



Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 05:34 AM EDT

PDB ID : 8G7R
EMDB ID : EMD-29821
Title : Structure of the Escherichia coli 70S ribosome in complex with A-site tRNA^{Ala}(LAU) bound to the cognate AUA codon (Structure III)
Authors : Rybak, M.Y.; Gagnon, M.G.
Deposited on : 2023-02-16
Resolution : 2.80 Å(reported)
Based on initial model : 7K00

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:

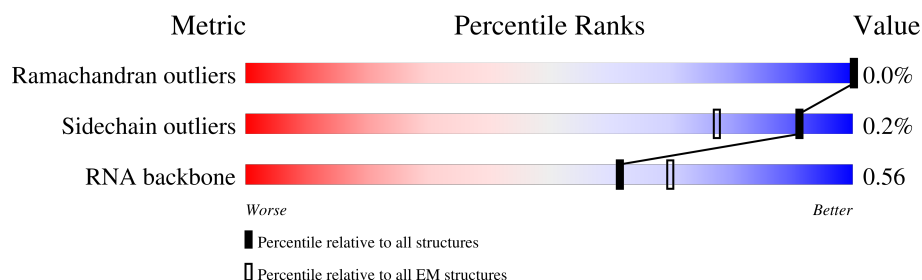
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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.



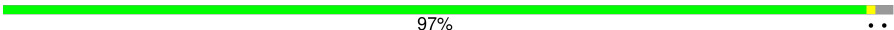


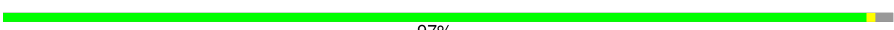






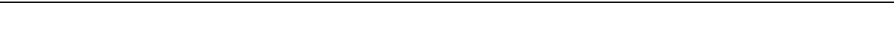

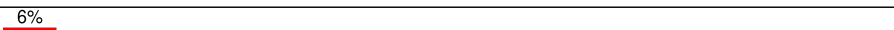
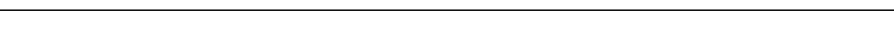






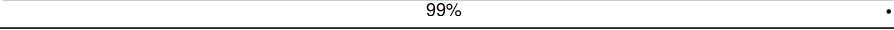
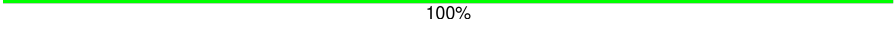
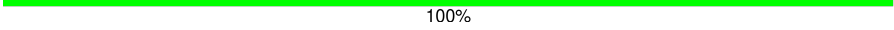
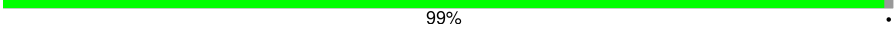
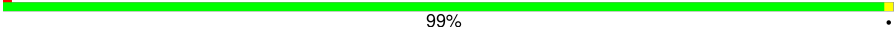
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	a	1542	
2	b	241	
3	c	233	
4	d	206	
5	e	167	
6	f	131	
7	g	156	
8	h	130	

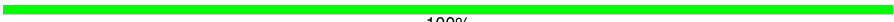










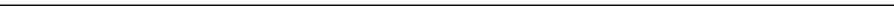



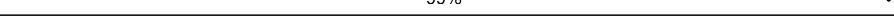
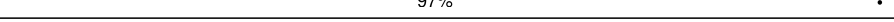
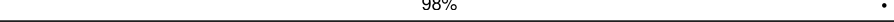

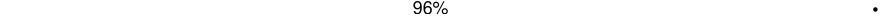

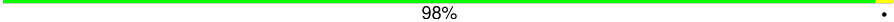
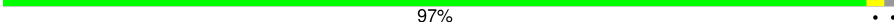
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Mol	Chain	Length	Quality of chain
9	i	130	 97% ..
10	j	103	 93% • 5%
11	k	129	 90% • 9%
12	l	124	 97% ..
13	m	118	 97% •
14	n	101	 99% •
15	o	89	 99% •
16	p	82	 99% •
17	q	84	 94% 6%
18	r	75	 72% 28%
19	s	92	 90% 10%
20	t	87	 99% •
21	u	71	 6% 77% 23%
22	w	76	 68% 24% 8%
22	y	76	 67% 22% 11%
23	x	77	 82% 17% •
24	v	27	 37% • 59%
25	A	2904	 86% 13%
26	B	120	 85% 14% •
27	C	273	 99% •
28	D	209	 100%
29	E	201	 100%
30	F	179	 99% •
31	G	177	 99% ..
32	H	149	 15% 28% 72%

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Mol	Chain	Length	Quality of chain
33	L	142	 100%
34	M	123	 100%
35	N	144	 100%
36	O	136	 99%
37	P	127	 93% 7%
38	Q	117	 99%
39	R	115	 99%
40	S	118	 99%
41	T	103	 100%
42	U	110	 100%
43	V	100	 93% 7%
44	W	104	 97% ..
45	X	94	 100%
46	Y	85	 87% • 11%
47	Z	78	 99% •
48	1	63	 97% •
49	2	59	 98% •
50	3	70	 84% • 14%
51	4	57	 96% •
52	5	55	 91% • 7%
53	6	46	 98% •
54	7	65	 97% • •
55	8	38	 100%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 147376 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1528	Total	C	N	O	P	0	0
			32803	14637	6019	10619	1528		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1754	1110	315	321	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	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	e	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

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

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

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

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	modified residue	UNP A0A0H3PWX2

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	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	n	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	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			446	283	85	78		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	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	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 22 is a RNA chain called Isoleucine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	w	76	Total	C	N	O	P	S	0	0
			1645	740	292	537	75	1		
22	y	76	Total	C	N	O	P	S	0	0
			1644	740	292	536	75	1		

- Molecule 23 is a RNA chain called P-site initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 24 is a RNA chain called M-I mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	11	Total	C	N	O	P	0	0
			239	108	49	71	11		

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	O	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	82	MS6	MET	modified residue	UNP E6BI61

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called Ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	60	Total	C	N	O	S	0	0
			468	290	87	85	6		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	5	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

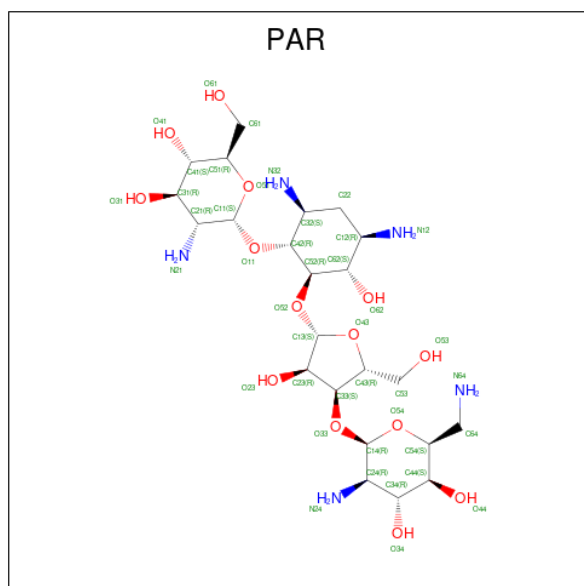
- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
56	a	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	a	91	Total	Mg	0
			91	91	
57	e	2	Total	Mg	0
			2	2	
57	l	1	Total	Mg	0
			1	1	
57	x	2	Total	Mg	0
			2	2	

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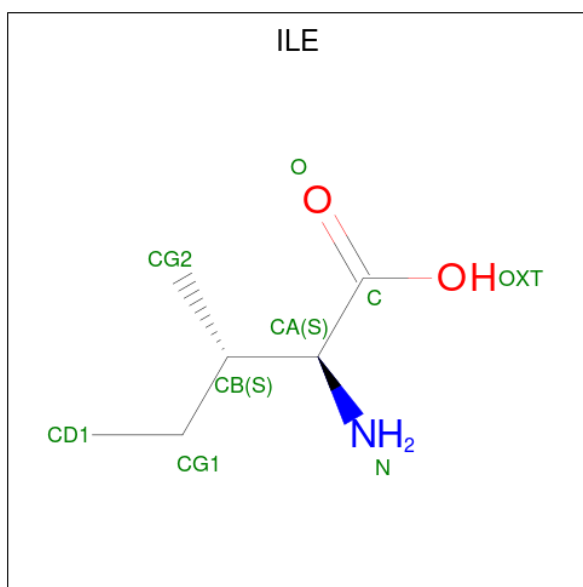
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Mol	Chain	Residues	Atoms		AltConf
57	v	2	Total 2	Mg 2	0
57	A	603	Total 603	Mg 603	0
57	B	6	Total 6	Mg 6	0
57	D	1	Total 1	Mg 1	0
57	E	2	Total 2	Mg 2	0
57	L	4	Total 4	Mg 4	0
57	N	2	Total 2	Mg 2	0
57	P	1	Total 1	Mg 1	0
57	R	1	Total 1	Mg 1	0
57	S	2	Total 2	Mg 2	0
57	U	1	Total 1	Mg 1	0
57	V	2	Total 2	Mg 2	0
57	Y	1	Total 1	Mg 1	0
57	4	7	Total 7	Mg 7	0
57	8	3	Total 3	Mg 3	0

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	a	1	Total 1	K 1	0
58	l	1	Total 1	K 1	0

- Molecule 59 is ISOLEUCINE (three-letter code: ILE) (formula: C₆H₁₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
59	y	1	Total	C	N	O	0
			8	6	1	1	

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	3	1	Total	Zn	0
			1	1	
60	8	1	Total	Zn	0
			1	1	

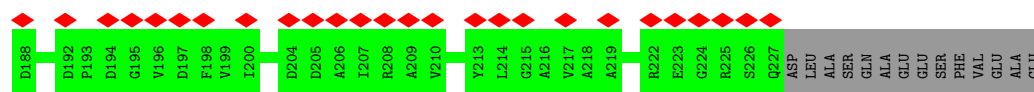
- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	a	31	Total	O	0
			31	31	
61	k	1	Total	O	0
			1	1	
61	l	2	Total	O	0
			2	2	
61	w	1	Total	O	0
			1	1	
61	A	278	Total	O	0
			278	278	
61	B	3	Total	O	0
			3	3	

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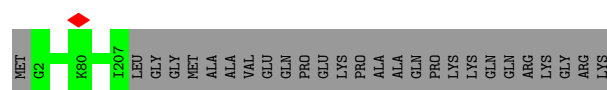
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
61	D	2	Total 2	O 2	0
61	L	2	Total 2	O 2	0
61	T	1	Total 1	O 1	0
61	U	2	Total 2	O 2	0
61	V	2	Total 2	O 2	0
61	Y	1	Total 1	O 1	0
61	Z	2	Total 2	O 2	0
61	4	3	Total 3	O 3	0



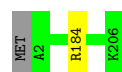
- Molecule 3: 30S ribosomal protein S3

Chain c: 88% 12%



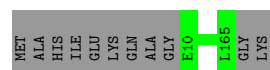
- Molecule 4: 30S ribosomal protein S4

Chain d: 99%



- Molecule 5: 30S ribosomal protein S5

Chain e: 93% 7%



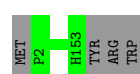
- Molecule 6: 30S ribosomal protein S6

Chain f: 79% 21%



- Molecule 7: 30S ribosomal protein S7

Chain g: 97%



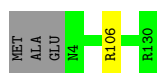
- Molecule 8: 30S ribosomal protein S8

Chain h: 99%

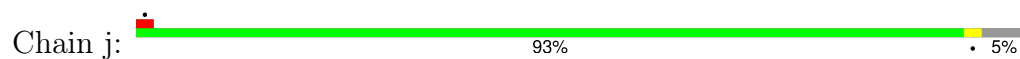


- Molecule 9: 30S ribosomal protein S9

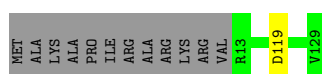
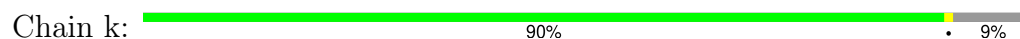
Chain i: 97%



- Molecule 10: 30S ribosomal protein S10



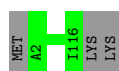
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



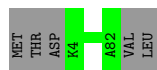
- Molecule 16: 30S ribosomal protein S16





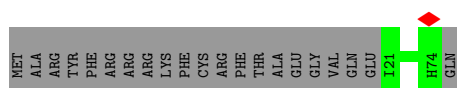
- Molecule 17: 30S ribosomal protein S17

Chain q: 94% 6%



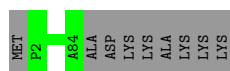
- Molecule 18: 30S ribosomal protein S18

Chain r: 72% 28%



- Molecule 19: 30S ribosomal protein S19

Chain s: 90% 10%



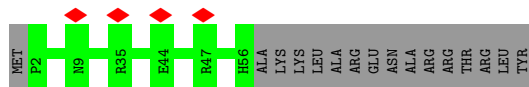
- Molecule 20: 30S ribosomal protein S20

Chain t: 99% .



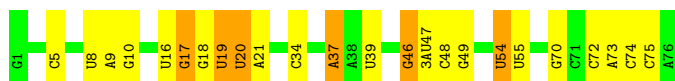
- Molecule 21: 30S ribosomal protein S21

Chain u: 6% 77% 23%



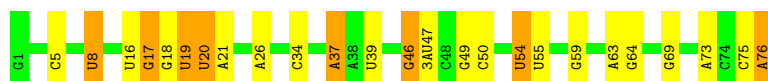
- Molecule 22: Isoleucine tRNA

Chain w: 68% 24% 8%



- Molecule 22: Isoleucine tRNA

Chain y: 67% 22% 11%



• Molecule 23: P-site initiator tRNA

Chain x: 82% 17%



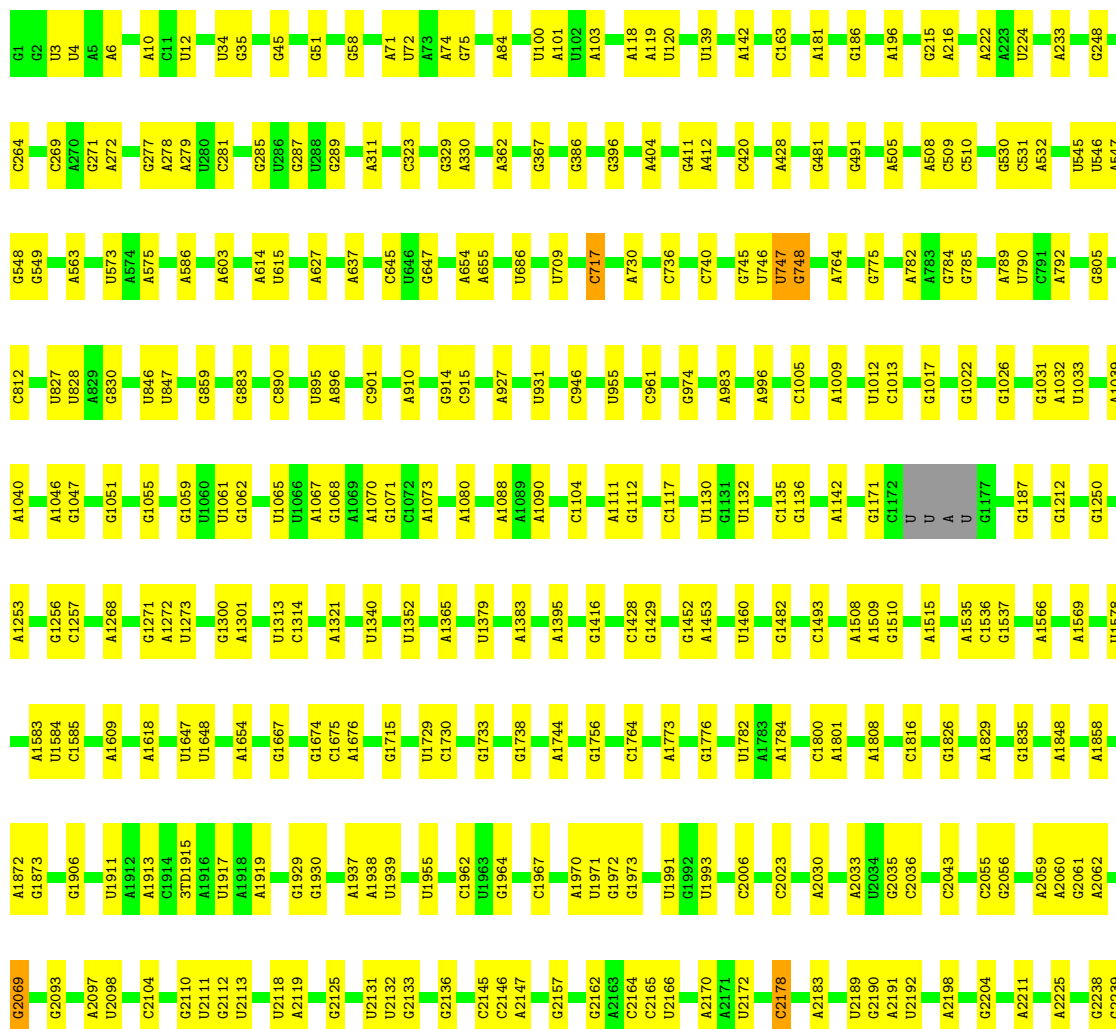
• Molecule 24: M-I mRNA

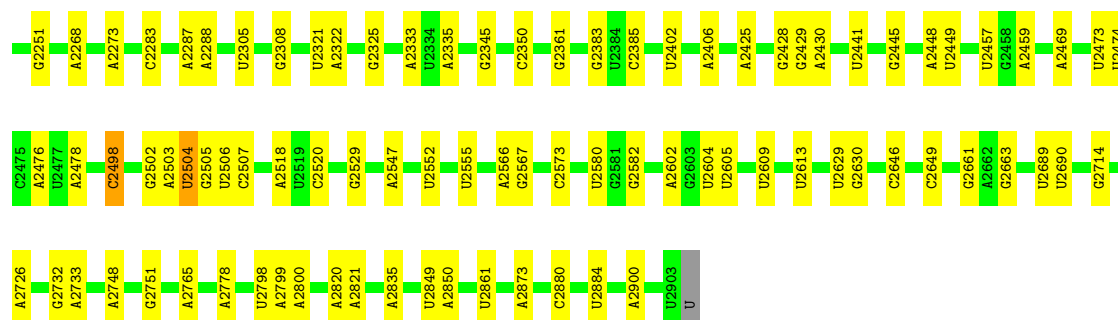
Chain v: 37% 59%



• Molecule 25: 23S Ribosomal RNA

Chain A: 86% 13%





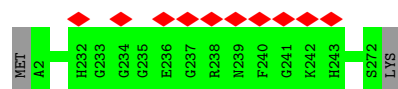
- Molecule 26: 5S Ribosomal RNA

Chain B: 85% 14%



- Molecule 27: 50S ribosomal protein L2

Chain C: 99%



- Molecule 28: 50S ribosomal protein L3

Chain D: 100%

There are no outlier residues recorded for this chain.

