.41
17:Q:108:LEU:HD12	17:Q:108:LEU:HA	1.94	0.41
23:W:3:ARG:NH1	23:W:9:ASP:OD2	2.53	0.41
26:Z:49:LEU:HA	26:Z:50:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:92:LYS:HG3	33:M:94:ILE:HD13	2.02	0.41
1:2:444:G:N1	1:2:460:A:OP1	2.50	0.41
1:2:615:G:P	14:N:13:ARG:CZ	3.09	0.41
1:2:1123:C:H2'	1:2:1124:G:O4'	2.21	0.41
4:C:222:ASP:OD1	4:C:222:ASP:N	2.54	0.41
5:D:111:LEU:HD21	5:D:190:VAL:HG21	2.03	0.41
7:F:122:ARG:HB2	7:F:189:ASN:ND2	2.36	0.41
8:G:47:LEU:HD12	8:G:47:LEU:N	2.36	0.41
13:L:115:ARG:HB3	13:L:199:PHE:HB3	2.03	0.41
16:P:109:PRO:N	16:P:110:PRO:HD2	2.36	0.41
17:Q:114:GLU:OE1	17:Q:115:ALA:N	2.54	0.41
19:S:102:ASN:OD1	19:S:102:ASN:C	2.64	0.41
22:V:73:ASP:OD1	22:V:73:ASP:N	2.51	0.41
30:d:109:ASN:O	30:d:110:SER:OG	2.37	0.41
33:M:28:ARG:O	33:M:28:ARG:HG2	2.20	0.41
1:2:576:G:H2'	1:2:577:G:O4'	2.21	0.41
6:E:161:LYS:HD3	6:E:171:GLU:OE1	2.21	0.41
7:F:120:VAL:O	7:F:121:ARG:C	2.64	0.41
17:Q:147:ARG:NH1	17:Q:153:ARG:HG3	2.36	0.41
21:U:63:ARG:CZ	21:U:84:GLU:OE1	2.69	0.41
31:f:98:TYR:CE2	31:f:106:GLU:HG3	2.56	0.41
32:g:6:A:C2	32:g:65:A:N1	2.89	0.41
32:g:12:G:C6	32:g:22:A:N1	2.89	0.41
33:M:44:LEU:HG	33:M:45:ALA:H	1.86	0.41
1:2:1066:C:C2	1:2:1067:G:C8	3.09	0.40
2:A:26:ALA:O	2:A:27:THR:OG1	2.30	0.40
5:D:37:ASP:OD1	5:D:37:ASP:N	2.45	0.40
13:L:186:GLU:OE2	13:L:186:GLU:HA	2.21	0.40
20:T:107:THR:CG2	20:T:108:PRO:HD2	2.50	0.40
31:f:130:CYS:O	31:f:131:GLY:C	2.63	0.40
11:J:69:ILE:HG23	11:J:70:LYS:N	2.36	0.40
20:T:158:LYS:HE3	20:T:158:LYS:HB3	1.94	0.40
25:Y:92:ILE:HG23	25:Y:99:ALA:HB2	2.03	0.40
26:Z:74:LYS:HD3	26:Z:75:SER:N	2.36	0.40
31:f:99:THR:HG21	31:f:103:ASP:O	2.22	0.40
1:2:901:A:H2'	1:2:902:C:H6	1.86	0.40
1:2:1186:A:H2'	1:2:1187:G:C8	2.56	0.40
5:D:168:HIS:N	5:D:169:PRO:CD	2.84	0.40
16:P:56:ARG:HH11	16:P:56:ARG:HG3	1.85	0.40
1:2:317:C:C2	1:2:318:C:C5	3.09	0.40
7:F:185:ILE:N	7:F:185:ILE:HD13	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:92:GLU:OE1	19:S:92:GLU:CA	2.69	0.40
20:T:45:ILE:HB	20:T:125:GLN:OE1	2.22	0.40
24:X:131:LEU:O	24:X:135:LEU:HD12	2.20	0.40
32:g:62:C:H2'	32:g:63:G:C8	2.56	0.40
33:M:67:HIS:O	33:M:67:HIS:CD2	2.75	0.40
1:2:808:C:C2'	1:2:809:C:H5'	2.51	0.40
1:2:1354:C:H2'	1:2:1355:G:O4'	2.21	0.40
9:H:91:LEU:HD23	9:H:92:ILE:HD13	2.03	0.40
12:K:44:LYS:O	12:K:45:LEU:HD23	2.21	0.40
13:L:165:ILE:HD12	13:L:188:VAL:CG2	2.52	0.40
14:N:38:CYS:HB2	14:N:78:LYS:HZ2	1.87	0.40
15:O:37:HIS:HD2	15:O:39:THR:HG23	1.87	0.40
27:a:94:ARG:CZ	27:a:94:ARG:HB2	2.51	0.40
29:c:39:ARG:HE	29:c:39:ARG:HB3	1.68	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	
2	A	197/245 (80%)	192 (98%)	5 (2%)	0	100	100
3	B	222/248 (90%)	216 (97%)	6 (3%)	0	100	100
4	C	207/242 (86%)	202 (98%)	5 (2%)	0	100	100
5	D	207/217 (95%)	190 (92%)	17 (8%)	0	100	100
6	E	256/268 (96%)	246 (96%)	10 (4%)	0	100	100
7	F	188/190 (99%)	173 (92%)	15 (8%)	0	100	100
8	G	208/248 (84%)	198 (95%)	10 (5%)	0	100	100
9	H	161/201 (80%)	155 (96%)	6 (4%)	0	100	100
10	I	163/174 (94%)	159 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	162/189 (86%)	158 (98%)	4 (2%)	0	100	100
12	K	103/134 (77%)	93 (90%)	9 (9%)	1 (1%)	12	31
13	L	168/199 (84%)	163 (97%)	5 (3%)	0	100	100
14	N	151/154 (98%)	149 (99%)	2 (1%)	0	100	100
15	O	137/145 (94%)	134 (98%)	3 (2%)	0	100	100
16	P	104/145 (72%)	99 (95%)	5 (5%)	0	100	100
17	Q	156/158 (99%)	142 (91%)	14 (9%)	0	100	100
18	R	79/137 (58%)	78 (99%)	1 (1%)	0	100	100
19	S	141/154 (92%)	122 (86%)	19 (14%)	0	100	100
20	T	135/158 (85%)	127 (94%)	8 (6%)	0	100	100
21	U	101/126 (80%)	94 (93%)	7 (7%)	0	100	100
22	V	79/89 (89%)	78 (99%)	1 (1%)	0	100	100
23	W	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
24	X	141/143 (99%)	133 (94%)	8 (6%)	0	100	100
25	Y	118/132 (89%)	110 (93%)	8 (7%)	0	100	100
26	Z	71/88 (81%)	63 (89%)	8 (11%)	0	100	100
27	a	94/109 (86%)	93 (99%)	1 (1%)	0	100	100
28	b	66/124 (53%)	63 (96%)	3 (4%)	0	100	100
29	c	58/64 (91%)	53 (91%)	5 (9%)	0	100	100
30	d	81/137 (59%)	66 (82%)	15 (18%)	0	100	100
31	f	29/137 (21%)	21 (72%)	7 (24%)	1 (3%)	3	7
33	M	97/125 (78%)	81 (84%)	16 (16%)	0	100	100
34	e	46/69 (67%)	45 (98%)	1 (2%)	0	100	100
All	All	4253/5079 (84%)	4011 (94%)	240 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	K	71	ALA
31	f	124	HIS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	175/217 (81%)	171 (98%)	4 (2%)	44	68
3	B	202/220 (92%)	198 (98%)	4 (2%)	48	70
4	C	173/201 (86%)	171 (99%)	2 (1%)	63	78
5	D	174/182 (96%)	171 (98%)	3 (2%)	53	73
6	E	227/232 (98%)	220 (97%)	7 (3%)	35	60
7	F	156/157 (99%)	152 (97%)	4 (3%)	40	65
8	G	185/213 (87%)	170 (92%)	15 (8%)	11	26
9	H	148/181 (82%)	141 (95%)	7 (5%)	23	48
10	I	141/148 (95%)	139 (99%)	2 (1%)	59	76
11	J	146/164 (89%)	143 (98%)	3 (2%)	47	70
12	K	94/119 (79%)	92 (98%)	2 (2%)	47	70
13	L	146/171 (85%)	140 (96%)	6 (4%)	27	52
14	N	129/130 (99%)	125 (97%)	4 (3%)	35	60
15	O	107/113 (95%)	103 (96%)	4 (4%)	30	55
16	P	97/128 (76%)	93 (96%)	4 (4%)	27	52
17	Q	130/130 (100%)	122 (94%)	8 (6%)	16	37
18	R	72/123 (58%)	66 (92%)	6 (8%)	10	26
19	S	122/131 (93%)	112 (92%)	10 (8%)	10	26
20	T	113/133 (85%)	107 (95%)	6 (5%)	20	43
21	U	92/110 (84%)	86 (94%)	6 (6%)	15	35
22	V	64/72 (89%)	61 (95%)	3 (5%)	23	48
23	W	114/115 (99%)	113 (99%)	1 (1%)	70	82
24	X	114/114 (100%)	111 (97%)	3 (3%)	40	65
25	Y	106/113 (94%)	104 (98%)	2 (2%)	50	71
26	Z	65/79 (82%)	62 (95%)	3 (5%)	24	49
27	a	90/103 (87%)	88 (98%)	2 (2%)	45	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	b	64/112 (57%)	63 (98%)	1 (2%)	55	74
29	c	53/57 (93%)	49 (92%)	4 (8%)	12	29
30	d	73/116 (63%)	72 (99%)	1 (1%)	59	76
31	f	28/112 (25%)	28 (100%)	0	100	100
33	M	93/112 (83%)	89 (96%)	4 (4%)	26	51
34	e	46/58 (79%)	46 (100%)	0	100	100
All	All	3739/4366 (86%)	3608 (96%)	131 (4%)	32	56

