



Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 03:49 PM EDT

PDB ID : 9N2B
EMDB ID : EMD-48830
Title : Impacts of ribosomal RNA sequence variation on gene expression and phenotype: Cryo-EM structure of the rrsB ribosome (BBB-70S)
Authors : Welfer, G.A.; Brady, R.A.; Natchiar, S.K.; Watson, Z.L.; Rundlet, E.J.; Alejo, J.L.; Singh, A.P.; Mishra, N.K.; Altman, R.B.; Blanchard, S.C.
Deposited on : 2025-01-28
Resolution : 2.20 Å (reported)
Based on initial model : 7N1P

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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

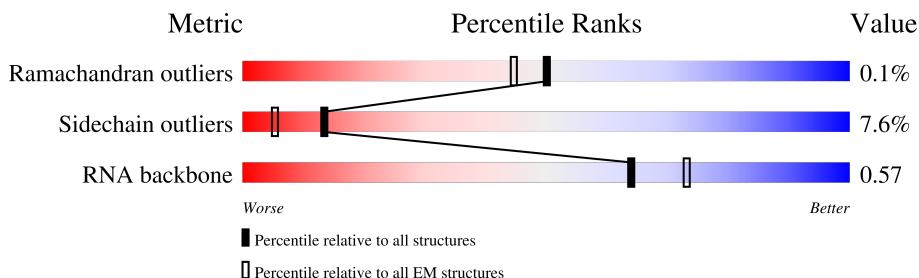
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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.



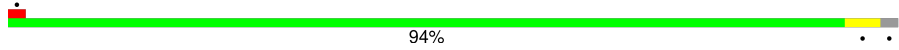


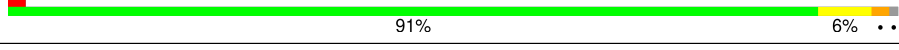

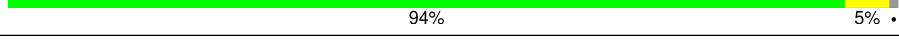
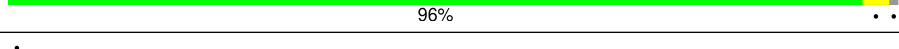
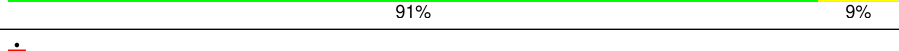
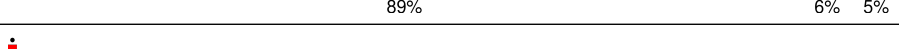
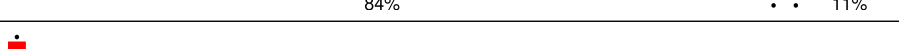
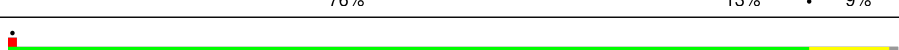

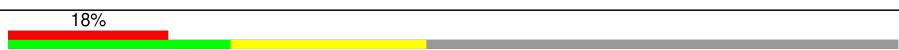

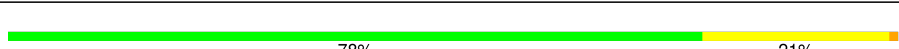
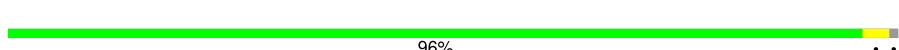

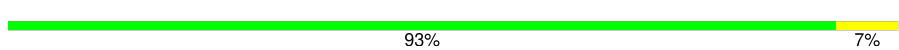


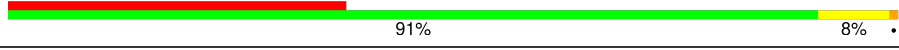
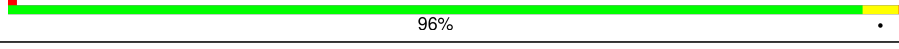
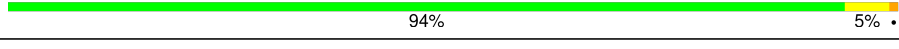
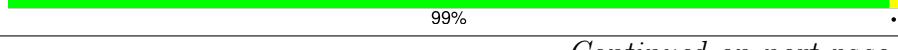

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	16	1542	
2	SB	241	
3	SC	233	
4	SD	206	
5	SE	167	
6	SF	135	
7	SG	179	
8	SH	130	

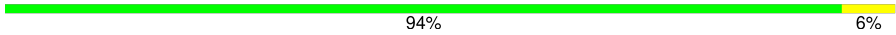


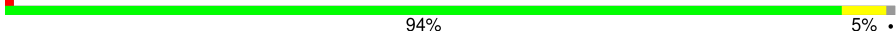
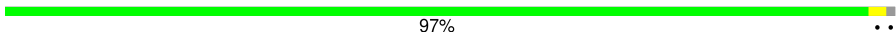



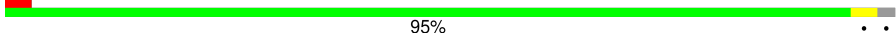



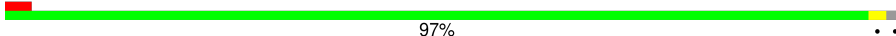


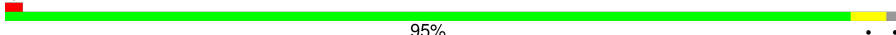





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Mol	Chain	Length	Quality of chain
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	91	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LB	273	
26	LC	209	
27	LD	201	
28	LE	179	
29	LF	177	
30	LI	149	
31	LM	142	
32	LN	123	
33	LO	144	

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Mol	Chain	Length	Quality of chain
34	LP	136	
35	LQ	127	
36	LR	117	
37	LS	115	
38	LT	118	
39	LU	103	
40	LV	110	
41	LW	100	
42	LX	104	
43	LY	94	
44	La	85	
45	Lb	78	
46	Lc	63	
47	Ld	59	
48	Le	70	
49	Lf	57	
50	Lg	55	
51	Lh	46	
52	Li	65	
53	Lj	38	
54	Pt	77	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 142763 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA (rRNA) from the rrnB operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	16	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SB	229	Total	C	N	O	S	0	0
			1787	1129	320	330	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SC	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SF	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SG	155	Total	C	N	O	S	1	0
			1236	772	240	220	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SI	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SK	118	Total	C	N	O	S	1	0
			895	551	178	163	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SK	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SL	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SM	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SO	88	Total	C	N	O	S	0	0
			713	439	144	129	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SR	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SU	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called Synthetic messenger RNA (mRNA) 60 bp in length.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	28	Total	C	N	O	P	1	0
			621	278	113	201	29		

- Molecule 23 is a RNA chain called 23S ribosomal RNA (rRNA) from the rrnB operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	23	2767	Total	C	N	O	P	0	0
			59424	26515	10941	19201	2767		

- Molecule 24 is a RNA chain called 5S ribosomal RNA (rRNA) from the B operon.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LC	209	Total	C	N	O	S	0	0
			1564	979	288	293	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LE	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LF	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LN	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LO	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LS	114	Total	C	N	O	S	0	0
			916	574	179	162	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LW	95	Total	C	N	O	S	0	0
			757	479	141	135	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	La	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lc	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Le	68	Total	C	N	O	S	0	0
			533	330	101	96	6		

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lg	52	Total	C	N	O	S	0	0
			426	275	78	73			

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

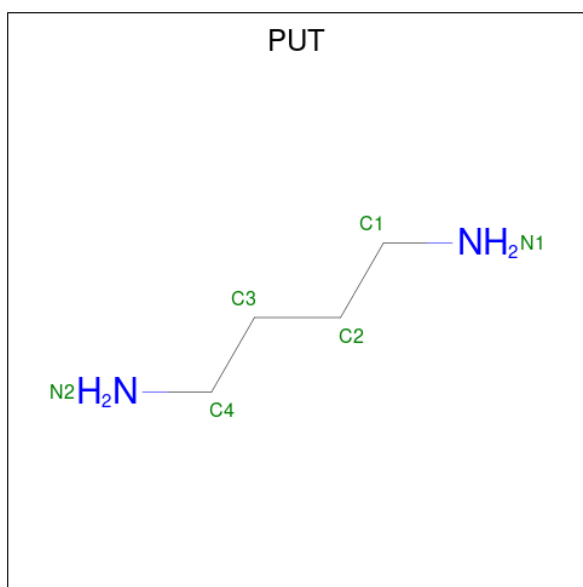
- Molecule 53 is a protein called 50S ribosomal protein L36.

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

- Molecule 54 is a RNA chain called N-formyl-methionine initiator tRNA (fMet-tRNA^{fMet}).

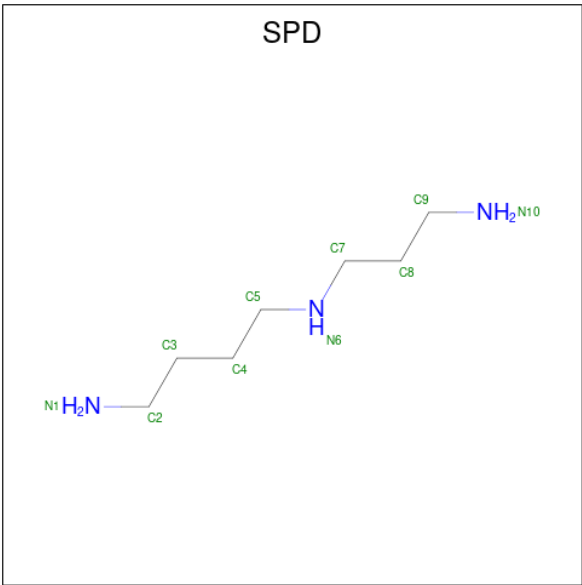
Mol	Chain	Residues	Atoms						AltConf	Trace
54	Pt	77	Total	C	N	O	P	S	0	0
			1646	734	298	536	77	1		

- Molecule 55 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C₄H₁₂N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
55	16	1	Total	C	N	0
			6	4	2	
55	23	1	Total	C	N	0
			6	4	2	
55	23	1	Total	C	N	0
			6	4	2	
55	23	1	Total	C	N	0
			6	4	2	
55	23	1	Total	C	N	0
			6	4	2	
55	23	1	Total	C	N	0
			6	4	2	
55	23	1	Total	C	N	0
			6	4	2	
55	23	1	Total	C	N	0
			6	4	2	

- Molecule 56 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
56	16	1	Total	C	N	0
			10	7	3	
56	23	1	Total	C	N	0
			10	7	3	
56	23	1	Total	C	N	0
			10	7	3	
56	23	1	Total	C	N	0
			10	7	3	
56	23	1	Total	C	N	0
			10	7	3	

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Lig- and of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
57	16	75	Total	Mg	0
			75	75	
57	mR	3	Total	Mg	0
			3	3	
57	23	185	Total	Mg	0
			185	185	
57	5	6	Total	Mg	0
			6	6	
57	LB	2	Total	Mg	0
			2	2	
57	LC	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
57	LD	1	Total 1	Mg 1	0
57	Lf	1	Total 1	Mg 1	0
57	Pt	2	Total 2	Mg 2	0

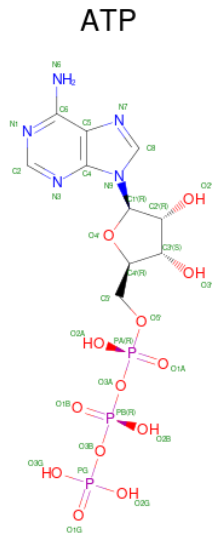
- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
58	16	8	Total 8	K 8	0
58	23	46	Total 46	K 46	0
58	LB	1	Total 1	K 1	0
58	LX	1	Total 1	K 1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

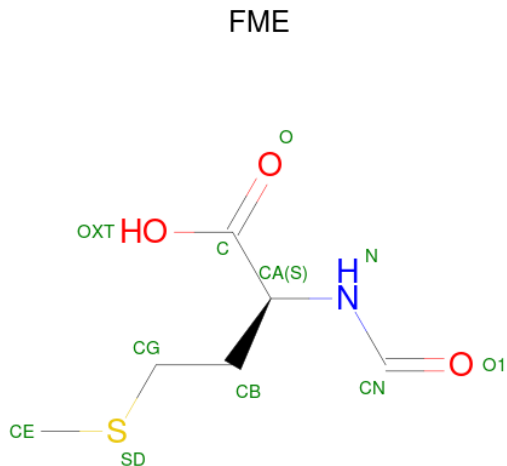
Mol	Chain	Residues	Atoms		AltConf
59	SB	1	Total 1	Zn 1	0
59	Le	1	Total 1	Zn 1	0
59	Lj	1	Total 1	Zn 1	0

- Molecule 60 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
60	23	1	Total 31	C 10	N 5	O 13	P 3	0
60	23	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $\text{C}_6\text{H}_{11}\text{NO}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).

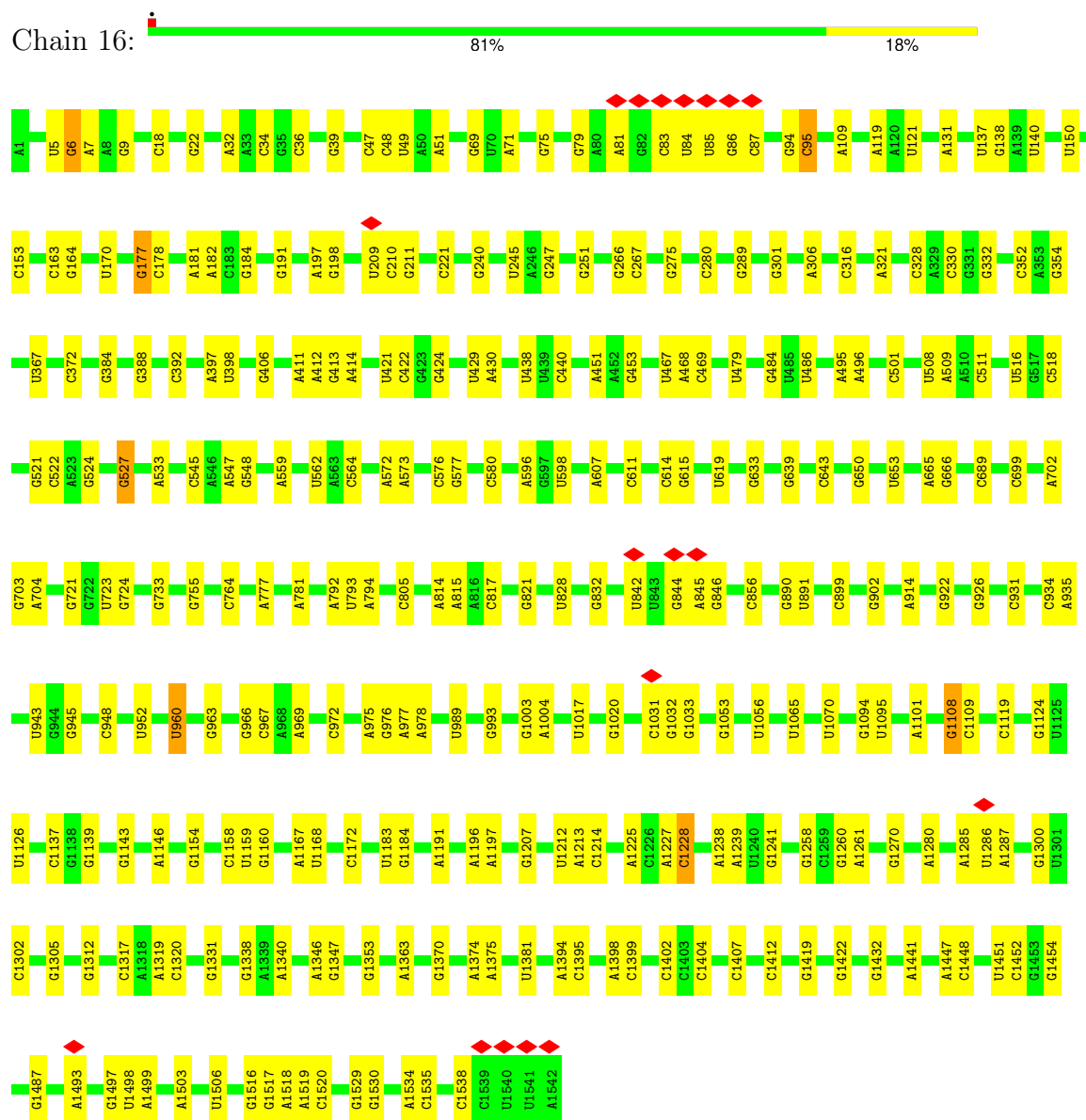



Mol	Chain	Residues	Atoms					AltConf
61	Pt	1	Total	C	N	O	S	0
			10	6	1	2	1	

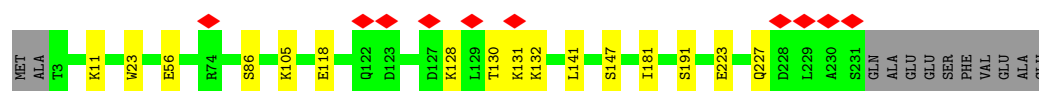
3 Residue-property plots

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: 16S ribosomal RNA (rRNA) from the *rrnB* operon



Chain SB:  88% 7% 5%



- Molecule 3: 30S ribosomal protein S3

Chain SC:  84% 6% 9%



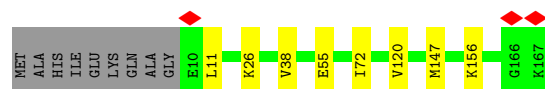
- Molecule 4: 30S ribosomal protein S4

Chain SD:  95% .



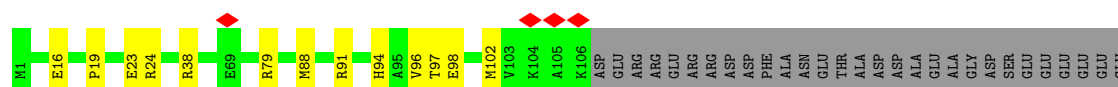
- Molecule 5: 30S ribosomal protein S5

Chain SE:  90% 5% 5%




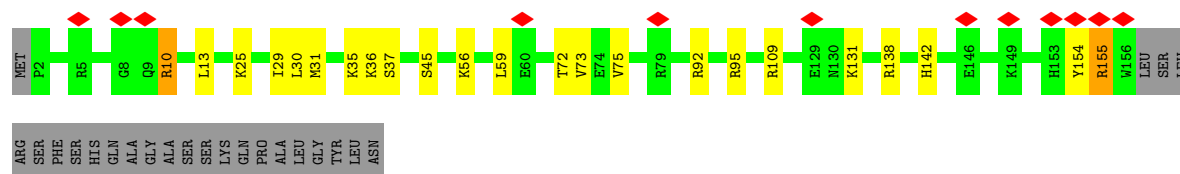
- Molecule 6: 30S ribosomal protein S6

Chain SF:  69% 10% 21%



- Molecule 7: 30S ribosomal protein S7

Chain SG:  74% 12% 13%

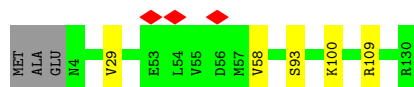


- Molecule 8: 30S ribosomal protein S8

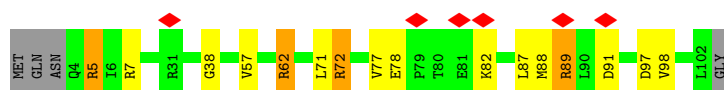
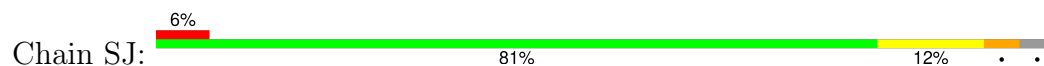
Chain SH:  95% . . .



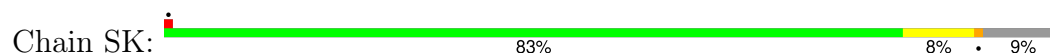
- Molecule 9: 30S ribosomal protein S9



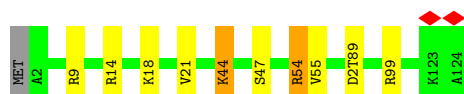
- Molecule 10: 30S ribosomal protein S10



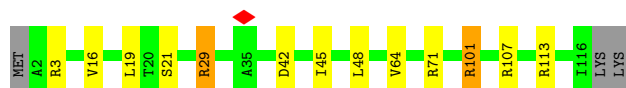
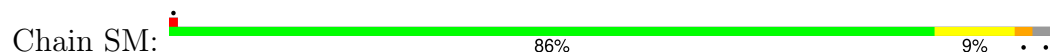
- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein uS12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



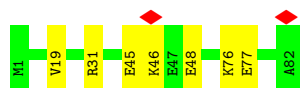
- Molecule 15: 30S ribosomal protein S15

Chain SO:  96% ..



- Molecule 16: 30S ribosomal protein S16

Chain SP:  91% 9%




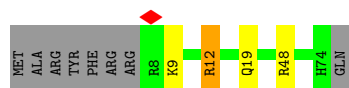
- Molecule 17: 30S ribosomal protein S17

Chain SQ:  89% 6% 5%



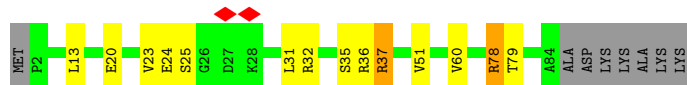
- Molecule 18: 30S ribosomal protein S18

Chain SR:  84% .. 11%




- Molecule 19: Small ribosomal subunit protein uS19

Chain SS:  76% 13% 9%




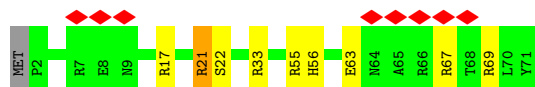
- Molecule 20: 30S ribosomal protein S20

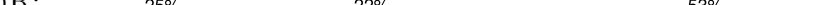
Chain ST:  90% 9% .



- Molecule 21: 30S ribosomal protein S21

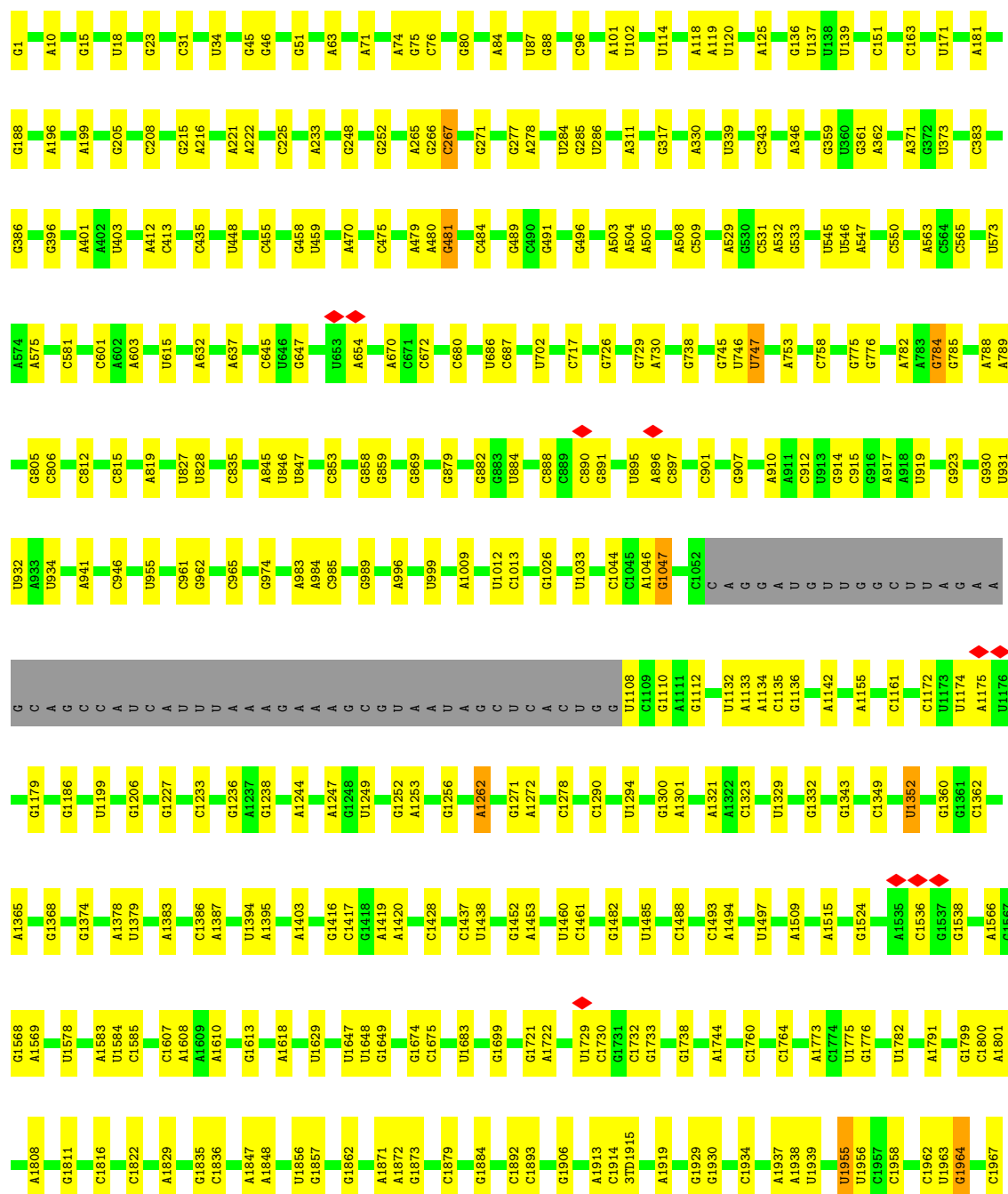
Chain SU:  11% 86% 11% ..

