



Full wwPDB EM Validation Report ⓘ

Sep 24, 2026 – 05:12 pm BST

PDB ID : 9TKP / pdb_00009tkp
EMDB ID : EMD-56036
Title : 70S Initiation Complex with extended IF2 bound (70S IC-I)
Authors : Guerra, G.S.; Demo, G.
Deposited on : 2025-12-10
Resolution : 3.00 Å(reported)
Based on initial model : 6WDD

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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 EMD 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) : 2.50

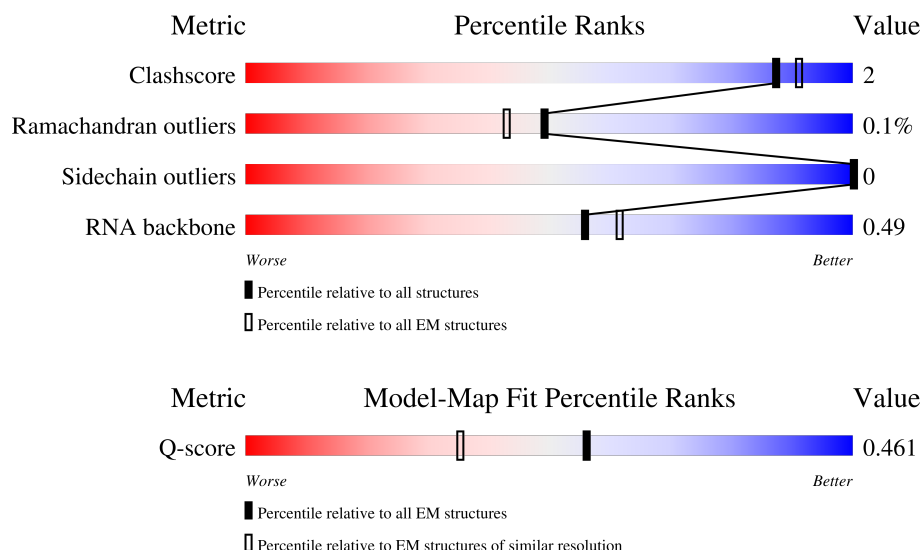
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



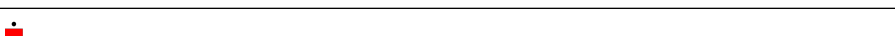
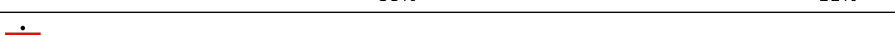
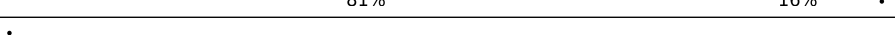
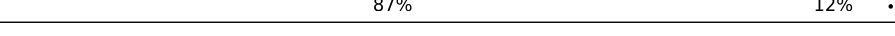
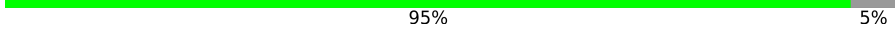
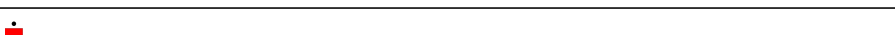
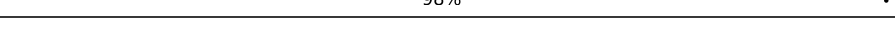
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	AA	241	
2	AB	233	
3	AC	206	

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Mol	Chain	Length	Quality of chain
4	AD	167	
5	AE	135	
6	AF	179	
7	AG	130	
8	AH	130	
9	AI	103	
10	AJ	129	
11	AK	124	
12	AL	118	
13	AM	101	
14	AN	89	
15	AO	82	
16	AP	84	
17	AQ	75	
18	AR	92	
19	AT	87	
20	AU	71	
21	B0	85	
22	B1	78	
23	B2	63	
24	B3	59	
25	B5	57	
26	B6	55	
27	B7	46	
28	B8	65	

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Mol	Chain	Length	Quality of chain
29	B9	38	
30	BA	234	
31	BB	273	
32	BC	209	
33	BD	201	
34	BE	179	
35	BF	177	
36	BI	149	
37	BK	142	
38	BM	142	
39	BN	123	
40	BO	144	
41	BP	136	
42	BQ	127	
43	BR	117	
44	BS	115	
45	BT	118	
46	BU	103	
47	BV	110	
48	BW	100	
49	BX	104	
50	BY	94	
51	D1	1540	
52	D2	2903	
53	D3	120	

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Mol	Chain	Length	Quality of chain
54	D4	56	9%91%
55	D5	77	68%30%
56	F2	896	60%6%33%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 150207 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 Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	225	Total	C	N	O	S	0	0
			1756	1111	315	322	8		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 5 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 7 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 19 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 20 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B0	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 25 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 26 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	B6	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 27 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BA	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BB	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BC	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BD	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BE	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BF	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BK	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 40 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BO	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BP	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 42 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BQ	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BR	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 44 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BS	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 45 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BT	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 46 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BU	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 47 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BV	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BX	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 50 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BY	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 51 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	D1	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 52 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	D2	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D2	747	C	U	conflict	GB CP194060.1

- Molecule 53 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	D3	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	120	A	U	conflict	GB CP076697.1

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	D4	5	Total	C	N	O	P	0	0
			109	49	22	33	5		

- Molecule 55 is a RNA chain called tRNA^fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	D5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

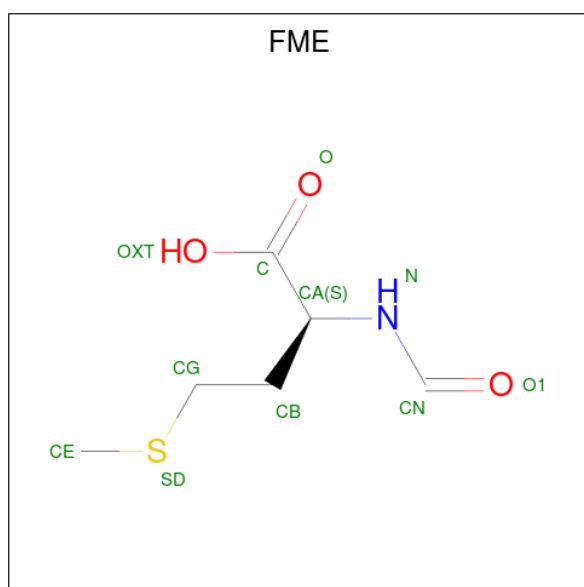
- Molecule 56 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	F2	596	Total	C	N	O	S	0	0
			4510	2818	794	877	21		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F2	-5	MET	-	initiating methionine	UNP P0A705
F2	-4	HIS	-	expression tag	UNP P0A705
F2	-3	HIS	-	expression tag	UNP P0A705
F2	-2	HIS	-	expression tag	UNP P0A705
F2	-1	HIS	-	expression tag	UNP P0A705
F2	0	HIS	-	expression tag	UNP P0A705
F2	1	HIS	-	expression tag	UNP P0A705

- Molecule 57 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S) (labeled as "Ligand of Interest" by depositor).

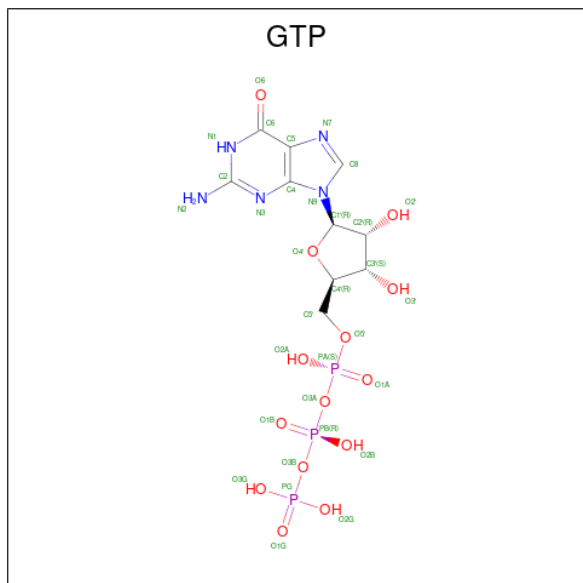


Mol	Chain	Residues	Atoms					AltConf
57	D5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
58	F2	1	Total	Mg	0
			1	1	

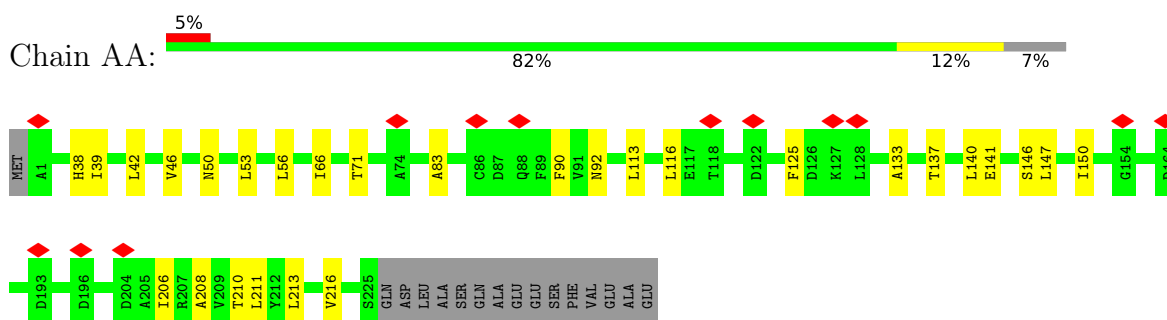
- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



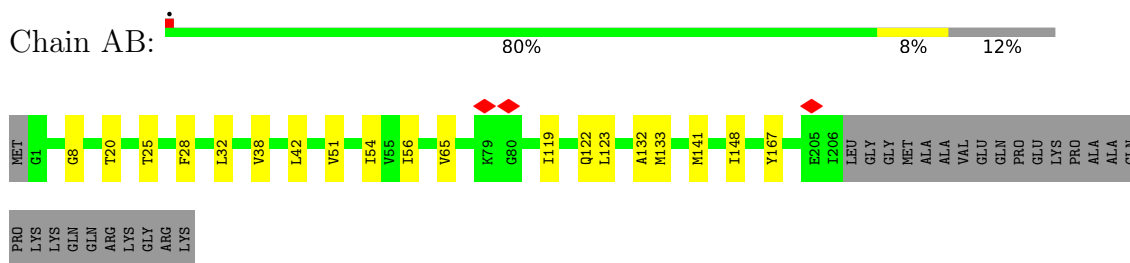
3 Residue-property plots

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.

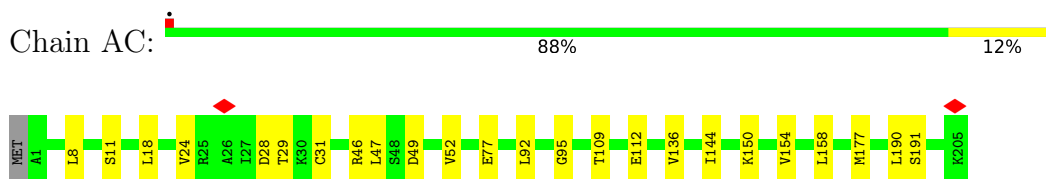
- Molecule 1: Small ribosomal subunit protein uS2



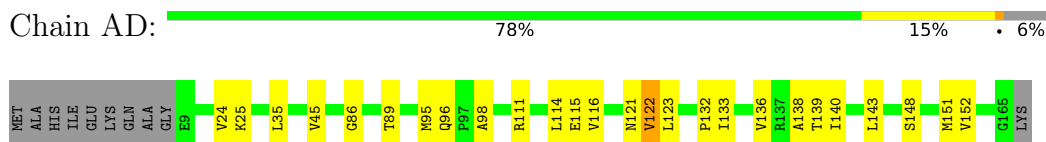
- Molecule 2: Small ribosomal subunit protein uS3



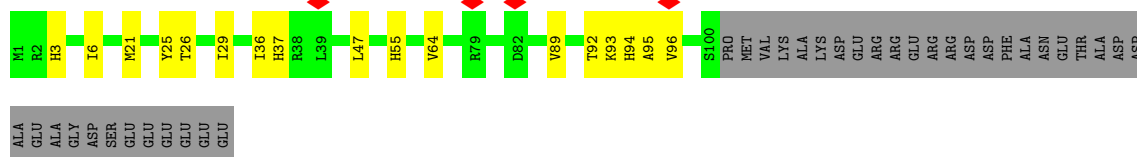
- Molecule 3: Small ribosomal subunit protein uS4



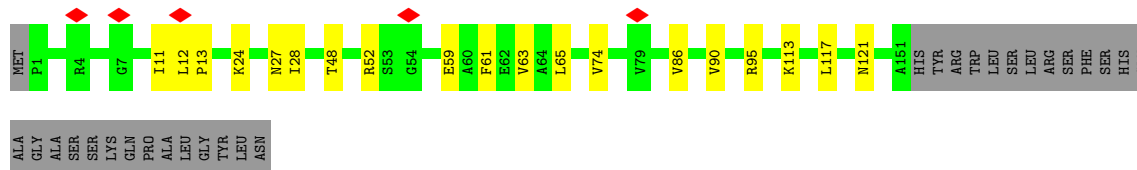
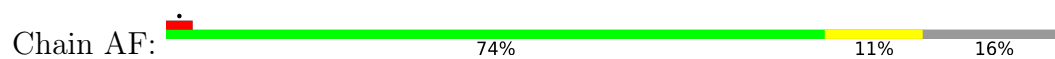
- Molecule 4: Small ribosomal subunit protein uS5



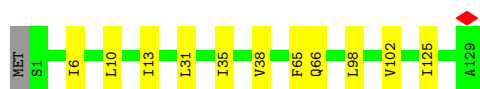
- Molecule 5: Small ribosomal subunit protein bS6, fully modified isoform



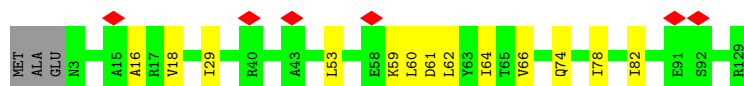
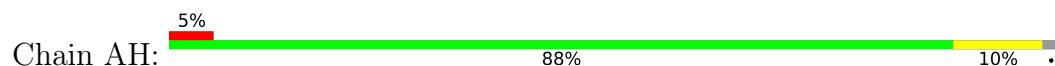
- Molecule 6: Small ribosomal subunit protein uS7



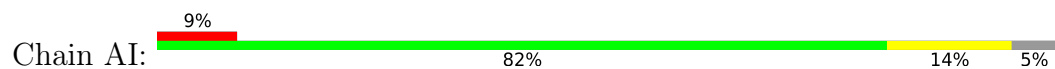
- Molecule 7: Small ribosomal subunit protein uS8



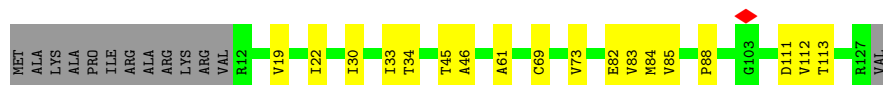
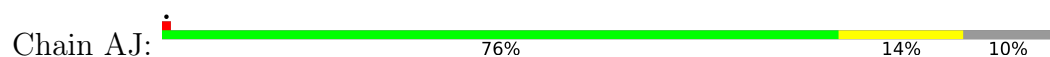
- Molecule 8: Small ribosomal subunit protein uS9



- Molecule 9: Small ribosomal subunit protein uS10



- Molecule 10: Small ribosomal subunit protein uS11



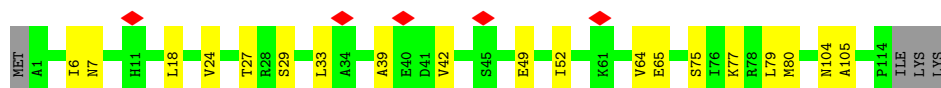
- Molecule 11: Small ribosomal subunit protein uS12

Chain AK:  88% 11%



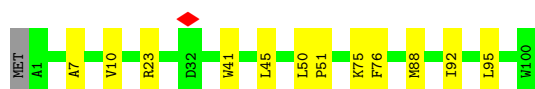
- Molecule 12: Small ribosomal subunit protein uS13

Chain AL:  81% 16%



- Molecule 13: Small ribosomal subunit protein uS14

Chain AM:  87% 12%



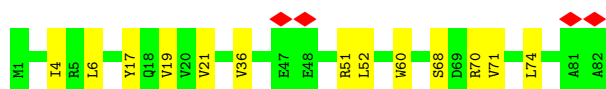
- Molecule 14: Small ribosomal subunit protein uS15

Chain AN:  88% 11%

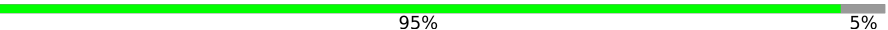


- Molecule 15: Small ribosomal subunit protein bS16

Chain AO:  84% 16%



- Molecule 16: Small ribosomal subunit protein uS17

Chain AP:  95% 5%

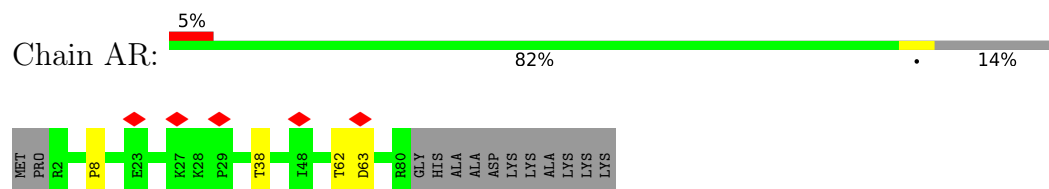


- Molecule 17: Small ribosomal subunit protein bS18

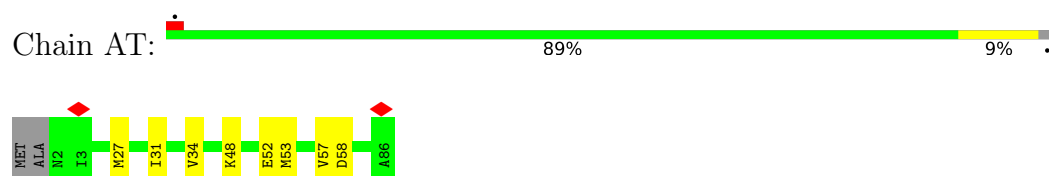
Chain AQ:  77% 9% 13%



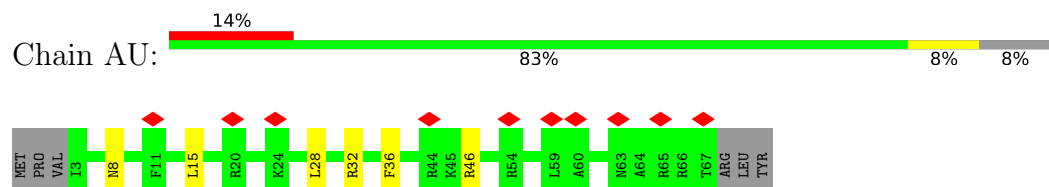
- Molecule 18: Small ribosomal subunit protein uS19



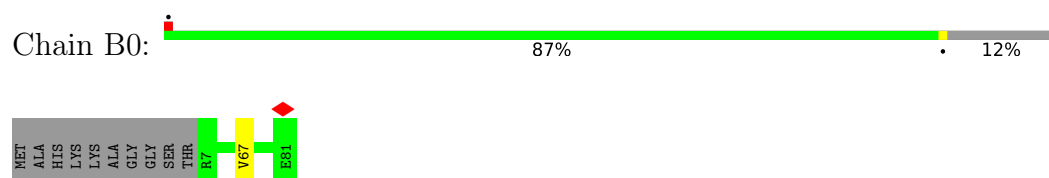
- Molecule 19: Small ribosomal subunit protein bS20



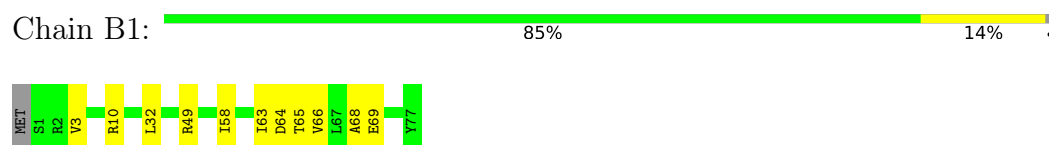
- Molecule 20: Small ribosomal subunit protein bS21