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	14	GLN
2	A	29	HIS
2	A	87	ASP
2	A	151	SER
3	B	135	LEU
3	B	171	THR
3	B	223	ASN
3	B	224	THR
4	C	115	VAL
4	C	217	SER
5	D	72	LEU
5	D	95	ASP
5	D	119	MET
6	E	98	THR
6	E	123	LEU
6	E	126	VAL
6	E	139	LEU
6	E	170	ASP
6	E	204	SER
6	E	220	THR
7	F	23	LEU
7	F	59	THR
7	F	142	THR
7	F	181	SER
8	G	12	SER
8	G	15	VAL
8	G	54	CYS
8	G	76	SER
8	G	89	CYS

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Mol	Chain	Res	Type
8	G	102	SER
8	G	118	VAL
8	G	120	VAL
8	G	126	THR
8	G	135	VAL
8	G	140	VAL
8	G	188	TYR
8	G	214	MET
8	G	218	LEU
8	G	240	TYR
9	H	155	THR
9	H	156	LEU
9	H	165	LEU
9	H	167	VAL
9	H	177	VAL
9	H	183	THR
9	H	196	THR
10	I	54	THR
10	I	97	ASN
11	J	116	VAL
11	J	129	ASN
11	J	147	SER
12	K	8	VAL
12	K	45	LEU
13	L	59	SER
13	L	63	GLN
13	L	67	LEU
13	L	108	SER
13	L	161	LYS
13	L	167	THR
14	N	19	THR
14	N	29	THR
14	N	48	SER
14	N	54	LEU
15	O	24	VAL
15	O	31	LYS
15	O	74	ASP
15	O	80	THR
16	P	31	THR
16	P	94	VAL
16	P	96	VAL
16	P	122	SER

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Mol	Chain	Res	Type
17	Q	8	ASP
17	Q	21	ASP
17	Q	44	LYS
17	Q	68	GLU
17	Q	79	LYS
17	Q	104	SER
17	Q	113	ASP
17	Q	133	VAL
18	R	16	ILE
18	R	28	ASP
18	R	41	VAL
18	R	61	MET
18	R	70	HIS
18	R	75	ARG
19	S	12	ASP
19	S	37	ILE
19	S	53	VAL
19	S	55	LYS
19	S	59	GLU
19	S	92	GLU
19	S	93	SER
19	S	107	THR
19	S	135	GLN
19	S	137	THR
20	T	23	VAL
20	T	68	ASP
20	T	91	VAL
20	T	124	SER
20	T	132	LEU
20	T	156	LEU
21	U	29	VAL
21	U	36	LEU
21	U	77	THR
21	U	101	ILE
21	U	102	SER
21	U	120	VAL
22	V	42	SER
22	V	78	LEU
22	V	81	GLN
23	W	25	VAL
24	X	24	ASP
24	X	51	VAL

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Mol	Chain	Res	Type
24	X	66	VAL
25	Y	46	GLN
25	Y	104	SER
26	Z	29	GLU
26	Z	31	LEU
26	Z	39	CYS
27	a	20	SER
27	a	87	SER
28	b	55	GLU
29	c	23	THR
29	c	25	VAL
29	c	27	VAL
29	c	30	MET
30	d	137	HIS
33	M	12	GLU
33	M	18	HIS
33	M	59	CYS
33	M	62	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	14	GLN
2	A	47	GLN
2	A	100	HIS
3	B	18	ASN
3	B	87	GLN
3	B	190	ASN
6	E	188	ASN
6	E	196	GLN
7	F	189	ASN
8	G	95	ASN
8	G	219	GLN
9	H	98	ASN
9	H	99	HIS
10	I	35	ASN
11	J	67	ASN
11	J	129	ASN
11	J	141	GLN
12	K	52	HIS
12	K	74	HIS
14	N	145	GLN

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Mol	Chain	Res	Type
15	O	70	GLN
19	S	128	HIS
23	W	5	ASN
23	W	56	HIS
24	X	97	ASN
26	Z	28	ASN
26	Z	42	HIS
27	a	81	GLN
33	M	18	HIS
33	M	105	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1437/1451 (99%)	249 (17%)	12 (0%)
32	g	73/74 (98%)	18 (24%)	0
All	All	1510/1525 (99%)	267 (17%)	12 (0%)

All (267) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	33	U
1	2	41	G
1	2	42	A
1	2	44	G
1	2	45	A
1	2	46	A
1	2	49	C
1	2	50	A
1	2	59	C
1	2	60	G
1	2	62	U
1	2	63	C
1	2	64	A
1	2	65	C
1	2	70	G
1	2	71	A
1	2	73	G

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Mol	Chain	Res	Type
1	2	80	A
1	2	89	G
1	2	91	C
1	2	92	A
1	2	101	A
1	2	114	G
1	2	116	C
1	2	117	C
1	2	124	G
1	2	125	C
1	2	136	U
1	2	137	G
1	2	138	G
1	2	144	C
1	2	149	C
1	2	151	A
1	2	160	G
1	2	171	G
1	2	174	G
1	2	186	G
1	2	198	A
1	2	204	G
1	2	206	C
1	2	216	C
1	2	226	A
1	2	227	U
1	2	228	C
1	2	230	C
1	2	234	G
1	2	249	G
1	2	250	C
1	2	257	A
1	2	258	G
1	2	273	C
1	2	283	G
1	2	313	A
1	2	314	C
1	2	328	A
1	2	329	A
1	2	330	G
1	2	336	C
1	2	337	A

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Mol	Chain	Res	Type
1	2	351	U
1	2	356	C
1	2	357	A
1	2	365	G
1	2	366	C
1	2	367	G
1	2	389	G
1	2	393	G
1	2	394	A
1	2	397	G
1	2	421	C
1	2	422	G
1	2	435	A
1	2	436	G
1	2	445	C
1	2	458	U
1	2	460	A
1	2	474	A
1	2	491	C
1	2	499	G
1	2	500	A
1	2	502	A
1	2	503	C
1	2	504	G
1	2	519	C
1	2	520	C
1	2	521	C
1	2	534	A
1	2	535	A
1	2	544	G
1	2	545	C
1	2	556	C
1	2	557	C
1	2	558	C
1	2	559	G
1	2	560	U
1	2	561	U
1	2	568	G
1	2	569	C
1	2	570	C
1	2	571	G
1	2	578	A

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Mol	Chain	Res	Type
1	2	584	C
1	2	586	G
1	2	592	G
1	2	593	C
1	2	602	G
1	2	603	C
1	2	604	G
1	2	605	G
1	2	607	A
1	2	608	G
1	2	614	A
1	2	615	G
1	2	616	G
1	2	624	G
1	2	627	G
1	2	637	U
1	2	665	G
1	2	680	G
1	2	681	C
1	2	684	G
1	2	685	C
1	2	686	C
1	2	711	U
1	2	717	A
1	2	721	A
1	2	739	C
1	2	740	U
1	2	756	A
1	2	777	A
1	2	779	C
1	2	782	U
1	2	783	G
1	2	790	C
1	2	807	U
1	2	809	C
1	2	810	C
1	2	832	G
1	2	833	G
1	2	838	U
1	2	879	A
1	2	891	G
1	2	892	A

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Mol	Chain	Res	Type
1	2	899	C
1	2	908	G
1	2	911	G
1	2	912	A
1	2	920	G
1	2	926	U
1	2	935	A
1	2	937	G
1	2	938	C
1	2	939	G
1	2	941	G
1	2	942	C
1	2	948	A
1	2	949	C
1	2	957	G
1	2	958	G
1	2	960	C
1	2	967	A
1	2	968	G
1	2	969	G
1	2	973	G
1	2	978	C
1	2	980	G
1	2	983	C
1	2	984	G
1	2	985	C
1	2	990	U
1	2	992	G
1	2	997	C
1	2	1004	G
1	2	1008	U
1	2	1014	A
1	2	1025	C
1	2	1027	G
1	2	1046	U
1	2	1052	A
1	2	1053	U
1	2	1054	U
1	2	1060	A
1	2	1069	G
1	2	1086	C
1	2	1087	C

