



Full wwPDB EM Validation Report ⓘ

Jul 10, 2023 – 02:53 PM EDT

PDB ID : 8FKV
EMDB ID : EMD-29258
Title : Human nucleolar pre-60S ribosomal subunit (State D1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.47 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

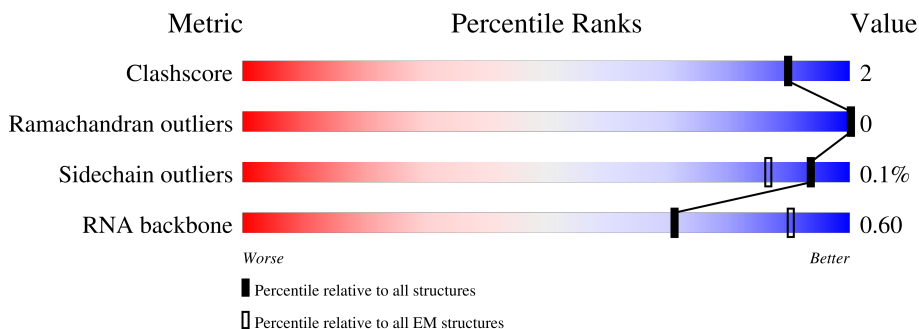
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

1 Overall quality at a glance

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

The reported resolution of this entry is 2.47 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.







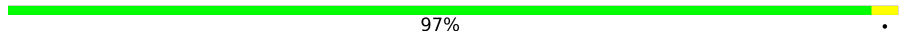








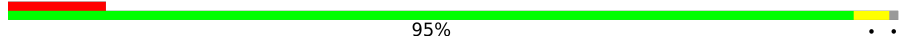
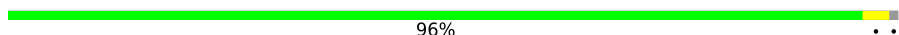
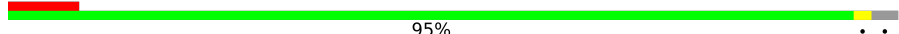






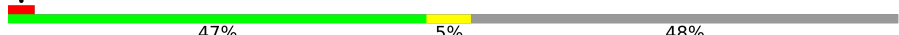


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	BA	165	
2	BB	217	
3	L1	157	
4	L2	1167	
5	L3	5070	
6	L6	211	
7	L7	203	

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Mol	Chain	Length	Quality of chain
8	L8	215	
9	L9	204	
10	LA	184	
11	LB	188	
12	LC	176	
13	LE	160	
14	LG	140	
15	LH	156	
16	LI	145	
17	LK	148	
18	LN	403	
19	LP	125	
20	LQ	135	
21	LS	123	
22	LT	110	
23	LU	105	
24	LW	97	
25	NA	749	
26	NB	549	
27	NF	260	
28	NH	180	
29	NI	881	
30	NK	129	
31	NM	300	
32	NO	461	

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Mol	Chain	Length	Quality of chain
33	NQ	385	81% 16%
34	NS	349	84% 13%
35	SA	427	80% 16%
36	SC	288	64% 6% 31%
37	SD	248	92%
38	SE	266	66% 30%
39	SG	192	92% 7%
40	SH	293	51% 49%
41	SI	255	85% 12%
42	SJ	847	8% 36% 60%
43	SK	245	93% 7%
44	SL	490	48% 50%
45	SM	588	11% 74% 23%
46	SN	306	55% 43%
47	SO	353	82% 5% 13%
48	SQ	239	6% 86% 5% 9%
49	SR	634	6% 67% 6% 27%
50	SS	746	30% 67%
51	ST	365	13% 30% 68%
52	SU	800	5% 66% 30%
53	SV	163	17% 74% 9% 16%
54	SW	670	21% 63% 34%
55	SY	812	44% 53%
56	SZ	178	87% 10%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 148975 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BA	160	1208	749	226	229	4	0	0

- Molecule 2 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	BB	213	1057	631	213	213	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L1	152	3234	1443	571	1068	152	0	0

- Molecule 4 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L2	69	1468	653	263	483	69	0	0

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L3	2213	47439	21130	8683	15413	2213	0	0

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L6	120	998	625	218	154	1	0	0

- Molecule 7 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L7	199	1634	1053	319	257	5	0	0

- Molecule 8 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L8	135	1111	713	213	178	7	0	0

- Molecule 9 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L9	183	1546	974	325	243	4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LA	160	1286	809	240	229	8	0	0

- Molecule 11 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LB	151	1223	768	247	203	5	0	0

- Molecule 12 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LC	176	1461	930	284	236	11	0	0

- Molecule 13 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LE	113	926	589	176	159	2	0	0

- Molecule 14 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LG	134	993	625	187	176	5	0	0

- Molecule 15 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LH	133	813	499	172	142		0	0

- Molecule 16 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LI	134	1115	700	226	186	3	0	0

- Molecule 17 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LK	108	642	388	137	115	2	0	0

- Molecule 18 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LN	358	2884	1834	531	506	13	0	0

- Molecule 19 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LP	106	526	314	106	106		0	0

- Molecule 20 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LQ	133	1096	690	225	176	5	0	0

- Molecule 21 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LS	122	1015	641	205	168	1	0	0

- Molecule 22 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	LT	109	876	555	174	144	3	0	0

- Molecule 23 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LU	102	832	521	177	129	5	0	0

- Molecule 24 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LW	74	612	379	134	94	5	0	0

- Molecule 25 is a protein called Nucleolar complex protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	NA	484	3658	2355	644	638	21	0	0

- Molecule 26 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	NB	387	2424	1493	475	450	6	0	0

- Molecule 27 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	NF	218	1783	1136	337	301	9	0	0

- Molecule 28 is a protein called 60S ribosome subunit biogenesis protein NIP7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	NH	180	1441	925	245	263	8	0	0

- Molecule 29 is a protein called ATP-dependent RNA helicase DDX54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	NI	647	5137	3254	934	934	15	0	0

- Molecule 30 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	NK	67	581	363	128	88	2	0	0

- Molecule 31 is a protein called Protein MAK16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	NM	182	1550	983	286	273	8	0	0

- Molecule 32 is a protein called Ribosomal RNA processing protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	NO	305	2487	1577	437	461	12	0	0

- Molecule 33 is a protein called WD repeat-containing protein 74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	NQ	324	2502	1559	471	457	15	0	0

- Molecule 34 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	NS	305	2529	1607	472	444	6	0	0

- Molecule 35 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	SA	360	2864	1803	572	475	14	0	0

- Molecule 36 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	SC	199	1627	1046	305	274	2	0	0

- Molecule 37 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	SD	239	1985	1275	381	320	9	0	0

- Molecule 38 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	SE	185	1491	946	289	252	4	0	0

- Molecule 39 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	SG	190	1526	961	287	272	6	1	0

- Molecule 40 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	SH	150	1267	819	224	220	4	0	0

- Molecule 41 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	SI	225	1864	1207	349	304	4	1	0

- Molecule 42 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SJ	340	Total	C	N	O	S	0	0
			2780	1777	507	489	7		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 44 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SL	243	Total	C	N	O	S	0	0
			1960	1254	344	356	6		

- Molecule 45 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SM	453	Total	C	N	O	S	0	0
			3735	2408	667	648	12		

- Molecule 46 is a protein called Probable rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SN	173	Total	C	N	O	S	0	0
			1350	849	251	243	7		

- Molecule 47 is a protein called Ribosome biogenesis protein BRX1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SO	307	Total	C	N	O	S	0	0
			2544	1637	458	434	15		

- Molecule 48 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SQ	217	Total	C	N	O	S	1	0
			1778	1134	313	320	11		

- Molecule 49 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	SR	462	3808	2417	677	696	18	0	0

- Molecule 50 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P S		
50	SS	243	2011	1271	357	374	2 7	0	0

- Molecule 51 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	ST	116	838	527	155	154	2	0	0

- Molecule 52 is a protein called Nucleolar complex protein 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	SU	561	4434	2842	761	810	21	0	0

- Molecule 53 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	SV	137	1171	745	227	189	10	0	0

- Molecule 54 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	SW	444	3549	2282	605	645	17	0	0