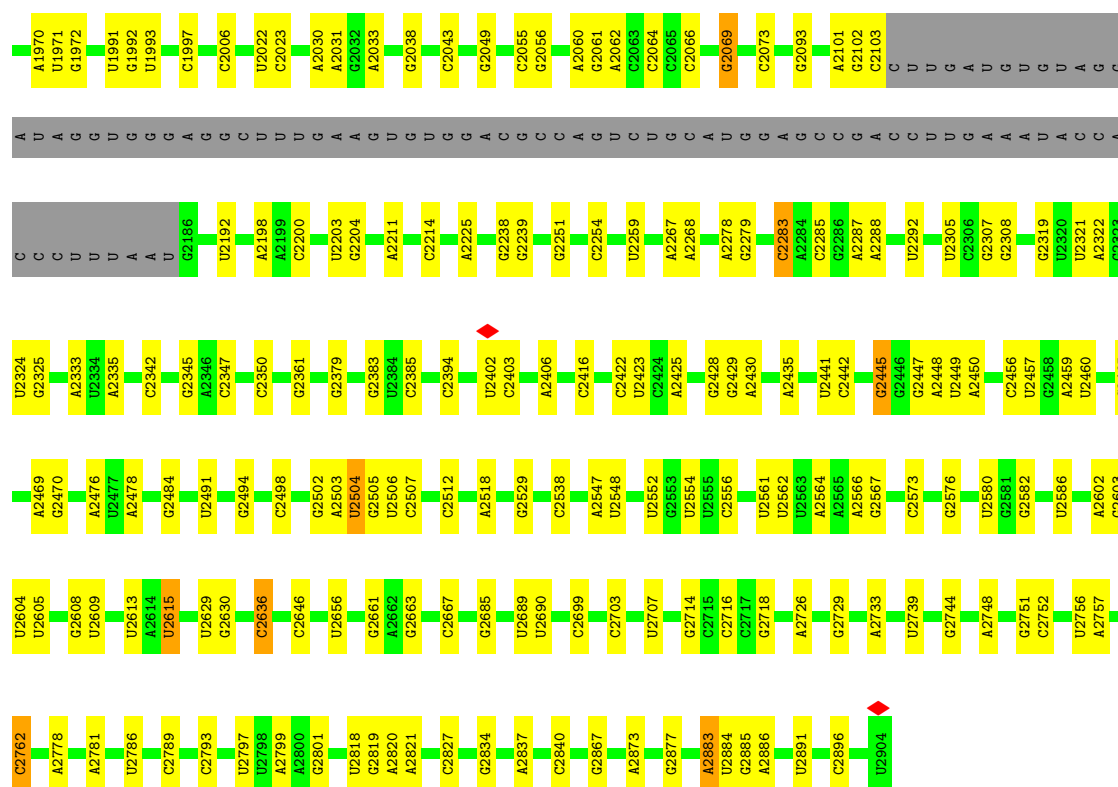


- Chain mR: 



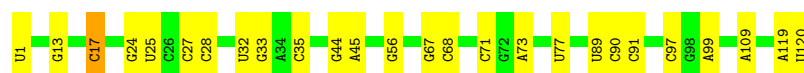
- Chain 23:  77% 18% • 5%





- Molecule 24: 5S ribosomal RNA (rRNA) from the B operon

Chain 5: 78% 21%



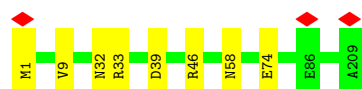
- Molecule 25: 50S ribosomal protein L2

Chain LB: 96%



- Molecule 26: 50S ribosomal protein L3

Chain LC: 96%

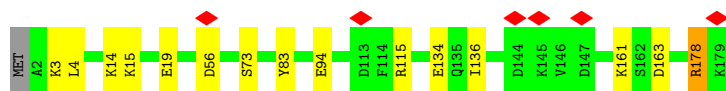
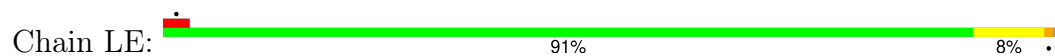


- Molecule 27: Large ribosomal subunit protein uL4

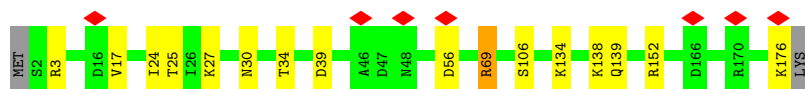
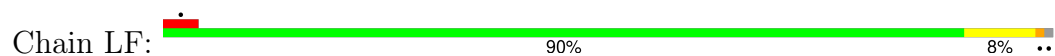
Chain LD: 93% 7%



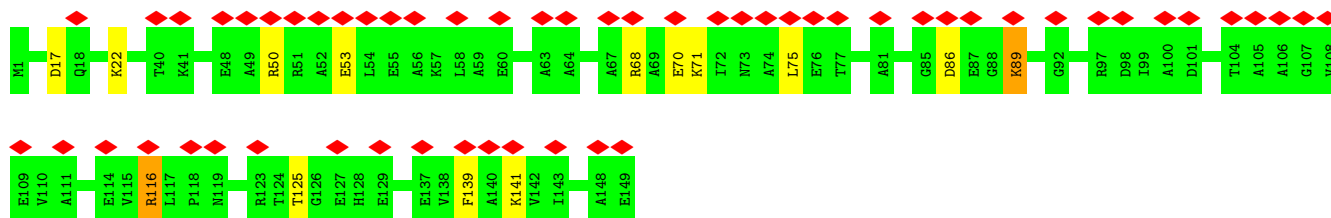
- Molecule 28: 50S ribosomal protein L5



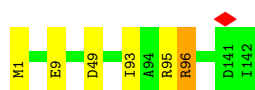
- Molecule 29: 50S ribosomal protein L6



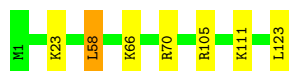
- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L13

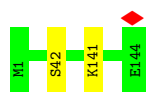


- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15





- Molecule 34: 50S ribosomal protein L16

Chain LP: 94% 6%



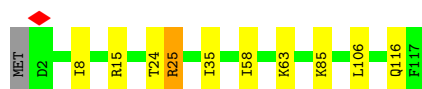
- Molecule 35: 50S ribosomal protein L17

Chain LQ: 90% 5% 6%



- Molecule 36: 50S ribosomal protein L18

Chain LR: 91% 8% ..



- Molecule 37: 50S ribosomal protein L19

Chain LS: 94% 5% •



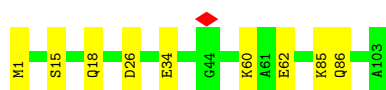
- Molecule 38: 50S ribosomal protein L20

Chain LT: 97% ..

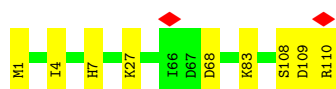


- Molecule 39: 50S ribosomal protein L21

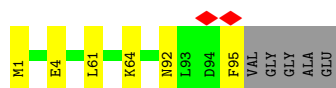
Chain LU: 91% 9%



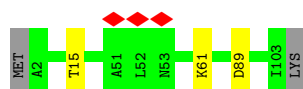
- Molecule 40: Large ribosomal subunit protein uL22



- Molecule 41: 50S ribosomal protein L23



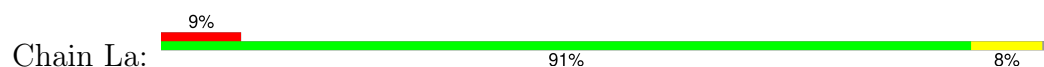
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25



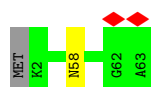
- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28

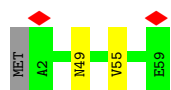


- Molecule 46: 50S ribosomal protein L29




- Molecule 47: 50S ribosomal protein L30

Chain Ld:  95%



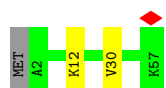
- Molecule 48: 50S ribosomal protein L31

Chain Le:  13% 76% 20%




- Molecule 49: 50S ribosomal protein L32

Chain Lf:  95%



- Molecule 50: 50S ribosomal protein L33

Chain Lg:  87% 7% 5%



- Molecule 51: 50S ribosomal protein L34

Chain Lh:  93% 7%




- Molecule 52: 50S ribosomal protein L35

Chain Li:  91% 6%

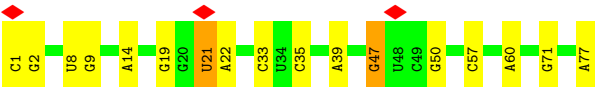
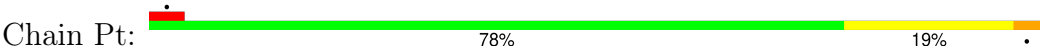


- Molecule 53: 50S ribosomal protein L36

Chain Lj:  87% 13%



- Molecule 54: N-formyl-methionine initiator tRNA (fMet-tRNA^{fMet})



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	555112	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 ($e^-/\text{\AA}^2$)	1.45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PUT, SPD, OMU, PSU, OMG, 1MG, FME, 2MA, 5MU, ATP, 4D4, 4SU, 4OC, MA6, MG, K, UR3, 6MZ, D2T, ZN, H2U, 5MC, 3TD, G7M, 2MG, OMC, IAS

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	16	0.49	0/36772	1.10	66/57358 (0.1%)
2	SB	0.38	0/1818	0.64	1/2450 (0.0%)
3	SC	0.35	0/1685	0.64	0/2270
4	SD	0.38	0/1665	0.65	0/2227
5	SE	0.39	0/1179	0.68	1/1584 (0.1%)
6	SF	0.43	0/881	0.68	0/1189
7	SG	0.41	0/1257	0.65	0/1686
8	SH	0.33	0/989	0.65	1/1326 (0.1%)
9	SI	0.37	0/1033	0.66	0/1375
10	SJ	0.43	0/805	0.80	1/1089 (0.1%)
11	SK	0.36	0/902	0.65	0/1215
12	SL	0.34	0/960	0.68	0/1286
13	SM	0.41	0/900	0.71	1/1204 (0.1%)
14	SN	0.32	0/817	0.58	0/1088
15	SO	0.36	0/721	0.61	0/964
16	SP	0.39	0/659	0.69	0/884
17	SQ	0.36	0/657	0.67	1/881 (0.1%)
18	SR	0.37	0/564	0.64	0/756
19	SS	0.36	0/680	0.62	0/915
20	ST	0.42	0/675	0.58	0/895
21	SU	0.36	0/597	0.61	0/792
22	mR	0.53	0/695	0.99	1/1081 (0.1%)
23	23	0.50	1/66023 (0.0%)	1.11	161/102992 (0.2%)
24	5	0.51	1/2876 (0.0%)	1.13	14/4483 (0.3%)
25	LB	0.34	0/2121	0.68	0/2852
26	LC	0.35	0/1585	0.64	0/2134
27	LD	0.32	0/1571	0.62	1/2113 (0.0%)
28	LE	0.43	0/1444	0.71	0/1937
29	LF	0.36	0/1333	0.61	0/1805
30	LI	0.38	0/1122	0.67	0/1515
31	LM	0.36	0/1152	0.65	1/1551 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LN	0.40	0/955	0.71	1/1279 (0.1%)
33	LO	0.33	0/1062	0.65	0/1413
34	LP	0.40	0/1080	0.67	0/1443
35	LQ	0.35	0/973	0.70	1/1301 (0.1%)
36	LR	0.43	0/902	0.75	1/1209 (0.1%)
37	LS	0.36	0/928	0.65	0/1242
38	LT	0.33	0/960	0.59	0/1278
39	LU	0.35	0/829	0.64	0/1107
40	LV	0.33	0/864	0.64	0/1156
41	LW	0.36	0/764	0.61	1/1021 (0.1%)
42	LX	0.33	0/787	0.58	0/1051
43	LY	0.35	0/766	0.64	0/1025
44	La	0.41	0/642	0.64	0/848
45	Lb	0.41	0/635	0.66	0/848
46	Lc	0.27	0/502	0.55	0/667
47	Ld	0.37	0/453	0.68	0/605
48	Le	0.36	0/543	0.63	0/726
49	Lf	0.31	0/450	0.65	0/599
50	Lg	0.34	0/433	0.67	0/576
51	Lh	0.32	0/380	0.70	0/498
52	Li	0.37	0/513	0.66	0/676
53	Lj	0.43	0/303	0.72	0/397
54	Pt	0.53	1/1744 (0.1%)	1.09	1/2716 (0.0%)
All	All	0.47	3/153606 (0.0%)	1.01	255/229578 (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
3	SC	0	4
6	SF	0	3
7	SG	0	2
8	SH	0	1
9	SI	0	1
10	SJ	0	4
11	SK	0	2
12	SL	0	1
13	SM	0	2
14	SN	0	2
16	SP	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	SR	0	2
19	SS	0	2
20	ST	0	1
21	SU	0	4
26	LC	0	1
28	LE	0	2
29	LF	0	2
30	LI	0	1
31	LM	0	2
32	LN	0	1
34	LP	0	1
35	LQ	0	2
36	LR	0	2
37	LS	0	2
38	LT	0	1
40	LV	0	1
43	LY	0	3
44	La	0	2
45	Lb	0	1
48	Le	0	2
51	Lh	0	1
52	Li	0	1
53	Lj	0	1
All	All	0	61

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	1	U	OP3-P	-7.57	1.52	1.61
23	23	1	G	OP3-P	-7.52	1.52	1.61
54	Pt	1	C	OP3-P	-7.50	1.52	1.61

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1955	U	C1'-O4'-C4'	-7.27	104.08	109.90
23	23	2819	G	OP2-P-O3'	6.05	118.50	105.20
1	16	611	C	N1-C2-O2	5.96	122.48	118.90
23	23	2073	C	C6-N1-C2	-5.96	117.92	120.30
23	23	901	C	N1-C2-O2	5.96	122.47	118.90
24	5	77	U	N3-C2-O2	-5.95	118.04	122.20
23	23	1488	C	C6-N1-C2	-5.94	117.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2762	C	C6-N1-C2	-5.94	117.92	120.30
23	23	680	C	C6-N1-C2	-5.93	117.93	120.30
23	23	2883	A	O5'-P-OP1	-5.93	100.36	105.70
36	LR	106	LEU	CA-CB-CG	5.93	128.94	115.30
23	23	2752	C	N1-C2-O2	5.93	122.46	118.90
23	23	1362	C	C6-N1-C2	-5.92	117.93	120.30
23	23	1760	C	N1-C2-O2	5.91	122.44	118.90
23	23	1836	C	C6-N1-C2	-5.90	117.94	120.30
23	23	1352	U	N3-C2-O2	-5.88	118.09	122.20
23	23	114	U	C2-N1-C1'	5.87	124.75	117.70
1	16	1538	C	C6-N1-C2	-5.87	117.95	120.30
23	23	1362	C	C5-C6-N1	5.87	123.93	121.00
23	23	484	C	C6-N1-C2	-5.87	117.95	120.30
23	23	2456	C	C6-N1-C2	-5.87	117.95	120.30
23	23	1323	C	N1-C2-O2	5.85	122.41	118.90
23	23	1629	U	N3-C2-O2	-5.83	118.12	122.20
5	SE	11	LEU	CA-CB-CG	5.82	128.68	115.30
1	16	1412	C	C6-N1-C2	-5.81	117.97	120.30
23	23	2656	U	N3-C2-O2	-5.81	118.13	122.20
23	23	171	U	N3-C2-O2	-5.81	118.13	122.20
23	23	2656	U	N1-C2-O2	5.81	126.86	122.80
23	23	601	C	C6-N1-C2	-5.81	117.98	120.30
23	23	343	C	N1-C2-O2	5.79	122.38	118.90
23	23	1290	C	C6-N1-C2	-5.79	117.98	120.30
23	23	806	C	C6-N1-C2	-5.78	117.99	120.30
23	23	2066	C	C6-N1-C2	-5.77	117.99	120.30
23	23	1485	U	C2-N1-C1'	5.76	124.61	117.70
22	mR	35	C	N1-C2-O2	5.76	122.35	118.90
24	5	28	C	C6-N1-C2	-5.75	118.00	120.30
23	23	1775	U	N3-C2-O2	-5.75	118.18	122.20
1	16	178	C	N1-C2-O2	5.74	122.35	118.90
23	23	2548	U	C5-C6-N1	5.73	125.56	122.70
23	23	2561	U	N3-C2-O2	-5.73	118.19	122.20
23	23	18	U	N3-C2-O2	-5.72	118.19	122.20
23	23	31	C	C5-C6-N1	5.72	123.86	121.00
23	23	484	C	C5-C6-N1	5.71	123.86	121.00
1	16	1520	C	C5-C6-N1	5.71	123.86	121.00
1	16	178	C	N3-C2-O2	-5.71	117.91	121.90
1	16	34	C	C6-N1-C2	-5.70	118.02	120.30
23	23	1934	C	C6-N1-C2	-5.70	118.02	120.30
1	16	960	U	C2-N1-C1'	5.70	124.53	117.70
23	23	2285	C	C6-N1-C2	-5.69	118.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	1109	C	N1-C2-O2	5.68	122.31	118.90
1	16	522	C	N1-C2-O2	5.67	122.31	118.90
23	23	76	C	C6-N1-C2	-5.67	118.03	120.30
23	23	581	C	C5-C6-N1	5.67	123.83	121.00
1	16	1109	C	C6-N1-C2	-5.67	118.03	120.30
23	23	225	C	C6-N1-C2	-5.67	118.03	120.30
23	23	475	C	C6-N1-C2	-5.66	118.04	120.30
23	23	343	C	C6-N1-C2	-5.63	118.05	120.30
23	23	343	C	N3-C2-O2	-5.63	117.96	121.90
23	23	1290	C	C5-C6-N1	5.63	123.81	121.00
23	23	758	C	C6-N1-C2	-5.62	118.05	120.30
23	23	2006	C	C6-N1-C2	-5.62	118.05	120.30
23	23	1776	G	N3-C4-C5	-5.62	125.79	128.60
24	5	27	C	N1-C2-O2	5.62	122.27	118.90
1	16	1108	G	N3-C4-N9	5.61	129.37	126.00
23	23	2512	C	C6-N1-C2	-5.61	118.06	120.30
23	23	1294	U	N3-C2-O2	-5.60	118.28	122.20
23	23	2460	U	N1-C2-O2	5.59	126.72	122.80
1	16	989	U	N3-C2-O2	-5.59	118.29	122.20
1	16	95	C	C6-N1-C2	-5.56	118.08	120.30
1	16	1119	C	C6-N1-C2	-5.56	118.08	120.30
23	23	96	C	C2-N1-C1'	5.56	124.92	118.80
24	5	71	C	C6-N1-C2	-5.56	118.08	120.30
23	23	2394	C	C6-N1-C2	-5.56	118.08	120.30
24	5	25	U	N1-C2-O2	5.55	126.69	122.80
23	23	1760	C	C6-N1-C2	-5.55	118.08	120.30
1	16	891	U	N1-C2-O2	5.54	126.68	122.80
23	23	1047	G	O4'-C1'-N9	5.54	112.64	108.20
23	23	2460	U	N3-C2-O2	-5.54	118.32	122.20
23	23	915	C	C2-N1-C1'	5.54	124.90	118.80
23	23	208	C	C6-N1-C2	-5.54	118.08	120.30
23	23	545	U	N1-C2-O2	5.54	126.68	122.80
1	16	614	C	C5-C6-N1	5.54	123.77	121.00
1	16	221	C	N1-C2-O2	5.54	122.22	118.90
24	5	77	U	N1-C2-O2	5.53	126.67	122.80
1	16	764	C	C6-N1-C2	-5.52	118.09	120.30
23	23	459	U	N3-C2-O2	-5.51	118.34	122.20
23	23	171	U	C2-N1-C1'	5.51	124.31	117.70
1	16	1395	C	C6-N1-C2	-5.50	118.10	120.30
23	23	2615	U	N1-C2-O2	5.50	126.65	122.80
23	23	2267	A	N1-C2-N3	-5.49	126.56	129.30
1	16	1109	C	N3-C2-O2	-5.48	118.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	545	C	C6-N1-C2	-5.47	118.11	120.30
24	5	68	C	N1-C2-O2	5.47	122.19	118.90
23	23	815	C	C6-N1-C2	-5.47	118.11	120.30
23	23	1323	C	N3-C2-O2	-5.47	118.07	121.90
1	16	943	U	N3-C2-O2	-5.47	118.37	122.20
23	23	1343	G	C4-N9-C1'	5.47	133.61	126.50
23	23	2615	U	N3-C2-O2	-5.47	118.37	122.20
23	23	2403	C	C6-N1-C2	-5.47	118.11	120.30
23	23	2667	C	N1-C2-O2	5.47	122.18	118.90
1	16	1395	C	N1-C2-O2	5.47	122.18	118.90
23	23	2636	C	N1-C2-O2	5.46	122.18	118.90
1	16	643	C	C6-N1-C2	-5.46	118.12	120.30
23	23	1349	C	N1-C2-O2	5.44	122.17	118.90
23	23	912	C	C2-N1-C1'	5.43	124.78	118.80
23	23	2576	G	C2-N3-C4	5.43	114.62	111.90
23	23	171	U	N1-C2-O2	5.43	126.60	122.80
1	16	1228	C	C6-N1-C2	-5.42	118.13	120.30
13	SM	48	LEU	CA-CB-CG	5.42	127.77	115.30
23	23	459	U	N1-C2-O2	5.42	126.59	122.80
23	23	151	C	C6-N1-C2	-5.42	118.13	120.30
23	23	2450	A	N1-C2-N3	-5.41	126.59	129.30
1	16	1172	C	C5-C6-N1	5.41	123.70	121.00
23	23	2729	G	N7-C8-N9	5.41	115.80	113.10
1	16	7	A	OP2-P-O3'	5.39	117.07	105.20
54	Pt	35	C	C6-N1-C2	-5.39	118.14	120.30
24	5	25	U	N3-C2-O2	-5.39	118.43	122.20
1	16	440	C	C6-N1-C2	-5.38	118.15	120.30
1	16	1070	U	N3-C2-O2	-5.38	118.44	122.20
23	23	2283	C	C6-N1-C2	-5.38	118.15	120.30
23	23	545	U	N3-C2-O2	-5.37	118.44	122.20
23	23	2703	C	C6-N1-C2	-5.37	118.15	120.30
23	23	2699	C	C6-N1-C2	-5.37	118.15	120.30
23	23	1387	A	N7-C8-N9	5.36	116.48	113.80
23	23	729	G	O4'-C1'-N9	5.36	112.49	108.20
1	16	36	C	C6-N1-C2	-5.36	118.16	120.30
23	23	1485	U	N1-C2-O2	5.36	126.55	122.80
23	23	784	G	OP1-P-O3'	5.35	116.97	105.20
23	23	1488	C	N1-C2-O2	5.35	122.11	118.90
23	23	339	U	C6-N1-C2	-5.34	117.79	121.00
23	23	1964	G	O4'-C1'-N9	-5.34	103.93	108.20
23	23	1776	G	C4-N9-C1'	5.34	133.44	126.50
23	23	339	U	N3-C2-O2	-5.34	118.46	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	SB	141	LEU	CA-CB-CG	5.33	127.57	115.30
23	23	1349	C	C6-N1-C2	-5.33	118.17	120.30
23	23	1488	C	C2-N1-C1'	5.33	124.67	118.80
23	23	2827	C	C6-N1-C2	-5.33	118.17	120.30
23	23	2416	C	C6-N1-C2	-5.33	118.17	120.30
23	23	1352	U	N1-C2-O2	5.32	126.53	122.80
23	23	2254	C	N1-C2-O2	5.32	122.09	118.90
23	23	985	C	C2-N1-C1'	5.32	124.65	118.80
23	23	1683	U	C5-C6-N1	5.31	125.36	122.70
23	23	2342	C	C6-N1-C2	-5.31	118.17	120.30
1	16	397	A	C2-N3-C4	5.31	113.25	110.60
1	16	963	G	N1-C6-O6	-5.31	116.72	119.90
23	23	2214	C	C6-N1-C2	-5.31	118.18	120.30
23	23	1262	A	C2-N3-C4	5.29	113.25	110.60
24	5	28	C	C5-C6-N1	5.29	123.64	121.00
23	23	2200	C	C6-N1-C2	-5.29	118.19	120.30
1	16	18	C	C6-N1-C2	-5.28	118.19	120.30
1	16	689	C	C6-N1-C2	-5.28	118.19	120.30
23	23	999	U	N3-C2-O2	-5.28	118.50	122.20
23	23	2456	C	C5-C6-N1	5.28	123.64	121.00
1	16	792	A	O4'-C1'-N9	5.28	112.42	108.20
1	16	611	C	C6-N1-C2	-5.28	118.19	120.30
1	16	972	C	C6-N1-C2	-5.27	118.19	120.30
23	23	2292	U	C5-C6-N1	5.27	125.33	122.70
24	5	17	C	C6-N1-C2	-5.27	118.19	120.30
27	LD	118	LEU	CA-CB-CG	5.27	127.42	115.30
23	23	702	U	N3-C2-O2	-5.27	118.51	122.20
35	LQ	44	LEU	CA-CB-CG	5.26	127.41	115.30
8	SH	121	LEU	CA-CB-CG	5.26	127.41	115.30
23	23	475	C	C5-C6-N1	5.26	123.63	121.00
1	16	316	C	C6-N1-C2	-5.26	118.19	120.30
41	LW	61	LEU	CA-CB-CG	5.26	127.40	115.30
1	16	899	C	C6-N1-C2	-5.26	118.20	120.30
1	16	1108	G	N3-C4-C5	-5.25	125.97	128.60
23	23	2667	C	C6-N1-C2	-5.25	118.20	120.30
23	23	2394	C	N1-C2-O2	5.24	122.05	118.90
23	23	2442	C	N3-C2-O2	-5.24	118.23	121.90
1	16	501	C	C5-C6-N1	5.23	123.62	121.00
1	16	891	U	N3-C2-O2	-5.23	118.54	122.20
1	16	1119	C	C5-C6-N1	5.23	123.62	121.00
23	23	1958	C	C6-N1-C2	-5.23	118.21	120.30
23	23	672	C	C5-C6-N1	5.22	123.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	1404	C	C6-N1-C2	-5.22	118.21	120.30
23	23	1438	U	N1-C2-O2	5.22	126.45	122.80
23	23	1568	G	C8-N9-C4	-5.21	104.31	106.40
23	23	2259	U	N3-C2-O2	-5.21	118.55	122.20
1	16	1520	C	C6-N1-C2	-5.21	118.22	120.30
1	16	49	U	OP2-P-O3'	5.20	116.64	105.20
23	23	2707	U	N3-C2-O2	-5.20	118.56	122.20
23	23	2507	C	C6-N1-C2	-5.20	118.22	120.30
23	23	2752	C	N3-C2-O2	-5.19	118.27	121.90
1	16	153	C	C6-N1-C2	-5.19	118.22	120.30
17	SQ	15	ASP	CB-CG-OD1	5.18	122.97	118.30
23	23	2416	C	C5-C6-N1	5.18	123.59	121.00
23	23	2465	C	C6-N1-C2	-5.18	118.23	120.30
23	23	2786	U	N3-C2-O2	-5.17	118.58	122.20
23	23	481	G	O4'-C1'-N9	5.16	112.33	108.20
1	16	469	C	N1-C2-O2	5.16	122.00	118.90
23	23	2789	C	C6-N1-C2	-5.16	118.24	120.30
23	23	2840	C	C5-C6-N1	5.15	123.58	121.00
1	16	1225	A	C2-N3-C4	5.15	113.17	110.60
23	23	267	C	C6-N1-C2	-5.15	118.24	120.30
23	23	1892	C	C6-N1-C2	-5.15	118.24	120.30
31	LM	49	ASP	CB-CG-OD1	5.15	122.94	118.30
23	23	835	C	C6-N1-C2	-5.15	118.24	120.30
1	16	501	C	C6-N1-C2	-5.15	118.24	120.30
23	23	2538	C	C6-N1-C2	-5.15	118.24	120.30
23	23	965	C	C6-N1-C2	-5.14	118.25	120.30
23	23	1963	U	N3-C2-O2	-5.13	118.61	122.20
23	23	1822	C	C6-N1-C2	-5.13	118.25	120.30
1	16	1395	C	N3-C2-O2	-5.13	118.31	121.90
1	16	611	C	N3-C2-O2	-5.12	118.31	121.90
32	LN	58	LEU	CA-CB-CG	5.12	127.09	115.30
23	23	1108	U	N1-C2-O2	5.12	126.38	122.80
24	5	17	C	N1-C2-O2	5.12	121.97	118.90
23	23	2699	C	C5-C6-N1	5.11	123.55	121.00
1	16	95	C	C2-N1-C1'	5.11	124.42	118.80
23	23	2896	C	C5-C6-N1	5.10	123.55	121.00
1	16	960	U	N1-C2-O2	5.09	126.37	122.80
23	23	1856	U	OP2-P-O3'	5.09	116.41	105.20
23	23	2064	C	C6-N1-C2	-5.09	118.26	120.30
23	23	225	C	C2-N1-C1'	5.09	124.40	118.80
23	23	2450	A	C6-N1-C2	5.09	121.66	118.60
23	23	1278	C	C6-N1-C2	-5.09	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2254	C	C6-N1-C2	-5.09	118.26	120.30
1	16	598	U	N3-C2-O2	-5.09	118.64	122.20
1	16	6	G	C2-N3-C4	5.08	114.44	111.90
23	23	1879	C	C6-N1-C2	-5.08	118.27	120.30
1	16	989	U	N1-C2-O2	5.08	126.36	122.80
23	23	1233	C	C6-N1-C2	-5.08	118.27	120.30
1	16	177	G	C4-N9-C1'	5.08	133.10	126.50
23	23	680	C	C5-C6-N1	5.07	123.54	121.00
24	5	17	C	C5-C6-N1	5.07	123.54	121.00
1	16	580	C	C6-N1-C2	-5.07	118.27	120.30
23	23	565	C	N1-C2-O2	5.07	121.94	118.90
1	16	1070	U	N1-C2-O2	5.07	126.35	122.80
23	23	853	C	C6-N1-C2	-5.07	118.27	120.30
23	23	1199	U	C5-C6-N1	5.07	125.23	122.70
23	23	31	C	C6-N1-C2	-5.07	118.27	120.30
23	23	1776	G	N3-C4-N9	5.07	129.04	126.00
24	5	68	C	C6-N1-C2	-5.06	118.28	120.30
23	23	985	C	C6-N1-C2	-5.05	118.28	120.30
23	23	1485	U	N3-C2-O2	-5.05	118.67	122.20
24	5	97	C	C6-N1-C2	-5.05	118.28	120.30
23	23	413	C	C6-N1-C2	-5.04	118.28	120.30
23	23	687	C	N1-C2-O2	5.04	121.92	118.90
23	23	2656	U	C2-N1-C1'	5.03	123.74	117.70
23	23	2006	C	C5-C6-N1	5.03	123.52	121.00
23	23	2442	C	N1-C2-O2	5.03	121.92	118.90
23	23	1760	C	N3-C2-O2	-5.03	118.38	121.90
23	23	1893	C	C6-N1-C2	-5.03	118.29	120.30
1	16	34	C	C5-C6-N1	5.02	123.51	121.00
1	16	699	C	C6-N1-C2	-5.02	118.29	120.30
23	23	435	C	C6-N1-C2	-5.02	118.29	120.30
23	23	1044	C	N1-C2-O2	5.02	121.91	118.90
10	SJ	71	LEU	CA-CB-CG	5.01	126.83	115.30
1	16	952	U	N3-C2-O2	-5.01	118.69	122.20
1	16	856	C	C6-N1-C2	-5.01	118.30	120.30
23	23	1108	U	N3-C2-O2	-5.01	118.69	122.20
23	23	2586	U	N3-C2-O2	-5.01	118.69	122.20
1	16	1172	C	C6-N1-C2	-5.01	118.30	120.30
23	23	137	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	LC	46	ARG	Sidechain
28	LE	115	ARG	Sidechain
28	LE	178	ARG	Sidechain
29	LF	3	ARG	Sidechain
29	LF	69	ARG	Sidechain
30	LI	116	ARG	Sidechain
31	LM	95	ARG	Sidechain
31	LM	96	ARG	Sidechain
32	LN	70	ARG	Sidechain
34	LP	10	ARG	Sidechain
35	LQ	69	ARG	Sidechain
35	LQ	8	ARG	Sidechain
36	LR	15	ARG	Sidechain
36	LR	25	ARG	Sidechain
37	LS	113	ARG	Sidechain
37	LS	51	ARG	Sidechain
38	LT	70	ARG	Sidechain
40	LV	110	ARG	Sidechain
43	LY	18	ARG	Sidechain
43	LY	21	ARG	Sidechain
43	LY	9	ARG	Sidechain
44	La	25	ARG	Sidechain
44	La	77	ARG	Sidechain
45	Lb	50	ARG	Sidechain
48	Le	25	ARG	Sidechain
48	Le	49	ARG	Sidechain
51	Lh	39	ARG	Sidechain
52	Li	45	ARG	Sidechain
53	Lj	36	ARG	Sidechain
3	SC	131	ARG	Sidechain
3	SC	136	ARG	Sidechain
3	SC	54	ARG	Sidechain
3	SC	59	ARG	Sidechain
6	SF	24	ARG	Sidechain
6	SF	38	ARG	Sidechain
6	SF	91	ARG	Sidechain
7	SG	10	ARG	Sidechain
7	SG	155	ARG	Sidechain
8	SH	114	ARG	Sidechain
9	SI	109	ARG	Sidechain
10	SJ	5	ARG	Sidechain
10	SJ	62	ARG	Sidechain
10	SJ	72	ARG	Sidechain