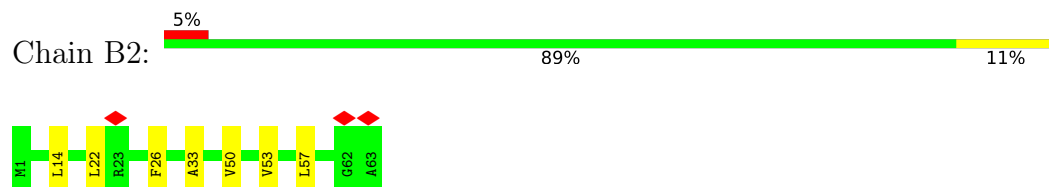
- Molecule 21: Large ribosomal subunit protein bL27



- Molecule 22: Large ribosomal subunit protein bL28

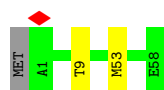


- Molecule 23: Large ribosomal subunit protein uL29



- Molecule 24: Large ribosomal subunit protein uL30





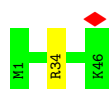
- Molecule 25: Large ribosomal subunit protein bL32



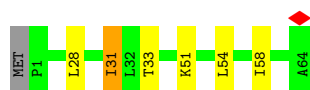
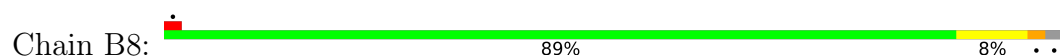
- Molecule 26: Large ribosomal subunit protein bL33



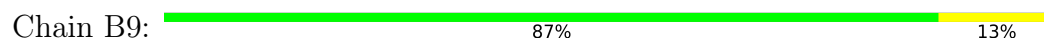
- Molecule 27: Large ribosomal subunit protein bL34



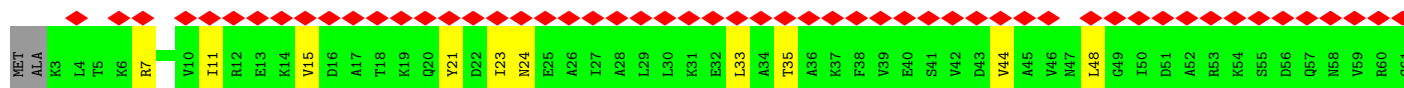
- Molecule 28: Large ribosomal subunit protein bL35

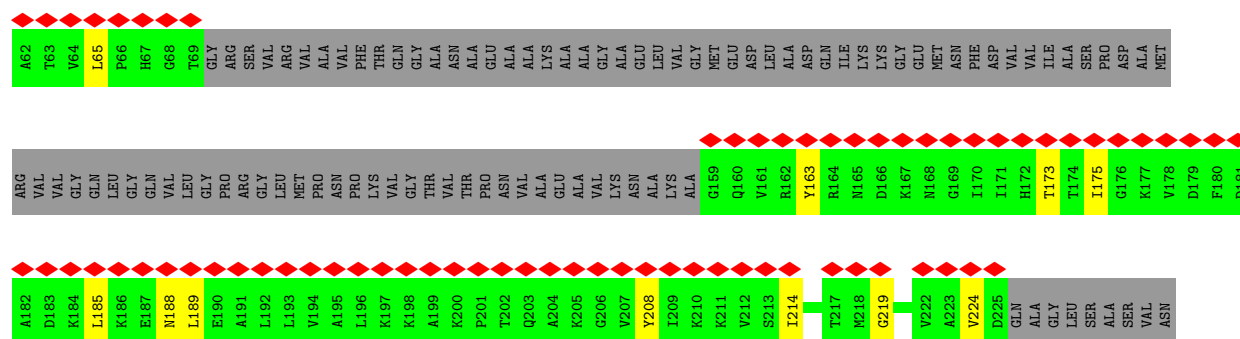


- Molecule 29: Large ribosomal subunit protein bL36A



- Molecule 30: Large ribosomal subunit protein uL1





• Molecule 31: Large ribosomal subunit protein uL2

Chain BB: 95%



• Molecule 32: 50S ribosomal protein L3

Chain BC: 98%



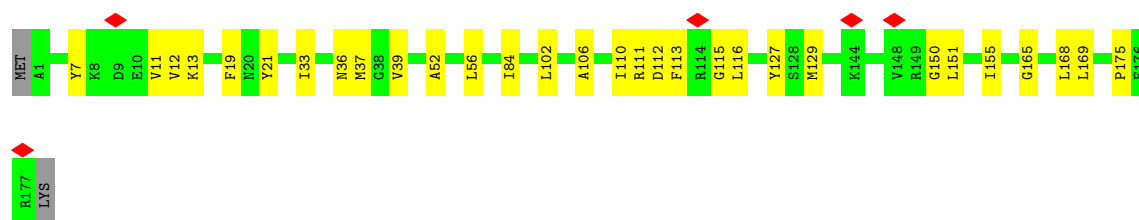
• Molecule 33: Large ribosomal subunit protein uL4

Chain BD: 95%



• Molecule 34: Large ribosomal subunit protein uL5

Chain BE: 82%

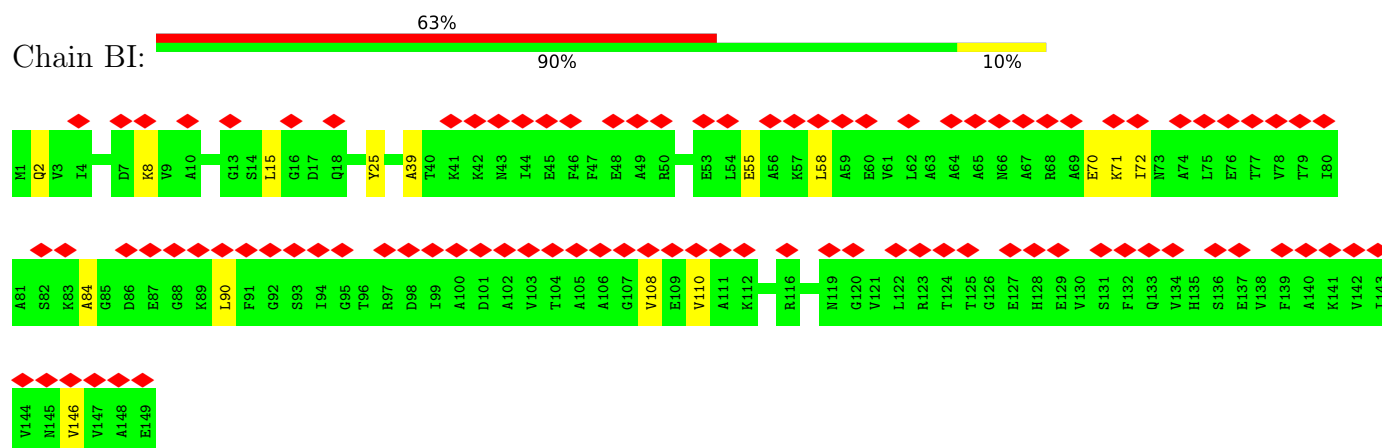


• Molecule 35: Large ribosomal subunit protein uL6

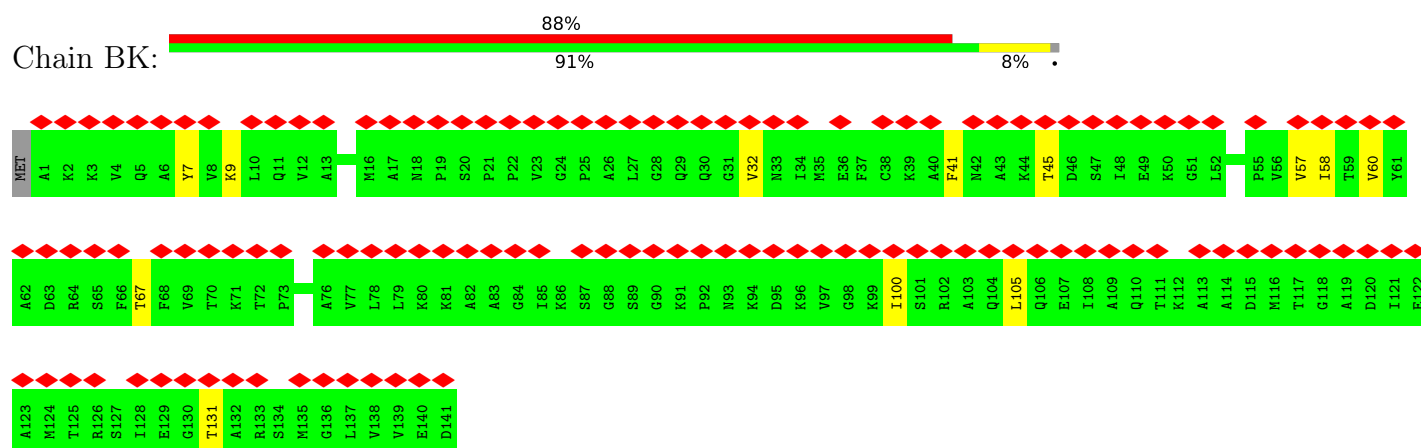
Chain BF: 89%



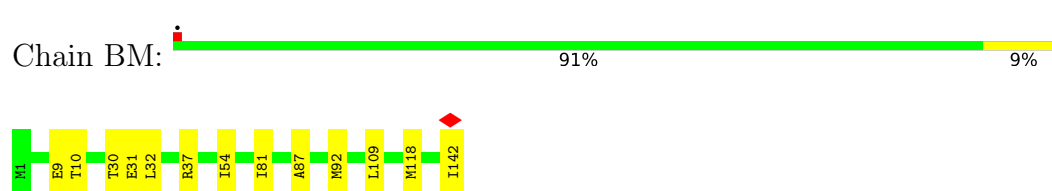
- Molecule 36: Large ribosomal subunit protein bL9



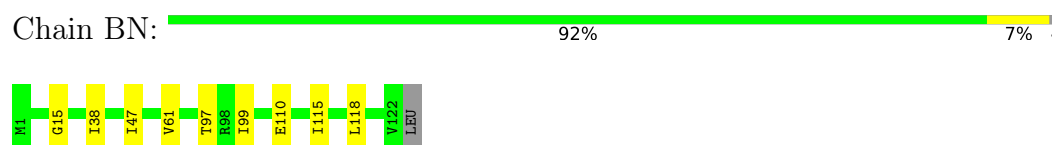
- Molecule 37: 50S ribosomal protein L11



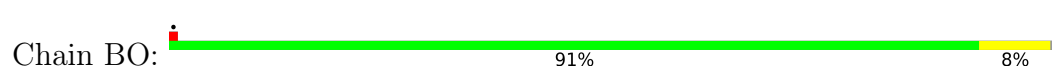
- Molecule 38: Large ribosomal subunit protein uL13



- Molecule 39: Large ribosomal subunit protein uL14



- Molecule 40: Large ribosomal subunit protein uL15





- Molecule 41: 50S ribosomal protein L16

Chain BP: 92% 8%



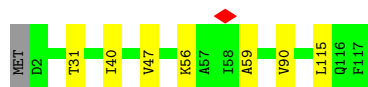
- Molecule 42: Large ribosomal subunit protein bL17

Chain BQ: 87% 7% 6%



- Molecule 43: Large ribosomal subunit protein uL18

Chain BR: 93% 6% .



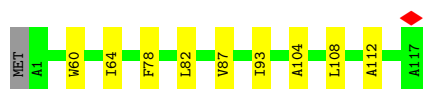
- Molecule 44: Large ribosomal subunit protein bL19

Chain BS: 90% 9% .



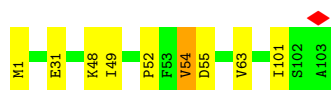
- Molecule 45: Large ribosomal subunit protein bL20

Chain BT: 92% 8% .



- Molecule 46: Large ribosomal subunit protein bL21

Chain BU: 91% 8% .



- Molecule 47: Large ribosomal subunit protein uL22

Chain BV:  90% 10%

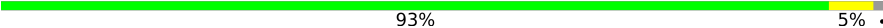


- Molecule 48: Large ribosomal subunit protein uL23

Chain BW:  82% 11% 7%



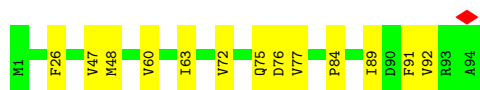
- Molecule 49: Large ribosomal subunit protein uL24

Chain BX:  93% 5%



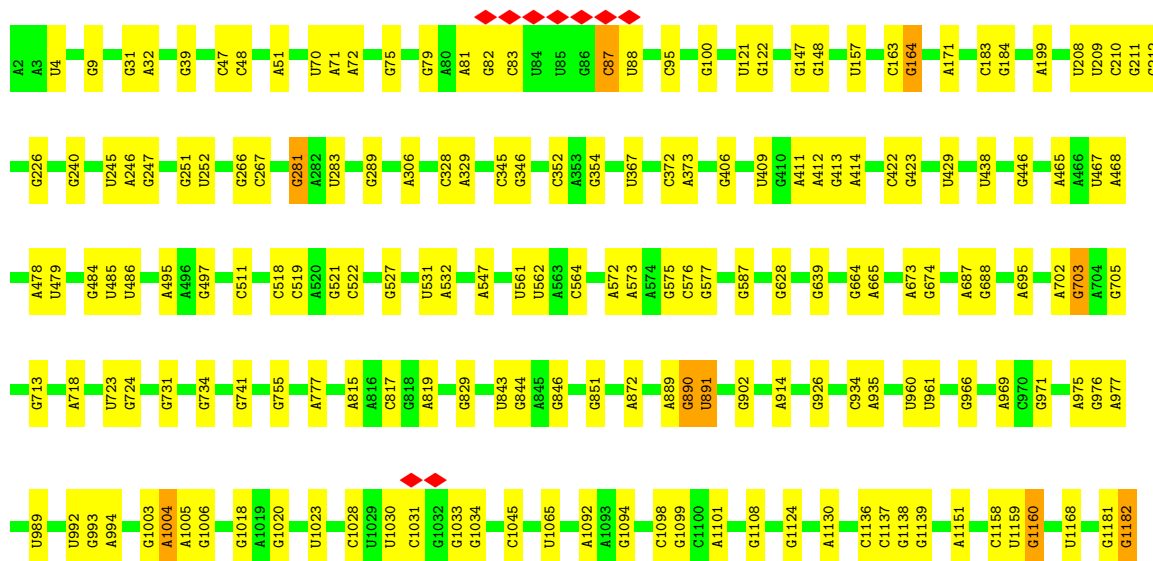
- Molecule 50: Large ribosomal subunit protein bL25

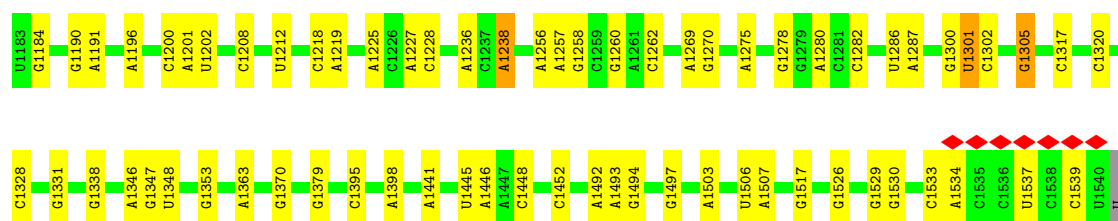
Chain BY:  86% 14%



- Molecule 51: 16S Ribosomal RNA

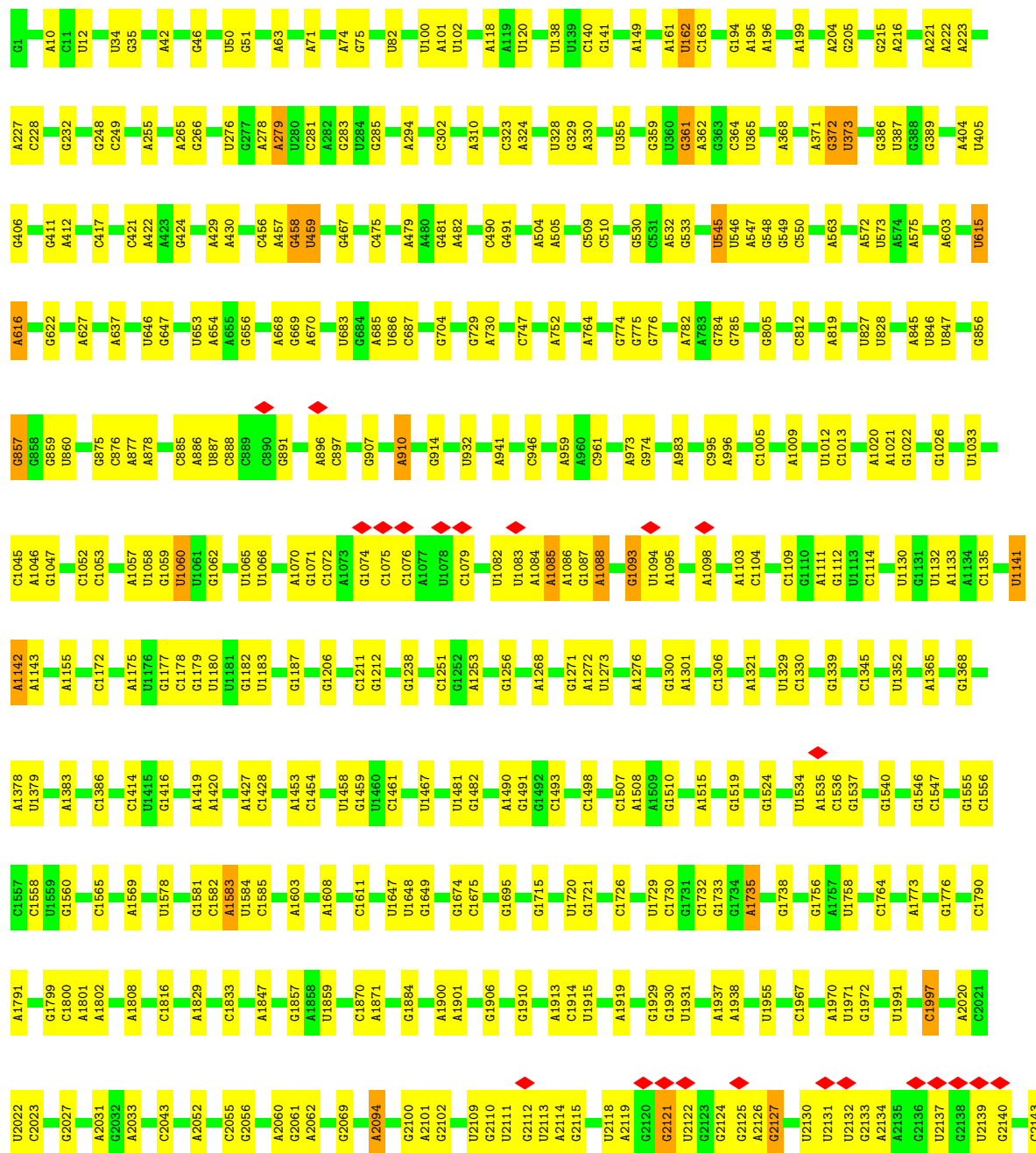
Chain D1:  84% 15%

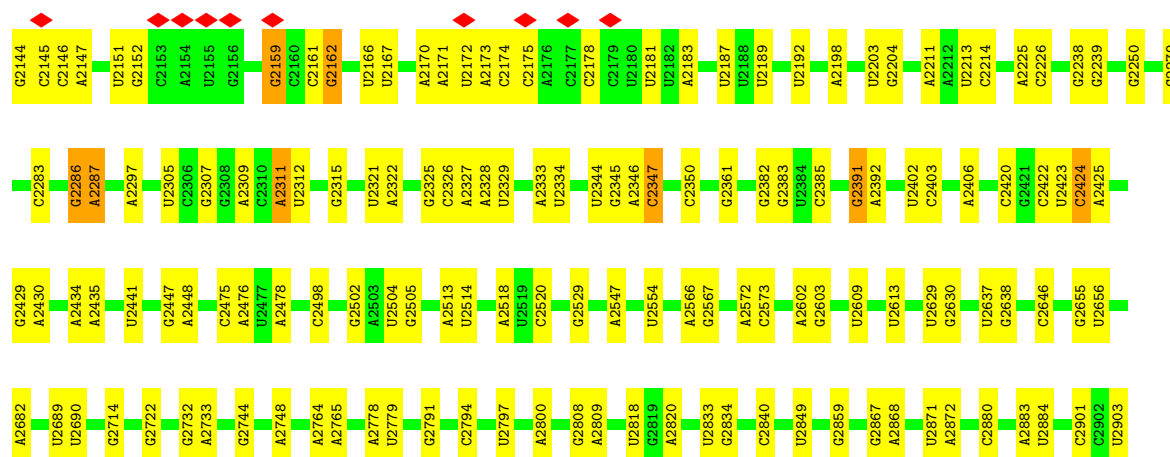




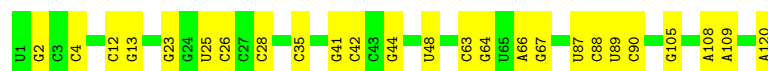
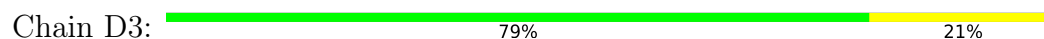
• Molecule 52: 23S Ribosomal RNA