- Molecule 55 is a protein called Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	SY	378	2985	1887	533	550	15	0	0

- Molecule 56 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	SZ	160	1338	835	260	238	5	0	0

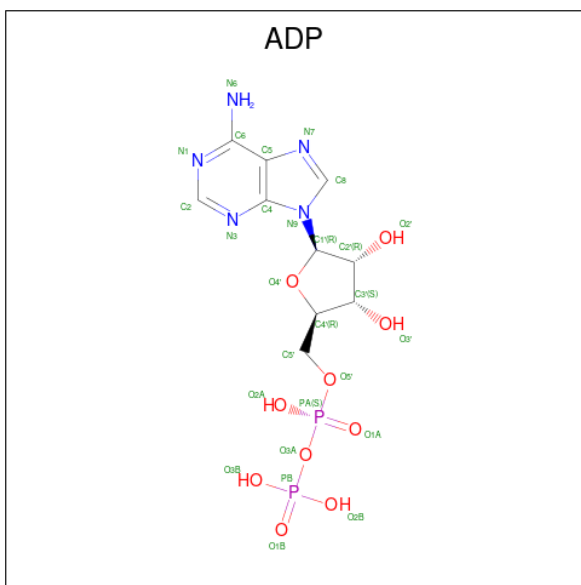
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	L1	4	Total	Mg	0
			4	4	
57	L2	1	Total	Mg	0
			1	1	
57	L3	51	Total	Mg	0
			51	51	
57	L9	1	Total	Mg	0
			1	1	
57	LN	1	Total	Mg	0
			1	1	
57	LQ	1	Total	Mg	0
			1	1	
57	LT	1	Total	Mg	0
			1	1	
57	NI	1	Total	Mg	0
			1	1	
57	SA	1	Total	Mg	0
			1	1	
57	SO	1	Total	Mg	0
			1	1	
57	SR	1	Total	Mg	0
			1	1	
57	SU	1	Total	Mg	0
			1	1	

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

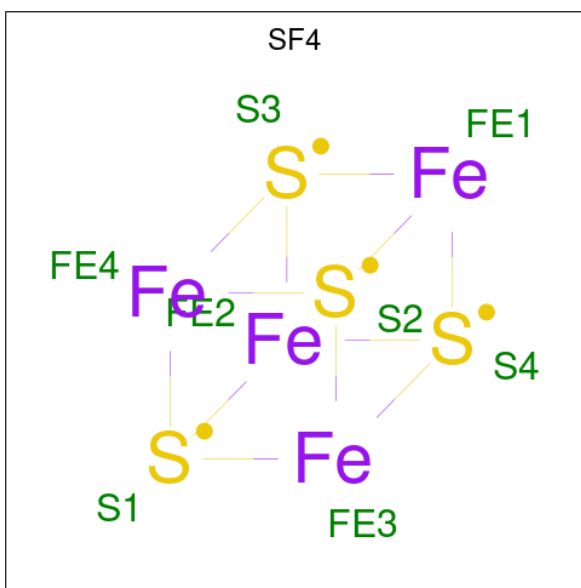
Mol	Chain	Residues	Atoms		AltConf
58	LW	1	Total	Zn	0
			1	1	
58	SV	1	Total	Zn	0
			1	1	

- Molecule 59 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



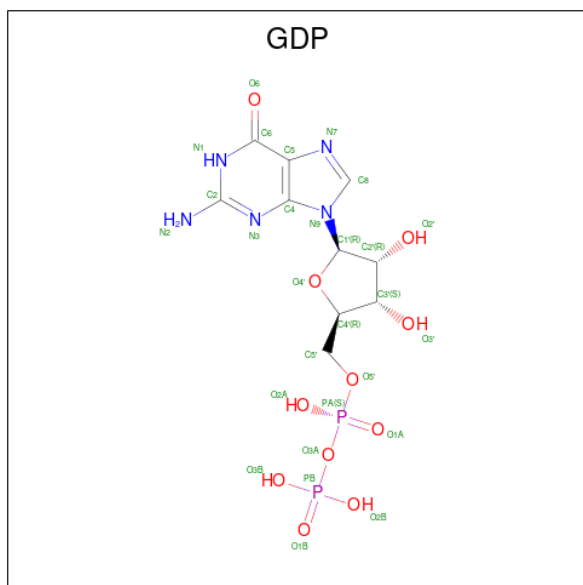
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	NI	1	27	10	5	10	2	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
60	NM	1	8	4	4	0

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
61	SR	1	28	10	5	11	2	0

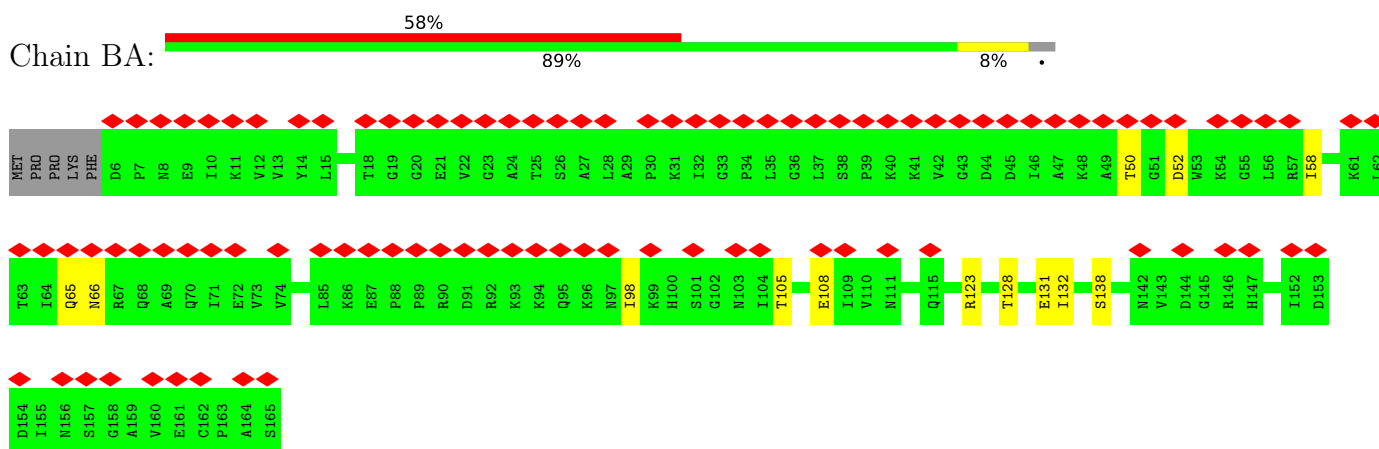
- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
62	SR	1	1	1	0

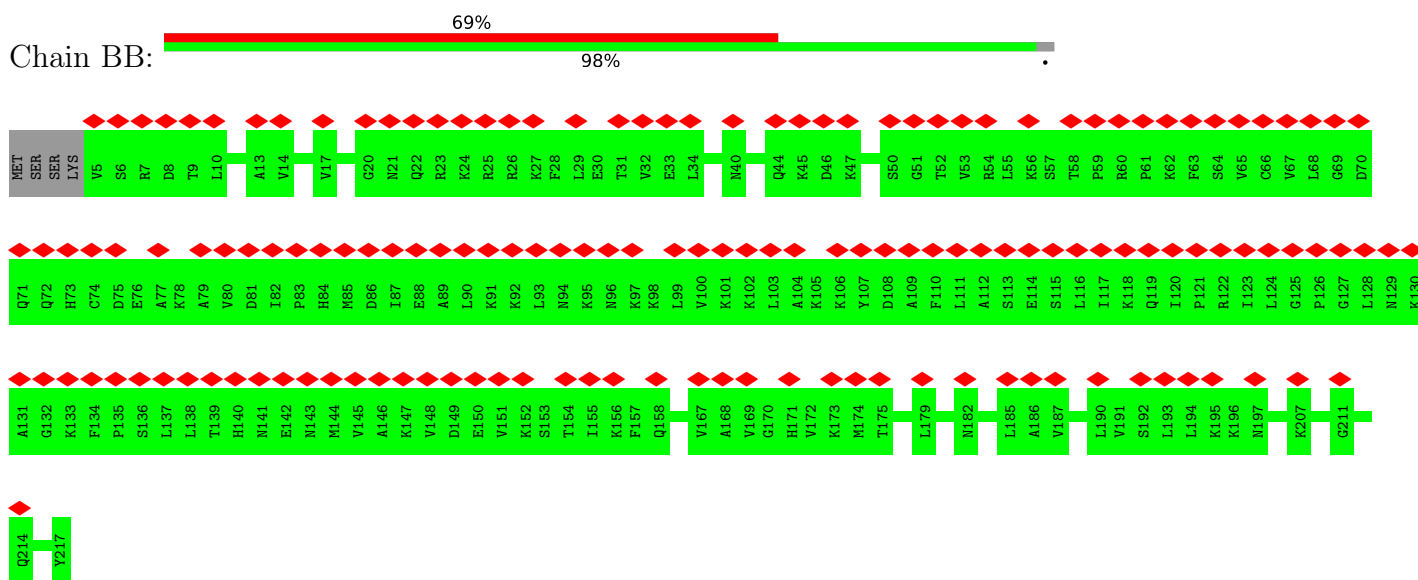
3 Residue-property plots [i](#)

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.