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Mol	Chain	Res	Type
1	2	1088	G
1	2	1095	G
1	2	1101	C
1	2	1107	C
1	2	1119	G
1	2	1130	A
1	2	1131	G
1	2	1139	A
1	2	1140	U
1	2	1145	U
1	2	1147	A
1	2	1148	G
1	2	1149	A
1	2	1150	C
1	2	1155	U
1	2	1160	C
1	2	1163	A
1	2	1167	G
1	2	1174	A
1	2	1177	G
1	2	1185	C
1	2	1189	C
1	2	1192	C
1	2	1196	C
1	2	1208	C
1	2	1210	G
1	2	1212	G
1	2	1235	G
1	2	1244	C
1	2	1247	C
1	2	1261	A
1	2	1269	G
1	2	1275	G
1	2	1278	C
1	2	1286	C
1	2	1297	A
1	2	1301	G
1	2	1320	A
1	2	1342	U
1	2	1343	G
1	2	1367	C
1	2	1368	G

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Mol	Chain	Res	Type
1	2	1370	G
1	2	1371	C
1	2	1372	G
1	2	1379	C
1	2	1383	A
1	2	1408	A
1	2	1409	G
1	2	1414	A
1	2	1418	A
1	2	1419	G
1	2	1421	U
1	2	1432	G
1	2	1435	C
1	2	1444	G
1	2	1445	G
1	2	1446	A
1	2	1447	U
1	2	1448	C
1	2	1451	U
32	g	2	G
32	g	10	G
32	g	12	G
32	g	16	U
32	g	17	U
32	g	18	G
32	g	20	U
32	g	22	A
32	g	32	U
32	g	33	C
32	g	34	U
32	g	35	C
32	g	44	G
32	g	46	G
32	g	57	C
32	g	58	G
32	g	59	A
32	g	74	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1	C

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Mol	Chain	Res	Type
1	2	115	U
1	2	123	A
1	2	312	G
1	2	392	C
1	2	393	G
1	2	421	C
1	2	558	C
1	2	604	G
1	2	679	C
1	2	891	G
1	2	989	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 24 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	$\# Z > 2$
36	YAT	2	1524	-	39,39,39	3.17	18 (46%)	51,56,56	2.50	17 (33%)

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
36	YAT	2	1524	-	-	8/14/49/49	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	2	1524	YAT	CAN-CAM	-10.81	1.31	1.51
36	2	1524	YAT	CAN-NBI	10.20	1.66	1.47
36	2	1524	YAT	CAQ-NBI	4.20	1.54	1.47
36	2	1524	YAT	OAT-CAZ	3.94	1.43	1.37
36	2	1524	YAT	CBC-CBG	3.80	1.55	1.52
36	2	1524	YAT	CAI-CBB	3.63	1.45	1.38
36	2	1524	YAT	CAF-CAW	3.56	1.45	1.39
36	2	1524	YAT	CAW-CBC	-3.33	1.34	1.40
36	2	1524	YAT	CAX-CBD	3.29	1.45	1.40
36	2	1524	YAT	CAH-CBC	2.96	1.44	1.39
36	2	1524	YAT	CAG-CAX	2.84	1.44	1.39
36	2	1524	YAT	CAG-CAZ	2.79	1.43	1.38
36	2	1524	YAT	OAS-CAY	2.70	1.41	1.37
36	2	1524	YAT	OAV-CBB	2.59	1.41	1.37
36	2	1524	YAT	OAU-CBA	2.50	1.41	1.37
36	2	1524	YAT	CBG-NAR	2.49	1.49	1.47
36	2	1524	YAT	CAI-CBD	2.13	1.43	1.39
36	2	1524	YAT	CAO-CBF	2.06	1.57	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	2	1524	YAT	CAN-NBI-CAQ	11.60	132.61	110.32
36	2	1524	YAT	CAQ-CBE-CBF	4.63	117.15	108.12
36	2	1524	YAT	CAP-CBH-CBD	-4.35	106.88	113.07
36	2	1524	YAT	CBE-CAQ-NBI	3.84	117.25	112.17
36	2	1524	YAT	CAL-CAK-NAR	3.47	113.73	109.02
36	2	1524	YAT	OAT-CAZ-CBB	3.39	120.00	115.40
36	2	1524	YAT	OAS-CAY-CBA	3.19	119.72	115.40
36	2	1524	YAT	OAU-CBA-CAY	2.98	119.45	115.40
36	2	1524	YAT	CAK-CAL-CAW	2.95	115.88	110.66
36	2	1524	YAT	CAJ-CBE-CAQ	-2.92	104.94	111.77
36	2	1524	YAT	CAB-OAS-CAY	-2.77	113.45	117.51
36	2	1524	YAT	CAP-CBF-CBE	2.68	114.97	110.57
36	2	1524	YAT	OAV-CBB-CAZ	2.67	119.02	115.40
36	2	1524	YAT	CAC-OAT-CAZ	-2.66	113.61	117.51
36	2	1524	YAT	OAT-CAZ-CAG	-2.49	119.78	124.08
36	2	1524	YAT	OAS-CAY-CAF	-2.22	120.25	124.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
36	2	1524	YAT	CAJ-CBE-CBF	-2.19	108.96	114.56

There are no chirality outliers.

All (8) torsion outliers are listed below:

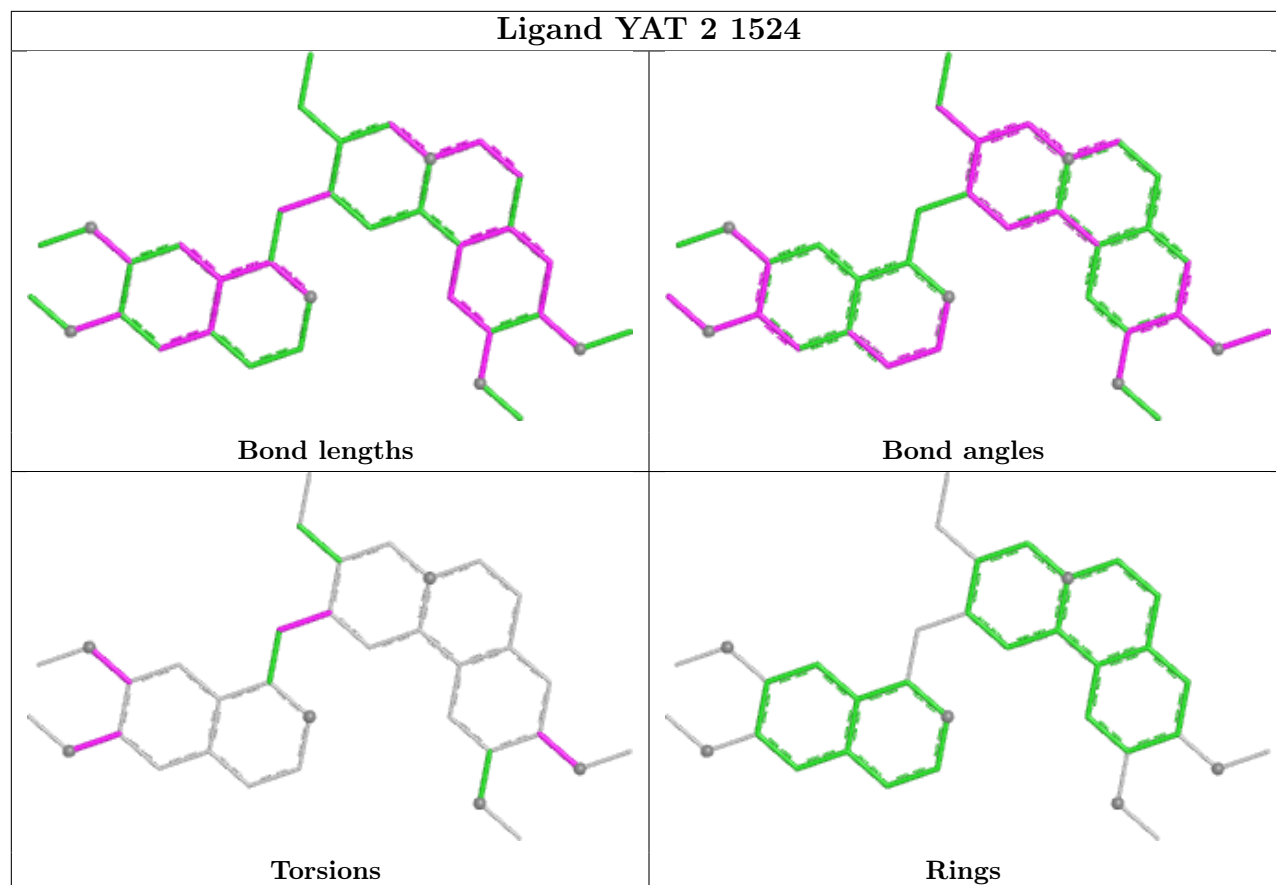
Mol	Chain	Res	Type	Atoms
36	2	1524	YAT	CAY-CBA-OAU-CAD
36	2	1524	YAT	CAG-CAZ-OAT-CAC
36	2	1524	YAT	CAF-CAY-OAS-CAB
36	2	1524	YAT	CBB-CAZ-OAT-CAC
36	2	1524	YAT	CAH-CBA-OAU-CAD
36	2	1524	YAT	CBA-CAY-OAS-CAB
36	2	1524	YAT	CBG-CAO-CBF-CBE
36	2	1524	YAT	CBG-CAO-CBF-CAP

