



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 02:21 AM EDT

PDB ID : 7TQL / pdb_00007tql
EMDB ID : EMD-26067
Title : CryoEM structure of the human 40S small ribosomal subunit in complex with translation initiation factors eIF1A and eIF5B.
Authors : Lapointe, C.P.; Grosely, R.; Sokabe, M.; Alvarado, C.; Wang, J.; Montabana, E.; Villa, N.; Shin, B.; Dever, T.; Fraser, C.; Fernandez, I.S.; Puglisi, J.D.
Deposited on : 2022-01-26
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

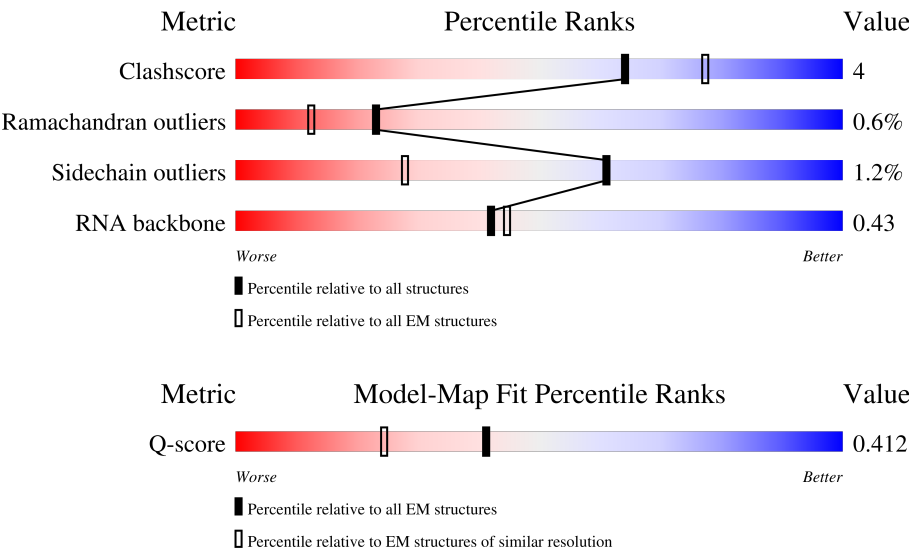
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



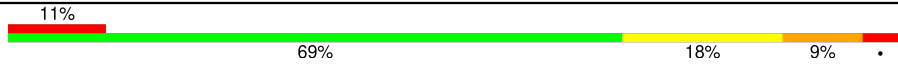
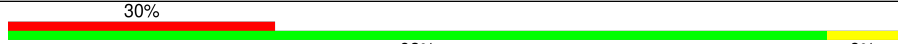
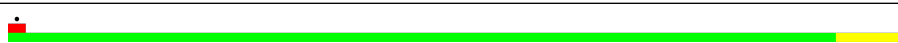
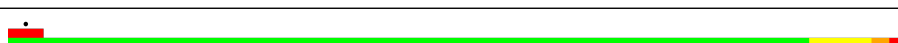
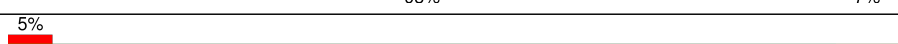
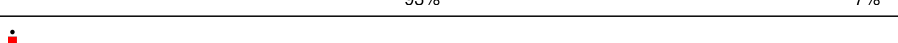
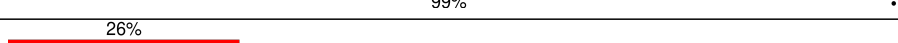
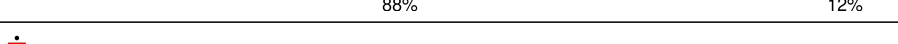
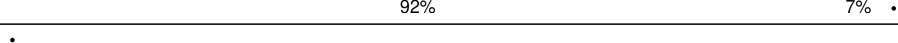
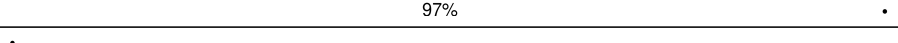
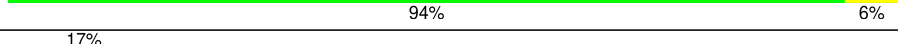
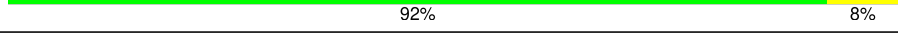
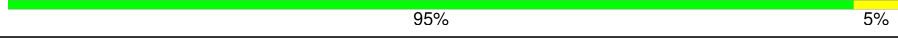
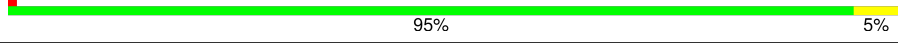
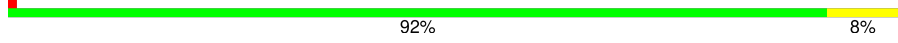
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	619	
2	2	1656	
3	3	75	

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Mol	Chain	Length	Quality of chain
4	4	90	
5	B	419	
5	C	419	
6	D	218	
7	E	258	
8	F	225	
9	G	226	
10	H	185	
11	I	205	
12	J	180	
13	K	189	
14	L	147	
15	M	97	
16	N	141	
17	O	120	
18	P	134	
19	Q	115	
20	R	139	
21	S	132	
22	T	140	
23	U	139	
24	V	101	
25	W	129	
26	X	141	
27	Y	123	

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Mol	Chain	Length	Quality of chain
28	Z	82	96%
29	a	72	79% 12%7%
30	b	82	83% 11%6%
31	c	99	98%
32	d	58	97%
33	e	51	10% 90%
34	f	54	98%
35	g	65	35% 95% 5%
36	h	19	5% 89% 11%
37	j	314	82% 13%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 80976 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	619	Total	C	N	O	S	0	0
			4901	3123	844	912	22		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	624	THR	ASN	engineered mutation	UNP O60841
1	625	GLU	-	insertion	UNP O60841
1	626	LYS	THR	engineered mutation	UNP O60841
1	627	ASP	GLU	engineered mutation	UNP O60841
1	906	THR	LEU	engineered mutation	UNP O60841

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1656	Total	C	N	O	P	0	0
			35361	15784	6351	11570	1656		

- Molecule 3 is a RNA chain called Human Met-tRNAiMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	75	Total	C	N	O	P	0	0
			1607	717	298	517	75		

- Molecule 4 is a protein called Translation initiation factor eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	90	Total	C	N	O	S	0	0
			727	459	132	132	4		

- Molecule 5 is a protein called ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	206	Total	C	N	O	S	0	0
			1624	1035	287	294	8		
5	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 6 is a protein called 40S ribosomal protein S2.

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

- Molecule 7 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	258	Total	C	N	O	S	0	0
			2050	1311	381	350	8		

- Molecule 8 is a protein called 40S ribosomal protein S3.

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

- Molecule 9 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	226	Total	C	N	O	S	0	0
			1831	1144	365	315	7		

- Molecule 10 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	185	Total	C	N	O	S	0	0
			1492	952	274	265	1		

- Molecule 11 is a protein called 40S ribosomal protein S8.

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

- Molecule 12 is a protein called 40S ribosomal protein S9.

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

- Molecule 13 is a protein called 40S ribosomal protein S5.

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

- Molecule 14 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	147	Total	C	N	O	S	0	0
			1204	767	225	206	6		

- Molecule 15 is a protein called 40S ribosomal protein S10.

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

- Molecule 16 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	141	Total	C	N	O	S	0	0
			1152	740	220	191	1		

- Molecule 17 is a protein called ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	120	Total	C	N	O	S	0	0
			929	583	164	174	8		

- Molecule 18 is a protein called ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	134	Total	C	N	O	S	0	0
			998	610	197	185	6		

- Molecule 19 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	115	Total	C	N	O	S	0	0
			950	604	176	163	7		

- Molecule 20 is a protein called 40S ribosomal protein S16.

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

- Molecule 21 is a protein called ribosomal protein eS17.

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

- Molecule 22 is a protein called ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	140	Total	C	N	O	S	0	0
			1162	731	234	196	1		

- Molecule 23 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	139	Total	C	N	O	S	0	0
			1083	678	208	194	3		

- Molecule 24 is a protein called ribosomal protein uS10.

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

- Molecule 25 is a protein called 40S ribosomal protein S15a.

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

- Molecule 26 is a protein called 40S ribosomal protein S23.

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

- Molecule 27 is a protein called Isoform 3 of 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	123	Total	C	N	O	S	0	0
			1006	637	197	167	5		

- Molecule 28 is a protein called 40S ribosomal protein S21.

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

- Molecule 29 is a protein called ribosomal protein eS25.

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

- Molecule 30 is a protein called 40S ribosomal protein S27.

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

- Molecule 31 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 32 is a protein called ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	58	Total	C	N	O	S	0	0
			449	274	86	87	2		

- Molecule 33 is a protein called ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	51	Total	C	N	O	S	0	0
			391	237	88	65	1		

- Molecule 34 is a protein called ribosomal protein uS14.

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

- Molecule 35 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	65	Total	C	N	O	S	0	0
			529	333	99	90	7		

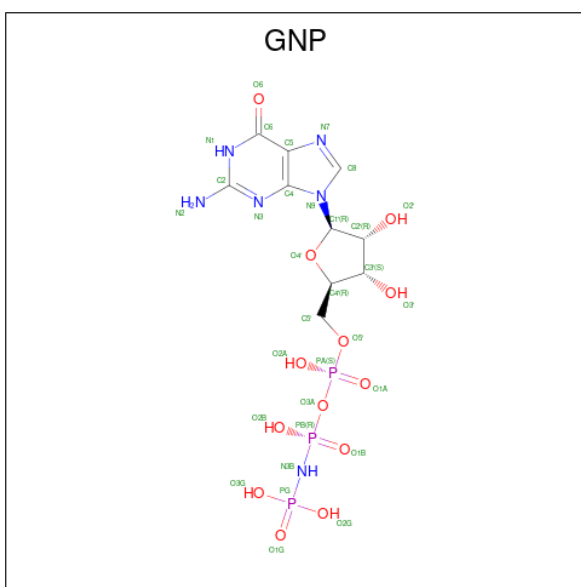
- Molecule 36 is a protein called ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	19	Total	C	N	O	S	0	0
			185	114	50	19	2		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

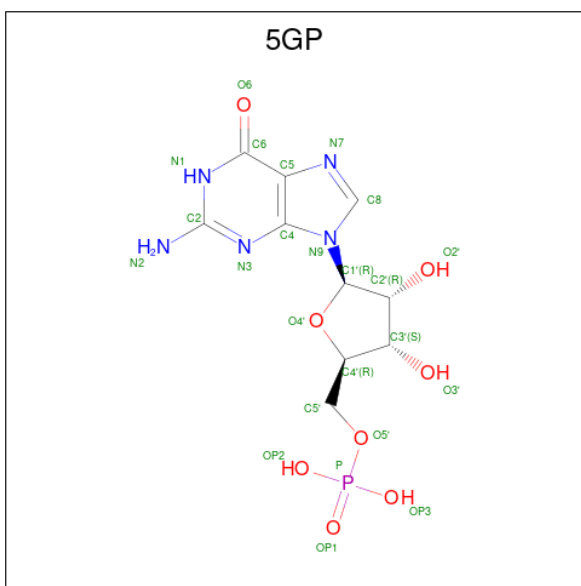
Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 38 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
38	1	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 39 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_8\text{P}$).



Mol	Chain	Residues	Atoms					AltConf
39	3	1	Total	C	N	O	P	0
			23	10	5	7	1	

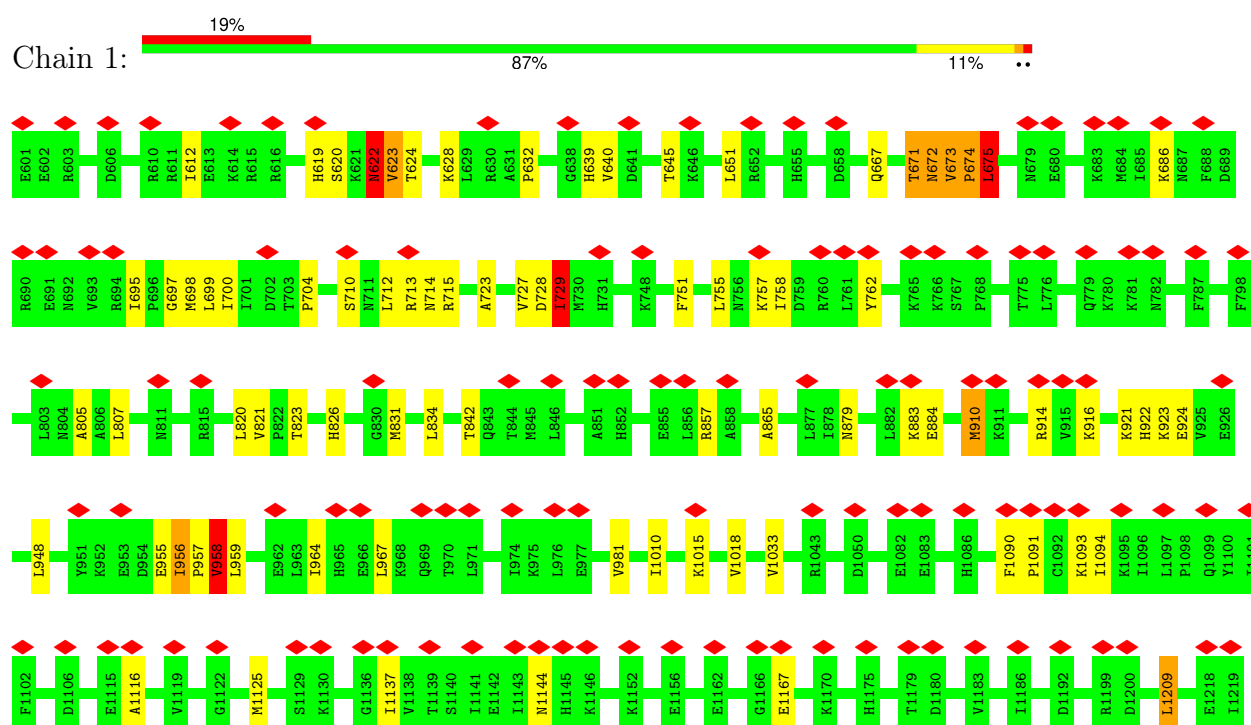
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

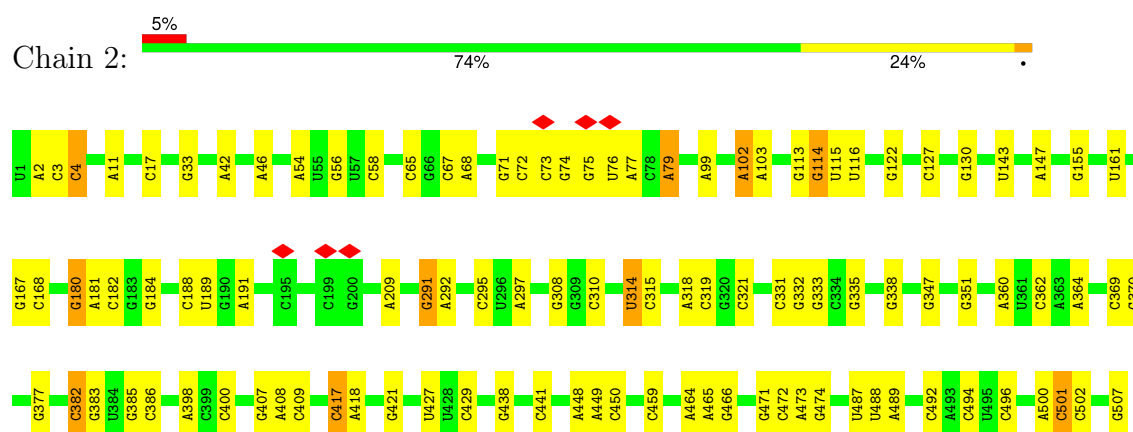
3 Residue-property plots

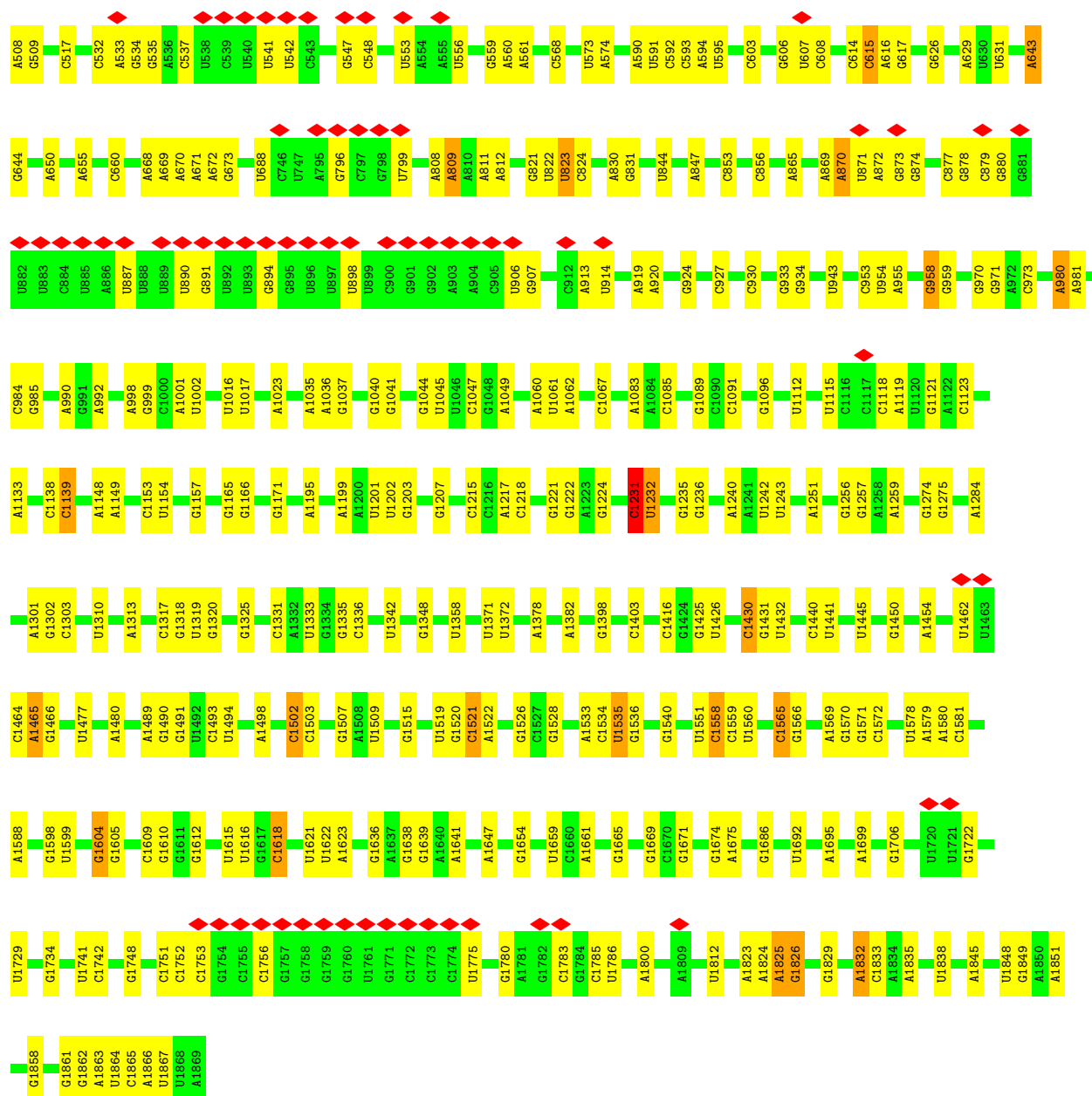
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Eukaryotic translation initiation factor 5B