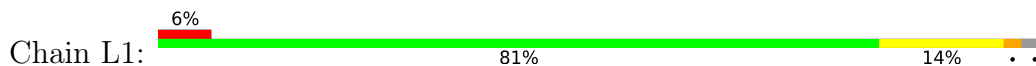
- Molecule 1: 60S ribosomal protein L12

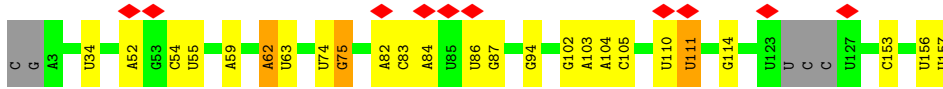


- Molecule 2: 60S ribosomal protein L10a

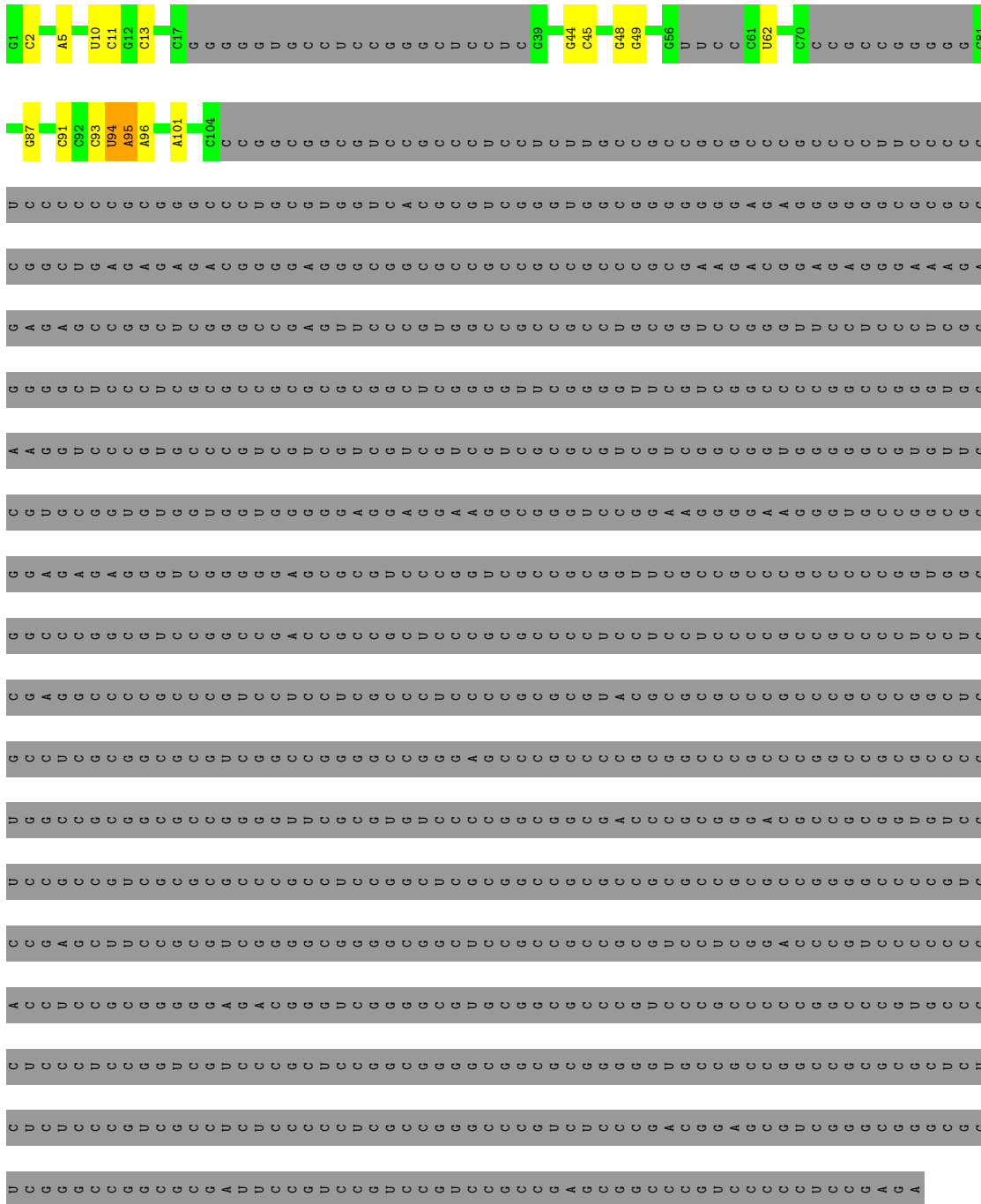


- Molecule 3: 5.8S rRNA

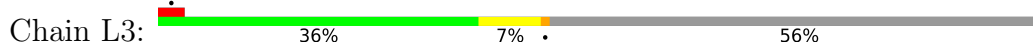


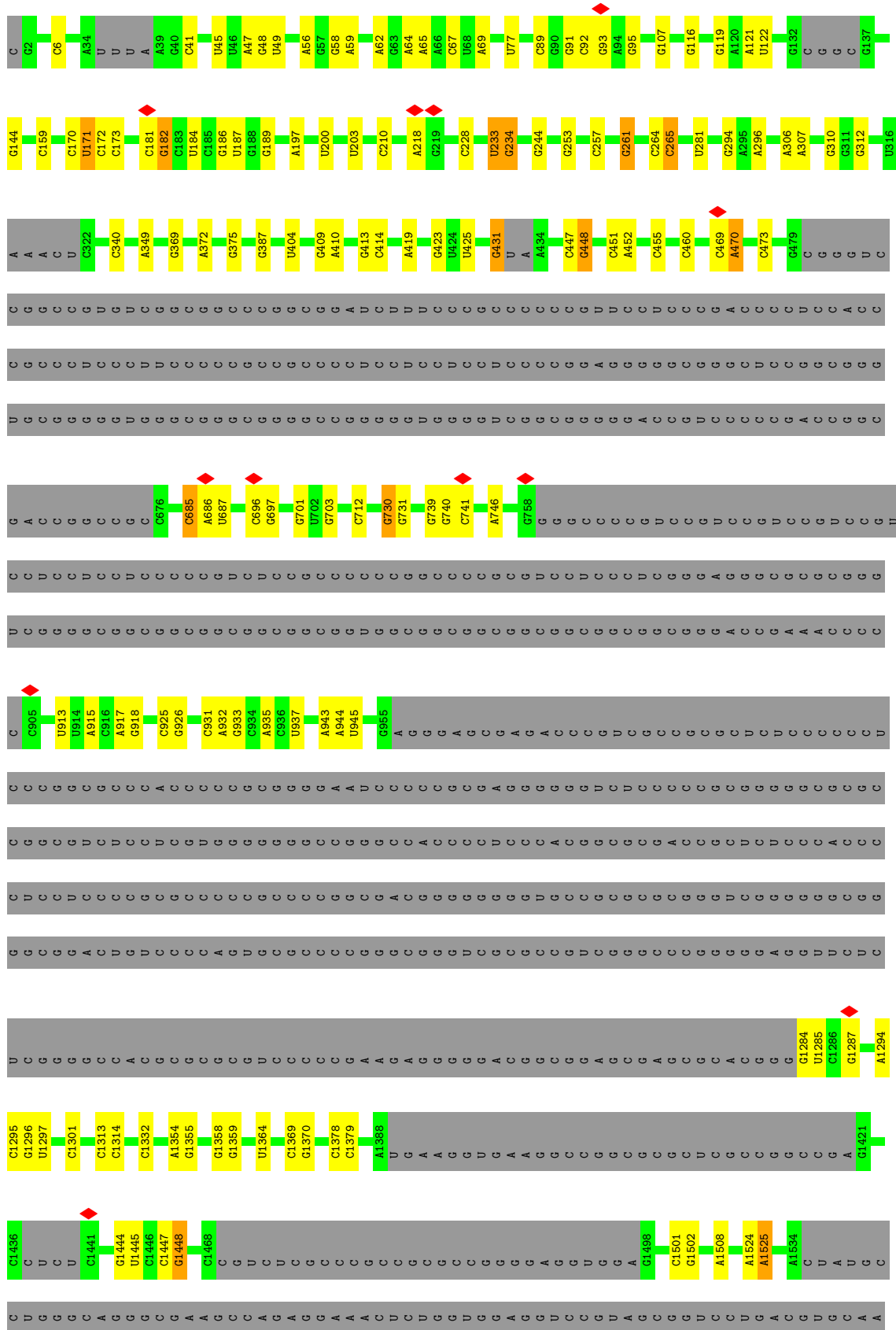


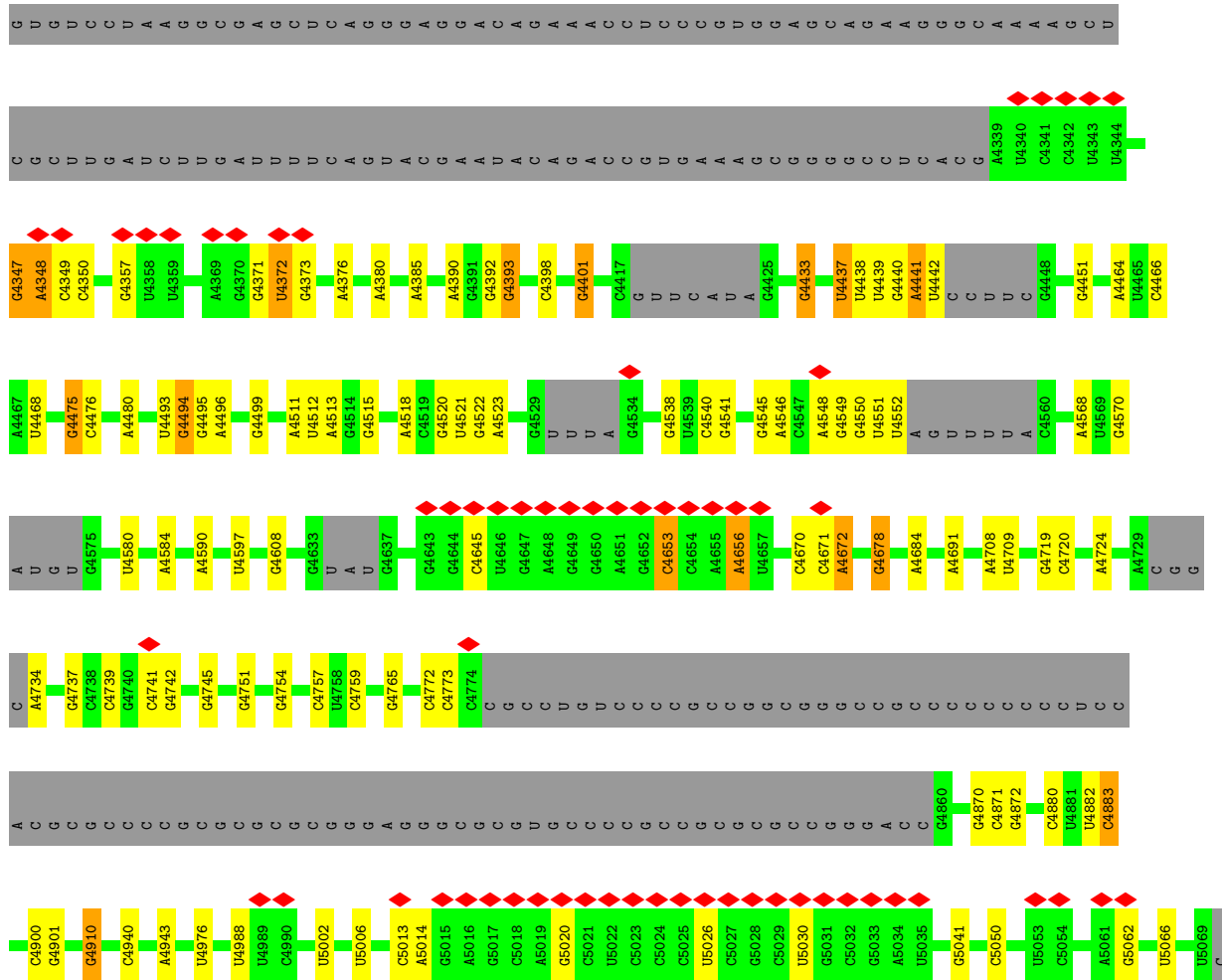
● Molecule 4: ITS2 rRNA



● Molecule 5: 28S rRNA