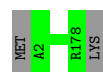
- Molecule 29: 50S ribosomal protein L4

Chain E: 100%

There are no outlier residues recorded for this chain.

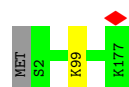
- Molecule 30: 50S ribosomal protein L5

Chain F: 99%

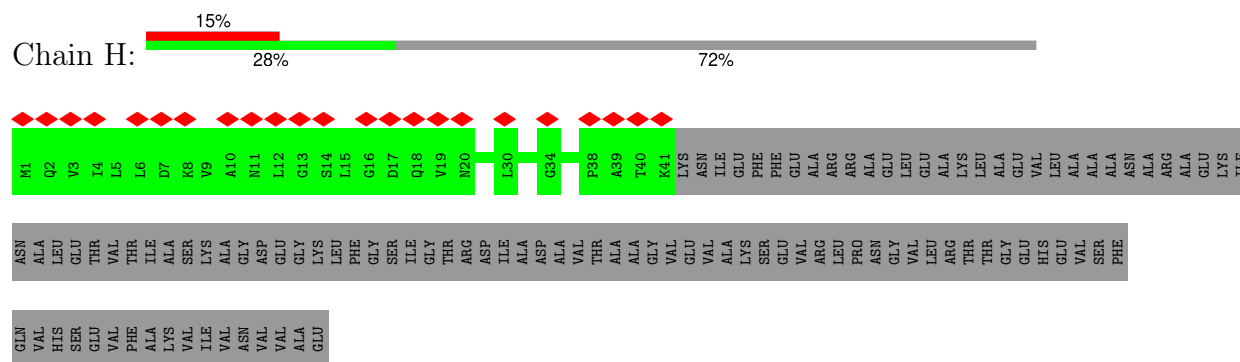


- Molecule 31: 50S ribosomal protein L6

Chain G: 99%



- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13



There are no outlier residues recorded for this chain.

- Molecule 34: 50S ribosomal protein L14



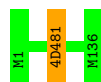
There are no outlier residues recorded for this chain.

- Molecule 35: 50S ribosomal protein L15

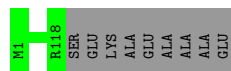


There are no outlier residues recorded for this chain.

- Molecule 36: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19

Chain R:  99% .



- Molecule 40: 50S ribosomal protein L20

Chain S:  99% .



- Molecule 41: Ribosomal protein L21

Chain T:  100%

There are no outlier residues recorded for this chain.

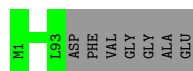
- Molecule 42: 50S ribosomal protein L22

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 50S ribosomal protein L23

Chain V:  93% 7%



- Molecule 44: 50S ribosomal protein L24

Chain W:  97% ..




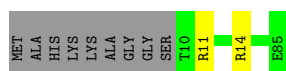
- Molecule 45: 50S ribosomal protein L25

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 50S ribosomal protein L27

Chain Y:  87% . 11%



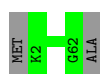
- Molecule 47: 50S ribosomal protein L28

Chain Z: 99%



- Molecule 48: 50S ribosomal protein L29

Chain 1: 97%



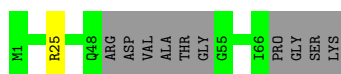
- Molecule 49: 50S ribosomal protein L30

Chain 2: 98%



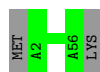
- Molecule 50: 50S ribosomal protein L31

Chain 3: 84% 14%



- Molecule 51: 50S ribosomal protein L32

Chain 4: 96%



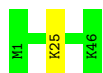
- Molecule 52: 50S ribosomal protein L33

Chain 5: 91% 7%



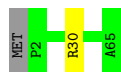
- Molecule 53: 50S ribosomal protein L34

Chain 6: 98%



- Molecule 54: 50S ribosomal protein L35

Chain 7:  97%



- Molecule 55: 50S ribosomal protein L36

Chain 8:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	466262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.865	Depositor
Minimum map value	-0.587	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 3TD, 2MA, OMC, 4OC, MS6, T6A, PAR, IAS, MA6, MG, K, UR3, PSU, 5MC, 6MZ, 1MG, 4D4, MEQ, 3AU, OMG, G7M, ZN, 4SU, OMU, H2U, 5MU, M3X, D2T

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	a	0.34	0/36450	0.79	4/56856 (0.0%)
2	b	0.25	0/1785	0.55	0/2404
3	c	0.25	0/1651	0.53	0/2225
4	d	0.25	0/1665	0.54	0/2227
5	e	0.26	0/1165	0.53	0/1568
6	f	0.25	0/858	0.54	0/1160
7	g	0.25	0/1206	0.57	0/1617
8	h	0.26	0/989	0.51	0/1326
9	i	0.26	0/1034	0.57	0/1375
10	j	0.23	0/796	0.58	0/1077
11	k	0.26	0/884	0.55	0/1191
12	l	0.28	0/945	0.60	0/1268
13	m	0.25	0/900	0.59	0/1204
14	n	0.24	0/817	0.54	0/1088
15	o	0.26	0/722	0.54	0/964
16	p	0.26	0/653	0.59	0/877
17	q	0.27	0/650	0.55	0/871
18	r	0.25	0/453	0.52	0/609
19	s	0.25	0/680	0.52	0/915
20	t	0.26	0/676	0.52	0/895
21	u	0.25	0/467	0.54	0/620
22	w	0.27	0/1550	0.83	0/2411
22	y	0.61	4/1549 (0.3%)	1.10	8/2408 (0.3%)
23	x	0.29	0/1725	0.80	0/2689
24	v	0.32	0/269	0.76	0/417
25	A	0.48	0/69147	0.85	15/107869 (0.0%)
26	B	0.42	1/2876 (0.0%)	0.87	3/4483 (0.1%)
27	C	0.29	0/2121	0.58	0/2852
28	D	0.30	0/1576	0.56	0/2119
29	E	0.27	0/1571	0.51	0/2113
30	F	0.25	0/1434	0.52	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	G	0.26	0/1343	0.53	0/1816
32	H	0.24	0/306	0.53	0/413
33	L	0.29	0/1152	0.53	0/1551
34	M	0.28	0/955	0.61	0/1279
35	N	0.27	0/1061	0.57	0/1412
36	O	0.29	0/1073	0.56	0/1433
37	P	0.29	0/958	0.59	0/1281
38	Q	0.26	0/902	0.55	0/1209
39	R	0.29	0/929	0.54	0/1242
40	S	0.32	0/960	0.53	0/1278
41	T	0.29	0/829	0.57	0/1107
42	U	0.27	0/864	0.54	0/1156
43	V	0.26	0/744	0.54	0/994
44	W	0.29	0/787	0.58	0/1051
45	X	0.28	0/766	0.51	0/1025
46	Y	0.28	0/589	0.60	0/779
47	Z	0.27	0/635	0.58	0/848
48	1	0.23	0/496	0.50	0/660
49	2	0.27	0/453	0.60	0/605
50	3	0.25	0/475	0.53	0/633
51	4	0.29	0/440	0.59	0/588
52	5	0.27	0/424	0.53	0/565
53	6	0.27	0/380	0.65	0/498
54	7	0.28	0/513	0.55	0/676
55	8	0.30	0/303	0.65	0/397
All	All	0.39	5/157601 (0.0%)	0.78	30/236120 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
36	O	0	1
54	7	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	76	A	C6-N6	17.53	1.48	1.33
26	B	1	U	OP3-P	-10.63	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	76	A	N7-C5	-7.78	1.34	1.39
22	y	76	A	N9-C8	-7.12	1.32	1.37
22	y	76	A	C6-N1	-5.04	1.32	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	76	A	C2-N3-C4	20.70	120.95	110.60
22	y	76	A	N1-C2-N3	-16.28	121.16	129.30
22	y	76	A	N3-C4-C5	-10.93	119.15	126.80
22	y	76	A	N3-C4-N9	7.98	133.79	127.40
22	y	76	A	C5-N7-C8	7.90	107.85	103.90
25	A	1313	U	C2-N1-C1'	7.82	127.08	117.70
22	y	76	A	N7-C8-N9	-7.71	109.94	113.80
25	A	2178	C	N3-C2-O2	-7.34	116.76	121.90
22	y	76	A	C4-C5-N7	-6.98	107.21	110.70
26	B	89	U	C2-N1-C1'	6.76	125.81	117.70
26	B	89	U	N1-C2-O2	6.61	127.43	122.80
1	a	754	C	C2-N1-C1'	6.60	126.06	118.80
25	A	790	U	C2-N1-C1'	6.60	125.62	117.70
26	B	89	U	N3-C2-O2	-6.12	117.92	122.20
25	A	748	G	O4'-C1'-N9	6.03	113.02	108.20
25	A	2321	U	C2-N1-C1'	6.02	124.92	117.70
25	A	1314	C	C2-N1-C1'	5.94	125.34	118.80
1	a	330	C	N1-C2-O2	5.88	122.43	118.90
25	A	2178	C	N1-C2-O2	5.52	122.21	118.90
1	a	330	C	C2-N1-C1'	5.45	124.79	118.80
25	A	1395	A	O4'-C1'-N9	5.41	112.53	108.20
25	A	717	C	N1-C2-O2	5.33	122.10	118.90
22	y	76	A	C8-N9-C4	5.33	107.93	105.80
25	A	1313	U	C6-N1-C1'	-5.26	113.84	121.20
25	A	323	C	C2-N1-C1'	5.22	124.55	118.80
25	A	1117	C	C2-N1-C1'	5.21	124.53	118.80
25	A	2321	U	N3-C2-O2	-5.18	118.57	122.20
25	A	717	C	C2-N1-C1'	5.13	124.44	118.80
1	a	993	G	C4-N9-C1'	5.07	133.09	126.50
25	A	790	U	N1-C2-O2	5.02	126.31	122.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	7	30	ARG	Peptide
36	O	81	4D4	Mainchain

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	b	222/241 (92%)	203 (91%)	19 (9%)	0	100	100
3	c	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
4	d	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	e	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	f	101/131 (77%)	95 (94%)	6 (6%)	0	100	100
7	g	150/156 (96%)	142 (95%)	8 (5%)	0	100	100
8	h	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	i	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
10	j	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	13	39
11	k	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
12	l	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
13	m	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	n	98/101 (97%)	98 (100%)	0	0	100	100
15	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	p	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
17	q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
18	r	52/75 (69%)	48 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	s	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
20	t	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	u	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
27	C	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
28	D	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
29	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
30	F	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
31	G	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
32	H	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
33	L	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	M	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
35	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
36	O	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
37	P	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
38	Q	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
39	R	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
40	S	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
41	T	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
42	U	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
43	V	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
44	W	100/104 (96%)	94 (94%)	5 (5%)	1 (1%)	13	39
45	X	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	Y	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
47	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
48	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
49	2	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	3	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
51	4	53/57 (93%)	53 (100%)	0	0	100	100
52	5	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
53	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	7	62/65 (95%)	57 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5446/5886 (92%)	5223 (96%)	221 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	j	57	VAL
44	W	99	ASN

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	b	186/199 (94%)	186 (100%)	0	100	100
3	c	170/190 (90%)	170 (100%)	0	100	100
4	d	172/173 (99%)	171 (99%)	1 (1%)	84	95
5	e	119/126 (94%)	119 (100%)	0	100	100
6	f	90/112 (80%)	90 (100%)	0	100	100
7	g	125/129 (97%)	125 (100%)	0	100	100
8	h	104/105 (99%)	104 (100%)	0	100	100
9	i	105/107 (98%)	104 (99%)	1 (1%)	73	91
10	j	86/90 (96%)	85 (99%)	1 (1%)	67	89
11	k	89/98 (91%)	89 (100%)	0	100	100
12	l	101/103 (98%)	101 (100%)	0	100	100
13	m	93/96 (97%)	93 (100%)	0	100	100
14	n	83/84 (99%)	83 (100%)	0	100	100
15	o	76/77 (99%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	73/78 (94%)	73 (100%)	0	100	100
18	r	47/65 (72%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	s	72/79 (91%)	72 (100%)	0	100	100
20	t	65/66 (98%)	65 (100%)	0	100	100
21	u	48/61 (79%)	48 (100%)	0	100	100
27	C	216/218 (99%)	216 (100%)	0	100	100
28	D	163/163 (100%)	163 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/150 (99%)	148 (100%)	0	100	100
31	G	137/138 (99%)	136 (99%)	1 (1%)	81	94
32	H	32/114 (28%)	32 (100%)	0	100	100
33	L	116/116 (100%)	116 (100%)	0	100	100
34	M	104/104 (100%)	104 (100%)	0	100	100
35	N	103/103 (100%)	103 (100%)	0	100	100
36	O	107/107 (100%)	107 (100%)	0	100	100
37	P	98/103 (95%)	98 (100%)	0	100	100
38	Q	86/87 (99%)	86 (100%)	0	100	100
39	R	99/100 (99%)	99 (100%)	0	100	100
40	S	89/90 (99%)	89 (100%)	0	100	100
41	T	84/84 (100%)	84 (100%)	0	100	100
42	U	93/93 (100%)	93 (100%)	0	100	100
43	V	80/84 (95%)	80 (100%)	0	100	100
44	W	83/85 (98%)	83 (100%)	0	100	100
45	X	78/78 (100%)	78 (100%)	0	100	100
46	Y	58/63 (92%)	56 (97%)	2 (3%)	32	66
47	Z	67/68 (98%)	67 (100%)	0	100	100
48	1	54/55 (98%)	54 (100%)	0	100	100
49	2	48/49 (98%)	48 (100%)	0	100	100
50	3	53/62 (86%)	52 (98%)	1 (2%)	52	82
51	4	46/48 (96%)	46 (100%)	0	100	100
52	5	46/49 (94%)	45 (98%)	1 (2%)	47	79
53	6	38/38 (100%)	37 (97%)	1 (3%)	41	75
54	7	51/52 (98%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	8	34/34 (100%)	34 (100%)	0	100	100
All	All	4545/4803 (95%)	4536 (100%)	9 (0%)	91	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	184	ARG
9	i	106	ARG
10	j	7	ARG
31	G	99	LYS
46	Y	11	ARG
46	Y	14	ARG
50	3	25	ARG
52	5	28	ARG
53	6	25	LYS

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

Mol	Chain	Res	Type
3	c	3	GLN
3	c	100	GLN
4	d	36	GLN
4	d	85	ASN
4	d	116	GLN
4	d	164	GLN
5	e	12	GLN
6	f	17	GLN
9	i	31	ASN
11	k	109	ASN
13	m	8	ASN
13	m	52	GLN
14	n	35	ASN
16	p	18	GLN
20	t	13	GLN
20	t	21	ASN
20	t	52	ASN
20	t	55	GLN
27	C	117	GLN
28	D	32	ASN
29	E	165	HIS
29	E	195	GLN

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Mol	Chain	Res	Type
33	L	128	ASN
36	O	22	GLN
36	O	60	GLN
39	R	7	GLN
39	R	41	GLN
39	R	75	GLN
40	S	44	GLN
43	V	70	HIS
44	W	45	HIS
44	W	53	ASN
50	3	41	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1523/1542 (98%)	193 (12%)	0
22	w	73/76 (96%)	19 (26%)	0
22	y	73/76 (96%)	21 (28%)	0
23	x	75/77 (97%)	9 (12%)	0
24	v	10/27 (37%)	1 (10%)	0
25	A	2893/2904 (99%)	364 (12%)	13 (0%)
26	B	119/120 (99%)	15 (12%)	2 (1%)
All	All	4766/4822 (98%)	622 (13%)	15 (0%)

