Full wwPDB EM Validation Report (i)

Nov 4, 2023 – 07:53 PM EDT

PDB ID	:	7S1K
EMDB ID	:	EMD-24804
Title	:	Cfr-modified Escherichia coli stalled ribosome with antibiotic radezolid
Authors	:	Tsai, K.; Stojkovic, V.; Lee, D.J.; Young, I.D.; Szal, T.; Vazquez-Laslop, N.; Mankin, A.S.; Fraser, J.S.; Galonic Fujimori, D.
Deposited on	:	2021-09-02
Resolution	:	2.42 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

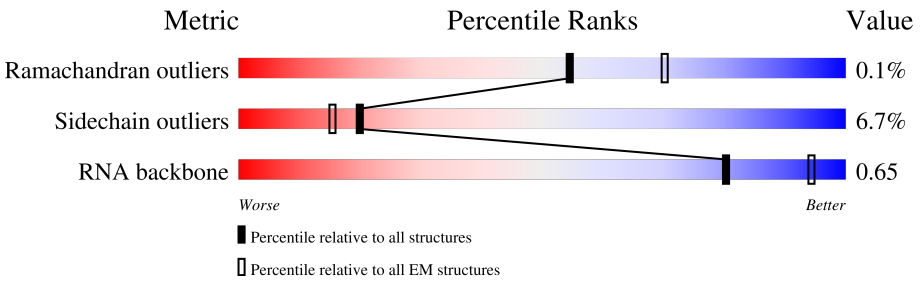
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.42 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	92	• 83% • 14%
2	2	87	5% 93% 5% •
3	3	71	23% 89% 10% •
4	4	15	40% 60%
5	A	76	• 72% 26% •
6	C	1540	• 87% 13%
7	D	240	7% 85% 5% 9%
8	E	233	• 82% 6% 12%

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Mol	Chain	Length	Quality of chain
9	F	206	6% 96%
10	G	167	84% 6% 10%
11	H	135	70% 26%
12	I	2904	85% 14%
13	J	120	89% 9%
14	K	273	95%
15	L	209	97%
16	M	201	97%
17	N	179	89% 9%
18	O	177	93% 7%
19	P	149	24% 95% 5%
20	Q	70	77% 9% 14%
21	R	142	96%
22	S	123	95%
23	T	144	98%
24	U	136	93% 7%
25	V	127	92% 6%
26	W	117	93% 6%
27	X	115	96%
28	Y	118	98%
29	Z	103	97%
30	a	110	95% 5%
31	b	100	85% 8% 7%
32	c	104	5% 93% 5%
33	d	94	89% 11%

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Mol	Chain	Length	Quality of chain
34	e	85	85% 12%
35	f	78	94% 5%
36	g	63	6% 87% 11%
37	h	59	93% 5%
38	i	57	93% 5%
39	j	55	13% 82% 9% 9%
40	k	46	98%
41	l	65	95%
42	m	38	5% 92% 8%
43	n	179	7% 81% 16%
44	o	130	92% 8%
45	p	130	8% 92% 6%
46	q	103	26% 87% 8% 5%
47	r	129	88% 9%
48	s	5	60% 100%
49	t	124	96%
50	u	118	93%
51	v	101	6% 76% 16% 5%
52	w	89	88% 11%
53	x	82	89% 11%
54	y	84	87% 8% 5%
55	z	75	72% 27%

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 240884 atoms, of which 96713 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	1	79	1303	408	666	120	107	2	0	0

- Molecule 2 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	2	85	1380	411	715	137	114	3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	3	70	1219	366	629	125	98	1	0	0

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
4	4	6	190	56	65	20	43	6	0	0

- Molecule 5 is a RNA chain called tRNA(PHE).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
5	A	76	2444	724	820	292	532	76	0	0

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	C	1540	49665	14735	16628	6057	10705	1540	0	0

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	D	218	3438	1081	1734	305	311	7	0	0

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	E	206	3321	1028	1697	305	288	3	0	0

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	F	205	3352	1026	1709	315	298	4	0	0

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	G	150	2255	687	1150	211	201	6	0	0

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	H	100	1625	515	808	148	148	6	0	0

- Molecule 12 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
12	I	2898	93582	27778	31332	11450	20123	2899	1	0

- Molecule 13 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
13	J	118	3809	1126	1280	464	821	118	0	0

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	K	271	4263	1294	2170	427	365	7	2	0

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	L	209	3184	979	1619	288	294	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	M	201	3172	974	1620	283	290	5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	N	177	2855	899	1445	249	256	6	0	0

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	O	176	2696	832	1373	243	246	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	P	149	2259	699	1148	197	214	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	Q	60	963	299	483	90	85	6	0	0

- Molecule 21 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	R	142	2292	714	1163	212	199	4	0	0

- Molecule 22 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	S	122	1950	587	1012	180	165	6	0	0

- Molecule 23 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	T	144	2182	654	1129	207	190	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	U	136	2231	686	1156	205	178	6	0	0

- Molecule 25 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	V	120	1960	593	1000	196	166	5	0	0

- Molecule 26 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
26	W	116	1817	552	925	178	162	0	0

- Molecule 27 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	X	114	1880	574	963	179	163	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
28	Y	117	1968	604	1021	192	151	0	0

- Molecule 29 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	Z	103	1657	516	841	153	145	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	a	110	1780	532	923	166	156	3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	b	93	1546	466	808	139	131	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
32	c	102	1612	492	833	146	141	0	0

- Molecule 33 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	d	94	1534	479	781	137	134	3	0	0

- Molecule 34 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	e	75	1168	356	593	116	102	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	f	77	1278	388	653	129	106	2	0	0

- Molecule 36 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	g	62	1033	308	532	98	94	1	0	0

- Molecule 37 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	h	58	938	281	489	87	79	2	0	0

- Molecule 38 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	i	56	904	269	460	94	80	1	0	0

- Molecule 39 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
39	j	50	851	263	442	75	71	0	0

- Molecule 40 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	k	46	795	228	418	90	57	2	0	0

- Molecule 41 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	l	64	1077	323	573	105	74	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	m	38	645	185	343	65	48	4	0	0

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	n	151	2419	735	1238	227	215	4	0	0

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	o	129	2011	616	1032	173	184	6	0	0

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	p	127	2093	634	1071	206	179	3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	q	98	1615	493	829	150	142	1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	r	117	1765	540	888	174	160	3	0	0

- Molecule 48 is a protein called nascent peptide chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	s	5	91	32	47	6	5	1	0	0

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	t	123	1972	590	1017	196	165	4	0	0

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	u	115	1845	552	954	179	157	3	0	0

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	v	96	1600	483	826	160	128	3	0	0

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	w	88	1441	437	731	143	129	1	0	0

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	x	82	1315	406	666	128	114	1	0	0

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	y	80	1341	411	693	121	113	3	0	0

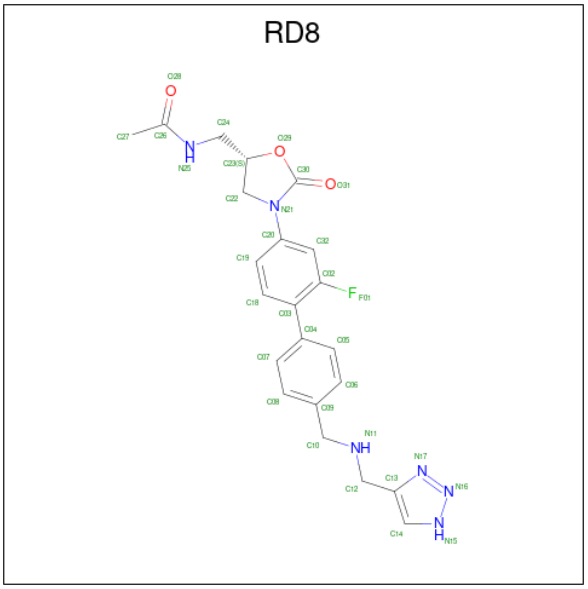
- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
55	z	55	934	288	479	86	81	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	C	90	90	90	0
56	I	112	112	112	0
56	K	2	2	2	0
56	L	1	1	1	0
56	V	1	1	1	0
56	v	1	1	1	0

- Molecule 57 is Radezolid (three-letter code: RD8) (formula: $C_{22}H_{23}FN_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
57	I	1	55	22	1	23	6	3	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
58	Q	1	1	1	0
58	m	1	1	1	0

- Molecule 59 is water.

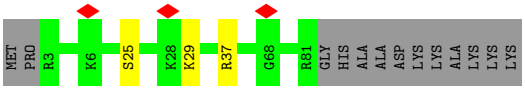
Mol	Chain	Residues	Atoms			AltConf
			Total	H	O	
59	C	3	9	6	3	0
59	I	32	96	64	32	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

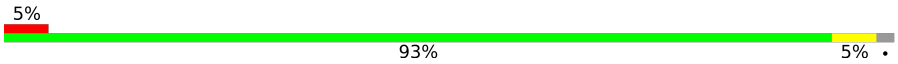
- Molecule 1: 30S ribosomal protein S19

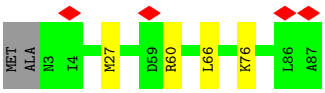
Chain 1:



- Molecule 2: 30S ribosomal protein S20

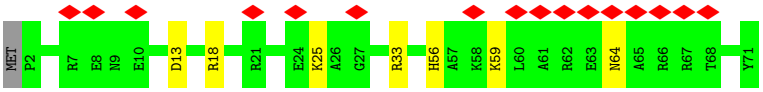
Chain 2:





- Molecule 3: 30S ribosomal protein S21

Chain 3:

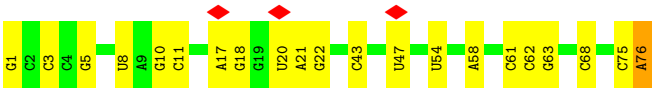


- Molecule 4: mRNA

Chain 4:

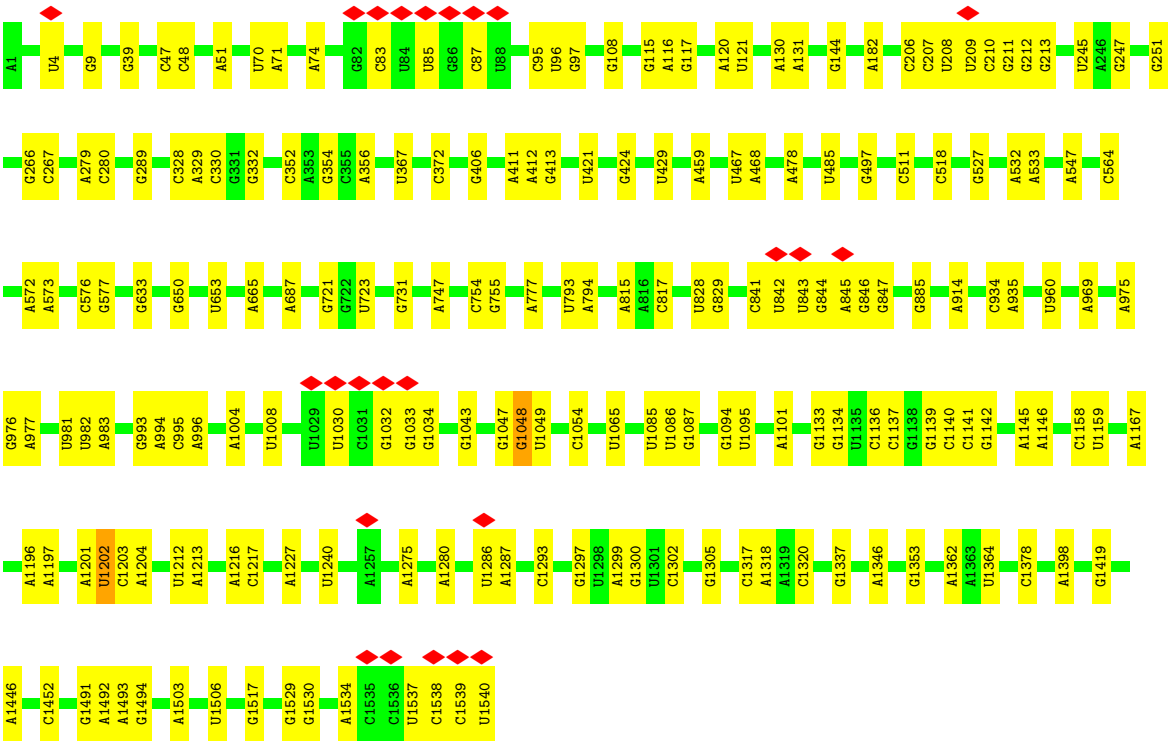
- Molecule 5: tRNA(PHE)

Chain A:



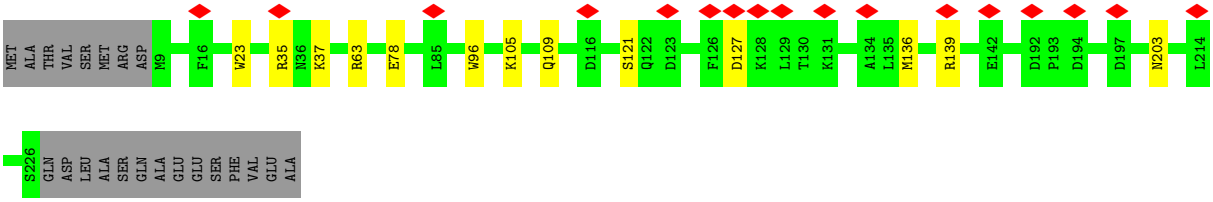
- Molecule 6: 16S rRNA

Chain C:



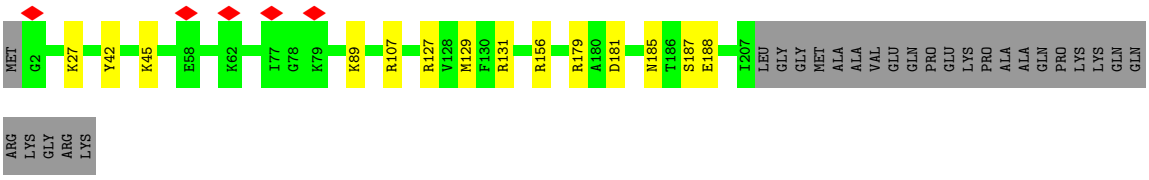
- Molecule 7: 30S ribosomal protein S2

Chain D:



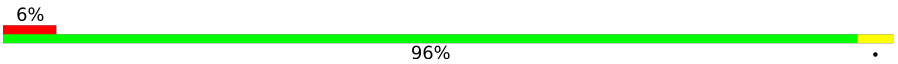
- Molecule 8: 30S ribosomal protein S3

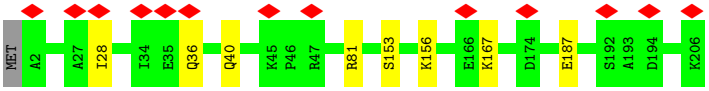
Chain E:



- Molecule 9: 30S ribosomal protein S4

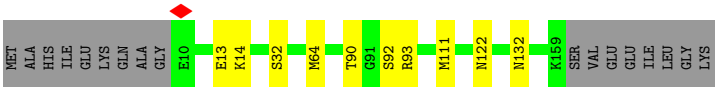
Chain F:





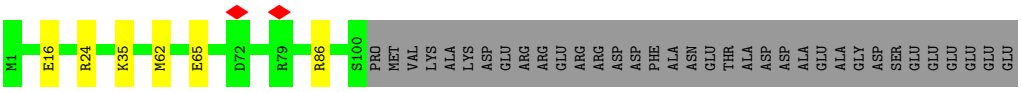
• Molecule 10: 30S ribosomal protein S5

Chain G:



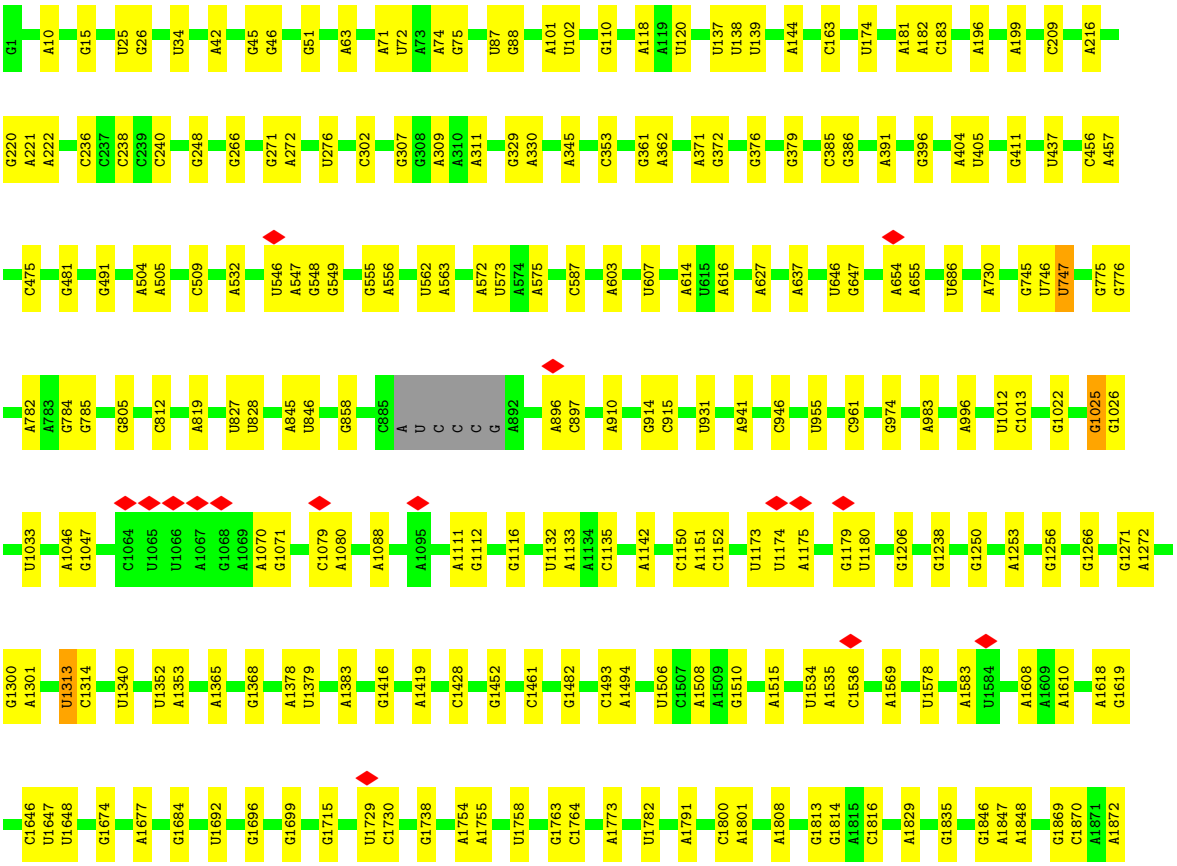
• Molecule 11: 30S ribosomal protein S6

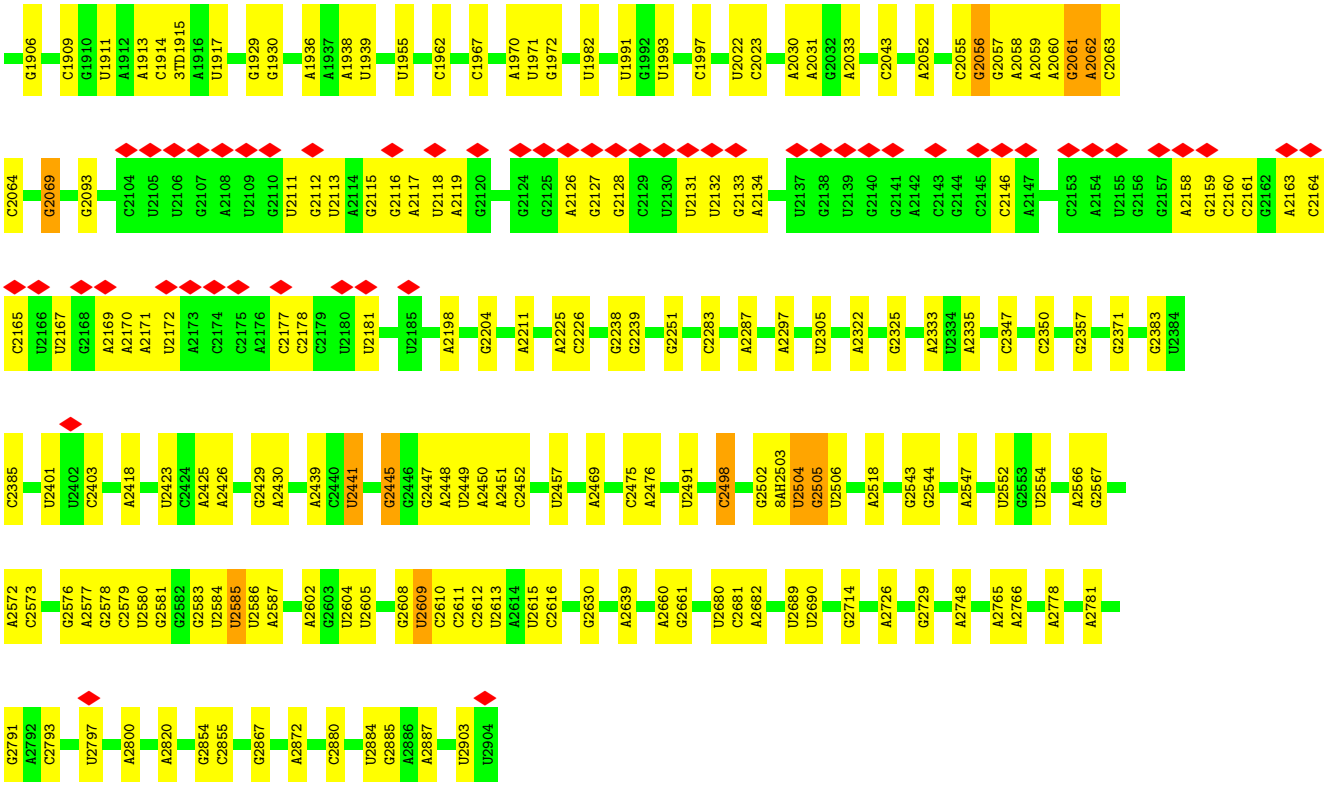
Chain H:



• Molecule 12: 23S rRNA

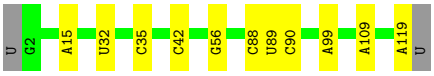
Chain I:





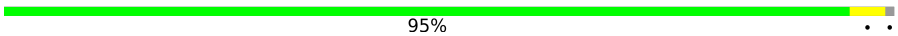
- Molecule 13: 5S rRNA

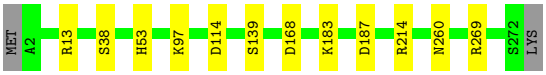
Chain J:



- Molecule 14: 50S ribosomal protein L2

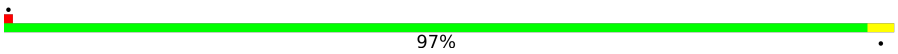
Chain K:

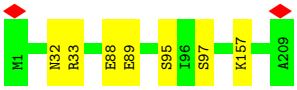




- Molecule 15: 50S ribosomal protein L3

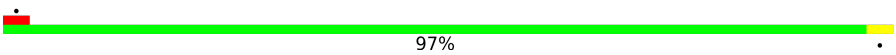
Chain L:

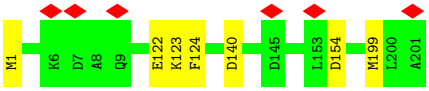




- Molecule 16: 50S ribosomal protein L4

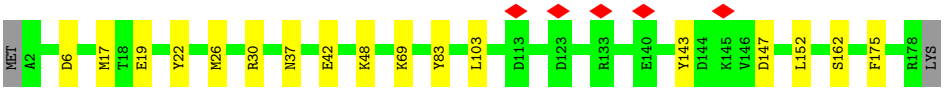
Chain M:





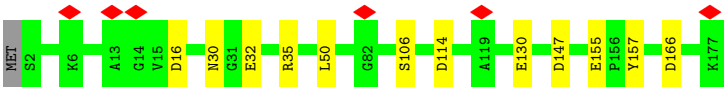
• Molecule 17: 50S ribosomal protein L5

Chain N:



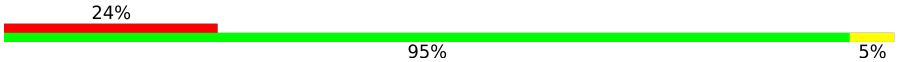
• Molecule 18: 50S ribosomal protein L6

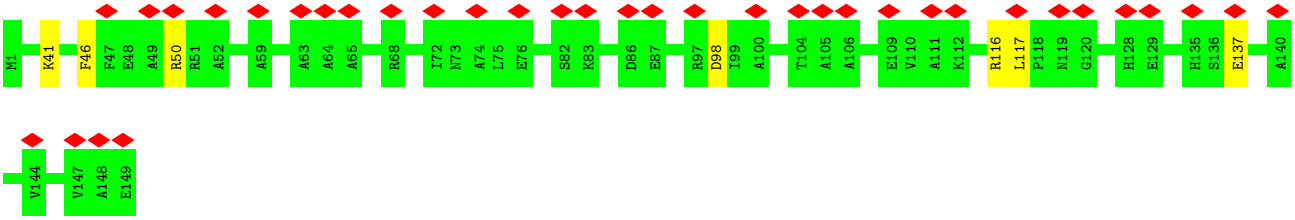
Chain O:



• Molecule 19: 50S ribosomal protein L9

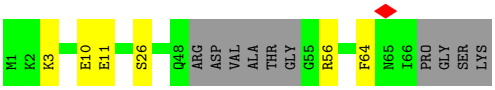
Chain P:





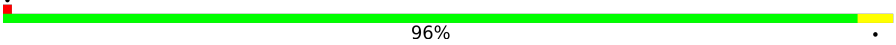
• Molecule 20: 50S ribosomal protein L31

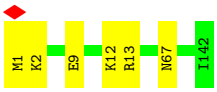
Chain Q:



• Molecule 21: 50S ribosomal protein L13

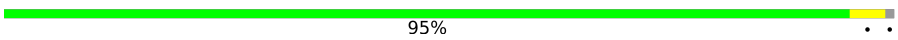
Chain R:

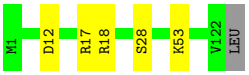




• Molecule 22: 50S ribosomal protein L14

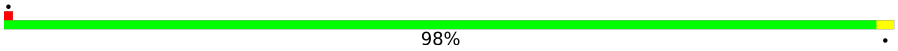
Chain S:

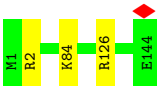




• Molecule 23: 50S ribosomal protein L15

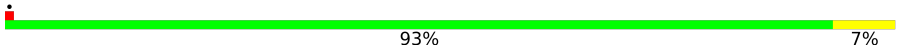
Chain T:

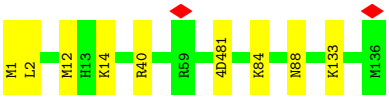




• Molecule 24: 50S ribosomal protein L16

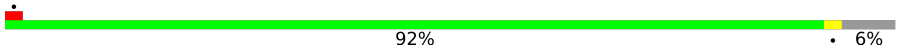
Chain U:

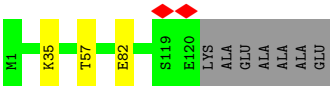




• Molecule 25: 50S ribosomal protein L17

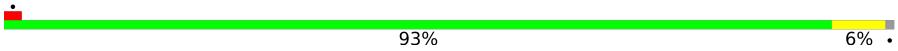
Chain V:

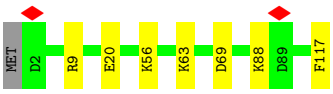




• Molecule 26: 50S ribosomal protein L18

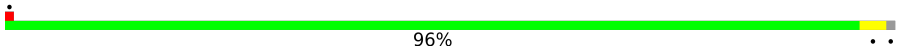
Chain W:

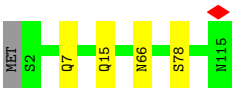




• Molecule 27: 50S ribosomal protein L19

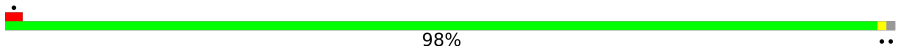
Chain X:

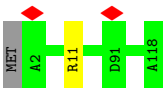




• Molecule 28: 50S ribosomal protein L20

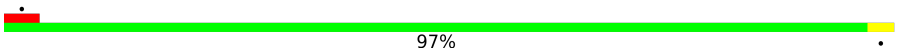
Chain Y:

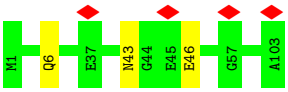




• Molecule 29: Ribosomal protein L21

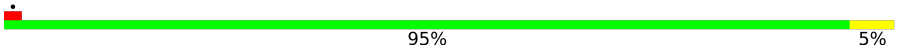
Chain Z:

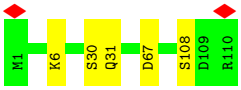




• Molecule 30: 50S ribosomal protein L22

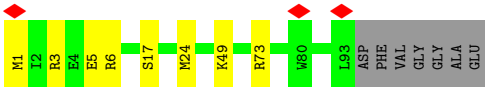
Chain a:





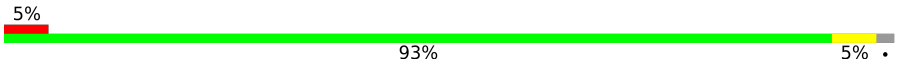
• Molecule 31: 50S ribosomal protein L23

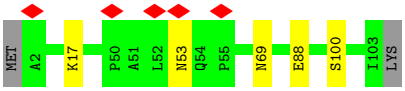
Chain b:



• Molecule 32: 50S ribosomal protein L24

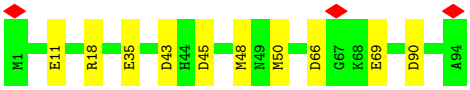
Chain c:





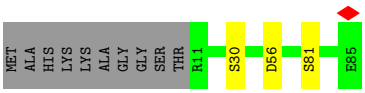
• Molecule 33: 50S ribosomal protein L25

Chain d:



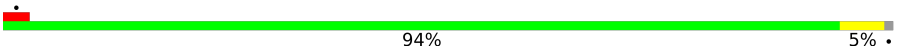
• Molecule 34: 50S ribosomal protein L27

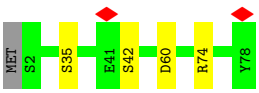
Chain e:



• Molecule 35: 50S ribosomal protein L28

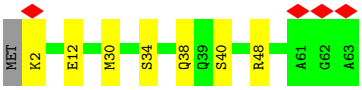
Chain f:





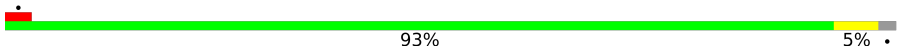
• Molecule 36: 50S ribosomal protein L29

Chain g:



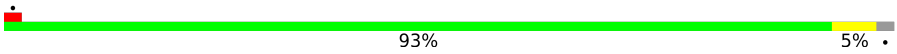
• Molecule 37: 50S ribosomal protein L30

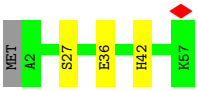
Chain h:



• Molecule 38: 50S ribosomal protein L32

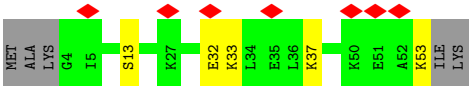
Chain i:





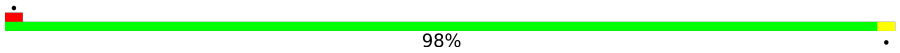
• Molecule 39: 50S ribosomal protein L33

Chain j:



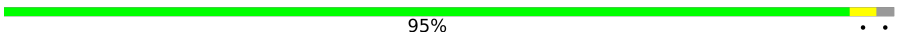
• Molecule 40: 50S ribosomal protein L34

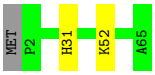
Chain k:



• Molecule 41: 50S ribosomal protein L35

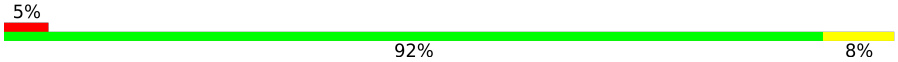
Chain l:





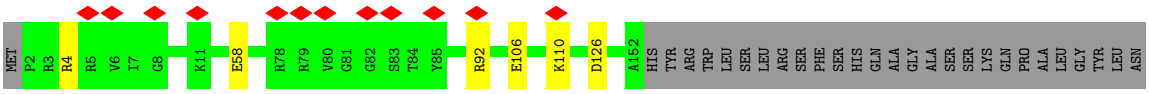
• Molecule 42: 50S ribosomal protein L36

Chain m:



• Molecule 43: 30S ribosomal protein S7

Chain n:

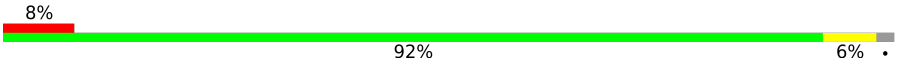


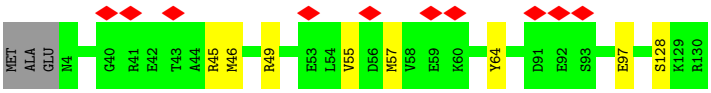
• Molecule 44: 30S ribosomal protein S8

Chain o:

• Molecule 45: 30S ribosomal protein S9

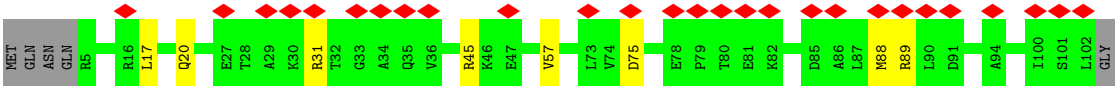
Chain p:





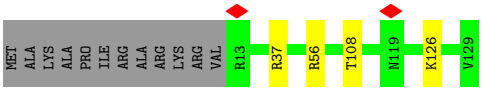
• Molecule 46: 30S ribosomal protein S10

Chain q:



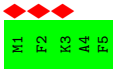
• Molecule 47: 30S ribosomal protein S11

Chain r:



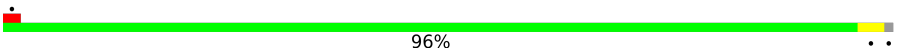
• Molecule 48: nascent peptide chain

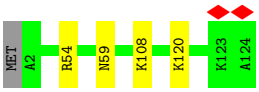
Chain s:



• Molecule 49: 30S ribosomal protein S12

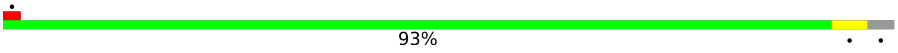
Chain t:

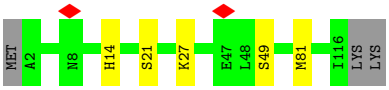




• Molecule 50: 30S ribosomal protein S13

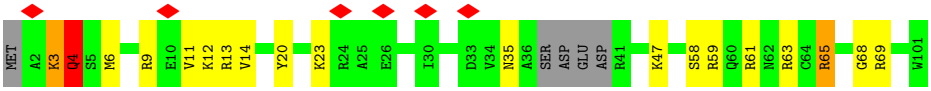
Chain u:





• Molecule 51: 30S ribosomal protein S14

Chain v:

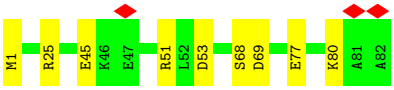


• Molecule 52: 30S ribosomal protein S15

Chain w:

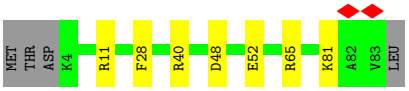
• Molecule 53: 30S ribosomal protein S16

Chain x:



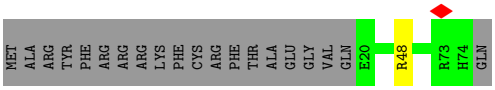
• Molecule 54: 30S ribosomal protein S17

Chain y:



• Molecule 55: 30S ribosomal protein S18

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	276799	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	69	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	23.504	Depositor
Minimum map value	-10.961	Depositor
Average map value	-0.028	Depositor
Map value standard deviation	0.776	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	422.9632, 422.9632, 422.9632	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8261, 0.8261, 0.8261	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, 5MU, 3TD, 8AH, OMC, 5MC, H2U, RD8, 2MG, 4D4, 1MG, OMG, OMU, ZN, G7M, MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	1	0.25	0/652	0.53	0/877
2	2	0.24	0/671	0.55	0/888
3	3	0.27	0/598	0.64	0/792
4	4	0.17	0/138	0.66	0/212
5	A	0.62	8/1815 (0.4%)	0.86	11/2828 (0.4%)
6	C	0.37	46/36991 (0.1%)	0.72	56/57705 (0.1%)
7	D	0.25	0/1735	0.51	0/2338
8	E	0.42	0/1651	0.61	0/2225
9	F	0.25	0/1665	0.55	0/2227
10	G	0.26	0/1118	0.57	0/1504
11	H	0.26	0/835	0.57	0/1128
12	I	0.41	117/69143 (0.2%)	0.73	139/107862 (0.1%)
13	J	0.15	0/2828	0.65	0/4410
14	K	0.25	0/2139	0.58	0/2876
15	L	0.26	0/1586	0.53	0/2134
16	M	0.26	0/1571	0.53	0/2113
17	N	0.26	0/1434	0.55	0/1926
18	O	0.25	0/1343	0.52	0/1816
19	P	0.26	0/1122	0.52	0/1515
20	Q	0.26	0/488	0.54	0/649
21	R	0.26	0/1152	0.52	0/1551
22	S	0.27	0/947	0.60	0/1268
23	T	0.26	0/1062	0.59	0/1413
24	U	0.26	0/1081	0.60	0/1443
25	V	0.24	0/973	0.57	0/1301
26	W	0.26	0/902	0.59	0/1209
27	X	0.25	0/929	0.56	0/1242
28	Y	0.25	0/960	0.54	0/1278
29	Z	0.27	0/829	0.56	0/1107
30	a	0.24	0/864	0.54	0/1156
31	b	0.24	0/744	0.54	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.25	0/787	0.53	0/1051
33	d	0.27	0/766	0.55	0/1025
34	e	0.26	0/582	0.57	0/769
35	f	0.24	0/635	0.58	0/848
36	g	0.27	0/502	0.55	0/667
37	h	0.24	0/453	0.56	0/605
38	i	0.23	0/450	0.57	0/599
39	j	0.27	0/416	0.55	0/554
40	k	0.25	0/380	0.67	0/498
41	l	0.24	0/513	0.57	0/676
42	m	0.27	0/303	0.64	0/397
43	n	0.24	0/1195	0.54	0/1602
44	o	0.25	0/989	0.53	0/1326
45	p	0.26	0/1034	0.64	0/1375
46	q	0.24	0/796	0.63	0/1077
47	r	0.26	0/893	0.57	0/1205
48	s	0.88	0/45	0.92	0/57
49	t	0.24	0/969	0.59	0/1300
50	u	0.23	0/900	0.60	0/1204
51	v	1.51	21/785 (2.7%)	1.31	10/1043 (1.0%)
52	w	0.23	0/718	0.54	0/959
53	x	0.27	0/659	0.57	0/884
54	y	0.26	0/657	0.58	0/881
55	z	0.25	0/462	0.54	0/621
All	All	0.38	192/155855 (0.1%)	0.69	216/233210 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
51	v	0	2

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1216	A	C6-N6	-11.51	1.24	1.33
6	C	1204	A	C6-N6	-11.45	1.24	1.33
6	C	994	A	C6-N6	-11.34	1.24	1.33
12	I	2450	A	C6-N6	-11.30	1.25	1.33
5	A	76	A	C6-N6	-11.27	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	2587	A	C6-N6	-11.24	1.25	1.33
12	I	2451	A	C6-N6	-11.23	1.25	1.33
12	I	2059	A	C6-N6	-11.21	1.25	1.33
12	I	2439	A	C6-N6	-11.17	1.25	1.33
12	I	2577	A	C6-N6	-11.12	1.25	1.33
12	I	2058	A	C6-N6	-11.06	1.25	1.33
12	I	2062	A	C6-N6	-10.97	1.25	1.33
6	C	996	A	C6-N6	-10.57	1.25	1.33
6	C	1203	C	C4-N4	-10.24	1.24	1.33
6	C	1217	C	C4-N4	-10.16	1.24	1.33
6	C	995	C	C4-N4	-10.15	1.24	1.33
12	I	2452	C	C4-N4	-10.03	1.25	1.33
12	I	2611	C	C4-N4	-9.94	1.25	1.33
12	I	2063	C	C4-N4	-9.91	1.25	1.33
12	I	2610	C	C4-N4	-9.89	1.25	1.33
5	A	75	C	C4-N4	-9.88	1.25	1.33
12	I	2612	C	C4-N4	-9.87	1.25	1.33
12	I	2579	C	C5-C6	-9.82	1.26	1.34
12	I	2579	C	C4-N4	-9.81	1.25	1.33
12	I	2452	C	C5-C6	-9.81	1.26	1.34
12	I	2063	C	C5-C6	-9.80	1.26	1.34
12	I	2064	C	C4-N4	-9.80	1.25	1.33
12	I	2610	C	C5-C6	-9.78	1.26	1.34
12	I	2611	C	C5-C6	-9.76	1.26	1.34
12	I	2612	C	C5-C6	-9.69	1.26	1.34
12	I	2064	C	C5-C6	-9.63	1.26	1.34
6	C	1203	C	C5-C6	-9.61	1.26	1.34
5	A	75	C	C5-C6	-9.51	1.26	1.34
6	C	1217	C	C5-C6	-9.49	1.26	1.34
6	C	995	C	C5-C6	-9.48	1.26	1.34
6	C	1047	G	C2-N2	-9.09	1.25	1.34
6	C	1048	G	C2-N2	-9.06	1.25	1.34
12	I	2056	G	C2-N2	-9.06	1.25	1.34
12	I	2583	G	C2-N2	-9.02	1.25	1.34
12	I	2608	G	C2-N2	-8.96	1.25	1.34
12	I	2057	G	C2-N2	-8.94	1.25	1.34
12	I	2581	G	C2-N2	-8.89	1.25	1.34
12	I	2061	G	C2-N2	-8.86	1.25	1.34
12	I	2576	G	C2-N2	-8.85	1.25	1.34
12	I	2505	G	C2-N2	-8.78	1.25	1.34
12	I	2586	U	C5-C6	-8.52	1.26	1.34
12	I	2584	U	C5-C6	-8.40	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	1782	U	C5-C6	-8.36	1.26	1.34
12	I	2585	U	C5-C6	-8.36	1.26	1.34
6	C	982	U	C5-C6	-8.32	1.26	1.34
6	C	981	U	C5-C6	-8.31	1.26	1.34
12	I	2441	U	C5-C6	-8.27	1.26	1.34
12	I	2609	U	C5-C6	-8.27	1.26	1.34
6	C	1049	U	C5-C6	-8.25	1.26	1.34
12	I	2506[A]	U	C5-C6	-8.19	1.26	1.34
12	I	2506[B]	U	C5-C6	-8.19	1.26	1.34
6	C	1202	U	C5-C6	-8.12	1.26	1.34
12	I	2061	G	C8-N7	-7.34	1.26	1.30
51	v	63	ARG	CZ-NH1	-7.29	1.23	1.33
51	v	9	ARG	CZ-NH1	-7.27	1.23	1.33
12	I	2576	G	C8-N7	-7.26	1.26	1.30
51	v	13	ARG	CZ-NH1	-7.26	1.23	1.33
51	v	61	ARG	CZ-NH1	-7.25	1.23	1.33
51	v	65	ARG	CZ-NH1	-7.23	1.23	1.33
12	I	2581	G	C8-N7	-7.20	1.26	1.30
51	v	69	ARG	CZ-NH1	-7.18	1.23	1.33
12	I	2056	G	C8-N7	-7.05	1.26	1.30
12	I	2057	G	C8-N7	-6.96	1.26	1.30
6	C	1048	G	C8-N7	-6.85	1.26	1.30
12	I	2608	G	C8-N7	-6.84	1.26	1.30
12	I	2583	G	C8-N7	-6.84	1.26	1.30
12	I	2505	G	C8-N7	-6.81	1.26	1.30
51	v	65	ARG	CZ-NH2	-6.78	1.24	1.33
51	v	69	ARG	CZ-NH2	-6.76	1.24	1.33
51	v	9	ARG	CZ-NH2	-6.76	1.24	1.33
51	v	13	ARG	CZ-NH2	-6.74	1.24	1.33
51	v	63	ARG	CZ-NH2	-6.74	1.24	1.33
51	v	61	ARG	CZ-NH2	-6.70	1.24	1.33
6	C	1047	G	C8-N7	-6.57	1.27	1.30
51	v	3	LYS	CE-NZ	-6.45	1.32	1.49
12	I	2061	G	N9-C8	-6.37	1.33	1.37
6	C	1217	C	N1-C6	-6.32	1.33	1.37
12	I	2612	C	N1-C6	-6.31	1.33	1.37
12	I	2610	C	N1-C6	-6.30	1.33	1.37
6	C	1203	C	N1-C6	-6.26	1.33	1.37
12	I	2579	C	N1-C6	-6.23	1.33	1.37
12	I	2611	C	N1-C6	-6.14	1.33	1.37
12	I	2608	G	N9-C8	-6.14	1.33	1.37
12	I	2583	G	N9-C8	-6.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	2056	G	N9-C8	-6.13	1.33	1.37
6	C	995	C	N1-C6	-6.12	1.33	1.37
12	I	2057	G	N9-C8	-6.08	1.33	1.37
12	I	2577	A	C8-N7	-6.08	1.27	1.31
12	I	2451	A	C8-N7	-6.06	1.27	1.31
12	I	2587	A	C8-N7	-6.05	1.27	1.31
5	A	76	A	C8-N7	-6.01	1.27	1.31
6	C	1047	G	N9-C8	-6.00	1.33	1.37
12	I	2064	C	N1-C6	-5.95	1.33	1.37
12	I	2058	A	C8-N7	-5.94	1.27	1.31
12	I	2062	A	C8-N7	-5.94	1.27	1.31
12	I	2581	G	N9-C8	-5.93	1.33	1.37
12	I	2452	C	N1-C6	-5.93	1.33	1.37
12	I	2439	A	C8-N7	-5.90	1.27	1.31
6	C	1048	G	N9-C8	-5.89	1.33	1.37
5	A	75	C	N1-C6	-5.89	1.33	1.37
12	I	2576	G	N9-C8	-5.88	1.33	1.37
12	I	2063	C	N1-C6	-5.86	1.33	1.37
12	I	2450	A	C8-N7	-5.84	1.27	1.31
12	I	2505	G	N9-C8	-5.83	1.33	1.37
6	C	1216	A	C8-N7	-5.75	1.27	1.31
12	I	2064	C	C5'-C4'	-5.71	1.44	1.51
6	C	1216	A	C5'-C4'	-5.69	1.44	1.51
12	I	2583	G	C5'-C4'	-5.69	1.44	1.51
12	I	2059	A	C8-N7	-5.69	1.27	1.31
6	C	994	A	C5'-C4'	-5.68	1.44	1.51
12	I	2063	C	C5'-C4'	-5.67	1.44	1.51
12	I	2579	C	C5'-C4'	-5.67	1.44	1.51
6	C	981	U	C5'-C4'	-5.67	1.44	1.51
5	A	76	A	N9-C8	-5.65	1.33	1.37
12	I	2587	A	C5'-C4'	-5.63	1.44	1.51
6	C	995	C	C5'-C4'	-5.62	1.44	1.51
12	I	1782	U	C5'-C4'	-5.62	1.44	1.51
6	C	1217	C	C5'-C4'	-5.61	1.44	1.51
6	C	1204	A	C5'-C4'	-5.61	1.44	1.51
6	C	1203	C	C5'-C4'	-5.60	1.44	1.51
6	C	1204	A	C8-N7	-5.60	1.27	1.31
12	I	2608	G	C5'-C4'	-5.59	1.44	1.51
6	C	996	A	C8-N7	-5.58	1.27	1.31
12	I	2058	A	C5'-C4'	-5.57	1.44	1.51
12	I	2576	G	C5'-C4'	-5.57	1.44	1.51
12	I	2586	U	C5'-C4'	-5.56	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	2057	G	C5'-C4'	-5.55	1.44	1.51
12	I	2612	C	C5'-C4'	-5.55	1.44	1.51
12	I	2062	A	C5'-C4'	-5.55	1.44	1.51
6	C	1048	G	C5'-C4'	-5.54	1.44	1.51
12	I	2611	C	C5'-C4'	-5.54	1.44	1.51
5	A	75	C	C5'-C4'	-5.52	1.44	1.51
12	I	2610	C	C5'-C4'	-5.51	1.44	1.51
12	I	2577	A	C5'-C4'	-5.50	1.44	1.51
12	I	2581	G	C5'-C4'	-5.50	1.44	1.51
12	I	2056	G	C5'-C4'	-5.49	1.44	1.51
12	I	2059	A	C5'-C4'	-5.49	1.44	1.51
6	C	1049	U	C5'-C4'	-5.48	1.44	1.51
6	C	1047	G	C5'-C4'	-5.47	1.44	1.51
6	C	996	A	C5'-C4'	-5.44	1.44	1.51
51	v	68	GLY	N-CA	-5.44	1.37	1.46
12	I	2450	A	C5'-C4'	-5.40	1.44	1.51
12	I	2452	C	C5'-C4'	-5.39	1.44	1.51
6	C	982	U	C5'-C4'	-5.38	1.44	1.51
12	I	2439	A	C5'-C4'	-5.37	1.45	1.51
6	C	994	A	C8-N7	-5.36	1.27	1.31
12	I	2584	U	C5'-C4'	-5.36	1.45	1.51
12	I	2585	U	C5'-C4'	-5.35	1.45	1.51
51	v	11	VAL	CB-CG1	-5.35	1.41	1.52
5	A	76	A	C5'-C4'	-5.34	1.45	1.51
12	I	2451	A	C5'-C4'	-5.34	1.45	1.51
51	v	11	VAL	CB-CG2	-5.33	1.41	1.52
6	C	1202	U	C5'-C4'	-5.33	1.45	1.51
51	v	12	LYS	CE-NZ	-5.30	1.35	1.49
12	I	2577	A	N9-C8	-5.30	1.33	1.37
12	I	2505	G	C5'-C4'	-5.29	1.45	1.51
12	I	2576	G	C6-N1	-5.27	1.35	1.39
12	I	2581	G	C6-N1	-5.26	1.35	1.39
6	C	1204	A	N9-C8	-5.23	1.33	1.37
51	v	14	VAL	CB-CG2	-5.23	1.41	1.52
12	I	2059	A	N9-C8	-5.23	1.33	1.37
51	v	14	VAL	CB-CG1	-5.21	1.42	1.52
12	I	2451	A	N9-C8	-5.21	1.33	1.37
6	C	994	A	N9-C8	-5.21	1.33	1.37
12	I	2062	A	N9-C8	-5.21	1.33	1.37
12	I	2441	U	C5'-C4'	-5.20	1.45	1.51
12	I	2506[A]	U	C5'-C4'	-5.20	1.45	1.51
12	I	2506[B]	U	C5'-C4'	-5.20	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	2450	A	N9-C8	-5.19	1.33	1.37
51	v	3	LYS	CD-CE	-5.19	1.38	1.51
12	I	2056	G	C6-N1	-5.18	1.35	1.39
6	C	1216	A	N9-C8	-5.16	1.33	1.37
12	I	2505	G	C6-N1	-5.15	1.35	1.39
12	I	2609	U	C5'-C4'	-5.15	1.45	1.51
12	I	2061	G	C6-N1	-5.13	1.35	1.39
12	I	2587	A	N9-C8	-5.12	1.33	1.37
12	I	2439	A	N9-C8	-5.11	1.33	1.37
6	C	1047	G	C6-N1	-5.09	1.35	1.39
12	I	2061	G	C5'-C4'	-5.09	1.45	1.51
12	I	2064	C	C4-C5	-5.07	1.38	1.43
51	v	4	GLN	CA-CB	-5.06	1.42	1.53
12	I	2608	G	C6-N1	-5.06	1.36	1.39
6	C	996	A	N9-C8	-5.04	1.33	1.37
12	I	2057	G	C6-N1	-5.04	1.36	1.39
12	I	2579	C	C4-C5	-5.01	1.39	1.43
6	C	1048	G	C6-N1	-5.00	1.36	1.39
12	I	2583	G	C6-N1	-5.00	1.36	1.39