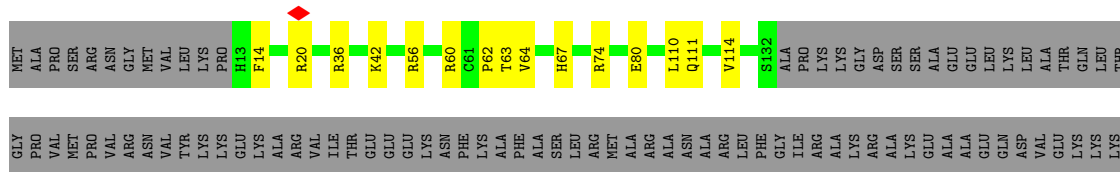






• Molecule 6: 60S ribosomal protein L13

Chain L6: 50% 7% 43%



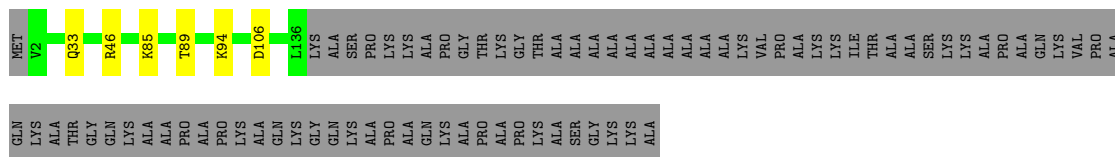
• Molecule 7: 60S ribosomal protein L13a

Chain L7: 94%

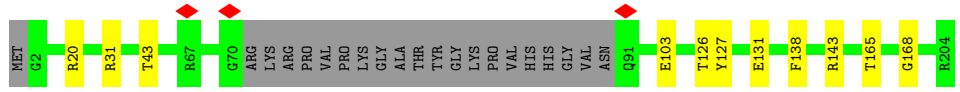
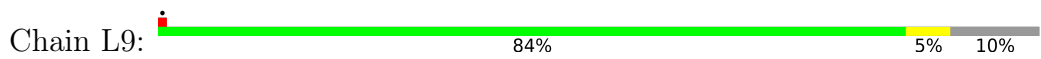


• Molecule 8: 60S ribosomal protein L14

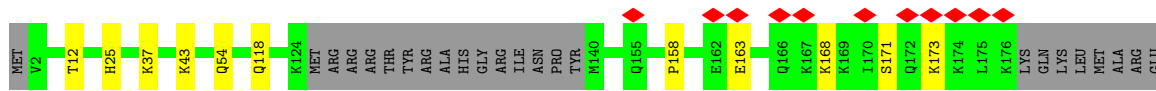
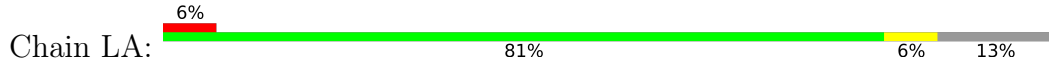
Chain L8: 60% 37%