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	2	1524	YAT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

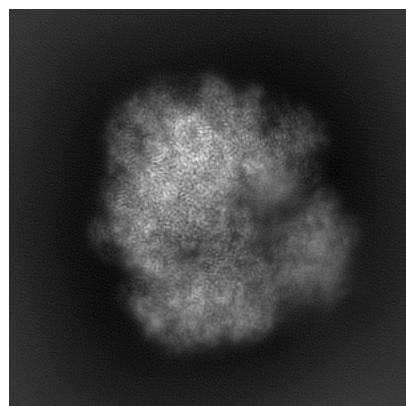
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29495. These allow visual inspection of the internal detail of the map and identification of artifacts.

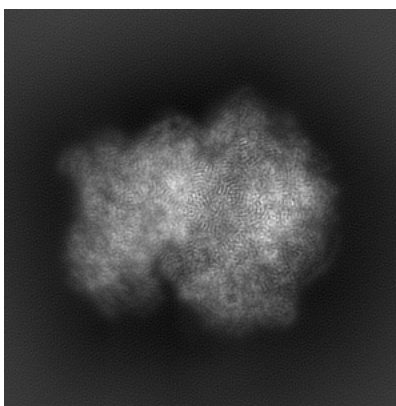
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

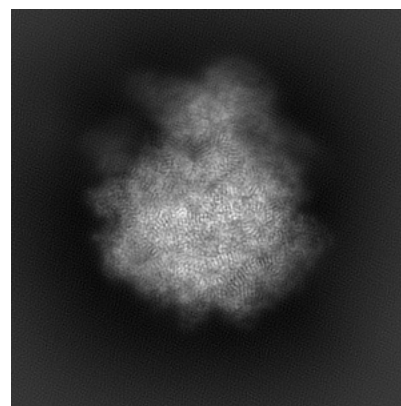
6.1.1 Primary map



X

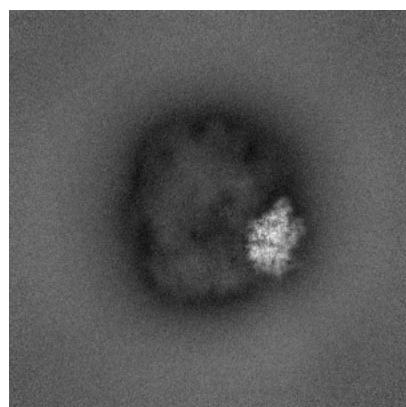


Y

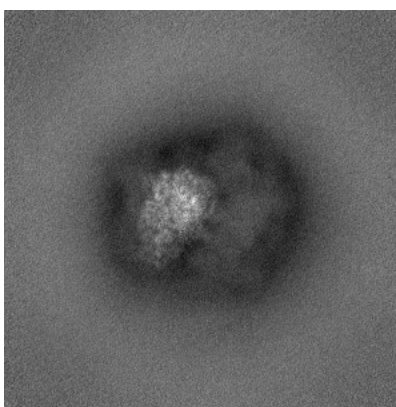


Z

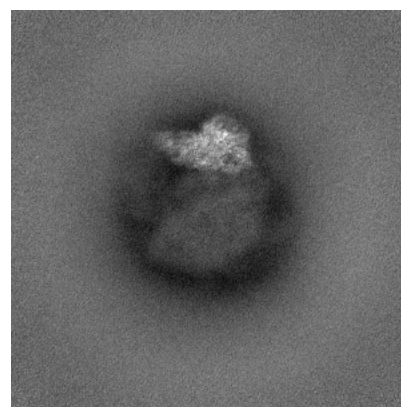
6.1.2 Raw map



X



Y

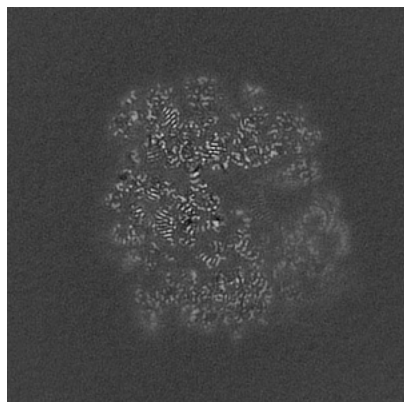


Z

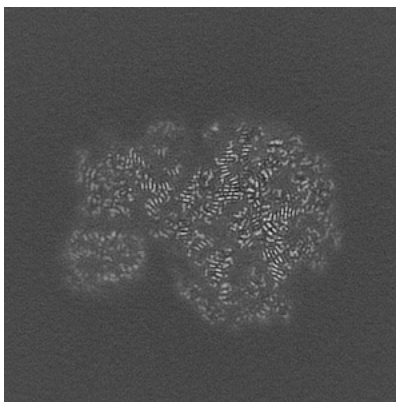
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

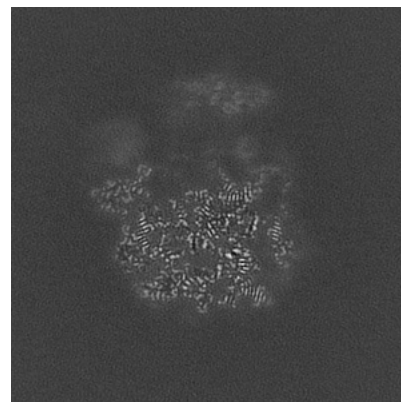
6.2.1 Primary map



X Index: 225

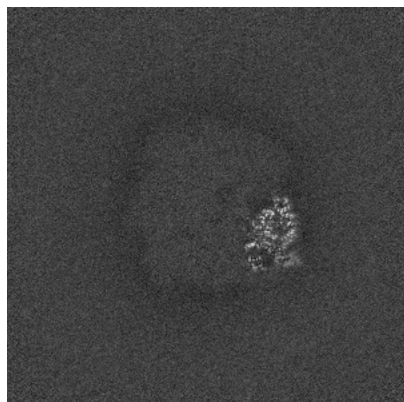


Y Index: 225

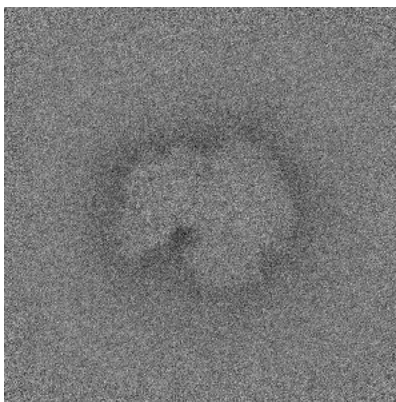


Z Index: 225

6.2.2 Raw map



X Index: 351



Y Index: 351

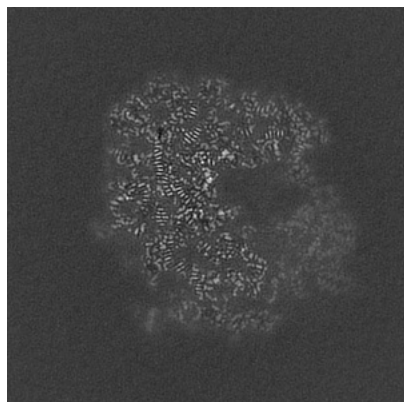


Z Index: 351

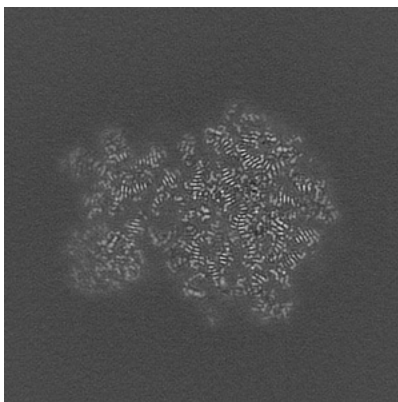
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