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	994	A	N1-C2-N3	12.82	135.71	129.30
12	I	2576	G	N7-C8-N9	12.10	119.15	113.10
12	I	2581	G	N7-C8-N9	11.83	119.02	113.10
12	I	2577	A	N1-C2-N3	11.77	135.19	129.30
12	I	2061	G	N7-C8-N9	11.62	118.91	113.10
5	A	76	A	N1-C2-N3	11.53	135.06	129.30
12	I	2439	A	N1-C2-N3	11.50	135.05	129.30
6	C	994	A	N7-C8-N9	11.49	119.55	113.80
12	I	2056	G	N7-C8-N9	11.45	118.83	113.10
12	I	2451	A	N1-C2-N3	11.45	135.02	129.30
12	I	2062	A	N1-C2-N3	11.42	135.01	129.30
6	C	1216	A	N1-C2-N3	11.41	135.01	129.30
12	I	2450	A	N1-C2-N3	11.41	135.00	129.30
6	C	1048	G	N7-C8-N9	11.40	118.80	113.10
6	C	1204	A	N1-C2-N3	11.39	135.00	129.30
12	I	2058	A	N1-C2-N3	11.32	134.96	129.30
12	I	2587	A	N1-C2-N3	11.31	134.96	129.30
12	I	2439	A	N7-C8-N9	11.29	119.45	113.80
12	I	2583	G	N7-C8-N9	11.27	118.74	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	2059	A	N1-C2-N3	11.26	134.93	129.30
12	I	2608	G	N7-C8-N9	11.22	118.71	113.10
12	I	2451	A	N7-C8-N9	11.20	119.40	113.80
6	C	996	A	N1-C2-N3	11.18	134.89	129.30
12	I	2057	G	N7-C8-N9	11.15	118.68	113.10
12	I	2505	G	N7-C8-N9	11.11	118.66	113.10
6	C	1047	G	N7-C8-N9	11.07	118.64	113.10
12	I	2450	A	N7-C8-N9	11.05	119.33	113.80
12	I	2058	A	N7-C8-N9	11.04	119.32	113.80
12	I	2577	A	N7-C8-N9	11.03	119.31	113.80
6	C	1216	A	N7-C8-N9	10.99	119.30	113.80
6	C	1204	A	N7-C8-N9	10.94	119.27	113.80
12	I	2587	A	N7-C8-N9	10.93	119.27	113.80
5	A	76	A	N7-C8-N9	10.90	119.25	113.80
12	I	2062	A	N7-C8-N9	10.87	119.24	113.80
12	I	2059	A	N7-C8-N9	10.84	119.22	113.80
6	C	996	A	N7-C8-N9	10.70	119.15	113.80
6	C	1048	G	C6-N1-C2	9.76	130.95	125.10
12	I	2506[A]	U	C2-N3-C4	9.65	132.79	127.00
12	I	2506[B]	U	C2-N3-C4	9.65	132.79	127.00
12	I	1782	U	C2-N3-C4	9.63	132.78	127.00
12	I	2609	U	C2-N3-C4	9.63	132.78	127.00
6	C	982	U	C2-N3-C4	9.59	132.75	127.00
12	I	2441	U	C2-N3-C4	9.56	132.74	127.00
6	C	981	U	C2-N3-C4	9.54	132.73	127.00
6	C	1049	U	C2-N3-C4	9.52	132.71	127.00
12	I	2586	U	C2-N3-C4	9.46	132.68	127.00
12	I	2505	G	C6-N1-C2	9.45	130.77	125.10
12	I	2583	G	C6-N1-C2	9.45	130.77	125.10
12	I	2056	G	C6-N1-C2	9.44	130.76	125.10
12	I	2584	U	C2-N3-C4	9.43	132.66	127.00
6	C	1202	U	C2-N3-C4	9.37	132.62	127.00
12	I	2585	U	C2-N3-C4	9.37	132.62	127.00
6	C	1047	G	C6-N1-C2	9.35	130.71	125.10
12	I	2057	G	C6-N1-C2	9.32	130.69	125.10
12	I	2608	G	C6-N1-C2	9.31	130.68	125.10
51	v	4	GLN	CB-CA-C	9.24	128.87	110.40
12	I	2581	G	C6-N1-C2	9.13	130.58	125.10
12	I	2576	G	C6-N1-C2	9.04	130.52	125.10
12	I	2061	G	C6-N1-C2	8.98	130.49	125.10
6	C	981	U	N3-C4-C5	-8.96	109.23	114.60
12	I	2585	U	N3-C4-C5	-8.90	109.26	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	2609	U	N3-C4-C5	-8.89	109.27	114.60
12	I	2441	U	N3-C4-C5	-8.83	109.30	114.60
12	I	2506[A]	U	N3-C4-C5	-8.81	109.31	114.60
12	I	2506[B]	U	N3-C4-C5	-8.81	109.31	114.60
6	C	1049	U	N3-C4-C5	-8.80	109.32	114.60
12	I	2586	U	N3-C4-C5	-8.79	109.33	114.60
12	I	1782	U	N3-C4-C5	-8.79	109.33	114.60
12	I	2584	U	N3-C4-C5	-8.70	109.38	114.60
6	C	1202	U	N3-C4-C5	-8.69	109.39	114.60
6	C	982	U	N3-C4-C5	-8.63	109.42	114.60
12	I	2610	C	C6-N1-C2	-7.92	117.13	120.30
12	I	2576	G	C8-N9-C4	-7.69	103.32	106.40
6	C	994	A	C8-N9-C4	-7.66	102.74	105.80
12	I	2581	G	C8-N9-C4	-7.54	103.38	106.40
12	I	2064	C	C6-N1-C2	-7.47	117.31	120.30
5	A	75	C	C6-N1-C2	-7.45	117.32	120.30
12	I	2063	C	C6-N1-C2	-7.41	117.34	120.30
51	v	4	GLN	N-CA-CB	-7.34	97.39	110.60
12	I	2611	C	C6-N1-C2	-7.18	117.43	120.30
6	C	1203	C	C6-N1-C2	-7.05	117.48	120.30
6	C	995	C	C6-N1-C2	-7.00	117.50	120.30
6	C	1217	C	C6-N1-C2	-6.99	117.51	120.30
12	I	2061	G	C8-N9-C4	-6.95	103.62	106.40
12	I	2452	C	C6-N1-C2	-6.92	117.53	120.30
6	C	1048	G	C8-N9-C4	-6.90	103.64	106.40
12	I	2579	C	C6-N1-C2	-6.88	117.55	120.30
12	I	2057	G	C8-N9-C4	-6.86	103.66	106.40
12	I	2418	A	OP1-P-OP2	-6.86	109.32	119.60
12	I	2612	C	C6-N1-C2	-6.86	117.56	120.30
12	I	2610	C	N3-C4-C5	-6.85	119.16	121.90
12	I	2058	A	C8-N9-C4	-6.84	103.06	105.80
12	I	2583	G	C8-N9-C4	-6.83	103.67	106.40
12	I	2451	A	C8-N9-C4	-6.82	103.07	105.80
12	I	2056	G	C8-N9-C4	-6.82	103.67	106.40
12	I	2608	G	C8-N9-C4	-6.79	103.69	106.40
12	I	2505	G	C8-N9-C4	-6.75	103.70	106.40
5	A	1	G	OP1-P-OP2	-6.74	109.49	119.60
6	C	1047	G	C8-N9-C4	-6.74	103.70	106.40
12	I	2401	U	OP1-P-OP2	-6.71	109.54	119.60
12	I	2611	C	N3-C4-C5	-6.70	119.22	121.90
12	I	2450	A	C8-N9-C4	-6.67	103.13	105.80
12	I	2063	C	N3-C4-C5	-6.67	119.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	1025	G	OP1-P-OP2	-6.66	109.61	119.60
6	C	1204	A	C8-N9-C4	-6.65	103.14	105.80
12	I	2616	C	OP1-P-OP2	-6.65	109.63	119.60
12	I	2064	C	N3-C4-C5	-6.64	119.24	121.90
6	C	1203	C	N3-C4-C5	-6.62	119.25	121.90
12	I	2612	C	N3-C4-C5	-6.61	119.26	121.90
5	A	75	C	N3-C4-C5	-6.60	119.26	121.90
12	I	2609	U	C5-C6-N1	6.59	126.00	122.70
12	I	2439	A	C8-N9-C4	-6.58	103.17	105.80
6	C	996	A	C8-N9-C4	-6.54	103.19	105.80
6	C	1217	C	N3-C4-C5	-6.52	119.29	121.90
12	I	2452	C	N3-C4-C5	-6.51	119.30	121.90
6	C	1216	A	C8-N9-C4	-6.48	103.21	105.80
51	v	3	LYS	CA-CB-CG	6.46	127.62	113.40
5	A	76	A	OP1-P-OP2	-6.46	109.92	119.60
6	C	1049	U	C5-C6-N1	6.45	125.92	122.70
6	C	995	C	N3-C4-C5	-6.44	119.32	121.90
12	I	2506[A]	U	C5-C6-N1	6.44	125.92	122.70
12	I	2506[B]	U	C5-C6-N1	6.44	125.92	122.70
12	I	2579	C	N3-C4-C5	-6.44	119.32	121.90
12	I	2587	A	C8-N9-C4	-6.42	103.23	105.80
12	I	1782	U	C5-C6-N1	6.42	125.91	122.70
12	I	2059	A	C8-N9-C4	-6.40	103.24	105.80
12	I	2577	A	C8-N9-C4	-6.34	103.26	105.80
5	A	76	A	C5-N7-C8	-6.34	100.73	103.90
6	C	981	U	C5-C6-N1	6.32	125.86	122.70
5	A	76	A	C2-N3-C4	-6.32	107.44	110.60
51	v	61	ARG	CD-NE-CZ	6.30	132.42	123.60
12	I	2584	U	C5-C6-N1	6.30	125.85	122.70
12	I	2439	A	C5-N7-C8	-6.29	100.76	103.90
51	v	13	ARG	CD-NE-CZ	6.28	132.40	123.60
6	C	982	U	C5-C6-N1	6.26	125.83	122.70
12	I	2441	U	C5-C6-N1	6.26	125.83	122.70
12	I	2586	U	C5-C6-N1	6.23	125.81	122.70
51	v	4	GLN	CB-CG-CD	6.22	127.76	111.60
12	I	2062	A	C8-N9-C4	-6.20	103.32	105.80
12	I	2576	G	C5-N7-C8	-6.16	101.22	104.30
51	v	9	ARG	CD-NE-CZ	6.15	132.21	123.60
12	I	2610	C	C5-C6-N1	6.12	124.06	121.00
6	C	1202	U	C5-C6-N1	6.07	125.74	122.70
6	C	1048	G	C5-N7-C8	-6.03	101.28	104.30
12	I	2056	G	C5-N7-C8	-6.01	101.30	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	2061	G	C5-N7-C8	-5.96	101.32	104.30
12	I	2450	A	C5-N7-C8	-5.95	100.93	103.90
12	I	2451	A	C5-N7-C8	-5.94	100.93	103.90
12	I	2439	A	C2-N3-C4	-5.91	107.64	110.60
12	I	2585	U	C5-C6-N1	5.90	125.65	122.70
12	I	2577	A	C5-N7-C8	-5.90	100.95	103.90
12	I	2611	C	C5-C6-N1	5.89	123.94	121.00
12	I	2577	A	C2-N3-C4	-5.87	107.67	110.60
12	I	2581	G	C5-N7-C8	-5.87	101.36	104.30
6	C	994	A	C2-N3-C4	-5.87	107.67	110.60
6	C	1203	C	C5-C6-N1	5.85	123.93	121.00
6	C	1216	A	C5-N7-C8	-5.85	100.98	103.90
5	A	75	C	C5-C6-N1	5.84	123.92	121.00
6	C	995	C	C5-C6-N1	5.84	123.92	121.00
6	C	1216	A	C2-N3-C4	-5.83	107.68	110.60
6	C	1048	G	C5-C6-N1	-5.83	108.59	111.50
6	C	754	C	C2-N1-C1'	5.82	125.20	118.80
12	I	2587	A	C5-N7-C8	-5.82	100.99	103.90
12	I	2583	G	C5-N7-C8	-5.80	101.40	104.30
12	I	2450	A	C2-N3-C4	-5.79	107.71	110.60
12	I	2059	A	C5-N7-C8	-5.79	101.01	103.90
12	I	2608	G	C5-N7-C8	-5.77	101.41	104.30
12	I	2451	A	C2-N3-C4	-5.77	107.72	110.60
12	I	2579	C	C5-C6-N1	5.76	123.88	121.00
12	I	2505	G	C5-N7-C8	-5.74	101.43	104.30
12	I	2058	A	C5-N7-C8	-5.74	101.03	103.90
6	C	1204	A	C2-N3-C4	-5.73	107.73	110.60
12	I	2062	A	C5-N7-C8	-5.73	101.03	103.90
12	I	2587	A	C2-N3-C4	-5.70	107.75	110.60
12	I	2062	A	C2-N3-C4	-5.68	107.76	110.60
12	I	2059	A	C2-N3-C4	-5.68	107.76	110.60
6	C	1158	C	C2-N1-C1'	5.68	125.05	118.80
12	I	2452	C	C5-C6-N1	5.67	123.84	121.00
12	I	2057	G	C5-N7-C8	-5.67	101.47	104.30
5	A	76	A	C8-N9-C4	-5.67	103.53	105.80
6	C	1204	A	C5-N7-C8	-5.67	101.07	103.90
12	I	2058	A	C2-N3-C4	-5.65	107.77	110.60
6	C	1047	G	C5-N7-C8	-5.65	101.47	104.30
12	I	2064	C	C5-C6-N1	5.65	123.82	121.00
12	I	2583	G	C5-C6-N1	-5.63	108.69	111.50
12	I	2063	C	C5-C6-N1	5.62	123.81	121.00
12	I	2056	G	C5-C6-N1	-5.60	108.70	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	1313	U	C2-N1-C1'	5.59	124.41	117.70
12	I	2612	C	C4-C5-C6	5.59	120.19	117.40
6	C	1217	C	C4-C5-C6	5.57	120.18	117.40
51	v	4	GLN	CG-CD-OE1	-5.55	110.49	121.60
12	I	2063	C	C4-C5-C6	5.55	120.18	117.40
6	C	1217	C	C5-C6-N1	5.53	123.77	121.00
12	I	2610	C	C4-C5-C6	5.51	120.16	117.40
12	I	2608	G	C5-C6-N1	-5.47	108.77	111.50
12	I	2064	C	C4-C5-C6	5.47	120.13	117.40
12	I	2057	G	C5-C6-N1	-5.46	108.77	111.50
6	C	996	A	C2-N3-C4	-5.44	107.88	110.60
12	I	2612	C	C5-C6-N1	5.43	123.72	121.00
12	I	2611	C	C4-C5-C6	5.41	120.11	117.40
6	C	996	A	C5-N7-C8	-5.41	101.20	103.90
12	I	2505	G	C5-C6-N1	-5.40	108.80	111.50
6	C	1203	C	C4-C5-C6	5.38	120.09	117.40
6	C	1047	G	C5-C6-N1	-5.32	108.84	111.50
12	I	2579	C	C4-C5-C6	5.31	120.06	117.40
51	v	3	LYS	C-N-CA	5.31	134.97	121.70
12	I	2452	C	C4-C5-C6	5.29	120.05	117.40
12	I	2609	U	C6-N1-C2	-5.24	117.86	121.00
12	I	2061	G	C5-C6-N1	-5.24	108.88	111.50
6	C	995	C	C4-C5-C6	5.19	120.00	117.40
12	I	2581	G	C5-C6-N1	-5.19	108.91	111.50
6	C	994	A	C5-N7-C8	-5.18	101.31	103.90
5	A	75	C	C4-C5-C6	5.18	119.99	117.40
12	I	2576	G	C5-C6-N1	-5.15	108.93	111.50
12	I	2577	A	C6-N1-C2	-5.06	115.56	118.60
51	v	61	ARG	CG-CD-NE	5.03	122.36	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	v	3	LYS	Mainchain
51	v	4	GLN	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
2	2	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
3	3	68/71 (96%)	68 (100%)	0	0	100	100
7	D	216/240 (90%)	207 (96%)	9 (4%)	0	100	100
8	E	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
9	F	203/206 (98%)	195 (96%)	7 (3%)	1 (0%)	29	40
10	G	148/167 (89%)	139 (94%)	8 (5%)	1 (1%)	22	31
11	H	98/135 (73%)	96 (98%)	2 (2%)	0	100	100
14	K	271/273 (99%)	261 (96%)	10 (4%)	0	100	100
15	L	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
16	M	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
17	N	175/179 (98%)	173 (99%)	2 (1%)	0	100	100
18	O	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
19	P	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
20	Q	56/70 (80%)	56 (100%)	0	0	100	100
21	R	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
22	S	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
23	T	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
24	U	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
25	V	118/127 (93%)	118 (100%)	0	0	100	100
26	W	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
27	X	112/115 (97%)	112 (100%)	0	0	100	100
28	Y	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
29	Z	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
30	a	108/110 (98%)	104 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	b	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
32	c	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
33	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
34	e	73/85 (86%)	73 (100%)	0	0	100	100
35	f	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
36	g	60/63 (95%)	60 (100%)	0	0	100	100
37	h	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
38	i	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
39	j	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
40	k	44/46 (96%)	44 (100%)	0	0	100	100
41	l	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
42	m	36/38 (95%)	36 (100%)	0	0	100	100
43	n	149/179 (83%)	147 (99%)	2 (1%)	0	100	100
44	o	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
45	p	125/130 (96%)	120 (96%)	4 (3%)	1 (1%)	19	27
46	q	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	15	22
47	r	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
48	s	3/5 (60%)	3 (100%)	0	0	100	100
49	t	121/124 (98%)	114 (94%)	7 (6%)	0	100	100
50	u	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
51	v	92/101 (91%)	87 (95%)	4 (4%)	1 (1%)	14	19
52	w	86/89 (97%)	86 (100%)	0	0	100	100
53	x	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
54	y	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
55	z	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
All	All	5558/5917 (94%)	5410 (97%)	143 (3%)	5 (0%)	54	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	F	28	ILE
46	q	57	VAL
45	p	55	VAL

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Mol	Chain	Res	Type
51	v	4	GLN
10	G	90	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	70/79 (89%)	67 (96%)	3 (4%)	29	44
2	2	65/66 (98%)	61 (94%)	4 (6%)	18	28
3	3	60/61 (98%)	53 (88%)	7 (12%)	5	6
7	D	180/198 (91%)	167 (93%)	13 (7%)	14	22
8	E	170/190 (90%)	156 (92%)	14 (8%)	11	16
9	F	172/173 (99%)	165 (96%)	7 (4%)	30	47
10	G	113/126 (90%)	104 (92%)	9 (8%)	12	18
11	H	87/116 (75%)	81 (93%)	6 (7%)	15	24
14	K	218/218 (100%)	206 (94%)	12 (6%)	21	33
15	L	164/164 (100%)	157 (96%)	7 (4%)	29	44
16	M	165/165 (100%)	158 (96%)	7 (4%)	30	46
17	N	148/150 (99%)	131 (88%)	17 (12%)	5	7
18	O	137/138 (99%)	125 (91%)	12 (9%)	10	14
19	P	114/114 (100%)	107 (94%)	7 (6%)	18	29
20	Q	55/62 (89%)	49 (89%)	6 (11%)	6	8
21	R	116/116 (100%)	110 (95%)	6 (5%)	23	37
22	S	103/104 (99%)	98 (95%)	5 (5%)	25	39
23	T	103/103 (100%)	100 (97%)	3 (3%)	42	61
24	U	108/108 (100%)	100 (93%)	8 (7%)	13	21
25	V	100/103 (97%)	97 (97%)	3 (3%)	41	59
26	W	86/87 (99%)	79 (92%)	7 (8%)	11	17
27	X	99/100 (99%)	95 (96%)	4 (4%)	31	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Y	89/90 (99%)	88 (99%)	1 (1%)	73	86
29	Z	84/84 (100%)	81 (96%)	3 (4%)	35	52
30	a	93/93 (100%)	88 (95%)	5 (5%)	22	34
31	b	80/84 (95%)	72 (90%)	8 (10%)	7	10
32	c	83/85 (98%)	78 (94%)	5 (6%)	19	30
33	d	78/78 (100%)	68 (87%)	10 (13%)	4	5
34	e	57/63 (90%)	54 (95%)	3 (5%)	22	36
35	f	67/68 (98%)	63 (94%)	4 (6%)	19	30
36	g	54/55 (98%)	47 (87%)	7 (13%)	4	4
37	h	48/49 (98%)	45 (94%)	3 (6%)	18	27
38	i	47/48 (98%)	44 (94%)	3 (6%)	17	27
39	j	45/49 (92%)	40 (89%)	5 (11%)	6	8
40	k	38/38 (100%)	37 (97%)	1 (3%)	46	64
41	l	51/52 (98%)	49 (96%)	2 (4%)	32	49
42	m	34/34 (100%)	31 (91%)	3 (9%)	10	14
43	n	124/147 (84%)	118 (95%)	6 (5%)	25	40
44	o	104/105 (99%)	94 (90%)	10 (10%)	8	11
45	p	105/107 (98%)	98 (93%)	7 (7%)	16	25
46	q	86/90 (96%)	79 (92%)	7 (8%)	11	17
47	r	90/99 (91%)	86 (96%)	4 (4%)	28	43
48	s	4/4 (100%)	4 (100%)	0	100	100
49	t	103/104 (99%)	99 (96%)	4 (4%)	32	49
50	u	93/96 (97%)	88 (95%)	5 (5%)	22	34
51	v	79/84 (94%)	71 (90%)	8 (10%)	7	10
52	w	75/77 (97%)	65 (87%)	10 (13%)	4	4
53	x	65/65 (100%)	56 (86%)	9 (14%)	3	4
54	y	74/78 (95%)	67 (90%)	7 (10%)	8	12
55	z	48/65 (74%)	47 (98%)	1 (2%)	53	71
All	All	4631/4832 (96%)	4323 (93%)	308 (7%)	20	25

