



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:05 PM UTC

PDB ID : 7PWG / pdb_00007pwg
EMDB ID : EMD-13681
Title : Cryo-EM structure of large subunit of Giardia lamblia ribosome at 2.7 Å resolution
Authors : Hiregange, D.G.; Rivalta, A.; Bose, T.; Breiner-Goldstein, E.; Samiya, S.; Cimicata, G.; Kulakova, L.; Zimmerman, E.; Bashan, A.; Herzberg, O.; Yonath, A.
Deposited on : 2021-10-06
Resolution : 2.75 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:

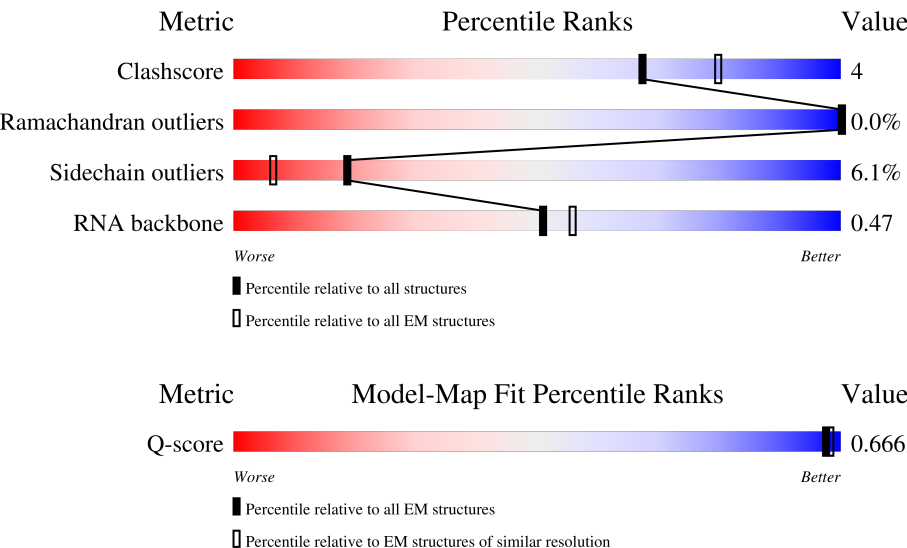
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.75 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	10570 (2.25 - 3.25)

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	1	2707	5% 66% 21% 9%
2	3	120	75% 17% 6%
3	4	139	12% 70% 26%

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Mol	Chain	Length	Quality of chain
4	A	251	
5	B	379	
6	C	316	
7	D	297	
8	F	235	
9	G	225	
10	H	185	
11	I	210	
12	J	173	
13	L	234	
14	M	131	
15	N	204	
16	O	197	
17	P	164	
18	Q	179	
19	R	196	
20	S	173	
21	T	159	
22	U	171	
23	V	142	
24	X	141	
25	Y	135	
26	Z	135	
27	a	149	
28	b	62	

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Mol	Chain	Length	Quality of chain
29	c	109	
30	d	106	
31	e	136	
32	f	123	
33	g	120	
34	h	124	
35	i	90	
36	j	89	
37	k	77	
38	l	51	
39	m	127	
40	o	106	
41	p	94	
42	w	76	
43	W	102	
44	E	3	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 109151 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called rRNA 28S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2450	Total	C	N	O	P	0	0
			52618	23393	9753	17022	2450		

- Molecule 2 is a RNA chain called rRNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	117	Total	C	N	O	P	0	0
			2501	1116	458	810	117		

- Molecule 3 is a RNA chain called rRNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	138	Total	C	N	O	P	0	0
			2958	1315	553	952	138		

- Molecule 4 is a protein called Ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	249	Total	C	N	O	S	0	0
			1865	1152	382	319	12		

- Molecule 5 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	378	Total	C	N	O	S	0	0
			2987	1886	566	514	21		

- Molecule 6 is a protein called Ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	314	Total	C	N	O	S	0	0
			2446	1539	474	424	9		

- Molecule 7 is a protein called Ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	266	Total	C	N	O	S	0	0
			2118	1342	392	376	8		

- Molecule 8 is a protein called Ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	214	Total	C	N	O	S	0	0
			1730	1100	315	310	5		

- Molecule 9 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	182	Total	C	N	O	S	0	0
			1450	923	264	257	6		

- Molecule 10 is a protein called Ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	184	Total	C	N	O	S	0	0
			1442	912	263	257	10		

- Molecule 11 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	200	Total	C	N	O	S	0	0
			1621	1019	321	273	8		

- Molecule 12 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	164	Total	C	N	O	S	0	0
			1305	821	246	233	5		

- Molecule 13 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	189	Total	C	N	O	S	0	0
			1512	942	309	255	6		

- Molecule 14 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	128	Total	C	N	O	S	0	0
			990	626	178	181	5		

- Molecule 15 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	204	Total	C	N	O	S	0	0
			1712	1083	358	265	6		

- Molecule 16 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	195	Total	C	N	O	S	0	0
			1587	997	310	267	13		

- Molecule 17 is a protein called Ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	154	Total	C	N	O	S	0	0
			1235	781	239	211	4		

- Molecule 18 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	178	Total	C	N	O	S	0	0
			1402	871	279	243	9		

- Molecule 19 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	177	Total	C	N	O	S	0	0
			1463	902	313	243	5		

- Molecule 20 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	173	Total	C	N	O	S	0	0
			1418	895	274	240	9		

- Molecule 21 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	153	Total	C	N	O	S	0	0
			1226	766	252	201	7		

- Molecule 22 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	98	Total	C	N	O	S	0	0
			802	513	138	149	2		

- Molecule 23 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	139	Total	C	N	O	S	0	0
			1057	665	204	183	5		

- Molecule 24 is a protein called Ribosomal protein L23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	116	Total	C	N	O	S	0	0
			936	601	169	163	3		

- Molecule 25 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	133	Total	C	N	O	S	0	0
			1076	665	219	184	8		

- Molecule 26 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	129	Total	C	N	O	S	0	0
			980	623	179	173	5		

- Molecule 27 is a protein called Ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	148	Total	C	N	O	S	0	0
			1201	759	240	199	3		

- Molecule 28 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	56	Total	C	N	O	S	0	0
			463	280	104	77	2		

- Molecule 29 is a protein called Ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	101	Total	C	N	O	S	0	0
			756	475	133	144	4		

- Molecule 30 is a protein called Ribosomal protein L31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	94	Total	C	N	O	S	0	0
			748	479	148	121			

- Molecule 31 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	126	Total	C	N	O	S	0	0
			1039	661	207	165	6		

- Molecule 32 is a protein called Ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	123	Total	C	N	O	S	0	0
			974	619	180	171	4		

- Molecule 33 is a protein called Ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	99	Total	C	N	O	S	0	0
			798	493	167	134	4		

- Molecule 34 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	116	Total	C	N	O	S	0	0
			926	589	178	154	5		

- Molecule 35 is a protein called Ribosomal protein L36-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	85	Total	C	N	O	S	0	0
			691	438	138	111	4		

- Molecule 36 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	87	Total	C	N	O	S	0	0
			692	423	146	116	7		

- Molecule 37 is a protein called Ribosomal L38e.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	66	Total	C	N	O	S	0	0
			500	317	85	94	4		

- Molecule 38 is a protein called Ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	l	50	Total	C	N	O	0	0
			434	278	91	65		

- Molecule 39 is a protein called Ubiquitin/Ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	51	Total	C	N	O	S	0	0
			421	257	88	69	7		

- Molecule 40 is a protein called Ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	94	Total	C	N	O	S	0	0
			762	474	157	126	5		

- Molecule 41 is a protein called Ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			708	436	144	122	6		

- Molecule 42 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	14	Total	C	N	O	P	0	0
			299	133	56	96	14		

- Molecule 43 is a protein called Ribosomal protein L24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	W	65	Total	C	N	O	S	0	0
			540	343	110	85	2		

- Molecule 44 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	E	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

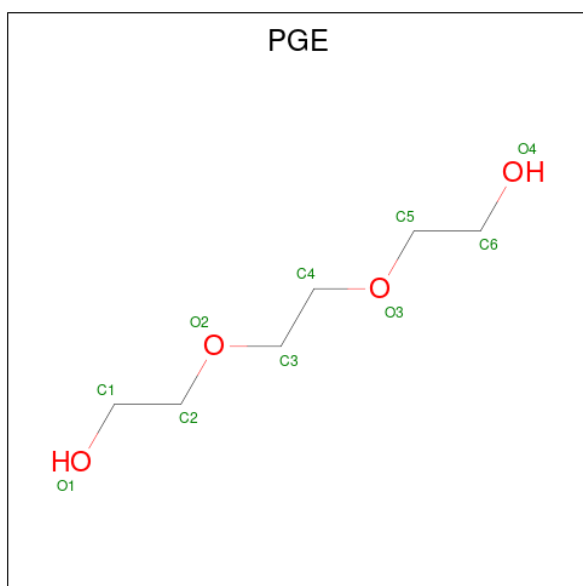
- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	1	99	Total	Mg	0
			99	99	
45	4	5	Total	Mg	0
			5	5	
45	C	1	Total	Mg	0
			1	1	
45	F	1	Total	Mg	0
			1	1	
45	I	1	Total	Mg	0
			1	1	
45	P	1	Total	Mg	0
			1	1	
45	V	1	Total	Mg	0
			1	1	
45	a	1	Total	Mg	0
			1	1	
45	b	1	Total	Mg	0
			1	1	
45	o	1	Total	Mg	0
			1	1	

- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
46	1	163	Total 163	K 163	0
46	3	1	Total 1	K 1	0
46	A	3	Total 3	K 3	0
46	B	3	Total 3	K 3	0
46	C	2	Total 2	K 2	0
46	I	1	Total 1	K 1	0
46	L	1	Total 1	K 1	0
46	N	2	Total 2	K 2	0
46	V	1	Total 1	K 1	0
46	a	1	Total 1	K 1	0
46	e	1	Total 1	K 1	0
46	j	1	Total 1	K 1	0
46	o	1	Total 1	K 1	0

- Molecule 47 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			AltConf
47	1	1	Total	C	O	0
			10	6	4	

- Molecule 48 is water.

Mol	Chain	Residues	Atoms			AltConf
48	1	3220	Total	O		0
			3220	3220		
48	3	71	Total	O		0
			71	71		
48	4	132	Total	O		0
			132	132		
48	A	54	Total	O		0
			54	54		
48	B	67	Total	O		0
			67	67		
48	C	57	Total	O		0
			57	57		
48	D	30	Total	O		0
			30	30		
48	F	23	Total	O		0
			23	23		
48	G	27	Total	O		0
			27	27		
48	H	15	Total	O		0
			15	15		
48	I	31	Total	O		0
			31	31		
48	J	19	Total	O		0
			19	19		
48	L	42	Total	O		0
			42	42		
48	M	7	Total	O		0
			7	7		
48	N	65	Total	O		0
			65	65		
48	O	35	Total	O		0
			35	35		
48	P	25	Total	O		0
			25	25		
48	Q	35	Total	O		0
			35	35		
48	R	19	Total	O		0
			19	19		

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Mol	Chain	Residues	Atoms		AltConf
48	S	27	Total 27	O 27	0
48	T	38	Total 38	O 38	0
48	U	9	Total 9	O 9	0
48	V	12	Total 12	O 12	0
48	X	30	Total 30	O 30	0
48	Y	18	Total 18	O 18	0
48	Z	23	Total 23	O 23	0
48	a	41	Total 41	O 41	0
48	b	19	Total 19	O 19	0
48	c	3	Total 3	O 3	0
48	d	12	Total 12	O 12	0
48	e	28	Total 28	O 28	0
48	f	15	Total 15	O 15	0
48	g	27	Total 27	O 27	0
48	h	14	Total 14	O 14	0
48	i	15	Total 15	O 15	0
48	j	28	Total 28	O 28	0
48	k	4	Total 4	O 4	0
48	l	7	Total 7	O 7	0
48	m	4	Total 4	O 4	0
48	o	15	Total 15	O 15	0

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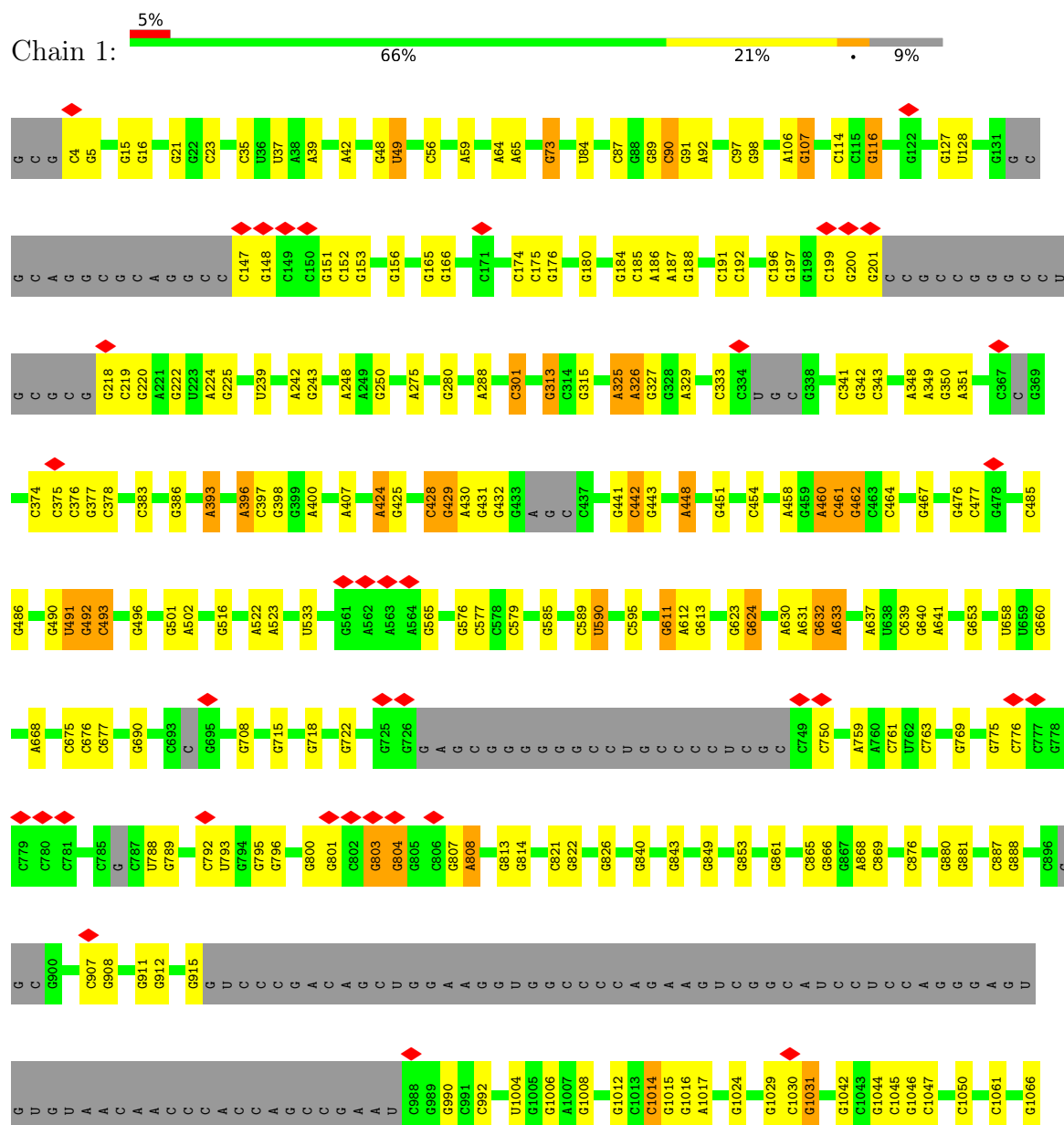
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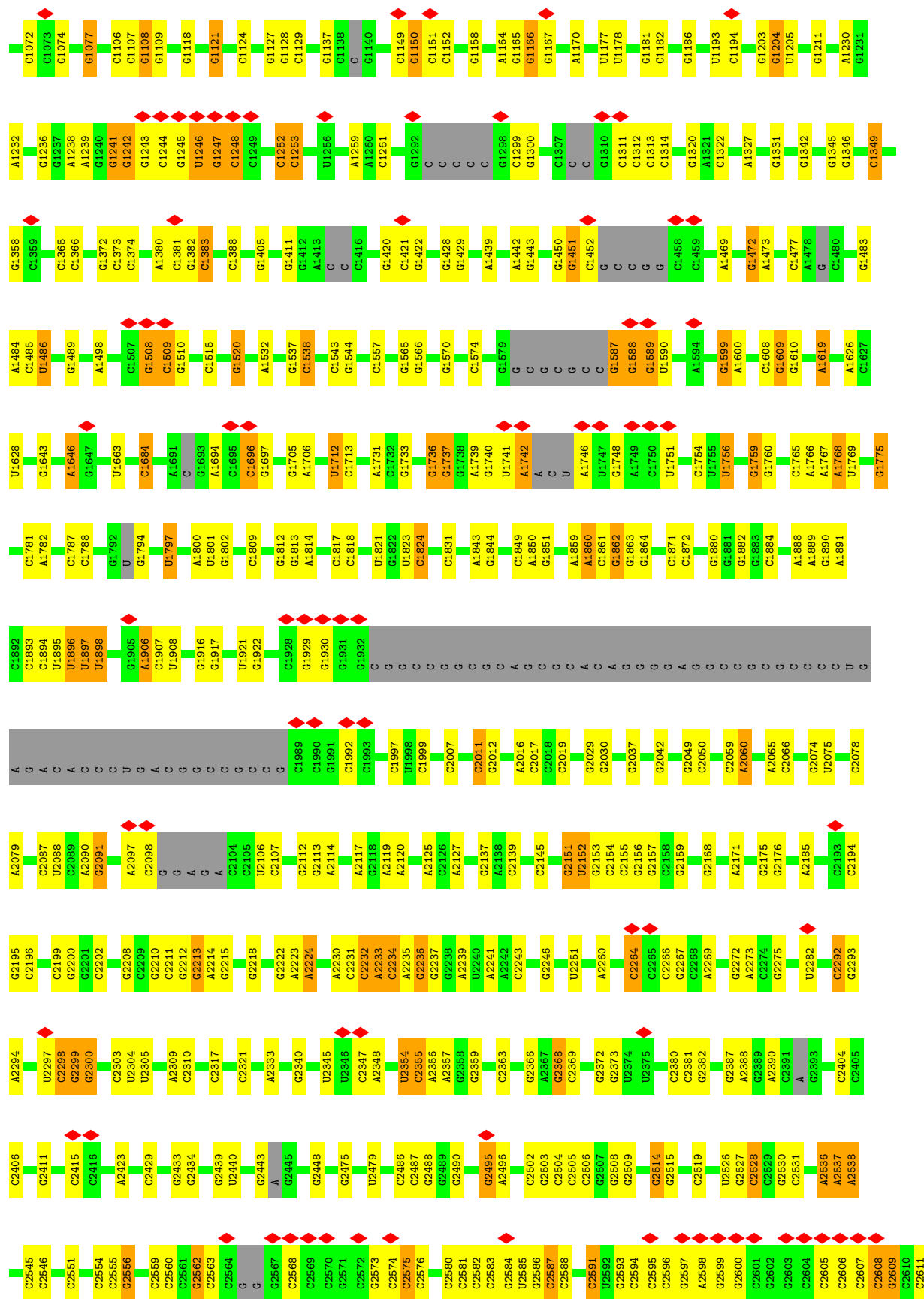
Mol	Chain	Residues	Atoms		AltConf
48	p	15	Total 15	O 15	0
48	w	6	Total 6	O 6	0
48	W	12	Total 12	O 12	0
48	E	1	Total 1	O 1	0

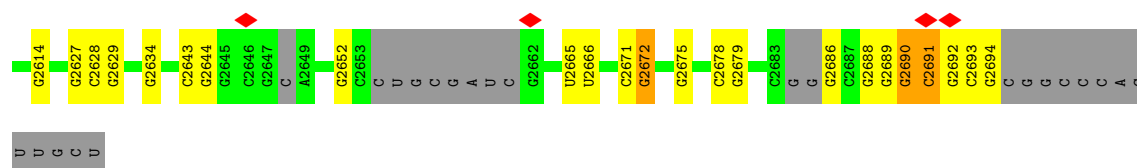
3 Residue-property plots

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.