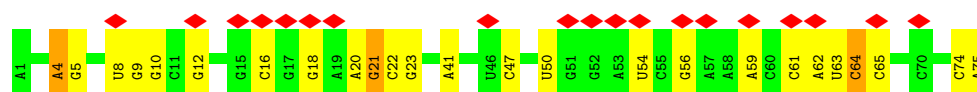


• Molecule 2: 18S ribosomal RNA

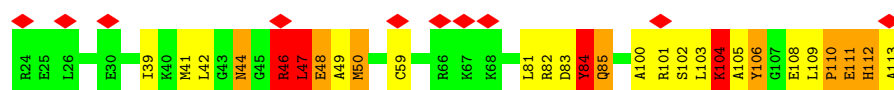




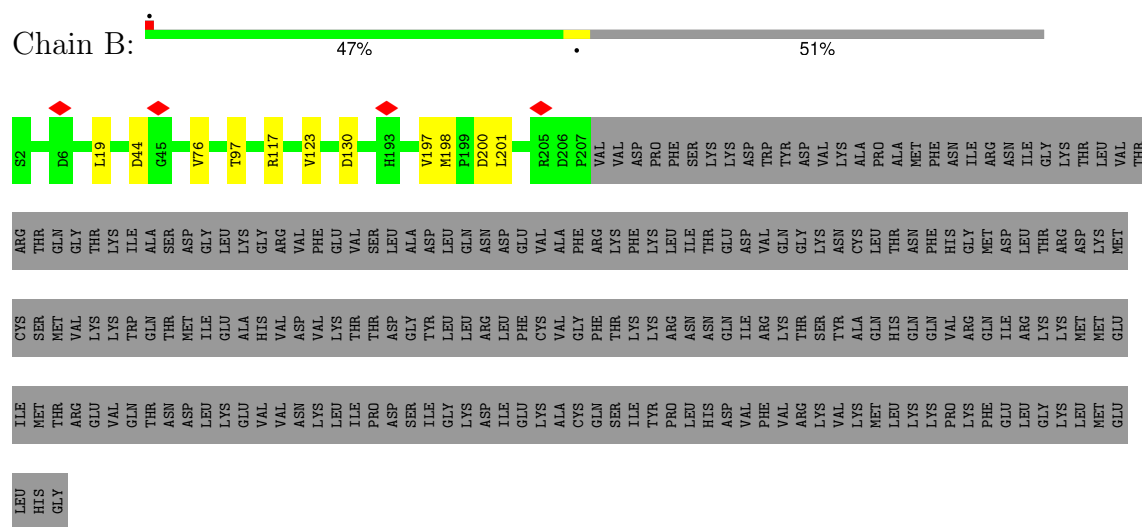
• Molecule 3: Human Met-tRNAⁱMet



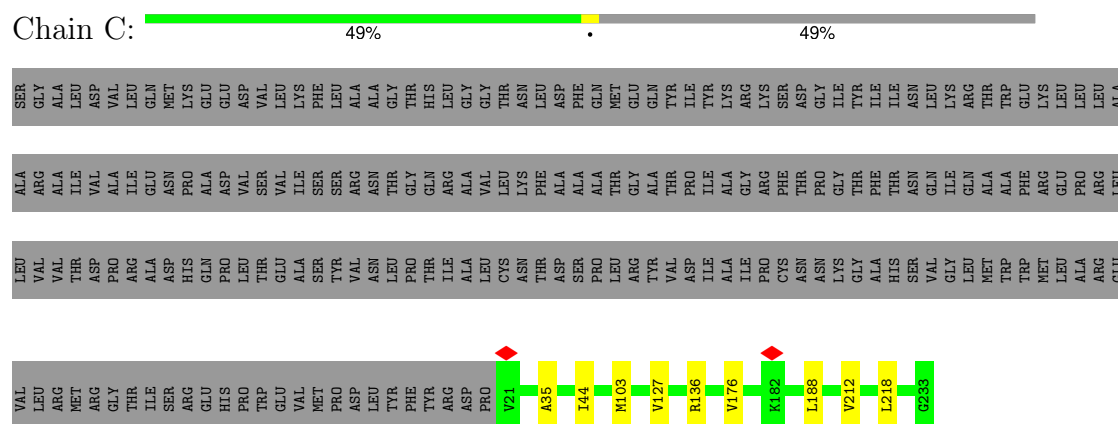
• Molecule 4: Translation initiation factor eIF1A



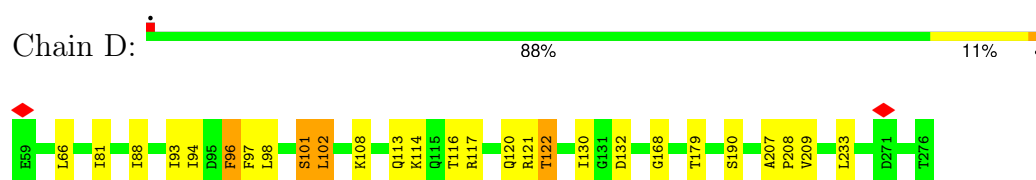
- Molecule 5: ribosomal protein uS2



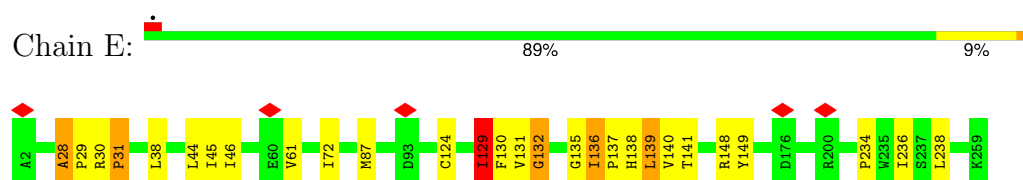
- Molecule 5: ribosomal protein uS2



- Molecule 6: 40S ribosomal protein S2

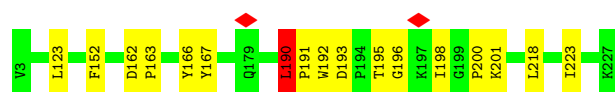


- Molecule 7: 40S ribosomal protein S4, X isoform

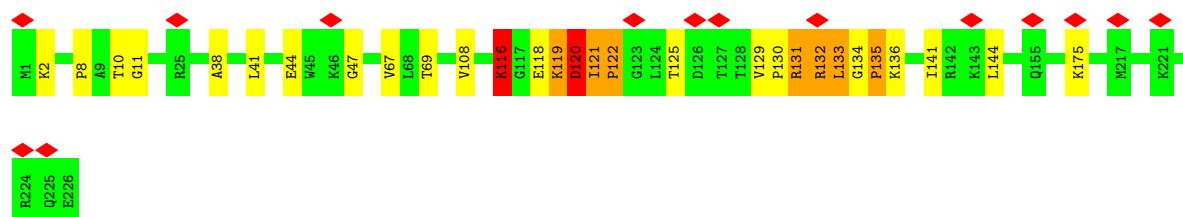
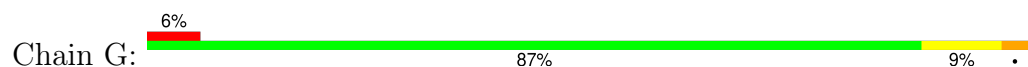


- Molecule 8: 40S ribosomal protein S3

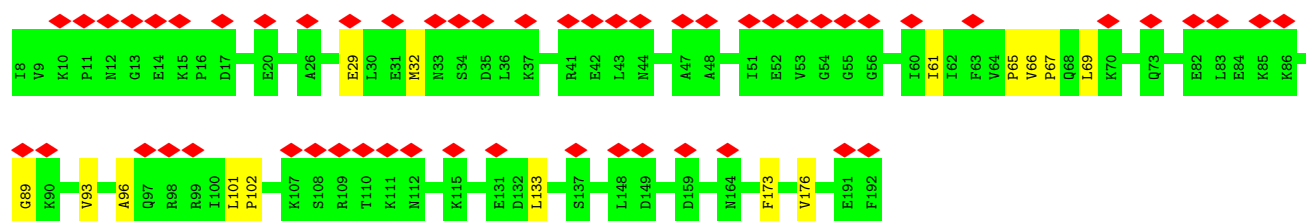




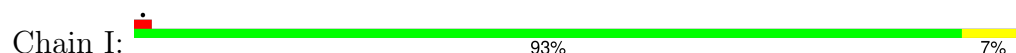
- Molecule 9: 40S ribosomal protein S6



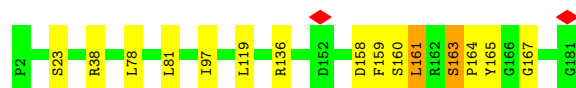
- Molecule 10: 40S ribosomal protein S7



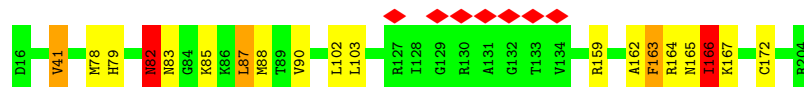
- Molecule 11: 40S ribosomal protein S8



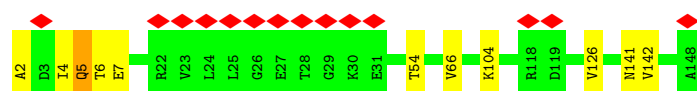
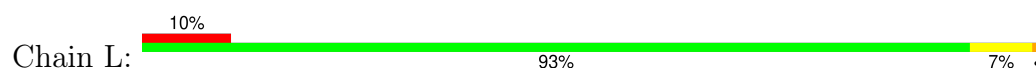
- Molecule 12: 40S ribosomal protein S9



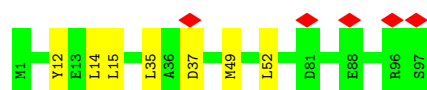
- Molecule 13: 40S ribosomal protein S5



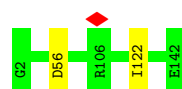
- Molecule 14: 40S ribosomal protein S11



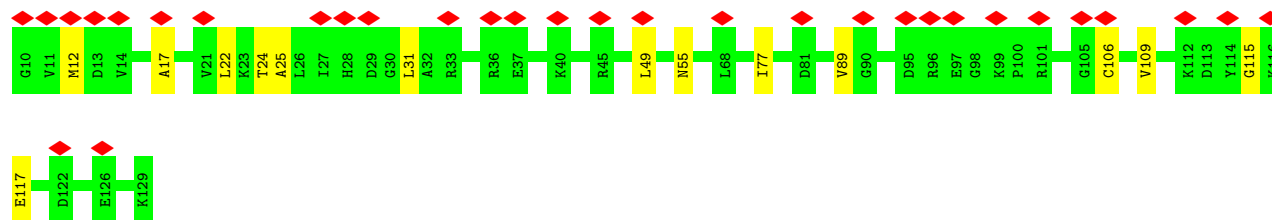
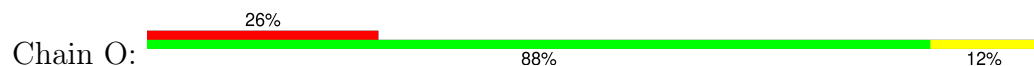
- Molecule 15: 40S ribosomal protein S10



- Molecule 16: ribosomal protein uS15



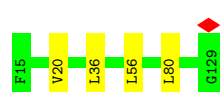
- Molecule 17: ribosomal protein eS12



- Molecule 18: ribosomal protein uS11



- Molecule 19: 40S ribosomal protein S15

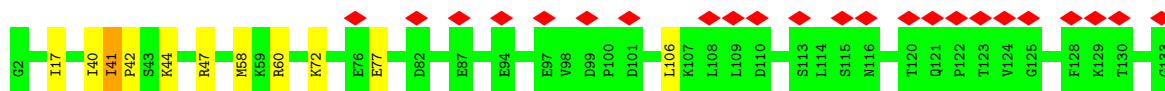
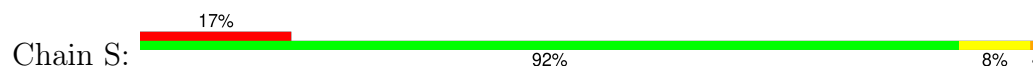


- Molecule 20: 40S ribosomal protein S16

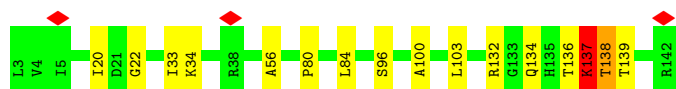
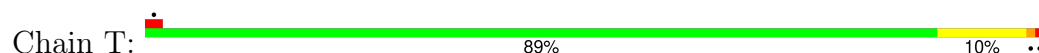




- Molecule 21: ribosomal protein eS17



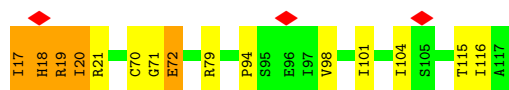
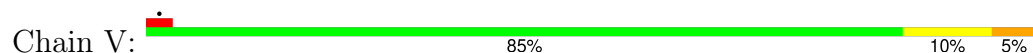
- Molecule 22: ribosomal protein uS13



- Molecule 23: 40S ribosomal protein S19



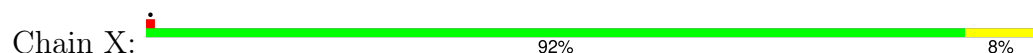
- Molecule 24: ribosomal protein uS10



- Molecule 25: 40S ribosomal protein S15a



- Molecule 26: 40S ribosomal protein S23



- Molecule 27: Isoform 3 of 40S ribosomal protein S24

Chain Y:  91% 7% .



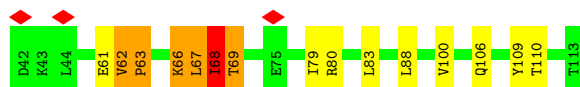
- Molecule 28: 40S ribosomal protein S21

Chain Z:  96% .



- Molecule 29: ribosomal protein eS25

Chain a:  79% 12% 7% .



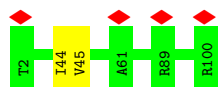
- Molecule 30: 40S ribosomal protein S27

Chain b:  83% 11% 6% .



- Molecule 31: 40S ribosomal protein S26

Chain c:  98% .



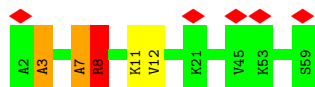
- Molecule 32: ribosomal protein eS28

Chain d:  97% .

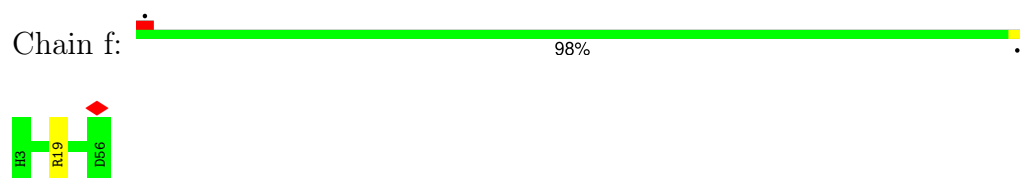


- Molecule 33: ribosomal protein eS30

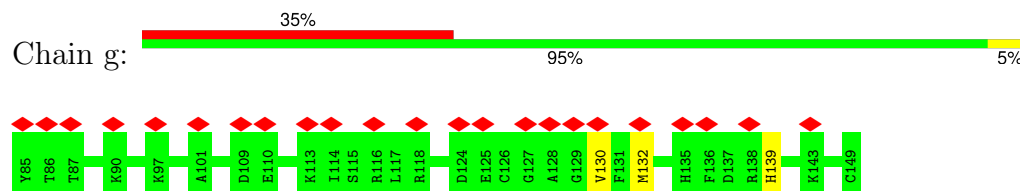
Chain e:  10% 90% . . .



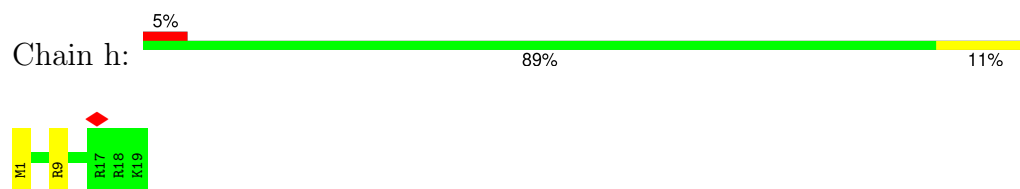
- Molecule 34: ribosomal protein uS14



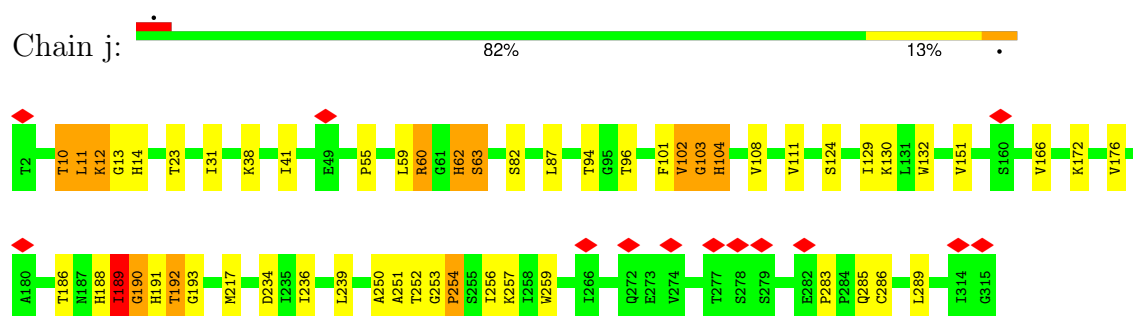
- Molecule 35: 40S ribosomal protein S27a



- Molecule 36: ribosomal protein eL41



- Molecule 37: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.534	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	628.8, 628.8, 628.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.31, 1.31, 1.31	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, 5GP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.10	1/4983 (0.0%)	1.50	11/6718 (0.2%)
2	2	0.52	0/39542	0.71	16/61622 (0.0%)
3	3	0.53	0/1798	0.69	2/2802 (0.1%)
4	4	1.12	0/737	1.56	14/986 (1.4%)
5	B	1.07	0/1661	1.51	0/2259
5	C	1.08	0/1756	1.46	0/2350
6	D	1.14	1/1718 (0.1%)	1.50	3/2322 (0.1%)
7	E	1.20	5/2092 (0.2%)	1.41	3/2816 (0.1%)
8	F	1.11	0/1776	1.54	2/2392 (0.1%)
9	G	1.11	1/1854 (0.1%)	1.64	13/2469 (0.5%)
10	H	1.11	0/1515	1.50	2/2030 (0.1%)
11	I	1.06	0/1711	1.42	1/2282 (0.0%)
12	J	1.11	0/1524	1.52	1/2035 (0.0%)
13	K	1.19	1/1516 (0.1%)	1.59	5/2037 (0.2%)
14	L	1.07	0/1225	1.34	4/1640 (0.2%)
15	M	1.06	0/840	1.48	0/1133
16	N	1.05	0/1176	1.57	0/1580
17	O	1.12	0/939	1.57	0/1261
18	P	1.14	1/1011 (0.1%)	1.63	4/1356 (0.3%)
19	Q	1.06	0/968	1.45	0/1294
20	R	1.08	0/1126	1.48	0/1506
21	S	1.16	2/1080 (0.2%)	1.58	5/1449 (0.3%)
22	T	1.11	1/1180 (0.1%)	1.54	0/1581
23	U	1.09	0/1101	1.61	0/1477
24	V	1.10	0/813	1.48	2/1092 (0.2%)
25	W	1.07	0/1051	1.47	1/1406 (0.1%)
26	X	1.08	0/1116	1.44	0/1490
27	Y	1.09	0/1023	1.47	0/1359
28	Z	1.09	0/631	1.52	0/844
29	a	1.11	0/580	1.83	7/780 (0.9%)
30	b	1.20	1/653 (0.2%)	1.51	3/876 (0.3%)
31	c	1.06	0/805	1.43	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	1.11	0/451	1.40	1/604 (0.2%)
33	e	1.09	0/393	1.59	4/516 (0.8%)
34	f	1.01	0/466	1.38	0/618
35	g	1.06	0/540	1.36	0/718
36	h	0.94	0/186	1.56	0/236
37	j	1.14	1/2497 (0.0%)	1.39	6/3399 (0.2%)
All	All	0.87	15/86034 (0.0%)	1.16	110/124414 (0.1%)