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Mol	Chain	Res	Type	Group
10	SJ	89	ARG	Sidechain
11	SK	122	ARG	Sidechain
11	SK	56	ARG	Sidechain
12	SL	54	ARG	Sidechain
13	SM	101	ARG	Sidechain
13	SM	29	ARG	Sidechain
14	SN	24	ARG	Sidechain
14	SN	41	ARG	Sidechain
16	SP	31	ARG	Sidechain
18	SR	12	ARG	Sidechain
18	SR	48	ARG	Sidechain
19	SS	37	ARG	Sidechain
19	SS	78	ARG	Sidechain
20	ST	24	ARG	Sidechain
21	SU	17	ARG	Sidechain
21	SU	21	ARG	Sidechain
21	SU	33	ARG	Sidechain
21	SU	55	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	227/241 (94%)	216 (95%)	11 (5%)	0	100	100
3	SC	210/233 (90%)	202 (96%)	8 (4%)	0	100	100
4	SD	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
5	SE	156/167 (93%)	153 (98%)	3 (2%)	0	100	100
6	SF	104/135 (77%)	103 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	SG	154/179 (86%)	149 (97%)	5 (3%)	0	100	100
8	SH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	SI	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	SJ	97/103 (94%)	91 (94%)	4 (4%)	2 (2%)	5	3
11	SK	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	117 (98%)	2 (2%)	1 (1%)	16	16
13	SM	113/118 (96%)	105 (93%)	8 (7%)	0	100	100
14	SN	98/101 (97%)	98 (100%)	0	0	100	100
15	SO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	SP	80/82 (98%)	76 (95%)	3 (4%)	1 (1%)	10	8
17	SQ	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
18	SR	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
19	SS	81/91 (89%)	80 (99%)	1 (1%)	0	100	100
20	ST	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	SU	68/71 (96%)	68 (100%)	0	0	100	100
25	LB	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
26	LC	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
27	LD	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
28	LE	176/179 (98%)	167 (95%)	9 (5%)	0	100	100
29	LF	173/177 (98%)	163 (94%)	10 (6%)	0	100	100
30	LI	147/149 (99%)	128 (87%)	18 (12%)	1 (1%)	19	19
31	LM	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
32	LN	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
33	LO	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
34	LP	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
35	LQ	118/127 (93%)	114 (97%)	4 (3%)	0	100	100
36	LR	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
37	LS	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
38	LT	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
39	LU	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
40	LV	108/110 (98%)	105 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	LW	93/100 (93%)	91 (98%)	2 (2%)	0	100	100
42	LX	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
43	LY	92/94 (98%)	92 (100%)	0	0	100	100
44	La	82/85 (96%)	78 (95%)	4 (5%)	0	100	100
45	Lb	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	Lc	60/63 (95%)	60 (100%)	0	0	100	100
47	Ld	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
48	Le	66/70 (94%)	60 (91%)	6 (9%)	0	100	100
49	Lf	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
50	Lg	50/55 (91%)	48 (96%)	2 (4%)	0	100	100
51	Lh	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	Li	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
53	Lj	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
All	All	5636/5912 (95%)	5440 (96%)	191 (3%)	5 (0%)	50	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	SJ	38	GLY
10	SJ	57	VAL
30	LI	89	LYS
12	SL	44	LYS
16	SP	48	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	190/199 (96%)	175 (92%)	15 (8%)	10	11
3	SC	172/190 (90%)	158 (92%)	14 (8%)	9	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	SD	172/173 (99%)	163 (95%)	9 (5%)	19	24
5	SE	120/126 (95%)	113 (94%)	7 (6%)	17	20
6	SF	92/116 (79%)	82 (89%)	10 (11%)	5	5
7	SG	129/147 (88%)	106 (82%)	23 (18%)	1	1
8	SH	104/105 (99%)	99 (95%)	5 (5%)	21	28
9	SI	105/107 (98%)	101 (96%)	4 (4%)	28	37
10	SJ	87/90 (97%)	74 (85%)	13 (15%)	2	2
11	SK	91/98 (93%)	82 (90%)	9 (10%)	6	6
12	SL	102/103 (99%)	93 (91%)	9 (9%)	8	8
13	SM	93/96 (97%)	81 (87%)	12 (13%)	3	3
14	SN	83/84 (99%)	80 (96%)	3 (4%)	30	40
15	SO	76/77 (99%)	73 (96%)	3 (4%)	27	37
16	SP	65/65 (100%)	60 (92%)	5 (8%)	10	11
17	SQ	74/78 (95%)	70 (95%)	4 (5%)	18	23
18	SR	58/65 (89%)	55 (95%)	3 (5%)	19	24
19	SS	72/78 (92%)	58 (81%)	14 (19%)	1	1
20	ST	65/66 (98%)	58 (89%)	7 (11%)	5	5
21	SU	60/61 (98%)	54 (90%)	6 (10%)	6	6
25	LB	216/218 (99%)	208 (96%)	8 (4%)	29	39
26	LC	164/164 (100%)	157 (96%)	7 (4%)	25	32
27	LD	165/165 (100%)	151 (92%)	14 (8%)	8	9
28	LE	149/150 (99%)	135 (91%)	14 (9%)	7	7
29	LF	136/138 (99%)	121 (89%)	15 (11%)	5	4
30	LI	114/114 (100%)	100 (88%)	14 (12%)	4	3
31	LM	116/116 (100%)	112 (97%)	4 (3%)	32	42
32	LN	104/104 (100%)	98 (94%)	6 (6%)	17	20
33	LO	103/103 (100%)	101 (98%)	2 (2%)	52	67
34	LP	108/108 (100%)	102 (94%)	6 (6%)	17	21
35	LQ	100/103 (97%)	97 (97%)	3 (3%)	36	48
36	LR	86/87 (99%)	78 (91%)	8 (9%)	7	7
37	LS	99/100 (99%)	95 (96%)	4 (4%)	27	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	LT	89/90 (99%)	88 (99%)	1 (1%)	70	82
39	LU	84/84 (100%)	75 (89%)	9 (11%)	5	5
40	LV	93/93 (100%)	85 (91%)	8 (9%)	8	9
41	LW	82/84 (98%)	77 (94%)	5 (6%)	15	18
42	LX	83/85 (98%)	80 (96%)	3 (4%)	30	40
43	LY	78/78 (100%)	72 (92%)	6 (8%)	10	11
44	La	62/63 (98%)	57 (92%)	5 (8%)	9	10
45	Lb	67/68 (98%)	63 (94%)	4 (6%)	16	19
46	Lc	54/55 (98%)	53 (98%)	1 (2%)	52	67
47	Ld	48/49 (98%)	46 (96%)	2 (4%)	25	33
48	Le	60/62 (97%)	46 (77%)	14 (23%)	0	0
49	Lf	47/48 (98%)	45 (96%)	2 (4%)	25	32
50	Lg	47/49 (96%)	43 (92%)	4 (8%)	8	9
51	Lh	38/38 (100%)	36 (95%)	2 (5%)	19	24
52	Li	51/52 (98%)	46 (90%)	5 (10%)	6	6
53	Lj	34/34 (100%)	30 (88%)	4 (12%)	4	4
All	All	4687/4826 (97%)	4332 (92%)	355 (8%)	13	12

All (355) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	11	LYS
2	SB	23	TRP
2	SB	56	GLU
2	SB	86	SER
2	SB	105	LYS
2	SB	118	GLU
2	SB	128	LYS
2	SB	130	THR
2	SB	131	LYS
2	SB	132	LYS
2	SB	147	SER
2	SB	181	ILE
2	SB	191	SER
2	SB	223	GLU
2	SB	227	GLN

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Mol	Chain	Res	Type
3	SC	35	SER
3	SC	54	ARG
3	SC	82	GLU
3	SC	86	LYS
3	SC	87	LEU
3	SC	93	ASP
3	SC	97	VAL
3	SC	121	THR
3	SC	128	VAL
3	SC	131	ARG
3	SC	147	LYS
3	SC	179	ARG
3	SC	185	ASN
3	SC	187	SER
4	SD	29	ASP
4	SD	44	ARG
4	SD	67	VAL
4	SD	104	ARG
4	SD	115	ARG
4	SD	138	SER
4	SD	143	VAL
4	SD	151	LYS
4	SD	179	GLU
5	SE	26	LYS
5	SE	38	VAL
5	SE	55	GLU
5	SE	72	ILE
5	SE	120	VAL
5	SE	147	MET
5	SE	156	LYS
6	SF	16	GLU
6	SF	19	PRO
6	SF	23	GLU
6	SF	79	ARG
6	SF	88	MET
6	SF	94	HIS
6	SF	96	VAL
6	SF	97	THR
6	SF	98	GLU
6	SF	102	MET
7	SG	10	ARG
7	SG	13	LEU

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Mol	Chain	Res	Type
7	SG	25	LYS
7	SG	29	ILE
7	SG	30	LEU
7	SG	31	MET
7	SG	35	LYS
7	SG	36	LYS
7	SG	37	SER
7	SG	45	SER
7	SG	56	LYS
7	SG	59	LEU
7	SG	72	THR
7	SG	73	VAL
7	SG	75	VAL
7	SG	92	ARG
7	SG	95	ARG
7	SG	109	ARG
7	SG	131	LYS
7	SG	138	ARG
7	SG	142	HIS
7	SG	154	TYR
7	SG	155	ARG
8	SH	54	ASP
8	SH	55	THR
8	SH	60	GLU
8	SH	114	ARG
8	SH	121	LEU
9	SI	29	VAL
9	SI	58	VAL
9	SI	93	SER
9	SI	100	LYS
10	SJ	5	ARG
10	SJ	7	ARG
10	SJ	62	ARG
10	SJ	72	ARG
10	SJ	77	VAL
10	SJ	78	GLU
10	SJ	82	LYS
10	SJ	87	LEU
10	SJ	88	MET
10	SJ	89	ARG
10	SJ	91	ASP
10	SJ	97	ASP

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Mol	Chain	Res	Type
10	SJ	98	VAL
11	SK	13	ARG
11	SK	14	LYS
11	SK	26	SER
11	SK	36	ASP
11	SK	56	ARG
11	SK	74	VAL
11	SK	75	LYS
11	SK	94	GLU
11	SK	98	ARG
12	SL	9	ARG
12	SL	14	ARG
12	SL	18	LYS
12	SL	21	VAL
12	SL	44	LYS
12	SL	47	SER
12	SL	54	ARG
12	SL	55	VAL
12	SL	99	ARG
13	SM	3	ARG
13	SM	16	VAL
13	SM	19	LEU
13	SM	21	SER
13	SM	29	ARG
13	SM	42	ASP
13	SM	45	ILE
13	SM	64	VAL
13	SM	71	ARG
13	SM	101	ARG
13	SM	107	ARG
13	SM	113	ARG
14	SN	10	GLU
14	SN	48	LEU
14	SN	51	LEU
15	SO	6	GLU
15	SO	61	SER
15	SO	73	LYS
16	SP	19	VAL
16	SP	45	GLU
16	SP	46	LYS
16	SP	76	LYS
16	SP	77	GLU

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Mol	Chain	Res	Type
17	SQ	27	ARG
17	SQ	41	THR
17	SQ	57	ASP
17	SQ	74	THR
18	SR	9	LYS
18	SR	12	ARG
18	SR	19	GLN
19	SS	13	LEU
19	SS	20	GLU
19	SS	23	VAL
19	SS	24	GLU
19	SS	25	SER
19	SS	31	LEU
19	SS	32	ARG
19	SS	35	SER
19	SS	36	ARG
19	SS	37	ARG
19	SS	51	VAL
19	SS	60	VAL
19	SS	78	ARG
19	SS	79	THR
20	ST	6	SER
20	ST	33	LYS
20	ST	34	LYS
20	ST	53	GLU
20	ST	54	MET
20	ST	59	ASP
20	ST	86	LEU
21	SU	21	ARG
21	SU	22	SER
21	SU	56	HIS
21	SU	63	GLU
21	SU	67	ARG
21	SU	69	ARG
25	LB	5	LYS
25	LB	71	LYS
25	LB	100	GLU
25	LB	130	LEU
25	LB	182	ARG
25	LB	216	VAL
25	LB	265	LYS
25	LB	272	SER

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Mol	Chain	Res	Type
26	LC	1	MET
26	LC	9	VAL
26	LC	32	ASN
26	LC	33	ARG
26	LC	39	ASP
26	LC	58	ASN
26	LC	74	GLU
27	LD	1	MET
27	LD	3	LEU
27	LD	4	VAL
27	LD	55	SER
27	LD	80	SER
27	LD	88	ARG
27	LD	116	ASP
27	LD	155	GLU
27	LD	163	ASN
27	LD	176	ASP
27	LD	184	ASP
27	LD	185	LYS
27	LD	194	LYS
27	LD	198	GLU
28	LE	3	LYS
28	LE	4	LEU
28	LE	14	LYS
28	LE	15	LYS
28	LE	19	GLU
28	LE	56	ASP
28	LE	73	SER
28	LE	83	TYR
28	LE	94	GLU
28	LE	134	GLU
28	LE	136	ILE
28	LE	161	LYS
28	LE	163	ASP
28	LE	178	ARG
29	LF	17	VAL
29	LF	24	ILE
29	LF	25	THR
29	LF	27	LYS
29	LF	30	ASN
29	LF	34	THR
29	LF	39	ASP

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Mol	Chain	Res	Type
29	LF	56	ASP
29	LF	69	ARG
29	LF	106	SER
29	LF	134	LYS
29	LF	138	LYS
29	LF	139	GLN
29	LF	152	ARG
29	LF	176	LYS
30	LI	17	ASP
30	LI	22	LYS
30	LI	50	ARG
30	LI	53	GLU
30	LI	68	ARG
30	LI	70	GLU
30	LI	71	LYS
30	LI	75	LEU
30	LI	86	ASP
30	LI	89	LYS
30	LI	116	ARG
30	LI	125	THR
30	LI	139	PHE
30	LI	141	LYS
31	LM	1	MET
31	LM	9	GLU
31	LM	93	ILE
31	LM	96	ARG
32	LN	23	LYS
32	LN	58	LEU
32	LN	66	LYS
32	LN	105	ARG
32	LN	111	LYS
32	LN	123	LEU
33	LO	42	SER
33	LO	141	LYS
34	LP	57	VAL
34	LP	60	GLN
34	LP	75	GLU
34	LP	110	GLU
34	LP	135	VAL
34	LP	136	MET
35	LQ	12	ARG
35	LQ	16	HIS

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Mol	Chain	Res	Type
35	LQ	65	LEU
36	LR	8	ILE
36	LR	24	THR
36	LR	25	ARG
36	LR	35	ILE
36	LR	58	ILE
36	LR	63	LYS
36	LR	85	LYS
36	LR	116	GLN
37	LS	10	GLN
37	LS	12	GLN
37	LS	16	ASP
37	LS	37	LYS
38	LT	13	ARG
39	LU	1	MET
39	LU	15	SER
39	LU	18	GLN
39	LU	26	ASP
39	LU	34	GLU
39	LU	60	LYS
39	LU	62	GLU
39	LU	85	LYS
39	LU	86	GLN
40	LV	1	MET
40	LV	4	ILE
40	LV	7	HIS
40	LV	27	LYS
40	LV	68	ASP
40	LV	83	LYS
40	LV	108	SER
40	LV	109	ASP
41	LW	1	MET
41	LW	4	GLU
41	LW	64	LYS
41	LW	92	ASN
41	LW	95	PHE
42	LX	15	THR
42	LX	61	LYS
42	LX	89	ASP
43	LY	1	MET
43	LY	34	LYS
43	LY	51	GLN

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Mol	Chain	Res	Type
43	LY	65	VAL
43	LY	66	ASP
43	LY	71	LYS
44	La	5	LYS
44	La	56	ASP
44	La	58	THR
44	La	68	LYS
44	La	83	GLU
45	Lb	17	ASN
45	Lb	22	LEU
45	Lb	35	SER
45	Lb	77	LYS
46	Lc	58	ASN
47	Ld	49	ASN
47	Ld	55	VAL
48	Le	4	ASP
48	Le	9	TYR
48	Le	10	GLU
48	Le	24	ILE
48	Le	25	ARG
48	Le	32	LEU
48	Le	35	ASP
48	Le	36	VAL
48	Le	40	CYS
48	Le	51	VAL
48	Le	59	ARG
48	Le	62	LYS
48	Le	63	ARG
48	Le	65	ASN
49	Lf	12	LYS
49	Lf	30	VAL
50	Lg	9	ILE
50	Lg	28	ARG
50	Lg	37	LYS
50	Lg	51	GLU
51	Lh	1	MET
51	Lh	25	LYS
52	Li	15	LYS
52	Li	19	LYS
52	Li	31	HIS
52	Li	45	ARG
52	Li	52	LYS

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Mol	Chain	Res	Type
53	Lj	2	LYS
53	Lj	7	VAL
53	Lj	19	ARG
53	Lj	20	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	120	GLN
3	SC	3	GLN
3	SC	6	HIS
3	SC	139	GLN
3	SC	140	ASN
3	SC	185	ASN
4	SD	116	GLN
7	SG	148	ASN
8	SH	18	GLN
8	SH	118	GLN
9	SI	32	GLN
9	SI	110	GLN
10	SJ	4	GLN
11	SK	64	GLN
11	SK	118	HIS
12	SL	5	ASN
12	SL	75	GLN
13	SM	105	ASN
14	SN	49	GLN
14	SN	62	ASN
15	SO	40	GLN
16	SP	18	GLN
16	SP	26	ASN
16	SP	79	ASN
17	SQ	51	ASN
18	SR	54	GLN
19	SS	69	HIS
20	ST	3	ASN
20	ST	70	ASN
20	ST	84	ASN
25	LB	115	GLN
25	LB	153	GLN
25	LB	230	HIS
25	LB	243	HIS

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Mol	Chain	Res	Type
26	LC	173	GLN
27	LD	41	GLN
27	LD	97	ASN
27	LD	163	ASN
27	LD	165	HIS
28	LE	23	ASN
28	LE	127	ASN
29	LF	38	ASN
29	LF	73	ASN
29	LF	116	GLN
29	LF	139	GLN
30	LI	2	GLN
30	LI	20	ASN
30	LI	28	ASN
31	LM	77	HIS
31	LM	80	HIS
31	LM	135	GLN
32	LN	82	ASN
32	LN	88	ASN
32	LN	93	GLN
34	LP	17	ASN
34	LP	22	GLN
35	LQ	11	ASN
36	LR	100	HIS
36	LR	116	GLN
38	LT	20	GLN
38	LT	44	GLN
39	LU	18	GLN
39	LU	86	GLN
40	LV	40	ASN
40	LV	57	ASN
40	LV	60	HIS
40	LV	61	ASN
42	LX	74	ASN
43	LY	12	GLN
43	LY	75	GLN
43	LY	78	GLN
43	LY	87	GLN
44	La	76	ASN
46	Lc	20	ASN
46	Lc	45	GLN
48	Le	61	ASN

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Mol	Chain	Res	Type
49	Lf	6	ASN
50	Lg	46	HIS
52	Li	28	ASN
53	Lj	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1538/1542 (99%)	238 (15%)	4 (0%)
22	mR	26/60 (43%)	12 (46%)	0
23	23	2760/2904 (95%)	404 (14%)	11 (0%)
24	5	119/120 (99%)	18 (15%)	0
54	Pt	76/77 (98%)	13 (17%)	0
All	All	4519/4703 (96%)	685 (15%)	15 (0%)