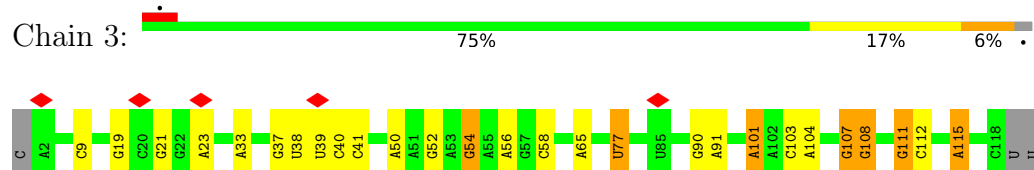
• Molecule 1: rRNA 28S



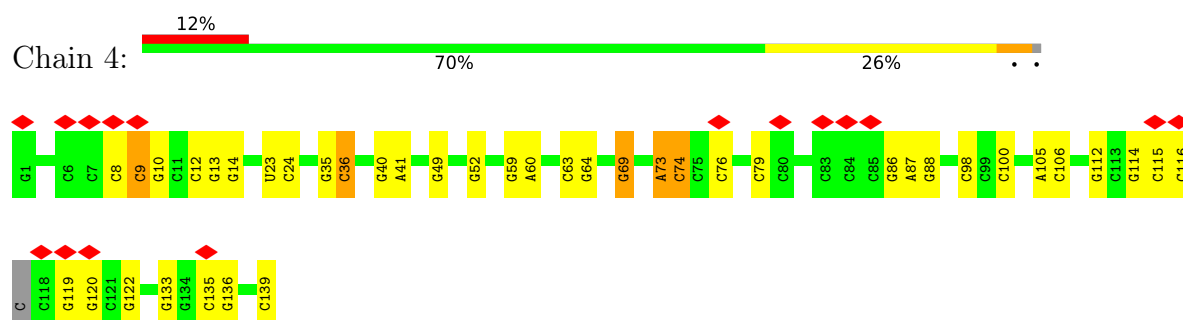




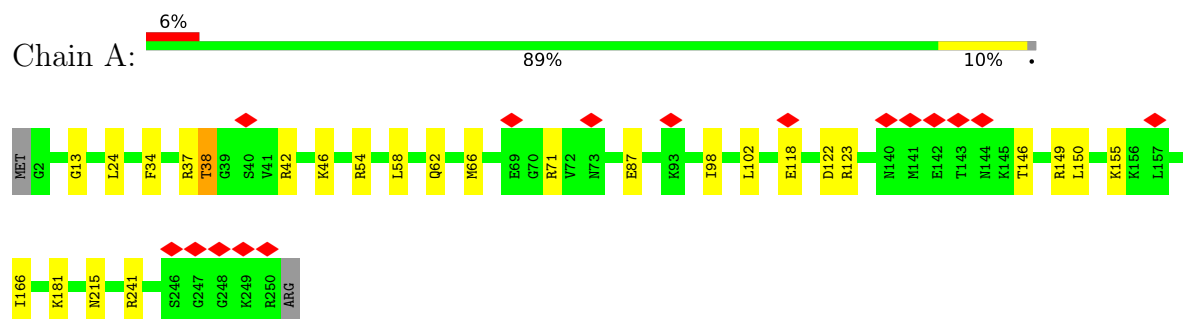
• Molecule 2: rRNA 5S



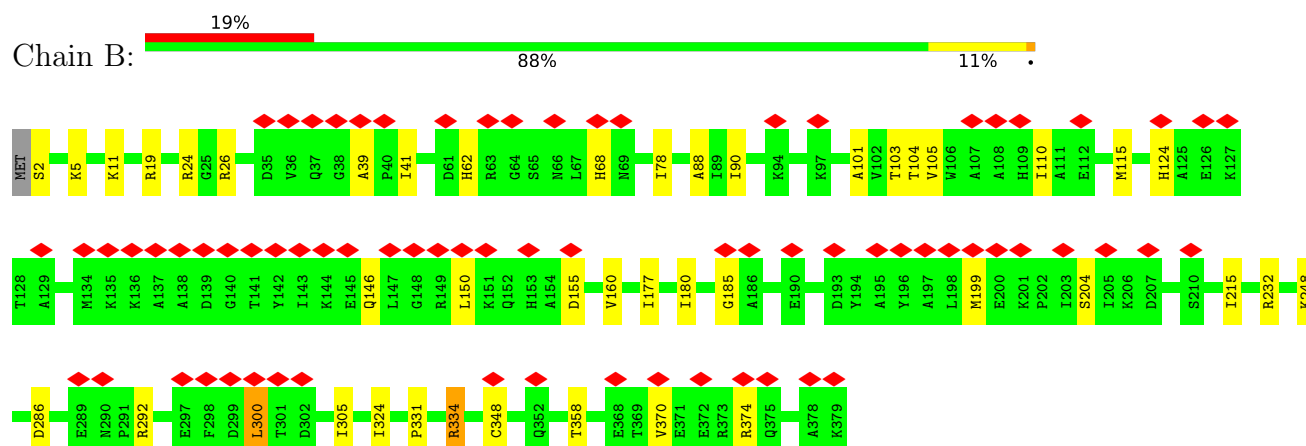
• Molecule 3: rRNA 5.8S



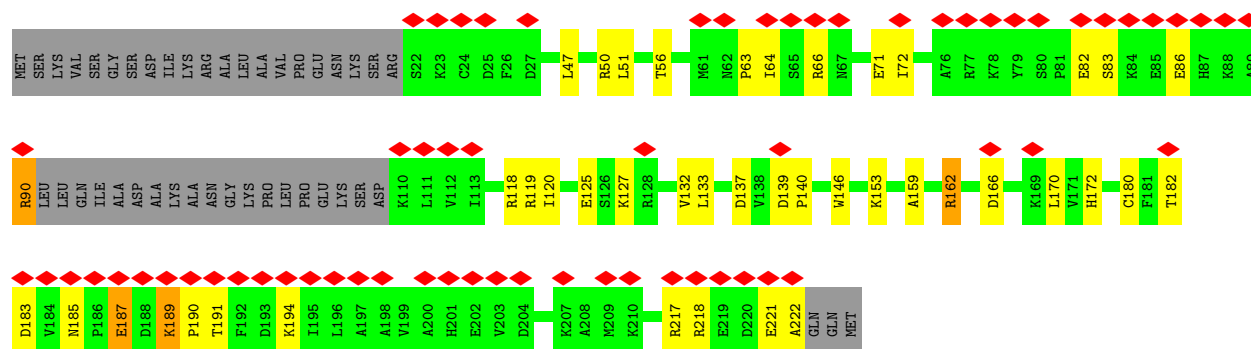
• Molecule 4: Ribosomal protein L2



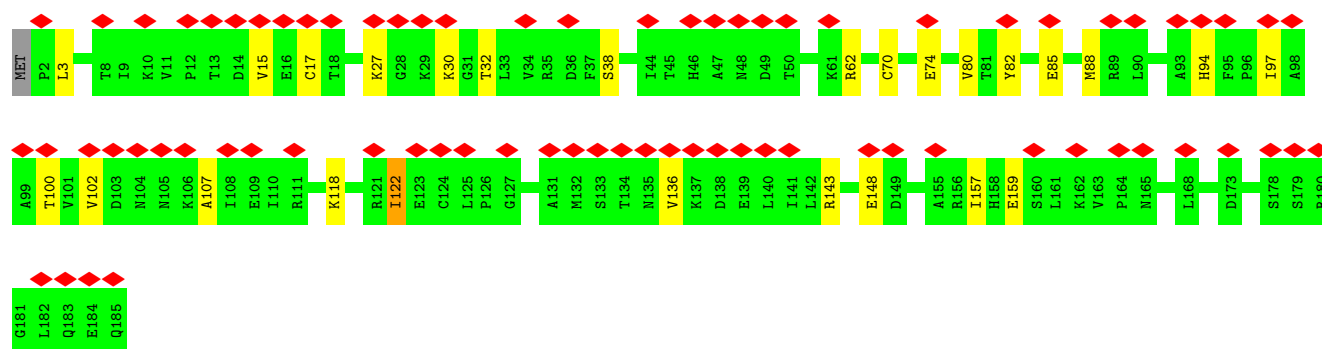
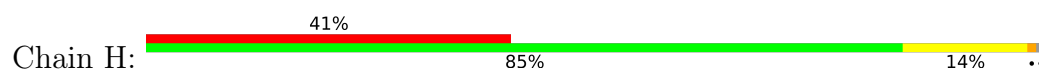
• Molecule 5: Ribosomal protein L3



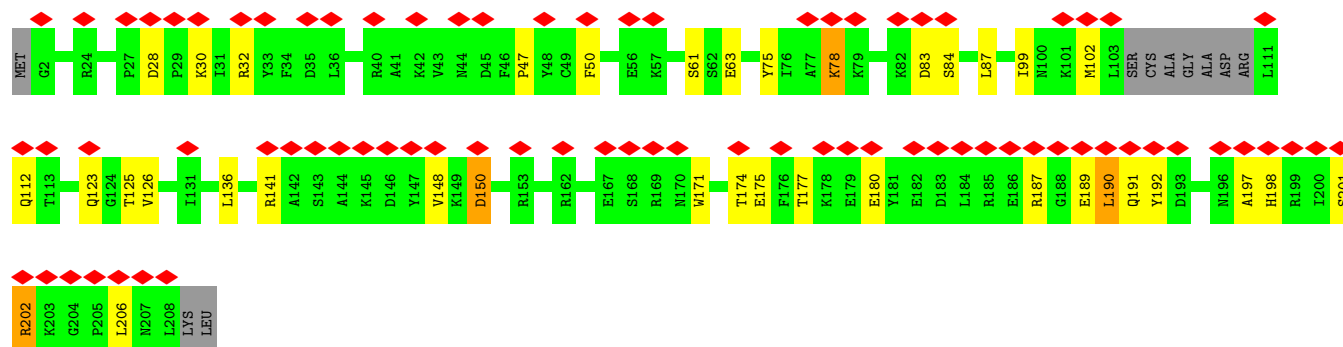
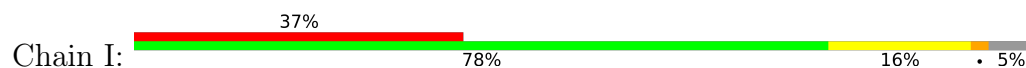




• Molecule 10: Ribosomal protein L6

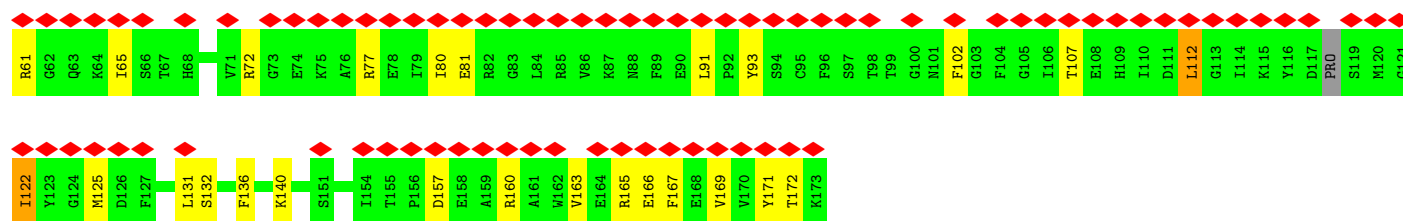


• Molecule 11: Ribosomal protein L10

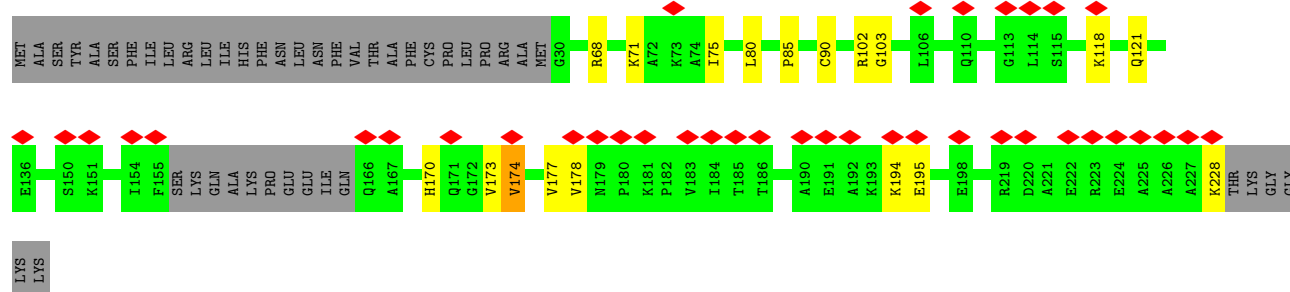
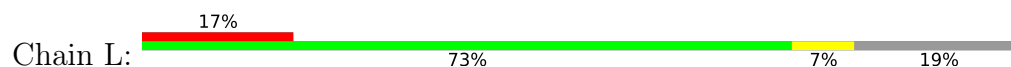


• Molecule 12: Ribosomal protein L11

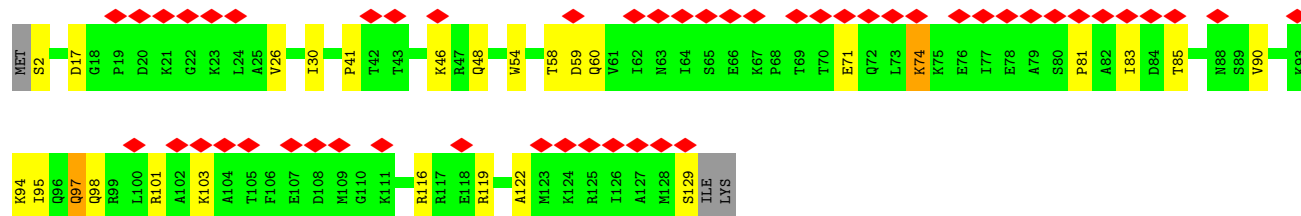
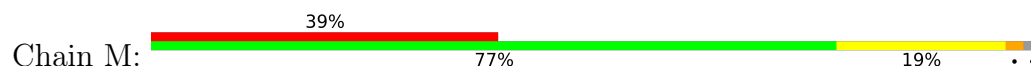




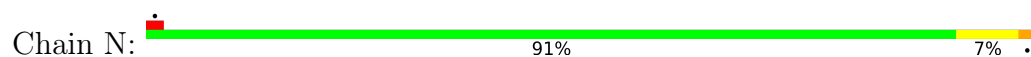
• Molecule 13: 60S ribosomal protein L13



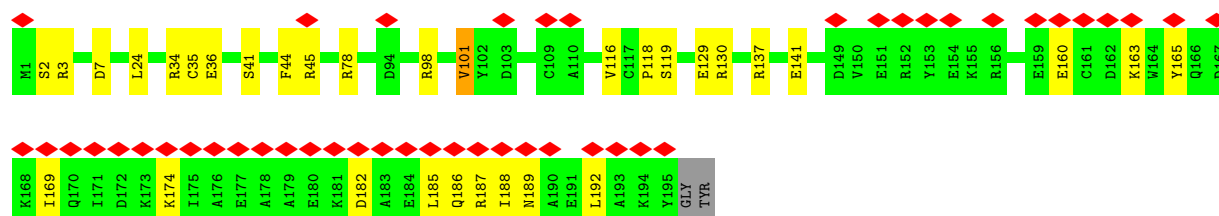
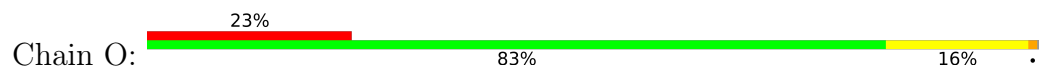
• Molecule 14: Ribosomal protein L14



• Molecule 15: Ribosomal protein L15

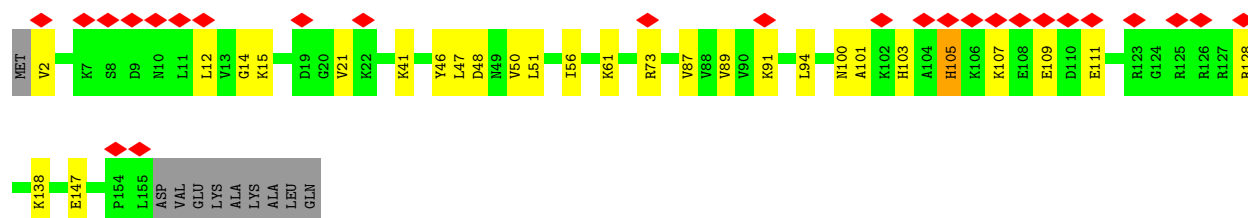


• Molecule 16: Ribosomal protein L13a



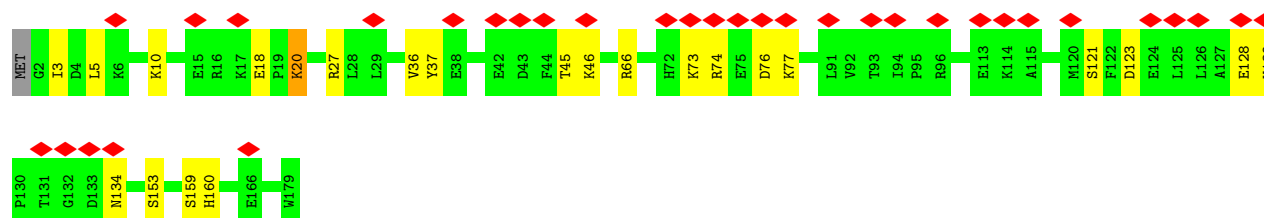
- Molecule 17: Ribosomal protein L17

Chain P: 



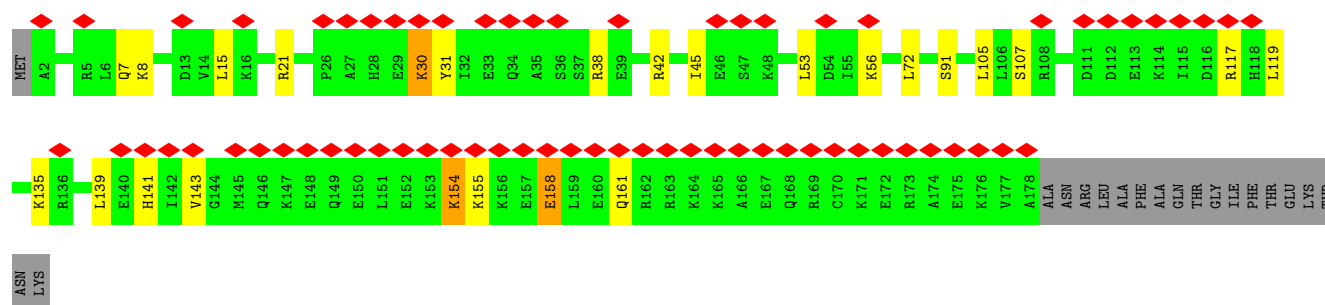
- Molecule 18: Ribosomal protein L18

Chain Q: 



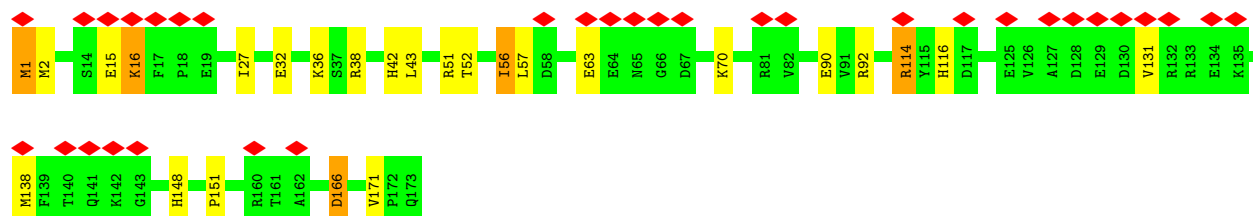
- Molecule 19: Ribosomal protein L19

Chain R: 



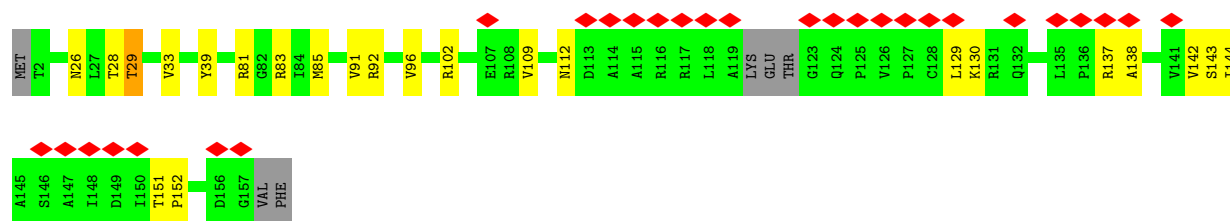
- Molecule 20: 60S ribosomal protein L18a

Chain S: 

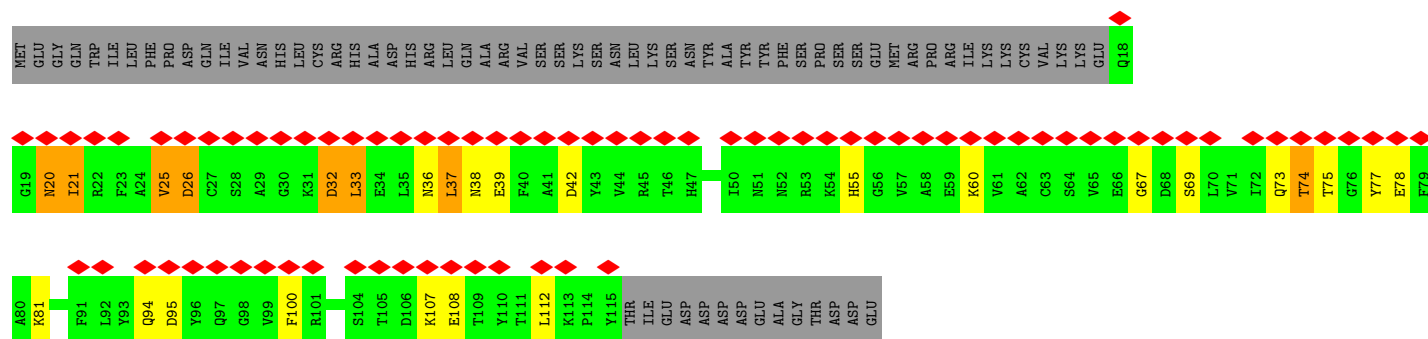


- Molecule 21: Ribosomal protein L21

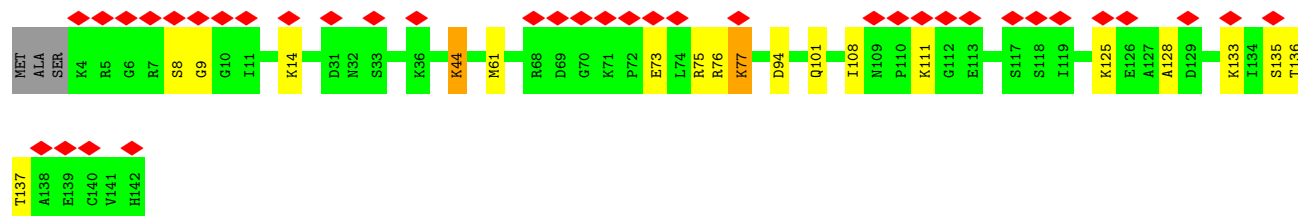
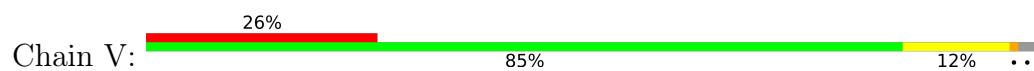
Chain T: 



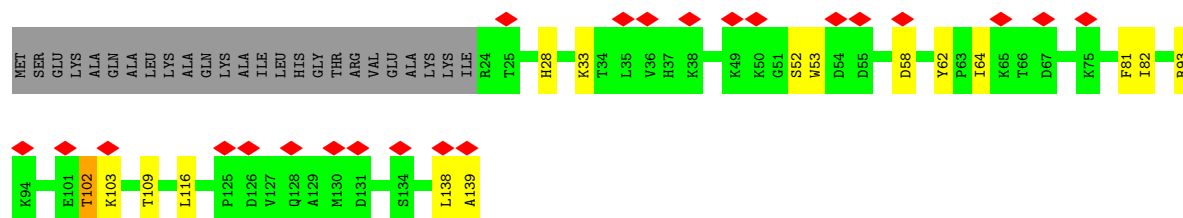
• Molecule 22: Ribosomal protein eL22



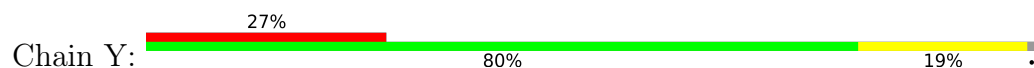
• Molecule 23: Ribosomal protein L23

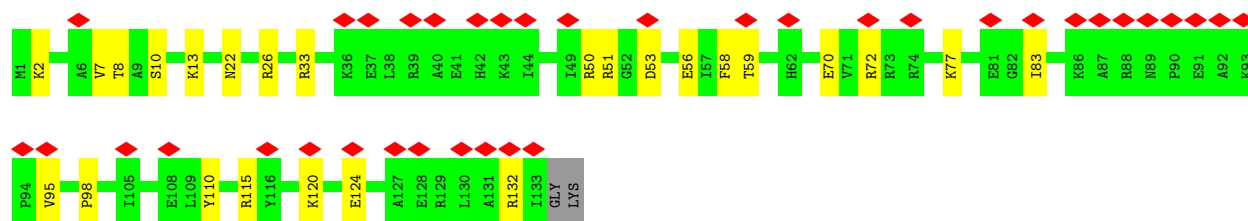


• Molecule 24: Ribosomal protein L23A

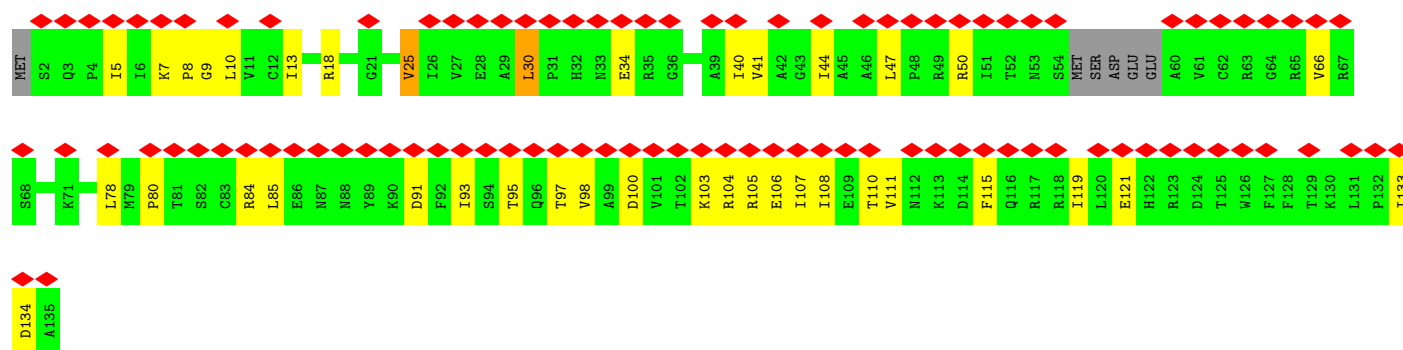
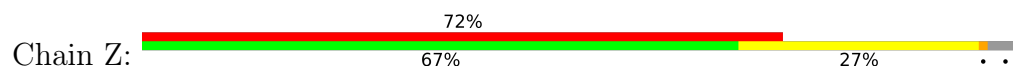


• Molecule 25: Ribosomal protein L26

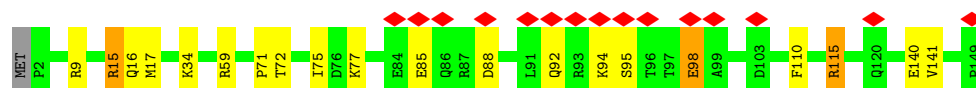
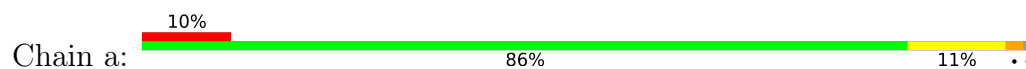




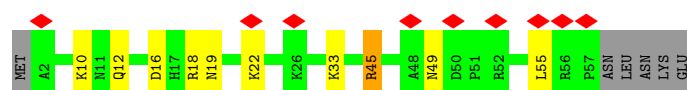
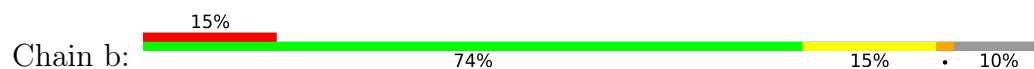
• Molecule 26: 60S ribosomal protein L27