Chain D2: 81% 18%





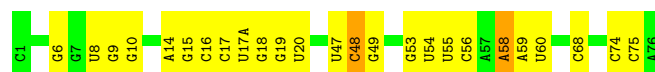
- Molecule 53: 5S Ribosomal RNA



- Molecule 54: mRNA

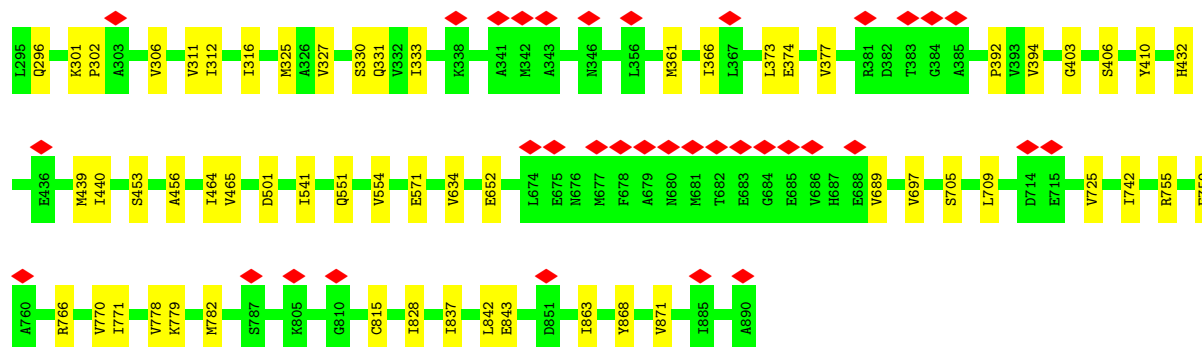


- Molecule 55: tRNA^{fMet}



- Molecule 56: Translation initiation factor IF-2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12354	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	19.959	Depositor
Minimum map value	-6.661	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.089	Depositor
Recommended contour level	2.6	Depositor
Map size (Å)	400.32, 400.32, 400.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FME, GTP

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	AA	0.18	0/1787	0.38	0/2408
2	AB	0.19	0/1651	0.37	0/2225
3	AC	0.19	0/1665	0.40	0/2227
4	AD	0.21	0/1169	0.45	0/1573
5	AE	0.21	0/835	0.50	0/1128
6	AF	0.18	0/1195	0.39	0/1602
7	AG	0.20	0/989	0.41	0/1326
8	AH	0.19	0/1034	0.43	0/1375
9	AI	0.20	0/796	0.49	0/1077
10	AJ	0.18	0/885	0.38	0/1195
11	AK	0.22	0/969	0.40	0/1300
12	AL	0.17	0/892	0.41	0/1193
13	AM	0.19	0/817	0.42	0/1088
14	AN	0.23	0/722	0.50	0/964
15	AO	0.19	0/659	0.38	0/884
16	AP	0.20	0/657	0.42	0/881
17	AQ	0.18	0/544	0.40	0/731
18	AR	0.18	0/652	0.40	0/877
19	AT	0.24	0/671	0.46	0/888
20	AU	0.23	0/550	0.58	0/728
21	B0	0.24	0/582	0.36	0/769
22	B1	0.24	0/635	0.36	0/848
23	B2	0.20	0/510	0.36	0/677
24	B3	0.21	0/453	0.34	0/605
25	B5	0.22	0/450	0.38	0/599
26	B6	0.21	0/416	0.38	0/554
27	B7	0.26	0/380	0.34	0/498
28	B8	0.24	0/513	0.35	0/676
29	B9	0.24	0/303	0.46	0/397
30	BA	0.13	0/1033	0.33	0/1387
31	BB	0.23	0/2121	0.37	0/2852
32	BC	0.24	0/1586	0.35	0/2134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BD	0.20	0/1571	0.37	0/2113
34	BE	0.19	0/1434	0.45	0/1926
35	BF	0.19	0/1343	0.42	0/1816
36	BI	0.18	0/1122	0.42	0/1515
37	BK	0.17	0/1046	0.37	0/1410
38	BM	0.23	0/1152	0.32	0/1551
39	BN	0.23	0/947	0.38	0/1268
40	BO	0.22	0/1054	0.39	0/1403
41	BP	0.24	0/1093	0.41	0/1460
42	BQ	0.24	0/973	0.46	0/1301
43	BR	0.18	0/902	0.37	0/1209
44	BS	0.22	0/929	0.32	0/1242
45	BT	0.26	0/960	0.35	0/1278
46	BU	0.23	0/829	0.45	0/1107
47	BV	0.23	0/864	0.39	0/1156
48	BW	0.22	0/744	0.41	0/994
49	BX	0.21	0/787	0.41	0/1051
50	BY	0.22	0/766	0.41	0/1025
51	D1	0.21	0/36963	0.29	0/57662
52	D2	0.26	0/69796	0.31	0/108888
53	D3	0.20	0/2872	0.29	0/4479
54	D4	0.14	0/122	0.20	0/188
55	D5	0.18	0/1832	0.32	0/2855
56	F2	0.19	0/4561	0.40	0/6158
All	All	0.23	0/162783	0.33	0/242721

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1756	0	1787	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1624	0	1699	11	0
3	AC	1643	0	1710	16	0
4	AD	1156	0	1199	18	0
5	AE	817	0	808	10	0
6	AF	1181	0	1240	11	0
7	AG	979	0	1034	7	0
8	AH	1022	0	1070	8	0
9	AI	786	0	828	10	0
10	AJ	869	0	878	14	0
11	AK	955	0	1019	8	0
12	AL	883	0	944	13	0
13	AM	805	0	847	8	0
14	AN	714	0	737	6	0
15	AO	649	0	666	9	0
16	AP	648	0	691	0	0
17	AQ	535	0	552	4	0
18	AR	637	0	665	2	0
19	AT	665	0	714	5	0
20	AU	544	0	579	6	0
21	B0	575	0	592	1	0
22	B1	625	0	655	6	0
23	B2	509	0	543	6	0
24	B3	449	0	491	1	0
25	B5	444	0	461	0	0
26	B6	409	0	440	3	0
27	B7	377	0	418	1	0
28	B8	504	0	574	7	0
29	B9	302	0	343	3	0
30	BA	1026	0	1092	16	0
31	BB	2082	0	2157	9	0
32	BC	1565	0	1616	3	0
33	BD	1552	0	1619	6	0
34	BE	1410	0	1447	22	0
35	BF	1323	0	1374	12	0
36	BI	1111	0	1148	9	0
37	BK	1032	0	1088	7	0
38	BM	1129	0	1162	10	0
39	BN	938	0	1012	6	0
40	BO	1045	0	1117	11	0
41	BP	1074	0	1157	9	0
42	BQ	960	0	1000	7	0
43	BR	892	0	923	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BS	917	0	965	6	0
45	BT	947	0	1022	6	0
46	BU	816	0	839	8	0
47	BV	857	0	922	6	0
48	BW	738	0	807	10	0
49	BX	779	0	834	3	0
50	BY	753	0	780	9	0
51	D1	33012	0	16618	23	0
52	D2	62317	0	31346	58	0
53	D3	2568	0	1303	1	0
54	D4	109	0	55	0	0
55	D5	1640	0	836	10	0
56	F2	4510	0	4599	40	0
57	D5	10	0	10	0	0
58	F2	1	0	0	0	0
59	F2	32	0	12	3	0
All	All	150207	0	103044	490	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 2.