All (685) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	5	U
1	16	6	G
1	16	9	G
1	16	22	G
1	16	32	A
1	16	39	G
1	16	47	C
1	16	48	C
1	16	51	A
1	16	69	G
1	16	71	A
1	16	75	G
1	16	79	G
1	16	81	A
1	16	83	C
1	16	84	U
1	16	85	U
1	16	86	G
1	16	87	C
1	16	94	G
1	16	95	C
1	16	109	A
1	16	119	A

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Mol	Chain	Res	Type
1	16	121	U
1	16	131	A
1	16	137	U
1	16	138	G
1	16	140	U
1	16	150	U
1	16	163	C
1	16	164	G
1	16	170	U
1	16	177	G
1	16	181	A
1	16	182	A
1	16	184	G
1	16	191	G
1	16	197	A
1	16	198	G
1	16	209	U
1	16	210	C
1	16	211	G
1	16	240	G
1	16	245	U
1	16	247	G
1	16	251	G
1	16	266	G
1	16	267	C
1	16	275	G
1	16	280	C
1	16	289	G
1	16	301	G
1	16	306	A
1	16	321	A
1	16	328	C
1	16	330	C
1	16	332	G
1	16	352	C
1	16	354	G
1	16	367	U
1	16	372	C
1	16	384	G
1	16	388	G
1	16	392	C
1	16	398	U

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Mol	Chain	Res	Type
1	16	406	G
1	16	411	A
1	16	412	A
1	16	413	G
1	16	414	A
1	16	421	U
1	16	422	C
1	16	424	G
1	16	429	U
1	16	430	A
1	16	451	A
1	16	453	G
1	16	467	U
1	16	468	A
1	16	479	U
1	16	484	G
1	16	486	U
1	16	495	A
1	16	496	A
1	16	508	U
1	16	509	A
1	16	511	C
1	16	518	C
1	16	521	G
1	16	524	G
1	16	527	G7M
1	16	533	A
1	16	547	A
1	16	548	G
1	16	559	A
1	16	562	U
1	16	564	C
1	16	572	A
1	16	573	A
1	16	576	C
1	16	577	G
1	16	596	A
1	16	607	A
1	16	615	G
1	16	619	U
1	16	633	G
1	16	639	G

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Mol	Chain	Res	Type
1	16	650	G
1	16	653	U
1	16	665	A
1	16	666	G
1	16	702	A
1	16	703	G
1	16	704	A
1	16	721	G
1	16	723	U
1	16	724	G
1	16	733	G
1	16	755	G
1	16	777	A
1	16	781	A
1	16	793	U
1	16	794	A
1	16	805	C
1	16	814	A
1	16	815	A
1	16	817	C
1	16	821	G
1	16	828	U
1	16	832	G
1	16	842	U
1	16	844	G
1	16	845	A
1	16	846	G
1	16	890	G
1	16	902	G
1	16	914	A
1	16	922	G
1	16	926	G
1	16	931	C
1	16	934	C
1	16	935	A
1	16	945	G
1	16	948	C
1	16	960	U
1	16	969	A
1	16	975	A
1	16	976	G
1	16	977	A

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Mol	Chain	Res	Type
1	16	978	A
1	16	993	G
1	16	1003	G
1	16	1004	A
1	16	1017	U
1	16	1020	G
1	16	1031	C
1	16	1032	G
1	16	1033	G
1	16	1053	G
1	16	1056	U
1	16	1065	U
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1108	G
1	16	1124	G
1	16	1126	U
1	16	1137	C
1	16	1139	G
1	16	1143	G
1	16	1146	A
1	16	1154	G
1	16	1158	C
1	16	1159	U
1	16	1160	G
1	16	1167	A
1	16	1168	U
1	16	1183	U
1	16	1184	G
1	16	1191	A
1	16	1196	A
1	16	1197	A
1	16	1212	U
1	16	1213	A
1	16	1214	C
1	16	1227	A
1	16	1228	C
1	16	1238	A
1	16	1239	A
1	16	1241	G
1	16	1258	G

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Mol	Chain	Res	Type
1	16	1260	G
1	16	1261	A
1	16	1270	G
1	16	1280	A
1	16	1285	A
1	16	1286	U
1	16	1287	A
1	16	1300	G
1	16	1302	C
1	16	1305	G
1	16	1312	G
1	16	1317	C
1	16	1320	C
1	16	1331	G
1	16	1338	G
1	16	1340	A
1	16	1346	A
1	16	1347	G
1	16	1353	G
1	16	1363	A
1	16	1370	G
1	16	1374	A
1	16	1375	A
1	16	1381	U
1	16	1394	A
1	16	1398	A
1	16	1399	C
1	16	1419	G
1	16	1422	G
1	16	1432	G
1	16	1441	A
1	16	1447	A
1	16	1448	C
1	16	1451	U
1	16	1452	C
1	16	1454	G
1	16	1487	G
1	16	1493	A
1	16	1497	G
1	16	1499	A
1	16	1503	A
1	16	1506	U

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Mol	Chain	Res	Type
1	16	1517	G
1	16	1529	G
1	16	1530	G
1	16	1534	A
1	16	1535	C
22	mR	23	U
22	mR	26	A
22	mR	28	G
22	mR	29	G
22	mR	30	A
22	mR	31	C
22	mR	40	U
22	mR	41	U
22	mR	42	C
22	mR	44	A
22	mR	48	C
22	mR	49	U
23	23	10	A
23	23	15	G
23	23	23	G
23	23	34	U
23	23	45	G
23	23	46	G
23	23	51	G
23	23	63	A
23	23	71	A
23	23	74	A
23	23	75	G
23	23	80	G
23	23	84	A
23	23	87	U
23	23	88	G
23	23	101	A
23	23	102	U
23	23	118	A
23	23	119	A
23	23	120	U
23	23	125	A
23	23	136	G
23	23	139	U
23	23	163	C
23	23	181	A

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Mol	Chain	Res	Type
23	23	188	G
23	23	196	A
23	23	199	A
23	23	205	G
23	23	215	G
23	23	216	A
23	23	221	A
23	23	222	A
23	23	233	A
23	23	248	G
23	23	252	G
23	23	265	A
23	23	266	G
23	23	267	C
23	23	271	G
23	23	277	G
23	23	278	A
23	23	284	U
23	23	285	G
23	23	286	U
23	23	311	A
23	23	317	G
23	23	330	A
23	23	346	A
23	23	359	G
23	23	361	G
23	23	362	A
23	23	371	A
23	23	373	U
23	23	383	C
23	23	386	G
23	23	396	G
23	23	401	A
23	23	403	U
23	23	412	A
23	23	448	U
23	23	455	C
23	23	458	G
23	23	470	A
23	23	479	A
23	23	480	A
23	23	481	G

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Mol	Chain	Res	Type
23	23	489	G
23	23	491	G
23	23	496	G
23	23	504	A
23	23	505	A
23	23	508	A
23	23	509	C
23	23	529	A
23	23	531	C
23	23	532	A
23	23	533	G
23	23	546	U
23	23	547	A
23	23	550	C
23	23	563	A
23	23	573	U
23	23	575	A
23	23	603	A
23	23	615	U
23	23	632	A
23	23	637	A
23	23	645	C
23	23	647	G
23	23	654	A
23	23	670	A
23	23	686	U
23	23	717	C
23	23	726	G
23	23	730	A
23	23	738	G
23	23	747	5MU
23	23	753	A
23	23	775	G
23	23	776	G
23	23	782	A
23	23	784	G
23	23	785	G
23	23	788	A
23	23	789	A
23	23	805	G
23	23	812	C
23	23	819	A

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Mol	Chain	Res	Type
23	23	827	U
23	23	828	U
23	23	845	A
23	23	846	U
23	23	847	U
23	23	859	G
23	23	869	G
23	23	879	G
23	23	882	G
23	23	884	U
23	23	888	C
23	23	890	C
23	23	891	G
23	23	895	U
23	23	896	A
23	23	897	C
23	23	907	G
23	23	910	A
23	23	914	G
23	23	917	A
23	23	919	U
23	23	923	G
23	23	930	G
23	23	931	U
23	23	932	U
23	23	934	U
23	23	941	A
23	23	946	C
23	23	961	C
23	23	962	G
23	23	974	G
23	23	983	A
23	23	989	G
23	23	996	A
23	23	1009	A
23	23	1012	U
23	23	1013	C
23	23	1026	G
23	23	1033	U
23	23	1046	A
23	23	1047	G
23	23	1110	G

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Mol	Chain	Res	Type
23	23	1112	G
23	23	1132	U
23	23	1133	A
23	23	1134	A
23	23	1135	C
23	23	1136	G
23	23	1142	A
23	23	1155	A
23	23	1161	C
23	23	1172	C
23	23	1174	U
23	23	1175	A
23	23	1179	G
23	23	1186	G
23	23	1206	G
23	23	1227	G
23	23	1236	G
23	23	1238	G
23	23	1244	A
23	23	1247	A
23	23	1249	U
23	23	1252	G
23	23	1253	A
23	23	1256	G
23	23	1262	A
23	23	1271	G
23	23	1272	A
23	23	1300	G
23	23	1301	A
23	23	1321	A
23	23	1329	U
23	23	1332	G
23	23	1352	U
23	23	1360	G
23	23	1365	A
23	23	1368	G
23	23	1374	G
23	23	1378	A
23	23	1379	U
23	23	1383	A
23	23	1386	C
23	23	1394	U

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Mol	Chain	Res	Type
23	23	1395	A
23	23	1403	A
23	23	1416	G
23	23	1417	C
23	23	1419	A
23	23	1420	A
23	23	1428	C
23	23	1437	C
23	23	1452	G
23	23	1453	A
23	23	1460	U
23	23	1461	C
23	23	1482	G
23	23	1493	C
23	23	1494	A
23	23	1497	U
23	23	1509	A
23	23	1515	A
23	23	1524	G
23	23	1536	C
23	23	1538	G
23	23	1566	A
23	23	1569	A
23	23	1578	U
23	23	1583	A
23	23	1584	U
23	23	1585	C
23	23	1607	C
23	23	1608	A
23	23	1610	A
23	23	1613	G
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1674	G
23	23	1675	C
23	23	1699	G
23	23	1721	G
23	23	1722	A
23	23	1729	U
23	23	1730	C
23	23	1732	C

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Mol	Chain	Res	Type
23	23	1733	G
23	23	1738	G
23	23	1744	A
23	23	1764	C
23	23	1773	A
23	23	1782	U
23	23	1791	A
23	23	1799	G
23	23	1800	C
23	23	1801	A
23	23	1808	A
23	23	1811	G
23	23	1816	C
23	23	1829	A
23	23	1847	A
23	23	1848	A
23	23	1857	G
23	23	1862	G
23	23	1871	A
23	23	1872	A
23	23	1873	G
23	23	1884	G
23	23	1906	G
23	23	1913	A
23	23	1914	C
23	23	1919	A
23	23	1929	G
23	23	1930	G
23	23	1937	A
23	23	1938	A
23	23	1955	U
23	23	1956	U
23	23	1964	G
23	23	1967	C
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1991	U
23	23	1992	G
23	23	1993	U
23	23	1997	C
23	23	2022	U

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Mol	Chain	Res	Type
23	23	2023	C
23	23	2031	A
23	23	2033	A
23	23	2038	G
23	23	2043	C
23	23	2049	G
23	23	2055	C
23	23	2056	G
23	23	2060	A
23	23	2061	G
23	23	2062	A
23	23	2069	G7M
23	23	2093	G
23	23	2101	A
23	23	2102	G
23	23	2103	C
23	23	2192	U
23	23	2198	A
23	23	2203	U
23	23	2204	G
23	23	2211	A
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2268	A
23	23	2278	A
23	23	2279	G
23	23	2283	C
23	23	2287	A
23	23	2288	A
23	23	2305	U
23	23	2307	G
23	23	2308	G
23	23	2319	G
23	23	2321	U
23	23	2322	A
23	23	2325	G
23	23	2333	A
23	23	2335	A
23	23	2345	G
23	23	2347	C
23	23	2350	C

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Mol	Chain	Res	Type
23	23	2361	G
23	23	2379	G
23	23	2383	G
23	23	2385	C
23	23	2402	U
23	23	2406	A
23	23	2422	C
23	23	2423	U
23	23	2425	A
23	23	2428	G
23	23	2429	G
23	23	2430	A
23	23	2435	A
23	23	2441	U
23	23	2445	2MG
23	23	2447	G
23	23	2448	A
23	23	2459	A
23	23	2469	A
23	23	2470	G
23	23	2476	A
23	23	2478	A
23	23	2484	G
23	23	2491	U
23	23	2494	G
23	23	2502	G
23	23	2504	PSU
23	23	2505	G
23	23	2506	U
23	23	2518	A
23	23	2529	G
23	23	2547	A
23	23	2554	U
23	23	2556	C
23	23	2562	U
23	23	2564	A
23	23	2566	A
23	23	2567	G
23	23	2573	C
23	23	2582	G
23	23	2602	A
23	23	2603	G

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Mol	Chain	Res	Type
23	23	2608	G
23	23	2609	U
23	23	2613	U
23	23	2615	U
23	23	2629	U
23	23	2630	G
23	23	2636	C
23	23	2646	C
23	23	2661	G
23	23	2663	G
23	23	2685	G
23	23	2689	U
23	23	2690	U
23	23	2714	G
23	23	2716	C
23	23	2718	G
23	23	2726	A
23	23	2733	A
23	23	2739	U
23	23	2744	G
23	23	2748	A
23	23	2751	G
23	23	2757	A
23	23	2762	C
23	23	2778	A
23	23	2781	A
23	23	2793	C
23	23	2797	U
23	23	2799	A
23	23	2801	G
23	23	2818	U
23	23	2820	A
23	23	2821	A
23	23	2834	G
23	23	2837	A
23	23	2867	G
23	23	2873	A
23	23	2877	G
23	23	2883	A
23	23	2884	U
23	23	2885	G
23	23	2886	A

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Mol	Chain	Res	Type
23	23	2891	U
24	5	13	G
24	5	17	C
24	5	24	G
24	5	32	U
24	5	33	G
24	5	35	C
24	5	44	G
24	5	45	A
24	5	56	G
24	5	67	G
24	5	73	A
24	5	89	U
24	5	90	C
24	5	91	C
24	5	99	A
24	5	109	A
24	5	119	A
24	5	120	U
54	Pt	2	G
54	Pt	9	G
54	Pt	14	A
54	Pt	19	G
54	Pt	21	H2U
54	Pt	22	A
54	Pt	39	A
54	Pt	47	G7M
54	Pt	50	G
54	Pt	57	C
54	Pt	60	A
54	Pt	71	G
54	Pt	77	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	429	U
1	16	438	U
1	16	1319	A
1	16	1447	A
23	23	479	A
23	23	503	A

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Mol	Chain	Res	Type
23	23	784	G
23	23	827	U
23	23	858	G
23	23	984	A
23	23	1955	U
23	23	2324	U
23	23	2430	A
23	23	2689	U
23	23	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	OMG	23	2251	54,23	19,26,27	0.93	1 (5%)	21,38,41	1.07	2 (9%)
1	MA6	16	1519	1	19,26,27	1.09	1 (5%)	18,38,41	2.11	3 (16%)
54	4SU	Pt	8	54	18,21,22	1.87	5 (27%)	25,30,33	2.30	5 (20%)
23	2MG	23	1835	23	18,26,27	0.91	1 (5%)	16,38,41	1.31	3 (18%)
23	5MU	23	747	23	19,22,23	1.41	5 (26%)	27,32,35	2.19	9 (33%)
1	PSU	16	516	57,1	18,21,22	1.36	3 (16%)	21,30,33	2.06	4 (19%)
23	5MC	23	1962	23,58	19,22,23	1.66	3 (15%)	26,32,35	1.08	2 (7%)
1	UR3	16	1498	1	19,22,23	0.94	0	26,32,35	1.70	4 (15%)
23	PSU	23	2580	23	18,21,22	1.39	3 (16%)	21,30,33	2.12	4 (19%)
23	PSU	23	2605	23	18,21,22	1.52	5 (27%)	21,30,33	2.31	4 (19%)
1	5MC	16	967	1	19,22,23	1.57	3 (15%)	26,32,35	1.12	2 (7%)
1	5MC	16	1407	1	19,22,23	1.54	3 (15%)	26,32,35	1.20	3 (11%)
54	H2U	Pt	21	54	18,21,22	0.96	2 (11%)	19,30,33	0.71	0
23	PSU	23	2457	23	18,21,22	1.39	3 (16%)	21,30,33	2.17	4 (19%)
23	OMC	23	2498	57,23	19,22,23	0.83	0	25,31,34	1.05	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	16	1402	57,1	20,23,24	0.78	0	25,32,35	2.08	7 (28%)
54	OMC	Pt	33	54	19,22,23	0.86	0	25,31,34	1.33	3 (12%)
1	2MG	16	966	1	18,26,27	0.91	1 (5%)	16,38,41	1.24	2 (12%)
23	PSU	23	2504	23,58	18,21,22	1.57	4 (22%)	21,30,33	2.15	4 (19%)
1	2MG	16	1207	1	18,26,27	0.90	1 (5%)	16,38,41	1.28	3 (18%)
1	2MG	16	1516	1	18,26,27	0.91	1 (5%)	16,38,41	1.34	3 (18%)
23	2MA	23	2503	57,23,58	18,25,26	0.75	0	20,37,40	2.07	4 (20%)
11	IAS	SK	119	11	6,7,8	1.34	1 (16%)	3,8,10	0.65	0
34	4D4	LP	81	34	9,11,12	2.03	2 (22%)	7,13,15	1.78	3 (42%)
23	G7M	23	2069	23	20,26,27	1.13	3 (15%)	16,39,42	0.45	0
54	G7M	Pt	47	54	20,26,27	1.15	3 (15%)	16,39,42	0.47	0
23	2MG	23	2445	23	18,26,27	0.90	1 (5%)	16,38,41	1.40	2 (12%)
12	D2T	SL	89	12	8,9,10	7.08	2 (25%)	6,11,13	2.60	3 (50%)
23	PSU	23	746	57,23	18,21,22	1.41	3 (16%)	21,30,33	2.04	4 (19%)
23	PSU	23	955	23	18,21,22	1.44	4 (22%)	21,30,33	2.06	3 (14%)
23	6MZ	23	2030	23	17,25,26	0.89	1 (5%)	15,36,39	2.87	4 (26%)
23	6MZ	23	1618	23	17,25,26	0.91	1 (5%)	15,36,39	2.19	4 (26%)
23	H2U	23	2449	23	18,21,22	1.09	3 (16%)	19,30,33	0.94	1 (5%)
1	MA6	16	1518	1	19,26,27	1.13	2 (10%)	18,38,41	2.21	4 (22%)
23	5MU	23	1939	23,58	19,22,23	1.54	4 (21%)	27,32,35	2.34	6 (22%)
23	3TD	23	1915	23	19,22,23	1.22	2 (10%)	23,32,35	2.07	3 (13%)
23	PSU	23	2604	23	18,21,22	1.68	5 (27%)	21,30,33	2.24	5 (23%)
23	1MG	23	745	23	19,26,27	0.90	1 (5%)	18,39,42	1.21	2 (11%)
23	OMU	23	2552	23	19,22,23	1.22	3 (15%)	25,31,34	1.80	6 (24%)
1	G7M	16	527	1	20,26,27	1.16	3 (15%)	16,39,42	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMG	23	2251	54,23	-	1/5/27/28	0/3/3/3
1	MA6	16	1519	1	-	4/7/29/30	0/3/3/3
54	4SU	Pt	8	54	-	0/7/25/26	0/2/2/2
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3
23	5MU	23	747	23	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	16	516	57,1	-	0/7/25/26	0/2/2/2
23	5MC	23	1962	23,58	-	0/7/25/26	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
54	H2U	Pt	21	54	-	2/7/38/39	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	57,23	-	0/9/27/28	0/2/2/2
1	4OC	16	1402	57,1	-	2/9/29/30	0/2/2/2
54	OMC	Pt	33	54	-	0/9/27/28	0/2/2/2
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3
23	PSU	23	2504	23,58	-	2/7/25/26	0/2/2/2
1	2MG	16	1207	1	-	0/5/27/28	0/3/3/3
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
23	2MA	23	2503	57,23,58	-	2/3/25/26	0/3/3/3
11	IAS	SK	119	11	-	0/7/7/8	-
34	4D4	LP	81	34	-	3/11/12/14	-
23	G7M	23	2069	23	-	1/3/25/26	0/3/3/3
54	G7M	Pt	47	54	-	2/3/25/26	0/3/3/3
23	2MG	23	2445	23	-	2/5/27/28	0/3/3/3
12	D2T	SL	89	12	-	4/7/12/14	-
23	PSU	23	746	57,23	-	2/7/25/26	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
23	6MZ	23	1618	23	-	2/5/27/28	0/3/3/3
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
1	MA6	16	1518	1	-	0/7/29/30	0/3/3/3
23	5MU	23	1939	23,58	-	0/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
23	PSU	23	2604	23	-	2/7/25/26	0/2/2/2
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
1	G7M	16	527	1	-	3/3/25/26	0/3/3/3

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	SL	89	D2T	CB-CA	-19.05	1.48	1.54
23	23	1962	5MC	C5-C4	6.12	1.48	1.44
1	16	967	5MC	C5-C4	5.71	1.48	1.44
1	16	1407	5MC	C5-C4	5.47	1.48	1.44
54	Pt	8	4SU	C4-S4	-5.11	1.59	1.68
12	SL	89	D2T	CB-SB	-5.08	1.77	1.82
34	LP	81	4D4	CZ-NE	5.02	1.43	1.33
23	23	2504	PSU	C6-C5	4.03	1.39	1.35
23	23	2604	PSU	C4-N3	-3.45	1.32	1.38
23	23	1939	5MU	C4-N3	-3.43	1.32	1.38
54	Pt	47	G7M	C8-N9	3.36	1.39	1.33
1	16	527	G7M	C8-N9	3.34	1.39	1.33
23	23	746	PSU	C6-C5	3.26	1.38	1.35
23	23	2069	G7M	C8-N9	3.26	1.39	1.33
23	23	2580	PSU	C6-C5	3.22	1.38	1.35
1	16	1518	MA6	C6-C5	3.21	1.49	1.44
23	23	955	PSU	C6-C5	3.19	1.38	1.35
1	16	1519	MA6	C6-C5	3.18	1.49	1.44
54	Pt	8	4SU	C4-N3	-3.18	1.34	1.37
23	23	1915	3TD	C6-C5	3.18	1.38	1.35
23	23	2605	PSU	C4-N3	-3.15	1.33	1.38
23	23	2457	PSU	C6-C5	3.13	1.38	1.35
23	23	1939	5MU	C2-N3	-3.12	1.32	1.38
23	23	747	5MU	C4-N3	-3.00	1.33	1.38
54	Pt	8	4SU	C5-C4	-2.98	1.38	1.42
23	23	2604	PSU	C6-C5	2.92	1.38	1.35
23	23	955	PSU	C4-N3	-2.87	1.33	1.38
23	23	2504	PSU	C4-N3	-2.84	1.33	1.38
1	16	516	PSU	C6-C5	2.84	1.38	1.35
23	23	2449	H2U	C2-N3	-2.81	1.33	1.38
23	23	2604	PSU	C2'-C1'	-2.79	1.50	1.53
23	23	2457	PSU	C4-N3	-2.77	1.33	1.38
23	23	746	PSU	C4-N3	-2.77	1.33	1.38
34	LP	81	4D4	CZ-NH1	2.74	1.44	1.34
23	23	2605	PSU	C6-C5	2.71	1.38	1.35
23	23	1962	5MC	C6-C5	2.71	1.39	1.34
23	23	2552	OMU	C4-N3	-2.69	1.34	1.38
1	16	966	2MG	C6-N1	-2.69	1.33	1.37
23	23	1939	5MU	C6-N1	-2.69	1.33	1.38
1	16	516	PSU	C4-N3	-2.68	1.33	1.38
23	23	2251	OMG	C6-N1	-2.65	1.33	1.37
23	23	2604	PSU	C2-N3	-2.65	1.33	1.37
23	23	2580	PSU	C4-N3	-2.62	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	SK	119	IAS	CB-CG	2.62	1.56	1.50
54	Pt	21	H2U	C2-N3	-2.61	1.33	1.38
23	23	1939	5MU	C6-C5	2.61	1.38	1.34
1	16	1407	5MC	C6-C5	2.60	1.38	1.34
23	23	1915	3TD	C2-N1	-2.55	1.34	1.37
23	23	747	5MU	C6-C5	2.52	1.38	1.34
23	23	1835	2MG	C6-N1	-2.49	1.34	1.37
23	23	745	1MG	C2-N1	2.49	1.41	1.37
1	16	1516	2MG	C6-N1	-2.46	1.34	1.37
1	16	1207	2MG	C6-N1	-2.43	1.34	1.37
23	23	2605	PSU	C2-N3	-2.43	1.33	1.37
1	16	967	5MC	C6-C5	2.43	1.38	1.34
23	23	747	5MU	C6-N1	-2.43	1.33	1.38
23	23	2449	H2U	C4-N3	-2.41	1.33	1.37
23	23	747	5MU	C2-N1	2.40	1.42	1.38
54	Pt	47	G7M	C8-N7	2.39	1.37	1.33
54	Pt	8	4SU	C2-N1	2.37	1.42	1.38
23	23	2445	2MG	C6-N1	-2.34	1.34	1.37
1	16	967	5MC	C6-N1	-2.33	1.34	1.38
23	23	1618	6MZ	C6-C5	2.33	1.48	1.44
54	Pt	21	H2U	C4-N3	-2.33	1.33	1.37
23	23	2552	OMU	C2-N3	-2.31	1.33	1.38
23	23	2552	OMU	C5-C4	-2.30	1.38	1.43
1	16	527	G7M	C5-C6	-2.28	1.39	1.45
1	16	527	G7M	C8-N7	2.26	1.37	1.33
23	23	1962	5MC	C6-N1	-2.21	1.34	1.38
23	23	2504	PSU	C2-N3	-2.20	1.33	1.37
23	23	2069	G7M	C8-N7	2.19	1.37	1.33
23	23	2030	6MZ	C6-C5	2.18	1.48	1.44
23	23	747	5MU	C2-N3	-2.17	1.34	1.38
1	16	1518	MA6	C6-N1	2.16	1.35	1.32
23	23	955	PSU	C2-N1	-2.14	1.33	1.36
23	23	2605	PSU	C2-N1	-2.14	1.33	1.36
23	23	2457	PSU	C2-N3	-2.13	1.34	1.37
23	23	2504	PSU	C2-N1	-2.11	1.33	1.36
23	23	955	PSU	C2-N3	-2.09	1.34	1.37
1	16	1407	5MC	C6-N1	-2.09	1.34	1.38
23	23	2605	PSU	C2'-C1'	-2.08	1.50	1.53
54	Pt	47	G7M	C5-C6	-2.08	1.40	1.45
23	23	2069	G7M	C5-C6	-2.08	1.40	1.45
23	23	2449	H2U	C2-N1	-2.07	1.32	1.35
23	23	2580	PSU	O4'-C1'	-2.06	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	516	PSU	C2-N3	-2.05	1.34	1.37
23	23	746	PSU	C2-N3	-2.04	1.34	1.37
54	Pt	8	4SU	C2-N3	-2.04	1.34	1.38
23	23	2604	PSU	C2-N1	-2.00	1.34	1.36