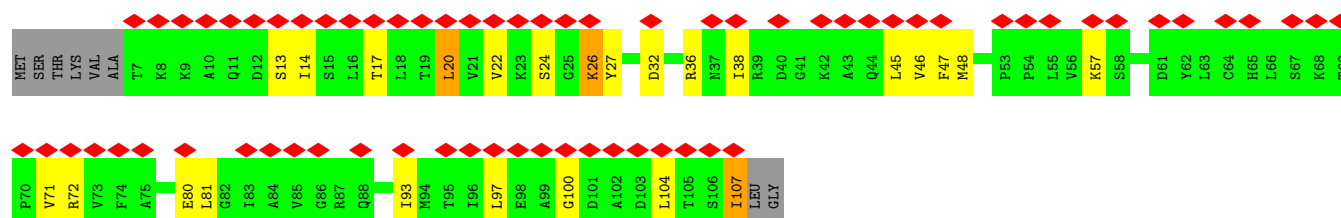
• Molecule 27: Ribosomal protein L27a



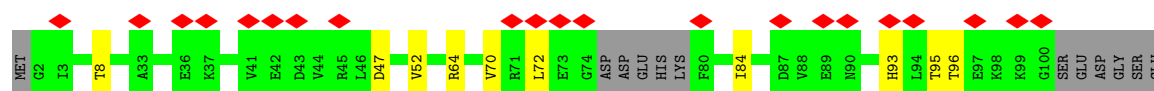
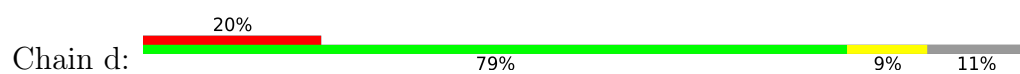
• Molecule 28: 60S ribosomal protein L29



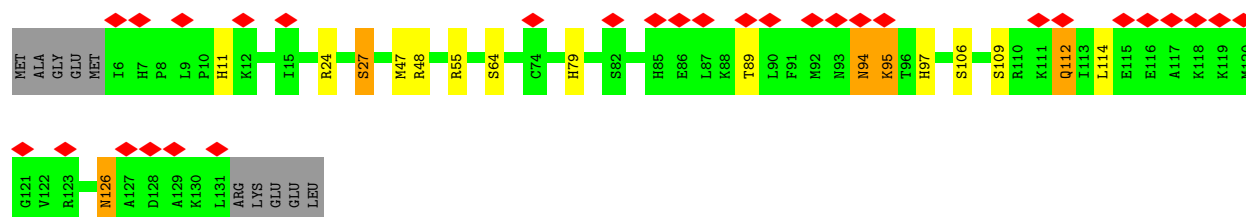
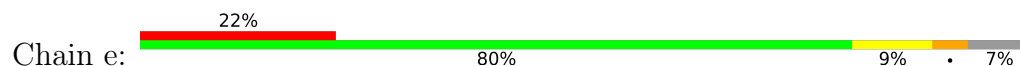
• Molecule 29: Ribosomal protein L30



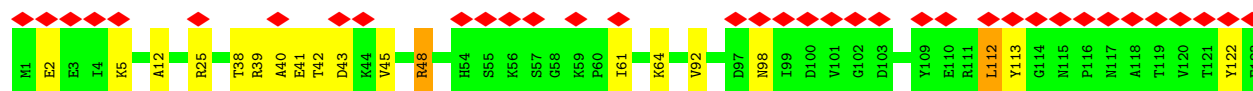
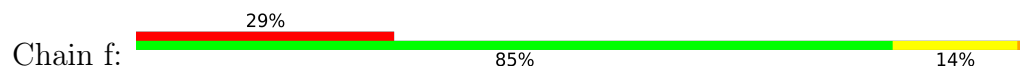
• Molecule 30: Ribosomal protein L31B



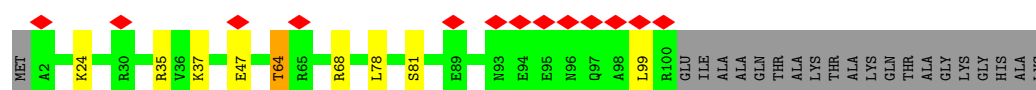
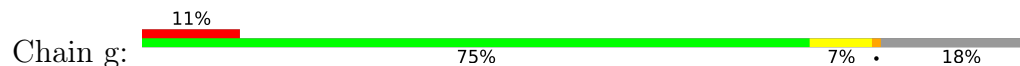
• Molecule 31: Ribosomal protein L32



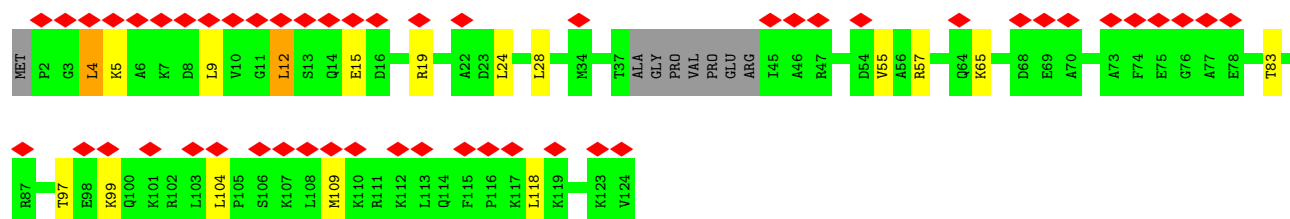
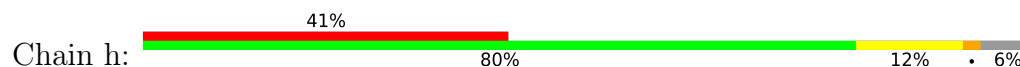
• Molecule 32: Ribosomal protein L35a



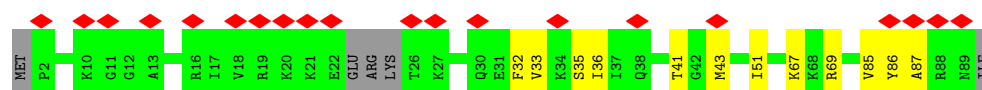
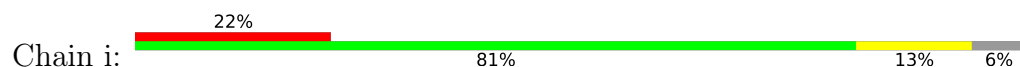
• Molecule 33: Ribosomal protein L34



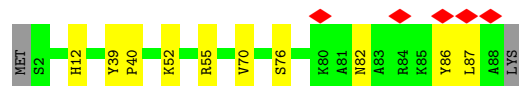
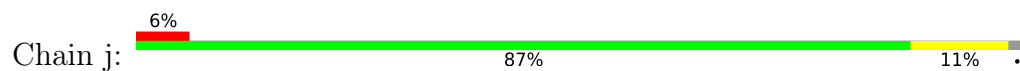
• Molecule 34: Ribosomal protein L29



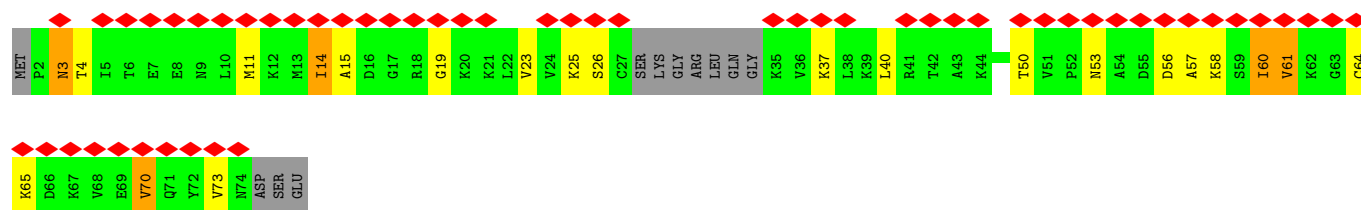
• Molecule 35: Ribosomal protein L36-1



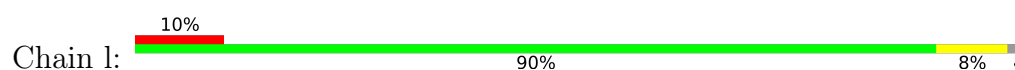
- Molecule 36: Ribosomal protein L37



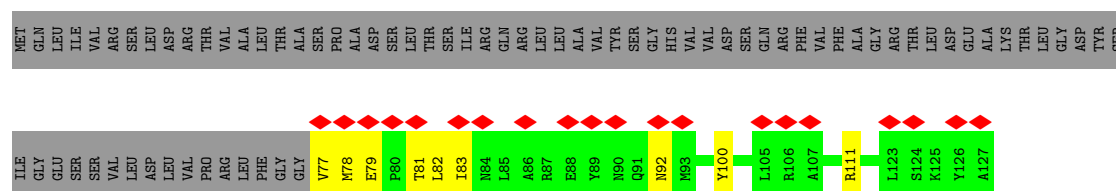
- Molecule 37: Ribosomal L38e



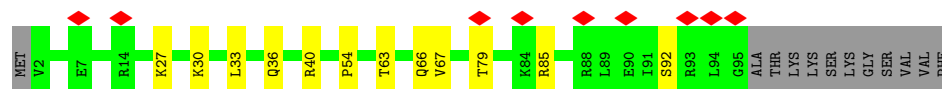
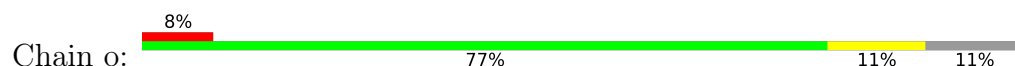
- Molecule 38: Ribosomal protein L39



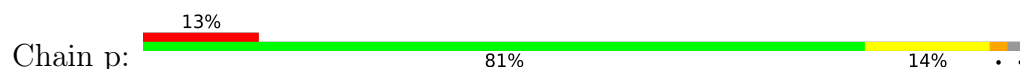
- Molecule 39: Ubiquitin/Ribosomal protein L40e

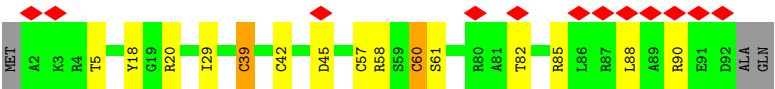


- Molecule 40: Ribosomal protein L44

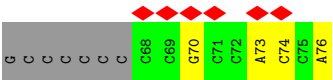


- Molecule 41: Ribosomal protein L37a

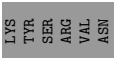
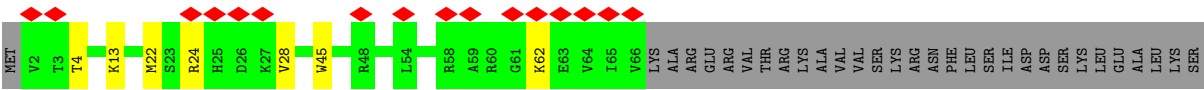




• Molecule 42: E-site tRNA



• Molecule 43: Ribosomal protein L24A



• Molecule 44: P-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.246	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, A2M, MG, OMC, K, PGE, OMU, OMG

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	1	0.53	2/58200 (0.0%)	0.53	31/90778 (0.0%)
2	3	0.43	0/2797	0.45	0/4359
3	4	0.49	0/3277	0.47	0/5109
4	A	0.39	0/1898	0.54	0/2551
5	B	0.37	0/3058	0.49	0/4129
6	C	0.38	0/2498	0.55	0/3388
7	D	0.32	0/2160	0.51	0/2903
8	F	0.37	0/1760	0.51	0/2374
9	G	0.35	0/1476	0.49	0/1994
10	H	0.32	0/1469	0.49	0/1985
11	I	0.31	0/1657	0.46	0/2219
12	J	0.29	0/1325	0.46	0/1776
13	L	0.38	0/1533	0.51	0/2052
14	M	0.31	0/1002	0.42	0/1349
15	N	0.44	0/1755	0.56	0/2353
16	O	0.37	0/1618	0.47	0/2169
17	P	0.37	0/1261	0.52	0/1688
18	Q	0.36	0/1425	0.49	0/1907
19	R	0.33	0/1478	0.46	0/1954
20	S	0.37	0/1452	0.50	0/1955
21	T	0.37	0/1251	0.54	0/1682
22	U	0.30	0/818	0.45	0/1101
23	V	0.35	0/1077	0.49	0/1451
24	X	0.37	0/956	0.52	0/1293
25	Y	0.36	0/1091	0.50	0/1454
26	Z	0.31	0/997	0.49	0/1352
27	a	0.42	0/1231	0.58	0/1647
28	b	0.37	0/471	0.54	0/624
29	c	0.28	0/764	0.43	0/1033
30	d	0.37	0/760	0.46	0/1022
31	e	0.38	0/1063	0.55	0/1418
32	f	0.38	0/994	0.50	0/1338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.35	0/813	0.51	0/1092
34	h	0.34	0/936	0.47	0/1247
35	i	0.35	0/700	0.48	0/927
36	j	0.41	0/708	0.52	0/941
37	k	0.27	0/503	0.43	0/675
38	l	0.36	0/445	0.51	0/594
39	m	0.33	0/426	0.46	0/568
40	o	0.38	0/773	0.52	0/1023
41	p	0.46	0/717	0.71	1/956 (0.1%)
42	w	0.40	0/332	0.46	0/511
43	W	0.36	0/551	0.46	0/738
44	E	0.28	0/68	0.38	0/103
All	All	0.46	2/111544 (0.0%)	0.52	32/163782 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
7	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1768	A2M	O3'-P	5.17	1.61	1.56
1	1	49	OMU	O3'-P	5.12	1.61	1.56