All (622) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	7	A
1	a	8	A
1	a	22	G
1	a	27	G
1	a	39	G
1	a	44	A
1	a	47	C
1	a	48	C
1	a	50	A
1	a	51	A
1	a	71	A

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Mol	Chain	Res	Type
1	a	76	G
1	a	77	A
1	a	79	G
1	a	80	A
1	a	82	G
1	a	84	U
1	a	85	U
1	a	86	G
1	a	88	U
1	a	90	C
1	a	92	U
1	a	95	C
1	a	110	C
1	a	121	U
1	a	130	A
1	a	131	A
1	a	163	C
1	a	164	G
1	a	174	A
1	a	183	C
1	a	184	G
1	a	197	A
1	a	207	C
1	a	208	U
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	289	G
1	a	321	A
1	a	324	G
1	a	328	C
1	a	344	A
1	a	345	C
1	a	351	G

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Mol	Chain	Res	Type
1	a	352	C
1	a	354	G
1	a	367	U
1	a	372	C
1	a	373	A
1	a	397	A
1	a	406	G
1	a	412	A
1	a	413	G
1	a	415	A
1	a	421	U
1	a	422	C
1	a	424	G
1	a	429	U
1	a	465	A
1	a	467	U
1	a	468	A
1	a	478	A
1	a	479	U
1	a	484	G
1	a	486	U
1	a	495	A
1	a	496	A
1	a	509	A
1	a	511	C
1	a	518	C
1	a	520	A
1	a	521	G
1	a	524	G
1	a	527	G7M
1	a	531	U
1	a	532	A
1	a	547	A
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	579	A
1	a	653	U
1	a	665	A
1	a	687	A

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Mol	Chain	Res	Type
1	a	702	A
1	a	721	G
1	a	723	U
1	a	742	G
1	a	747	A
1	a	755	G
1	a	758	C
1	a	760	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	802	A
1	a	815	A
1	a	817	C
1	a	890	G
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	966	2MG
1	a	969	A
1	a	971	G
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1003	G
1	a	1004	A
1	a	1009	U
1	a	1017	U
1	a	1027	C
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1036	A
1	a	1039	G
1	a	1044	A
1	a	1053	G

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Mol	Chain	Res	Type
1	a	1065	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1137	C
1	a	1139	G
1	a	1152	A
1	a	1159	U
1	a	1167	A
1	a	1168	U
1	a	1196	A
1	a	1197	A
1	a	1213	A
1	a	1214	C
1	a	1227	A
1	a	1228	C
1	a	1238	A
1	a	1241	G
1	a	1258	G
1	a	1260	G
1	a	1275	A
1	a	1280	A
1	a	1285	A
1	a	1286	U
1	a	1287	A
1	a	1300	G
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1335	U
1	a	1338	G
1	a	1346	A
1	a	1363	A
1	a	1379	G
1	a	1381	U
1	a	1419	G
1	a	1432	G
1	a	1441	A
1	a	1446	A
1	a	1448	C
1	a	1452	C
1	a	1453	G

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Mol	Chain	Res	Type
1	a	1487	G
1	a	1492	A
1	a	1493	A
1	a	1494	G
1	a	1497	G
1	a	1499	A
1	a	1506	U
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1534	A
22	w	5	C
22	w	9	A
22	w	10	G
22	w	16	U
22	w	17	OMG
22	w	18	G
22	w	19	H2U
22	w	20	H2U
22	w	21	A
22	w	37	T6A
22	w	46	G7M
22	w	48	C
22	w	49	G
22	w	54	5MU
22	w	70	G
22	w	72	C
22	w	73	A
22	w	74	C
22	w	75	C
23	x	9	G
23	x	18	G
23	x	19	G
23	x	21	A
23	x	26	G
23	x	47	U
23	x	58	A
23	x	74	C
23	x	76	A
22	y	5	C
22	y	8	4SU
22	y	16	U

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Mol	Chain	Res	Type
22	y	17	OMG
22	y	18	G
22	y	19	H2U
22	y	20	H2U
22	y	21	A
22	y	26	A
22	y	37	T6A
22	y	46	G7M
22	y	49	G
22	y	50	C
22	y	54	5MU
22	y	59	G
22	y	63	A
22	y	64	G
22	y	69	G
22	y	73	A
22	y	75	C
22	y	76	A
24	v	23	A
25	A	4	U
25	A	6	A
25	A	10	A
25	A	12	U
25	A	34	U
25	A	35	G
25	A	45	G
25	A	51	G
25	A	58	G
25	A	71	A
25	A	72	U
25	A	74	A
25	A	75	G
25	A	84	A
25	A	100	U
25	A	101	A
25	A	103	A
25	A	118	A
25	A	119	A
25	A	120	U
25	A	139	U
25	A	142	A
25	A	163	C

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Mol	Chain	Res	Type
25	A	181	A
25	A	186	G
25	A	196	A
25	A	215	G
25	A	216	A
25	A	222	A
25	A	224	U
25	A	233	A
25	A	248	G
25	A	264	C
25	A	269	C
25	A	271	G
25	A	272	A
25	A	277	G
25	A	278	A
25	A	279	A
25	A	281	C
25	A	285	G
25	A	287	G
25	A	289	G
25	A	311	A
25	A	329	G
25	A	330	A
25	A	362	A
25	A	367	G
25	A	386	G
25	A	396	G
25	A	404	A
25	A	411	G
25	A	412	A
25	A	420	C
25	A	428	A
25	A	481	G
25	A	491	G
25	A	505	A
25	A	508	A
25	A	509	C
25	A	510	C
25	A	530	G
25	A	531	C
25	A	532	A
25	A	545	U

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Mol	Chain	Res	Type
25	A	546	U
25	A	547	A
25	A	548	G
25	A	549	G
25	A	563	A
25	A	573	U
25	A	575	A
25	A	586	A
25	A	603	A
25	A	614	A
25	A	615	U
25	A	627	A
25	A	637	A
25	A	645	C
25	A	647	G
25	A	654	A
25	A	655	A
25	A	686	U
25	A	709	U
25	A	717	C
25	A	730	A
25	A	736	C
25	A	740	C
25	A	747	5MU
25	A	748	G
25	A	764	A
25	A	775	G
25	A	782	A
25	A	784	G
25	A	785	G
25	A	789	A
25	A	792	A
25	A	805	G
25	A	812	C
25	A	827	U
25	A	828	U
25	A	830	G
25	A	846	U
25	A	847	U
25	A	859	G
25	A	883	G
25	A	890	C

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Mol	Chain	Res	Type
25	A	895	U
25	A	896	A
25	A	901	C
25	A	910	A
25	A	914	G
25	A	915	C
25	A	927	A
25	A	931	U
25	A	946	C
25	A	961	C
25	A	974	G
25	A	983	A
25	A	996	A
25	A	1005	C
25	A	1009	A
25	A	1012	U
25	A	1013	C
25	A	1017	G
25	A	1022	G
25	A	1026	G
25	A	1032	A
25	A	1033	U
25	A	1039	A
25	A	1040	A
25	A	1046	A
25	A	1047	G
25	A	1051	G
25	A	1055	G
25	A	1059	G
25	A	1061	U
25	A	1062	G
25	A	1065	U
25	A	1067	A
25	A	1068	G
25	A	1070	A
25	A	1071	G
25	A	1073	A
25	A	1080	A
25	A	1088	A
25	A	1090	A
25	A	1104	C
25	A	1111	A

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Mol	Chain	Res	Type
25	A	1112	G
25	A	1130	U
25	A	1132	U
25	A	1135	C
25	A	1136	G
25	A	1142	A
25	A	1171	G
25	A	1187	G
25	A	1212	G
25	A	1250	G
25	A	1253	A
25	A	1256	G
25	A	1257	C
25	A	1268	A
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1300	G
25	A	1301	A
25	A	1321	A
25	A	1340	U
25	A	1352	U
25	A	1365	A
25	A	1379	U
25	A	1383	A
25	A	1416	G
25	A	1428	C
25	A	1429	G
25	A	1452	G
25	A	1453	A
25	A	1460	U
25	A	1482	G
25	A	1493	C
25	A	1508	A
25	A	1509	A
25	A	1510	G
25	A	1515	A
25	A	1535	A
25	A	1536	C
25	A	1537	G
25	A	1566	A
25	A	1569	A

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Mol	Chain	Res	Type
25	A	1578	U
25	A	1583	A
25	A	1584	U
25	A	1585	C
25	A	1609	A
25	A	1647	U
25	A	1648	U
25	A	1654	A
25	A	1667	G
25	A	1674	G
25	A	1675	C
25	A	1676	A
25	A	1715	G
25	A	1729	U
25	A	1730	C
25	A	1733	G
25	A	1738	G
25	A	1744	A
25	A	1756	G
25	A	1764	C
25	A	1773	A
25	A	1776	G
25	A	1782	U
25	A	1784	A
25	A	1800	C
25	A	1801	A
25	A	1808	A
25	A	1816	C
25	A	1826	G
25	A	1829	A
25	A	1848	A
25	A	1858	A
25	A	1872	A
25	A	1873	G
25	A	1906	G
25	A	1913	A
25	A	1919	A
25	A	1929	G
25	A	1930	G
25	A	1937	A
25	A	1938	A
25	A	1955	U

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Mol	Chain	Res	Type
25	A	1964	G
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1973	G
25	A	1991	U
25	A	1993	U
25	A	2006	C
25	A	2023	C
25	A	2033	A
25	A	2035	G
25	A	2036	C
25	A	2043	C
25	A	2055	C
25	A	2056	G
25	A	2059	A
25	A	2060	A
25	A	2061	G
25	A	2062	A
25	A	2069	G7M
25	A	2093	G
25	A	2098	U
25	A	2104	C
25	A	2110	G
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2118	U
25	A	2119	A
25	A	2125	G
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2136	G
25	A	2145	C
25	A	2146	C
25	A	2147	A
25	A	2157	G
25	A	2162	G
25	A	2164	C
25	A	2165	C

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Mol	Chain	Res	Type
25	A	2166	U
25	A	2170	A
25	A	2172	U
25	A	2178	C
25	A	2183	A
25	A	2189	U
25	A	2190	G
25	A	2192	U
25	A	2198	A
25	A	2204	G
25	A	2211	A
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2268	A
25	A	2273	A
25	A	2283	C
25	A	2287	A
25	A	2288	A
25	A	2305	U
25	A	2308	G
25	A	2322	A
25	A	2325	G
25	A	2333	A
25	A	2335	A
25	A	2345	G
25	A	2350	C
25	A	2361	G
25	A	2383	G
25	A	2385	C
25	A	2402	U
25	A	2406	A
25	A	2425	A
25	A	2428	G
25	A	2429	G
25	A	2430	A
25	A	2441	U
25	A	2448	A
25	A	2459	A
25	A	2469	A
25	A	2474	U
25	A	2476	A

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Mol	Chain	Res	Type
25	A	2478	A
25	A	2498	OMC
25	A	2502	G
25	A	2504	PSU
25	A	2505	G
25	A	2506	U
25	A	2507	C
25	A	2518	A
25	A	2520	C
25	A	2529	G
25	A	2547	A
25	A	2555	U
25	A	2566	A
25	A	2567	G
25	A	2573	C
25	A	2582	G
25	A	2602	A
25	A	2609	U
25	A	2613	U
25	A	2629	U
25	A	2630	G
25	A	2646	C
25	A	2649	C
25	A	2661	G
25	A	2663	G
25	A	2689	U
25	A	2690	U
25	A	2714	G
25	A	2726	A
25	A	2732	G
25	A	2733	A
25	A	2748	A
25	A	2751	G
25	A	2765	A
25	A	2778	A
25	A	2798	U
25	A	2800	A
25	A	2820	A
25	A	2821	A
25	A	2835	A
25	A	2849	U
25	A	2850	A

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Mol	Chain	Res	Type
25	A	2861	U
25	A	2873	A
25	A	2880	C
25	A	2884	U
25	A	2900	A
26	B	4	C
26	B	24	G
26	B	35	C
26	B	36	C
26	B	44	G
26	B	45	A
26	B	52	A
26	B	53	A
26	B	56	G
26	B	65	U
26	B	67	G
26	B	89	U
26	B	108	A
26	B	109	A
26	B	119	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	3	U
25	A	271	G
25	A	277	G
25	A	784	G
25	A	1026	G
25	A	1031	G
25	A	1111	A
25	A	1583	A
25	A	2097	A
25	A	2189	U
25	A	2191	A
25	A	2473	U
25	A	2799	A
26	B	3	C
26	B	66	A

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

65 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
25	H2U	A	2449	25	18,21,22	1.16	2 (11%)	19,30,33	0.78	0
12	D2T	l	89	12	8,9,10	1.75	1 (12%)	6,11,13	2.48	2 (33%)
23	5MC	x	32	23	19,22,23	1.42	3 (15%)	26,32,35	1.31	4 (15%)
22	T6A	w	37	22	26,34,35	0.94	1 (3%)	28,49,52	1.88	5 (17%)
25	PSU	A	2604	25	18,21,22	1.43	3 (16%)	21,30,33	2.17	4 (19%)
22	M3X	w	34	22,24	24,30,31	2.19	4 (16%)	24,41,44	1.00	2 (8%)
22	4SU	y	8	22	18,21,22	1.87	4 (22%)	25,30,33	2.38	5 (20%)
22	M3X	y	34	22	24,30,31	2.23	3 (12%)	24,41,44	0.99	2 (8%)
25	1MG	A	745	25	19,26,27	0.83	1 (5%)	18,39,42	1.12	2 (11%)
25	5MU	A	1939	25	19,22,23	1.39	4 (21%)	27,32,35	2.12	6 (22%)
1	MA6	a	1518	1	19,26,27	0.91	0	18,38,41	2.28	7 (38%)
22	PSU	w	39	22	18,21,22	1.36	2 (11%)	21,30,33	2.07	3 (14%)
22	H2U	y	20	22	18,21,22	0.98	2 (11%)	19,30,33	0.86	1 (5%)
25	OMG	A	2251	23,57,25	19,26,27	0.90	1 (5%)	21,38,41	1.07	2 (9%)
1	5MC	a	967	1	19,22,23	1.54	3 (15%)	26,32,35	1.14	2 (7%)
22	T6A	y	37	22	26,34,35	0.99	1 (3%)	28,49,52	1.90	4 (14%)
25	2MG	A	1835	25	18,26,27	0.91	1 (5%)	16,38,41	1.27	2 (12%)
22	H2U	w	19	22	18,21,22	1.02	2 (11%)	19,30,33	0.82	1 (5%)
22	5MU	y	54	22	19,22,23	1.43	5 (26%)	27,32,35	2.13	8 (29%)
23	4SU	x	8	23	18,21,22	1.83	4 (22%)	25,30,33	2.24	5 (20%)
1	MA6	a	1519	1	19,26,27	0.94	1 (5%)	18,38,41	2.54	7 (38%)
25	PSU	A	2580	25	18,21,22	1.43	5 (27%)	21,30,33	2.21	4 (19%)
11	IAS	k	119	11	6,7,8	0.95	0	3,8,10	1.46	1 (33%)
25	2MA	A	2503	57,25	18,25,26	0.69	0	20,37,40	1.99	4 (20%)
22	OMG	y	17	22	19,26,27	0.92	1 (5%)	21,38,41	1.09	2 (9%)
22	H2U	y	19	22	18,21,22	1.02	2 (11%)	19,30,33	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	w	55	22	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
1	5MC	a	1407	1	19,22,23	1.54	3 (15%)	26,32,35	1.17	3 (11%)
25	5MU	A	747	25	19,22,23	1.43	6 (31%)	27,32,35	2.08	6 (22%)
25	PSU	A	955	25	18,21,22	1.46	3 (16%)	21,30,33	2.15	4 (19%)
22	3AU	w	47	22	24,28,29	2.70	9 (37%)	30,40,43	1.37	4 (13%)
22	G7M	w	46	22	20,26,27	1.18	2 (10%)	16,39,42	0.70	0
22	OMG	w	17	22	19,26,27	0.89	1 (5%)	21,38,41	1.15	1 (4%)
25	PSU	A	746	25	18,21,22	1.44	5 (27%)	21,30,33	2.17	5 (23%)
25	PSU	A	1917	25	18,21,22	1.40	3 (16%)	21,30,33	2.03	3 (14%)
25	OMU	A	2552	57,25	19,22,23	1.31	3 (15%)	25,31,34	1.88	5 (20%)
1	2MG	a	1516	1	18,26,27	0.92	1 (5%)	16,38,41	1.38	3 (18%)
25	G7M	A	2069	57,25	20,26,27	1.15	2 (10%)	16,39,42	0.58	0
22	PSU	y	55	22	18,21,22	1.35	2 (11%)	21,30,33	2.04	3 (14%)
25	PSU	A	1911	25	18,21,22	1.42	3 (16%)	21,30,33	2.13	4 (19%)
25	PSU	A	2504	25	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
28	MEQ	D	150	28	8,9,10	0.52	0	5,10,12	0.33	0
1	4OC	a	1402	1,57	20,23,24	0.74	0	25,32,35	1.00	1 (4%)
23	5MU	x	54	23	19,22,23	1.39	6 (31%)	27,32,35	2.10	6 (22%)
25	PSU	A	2605	25	18,21,22	1.43	4 (22%)	21,30,33	2.09	4 (19%)
25	OMC	A	2498	57,25	19,22,23	0.82	0	25,31,34	0.98	1 (4%)
25	6MZ	A	1618	25	17,25,26	0.85	1 (5%)	15,36,39	2.23	4 (26%)
1	2MG	a	966	1	18,26,27	0.88	1 (5%)	16,38,41	1.33	3 (18%)
1	2MG	a	1207	1	18,26,27	0.90	1 (5%)	16,38,41	1.21	2 (12%)
22	3AU	y	47	22	24,28,29	2.72	9 (37%)	30,40,43	1.40	5 (16%)
25	3TD	A	1915	25	19,22,23	4.18	7 (36%)	23,32,35	1.79	3 (13%)
22	4SU	w	8	22	18,21,22	1.84	4 (22%)	25,30,33	2.26	4 (16%)
22	PSU	y	39	22	18,21,22	1.46	3 (16%)	21,30,33	1.79	3 (14%)
1	PSU	a	516	1	18,21,22	1.41	4 (22%)	21,30,33	2.07	4 (19%)
1	UR3	a	1498	1	19,22,23	0.96	0	26,32,35	1.82	3 (11%)
22	G7M	y	46	22	20,26,27	1.24	2 (10%)	16,39,42	0.56	0
25	6MZ	A	2030	25	17,25,26	0.84	1 (5%)	15,36,39	2.43	4 (26%)
36	4D4	O	81	36	9,11,12	2.60	3 (33%)	7,13,15	0.98	0
25	5MC	A	1962	25	19,22,23	1.45	3 (15%)	26,32,35	1.09	2 (7%)
22	H2U	w	20	22	18,21,22	1.03	2 (11%)	19,30,33	0.86	1 (5%)
25	2MG	A	2445	57,25	18,26,27	0.98	1 (5%)	16,38,41	1.27	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	A	2457	25	18,21,22	1.43	4 (22%)	21,30,33	2.16	5 (23%)
1	G7M	a	527	1	20,26,27	1.20	2 (10%)	16,39,42	0.56	0
23	PSU	x	55	23	18,21,22	1.39	2 (11%)	21,30,33	2.06	3 (14%)
22	5MU	w	54	22	19,22,23	1.42	6 (31%)	27,32,35	2.23	6 (22%)