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	25	SER
1	1	29	LYS
1	1	37	ARG
2	2	27	MET
2	2	60	ARG
2	2	66	LEU
2	2	76	LYS
3	3	13	ASP
3	3	18	ARG
3	3	25	LYS
3	3	33	ARG
3	3	56	HIS
3	3	59	LYS
3	3	64	ASN
7	D	23	TRP
7	D	35	ARG
7	D	37	LYS
7	D	63	ARG
7	D	78	GLU
7	D	96	TRP
7	D	105	LYS
7	D	109	GLN
7	D	121	SER
7	D	127	ASP
7	D	136	MET
7	D	139	ARG
7	D	203	ASN
8	E	27	LYS
8	E	42	TYR
8	E	45	LYS
8	E	89	LYS
8	E	107	ARG
8	E	127	ARG
8	E	129	MET
8	E	131	ARG
8	E	156	ARG
8	E	179	ARG
8	E	181	ASP
8	E	185	ASN
8	E	187	SER
8	E	188	GLU
9	F	36	GLN
9	F	40	GLN

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Mol	Chain	Res	Type
9	F	81	ARG
9	F	153	SER
9	F	156	LYS
9	F	167	LYS
9	F	187	GLU
10	G	13	GLU
10	G	14	LYS
10	G	32	SER
10	G	64	MET
10	G	92	SER
10	G	93	ARG
10	G	111	MET
10	G	122	ASN
10	G	132	ASN
11	H	16	GLU
11	H	24	ARG
11	H	35	LYS
11	H	62	MET
11	H	65	GLU
11	H	86	ARG
14	K	13	ARG
14	K	38	SER
14	K	53	HIS
14	K	97	LYS
14	K	114	ASP
14	K	139	SER
14	K	168	ASP
14	K	183	LYS
14	K	187	ASP
14	K	214	ARG
14	K	260	ASN
14	K	269	ARG
15	L	32	ASN
15	L	33	ARG
15	L	88	GLU
15	L	89	GLU
15	L	95	SER
15	L	97	SER
15	L	157	LYS
16	M	1	MET
16	M	122	GLU
16	M	123	LYS

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Mol	Chain	Res	Type
16	M	124	PHE
16	M	140	ASP
16	M	154	ASP
16	M	199	MET
17	N	6	ASP
17	N	17	MET
17	N	19	GLU
17	N	22	TYR
17	N	26	MET
17	N	30	ARG
17	N	37	ASN
17	N	42	GLU
17	N	48	LYS
17	N	69	LYS
17	N	83	TYR
17	N	103	LEU
17	N	143	TYR
17	N	147	ASP
17	N	152	LEU
17	N	162	SER
17	N	175	PHE
18	O	16	ASP
18	O	30	ASN
18	O	32	GLU
18	O	35	ARG
18	O	50	LEU
18	O	106	SER
18	O	114	ASP
18	O	130	GLU
18	O	147	ASP
18	O	155	GLU
18	O	157	TYR
18	O	166	ASP
19	P	41	LYS
19	P	46	PHE
19	P	50	ARG
19	P	98	ASP
19	P	116	ARG
19	P	117	LEU
19	P	137	GLU
20	Q	3	LYS
20	Q	10	GLU

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Mol	Chain	Res	Type
20	Q	11	GLU
20	Q	26	SER
20	Q	56	ARG
20	Q	64	PHE
21	R	1	MET
21	R	2	LYS
21	R	9	GLU
21	R	12	LYS
21	R	13	ARG
21	R	67	ASN
22	S	12	ASP
22	S	17	ARG
22	S	18	ARG
22	S	28	SER
22	S	53	LYS
23	T	2	ARG
23	T	84	LYS
23	T	126	ARG
24	U	1	MET
24	U	2	LEU
24	U	12	MET
24	U	14	LYS
24	U	40	ARG
24	U	84	LYS
24	U	88	ASN
24	U	133	LYS
25	V	35	LYS
25	V	57	THR
25	V	82	GLU
26	W	9	ARG
26	W	20	GLU
26	W	56	LYS
26	W	63	LYS
26	W	69	ASP
26	W	88	LYS
26	W	117	PHE
27	X	7	GLN
27	X	15	GLN
27	X	66	ASN
27	X	78	SER
28	Y	11	ARG
29	Z	6	GLN

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Mol	Chain	Res	Type
29	Z	43	ASN
29	Z	46	GLU
30	a	6	LYS
30	a	30	SER
30	a	31	GLN
30	a	67	ASP
30	a	108	SER
31	b	1	MET
31	b	3	ARG
31	b	5	GLU
31	b	6	ARG
31	b	17	SER
31	b	24	MET
31	b	49	LYS
31	b	73	ARG
32	c	17	LYS
32	c	53	ASN
32	c	69	ASN
32	c	88	GLU
32	c	100	SER
33	d	11	GLU
33	d	18	ARG
33	d	35	GLU
33	d	43	ASP
33	d	45	ASP
33	d	48	MET
33	d	50	MET
33	d	66	ASP
33	d	69	GLU
33	d	90	ASP
34	e	30	SER
34	e	56	ASP
34	e	81	SER
35	f	35	SER
35	f	42	SER
35	f	60	ASP
35	f	74	ARG
36	g	2	LYS
36	g	12	GLU
36	g	30	MET
36	g	34	SER
36	g	38	GLN

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Mol	Chain	Res	Type
36	g	40	SER
36	g	48	ARG
37	h	31	ARG
37	h	39	GLU
37	h	47	MET
38	i	27	SER
38	i	36	GLU
38	i	42	HIS
39	j	13	SER
39	j	32	GLU
39	j	33	LYS
39	j	37	LYS
39	j	53	LYS
40	k	45	SER
41	l	31	HIS
41	l	52	LYS
42	m	1	MET
42	m	4	ARG
42	m	34	LYS
43	n	4	ARG
43	n	58	GLU
43	n	92	ARG
43	n	106	GLU
43	n	110	LYS
43	n	126	ASP
44	o	5	ASP
44	o	29	SER
44	o	41	LYS
44	o	48	ASP
44	o	54	ASP
44	o	74	SER
44	o	87	LYS
44	o	90	ASP
44	o	105	SER
44	o	118	GLN
45	p	45	ARG
45	p	46	MET
45	p	49	ARG
45	p	57	MET
45	p	64	TYR
45	p	97	GLU
45	p	128	SER

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Mol	Chain	Res	Type
46	q	17	LEU
46	q	20	GLN
46	q	31	ARG
46	q	45	ARG
46	q	75	ASP
46	q	88	MET
46	q	89	ARG
47	r	37	ARG
47	r	56	ARG
47	r	108	THR
47	r	126	LYS
49	t	54	ARG
49	t	59	ASN
49	t	108	LYS
49	t	120	LYS
50	u	14	HIS
50	u	21	SER
50	u	27	LYS
50	u	49	SER
50	u	81	MET
51	v	6	MET
51	v	20	TYR
51	v	23	LYS
51	v	35	ASN
51	v	47	LYS
51	v	58	SER
51	v	59	ARG
51	v	65	ARG
52	w	14	GLU
52	w	17	ARG
52	w	45	GLU
52	w	58	ARG
52	w	61	SER
52	w	64	ARG
52	w	73	LYS
52	w	77	ARG
52	w	84	ARG
52	w	88	ARG
53	x	1	MET
53	x	25	ARG
53	x	45	GLU
53	x	51	ARG

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Mol	Chain	Res	Type
53	x	53	ASP
53	x	68	SER
53	x	69	ASP
53	x	77	GLU
53	x	80	LYS
54	y	11	ARG
54	y	28	PHE
54	y	40	ARG
54	y	48	ASP
54	y	52	GLU
54	y	65	ARG
54	y	81	LYS
55	z	48	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	64	ASN
7	D	94	HIS
16	M	92	HIS
17	N	81	GLN
21	R	132	HIS
44	o	118	GLN
50	u	105	ASN
52	w	28	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	I	2891/2904 (99%)	355 (12%)	30 (1%)
13	J	117/120 (97%)	11 (9%)	0
4	4	5/15 (33%)	0	0
5	A	75/76 (98%)	18 (24%)	3 (4%)
6	C	1539/1540 (99%)	176 (11%)	8 (0%)
All	All	4627/4655 (99%)	560 (12%)	41 (0%)

All (560) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	3	C

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Mol	Chain	Res	Type
5	A	5	G
5	A	8	U
5	A	11	C
5	A	17	A
5	A	18	G
5	A	20	U
5	A	21	A
5	A	22	G
5	A	43	C
5	A	47	U
5	A	54	U
5	A	58	A
5	A	61	C
5	A	62	C
5	A	63	G
5	A	68	C
5	A	76	A
6	C	4	U
6	C	9	G
6	C	39	G
6	C	47	C
6	C	48	C
6	C	51	A
6	C	70	U
6	C	71	A
6	C	74	A
6	C	83	C
6	C	85	U
6	C	87	C
6	C	95	C
6	C	97	G
6	C	108	G
6	C	116	A
6	C	117	G
6	C	120	A
6	C	121	U
6	C	130	A
6	C	131	A
6	C	144	G
6	C	182	A
6	C	207	C
6	C	208	U

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Mol	Chain	Res	Type
6	C	209	U
6	C	210	C
6	C	211	G
6	C	213	G
6	C	245	U
6	C	247	G
6	C	251	G
6	C	266	G
6	C	267	C
6	C	279	A
6	C	280	C
6	C	289	G
6	C	328	C
6	C	329	A
6	C	330	C
6	C	332	G
6	C	352	C
6	C	354	G
6	C	356	A
6	C	367	U
6	C	372	C
6	C	406	G
6	C	411	A
6	C	412	A
6	C	413	G
6	C	421	U
6	C	424	G
6	C	429	U
6	C	459	A
6	C	467	U
6	C	468	A
6	C	478	A
6	C	485	U
6	C	497	G
6	C	511	C
6	C	518	C
6	C	527	G
6	C	532	A
6	C	533	A
6	C	547	A
6	C	564	C
6	C	572	A

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Mol	Chain	Res	Type
6	C	573	A
6	C	576	C
6	C	577	G
6	C	633	G
6	C	650	G
6	C	653	U
6	C	665	A
6	C	687	A
6	C	721	G
6	C	723	U
6	C	731	G
6	C	747	A
6	C	755	G
6	C	777	A
6	C	793	U
6	C	794	A
6	C	815	A
6	C	817	C
6	C	828	U
6	C	829	G
6	C	841	C
6	C	842	U
6	C	843	U
6	C	844	G
6	C	845	A
6	C	846	G
6	C	847	G
6	C	885	G
6	C	914	A
6	C	934	C
6	C	935	A
6	C	960	U
6	C	969	A
6	C	975	A
6	C	976	G
6	C	977	A
6	C	983	A
6	C	993	G
6	C	1004	A
6	C	1008	U
6	C	1030	U
6	C	1032	G

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Mol	Chain	Res	Type
6	C	1033	G
6	C	1034	G
6	C	1043	G
6	C	1048	G
6	C	1054	C
6	C	1065	U
6	C	1085	U
6	C	1086	U
6	C	1087	G
6	C	1094	G
6	C	1095	U
6	C	1101	A
6	C	1133	G
6	C	1134	G
6	C	1136	C
6	C	1137	C
6	C	1139	G
6	C	1140	C
6	C	1141	C
6	C	1142	G
6	C	1145	A
6	C	1146	A
6	C	1159	U
6	C	1167	A
6	C	1196	A
6	C	1197	A
6	C	1202	U
6	C	1212	U
6	C	1213	A
6	C	1227	A
6	C	1240	U
6	C	1275	A
6	C	1280	A
6	C	1286	U
6	C	1287	A
6	C	1293	C
6	C	1297	G
6	C	1299	A
6	C	1300	G
6	C	1302	C
6	C	1305	G
6	C	1317	C

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Mol	Chain	Res	Type
6	C	1318	A
6	C	1320	C
6	C	1337	G
6	C	1346	A
6	C	1353	G
6	C	1362	A
6	C	1364	U
6	C	1378	C
6	C	1398	A
6	C	1419	G
6	C	1446	A
6	C	1452	C
6	C	1492	A
6	C	1493	A
6	C	1494	G
6	C	1503	A
6	C	1506	U
6	C	1517	G
6	C	1529	G
6	C	1530	G
6	C	1534	A
6	C	1537	U
6	C	1538	C
6	C	1539	C
6	C	1540	U
12	I	10	A
12	I	15	G
12	I	26	G
12	I	34	U
12	I	42	A
12	I	45	G
12	I	46	G
12	I	51	G
12	I	63	A
12	I	71	A
12	I	72	U
12	I	74	A
12	I	75	G
12	I	88	G
12	I	101	A
12	I	102	U
12	I	110	G

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Mol	Chain	Res	Type
12	I	118	A
12	I	120	U
12	I	137	U
12	I	139	U
12	I	144	A
12	I	163	C
12	I	174	U
12	I	181	A
12	I	183	C
12	I	196	A
12	I	199	A
12	I	209	C
12	I	216	A
12	I	220	G
12	I	221	A
12	I	222	A
12	I	236	C
12	I	238	C
12	I	240	C
12	I	248	G
12	I	266	G
12	I	272	A
12	I	276	U
12	I	302	C
12	I	307	G
12	I	309	A
12	I	311	A
12	I	329	G
12	I	330	A
12	I	345	A
12	I	353	C
12	I	361	G
12	I	362	A
12	I	371	A
12	I	372	G
12	I	376	G
12	I	379	G
12	I	385	C
12	I	386	G
12	I	391	A
12	I	396	G
12	I	404	A

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Mol	Chain	Res	Type
12	I	405	U
12	I	411	G
12	I	437	U
12	I	456	C
12	I	457	A
12	I	475	C
12	I	481	G
12	I	491	G
12	I	504	A
12	I	505	A
12	I	509	C
12	I	532	A
12	I	546	U
12	I	548	G
12	I	549	G
12	I	556	A
12	I	562	U
12	I	563	A
12	I	572	A
12	I	573	U
12	I	575	A
12	I	587	C
12	I	603	A
12	I	607	U
12	I	614	A
12	I	616	A
12	I	627	A
12	I	637	A
12	I	646	U
12	I	647	G
12	I	654	A
12	I	655	A
12	I	686	U
12	I	730	A
12	I	747	5MU
12	I	775	G
12	I	776	G
12	I	782	A
12	I	784	G
12	I	785	G
12	I	805	G
12	I	812	C

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Mol	Chain	Res	Type
12	I	819	A
12	I	827	U
12	I	828	U
12	I	845	A
12	I	846	U
12	I	858	G
12	I	896	A
12	I	897	C
12	I	910	A
12	I	914	G
12	I	915	C
12	I	931	U
12	I	941	A
12	I	946	C
12	I	961	C
12	I	974	G
12	I	983	A
12	I	996	A
12	I	1012	U
12	I	1013	C
12	I	1022	G
12	I	1025	G
12	I	1026	G
12	I	1033	U
12	I	1046	A
12	I	1047	G
12	I	1070	A
12	I	1071	G
12	I	1080	A
12	I	1088	A
12	I	1111	A
12	I	1112	G
12	I	1116	G
12	I	1132	U
12	I	1133	A
12	I	1135	C
12	I	1142	A
12	I	1150	C
12	I	1151	A
12	I	1152	C
12	I	1173	U
12	I	1174	U

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Mol	Chain	Res	Type
12	I	1175	A
12	I	1179	G
12	I	1180	U
12	I	1206	G
12	I	1238	G
12	I	1250	G
12	I	1253	A
12	I	1256	G
12	I	1266	G
12	I	1271	G
12	I	1272	A
12	I	1300	G
12	I	1301	A
12	I	1314	C
12	I	1340	U
12	I	1353	A
12	I	1365	A
12	I	1368	G
12	I	1378	A
12	I	1379	U
12	I	1383	A
12	I	1416	G
12	I	1419	A
12	I	1428	C
12	I	1452	G
12	I	1461	C
12	I	1482	G
12	I	1493	C
12	I	1494	A
12	I	1506	U
12	I	1508	A
12	I	1510	G
12	I	1515	A
12	I	1534	U
12	I	1535	A
12	I	1536	C
12	I	1569	A
12	I	1578	U
12	I	1583	A
12	I	1608	A
12	I	1610	A
12	I	1619	G

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Mol	Chain	Res	Type
12	I	1646	C
12	I	1647	U
12	I	1648	U
12	I	1674	G
12	I	1677	A
12	I	1684	G
12	I	1692	U
12	I	1696	G
12	I	1699	G
12	I	1715	G
12	I	1729	U
12	I	1730	C
12	I	1738	G
12	I	1755	A
12	I	1758	U
12	I	1763	G
12	I	1764	C
12	I	1773	A
12	I	1791	A
12	I	1800	C
12	I	1801	A
12	I	1808	A
12	I	1814	G
12	I	1816	C
12	I	1829	A
12	I	1847	A
12	I	1848	A
12	I	1869	G
12	I	1870	C
12	I	1872	A
12	I	1906	G
12	I	1909	C
12	I	1913	A
12	I	1914	C
12	I	1929	G
12	I	1930	G
12	I	1936	A
12	I	1938	A
12	I	1955	U
12	I	1967	C
12	I	1970	A
12	I	1971	U