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2156	G	P-O3'-C3'	-7.87	108.39	120.20
1	1	2154	C	P-O3'-C3'	-7.43	109.05	120.20
1	1	1813	G	P-O3'-C3'	-7.28	109.28	120.20
1	1	2152	U	P-O3'-C3'	-6.91	109.83	120.20
1	1	2212	G	P-O3'-C3'	-6.82	109.97	120.20
1	1	2298	C	P-O3'-C3'	-6.78	110.03	120.20
1	1	2213	G	P-O3'-C3'	-6.68	110.18	120.20
1	1	2230	A	P-O3'-C3'	-6.51	110.43	120.20
1	1	2211	C	P-O3'-C3'	-6.47	110.50	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1814	A	P-O3'-C3'	-6.40	110.59	120.20
1	1	2155	C	P-O3'-C3'	-6.26	110.80	120.20
1	1	2157	G	P-O3'-C3'	-6.23	110.86	120.20
1	1	1812	G	P-O3'-C3'	-6.15	110.98	120.20
1	1	2214	A	P-O3'-C3'	-6.01	111.18	120.20
1	1	37	U	P-O3'-C3'	-5.92	111.32	120.20
1	1	1882	OMG	P-O3'-C3'	-5.89	111.36	120.20
1	1	1483	G	P-O3'-C3'	-5.87	111.39	120.20
41	p	60	CYS	CA-CB-SG	5.84	127.84	114.40
1	1	2231	C	P-O3'-C3'	-5.82	111.48	120.20
1	1	1485	C	P-O3'-C3'	-5.79	111.51	120.20
1	1	2153	G	P-O3'-C3'	-5.78	111.54	120.20
1	1	2299	G	P-O3'-C3'	-5.77	111.55	120.20
1	1	2215	G	P-O3'-C3'	-5.70	111.65	120.20
1	1	1486	U	P-O3'-C3'	-5.62	111.77	120.20
1	1	1484	A	P-O3'-C3'	-5.61	111.78	120.20
1	1	1809	C	P-O3'-C3'	-5.57	111.85	120.20
1	1	2232	C	P-O3'-C3'	-5.32	112.23	120.20
1	1	2234	C	P-O3'-C3'	-5.21	112.39	120.20
1	1	2210	G	P-O3'-C3'	-5.15	112.48	120.20
1	1	35	C	P-O3'-C3'	-5.14	112.49	120.20
1	1	1489	G	P-O3'-C3'	-5.09	112.56	120.20
1	1	2300	G	P-O3'-C3'	-5.02	112.67	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	13	GLY	Peptide
7	D	42	LYS	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	1	52618	0	26760	245	0
2	3	2501	0	1269	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4	2958	0	1517	13	0
4	A	1865	0	1920	15	0
5	B	2987	0	3022	21	0
6	C	2446	0	2535	30	0
7	D	2118	0	2139	22	0
8	F	1730	0	1766	22	0
9	G	1450	0	1512	25	0
10	H	1442	0	1480	13	0
11	I	1621	0	1635	22	0
12	J	1305	0	1318	19	0
13	L	1512	0	1607	10	0
14	M	990	0	1022	18	0
15	N	1712	0	1790	16	0
16	O	1587	0	1634	22	0
17	P	1235	0	1265	13	0
18	Q	1402	0	1478	14	0
19	R	1463	0	1567	10	0
20	S	1418	0	1410	17	0
21	T	1226	0	1256	17	0
22	U	802	0	787	18	0
23	V	1057	0	1099	10	0
24	X	936	0	984	7	0
25	Y	1076	0	1140	13	0
26	Z	980	0	974	17	0
27	a	1201	0	1233	11	0
28	b	463	0	489	7	0
29	c	756	0	781	11	0
30	d	748	0	793	4	0
31	e	1039	0	1095	9	0
32	f	974	0	995	10	0
33	g	798	0	832	4	0
34	h	926	0	1011	9	0
35	i	691	0	748	5	0
36	j	692	0	680	7	0
37	k	500	0	524	10	0
38	l	434	0	468	1	0
39	m	421	0	441	5	0
40	o	762	0	805	6	0
41	p	708	0	745	9	0
42	w	299	0	156	2	0
43	W	540	0	575	4	0
44	E	62	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1	99	0	0	1	0
45	4	5	0	0	0	0
45	C	1	0	0	0	0
45	F	1	0	0	0	0
45	I	1	0	0	0	0
45	P	1	0	0	0	0
45	V	1	0	0	0	0
45	a	1	0	0	0	0
45	b	1	0	0	0	0
45	o	1	0	0	0	0
46	1	163	0	0	1	0
46	3	1	0	0	0	0
46	A	3	0	0	0	0
46	B	3	0	0	0	0
46	C	2	0	0	0	0
46	I	1	0	0	0	0
46	L	1	0	0	0	0
46	N	2	0	0	0	0
46	V	1	0	0	0	0
46	a	1	0	0	0	0
46	e	1	0	0	0	0
46	j	1	0	0	0	0
46	o	1	0	0	0	0
47	1	10	0	14	0	0
48	1	3220	0	0	36	0
48	3	71	0	0	1	0
48	4	132	0	0	3	0
48	A	54	0	0	0	0
48	B	67	0	0	2	0
48	C	57	0	0	1	0
48	D	30	0	0	0	0
48	E	1	0	0	0	0
48	F	23	0	0	1	0
48	G	27	0	0	1	0
48	H	15	0	0	0	0
48	I	31	0	0	0	0
48	J	19	0	0	0	0
48	L	42	0	0	0	0
48	M	7	0	0	1	0
48	N	65	0	0	3	0
48	O	35	0	0	1	0
48	P	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Q	35	0	0	0	0
48	R	19	0	0	0	0
48	S	27	0	0	0	0
48	T	38	0	0	0	0
48	U	9	0	0	1	0
48	V	12	0	0	0	0
48	W	12	0	0	0	0
48	X	30	0	0	0	0
48	Y	18	0	0	0	0
48	Z	23	0	0	0	0
48	a	41	0	0	0	0
48	b	19	0	0	0	0
48	c	3	0	0	0	0
48	d	12	0	0	1	0
48	e	28	0	0	0	0
48	f	15	0	0	0	0
48	g	27	0	0	0	0
48	h	14	0	0	1	0
48	i	15	0	0	0	0
48	j	28	0	0	2	0
48	k	4	0	0	0	0
48	l	7	0	0	0	0
48	m	4	0	0	1	0
48	o	15	0	0	0	0
48	p	15	0	0	0	0
48	w	6	0	0	0	0
All	All	109151	0	77305	673	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 (673) 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)
1:1:2011:C:OP1	4:A:37:ARG:NH1	2.05	0.88
1:1:2479:U:H3	1:1:2496:A:H61	1.27	0.81
1:1:329:A:N6	1:1:342:G:O2'	2.15	0.80
32:f:38:THR:HG22	32:f:40:ALA:H	1.48	0.78
1:1:451:G:N2	1:1:454:C:OP2	2.18	0.77
9:G:189:LYS:HG3	9:G:190:PRO:HD3	1.65	0.77
41:p:82:THR:HG23	41:p:85:ARG:HH11	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:843:G:N7	48:1:3113:HOH:O	2.17	0.76
14:M:2:SER:N	48:M:201:HOH:O	2.19	0.76
1:1:611:G:O2'	1:1:613:G:OP2	2.04	0.75
28:b:19:ASN:O	28:b:22:LYS:NZ	2.20	0.75
1:1:1508:G:C8	1:1:1509:C:H2'	2.22	0.74
11:I:102:MET:SD	11:I:112:GLN:NE2	2.59	0.73
5:B:331:PRO:HD2	5:B:334:ARG:HG3	1.70	0.73
6:C:4:THR:OG1	6:C:17:GLU:OE1	2.06	0.72
1:1:1849:C:H5	1:1:1863:G:H1	1.35	0.72
25:Y:2:LYS:NZ	25:Y:7:VAL:O	2.23	0.72
40:o:36:GLN:OE1	40:o:40:ARG:NH2	2.22	0.71
34:h:12:LEU:O	34:h:65:LYS:NZ	2.23	0.71
1:1:2536:A:H1'	1:1:2537:A:H5''	1.73	0.71
1:1:1243:G:H1	1:1:1248:C:H42	1.39	0.70
36:j:82:ASN:OD1	48:j:201:HOH:O	2.08	0.70
1:1:632:G:OP1	48:1:3101:HOH:O	2.08	0.70
7:D:54:ARG:HG3	7:D:59:ILE:HG12	1.73	0.70
34:h:28:LEU:HD11	34:h:55:VAL:HG21	1.73	0.70
1:1:2059:C:OP1	48:1:3102:HOH:O	2.09	0.70
26:Z:133:ILE:HG22	26:Z:134:ASP:HB2	1.72	0.70
7:D:90:GLY:O	7:D:93:ASN:ND2	2.25	0.69
16:O:44:PHE:HZ	16:O:141:GLU:HG3	1.57	0.68
6:C:76:HIS:O	48:C:501:HOH:O	2.12	0.68
22:U:73:GLN:NE2	22:U:74:THR:O	2.25	0.68
1:1:2487:C:OP2	48:1:3103:HOH:O	2.10	0.68
1:1:2643:C:H41	1:1:2671:C:N4	1.92	0.68
17:P:41:LYS:NZ	17:P:109:GLU:OE2	2.27	0.68
2:3:41:C:O2	12:J:72:ARG:NH1	2.27	0.68
8:F:112:MET:HE2	8:F:118:THR:HB	1.76	0.68
8:F:160:ASP:OD2	8:F:162:ASN:ND2	2.27	0.68
1:1:2514:G:O2'	48:1:3104:HOH:O	2.10	0.67
1:1:2490:G:N7	48:1:3153:HOH:O	2.27	0.67
1:1:1300:G:OP1	26:Z:105:ARG:NH2	2.25	0.67
1:1:865:C:OP2	48:1:3105:HOH:O	2.12	0.66
2:3:9:C:OP1	21:T:28:THR:OG1	2.14	0.66
8:F:75:GLU:OE2	21:T:137:ARG:NH1	2.28	0.66
1:1:1498:A:OP1	48:1:3107:HOH:O	2.14	0.66
6:C:118:LEU:O	6:C:121:SER:OG	2.14	0.66
1:1:2264:C:OP1	1:1:2266:C:N4	2.28	0.66
1:1:1557:C:OP2	41:p:20:ARG:NH1	2.29	0.65
19:R:105:LEU:HD22	19:R:135:LYS:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:20:ASN:N	22:U:20:ASN:OD1	2.30	0.65
1:1:2502:C:H3'	1:1:2503:G:H21	1.61	0.65
45:1:2809:MG:MG	48:1:3115:HOH:O	1.38	0.65
1:1:1782:A:OP2	23:V:76:ARG:NH1	2.30	0.65
1:1:1742:A:H5'	1:1:1748:G:H22	1.61	0.64
1:1:2536:A:N6	1:1:2538:A:H62	1.95	0.64
14:M:17:ASP:HB3	14:M:54:TRP:CD1	2.32	0.64
3:4:73:A:H5''	25:Y:50:ARG:HG3	1.79	0.64
12:J:21:ILE:HD11	12:J:125:MET:HE2	1.78	0.64
18:Q:74:ARG:HB2	18:Q:77:LYS:HD2	1.79	0.64
1:1:1241:G:N7	24:X:33:LYS:NZ	2.45	0.64
3:4:41:A:OP1	48:4:301:HOH:O	2.15	0.64
10:H:62:ARG:NH1	16:O:129:GLU:OE2	2.30	0.64
1:1:2260:A:N6	1:1:2272:G:O2'	2.31	0.64
5:B:26:ARG:NH2	5:B:177:ILE:O	2.31	0.64
8:F:76:PRO:HB3	8:F:133:GLU:HG2	1.78	0.64
15:N:12:ARG:NH1	48:N:1201:HOH:O	2.30	0.64
18:Q:121:SER:OG	18:Q:123:ASP:OD1	2.14	0.64
2:3:111:G:H2'	2:3:112:C:C6	2.34	0.63
1:1:2672:G:OP2	43:W:62:LYS:NZ	2.32	0.63
10:H:3:LEU:HG	20:S:138:MET:HE3	1.81	0.63
23:V:128:ALA:O	23:V:135:SER:OG	2.15	0.63
7:D:262:LYS:H	7:D:262:LYS:HD2	1.63	0.63
23:V:8:SER:OG	23:V:9:GLY:N	2.31	0.63
6:C:26:VAL:HG13	6:C:260:PRO:HG2	1.80	0.63
8:F:70:LEU:HG	21:T:144:ILE:HD13	1.81	0.62
26:Z:104:ARG:HA	26:Z:107:ILE:HD12	1.81	0.62
22:U:20:ASN:HB3	22:U:75:THR:HA	1.82	0.62
27:a:15:ARG:HD2	27:a:15:ARG:O	1.99	0.62
18:Q:18:GLU:OE2	18:Q:27:ARG:NH2	2.32	0.62
26:Z:103:LYS:O	26:Z:106:GLU:HG2	2.00	0.62
18:Q:128:GLU:HG2	18:Q:129:LYS:HG3	1.81	0.61
2:3:54:G:H21	2:3:56:A:H62	1.48	0.61
1:1:107:G:OP2	13:L:102:ARG:NH2	2.31	0.61
1:1:1599:G:HO2'	43:W:45:TRP:CD1	2.19	0.61
11:I:150:ASP:OD1	11:I:150:ASP:N	2.33	0.61
37:k:3:ASN:HD22	37:k:4:THR:H	1.48	0.61
13:L:71:LYS:HE3	13:L:80:LEU:HD22	1.83	0.61
2:3:115:A:N7	48:3:302:HOH:O	2.31	0.60
1:1:114:C:P	15:N:1:MET:HA	2.41	0.60
1:1:1428:G:H2'	1:1:1429:G:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2275:G:OP1	11:I:30:LYS:NZ	2.32	0.60
1:1:808:A:OP2	21:T:130:LYS:HA	2.01	0.60
6:C:123:ASN:HD22	6:C:126:LEU:HD12	1.66	0.59
22:U:55:HIS:O	22:U:55:HIS:ND1	2.32	0.59
14:M:119:ARG:HH11	16:O:188:ILE:HD12	1.67	0.59
1:1:2536:A:H62	1:1:2538:A:H62	1.48	0.59
1:1:2443:G:O6	48:1:3111:HOH:O	2.17	0.59
9:G:194:LYS:NZ	48:G:302:HOH:O	2.36	0.59
1:1:1663:U:OP1	4:A:54:ARG:NH2	2.36	0.58
6:C:292:GLU:OE2	6:C:306:ARG:NH1	2.33	0.58
18:Q:153:SER:O	18:Q:159:SER:OG	2.10	0.58
20:S:166:ASP:OD1	20:S:166:ASP:N	2.34	0.58
1:1:2607:C:H2'	1:1:2608:C:C5	2.39	0.58
1:1:1127:G:O6	48:1:3108:HOH:O	2.14	0.58
1:1:1014:C:H2'	16:O:130:ARG:NH1	2.19	0.58
16:O:185:LEU:O	16:O:189:ASN:ND2	2.36	0.58
1:1:2609:G:O6	48:1:3106:HOH:O	2.13	0.58
1:1:1843:A:H5'	17:P:138:LYS:HE3	1.85	0.57
1:1:1794:G:O2'	1:1:1797:U:OP2	2.23	0.57
5:B:110:ILE:HB	5:B:115:MET:HE2	1.86	0.57
11:I:190:LEU:HD11	11:I:197:ALA:HB1	1.85	0.57
29:c:72:ARG:HG3	29:c:107:ILE:HG23	1.86	0.57
1:1:2475:G:OP2	30:d:64:ARG:NH2	2.37	0.57
1:1:2690:G:O2'	5:B:124:HIS:NE2	2.36	0.57
34:h:5:LYS:NZ	48:h:201:HOH:O	2.37	0.57
1:1:1587:G:O2'	1:1:1588:G:OP1	2.21	0.57
1:1:1170:A:N1	1:1:1486:U:H5	2.02	0.57
1:1:1626:A:N6	48:1:3216:HOH:O	2.38	0.57
1:1:1754:C:O2	48:1:3109:HOH:O	2.15	0.57
1:1:2439:G:O2'	1:1:2448:G:O6	2.18	0.57
5:B:370:VAL:O	5:B:374:ARG:HD3	2.05	0.57
32:f:39:ARG:O	32:f:42:THR:OG1	2.19	0.57
23:V:75:ARG:O	23:V:77:LYS:NZ	2.38	0.56
1:1:1342:G:OP1	22:U:81:LYS:NZ	2.27	0.56
4:A:149:ARG:HG3	4:A:155:LYS:HE3	1.87	0.56
1:1:432:G:OP1	13:L:68:ARG:NH2	2.36	0.56
1:1:750:C:HO2'	7:D:2:TRP:N	2.04	0.56
1:1:888:G:OP2	48:1:3114:HOH:O	2.18	0.56
6:C:307:LEU:O	8:F:161:ASN:ND2	2.37	0.56
25:Y:8:THR:HG21	25:Y:13:LYS:HD3	1.88	0.56
10:H:85:GLU:HG3	10:H:143:ARG:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:75:TYR:CE1	11:I:150:ASP:HB2	2.40	0.56
26:Z:9:GLY:HA3	26:Z:84:ARG:HH21	1.69	0.56
32:f:38:THR:HB	32:f:41:GLU:HG2	1.86	0.56
1:1:2555:C:H5	5:B:24:ARG:HH22	1.54	0.56
11:I:191:GLN:N	11:I:198:HIS:O	2.38	0.56
8:F:106:ILE:HG12	8:F:106:ILE:O	2.06	0.56
24:X:52:SER:OG	24:X:53:TRP:N	2.37	0.55
6:C:96:THR:HG22	6:C:98:ILE:H	1.71	0.55
1:1:631:A:OP2	48:1:3115:HOH:O	2.18	0.55
7:D:110:GLU:HG3	7:D:256:PRO:HG2	1.88	0.55
40:o:63:THR:HG21	40:o:85:ARG:HB3	1.87	0.55
1:1:492:G:OP1	28:b:45:ARG:NH1	2.39	0.55
6:C:35:PHE:O	6:C:39:GLN:HG2	2.06	0.55
9:G:120:ILE:HG13	9:G:180:CYS:SG	2.46	0.55
1:1:861:G:OP2	1:1:861:G:N2	2.33	0.55
1:1:1108:G:H2'	1:1:1109:G:C8	2.41	0.55
1:1:1245:G:O2'	1:1:1246:U:OP2	2.25	0.55
1:1:887:C:OP2	48:1:3114:HOH:O	2.18	0.55
1:1:2526:U:O2'	10:H:148:GLU:OE2	2.25	0.55
29:c:48:MET:HE1	29:c:57:LYS:HG3	1.87	0.55
1:1:814:G:OP1	18:Q:10:LYS:NZ	2.40	0.55
7:D:71:ASP:OD1	7:D:71:ASP:N	2.39	0.55
9:G:125:GLU:OE2	15:N:1:MET:N	2.30	0.55
22:U:38:ASN:O	22:U:42:ASP:N	2.33	0.54
5:B:300:LEU:H	5:B:300:LEU:HD23	1.71	0.54
21:T:81:ARG:NH1	28:b:12:GLN:OE1	2.37	0.54
9:G:185:ASN:ND2	9:G:187:GLU:OE2	2.41	0.54
1:1:2087:C:OP1	48:1:3116:HOH:O	2.18	0.54
11:I:174:THR:HG22	11:I:175:GLU:H	1.73	0.54
9:G:132:VAL:HG22	9:G:180:CYS:SG	2.48	0.54
17:P:105:HIS:O	17:P:107:LYS:N	2.41	0.54
26:Z:98:VAL:C	26:Z:100:ASP:H	2.14	0.54
1:1:624:OMG:HM22	1:1:624:OMG:N3	2.22	0.54
1:1:715:G:N2	1:1:763:C:OP1	2.37	0.54
3:4:36:C:H5'	36:j:70:VAL:HG11	1.89	0.54
1:1:502:A:OP1	48:1:3117:HOH:O	2.19	0.54
1:1:2208:G:N7	48:1:3183:HOH:O	2.33	0.54
1:1:200:G:C5	1:1:201:G:H2'	2.43	0.54
1:1:393:A2M:HM'3	48:1:4625:HOH:O	2.07	0.54
12:J:91:LEU:O	12:J:171:TYR:HA	2.08	0.54
37:k:11:MET:O	37:k:15:ALA:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1245:G:OP1	1:1:1245:G:N2	2.37	0.53
13:L:85:PRO:HG3	13:L:103:GLY:O	2.08	0.53
37:k:23:VAL:HG22	37:k:70:VAL:HG22	1.90	0.53
1:1:1643:G:OP1	4:A:241:ARG:HD3	2.08	0.53
7:D:94:TYR:CZ	7:D:168:ALA:HB2	2.43	0.53
1:1:196:C:O2	25:Y:132:ARG:NH2	2.40	0.53
1:1:1894:C:H2'	1:1:1895:U:C6	2.43	0.53
8:F:22:ALA:N	48:F:401:HOH:O	2.42	0.53
25:Y:120:LYS:O	25:Y:124:GLU:HG3	2.08	0.53
33:g:35:ARG:HH21	33:g:37:LYS:HE2	1.72	0.53
16:O:45:ARG:NH1	16:O:45:ARG:HB3	2.23	0.53
31:e:109:SER:HA	31:e:112:GLN:HG3	1.89	0.53
11:I:84:SER:OG	11:I:141:ARG:NH1	2.42	0.53
23:V:94:ASP:OD1	23:V:94:ASP:N	2.40	0.53
9:G:83:SER:HB3	9:G:172:HIS:CE1	2.44	0.53
26:Z:93:ILE:HG23	26:Z:97:THR:HG21	1.91	0.53
41:p:39:CYS:HB3	41:p:42:CYS:N	2.24	0.53
17:P:12:LEU:HB3	17:P:105:HIS:CD2	2.43	0.53
18:Q:37:TYR:CE1	18:Q:46:LYS:HB2	2.44	0.53
31:e:126:ASN:N	31:e:126:ASN:OD1	2.41	0.53
1:1:1746:A:H8	1:1:1746:A:P	2.33	0.53
7:D:102:LEU:HD12	7:D:176:ALA:HB2	1.90	0.53
7:D:66:ALA:HA	7:D:71:ASP:HB3	1.91	0.52
16:O:78:ARG:HB2	16:O:101:VAL:HG21	1.92	0.52
36:j:39:TYR:CD1	36:j:40:PRO:HA	2.44	0.52
1:1:1896:OMU:HM21	1:1:1898:U:H5'	1.92	0.52
2:3:77:U:H5	2:3:101:A:N7	2.07	0.52
14:M:81:PRO:O	14:M:85:THR:HG23	2.10	0.52
20:S:148:HIS:HB3	20:S:151:PRO:HG3	1.92	0.52
37:k:57:ALA:O	37:k:61:VAL:HG23	2.08	0.52
9:G:187:GLU:CD	9:G:187:GLU:H	2.18	0.52
11:I:201:SER:OG	11:I:202:ARG:N	2.42	0.52
12:J:77:ARG:HA	12:J:80:ILE:HG22	1.92	0.52
14:M:30:ILE:O	20:S:92:ARG:NH1	2.42	0.52
4:A:24:LEU:HD12	4:A:58:LEU:HD12	1.91	0.52
1:1:476:G:H1	1:1:491:U:H3	1.58	0.52
16:O:165:TYR:O	16:O:169:ILE:HG13	2.10	0.52
1:1:1646:A:O2'	4:A:118:GLU:OE2	2.26	0.51
2:3:40:C:H4'	12:J:44:GLU:HG3	1.92	0.51
1:1:1345:G:H2'	1:1:1346:G:C8	2.45	0.51
23:V:101:GLN:HG3	43:W:22:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:i:32:PHE:CZ	35:i:36:ILE:HD11	2.45	0.51
37:k:14:ILE:HG23	37:k:64:CYS:HB2	1.92	0.51
1:l:1150:G:O2'	48:l:3118:HOH:O	2.19	0.51
4:A:62:GLN:OE1	4:A:71:ARG:NH1	2.44	0.51
15:N:202:ARG:NH1	48:N:1203:HOH:O	2.39	0.51
28:b:45:ARG:O	28:b:49:ASN:ND2	2.42	0.51
1:l:775:G:C6	21:T:109:VAL:HG22	2.45	0.51
34:h:97:THR:HG22	34:h:99:LYS:H	1.75	0.51
1:l:2555:C:H2'	1:l:2556:G:N2	2.25	0.51
1:l:1312:C:H2'	1:l:1313:C:C6	2.45	0.51
1:l:2106:U:H2'	1:l:2107:C:C6	2.46	0.51
5:B:103:THR:HG22	5:B:150:LEU:HD21	1.93	0.51
15:N:153:ASN:HD21	15:N:155:VAL:HG22	1.75	0.51
19:R:7:GLN:OE1	19:R:7:GLN:N	2.43	0.51
1:l:1383:C:OP1	19:R:117:ARG:NE	2.41	0.51
1:l:2415:C:O2'	17:P:73:ARG:NH1	2.44	0.51
1:l:2159:G:OP1	21:T:92:ARG:NH1	2.43	0.50
6:C:136:ASP:N	6:C:136:ASP:OD1	2.44	0.50
9:G:83:SER:HB3	9:G:172:HIS:NE2	2.25	0.50
34:h:24:LEU:HB3	34:h:55:VAL:HG22	1.93	0.50
1:l:301:C:H5	48:4:379:HOH:O	1.94	0.50
11:I:191:GLN:HG3	11:I:192:TYR:N	2.26	0.50
1:l:448:A:OP2	27:a:115:ARG:NH2	2.44	0.50
3:4:9:C:H2'	3:4:10:G:O4'	2.12	0.50
6:C:307:LEU:HD22	8:F:176:ALA:HB2	1.94	0.50
7:D:55:THR:OG1	7:D:56:ASN:O	2.29	0.50
39:m:78:MET:HB3	39:m:83:ILE:HD11	1.94	0.50
1:l:668:A:OP1	28:b:18:ARG:NH2	2.42	0.50
5:B:39:ALA:O	5:B:185:GLY:N	2.39	0.50
35:i:85:VAL:HG13	35:i:86:TYR:CD1	2.45	0.50
1:l:114:C:OP1	15:N:1:MET:HA	2.12	0.50
1:l:496:G:OP1	18:Q:160:HIS:HA	2.11	0.50
1:l:2304:U:H2'	1:l:2305:U:C6	2.46	0.50
6:C:159:ILE:HB	6:C:164:VAL:HG23	1.93	0.50
7:D:184:MET:HA	7:D:184:MET:HE2	1.93	0.50
29:c:38:ILE:HD11	29:c:46:VAL:HG21	1.94	0.50
1:l:2390:A:N7	4:A:215:ASN:ND2	2.60	0.49
8:F:23:GLU:O	8:F:27:GLU:HG2	2.11	0.49
12:J:57:PHE:HD2	12:J:59:ILE:HG12	1.77	0.49
20:S:38:ARG:HH21	20:S:116:HIS:CD2	2.30	0.49
20:S:114:ARG:HD3	20:S:114:ARG:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:12:ALA:HB3	32:f:92:VAL:HB	1.94	0.49
12:J:54:ILE:HG22	12:J:57:PHE:H	1.77	0.49
19:R:38:ARG:O	19:R:42:ARG:HG3	2.12	0.49
26:Z:30:LEU:HD21	26:Z:40:ILE:HG12	1.94	0.49
9:G:64:ILE:HG13	9:G:159:ALA:HB1	1.94	0.49
26:Z:25:VAL:HG21	26:Z:85:LEU:HD22	1.94	0.49
1:1:492:G:O2'	1:1:493:C:OP1	2.26	0.49
1:1:1252:C:H5'	24:X:28:HIS:CE1	2.46	0.49
22:U:26:ASP:OD1	22:U:69:SER:OG	2.26	0.49
1:1:1077:G:H5'	31:e:106:SER:HB3	1.93	0.49
1:1:2643:C:H41	1:1:2671:C:H41	1.58	0.49
3:4:14:G:OP1	17:P:2:VAL:HB	2.12	0.49
11:I:50:PHE:CE1	11:I:148:VAL:HG21	2.48	0.49
14:M:58:THR:HG22	14:M:59:ASP:H	1.78	0.49
15:N:4:TYR:HE2	15:N:49:ARG:HD3	1.77	0.49
1:1:429:G:H22	1:1:441:G:H2'	1.76	0.49
1:1:1107:C:C5	6:C:179:ALA:HA	2.47	0.49
4:A:102:LEU:HD13	4:A:166:ILE:HD11	1.95	0.49
9:G:63:PRO:HG2	9:G:162:ARG:HE	1.76	0.49
8:F:173:ILE:HG23	8:F:178:ASP:HB3	1.94	0.49
16:O:35:CYS:SG	16:O:101:VAL:HG12	2.52	0.49
1:1:1705:G:H2'	1:1:1706:A:C8	2.47	0.49
1:1:789:G:N1	1:1:792:C:OP2	2.36	0.48
1:1:1420:G:H4'	1:1:1588:G:OP1	2.13	0.48
1:1:2233:A:N3	1:1:2233:A:H2'	2.27	0.48
8:F:37:ASP:O	8:F:41:LYS:HG3	2.12	0.48
9:G:50:ARG:HH21	9:G:218:ARG:HG2	1.78	0.48
20:S:57:LEU:HD22	21:T:142:VAL:HG11	1.95	0.48
33:g:64:THR:O	33:g:68:ARG:HG3	2.13	0.48
41:p:42:CYS:N	41:p:60:CYS:SG	2.86	0.48
12:J:93:TYR:O	12:J:160:ARG:NH2	2.42	0.48
1:1:1108:G:H2'	1:1:1109:G:N7	2.28	0.48
7:D:162:THR:HA	7:D:186:ARG:HA	1.94	0.48
2:3:90:G:H2'	2:3:91:A:C8	2.49	0.48
29:c:32:ASP:O	29:c:36:ARG:HG3	2.13	0.48
1:1:73:G:O2'	13:L:90:CYS:HB3	2.14	0.48
1:1:224:A:H2'	1:1:225:G:O4'	2.13	0.48
1:1:424:A:H4'	1:1:425:G:O5'	2.13	0.48
11:I:28:ASP:HB2	11:I:32:ARG:HH21	1.78	0.48
23:V:133:LYS:O	23:V:137:THR:HG22	2.13	0.48
31:e:11:HIS:CD2	32:f:122:TYR:HE2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2415:C:H1'	17:P:73:ARG:HD2	1.95	0.48
6:C:160:LYS:HG3	6:C:165:LEU:HD22	1.96	0.48
1:1:4:C:H2'	1:1:5:G:C8	2.49	0.48
1:1:2487:C:H3'	1:1:2488:G:H21	1.79	0.48
17:P:47:LEU:HD22	17:P:87:VAL:HG13	1.96	0.48
42:w:1:A:N6	42:w:73:A:C6	2.82	0.48
4:A:42:ARG:HH11	4:A:87:GLU:CD	2.21	0.48
20:S:38:ARG:HH21	20:S:116:HIS:HD2	1.60	0.48
26:Z:44:ILE:HD12	26:Z:47:LEU:HD21	1.96	0.48
1:1:1741:U:H2'	1:1:1748:G:N2	2.29	0.47
18:Q:36:VAL:HG12	18:Q:45:THR:HG21	1.96	0.47
19:R:154:LYS:O	19:R:158:GLU:N	2.45	0.47
26:Z:115:PHE:O	26:Z:119:ILE:HG13	2.14	0.47
42:w:1:A:H1'	42:w:2:G:H5'	1.96	0.47
1:1:1178:U:H5	1:1:1469:A:N1	2.12	0.47
8:F:231:VAL:O	8:F:235:ILE:HG13	2.14	0.47
14:M:129:SER:HA	16:O:174:LYS:NZ	2.30	0.47
1:1:49:OMU:HM23	1:1:49:OMU:H1'	1.45	0.47
14:M:98:GLN:HA	14:M:101:ARG:HG2	1.95	0.47
34:h:4:LEU:O	34:h:57:ARG:HD3	2.14	0.47
9:G:139:ASP:HB3	9:G:140:PRO:HD3	1.96	0.47
39:m:79:GLU:HG2	39:m:81:THR:HG22	1.96	0.47
1:1:2439:G:H1'	1:1:2440:U:H5	1.80	0.47
9:G:125:GLU:OE1	15:N:6:TYR:OH	2.25	0.47
1:1:869:C:OP1	1:1:1031:G:H5''	2.15	0.47
1:1:1589:G:H2'	1:1:1590:U:C6	2.50	0.47
1:1:2354:U:O2'	1:1:2355:C:OP1	2.29	0.47
2:3:54:G:N2	2:3:56:A:H62	2.10	0.47
16:O:160:GLU:HA	16:O:163:LYS:HE2	1.97	0.47
20:S:90:GLU:OE1	20:S:131:VAL:HG13	2.14	0.47
36:j:12:HIS:ND1	48:j:202:HOH:O	2.25	0.47
1:1:1916:G:H2'	1:1:1917:G:C8	2.50	0.47
1:1:428:C:H5	6:C:104:LYS:HA	1.80	0.47
10:H:85:GLU:OE2	10:H:143:ARG:NH2	2.39	0.47
10:H:94:HIS:O	10:H:94:HIS:ND1	2.48	0.47
31:e:47:MET:HE1	31:e:55:ARG:HB2	1.97	0.47
41:p:42:CYS:SG	41:p:60:CYS:N	2.88	0.47
1:1:1508:G:H1'	1:1:1509:C:H5'	1.97	0.47
1:1:1736:G:O2'	1:1:1737:G:P	2.73	0.47
1:1:1850:A:H2'	1:1:1851:G:O4'	2.15	0.47
1:1:1862:G:O2'	1:1:1864:G:OP2	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:23:U:OP2	6:C:184:MET:HE2	2.15	0.47
6:C:140:ILE:HD13	6:C:140:ILE:HA	1.61	0.46
10:H:102:VAL:HG23	10:H:107:ALA:HB3	1.96	0.46
11:I:47:PRO:HB3	11:I:171:TRP:CZ2	2.50	0.46
12:J:29:ALA:O	12:J:33:ALA:N	2.39	0.46
20:S:1:MET:HE3	20:S:2:MET:HE2	1.96	0.46
1:1:2151:G:H5''	21:T:83:ARG:NH2	2.30	0.46
1:1:325:A:H1'	1:1:326:A:H5''	1.96	0.46
1:1:1472:G:OP2	48:1:3126:HOH:O	2.21	0.46
1:1:2317:C:O2'	39:m:100:TYR:O	2.32	0.46
9:G:146:TRP:CD1	9:G:146:TRP:H	2.33	0.46
1:1:15:G:H2'	1:1:16:G:C8	2.50	0.46
1:1:2368:G:H4'	1:1:2368:G:OP2	2.14	0.46
7:D:113:SER:HB2	7:D:120:ALA:HB1	1.96	0.46
16:O:24:LEU:O	16:O:98:ARG:NH2	2.33	0.46
29:c:22:VAL:HG12	29:c:27:TYR:CZ	2.51	0.46
1:1:2591:C:H2'	14:M:116:ARG:NH2	2.31	0.46
8:F:26:THR:O	8:F:30:LYS:HG3	2.15	0.46
16:O:116:VAL:HG23	16:O:118:PRO:HD3	1.97	0.46
29:c:24:SER:O	29:c:100:GLY:HA3	2.16	0.46
10:H:27:LYS:HB2	10:H:32:THR:HG23	1.97	0.46
5:B:62:HIS:O	5:B:68:HIS:ND1	2.48	0.46
11:I:50:PHE:CD1	11:I:148:VAL:HG21	2.51	0.46
22:U:33:LEU:HD22	22:U:33:LEU:HA	1.81	0.46
3:4:116:C:O2'	3:4:119:G:O6	2.26	0.46
6:C:123:ASN:ND2	6:C:126:LEU:HD12	2.31	0.46
12:J:51:ARG:O	12:J:61:ARG:HD2	2.16	0.46
1:1:462:G:H2'	1:1:462:G:N3	2.31	0.46
1:1:821:C:H2'	1:1:822:G:C8	2.51	0.46
1:1:1451:G:OP1	26:Z:50:ARG:HD3	2.16	0.46
5:B:88:ALA:HB3	5:B:160:VAL:HB	1.98	0.46
16:O:165:TYR:CE2	16:O:169:ILE:HD11	2.51	0.46
1:1:1365:C:H2'	1:1:1366:C:C6	2.51	0.45
7:D:191:SER:C	7:D:193:ASP:H	2.24	0.45
12:J:163:VAL:O	12:J:167:PHE:N	2.44	0.45
1:1:1311:C:H2'	1:1:1312:C:C6	2.51	0.45
5:B:292:ARG:NH2	48:B:508:HOH:O	2.49	0.45
16:O:182:ASP:O	16:O:185:LEU:N	2.50	0.45
17:P:14:GLY:HA3	17:P:101:ALA:HB2	1.98	0.45
19:R:154:LYS:HB3	19:R:158:GLU:HG2	1.97	0.45
31:e:94:ASN:O	31:e:95:LYS:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1787:C:H2'	1:1:1788:C:C6	2.51	0.45
1:1:2643:C:H2'	1:1:2644:G:O4'	2.16	0.45
6:C:294:LYS:NZ	8:F:158:ILE:O	2.49	0.45
7:D:132:THR:HB	7:D:134:GLU:HG3	1.98	0.45
1:1:23:C:OP2	48:1:3125:HOH:O	2.20	0.45
1:1:91:G:H2'	1:1:92:A:C8	2.51	0.45
1:1:1781:C:H3'	23:V:76:ARG:HH12	1.81	0.45
6:C:149:VAL:HG23	6:C:204:VAL:HG12	1.98	0.45
6:C:268:ASP:O	6:C:272:ILE:HG13	2.16	0.45
14:M:41:PRO:HB2	14:M:74:LYS:HG3	1.99	0.45
32:f:112:LEU:HD12	32:f:113:TYR:CE2	2.51	0.45
8:F:58:LYS:HB2	8:F:58:LYS:HE3	1.72	0.45
1:1:658:U:OP2	27:a:15:ARG:HD3	2.16	0.45
1:1:2686:G:O2'	30:d:96:THR:O	2.34	0.45
6:C:9:GLY:C	6:C:11:THR:H	2.23	0.45
10:H:88:MET:HE1	10:H:157:ILE:HD12	1.97	0.45
15:N:13:LYS:HD3	35:i:41:THR:HG21	1.99	0.45
19:R:30:LYS:HG3	19:R:31:TYR:N	2.32	0.45
1:1:590:U:OP2	1:1:1538:C:O2'	2.32	0.45
1:1:2611:C:C2	1:1:2691:C:N4	2.84	0.45
7:D:91:LEU:O	7:D:92:THR:OG1	2.24	0.45
1:1:2559:C:H2'	1:1:2560:C:C6	2.52	0.45
48:1:5328:HOH:O	15:N:93:LYS:HE3	2.16	0.45
11:I:30:LYS:HD2	11:I:63:GLU:HA	1.99	0.45
21:T:83:ARG:HH21	21:T:85:MET:HE3	1.82	0.45
41:p:39:CYS:HB3	41:p:42:CYS:H	1.82	0.45
1:1:1860:A:N3	1:1:2246:G:O2'	2.36	0.45
1:1:2145:C:OP1	28:b:33:LYS:NZ	2.30	0.45
15:N:185:ARG:HA	15:N:185:ARG:HD3	1.42	0.45
20:S:42:HIS:CE1	21:T:152:PRO:HG3	2.52	0.45
1:1:2303:C:H2'	1:1:2304:U:C6	2.52	0.44
15:N:38:ARG:HD2	15:N:62:TYR:CE1	2.52	0.44
16:O:192:LEU:HD23	16:O:192:LEU:HA	1.75	0.44
18:Q:129:LYS:NZ	18:Q:134:ASN:HB3	2.32	0.44
22:U:60:LYS:HD3	22:U:77:TYR:HB2	1.99	0.44
32:f:45:VAL:HA	32:f:48:ARG:HD2	1.99	0.44
33:g:24:LYS:HA	33:g:24:LYS:HD2	1.79	0.44
1:1:2168:G:N2	1:1:2171:A:OP2	2.40	0.44
1:1:2347:C:H2'	1:1:2348:A:O4'	2.17	0.44
11:I:61:SER:HA	11:I:126:VAL:HG12	1.98	0.44
14:M:122:ALA:HB2	16:O:187:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:67:GLY:N	48:U:201:HOH:O	2.50	0.44
1:1:442:C:H2'	1:1:443:G:O4'	2.17	0.44
9:G:47:LEU:O	9:G:51:LEU:HG	2.18	0.44
22:U:36:ASN:OD1	22:U:37:LEU:N	2.51	0.44
34:h:4:LEU:HD13	34:h:4:LEU:HA	1.68	0.44
1:1:2373:G:OP2	48:1:3130:HOH:O	2.21	0.44
1:1:2587:C:N4	20:S:166:ASP:OD1	2.36	0.44
5:B:215:ILE:HD11	5:B:324:ILE:HG21	2.00	0.44
31:e:114:LEU:HD23	31:e:114:LEU:HA	1.79	0.44
1:1:275:A:OP2	48:1:3131:HOH:O	2.21	0.44
1:1:2366:G:O2'	1:1:2369:C:OP2	2.27	0.44
1:1:2588:C:OP1	14:M:94:LYS:NZ	2.46	0.44
10:H:70:CYS:O	10:H:74:GLU:HG3	2.18	0.44
12:J:140:LYS:HA	12:J:140:LYS:HD3	1.80	0.44
22:U:100:PHE:CD2	22:U:112:LEU:HB3	2.52	0.44
26:Z:7:LYS:HB2	26:Z:7:LYS:HE2	1.80	0.44
43:W:24:ARG:HH21	43:W:28:VAL:HG11	1.82	0.44
1:1:147:C:H2'	1:1:148:G:C8	2.53	0.44
1:1:1349:C:H42	1:1:2486:C:N4	2.16	0.44
1:1:1619:A:N6	41:p:18:TYR:HA	2.32	0.44
1:1:1756:U:H5	1:1:1759:G:OP2	2.00	0.44
1:1:2575:C:H2'	1:1:2576:C:O4'	2.18	0.44
6:C:292:GLU:O	8:F:157:PRO:HG2	2.18	0.44
25:Y:77:LYS:HG2	25:Y:98:PRO:HB2	2.00	0.44
1:1:197:G:H4'	25:Y:132:ARG:HD2	1.99	0.44
1:1:2527:G:H2'	1:1:2528:C:H5''	2.00	0.44
3:4:135:C:H5''	3:4:136:G:OP1	2.18	0.44
23:V:44:LYS:HD2	23:V:61:MET:HG2	1.99	0.44
37:k:60:ILE:HD13	37:k:60:ILE:HA	1.69	0.44
1:1:1906:A:H2'	1:1:1907:C:C6	2.53	0.44
1:1:2479:U:H3	1:1:2496:A:N6	2.06	0.44
1:1:2504:C:H2'	1:1:2505:C:C6	2.53	0.44
31:e:24:ARG:O	31:e:27:SER:OG	2.33	0.44
39:m:81:THR:HG23	39:m:82:LEU:HD22	1.99	0.44
1:1:1831:C:H1'	1:1:2495:G:H1	1.81	0.44
1:1:2607:C:H5''	1:1:2608:C:OP1	2.17	0.44
13:L:75:ILE:HD11	13:L:80:LEU:HD23	2.00	0.44
14:M:103:LYS:HE2	14:M:103:LYS:HB3	1.84	0.44
17:P:15:LYS:O	17:P:100:ASN:ND2	2.45	0.44
18:Q:129:LYS:HZ3	18:Q:134:ASN:HB3	1.83	0.44
25:Y:22:ASN:O	25:Y:26:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:107:ILE:O	26:Z:111:VAL:HG23	2.18	0.44
37:k:26:SER:HB3	37:k:73:VAL:HG23	1.99	0.44
37:k:53:ASN:HA	37:k:56:ASP:OD2	2.18	0.44
1:1:803:G:H5'	1:1:804:G:OP2	2.17	0.43
25:Y:58:PHE:HD1	25:Y:59:THR:HB	1.83	0.43
1:1:632:G:H5'	1:1:633:A:OP1	2.17	0.43
1:1:1893:C:H2'	1:1:1894:C:C6	2.52	0.43
6:C:136:ASP:O	6:C:163:GLY:HA3	2.17	0.43
10:H:30:LYS:HE3	10:H:82:TYR:O	2.18	0.43
27:a:95:SER:HB3	27:a:98:GLU:H	1.82	0.43
37:k:25:LYS:HB3	37:k:37:LYS:HB2	1.99	0.43
1:1:90:C:H5	27:a:59:ARG:HH12	1.66	0.43
1:1:1320:G:O6	48:1:3127:HOH:O	2.21	0.43
1:1:1619:A:H61	41:p:18:TYR:HA	1.83	0.43
1:1:2234:C:H2'	1:1:2235:A:C8	2.53	0.43
2:3:58:C:O5'	2:3:58:C:H6	2.02	0.43
6:C:310:SER:HB2	8:F:40:VAL:HG13	2.00	0.43
21:T:112:ASN:HB3	21:T:129:LEU:HD13	2.00	0.43
27:a:85:GLU:CD	27:a:85:GLU:H	2.26	0.43
1:1:2562:G:C6	1:1:2563:C:N4	2.86	0.43
3:4:69:G:N7	48:4:306:HOH:O	2.37	0.43
21:T:81:ARG:NH2	28:b:16:ASP:OD1	2.50	0.43
1:1:1252:C:HO2'	1:1:1253:C:H6	1.62	0.43
1:1:2502:C:H3'	1:1:2503:G:N2	2.32	0.43
1:1:2536:A:H4'	1:1:2537:A:OP1	2.15	0.43
11:I:191:GLN:HB3	11:I:198:HIS:C	2.44	0.43
16:O:7:ASP:OD1	16:O:34:ARG:HD3	2.19	0.43
30:d:93:HIS:ND1	48:d:202:HOH:O	2.37	0.43
31:e:94:ASN:OD1	31:e:97:HIS:N	2.44	0.43
1:1:1543:C:O2'	1:1:1609:G:N7	2.47	0.43
5:B:78:ILE:HD13	5:B:305:ILE:HD11	2.01	0.43
11:I:187:ARG:NH2	11:I:189:GLU:OE2	2.51	0.43
1:1:152:C:H2'	1:1:153:G:O4'	2.19	0.43
1:1:2381:C:H2'	1:1:2382:G:C8	2.54	0.43
5:B:105:VAL:CG2	5:B:146:GLN:HB3	2.49	0.43
14:M:46:LYS:O	14:M:48:GLN:NE2	2.47	0.43
16:O:2:SER:OG	16:O:3:ARG:N	2.52	0.43
20:S:15:GLU:CD	20:S:15:GLU:H	2.27	0.43
29:c:104:LEU:O	29:c:107:ILE:HG13	2.18	0.43
1:1:876:C:O2	8:F:204:SER:OG	2.31	0.43
1:1:2554:C:H2'	1:1:2555:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:34:PHE:O	4:A:38:THR:HG23	2.18	0.43
8:F:69:GLN:HG2	21:T:143:SER:HA	2.01	0.43
20:S:32:GLU:O	20:S:36:LYS:NZ	2.51	0.43
22:U:25:VAL:O	22:U:69:SER:HB3	2.18	0.43
36:j:39:TYR:CG	36:j:40:PRO:HA	2.54	0.43
41:p:60:CYS:O	41:p:61:SER:HB2	2.19	0.43
5:B:11:LYS:HE3	48:B:507:HOH:O	2.19	0.43
7:D:56:ASN:O	7:D:57:LYS:HB2	2.19	0.43
12:J:21:ILE:HG12	12:J:125:MET:HG2	2.01	0.43
24:X:102:THR:OG1	24:X:103:LYS:N	2.52	0.43
25:Y:58:PHE:O	25:Y:59:THR:HG22	2.18	0.43
26:Z:10:LEU:HD21	26:Z:80:PRO:HB3	2.00	0.43
5:B:90:ILE:HD11	5:B:101:ALA:HB1	2.01	0.42
10:H:38:SER:O	10:H:38:SER:OG	2.36	0.42
17:P:21:VAL:HG11	17:P:89:VAL:HG11	2.01	0.42
1:1:677:C:OP2	48:1:3133:HOH:O	2.21	0.42
1:1:750:C:OP2	48:1:3129:HOH:O	2.21	0.42
1:1:1544:G:N3	1:1:1608:C:H2'	2.34	0.42
4:A:46:LYS:HA	4:A:46:LYS:HD3	1.77	0.42
4:A:122:ASP:O	4:A:123:ARG:HB2	2.19	0.42
1:1:174:C:H2'	1:1:175:C:O4'	2.19	0.42
1:1:242:A:H2'	1:1:243:G:C8	2.54	0.42
1:1:341:C:H2'	1:1:342:G:O4'	2.18	0.42
2:3:107:G:O2'	2:3:108:G:OP1	2.28	0.42
3:4:8:C:H1'	3:4:9:C:H5	1.85	0.42
3:4:74:C:OP2	25:Y:51:ARG:NE	2.38	0.42
5:B:358:THR:HG22	5:B:358:THR:O	2.19	0.42
27:a:88:ASP:O	27:a:92:GLN:HG3	2.19	0.42
1:1:788:U:O3'	7:D:42:LYS:HE3	2.18	0.42
1:1:1696:C:H2'	1:1:1697:G:C8	2.54	0.42
46:1:3017:K:K	15:N:81:TYR:HB3	2.12	0.42
6:C:197:VAL:HG22	6:C:238:LEU:HD22	2.01	0.42
13:L:170:HIS:CD2	13:L:174:VAL:HG12	2.54	0.42
22:U:32:ASP:OD1	22:U:32:ASP:N	2.49	0.42
1:1:97:C:H2'	1:1:98:G:C8	2.54	0.42
1:1:460:A:H4'	1:1:461:C:H5'	2.02	0.42
14:M:122:ALA:HB2	16:O:187:ARG:HH11	1.83	0.42
1:1:151:G:H2'	1:1:152:C:C6	2.54	0.42
1:1:315:G:OP2	36:j:52:LYS:NZ	2.34	0.42
1:1:1712:U:H2'	1:1:1713:C:C6	2.54	0.42
1:1:2235:A:H2'	1:1:2236:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:103:C:H2'	2:3:104:A:O4'	2.19	0.42
10:H:122:ILE:HD13	10:H:157:ILE:HG12	2.01	0.42
13:L:121:GLN:HG2	34:h:118:LEU:HD12	2.02	0.42
1:1:2300:G:H5''	5:B:5:LYS:NZ	2.35	0.42
3:4:59:G:OP1	3:4:98:C:H5	2.01	0.42
13:L:228:LYS:HB3	13:L:228:LYS:HE3	1.73	0.42
18:Q:20:LYS:HB2	18:Q:20:LYS:HE3	1.81	0.42
33:g:47:GLU:HG2	33:g:78:LEU:HD22	2.02	0.42
40:o:63:THR:O	40:o:85:ARG:NH2	2.52	0.42
1:1:462:G:O2'	1:1:464:C:OP2	2.37	0.42
1:1:1211:G:OP2	48:1:3132:HOH:O	2.21	0.42
1:1:2060:A:OP1	48:1:3128:HOH:O	2.21	0.42
4:A:66:MET:HE2	4:A:66:MET:HA	2.01	0.42
18:Q:76:ASP:OD1	18:Q:76:ASP:N	2.47	0.42
1:1:576:G:C5	4:A:181:LYS:HB3	2.55	0.42
1:1:1442:A:H2'	1:1:1443:G:O4'	2.19	0.42
1:1:1736:G:O2'	1:1:1737:G:OP2	2.35	0.42
1:1:1817:C:H2'	1:1:1818:C:H6	1.85	0.42
1:1:1997:C:O2'	9:G:217:ARG:NH1	2.53	0.42
15:N:63:ARG:HD2	48:N:1242:HOH:O	2.19	0.42
35:i:51:ILE:HG23	35:i:87:ALA:HB2	2.01	0.42
1:1:191:C:OP1	25:Y:33:ARG:NE	2.52	0.42
1:1:397:C:H2'	1:1:398:G:C8	2.55	0.42
1:1:880:G:H2'	1:1:881:G:O4'	2.20	0.42
1:1:1311:C:H2'	1:1:1312:C:H6	1.84	0.42
7:D:191:SER:OG	7:D:193:ASP:OD1	2.27	0.42
12:J:102:PHE:CE1	12:J:163:VAL:HG11	2.54	0.42
36:j:86:TYR:HD2	36:j:87:LEU:HD22	1.84	0.42
1:1:2194:C:H2'	1:1:2195:G:O4'	2.20	0.41
14:M:58:THR:HG22	14:M:59:ASP:N	2.35	0.41
22:U:107:LYS:O	22:U:108:GLU:HG2	2.19	0.41
1:1:1450:G:O2'	1:1:1451:G:H5'	2.20	0.41
1:1:1896:OMU:HM22	1:1:1897:OMU:H4'	2.02	0.41
3:4:139:C:H5''	9:G:66:ARG:HD3	2.02	0.41
14:M:94:LYS:HA	14:M:97:GLN:HG3	2.02	0.41
29:c:20:LEU:HD13	29:c:20:LEU:HA	1.80	0.41
29:c:26:LYS:HE2	29:c:26:LYS:HB3	1.88	0.41
1:1:2087:C:O2'	1:1:2088:U:H5'	2.19	0.41
6:C:175:ARG:HA	6:C:190:ILE:O	2.20	0.41
7:D:59:ILE:HG13	7:D:92:THR:HG22	2.01	0.41
9:G:194:LYS:HB2	9:G:194:LYS:HE3	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:28:ASP:O	12:J:32:LYS:HD2	2.21	0.41
19:R:155:LYS:HD2	19:R:155:LYS:N	2.35	0.41
21:T:39:TYR:CE1	21:T:102:ARG:HD2	2.56	0.41
30:d:47:ASP:CB	30:d:84:ILE:HG22	2.50	0.41
32:f:43:ASP:OD1	32:f:43:ASP:N	2.52	0.41
1:1:1824:OMC:O3'	1:1:1824:OMC:HM23	2.19	0.41
1:1:2090:A:H2'	1:1:2091:G:O4'	2.20	0.41
5:B:19:ARG:HB2	5:B:232:ARG:NH1	2.35	0.41
6:C:316:LYS:HB2	6:C:316:LYS:HE3	1.74	0.41
11:I:83:ASP:OD1	11:I:83:ASP:N	2.53	0.41
21:T:26:ASN:O	21:T:29:THR:OG1	2.31	0.41
23:V:111:LYS:HB3	23:V:111:LYS:HE3	1.80	0.41
1:1:1165:G:H3'	1:1:1166:G:C5'	2.51	0.41
1:1:1177:U:H4'	1:1:1178:U:O5'	2.21	0.41
1:1:1241:G:O2'	1:1:1242:G:OP2	2.29	0.41
1:1:1421:C:N3	48:1:3209:HOH:O	2.37	0.41
9:G:63:PRO:HG2	9:G:162:ARG:NE	2.34	0.41
20:S:36:LYS:HG2	20:S:56:ILE:HD13	2.02	0.41
22:U:36:ASN:ND2	22:U:39:GLU:HG2	2.35	0.41
24:X:62:TYR:HE1	24:X:64:ILE:HD11	1.85	0.41
32:f:98:ASN:OD1	32:f:98:ASN:N	2.52	0.41
1:1:1247:G:C6	1:1:1248:C:C4	3.08	0.41
1:1:1372:G:H2'	1:1:1373:C:C6	2.55	0.41
1:1:2551:C:OP2	48:1:3135:HOH:O	2.22	0.41
8:F:83:ARG:O	8:F:106:ILE:O	2.38	0.41
9:G:221:GLU:HG3	9:G:222:ALA:N	2.34	0.41
27:a:16:GLN:O	27:a:16:GLN:HG2	2.19	0.41
7:D:216:LEU:HA	7:D:216:LEU:HD12	1.84	0.41
8:F:74:ASP:OD1	21:T:138:ALA:HA	2.20	0.41
9:G:72:ILE:HG21	9:G:133:LEU:HD11	2.01	0.41
20:S:43:LEU:HD12	20:S:43:LEU:HA	1.75	0.41
26:Z:98:VAL:C	26:Z:100:ASP:N	2.79	0.41
38:l:50:LYS:C	38:l:51:LEU:HD22	2.45	0.41
1:1:428:C:H5	6:C:105:VAL:H	1.64	0.41
1:1:1193:U:O2'	1:1:1194:C:H2'	2.20	0.41
1:1:2224:A:C8	40:o:54:PRO:HB3	2.56	0.41
15:N:5:LYS:HA	15:N:5:LYS:HD2	1.88	0.41
17:P:46:TYR:O	17:P:50:VAL:HG23	2.21	0.41
18:Q:3:ILE:HG13	18:Q:5:LEU:HG	2.03	0.41
29:c:104:LEU:HD23	29:c:104:LEU:HA	1.91	0.41
1:1:1128:G:H2'	1:1:1129:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1532:A:O2'	1:1:2340:G:OP1	2.36	0.41
1:1:1684:OMC:HM23	1:1:1684:OMC:C6	2.56	0.41
1:1:1929:G:H2'	1:1:1930:G:O4'	2.21	0.41
5:B:90:ILE:HD13	5:B:104:THR:OG1	2.20	0.41
6:C:8:PHE:CZ	6:C:138:PRO:HB2	2.56	0.41
12:J:112:LEU:H	12:J:112:LEU:HD22	1.85	0.41
13:L:194:LYS:HE3	13:L:194:LYS:HB2	1.64	0.41
15:N:6:TYR:CE1	35:i:33:VAL:HG22	2.56	0.41
19:R:15:LEU:HD21	19:R:45:ILE:HD13	2.03	0.41
22:U:21:ILE:HD11	22:U:78:GLU:HA	2.02	0.41
24:X:138:LEU:O	24:X:139:ALA:HB3	2.21	0.41
27:a:71:PRO:HD2	27:a:110:PHE:CD2	2.56	0.41
27:a:77:LYS:HE2	27:a:77:LYS:HB3	1.98	0.41
37:k:19:GLY:HA3	37:k:40:LEU:HD11	2.02	0.41
40:o:27:LYS:HD3	40:o:27:LYS:HA	1.72	0.41
1:1:116:G:N3	9:G:119:ARG:HD2	2.36	0.41
1:1:429:G:H2'	1:1:430:A:O4'	2.21	0.41
1:1:1706:A:O5'	1:1:1706:A:H8	2.04	0.41
1:1:2605:C:H2'	1:1:2606:C:O4'	2.21	0.41
48:1:3156:HOH:O	7:D:4:LYS:HB2	2.21	0.41
12:J:132:SER:HB2	12:J:136:PHE:CD2	2.56	0.41
14:M:129:SER:HA	16:O:174:LYS:HZ2	1.85	0.41
25:Y:53:ASP:OD1	25:Y:110:TYR:N	2.46	0.41
29:c:26:LYS:HB2	29:c:97:LEU:HB2	2.02	0.41
40:o:33:LEU:HD23	40:o:33:LEU:HA	1.79	0.41
1:1:87:C:OP2	27:a:59:ARG:NH1	2.53	0.40
1:1:1181:G:H2'	1:1:1182:C:C6	2.55	0.40
1:1:2675:G:OP2	48:1:3121:HOH:O	2.20	0.40
11:I:99:ILE:HG22	11:I:123:GLN:HB2	2.03	0.40
16:O:137:ARG:NH1	48:O:201:HOH:O	2.32	0.40
20:S:15:GLU:HG2	20:S:16:LYS:N	2.37	0.40
1:1:2119:A:H2'	1:1:2120:A:C8	2.56	0.40
12:J:122:ILE:H	12:J:122:ILE:HG12	1.64	0.40
11:I:177:THR:OG1	11:I:180:GLU:HB2	2.22	0.40
26:Z:8:PRO:O	26:Z:84:ARG:NH2	2.53	0.40
1:1:2065:A:H2'	1:1:2066:C:C6	2.57	0.40
1:1:2387:G:H2'	1:1:2388:A:C8	2.57	0.40
9:G:90:ARG:HD3	9:G:90:ARG:N	2.36	0.40
12:J:35:LYS:HA	12:J:38:GLN:HB3	2.03	0.40
19:R:21:ARG:NH1	19:R:53:LEU:O	2.51	0.40
24:X:62:TYR:CE1	24:X:82:ILE:HG13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:104:LEU:HB2	34:h:109:MET:HE2	2.04	0.40
1:1:795:G:H2'	1:1:796:G:C8	2.57	0.40
1:1:1243:G:H1	1:1:1248:C:N4	2.11	0.40
1:1:2665:U:H2'	1:1:2666:U:O4'	2.22	0.40
9:G:137:ASP:OD1	9:G:137:ASP:N	2.55	0.40
11:I:78:LYS:HB2	11:I:78:LYS:HE2	1.59	0.40
17:P:48:ASP:OD1	17:P:91:LYS:HE3	2.21	0.40
22:U:21:ILE:O	22:U:74:THR:HG23	2.22	0.40
32:f:5:LYS:HB3	32:f:5:LYS:HE3	1.95	0.40
39:m:111:ARG:HD2	48:m:202:HOH:O	2.21	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	
4	A	247/251 (98%)	236 (96%)	11 (4%)	0	100	100
5	B	376/379 (99%)	366 (97%)	10 (3%)	0	100	100
6	C	312/316 (99%)	290 (93%)	22 (7%)	0	100	100
7	D	264/297 (89%)	245 (93%)	19 (7%)	0	100	100
8	F	212/235 (90%)	208 (98%)	4 (2%)	0	100	100
9	G	178/225 (79%)	169 (95%)	9 (5%)	0	100	100
10	H	182/185 (98%)	173 (95%)	9 (5%)	0	100	100
11	I	196/210 (93%)	186 (95%)	10 (5%)	0	100	100
12	J	158/173 (91%)	145 (92%)	13 (8%)	0	100	100
13	L	185/234 (79%)	179 (97%)	6 (3%)	0	100	100
14	M	126/131 (96%)	121 (96%)	5 (4%)	0	100	100
15	N	202/204 (99%)	192 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	O	193/197 (98%)	188 (97%)	5 (3%)	0	100	100
17	P	152/164 (93%)	143 (94%)	9 (6%)	0	100	100
18	Q	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
19	R	175/196 (89%)	170 (97%)	5 (3%)	0	100	100
20	S	171/173 (99%)	166 (97%)	5 (3%)	0	100	100
21	T	149/159 (94%)	145 (97%)	4 (3%)	0	100	100
22	U	96/171 (56%)	90 (94%)	6 (6%)	0	100	100
23	V	137/142 (96%)	131 (96%)	6 (4%)	0	100	100
24	X	114/141 (81%)	107 (94%)	7 (6%)	0	100	100
25	Y	131/135 (97%)	126 (96%)	5 (4%)	0	100	100
26	Z	125/135 (93%)	113 (90%)	12 (10%)	0	100	100
27	a	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
28	b	54/62 (87%)	54 (100%)	0	0	100	100
29	c	99/109 (91%)	95 (96%)	4 (4%)	0	100	100
30	d	90/106 (85%)	85 (94%)	5 (6%)	0	100	100
31	e	124/136 (91%)	117 (94%)	6 (5%)	1 (1%)	16	30
32	f	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
33	g	97/120 (81%)	95 (98%)	2 (2%)	0	100	100
34	h	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
35	i	81/90 (90%)	78 (96%)	3 (4%)	0	100	100
36	j	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
37	k	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
38	l	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
39	m	49/127 (39%)	47 (96%)	2 (4%)	0	100	100
40	o	92/106 (87%)	90 (98%)	2 (2%)	0	100	100
41	p	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
43	W	63/102 (62%)	61 (97%)	2 (3%)	0	100	100
All	All	5669/6297 (90%)	5420 (96%)	248 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	e	95	LYS