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2030	6MZ	C2-N1-C6	7.69	122.57	116.60
23	23	2503	2MA	C2-N3-C4	7.57	121.57	115.46
23	23	2605	PSU	N1-C2-N3	7.18	122.74	115.17
23	23	2604	PSU	N1-C2-N3	7.15	122.71	115.17
23	23	1915	3TD	N1-C2-N3	7.02	121.23	116.13
1	16	1518	MA6	C2-N1-C6	6.83	123.54	116.84
23	23	2504	PSU	N1-C2-N3	6.76	122.30	115.17
23	23	2457	PSU	N1-C2-N3	6.75	122.29	115.17
23	23	746	PSU	N1-C2-N3	6.59	122.12	115.17
1	16	1498	UR3	C4-N3-C2	-6.54	119.31	124.58
23	23	1618	6MZ	C2-N1-C6	6.51	121.65	116.60
23	23	2580	PSU	N1-C2-N3	6.50	122.03	115.17
23	23	955	PSU	N1-C2-N3	6.44	121.96	115.17
54	Pt	8	4SU	C4-N3-C2	-6.41	121.17	127.31
1	16	516	PSU	N1-C2-N3	6.37	121.89	115.17
1	16	1519	MA6	C2-N1-C6	6.32	123.04	116.84
23	23	747	5MU	N3-C2-N1	5.99	122.68	114.89
54	Pt	8	4SU	C5-C4-N3	5.89	120.22	114.75
23	23	1939	5MU	N3-C2-N1	5.88	122.55	114.89
23	23	1939	5MU	C4-N3-C2	-5.76	119.79	127.34
1	16	1402	4OC	O2-C2-N3	-5.59	113.51	122.33
23	23	2030	6MZ	C9-N6-C6	-5.43	117.81	122.85
1	16	1402	4OC	C1'-N1-C2	5.10	129.70	118.44
23	23	747	5MU	C4-N3-C2	-5.05	120.72	127.34
23	23	1915	3TD	C4-N3-C2	-5.04	119.28	124.61
23	23	2605	PSU	C4-N3-C2	-4.78	119.79	126.37
23	23	1939	5MU	C5-C6-N1	-4.75	118.16	123.31
23	23	1939	5MU	C5-C4-N3	4.75	119.45	115.32
54	Pt	8	4SU	C5-C4-S4	-4.66	118.98	124.31
23	23	2604	PSU	C4-N3-C2	-4.49	120.19	126.37
23	23	2552	OMU	N3-C2-N1	4.47	120.71	114.89
23	23	2457	PSU	C4-N3-C2	-4.33	120.41	126.37
23	23	2030	6MZ	N3-C2-N1	-4.30	122.84	128.67
23	23	2552	OMU	C4-N3-C2	-4.26	121.33	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	SL	89	D2T	CB1-SB-CB	4.23	109.98	102.36
1	16	1519	MA6	C4-C5-N7	-4.21	104.89	109.34
23	23	746	PSU	C4-N3-C2	-4.21	120.57	126.37
23	23	2457	PSU	O2-C2-N1	-4.19	118.47	122.79
1	16	1518	MA6	C4-C5-N7	-4.15	104.95	109.34
1	16	516	PSU	C4-N3-C2	-4.12	120.69	126.37
23	23	2580	PSU	C4-N3-C2	-4.12	120.69	126.37
1	16	1518	MA6	N3-C2-N1	-4.01	123.22	128.67
23	23	955	PSU	C4-N3-C2	-4.00	120.86	126.37
23	23	2580	PSU	O2-C2-N1	-3.96	118.71	122.79
54	Pt	8	4SU	N3-C2-N1	3.93	120.01	114.89
23	23	2504	PSU	C4-N3-C2	-3.93	120.96	126.37
54	Pt	33	OMC	O2-C2-N3	-3.90	116.18	122.33
23	23	2605	PSU	O2-C2-N1	-3.89	118.77	122.79
23	23	2504	PSU	O2-C2-N1	-3.82	118.85	122.79
23	23	1618	6MZ	N3-C2-N1	-3.76	123.57	128.67
23	23	747	5MU	O4-C4-C5	-3.74	120.64	124.92
23	23	2552	OMU	C5-C4-N3	3.69	119.97	114.80
23	23	955	PSU	O2-C2-N1	-3.69	118.98	122.79
1	16	1519	MA6	N3-C2-N1	-3.68	123.68	128.67
1	16	516	PSU	O2-C2-N1	-3.65	119.02	122.79
23	23	1939	5MU	O4-C4-C5	-3.52	120.89	124.92
34	LP	81	4D4	NE-CZ-NH2	3.50	126.68	120.67
23	23	2498	OMC	C2'-C1'-N1	-3.46	107.68	114.24
1	16	1402	4OC	O2-C2-N1	3.43	125.62	118.90
12	SL	89	D2T	OD2-CG-CB	3.39	120.48	113.15
23	23	747	5MU	C5-C6-N1	-3.34	119.69	123.31
1	16	1402	4OC	C1'-N1-C6	-3.34	113.64	120.78
23	23	746	PSU	O2-C2-N1	-3.31	119.37	122.79
23	23	2030	6MZ	C4-C5-N7	-3.28	105.87	109.34
1	16	1498	UR3	C5-C4-N3	3.23	119.29	115.04
1	16	1407	5MC	O2-C2-N3	-3.21	117.28	122.33
23	23	2604	PSU	O2-C2-N1	-3.18	119.51	122.79
23	23	1962	5MC	C5-C6-N1	-3.12	119.93	123.31
23	23	2552	OMU	O4-C4-C5	-3.09	119.83	125.16
23	23	2445	2MG	N1-C2-N2	3.06	119.69	116.56
23	23	747	5MU	C5-C4-N3	3.03	117.96	115.32
1	16	1407	5MC	C5-C4-N3	-3.03	118.65	121.75
23	23	745	1MG	C8-N7-C5	2.97	107.61	102.55
1	16	1516	2MG	C8-N7-C5	2.97	107.60	102.55
23	23	1835	2MG	C8-N7-C5	2.92	107.51	102.55
1	16	1207	2MG	C8-N7-C5	2.90	107.48	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Pt	33	OMC	C1'-N1-C2	2.88	124.80	118.44
23	23	2445	2MG	C8-N7-C5	2.88	107.45	102.55
1	16	967	5MC	C5-C6-N1	-2.87	120.20	123.31
23	23	1939	5MU	O2-C2-N1	-2.84	119.10	122.80
23	23	2504	PSU	C6-C5-C4	-2.84	116.26	118.17
1	16	966	2MG	C8-N7-C5	2.82	107.36	102.55
1	16	967	5MC	C5-C4-N3	-2.81	118.87	121.75
23	23	2251	OMG	C8-N7-C5	2.77	107.27	102.55
23	23	2604	PSU	C5-C6-N1	-2.68	118.41	122.14
54	Pt	8	4SU	C1'-N1-C2	2.68	122.40	117.59
23	23	1618	6MZ	C4-C5-N7	-2.68	106.51	109.34
23	23	1915	3TD	C1'-C5-C4	2.66	121.64	117.61
23	23	745	1MG	C5-C6-N1	2.64	117.78	113.96
23	23	1962	5MC	C5-C4-N3	-2.63	119.06	121.75
1	16	1402	4OC	C6-C5-C4	2.58	120.11	117.00
23	23	747	5MU	C1'-N1-C2	2.57	122.20	117.59
54	Pt	33	OMC	O2-C2-N1	2.54	123.88	118.90
1	16	1402	4OC	C5-C4-N3	-2.53	118.65	122.60
23	23	2503	2MA	C4-C5-N7	-2.51	106.69	109.34
23	23	2552	OMU	C6-N1-C2	-2.49	117.96	121.00
23	23	2251	OMG	C5-C6-N1	2.41	118.67	114.07
23	23	747	5MU	O2-C2-N3	-2.40	117.05	121.49
23	23	2580	PSU	O4'-C1'-C2'	2.36	108.42	105.15
23	23	2503	2MA	C2-N1-C6	2.35	121.71	118.10
23	23	2605	PSU	C5-C6-N1	-2.34	118.89	122.14
23	23	747	5MU	C6-C5-C4	2.32	119.93	118.02
23	23	747	5MU	C6-N1-C2	-2.30	119.01	121.30
23	23	2604	PSU	O2-C2-N3	-2.30	117.77	121.86
23	23	2503	2MA	C5-C6-N1	-2.26	118.17	120.84
1	16	1402	4OC	C6-N1-C2	-2.25	116.65	120.46
23	23	746	PSU	C5-C6-N1	-2.24	119.04	122.14
1	16	1516	2MG	N1-C2-N2	2.22	118.82	116.56
1	16	516	PSU	O4'-C1'-C2'	2.22	108.22	105.15
1	16	1207	2MG	N1-C2-N2	2.20	118.81	116.56
1	16	1498	UR3	C6-N1-C2	-2.20	120.00	121.80
23	23	1835	2MG	N1-C2-N2	2.19	118.80	116.56
1	16	1207	2MG	C5-C6-N1	2.16	118.20	114.07
12	SL	89	D2T	OD1-CG-CB	-2.16	117.91	122.44
23	23	1835	2MG	C5-C6-N1	2.16	118.19	114.07
1	16	1407	5MC	C5-C6-N1	-2.14	120.98	123.31
1	16	966	2MG	C5-C6-N1	2.11	118.10	114.07
34	LP	81	4D4	O-C-CA	-2.11	119.34	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	1516	2MG	C5-C6-N1	2.11	118.10	114.07
23	23	1618	6MZ	C9-N6-C6	-2.09	120.91	122.85
34	LP	81	4D4	NH1-CZ-NE	-2.07	114.56	119.27
23	23	2457	PSU	C5-C6-N1	-2.07	119.27	122.14
1	16	1518	MA6	C9-N6-C6	2.04	125.03	119.40
23	23	2449	H2U	C5-C4-N3	2.02	118.84	116.69
23	23	2552	OMU	O2-C2-N1	-2.01	120.17	122.80
1	16	1498	UR3	C3U-N3-C2	2.01	120.83	117.33

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	1402	4OC	O4'-C1'-N1-C2
1	16	1402	4OC	O4'-C1'-N1-C6
1	16	1519	MA6	O4'-C4'-C5'-O5'
1	16	1519	MA6	C5-C6-N6-C9
12	SL	89	D2T	CA-CB-CG-OD1
12	SL	89	D2T	CA-CB-CG-OD2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	2251	OMG	C1'-C2'-O2'-CM2
23	23	2504	PSU	O4'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
23	23	2445	2MG	C3'-C4'-C5'-O5'
23	23	2604	PSU	O4'-C4'-C5'-O5'
1	16	1519	MA6	C3'-C4'-C5'-O5'
23	23	1618	6MZ	C3'-C4'-C5'-O5'
23	23	2030	6MZ	C3'-C4'-C5'-O5'
1	16	527	G7M	C3'-C4'-C5'-O5'
54	Pt	21	H2U	O4'-C4'-C5'-O5'
23	23	1915	3TD	C3'-C4'-C5'-O5'
54	Pt	47	G7M	O4'-C4'-C5'-O5'
54	Pt	47	G7M	C3'-C4'-C5'-O5'
23	23	2503	2MA	O4'-C4'-C5'-O5'
23	23	2504	PSU	C3'-C4'-C5'-O5'
23	23	1915	3TD	O4'-C4'-C5'-O5'
23	23	2503	2MA	C3'-C4'-C5'-O5'
1	16	527	G7M	O4'-C4'-C5'-O5'
23	23	2445	2MG	O4'-C4'-C5'-O5'
34	LP	81	4D4	OB-CB-CG-CD
12	SL	89	D2T	CG-CB-SB-CB1
34	LP	81	4D4	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
54	Pt	21	H2U	C3'-C4'-C5'-O5'
1	16	527	G7M	C4'-C5'-O5'-P
1	16	1519	MA6	C4'-C5'-O5'-P
23	23	2069	G7M	C4'-C5'-O5'-P
12	SL	89	D2T	SB-CB-CG-OD2
23	23	746	PSU	O4'-C1'-C5-C6
23	23	746	PSU	C2'-C1'-C5-C6
23	23	747	5MU	C3'-C4'-C5'-O5'
34	LP	81	4D4	CG-CD-NE-CZ
23	23	2604	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 352 ligands modelled in this entry, 335 are monoatomic - leaving 17 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	$\# Z > 2$
55	PUT	23	3008	-	5,5,5	0.14	0	4,4,4	0.20	0
56	SPD	16	1602	-	9,9,9	0.16	0	8,8,8	0.20	0
55	PUT	16	1601	-	5,5,5	0.13	0	4,4,4	0.23	0
56	SPD	23	3014	-	9,9,9	0.26	0	8,8,8	0.20	0
56	SPD	23	3012	-	9,9,9	0.24	0	8,8,8	0.30	0
56	SPD	23	3011	-	9,9,9	0.27	0	8,8,8	0.27	0
55	PUT	23	3007	-	5,5,5	0.10	0	4,4,4	0.28	0
60	ATP	23	3001	-	28,33,33	0.66	0	34,52,52	0.61	1 (2%)
61	FME	Pt	101	54	8,9,10	0.59	0	8,9,11	1.14	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	ATP	23	3002	-	28,33,33	0.61	0	34,52,52	0.70	2 (5%)
55	PUT	23	3010	-	5,5,5	0.14	0	4,4,4	0.19	0
55	PUT	23	3006	-	5,5,5	0.11	0	4,4,4	0.20	0
55	PUT	23	3005	-	5,5,5	0.18	0	4,4,4	0.24	0
55	PUT	23	3009	-	5,5,5	0.11	0	4,4,4	0.17	0
55	PUT	23	3004	-	5,5,5	0.13	0	4,4,4	0.22	0
55	PUT	23	3003	-	5,5,5	0.14	0	4,4,4	0.15	0
56	SPD	23	3013	-	9,9,9	0.27	0	8,8,8	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PUT	23	3008	-	-	0/3/3/3	-
56	SPD	16	1602	-	-	3/7/7/7	-
55	PUT	16	1601	-	-	2/3/3/3	-
56	SPD	23	3014	-	-	2/7/7/7	-
56	SPD	23	3012	-	-	2/7/7/7	-
56	SPD	23	3011	-	-	2/7/7/7	-
55	PUT	23	3007	-	-	1/3/3/3	-
60	ATP	23	3001	-	-	4/18/38/38	0/3/3/3
61	FME	Pt	101	54	-	4/7/9/11	-
60	ATP	23	3002	-	-	3/18/38/38	0/3/3/3
55	PUT	23	3010	-	-	1/3/3/3	-
55	PUT	23	3006	-	-	2/3/3/3	-
55	PUT	23	3005	-	-	1/3/3/3	-
55	PUT	23	3009	-	-	1/3/3/3	-
55	PUT	23	3004	-	-	1/3/3/3	-
55	PUT	23	3003	-	-	1/3/3/3	-
56	SPD	23	3013	-	-	2/7/7/7	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	Pt	101	FME	O-C-CA	-2.85	117.43	124.77
60	23	3001	ATP	C5-C6-N6	2.32	123.84	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	23	3002	ATP	C5-C6-N6	2.27	123.78	120.31
60	23	3002	ATP	C4'-O4'-C1'	-2.13	107.98	109.92

There are no chirality outliers.

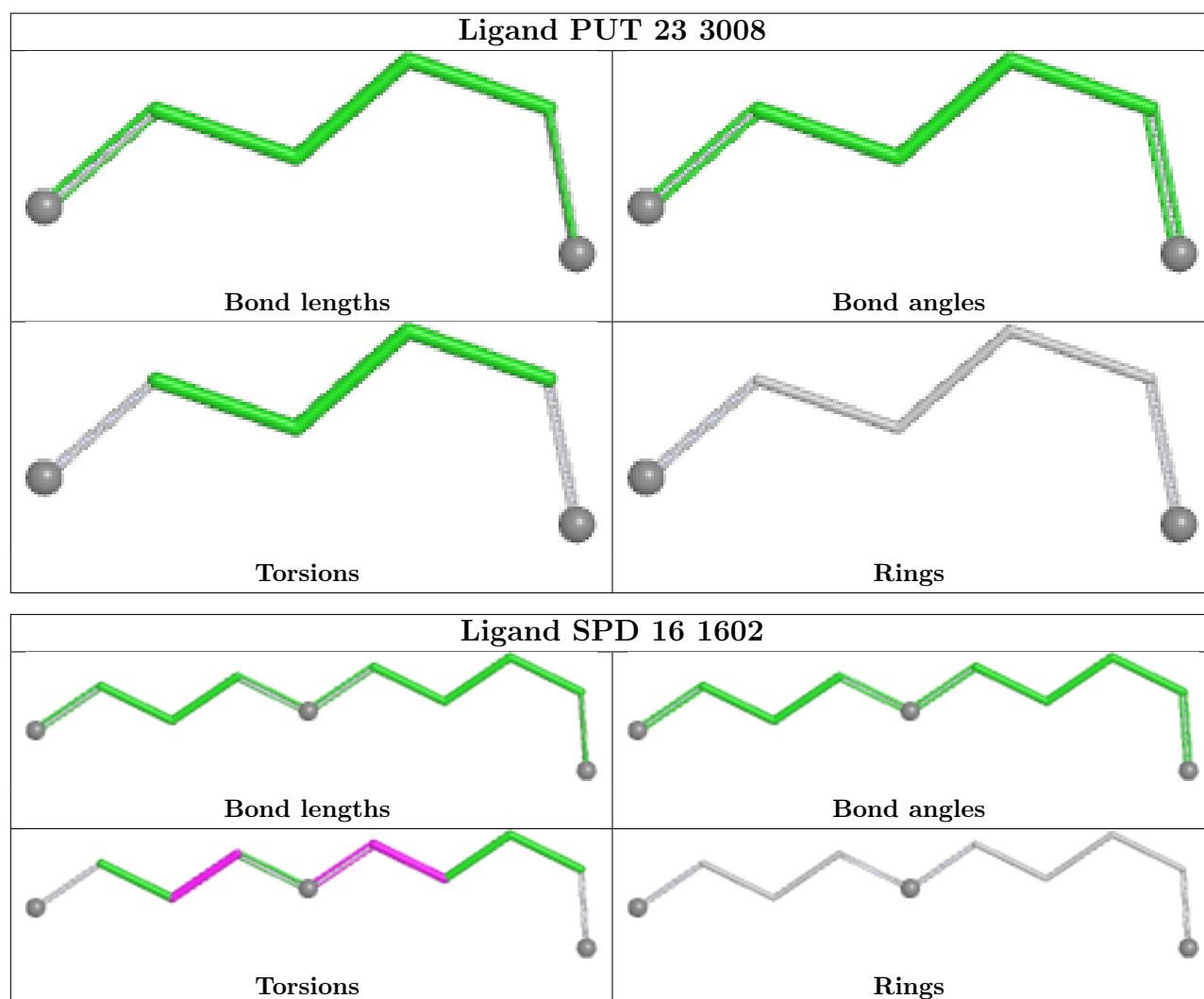
All (32) torsion outliers are listed below:

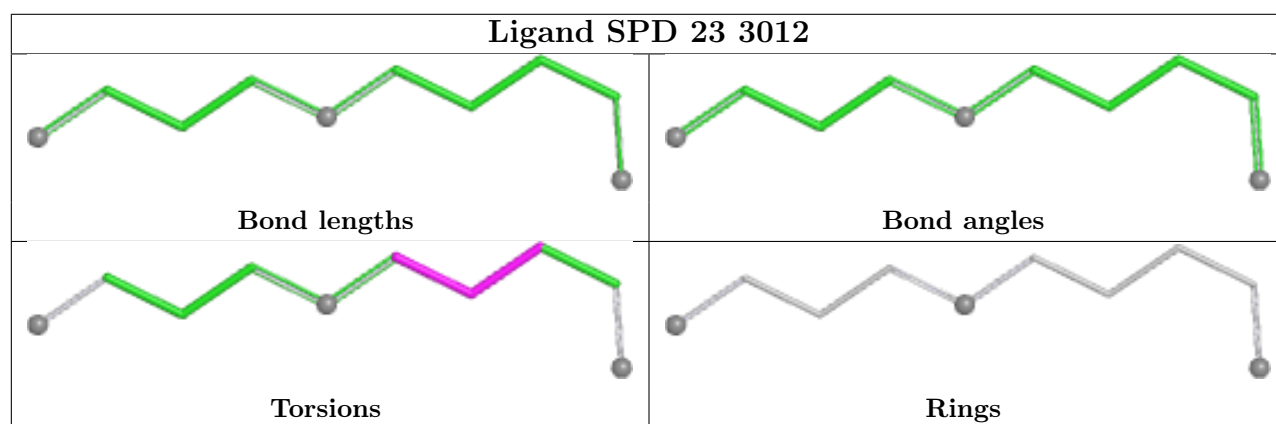
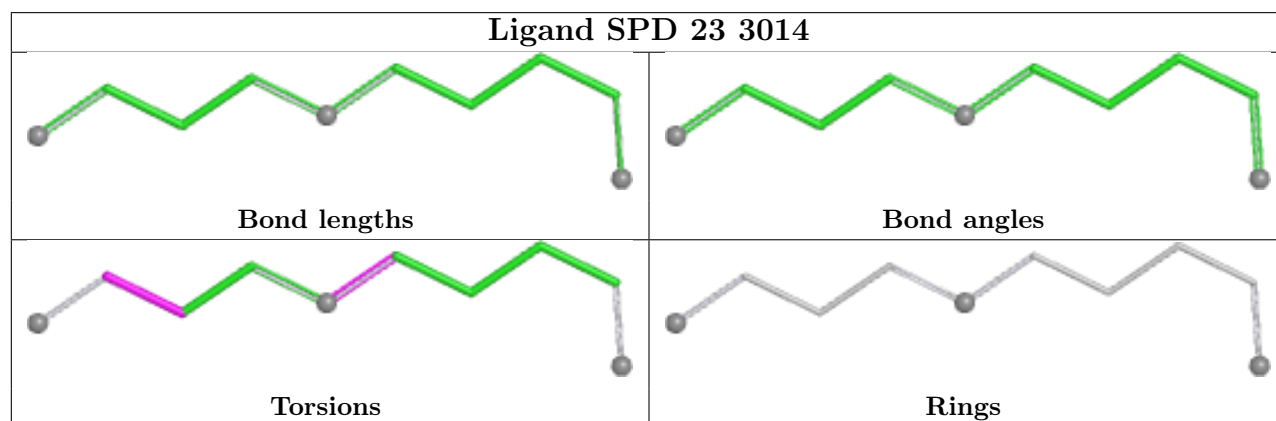
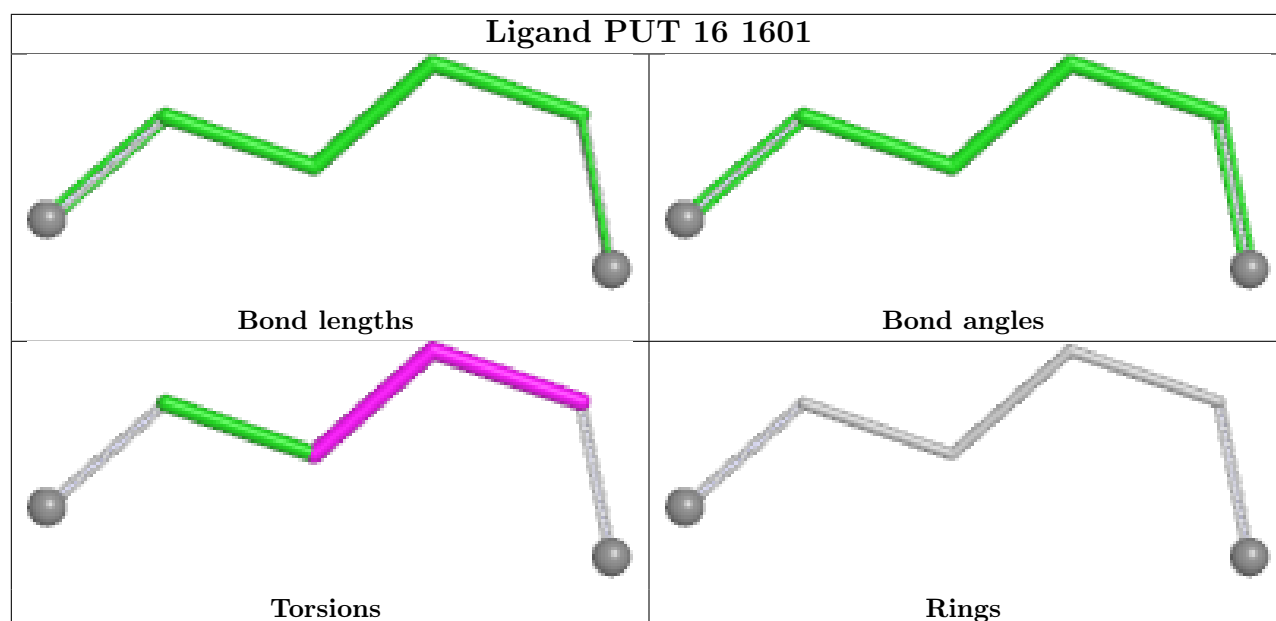
Mol	Chain	Res	Type	Atoms
60	23	3001	ATP	PB-O3B-PG-O2G
61	Pt	101	FME	O1-CN-N-CA
61	Pt	101	FME	N-CA-CB-CG
56	16	1602	SPD	N6-C7-C8-C9
55	23	3005	PUT	C1-C2-C3-C4
56	16	1602	SPD	C3-C4-C5-N6
56	23	3012	SPD	C3-C4-C5-N6
56	23	3013	SPD	N6-C7-C8-C9
56	23	3011	SPD	C3-C4-C5-N6
56	16	1602	SPD	C4-C5-N6-C7
61	Pt	101	FME	CB-CG-SD-CE
60	23	3001	ATP	PB-O3B-PG-O1G
55	23	3007	PUT	C1-C2-C3-C4
55	16	1601	PUT	C1-C2-C3-C4
55	23	3006	PUT	C1-C2-C3-C4
56	23	3014	SPD	C4-C5-N6-C7
56	23	3013	SPD	C7-C8-C9-N10
61	Pt	101	FME	C-CA-CB-CG
55	16	1601	PUT	C2-C3-C4-N2
56	23	3012	SPD	C2-C3-C4-C5
55	23	3009	PUT	C1-C2-C3-C4
56	23	3014	SPD	C7-C8-C9-N10
56	23	3011	SPD	C2-C3-C4-C5
60	23	3001	ATP	PG-O3B-PB-O2B
55	23	3006	PUT	C2-C3-C4-N2
60	23	3002	ATP	C3'-C4'-C5'-O5'
60	23	3001	ATP	C4'-C5'-O5'-PA
55	23	3003	PUT	C2-C3-C4-N2
55	23	3004	PUT	N1-C1-C2-C3
55	23	3010	PUT	C2-C3-C4-N2
60	23	3002	ATP	PG-O3B-PB-O1B
60	23	3002	ATP	PG-O3B-PB-O2B