All (490) 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)
55:D5:6:G:N2	55:D5:68:C:C2	2.44	0.86
55:D5:8:U:O2	55:D5:14:A:N7	2.10	0.84
52:D2:285:G:O6	52:D2:355:U:O2	1.97	0.82
52:D2:2139:U:O2	52:D2:2152:G:O6	1.96	0.82
15:AO:4:ILE:HG22	15:AO:21:VAL:HG22	1.59	0.82
55:D5:54:U:O2	55:D5:58:A:N7	2.12	0.82
46:BU:54:VAL:HG12	46:BU:55:ASP:H	1.46	0.81
51:D1:1006:G:O6	51:D1:1023:U:O2	2.00	0.78
1:AA:56:LEU:HD21	1:AA:216:VAL:HG23	1.68	0.76
50:BY:77:VAL:HG22	50:BY:89:ILE:HD13	1.68	0.75
42:BQ:53:THR:HG21	52:D2:2840:C:H5''	1.69	0.75
43:BR:31:THR:HG21	53:D3:28:C:OP1	1.88	0.74
51:D1:157:U:O2	51:D1:164:G:O6	2.08	0.71
8:AH:74:GLN:O	8:AH:78:ILE:HD12	1.90	0.71
55:D5:6:G:C2	55:D5:68:C:C2	2.79	0.71
36:BI:90:LEU:HD11	36:BI:146:VAL:HG21	1.71	0.70
28:B8:28:LEU:O	28:B8:28:LEU:HD12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:133:MET:HE2	2:AB:167:TYR:HB3	1.76	0.68
17:AQ:54:LEU:O	17:AQ:58:ILE:HD12	1.93	0.68
49:BX:35:VAL:HG13	49:BX:38:ILE:HD13	1.74	0.68
52:D2:545:U:O2	52:D2:548:G:O6	2.12	0.68
52:D2:1481:U:O2	52:D2:1510:G:O6	2.13	0.66
45:BT:82:LEU:HD22	45:BT:112:ALA:HB2	1.77	0.65
28:B8:33:THR:HG23	52:D2:2420:C:OP1	1.95	0.65
35:BF:51:PHE:HZ	35:BF:71:LEU:HD22	1.60	0.65
5:AE:36:ILE:HD13	5:AE:64:VAL:HG23	1.79	0.64
38:BM:9:GLU:HG2	38:BM:10:THR:HG23	1.80	0.63
56:F2:689:VAL:HG21	56:F2:782:MET:HB3	1.80	0.63
39:BN:99:ILE:HD13	39:BN:115:ILE:HG23	1.78	0.63
46:BU:49:ILE:HD12	46:BU:52:PRO:HA	1.80	0.63
4:AD:121:ASN:O	4:AD:122:VAL:HG12	1.99	0.63
29:B9:36:ARG:HG2	29:B9:37:GLN:H	1.64	0.63
30:BA:15:VAL:HG13	30:BA:21:TYR:HE2	1.62	0.63
37:BK:41:PHE:O	37:BK:45:THR:HG23	1.99	0.63
42:BQ:20:MET:HE1	52:D2:1276:A:O2'	1.99	0.62
8:AH:53:LEU:HD23	8:AH:53:LEU:O	1.99	0.62
8:AH:78:ILE:O	8:AH:82:ILE:HD12	1.98	0.62
45:BT:60:TRP:O	45:BT:64:ILE:HD12	1.99	0.62
6:AF:48:THR:HG22	6:AF:52:ARG:HE	1.64	0.62
56:F2:778:VAL:HG12	56:F2:782:MET:HE1	1.82	0.62
1:AA:42:LEU:O	1:AA:46:VAL:HG23	1.99	0.62
4:AD:152:VAL:HG21	7:AG:98:LEU:HD12	1.80	0.61
21:B0:67:VAL:HG12	21:B0:67:VAL:O	2.00	0.61
32:BC:129:THR:HG22	52:D2:1997:C:OP2	2.01	0.61
52:D2:285:G:C6	52:D2:355:U:O2	2.52	0.61
30:BA:48:LEU:HD11	30:BA:208:TYR:CZ	2.36	0.60
55:D5:8:U:C2	55:D5:14:A:N7	2.70	0.60
13:AM:76:PHE:HE2	13:AM:92:ILE:HD13	1.66	0.60
56:F2:406:SER:OG	59:F2:902:GTP:H5'	2.02	0.60
34:BE:33:ILE:HG12	34:BE:155:ILE:HG22	1.83	0.59
6:AF:59:GLU:O	6:AF:63:VAL:HG13	2.02	0.59
3:AC:77:GLU:OE1	3:AC:92:LEU:HD21	2.02	0.59
36:BI:72:ILE:HB	36:BI:108:VAL:HG22	1.84	0.59
56:F2:432:HIS:CE1	56:F2:439:MET:HE3	2.38	0.59
30:BA:185:LEU:O	30:BA:189:LEU:HD13	2.03	0.58
50:BY:77:VAL:CG2	50:BY:89:ILE:HD13	2.34	0.58
34:BE:168:LEU:HD12	34:BE:169:LEU:HD22	1.84	0.58
38:BM:37:ARG:HA	38:BM:118:MET:HE1	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BT:87:VAL:HG21	46:BU:48:LYS:NZ	2.19	0.57
37:BK:32:VAL:HG22	37:BK:60:VAL:HG21	1.87	0.57
7:AG:102:VAL:HG23	7:AG:125:ILE:HB	1.86	0.57
41:BP:17:ASN:CG	41:BP:95:LEU:HD12	2.30	0.57
50:BY:76:ASP:O	50:BY:89:ILE:HD12	2.04	0.57
8:AH:16:ALA:CB	8:AH:66:VAL:HG12	2.35	0.57
3:AC:109:THR:HG23	3:AC:112:GLU:H	1.69	0.57
36:BI:84:ALA:HB2	36:BI:90:LEU:HD23	1.87	0.57
52:D2:279:A:H61	52:D2:361:G:C2'	2.18	0.57
22:B1:58:ILE:CD1	22:B1:66:VAL:HG11	2.34	0.57
2:AB:141:MET:HE2	2:AB:148:ILE:HG22	1.86	0.57
38:BM:109:LEU:CD1	38:BM:118:MET:HE2	2.35	0.57
1:AA:71:THR:HG22	1:AA:92:ASN:C	2.30	0.56
22:B1:32:LEU:HD21	22:B1:49:ARG:HB3	1.88	0.56
35:BF:71:LEU:HG	35:BF:74:MET:HE2	1.87	0.56
44:BS:59:THR:OG1	44:BS:72:VAL:HG12	2.04	0.56
3:AC:95:GLY:O	3:AC:136:VAL:HG22	2.05	0.56
37:BK:58:ILE:HD12	37:BK:67:THR:O	2.05	0.56
4:AD:35:LEU:HD22	4:AD:133:ILE:HG22	1.87	0.56
20:AU:15:LEU:HD23	20:AU:15:LEU:O	2.05	0.56
31:BB:174:ARG:HB2	31:BB:180:MET:HE1	1.87	0.56
37:BK:100:ILE:HG21	37:BK:105:LEU:HD21	1.87	0.56
56:F2:373:LEU:HD22	56:F2:652:GLU:CD	2.29	0.56
13:AM:50:LEU:HD12	13:AM:51:PRO:O	2.04	0.56
30:BA:175:ILE:CD1	30:BA:189:LEU:HD11	2.35	0.56
35:BF:51:PHE:CZ	35:BF:71:LEU:HD22	2.40	0.56
9:AI:6:ILE:HD12	9:AI:102:LEU:HD13	1.87	0.56
14:AN:77:TYR:O	14:AN:81:ILE:HD12	2.05	0.56
18:AR:62:THR:HG22	18:AR:63:ASP:H	1.70	0.56
30:BA:175:ILE:HD13	30:BA:189:LEU:HD11	1.87	0.56
51:D1:1160:G:O6	51:D1:1182:G:O6	2.24	0.56
29:B9:1:MET:HE2	29:B9:36:ARG:HB2	1.87	0.56
52:D2:1093:G:H1'	52:D2:1098:A:H61	1.71	0.56
56:F2:432:HIS:HE1	56:F2:439:MET:HE3	1.69	0.56
3:AC:8:LEU:HD23	3:AC:31:CYS:HB3	1.88	0.56
43:BR:90:VAL:CG1	43:BR:115:LEU:HD21	2.36	0.55
56:F2:394:VAL:HG12	56:F2:464:ILE:HB	1.88	0.55
44:BS:9:GLN:HA	44:BS:12:MET:HE3	1.87	0.55
2:AB:25:THR:HG22	13:AM:75:LYS:HE3	1.88	0.55
48:BW:23:ALA:HB1	48:BW:29:THR:HG23	1.89	0.55
2:AB:28:PHE:CE2	2:AB:32:LEU:HD11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BE:115:GLY:C	34:BE:116:LEU:HD22	2.32	0.55
40:BO:91:ASP:O	40:BO:95:LEU:HD23	2.07	0.55
7:AG:31:LEU:O	7:AG:35:ILE:HD12	2.07	0.54
11:AK:33:CYS:HA	11:AK:54:VAL:HG22	1.89	0.54
38:BM:87:ALA:HB3	38:BM:92:MET:HE3	1.88	0.54
7:AG:6:ILE:O	7:AG:10:LEU:HD23	2.07	0.54
52:D2:2127:G:H22	52:D2:2162:G:H1'	1.72	0.54
28:B8:54:LEU:O	28:B8:58:ILE:HD12	2.08	0.54
40:BO:95:LEU:HD12	40:BO:100:ILE:HD11	1.88	0.54
48:BW:8:LEU:HD23	48:BW:50:LEU:HD21	1.90	0.54
52:D2:285:G:O6	52:D2:355:U:C2	2.61	0.54
4:AD:136:VAL:O	4:AD:140:ILE:HD12	2.08	0.54
32:BC:78:GLY:C	32:BC:79:LEU:HD22	2.33	0.54
33:BD:1:MET:CE	33:BD:113:VAL:HG11	2.38	0.54
1:AA:146:SER:C	1:AA:147:LEU:HD22	2.33	0.54
38:BM:109:LEU:HD11	38:BM:118:MET:HE2	1.90	0.54
3:AC:154:VAL:HG22	3:AC:158:LEU:HD23	1.90	0.53
14:AN:28:VAL:HG11	14:AN:66:LEU:HD22	1.90	0.53
55:D5:6:G:N1	55:D5:68:C:N3	2.57	0.53
15:AO:19:VAL:HG13	15:AO:36:VAL:O	2.07	0.53
43:BR:40:ILE:HG22	43:BR:47:VAL:HG12	1.90	0.53
1:AA:71:THR:HG22	1:AA:92:ASN:O	2.09	0.53
30:BA:7:ARG:NH1	30:BA:11:ILE:HD11	2.24	0.53
30:BA:35:THR:HG23	30:BA:35:THR:O	2.09	0.53
38:BM:81:ILE:HD11	52:D2:2514:U:H4'	1.90	0.53
15:AO:21:VAL:HG21	15:AO:60:TRP:CD1	2.43	0.53
1:AA:38:HIS:O	1:AA:39:ILE:HD13	2.09	0.53
4:AD:95:MET:HE1	4:AD:143:LEU:HD22	1.91	0.53
34:BE:165:GLY:O	34:BE:169:LEU:HD23	2.09	0.53
36:BI:8:LYS:HE3	36:BI:15:LEU:HD21	1.91	0.53
38:BM:30:THR:HG21	52:D2:1005:C:O2'	2.09	0.52
56:F2:311:VAL:HG12	56:F2:366:ILE:HB	1.91	0.52
6:AF:24:LYS:O	6:AF:28:ILE:HD12	2.09	0.52
11:AK:86:VAL:HG23	11:AK:88:ASP:H	1.75	0.52
30:BA:44:VAL:HG22	30:BA:214:ILE:HG22	1.90	0.52
34:BE:84:ILE:HD11	52:D2:2311:A:N3	2.23	0.52
14:AN:11:VAL:HG22	14:AN:26:VAL:HG21	1.92	0.52
41:BP:105:MET:HE1	41:BP:108:VAL:CG2	2.40	0.52
35:BF:173:ALA:O	35:BF:174:LYS:HG3	2.09	0.52
56:F2:403:GLY:HA2	59:F2:902:GTP:H5''	1.91	0.52
56:F2:501:ASP:HB3	59:F2:902:GTP:HN1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:81:ILE:HD12	11:AK:95:HIS:O	2.10	0.52
30:BA:163:TYR:CB	30:BA:173:THR:HG22	2.40	0.52
35:BF:120:ILE:HD11	35:BF:140:ILE:HG22	1.91	0.52
14:AN:62:ARG:O	14:AN:66:LEU:HD23	2.10	0.52
40:BO:135:ILE:CD1	40:BO:142:ILE:HD11	2.40	0.51
22:B1:3:VAL:HG22	22:B1:10:ARG:HG2	1.91	0.51
31:BB:92:LEU:HD11	31:BB:100:ARG:HB3	1.92	0.51
45:BT:104:ALA:O	45:BT:108:LEU:HD23	2.10	0.51
5:AE:6:ILE:HG22	5:AE:89:VAL:HG22	1.93	0.51
12:AL:27:THR:HG21	51:D1:1328:C:H5''	1.92	0.51
39:BN:38:ILE:CD1	39:BN:61:VAL:HG22	2.40	0.51
50:BY:63:ILE:HD12	50:BY:72:VAL:HG11	1.92	0.51
51:D1:1006:G:O6	51:D1:1023:U:C2	2.64	0.51
56:F2:815:CYS:SG	56:F2:863:ILE:HD12	2.51	0.51
10:AJ:22:ILE:HD11	10:AJ:85:VAL:HG12	1.91	0.51
17:AQ:29:LYS:HA	17:AQ:32:ILE:HD13	1.93	0.51
1:AA:206:ILE:O	1:AA:210:THR:HG23	2.11	0.51
7:AG:65:PHE:O	7:AG:66:GLN:NE2	2.43	0.51
12:AL:64:VAL:HG12	12:AL:65:GLU:H	1.76	0.51
2:AB:51:VAL:HG21	2:AB:54:ILE:HD11	1.91	0.51
13:AM:41:TRP:O	13:AM:45:LEU:HD13	2.11	0.51
40:BO:85:VAL:HG23	40:BO:86:GLU:H	1.75	0.51
44:BS:83:ILE:HG22	44:BS:83:ILE:O	2.11	0.51
4:AD:139:THR:O	4:AD:143:LEU:HD23	2.10	0.50
6:AF:113:LYS:HB3	6:AF:117:LEU:HD13	1.92	0.50
9:AI:57:VAL:HG12	9:AI:58:ASN:H	1.76	0.50
37:BK:7:TYR:CE1	37:BK:57:VAL:HG13	2.46	0.50
56:F2:842:LEU:HD23	56:F2:843:GLU:O	2.11	0.50
3:AC:150:LYS:HD2	3:AC:150:LYS:O	2.12	0.50
23:B2:26:PHE:CE2	48:BW:50:LEU:HD23	2.47	0.50
37:BK:131:THR:HG23	52:D2:1060:U:O4	2.11	0.50
47:BV:36:LEU:HD11	47:BV:47:VAL:HG13	1.93	0.50
51:D1:1006:G:C6	51:D1:1023:U:O2	2.63	0.50
52:D2:2127:G:H22	52:D2:2162:G:C1'	2.24	0.50
56:F2:325:MET:HB2	56:F2:327:VAL:HG22	1.93	0.50
26:B6:21:THR:CG2	28:B8:33:THR:HG22	2.40	0.50
6:AF:12:LEU:HD23	6:AF:13:PRO:O	2.11	0.50
12:AL:75:SER:O	12:AL:79:LEU:HD23	2.10	0.50
26:B6:21:THR:HG21	28:B8:33:THR:HG22	1.94	0.50
1:AA:137:THR:O	1:AA:141:GLU:OE1	2.30	0.50
30:BA:185:LEU:HD12	30:BA:188:ASN:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BB:32:LEU:O	31:BB:33:LEU:HD12	2.12	0.50
34:BE:150:GLY:O	34:BE:151:LEU:HD12	2.12	0.50
40:BO:26:GLY:C	40:BO:27:LEU:HD22	2.36	0.50
41:BP:57:VAL:HG12	41:BP:112:LEU:CD2	2.42	0.50
56:F2:501:ASP:OD1	56:F2:501:ASP:O	2.30	0.50
2:AB:122:GLN:NE2	2:AB:132:ALA:HB1	2.26	0.49
56:F2:306:VAL:HG13	56:F2:306:VAL:O	2.12	0.49
48:BW:67:VAL:HG22	48:BW:76:ARG:HG2	1.94	0.49
9:AI:15:HIS:HA	9:AI:18:ILE:HG22	1.95	0.49
34:BE:110:ILE:HD11	34:BE:113:PHE:HD1	1.76	0.49
34:BE:102:LEU:HA	34:BE:106:ALA:HB3	1.95	0.49
35:BF:10:VAL:HG12	35:BF:47:ASN:O	2.12	0.49
52:D2:2328:A:H2'	52:D2:2329:U:C6	2.47	0.49
6:AF:61:PHE:O	6:AF:65:LEU:HD13	2.13	0.49
52:D2:1079:C:H41	52:D2:1088:A:P	2.36	0.49
13:AM:7:ALA:HA	13:AM:10:VAL:HG12	1.94	0.48
43:BR:90:VAL:HG12	43:BR:115:LEU:HD21	1.94	0.48
2:AB:20:THR:HG23	2:AB:20:THR:O	2.13	0.48
3:AC:154:VAL:HG22	3:AC:158:LEU:CD2	2.43	0.48
28:B8:51:LYS:HA	28:B8:54:LEU:HD23	1.94	0.48
55:D5:54:U:O2	55:D5:58:A:C5	2.67	0.48
52:D2:2139:U:C2	52:D2:2152:G:O6	2.65	0.48
52:D2:2391:G:H2'	52:D2:2424:C:H41	1.79	0.48
1:AA:50:ASN:HA	1:AA:53:LEU:HD12	1.94	0.48
2:AB:38:VAL:O	2:AB:42:LEU:HD23	2.14	0.48
4:AD:148:SER:O	4:AD:152:VAL:HG22	2.13	0.48
17:AQ:17:VAL:HG13	17:AQ:17:VAL:O	2.13	0.48
42:BQ:116:VAL:HG13	42:BQ:116:VAL:O	2.14	0.48
10:AJ:112:VAL:HG12	10:AJ:112:VAL:O	2.13	0.48
40:BO:85:VAL:HG23	40:BO:86:GLU:N	2.29	0.48
52:D2:2143:C:H2'	52:D2:2144:G:O4'	2.14	0.48
50:BY:72:VAL:HG22	50:BY:91:PHE:HB3	1.95	0.48
10:AJ:30:ILE:HG13	10:AJ:45:THR:HG22	1.94	0.48
31:BB:92:LEU:HD12	31:BB:101:ARG:O	2.13	0.48
2:AB:56:ILE:HG12	2:AB:65:VAL:HG12	1.96	0.48
4:AD:98:ALA:HB2	4:AD:123:LEU:HD23	1.96	0.48
1:AA:83:ALA:HB3	1:AA:90:PHE:HD2	1.78	0.47
33:BD:132:LYS:O	33:BD:136:GLN:OE1	2.32	0.47
34:BE:116:LEU:HD12	34:BE:127:TYR:OH	2.14	0.47
34:BE:116:LEU:HD23	34:BE:175:PRO:HD2	1.95	0.47
41:BP:105:MET:HE1	41:BP:108:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D5:6:G:C2	55:D5:68:C:O2	2.67	0.47
5:AE:3:HIS:N	5:AE:92:THR:HG22	2.29	0.47
10:AJ:111:ASP:OD1	10:AJ:113:THR:HG23	2.14	0.47
31:BB:207:ALA:HB2	52:D2:1790:C:O2'	2.13	0.47
11:AK:49:ARG:NH2	51:D1:522:C:H41	2.13	0.47
34:BE:37:MET:HE1	34:BE:39:VAL:HB	1.96	0.47
41:BP:26:VAL:HG13	41:BP:26:VAL:O	2.14	0.47
12:AL:6:ILE:HG23	12:AL:7:ASN:N	2.29	0.47
22:B1:65:THR:O	22:B1:68:ALA:HB3	2.15	0.47
35:BF:103:ASN:C	35:BF:104:LEU:HD22	2.39	0.47
52:D2:2130:U:C4'	52:D2:2159:G:H22	2.27	0.47
3:AC:24:VAL:HG21	56:F2:296:GLN:HG3	1.97	0.47
34:BE:150:GLY:C	34:BE:151:LEU:HD12	2.39	0.47
29:B9:19:ARG:O	29:B9:22:VAL:HG12	2.15	0.47
46:BU:31:GLU:O	46:BU:63:VAL:HG12	2.14	0.47
34:BE:111:ARG:HE	34:BE:112:ASP:H	1.63	0.47
46:BU:54:VAL:HG12	46:BU:55:ASP:N	2.23	0.47
12:AL:39:ALA:O	12:AL:42:VAL:HG22	2.14	0.46
12:AL:77:LYS:HA	12:AL:80:MET:HG3	1.96	0.46
51:D1:1238:A:N7	51:D1:1301:U:O4	2.48	0.46
56:F2:755:ARG:O	56:F2:759:GLU:OE1	2.33	0.46
3:AC:11:SER:HA	3:AC:18:LEU:HD23	1.98	0.46
12:AL:49:GLU:OE1	12:AL:52:ILE:HD12	2.15	0.46
4:AD:24:VAL:HG22	4:AD:25:LYS:H	1.80	0.46
4:AD:111:ARG:HA	4:AD:114:LEU:HD12	1.96	0.46
4:AD:111:ARG:O	4:AD:115:GLU:OE1	2.33	0.46
38:BM:32:LEU:HD22	38:BM:54:ILE:HG21	1.96	0.46
15:AO:68:SER:HB2	15:AO:71:VAL:HG12	1.96	0.46
34:BE:116:LEU:HD11	34:BE:129:MET:SD	2.55	0.46
48:BW:10:VAL:HG23	48:BW:11:LEU:HD22	1.97	0.46
52:D2:2139:U:O2	52:D2:2152:G:C6	2.67	0.46
56:F2:301:LYS:HD3	56:F2:302:PRO:HD2	1.98	0.46
12:AL:6:ILE:HG23	12:AL:7:ASN:H	1.80	0.46
32:BC:110:THR:HG22	32:BC:171:THR:OG1	2.15	0.46
51:D1:664:G:H22	51:D1:741:G:H1	1.62	0.46
55:D5:15:G:N2	55:D5:48:C:C2	2.84	0.46
56:F2:868:TYR:CZ	56:F2:871:VAL:HG12	2.50	0.46
52:D2:1141:U:H4'	52:D2:1142:A:O4'	2.16	0.46
31:BB:153:LEU:HD13	31:BB:175:LEU:HD11	1.97	0.46
36:BI:108:VAL:HG12	36:BI:110:VAL:HG23	1.97	0.46
5:AE:21:MET:HE3	5:AE:25:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:D1:1305:G:H22	51:D1:1331:G:H2'	1.81	0.46
8:AH:61:ASP:C	8:AH:62:LEU:HD12	2.41	0.45
10:AJ:88:PRO:CD	20:AU:28:LEU:HD11	2.45	0.45
13:AM:92:ILE:HG21	13:AM:95:LEU:HD22	1.97	0.45
15:AO:6:LEU:HD12	15:AO:17:TYR:HB3	1.98	0.45
23:B2:22:LEU:HA	48:BW:8:LEU:HD11	1.97	0.45
31:BB:32:LEU:C	31:BB:33:LEU:HD12	2.41	0.45
3:AC:46:ARG:C	3:AC:47:LEU:HD23	2.42	0.45
7:AG:38:VAL:HG11	7:AG:102:VAL:HG12	1.98	0.45
11:AK:74:GLN:O	11:AK:74:GLN:HG2	2.16	0.45
22:B1:65:THR:O	22:B1:69:GLU:OE1	2.35	0.45
30:BA:48:LEU:HD11	30:BA:208:TYR:CE1	2.50	0.45
38:BM:31:GLU:CD	38:BM:142:ILE:HG21	2.42	0.45
40:BO:135:ILE:HD11	40:BO:142:ILE:HD11	1.98	0.45
41:BP:26:VAL:HG11	41:BP:133:LYS:HA	1.98	0.45
44:BS:113:LEU:HD12	44:BS:113:LEU:O	2.16	0.45
1:AA:116:LEU:HD22	1:AA:140:LEU:HD13	1.98	0.45
13:AM:23:ARG:HH22	13:AM:50:LEU:HD22	1.81	0.45
56:F2:453:SER:O	56:F2:456:ALA:HB3	2.17	0.45
33:BD:118:LEU:HD13	33:BD:186:VAL:HG13	1.99	0.45
38:BM:37:ARG:HD2	38:BM:118:MET:HE1	1.98	0.45
56:F2:312:ILE:HG23	56:F2:316:ILE:HG21	1.98	0.45
4:AD:89:THR:HG23	4:AD:89:THR:O	2.17	0.45
20:AU:46:ARG:HD3	20:AU:46:ARG:C	2.42	0.45
26:B6:16:THR:HG21	26:B6:41:VAL:HG21	1.99	0.45
52:D2:475:C:O2	52:D2:479:A:N6	2.50	0.45
1:AA:213:LEU:HA	1:AA:216:VAL:HG12	1.99	0.45
56:F2:330:SER:HA	56:F2:333:ILE:HG22	1.98	0.45
1:AA:125:PHE:HB3	1:AA:133:ALA:HB1	1.98	0.45
6:AF:86:VAL:O	6:AF:86:VAL:HG13	2.17	0.45
52:D2:615:U:H4'	52:D2:616:A:OP2	2.17	0.45
56:F2:778:VAL:HG12	56:F2:782:MET:CE	2.46	0.45
23:B2:50:VAL:HA	23:B2:53:VAL:HG12	1.99	0.44
42:BQ:79:LEU:HD23	42:BQ:83:LEU:HB2	1.99	0.44
51:D1:81:A:N6	51:D1:87:C:H41	2.15	0.44
3:AC:154:VAL:O	3:AC:158:LEU:HD23	2.17	0.44
9:AI:52:LEU:HD11	9:AI:59:LYS:HG3	1.98	0.44
10:AJ:33:ILE:HG21	10:AJ:73:VAL:CG1	2.47	0.44
10:AJ:46:ALA:HB1	10:AJ:61:ALA:HB1	1.98	0.44
10:AJ:88:PRO:HD3	20:AU:28:LEU:HD11	1.98	0.44
17:AQ:49:LYS:O	17:AQ:53:GLN:OE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BT:78:PHE:O	45:BT:82:LEU:HD23	2.17	0.44
55:D5:54:U:C2	55:D5:58:A:N7	2.84	0.44
56:F2:868:TYR:OH	56:F2:871:VAL:HG12	2.17	0.44
39:BN:38:ILE:HD13	39:BN:61:VAL:HG22	1.99	0.44
42:BQ:32:GLU:OE1	42:BQ:115:LEU:HD12	2.17	0.44
56:F2:778:VAL:O	56:F2:782:MET:CE	2.65	0.44
6:AF:74:VAL:HG13	6:AF:74:VAL:O	2.17	0.44
40:BO:29:LYS:O	40:BO:30:THR:OG1	2.32	0.44
3:AC:24:VAL:HG22	51:D1:409:U:H5''	2.00	0.44
47:BV:42:LYS:O	47:BV:45:VAL:HG12	2.17	0.44
56:F2:392:PRO:HG2	56:F2:440:ILE:HD12	2.00	0.44
33:BD:164:LEU:HB3	33:BD:167:VAL:HG22	1.99	0.44
36:BI:2:GLN:OE1	36:BI:39:ALA:HB3	2.18	0.44
40:BO:90:VAL:HG23	40:BO:95:LEU:HD21	1.99	0.44
30:BA:65:LEU:HD22	30:BA:188:ASN:HB2	2.00	0.43
36:BI:25:TYR:OH	52:D2:2094:A:H4'	2.18	0.43
42:BQ:97:ILE:HD11	42:BQ:113:ILE:HD12	2.00	0.43
46:BU:49:ILE:HG22	46:BU:54:VAL:H	1.83	0.43
1:AA:208:ALA:O	1:AA:211:LEU:HD23	2.18	0.43
9:AI:57:VAL:HG12	9:AI:58:ASN:N	2.33	0.43
19:AT:27:MET:HE3	19:AT:57:VAL:HA	2.00	0.43
42:BQ:83:LEU:HD11	42:BQ:115:LEU:HD13	2.00	0.43
46:BU:49:ILE:HG22	46:BU:54:VAL:N	2.32	0.43
56:F2:551:GLN:O	56:F2:554:VAL:HG12	2.18	0.43
30:BA:23:ILE:HD13	30:BA:224:VAL:HG21	1.99	0.43
51:D1:157:U:O2	51:D1:164:G:C6	2.72	0.43
52:D2:668:A:H2'	52:D2:670:A:H62	1.82	0.43
56:F2:634:VAL:HG11	56:F2:725:VAL:HG21	1.99	0.43
5:AE:26:THR:HA	5:AE:29:ILE:HG22	2.01	0.43
56:F2:571:GLU:OE2	56:F2:697:VAL:HG22	2.18	0.43
56:F2:742:ILE:HG21	56:F2:766:ARG:NH2	2.34	0.43
4:AD:151:MET:SD	4:AD:152:VAL:HG13	2.59	0.43
33:BD:132:LYS:O	33:BD:135:ALA:HB3	2.18	0.43
35:BF:85:LYS:C	35:BF:86:LEU:HD22	2.44	0.43
52:D2:1720:U:H2'	52:D2:1721:G:O4'	2.18	0.43
44:BS:24:THR:HG22	44:BS:87:ARG:HB2	2.00	0.43
46:BU:1:MET:SD	46:BU:101:ILE:HD11	2.58	0.43
8:AH:18:VAL:HG23	8:AH:64:ILE:HG22	2.00	0.43
14:AN:32:THR:HG21	14:AN:84:LEU:HD23	2.00	0.43
35:BF:19:ASN:O	35:BF:22:VAL:HG12	2.19	0.43
40:BO:26:GLY:O	40:BO:27:LEU:HD22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BX:11:ILE:HD13	49:BX:21:ARG:CG	2.48	0.43
1:AA:113:LEU:HD23	1:AA:113:LEU:C	2.44	0.43
10:AJ:30:ILE:CD1	51:D1:705:G:H21	2.31	0.43
37:BK:9:LYS:HZ1	52:D2:1060:U:H5''	1.83	0.43
52:D2:458:G:O2'	52:D2:459:U:P	2.76	0.43
52:D2:875:G:C5	52:D2:876:C:N3	2.86	0.43
56:F2:842:LEU:HD23	56:F2:843:GLU:N	2.34	0.43
9:AI:52:LEU:HD13	9:AI:62:ARG:HG3	2.00	0.42
15:AO:51:ARG:C	15:AO:52:LEU:HD12	2.44	0.42
51:D1:75:G:H22	51:D1:95:C:H42	1.67	0.42
10:AJ:33:ILE:HG23	10:AJ:69:CYS:SG	2.59	0.42
51:D1:147:G:H2'	51:D1:148:G:C8	2.54	0.42
52:D2:1339:G:H21	52:D2:1603:A:H1'	1.84	0.42
52:D2:2637:U:H2'	52:D2:2638:G:O4'	2.19	0.42
4:AD:132:PRO:O	4:AD:136:VAL:HG23	2.19	0.42
5:AE:47:LEU:HD21	5:AE:55:HIS:HA	2.01	0.42
35:BF:136:ASP:OD1	35:BF:139:VAL:HG22	2.19	0.42
1:AA:66:ILE:H	1:AA:66:ILE:HD12	1.84	0.42
5:AE:3:HIS:ND1	5:AE:95:ALA:HB3	2.34	0.42
12:AL:64:VAL:HG12	12:AL:65:GLU:N	2.34	0.42
28:B8:31:ILE:O	28:B8:31:ILE:HG13	2.19	0.42
34:BE:56:LEU:CD2	34:BE:151:LEU:HD21	2.50	0.42
41:BP:12:MET:HA	52:D2:910:A:H62	1.84	0.42
52:D2:2114:A:H62	52:D2:2115:G:H21	1.68	0.42
52:D2:2286:G:H4'	52:D2:2287:A:O4'	2.19	0.42
4:AD:98:ALA:CB	4:AD:123:LEU:HD23	2.49	0.42
19:AT:48:LYS:O	19:AT:52:GLU:OE1	2.37	0.42
47:BV:29:VAL:HG13	47:BV:69:LEU:O	2.20	0.42
51:D1:1004:A:H2'	51:D1:1005:A:O4'	2.20	0.42
52:D2:2346:A:H3'	52:D2:2347:C:C5'	2.50	0.42
3:AC:190:LEU:HD12	3:AC:191:SER:N	2.34	0.42
11:AK:47:ALA:C	11:AK:48:LEU:HD22	2.45	0.42
14:AN:84:LEU:HB3	14:AN:86:LEU:HD13	2.01	0.42
56:F2:837:ILE:HG22	56:F2:837:ILE:O	2.20	0.42
24:B3:9:THR:HG22	24:B3:53:MET:O	2.19	0.42
50:BY:26:PHE:CE1	50:BY:47:VAL:HG21	2.55	0.42
41:BP:26:VAL:HG23	41:BP:104:GLU:OE1	2.20	0.42
50:BY:75:GLN:HG3	50:BY:92:VAL:HG23	2.01	0.42
52:D2:2167:U:H3	52:D2:2170:A:H62	1.67	0.42
23:B2:14:LEU:HD22	23:B2:57:LEU:HD11	2.02	0.42
30:BA:33:LEU:HD22	30:BA:219:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BE:7:TYR:CD1	34:BE:11:VAL:HG21	2.55	0.42
52:D2:100:U:H4'	52:D2:101:A:O4'	2.20	0.42
52:D2:1582:C:H2'	52:D2:1583:A:N9	2.34	0.42
56:F2:705:SER:O	56:F2:709:LEU:HD23	2.20	0.42
3:AC:144:ILE:HD11	3:AC:177:MET:HG3	2.02	0.41
52:D2:2121:G:H2'	52:D2:2122:U:C6	2.55	0.41
6:AF:11:ILE:HD11	6:AF:27:ASN:HD22	1.83	0.41
8:AH:29:ILE:O	8:AH:29:ILE:HG23	2.19	0.41
12:AL:29:SER:O	12:AL:33:LEU:HD23	2.18	0.41
35:BF:9:VAL:O	35:BF:9:VAL:HG13	2.20	0.41
39:BN:110:GLU:HG3	39:BN:110:GLU:O	2.19	0.41
51:D1:687:A:H62	51:D1:703:G:H21	1.68	0.41
9:AI:57:VAL:O	9:AI:58:ASN:HB2	2.20	0.41
35:BF:120:ILE:HD12	35:BF:134:GLY:HA3	2.02	0.41
39:BN:97:THR:O	39:BN:118:LEU:HD13	2.20	0.41
52:D2:161:A:H3'	52:D2:162:U:H5''	2.02	0.41
52:D2:194:G:H2'	52:D2:195:A:O4'	2.21	0.41
56:F2:828:ILE:HG21	56:F2:842:LEU:HD12	2.01	0.41
9:AI:77:VAL:HG23	9:AI:78:GLU:N	2.36	0.41
11:AK:115:LYS:O	11:AK:116:TYR:HB2	2.20	0.41
52:D2:372:G:O2'	52:D2:373:U:P	2.78	0.41
3:AC:28:ASP:OD1	3:AC:29:THR:N	2.53	0.41
9:AI:50:THR:HG21	9:AI:62:ARG:HH21	1.85	0.41
15:AO:70:ARG:O	15:AO:74:LEU:HD23	2.21	0.41
20:AU:32:ARG:O	20:AU:32:ARG:HD3	2.20	0.41
41:BP:101:VAL:O	41:BP:101:VAL:HG13	2.20	0.41
43:BR:56:LYS:HA	43:BR:59:ALA:HB3	2.02	0.41
47:BV:34:ASP:O	47:BV:37:THR:HG22	2.20	0.41
52:D2:1182:G:H2'	52:D2:1183:U:O4'	2.21	0.41
52:D2:2124:G:H2'	52:D2:2125:G:C4'	2.50	0.41
5:AE:93:LYS:HG3	5:AE:93:LYS:O	2.20	0.41
36:BI:55:GLU:HA	36:BI:58:LEU:HD13	2.01	0.41
52:D2:856:G:H2'	52:D2:857:G:C8	2.56	0.41
52:D2:1085:A:H2'	52:D2:1086:A:N3	2.35	0.41
1:AA:56:LEU:HD11	1:AA:66:ILE:HG12	2.03	0.41
12:AL:18:LEU:O	12:AL:24:VAL:HG11	2.20	0.41
23:B2:26:PHE:CZ	48:BW:50:LEU:HD23	2.55	0.41
30:BA:163:TYR:HB3	30:BA:173:THR:HG22	2.02	0.41
40:BO:90:VAL:CG2	40:BO:95:LEU:HD21	2.50	0.41
47:BV:37:THR:HG23	47:BV:38:TYR:CD1	2.55	0.41
12:AL:104:ASN:O	12:AL:105:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BB:153:LEU:HD23	52:D2:1799:G:N2	2.36	0.41
34:BE:19:PHE:HB2	34:BE:21:TYR:CZ	2.56	0.41
48:BW:47:VAL:CG2	48:BW:55:VAL:HG21	2.51	0.41
2:AB:8:GLY:HA3	13:AM:88:MET:HE3	2.03	0.41
4:AD:96:GLN:O	4:AD:122:VAL:HG23	2.20	0.41
5:AE:36:ILE:HG22	5:AE:37:HIS:N	2.36	0.41
6:AF:90:VAL:HG13	6:AF:95:ARG:CG	2.51	0.41
10:AJ:19:VAL:CG2	10:AJ:34:THR:HG23	2.50	0.41
34:BE:12:VAL:HG23	34:BE:13:LYS:HD3	2.03	0.41
34:BE:168:LEU:CD1	34:BE:169:LEU:HD22	2.50	0.41
48:BW:23:ALA:HB1	48:BW:29:THR:CG2	2.51	0.41
49:BX:98:ASN:O	49:BX:98:ASN:OD1	2.39	0.41
51:D1:246:A:H62	51:D1:281:G:N2	2.19	0.41
1:AA:150:ILE:O	1:AA:150:ILE:HG22	2.20	0.41
2:AB:119:ILE:O	2:AB:123:LEU:HD23	2.21	0.41
7:AG:10:LEU:O	7:AG:13:ILE:HG22	2.21	0.41
8:AH:59:LYS:O	8:AH:60:LEU:HD22	2.21	0.41
9:AI:88:MET:O	9:AI:89:ARG:HD3	2.21	0.41
50:BY:60:VAL:HG23	50:BY:60:VAL:O	2.20	0.41
52:D2:876:C:H2'	52:D2:877:A:O4'	2.21	0.41
52:D2:1726:C:N4	52:D2:1735:A:H61	2.19	0.41
3:AC:49:ASP:O	3:AC:52:VAL:HG22	2.21	0.40
4:AD:86:GLY:O	4:AD:138:ALA:HB1	2.21	0.40
10:AJ:19:VAL:HG12	10:AJ:82:GLU:HB2	2.03	0.40
10:AJ:88:PRO:CG	20:AU:28:LEU:HD11	2.51	0.40
51:D1:890:G:O2'	51:D1:891:U:P	2.79	0.40
56:F2:410:TYR:CE2	56:F2:541:ILE:HG21	2.56	0.40
56:F2:779:LYS:HA	56:F2:782:MET:SD	2.61	0.40
15:AO:19:VAL:HG13	15:AO:19:VAL:O	2.21	0.40
18:AR:8:PRO:HB2	18:AR:38:THR:HG21	2.02	0.40
39:BN:15:GLY:O	39:BN:47:ILE:HD12	2.21	0.40
50:BY:48:MET:HE2	50:BY:84:PRO:O	2.21	0.40
51:D1:673:A:H2'	51:D1:674:G:C8	2.56	0.40
52:D2:364:C:C2	52:D2:365:U:C5	3.10	0.40
11:AK:64:SER:OG	11:AK:96:THR:HG23	2.21	0.40
12:AL:27:THR:HG21	51:D1:1328:C:C5'	2.50	0.40
30:BA:23:ILE:HG23	30:BA:24:ASN:N	2.37	0.40
34:BE:36:ASN:OD1	34:BE:37:MET:N	2.54	0.40
36:BI:70:GLU:HG2	36:BI:71:LYS:HG2	2.04	0.40
45:BT:93:ILE:HD12	45:BT:93:ILE:H	1.87	0.40
56:F2:464:ILE:HG22	56:F2:465:VAL:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:45:VAL:HG12	4:AD:116:VAL:HG23	2.04	0.40
10:AJ:83:VAL:HG12	10:AJ:84:MET:N	2.36	0.40
15:AO:4:ILE:HD12	15:AO:71:VAL:HG21	2.03	0.40
19:AT:31:ILE:HD13	19:AT:53:MET:HE2	2.03	0.40
22:B1:63:ILE:HG23	22:B1:64:ASP:N	2.36	0.40
23:B2:33:ALA:HB1	48:BW:13:ALA:HB1	2.03	0.40
27:B7:34:ARG:HD3	52:D2:467:G:OP2	2.22	0.40
31:BB:131:MET:HE1	31:BB:187:CYS:HB2	2.04	0.40
56:F2:331:GLN:O	56:F2:361:MET:HE1	2.22	0.40
5:AE:94:HIS:O	5:AE:96:VAL:HG13	2.21	0.40
6:AF:117:LEU:HD23	6:AF:121:ASN:ND2	2.37	0.40
19:AT:31:ILE:O	19:AT:34:VAL:HG12	2.22	0.40
19:AT:57:VAL:HG23	19:AT:58:ASP:N	2.37	0.40
33:BD:164:LEU:CB	33:BD:167:VAL:HG22	2.52	0.40
34:BE:37:MET:O	34:BE:37:MET:SD	2.80	0.40
34:BE:37:MET:SD	34:BE:52:ALA:HB1	2.62	0.40
44:BS:50:ARG:NH2	44:BS:52:ARG:HE	2.19	0.40
47:BV:4:ILE:HG22	47:BV:106:VAL:HG22	2.04	0.40
51:D1:1218:C:H2'	51:D1:1219:A:C8	2.55	0.40
52:D2:278:A:H2	52:D2:279:A:H62	1.70	0.40
56:F2:374:GLU:O	56:F2:377:VAL:HG22	2.20	0.40
56:F2:770:VAL:HG12	56:F2:771:ILE:N	2.37	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	AA	223/241 (92%)	205 (92%)	18 (8%)	0	100	100
2	AB	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
3	AC	203/206 (98%)	179 (88%)	24 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	155/167 (93%)	133 (86%)	21 (14%)	1 (1%)	21	56
5	AE	98/135 (73%)	81 (83%)	17 (17%)	0	100	100
6	AF	149/179 (83%)	136 (91%)	13 (9%)	0	100	100
7	AG	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AH	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
9	AI	96/103 (93%)	77 (80%)	19 (20%)	0	100	100
10	AJ	114/129 (88%)	93 (82%)	21 (18%)	0	100	100
11	AK	121/124 (98%)	99 (82%)	22 (18%)	0	100	100
12	AL	112/118 (95%)	101 (90%)	11 (10%)	0	100	100
13	AM	98/101 (97%)	84 (86%)	14 (14%)	0	100	100
14	AN	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	AO	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
16	AP	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
17	AQ	63/75 (84%)	55 (87%)	8 (13%)	0	100	100
18	AR	77/92 (84%)	68 (88%)	9 (12%)	0	100	100
19	AT	83/87 (95%)	76 (92%)	7 (8%)	0	100	100
20	AU	63/71 (89%)	40 (64%)	21 (33%)	2 (3%)	3	18
21	B0	73/85 (86%)	64 (88%)	9 (12%)	0	100	100
22	B1	75/78 (96%)	68 (91%)	7 (9%)	0	100	100
23	B2	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
24	B3	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
25	B5	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
26	B6	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
27	B7	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
28	B8	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	7	34
29	B9	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
30	BA	130/234 (56%)	126 (97%)	4 (3%)	0	100	100
31	BB	269/273 (98%)	246 (91%)	23 (9%)	0	100	100
32	BC	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
33	BD	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	24	60
34	BE	175/179 (98%)	157 (90%)	18 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BF	174/177 (98%)	157 (90%)	17 (10%)	0	100	100
36	BI	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
37	BK	139/142 (98%)	126 (91%)	13 (9%)	0	100	100
38	BM	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
39	BN	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
40	BO	141/144 (98%)	122 (86%)	19 (14%)	0	100	100
41	BP	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
42	BQ	118/127 (93%)	106 (90%)	12 (10%)	0	100	100
43	BR	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
44	BS	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
45	BT	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
46	BU	101/103 (98%)	89 (88%)	11 (11%)	1 (1%)	12	45
47	BV	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
48	BW	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
49	BX	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
50	BY	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
56	F2	594/896 (66%)	548 (92%)	46 (8%)	0	100	100
All	All	6384/7115 (90%)	5771 (90%)	607 (10%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	AU	8	ASN
46	BU	54	VAL
4	AD	122	VAL
20	AU	36	PHE
33	BD	83	VAL
28	B8	31	ILE