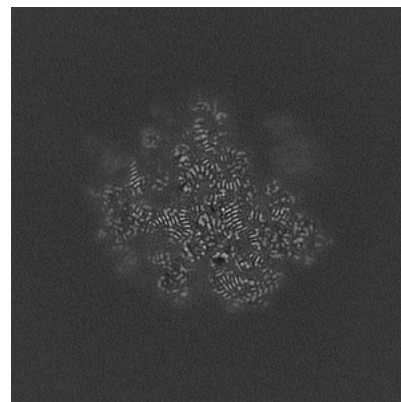
6.3.1 Primary map



X Index: 239

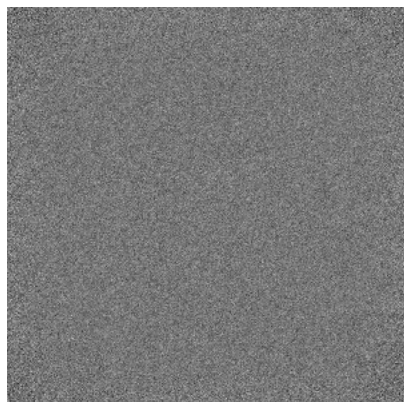


Y Index: 217

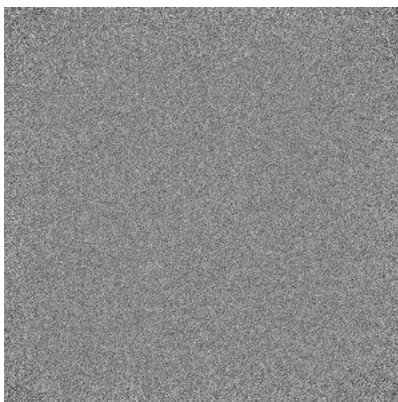


Z Index: 280

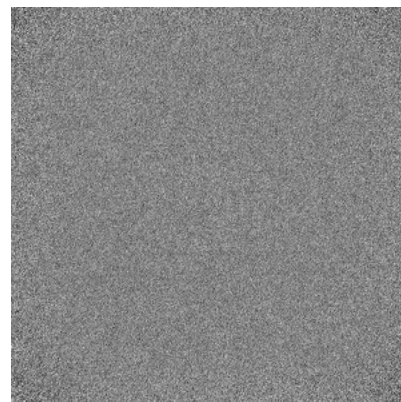
6.3.2 Raw map



X Index: 0



Y Index: 0

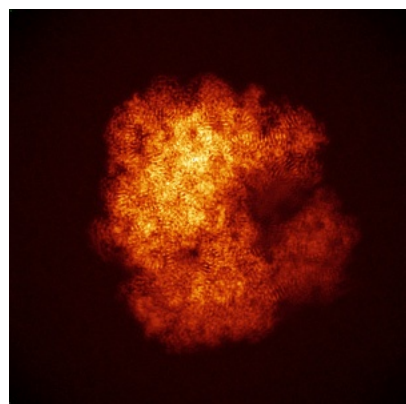


Z Index: 0

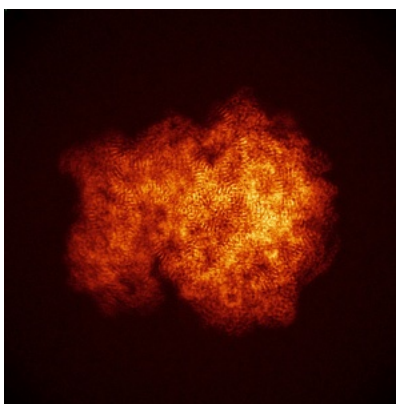
The images above show the largest variance slices of the map in three orthogonal directions.

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

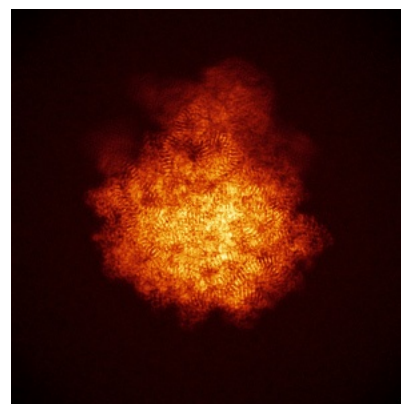
6.4.1 Primary map



X

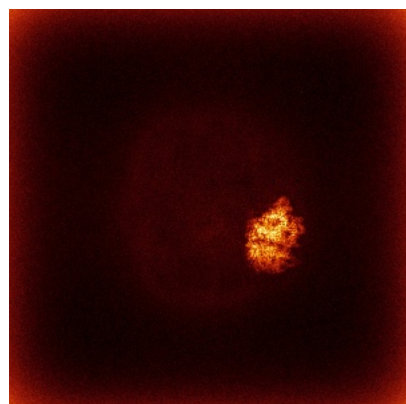


Y

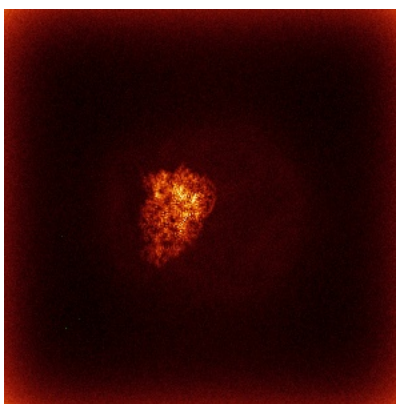


Z

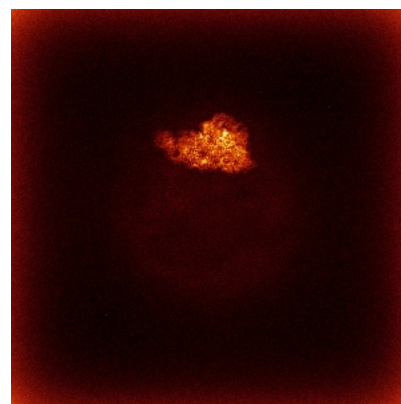
6.4.2 Raw map



X



Y

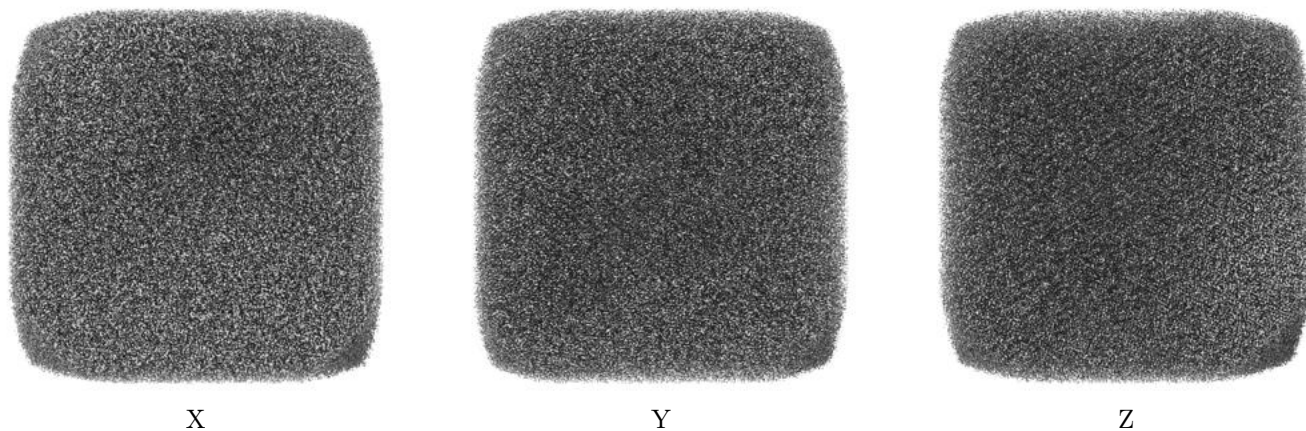


Z

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

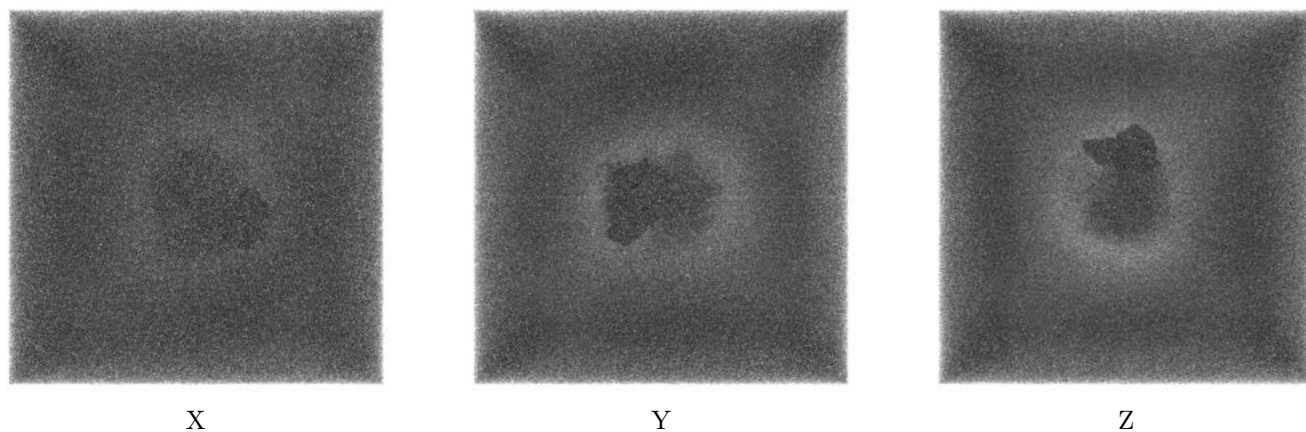
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0895. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