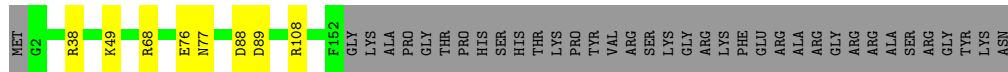
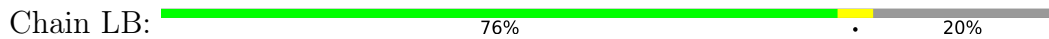
• Molecule 9: 60S ribosomal protein L15



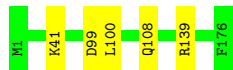
• Molecule 10: 60S ribosomal protein L17



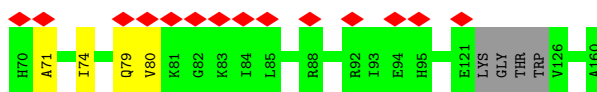
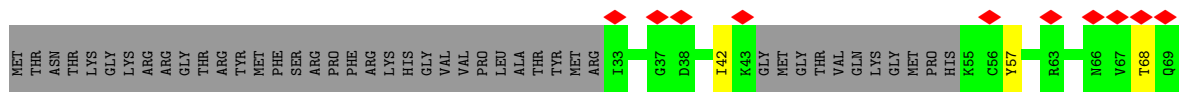
• Molecule 11: 60S ribosomal protein L18



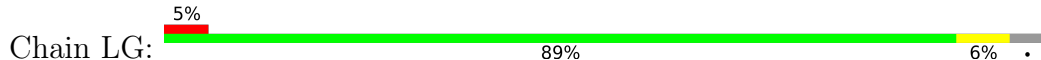
• Molecule 12: 60S ribosomal protein L18a

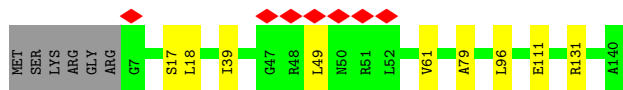


• Molecule 13: 60S ribosomal protein L21

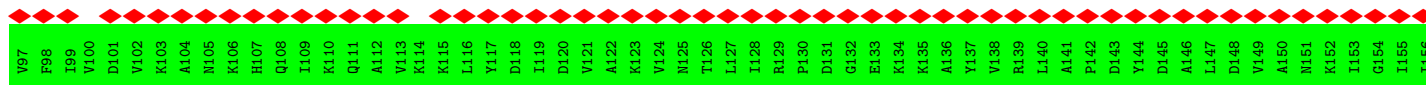
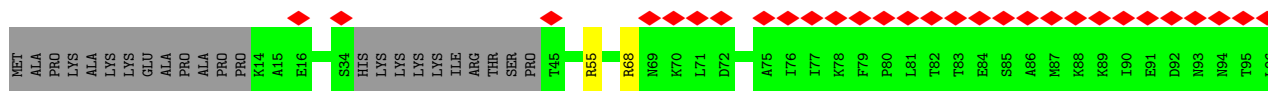
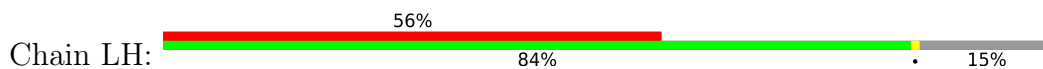


• Molecule 14: 60S ribosomal protein L23

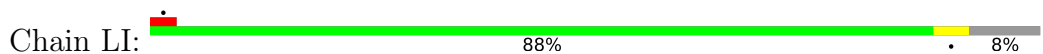




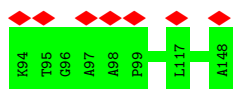
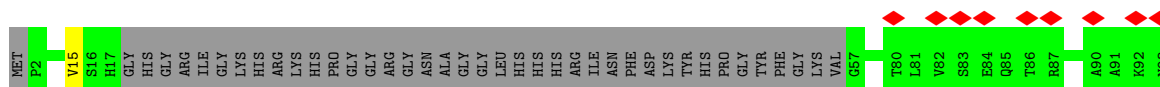
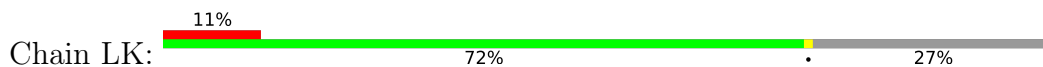
• Molecule 15: 60S ribosomal protein L23a



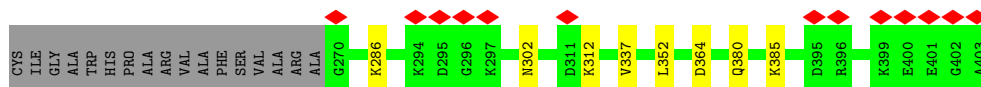
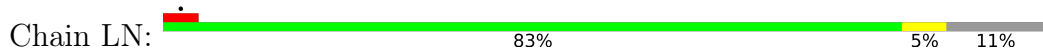
• Molecule 16: 60S ribosomal protein L26



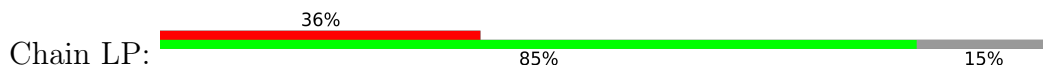
• Molecule 17: 60S ribosomal protein L27a

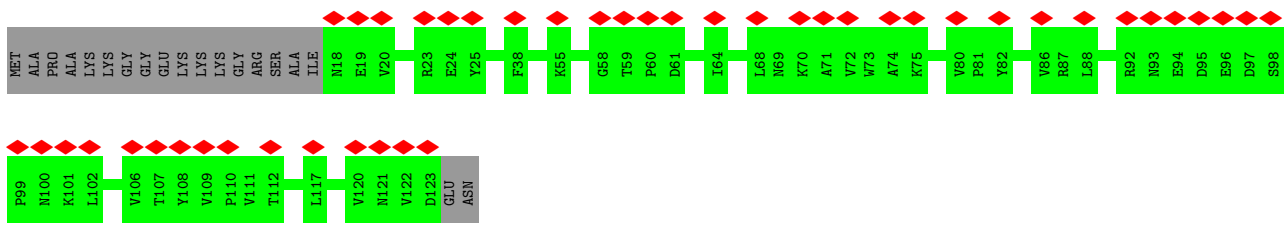


• Molecule 18: 60S ribosomal protein L3



• Molecule 19: 60S ribosomal protein L31

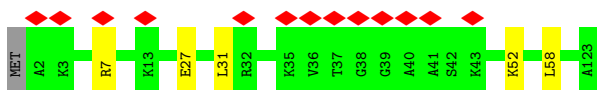




● Molecule 20: 60S ribosomal protein L32



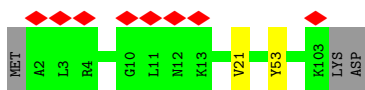
● Molecule 21: 60S ribosomal protein L35



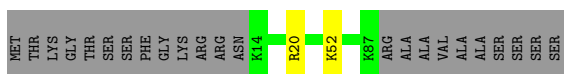
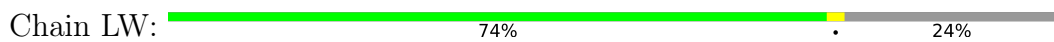
● Molecule 22: 60S ribosomal protein L35a



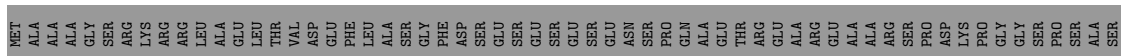
● Molecule 23: 60S ribosomal protein L36