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
1	1	0	2
33	e	0	1
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	137	LYS	CA-C	-8.05	1.47	1.52
7	E	136	ILE	N-CA	-7.51	1.40	1.46
7	E	132	GLY	C-O	-7.46	1.16	1.24
6	D	122	THR	CA-C	-6.87	1.44	1.52
7	E	31	PRO	CA-C	-6.68	1.44	1.52
7	E	129	ILE	C-O	-6.03	1.16	1.24
7	E	136	ILE	CA-C	-5.69	1.48	1.53
18	P	140	THR	C-O	-5.58	1.16	1.23
9	G	121	ILE	CA-C	-5.25	1.47	1.53
21	S	41	ILE	CA-CB	-5.21	1.47	1.54
21	S	40	ILE	N-CA	-5.13	1.40	1.46
37	j	191	HIS	CA-C	-5.11	1.46	1.53
30	b	49	HIS	CA-C	-5.03	1.46	1.52
1	1	821	VAL	N-CA	5.03	1.50	1.46
13	K	82	ASN	CA-C	-5.02	1.44	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	134	GLY	CA-C-N	20.35	145.28	119.84
9	G	134	GLY	C-N-CA	20.35	145.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	j	103	GLY	N-CA-C	15.28	131.07	112.73
8	F	190	LEU	CA-C-N	13.60	133.50	120.03
8	F	190	LEU	C-N-CA	13.60	133.50	120.03
29	a	62	VAL	CA-C-N	13.10	136.22	119.84
29	a	62	VAL	C-N-CA	13.10	136.22	119.84
9	G	132	ARG	N-CA-C	11.63	123.96	111.28
14	L	5	GLN	N-CA-C	11.47	126.62	110.68
29	a	62	VAL	O-C-N	11.20	127.59	120.42
13	K	166	ILE	N-CA-C	11.02	121.86	110.62
37	j	190	GLY	N-CA-C	10.83	125.73	112.73
18	P	137	SER	N-CA-C	10.74	122.74	111.14
7	E	136	ILE	N-CA-C	-10.54	97.11	107.55
1	1	673	VAL	CA-C-N	10.38	132.82	119.84
1	1	673	VAL	C-N-CA	10.38	132.82	119.84
14	L	6	THR	N-CA-C	10.21	122.49	111.36
4	4	83	ASP	N-CA-C	9.79	124.96	109.39
37	j	189	ILE	N-CA-C	9.69	121.85	111.77
4	4	46	ARG	N-CA-C	9.11	121.21	111.28
29	a	69	THR	CB-CA-C	-8.36	98.55	109.92
37	j	102	VAL	N-CA-C	8.30	120.09	112.29
14	L	7	GLU	N-CA-C	8.10	122.43	109.79
1	1	956	ILE	CA-C-N	8.07	129.93	119.84
1	1	956	ILE	C-N-CA	8.07	129.93	119.84
1	1	672	ASN	N-CA-C	7.93	122.45	111.74
4	4	48	GLU	N-CA-C	7.88	122.27	111.39
21	S	40	ILE	N-CA-C	-7.84	96.93	108.54
33	e	8	ARG	N-CA-C	7.70	120.64	111.02
13	K	83	ASN	N-CA-C	7.69	119.66	111.28
9	G	118	GLU	N-CA-C	7.62	119.22	111.07
9	G	134	GLY	C-N-CD	-7.49	94.30	125.00
1	1	622	ASN	N-CA-C	-7.45	99.49	111.04
29	a	69	THR	CA-C-N	7.40	127.26	119.05
29	a	69	THR	C-N-CA	7.40	127.26	119.05
13	K	163	PHE	N-CA-C	7.06	118.62	111.07
10	H	65	PRO	CA-C-N	6.98	125.91	120.33
10	H	65	PRO	C-N-CA	6.98	125.91	120.33
24	V	19	ARG	N-CA-C	6.91	120.94	111.54
2	2	870	A	C4'-C3'-O3'	6.86	119.69	109.40
1	1	728	ASP	N-CA-C	6.86	120.85	111.39
1	1	675	LEU	N-CA-C	6.85	125.39	110.80
30	b	53	VAL	N-CA-C	-6.80	100.80	109.30
24	V	18	HIS	N-CA-C	6.76	119.74	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	111	GLU	N-CA-C	6.69	121.45	113.16
1	1	729	ILE	N-CA-C	6.60	123.07	109.34
1	1	623	VAL	N-CA-C	6.48	122.81	109.34
2	2	1832	A	C2'-C3'-O3'	6.48	123.42	113.70
2	2	1231	C	C2'-C3'-O3'	6.42	123.34	113.70
6	D	208	PRO	CA-C-N	6.40	125.45	120.33
6	D	208	PRO	C-N-CA	6.40	125.45	120.33
9	G	131	ARG	N-CA-C	-6.30	98.26	108.41
9	G	121	ILE	CA-C-N	6.30	127.72	119.84
9	G	121	ILE	C-N-CA	6.30	127.72	119.84
4	4	84	TYR	N-CA-C	-6.22	97.56	110.80
2	2	382	C	C2'-C3'-O3'	6.19	122.98	113.70
37	j	191	HIS	N-CA-C	6.16	117.99	110.41
30	b	49	HIS	N-CA-C	-6.16	97.10	107.99
2	2	1502	C	C2'-C3'-O3'	6.11	122.86	113.70
32	d	22	GLY	CA-C-O	-6.10	118.02	122.23
14	L	5	GLN	N-CA-CB	-6.09	102.78	110.45
4	4	47	LEU	N-CA-C	6.02	123.62	110.80
2	2	958	G	C2'-C3'-O3'	5.99	122.68	113.70
9	G	121	ILE	N-CA-C	-5.97	103.10	108.95
1	1	958	VAL	N-CA-C	5.96	121.75	109.34
2	2	314	U	C2'-C3'-O3'	5.94	122.61	113.70
18	P	139	SER	N-CA-C	5.88	118.12	110.53
33	e	7	ALA	N-CA-C	-5.87	98.87	108.67
4	4	85	GLN	N-CA-C	5.85	117.73	111.36
18	P	135	ILE	CA-C-N	5.83	127.13	119.84
18	P	135	ILE	C-N-CA	5.83	127.13	119.84
4	4	49	ALA	N-CA-C	5.77	117.97	110.53
30	b	3	LEU	N-CA-C	5.77	123.08	110.80
11	I	126	GLY	N-CA-C	5.71	125.73	115.80
9	G	121	ILE	CB-CA-C	-5.68	104.75	110.89
9	G	120	ASP	N-CA-C	5.65	118.44	109.96
4	4	50	MET	CA-C-N	5.60	128.82	120.87
4	4	50	MET	C-N-CA	5.60	128.82	120.87
4	4	103	LEU	O-C-N	5.55	128.72	122.22
2	2	180	G	C2'-C3'-O3'	5.52	121.98	113.70
2	2	291	G	C2'-C3'-O3'	5.46	121.89	113.70
2	2	114	G	C2'-C3'-O3'	5.45	117.68	109.50
37	j	104	HIS	N-CA-C	5.45	117.72	110.53
2	2	980	A	C2'-C3'-O3'	5.43	121.85	113.70
3	3	4	A	C2'-C3'-O3'	5.43	121.84	113.70
7	E	28	ALA	CA-C-N	5.40	124.74	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	28	ALA	C-N-CA	5.40	124.74	118.85
4	4	44	ASN	N-CA-C	-5.39	99.31	110.80
13	K	79	HIS	CA-C-N	5.37	126.05	120.03
13	K	79	HIS	C-N-CA	5.37	126.05	120.03
2	2	102	A	C2'-C3'-O3'	5.36	117.54	109.50
9	G	116	LYS	CA-C-N	5.30	130.69	121.15
9	G	116	LYS	C-N-CA	5.30	130.69	121.15
29	a	68	ILE	N-CA-C	5.25	115.41	107.80
2	2	1565	C	C2'-C3'-O3'	5.22	121.52	113.70
2	2	1558	C	C2'-C3'-O3'	5.19	117.29	109.50
2	2	417	C	C2'-C3'-O3'	5.19	121.48	113.70
6	D	101	SER	N-CA-C	5.17	118.89	112.59
21	S	41	ILE	CA-C-N	5.13	124.75	119.05
21	S	41	ILE	C-N-CA	5.13	124.75	119.05
25	W	100	GLY	CA-C-O	-5.12	117.89	121.88
4	4	104	LYS	N-CA-C	-5.10	105.72	111.28
12	J	163	SER	N-CA-C	5.08	121.04	109.81
2	2	1430	C	C2'-C3'-O3'	5.04	121.26	113.70
3	3	64	C	C2'-C3'-O3'	5.03	121.25	113.70
33	e	3	ALA	CA-C-N	5.03	130.75	121.70
33	e	3	ALA	C-N-CA	5.03	130.75	121.70
4	4	108	GLU	N-CA-C	-5.02	100.11	110.80
21	S	42	PRO	N-CA-C	5.02	120.50	113.53
21	S	40	ILE	CB-CA-C	-5.02	105.21	111.08