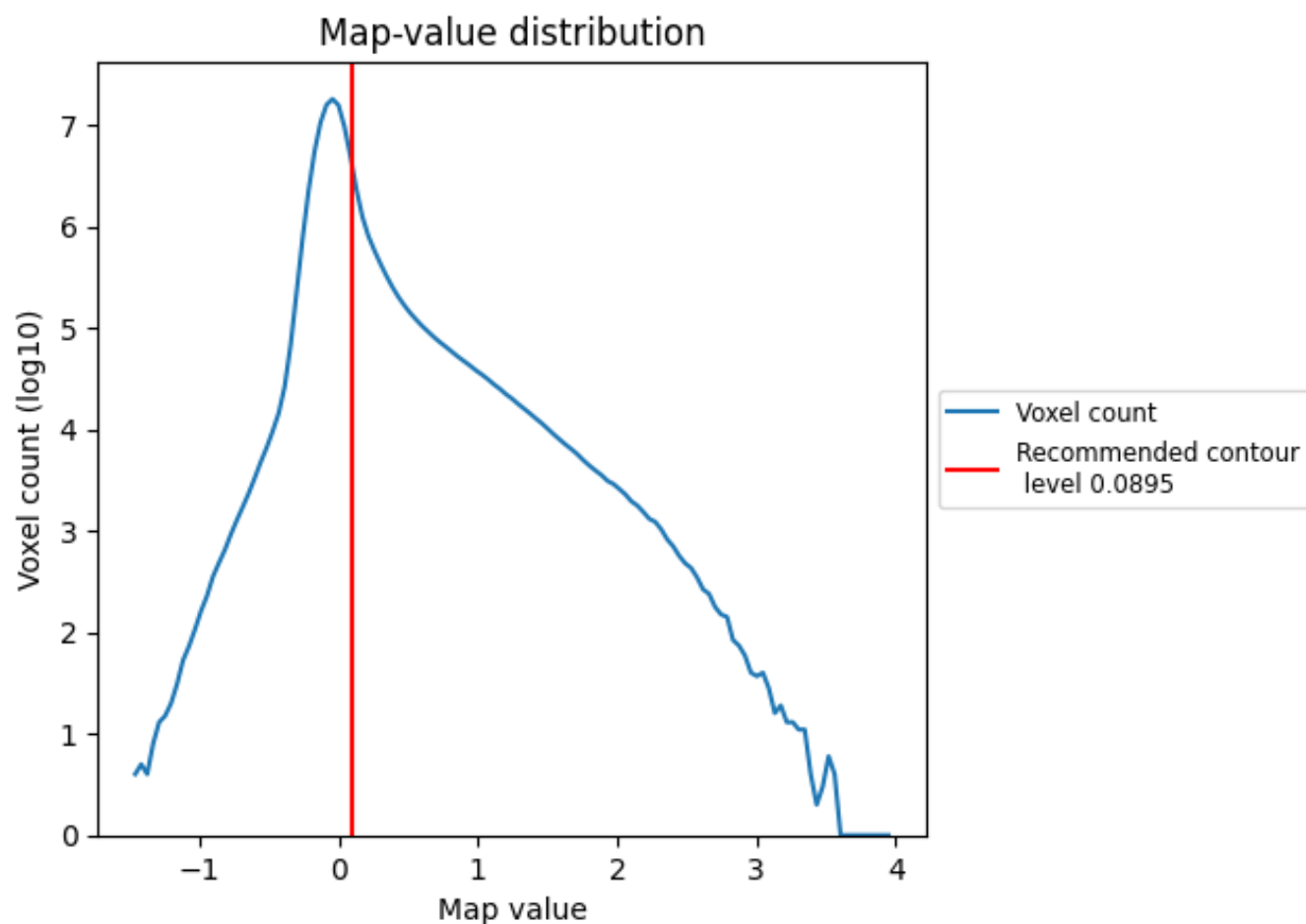
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

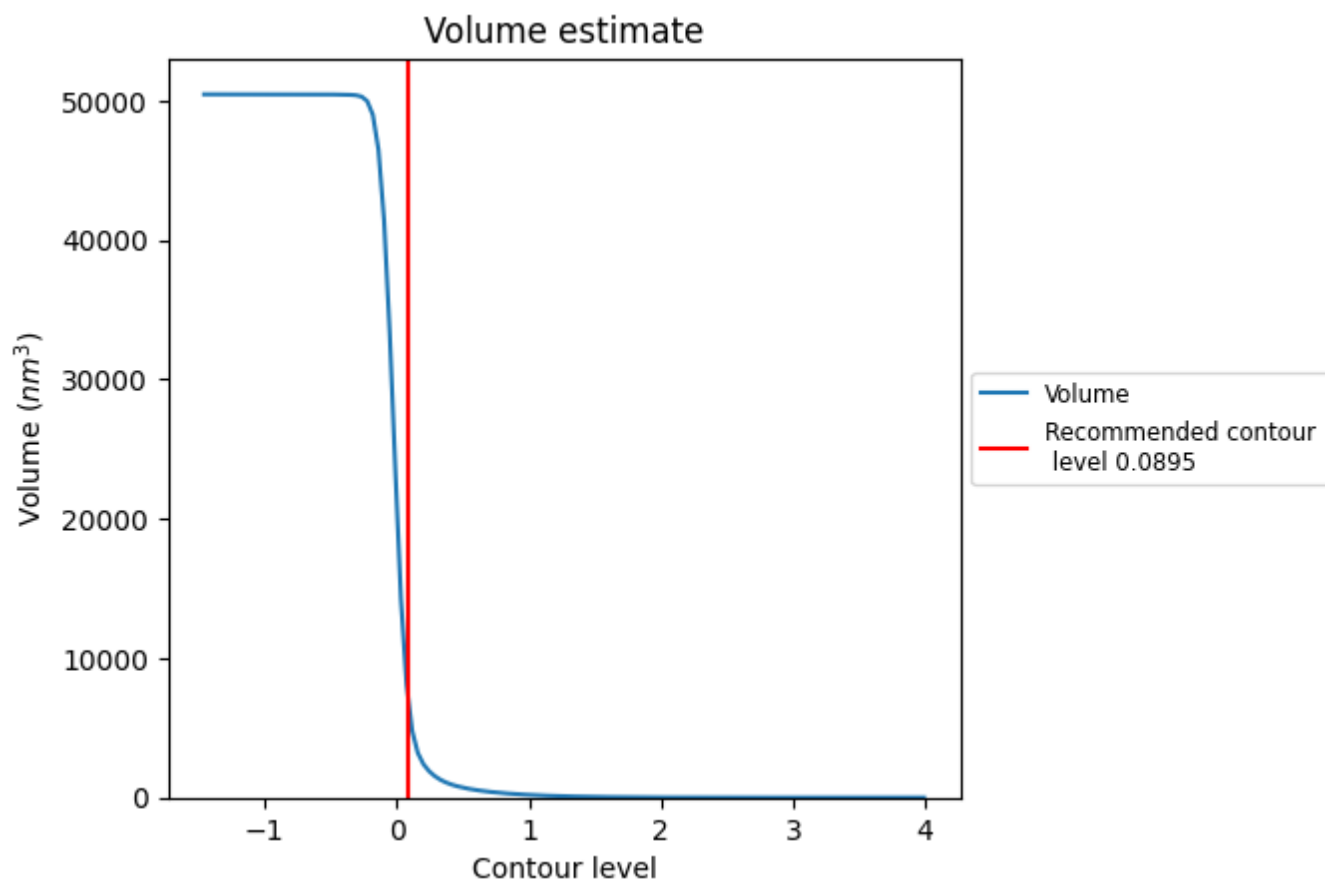
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