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	AA	186/199 (94%)	186 (100%)	0	100	100
2	AB	170/190 (90%)	170 (100%)	0	100	100
3	AC	172/173 (99%)	172 (100%)	0	100	100
4	AD	119/126 (94%)	119 (100%)	0	100	100
5	AE	87/116 (75%)	87 (100%)	0	100	100
6	AF	124/147 (84%)	124 (100%)	0	100	100
7	AG	104/105 (99%)	104 (100%)	0	100	100
8	AH	105/107 (98%)	105 (100%)	0	100	100
9	AI	86/90 (96%)	86 (100%)	0	100	100
10	AJ	89/99 (90%)	89 (100%)	0	100	100
11	AK	103/104 (99%)	103 (100%)	0	100	100
12	AL	92/96 (96%)	92 (100%)	0	100	100
13	AM	83/84 (99%)	83 (100%)	0	100	100
14	AN	76/77 (99%)	76 (100%)	0	100	100
15	AO	65/65 (100%)	65 (100%)	0	100	100
16	AP	74/78 (95%)	74 (100%)	0	100	100
17	AQ	56/65 (86%)	56 (100%)	0	100	100
18	AR	70/79 (89%)	70 (100%)	0	100	100
19	AT	65/66 (98%)	65 (100%)	0	100	100
20	AU	55/61 (90%)	55 (100%)	0	100	100
21	B0	57/63 (90%)	57 (100%)	0	100	100
22	B1	67/68 (98%)	67 (100%)	0	100	100
23	B2	55/55 (100%)	55 (100%)	0	100	100
24	B3	48/49 (98%)	48 (100%)	0	100	100
25	B5	47/48 (98%)	47 (100%)	0	100	100
26	B6	45/49 (92%)	45 (100%)	0	100	100
27	B7	38/38 (100%)	38 (100%)	0	100	100
28	B8	51/52 (98%)	51 (100%)	0	100	100
29	B9	34/34 (100%)	34 (100%)	0	100	100
30	BA	110/181 (61%)	110 (100%)	0	100	100
31	BB	216/218 (99%)	216 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	BC	164/164 (100%)	164 (100%)	0	100	100
33	BD	165/165 (100%)	165 (100%)	0	100	100
34	BE	148/150 (99%)	148 (100%)	0	100	100
35	BF	137/138 (99%)	137 (100%)	0	100	100
36	BI	114/114 (100%)	114 (100%)	0	100	100
37	BK	109/110 (99%)	109 (100%)	0	100	100
38	BM	116/116 (100%)	116 (100%)	0	100	100
39	BN	103/104 (99%)	103 (100%)	0	100	100
40	BO	102/103 (99%)	102 (100%)	0	100	100
41	BP	109/109 (100%)	109 (100%)	0	100	100
42	BQ	100/103 (97%)	100 (100%)	0	100	100
43	BR	86/87 (99%)	86 (100%)	0	100	100
44	BS	99/100 (99%)	99 (100%)	0	100	100
45	BT	89/90 (99%)	89 (100%)	0	100	100
46	BU	84/84 (100%)	84 (100%)	0	100	100
47	BV	93/93 (100%)	93 (100%)	0	100	100
48	BW	80/84 (95%)	80 (100%)	0	100	100
49	BX	83/85 (98%)	83 (100%)	0	100	100
50	BY	78/78 (100%)	78 (100%)	0	100	100
56	F2	480/719 (67%)	480 (100%)	0	100	100
All	All	5288/5778 (92%)	5288 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	23	ASN
1	AA	88	GLN
2	AB	18	ASN
3	AC	70	GLN
4	AD	77	ASN
4	AD	120	HIS
5	AE	14	GLN
9	AI	58	ASN

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Mol	Chain	Res	Type
9	AI	99	GLN
10	AJ	117	HIS
14	AN	45	HIS
15	AO	63	GLN
16	AP	44	HIS
19	AT	12	GLN
19	AT	81	GLN
23	B2	25	GLN
31	BB	36	ASN
31	BB	44	ASN
31	BB	52	HIS
32	BC	67	HIS
32	BC	173	GLN
34	BE	4	HIS
35	BF	21	GLN
35	BF	138	GLN
37	BK	106	GLN
40	BO	38	GLN
40	BO	99	ASN
42	BQ	9	GLN
42	BQ	23	ASN
43	BR	29	HIS
43	BR	104	GLN
56	F2	432	HIS
56	F2	485	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	D1	1538/1540 (99%)	222 (14%)	8 (0%)
52	D2	2902/2903 (99%)	486 (16%)	22 (0%)
53	D3	119/120 (99%)	24 (20%)	1 (0%)
54	D4	4/56 (7%)	0	0
55	D5	76/77 (98%)	19 (25%)	0
All	All	4639/4696 (98%)	751 (16%)	31 (0%)

All (751) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	D1	4	U
51	D1	9	G

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Mol	Chain	Res	Type
51	D1	31	G
51	D1	32	A
51	D1	39	G
51	D1	47	C
51	D1	48	C
51	D1	51	A
51	D1	71	A
51	D1	72	A
51	D1	79	G
51	D1	82	G
51	D1	83	C
51	D1	87	C
51	D1	88	U
51	D1	100	G
51	D1	121	U
51	D1	122	G
51	D1	163	C
51	D1	164	G
51	D1	171	A
51	D1	183	C
51	D1	184	G
51	D1	199	A
51	D1	208	U
51	D1	209	U
51	D1	210	C
51	D1	211	G
51	D1	212	G
51	D1	226	G
51	D1	240	G
51	D1	245	U
51	D1	247	G
51	D1	251	G
51	D1	252	U
51	D1	266	G
51	D1	267	C
51	D1	281	G
51	D1	283	U
51	D1	289	G
51	D1	306	A
51	D1	328	C
51	D1	329	A
51	D1	345	C

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Mol	Chain	Res	Type
51	D1	346	G
51	D1	352	C
51	D1	354	G
51	D1	367	U
51	D1	372	C
51	D1	373	A
51	D1	406	G
51	D1	411	A
51	D1	412	A
51	D1	413	G
51	D1	414	A
51	D1	422	C
51	D1	423	G
51	D1	429	U
51	D1	438	U
51	D1	446	G
51	D1	465	A
51	D1	467	U
51	D1	468	A
51	D1	478	A
51	D1	479	U
51	D1	484	G
51	D1	485	U
51	D1	486	U
51	D1	495	A
51	D1	497	G
51	D1	511	C
51	D1	518	C
51	D1	519	C
51	D1	521	G
51	D1	527	G
51	D1	531	U
51	D1	532	A
51	D1	547	A
51	D1	561	U
51	D1	562	U
51	D1	564	C
51	D1	572	A
51	D1	573	A
51	D1	575	G
51	D1	576	C
51	D1	577	G

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Mol	Chain	Res	Type
51	D1	587	G
51	D1	628	G
51	D1	639	G
51	D1	665	A
51	D1	688	G
51	D1	695	A
51	D1	702	A
51	D1	703	G
51	D1	713	G
51	D1	718	A
51	D1	723	U
51	D1	724	G
51	D1	731	G
51	D1	734	G
51	D1	755	G
51	D1	777	A
51	D1	815	A
51	D1	817	C
51	D1	819	A
51	D1	829	G
51	D1	843	U
51	D1	844	G
51	D1	846	G
51	D1	851	G
51	D1	872	A
51	D1	889	A
51	D1	890	G
51	D1	891	U
51	D1	902	G
51	D1	914	A
51	D1	926	G
51	D1	934	C
51	D1	935	A
51	D1	960	U
51	D1	961	U
51	D1	966	G
51	D1	969	A
51	D1	971	G
51	D1	975	A
51	D1	976	G
51	D1	977	A
51	D1	989	U

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Mol	Chain	Res	Type
51	D1	992	U
51	D1	993	G
51	D1	994	A
51	D1	1003	G
51	D1	1004	A
51	D1	1018	G
51	D1	1020	G
51	D1	1028	C
51	D1	1030	U
51	D1	1031	C
51	D1	1033	G
51	D1	1034	G
51	D1	1045	C
51	D1	1065	U
51	D1	1092	A
51	D1	1094	G
51	D1	1098	C
51	D1	1099	G
51	D1	1101	A
51	D1	1108	G
51	D1	1124	G
51	D1	1130	A
51	D1	1136	C
51	D1	1137	C
51	D1	1138	G
51	D1	1139	G
51	D1	1151	A
51	D1	1158	C
51	D1	1159	U
51	D1	1160	G
51	D1	1168	U
51	D1	1181	G
51	D1	1182	G
51	D1	1184	G
51	D1	1191	A
51	D1	1196	A
51	D1	1200	C
51	D1	1201	A
51	D1	1202	U
51	D1	1208	C
51	D1	1212	U
51	D1	1225	A