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
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
12	D2T	l	89	12	-	2/7/12/14	-
23	5MC	x	32	23	-	1/7/25/26	0/2/2/2
22	T6A	w	37	22	-	2/19/41/42	0/3/3/3
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
22	M3X	w	34	22,24	-	10/17/37/38	0/2/2/2
22	4SU	y	8	22	-	1/7/25/26	0/2/2/2
22	M3X	y	34	22	-	6/17/37/38	0/2/2/2
25	1MG	A	745	25	-	0/3/25/26	0/3/3/3
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/7/29/30	0/3/3/3
22	PSU	w	39	22	-	2/7/25/26	0/2/2/2
22	H2U	y	20	22	-	3/7/38/39	0/2/2/2
25	OMG	A	2251	23,57,25	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
22	T6A	y	37	22	-	9/19/41/42	0/3/3/3
25	2MG	A	1835	25	-	0/5/27/28	0/3/3/3
22	H2U	w	19	22	-	3/7/38/39	0/2/2/2
22	5MU	y	54	22	-	1/7/25/26	0/2/2/2
23	4SU	x	8	23	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	5/7/29/30	0/3/3/3
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
11	IAS	k	119	11	-	0/7/7/8	-
25	2MA	A	2503	57,25	-	2/3/25/26	0/3/3/3
22	OMG	y	17	22	-	0/5/27/28	0/3/3/3
22	H2U	y	19	22	-	3/7/38/39	0/2/2/2
22	PSU	w	55	22	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	5MU	A	747	25	-	2/7/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
22	3AU	w	47	22	-	4/16/34/35	0/2/2/2
22	G7M	w	46	22	-	0/3/25/26	0/3/3/3
22	OMG	w	17	22	-	0/5/27/28	0/3/3/3
25	PSU	A	746	25	-	1/7/25/26	0/2/2/2
25	PSU	A	1917	25	-	2/7/25/26	0/2/2/2
25	OMU	A	2552	57,25	-	2/9/27/28	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
25	G7M	A	2069	57,25	-	1/3/25/26	0/3/3/3
22	PSU	y	55	22	-	0/7/25/26	0/2/2/2
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2504	25	-	2/7/25/26	0/2/2/2
28	MEQ	D	150	28	-	3/8/9/11	-
1	4OC	a	1402	1,57	-	2/9/29/30	0/2/2/2
23	5MU	x	54	23	-	0/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	OMC	A	2498	57,25	-	3/9/27/28	0/2/2/2
25	6MZ	A	1618	25	-	0/5/27/28	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
22	3AU	y	47	22	-	4/16/34/35	0/2/2/2
25	3TD	A	1915	25	-	0/7/25/26	0/2/2/2
22	4SU	w	8	22	-	0/7/25/26	0/2/2/2
22	PSU	y	39	22	-	3/7/25/26	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
22	G7M	y	46	22	-	2/3/25/26	0/3/3/3
25	6MZ	A	2030	25	-	2/5/27/28	0/3/3/3
36	4D4	O	81	36	-	0/11/12/14	-
25	5MC	A	1962	25	-	0/7/25/26	0/2/2/2
22	H2U	w	20	22	-	1/7/38/39	0/2/2/2
25	2MG	A	2445	57,25	-	0/5/27/28	0/3/3/3
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	-	2/3/25/26	0/3/3/3
23	PSU	x	55	23	-	0/7/25/26	0/2/2/2
22	5MU	w	54	22	-	0/7/25/26	0/2/2/2

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	12.32	1.48	1.35
25	A	1915	3TD	C2-N1	9.73	1.49	1.37
22	y	34	M3X	C2-N2	8.86	1.47	1.34
22	w	34	M3X	C2-N2	8.53	1.47	1.34
22	y	47	3AU	C2-N1	6.50	1.47	1.38
22	w	47	3AU	C2-N1	6.33	1.47	1.38
22	w	47	3AU	C2-N3	6.21	1.49	1.38
22	y	47	3AU	C2-N3	6.12	1.49	1.38
22	y	47	3AU	C6-C5	6.09	1.49	1.35
22	w	47	3AU	C6-C5	6.05	1.49	1.35
36	O	81	4D4	CZ-NE	5.94	1.44	1.33
25	A	1915	3TD	C6-N1	5.69	1.45	1.36
1	a	1407	5MC	C5-C4	5.47	1.48	1.44
1	a	967	5MC	C5-C4	5.43	1.48	1.44
25	A	1962	5MC	C5-C4	5.08	1.48	1.44
23	x	8	4SU	C4-S4	-5.05	1.59	1.68
22	w	8	4SU	C4-S4	-5.01	1.59	1.68
22	y	8	4SU	C4-S4	-5.01	1.59	1.68
25	A	1915	3TD	C2-N3	4.97	1.49	1.38
23	x	32	5MC	C5-C4	4.76	1.47	1.44
12	l	89	D2T	CB-CA	-4.00	1.53	1.54
22	w	34	M3X	C4-N4	-3.77	1.24	1.35
22	y	34	M3X	C4-N4	-3.76	1.24	1.35
22	y	46	G7M	C5-C4	3.68	1.46	1.39
36	O	81	4D4	CZ-NH2	3.65	1.45	1.32
1	a	527	G7M	C5-C4	3.57	1.46	1.39
22	y	47	3AU	C6-N1	3.56	1.46	1.38
22	w	47	3AU	O2-C2	-3.52	1.16	1.22
22	w	46	G7M	C5-C4	3.52	1.46	1.39
22	w	47	3AU	C6-N1	3.49	1.46	1.38
22	y	47	3AU	O2-C2	-3.49	1.16	1.22
23	x	8	4SU	C4-N3	-3.47	1.34	1.37
22	y	39	PSU	C6-C5	3.46	1.39	1.35
22	y	47	3AU	C4-N3	3.46	1.46	1.40
22	y	8	4SU	C4-N3	-3.39	1.34	1.37
22	w	47	3AU	C4-N3	3.37	1.46	1.40
22	y	55	PSU	C6-C5	3.37	1.39	1.35
25	A	2504	PSU	C6-C5	3.35	1.39	1.35
23	x	55	PSU	C6-C5	3.32	1.39	1.35
22	w	34	M3X	C6-N1	-3.28	1.31	1.36
25	A	2552	OMU	C4-N3	-3.26	1.33	1.38
25	A	2069	G7M	C5-C4	3.22	1.45	1.39
22	w	8	4SU	C4-N3	-3.17	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	55	PSU	C6-C5	3.17	1.38	1.35
1	a	516	PSU	C6-C5	3.14	1.38	1.35
25	A	1911	PSU	C6-C5	3.14	1.38	1.35
25	A	2604	PSU	C4-N3	-3.14	1.33	1.38
22	w	39	PSU	C6-C5	3.10	1.38	1.35
22	y	34	M3X	C6-N1	-3.10	1.32	1.36
25	A	955	PSU	C4-N3	-3.09	1.33	1.38
25	A	2605	PSU	C4-N3	-3.08	1.33	1.38
25	A	2445	2MG	C6-N1	-3.07	1.33	1.37
25	A	2604	PSU	C6-C5	3.05	1.38	1.35
25	A	1917	PSU	C6-C5	3.03	1.38	1.35
25	A	2449	H2U	C2-N3	-3.02	1.32	1.38
25	A	2457	PSU	C4-N3	-3.01	1.33	1.38
25	A	1939	5MU	C4-N3	-3.00	1.33	1.38
25	A	955	PSU	C6-C5	2.94	1.38	1.35
25	A	1911	PSU	C4-N3	-2.94	1.33	1.38
25	A	747	5MU	C4-N3	-2.93	1.33	1.38
22	y	39	PSU	C4-N3	-2.93	1.33	1.38
25	A	746	PSU	C6-C5	2.92	1.38	1.35
25	A	746	PSU	C4-N3	-2.90	1.33	1.38
25	A	1917	PSU	C4-N3	-2.88	1.33	1.38
25	A	1915	3TD	C4-N3	2.88	1.46	1.40
22	w	8	4SU	C5-C4	-2.87	1.39	1.42
25	A	2552	OMU	C2-N3	-2.86	1.33	1.38
25	A	2449	H2U	C4-N3	-2.86	1.32	1.37
22	w	55	PSU	C4-N3	-2.83	1.33	1.38
25	A	2251	OMG	C6-N1	-2.82	1.33	1.37
22	y	8	4SU	C5-C4	-2.81	1.39	1.42
1	a	516	PSU	C4-N3	-2.77	1.33	1.38
25	A	2605	PSU	C6-C5	2.76	1.38	1.35
25	A	2580	PSU	C4-N3	-2.76	1.33	1.38
22	y	54	5MU	C2-N1	2.74	1.42	1.38
22	w	54	5MU	C4-N3	-2.74	1.33	1.38
25	A	2580	PSU	C6-C5	2.72	1.38	1.35
25	A	1835	2MG	C6-N1	-2.71	1.33	1.37
22	w	54	5MU	C6-C5	2.71	1.39	1.34
23	x	55	PSU	C4-N3	-2.70	1.33	1.38
25	A	2504	PSU	C4-N3	-2.69	1.33	1.38
22	w	19	H2U	C2-N3	-2.69	1.33	1.38
22	y	54	5MU	C6-C5	2.69	1.39	1.34
25	A	2069	G7M	C6-N1	-2.69	1.33	1.37
23	x	54	5MU	C4-N3	-2.66	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	967	5MC	C6-C5	2.66	1.38	1.34
25	A	2457	PSU	C6-C5	2.65	1.38	1.35
22	y	19	H2U	C2-N3	-2.64	1.33	1.38
22	y	37	T6A	C6-C5	2.63	1.48	1.44
25	A	1915	3TD	O2-C2	-2.63	1.18	1.23
23	x	54	5MU	C6-C5	2.62	1.38	1.34
22	w	20	H2U	C2-N3	-2.61	1.33	1.38
1	a	1407	5MC	C6-C5	2.60	1.38	1.34
1	a	966	2MG	C6-N1	-2.60	1.33	1.37
1	a	1516	2MG	C6-N1	-2.59	1.33	1.37
22	y	54	5MU	C4-N3	-2.59	1.34	1.38
23	x	8	4SU	C5-C4	-2.58	1.39	1.42
22	y	8	4SU	C2-N1	2.56	1.42	1.38
25	A	747	5MU	C6-C5	2.55	1.38	1.34
1	a	1207	2MG	C6-N1	-2.55	1.33	1.37
22	y	20	H2U	C2-N3	-2.55	1.33	1.38
23	x	32	5MC	C6-C5	2.52	1.38	1.34
25	A	1939	5MU	C2-N3	-2.51	1.33	1.38
25	A	2580	PSU	O4'-C1'	-2.50	1.40	1.43
1	a	527	G7M	C6-N1	-2.50	1.34	1.37
25	A	2605	PSU	C2-N3	-2.49	1.33	1.37
22	w	39	PSU	C4-N3	-2.49	1.34	1.38
25	A	1939	5MU	C6-C5	2.49	1.38	1.34
22	w	47	3AU	O4-C4	-2.48	1.18	1.23
25	A	1962	5MC	C6-C5	2.48	1.38	1.34
22	y	55	PSU	C4-N3	-2.48	1.34	1.38
25	A	955	PSU	C2-N3	-2.48	1.33	1.37
23	x	32	5MC	C6-N1	-2.47	1.33	1.38
25	A	1939	5MU	C6-N1	-2.44	1.33	1.38
25	A	747	5MU	C6-N1	-2.43	1.33	1.38
22	y	47	3AU	O4-C4	-2.42	1.18	1.23
22	y	19	H2U	C4-N3	-2.42	1.33	1.37
22	w	19	H2U	C4-N3	-2.41	1.33	1.37
25	A	1962	5MC	C6-N1	-2.41	1.33	1.38
36	O	81	4D4	CZ-NH1	-2.40	1.25	1.34
1	a	967	5MC	C6-N1	-2.38	1.34	1.38
1	a	1519	MA6	C6-C5	2.38	1.48	1.44
1	a	1407	5MC	C6-N1	-2.37	1.34	1.38
22	w	54	5MU	C6-N1	-2.36	1.34	1.38
22	w	46	G7M	C6-N1	-2.35	1.34	1.37
25	A	747	5MU	C2-N3	-2.35	1.33	1.38
22	y	54	5MU	C6-N1	-2.35	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	47	3AU	O30-C13	2.34	1.29	1.22
23	x	54	5MU	C4-C5	2.34	1.48	1.44
22	w	17	OMG	C6-N1	-2.33	1.34	1.37
22	y	46	G7M	C6-N1	-2.33	1.34	1.37
25	A	2457	PSU	C2-N3	-2.32	1.33	1.37
22	y	17	OMG	C6-N1	-2.31	1.34	1.37
22	w	54	5MU	C4-C5	2.31	1.48	1.44
22	w	47	3AU	O30-C13	2.31	1.28	1.22
22	y	20	H2U	C4-N3	-2.31	1.33	1.37
22	w	20	H2U	C4-N3	-2.29	1.33	1.37
25	A	2604	PSU	C2-N3	-2.26	1.33	1.37
22	y	54	5MU	C4-C5	2.25	1.48	1.44
25	A	2030	6MZ	C6-C5	2.24	1.48	1.44
23	x	54	5MU	C6-N1	-2.23	1.34	1.38
25	A	1911	PSU	C2-N3	-2.21	1.33	1.37
23	x	8	4SU	C2-N3	-2.21	1.34	1.38
22	w	8	4SU	C2-N3	-2.18	1.34	1.38
25	A	747	5MU	C2-N1	2.18	1.41	1.38
25	A	1915	3TD	O4-C4	-2.18	1.18	1.23
25	A	747	5MU	C4-C5	2.18	1.48	1.44
25	A	745	1MG	C2-N1	2.18	1.41	1.37
25	A	746	PSU	O4'-C1'	-2.17	1.40	1.43
25	A	2457	PSU	C2-N1	-2.17	1.33	1.36
22	w	54	5MU	C2-N1	2.17	1.41	1.38
25	A	1917	PSU	C2-N3	-2.16	1.33	1.37
25	A	2580	PSU	C2-N1	-2.16	1.33	1.36
22	w	54	5MU	C2-N3	-2.15	1.34	1.38
25	A	2552	OMU	C5-C4	-2.12	1.39	1.43
23	x	54	5MU	C2-N1	2.10	1.41	1.38
25	A	746	PSU	C2-N1	-2.10	1.33	1.36
22	y	47	3AU	C11-C10	2.10	1.59	1.52
23	x	54	5MU	C2-N3	-2.09	1.34	1.38
25	A	746	PSU	C2-N3	-2.08	1.34	1.37
25	A	2605	PSU	C2-N1	-2.06	1.34	1.36
25	A	1618	6MZ	C6-C5	2.05	1.48	1.44
22	y	39	PSU	C2-N3	-2.05	1.34	1.37
25	A	2580	PSU	C2-N3	-2.05	1.34	1.37
22	w	55	PSU	C2-N3	-2.05	1.34	1.37
1	a	516	PSU	C2-N3	-2.04	1.34	1.37
22	w	47	3AU	C11-C10	2.04	1.58	1.52
1	a	516	PSU	O4'-C1'	-2.04	1.41	1.43
22	w	37	T6A	C10-N6	-2.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	34	M3X	O-C	-2.02	1.24	1.30