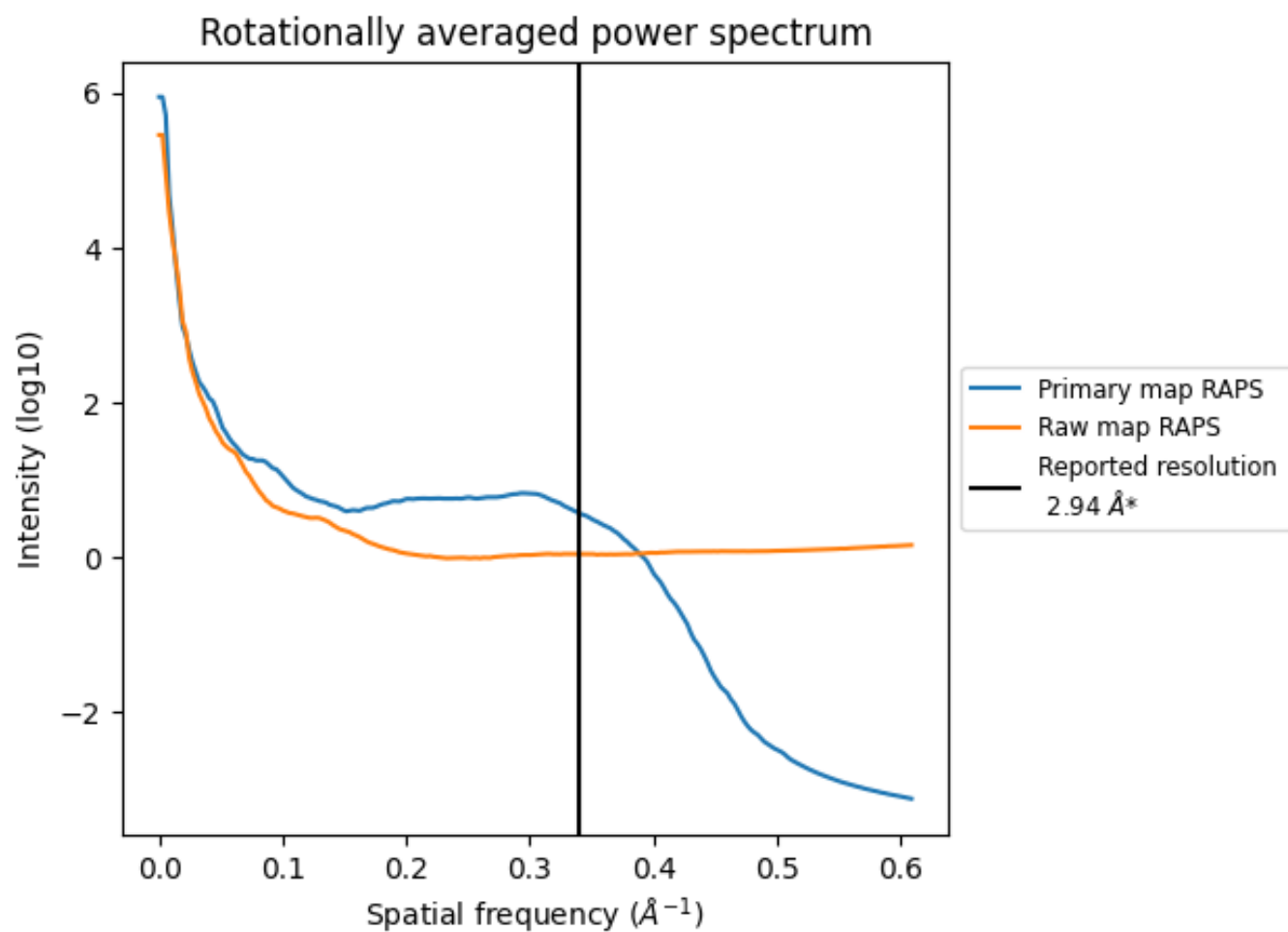
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6823 nm³; this corresponds to an approximate mass of 6164 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 ⓘ

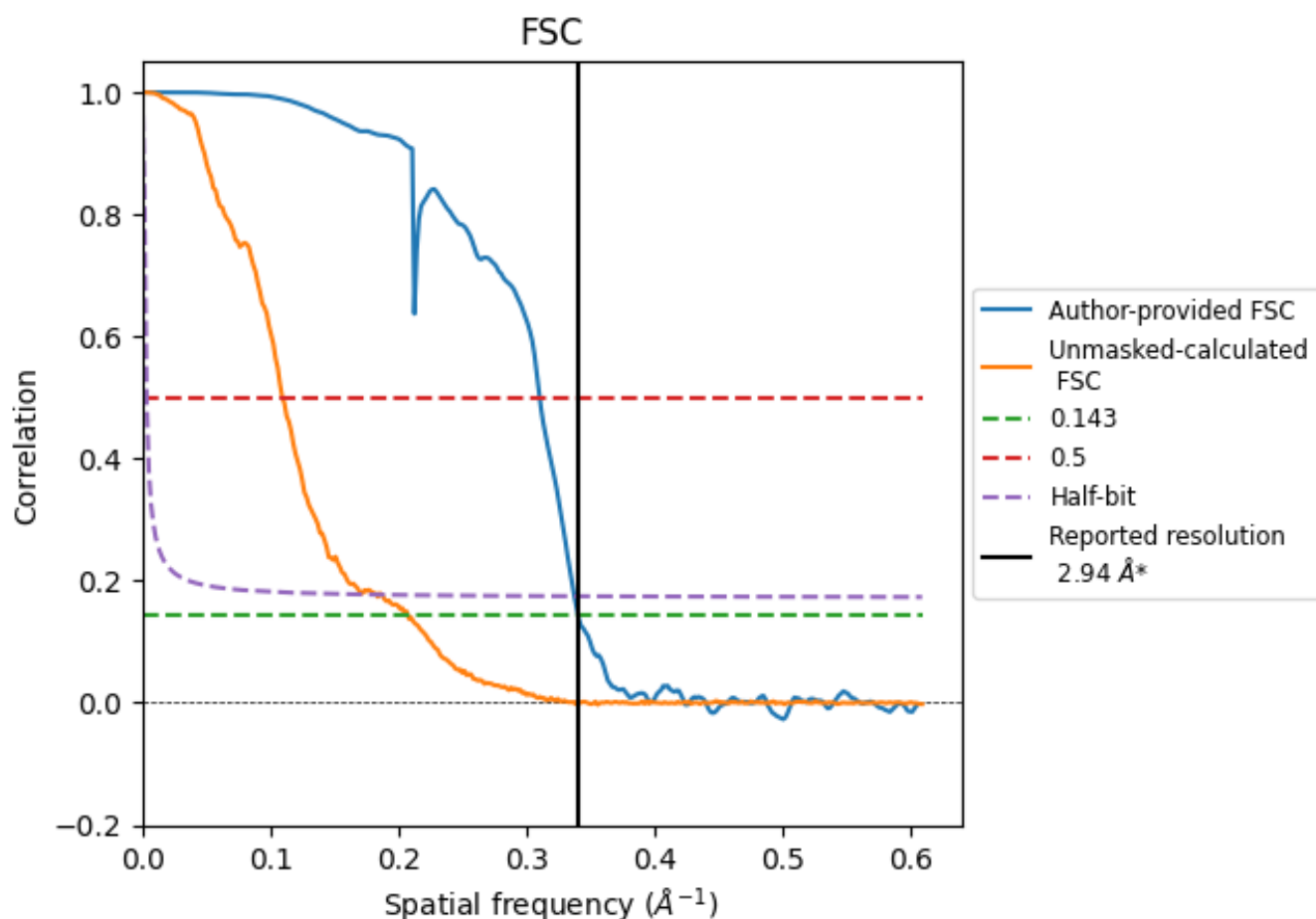


*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

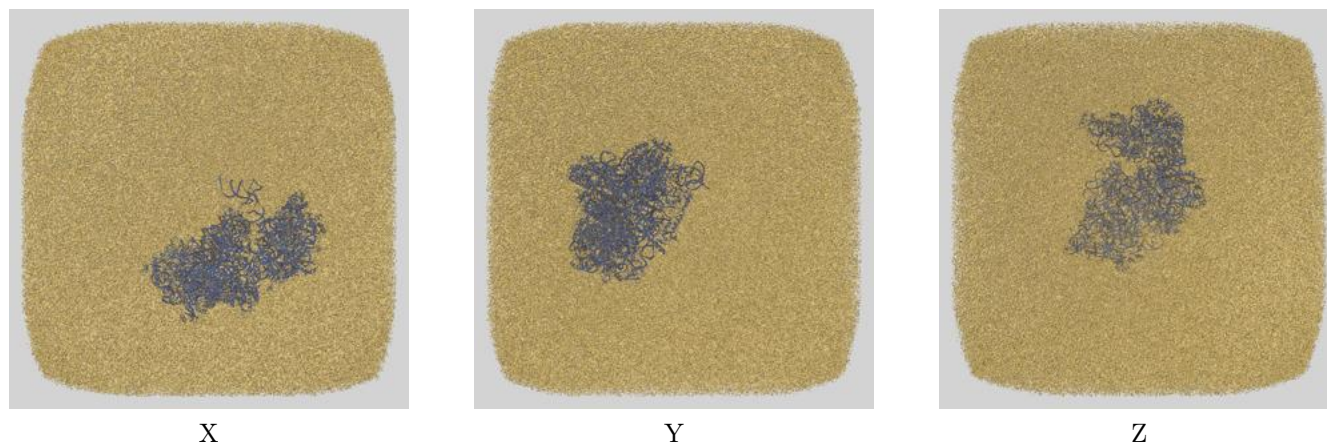
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.94	3.22	2.96
Unmasked-calculated*	4.82	9.13	5.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.82 differs from the reported value 2.94 by more than 10 %