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Mol	Chain	Res	Type
12	I	1972	G
12	I	1982	U
12	I	1991	U
12	I	1993	U
12	I	1997	C
12	I	2022	U
12	I	2023	C
12	I	2031	A
12	I	2033	A
12	I	2043	C
12	I	2052	A
12	I	2055	C
12	I	2056	G
12	I	2060	A
12	I	2061	G
12	I	2062	A
12	I	2069	G7M
12	I	2093	G
12	I	2111	U
12	I	2112	G
12	I	2113	U
12	I	2115	G
12	I	2116	G
12	I	2117	A
12	I	2118	U
12	I	2119	A
12	I	2126	A
12	I	2128	G
12	I	2131	U
12	I	2132	U
12	I	2133	G
12	I	2134	A
12	I	2146	C
12	I	2159	G
12	I	2160	C
12	I	2161	C
12	I	2163	A
12	I	2164	C
12	I	2165	C
12	I	2167	U
12	I	2169	A
12	I	2170	A

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Mol	Chain	Res	Type
12	I	2171	A
12	I	2172	U
12	I	2177	C
12	I	2178	C
12	I	2181	U
12	I	2198	A
12	I	2204	G
12	I	2211	A
12	I	2225	A
12	I	2226	C
12	I	2238	G
12	I	2239	G
12	I	2283	C
12	I	2287	A
12	I	2297	A
12	I	2305	U
12	I	2322	A
12	I	2325	G
12	I	2333	A
12	I	2335	A
12	I	2347	C
12	I	2350	C
12	I	2357	G
12	I	2371	G
12	I	2383	G
12	I	2385	C
12	I	2403	C
12	I	2423	U
12	I	2425	A
12	I	2426	A
12	I	2429	G
12	I	2430	A
12	I	2441	U
12	I	2445	2MG
12	I	2448	A
12	I	2469	A
12	I	2475	C
12	I	2476	A
12	I	2491	U
12	I	2498	OMC
12	I	2502	G
12	I	2504	PSU

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Mol	Chain	Res	Type
12	I	2505	G
12	I	2518	A
12	I	2543	G
12	I	2544	G
12	I	2547	A
12	I	2554	U
12	I	2566	A
12	I	2567	G
12	I	2572	A
12	I	2573	C
12	I	2578	G
12	I	2585	U
12	I	2602	A
12	I	2609	U
12	I	2613	U
12	I	2615	U
12	I	2630	G
12	I	2639	A
12	I	2661	G
12	I	2681	C
12	I	2682	A
12	I	2689	U
12	I	2690	U
12	I	2714	G
12	I	2726	A
12	I	2729	G
12	I	2748	A
12	I	2765	A
12	I	2766	A
12	I	2778	A
12	I	2781	A
12	I	2791	G
12	I	2793	C
12	I	2797	U
12	I	2800	A
12	I	2820	A
12	I	2855	C
12	I	2867	G
12	I	2872	A
12	I	2880	C
12	I	2884	U
12	I	2885	G

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Mol	Chain	Res	Type
12	I	2887	A
12	I	2903	U
13	J	15	A
13	J	32	U
13	J	35	C
13	J	42	C
13	J	56	G
13	J	88	C
13	J	89	U
13	J	90	C
13	J	99	A
13	J	109	A
13	J	119	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	10	G
5	A	21	A
5	A	61	C
6	C	96	U
6	C	115	G
6	C	206	C
6	C	212	G
6	C	846	G
6	C	1145	A
6	C	1201	A
6	C	1491	G
12	I	25	U
12	I	87	U
12	I	138	U
12	I	182	A
12	I	271	G
12	I	404	A
12	I	504	A
12	I	547	A
12	I	548	G
12	I	555	G
12	I	784	G
12	I	1025	G
12	I	1079	C
12	I	1313	U

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Mol	Chain	Res	Type
12	I	1352	U
12	I	1754	A
12	I	1813	G
12	I	1846	G
12	I	1847	A
12	I	1913	A
12	I	2127	G
12	I	2158	A
12	I	2159	G
12	I	2225	A
12	I	2425	A
12	I	2447	G
12	I	2543	G
12	I	2660	A
12	I	2680	U
12	I	2854	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	5MU	I	1939	12	19,22,23	1.03	2 (10%)	28,32,35	2.08	6 (21%)
12	PSU	I	2580	56,12	18,21,22	0.96	0	22,30,33	1.86	5 (22%)
12	PSU	I	2604	12	18,21,22	0.94	1 (5%)	22,30,33	1.83	4 (18%)
12	PSU	I	955	12	18,21,22	0.94	0	22,30,33	1.83	4 (18%)
12	5MU	I	747	12	19,22,23	1.03	2 (10%)	28,32,35	2.11	6 (21%)
12	PSU	I	1911	12	18,21,22	0.92	0	22,30,33	1.81	3 (13%)
12	PSU	I	2605	12	18,21,22	0.95	1 (5%)	22,30,33	1.84	4 (18%)
12	2MG	I	2445	12	18,26,27	1.25	2 (11%)	16,38,41	1.30	3 (18%)
12	3TD	I	1915	12	18,22,23	0.95	1 (5%)	22,32,35	1.77	2 (9%)
12	PSU	I	2457	12	18,21,22	0.94	1 (5%)	22,30,33	1.85	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	G7M	I	2069	12	20,26,27	0.95	1 (5%)	17,39,42	0.51	0
12	OMC	I	2498	56,12	19,22,23	0.91	1 (5%)	26,31,34	0.94	1 (3%)
12	5MC	I	1962	12	18,22,23	0.85	1 (5%)	26,32,35	1.11	3 (11%)
12	OMG	I	2251	5,12	18,26,27	1.22	2 (11%)	19,38,41	1.41	4 (21%)
12	PSU	I	746	56,12	18,21,22	2.59	10 (55%)	22,30,33	1.16	1 (4%)
12	PSU	I	2504	56,12	18,21,22	2.59	9 (50%)	22,30,33	1.07	1 (4%)
12	6MZ	I	2030	12	18,25,26	1.03	2 (11%)	16,36,39	2.08	4 (25%)
12	1MG	I	745	12	18,26,27	1.21	2 (11%)	19,39,42	1.32	3 (15%)
12	OMU	I	2552	12	19,22,23	0.94	1 (5%)	26,31,34	1.85	6 (23%)
12	8AH	I	2503	56,12	20,26,27	1.12	1 (5%)	23,39,42	2.56	3 (13%)
12	H2U	I	2449	12	18,21,22	0.46	0	21,30,33	0.88	1 (4%)
12	2MG	I	1835	12	18,26,27	1.23	2 (11%)	16,38,41	1.27	2 (12%)
12	6MZ	I	1618	12	18,25,26	1.03	2 (11%)	16,36,39	1.95	4 (25%)
12	PSU	I	1917	12	18,21,22	0.91	0	22,30,33	1.83	4 (18%)
24	4D4	U	81	24	9,11,12	2.15	2 (22%)	8,13,15	2.16	4 (50%)

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
12	5MU	I	1939	12	-	0/7/25/26	0/2/2/2
12	PSU	I	2580	56,12	-	0/7/25/26	0/2/2/2
12	PSU	I	2604	12	-	0/7/25/26	0/2/2/2
12	PSU	I	955	12	-	0/7/25/26	0/2/2/2
12	5MU	I	747	12	-	0/7/25/26	0/2/2/2
12	PSU	I	1911	12	-	0/7/25/26	0/2/2/2
12	PSU	I	2605	12	-	2/7/25/26	0/2/2/2
12	2MG	I	2445	12	-	2/5/27/28	0/3/3/3
12	3TD	I	1915	12	-	2/7/25/26	0/2/2/2
12	PSU	I	2457	12	-	0/7/25/26	0/2/2/2
12	G7M	I	2069	12	-	1/3/25/26	0/3/3/3
12	OMC	I	2498	56,12	-	1/9/27/28	0/2/2/2
12	5MC	I	1962	12	-	0/7/25/26	0/2/2/2
12	OMG	I	2251	5,12	-	0/5/27/28	0/3/3/3
12	PSU	I	746	56,12	-	0/7/25/26	0/2/2/2
12	PSU	I	2504	56,12	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	6MZ	I	2030	12	-	2/5/27/28	0/3/3/3
12	1MG	I	745	12	-	0/3/25/26	0/3/3/3
12	OMU	I	2552	12	-	0/9/27/28	0/2/2/2
12	8AH	I	2503	56,12	-	1/3/25/26	0/3/3/3
12	H2U	I	2449	12	-	0/7/38/39	0/2/2/2
12	2MG	I	1835	12	-	0/5/27/28	0/3/3/3
12	6MZ	I	1618	12	-	2/5/27/28	0/3/3/3
12	PSU	I	1917	12	-	0/7/25/26	0/2/2/2
24	4D4	U	81	24	-	1/11/12/14	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	81	4D4	CZ-NE	5.24	1.43	1.33
12	I	2504	PSU	C2-N1	-4.24	1.31	1.36
12	I	746	PSU	C2-N1	-4.21	1.31	1.36
12	I	2504	PSU	C6-N1	-4.01	1.29	1.36
12	I	2504	PSU	C4-N3	-3.97	1.31	1.38
12	I	746	PSU	C6-N1	-3.97	1.29	1.36
12	I	746	PSU	C4-N3	-3.94	1.31	1.38
12	I	746	PSU	C2-N3	-3.73	1.31	1.37
12	I	2504	PSU	C2-N3	-3.72	1.31	1.37
12	I	746	PSU	C2'-C1'	-3.62	1.49	1.53
12	I	2503	8AH	C6-N1	3.55	1.40	1.33
12	I	746	PSU	O4'-C1'	-3.44	1.39	1.43
12	I	2504	PSU	C2'-C1'	-3.38	1.49	1.53
12	I	746	PSU	C6-C5	-3.13	1.31	1.35
12	I	2504	PSU	C6-C5	-3.13	1.31	1.35
24	U	81	4D4	CZ-NH2	3.10	1.44	1.32
12	I	2504	PSU	O4'-C1'	-2.96	1.39	1.43
12	I	2069	G7M	C8-N9	2.95	1.38	1.33
12	I	2445	2MG	C5-C6	-2.88	1.41	1.47
12	I	2504	PSU	O5'-C5'	-2.84	1.37	1.44
12	I	1835	2MG	C5-C6	-2.84	1.41	1.47
12	I	2251	OMG	C5-C6	-2.83	1.41	1.47
12	I	2251	OMG	C8-N7	-2.82	1.30	1.35
12	I	745	1MG	C8-N7	-2.73	1.30	1.35
12	I	1835	2MG	C8-N7	-2.72	1.30	1.35
12	I	746	PSU	O5'-C5'	-2.68	1.38	1.44
12	I	2445	2MG	C8-N7	-2.67	1.30	1.35
12	I	2498	OMC	C2-N1	-2.53	1.34	1.40
12	I	1618	6MZ	C8-N7	-2.46	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	1915	3TD	C4-N3	-2.43	1.35	1.40
12	I	747	5MU	C2-N1	-2.40	1.34	1.38
12	I	2030	6MZ	C8-N7	-2.38	1.30	1.34
12	I	1962	5MC	C2-N1	-2.38	1.34	1.40
12	I	2552	OMU	C2-N1	-2.36	1.34	1.38
12	I	1939	5MU	C2-N1	-2.30	1.34	1.38
12	I	2504	PSU	C5'-C4'	-2.25	1.44	1.51
12	I	746	PSU	C5'-C4'	-2.18	1.44	1.51
12	I	746	PSU	O2'-C2'	-2.17	1.37	1.43
12	I	1618	6MZ	C6-N6	2.16	1.38	1.35
12	I	745	1MG	C6-N1	-2.12	1.35	1.39
12	I	2030	6MZ	C6-N6	2.11	1.38	1.35
12	I	1939	5MU	C4-N3	-2.11	1.34	1.38
12	I	2604	PSU	C4-N3	-2.06	1.35	1.38
12	I	2457	PSU	C4-N3	-2.04	1.35	1.38
12	I	747	5MU	C4-N3	-2.03	1.35	1.38
12	I	2605	PSU	C4-N3	-2.01	1.35	1.38

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	2503	8AH	C5-C6-N1	-10.12	114.36	121.01
12	I	1915	3TD	N1-C2-N3	6.11	120.96	116.14
12	I	747	5MU	C4-N3-C2	-5.52	120.20	127.35
12	I	1939	5MU	C4-N3-C2	-5.44	120.31	127.35
12	I	2503	8AH	C2-N3-C4	5.34	119.86	115.52
12	I	2030	6MZ	C2-N1-C6	5.27	121.11	116.59
12	I	2605	PSU	N1-C2-N3	5.27	121.10	115.13
12	I	2580	PSU	N1-C2-N3	5.26	121.09	115.13
12	I	2457	PSU	N1-C2-N3	5.24	121.07	115.13
12	I	955	PSU	N1-C2-N3	5.23	121.06	115.13
12	I	2604	PSU	N1-C2-N3	5.19	121.01	115.13
12	I	1917	PSU	N1-C2-N3	5.17	120.98	115.13
12	I	1618	6MZ	C2-N1-C6	5.15	121.00	116.59
12	I	1911	PSU	N1-C2-N3	5.13	120.94	115.13
12	I	2552	OMU	C4-N3-C2	-4.94	120.06	126.58
12	I	2552	OMU	N3-C2-N1	4.74	121.19	114.89
12	I	747	5MU	C5-C4-N3	4.72	119.34	115.31
12	I	1939	5MU	C5-C4-N3	4.72	119.34	115.31
12	I	747	5MU	N3-C2-N1	4.71	121.15	114.89
12	I	1939	5MU	N3-C2-N1	4.64	121.05	114.89
12	I	2605	PSU	C4-N3-C2	-4.35	120.06	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	1917	PSU	C4-N3-C2	-4.32	120.11	126.34
12	I	2457	PSU	C4-N3-C2	-4.30	120.14	126.34
12	I	955	PSU	C4-N3-C2	-4.27	120.18	126.34
12	I	2604	PSU	C4-N3-C2	-4.26	120.20	126.34
12	I	2580	PSU	C4-N3-C2	-4.25	120.22	126.34
12	I	1911	PSU	C4-N3-C2	-4.23	120.24	126.34
12	I	1915	3TD	C4-N3-C2	-4.15	120.11	124.61
12	I	1939	5MU	O4-C4-C5	-4.01	120.25	124.90
12	I	2030	6MZ	N3-C2-N1	-4.00	122.42	128.68
12	I	1618	6MZ	N3-C2-N1	-3.95	122.51	128.68
12	I	747	5MU	O4-C4-C5	-3.94	120.33	124.90
12	I	2030	6MZ	C9-N6-C6	-3.87	119.53	122.87
12	I	747	5MU	C5-C6-N1	-3.71	119.52	123.34
24	U	81	4D4	NE-CZ-NH2	-3.61	114.36	120.70
12	I	1939	5MU	C5-C6-N1	-3.60	119.63	123.34
24	U	81	4D4	NH1-CZ-NE	3.56	127.40	119.19
12	I	1962	5MC	C5-C6-N1	-3.39	119.85	123.34
12	I	1618	6MZ	C9-N6-C6	-3.37	119.97	122.87
12	I	746	PSU	C6-C5-C4	-3.35	115.86	118.20
12	I	2251	OMG	C8-N7-C5	3.30	109.28	102.99
12	I	1835	2MG	C8-N7-C5	3.29	109.25	102.99
12	I	2445	2MG	C8-N7-C5	3.28	109.24	102.99
12	I	745	1MG	C8-N7-C5	3.27	109.22	102.99
12	I	2552	OMU	CM2-O2'-C2'	-3.08	106.44	114.52
12	I	2552	OMU	C5-C4-N3	3.08	119.44	114.84
12	I	745	1MG	C5-C6-N1	3.07	118.52	113.90
12	I	2580	PSU	O2-C2-N1	-3.02	119.47	122.79
12	I	2457	PSU	O2-C2-N1	-2.98	119.51	122.79
12	I	955	PSU	O2-C2-N1	-2.95	119.54	122.79
12	I	1917	PSU	O2-C2-N1	-2.90	119.60	122.79
12	I	2604	PSU	O2-C2-N1	-2.90	119.60	122.79
12	I	1911	PSU	O2-C2-N1	-2.90	119.60	122.79
12	I	2605	PSU	O2-C2-N1	-2.90	119.60	122.79
12	I	2449	H2U	C4-N3-C2	2.72	128.05	125.79
12	I	2504	PSU	C6-C5-C4	-2.72	116.30	118.20
12	I	2552	OMU	O4-C4-C5	-2.71	120.39	125.16
12	I	747	5MU	O2-C2-N1	-2.69	119.21	122.79
12	I	2251	OMG	C2-N1-C6	-2.65	120.21	125.10
12	I	2552	OMU	O2-C2-N1	-2.58	119.36	122.79
12	I	2445	2MG	C5-C6-N1	2.53	118.43	113.95
12	I	2251	OMG	C5-C6-N1	2.50	118.36	113.95
12	I	1835	2MG	C5-C6-N1	2.49	118.35	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	2030	6MZ	C4-C5-N7	-2.44	106.86	109.40
24	U	81	4D4	CB-CA-C	-2.39	107.96	111.77
12	I	2498	OMC	CM2-O2'-C2'	-2.37	108.31	114.52
12	I	2251	OMG	CM2-O2'-C2'	-2.27	108.56	114.52
12	I	1939	5MU	O2-C2-N1	-2.24	119.81	122.79
12	I	1962	5MC	O2-C2-N3	-2.22	118.72	122.33
24	U	81	4D4	O-C-CA	-2.18	119.08	124.78
12	I	745	1MG	O6-C6-C5	-2.17	120.34	124.19
12	I	2503	8AH	N6-C6-N1	2.17	122.98	117.07
12	I	2580	PSU	C6-N1-C2	-2.16	120.47	122.68
12	I	2445	2MG	CM2-N2-C2	-2.15	119.10	123.86
12	I	1618	6MZ	C4-C5-N7	-2.13	107.18	109.40
12	I	1962	5MC	C5-C4-N3	-2.11	119.39	121.67
12	I	2580	PSU	O4'-C1'-C2'	2.10	108.11	105.14
12	I	955	PSU	C6-N1-C2	-2.07	120.57	122.68
12	I	2457	PSU	C6-N1-C2	-2.07	120.57	122.68
12	I	2604	PSU	C6-N1-C2	-2.01	120.62	122.68
12	I	2605	PSU	C6-N1-C2	-2.00	120.64	122.68
12	I	1917	PSU	C6-N1-C2	-2.00	120.64	122.68

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	1618	6MZ	O4'-C4'-C5'-O5'
12	I	1618	6MZ	C3'-C4'-C5'-O5'
12	I	1915	3TD	C3'-C4'-C5'-O5'
12	I	1915	3TD	O4'-C4'-C5'-O5'
12	I	2445	2MG	C3'-C4'-C5'-O5'
12	I	2605	PSU	C3'-C4'-C5'-O5'
12	I	2030	6MZ	O4'-C4'-C5'-O5'
12	I	2030	6MZ	C3'-C4'-C5'-O5'
12	I	2605	PSU	O4'-C4'-C5'-O5'
12	I	2445	2MG	O4'-C4'-C5'-O5'
12	I	2503	8AH	O4'-C4'-C5'-O5'
12	I	2504	PSU	C3'-C4'-C5'-O5'
12	I	2498	OMC	C4'-C5'-O5'-P
12	I	2504	PSU	O4'-C4'-C5'-O5'
12	I	2069	G7M	O4'-C4'-C5'-O5'
24	U	81	4D4	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 210 ligands modelled in this entry, 209 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	RD8	I	3113	56	34,35,35	1.26	3 (8%)	45,48,48	1.84	10 (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
57	RD8	I	3113	56	-	0/17/31/31	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	I	3113	RD8	C30-N21	4.11	1.40	1.36
57	I	3113	RD8	O29-C23	-3.38	1.41	1.46
57	I	3113	RD8	C24-C23	3.20	1.55	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	I	3113	RD8	C22-N21-C30	-5.29	108.22	111.28
57	I	3113	RD8	C23-O29-C30	4.66	113.82	110.15
57	I	3113	RD8	N17-N16-N15	3.97	116.19	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	I	3113	RD8	O29-C30-N21	-3.33	107.53	109.83
57	I	3113	RD8	C23-C22-N21	2.93	104.76	101.81
57	I	3113	RD8	O31-C30-N21	2.87	131.19	128.91
57	I	3113	RD8	C14-N15-N16	-2.81	101.92	107.97
57	I	3113	RD8	C22-C23-C24	2.76	116.14	113.08
57	I	3113	RD8	O29-C23-C22	-2.73	101.82	104.57
57	I	3113	RD8	C14-C13-N17	-2.01	108.35	111.34

There are no chirality outliers.