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	807	LEU	Peptide
1	1	921	LYS	Mainchain
33	e	3	ALA	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	4901	0	5072	87	0
2	2	35361	0	17850	91	0
3	3	1607	0	815	1	0
4	4	727	0	741	43	0
5	B	1624	0	1634	5	0
5	C	1729	0	1803	5	0
6	D	1682	0	1769	23	0
7	E	2050	0	2156	27	0
8	F	1748	0	1844	20	0
9	G	1831	0	1977	41	0
10	H	1492	0	1585	8	0
11	I	1682	0	1769	13	0
12	J	1499	0	1618	14	0
13	K	1495	0	1549	27	0
14	L	1204	0	1274	16	0
15	M	816	0	841	3	0
16	N	1152	0	1237	2	0
17	O	929	0	959	9	0
18	P	998	0	1019	11	0
19	Q	950	0	991	2	0
20	R	1109	0	1174	17	0
21	S	1066	0	1116	9	0
22	T	1162	0	1221	21	0
23	U	1083	0	1109	5	0
24	V	803	0	873	14	0
25	W	1034	0	1080	5	0
26	X	1098	0	1167	7	0
27	Y	1006	0	1078	24	0
28	Z	625	0	628	4	0
29	a	574	0	627	23	0
30	b	640	0	664	31	0
31	c	792	0	842	1	0
32	d	449	0	470	0	0
33	e	391	0	420	12	0
34	f	455	0	446	1	0
35	g	529	0	536	2	0
36	h	185	0	228	2	0
37	j	2440	0	2396	74	0
38	1	32	0	13	2	0
39	3	23	0	12	0	0
40	c	1	0	0	0	0
40	f	1	0	0	0	0
40	g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	80976	0	64603	593	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 (593) 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)
14:L:4:ILE:CD1	14:L:54:THR:HG22	1.25	1.60
1:1:673:VAL:HG22	1:1:910:MET:CE	1.37	1.52
14:L:4:ILE:HD11	14:L:54:THR:CG2	1.40	1.52
2:2:1521:C:C5	22:T:137:LYS:HG2	1.51	1.44
1:1:884:GLU:OE2	1:1:923:LYS:HB3	1.15	1.30
30:b:6:ASP:OD2	30:b:9:HIS:N	1.60	1.29
37:j:38:LYS:HD2	37:j:63:SER:O	1.27	1.29
29:a:62:VAL:N	29:a:63:PRO:HD2	1.33	1.29
1:1:619:HIS:HA	1:1:622:ASN:OD1	1.14	1.25
1:1:883:LYS:HA	1:1:924:GLU:OE1	1.34	1.24
1:1:883:LYS:HA	1:1:924:GLU:CD	1.63	1.22
2:2:1521:C:C5	22:T:137:LYS:CG	2.22	1.22
30:b:6:ASP:OD2	30:b:9:HIS:CA	1.89	1.21
16:N:56:ASP:OD1	30:b:52:THR:HG22	1.39	1.21
1:1:884:GLU:OE1	1:1:923:LYS:HA	1.42	1.19
13:K:162:ALA:HB2	13:K:172:CYS:SG	1.85	1.17
2:2:1826:G:O2'	4:4:42:LEU:CD2	1.94	1.16
1:1:620:SER:O	1:1:623:VAL:CG1	1.93	1.15
37:j:38:LYS:CD	37:j:63:SER:O	1.95	1.14
8:F:223:ILE:O	37:j:189:ILE:CD1	1.95	1.13
1:1:675:LEU:HD21	1:1:697:GLY:HA2	1.14	1.11
27:Y:12:PHE:CE1	27:Y:48:TYR:OH	2.03	1.11
1:1:673:VAL:CG2	1:1:910:MET:HE1	1.80	1.11
1:1:620:SER:O	1:1:623:VAL:HG13	1.52	1.09
1:1:675:LEU:HD21	1:1:697:GLY:CA	1.84	1.08
1:1:619:HIS:CA	1:1:622:ASN:OD1	2.01	1.07
8:F:223:ILE:O	37:j:189:ILE:HD13	1.53	1.06
9:G:120:ASP:HB3	9:G:125:THR:OG1	1.54	1.06
1:1:673:VAL:CG2	1:1:910:MET:CE	2.32	1.06
2:2:561:A:H4'	12:J:165:TYR:HE1	1.16	1.05
1:1:884:GLU:CD	1:1:923:LYS:HB3	1.81	1.04
14:L:4:ILE:CD1	14:L:54:THR:O	2.05	1.04
12:J:161:LEU:O	12:J:167:GLY:HA3	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1826:G:O2'	4:4:42:LEU:HD23	1.53	1.02
1:1:673:VAL:HG22	1:1:910:MET:HE1	1.03	1.01
29:a:62:VAL:N	29:a:63:PRO:CD	2.24	1.01
33:e:8:ARG:HB3	33:e:8:ARG:HH11	1.26	1.00
24:V:20:ILE:HD12	24:V:20:ILE:H	1.25	0.99
37:j:62:HIS:CE1	37:j:82:SER:HB3	1.98	0.99
2:2:168:C:OP1	9:G:131:ARG:HD3	1.61	0.98
1:1:948:LEU:CD1	1:1:959:LEU:HD12	1.93	0.98
9:G:47:GLY:O	9:G:116:LYS:O	1.80	0.97
30:b:6:ASP:OD1	30:b:8:LEU:HB2	1.64	0.97
8:F:218:LEU:HD12	37:j:192:THR:CG2	1.95	0.97
1:1:884:GLU:OE2	1:1:923:LYS:CB	2.11	0.97
2:2:561:A:H4'	12:J:165:TYR:CE1	2.00	0.97
4:4:84:TYR:OH	33:e:7:ALA:HB1	1.65	0.97
27:Y:12:PHE:HE1	27:Y:48:TYR:HH	1.08	0.96
20:R:97:GLN:NE2	37:j:60:ARG:NH1	2.13	0.96
8:F:218:LEU:HD12	37:j:192:THR:HG23	1.48	0.96
27:Y:10:ARG:HH11	27:Y:10:ARG:HB2	1.29	0.96
30:b:6:ASP:CG	30:b:9:HIS:N	2.25	0.95
6:D:98:LEU:HD13	6:D:132:ASP:OD1	1.66	0.94
29:a:62:VAL:H	29:a:63:PRO:HD2	1.30	0.93
20:R:97:GLN:HE22	37:j:60:ARG:NH1	1.66	0.93
8:F:223:ILE:O	37:j:189:ILE:HD12	1.67	0.93
14:L:4:ILE:HD13	14:L:54:THR:O	1.68	0.93
37:j:256:ILE:HD13	37:j:289:LEU:HD21	1.49	0.91
2:2:167:G:O2'	9:G:131:ARG:HG2	1.68	0.91
1:1:884:GLU:OE1	1:1:923:LYS:CA	2.18	0.91
30:b:5:LYS:HE3	30:b:5:LYS:HA	1.52	0.90
7:E:136:ILE:HG23	7:E:149:TYR:CE1	2.07	0.89
1:1:883:LYS:CA	1:1:924:GLU:OE1	2.21	0.89
1:1:673:VAL:HG22	1:1:910:MET:HE3	1.49	0.89
29:a:68:ILE:O	29:a:109:TYR:N	2.06	0.89
37:j:190:GLY:HA3	37:j:217:MET:HE1	1.55	0.88
1:1:729:ILE:HD11	1:1:757:LYS:C	2.00	0.87
20:R:97:GLN:NE2	37:j:60:ARG:HD2	1.89	0.87
12:J:136:ARG:HG2	12:J:160:SER:HA	1.55	0.87
2:2:1534:C:OP1	13:K:163:PHE:CD1	2.28	0.86
2:2:167:G:O3'	9:G:131:ARG:NE	2.08	0.86
2:2:1521:C:C4	22:T:137:LYS:HG2	2.10	0.86
20:R:97:GLN:HE22	37:j:60:ARG:HH11	1.19	0.86
1:1:948:LEU:HD11	1:1:959:LEU:HD12	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1521:C:H5	22:T:137:LYS:CG	1.88	0.86
14:L:4:ILE:HD12	14:L:54:THR:HG22	1.53	0.85
4:4:104:LYS:HE3	4:4:104:LYS:HA	1.56	0.85
1:1:675:LEU:CD2	1:1:697:GLY:HA2	2.02	0.85
13:K:166:ILE:H	13:K:166:ILE:HD12	1.42	0.84
30:b:6:ASP:OD2	30:b:9:HIS:CB	2.25	0.83
37:j:87:LEU:HD12	37:j:101:PHE:HD2	1.43	0.83
4:4:104:LYS:HE3	4:4:104:LYS:CA	2.08	0.83
9:G:44:GLU:HG3	9:G:121:ILE:HD12	1.59	0.83
30:b:6:ASP:OD2	30:b:9:HIS:C	2.21	0.82
8:F:190:LEU:HB3	8:F:191:PRO:HD2	1.59	0.82
7:E:28:ALA:HB1	7:E:29:PRO:HD2	1.60	0.82
8:F:167:TYR:O	8:F:190:LEU:HD12	1.80	0.82
1:1:624:THR:HG21	1:1:628:LYS:HE2	1.62	0.82
2:2:168:C:OP1	9:G:131:ARG:CD	2.28	0.81
2:2:1521:C:C5	22:T:137:LYS:HG3	2.15	0.81
37:j:62:HIS:CE1	37:j:82:SER:CB	2.63	0.81
1:1:948:LEU:HD13	1:1:959:LEU:HD12	1.60	0.81
14:L:4:ILE:HD11	14:L:54:THR:CB	2.11	0.81
33:e:8:ARG:HH11	33:e:8:ARG:CB	1.93	0.80
13:K:162:ALA:HB2	13:K:172:CYS:HG	1.43	0.80
7:E:28:ALA:HB1	7:E:29:PRO:CD	2.11	0.80
27:Y:10:ARG:HB2	27:Y:10:ARG:NH1	1.96	0.80
4:4:46:ARG:HE	4:4:46:ARG:HA	1.46	0.80
21:S:41:ILE:HD13	21:S:47:ARG:HB2	1.65	0.79
30:b:6:ASP:OD1	30:b:8:LEU:N	2.17	0.78
2:2:1521:C:C4	22:T:137:LYS:CG	2.65	0.78
37:j:12:LYS:HD3	37:j:12:LYS:H	1.47	0.78
13:K:82:ASN:HA	13:K:85:LYS:HD2	1.64	0.77
11:I:120:PRO:HB3	11:I:123:ARG:HG3	1.64	0.77
7:E:136:ILE:HG23	7:E:149:TYR:CZ	2.19	0.77
14:L:4:ILE:CD1	14:L:54:THR:CG2	2.22	0.77
1:1:620:SER:O	1:1:623:VAL:HG11	1.85	0.77
4:4:41:MET:HG3	4:4:47:LEU:CD1	2.16	0.76
2:2:985:G:C4'	18:P:138:ASP:CG	2.42	0.76
9:G:133:LEU:N	9:G:133:LEU:HD22	2.01	0.76
30:b:6:ASP:OD1	30:b:8:LEU:CB	2.34	0.76
30:b:47:PHE:CD2	30:b:49:HIS:O	2.39	0.76
37:j:253:GLY:O	37:j:285:GLN:HA	1.86	0.76
37:j:186:THR:OG1	37:j:188:HIS:NE2	2.19	0.76
10:H:61:ILE:HD11	10:H:176:VAL:HG21	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:97:GLN:HE22	37:j:60:ARG:HD2	1.49	0.75
12:J:161:LEU:O	12:J:167:GLY:CA	2.33	0.75
27:Y:10:ARG:NH1	27:Y:26:ASP:OD1	2.20	0.75
29:a:68:ILE:N	29:a:109:TYR:O	2.18	0.75
1:1:884:GLU:CD	1:1:923:LYS:CB	2.57	0.75
5:C:127:VAL:HG11	5:C:176:VAL:HG13	1.69	0.74
4:4:41:MET:HG3	4:4:47:LEU:HD12	1.69	0.74
1:1:883:LYS:CA	1:1:924:GLU:CD	2.55	0.74
13:K:166:ILE:HD12	13:K:166:ILE:N	2.02	0.74
20:R:97:GLN:NE2	37:j:60:ARG:CZ	2.51	0.74
20:R:97:GLN:HE22	37:j:60:ARG:CD	2.01	0.73
9:G:11:GLY:HA3	9:G:129:VAL:HG11	1.71	0.73
6:D:120:GLN:OE1	6:D:120:GLN:N	2.21	0.73
6:D:102:LEU:HD13	6:D:130:ILE:CD1	2.18	0.72
1:1:675:LEU:HD23	1:1:675:LEU:N	2.03	0.72
33:e:8:ARG:HD2	33:e:8:ARG:O	1.88	0.72
2:2:1534:C:OP1	13:K:163:PHE:HD1	1.71	0.72
27:Y:12:PHE:HE1	27:Y:48:TYR:OH	1.53	0.72
37:j:12:LYS:HD3	37:j:12:LYS:N	2.05	0.71
4:4:109:LEU:N	4:4:109:LEU:HD23	2.04	0.71
4:4:84:TYR:OH	26:X:68:LYS:HE3	1.89	0.71
29:a:67:LEU:HD23	29:a:67:LEU:O	1.91	0.71
9:G:121:ILE:CG2	9:G:122:PRO:HD2	2.21	0.70
24:V:20:ILE:HG23	24:V:116:ILE:HG12	1.74	0.70
37:j:186:THR:CG2	37:j:188:HIS:NE2	2.54	0.70
37:j:256:ILE:HD11	37:j:286:CYS:SG	2.32	0.70
2:2:168:C:O2'	9:G:133:LEU:O	2.08	0.70
15:M:15:LEU:HD22	15:M:49:MET:HE1	1.73	0.70
1:1:673:VAL:HG22	1:1:910:MET:HE2	1.66	0.69
37:j:11:LEU:HD23	37:j:11:LEU:N	2.07	0.69
7:E:29:PRO:HG2	7:E:46:ILE:HD11	1.74	0.69
26:X:51:VAL:HG13	26:X:70:VAL:HG13	1.75	0.69
29:a:68:ILE:HG12	29:a:110:THR:HA	1.74	0.69
27:Y:10:ARG:NH1	27:Y:26:ASP:CG	2.51	0.68
37:j:186:THR:OG1	37:j:188:HIS:CE1	2.46	0.68
11:I:124:LYS:HD3	11:I:124:LYS:N	2.08	0.68
14:L:4:ILE:HD11	14:L:54:THR:O	1.92	0.68
4:4:104:LYS:HA	4:4:104:LYS:CE	2.24	0.67
4:4:109:LEU:O	4:4:111:GLU:N	2.25	0.67
1:1:673:VAL:HA	1:1:910:MET:HE3	1.77	0.67
1:1:729:ILE:HG23	1:1:755:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:6:ASP:OD2	30:b:9:HIS:HB2	1.95	0.67
29:a:61:GLU:C	29:a:63:PRO:HD2	2.16	0.66
29:a:68:ILE:HG12	29:a:110:THR:CA	1.76	0.66
2:2:1636:G:O2'	13:K:164:ARG:NH1	2.29	0.66
1:1:826:HIS:CE1	38:1:1301:GNP:HN22	2.13	0.66
1:1:884:GLU:CD	1:1:923:LYS:CA	2.68	0.66
2:2:1826:G:O2'	4:4:42:LEU:HD21	1.94	0.66
37:j:104:HIS:CE1	37:j:124:SER:HB3	2.30	0.66
6:D:102:LEU:HD13	6:D:130:ILE:HD11	1.78	0.65
2:2:1521:C:H5	22:T:137:LYS:HG3	1.58	0.65
6:D:98:LEU:CD1	6:D:132:ASP:OD1	2.44	0.65
30:b:6:ASP:OD1	30:b:8:LEU:CA	2.44	0.65
1:1:673:VAL:O	1:1:698:MET:O	2.14	0.65
28:Z:64:GLU:HG3	30:b:3:LEU:HD13	1.79	0.65
27:Y:10:ARG:NH1	27:Y:26:ASP:OD2	2.28	0.65
37:j:186:THR:HG21	37:j:188:HIS:NE2	2.11	0.65
1:1:883:LYS:HA	1:1:924:GLU:OE2	1.97	0.65
2:2:1534:C:OP1	13:K:163:PHE:CE1	2.49	0.64
30:b:54:VAL:CG1	30:b:63:LEU:HB2	2.28	0.64
24:V:20:ILE:HG21	24:V:98:VAL:HG11	1.80	0.64
37:j:59:LEU:N	37:j:59:LEU:HD23	2.12	0.64
9:G:44:GLU:CG	9:G:121:ILE:HD12	2.27	0.64
1:1:956:ILE:O	1:1:956:ILE:HG13	1.97	0.63
27:Y:9:THR:CG2	27:Y:23:MET:HB2	2.28	0.63
2:2:1521:C:C6	22:T:137:LYS:HG2	2.26	0.63
9:G:121:ILE:HG23	9:G:122:PRO:HD2	1.80	0.63
13:K:166:ILE:H	13:K:166:ILE:CD1	2.12	0.63
8:F:218:LEU:HD12	37:j:192:THR:HG22	1.79	0.63
27:Y:12:PHE:CZ	27:Y:48:TYR:CE2	2.86	0.63
30:b:5:LYS:HD2	30:b:5:LYS:N	2.14	0.63
18:P:44:VAL:HG11	18:P:85:CYS:SG	2.39	0.63
27:Y:12:PHE:CZ	27:Y:48:TYR:CZ	2.86	0.63
1:1:727:VAL:HB	1:1:755:LEU:HD13	1.81	0.62
4:4:82:ARG:O	4:4:82:ARG:HG2	1.99	0.62
10:H:101:LEU:HD12	10:H:102:PRO:HD2	1.80	0.62
1:1:729:ILE:HD11	1:1:758:ILE:N	2.13	0.62
9:G:132:ARG:HE	9:G:133:LEU:HD21	1.64	0.62
30:b:6:ASP:OD1	30:b:9:HIS:N	2.33	0.62
2:2:985:G:H4'	18:P:138:ASP:OD1	1.98	0.62
27:Y:12:PHE:HZ	27:Y:48:TYR:CE2	2.17	0.62
2:2:1823:A:H2'	4:4:44:ASN:HD21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:20:ILE:HD12	24:V:20:ILE:N	2.07	0.61
11:I:129:LEU:HD23	11:I:134:GLU:HB3	1.83	0.61
4:4:104:LYS:HE3	4:4:104:LYS:O	2.00	0.61
20:R:97:GLN:NE2	37:j:60:ARG:CD	2.58	0.61
1:1:675:LEU:HD23	1:1:675:LEU:H	1.64	0.61
7:E:129:ILE:HD12	7:E:139:LEU:HD23	1.83	0.61
21:S:58:MET:HE2	21:S:58:MET:HA	1.83	0.61
2:2:985:G:H4'	18:P:138:ASP:CG	2.26	0.61
13:K:102:LEU:O	29:a:66:LYS:HD2	2.01	0.60
2:2:984:C:H1'	18:P:138:ASP:O	2.01	0.60
4:4:109:LEU:HB3	4:4:110:PRO:HD2	1.83	0.60
9:G:120:ASP:CB	9:G:125:THR:OG1	2.40	0.60
13:K:165:ASN:HD21	13:K:167:LYS:HG2	1.66	0.60
21:S:17:ILE:HD12	21:S:58:MET:HE3	1.83	0.60
11:I:121:LEU:O	11:I:123:ARG:CD	2.50	0.60
37:j:102:VAL:O	37:j:102:VAL:HG22	2.01	0.60
37:j:256:ILE:HD13	37:j:289:LEU:CD2	2.26	0.60
37:j:236:ILE:HA	37:j:251:ALA:O	2.02	0.60
5:B:198:MET:HE2	5:B:200:ASP:HB2	1.84	0.60
37:j:189:ILE:HG22	37:j:189:ILE:O	2.01	0.60
4:4:104:LYS:HE3	4:4:104:LYS:C	2.27	0.59
9:G:135:PRO:HB2	9:G:141:ILE:HG12	1.83	0.59
12:J:78:LEU:HD23	12:J:97:ILE:HD11	1.84	0.59
1:1:623:VAL:HG23	1:1:623:VAL:O	2.03	0.59
2:2:496:C:H4'	7:E:28:ALA:O	2.02	0.59
30:b:54:VAL:HG13	30:b:63:LEU:HD12	1.84	0.59
2:2:1450:G:OP2	21:S:44:LYS:NZ	2.35	0.59
30:b:47:PHE:HD2	30:b:49:HIS:O	1.84	0.59
37:j:104:HIS:CD2	37:j:130:LYS:HG3	2.36	0.59
2:2:71:G:N2	2:2:79:A:N7	2.51	0.59
7:E:131:VAL:HG23	7:E:137:PRO:HA	1.85	0.59
2:2:168:C:P	9:G:131:ARG:HD3	2.42	0.58
37:j:234:ASP:H	37:j:252:THR:HG23	1.69	0.58
1:1:923:LYS:N	1:1:923:LYS:HD3	2.18	0.58
37:j:23:THR:HG22	37:j:31:ILE:HG22	1.85	0.58
2:2:615:C:O2	33:e:11:LYS:HE3	2.04	0.58
4:4:48:GLU:O	4:4:48:GLU:HG3	2.03	0.58
1:1:958:VAL:HG23	1:1:958:VAL:O	2.03	0.58
1:1:612:ILE:HD11	1:1:956:ILE:CG2	2.34	0.58
37:j:10:THR:HG23	37:j:10:THR:O	2.02	0.57
4:4:46:ARG:HE	4:4:46:ARG:CA	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:103:GLY:H	37:j:132:TRP:HH2	1.51	0.57
1:1:729:ILE:CD1	1:1:757:LYS:O	2.53	0.57
2:2:1618:C:O4'	2:2:1618:C:O2	2.23	0.57
30:b:5:LYS:HE3	30:b:5:LYS:CA	2.22	0.57
4:4:106:TYR:HD2	4:4:106:TYR:N	2.02	0.57
4:4:82:ARG:HG3	33:e:7:ALA:CB	2.35	0.57
24:V:20:ILE:H	24:V:20:ILE:CD1	1.97	0.57
10:H:61:ILE:HD11	10:H:176:VAL:CG2	2.36	0.56
12:J:136:ARG:HG3	12:J:158:ASP:O	2.05	0.56
37:j:189:ILE:HD12	37:j:189:ILE:N	2.20	0.56
1:1:624:THR:CG2	1:1:628:LYS:HE2	2.35	0.56
2:2:1091:C:HO2'	25:W:2:VAL:N	2.03	0.56
9:G:119:LYS:HB2	9:G:119:LYS:NZ	2.17	0.56
4:4:39:ILE:HG13	4:4:39:ILE:O	2.05	0.56
24:V:20:ILE:HG12	24:V:98:VAL:HG21	1.86	0.56
7:E:129:ILE:HG23	7:E:129:ILE:O	2.05	0.56
20:R:97:GLN:HE22	37:j:60:ARG:CZ	2.15	0.56
28:Z:55:ILE:HD11	28:Z:69:ILE:HD11	1.86	0.56
6:D:96:PHE:C	6:D:96:PHE:CD2	2.84	0.56
1:1:729:ILE:HD13	1:1:758:ILE:HG22	1.87	0.56
8:F:190:LEU:CB	8:F:191:PRO:HD2	2.23	0.56
4:4:50:MET:HG3	4:4:50:MET:O	2.04	0.56
25:W:111:MET:HE3	25:W:116:ALA:HA	1.87	0.56
2:2:808:A:O2'	2:2:809:A:O4'	2.24	0.56
9:G:8:PRO:O	9:G:131:ARG:NH2	2.39	0.56
4:4:109:LEU:C	4:4:111:GLU:H	2.11	0.55
17:O:12:MET:HE1	17:O:17:ALA:HB2	1.88	0.55
37:j:14:HIS:NE2	37:j:41:ILE:HG22	2.21	0.55
37:j:234:ASP:H	37:j:252:THR:CG2	2.18	0.55
13:K:87:LEU:HD11	20:R:47:LEU:HD11	1.88	0.55
1:1:729:ILE:HD11	1:1:757:LYS:O	2.06	0.55
16:N:56:ASP:OD1	30:b:52:THR:CG2	2.33	0.55
2:2:1521:C:N4	22:T:137:LYS:HD3	2.22	0.55
4:4:112:HIS:C	4:4:112:HIS:CD2	2.85	0.55
17:O:49:LEU:HD11	17:O:77:ILE:HG12	1.89	0.55
24:V:21:ARG:HG2	24:V:115:THR:OG1	2.07	0.55
30:b:5:LYS:HA	30:b:5:LYS:CE	2.29	0.55
7:E:138:HIS:CE1	7:E:148:ARG:HG2	2.42	0.55
37:j:166:VAL:HG12	37:j:176:VAL:HG22	1.88	0.54
2:2:615:C:O2	33:e:11:LYS:CE	2.55	0.54
11:I:123:ARG:HD2	11:I:123:ARG:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:168:C:P	9:G:131:ARG:HE	2.30	0.54
2:2:297:A:H5'	7:E:132:GLY:HA2	1.90	0.54
37:j:190:GLY:HA3	37:j:217:MET:CE	2.34	0.54
1:1:729:ILE:CD1	1:1:758:ILE:HG22	2.38	0.54
37:j:11:LEU:HD23	37:j:11:LEU:H	1.72	0.54
2:2:297:A:C5'	7:E:132:GLY:HA2	2.38	0.54
4:4:106:TYR:N	4:4:106:TYR:CD2	2.73	0.54
6:D:88:ILE:HG21	6:D:94:ILE:HD11	1.88	0.54
13:K:82:ASN:OD1	13:K:82:ASN:N	2.41	0.54
29:a:66:LYS:HB2	29:a:66:LYS:NZ	2.23	0.54
37:j:103:GLY:HA3	37:j:132:TRP:HH2	1.72	0.54
6:D:113:GLN:HA	6:D:121:ARG:O	2.07	0.54
6:D:101:SER:O	6:D:132:ASP:HB3	2.08	0.54
7:E:30:ARG:O	7:E:30:ARG:HG3	2.07	0.53
7:E:136:ILE:CG2	7:E:149:TYR:CZ	2.91	0.53
2:2:561:A:C4'	12:J:165:TYR:CE1	2.86	0.53
4:4:41:MET:O	4:4:41:MET:HG2	2.08	0.53
14:L:4:ILE:HD11	14:L:54:THR:HG22	0.55	0.53
9:G:120:ASP:N	9:G:120:ASP:OD1	2.41	0.53
9:G:135:PRO:HB2	9:G:141:ILE:CG1	2.39	0.53
24:V:17:ILE:HA	24:V:94:PRO:HA	1.90	0.53
27:Y:12:PHE:CZ	27:Y:48:TYR:OH	2.47	0.53
2:2:615:C:O2	33:e:11:LYS:NZ	2.42	0.53
17:O:24:THR:HG21	17:O:117:GLU:HG2	1.90	0.53
37:j:104:HIS:CE1	37:j:124:SER:CB	2.91	0.53
2:2:616:A:N3	33:e:12:VAL:HG21	2.23	0.52
6:D:66:LEU:HD11	6:D:81:ILE:HD12	1.90	0.52
9:G:67:VAL:HG12	9:G:69:THR:HG22	1.92	0.52
17:O:25:ALA:HB3	17:O:31:LEU:HD21	1.92	0.52
18:P:102:GLY:O	18:P:136:PRO:HG3	2.10	0.52
4:4:84:TYR:OH	26:X:68:LYS:CE	2.58	0.52
11:I:120:PRO:CB	11:I:123:ARG:HG3	2.36	0.52
24:V:101:ILE:HD12	24:V:104:ILE:HD11	1.92	0.52
29:a:66:LYS:NZ	29:a:66:LYS:CB	2.73	0.52
6:D:96:PHE:C	6:D:96:PHE:HD2	2.18	0.52
2:2:927:C:O2	30:b:51:GLN:OE1	2.27	0.52
7:E:87:MET:HE1	7:E:236:ILE:HD13	1.90	0.52
26:X:100:VAL:HG13	26:X:122:VAL:HG13	1.92	0.52
2:2:1521:C:H2'	22:T:136:THR:O	2.09	0.51
5:C:103:MET:HE1	5:C:212:VAL:O	2.10	0.51
8:F:192:TRP:O	8:F:200:PRO:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:704:PRO:HD2	1:1:712:LEU:HD22	1.92	0.51
1:1:957:PRO:HB2	1:1:958:VAL:HG13	1.91	0.51
1:1:884:GLU:OE1	1:1:923:LYS:CB	2.58	0.51
2:2:1540:G:OP1	23:U:39:LEU:HD12	2.11	0.51
4:4:109:LEU:C	4:4:111:GLU:N	2.69	0.51
9:G:133:LEU:HD22	9:G:133:LEU:H	1.76	0.51
37:j:87:LEU:HD21	37:j:108:VAL:HG11	1.92	0.51
2:2:1491:G:H1'	24:V:72:GLU:HG2	1.93	0.51
37:j:38:LYS:HD3	37:j:63:SER:O	2.01	0.51
1:1:823:THR:HG21	1:1:834:LEU:HD11	1.93	0.51
1:1:622:ASN:ND2	1:1:622:ASN:N	2.59	0.50
2:2:1139:C:O4'	2:2:1139:C:O2	2.28	0.50
2:2:1535:U:O3'	13:K:88:MET:HE1	2.11	0.50
7:E:130:PHE:HE1	7:E:140:VAL:HG23	1.76	0.50
14:L:4:ILE:CG1	14:L:54:THR:O	2.59	0.50
20:R:97:GLN:NE2	37:j:60:ARG:HH11	1.87	0.50
2:2:4:C:H4'	6:D:207:ALA:HB2	1.93	0.50
37:j:256:ILE:CD1	37:j:289:LEU:HD21	2.33	0.50
1:1:675:LEU:HD13	1:1:695:ILE:HG23	1.94	0.50
13:K:78:MET:HG3	13:K:159:ARG:NH2	2.26	0.50
22:T:80:PRO:HG2	23:U:36:THR:HG21	1.93	0.50
1:1:667:GLN:HE22	1:1:914:ARG:HA	1.76	0.50
1:1:805:ALA:HB1	1:1:820:LEU:CD2	2.41	0.50
13:K:87:LEU:O	13:K:90:VAL:HG12	2.12	0.50
8:F:196:GLY:O	8:F:201:LYS:NZ	2.45	0.50
2:2:1521:C:N4	22:T:137:LYS:CG	2.74	0.50
21:S:41:ILE:HG21	21:S:47:ARG:HB2	1.92	0.49
4:4:102:SER:O	4:4:105:ALA:HB3	2.11	0.49
2:2:168:C:P	9:G:131:ARG:NE	2.84	0.49
18:P:44:VAL:HG13	18:P:53:ILE:HB	1.93	0.49
37:j:62:HIS:CE1	37:j:82:SER:HB2	2.45	0.49
37:j:189:ILE:HD12	37:j:189:ILE:H	1.76	0.49
5:B:97:THR:HG21	5:B:117:ARG:HD3	1.93	0.49
12:J:136:ARG:HB3	12:J:160:SER:OG	2.12	0.49
27:Y:9:THR:HG21	27:Y:12:PHE:CE1	2.47	0.49
9:G:119:LYS:NZ	9:G:119:LYS:CB	2.73	0.49
15:M:14:LEU:HD22	15:M:35:LEU:HD21	1.94	0.49
1:1:884:GLU:N	1:1:924:GLU:OE1	2.44	0.49
8:F:195:THR:HG22	8:F:195:THR:O	2.13	0.49
37:j:41:ILE:HD11	37:j:55:PRO:HB3	1.94	0.49
2:2:1534:C:OP2	13:K:163:PHE:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:22:LEU:HD13	17:O:31:LEU:HD22	1.95	0.49
27:Y:9:THR:HG22	27:Y:23:MET:HB2	1.95	0.49
12:J:136:ARG:HG2	12:J:160:SER:CA	2.37	0.49
2:2:984:C:O2	18:P:138:ASP:HB3	2.13	0.48
14:L:2:ALA:HB3	14:L:5:GLN:HB2	1.95	0.48
27:Y:12:PHE:HZ	27:Y:48:TYR:CZ	2.30	0.48
30:b:54:VAL:HG12	30:b:63:LEU:HB2	1.95	0.48
14:L:4:ILE:O	14:L:4:ILE:HG22	2.14	0.48
37:j:103:GLY:N	37:j:132:TRP:HH2	2.11	0.48
2:2:1222:G:H5''	13:K:78:MET:HE1	1.94	0.48
11:I:121:LEU:O	11:I:123:ARG:HD2	2.13	0.48
11:I:121:LEU:O	11:I:123:ARG:HD3	2.13	0.48
26:X:101:LEU:HB3	26:X:124:LYS:HB2	1.95	0.48
28:Z:64:GLU:HG3	30:b:3:LEU:CD1	2.44	0.48
2:2:984:C:O2	18:P:138:ASP:CB	2.61	0.48
37:j:11:LEU:H	37:j:11:LEU:CD2	2.25	0.48
29:a:79:ILE:HG23	29:a:83:LEU:HD23	1.96	0.48
1:1:632:PRO:HG3	1:1:842:THR:HG21	1.96	0.48
7:E:44:LEU:HD11	7:E:72:ILE:HD11	1.96	0.48
27:Y:12:PHE:CZ	27:Y:23:MET:HE3	2.49	0.48
31:c:44:ILE:HG23	31:c:45:VAL:HG23	1.94	0.48
1:1:910:MET:HE2	1:1:910:MET:HA	1.96	0.47
2:2:853:C:O4'	2:2:853:C:O2	2.29	0.47
2:2:1706:G:H4'	36:h:1:MET:HE2	1.95	0.47
35:g:132:MET:HE3	35:g:139:HIS:HB3	1.96	0.47
1:1:729:ILE:H	1:1:755:LEU:HD12	1.79	0.47
21:S:41:ILE:HD13	21:S:47:ARG:CB	2.39	0.47
1:1:884:GLU:HB3	1:1:923:LYS:O	2.15	0.47
22:T:34:LYS:HG2	22:T:103:LEU:HD23	1.95	0.47
7:E:31:PRO:CG	7:E:38:LEU:HG	2.45	0.47
27:Y:10:ARG:NH1	27:Y:10:ARG:CB	2.73	0.47
1:1:671:THR:HB	1:1:700:ILE:HG13	1.95	0.47
1:1:981:VAL:HG13	1:1:1033:VAL:HG23	1.97	0.47
2:2:1826:G:HO2'	4:4:42:LEU:HD23	1.72	0.47
2:2:1598:G:H3'	29:a:80:ARG:HD2	1.96	0.47
7:E:136:ILE:HD13	7:E:136:ILE:N	2.30	0.47
13:K:103:LEU:HA	29:a:66:LYS:HG3	1.95	0.47
24:V:18:HIS:CE1	24:V:19:ARG:HD3	2.49	0.47
37:j:254:PRO:HB3	37:j:283:PRO:CG	2.45	0.47
37:j:101:PHE:N	37:j:101:PHE:CD1	2.79	0.47
10:H:173:PHE:HA	10:H:176:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:138:THR:HG23	22:T:139:THR:HG23	1.97	0.47
11:I:124:LYS:N	11:I:124:LYS:CD	2.72	0.46
12:J:119:LEU:HD23	12:J:159:PHE:CE2	2.50	0.46
2:2:643:A:OP1	12:J:38:ARG:NH1	2.47	0.46
22:T:20:ILE:HD11	22:T:33:ILE:HG13	1.96	0.46
1:1:826:HIS:CE1	38:1:1301:GNP:N2	2.81	0.46
4:4:47:LEU:HB3	4:4:59:CYS:SG	2.54	0.46
1:1:1094:ILE:HD12	1:1:1125:MET:HE2	1.96	0.46
22:T:137:LYS:HB3	22:T:137:LYS:HE2	1.52	0.46
24:V:18:HIS:NE2	24:V:19:ARG:HD3	2.31	0.46
37:j:254:PRO:HB3	37:j:283:PRO:HG2	1.97	0.46
1:1:865:ALA:HB2	1:1:1010:ILE:HG22	1.98	0.46
2:2:1848:U:O2	2:2:1848:U:O4'	2.33	0.46
8:F:123:LEU:HD11	8:F:152:PHE:HB3	1.97	0.46
11:I:128:LYS:HA	11:I:128:LYS:HD2	1.74	0.46
14:L:2:ALA:N	14:L:5:GLN:HB2	2.31	0.46
20:R:32:ILE:HD13	20:R:68:ILE:HG12	1.98	0.46
9:G:10:THR:HB	9:G:129:VAL:HG23	1.98	0.46
13:K:41:VAL:HG13	13:K:41:VAL:O	2.16	0.46
3:3:12:G:H1	3:3:21:G:H22	1.62	0.46
30:b:5:LYS:CA	30:b:5:LYS:CE	2.86	0.46
4:4:100:ALA:HB1	4:4:113:ALA:HB1	1.98	0.46
6:D:98:LEU:HA	6:D:98:LEU:HD23	1.56	0.46
10:H:66:VAL:N	10:H:67:PRO:HD2	2.30	0.46
29:a:88:LEU:HD12	29:a:109:TYR:CD2	2.51	0.46
2:2:1599:U:C5	13:K:166:ILE:HG13	2.51	0.46
6:D:209:VAL:HG21	6:D:233:LEU:HD22	1.98	0.46
8:F:193:ASP:OD2	8:F:198:ILE:N	2.48	0.46
37:j:234:ASP:N	37:j:252:THR:HG23	2.30	0.45
4:4:84:TYR:CZ	33:e:7:ALA:HB1	2.50	0.45
17:O:106:CYS:SG	17:O:109:VAL:HG22	2.56	0.45
7:E:131:VAL:HG23	7:E:137:PRO:CA	2.45	0.45
37:j:94:THR:HG23	37:j:96:THR:HG22	1.98	0.45
2:2:1858:G:OP2	18:P:146:ARG:NH2	2.45	0.45
37:j:87:LEU:HD12	37:j:101:PHE:CD2	2.35	0.45
4:4:101:ARG:O	4:4:104:LYS:HB3	2.16	0.45
7:E:31:PRO:O	7:E:31:PRO:HG2	2.15	0.45
8:F:192:TRP:O	8:F:192:TRP:CD1	2.70	0.45
13:K:78:MET:HG3	13:K:159:ARG:HH22	1.82	0.45
1:1:714:ASN:HA	1:1:715:ARG:C	2.42	0.45
11:I:29:LEU:HD12	11:I:29:LEU:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:119:LYS:HB2	9:G:119:LYS:HZ3	1.79	0.45
9:G:133:LEU:N	9:G:133:LEU:CD2	2.71	0.45
5:B:19:LEU:HD11	21:S:106:LEU:HD11	1.99	0.45
10:H:29:GLU:HA	10:H:32:MET:HE2	1.99	0.45
13:K:166:ILE:O	13:K:166:ILE:HG22	2.16	0.45
14:L:126:VAL:CG2	14:L:142:VAL:HG13	2.47	0.45
27:Y:10:ARG:HH12	27:Y:26:ASP:CG	2.16	0.44
2:2:1149:A:H2'	2:2:1149:A:N3	2.32	0.44
19:Q:20:VAL:HG21	19:Q:36:LEU:HD21	1.99	0.44
24:V:70:CYS:SG	24:V:71:GLY:N	2.90	0.44
25:W:104:LEU:HD23	25:W:125:ILE:HA	1.99	0.44
2:2:1661:A:OP1	34:f:19:ARG:NH2	2.49	0.44
4:4:109:LEU:CB	4:4:111:GLU:OE2	2.66	0.44
1:1:675:LEU:CD1	1:1:695:ILE:HG23	2.47	0.44
1:1:1091:PRO:HB2	1:1:1209:LEU:HD21	2.00	0.44
2:2:1753:C:O2	2:2:1780:G:N2	2.51	0.44
8:F:192:TRP:CD1	8:F:192:TRP:C	2.90	0.44
11:I:78:ILE:HG23	11:I:102:VAL:CG1	2.47	0.44
25:W:53:ILE:HD13	30:b:24:LEU:HD11	1.98	0.44
1:1:672:ASN:OD1	1:1:699:LEU:HD13	2.18	0.44
1:1:675:LEU:CD2	1:1:675:LEU:H	2.27	0.44
2:2:1604:G:H2'	2:2:1604:G:N3	2.32	0.44
4:4:41:MET:HG3	4:4:47:LEU:HD11	1.96	0.44
14:L:66:VAL:HG11	14:L:141:ASN:HD22	1.83	0.44
23:U:37:VAL:HG12	23:U:38:LYS:O	2.18	0.44
1:1:651:LEU:HD22	1:1:673:VAL:HG21	1.98	0.44
29:a:66:LYS:CB	29:a:66:LYS:HZ2	2.31	0.44
22:T:84:LEU:HD12	22:T:96:SER:C	2.43	0.43
1:1:673:VAL:HA	1:1:674:PRO:HD3	1.62	0.43
2:2:1310:U:H5''	35:g:130:VAL:HG13	1.99	0.43
20:R:51:LEU:HD11	20:R:81:ILE:HG23	1.99	0.43
33:e:11:LYS:HZ2	33:e:11:LYS:HG2	1.59	0.43
2:2:1465:A:OP1	21:S:60:ARG:NH1	2.52	0.43
2:2:1521:C:H41	22:T:137:LYS:HG3	1.84	0.43
9:G:10:THR:HB	9:G:129:VAL:CG2	2.49	0.43
22:T:22:GLY:HA2	22:T:56:ALA:HB3	2.00	0.43
28:Z:64:GLU:CG	30:b:3:LEU:HD13	2.46	0.43
1:1:729:ILE:HG23	1:1:755:LEU:CD1	2.46	0.43
6:D:102:LEU:HD13	6:D:130:ILE:HG12	2.00	0.43
6:D:102:LEU:HD23	6:D:102:LEU:HA	1.56	0.43
37:j:87:LEU:HD22	37:j:111:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:964:ILE:HD13	1:1:967:LEU:HD11	2.01	0.43
20:R:39:LEU:HD22	20:R:51:LEU:HD23	2.00	0.43
8:F:162:ASP:N	8:F:163:PRO:CD	2.82	0.43
10:H:69:LEU:HD13	10:H:96:ALA:HB2	2.00	0.43
6:D:102:LEU:HD13	6:D:130:ILE:CG1	2.49	0.43
7:E:45:ILE:HA	7:E:61:VAL:HG11	2.00	0.43
1:1:1015:LYS:HA	1:1:1018:VAL:HG12	2.01	0.43
5:C:136:ARG:HB2	5:C:218:LEU:HD11	2.01	0.43
9:G:2:LYS:HB2	9:G:108:VAL:HG12	2.01	0.43
1:1:857:ARG:N	1:1:879:ASN:O	2.47	0.42
17:O:24:THR:HG22	17:O:115:GLY:HA3	2.00	0.42
20:R:97:GLN:NE2	37:j:60:ARG:NE	2.67	0.42
37:j:14:HIS:CE1	37:j:41:ILE:HB	2.54	0.42
4:4:46:ARG:CA	4:4:46:ARG:NE	2.82	0.42
7:E:124:CYS:HB3	7:E:141:THR:OG1	2.18	0.42
27:Y:55:ILE:HD12	27:Y:75:ILE:HG22	2.01	0.42
29:a:66:LYS:HD3	29:a:66:LYS:HA	1.68	0.42
37:j:129:ILE:CD1	37:j:151:VAL:HG11	2.48	0.42
2:2:167:G:HO2'	9:G:131:ARG:HG2	1.78	0.42
2:2:168:C:O2	9:G:133:LEU:HD23	2.19	0.42
2:2:494:C:N4	2:2:509:G:H21	2.17	0.42
4:4:39:ILE:HD13	4:4:50:MET:CB	2.49	0.42
7:E:234:PRO:HG3	7:E:238:LEU:HD11	2.01	0.42
8:F:190:LEU:HB3	8:F:191:PRO:CD	2.42	0.42
1:1:639:HIS:CD2	1:1:640:VAL:HG22	2.53	0.42
1:1:729:ILE:HD11	1:1:758:ILE:CA	2.49	0.42
1:1:1116:ALA:HB1	1:1:1209:LEU:HD13	2.00	0.42
13:K:163:PHE:CD2	13:K:164:ARG:HG3	2.53	0.42
22:T:132:ARG:HB2	22:T:134:GLN:HE22	1.83	0.42
11:I:90:LEU:HD23	11:I:95:THR:HB	2.01	0.42
1:1:1093:LYS:HB3	1:1:1116:ALA:HB3	2.01	0.42
7:E:131:VAL:HG22	7:E:135:GLY:HA2	2.02	0.42
17:O:89:VAL:HG21	17:O:109:VAL:HG21	2.02	0.42
26:X:46:HIS:CD2	26:X:103:ALA:HB2	2.54	0.42
1:1:673:VAL:CA	1:1:910:MET:HE3	2.45	0.42
12:J:81:LEU:CD1	12:J:97:ILE:HD12	2.49	0.42
20:R:51:LEU:CD1	20:R:81:ILE:HG23	2.49	0.42
2:2:1231:C:H2'	2:2:1232:U:O4'	2.18	0.42
4:4:109:LEU:HB2	4:4:111:GLU:OE2	2.19	0.42
6:D:120:GLN:N	6:D:120:GLN:CD	2.73	0.42
15:M:12:TYR:CE1	15:M:52:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:10:ARG:HB3	27:Y:24:VAL:HB	2.01	0.42
2:2:1521:C:N4	22:T:137:LYS:HG3	2.35	0.42
9:G:11:GLY:CA	9:G:129:VAL:HG11	2.45	0.42
19:Q:56:LEU:HD22	19:Q:80:LEU:HD12	2.01	0.42
23:U:39:LEU:HD21	23:U:52:TRP:CZ3	2.54	0.42
6:D:168:GLY:N	6:D:179:THR:O	2.48	0.42
1:1:831:MET:HA	1:1:834:LEU:HD12	2.02	0.41
2:2:168:C:P	9:G:131:ARG:CD	3.06	0.41
2:2:1647:A:OP1	20:R:138:ARG:NH2	2.53	0.41
6:D:108:LYS:HD2	6:D:233:LEU:HD12	2.01	0.41
29:a:68:ILE:HB	29:a:109:TYR:HB2	1.23	0.41
37:j:12:LYS:N	37:j:12:LYS:CD	2.75	0.41
1:1:729:ILE:HG13	1:1:757:LYS:O	2.20	0.41
9:G:38:ALA:HB1	9:G:41:LEU:HD13	2.01	0.41
37:j:172:LYS:HD2	37:j:193:GLY:H	1.85	0.41
5:C:35:ALA:HB2	5:C:44:ILE:HD11	2.01	0.41
9:G:135:PRO:HG3	9:G:144:LEU:HD22	2.02	0.41
27:Y:12:PHE:CE1	27:Y:48:TYR:CZ	2.98	0.41
2:2:1520:G:N3	2:2:1520:G:H2'	2.34	0.41
9:G:116:LYS:HA	9:G:116:LYS:HD2	1.52	0.41
5:B:76:VAL:HG12	5:B:123:VAL:HB	2.03	0.41
7:E:130:PHE:CD1	7:E:130:PHE:N	2.87	0.41
2:2:953:C:H2'	2:2:954:U:O4'	2.20	0.41
2:2:1825:A:C8	4:4:41:MET:CE	3.03	0.41
29:a:88:LEU:HD12	29:a:109:TYR:CG	2.55	0.41
30:b:53:VAL:HG13	30:b:62:VAL:HG23	2.02	0.41
37:j:257:LYS:HD3	37:j:259:TRP:CZ2	2.55	0.41
4:4:84:TYR:HB2	4:4:85:GLN:H	1.57	0.41
6:D:117:ARG:H	6:D:117:ARG:HG3	1.55	0.41
21:S:41:ILE:HD13	21:S:41:ILE:HG21	1.82	0.41
29:a:69:THR:HG22	29:a:106:GLN:NE2	2.35	0.41
30:b:6:ASP:OD2	30:b:9:HIS:O	2.37	0.41
2:2:1284:A:HO2'	17:O:106:CYS:HG	1.68	0.41
1:1:723:ALA:HB3	1:1:751:PHE:HB3	2.02	0.41
2:2:427:U:O2	2:2:427:U:O4'	2.38	0.41
2:2:1035:A:H2'	2:2:1036:A:O4'	2.20	0.41
2:2:1669:G:OP1	24:V:79:ARG:NH1	2.53	0.41
2:2:1741:U:H2'	2:2:1742:C:O4'	2.21	0.41
5:B:197:VAL:HG13	5:B:201:LEU:HD23	2.02	0.41
8:F:163:PRO:HA	8:F:166:TYR:CE2	2.55	0.41
9:G:120:ASP:HB3	9:G:125:THR:CB	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:93:VAL:HG21	10:H:133:LEU:HD12	2.02	0.41
26:X:68:LYS:HB3	26:X:91:LEU:HD22	2.02	0.41
33:e:8:ARG:CB	33:e:8:ARG:NH1	2.72	0.41
2:2:823:U:O2	2:2:823:U:O4'	2.37	0.41
2:2:831:G:N7	27:Y:11:LYS:NZ	2.66	0.41
6:D:114:LYS:HE3	6:D:121:ARG:HH21	1.85	0.41
9:G:136:LYS:HE2	9:G:175:LYS:O	2.21	0.41
36:h:1:MET:HE1	36:h:9:ARG:CZ	2.51	0.41
37:j:104:HIS:ND1	37:j:124:SER:CB	2.84	0.41
2:2:984:C:C2'	18:P:138:ASP:HB3	2.51	0.40
13:K:102:LEU:HD11	29:a:100:VAL:HG21	2.03	0.40
13:K:165:ASN:ND2	13:K:167:LYS:HG2	2.33	0.40
29:a:62:VAL:HB	29:a:63:PRO:CD	2.51	0.40
1:1:729:ILE:CD1	1:1:758:ILE:HA	2.52	0.40
2:2:1037:G:H4'	2:2:1845:A:H4'	2.02	0.40
5:C:103:MET:HE2	5:C:188:LEU:HD22	2.03	0.40
6:D:93:ILE:HG23	6:D:97:PHE:HE2	1.87	0.40
9:G:44:GLU:CG	9:G:121:ILE:CD1	2.97	0.40
27:Y:12:PHE:CZ	27:Y:23:MET:CE	3.04	0.40
25:W:53:ILE:CD1	30:b:24:LEU:HD11	2.52	0.40
2:2:501:C:O2	2:2:501:C:H2'	2.21	0.40
7:E:129:ILE:O	7:E:129:ILE:CG2	2.70	0.40
8:F:190:LEU:CB	8:F:191:PRO:CD	2.95	0.40
23:U:76:THR:HG22	23:U:94:ARG:HB3	2.04	0.40
12:J:163:SER:HA	12:J:164:PRO:HD3	1.92	0.40
14:L:2:ALA:HB3	14:L:5:GLN:CG	2.51	0.40
37:j:239:LEU:HD23	37:j:250:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	617/619 (100%)	518 (84%)	87 (14%)	12 (2%)	6	33
4	4	88/90 (98%)	72 (82%)	14 (16%)	2 (2%)	5	29
5	B	204/419 (49%)	196 (96%)	7 (3%)	1 (0%)	24	59
5	C	211/419 (50%)	198 (94%)	13 (6%)	0	100	100
6	D	216/218 (99%)	207 (96%)	8 (4%)	1 (0%)	24	59
7	E	256/258 (99%)	240 (94%)	16 (6%)	0	100	100
8	F	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
9	G	224/226 (99%)	211 (94%)	10 (4%)	3 (1%)	9	40
10	H	183/185 (99%)	174 (95%)	8 (4%)	1 (0%)	24	59
11	I	203/205 (99%)	186 (92%)	15 (7%)	2 (1%)	12	45
12	J	178/180 (99%)	168 (94%)	9 (5%)	1 (1%)	21	56
13	K	187/189 (99%)	173 (92%)	13 (7%)	1 (0%)	24	59
14	L	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
15	M	95/97 (98%)	86 (90%)	8 (8%)	1 (1%)	11	43
16	N	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
17	O	118/120 (98%)	111 (94%)	6 (5%)	1 (1%)	16	50
18	P	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	16	50
19	Q	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
20	R	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
21	S	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	16	50
22	T	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	52
23	U	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
24	V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
25	W	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
26	X	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	18	52
27	Y	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
28	Z	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
29	a	70/72 (97%)	66 (94%)	3 (4%)	1 (1%)	9	39
30	b	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
31	c	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
32	d	56/58 (97%)	56 (100%)	0	0	100	100
33	e	47/51 (92%)	45 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	f	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
35	g	63/65 (97%)	54 (86%)	9 (14%)	0	100	100
36	h	17/19 (90%)	17 (100%)	0	0	100	100
37	j	312/314 (99%)	284 (91%)	25 (8%)	3 (1%)	12	45
All	All	5434/5927 (92%)	5044 (93%)	356 (7%)	34 (1%)	23	56