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1498	UR3	C4-N3-C2	-7.27	118.73	124.58
25	A	2503	2MA	C2-N3-C4	7.02	121.13	115.46
22	y	8	4SU	C4-N3-C2	-6.95	120.65	127.31
23	x	8	4SU	C4-N3-C2	-6.91	120.69	127.31
25	A	2604	PSU	N1-C2-N3	6.88	122.42	115.17
22	w	8	4SU	C4-N3-C2	-6.81	120.79	127.31
25	A	955	PSU	N1-C2-N3	6.75	122.29	115.17
25	A	746	PSU	N1-C2-N3	6.70	122.24	115.17
25	A	2457	PSU	N1-C2-N3	6.69	122.23	115.17
25	A	2030	6MZ	C2-N1-C6	6.66	121.77	116.60
25	A	1911	PSU	N1-C2-N3	6.63	122.16	115.17
25	A	2580	PSU	N1-C2-N3	6.57	122.09	115.17
22	y	37	T6A	C2-N1-C6	6.50	121.64	116.60
25	A	2605	PSU	N1-C2-N3	6.49	122.01	115.17
22	y	55	PSU	N1-C2-N3	6.44	121.96	115.17
23	x	55	PSU	N1-C2-N3	6.44	121.96	115.17
22	w	55	PSU	N1-C2-N3	6.43	121.95	115.17
25	A	1917	PSU	N1-C2-N3	6.38	121.89	115.17
25	A	1618	6MZ	C2-N1-C6	6.34	121.52	116.60
22	w	39	PSU	N1-C2-N3	6.33	121.84	115.17
1	a	516	PSU	N1-C2-N3	6.33	121.84	115.17
22	w	37	T6A	C2-N1-C6	6.23	121.43	116.60
25	A	2504	PSU	N1-C2-N3	6.20	121.71	115.17
22	y	8	4SU	C5-C4-N3	5.95	120.28	114.75
1	a	1519	MA6	C2-N1-C6	5.82	122.55	116.84
22	y	39	PSU	N1-C2-N3	5.81	121.30	115.17
22	w	8	4SU	C5-C4-N3	5.81	120.15	114.75
22	w	54	5MU	C4-N3-C2	-5.61	119.99	127.34
23	x	8	4SU	C5-C4-N3	5.57	119.93	114.75
22	w	54	5MU	N3-C2-N1	5.46	122.00	114.89
25	A	1915	3TD	N1-C2-N3	5.44	120.09	116.13
25	A	1939	5MU	C4-N3-C2	-5.18	120.55	127.34
22	y	54	5MU	N3-C2-N1	5.18	121.63	114.89
23	x	54	5MU	C4-N3-C2	-5.14	120.60	127.34
25	A	1939	5MU	N3-C2-N1	5.14	121.58	114.89
25	A	2552	OMU	C4-N3-C2	-5.14	120.23	126.61
25	A	747	5MU	N3-C2-N1	5.10	121.53	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	54	5MU	C4-N3-C2	-5.06	120.71	127.34
23	x	54	5MU	N3-C2-N1	5.00	121.40	114.89
25	A	747	5MU	C4-N3-C2	-4.97	120.82	127.34
1	a	1518	MA6	C2-N1-C6	4.86	121.60	116.84
22	w	54	5MU	C5-C4-N3	4.71	119.42	115.32
22	y	8	4SU	C5-C4-S4	-4.52	119.14	124.31
25	A	2552	OMU	N3-C2-N1	4.52	120.77	114.89
25	A	1939	5MU	C5-C4-N3	4.48	119.22	115.32
23	x	54	5MU	C5-C4-N3	4.44	119.18	115.32
25	A	2580	PSU	C4-N3-C2	-4.42	120.29	126.37
25	A	2457	PSU	C4-N3-C2	-4.40	120.30	126.37
23	x	8	4SU	N3-C2-N1	4.39	120.60	114.89
25	A	1915	3TD	C4-N3-C2	-4.38	119.98	124.61
25	A	955	PSU	C4-N3-C2	-4.36	120.36	126.37
25	A	2604	PSU	C4-N3-C2	-4.34	120.39	126.37
25	A	2605	PSU	C4-N3-C2	-4.34	120.40	126.37
22	w	55	PSU	C4-N3-C2	-4.30	120.44	126.37
22	w	39	PSU	C4-N3-C2	-4.30	120.45	126.37
25	A	1911	PSU	C4-N3-C2	-4.30	120.45	126.37
1	a	1519	MA6	N3-C2-N1	-4.29	122.84	128.67
25	A	746	PSU	C4-N3-C2	-4.29	120.46	126.37
25	A	2580	PSU	O2-C2-N1	-4.29	118.37	122.79
1	a	1518	MA6	N1-C6-N6	4.25	121.74	116.83
25	A	747	5MU	C5-C4-N3	4.21	118.98	115.32
22	y	54	5MU	C5-C4-N3	4.18	118.95	115.32
22	y	54	5MU	O4-C4-C5	-4.16	120.16	124.92
25	A	2030	6MZ	C9-N6-C6	-4.14	119.01	122.85
25	A	2504	PSU	C4-N3-C2	-4.11	120.70	126.37
22	w	8	4SU	C5-C4-S4	-4.10	119.62	124.31
22	y	37	T6A	N6-C10-N11	4.09	119.40	113.77
12	l	89	D2T	CB1-SB-CB	4.08	109.70	102.36
25	A	2552	OMU	C5-C4-N3	4.08	120.51	114.80
22	w	37	T6A	N6-C10-N11	4.08	119.38	113.77
25	A	1939	5MU	O4-C4-C5	-4.08	120.25	124.92
22	w	8	4SU	N3-C2-N1	4.07	120.19	114.89
23	x	55	PSU	C4-N3-C2	-4.06	120.77	126.37
22	y	8	4SU	N3-C2-N1	4.06	120.18	114.89
25	A	746	PSU	O2-C2-N1	-4.00	118.67	122.79
25	A	1917	PSU	C4-N3-C2	-3.98	120.89	126.37
1	a	516	PSU	C4-N3-C2	-3.95	120.92	126.37
25	A	2457	PSU	O2-C2-N1	-3.95	118.72	122.79
22	y	55	PSU	O2-C2-N1	-3.95	118.72	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	x	54	5MU	O4-C4-C5	-3.94	120.41	124.92
22	y	55	PSU	C4-N3-C2	-3.93	120.96	126.37
22	w	54	5MU	O4-C4-C5	-3.91	120.44	124.92
1	a	1518	MA6	C10-N6-C6	-3.91	108.63	119.40
1	a	1519	MA6	C10-N6-C6	-3.90	108.64	119.40
1	a	1519	MA6	C9-N6-C6	-3.89	108.68	119.40
23	x	55	PSU	O2-C2-N1	-3.84	118.83	122.79
22	w	47	3AU	C4-N3-C2	-3.83	120.17	124.66
25	A	1939	5MU	C5-C6-N1	-3.79	119.20	123.31
1	a	516	PSU	O2-C2-N1	-3.79	118.88	122.79
25	A	1911	PSU	O2-C2-N1	-3.78	118.89	122.79
25	A	747	5MU	O4-C4-C5	-3.77	120.60	124.92
22	w	54	5MU	C5-C6-N1	-3.77	119.22	123.31
22	y	47	3AU	C4-N3-C2	-3.76	120.24	124.66
22	w	39	PSU	O2-C2-N1	-3.75	118.92	122.79
25	A	1618	6MZ	N3-C2-N1	-3.66	123.71	128.67
25	A	2030	6MZ	N3-C2-N1	-3.65	123.72	128.67
23	x	8	4SU	C5-C4-S4	-3.65	120.14	124.31
1	a	1518	MA6	N3-C2-N1	-3.63	123.74	128.67
22	w	37	T6A	N6-C6-N1	3.63	122.79	118.71
22	y	37	T6A	N3-C2-N1	-3.63	123.75	128.67
25	A	2604	PSU	O2-C2-N1	-3.62	119.05	122.79
25	A	1917	PSU	O2-C2-N1	-3.58	119.10	122.79
25	A	955	PSU	O2-C2-N1	-3.54	119.13	122.79
22	w	37	T6A	N3-C2-N1	-3.54	123.87	128.67
23	x	54	5MU	C5-C6-N1	-3.53	119.48	123.31
22	w	55	PSU	O2-C2-N1	-3.44	119.24	122.79
25	A	1618	6MZ	C9-N6-C6	-3.40	119.69	122.85
25	A	747	5MU	C5-C6-N1	-3.40	119.62	123.31
1	a	1498	UR3	C5-C4-N3	3.39	119.50	115.04
1	a	967	5MC	C5-C6-N1	-3.37	119.66	123.31
25	A	2504	PSU	O2-C2-N1	-3.37	119.32	122.79
12	l	89	D2T	OD2-CG-CB	3.35	120.39	113.15
25	A	2605	PSU	O2-C2-N1	-3.33	119.36	122.79
1	a	1518	MA6	C9-N6-C6	-3.27	110.39	119.40
23	x	32	5MC	C5-C6-N1	-3.23	119.80	123.31
1	a	1519	MA6	C4-C5-N7	-3.20	105.95	109.34
22	y	39	PSU	C4-N3-C2	-3.15	122.04	126.37
22	y	8	4SU	C1'-N1-C2	3.09	123.14	117.59
22	y	37	T6A	C4-C5-N7	-3.08	106.08	109.34
1	a	1407	5MC	C5-C6-N1	-3.07	119.98	123.31
1	a	1519	MA6	C10-N6-C9	-3.06	106.35	116.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1407	5MC	C5-C4-N3	-3.01	118.67	121.75
22	w	47	3AU	C5-C4-N3	3.00	119.78	115.64
23	x	32	5MC	C5-C4-N3	-2.98	118.70	121.75
1	a	966	2MG	C8-N7-C5	2.95	107.57	102.55
25	A	1962	5MC	C5-C4-N3	-2.92	118.76	121.75
25	A	2251	OMG	C8-N7-C5	2.92	107.53	102.55
1	a	1516	2MG	C8-N7-C5	2.92	107.52	102.55
25	A	2445	2MG	C8-N7-C5	2.91	107.51	102.55
25	A	1962	5MC	C5-C6-N1	-2.90	120.16	123.31
22	w	17	OMG	C8-N7-C5	2.88	107.46	102.55
22	y	47	3AU	C5-C4-N3	2.86	119.60	115.64
23	x	32	5MC	O2-C2-N3	-2.85	117.83	122.33
22	y	47	3AU	C6-N1-C2	-2.83	119.48	121.80
1	a	1207	2MG	C8-N7-C5	2.83	107.37	102.55
22	y	39	PSU	O2-C2-N1	-2.78	119.92	122.79
22	w	54	5MU	O2-C2-N1	-2.77	119.19	122.80
22	y	17	OMG	C8-N7-C5	2.77	107.26	102.55
25	A	2030	6MZ	C4-C5-N7	-2.76	106.42	109.34
25	A	2503	2MA	C2-N1-C6	2.75	122.33	118.10
22	y	54	5MU	C1'-N1-C2	2.75	122.54	117.59
1	a	967	5MC	C5-C4-N3	-2.74	118.95	121.75
25	A	745	1MG	C8-N7-C5	2.73	107.20	102.55
25	A	1835	2MG	C8-N7-C5	2.72	107.19	102.55
25	A	2498	OMC	O2-C2-N3	-2.69	118.10	122.33
25	A	1939	5MU	O2-C2-N1	-2.68	119.31	122.80
25	A	745	1MG	C5-C6-N1	2.64	117.78	113.96
22	y	54	5MU	C5-C6-N1	-2.60	120.49	123.31
1	a	1402	4OC	C6-C5-C4	2.58	120.11	117.00
25	A	2552	OMU	O4-C4-C5	-2.58	120.72	125.16
25	A	1618	6MZ	C4-C5-N7	-2.57	106.62	109.34
22	w	47	3AU	C6-N1-C2	-2.56	119.71	121.80
22	y	20	H2U	C5-C6-N1	-2.54	103.83	111.52
23	x	54	5MU	O2-C2-N1	-2.54	119.49	122.80
22	y	47	3AU	C1'-N1-C2	2.48	121.10	117.04
25	A	2552	OMU	O2-C2-N1	-2.45	119.61	122.80
1	a	1519	MA6	N1-C6-N6	2.44	119.66	116.83
25	A	2580	PSU	O4'-C1'-C2'	2.43	108.52	105.15
11	k	119	IAS	OD1-CG-CB	-2.42	118.32	125.38
25	A	2604	PSU	C5-C6-N1	-2.40	118.81	122.14
25	A	2503	2MA	C4-C5-N7	-2.40	106.81	109.34
22	w	20	H2U	C5-C6-N1	-2.39	104.29	111.52
1	a	1407	5MC	O2-C2-N3	-2.38	118.58	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	516	PSU	O4'-C1'-C2'	2.37	108.43	105.15
25	A	1915	3TD	C1'-C5-C4	2.37	121.20	117.61
25	A	746	PSU	O4'-C1'-C2'	2.34	108.38	105.15
1	a	1518	MA6	C10-N6-C9	-2.32	108.73	116.18
22	w	34	M3X	C5-C4-N3	-2.32	119.04	121.83
1	a	1516	2MG	N1-C2-N2	2.30	118.91	116.56
25	A	2251	OMG	C5-C6-N1	2.29	118.44	114.07
22	y	34	M3X	N4-C4-N3	2.29	120.27	116.59
22	w	37	T6A	O10-C10-N6	-2.29	119.57	123.64
1	a	1518	MA6	C4-C5-N7	-2.28	106.92	109.34
22	w	19	H2U	C5-C6-N1	-2.28	104.63	111.52
22	y	34	M3X	C5-C4-N3	-2.26	119.11	121.83
22	w	47	3AU	C1'-N1-C2	2.23	120.70	117.04
25	A	955	PSU	C5-C6-N1	-2.23	119.05	122.14
25	A	2457	PSU	C5-C6-N1	-2.22	119.06	122.14
22	w	34	M3X	N4-C4-N3	2.21	120.14	116.59
22	y	47	3AU	O2-C2-N3	-2.20	119.02	121.98
25	A	1835	2MG	C5-C6-N1	2.20	118.27	114.07
25	A	2605	PSU	C5-C6-N1	-2.20	119.09	122.14
25	A	2445	2MG	C5-C6-N1	2.20	118.26	114.07
22	y	17	OMG	C5-C6-N1	2.19	118.25	114.07
25	A	2503	2MA	C5-C6-N1	-2.15	118.29	120.84
1	a	966	2MG	C5-C6-N1	2.14	118.16	114.07
1	a	1207	2MG	C5-C6-N1	2.13	118.13	114.07
25	A	746	PSU	C5-C6-N1	-2.12	119.20	122.14
25	A	2457	PSU	O4'-C1'-C2'	2.12	108.08	105.15
22	w	55	PSU	C5-C6-N1	-2.12	119.20	122.14
25	A	1911	PSU	C5-C6-N1	-2.11	119.20	122.14
23	x	8	4SU	O2-C2-N1	-2.11	120.05	122.80
25	A	747	5MU	O2-C2-N1	-2.11	120.05	122.80
1	a	1516	2MG	C5-C6-N1	2.09	118.05	114.07
1	a	1498	UR3	C3U-N3-C2	2.08	120.96	117.33
23	x	32	5MC	C1'-N1-C6	-2.08	117.73	121.15
22	y	54	5MU	O2-C2-N3	-2.06	117.69	121.49
1	a	966	2MG	CM2-N2-C2	-2.04	119.27	123.65
22	y	54	5MU	C1'-N1-C6	-2.04	117.80	121.15
22	y	19	H2U	C5-C6-N1	-2.01	105.43	111.52