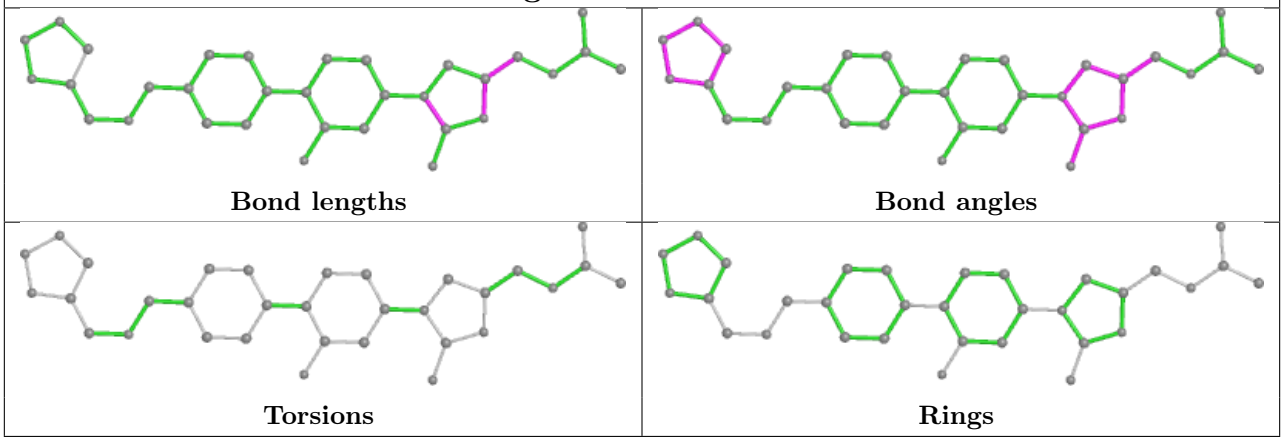
There are no torsion outliers.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand RD8 I 3113



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

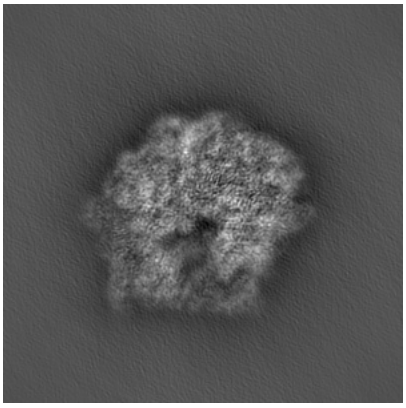
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24804. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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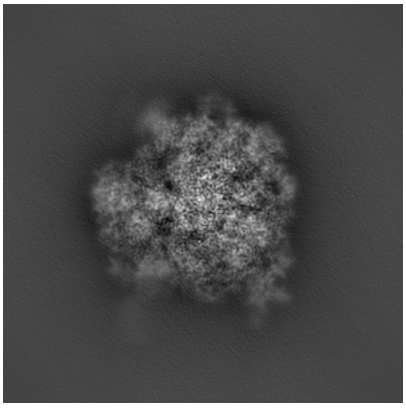
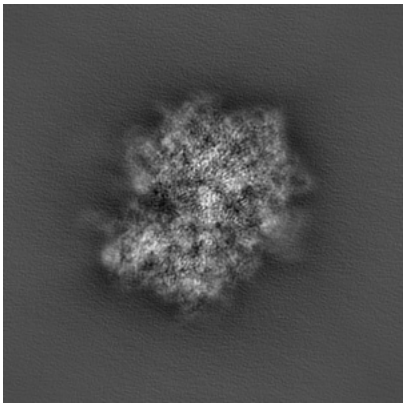


Y

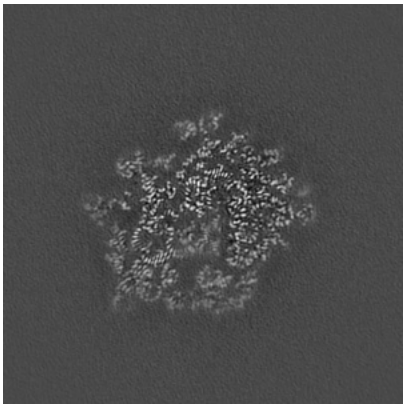


Z

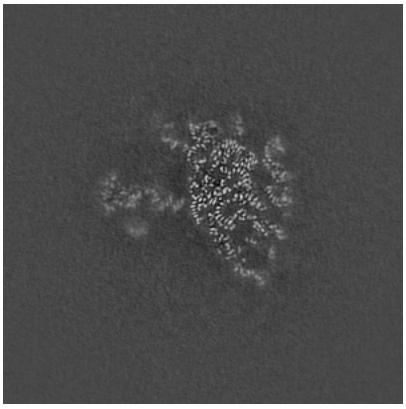
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

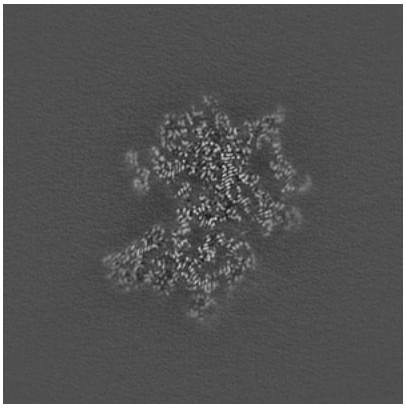
6.2.1 Primary map



X Index: 256



Y Index: 256

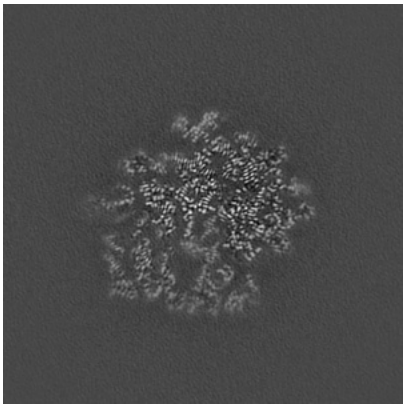


Z Index: 256

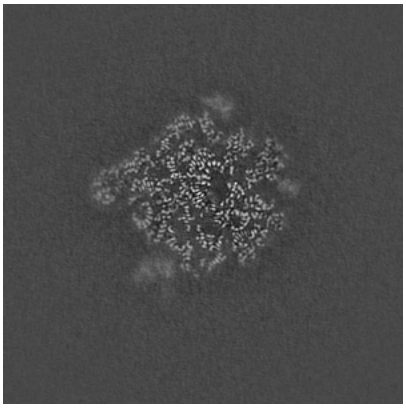
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

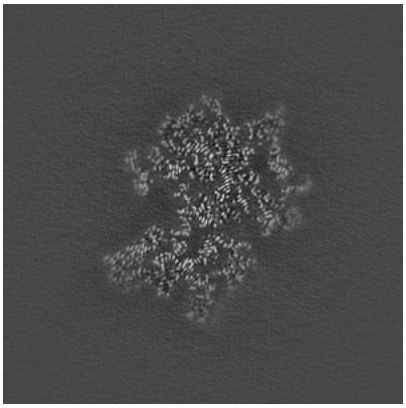
6.3.1 Primary map



X Index: 263



Y Index: 292

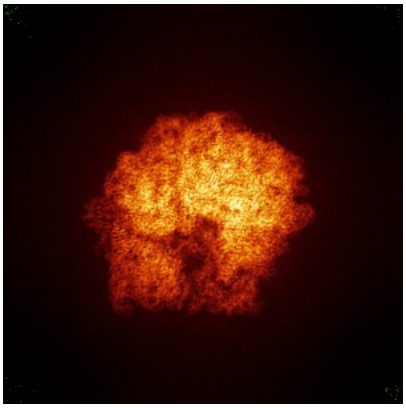


Z Index: 254

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



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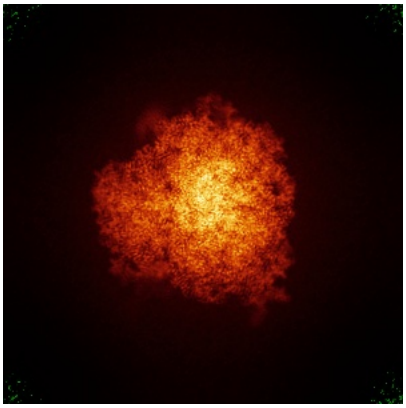
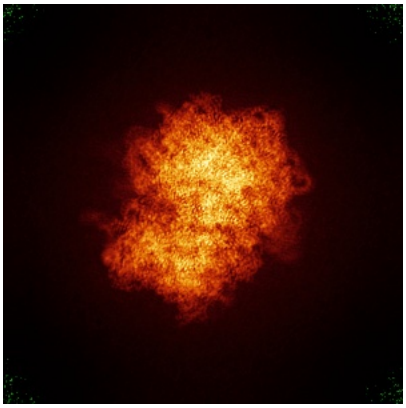


Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

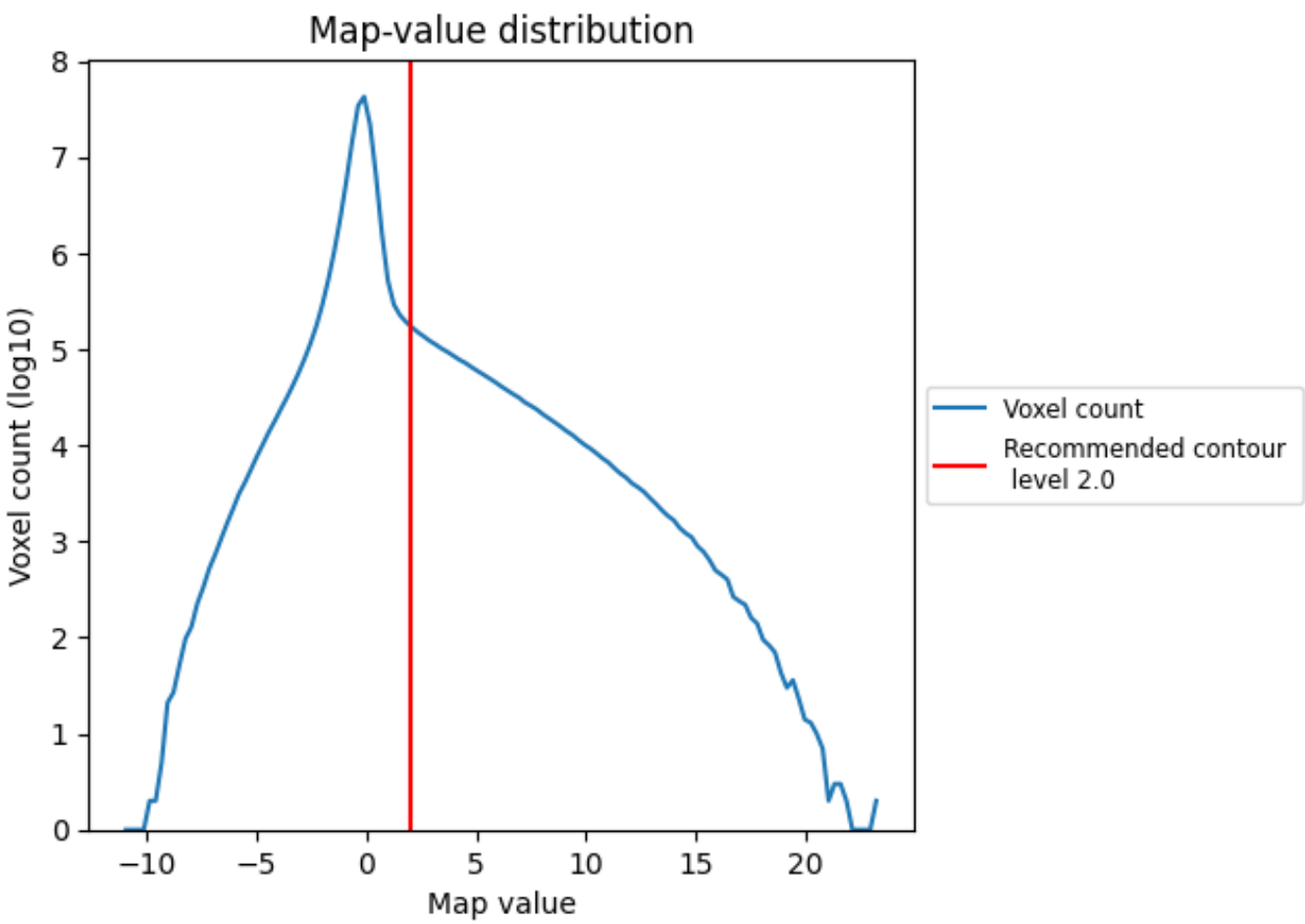
6.6 Mask visualisation (i)

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

7 Map analysis (i)

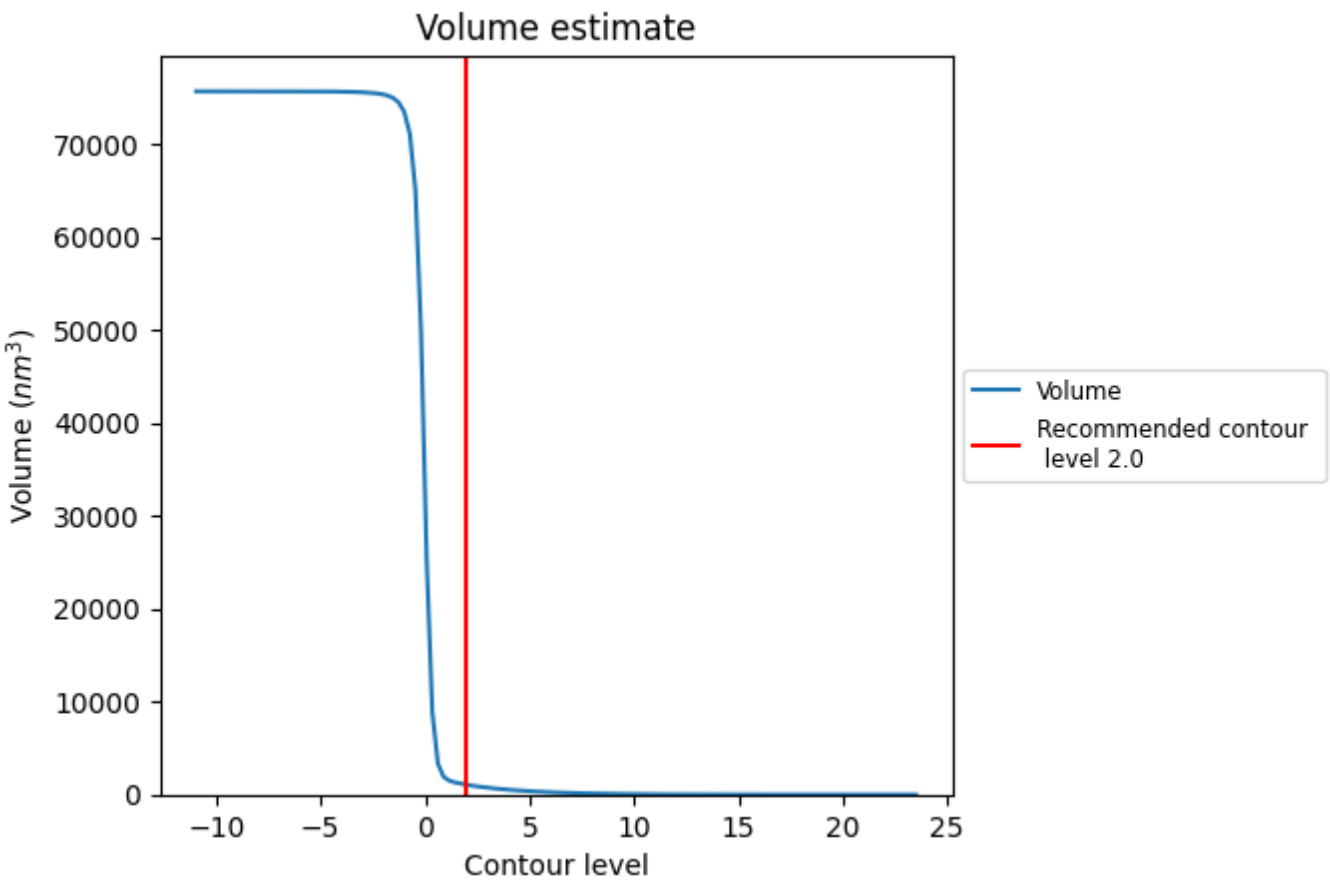
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