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	
4	A	188/192 (98%)	184 (98%)	4 (2%)	47	67
5	B	312/313 (100%)	301 (96%)	11 (4%)	32	56
6	C	261/263 (99%)	246 (94%)	15 (6%)	18	35
7	D	211/242 (87%)	201 (95%)	10 (5%)	23	45
8	F	184/204 (90%)	177 (96%)	7 (4%)	29	52
9	G	160/198 (81%)	144 (90%)	16 (10%)	7	14
10	H	160/164 (98%)	151 (94%)	9 (6%)	19	36
11	I	166/177 (94%)	158 (95%)	8 (5%)	23	44
12	J	137/149 (92%)	121 (88%)	16 (12%)	5	9
13	L	159/197 (81%)	153 (96%)	6 (4%)	29	52
14	M	103/111 (93%)	95 (92%)	8 (8%)	11	21
15	N	174/175 (99%)	167 (96%)	7 (4%)	28	50
16	O	164/165 (99%)	159 (97%)	5 (3%)	36	60
17	P	130/139 (94%)	121 (93%)	9 (7%)	14	26
18	Q	154/155 (99%)	151 (98%)	3 (2%)	50	70
19	R	149/167 (89%)	136 (91%)	13 (9%)	9	18
20	S	147/154 (96%)	136 (92%)	11 (8%)	12	24
21	T	126/133 (95%)	121 (96%)	5 (4%)	28	50
22	U	85/153 (56%)	75 (88%)	10 (12%)	5	9
23	V	111/114 (97%)	104 (94%)	7 (6%)	16	30
24	X	104/123 (85%)	98 (94%)	6 (6%)	18	34
25	Y	114/115 (99%)	107 (94%)	7 (6%)	17	31
26	Z	101/119 (85%)	87 (86%)	14 (14%)	3	6
27	a	126/127 (99%)	115 (91%)	11 (9%)	9	18
28	b	51/57 (90%)	48 (94%)	3 (6%)	18	33
29	c	84/92 (91%)	72 (86%)	12 (14%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d	77/92 (84%)	72 (94%)	5 (6%)	15	29
31	e	112/120 (93%)	104 (93%)	8 (7%)	13	25
32	f	102/103 (99%)	96 (94%)	6 (6%)	18	33
33	g	87/100 (87%)	84 (97%)	3 (3%)	32	57
34	h	98/107 (92%)	92 (94%)	6 (6%)	17	31
35	i	72/78 (92%)	68 (94%)	4 (6%)	19	36
36	j	70/74 (95%)	68 (97%)	2 (3%)	37	61
37	k	55/68 (81%)	47 (86%)	8 (14%)	3	5
38	l	46/48 (96%)	44 (96%)	2 (4%)	26	47
39	m	46/110 (42%)	44 (96%)	2 (4%)	26	47
40	o	81/93 (87%)	76 (94%)	5 (6%)	16	31
41	p	71/73 (97%)	63 (89%)	8 (11%)	5	11
43	W	58/92 (63%)	56 (97%)	2 (3%)	32	57
All	All	4836/5356 (90%)	4542 (94%)	294 (6%)	19	31