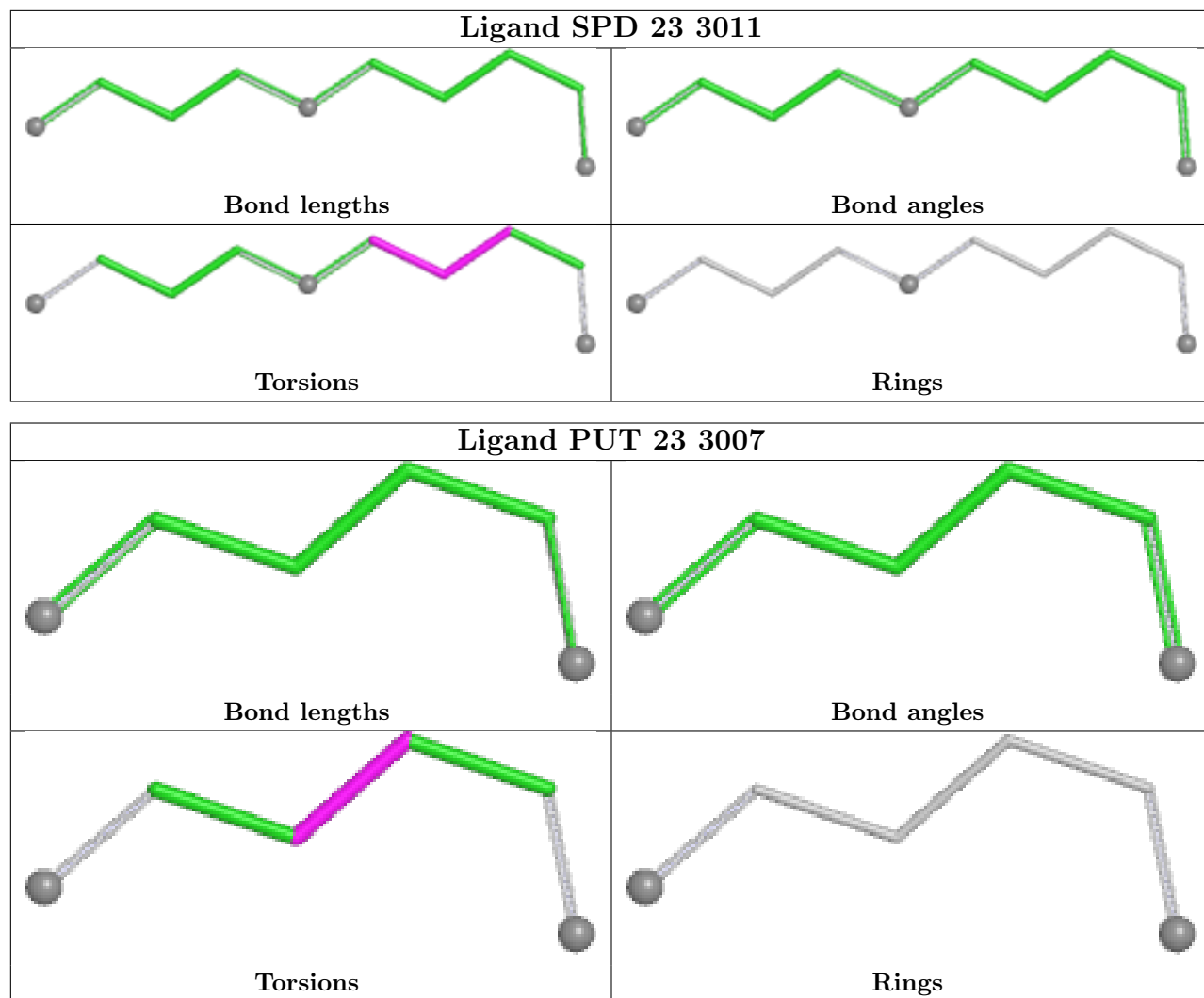
There are no ring outliers.

No monomer is involved in short contacts.

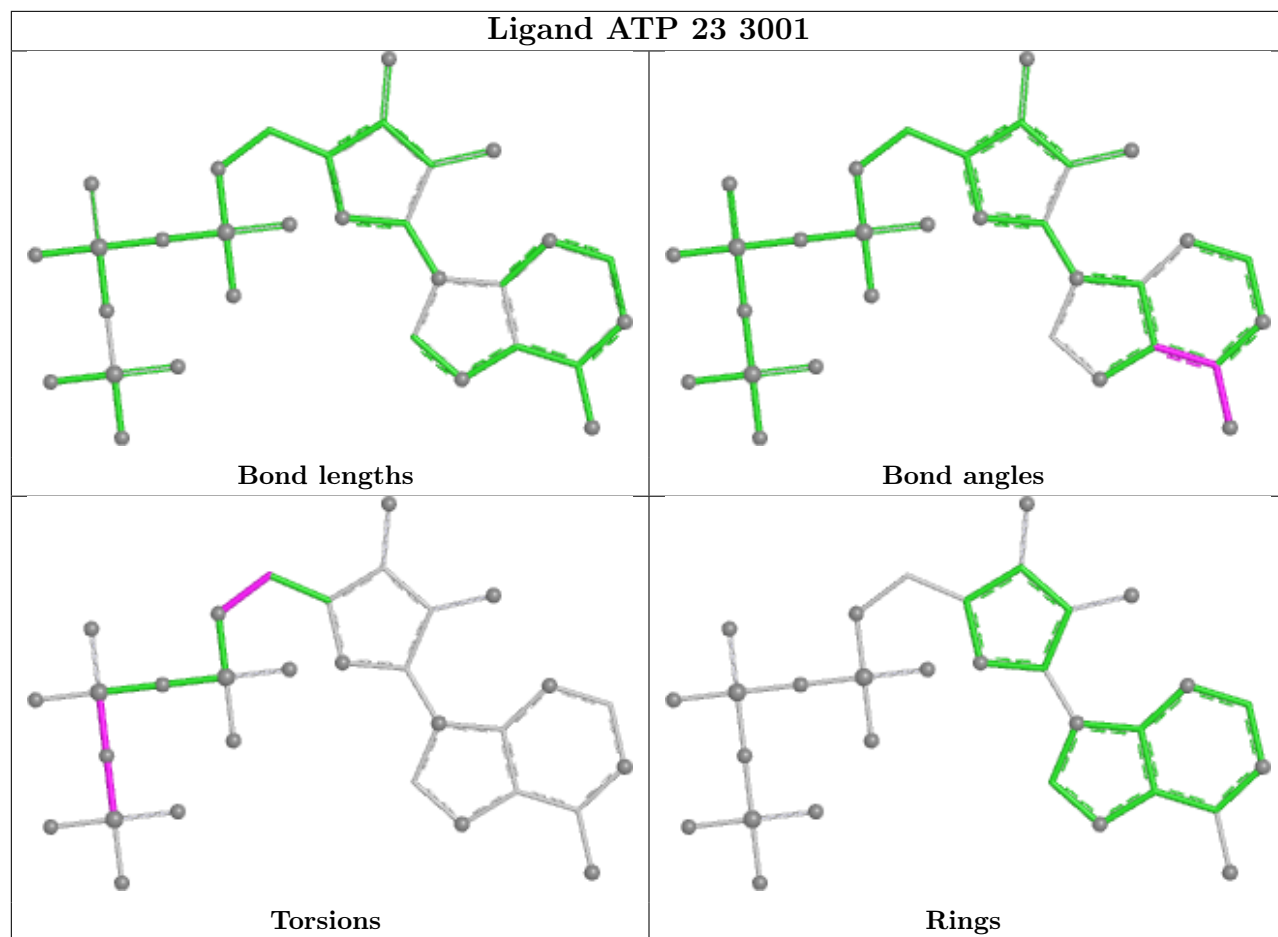
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



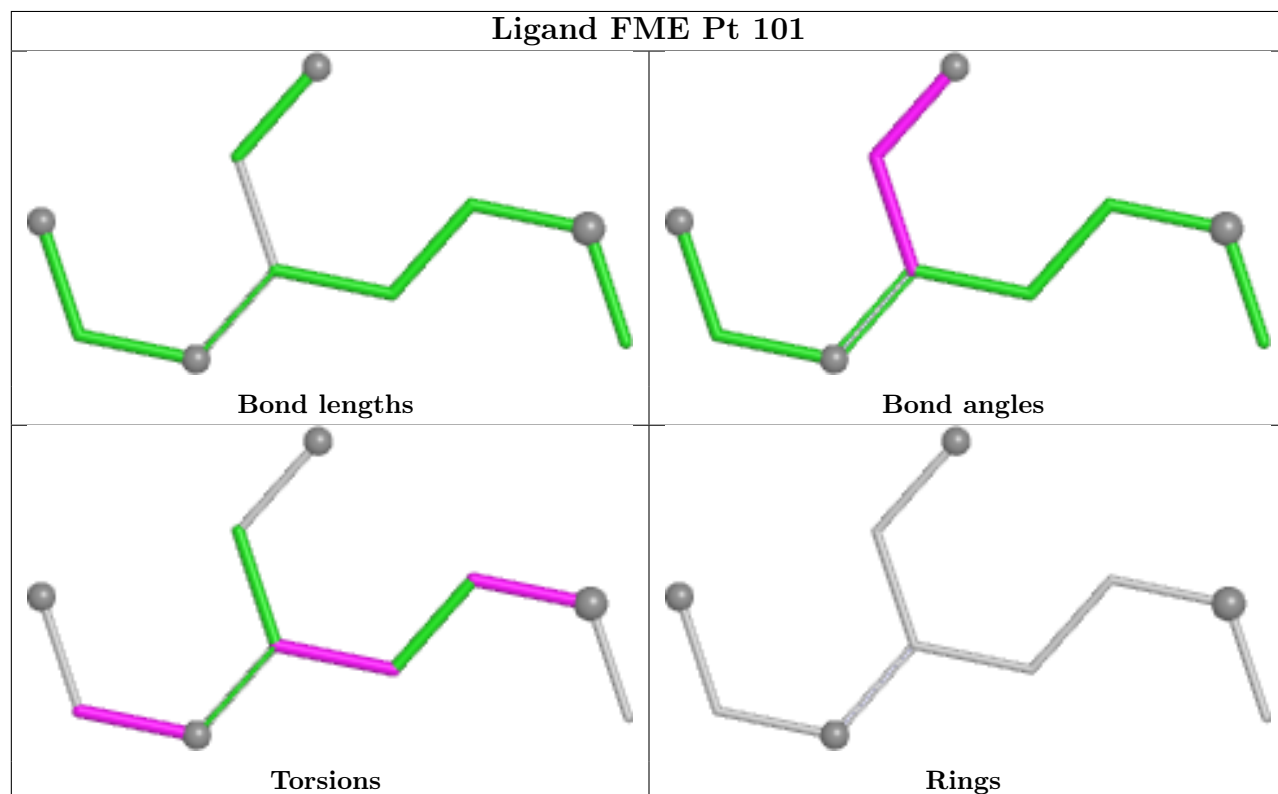




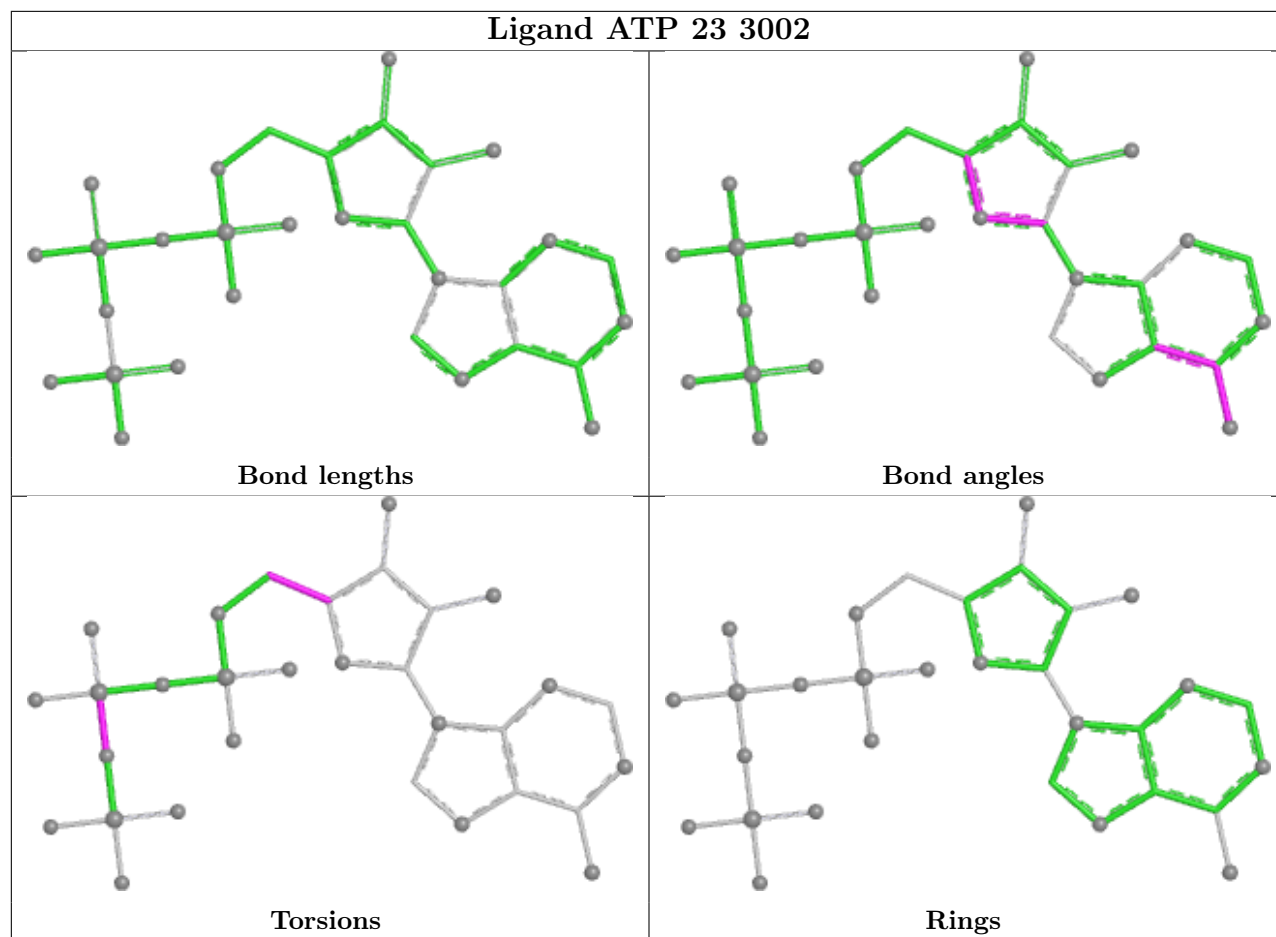
Ligand ATP 23 3001



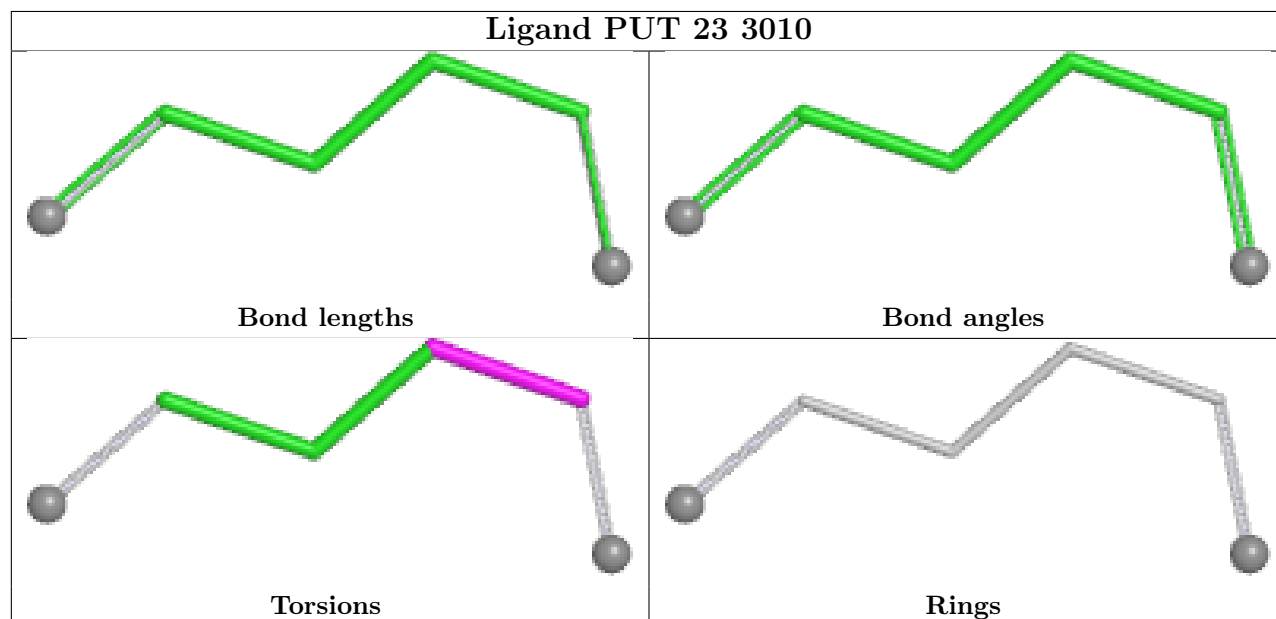
Ligand FME Pt 101

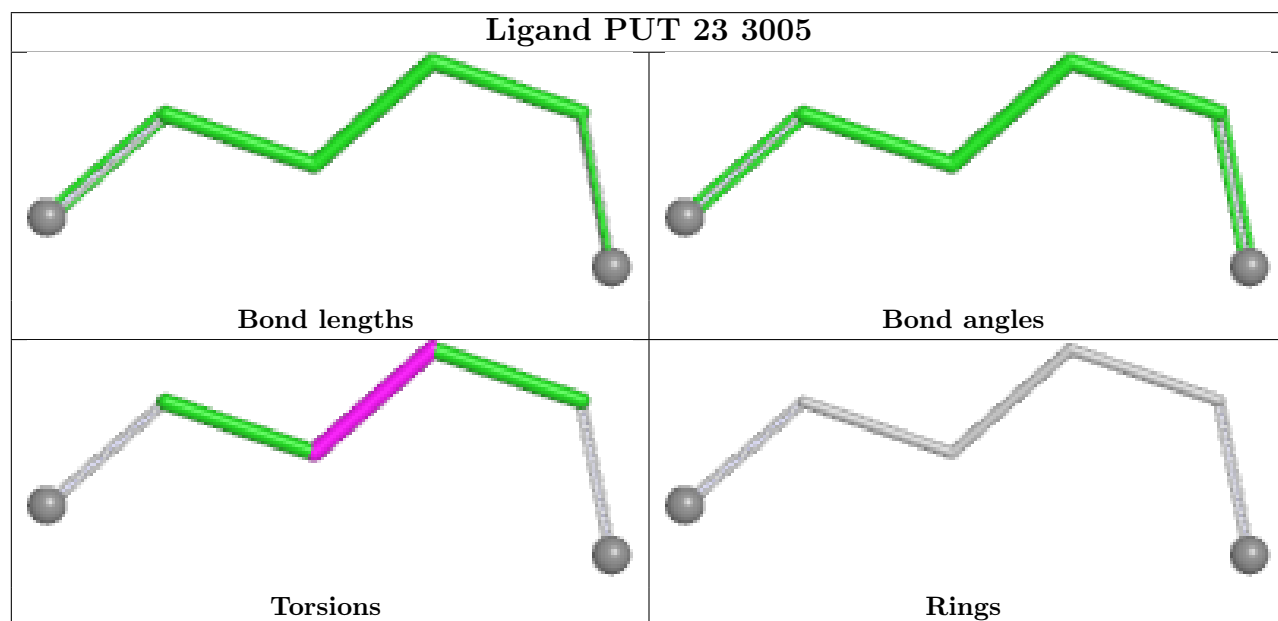
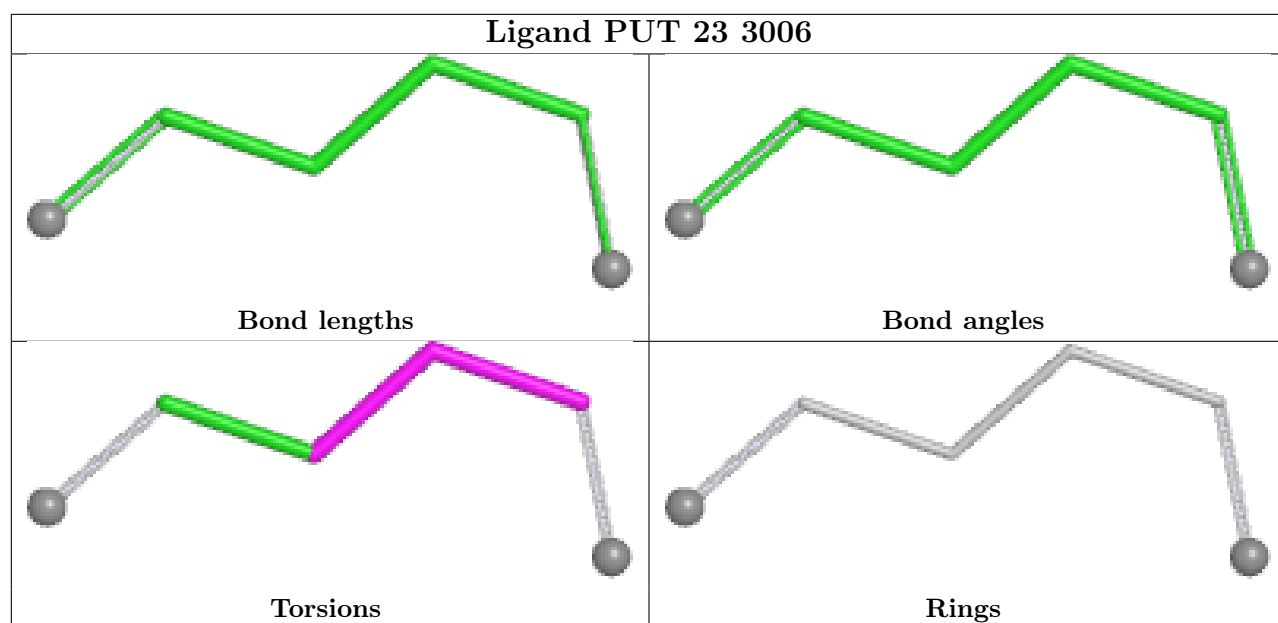