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
1	a	1519	MA6	N1-C6-N6-C9
12	l	89	D2T	CA-CB-SB-CB1
12	l	89	D2T	CG-CB-SB-CB1
22	y	20	H2U	O4'-C4'-C5'-O5'
22	y	20	H2U	C3'-C4'-C5'-O5'
22	w	34	M3X	N1-C2-N2-CE
22	w	34	M3X	N3-C2-N2-CE
22	w	34	M3X	OXT-C-CZ-N
22	y	34	M3X	CG-CB-CZ-N
22	y	37	T6A	O10-C10-N6-C6
22	y	37	T6A	N11-C10-N6-C6
22	y	37	T6A	C13-C12-C14-O14
22	y	37	T6A	C13-C12-C14-C15
22	y	39	PSU	C2'-C1'-C5-C4
22	w	47	3AU	C10-C11-C12-C13
22	w	47	3AU	C10-C11-C12-N40
22	y	47	3AU	N40-C12-C13-O30
25	A	2504	PSU	O4'-C4'-C5'-O5'
22	y	37	T6A	N6-C10-N11-C12
22	w	34	M3X	CE-CD-CG-CB
1	a	527	G7M	C3'-C4'-C5'-O5'
22	y	19	H2U	C3'-C4'-C5'-O5'
22	w	39	PSU	C3'-C4'-C5'-O5'
25	A	1917	PSU	O4'-C4'-C5'-O5'
22	w	47	3AU	N40-C12-C13-O31
22	y	37	T6A	O10-C10-N11-C12
1	a	1402	4OC	O4'-C4'-C5'-O5'
22	y	19	H2U	O4'-C4'-C5'-O5'
22	w	39	PSU	O4'-C4'-C5'-O5'
25	A	1917	PSU	C3'-C4'-C5'-O5'
25	A	2552	OMU	O4'-C4'-C5'-O5'
22	w	34	M3X	O-C-CZ-N
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	N1-C6-N6-C10
22	y	37	T6A	C5-C6-N6-C10
22	y	47	3AU	N40-C12-C13-O31
25	A	2030	6MZ	O4'-C4'-C5'-O5'
25	A	2504	PSU	C3'-C4'-C5'-O5'
28	D	150	MEQ	NE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
28	D	150	MEQ	OE1-CD-CG-CB
22	y	37	T6A	N11-C12-C14-O14
22	y	46	G7M	O4'-C4'-C5'-O5'
25	A	2498	OMC	O4'-C4'-C5'-O5'
22	w	19	H2U	O4'-C4'-C5'-O5'
22	y	46	G7M	C3'-C4'-C5'-O5'
25	A	2030	6MZ	C3'-C4'-C5'-O5'
22	w	19	H2U	C3'-C4'-C5'-O5'
22	y	34	M3X	CG-CD-CE-N2
1	a	1402	4OC	C3'-C4'-C5'-O5'
22	w	19	H2U	C4'-C5'-O5'-P
22	w	34	M3X	CZ-CB-CG-CD
25	A	747	5MU	C3'-C4'-C5'-O5'
22	y	37	T6A	N11-C12-C14-C15
22	y	34	M3X	CG-CB-CZ-C
22	y	34	M3X	OXT-C-CZ-CB
22	y	39	PSU	C3'-C4'-C5'-O5'
28	D	150	MEQ	C-CA-CB-CG
22	y	34	M3X	O-C-CZ-CB
1	a	1519	MA6	O4'-C4'-C5'-O5'
22	w	34	M3X	OXT-C-CZ-CB
22	w	37	T6A	N6-C10-N11-C12
22	y	19	H2U	C4'-C5'-O5'-P
22	w	20	H2U	C4'-C5'-O5'-P
22	w	34	M3X	O-C-CZ-CB
25	A	2498	OMC	C3'-C2'-O2'-CM2
22	y	20	H2U	C4'-C5'-O5'-P
22	y	54	5MU	C4'-C5'-O5'-P
25	A	746	PSU	O4'-C1'-C5-C4
22	w	34	M3X	C3'-C4'-C5'-O5'
22	w	37	T6A	O10-C10-N11-C12
22	y	47	3AU	C11-C12-C13-O31
25	A	2552	OMU	C3'-C4'-C5'-O5'
25	A	747	5MU	O4'-C4'-C5'-O5'
22	y	47	3AU	C11-C12-C13-O30
22	y	34	M3X	CZ-CB-CG-CD
22	w	34	M3X	O4'-C4'-C5'-O5'
22	y	39	PSU	O4'-C4'-C5'-O5'
25	A	2498	OMC	C3'-C4'-C5'-O5'
25	A	2503	2MA	C4'-C5'-O5'-P
25	A	2503	2MA	O4'-C4'-C5'-O5'
23	x	32	5MC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
22	y	8	4SU	C2'-C1'-N1-C2
22	w	47	3AU	N40-C12-C13-O30
25	A	2069	G7M	O4'-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 740 ligands modelled in this entry, 738 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	ILE	y	101	-	6,7,8	0.55	0	4,8,10	1.10	0
56	PAR	a	1601	-	44,45,45	3.17	12 (27%)	63,67,67	1.08	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	ILE	y	101	-	-	1/7/8/10	-
56	PAR	a	1601	-	-	5/18/94/94	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	a	1601	PAR	C23-C33	-12.11	1.26	1.53
56	a	1601	PAR	C13-C23	10.88	1.66	1.52
56	a	1601	PAR	O43-C13	-7.07	1.29	1.41
56	a	1601	PAR	O43-C43	4.67	1.55	1.45
56	a	1601	PAR	C31-C21	-4.14	1.48	1.53
56	a	1601	PAR	C53-C43	-3.85	1.38	1.51
56	a	1601	PAR	C34-C24	-3.55	1.49	1.53
56	a	1601	PAR	C24-N24	3.05	1.51	1.47
56	a	1601	PAR	O33-C33	2.90	1.51	1.43
56	a	1601	PAR	C21-N21	2.23	1.50	1.47
56	a	1601	PAR	O51-C51	2.18	1.49	1.44
56	a	1601	PAR	O51-C11	2.09	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	a	1601	PAR	C14-O33-C33	-2.97	110.94	117.98
56	a	1601	PAR	O11-C42-C32	-2.14	104.07	109.18
56	a	1601	PAR	C13-O52-C52	-2.13	112.92	117.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

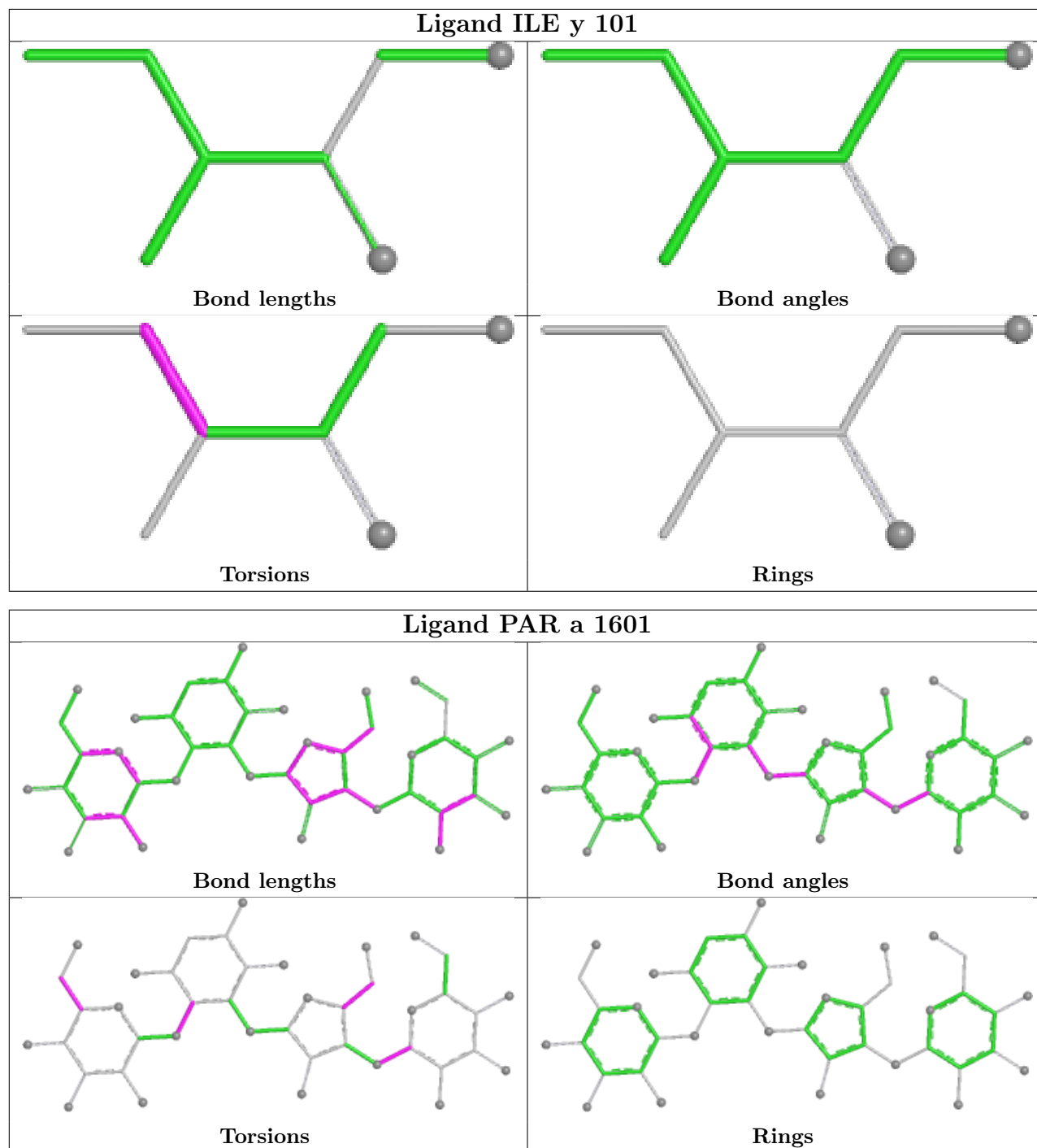
Mol	Chain	Res	Type	Atoms
56	a	1601	PAR	O43-C43-C53-O53
56	a	1601	PAR	C33-C43-C53-O53
56	a	1601	PAR	O51-C51-C61-O61
56	a	1601	PAR	O54-C14-O33-C33
56	a	1601	PAR	C52-C42-O11-C11
59	y	101	ILE	CG2-CB-CG1-CD1

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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

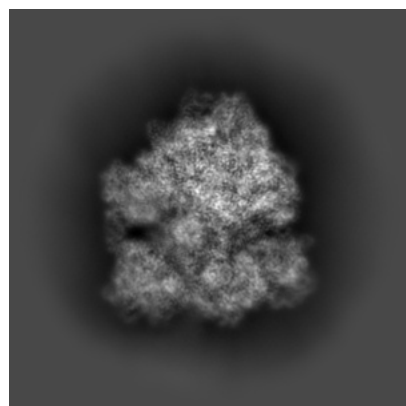
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29821. These allow visual inspection of the internal detail of the map and identification of artifacts.

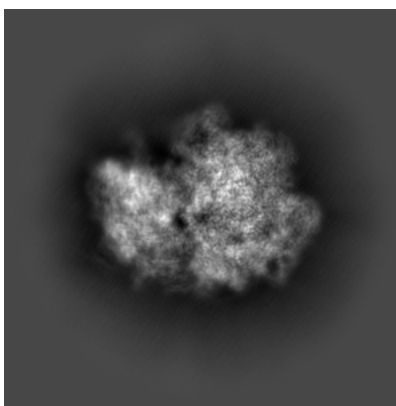
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

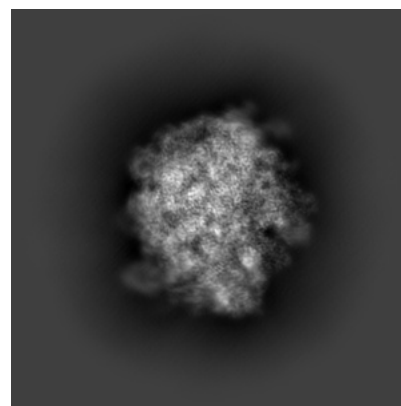
6.1.1 Primary map



X

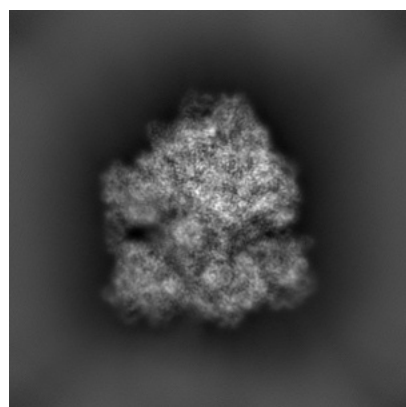


Y

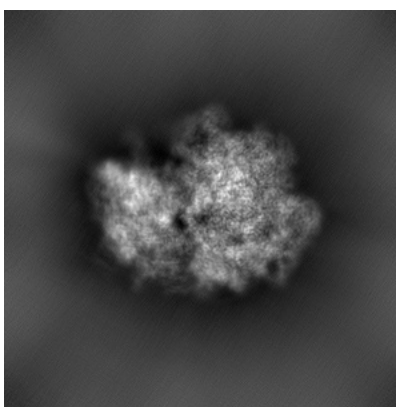


Z

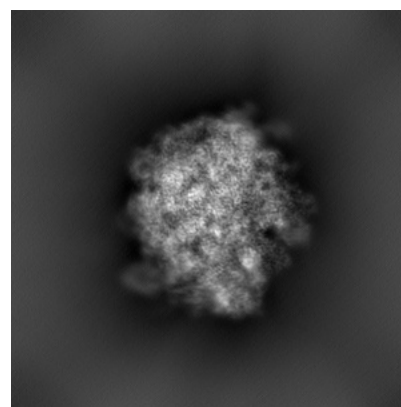
6.1.2 Raw map



X



Y

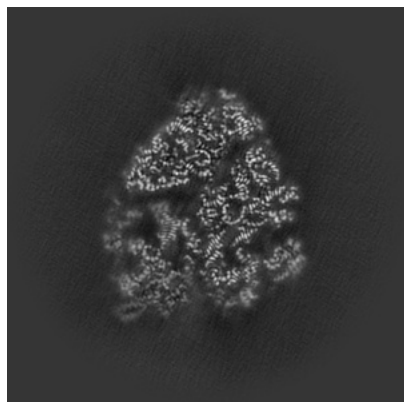


Z

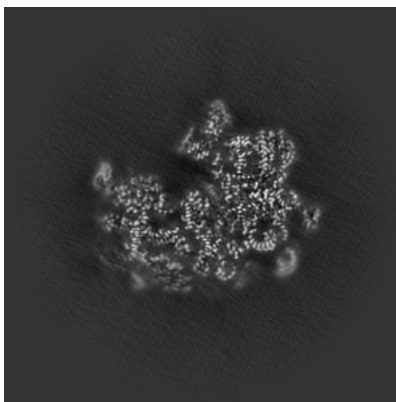
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

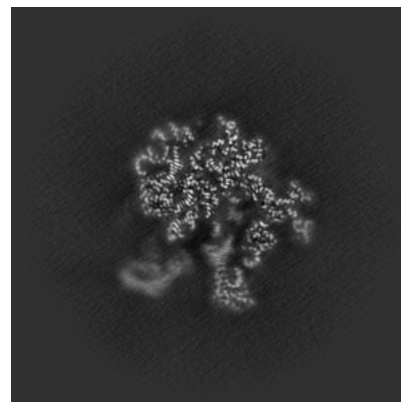
6.2.1 Primary map



X Index: 256

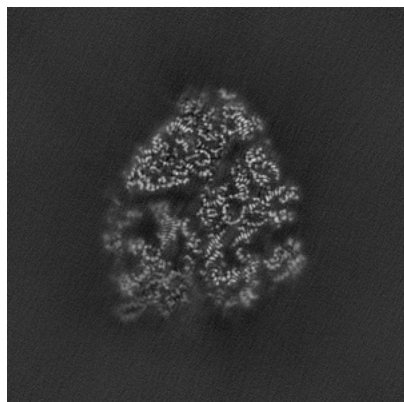


Y Index: 256

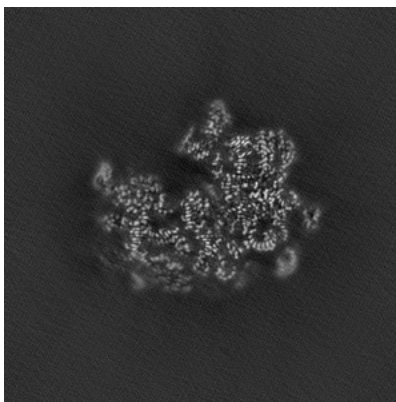


Z Index: 256

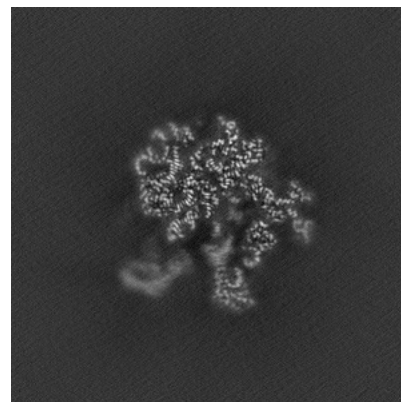
6.2.2 Raw map



X Index: 256



Y Index: 256

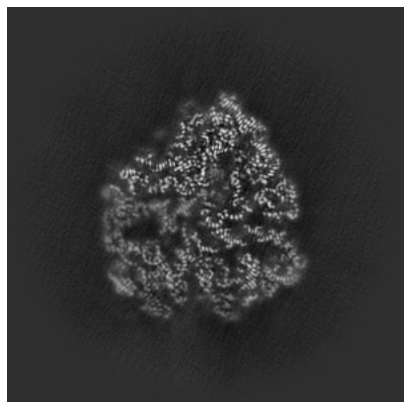


Z Index: 256

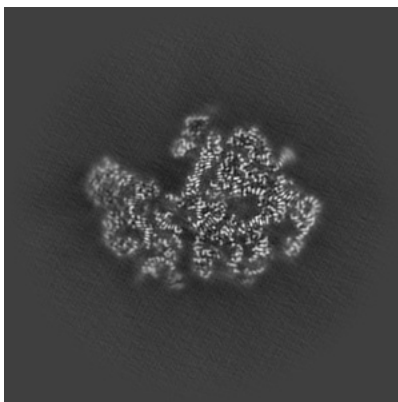
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