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	38	THR
4	A	98	ILE
4	A	146	THR
4	A	150	LEU
5	B	2	SER
5	B	41	ILE
5	B	155	ASP
5	B	180	ILE
5	B	199	MET
5	B	204	SER
5	B	248	LYS
5	B	286	ASP
5	B	300	LEU
5	B	334	ARG
5	B	348	CYS
6	C	14	GLN
6	C	15	VAL
6	C	82	TYR
6	C	93	HIS

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Mol	Chain	Res	Type
6	C	130	ARG
6	C	140	ILE
6	C	144	VAL
6	C	147	ASP
6	C	177	ILE
6	C	202	GLU
6	C	216	LEU
6	C	217	CYS
6	C	265	THR
6	C	287	ASP
6	C	289	LEU
7	D	41	ASN
7	D	55	THR
7	D	67	GLU
7	D	70	LYS
7	D	84	ARG
7	D	124	LEU
7	D	132	THR
7	D	204	ILE
7	D	236	VAL
7	D	263	PHE
8	F	28	LYS
8	F	56	SER
8	F	57	GLU
8	F	106	ILE
8	F	112	MET
8	F	129	VAL
8	F	204	SER
9	G	56	THR
9	G	71	GLU
9	G	82	GLU
9	G	86	GLU
9	G	90	ARG
9	G	118	ARG
9	G	127	LYS
9	G	153	LYS
9	G	162	ARG
9	G	166	ASP
9	G	170	LEU
9	G	182	THR
9	G	183	ASP
9	G	187	GLU

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Mol	Chain	Res	Type
9	G	189	LYS
9	G	191	THR
10	H	15	VAL
10	H	17	CYS
10	H	80	VAL
10	H	97	ILE
10	H	100	THR
10	H	118	LYS
10	H	122	ILE
10	H	136	VAL
10	H	159	GLU
11	I	78	LYS
11	I	87	LEU
11	I	125	THR
11	I	136	LEU
11	I	150	ASP
11	I	190	LEU
11	I	202	ARG
11	I	206	LEU
12	J	15	GLU
12	J	19	LEU
12	J	46	THR
12	J	52	LEU
12	J	54	ILE
12	J	65	ILE
12	J	81	GLU
12	J	107	THR
12	J	112	LEU
12	J	122	ILE
12	J	131	LEU
12	J	157	ASP
12	J	165	ARG
12	J	166	GLU
12	J	169	VAL
12	J	172	THR
13	L	118	LYS
13	L	173	VAL
13	L	174	VAL
13	L	177	VAL
13	L	178	VAL
13	L	195	GLU
14	M	26	VAL

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Mol	Chain	Res	Type
14	M	60	GLN
14	M	71	GLU
14	M	74	LYS
14	M	83	ILE
14	M	90	VAL
14	M	95	ILE
14	M	97	GLN
15	N	12	ARG
15	N	13	LYS
15	N	27	THR
15	N	80	SER
15	N	153	ASN
15	N	184	LEU
15	N	185	ARG
16	O	36	GLU
16	O	41	SER
16	O	101	VAL
16	O	119	SER
16	O	186	GLN
17	P	51	LEU
17	P	56	ILE
17	P	61	LYS
17	P	94	LEU
17	P	103	HIS
17	P	105	HIS
17	P	111	GLU
17	P	128	ARG
17	P	147	GLU
18	Q	20	LYS
18	Q	66	ARG
18	Q	73	LYS
19	R	8	LYS
19	R	30	LYS
19	R	56	LYS
19	R	72	LEU
19	R	91	SER
19	R	107	SER
19	R	119	LEU
19	R	139	LEU
19	R	141	HIS
19	R	143	VAL
19	R	154	LYS

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Mol	Chain	Res	Type
19	R	158	GLU
19	R	161	GLN
20	S	1	MET
20	S	16	LYS
20	S	27	ILE
20	S	51	ARG
20	S	52	THR
20	S	56	ILE
20	S	63	GLU
20	S	70	LYS
20	S	114	ARG
20	S	166	ASP
20	S	171	VAL
21	T	29	THR
21	T	33	VAL
21	T	91	VAL
21	T	96	VAL
21	T	151	THR
22	U	20	ASN
22	U	21	ILE
22	U	25	VAL
22	U	26	ASP
22	U	32	ASP
22	U	33	LEU
22	U	37	LEU
22	U	74	THR
22	U	94	GLN
22	U	95	ASP
23	V	14	LYS
23	V	44	LYS
23	V	73	GLU
23	V	77	LYS
23	V	108	ILE
23	V	125	LYS
23	V	136	THR
24	X	58	ASP
24	X	81	PHE
24	X	93	ARG
24	X	102	THR
24	X	109	THR
24	X	116	LEU
25	Y	10	SER

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Mol	Chain	Res	Type
25	Y	56	GLU
25	Y	70	GLU
25	Y	72	ARG
25	Y	83	ILE
25	Y	95	VAL
25	Y	115	ARG
26	Z	5	ILE
26	Z	13	ILE
26	Z	18	ARG
26	Z	25	VAL
26	Z	30	LEU
26	Z	34	GLU
26	Z	41	VAL
26	Z	66	VAL
26	Z	78	LEU
26	Z	91	ASP
26	Z	95	THR
26	Z	108	ILE
26	Z	110	THR
26	Z	121	GLU
27	a	9	ARG
27	a	15	ARG
27	a	17	MET
27	a	34	LYS
27	a	72	THR
27	a	75	ILE
27	a	94	LYS
27	a	98	GLU
27	a	115	ARG
27	a	140	GLU
27	a	141	VAL
28	b	10	LYS
28	b	45	ARG
28	b	55	LEU
29	c	13	SER
29	c	14	ILE
29	c	17	THR
29	c	20	LEU
29	c	26	LYS
29	c	45	LEU
29	c	47	PHE
29	c	71	VAL

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Mol	Chain	Res	Type
29	c	80	GLU
29	c	81	LEU
29	c	93	ILE
29	c	107	ILE
30	d	8	THR
30	d	52	VAL
30	d	70	VAL
30	d	72	LEU
30	d	95	THR
31	e	27	SER
31	e	48	ARG
31	e	64	SER
31	e	79	HIS
31	e	89	THR
31	e	94	ASN
31	e	112	GLN
31	e	126	ASN
32	f	2	GLU
32	f	25	ARG
32	f	48	ARG
32	f	61	ILE
32	f	64	LYS
32	f	112	LEU
33	g	64	THR
33	g	81	SER
33	g	99	LEU
34	h	4	LEU
34	h	9	LEU
34	h	12	LEU
34	h	15	GLU
34	h	19	ARG
34	h	83	THR
35	i	35	SER
35	i	43	MET
35	i	67	LYS
35	i	69	ARG
36	j	55	ARG
36	j	76	SER
37	k	3	ASN
37	k	14	ILE
37	k	50	THR
37	k	58	LYS

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Mol	Chain	Res	Type
37	k	60	ILE
37	k	61	VAL
37	k	65	LYS
37	k	70	VAL
38	l	34	LYS
38	l	46	ARG
39	m	77	VAL
39	m	92	ASN
40	o	30	LYS
40	o	66	GLN
40	o	67	VAL
40	o	79	THR
40	o	92	SER
41	p	5	THR
41	p	29	ILE
41	p	39	CYS
41	p	45	ASP
41	p	57	CYS
41	p	58	ARG
41	p	88	LEU
41	p	90	ARG
43	W	4	THR
43	W	13	LYS

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

Mol	Chain	Res	Type
4	A	50	HIS
6	C	132	HIS
8	F	105	GLN
9	G	172	HIS
12	J	145	GLN
13	L	98	GLN
15	N	176	ASN
16	O	189	ASN
17	P	69	HIS
17	P	96	GLN
17	P	133	HIS
18	Q	177	HIS
20	S	3	GLN
20	S	71	ASN
20	S	122	ASN

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Mol	Chain	Res	Type
25	Y	62	HIS
25	Y	84	ASN
26	Z	112	ASN
27	a	14	HIS
27	a	39	GLN
29	c	37	ASN
32	f	90	HIS
33	g	41	ASN
33	g	86	HIS
34	h	90	HIS
35	i	72	ASN
36	j	48	ASN
37	k	9	ASN
39	m	92	ASN
43	W	25	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2423/2707 (89%)	395 (16%)	20 (0%)
2	3	116/120 (96%)	17 (14%)	2 (1%)
3	4	136/139 (97%)	28 (20%)	1 (0%)
42	w	12/76 (15%)	5 (41%)	0
44	E	2/3 (66%)	1 (50%)	0
All	All	2689/3045 (88%)	446 (16%)	23 (0%)

All (446) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	21	G
1	1	39	A
1	1	42	A
1	1	48	G
1	1	56	C
1	1	59	A
1	1	64	A
1	1	65	A
1	1	73	G
1	1	84	U
1	1	89	G
1	1	90	C

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Mol	Chain	Res	Type
1	1	106	A
1	1	107	G
1	1	116	G
1	1	127	G
1	1	128	U
1	1	156	G
1	1	165	G
1	1	166	G
1	1	176	G
1	1	180	G
1	1	184	G
1	1	185	C
1	1	186	A
1	1	187	A
1	1	188	G
1	1	192	C
1	1	199	C
1	1	219	C
1	1	220	G
1	1	222	G
1	1	239	U
1	1	248	A
1	1	250	G
1	1	280	G
1	1	288	A
1	1	301	C
1	1	313	OMG
1	1	326	A
1	1	327	G
1	1	333	C
1	1	343	C
1	1	348	A
1	1	349	A
1	1	350	G
1	1	351	A
1	1	374	C
1	1	375	C
1	1	376	C
1	1	377	G
1	1	378	C
1	1	383	C
1	1	396	A2M

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Mol	Chain	Res	Type
1	1	400	A
1	1	407	A
1	1	424	A
1	1	428	C
1	1	429	G
1	1	431	G
1	1	442	C
1	1	448	A
1	1	458	A
1	1	460	A
1	1	461	C
1	1	462	G
1	1	467	G
1	1	477	C
1	1	485	C
1	1	486	G
1	1	490	G
1	1	491	U
1	1	492	G
1	1	493	C
1	1	501	G
1	1	522	A
1	1	533	U
1	1	565	G
1	1	577	C
1	1	579	C
1	1	585	G
1	1	590	U
1	1	595	C
1	1	611	G
1	1	612	A
1	1	623	G
1	1	630	A
1	1	632	G
1	1	633	A
1	1	637	A
1	1	639	C
1	1	640	G
1	1	641	A
1	1	653	G
1	1	660	G
1	1	675	C

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Mol	Chain	Res	Type
1	1	676	C
1	1	690	G
1	1	708	G
1	1	718	G
1	1	722	G
1	1	759	A
1	1	761	C
1	1	769	G
1	1	776	C
1	1	793	U
1	1	800	G
1	1	801	G
1	1	803	G
1	1	804	G
1	1	807	G
1	1	808	A
1	1	813	G
1	1	826	G
1	1	840	G
1	1	849	G
1	1	853	G
1	1	866	G
1	1	868	A
1	1	907	C
1	1	908	G
1	1	911	G
1	1	912	G
1	1	915	G
1	1	990	G
1	1	992	C
1	1	1004	U
1	1	1006	G
1	1	1008	G
1	1	1012	G
1	1	1014	C
1	1	1015	G
1	1	1016	G
1	1	1017	A
1	1	1024	G
1	1	1029	G
1	1	1030	C
1	1	1031	G

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Mol	Chain	Res	Type
1	1	1042	G
1	1	1044	G
1	1	1045	C
1	1	1046	G
1	1	1047	C
1	1	1050	C
1	1	1061	C
1	1	1066	G
1	1	1072	C
1	1	1074	G
1	1	1077	G
1	1	1106	C
1	1	1108	G
1	1	1118	G
1	1	1121	OMG
1	1	1124	C
1	1	1137	G
1	1	1149	C
1	1	1150	G
1	1	1151	C
1	1	1152	C
1	1	1158	G
1	1	1164	A
1	1	1166	G
1	1	1167	G
1	1	1186	G
1	1	1203	G
1	1	1205	U
1	1	1230	A
1	1	1232	A
1	1	1236	G
1	1	1238	A
1	1	1239	A
1	1	1241	G
1	1	1242	G
1	1	1244	C
1	1	1246	U
1	1	1247	G
1	1	1248	C
1	1	1252	C
1	1	1253	C
1	1	1259	A

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Mol	Chain	Res	Type
1	1	1261	C
1	1	1299	C
1	1	1314	C
1	1	1322	C
1	1	1327	A
1	1	1331	G
1	1	1349	C
1	1	1358	G
1	1	1374	C
1	1	1380	A
1	1	1381	C
1	1	1382	G
1	1	1383	C
1	1	1388	C
1	1	1405	G
1	1	1411	G
1	1	1422	G
1	1	1439	A
1	1	1451	G
1	1	1452	C
1	1	1472	G
1	1	1473	A
1	1	1508	G
1	1	1509	C
1	1	1510	G
1	1	1515	C
1	1	1520	OMG
1	1	1537	G
1	1	1538	C
1	1	1565	G
1	1	1566	G
1	1	1570	G
1	1	1574	C
1	1	1588	G
1	1	1589	G
1	1	1599	G
1	1	1600	A
1	1	1609	G
1	1	1610	G
1	1	1619	A
1	1	1628	U
1	1	1646	A

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Mol	Chain	Res	Type
1	1	1694	A
1	1	1696	C
1	1	1712	U
1	1	1731	A
1	1	1733	G
1	1	1736	G
1	1	1737	G
1	1	1739	A
1	1	1740	G
1	1	1742	A
1	1	1751	U
1	1	1756	U
1	1	1759	G
1	1	1760	G
1	1	1766	A
1	1	1767	A
1	1	1768	A2M
1	1	1769	U
1	1	1775	OMG
1	1	1797	U
1	1	1800	A
1	1	1801	U
1	1	1802	G
1	1	1821	U
1	1	1823	U
1	1	1844	G
1	1	1859	A
1	1	1860	A
1	1	1861	C
1	1	1862	G
1	1	1872	C
1	1	1880	G
1	1	1884	C
1	1	1888	A
1	1	1889	A
1	1	1890	G
1	1	1891	A
1	1	1898	U
1	1	1906	A
1	1	1922	G
1	1	1992	C
1	1	1999	C

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Mol	Chain	Res	Type
1	1	2007	C
1	1	2011	C
1	1	2012	G
1	1	2016	A
1	1	2017	C
1	1	2019	C
1	1	2029	G
1	1	2030	G
1	1	2037	G
1	1	2049	G
1	1	2050	C
1	1	2060	A
1	1	2075	U
1	1	2078	C
1	1	2079	A
1	1	2091	G
1	1	2097	A
1	1	2098	C
1	1	2112	G
1	1	2113	G
1	1	2114	A
1	1	2117	A
1	1	2125	A
1	1	2127	A
1	1	2137	G
1	1	2139	C
1	1	2151	G
1	1	2152	U
1	1	2175	G
1	1	2176	G
1	1	2185	A
1	1	2196	C
1	1	2199	C
1	1	2200	G
1	1	2202	C
1	1	2213	G
1	1	2218	G
1	1	2222	G
1	1	2223	A
1	1	2224	A
1	1	2232	C
1	1	2233	A

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Mol	Chain	Res	Type
1	1	2236	G
1	1	2239	A
1	1	2241	A
1	1	2243	C
1	1	2251	U
1	1	2264	C
1	1	2267	G
1	1	2269	A
1	1	2273	A
1	1	2282	U
1	1	2292	5MC
1	1	2293	G
1	1	2294	A
1	1	2297	U
1	1	2298	C
1	1	2299	G
1	1	2309	A
1	1	2310	C
1	1	2321	C
1	1	2333	A
1	1	2345	U
1	1	2355	C
1	1	2356	A
1	1	2357	A
1	1	2359	G
1	1	2363	C
1	1	2368	G
1	1	2372	G
1	1	2404	C
1	1	2406	C
1	1	2411	G
1	1	2423	A
1	1	2429	C
1	1	2433	G
1	1	2434	G
1	1	2495	G
1	1	2506	C
1	1	2508	G
1	1	2509	G
1	1	2514	G
1	1	2515	G
1	1	2519	C

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Mol	Chain	Res	Type
1	1	2528	C
1	1	2531	C
1	1	2537	A
1	1	2538	A
1	1	2545	C
1	1	2546	C
1	1	2556	G
1	1	2562	G
1	1	2568	C
1	1	2573	G
1	1	2574	C
1	1	2575	C
1	1	2580	C
1	1	2581	C
1	1	2582	C
1	1	2583	C
1	1	2584	G
1	1	2585	U
1	1	2586	G
1	1	2587	C
1	1	2591	C
1	1	2593	G
1	1	2594	C
1	1	2595	C
1	1	2596	C
1	1	2597	G
1	1	2598	A
1	1	2599	G
1	1	2600	G
1	1	2608	C
1	1	2609	G
1	1	2614	G
1	1	2627	G
1	1	2628	C
1	1	2629	G
1	1	2634	G
1	1	2652	G
1	1	2672	G
1	1	2678	C
1	1	2679	G
1	1	2688	G
1	1	2689	G

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Mol	Chain	Res	Type
1	1	2690	G
1	1	2691	C
1	1	2692	G
1	1	2693	C
1	1	2694	G
2	3	19	G
2	3	21	G
2	3	23	A
2	3	33	A
2	3	37	G
2	3	38	U
2	3	39	U
2	3	50	A
2	3	52	G
2	3	54	G
2	3	65	A
2	3	77	U
2	3	101	A
2	3	107	G
2	3	108	G
2	3	111	G
2	3	115	A
3	4	9	C
3	4	12	C
3	4	13	G
3	4	24	C
3	4	35	G
3	4	36	C
3	4	40	G
3	4	49	G
3	4	52	G
3	4	60	A
3	4	63	C
3	4	64	G
3	4	69	G
3	4	73	A
3	4	74	C
3	4	76	C
3	4	79	C
3	4	86	G
3	4	87	A
3	4	88	G