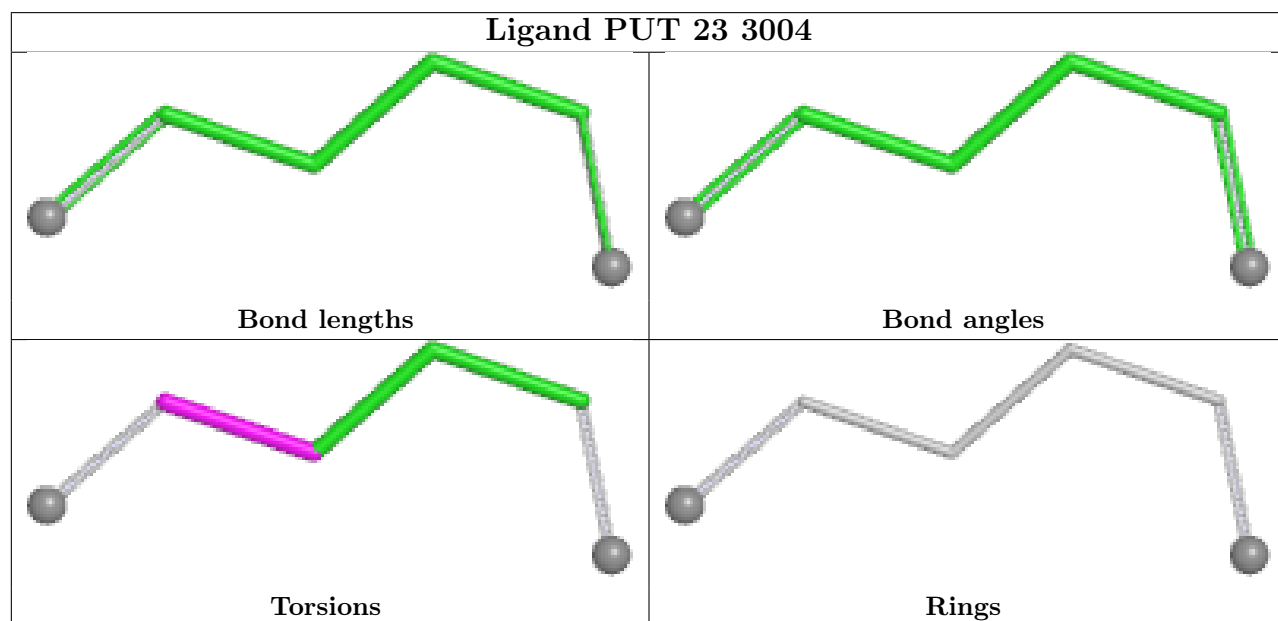
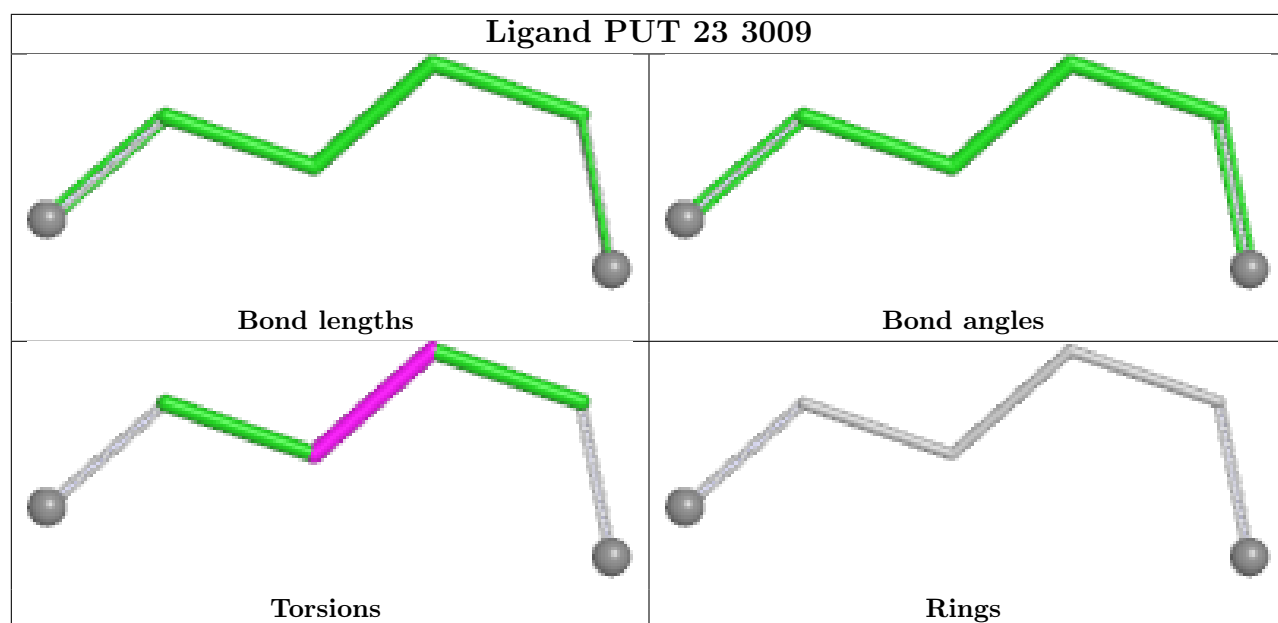
Ligand ATP 23 3002

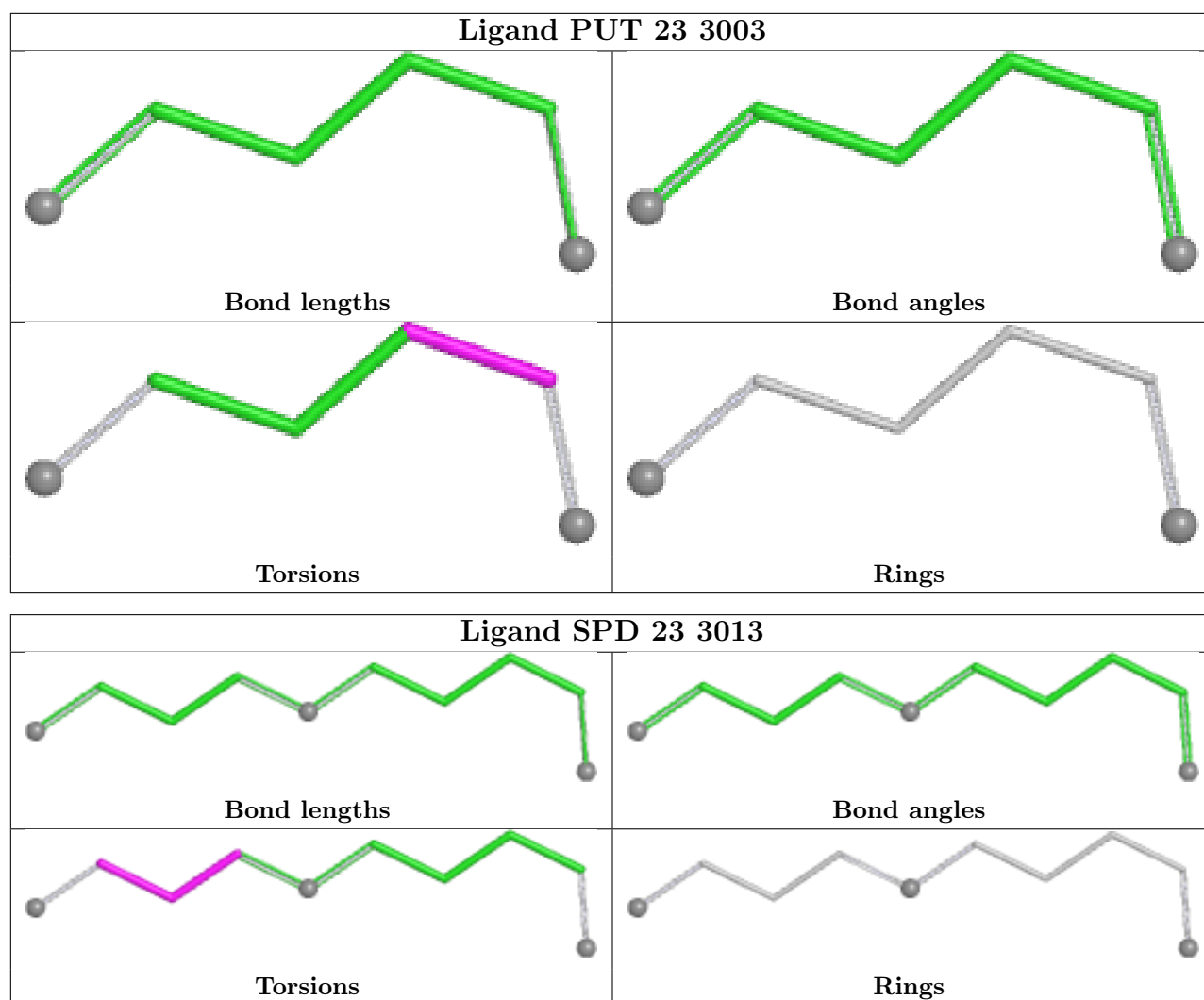


Ligand PUT 23 3010









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.

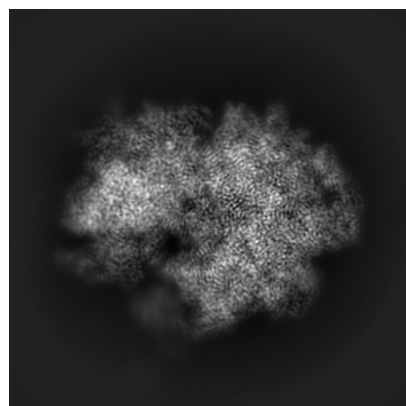
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48830. These allow visual inspection of the internal detail of the map and identification of artifacts.

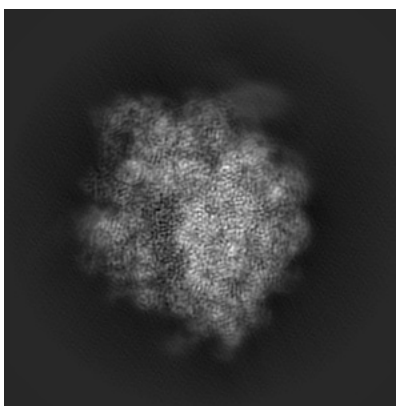
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

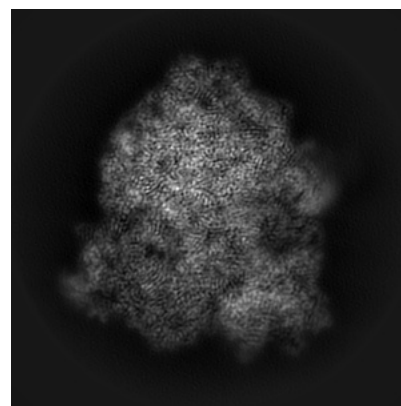
6.1.1 Primary map



X

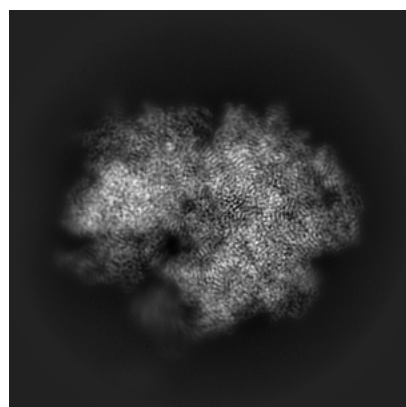


Y

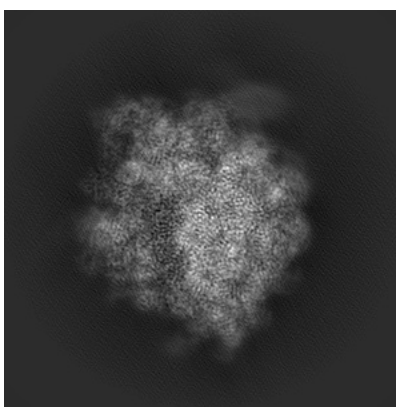


Z

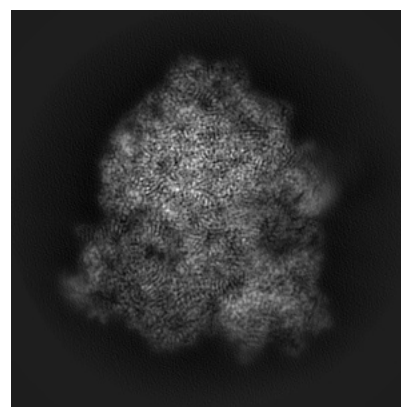
6.1.2 Raw map



X



Y

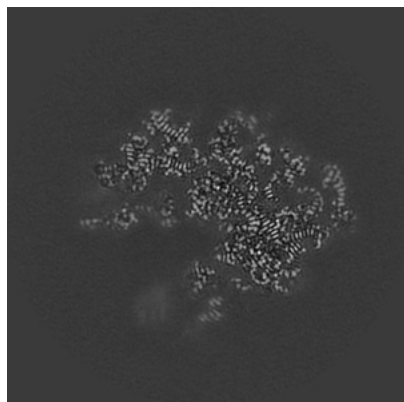


Z

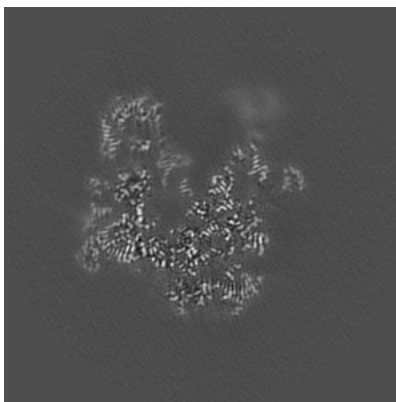
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

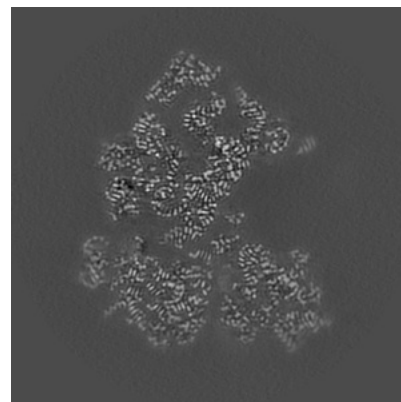
6.2.1 Primary map



X Index: 160

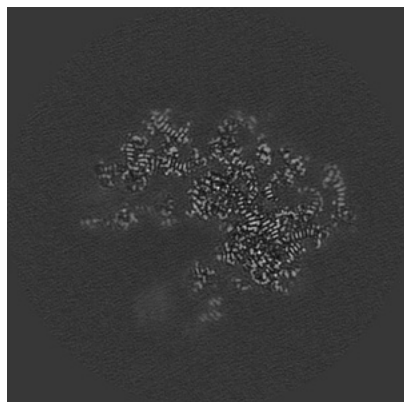


Y Index: 160

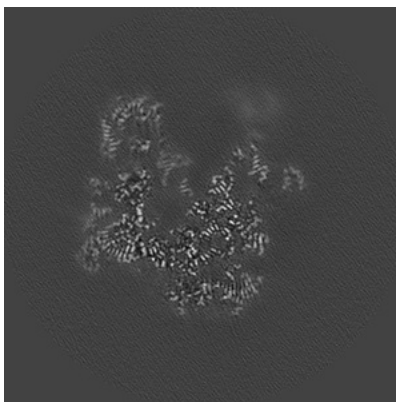


Z Index: 160

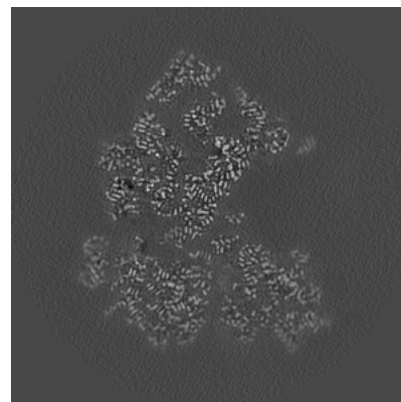
6.2.2 Raw map



X Index: 160



Y Index: 160

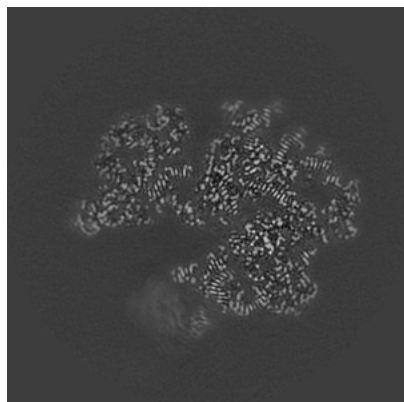


Z Index: 160

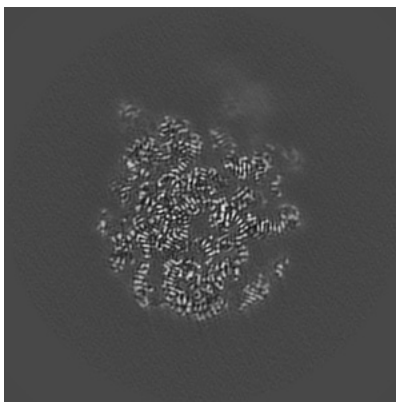
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

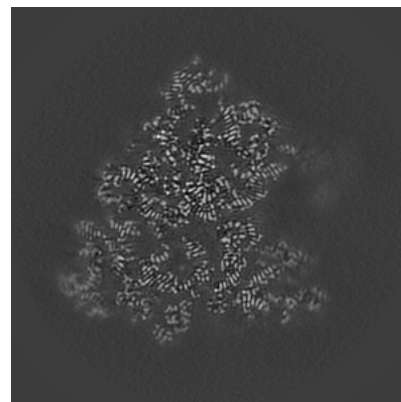
6.3.1 Primary map



X Index: 147

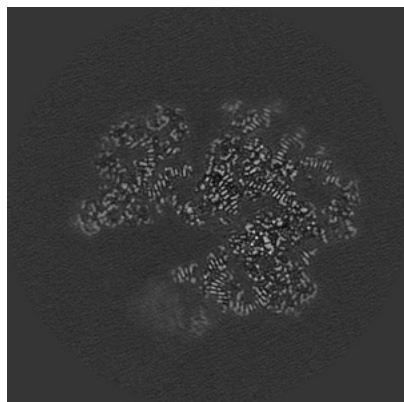


Y Index: 195

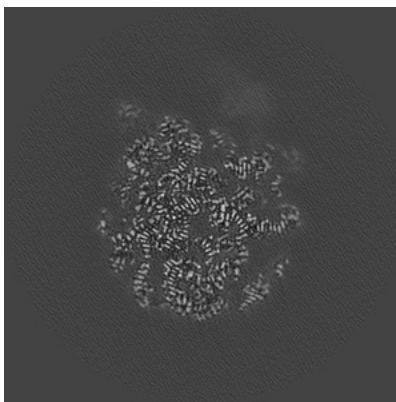


Z Index: 179

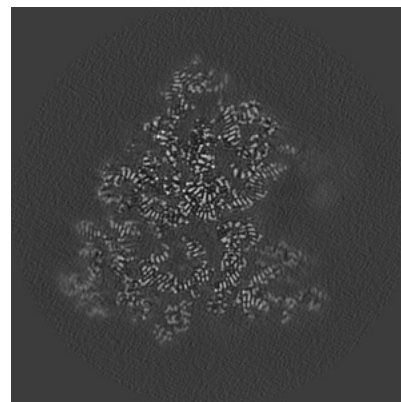
6.3.2 Raw map



X Index: 147



Y Index: 195

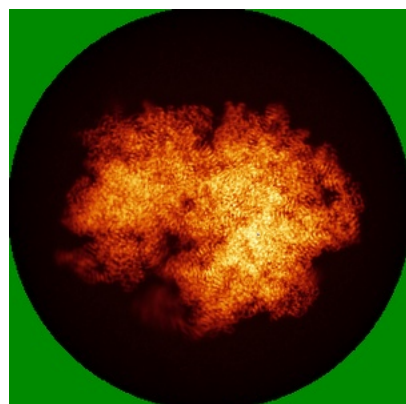


Z Index: 179

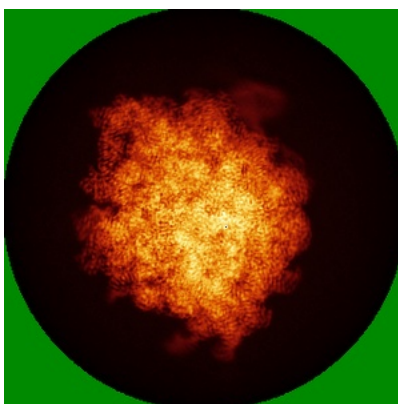
The images above show the largest variance slices of the map in three orthogonal directions.

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

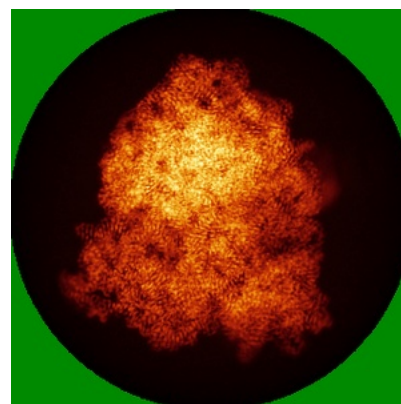
6.4.1 Primary map



X

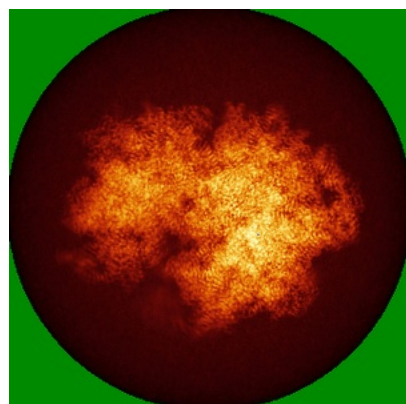


Y

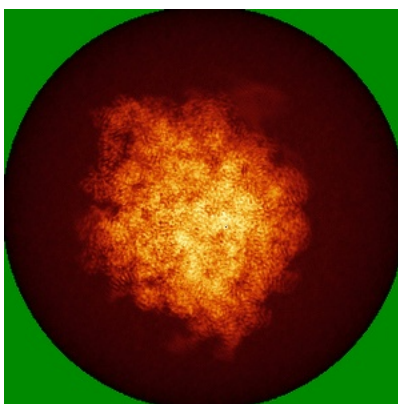


Z

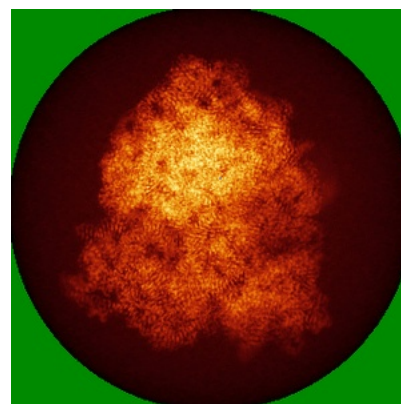
6.4.2 Raw map



X



Y

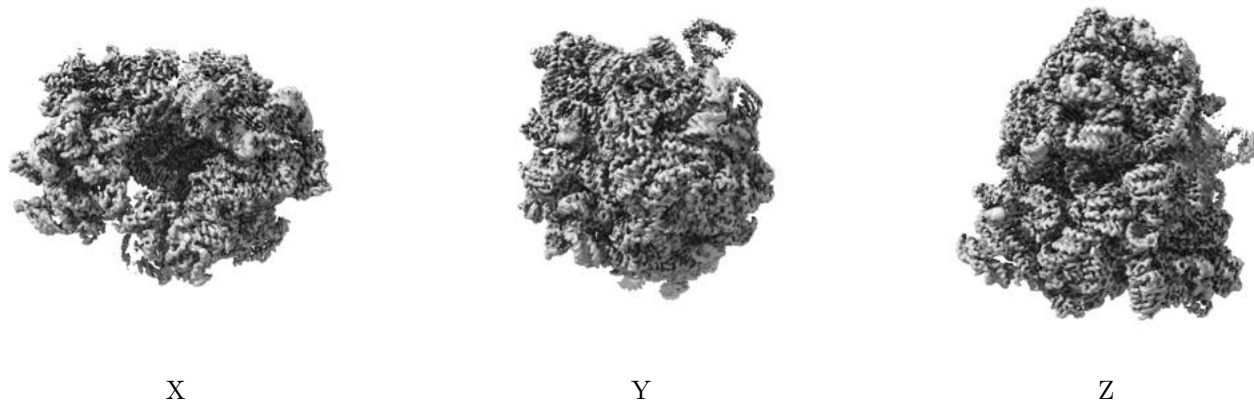


Z

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.