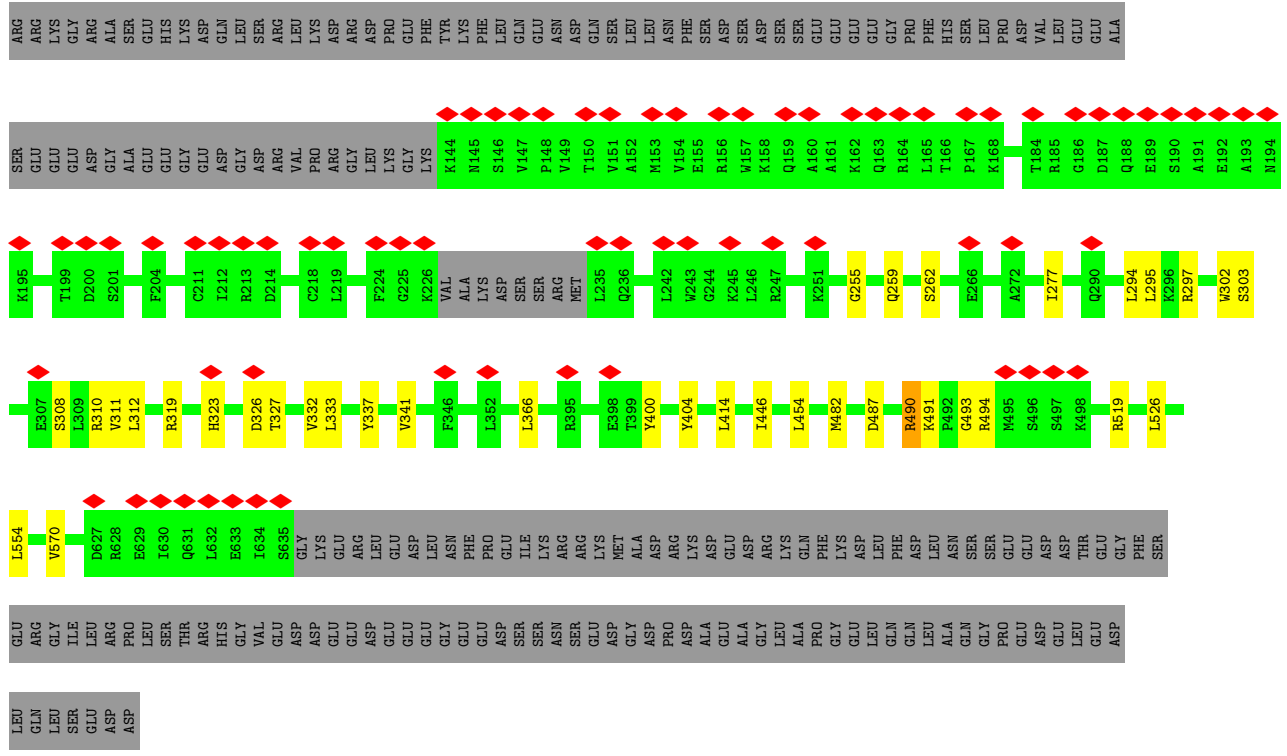


● Molecule 24: 60S ribosomal protein L37

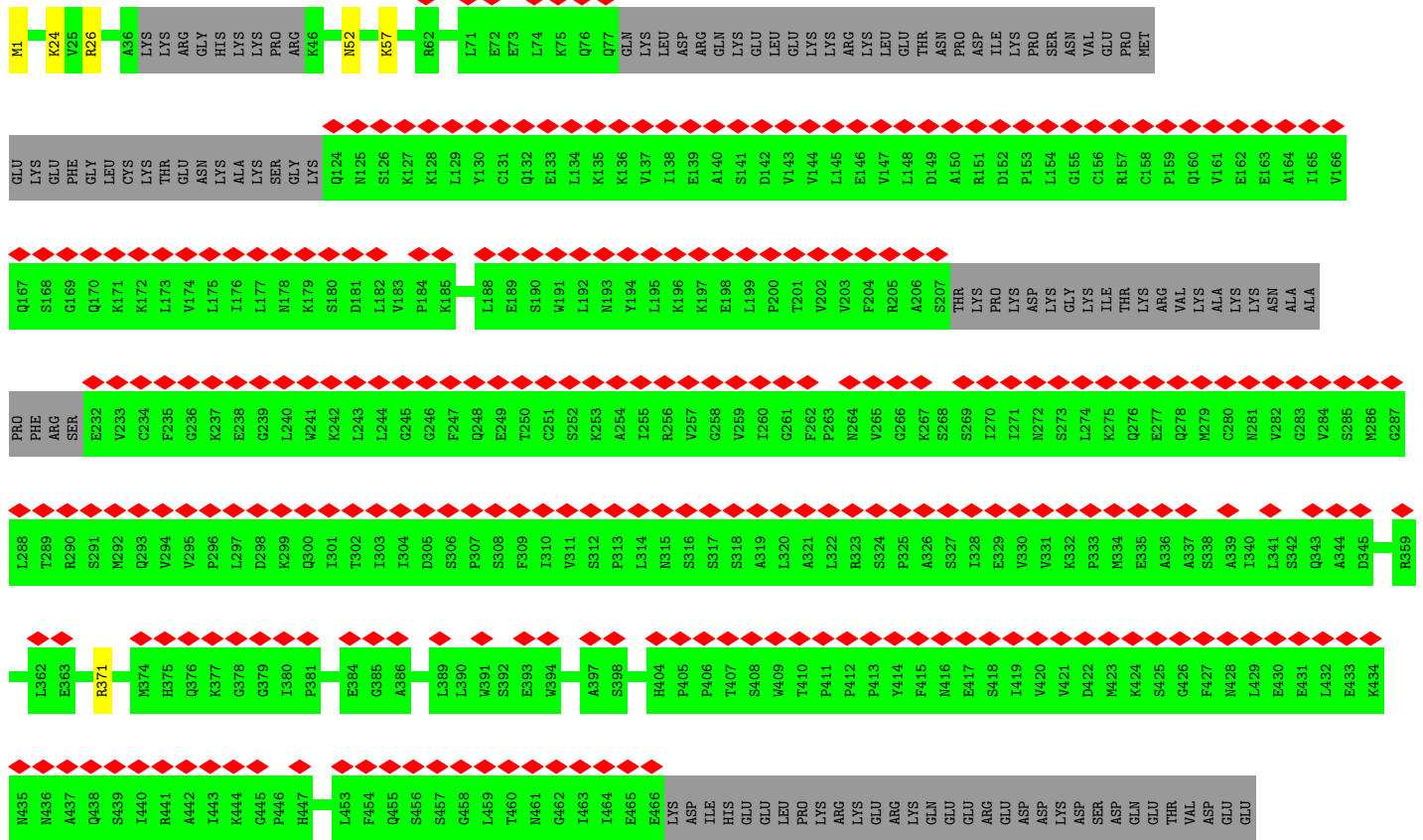


● Molecule 25: Nucleolar complex protein 2 homolog

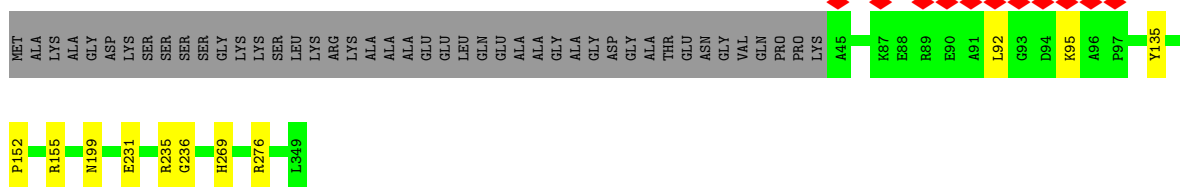




• Molecule 26: Guanine nucleotide-binding protein-like 3

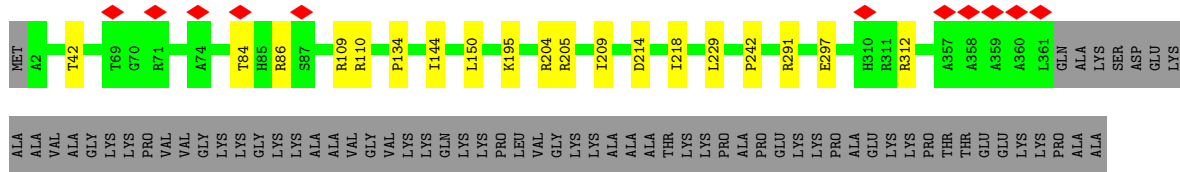


Chain NS: 84% 13%



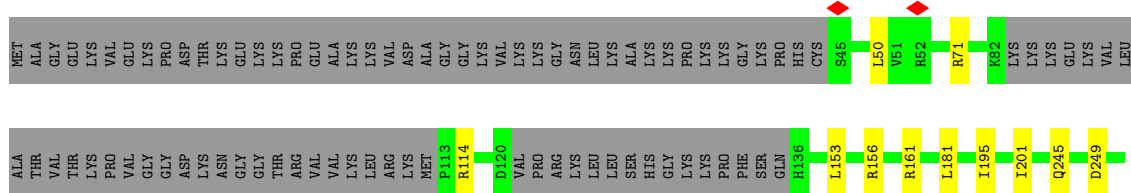
- Molecule 35: 60S ribosomal protein L4

Chain SA: 80% 16%



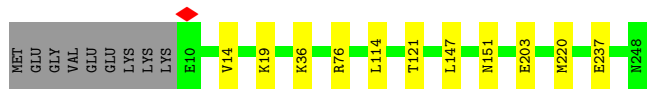
- Molecule 36: 60S ribosomal protein L6

Chain SC: 64% 6% 31%



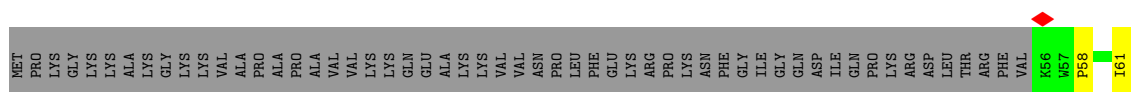
- Molecule 37: 60S ribosomal protein L7

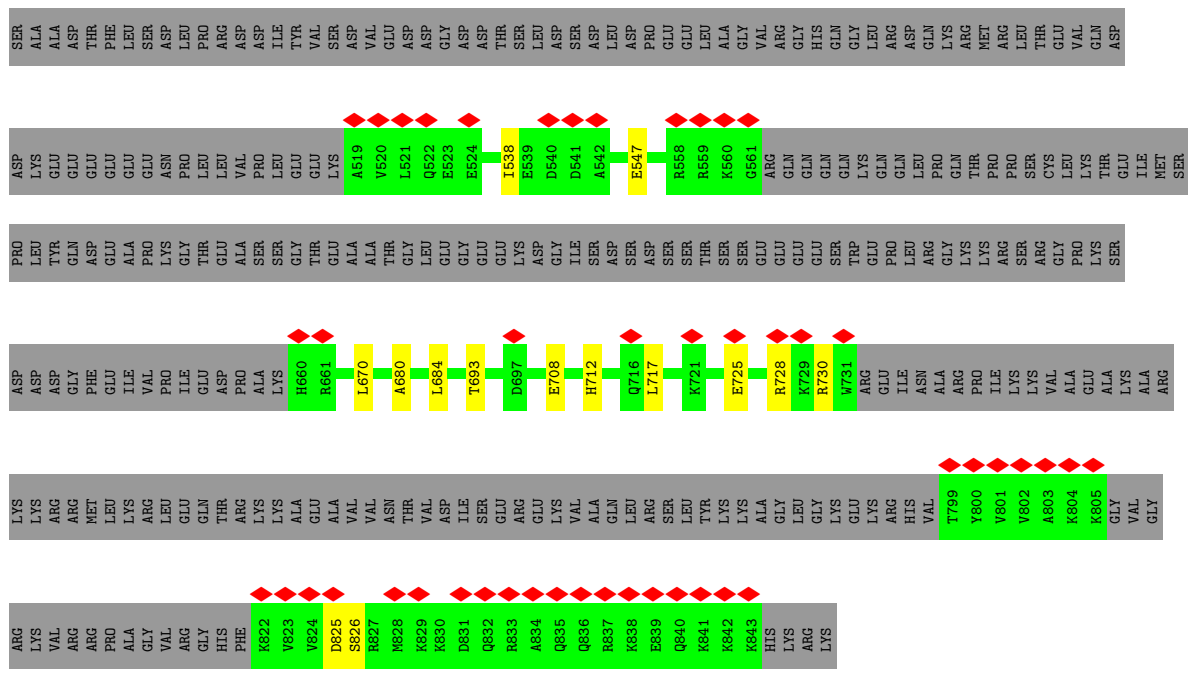
Chain SD: 92%



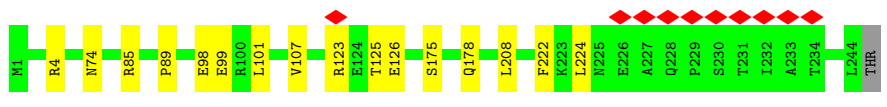