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Mol	Chain	Res	Type
51	D1	1227	A
51	D1	1228	C
51	D1	1236	A
51	D1	1238	A
51	D1	1257	A
51	D1	1258	G
51	D1	1260	G
51	D1	1262	C
51	D1	1269	A
51	D1	1270	G
51	D1	1275	A
51	D1	1278	G
51	D1	1280	A
51	D1	1282	C
51	D1	1286	U
51	D1	1287	A
51	D1	1300	G
51	D1	1301	U
51	D1	1302	C
51	D1	1305	G
51	D1	1317	C
51	D1	1320	C
51	D1	1338	G
51	D1	1346	A
51	D1	1347	G
51	D1	1348	U
51	D1	1353	G
51	D1	1363	A
51	D1	1370	G
51	D1	1379	G
51	D1	1395	C
51	D1	1398	A
51	D1	1441	A
51	D1	1445	U
51	D1	1446	A
51	D1	1448	C
51	D1	1452	C
51	D1	1492	A
51	D1	1493	A
51	D1	1494	G
51	D1	1497	G
51	D1	1503	A

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Mol	Chain	Res	Type
51	D1	1506	U
51	D1	1507	A
51	D1	1517	G
51	D1	1526	G
51	D1	1529	G
51	D1	1530	G
51	D1	1533	C
51	D1	1534	A
51	D1	1537	U
51	D1	1539	C
52	D2	10	A
52	D2	12	U
52	D2	34	U
52	D2	35	G
52	D2	42	A
52	D2	46	G
52	D2	50	U
52	D2	51	G
52	D2	63	A
52	D2	71	A
52	D2	74	A
52	D2	75	G
52	D2	82	U
52	D2	102	U
52	D2	118	A
52	D2	120	U
52	D2	138	U
52	D2	140	C
52	D2	141	G
52	D2	149	A
52	D2	162	U
52	D2	163	C
52	D2	196	A
52	D2	199	A
52	D2	204	A
52	D2	205	G
52	D2	215	G
52	D2	216	A
52	D2	221	A
52	D2	222	A
52	D2	223	A
52	D2	228	C

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Mol	Chain	Res	Type
52	D2	232	G
52	D2	248	G
52	D2	249	C
52	D2	255	A
52	D2	265	A
52	D2	266	G
52	D2	276	U
52	D2	279	A
52	D2	281	C
52	D2	283	G
52	D2	294	A
52	D2	302	C
52	D2	310	A
52	D2	323	C
52	D2	324	A
52	D2	329	G
52	D2	330	A
52	D2	359	G
52	D2	361	G
52	D2	362	A
52	D2	368	A
52	D2	371	A
52	D2	372	G
52	D2	373	U
52	D2	386	G
52	D2	387	U
52	D2	389	G
52	D2	404	A
52	D2	405	U
52	D2	406	G
52	D2	411	G
52	D2	412	A
52	D2	417	C
52	D2	422	A
52	D2	424	G
52	D2	429	A
52	D2	430	A
52	D2	456	C
52	D2	457	A
52	D2	458	G
52	D2	459	U
52	D2	481	G

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Mol	Chain	Res	Type
52	D2	482	A
52	D2	491	G
52	D2	504	A
52	D2	505	A
52	D2	509	C
52	D2	510	C
52	D2	530	G
52	D2	532	A
52	D2	533	G
52	D2	545	U
52	D2	546	U
52	D2	547	A
52	D2	549	G
52	D2	550	C
52	D2	563	A
52	D2	572	A
52	D2	573	U
52	D2	575	A
52	D2	603	A
52	D2	615	U
52	D2	616	A
52	D2	622	G
52	D2	627	A
52	D2	637	A
52	D2	646	U
52	D2	647	G
52	D2	653	U
52	D2	654	A
52	D2	656	G
52	D2	669	G
52	D2	683	U
52	D2	685	A
52	D2	686	U
52	D2	687	C
52	D2	704	G
52	D2	729	G
52	D2	730	A
52	D2	747	C
52	D2	752	A
52	D2	764	A
52	D2	775	G
52	D2	776	G

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Mol	Chain	Res	Type
52	D2	782	A
52	D2	784	G
52	D2	785	G
52	D2	805	G
52	D2	812	C
52	D2	819	A
52	D2	827	U
52	D2	828	U
52	D2	845	A
52	D2	846	U
52	D2	847	U
52	D2	857	G
52	D2	859	G
52	D2	860	U
52	D2	878	A
52	D2	885	C
52	D2	886	A
52	D2	887	U
52	D2	888	C
52	D2	891	G
52	D2	896	A
52	D2	897	C
52	D2	907	G
52	D2	910	A
52	D2	914	G
52	D2	932	U
52	D2	941	A
52	D2	946	C
52	D2	959	A
52	D2	961	C
52	D2	973	A
52	D2	974	G
52	D2	983	A
52	D2	995	C
52	D2	996	A
52	D2	1009	A
52	D2	1012	U
52	D2	1013	C
52	D2	1021	A
52	D2	1022	G
52	D2	1026	G
52	D2	1033	U

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Mol	Chain	Res	Type
52	D2	1045	C
52	D2	1046	A
52	D2	1047	G
52	D2	1053	C
52	D2	1057	A
52	D2	1058	U
52	D2	1059	G
52	D2	1060	U
52	D2	1062	G
52	D2	1065	U
52	D2	1066	U
52	D2	1070	A
52	D2	1071	G
52	D2	1072	C
52	D2	1074	G
52	D2	1075	C
52	D2	1076	C
52	D2	1082	U
52	D2	1083	U
52	D2	1084	A
52	D2	1085	A
52	D2	1087	G
52	D2	1088	A
52	D2	1093	G
52	D2	1094	U
52	D2	1095	A
52	D2	1103	A
52	D2	1104	C
52	D2	1109	C
52	D2	1111	A
52	D2	1112	G
52	D2	1114	C
52	D2	1130	U
52	D2	1132	U
52	D2	1133	A
52	D2	1135	C
52	D2	1141	U
52	D2	1142	A
52	D2	1143	A
52	D2	1155	A
52	D2	1172	C
52	D2	1175	A

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Mol	Chain	Res	Type
52	D2	1177	G
52	D2	1178	C
52	D2	1179	G
52	D2	1180	U
52	D2	1187	G
52	D2	1206	G
52	D2	1211	C
52	D2	1212	G
52	D2	1238	G
52	D2	1251	C
52	D2	1253	A
52	D2	1256	G
52	D2	1268	A
52	D2	1271	G
52	D2	1272	A
52	D2	1273	U
52	D2	1300	G
52	D2	1301	A
52	D2	1306	C
52	D2	1321	A
52	D2	1329	U
52	D2	1330	C
52	D2	1345	C
52	D2	1352	U
52	D2	1365	A
52	D2	1368	G
52	D2	1378	A
52	D2	1379	U
52	D2	1383	A
52	D2	1386	C
52	D2	1414	C
52	D2	1416	G
52	D2	1419	A
52	D2	1420	A
52	D2	1427	A
52	D2	1428	C
52	D2	1453	A
52	D2	1454	C
52	D2	1458	U
52	D2	1459	G
52	D2	1461	C
52	D2	1467	U

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Mol	Chain	Res	Type
52	D2	1482	G
52	D2	1490	A
52	D2	1491	G
52	D2	1493	C
52	D2	1498	C
52	D2	1507	C
52	D2	1508	A
52	D2	1515	A
52	D2	1519	G
52	D2	1524	G
52	D2	1534	U
52	D2	1535	A
52	D2	1536	C
52	D2	1537	G
52	D2	1540	G
52	D2	1546	G
52	D2	1547	C
52	D2	1555	G
52	D2	1556	C
52	D2	1558	C
52	D2	1560	G
52	D2	1565	C
52	D2	1569	A
52	D2	1578	U
52	D2	1581	G
52	D2	1583	A
52	D2	1584	U
52	D2	1585	C
52	D2	1608	A
52	D2	1611	C
52	D2	1647	U
52	D2	1648	U
52	D2	1649	G
52	D2	1674	G
52	D2	1675	C
52	D2	1695	G
52	D2	1715	G
52	D2	1729	U
52	D2	1730	C
52	D2	1732	C
52	D2	1733	G
52	D2	1735	A

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Mol	Chain	Res	Type
52	D2	1738	G
52	D2	1756	G
52	D2	1758	U
52	D2	1764	C
52	D2	1773	A
52	D2	1776	G
52	D2	1791	A
52	D2	1800	C
52	D2	1801	A
52	D2	1802	A
52	D2	1808	A
52	D2	1816	C
52	D2	1829	A
52	D2	1833	C
52	D2	1847	A
52	D2	1857	G
52	D2	1859	U
52	D2	1870	C
52	D2	1871	A
52	D2	1884	G
52	D2	1901	A
52	D2	1906	G
52	D2	1910	G
52	D2	1913	A
52	D2	1914	C
52	D2	1915	U
52	D2	1919	A
52	D2	1929	G
52	D2	1930	G
52	D2	1931	U
52	D2	1937	A
52	D2	1938	A
52	D2	1955	U
52	D2	1967	C
52	D2	1970	A
52	D2	1971	U
52	D2	1972	G
52	D2	1991	U
52	D2	1997	C
52	D2	2020	A
52	D2	2022	U
52	D2	2023	C

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Mol	Chain	Res	Type
52	D2	2027	G
52	D2	2031	A
52	D2	2033	A
52	D2	2043	C
52	D2	2052	A
52	D2	2055	C
52	D2	2056	G
52	D2	2060	A
52	D2	2061	G
52	D2	2062	A
52	D2	2069	G
52	D2	2094	A
52	D2	2100	G
52	D2	2101	A
52	D2	2102	G
52	D2	2110	G
52	D2	2111	U
52	D2	2112	G
52	D2	2113	U
52	D2	2118	U
52	D2	2119	A
52	D2	2121	G
52	D2	2126	A
52	D2	2127	G
52	D2	2131	U
52	D2	2132	U
52	D2	2133	G
52	D2	2134	A
52	D2	2137	U
52	D2	2140	G
52	D2	2145	C
52	D2	2146	C
52	D2	2147	A
52	D2	2151	U
52	D2	2159	G
52	D2	2161	C
52	D2	2162	G
52	D2	2166	U
52	D2	2171	A
52	D2	2172	U
52	D2	2173	A
52	D2	2174	C

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Mol	Chain	Res	Type
52	D2	2175	C
52	D2	2178	C
52	D2	2181	U
52	D2	2183	A
52	D2	2187	U
52	D2	2189	U
52	D2	2192	U
52	D2	2198	A
52	D2	2203	U
52	D2	2204	G
52	D2	2211	A
52	D2	2213	U
52	D2	2214	C
52	D2	2225	A
52	D2	2226	C
52	D2	2238	G
52	D2	2239	G
52	D2	2250	G
52	D2	2279	G
52	D2	2283	C
52	D2	2286	G
52	D2	2287	A
52	D2	2297	A
52	D2	2305	U
52	D2	2307	G
52	D2	2309	A
52	D2	2311	A
52	D2	2312	U
52	D2	2315	G
52	D2	2321	U
52	D2	2322	A
52	D2	2325	G
52	D2	2327	A
52	D2	2334	U
52	D2	2344	U
52	D2	2345	G
52	D2	2347	C
52	D2	2350	C
52	D2	2361	G
52	D2	2382	G
52	D2	2383	G
52	D2	2385	C

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Mol	Chain	Res	Type
52	D2	2391	G
52	D2	2392	A
52	D2	2402	U
52	D2	2403	C
52	D2	2406	A
52	D2	2422	C
52	D2	2423	U
52	D2	2424	C
52	D2	2425	A
52	D2	2429	G
52	D2	2430	A
52	D2	2434	A
52	D2	2435	A
52	D2	2441	U
52	D2	2447	G
52	D2	2448	A
52	D2	2475	C
52	D2	2476	A
52	D2	2478	A
52	D2	2498	C
52	D2	2502	G
52	D2	2504	U
52	D2	2505	G
52	D2	2513	A
52	D2	2518	A
52	D2	2520	C
52	D2	2529	G
52	D2	2547	A
52	D2	2554	U
52	D2	2566	A
52	D2	2567	G
52	D2	2572	A
52	D2	2573	C
52	D2	2602	A
52	D2	2603	G
52	D2	2609	U
52	D2	2613	U
52	D2	2629	U
52	D2	2630	G
52	D2	2646	C
52	D2	2655	G
52	D2	2656	U

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Mol	Chain	Res	Type
52	D2	2682	A
52	D2	2689	U
52	D2	2690	U
52	D2	2714	G
52	D2	2722	G
52	D2	2732	G
52	D2	2733	A
52	D2	2744	G
52	D2	2748	A
52	D2	2764	A
52	D2	2765	A
52	D2	2778	A
52	D2	2779	U
52	D2	2791	G
52	D2	2794	C
52	D2	2797	U
52	D2	2800	A
52	D2	2808	G
52	D2	2809	A
52	D2	2818	U
52	D2	2820	A
52	D2	2833	U
52	D2	2834	G
52	D2	2849	U
52	D2	2859	G
52	D2	2867	G
52	D2	2868	A
52	D2	2871	U
52	D2	2872	A
52	D2	2880	C
52	D2	2883	A
52	D2	2884	U
52	D2	2901	C
52	D2	2903	U
53	D3	2	G
53	D3	4	C
53	D3	12	C
53	D3	13	G
53	D3	23	G
53	D3	25	U
53	D3	26	C
53	D3	35	C

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Mol	Chain	Res	Type
53	D3	41	G
53	D3	42	C
53	D3	44	G
53	D3	48	U
53	D3	63	C
53	D3	64	G
53	D3	66	A
53	D3	67	G
53	D3	87	U
53	D3	88	C
53	D3	89	U
53	D3	90	C
53	D3	105	G
53	D3	108	A
53	D3	109	A
53	D3	120	A
55	D5	9	G
55	D5	10	G
55	D5	16	C
55	D5	17	C
55	D5	17(A)	U
55	D5	18	G
55	D5	19	G
55	D5	20	U
55	D5	47	U
55	D5	48	C
55	D5	49	G
55	D5	53	G
55	D5	55	U
55	D5	56	C
55	D5	58	A
55	D5	59	A
55	D5	60	U
55	D5	74	C
55	D5	75	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	D1	70	U
51	D1	890	G
51	D1	1190	G

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Mol	Chain	Res	Type
51	D1	1201	A
51	D1	1256	A
51	D1	1257	A
51	D1	1300	G
51	D1	1347	G
52	D2	227	A
52	D2	328	U
52	D2	372	G
52	D2	421	C
52	D2	458	G
52	D2	481	G
52	D2	490	C
52	D2	615	U
52	D2	774	G
52	D2	859	G
52	D2	1020	A
52	D2	1052	C
52	D2	1900	A
52	D2	1930	G
52	D2	2109	U
52	D2	2286	G
52	D2	2326	C
52	D2	2333	A
52	D2	2391	G
52	D2	2423	U
52	D2	2655	G
52	D2	2808	G
53	D3	88	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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$
57	FME	D5	101	55	8,9,10	0.31	0	7,9,11	1.13	1 (14%)
59	GTP	F2	902	58	30,34,34	0.88	2 (6%)	46,54,54	1.78	11 (23%)

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
57	FME	D5	101	55	-	1/7/9/11	-
59	GTP	F2	902	58	-	6/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	F2	902	GTP	C2-N3	2.17	1.38	1.33
59	F2	902	GTP	C5-N7	-2.09	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	F2	902	GTP	C5-C4-N3	-5.25	119.95	128.46
59	F2	902	GTP	C2-N3-C4	4.56	120.43	112.30
59	F2	902	GTP	PB-O3B-PG	-3.77	119.89	132.83
59	F2	902	GTP	C2-N1-C6	-3.56	118.62	125.10
59	F2	902	GTP	N9-C4-N3	3.35	132.66	125.94
59	F2	902	GTP	C5-C6-N1	2.73	120.14	113.19
59	F2	902	GTP	O6-C6-C5	-2.72	119.38	126.60
59	F2	902	GTP	N9-C8-N7	-2.63	108.44	113.39
59	F2	902	GTP	C8-N7-C5	2.58	108.90	104.24
57	D5	101	FME	CA-N-CN	2.38	126.48	122.82
59	F2	902	GTP	PA-O3A-PB	-2.31	124.89	132.83
59	F2	902	GTP	C3'-C2'-C1'	2.06	105.34	101.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

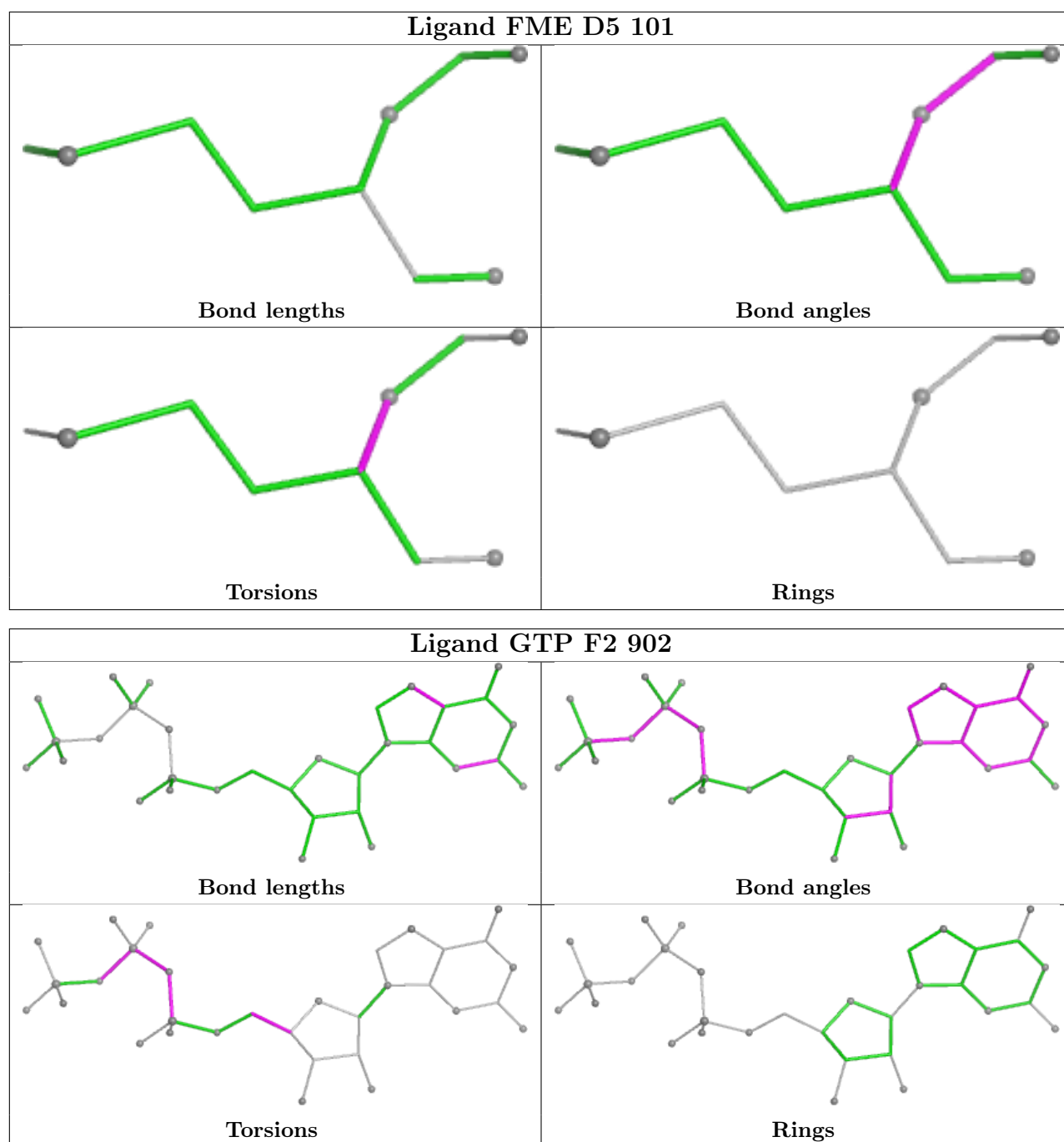
Mol	Chain	Res	Type	Atoms
59	F2	902	GTP	O4'-C4'-C5'-O5'
59	F2	902	GTP	C3'-C4'-C5'-O5'
59	F2	902	GTP	PA-O3A-PB-O3B
59	F2	902	GTP	PG-O3B-PB-O2B
59	F2	902	GTP	PB-O3A-PA-O1A
59	F2	902	GTP	PB-O3A-PA-O2A
57	D5	101	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	F2	902	GTP	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

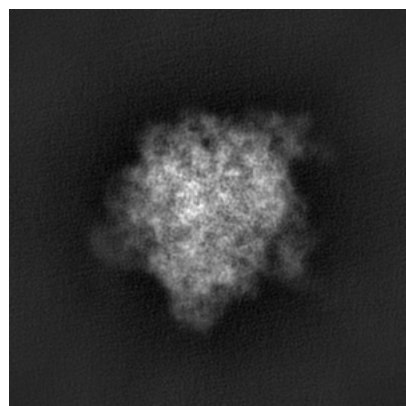
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56036. These allow visual inspection of the internal detail of the map and identification of artifacts.