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	675	LEU
1	1	729	ILE
9	G	130	PRO
9	G	135	PRO
26	X	86	PRO
37	j	63	SER
1	1	710	SER
1	1	916	LYS
12	J	23	SER
1	1	674	PRO
6	D	190	SER
11	I	156	ALA
13	K	41	VAL
15	M	37	ASP
1	1	686	LYS
1	1	762	TYR
4	4	81	LEU
5	B	44	ASP
21	S	72	LYS
22	T	100	ALA
37	j	13	GLY
1	1	713	ARG
1	1	955	GLU
1	1	1090	PHE
1	1	1137	ILE
1	1	1144	ASN
9	G	122	PRO
10	H	89	GLY
11	I	132	GLU
17	O	55	ASN
29	a	63	PRO
18	P	136	PRO

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Mol	Chain	Res	Type
37	j	254	PRO
4	4	110	PRO

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	
1	1	544/544 (100%)	535 (98%)	9 (2%)	53	75
4	4	76/76 (100%)	70 (92%)	6 (8%)	11	40
5	B	172/366 (47%)	171 (99%)	1 (1%)	78	84
5	C	194/366 (53%)	194 (100%)	0	100	100
6	D	182/184 (99%)	178 (98%)	4 (2%)	45	71
7	E	221/221 (100%)	219 (99%)	2 (1%)	70	81
8	F	188/189 (100%)	187 (100%)	1 (0%)	81	85
9	G	197/197 (100%)	193 (98%)	4 (2%)	48	72
10	H	166/166 (100%)	166 (100%)	0	100	100
11	I	178/178 (100%)	178 (100%)	0	100	100
12	J	160/160 (100%)	159 (99%)	1 (1%)	78	84
13	K	159/159 (100%)	156 (98%)	3 (2%)	50	73
14	L	133/133 (100%)	132 (99%)	1 (1%)	73	82
15	M	88/88 (100%)	88 (100%)	0	100	100
16	N	124/124 (100%)	123 (99%)	1 (1%)	73	82
17	O	101/101 (100%)	101 (100%)	0	100	100
18	P	103/104 (99%)	103 (100%)	0	100	100
19	Q	104/104 (100%)	104 (100%)	0	100	100
20	R	115/115 (100%)	115 (100%)	0	100	100
21	S	118/119 (99%)	117 (99%)	1 (1%)	73	82
22	T	122/122 (100%)	120 (98%)	2 (2%)	55	75
23	U	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	V	93/93 (100%)	90 (97%)	3 (3%)	34	65
25	W	112/112 (100%)	112 (100%)	0	100	100
26	X	113/113 (100%)	113 (100%)	0	100	100
27	Y	107/107 (100%)	104 (97%)	3 (3%)	38	68
28	Z	66/66 (100%)	66 (100%)	0	100	100
29	a	64/64 (100%)	61 (95%)	3 (5%)	23	57
30	b	74/74 (100%)	72 (97%)	2 (3%)	39	68
31	c	86/86 (100%)	86 (100%)	0	100	100
32	d	51/51 (100%)	50 (98%)	1 (2%)	48	72
33	e	36/37 (97%)	35 (97%)	1 (3%)	38	68
34	f	48/48 (100%)	48 (100%)	0	100	100
35	g	58/58 (100%)	58 (100%)	0	100	100
36	h	18/18 (100%)	18 (100%)	0	100	100
37	j	272/272 (100%)	265 (97%)	7 (3%)	40	69
All	All	4753/5125 (93%)	4697 (99%)	56 (1%)	61	79