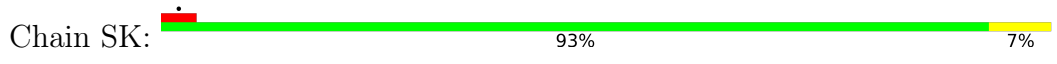
- Molecule 38: 60S ribosomal protein L7a

Chain SE: 66% 30%

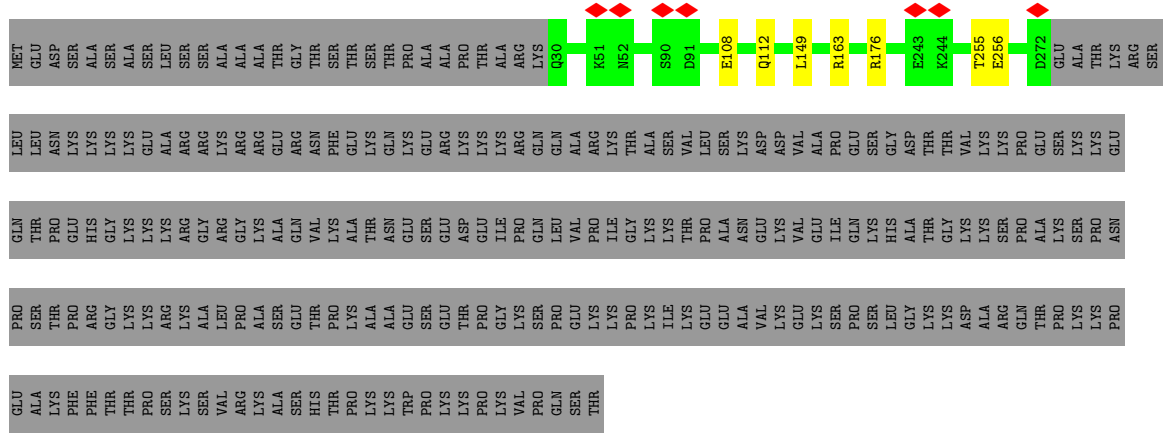




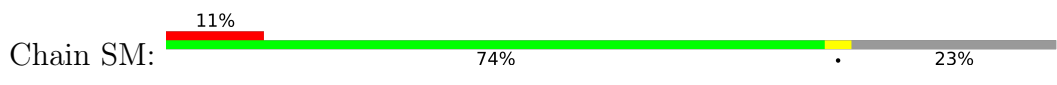
● Molecule 43: Eukaryotic translation initiation factor 6



● Molecule 44: Ribosomal L1 domain-containing protein 1



● Molecule 45: Pescadillo homolog



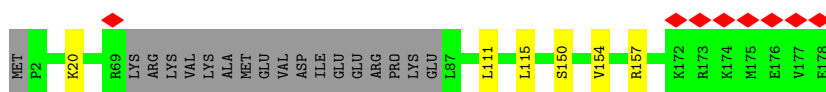
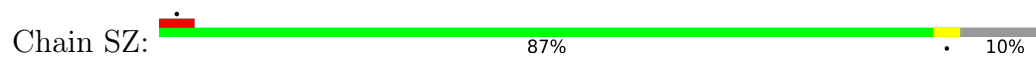
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GLY
ALA
LYS
THR
LYS
GLN
GLN
LEU
GLY
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LYS
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GLN
HIS
PRO
LYS
LYS
LYS
ALA
PHE
GLN
LYS
LYS
LEU
ASN
GLY
ILE
SER
LYS
GLY
ALA
ASP
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LEU
SER