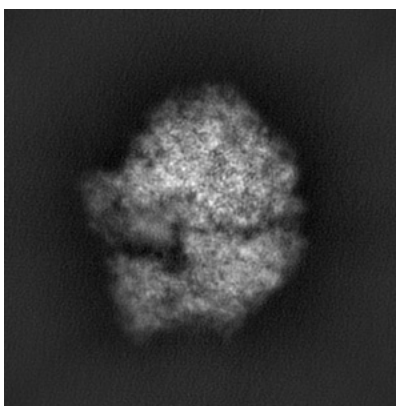
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

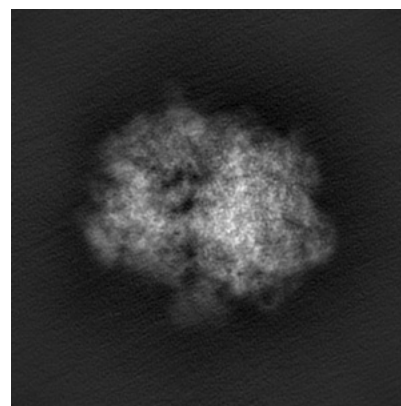
6.1.1 Primary map



X

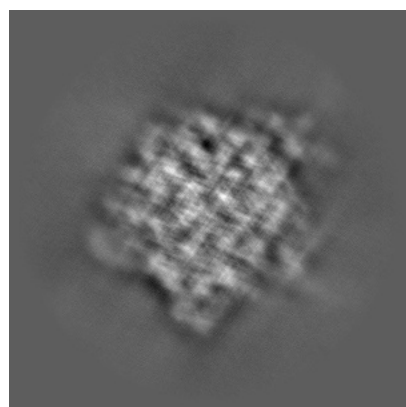


Y

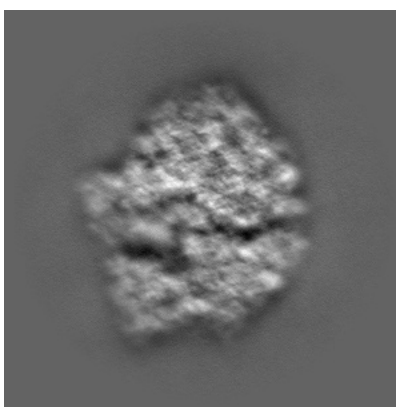


Z

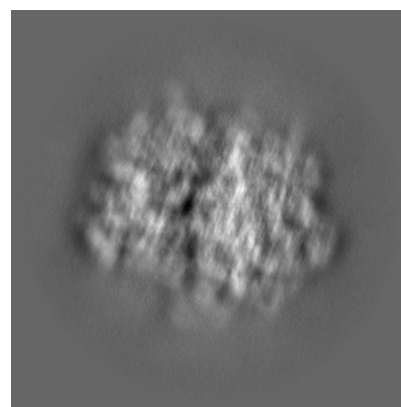
6.1.2 Raw map



X



Y

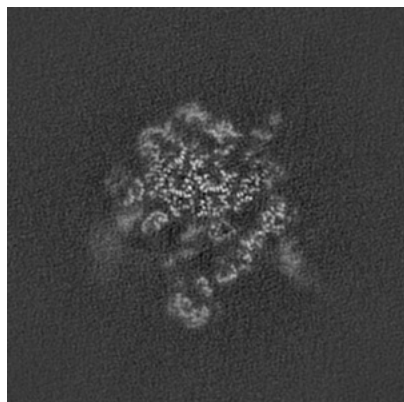


Z

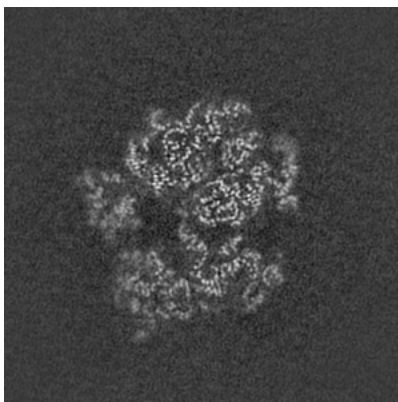
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

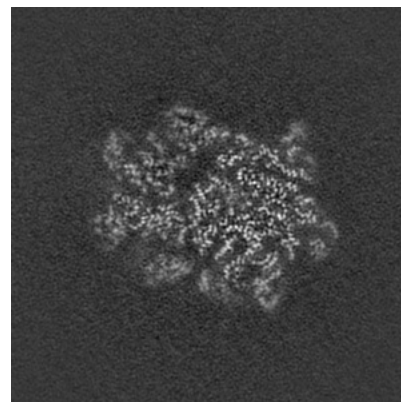
6.2.1 Primary map



X Index: 240

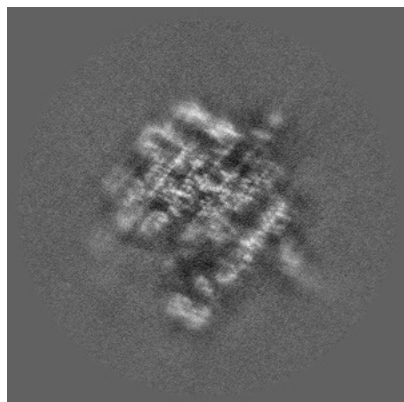


Y Index: 240

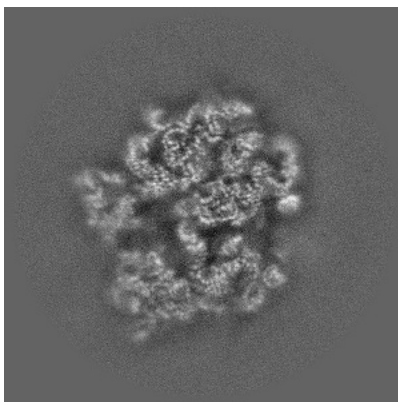


Z Index: 240

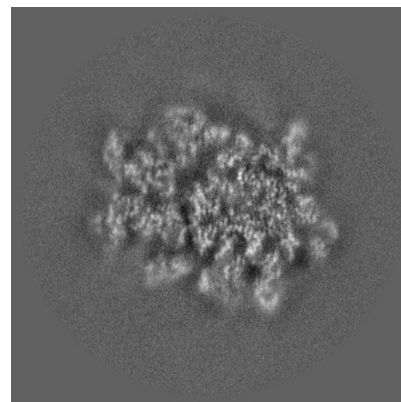
6.2.2 Raw map



X Index: 240



Y Index: 240

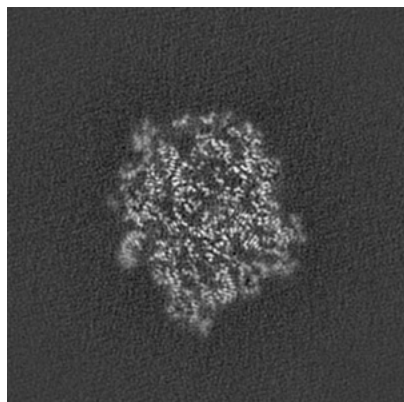


Z Index: 240

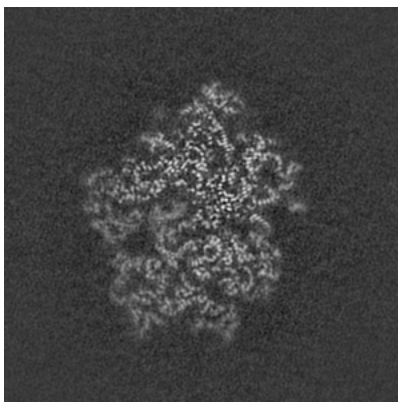
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

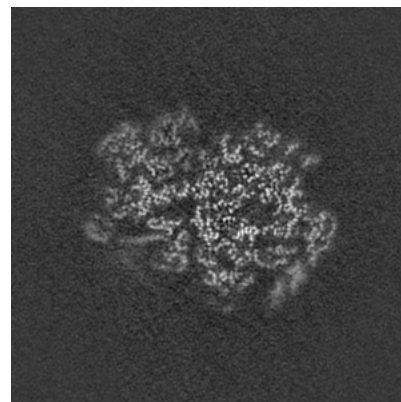
6.3.1 Primary map



X Index: 271

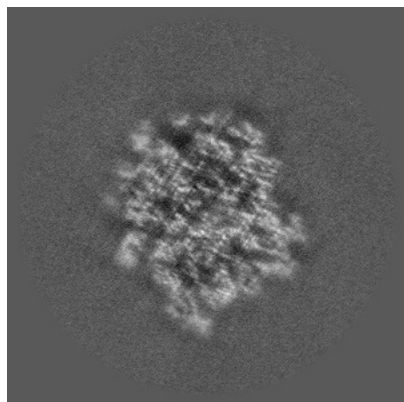


Y Index: 220

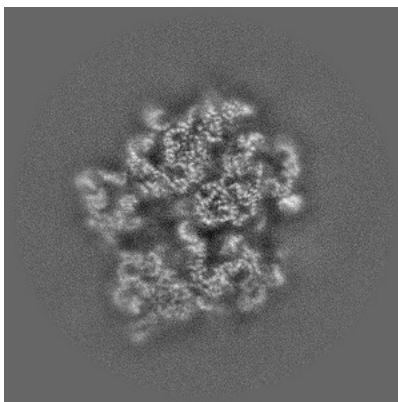


Z Index: 256

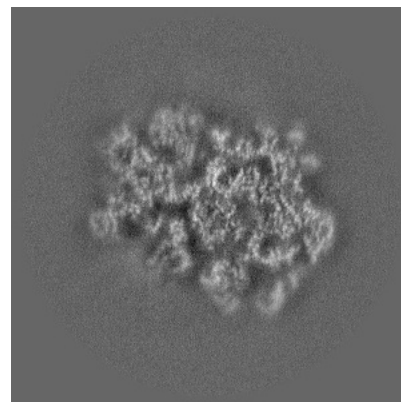
6.3.2 Raw map



X Index: 270



Y Index: 237

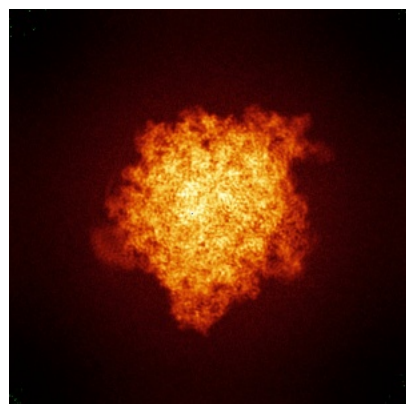


Z Index: 249

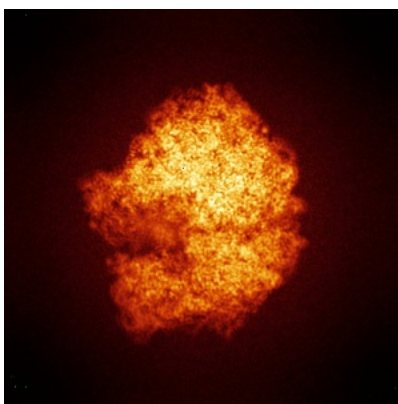
The images above show the largest variance slices of the map in three orthogonal directions.

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

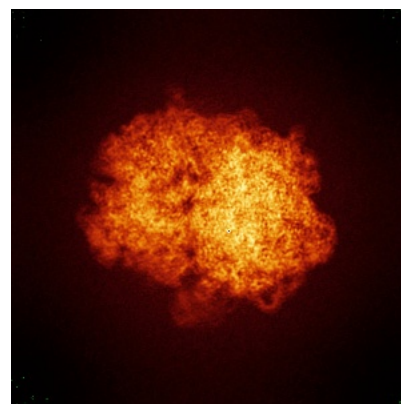
6.4.1 Primary map



X

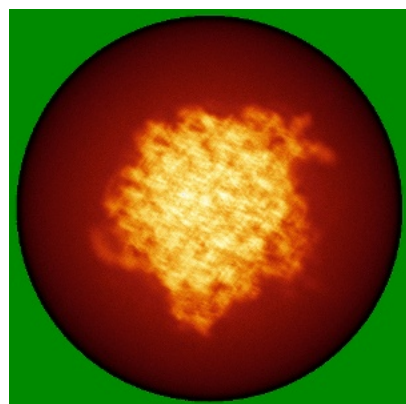


Y

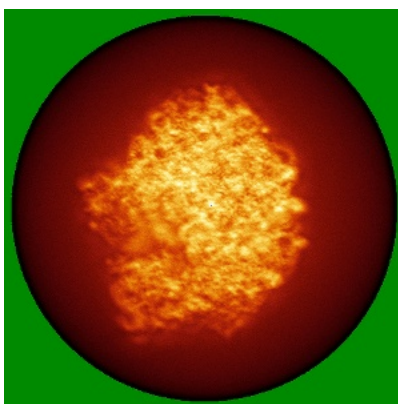


Z

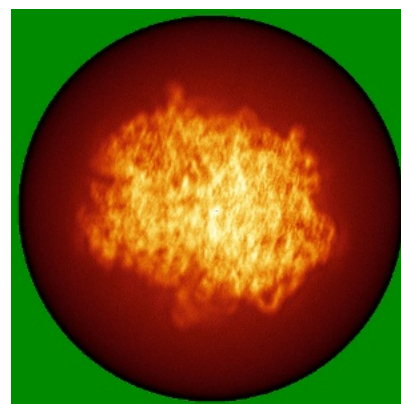
6.4.2 Raw map



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



X



Y



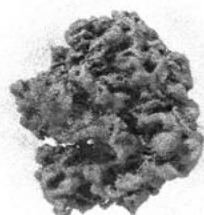
Z

The images above show the 3D surface view of the map at the recommended contour level 2.6. 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



X



Y



Z

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

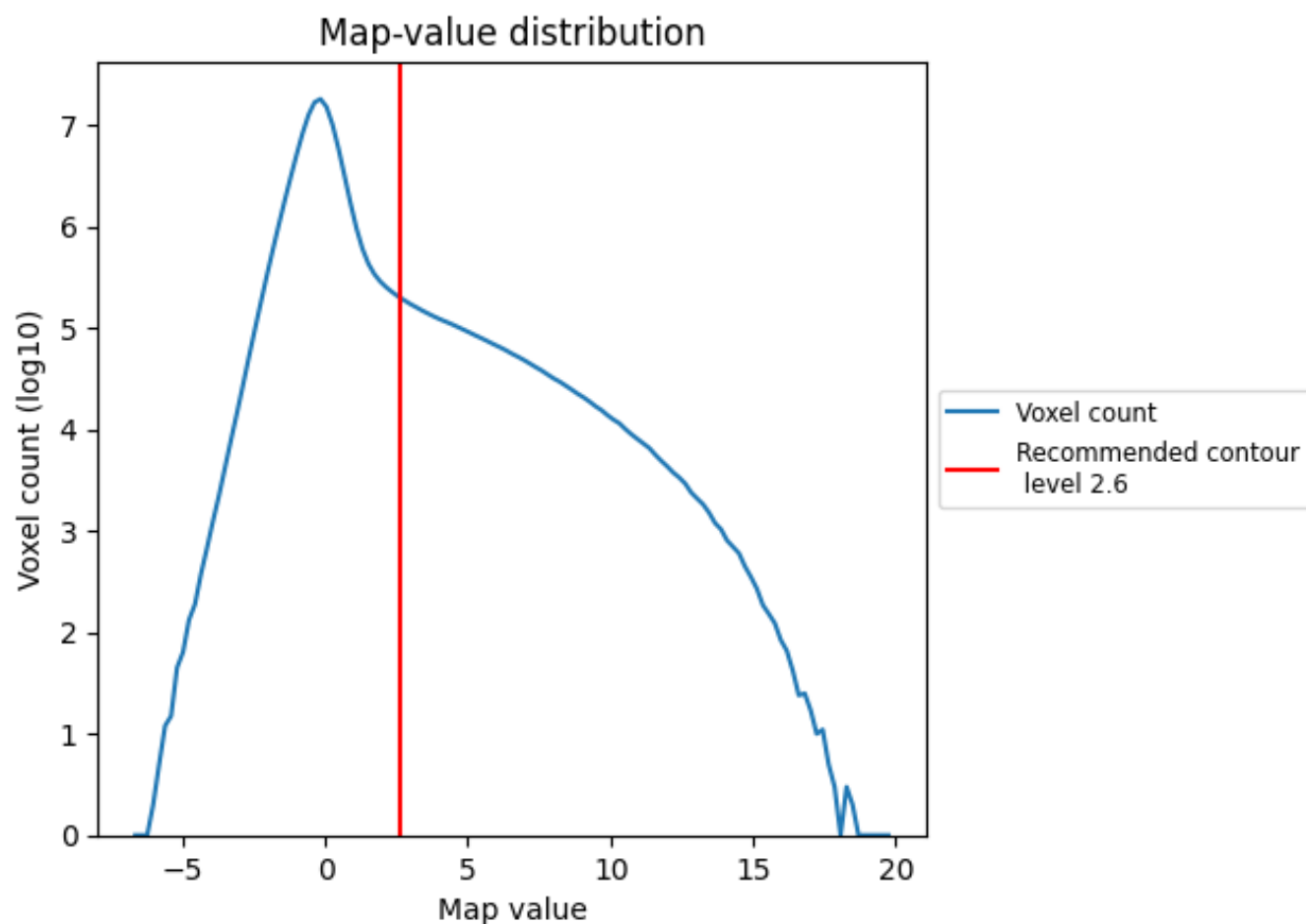
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

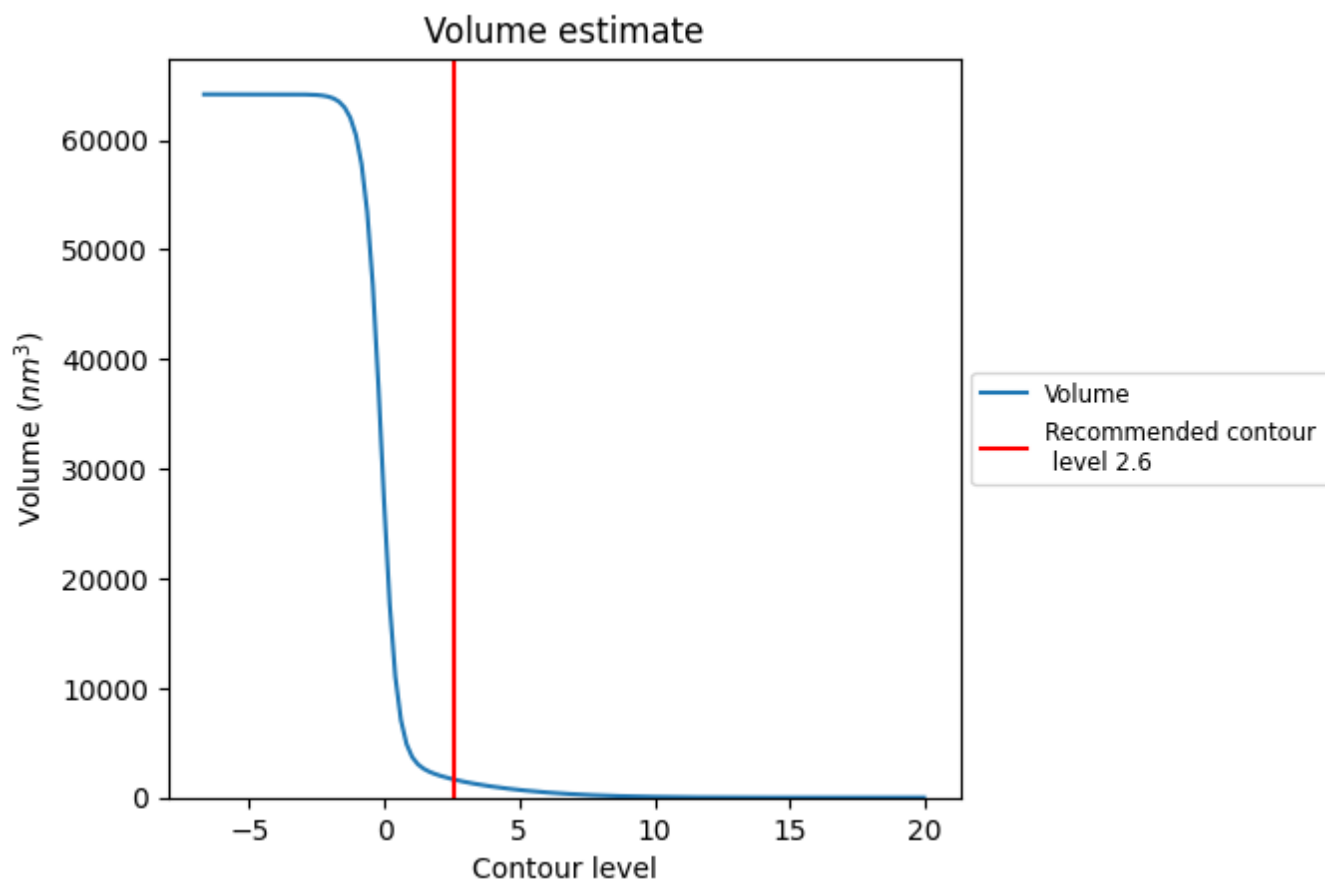
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