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	622	ASN
1	1	645	THR
1	1	671	THR
1	1	729	ILE
1	1	910	MET
1	1	922	HIS
1	1	958	VAL
1	1	1167	GLU
1	1	1209	LEU
4	4	46	ARG
4	4	47	LEU
4	4	84	TYR
4	4	104	LYS
4	4	106	TYR
4	4	112	HIS
5	B	130	ASP
6	D	96	PHE
6	D	102	LEU

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Mol	Chain	Res	Type
6	D	116	THR
6	D	122	THR
7	E	129	ILE
7	E	139	LEU
8	F	190	LEU
9	G	116	LYS
9	G	119	LYS
9	G	120	ASP
9	G	133	LEU
12	J	161	LEU
13	K	82	ASN
13	K	87	LEU
13	K	166	ILE
14	L	104	LYS
16	N	122	ILE
21	S	77	GLU
22	T	137	LYS
22	T	138	THR
24	V	17	ILE
24	V	20	ILE
24	V	72	GLU
27	Y	10	ARG
27	Y	12	PHE
27	Y	51	THR
29	a	66	LYS
29	a	67	LEU
29	a	68	ILE
30	b	6	ASP
30	b	52	THR
32	d	57	THR
33	e	8	ARG
37	j	10	THR
37	j	11	LEU
37	j	12	LYS
37	j	60	ARG
37	j	62	HIS
37	j	189	ILE
37	j	192	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	667	GLN
1	1	731	HIS
1	1	742	ASN
1	1	811	ASN
1	1	1074	GLN
1	1	1079	GLN
1	1	1081	GLN
1	1	1103	ASN
1	1	1189	GLN
4	4	33	GLN
4	4	85	GLN
4	4	112	HIS
5	B	113	GLN
5	C	75	GLN
5	C	157	GLN
5	C	186	ASN
7	E	67	GLN
7	E	138	HIS
8	F	101	GLN
8	F	226	GLN
9	G	56	ASN
9	G	65	GLN
9	G	163	ASN
9	G	177	GLN
12	J	75	ASN
12	J	154	GLN
12	J	177	ASN
13	K	31	ASN
13	K	114	ASN
13	K	118	ASN
14	L	18	GLN
14	L	108	ASN
14	L	141	ASN
15	M	39	ASN
15	M	42	ASN
16	N	49	GLN
17	O	28	HIS
18	P	20	GLN
18	P	38	ASN
20	R	77	HIS
20	R	80	GLN
20	R	97	GLN
21	S	62	GLN

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Mol	Chain	Res	Type
22	T	11	HIS
24	V	85	HIS
25	W	120	HIS
26	X	31	HIS
26	X	63	ASN
26	X	73	GLN
27	Y	85	ASN
28	Z	35	ASN
30	b	9	HIS
30	b	51	GLN
33	e	22	GLN
35	g	111	ASN
37	j	4	GLN
37	j	76	GLN
37	j	215	GLN
37	j	244	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1646/1656 (99%)	363 (22%)	36 (2%)
3	3	74/75 (98%)	22 (29%)	2 (2%)
All	All	1720/1731 (99%)	385 (22%)	38 (2%)

All (385) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	2	A
2	2	3	C
2	2	4	C
2	2	11	A
2	2	17	C
2	2	33	G
2	2	42	A
2	2	46	A
2	2	54	A
2	2	56	G
2	2	58	C
2	2	65	C
2	2	67	C
2	2	68	A

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Mol	Chain	Res	Type
2	2	72	C
2	2	73	C
2	2	74	G
2	2	75	G
2	2	76	U
2	2	77	A
2	2	79	A
2	2	99	A
2	2	103	A
2	2	113	G
2	2	115	U
2	2	116	U
2	2	122	G
2	2	127	C
2	2	130	G
2	2	143	U
2	2	147	A
2	2	155	G
2	2	161	U
2	2	181	A
2	2	182	C
2	2	184	G
2	2	188	C
2	2	189	U
2	2	191	A
2	2	209	A
2	2	291	G
2	2	292	A
2	2	295	C
2	2	308	G
2	2	310	C
2	2	315	C
2	2	318	A
2	2	319	C
2	2	321	C
2	2	331	C
2	2	333	G
2	2	335	G
2	2	338	G
2	2	347	G
2	2	351	G
2	2	360	A

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Mol	Chain	Res	Type
2	2	362	C
2	2	364	A
2	2	369	C
2	2	370	G
2	2	377	G
2	2	382	C
2	2	383	G
2	2	385	G
2	2	386	C
2	2	398	A
2	2	400	C
2	2	407	G
2	2	408	A
2	2	409	C
2	2	418	A
2	2	421	G
2	2	429	C
2	2	438	G
2	2	441	C
2	2	448	A
2	2	449	A
2	2	450	C
2	2	459	C
2	2	464	A
2	2	465	A
2	2	466	G
2	2	471	G
2	2	472	C
2	2	473	A
2	2	474	G
2	2	487	U
2	2	488	U
2	2	489	A
2	2	492	C
2	2	500	A
2	2	501	C
2	2	502	C
2	2	507	G
2	2	508	A
2	2	517	C
2	2	532	C
2	2	533	A

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Mol	Chain	Res	Type
2	2	534	G
2	2	535	G
2	2	537	C
2	2	541	U
2	2	542	U
2	2	547	G
2	2	548	C
2	2	553	U
2	2	556	U
2	2	559	G
2	2	560	A
2	2	568	C
2	2	573	U
2	2	574	A
2	2	590	A
2	2	591	U
2	2	592	C
2	2	593	C
2	2	594	A
2	2	595	U
2	2	603	C
2	2	606	G
2	2	607	U
2	2	608	C
2	2	614	C
2	2	615	C
2	2	617	G
2	2	626	G
2	2	629	A
2	2	631	U
2	2	643	A
2	2	644	G
2	2	650	A
2	2	655	A
2	2	660	C
2	2	668	A
2	2	669	A
2	2	670	A
2	2	671	A
2	2	672	A
2	2	673	G
2	2	688	U

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Mol	Chain	Res	Type
2	2	796	G
2	2	799	U
2	2	809	A
2	2	812	A
2	2	821	G
2	2	822	U
2	2	823	U
2	2	824	C
2	2	830	A
2	2	844	U
2	2	847	A
2	2	856	C
2	2	865	A
2	2	869	A
2	2	870	A
2	2	871	U
2	2	872	A
2	2	873	G
2	2	874	G
2	2	877	C
2	2	878	G
2	2	879	C
2	2	880	G
2	2	887	U
2	2	890	U
2	2	891	G
2	2	894	G
2	2	898	U
2	2	906	U
2	2	907	G
2	2	913	A
2	2	914	U
2	2	919	A
2	2	920	A
2	2	924	G
2	2	930	C
2	2	933	G
2	2	934	G
2	2	943	U
2	2	955	A
2	2	958	G
2	2	959	G

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Mol	Chain	Res	Type
2	2	970	G
2	2	971	G
2	2	973	C
2	2	981	A
2	2	990	A
2	2	992	A
2	2	998	A
2	2	999	G
2	2	1001	A
2	2	1002	U
2	2	1016	U
2	2	1017	U
2	2	1023	A
2	2	1040	G
2	2	1041	G
2	2	1044	G
2	2	1045	U
2	2	1047	C
2	2	1049	A
2	2	1060	A
2	2	1061	U
2	2	1062	A
2	2	1067	C
2	2	1083	A
2	2	1085	C
2	2	1089	G
2	2	1096	G
2	2	1112	U
2	2	1115	U
2	2	1118	C
2	2	1119	A
2	2	1121	G
2	2	1123	C
2	2	1133	A
2	2	1138	C
2	2	1139	C
2	2	1148	A
2	2	1153	C
2	2	1154	U
2	2	1157	G
2	2	1165	G
2	2	1166	G

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Mol	Chain	Res	Type
2	2	1171	G
2	2	1195	A
2	2	1199	A
2	2	1201	U
2	2	1202	U
2	2	1203	G
2	2	1207	G
2	2	1215	C
2	2	1217	A
2	2	1218	C
2	2	1221	G
2	2	1224	G
2	2	1232	U
2	2	1235	G
2	2	1236	G
2	2	1240	A
2	2	1242	U
2	2	1243	U
2	2	1251	A
2	2	1256	G
2	2	1257	G
2	2	1259	A
2	2	1274	G
2	2	1275	G
2	2	1301	A
2	2	1302	G
2	2	1303	C
2	2	1313	A
2	2	1317	C
2	2	1318	G
2	2	1319	U
2	2	1320	G
2	2	1325	G
2	2	1331	C
2	2	1333	U
2	2	1335	G
2	2	1336	C
2	2	1342	U
2	2	1348	G
2	2	1358	U
2	2	1371	U
2	2	1372	U

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Mol	Chain	Res	Type
2	2	1378	A
2	2	1382	A
2	2	1398	G
2	2	1403	C
2	2	1416	C
2	2	1426	U
2	2	1431	G
2	2	1432	U
2	2	1440	C
2	2	1441	U
2	2	1445	U
2	2	1454	A
2	2	1462	U
2	2	1464	C
2	2	1465	A
2	2	1466	G
2	2	1477	U
2	2	1480	A
2	2	1489	A
2	2	1490	G
2	2	1493	C
2	2	1494	U
2	2	1498	A
2	2	1503	C
2	2	1507	G
2	2	1509	U
2	2	1515	G
2	2	1521	C
2	2	1522	A
2	2	1526	G
2	2	1528	G
2	2	1533	A
2	2	1536	G
2	2	1551	U
2	2	1559	C
2	2	1560	U
2	2	1566	G
2	2	1569	A
2	2	1570	G
2	2	1571	G
2	2	1572	C
2	2	1578	U

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Mol	Chain	Res	Type
2	2	1579	A
2	2	1580	A
2	2	1581	C
2	2	1588	A
2	2	1604	G
2	2	1605	G
2	2	1609	C
2	2	1610	G
2	2	1612	G
2	2	1615	U
2	2	1616	U
2	2	1618	C
2	2	1621	U
2	2	1623	A
2	2	1638	G
2	2	1639	G
2	2	1641	A
2	2	1654	G
2	2	1659	U
2	2	1665	G
2	2	1671	G
2	2	1674	G
2	2	1675	A
2	2	1686	G
2	2	1692	U
2	2	1695	A
2	2	1699	A
2	2	1722	G
2	2	1729	U
2	2	1748	G
2	2	1751	C
2	2	1752	C
2	2	1756	C
2	2	1775	U
2	2	1783	C
2	2	1785	C
2	2	1786	U
2	2	1800	A
2	2	1812	U
2	2	1824	A
2	2	1825	A
2	2	1826	G

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Mol	Chain	Res	Type
2	2	1829	G
2	2	1833	C
2	2	1835	A
2	2	1838	U
2	2	1849	G
2	2	1851	A
2	2	1861	G
2	2	1862	G
2	2	1863	A
2	2	1864	U
2	2	1865	C
2	2	1866	A
2	2	1867	U
3	3	5	G
3	3	8	U
3	3	9	G
3	3	10	G
3	3	16	C
3	3	18	G
3	3	20	A
3	3	21	G
3	3	22	C
3	3	23	G
3	3	41	A
3	3	47	C
3	3	50	U
3	3	54	U
3	3	56	G
3	3	59	A
3	3	61	C
3	3	62	A
3	3	63	U
3	3	65	C
3	3	74	C
3	3	75	A

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	72	C
2	2	102	A
2	2	114	G

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Mol	Chain	Res	Type
2	2	180	G
2	2	291	G
2	2	314	U
2	2	332	G
2	2	382	C
2	2	417	C
2	2	448	A
2	2	465	A
2	2	488	U
2	2	500	A
2	2	593	C
2	2	594	A
2	2	655	A
2	2	670	A
2	2	811	A
2	2	870	A
2	2	958	G
2	2	980	A
2	2	1016	U
2	2	1165	G
2	2	1231	C
2	2	1425	G
2	2	1430	C
2	2	1440	C
2	2	1464	C
2	2	1502	C
2	2	1519	U
2	2	1535	U
2	2	1558	C
2	2	1565	C
2	2	1622	U
2	2	1734	G
2	2	1832	A
3	3	4	A
3	3	64	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
39	5GP	3	101	-	22,25,26	0.37	0	32,37,40	0.32	0
38	GNP	1	1301	-	34,34,34	1.15	5 (14%)	47,54,54	0.87	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	5GP	3	101	-	-	2/7/25/26	0/3/3/3
38	GNP	1	1301	-	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	1301	GNP	PG-O1G	3.37	1.51	1.46
38	1	1301	GNP	PB-O1B	2.98	1.50	1.46
38	1	1301	GNP	PB-O2B	-2.29	1.50	1.56
38	1	1301	GNP	PG-O2G	-2.15	1.51	1.56
38	1	1301	GNP	PG-O3G	-2.12	1.51	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	1301	GNP	O2B-PB-O1B	3.85	118.12	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	1301	GNP	O3G-PG-O1G	-2.01	108.41	113.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	1	1301	GNP	PB-N3B-PG-O1G
38	1	1301	GNP	PG-N3B-PB-O1B
38	1	1301	GNP	C5'-O5'-PA-O3A
38	1	1301	GNP	C5'-O5'-PA-O2A
39	3	101	5GP	O4'-C4'-C5'-O5'
39	3	101	5GP	C3'-C4'-C5'-O5'
38	1	1301	GNP	PG-N3B-PB-O3A

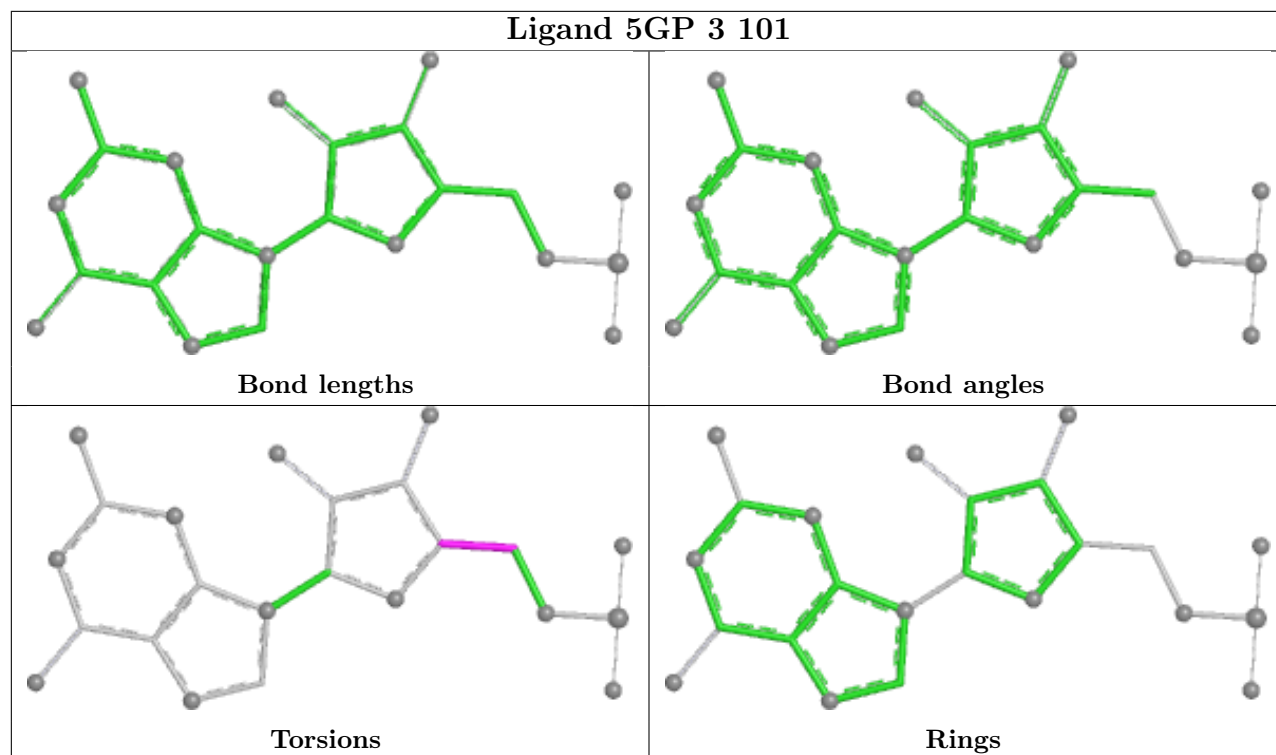
There are no ring outliers.

1 monomer is involved in 2 short contacts:

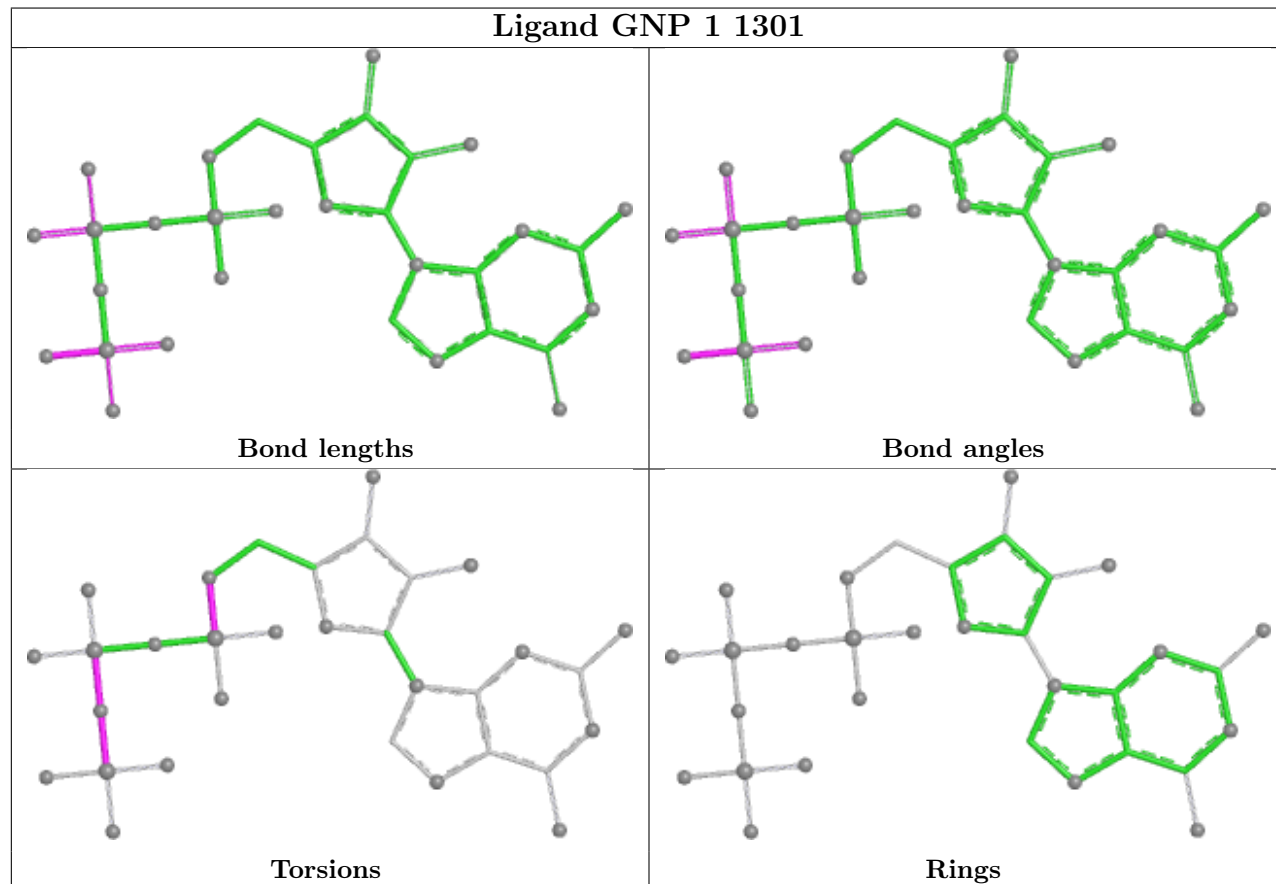
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	1	1301	GNP	2	0

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

Ligand 5GP 3 101



Ligand GNP 1 1301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	10
33	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	834:C	O3'	841:G	P	18.33
1	2	130:G	O3'	140:U	P	17.28
1	2	1416:C	O3'	1424:G	P	17.27
1	2	747:U	O3'	795:A	P	16.72
1	2	1761:U	O3'	1771:G	P	15.57
1	2	688:U	O3'	746:C	P	15.21
1	2	322:C	O3'	329:G	P	15.08
1	e	45:VAL	C	53:LYS	N	12.35
1	2	1551:U	O3'	1558:C	P	8.82
1	2	225:G	O3'	287:U	P	7.52
1	2	1432:U	O3'	1438:A	P	5.22

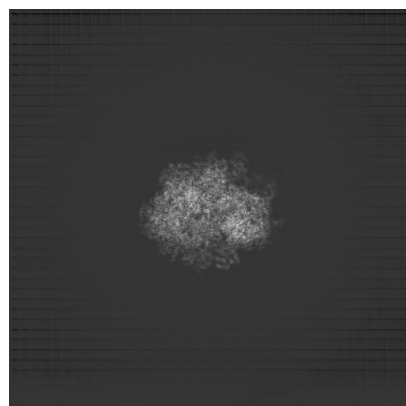
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26067. These allow visual inspection of the internal detail of the map and identification of artifacts.