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Mol	Chain	Res	Type
3	4	100	C
3	4	105	A
3	4	106	C
3	4	112	G
3	4	114	G
3	4	115	C
3	4	120	G
3	4	122	G
42	w	2	G
42	w	4	G
42	w	70	G
42	w	74	C
42	w	76	A
44	E	76	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	218	G
1	1	325	A
1	1	492	G
1	1	516	G
1	1	589	C
1	1	632	G
1	1	675	C
1	1	807	G
1	1	1017	A
1	1	1204	OMG
1	1	1382	G
1	1	1477	C
1	1	1587	G
1	1	1860	A
1	1	1871	C
1	1	1921	U
1	1	2151	G
1	1	2354	U
1	1	2530	G
1	1	2536	A
2	3	38	U
2	3	107	G
3	4	114	G

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	A2M	1	393	1	22,25,26	1.35	3 (13%)	30,36,39	1.20	4 (13%)
1	OMG	1	1775	1	23,26,27	0.92	0	32,38,41	1.18	4 (12%)
1	OMG	1	2074	1	23,26,27	0.94	3 (13%)	32,38,41	1.00	2 (6%)
1	OMC	1	2380	1	19,22,23	0.88	1 (5%)	25,31,34	1.19	4 (16%)
1	A2M	1	396	46,1	22,25,26	1.42	1 (4%)	30,36,39	0.90	1 (3%)
1	OMG	1	1882	1	23,26,27	1.23	3 (13%)	32,38,41	2.22	7 (21%)
1	OMU	1	1896	46,1	19,22,23	0.82	1 (5%)	25,31,34	1.04	2 (8%)
1	OMG	1	624	1	23,26,27	0.84	0	32,38,41	1.31	7 (21%)
1	OMG	1	1204	1	23,26,27	0.93	1 (4%)	32,38,41	1.48	6 (18%)
1	OMG	1	1520	1	23,26,27	0.87	0	32,38,41	1.19	5 (15%)
1	5MC	1	1765	1	19,22,23	1.54	5 (26%)	26,32,35	1.12	3 (11%)
1	OMC	1	1684	46,1	19,22,23	0.94	1 (5%)	25,31,34	1.25	4 (16%)
1	OMU	1	1897	46,1	19,22,23	0.82	0	25,31,34	0.97	1 (4%)
3	OMG	4	133	3,1	23,26,27	0.95	2 (8%)	32,38,41	0.99	1 (3%)
1	OMG	1	2042	44,1	23,26,27	0.93	1 (4%)	32,38,41	1.13	4 (12%)
1	OMU	1	49	46,1	19,22,23	0.91	1 (5%)	25,31,34	0.95	1 (4%)
1	OMC	1	1824	1	19,22,23	0.79	1 (5%)	25,31,34	1.26	4 (16%)
1	OMG	1	1121	45,1	23,26,27	0.89	1 (4%)	32,38,41	1.17	3 (9%)
1	OMU	1	1908	1	19,22,23	1.86	5 (26%)	25,31,34	1.38	4 (16%)
1	5MC	1	2292	46,1	19,22,23	1.79	7 (36%)	26,32,35	1.47	3 (11%)
1	A2M	1	523	1	22,25,26	1.38	3 (13%)	30,36,39	1.04	2 (6%)
1	A2M	1	1768	1	22,25,26	1.22	1 (4%)	30,36,39	1.63	4 (13%)
1	OMG	1	2237	46,1	23,26,27	0.81	0	32,38,41	1.13	3 (9%)
1	OMG	1	386	1	23,26,27	0.98	1 (4%)	32,38,41	1.20	3 (9%)
1	OMG	1	313	1	23,26,27	0.91	1 (4%)	32,38,41	1.16	3 (9%)

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
1	A2M	1	393	1	-	2/9/27/28	0/3/3/3
1	OMG	1	1775	1	-	2/9/27/28	0/3/3/3
1	OMG	1	2074	1	-	1/9/27/28	0/3/3/3
1	OMC	1	2380	1	-	0/9/27/28	0/2/2/2
1	A2M	1	396	46,1	-	0/9/27/28	0/3/3/3
1	OMG	1	1882	1	-	3/9/27/28	0/3/3/3
1	OMU	1	1896	46,1	-	0/9/27/28	0/2/2/2
1	OMG	1	624	1	-	1/9/27/28	0/3/3/3
1	OMG	1	1204	1	-	0/9/27/28	0/3/3/3
1	OMG	1	1520	1	-	2/9/27/28	0/3/3/3
1	5MC	1	1765	1	-	0/7/25/26	0/2/2/2
1	OMC	1	1684	46,1	-	5/9/27/28	0/2/2/2
1	OMU	1	1897	46,1	-	0/9/27/28	0/2/2/2
3	OMG	4	133	3,1	-	1/9/27/28	0/3/3/3
1	OMG	1	2042	44,1	-	0/9/27/28	0/3/3/3
1	OMU	1	49	46,1	-	1/9/27/28	0/2/2/2
1	OMC	1	1824	1	-	1/9/27/28	0/2/2/2
1	OMG	1	1121	45,1	-	2/9/27/28	0/3/3/3
1	OMU	1	1908	1	-	2/9/27/28	0/2/2/2
1	5MC	1	2292	46,1	-	5/7/25/26	0/2/2/2
1	A2M	1	523	1	-	1/9/27/28	0/3/3/3
1	A2M	1	1768	1	-	3/9/27/28	0/3/3/3
1	OMG	1	2237	46,1	-	0/9/27/28	0/3/3/3
1	OMG	1	386	1	-	0/9/27/28	0/3/3/3
1	OMG	1	313	1	-	2/9/27/28	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1908	OMU	O5'-C5'	-5.36	1.28	1.44
1	1	393	A2M	O5'-C5'	-4.19	1.32	1.44
1	1	396	A2M	O5'-C5'	-4.07	1.32	1.44
1	1	2292	5MC	C2-N1	4.04	1.48	1.40
1	1	1768	A2M	O5'-C5'	-3.89	1.32	1.44
1	1	523	A2M	O5'-C5'	-3.81	1.33	1.44
1	1	1765	5MC	C2-N1	3.32	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2292	5MC	O2-C2	-3.07	1.18	1.23
1	1	2292	5MC	C4-N3	-2.93	1.29	1.34
1	1	1908	OMU	O2'-C2'	-2.88	1.35	1.42
1	1	1765	5MC	O2-C2	-2.87	1.18	1.23
1	1	1882	OMG	C6-N1	-2.85	1.33	1.38
1	1	1882	OMG	C5-C4	2.85	1.46	1.38
1	1	1765	5MC	C6-N1	-2.78	1.33	1.38
1	1	523	A2M	O2'-C2'	-2.63	1.36	1.42
1	1	523	A2M	O4'-C4'	-2.59	1.39	1.45
1	1	1908	OMU	O4-C4	-2.44	1.19	1.24
1	1	2292	5MC	C6-N1	-2.42	1.33	1.38
1	1	1204	OMG	C6-N1	2.38	1.43	1.38
1	1	2380	OMC	C2-N1	2.37	1.45	1.40
1	1	1882	OMG	C5-N7	-2.28	1.34	1.39
1	1	1765	5MC	C2-N3	2.27	1.40	1.36
1	1	1908	OMU	O3'-C3'	-2.22	1.37	1.43
1	1	2074	OMG	C4-N3	2.19	1.39	1.34
1	1	1765	5MC	C4-N3	-2.18	1.30	1.34
3	4	133	OMG	C4-N3	2.17	1.39	1.34
1	1	2292	5MC	CM5-C5	-2.16	1.45	1.50
1	1	386	OMG	O6-C6	-2.16	1.19	1.23
3	4	133	OMG	C6-N1	2.15	1.42	1.38
1	1	1684	OMC	C2-N1	2.14	1.44	1.40
1	1	1824	OMC	C2-N1	2.12	1.44	1.40
1	1	393	A2M	C5'-C4'	2.08	1.57	1.51
1	1	393	A2M	O3'-C3'	-2.06	1.37	1.43
1	1	49	OMU	C2-N1	2.06	1.41	1.38
1	1	2292	5MC	C2-N3	2.05	1.40	1.36
1	1	1896	OMU	C2-N1	2.05	1.41	1.38
1	1	1908	OMU	C3'-C4'	-2.04	1.47	1.53
1	1	2292	5MC	C6-C5	2.04	1.37	1.34
1	1	313	OMG	C4-N3	2.03	1.38	1.34
1	1	2074	OMG	C6-N1	2.02	1.42	1.38
1	1	2042	OMG	C4-N3	2.02	1.38	1.34
1	1	1121	OMG	C6-N1	2.01	1.42	1.38
1	1	2074	OMG	C8-N9	2.00	1.42	1.37

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1882	OMG	C5-C4-N3	-6.39	118.22	128.39
1	1	1882	OMG	C2-N3-C4	5.25	121.33	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1768	A2M	C2'-C1'-N9	-4.80	105.86	113.75
1	1	1882	OMG	N9-C4-N3	4.67	135.30	125.95
1	1	1882	OMG	C2'-C1'-N9	-4.45	105.80	114.24
1	1	2292	5MC	C1'-N1-C6	4.37	128.34	121.15
1	1	1882	OMG	C6-C5-N7	3.49	136.63	130.29
1	1	1768	A2M	C4'-O4'-C1'	-3.33	102.11	109.47
1	1	2380	OMC	C5-C4-N3	3.25	126.80	121.32
1	1	1765	5MC	C5-C4-N3	3.24	125.07	121.75
1	1	1824	OMC	CM2-O2'-C2'	3.20	122.70	114.47
1	1	1768	A2M	O4'-C1'-N9	3.11	114.07	108.09
1	1	624	OMG	O2'-C2'-C1'	3.10	114.87	108.99
1	1	2292	5MC	C1'-N1-C2	-3.08	111.63	118.44
1	1	1204	OMG	C2'-C1'-N9	-3.06	108.43	114.24
1	1	1204	OMG	O3'-C3'-C4'	3.04	119.83	111.08
1	1	1684	OMC	C5-C4-N3	2.98	126.33	121.32
1	1	1882	OMG	C4-C5-N7	-2.87	106.12	110.67
1	1	1768	A2M	O3'-C3'-C4'	2.86	119.31	111.08
1	1	1204	OMG	O3'-C3'-C2'	2.85	119.17	111.19
1	1	393	A2M	N3-C4-N9	2.81	131.95	127.17
1	1	386	OMG	CM2-O2'-C2'	-2.81	107.26	114.47
1	1	1824	OMC	C5-C4-N3	2.77	125.98	121.32
1	1	1520	OMG	C6-C5-N7	-2.71	125.36	130.29
1	1	2292	5MC	C5-C4-N3	2.69	124.51	121.75
1	1	624	OMG	O6-C6-N1	-2.60	115.22	120.11
1	1	1908	OMU	CM2-O2'-C2'	-2.59	107.82	114.47
1	1	2237	OMG	N1-C2-N3	2.59	128.06	123.32
1	1	2380	OMC	N4-C4-N3	-2.58	113.29	117.91
1	1	313	OMG	CM2-O2'-C2'	-2.56	107.90	114.47
1	1	624	OMG	C5-C4-N3	-2.56	124.32	128.39
1	1	1896	OMU	CM2-O2'-C2'	-2.55	107.93	114.47
1	1	393	A2M	C2'-C1'-N9	2.54	117.94	113.75
1	1	1121	OMG	C2-N1-C6	-2.54	120.50	125.11
1	1	386	OMG	C2'-C1'-N9	-2.53	109.44	114.24
1	1	1896	OMU	C4-N3-C2	-2.52	123.48	126.61
1	1	386	OMG	C2-N1-C6	-2.51	120.57	125.11
1	1	1684	OMC	CM2-O2'-C2'	-2.50	108.04	114.47
1	1	523	A2M	N3-C4-N9	2.46	131.36	127.17
1	1	1908	OMU	C5'-C4'-C3'	-2.45	106.38	115.21
1	1	1824	OMC	N4-C4-N3	-2.44	113.54	117.91
1	1	1520	OMG	C6-C5-C4	2.41	122.45	118.83
1	1	1204	OMG	O6-C6-N1	-2.38	115.63	120.11
1	1	1121	OMG	N1-C2-N3	2.38	127.67	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2042	OMG	N1-C2-N3	2.37	127.66	123.32
1	1	1684	OMC	C4-N3-C2	-2.32	116.62	120.26
1	1	1775	OMG	C6-C5-N7	-2.29	126.13	130.29
1	1	1775	OMG	C2-N1-C6	-2.28	120.98	125.11
1	1	2380	OMC	C4-N3-C2	-2.27	116.69	120.26
1	1	1520	OMG	C2-N1-C6	-2.27	121.00	125.11
1	1	1897	OMU	C4-N3-C2	-2.27	123.80	126.61
1	1	396	A2M	N3-C2-N1	2.26	132.01	128.58
1	1	1775	OMG	N1-C2-N3	2.26	127.46	123.32
1	1	313	OMG	N1-C2-N3	2.25	127.43	123.32
1	1	1684	OMC	N4-C4-N3	-2.23	113.92	117.91
1	1	2042	OMG	C2-N1-C6	-2.22	121.09	125.11
1	1	2074	OMG	N1-C2-N3	2.20	127.36	123.32
1	1	624	OMG	C6-C5-C4	2.20	122.14	118.83
1	1	1908	OMU	C2'-C3'-C4'	-2.20	97.26	101.99
1	1	1121	OMG	N2-C2-N3	-2.19	115.39	119.67
1	1	1204	OMG	C2-N1-C6	-2.19	121.13	125.11
1	1	523	A2M	C5-C4-N3	-2.19	123.70	126.72
1	1	2237	OMG	O6-C6-N1	-2.19	116.00	120.11
1	1	1882	OMG	C8-N7-C5	2.19	108.16	104.26
1	1	49	OMU	C4-N3-C2	-2.18	123.90	126.61
1	1	2042	OMG	O6-C6-N1	-2.17	116.04	120.11
1	1	1520	OMG	C5-C4-N3	-2.17	124.94	128.39
1	1	313	OMG	C2-N1-C6	-2.16	121.19	125.11
1	1	2042	OMG	C6-C5-C4	2.15	122.06	118.83
1	1	1520	OMG	N1-C2-N3	2.15	127.25	123.32
1	1	624	OMG	C2-N1-C6	-2.15	121.22	125.11
1	1	624	OMG	N1-C2-N3	2.12	127.20	123.32
1	1	1908	OMU	O4-C4-N3	-2.11	116.21	119.27
1	1	624	OMG	O6-C6-C5	2.11	132.11	126.53
1	1	1765	5MC	O2-C2-N1	2.11	123.03	118.90
1	1	393	A2M	C5-C4-N3	-2.11	123.81	126.72
1	1	1765	5MC	N1-C2-N3	-2.09	115.17	118.80
1	1	2237	OMG	O6-C6-C5	2.08	132.02	126.53
3	4	133	OMG	N1-C2-N3	2.06	127.10	123.32
1	1	1824	OMC	C2'-C1'-N1	-2.06	110.33	114.24
1	1	1204	OMG	C3'-C2'-C1'	-2.06	98.87	102.81
1	1	1775	OMG	C6-C5-C4	2.04	121.90	118.83
1	1	393	A2M	C2-N1-C6	-2.04	115.38	118.73
1	1	2074	OMG	C2-N1-C6	-2.02	121.44	125.11
1	1	2380	OMC	CM2-O2'-C2'	-2.01	109.33	114.47

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	4	133	OMG	C1'-C2'-O2'-CM2
1	1	49	OMU	C1'-C2'-O2'-CM2
1	1	313	OMG	O4'-C4'-C5'-O5'
1	1	624	OMG	C1'-C2'-O2'-CM2
1	1	1684	OMC	C2'-C1'-N1-C6
1	1	1775	OMG	O4'-C4'-C5'-O5'
1	1	1824	OMC	C3'-C2'-O2'-CM2
1	1	1882	OMG	C1'-C2'-O2'-CM2
1	1	1684	OMC	C2'-C1'-N1-C2
1	1	1520	OMG	O4'-C4'-C5'-O5'
1	1	1768	A2M	C3'-C4'-C5'-O5'
1	1	1775	OMG	C3'-C4'-C5'-O5'
1	1	1882	OMG	O4'-C4'-C5'-O5'
1	1	2292	5MC	O4'-C4'-C5'-O5'
1	1	313	OMG	C3'-C4'-C5'-O5'
1	1	1121	OMG	C3'-C4'-C5'-O5'
1	1	1908	OMU	C3'-C4'-C5'-O5'
1	1	1520	OMG	C3'-C4'-C5'-O5'
1	1	1768	A2M	O4'-C4'-C5'-O5'
1	1	2292	5MC	C3'-C4'-C5'-O5'
1	1	1882	OMG	C3'-C4'-C5'-O5'
1	1	1908	OMU	O4'-C4'-C5'-O5'
1	1	1768	A2M	C2'-C1'-N9-C8
1	1	1684	OMC	O4'-C1'-N1-C6
1	1	393	A2M	C3'-C2'-O2'-CM'
1	1	1684	OMC	O4'-C1'-N1-C2
1	1	2292	5MC	O4'-C1'-N1-C6
1	1	1684	OMC	C3'-C2'-O2'-CM2
1	1	393	A2M	O4'-C4'-C5'-O5'
1	1	2292	5MC	C2'-C1'-N1-C6
1	1	523	A2M	O4'-C1'-N9-C8
1	1	2074	OMG	C3'-C2'-O2'-CM2
1	1	1121	OMG	O4'-C4'-C5'-O5'
1	1	2292	5MC	O4'-C1'-N1-C2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	393	A2M	1	0
1	1	1896	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	624	OMG	1	0
1	1	1684	OMC	1	0
1	1	1897	OMU	1	0
1	1	49	OMU	1	0
1	1	1824	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 294 ligands modelled in this entry, 293 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	$\# Z > 2$
47	PGE	1	3063	46	9,9,9	0.29	0	8,8,8	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PGE	1	3063	46	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	1	3063	PGE	O3-C5-C6-O4
47	1	3063	PGE	C6-C5-O3-C4
47	1	3063	PGE	O1-C1-C2-O2
47	1	3063	PGE	O2-C3-C4-O3

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](#)

There are no chain breaks in this entry.

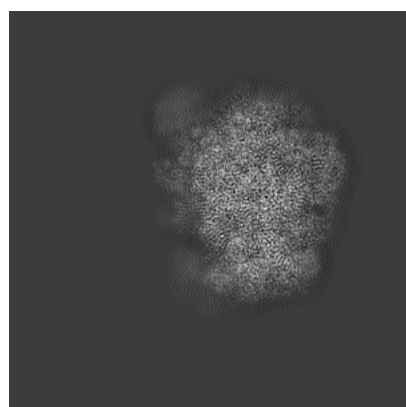
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13681. These allow visual inspection of the internal detail of the map and identification of artifacts.

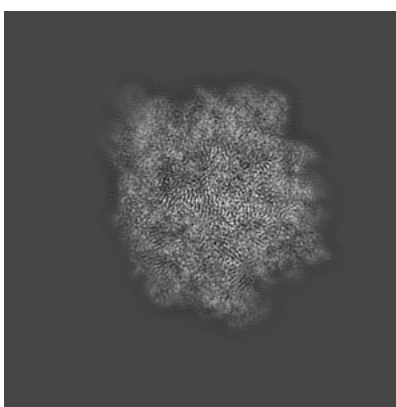
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

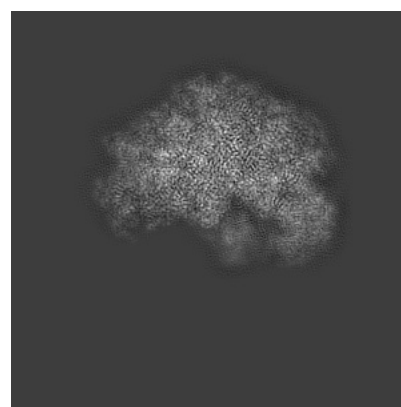
6.1.1 Primary map



X



Y

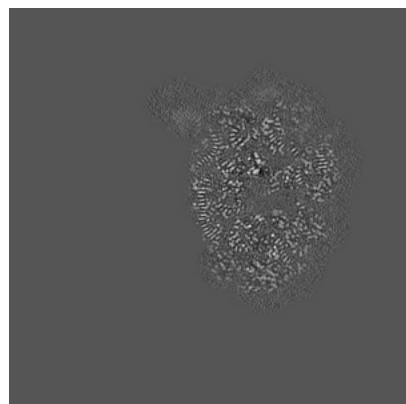


Z

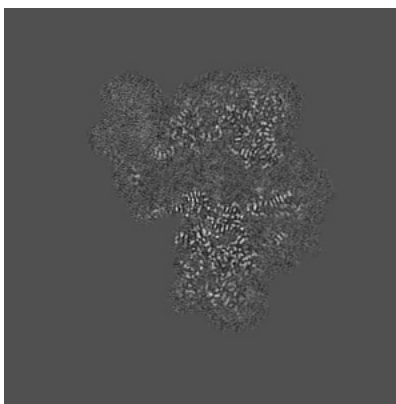
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

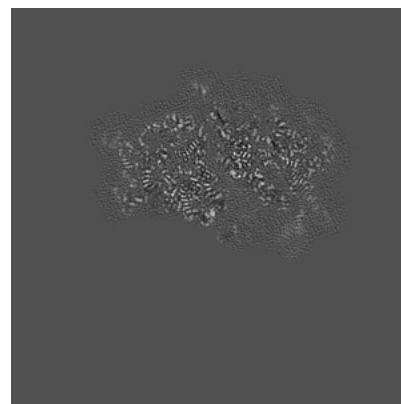
6.2.1 Primary map



X Index: 220



Y Index: 220

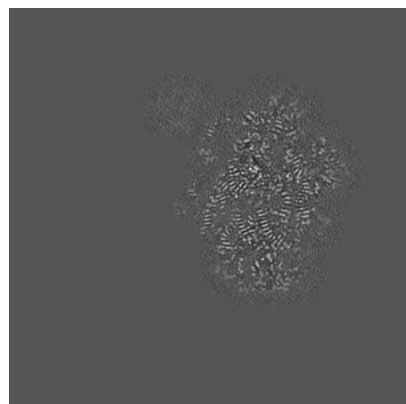


Z Index: 220

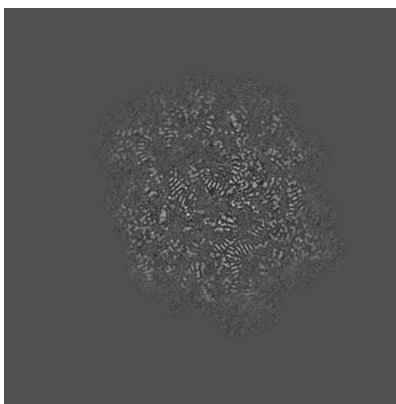
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

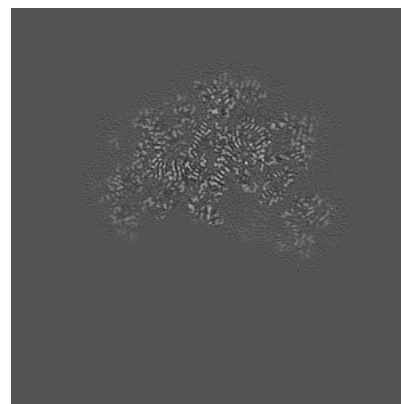
6.3.1 Primary map



X Index: 230



Y Index: 264

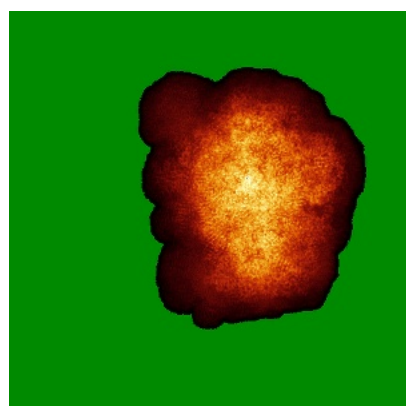


Z Index: 245

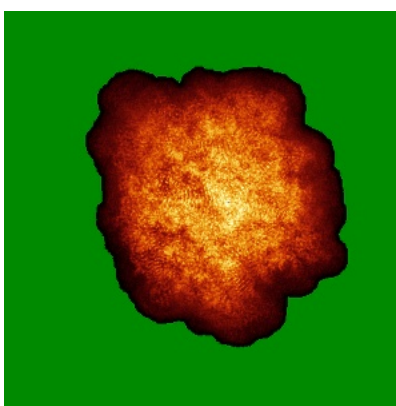
The images above show the largest variance slices of the map in three orthogonal directions.