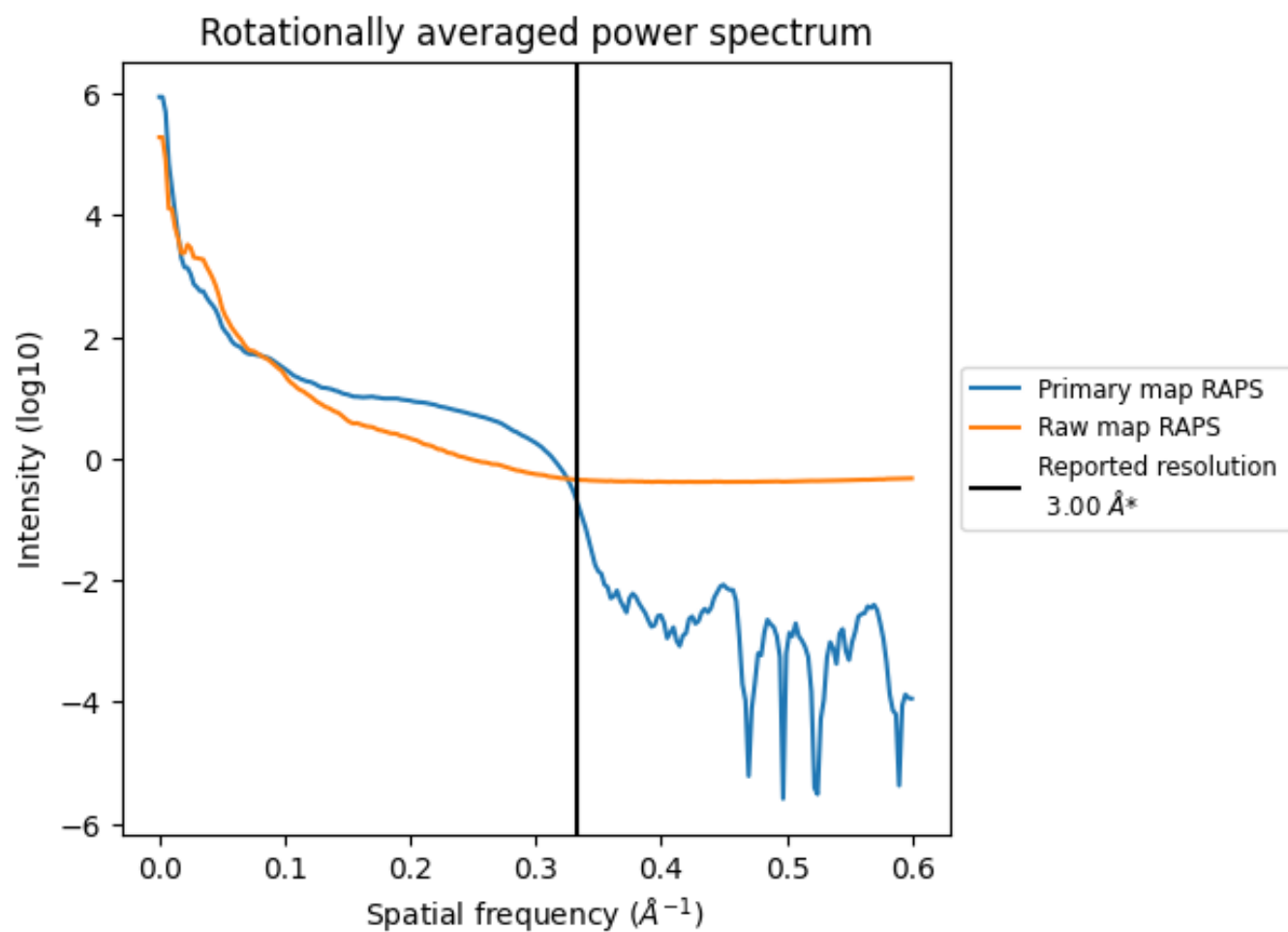
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1635 nm³; this corresponds to an approximate mass of 1477 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 ⓘ

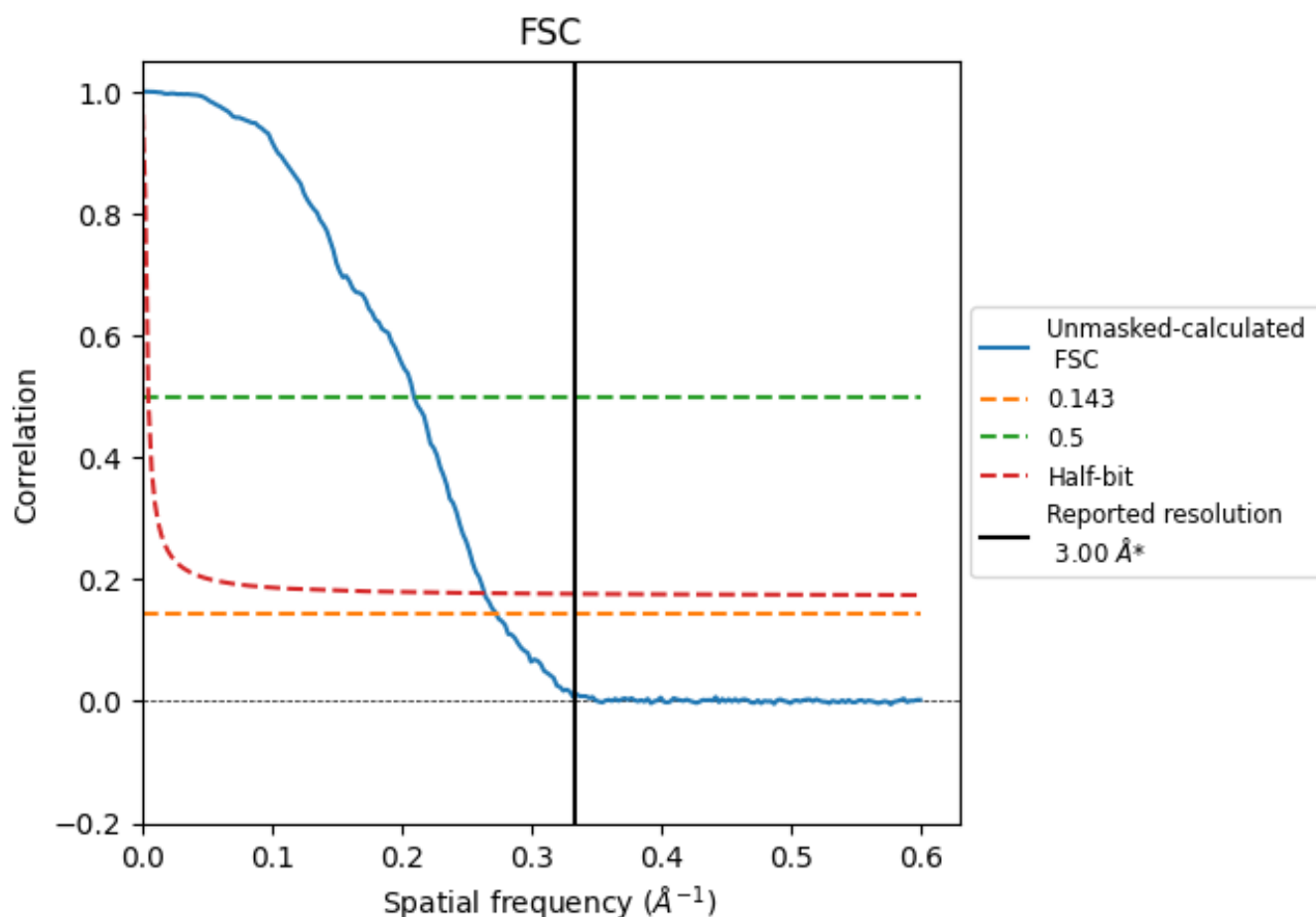


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

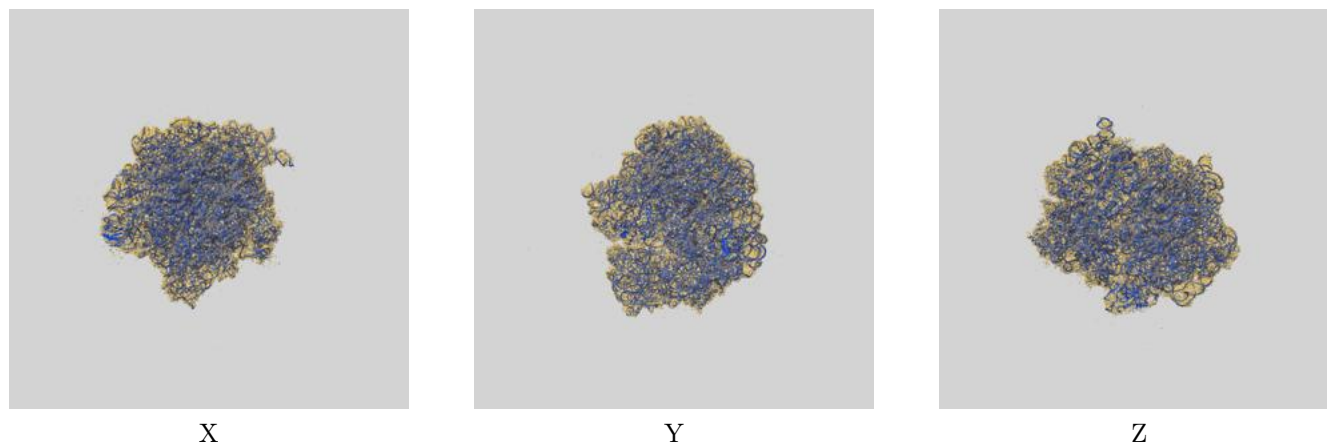
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.77	3.79

*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 3.66 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

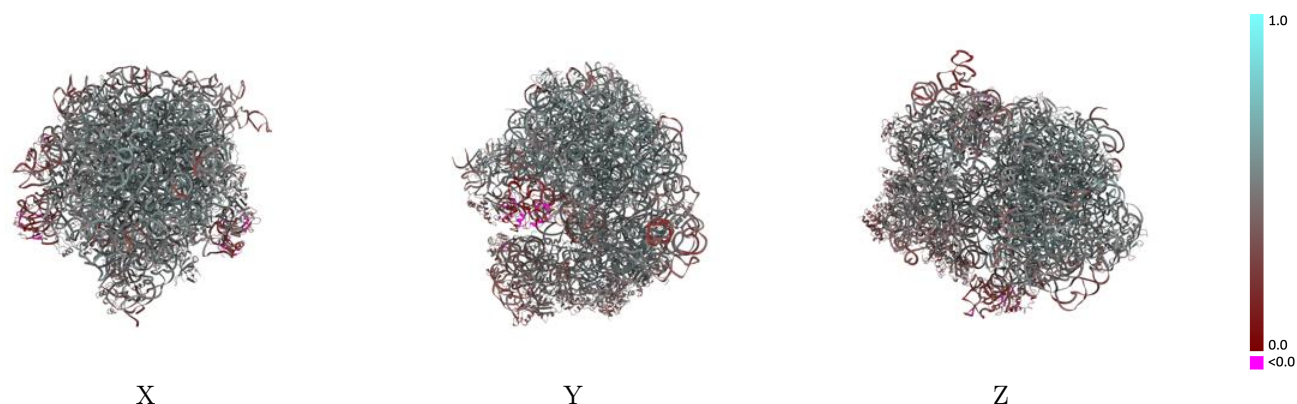
This section contains information regarding the fit between EMDB map EMD-56036 and PDB model 9TKP. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



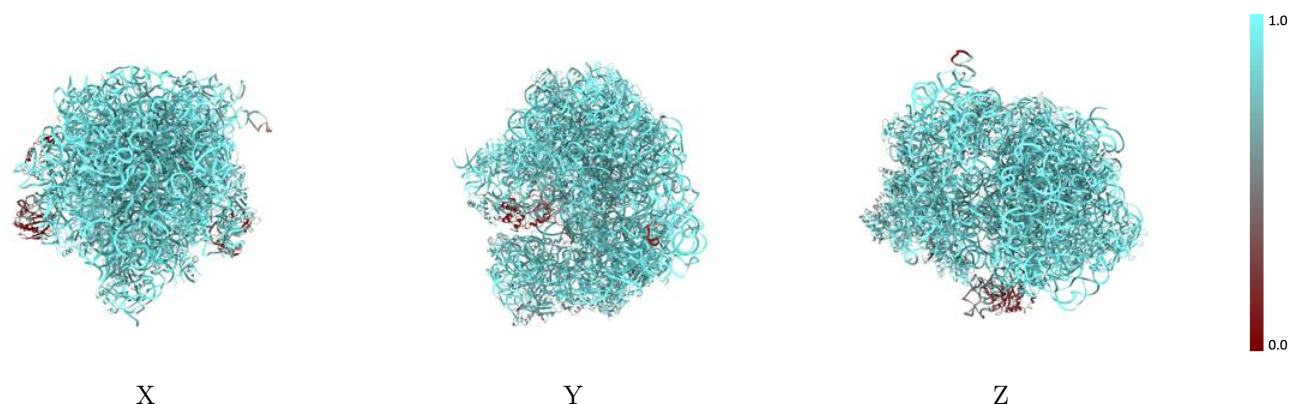
The images above show the 3D surface view of the map at the recommended contour level 2.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



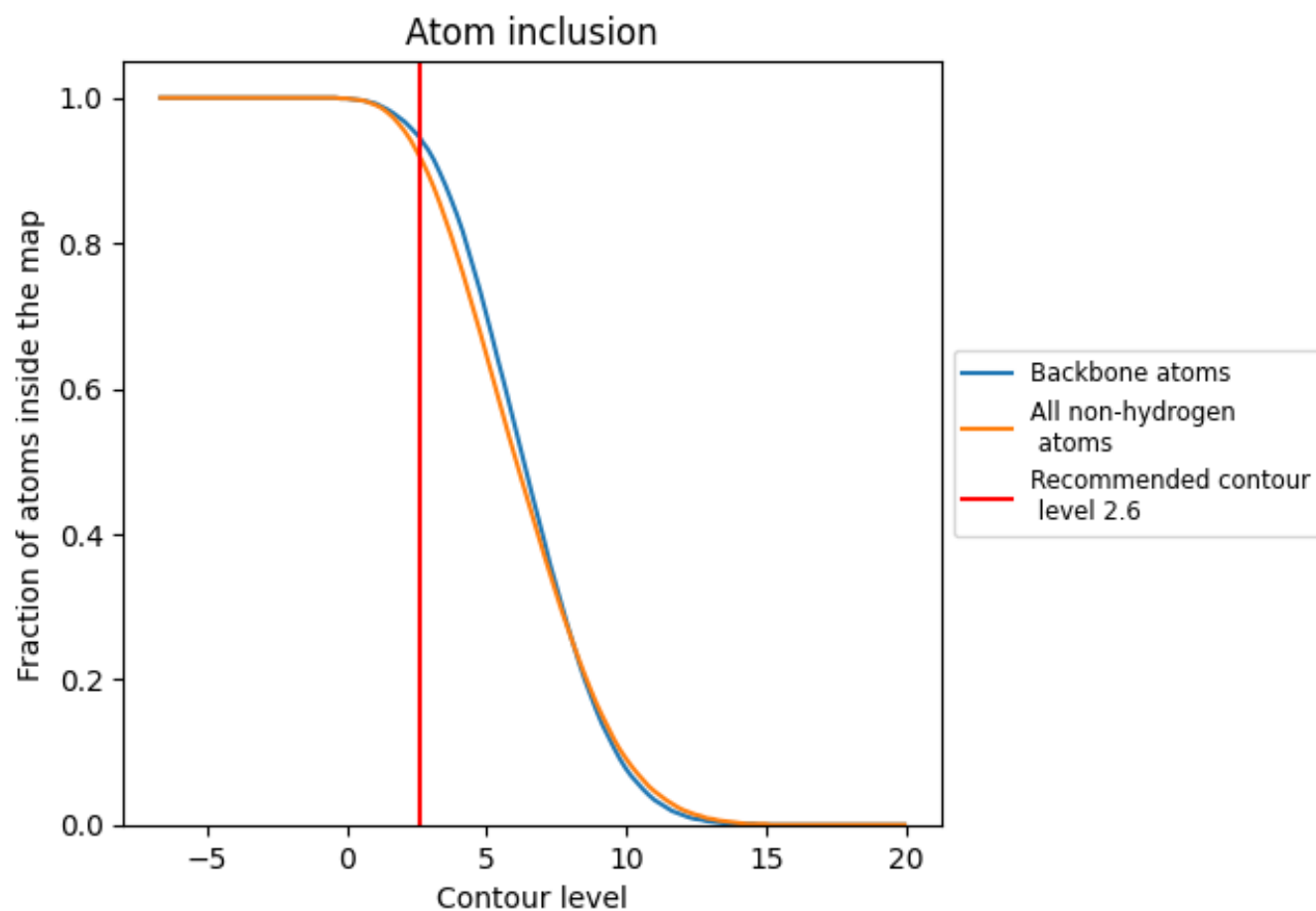
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (2.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9200	0.4610
AA	0.7450	0.3800
AB	0.8400	0.4360
AC	0.8530	0.4260
AD	0.8940	0.4630
AE	0.7940	0.3620
AF	0.7880	0.3590
AG	0.8800	0.4590
AH	0.7950	0.3810
AI	0.7420	0.3880
AJ	0.8890	0.3940
AK	0.8920	0.4800
AL	0.8160	0.3590
AM	0.8490	0.3900
AN	0.8880	0.4230
AO	0.8790	0.4660
AP	0.9020	0.4670
AQ	0.8830	0.4110
AR	0.7660	0.3620
AT	0.8520	0.4310
AU	0.6750	0.3070
B0	0.9450	0.5330
B1	0.9300	0.4960
B2	0.8710	0.4370
B3	0.9270	0.5130
B5	0.9350	0.5200
B6	0.9230	0.4900
B7	0.9580	0.5250
B8	0.9550	0.5420
B9	0.9210	0.5140
BA	0.1160	0.2140
BB	0.9420	0.5270
BC	0.9550	0.5280
BD	0.8850	0.4920
BE	0.7970	0.3660



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Chain	Atom inclusion	Q-score
BF	 0.8640	 0.4570
BI	 0.3610	 0.3100
BK	 0.1610	 0.1160
BM	 0.9330	 0.5200
BN	 0.9300	 0.5310
BO	 0.9270	 0.5020
BP	 0.9380	 0.5110
BQ	 0.9510	 0.5190
BR	 0.8790	 0.4410
BS	 0.9040	 0.5090
BT	 0.9350	 0.5210
BU	 0.8830	 0.5020
BV	 0.9200	 0.5140
BW	 0.8840	 0.4860
BX	 0.8900	 0.4650
BY	 0.8870	 0.4680
D1	 0.9660	 0.4510
D2	 0.9690	 0.4870
D3	 0.9750	 0.4500
D4	 0.6880	 0.4000
D5	 0.9340	 0.3340
F2	 0.7940	 0.4200