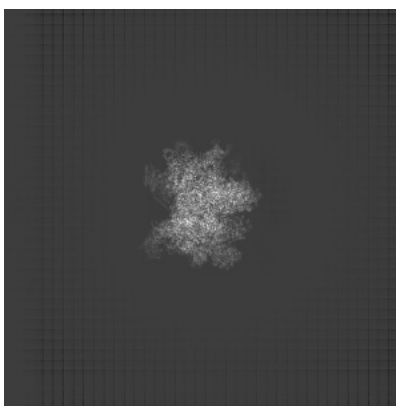
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

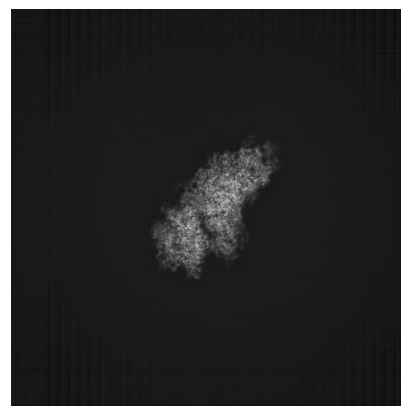
6.1.1 Primary map



X

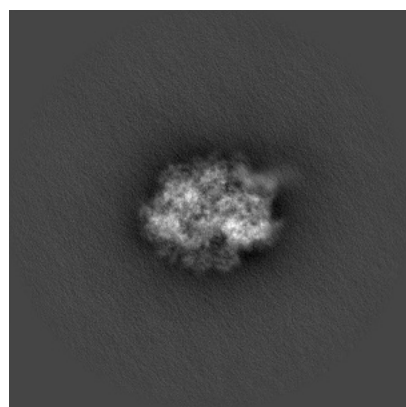


Y

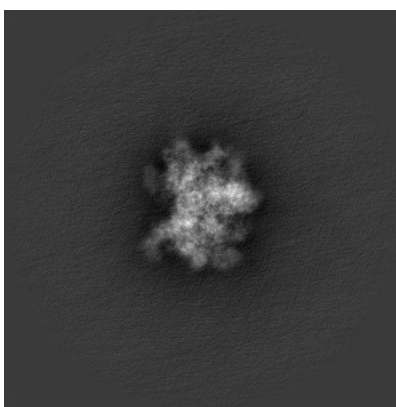


Z

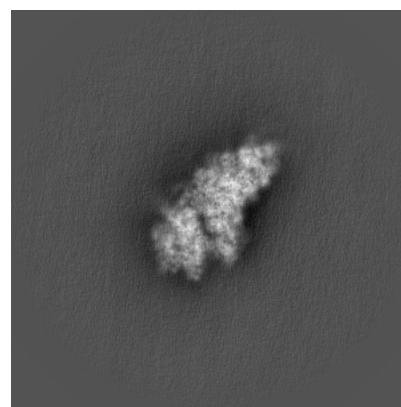
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

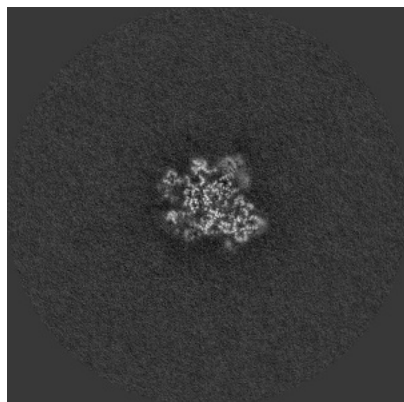


Y Index: 240

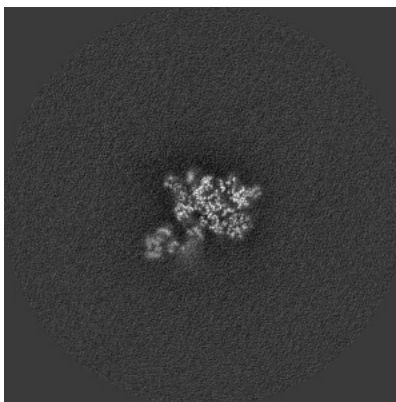


Z Index: 240

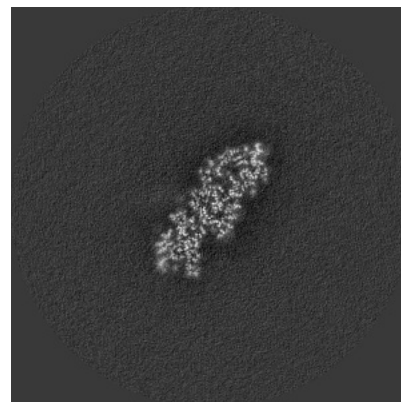
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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: 259

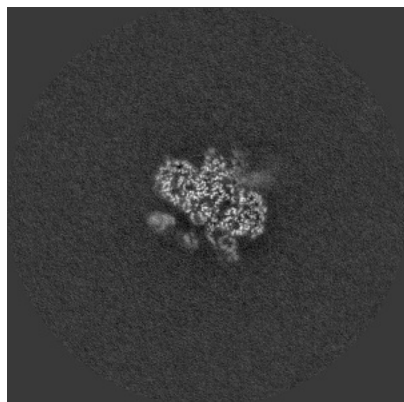


Y Index: 238

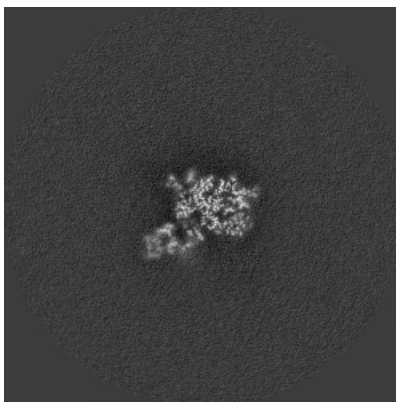


Z Index: 252

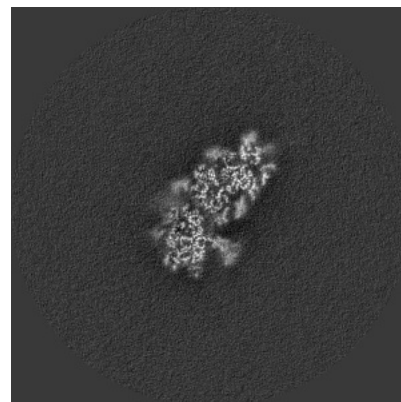
6.3.2 Raw map



X Index: 259



Y Index: 238

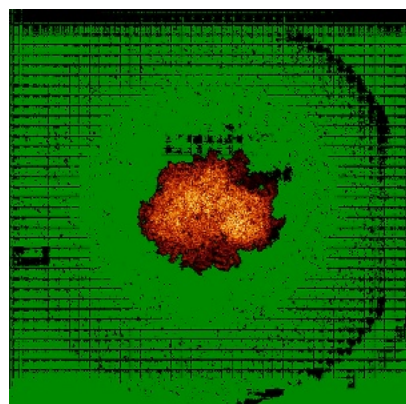


Z Index: 223

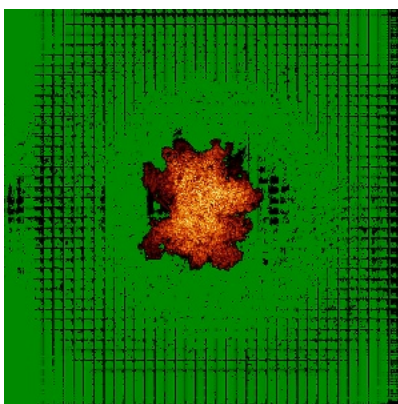
The images above show the largest variance slices of the map in three orthogonal directions.

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

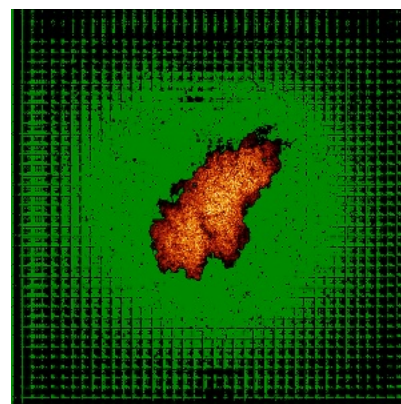
6.4.1 Primary map



X

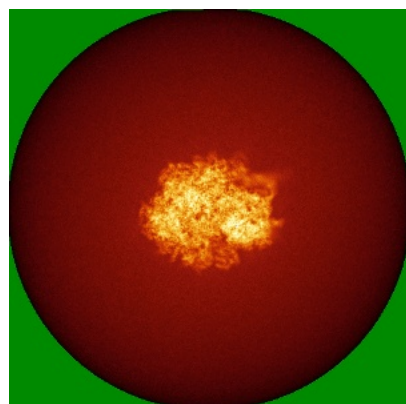


Y

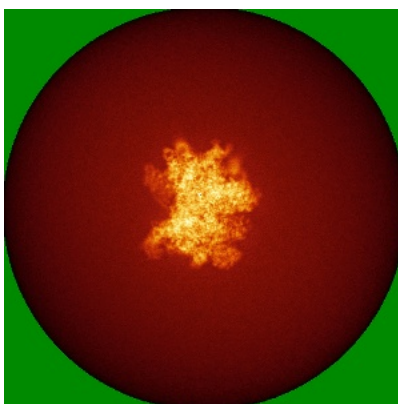


Z

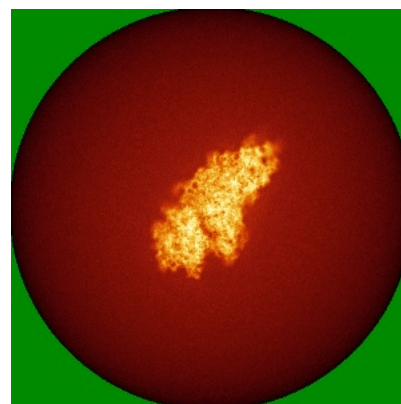
6.4.2 Raw map



X



Y

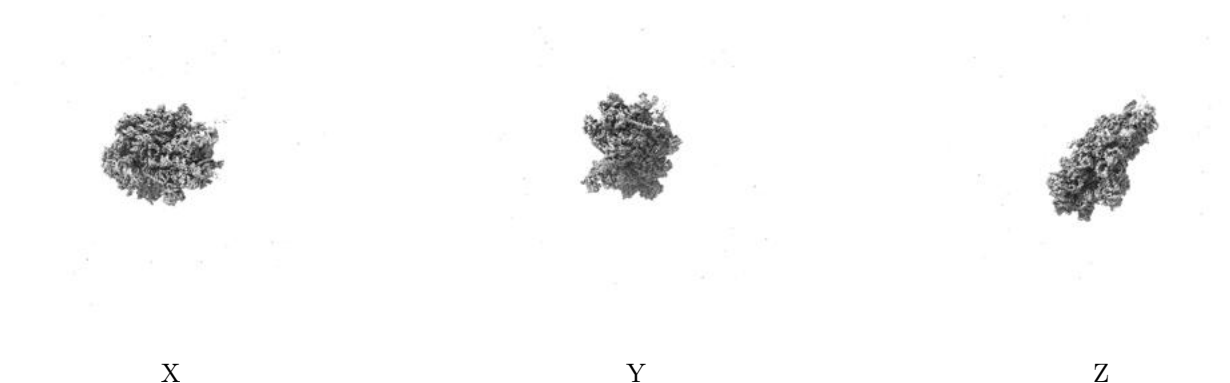


Z

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

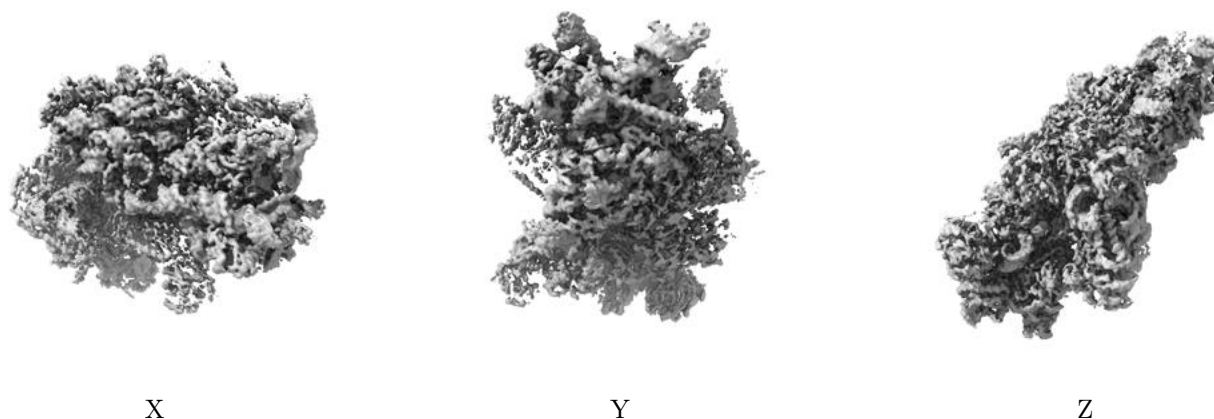
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

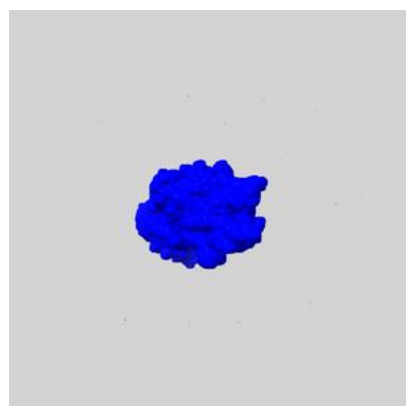
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

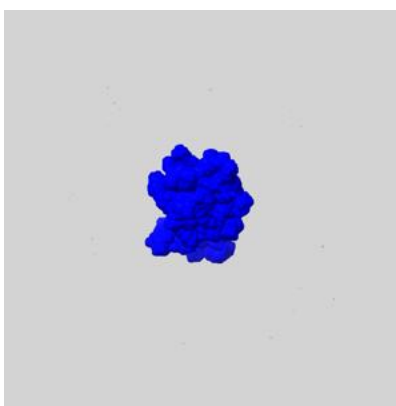
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

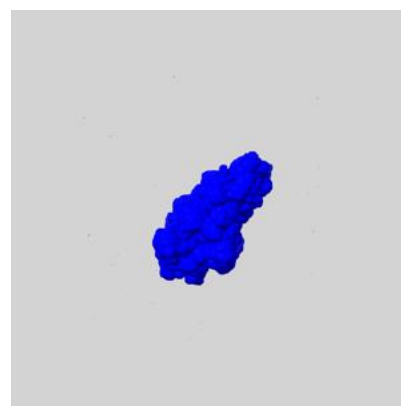
6.6.1 emd_26067_msk_1.map [i](#)



X



Y

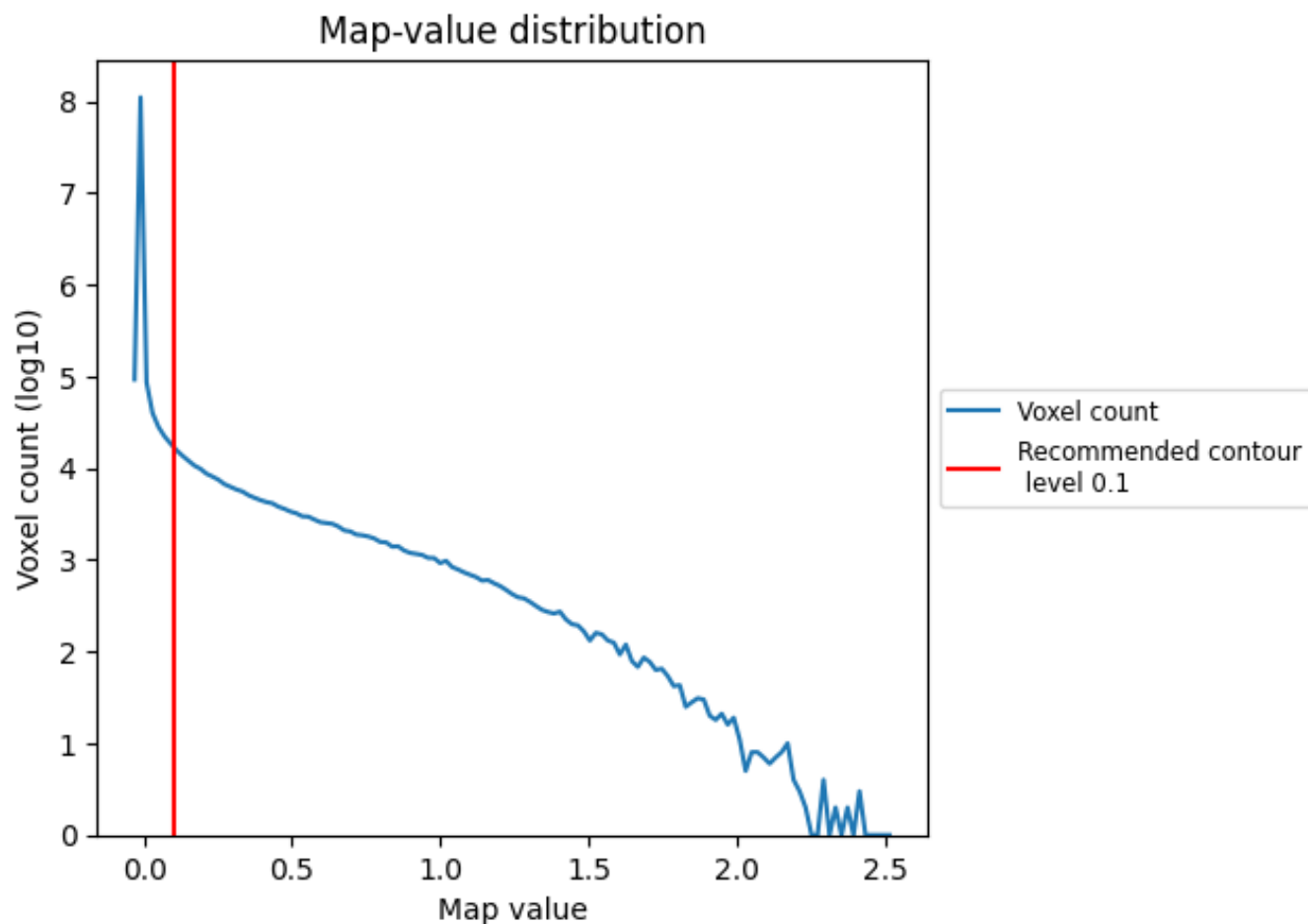


Z

7 Map analysis [i](#)

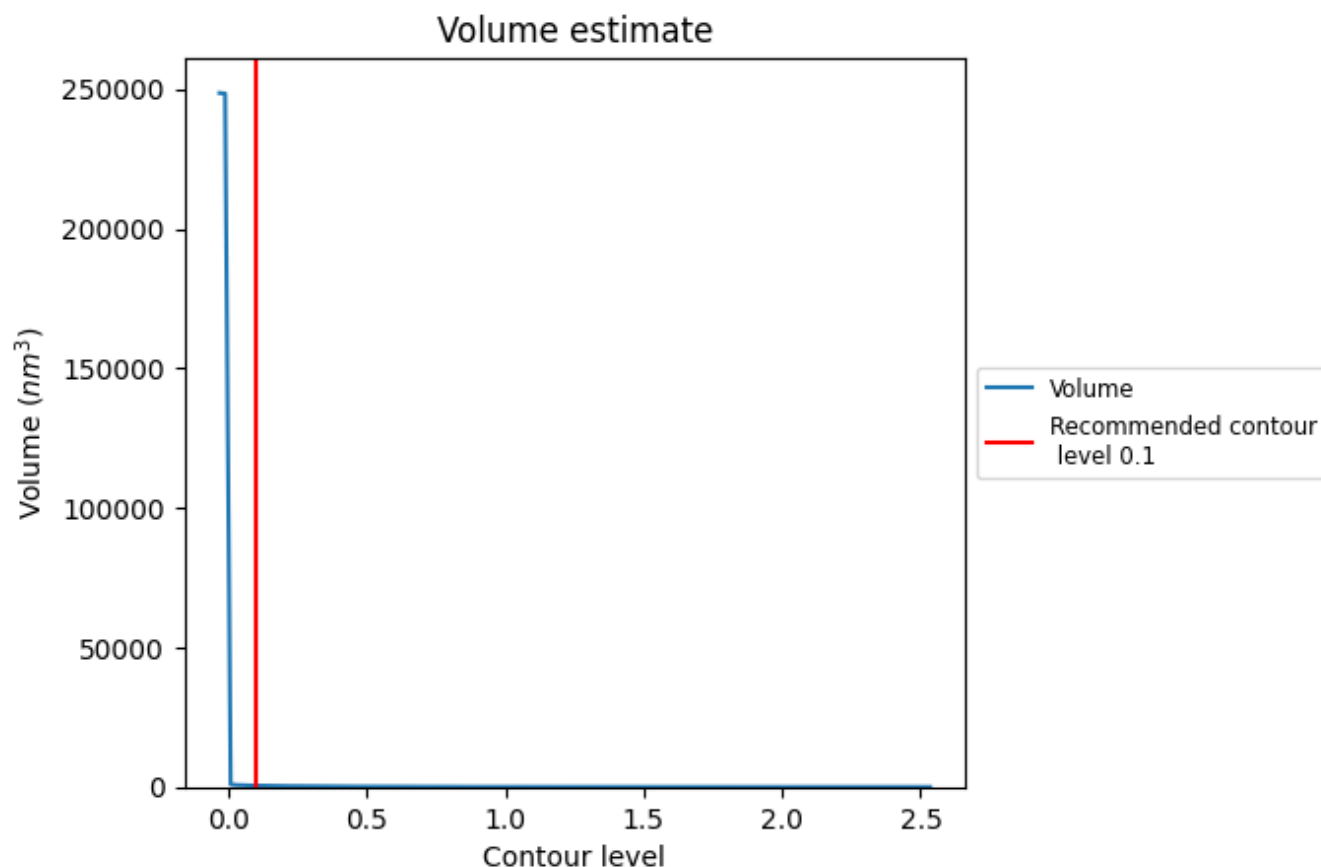
This section contains the results of statistical analysis of the map.