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

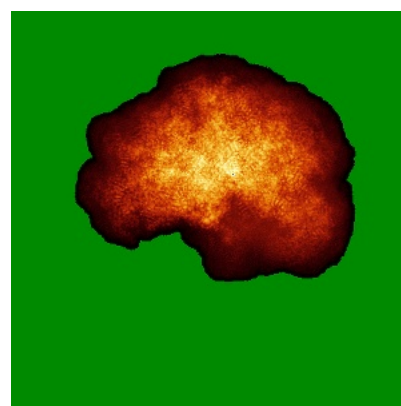
6.4.1 Primary map



X



Y

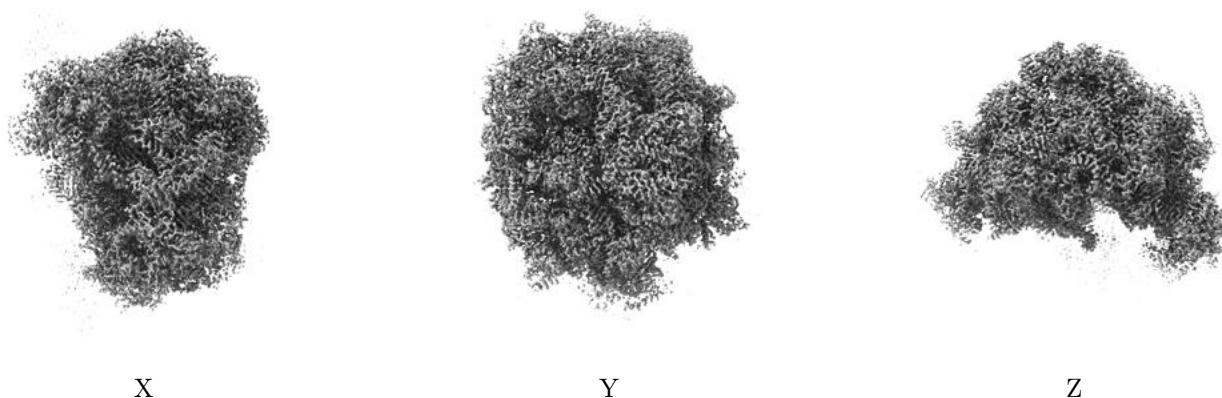


Z

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

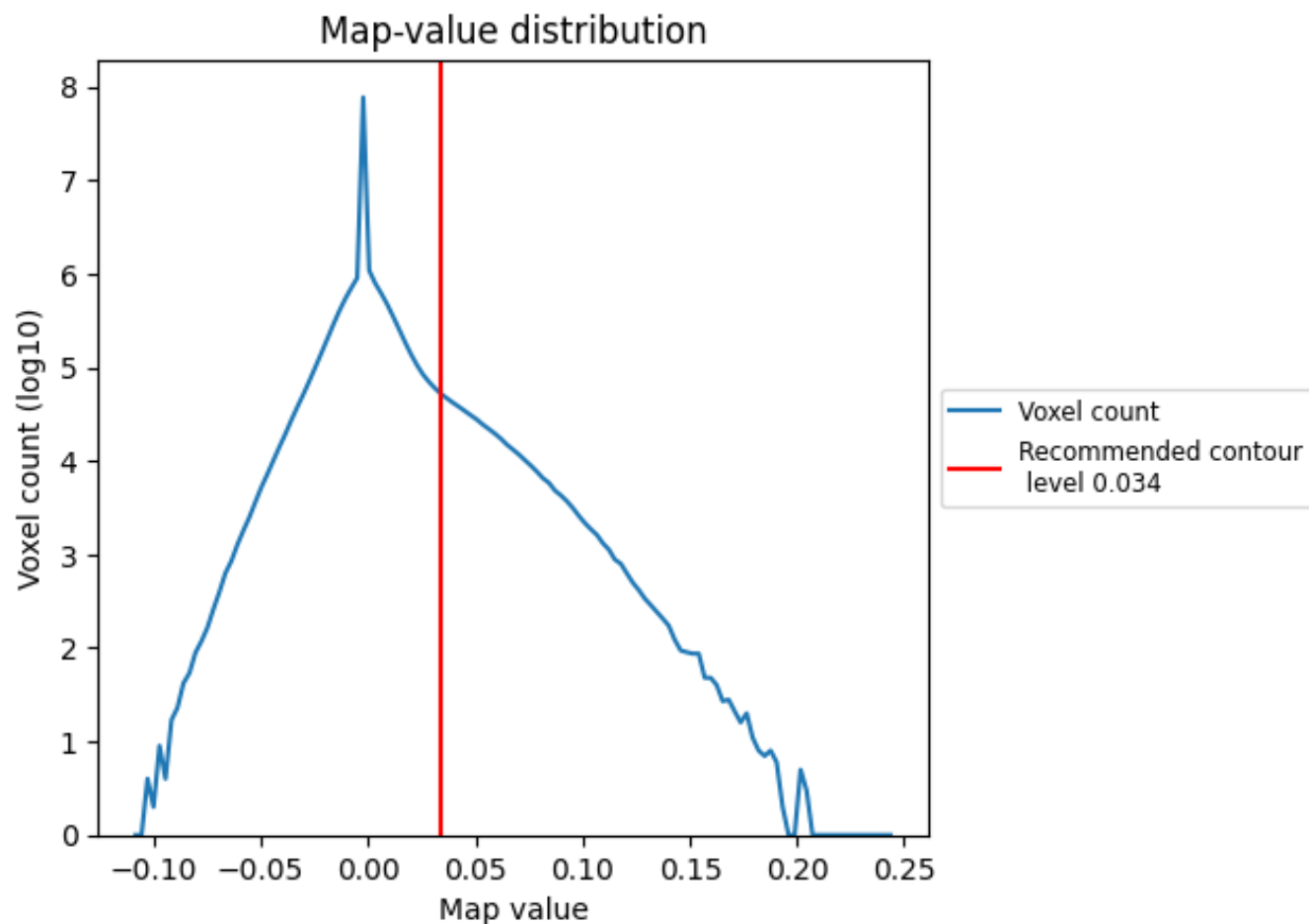
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

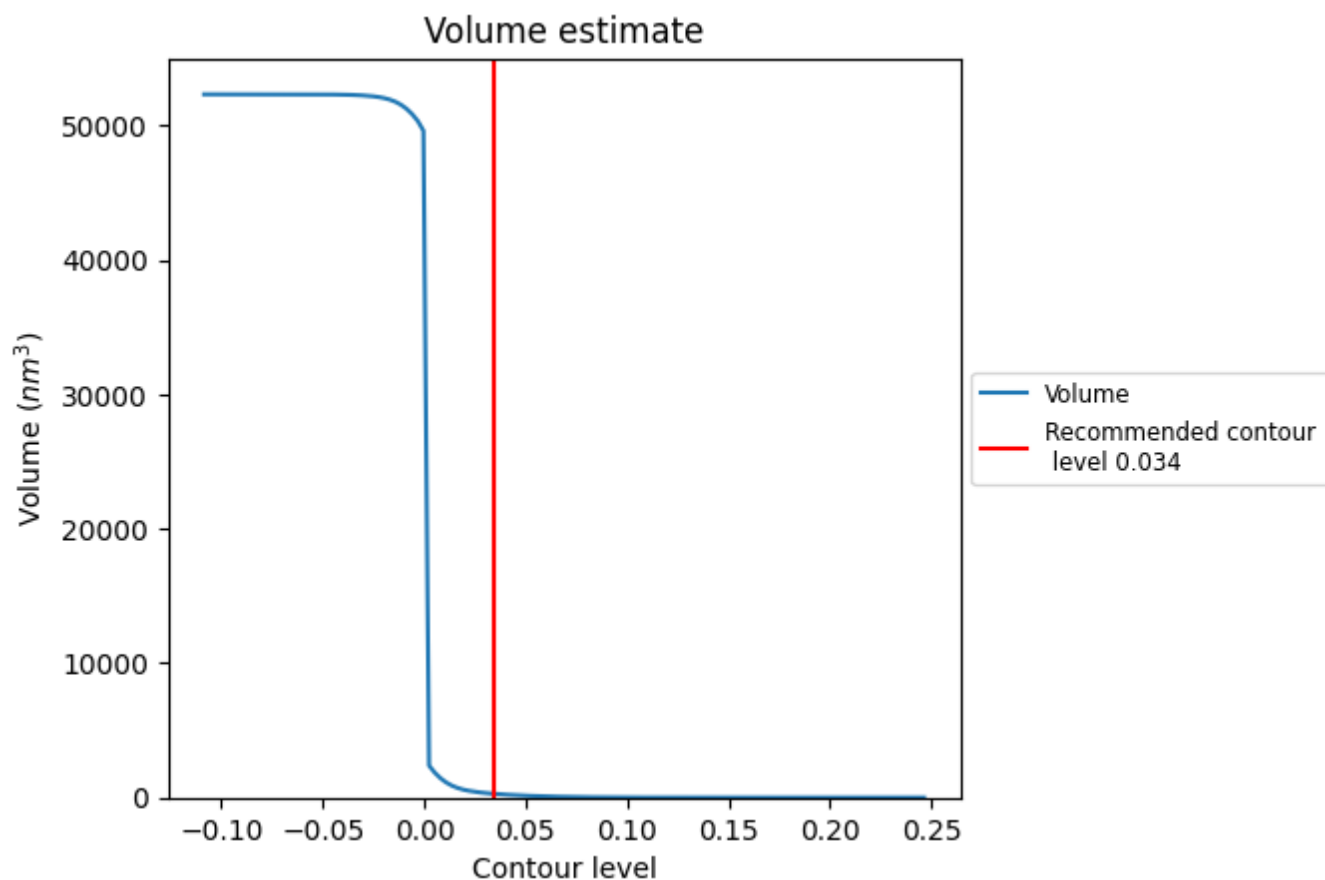
This section contains the results of statistical analysis of the map.

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.

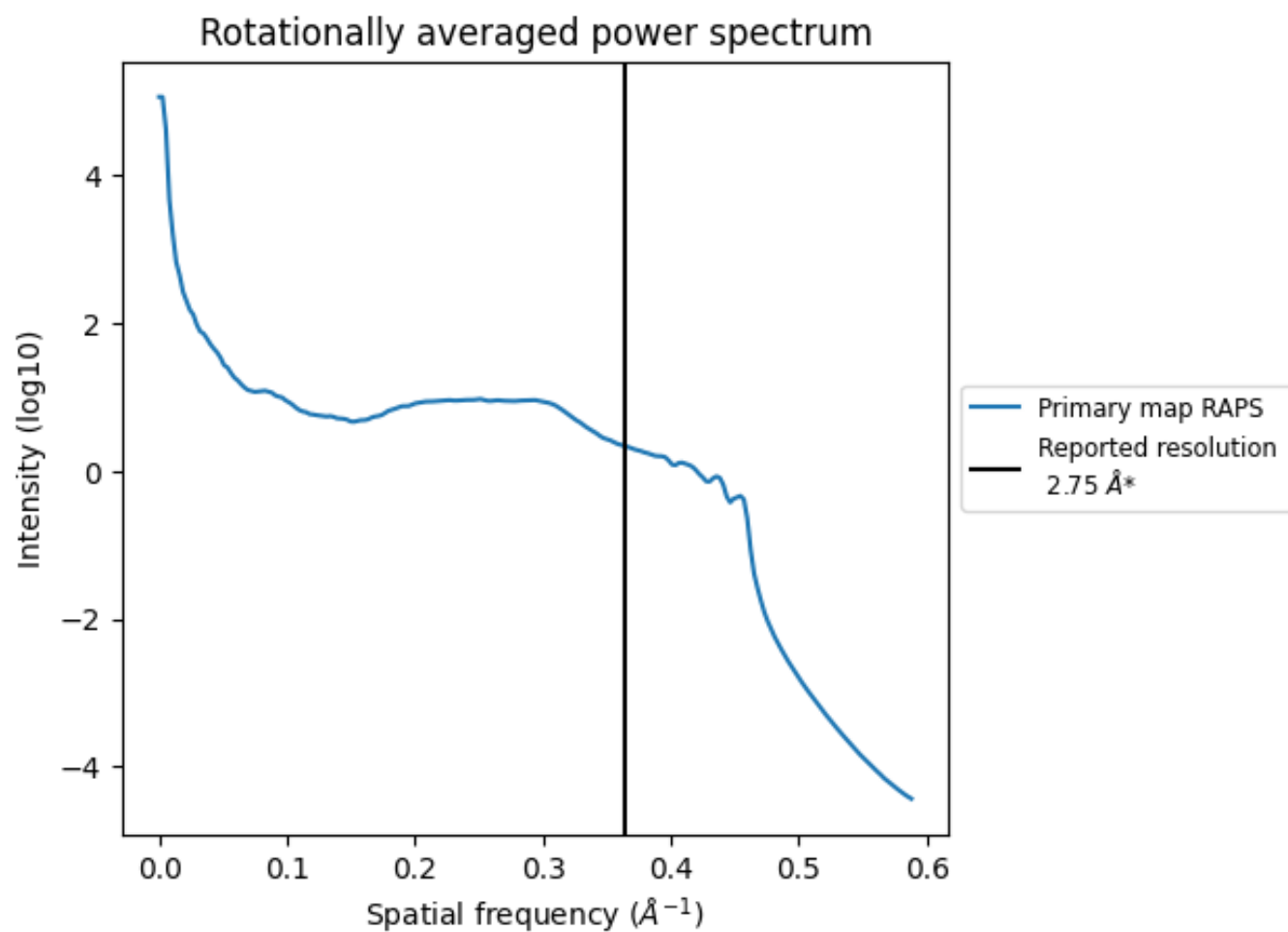
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm^3 ; this corresponds to an approximate mass of 258 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 0.364 Å⁻¹

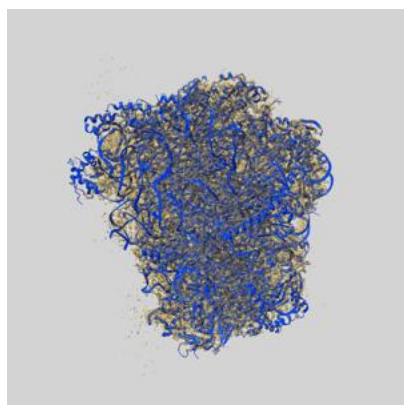
8 Fourier-Shell correlation

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

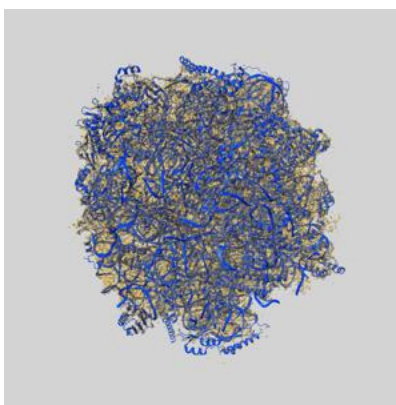
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13681 and PDB model 7PWG. Per-residue inclusion information can be found in section [3](#) on page [16](#).

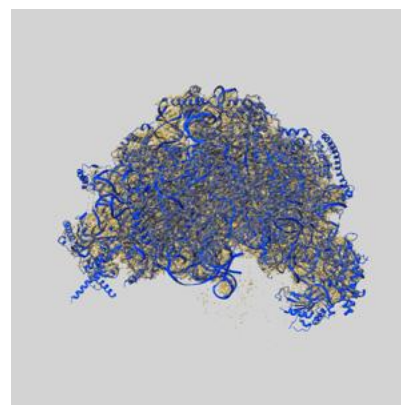
9.1 Map-model overlay [i](#)



X



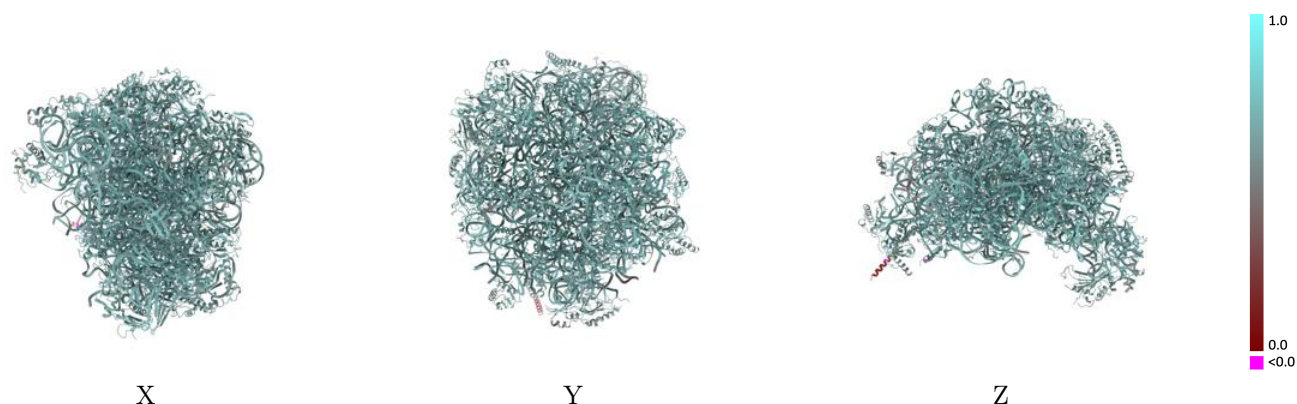
Y



Z

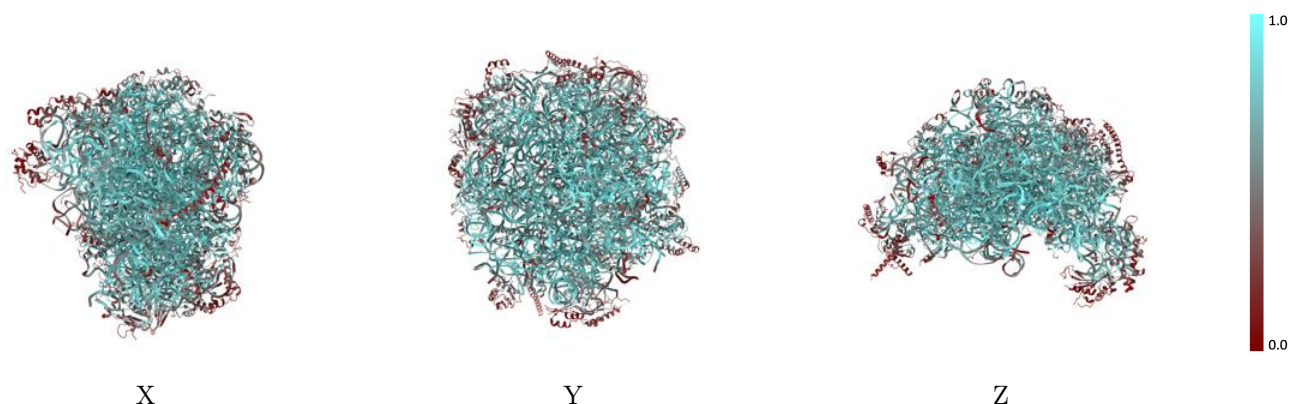
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



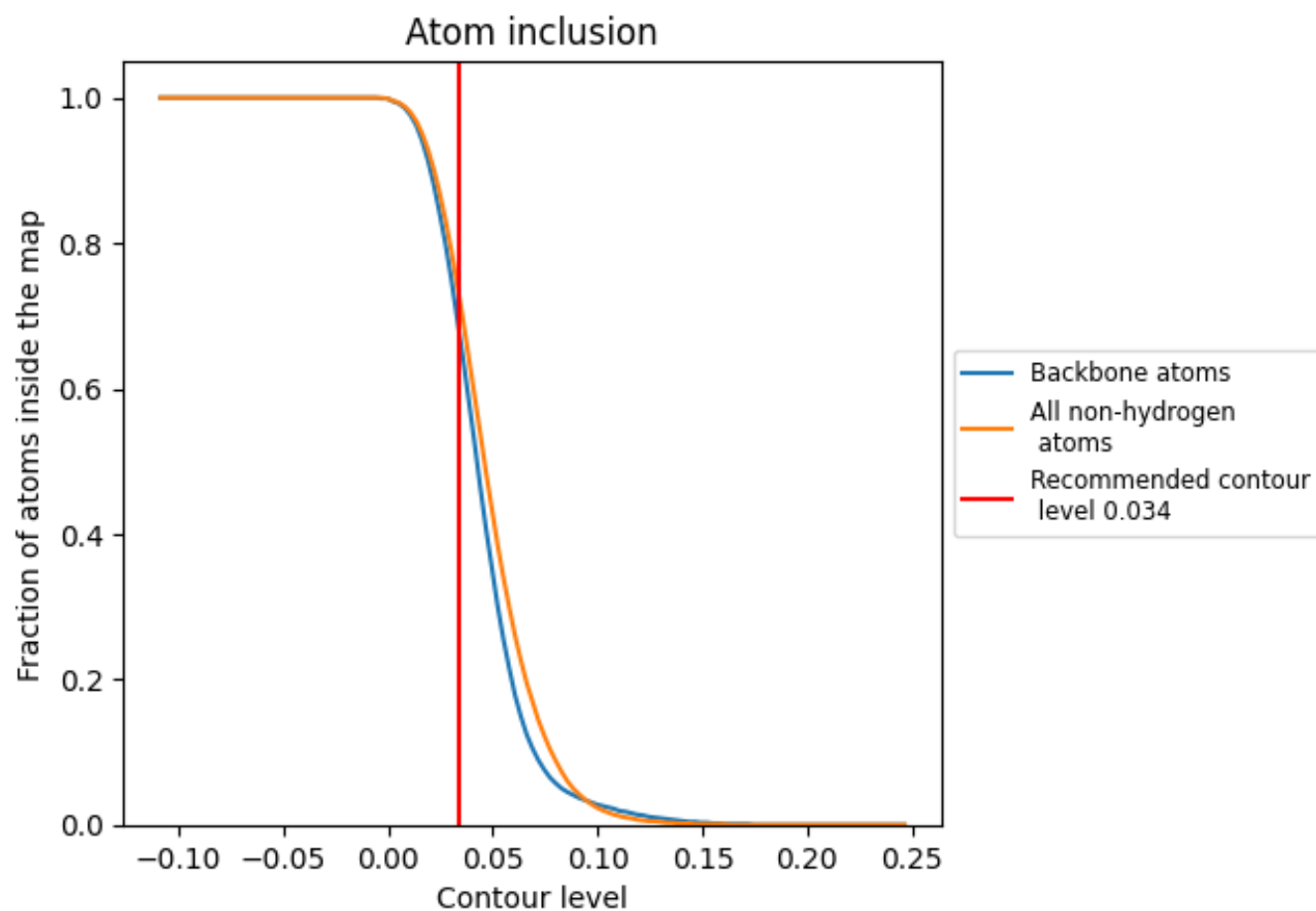
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 73% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7270	 0.6660
1	 0.8370	 0.6760
3	 0.7150	 0.6500
4	 0.7810	 0.6650
A	 0.7840	 0.6970
B	 0.6880	 0.6730
C	 0.6300	 0.6560
D	 0.4610	 0.6330
E	 0.1770	 0.5740
F	 0.6040	 0.6590
G	 0.5300	 0.6420
H	 0.4830	 0.6410
I	 0.5320	 0.6550
J	 0.2450	 0.5980
L	 0.6500	 0.6670
M	 0.4950	 0.6390
N	 0.8660	 0.7030
O	 0.6440	 0.6580
P	 0.7040	 0.6700
Q	 0.6250	 0.6670
R	 0.5390	 0.5930
S	 0.6700	 0.6630
T	 0.7160	 0.6760
U	 0.2330	 0.5810
V	 0.6100	 0.6690
W	 0.6340	 0.6420
X	 0.6440	 0.6640
Y	 0.5730	 0.6510
Z	 0.2840	 0.5950
a	 0.7840	 0.6840
b	 0.6970	 0.6770
c	 0.3150	 0.6240
d	 0.6270	 0.6640
e	 0.6330	 0.6580
f	 0.5940	 0.6510



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Chain	Atom inclusion	Q-score
g	 0.7080	 0.6770
h	 0.5240	 0.6440
i	 0.5850	 0.6520
j	 0.8390	 0.7020
k	 0.2210	 0.5850
l	 0.7310	 0.6830
m	 0.5070	 0.6540
o	 0.7380	 0.6870
p	 0.6910	 0.6770
w	 0.3310	 0.6040