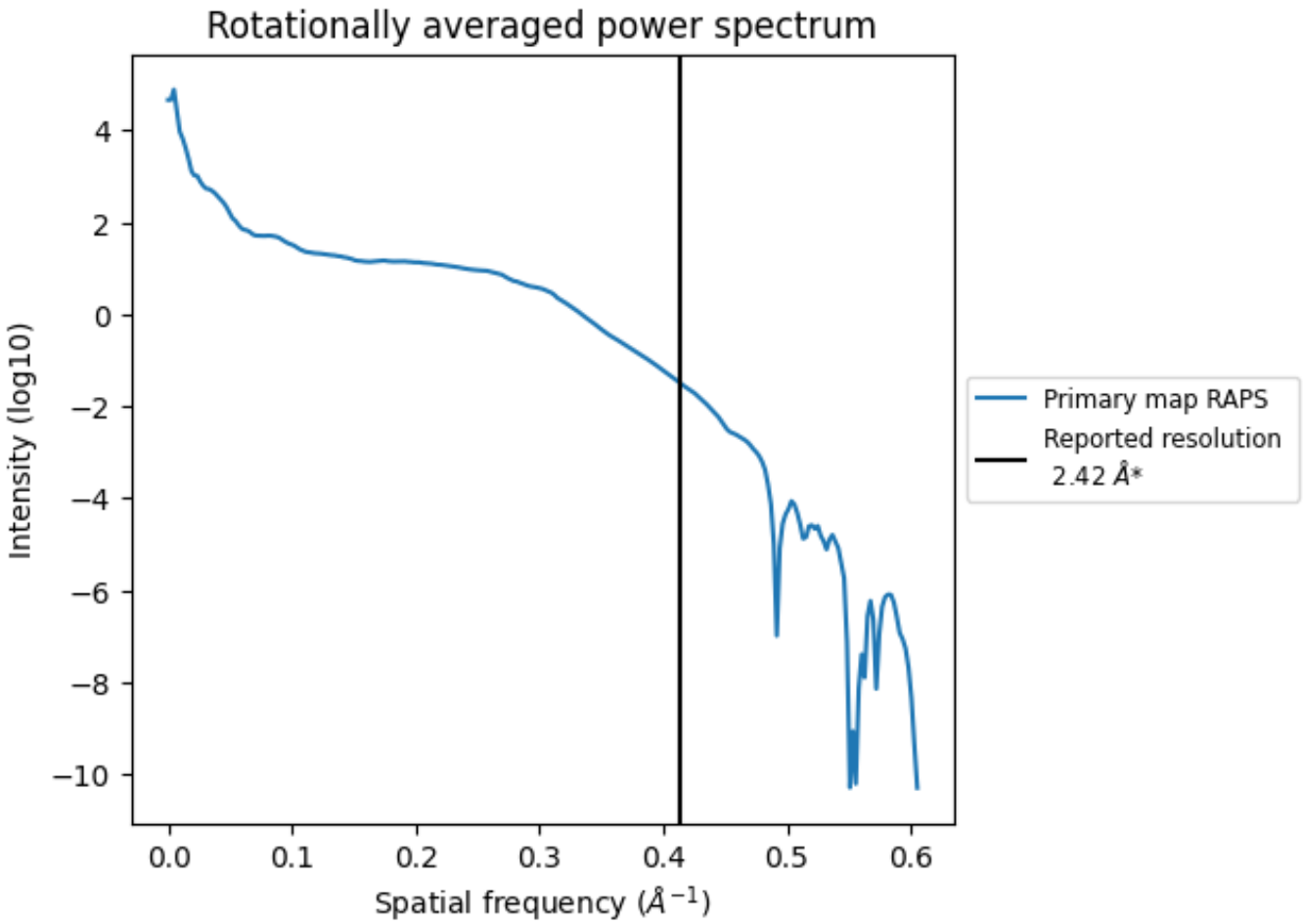
7.2 Volume estimate (i)



The volume at the recommended contour level is 1050 nm^3; this corresponds to an approximate mass of 948 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 (i)

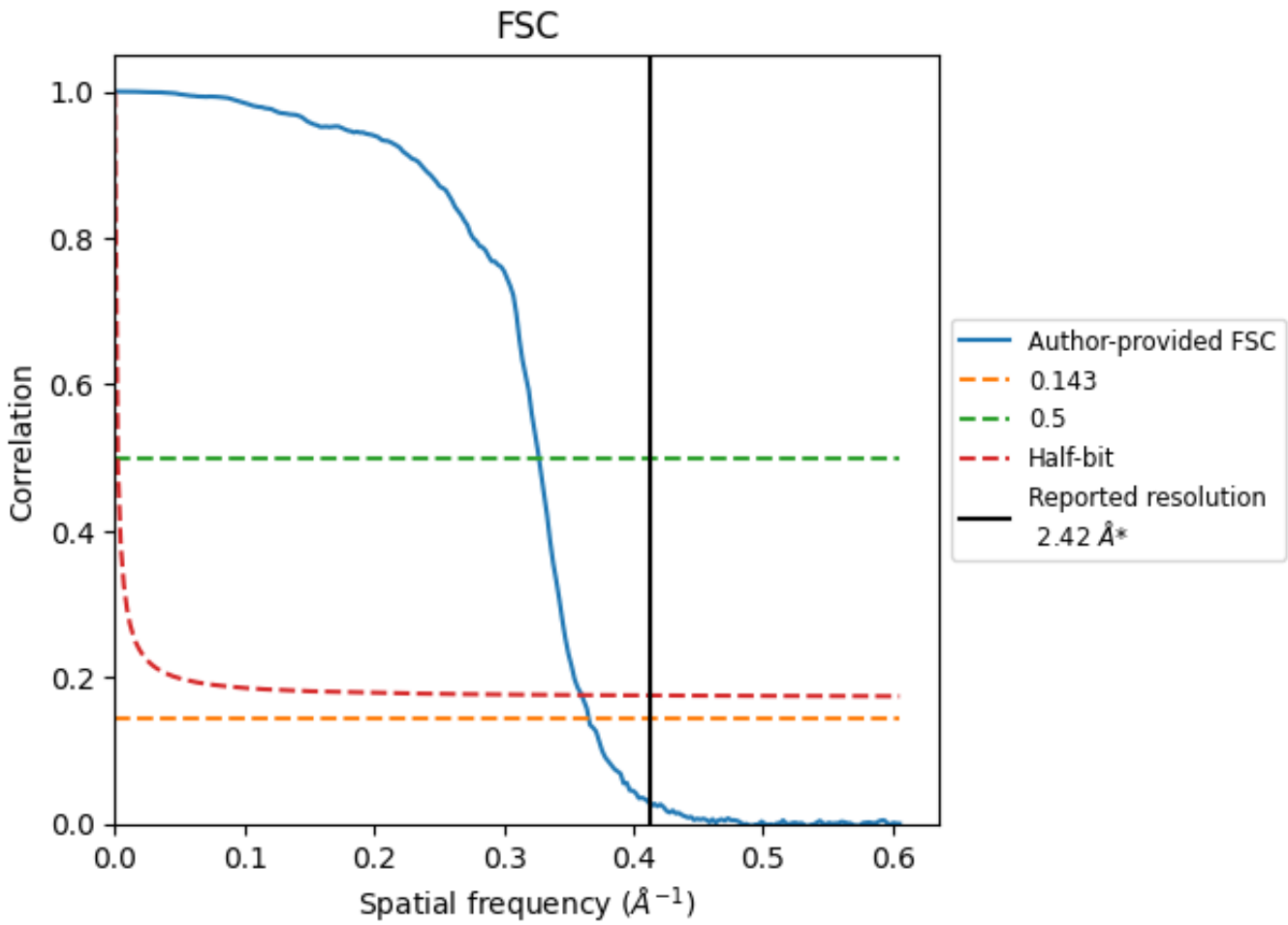


*Reported resolution corresponds to spatial frequency of 0.413 Å^{-1}

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 0.413 Å^{-1}

8.2 Resolution estimates (i)

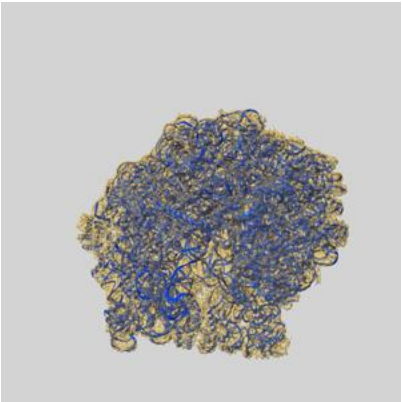
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.74	3.06	2.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.74 differs from the reported value 2.42 by more than 10 %

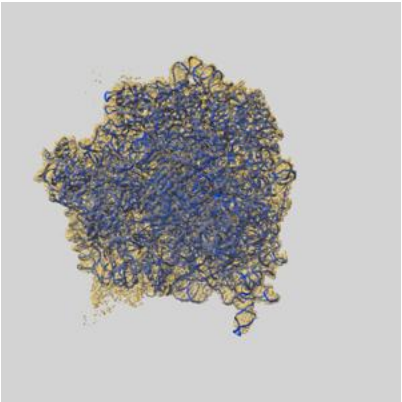
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24804 and PDB model 7S1K. Per-residue inclusion information can be found in section 3 on page 15.

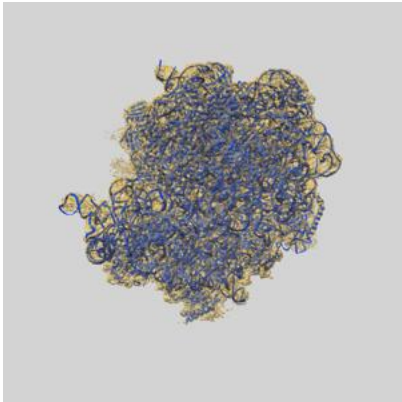
9.1 Map-model overlay (i)



X



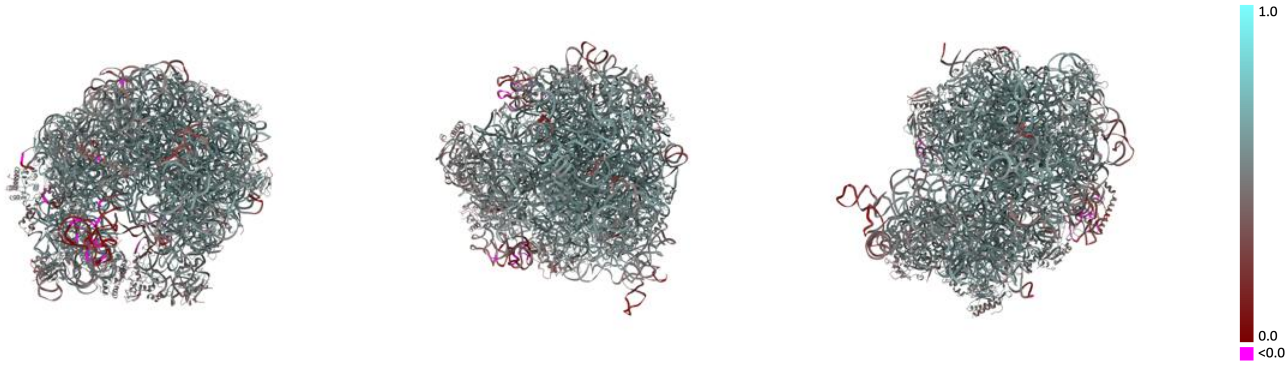
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

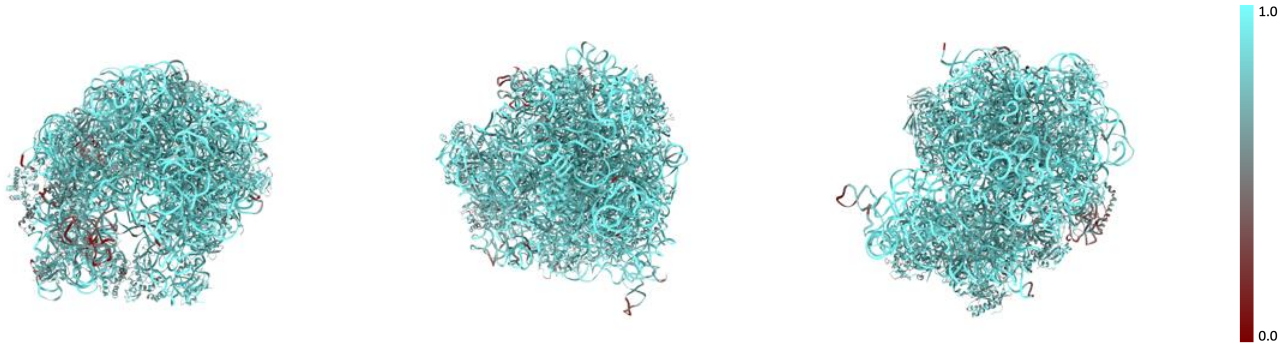
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

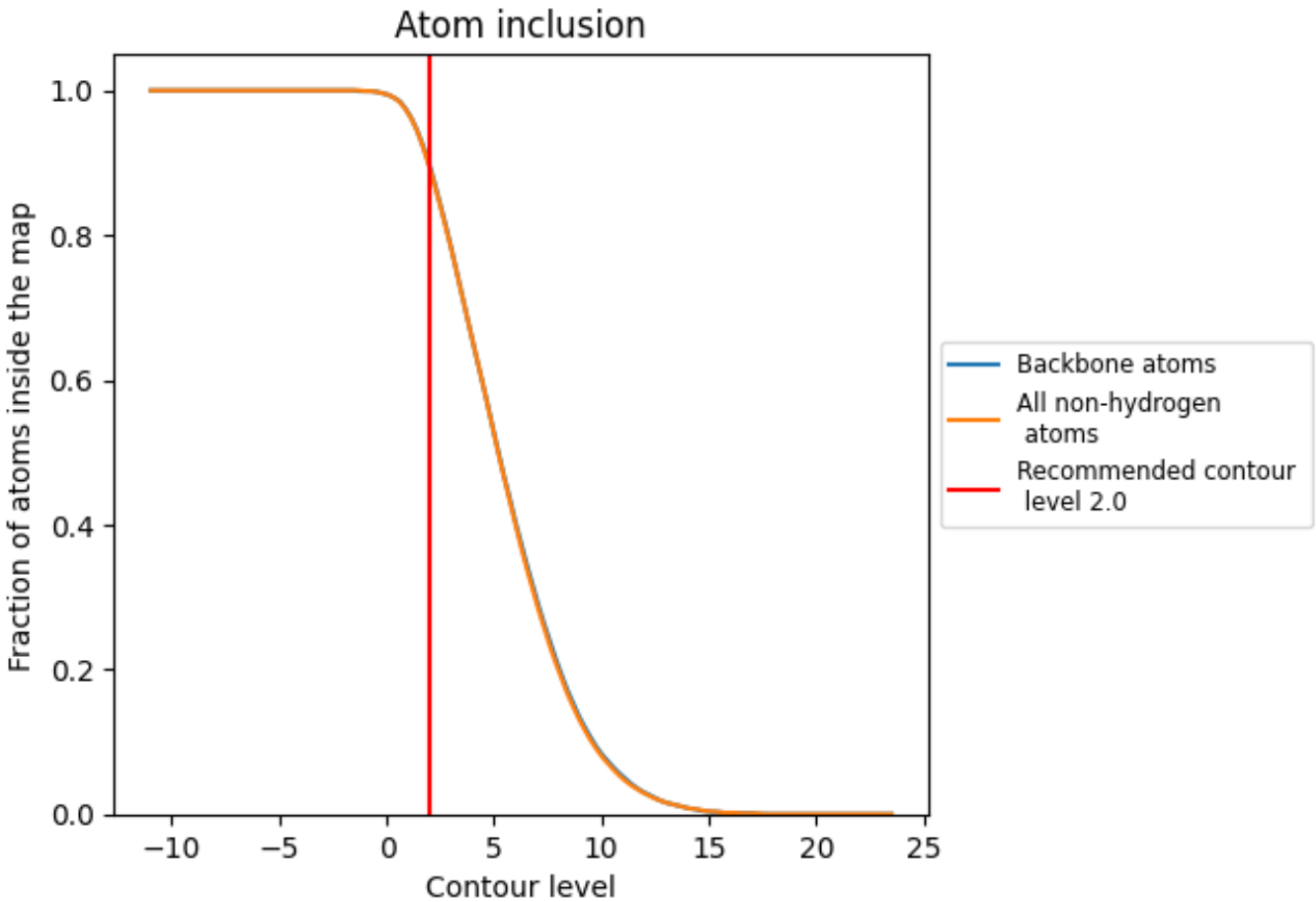
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.5310
1	0.7830	0.4670
2	0.7680	0.4910
3	0.5680	0.4300
4	0.9200	0.5580
A	0.9000	0.4950
C	0.9390	0.5360
D	0.6930	0.4690
E	0.7780	0.5130
F	0.7550	0.4860
G	0.8240	0.5410
H	0.8000	0.4840
I	0.9420	0.5410
J	0.9410	0.4930
K	0.8940	0.5810
L	0.8610	0.5630
M	0.8050	0.5310
N	0.7490	0.4540
O	0.7540	0.4420
P	0.5460	0.3740
Q	0.7120	0.4250
R	0.8520	0.5590
S	0.8610	0.5820
T	0.8350	0.5410
U	0.8330	0.5510
V	0.8890	0.5810
W	0.7890	0.4760
X	0.8360	0.5650
Y	0.8920	0.5770
Z	0.8570	0.5520
a	0.8420	0.5790
b	0.7670	0.5170
c	0.8120	0.5060
d	0.7910	0.5030
e	0.8710	0.5850

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Chain	Atom inclusion	Q-score
f	0.8340	0.5390
g	0.7730	0.4820
h	0.8440	0.5410
i	0.8510	0.5730
j	0.7110	0.4950
k	0.8790	0.5990
l	0.8920	0.5970
m	0.8360	0.5390
n	0.7400	0.4690
o	0.8270	0.5510
p	0.7510	0.4740
q	0.5830	0.4390
r	0.8230	0.5200
s	0.3860	0.5040
t	0.8660	0.5510
u	0.8040	0.4980
v	0.7540	0.4880
w	0.8670	0.5340
x	0.7860	0.5010
y	0.7880	0.5260
z	0.8560	0.5320