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.

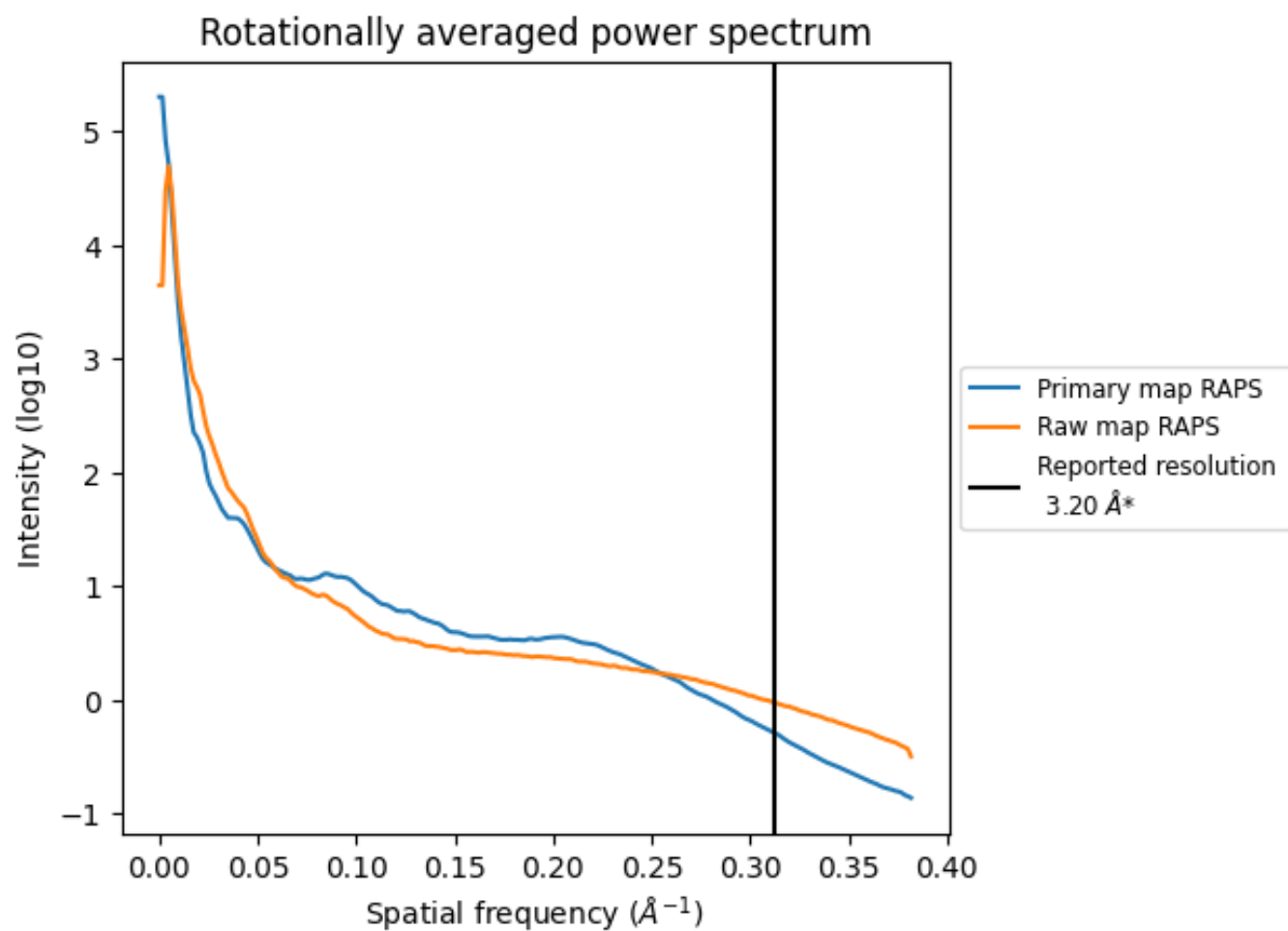
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 478 nm³; this corresponds to an approximate mass of 432 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 ⓘ

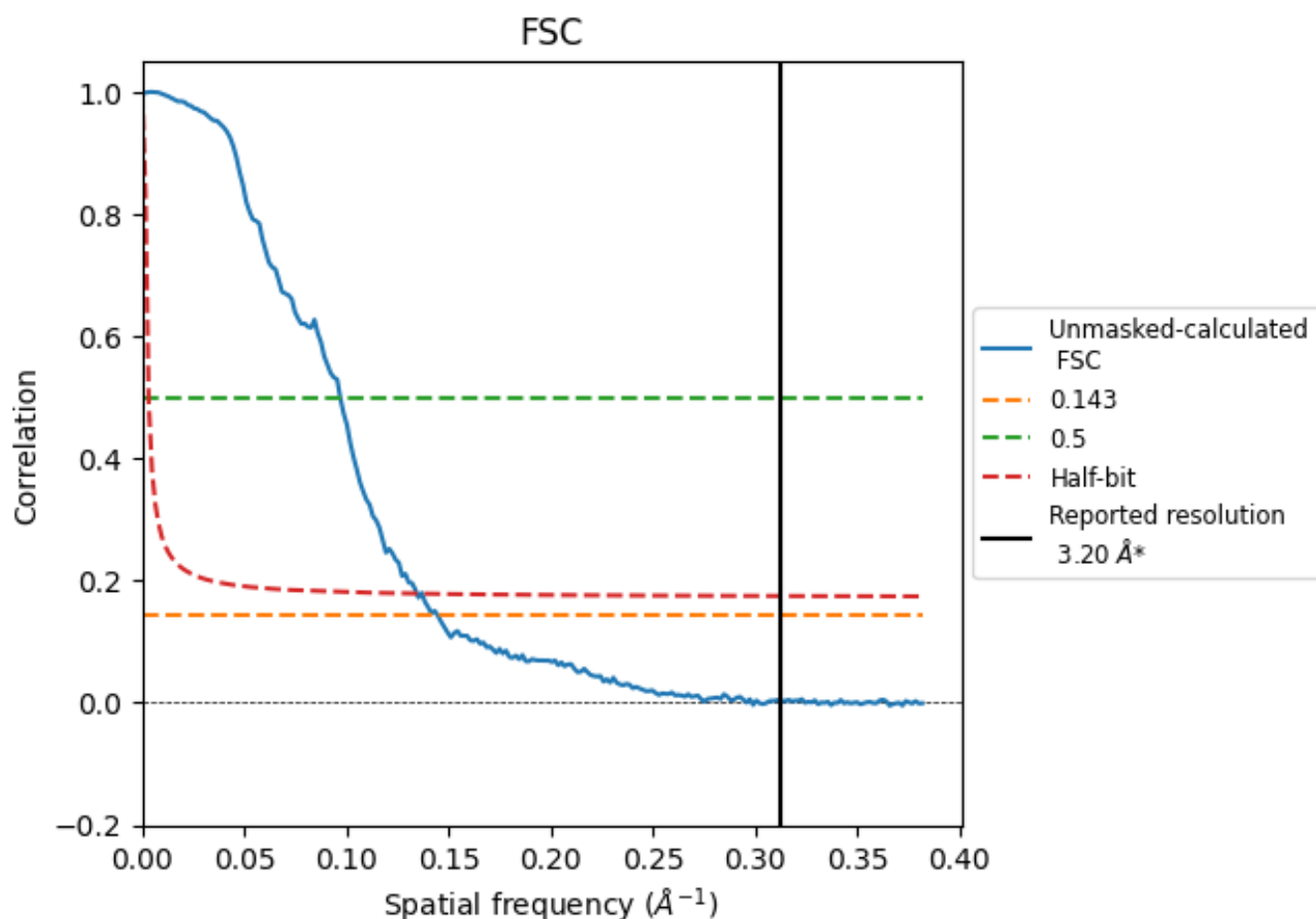


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

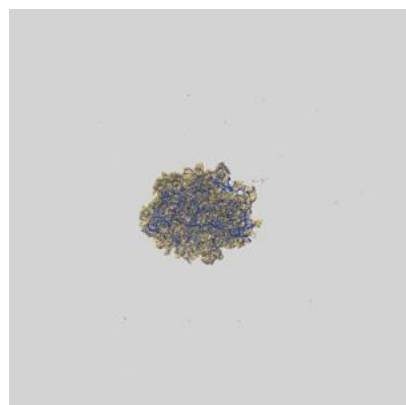
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.92	10.32	7.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.92 differs from the reported value 3.2 by more than 10 %

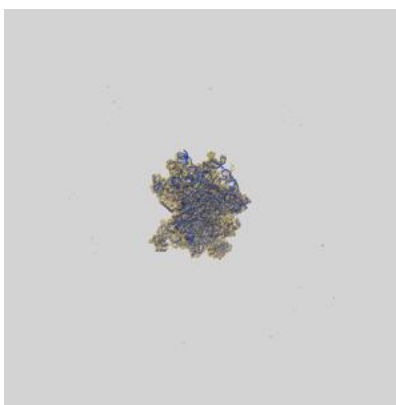
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26067 and PDB model 7TQL. Per-residue inclusion information can be found in section 3 on page 13.

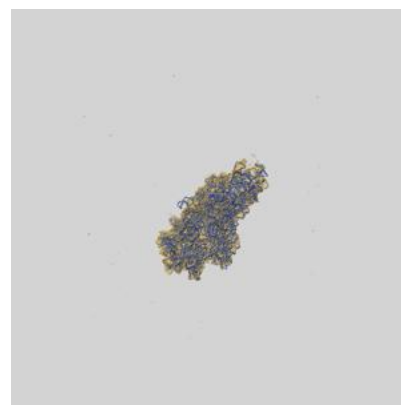
9.1 Map-model overlay [i](#)



X



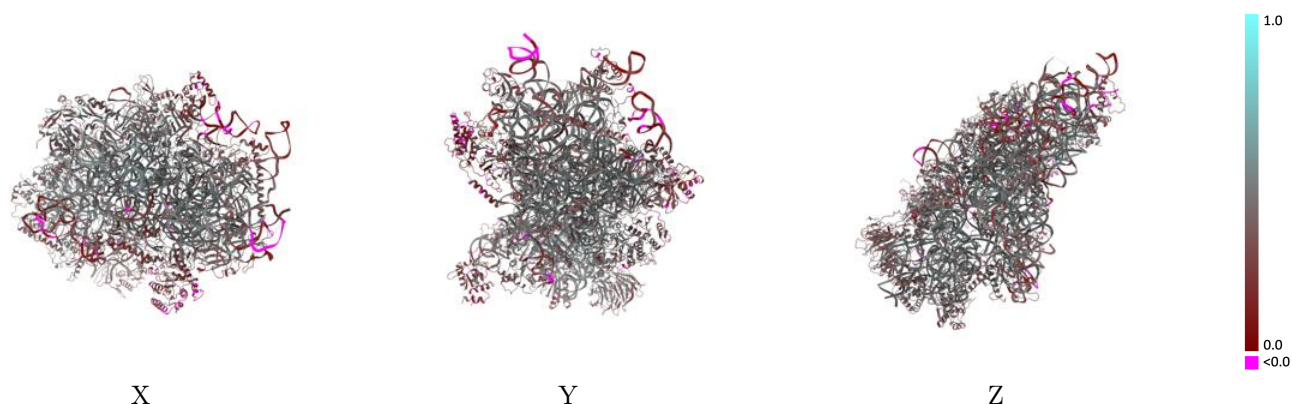
Y



Z

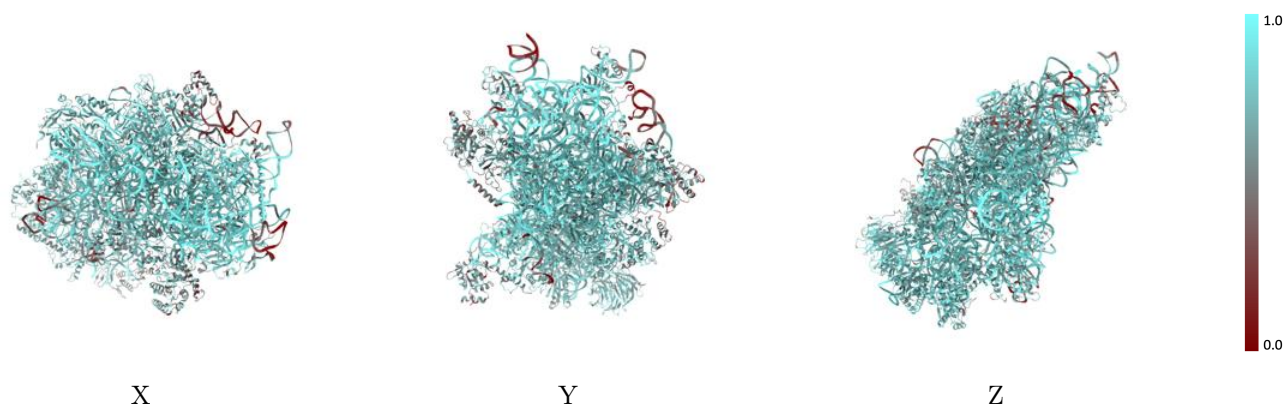
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



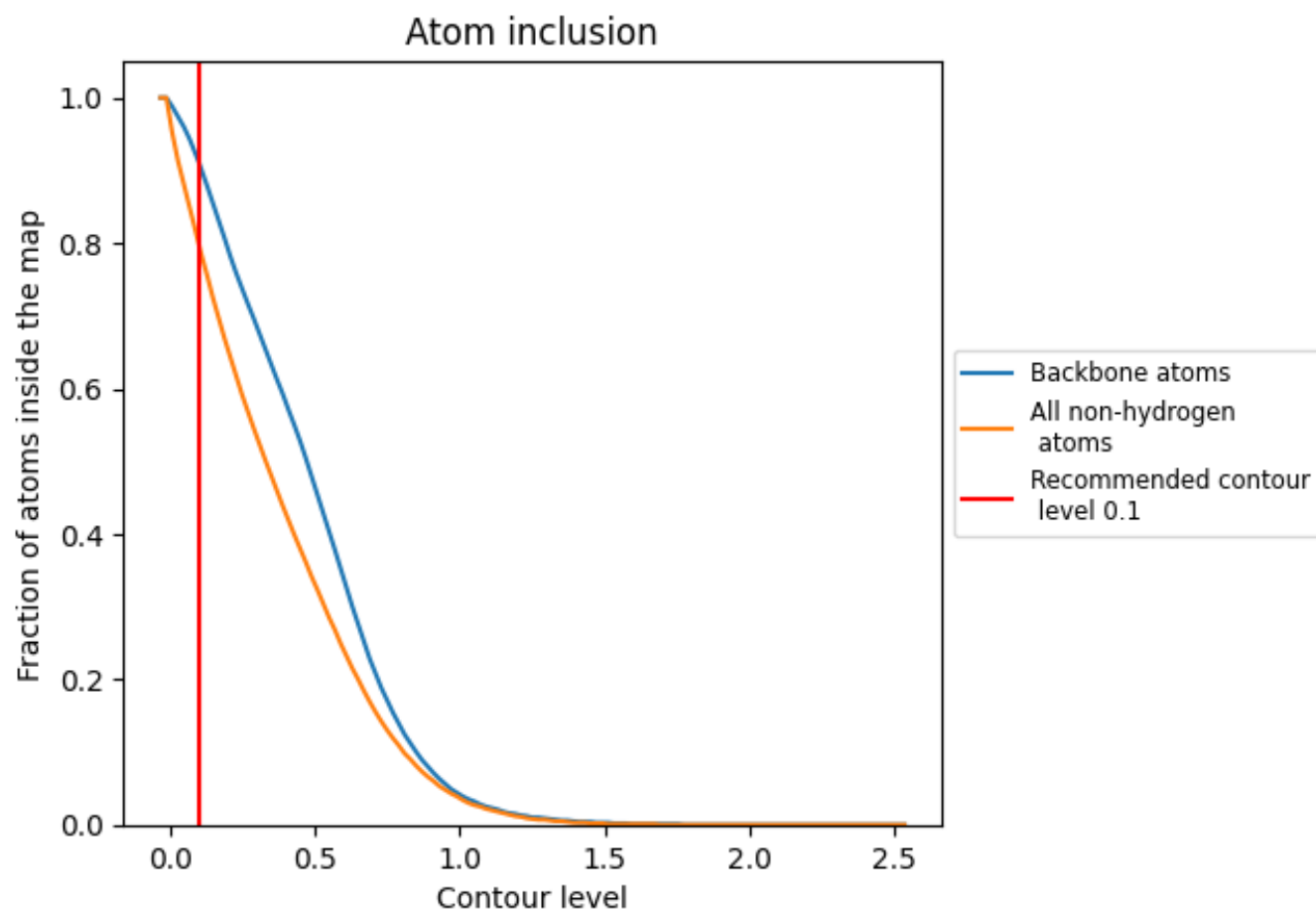
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 80% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.4120
1	 0.5780	 0.2370
2	 0.8910	 0.4520
3	 0.6060	 0.2690
4	 0.6200	 0.3420
B	 0.7920	 0.4240
C	 0.7600	 0.4190
D	 0.8070	 0.4500
E	 0.7910	 0.4410
F	 0.7740	 0.4140
G	 0.7030	 0.3630
H	 0.5190	 0.2560
I	 0.7750	 0.4120
J	 0.7730	 0.4210
K	 0.8010	 0.4380
L	 0.7380	 0.4230
M	 0.7700	 0.3900
N	 0.7770	 0.4200
O	 0.5200	 0.2170
P	 0.7980	 0.4340
Q	 0.7880	 0.4150
R	 0.8300	 0.4440
S	 0.6520	 0.3360
T	 0.7650	 0.4100
U	 0.8020	 0.4380
V	 0.7480	 0.4080
W	 0.8140	 0.4520
X	 0.8070	 0.4540
Y	 0.7610	 0.4110
Z	 0.7540	 0.4130
a	 0.7270	 0.4050
b	 0.7980	 0.4320
c	 0.8110	 0.4510
d	 0.7820	 0.4320
e	 0.7420	 0.4190



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Chain	Atom inclusion	Q-score
f	 0.8400	 0.4590
g	 0.4890	 0.2410
h	 0.7320	 0.4340
j	 0.7560	 0.3800