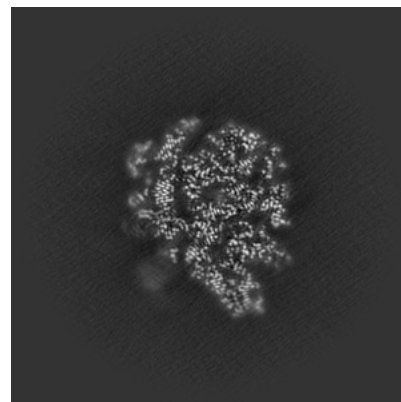
6.3.1 Primary map



X Index: 265

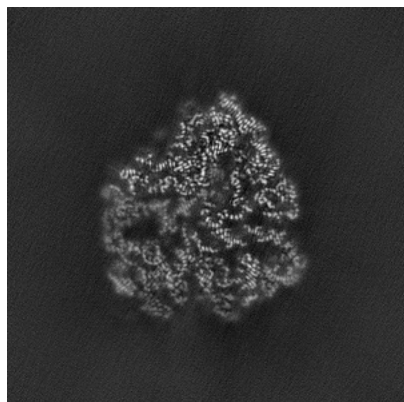


Y Index: 278

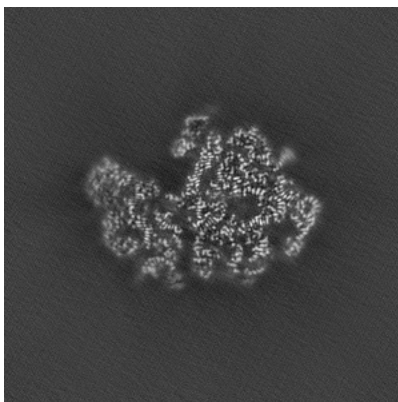


Z Index: 299

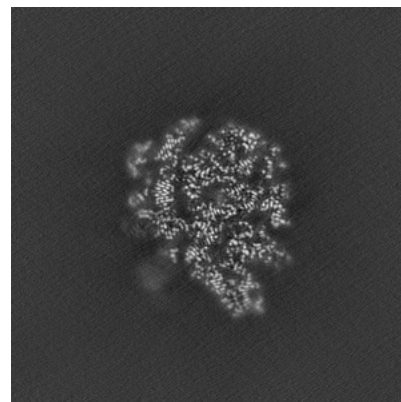
6.3.2 Raw map



X Index: 265



Y Index: 278

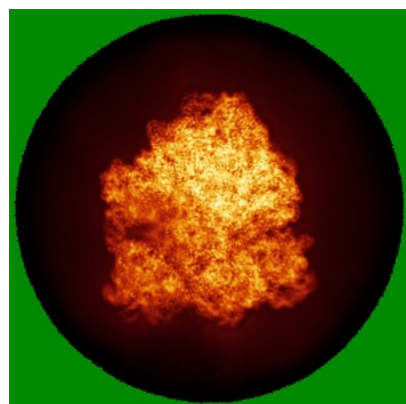


Z Index: 299

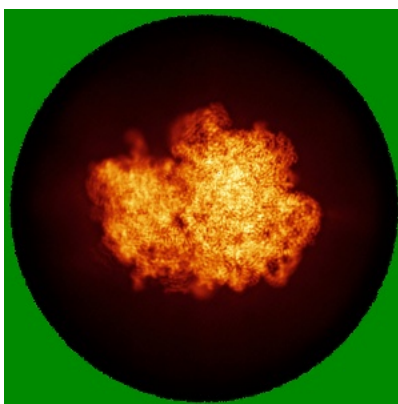
The images above show the largest variance slices of the map in three orthogonal directions.

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

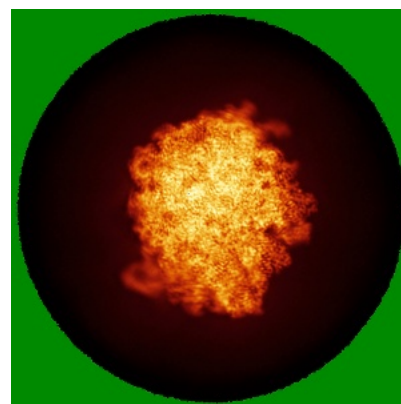
6.4.1 Primary map



X



Y

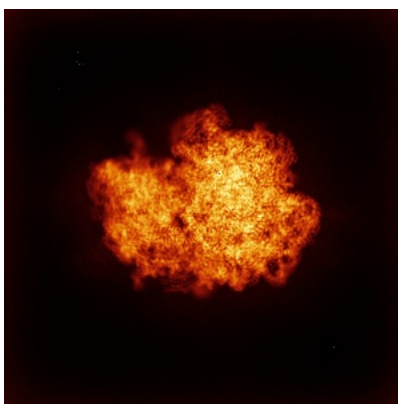


Z

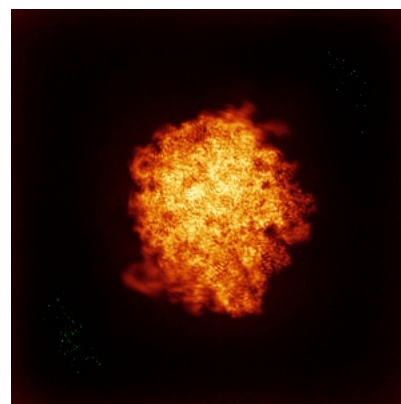
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



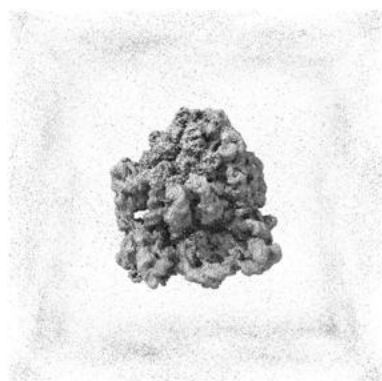
Y



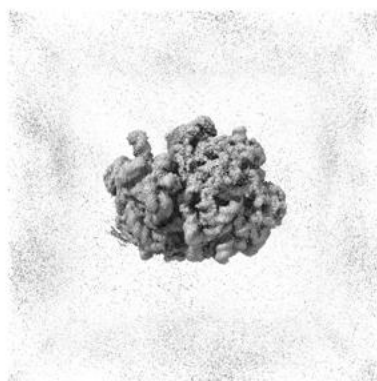
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

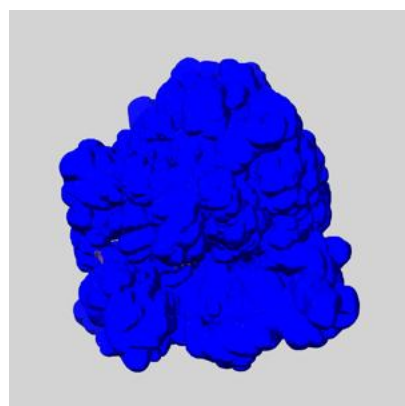
6.6 Mask visualisation [i](#)

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

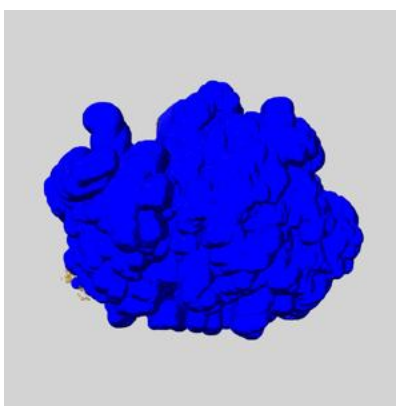
A mask typically either:

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

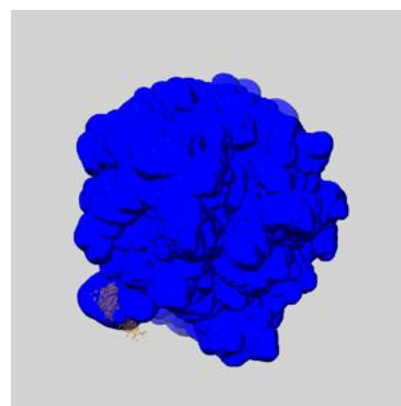
6.6.1 emd_29821_msk_1.map [i](#)



X



Y

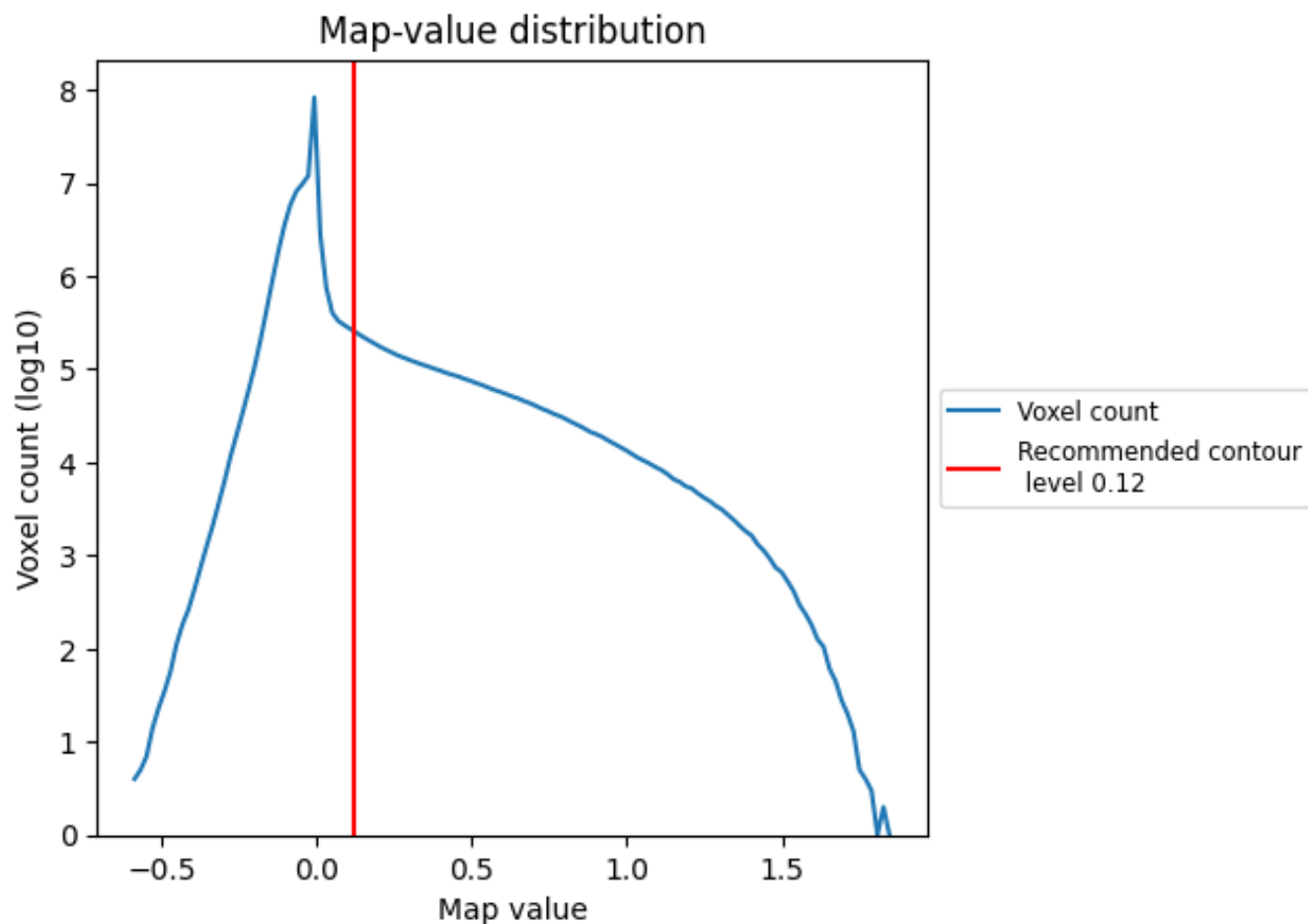


Z

7 Map analysis [i](#)

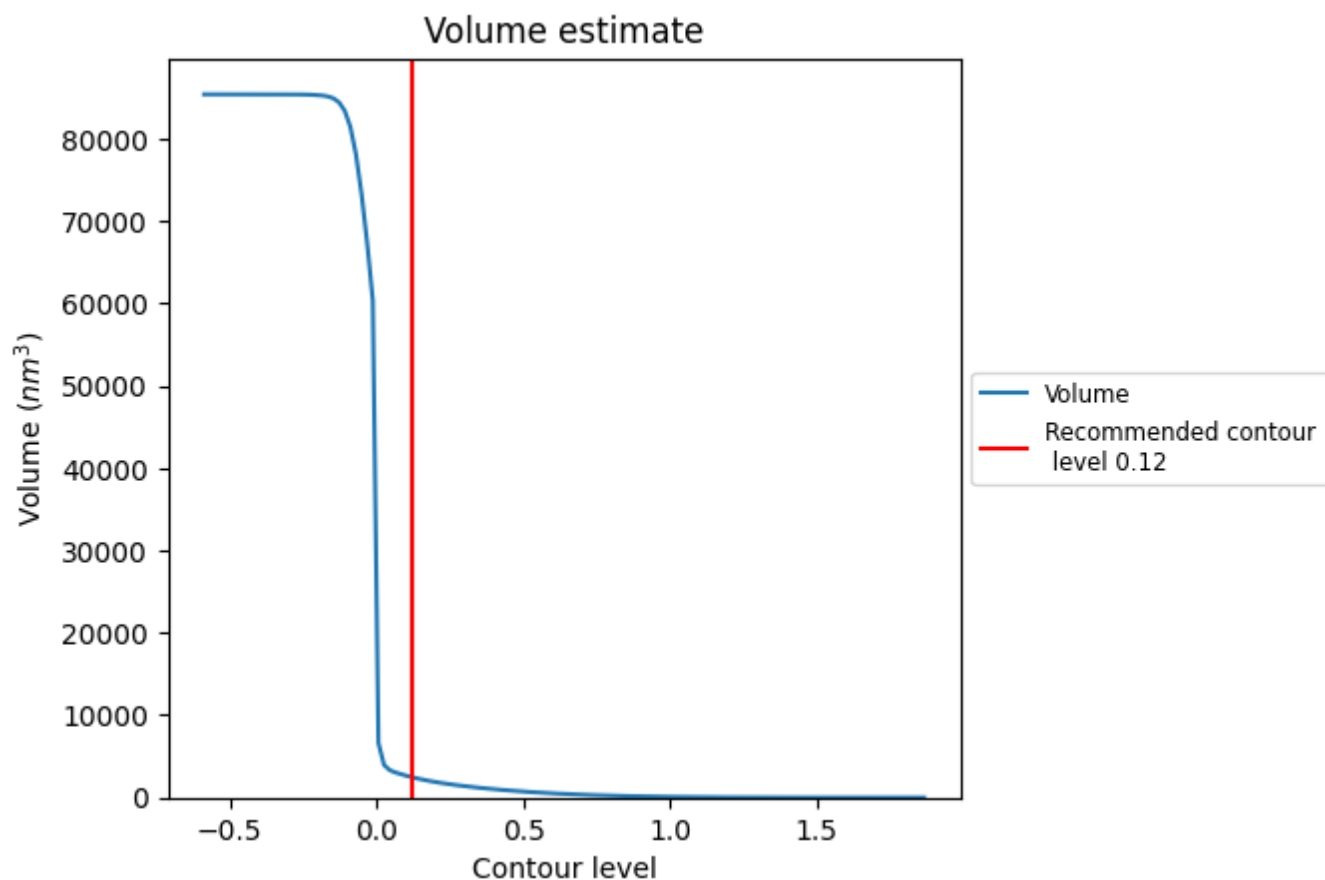
This section contains the results of statistical analysis of the map.

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.