9 Map-model fit [i](#)

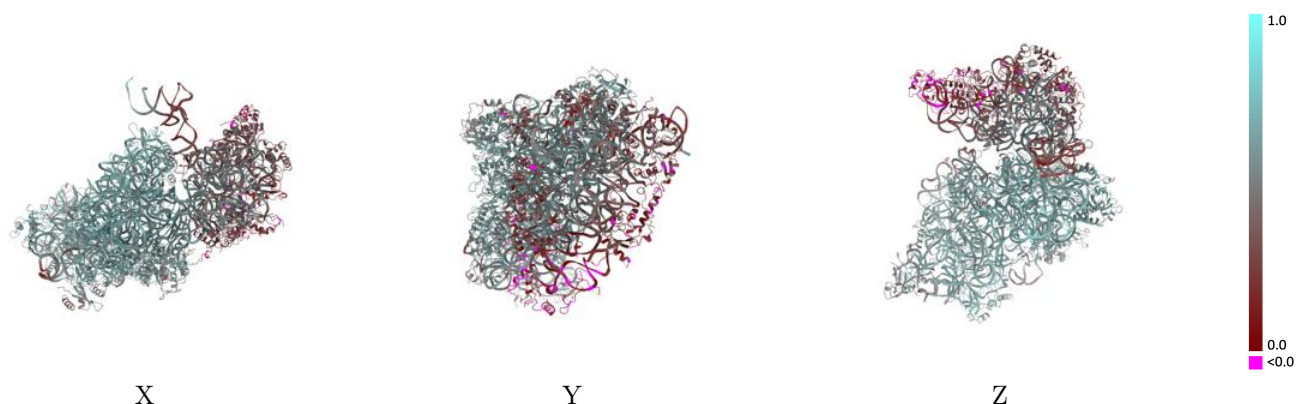
This section contains information regarding the fit between EMDB map EMD-29495 and PDB model 8FVY. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



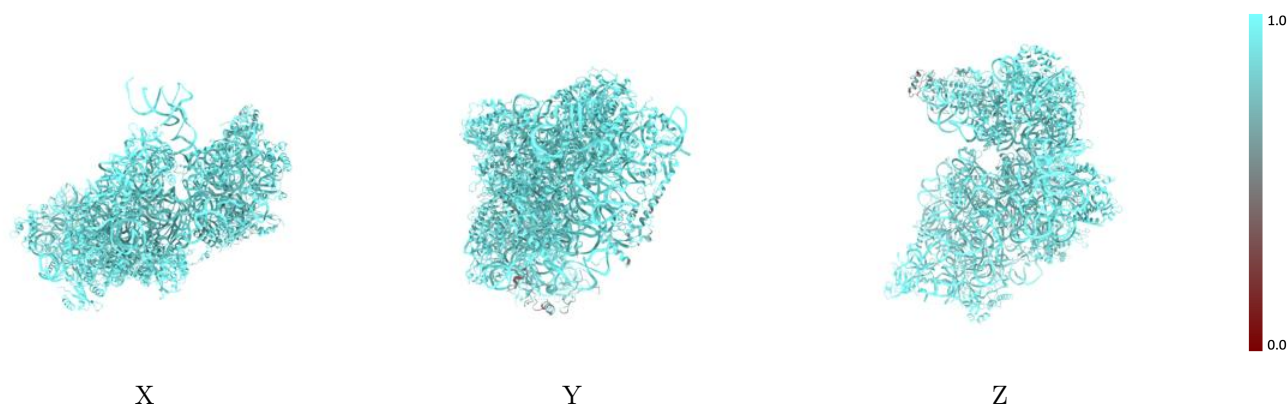
The images above show the 3D surface view of the map at the recommended contour level 0.0895 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



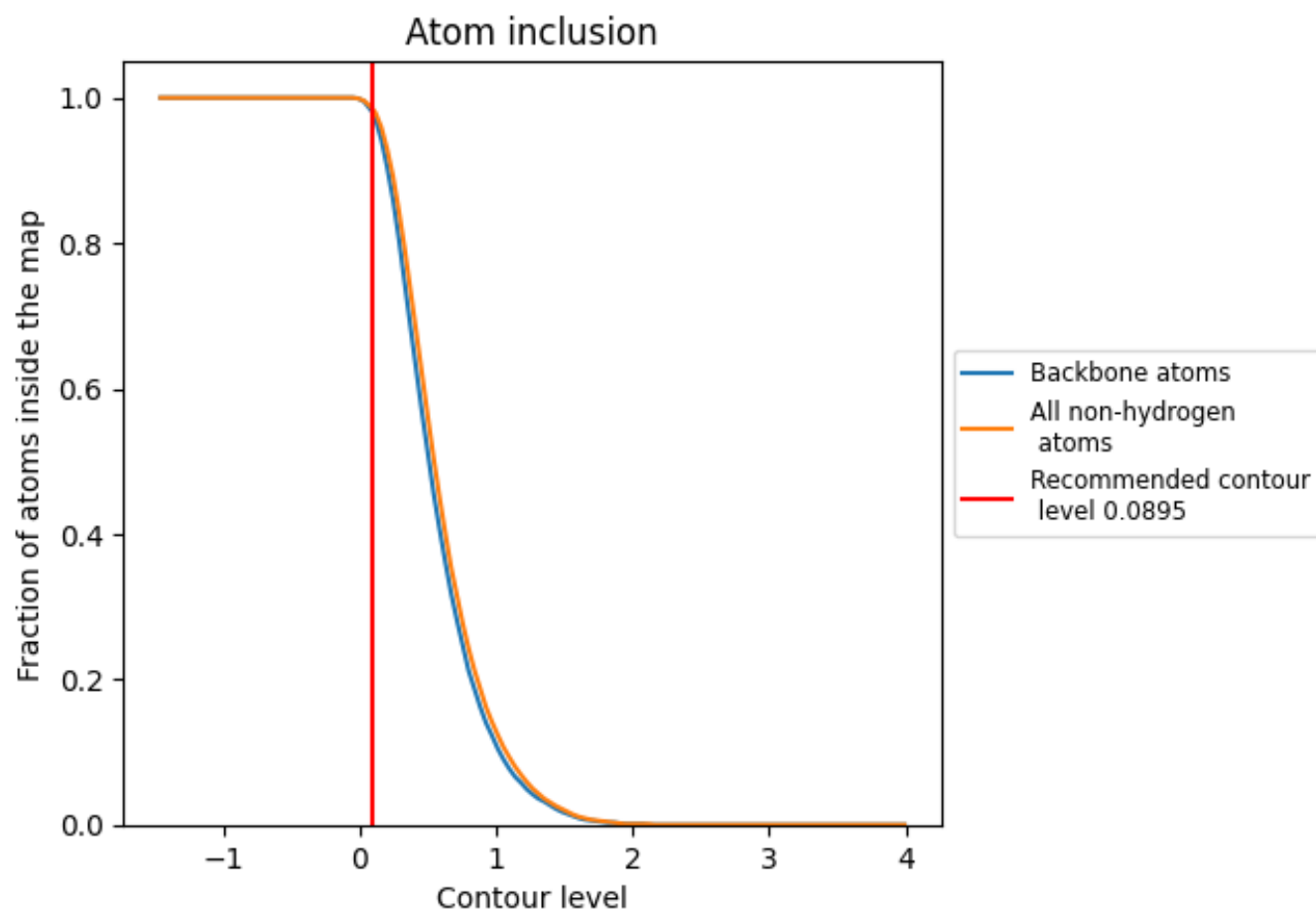
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0895).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 99% 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 (0.0895) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9860	 0.5100
2	 0.9980	 0.5630
A	 0.9970	 0.5450
B	 0.9960	 0.5910
C	 0.9980	 0.5950
D	 0.9580	 0.3470
E	 1.0000	 0.5950
F	 0.9860	 0.4100
G	 0.9900	 0.5010
H	 0.9950	 0.5190
I	 0.9960	 0.6120
J	 0.9980	 0.5700
K	 0.9250	 0.2060
L	 0.9960	 0.6260
M	 0.6630	 0.0740
N	 0.9990	 0.5970
O	 0.9980	 0.6060
P	 0.9350	 0.2040
Q	 0.9850	 0.3720
R	 0.9750	 0.3270
S	 0.9370	 0.1920
T	 0.9910	 0.3780
U	 0.9540	 0.3480
V	 0.9920	 0.5600
W	 0.9980	 0.6180
X	 0.9920	 0.5800
Y	 0.9940	 0.5060
Z	 0.9580	 0.2960
a	 1.0000	 0.6300
b	 0.9940	 0.5620
c	 0.9760	 0.4110
d	 0.9560	 0.2930
e	 0.9300	 0.3190
f	 0.6720	 0.0420
g	 0.9640	 0.3130