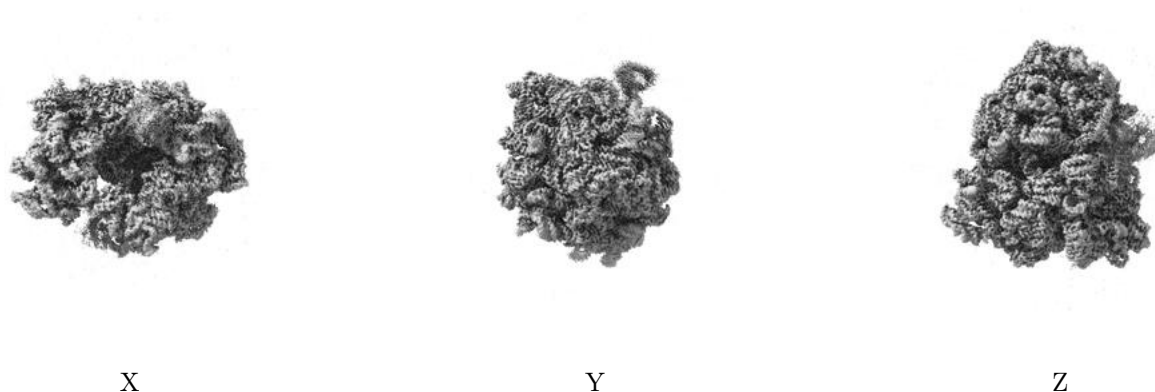
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

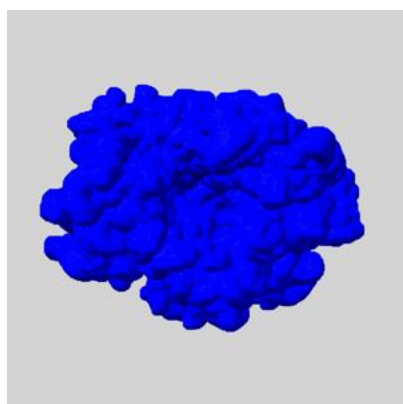
6.6 Mask visualisation [i](#)

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

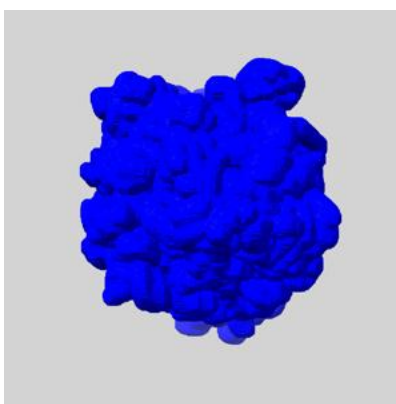
A mask typically either:

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

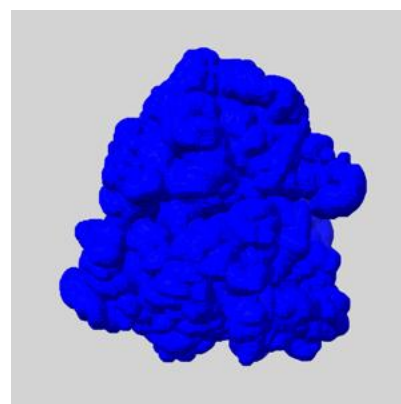
6.6.1 emd_48830_msk_1.map [i](#)



X



Y

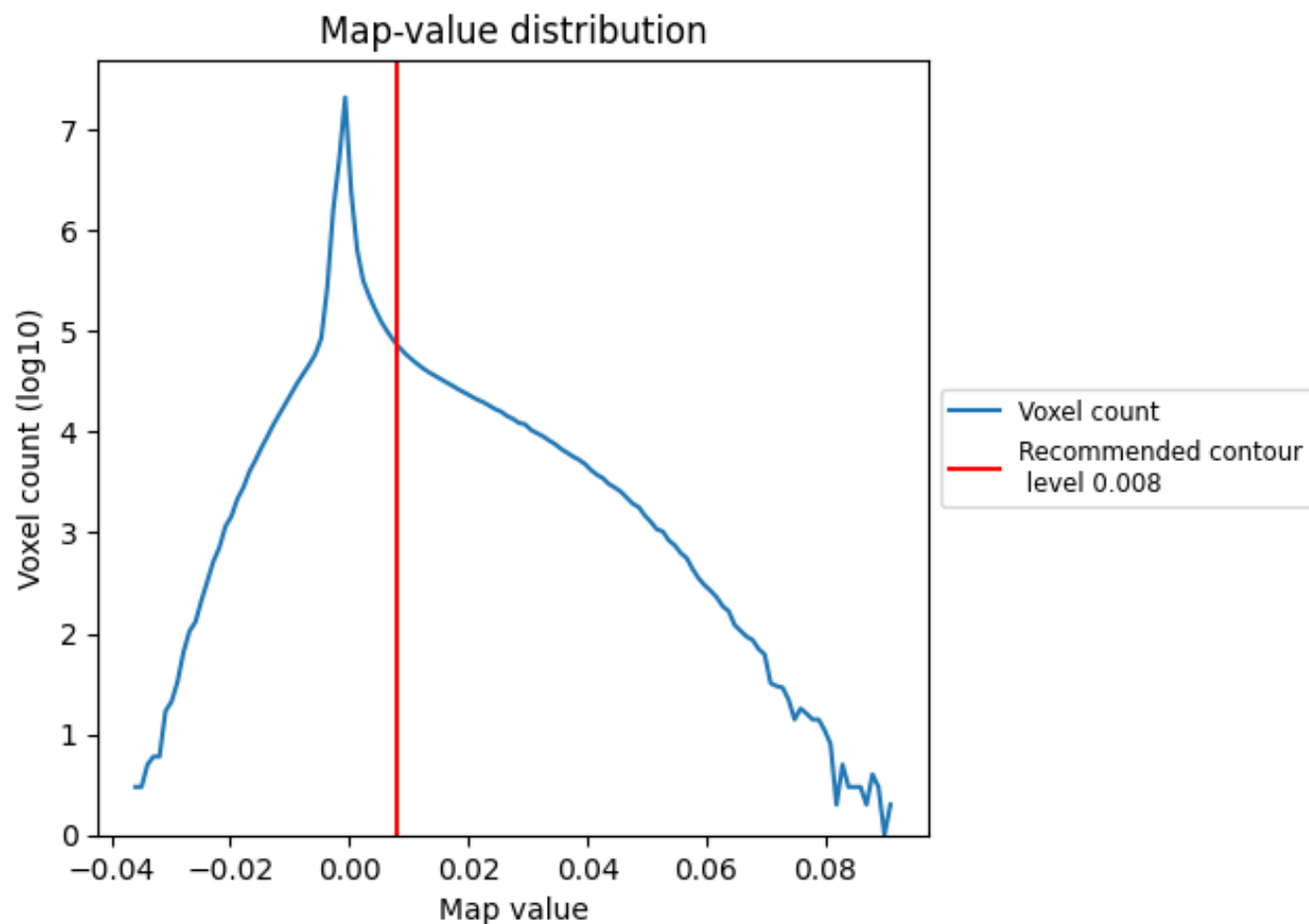


Z

7 Map analysis [i](#)

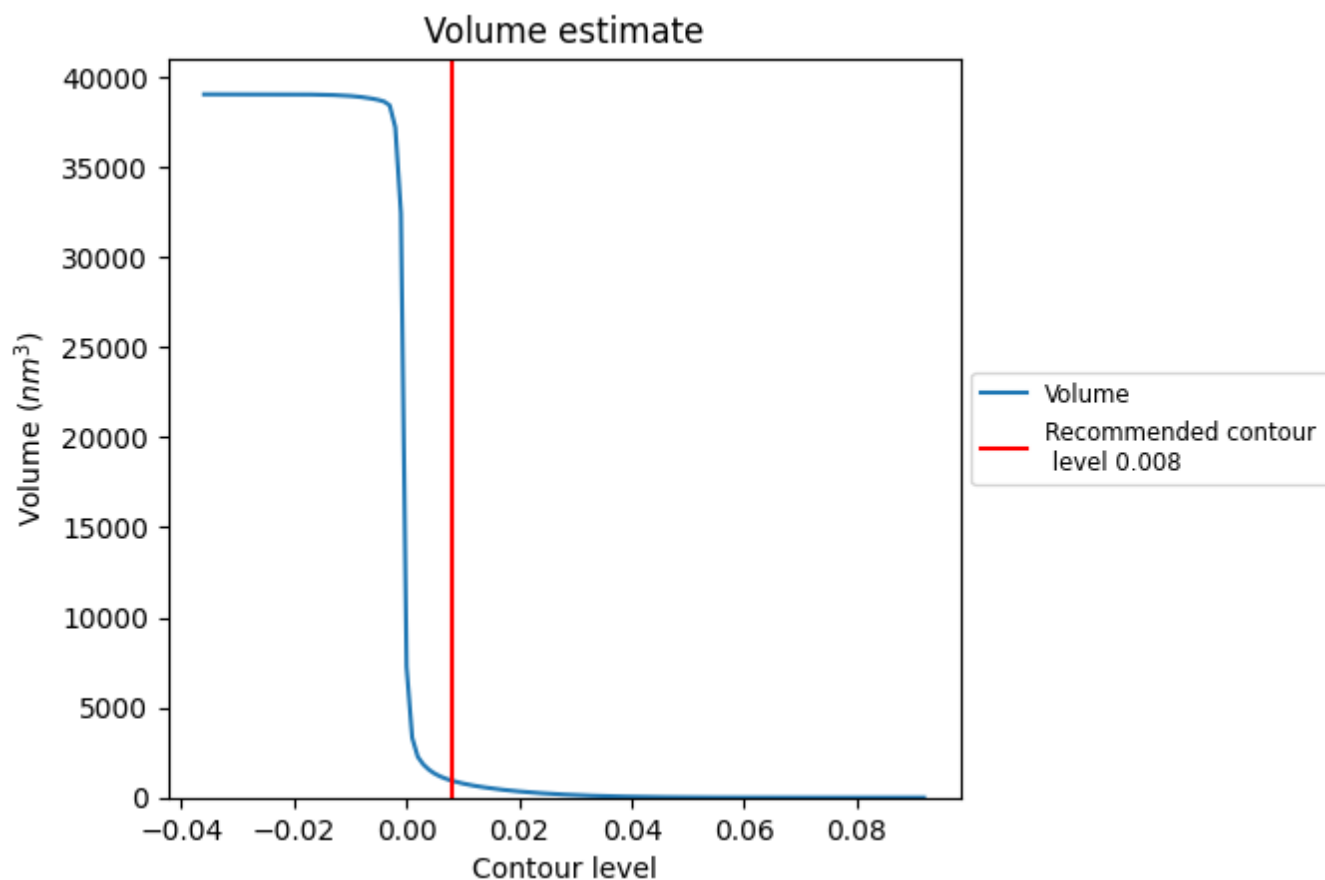
This section contains the results of statistical analysis of the map.

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.

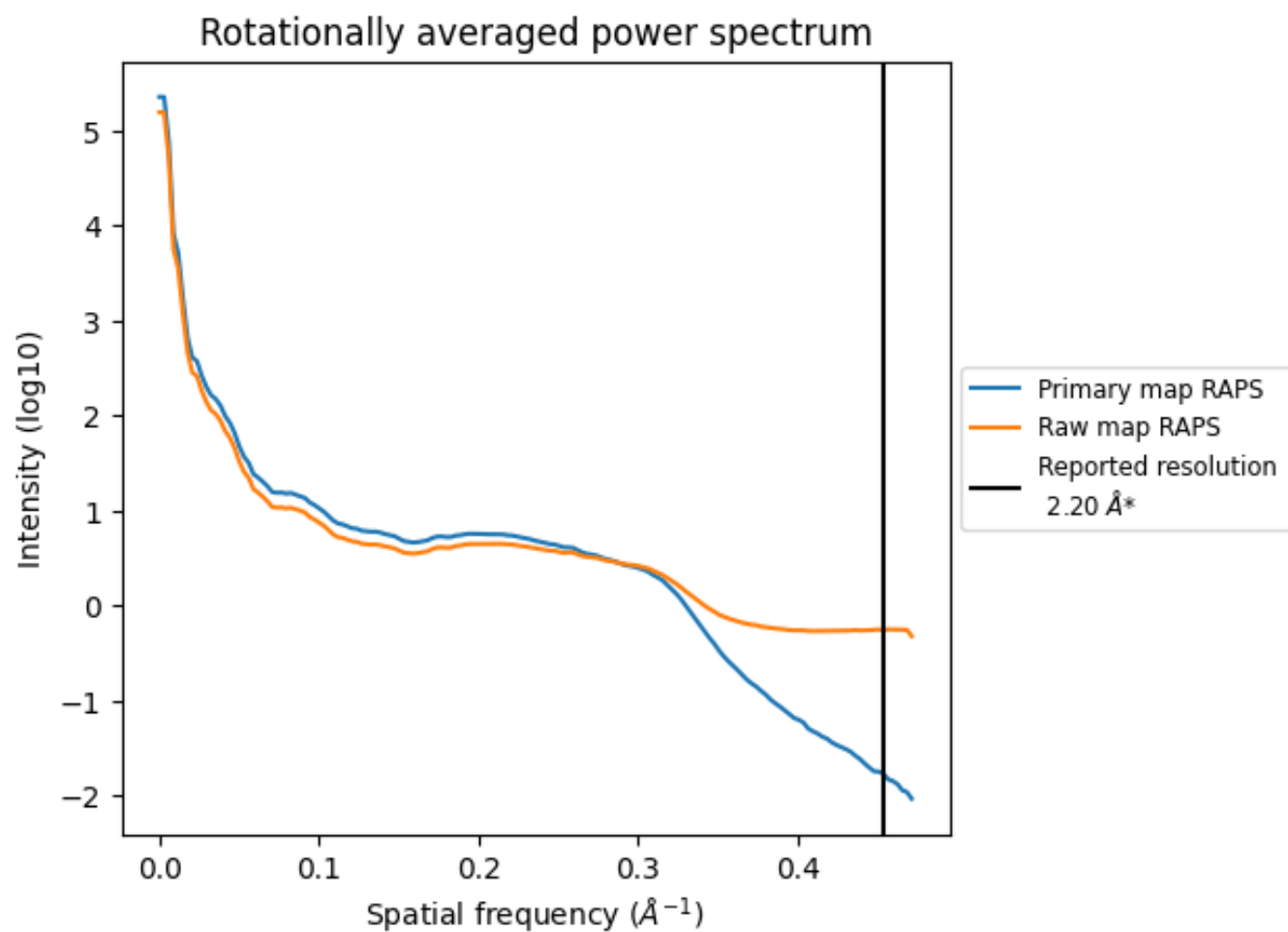
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 945 nm^3 ; this corresponds to an approximate mass of 854 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 ⓘ

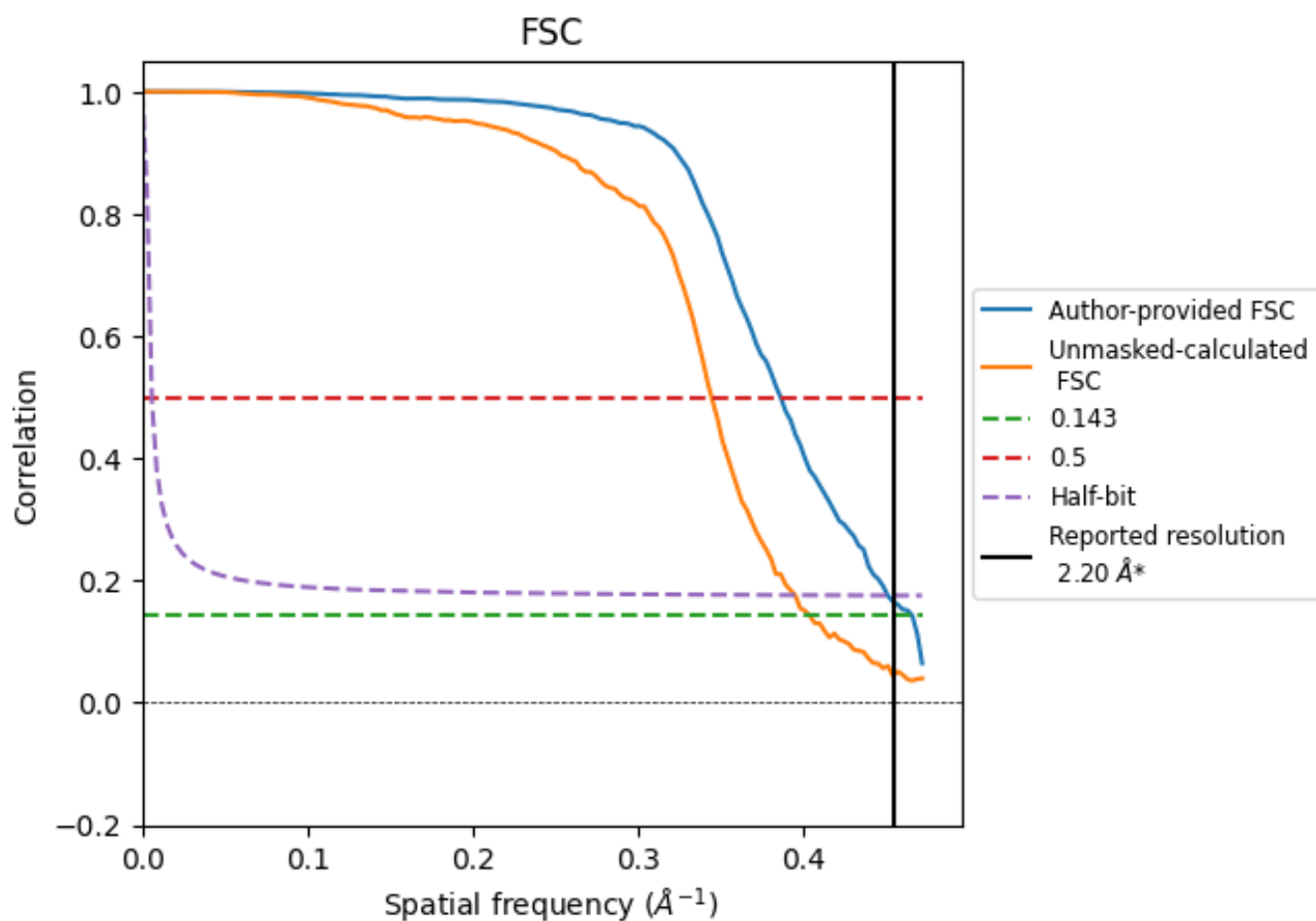


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 \AA^{-1}

8.2 Resolution estimates [i](#)

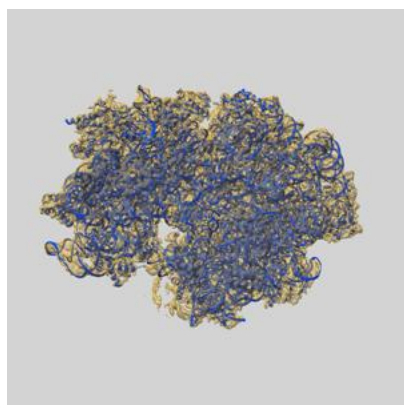
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.15	2.59	2.22
Unmasked-calculated*	2.48	2.90	2.53

*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 2.48 differs from the reported value 2.2 by more than 10 %

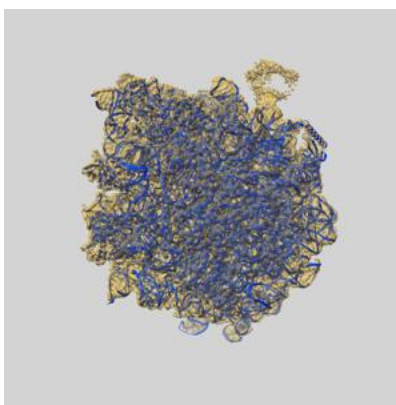
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48830 and PDB model 9N2B. Per-residue inclusion information can be found in section [3](#) on page [17](#).

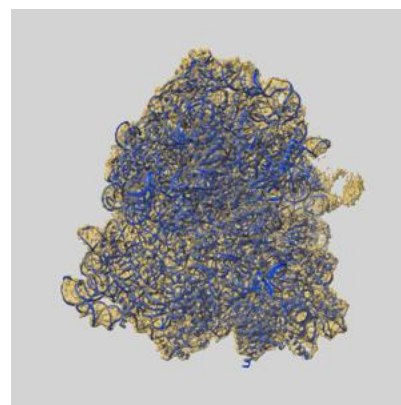
9.1 Map-model overlay [i](#)



X



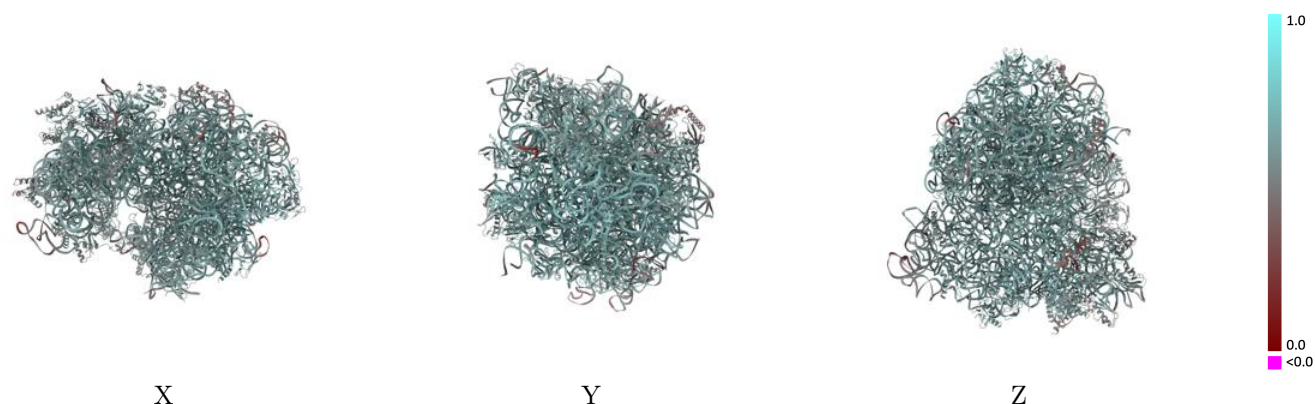
Y



Z

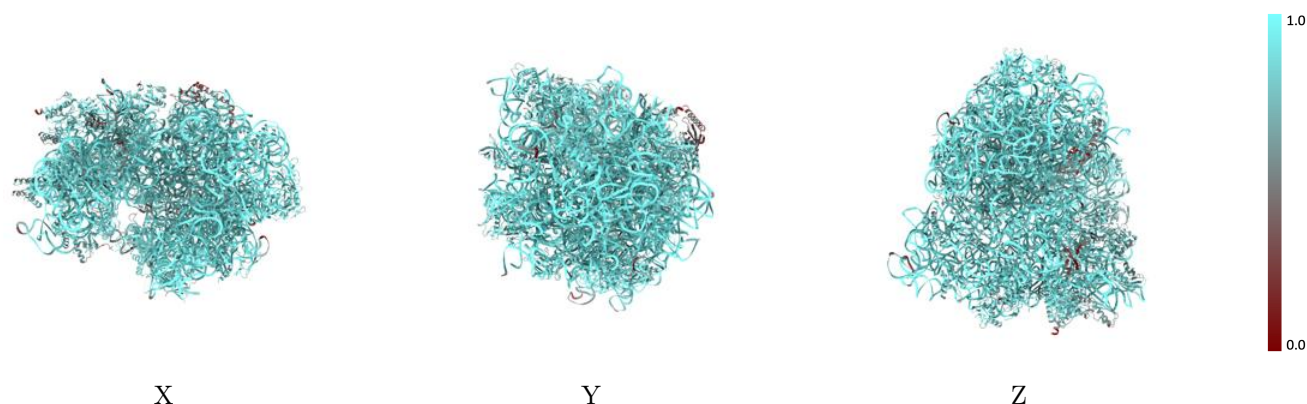
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



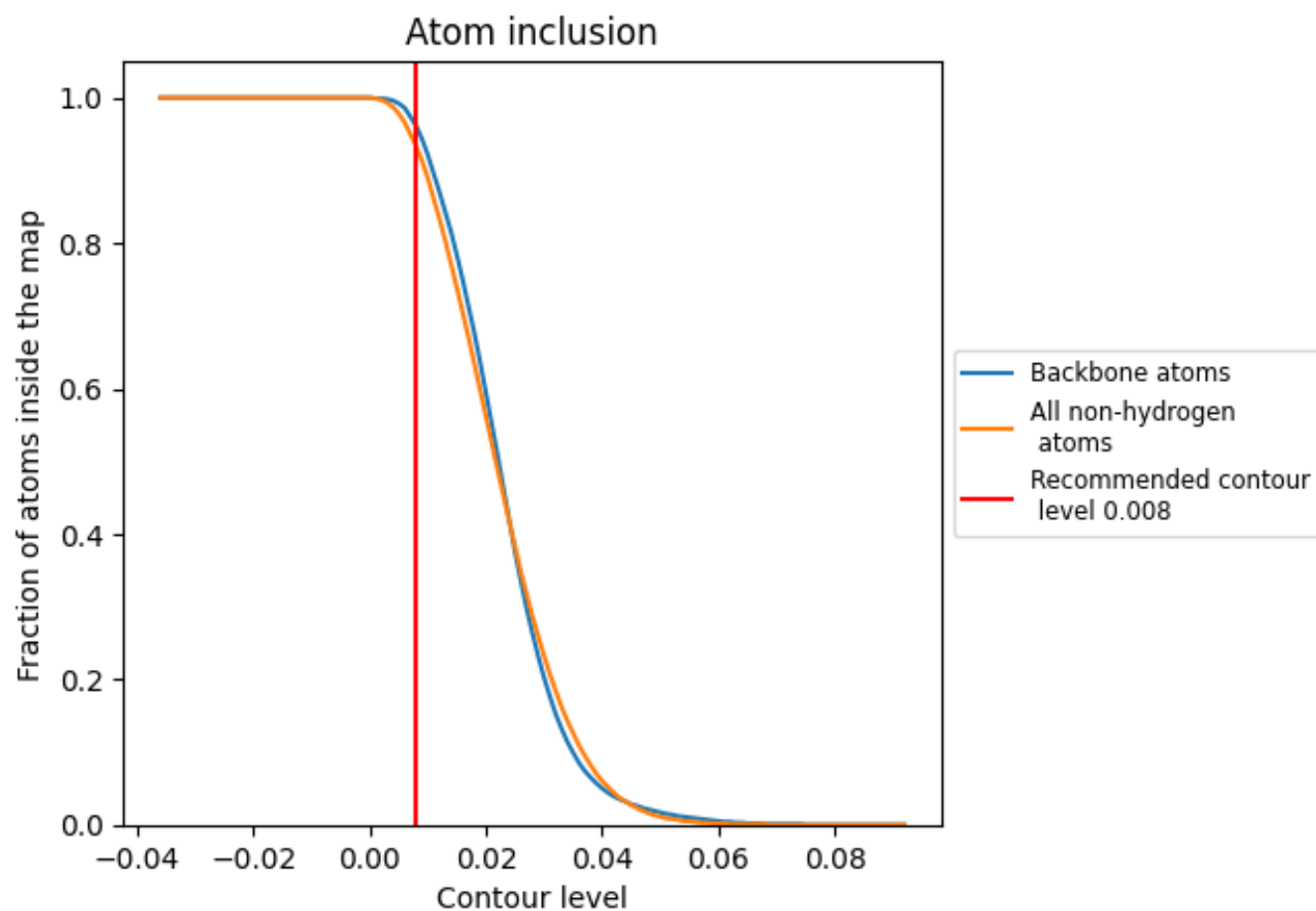
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.6070
16	 0.9630	 0.5960
23	 0.9770	 0.6260
5	 0.9650	 0.5850
LB	 0.9530	 0.6530
LC	 0.9210	 0.6250
LD	 0.8940	 0.6120
LE	 0.7840	 0.5360
LF	 0.8020	 0.5540
LI	 0.4980	 0.4780
LM	 0.9320	 0.6330
LN	 0.9170	 0.6300
LO	 0.9140	 0.6190
LP	 0.9230	 0.6350
LQ	 0.9390	 0.6240
LR	 0.8710	 0.5640
LS	 0.8890	 0.6140
LT	 0.9620	 0.6540
LU	 0.9070	 0.6250
LV	 0.9100	 0.6240
LW	 0.8680	 0.6150
LX	 0.8850	 0.6130
LY	 0.8600	 0.5930
La	 0.8460	 0.6120
Lb	 0.9320	 0.6280
Lc	 0.8590	 0.5920
Ld	 0.8860	 0.6110
Le	 0.6830	 0.5140
Lf	 0.9070	 0.6320
Lg	 0.8590	 0.5930
Lh	 0.9410	 0.6660
Li	 0.9290	 0.6400
Lj	 0.9520	 0.6280
Pt	 0.8910	 0.5800
SB	 0.7910	 0.5600



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Chain	Atom inclusion	Q-score
SC	 0.8480	 0.5890
SD	 0.8610	 0.5940
SE	 0.9060	 0.6200
SF	 0.8230	 0.5690
SG	 0.7270	 0.5300
SH	 0.8970	 0.6170
SI	 0.8350	 0.5620
SJ	 0.7570	 0.5320
SK	 0.8550	 0.5810
SL	 0.9090	 0.6270
SM	 0.8300	 0.5670
SN	 0.8610	 0.5870
SO	 0.8900	 0.6070
SP	 0.8660	 0.5830
SQ	 0.8340	 0.5920
SR	 0.8550	 0.5990
SS	 0.8250	 0.5680
ST	 0.8500	 0.5670
SU	 0.7320	 0.5430
mR	 0.5680	 0.4780