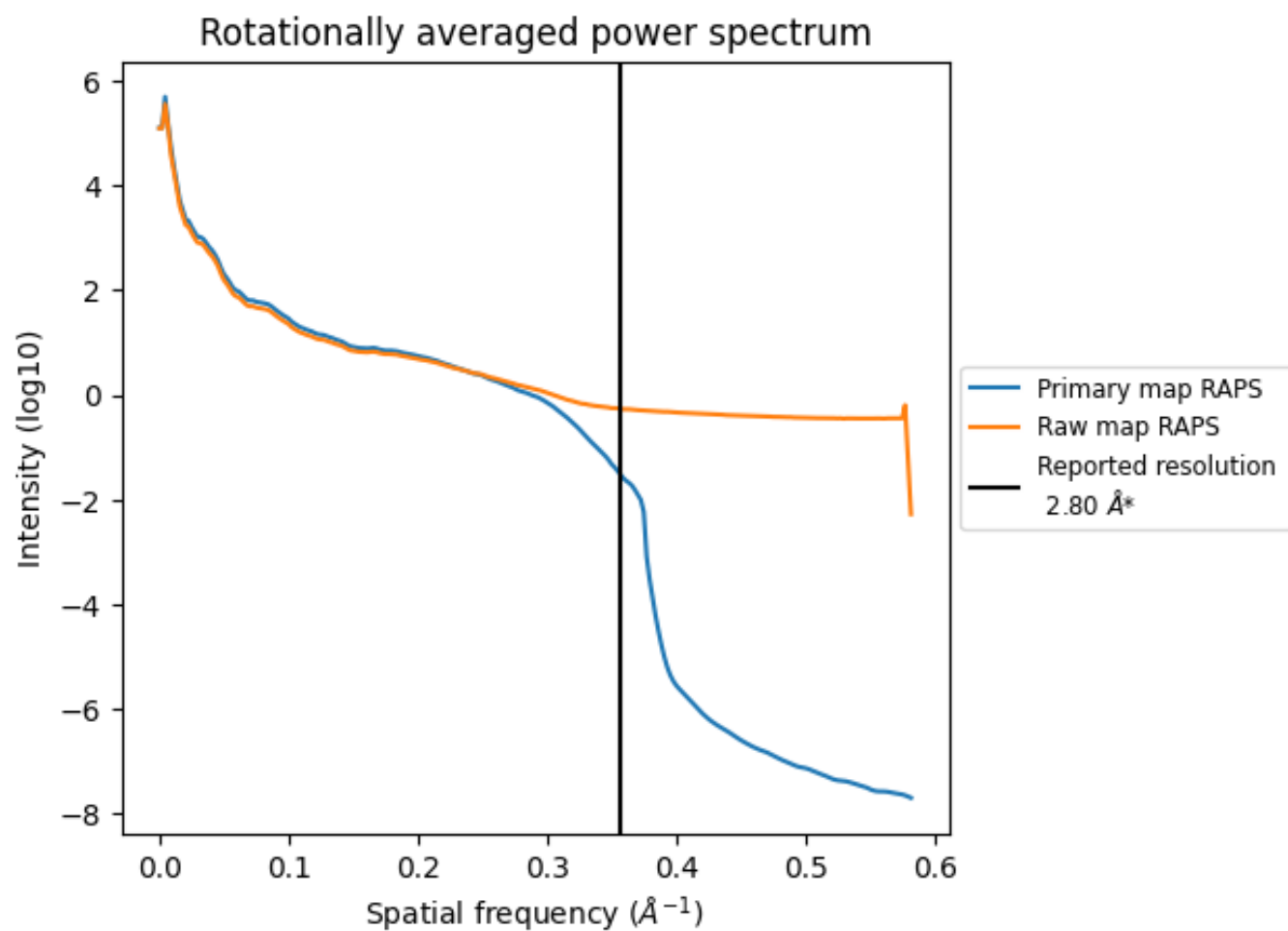
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2483 nm³; this corresponds to an approximate mass of 2243 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 ⓘ

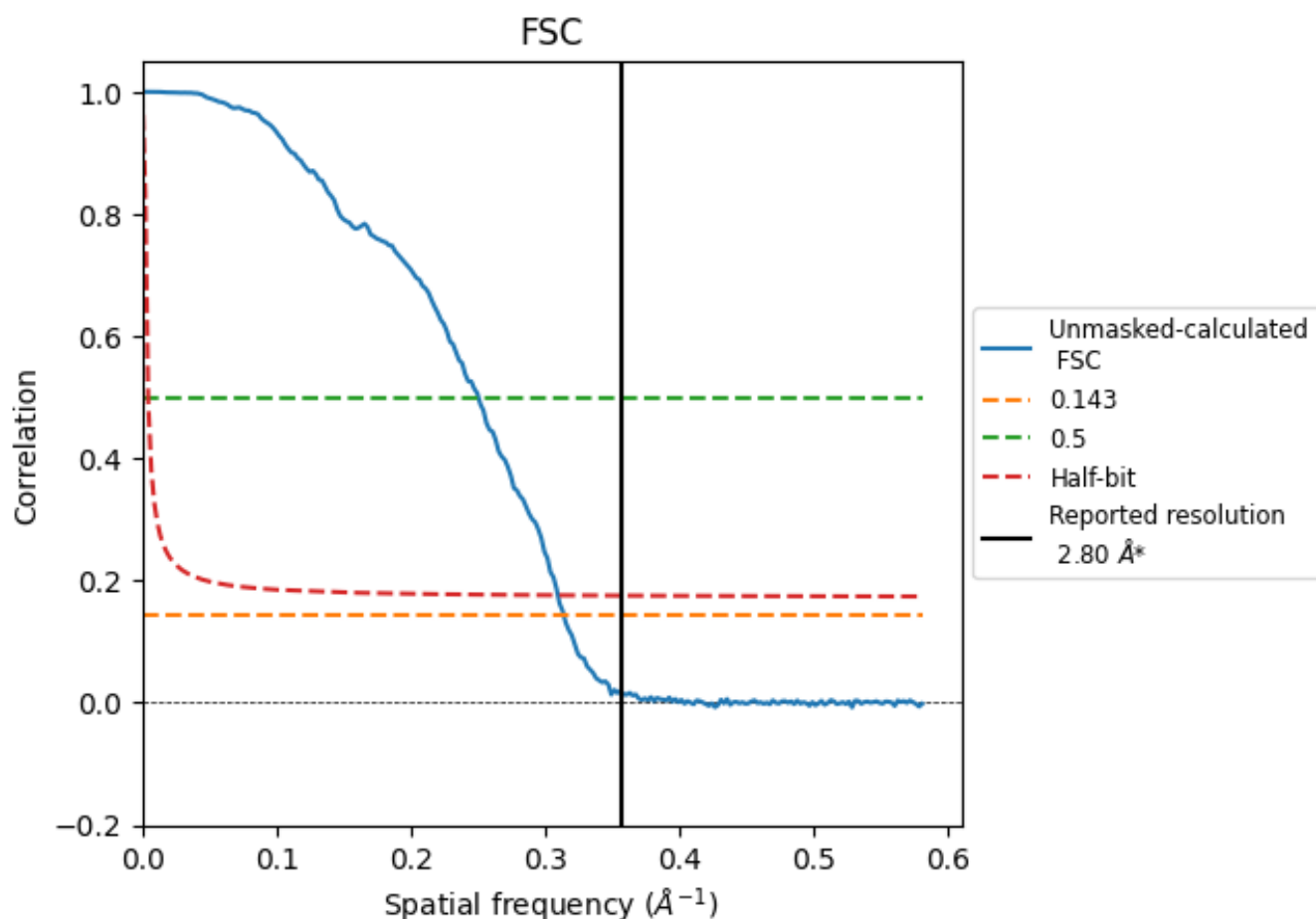


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

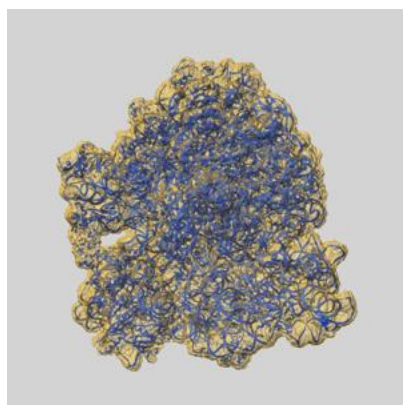
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.99	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.8 by more than 10 %

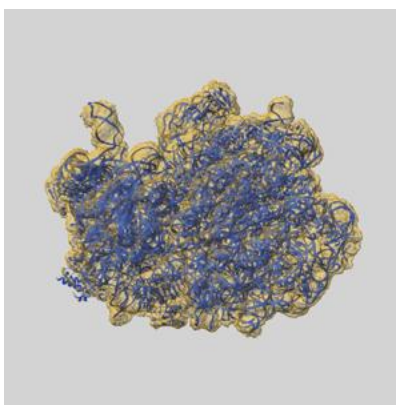
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29821 and PDB model 8G7R. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

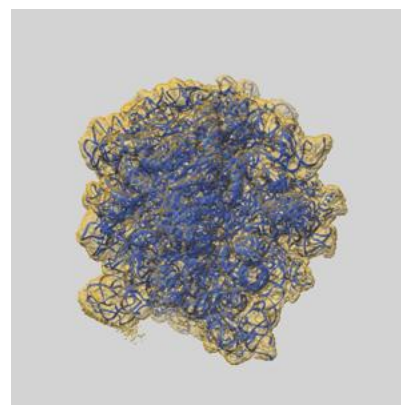
9.1 Map-model overlay [i](#)



X



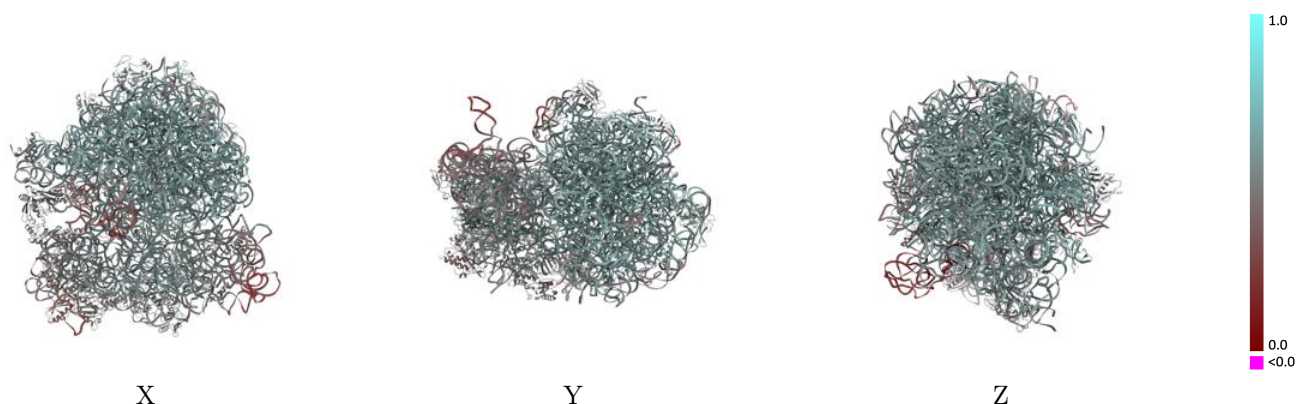
Y



Z

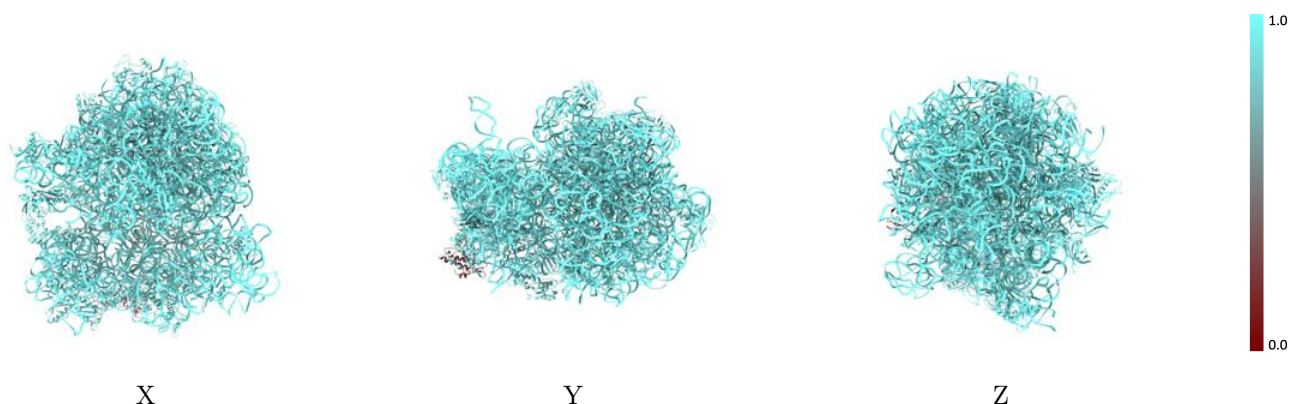
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



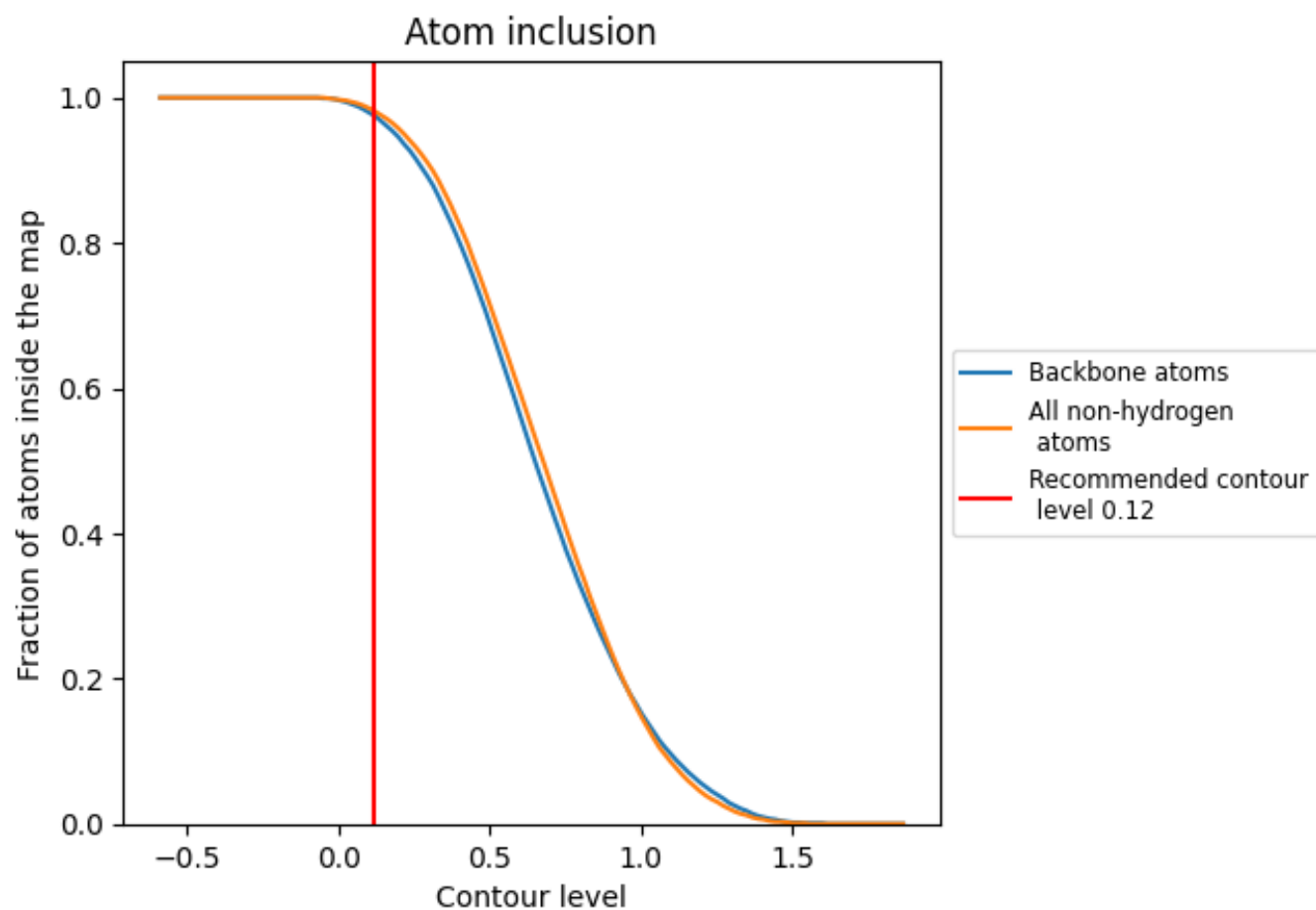
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9820	 0.5340
1	 0.9900	 0.5200
2	 0.9860	 0.5690
3	 0.9570	 0.4440
4	 0.9950	 0.5910
5	 0.9780	 0.5640
6	 0.9830	 0.6030
7	 0.9880	 0.6040
8	 0.9900	 0.5770
A	 0.9990	 0.5640
B	 0.9980	 0.5310
C	 0.9480	 0.5780
D	 0.9960	 0.5880
E	 0.9720	 0.5420
F	 0.9860	 0.4840
G	 0.9820	 0.5160
H	 0.4100	 0.3960
L	 0.9950	 0.5880
M	 0.9880	 0.5880
N	 0.9880	 0.5790
O	 0.9820	 0.5900
P	 0.9980	 0.6020
Q	 0.9940	 0.5280
R	 0.9850	 0.5780
S	 0.9960	 0.5960
T	 0.9770	 0.5710
U	 0.9890	 0.5760
V	 0.9780	 0.5490
W	 0.9940	 0.5310
X	 0.9840	 0.5550
Y	 0.9810	 0.5840
Z	 0.9850	 0.5780
a	 0.9980	 0.5050
b	 0.4140	 0.3940
c	 0.9350	 0.5040



Continued on next page...

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Chain	Atom inclusion	Q-score
d	 0.9650	 0.4770
e	 0.9810	 0.5340
f	 0.9070	 0.4430
g	 0.9710	 0.4350
h	 0.9810	 0.5200
i	 0.9840	 0.4610
j	 0.8870	 0.4450
k	 0.9750	 0.4900
l	 0.9800	 0.5600
m	 0.9830	 0.4720
n	 0.9740	 0.4910
o	 0.9810	 0.4790
p	 0.9840	 0.4920
q	 0.9840	 0.5050
r	 0.9180	 0.4850
s	 0.9910	 0.4720
t	 0.9880	 0.4500
u	 0.7180	 0.4540
v	 1.0000	 0.5510
w	 0.9760	 0.4850
x	 0.9930	 0.4960
y	 0.9550	 0.2960