• Molecule 56: Nucleolar protein 16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	209464	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.435	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.039	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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: SF4, SEP, GDP, ZN, MG, AME, K, ADP

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	BA	0.24	0/1224	0.50	0/1651
2	BB	0.24	0/1056	0.45	0/1472
3	L1	0.24	0/3611	0.74	0/5623
4	L2	0.24	0/1634	0.78	0/2538
5	L3	0.25	0/53038	0.78	2/82653 (0.0%)
6	L6	0.25	0/1020	0.64	0/1367
7	L7	0.26	0/1666	0.55	0/2228
8	L8	0.26	0/1133	0.53	0/1516
9	L9	0.25	0/1584	0.63	0/2117
10	LA	0.24	0/1309	0.47	0/1752
11	LB	0.24	0/1239	0.62	0/1658
12	LC	0.25	0/1501	0.57	0/2013
13	LE	0.25	0/941	0.52	0/1254
14	LG	0.26	0/1007	0.55	0/1350
15	LH	0.23	0/818	0.51	0/1111
16	LI	0.26	0/1132	0.61	1/1504 (0.1%)
17	LK	0.23	0/648	0.52	0/880
18	LN	0.25	0/2938	0.52	0/3923
19	LP	0.22	0/525	0.43	0/731
20	LQ	0.24	0/1114	0.58	0/1486
21	LS	0.25	0/1023	0.56	0/1351
22	LT	0.25	0/895	0.61	0/1198
23	LU	0.25	0/843	0.62	0/1115
24	LW	0.25	0/626	0.64	0/829
25	NA	0.26	0/3734	0.47	0/5079
26	NB	0.24	0/2449	0.46	0/3335
27	NF	0.25	0/1816	0.52	0/2420
28	NH	0.26	0/1473	0.50	0/1988
29	NI	0.24	0/5222	0.52	0/7025
30	NK	0.23	0/587	0.58	0/767
31	NM	0.25	0/1566	0.54	0/2097
32	NO	0.24	0/2530	0.49	0/3412

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	NQ	0.24	0/2556	0.54	0/3466
34	NS	0.25	0/2592	0.53	0/3487
35	SA	0.24	0/2918	0.57	0/3920
36	SC	0.25	0/1657	0.55	0/2219
37	SD	0.25	0/2022	0.56	0/2696
38	SE	0.24	0/1517	0.54	0/2046
39	SG	0.25	0/1548	0.54	0/2081
40	SH	0.26	0/1298	0.50	0/1742
41	SI	0.24	0/1906	0.51	0/2561
42	SJ	0.24	0/2833	0.49	0/3801
43	SK	0.24	0/1877	0.52	0/2554
44	SL	0.24	0/1994	0.50	0/2684
45	SM	0.25	0/3819	0.49	0/5139
46	SN	0.24	0/1368	0.48	0/1830
47	SO	0.25	0/2608	0.51	0/3506
48	SQ	0.25	0/1817	0.51	0/2435
49	SR	0.25	0/3882	0.51	0/5237
50	SS	0.25	0/2052	0.52	0/2786
51	ST	0.24	0/851	0.45	0/1149
52	SU	0.25	0/4510	0.45	0/6082
53	SV	0.26	0/1194	0.53	0/1582
54	SW	0.24	0/3620	0.47	0/4886
55	SY	0.24	0/3046	0.52	0/4117
56	SZ	0.24	0/1364	0.53	0/1826
All	All	0.25	0/156751	0.64	3/223275 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L3	4653	C	C2-N1-C1'	5.44	124.78	118.80
16	LI	53	ASP	CB-CG-OD1	5.15	122.94	118.30
5	L3	2266	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1208	0	1257	10	0
2	BB	1057	0	464	0	0
3	L1	3234	0	1639	6	0
4	L2	1468	0	755	6	0
5	L3	47439	0	24001	139	0
6	L6	998	0	1067	11	0
7	L7	1634	0	1779	5	0
8	L8	1111	0	1174	6	0
9	L9	1546	0	1585	9	0
10	LA	1286	0	1338	10	0
11	LB	1223	0	1330	6	0
12	LC	1461	0	1502	4	0
13	LE	926	0	979	4	0
14	LG	993	0	1050	9	0
15	LH	813	0	640	2	0
16	LI	1115	0	1205	4	0
17	LK	642	0	455	1	0
18	LN	2884	0	3000	19	0
19	LP	526	0	225	0	0
20	LQ	1096	0	1183	7	0
21	LS	1015	0	1148	4	0
22	LT	876	0	912	2	0
23	LU	832	0	917	2	0
24	LW	612	0	640	2	0
25	NA	3658	0	3564	23	0
26	NB	2424	0	1868	5	0
27	NF	1783	0	1896	11	0
28	NH	1441	0	1448	16	0
29	NI	5137	0	5294	22	0
30	NK	581	0	656	7	0
31	NM	1550	0	1599	12	0
32	NO	2487	0	2506	8	0
33	NQ	2502	0	2481	7	0
34	NS	2529	0	2563	9	0
35	SA	2864	0	3038	13	0
36	SC	1627	0	1751	11	0
37	SD	1985	0	2128	8	0
38	SE	1491	0	1592	6	0
39	SG	1526	0	1614	8	0
40	SH	1267	0	1291	0	0
41	SI	1864	0	1982	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	SJ	2780	0	2826	25	0
43	SK	1852	0	1828	9	0
44	SL	1960	0	2052	5	0
45	SM	3735	0	3830	11	0
46	SN	1350	0	1345	6	0
47	SO	2544	0	2631	15	0
48	SQ	1778	0	1817	8	0
49	SR	3808	0	3873	24	0
50	SS	2011	0	1919	14	0
51	ST	838	0	781	5	0
52	SU	4434	0	4551	31	0
53	SV	1171	0	1232	12	0
54	SW	3549	0	3628	15	0
55	SY	2985	0	3004	11	0
56	SZ	1338	0	1352	5	0
57	L1	4	0	0	0	0
57	L2	1	0	0	0	0
57	L3	51	0	0	0	0
57	L9	1	0	0	0	0
57	LN	1	0	0	0	0
57	LQ	1	0	0	0	0
57	LT	1	0	0	0	0
57	NI	1	0	0	0	0
57	SA	1	0	0	0	0
57	SO	1	0	0	0	0
57	SR	1	0	0	0	0
57	SU	1	0	0	0	0
58	LW	1	0	0	0	0
58	SV	1	0	0	0	0
59	NI	27	0	12	0	0
60	NM	8	0	0	0	0
61	SR	28	0	12	0	0
62	SR	1	0	0	0	0
All	All	148975	0	124209	466	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (466) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:712:C:O2	5:L3:1284:G:N2	2.01	0.93
25:NA:302:TRP:O	25:NA:310:ARG:NH1	2.11	0.84
1:BA:105:THR:OG1	1:BA:108:GLU:OE1	1.97	0.82
5:L3:2338:C:OP1	31:NM:22:ARG:NH1	2.13	0.82
54:SW:238:VAL:HG21	54:SW:274:LEU:HD22	1.61	0.82
5:L3:1501:C:O2'	11:LB:68:ARG:NH2	2.14	0.80
5:L3:4468:U:HO2'	30:NK:2:ALA:N	1.80	0.80
5:L3:3890:A:OP2	5:L3:4570:G:N2	2.15	0.79
5:L3:184:U:O2'	5:L3:189:G:OP2	1.99	0.79
5:L3:4678:G:OP1	30:NK:14:ARG:NH1	2.16	0.79
25:NA:303:SER:O	25:NA:310:ARG:NH2	2.16	0.79
25:NA:311:VAL:HG21	52:SU:775:LEU:HD22	1.65	0.79
31:NM:23:THR:OG1	31:NM:26:GLN:O	2.01	0.78
5:L3:712:C:N3	5:L3:1284:G:N1	2.30	0.78
43:SK:99:GLU:OE1	43:SK:125:THR:OG1	1.99	0.77
55:SY:227:MET:SD	55:SY:269:ARG:NH1	2.58	0.77
47:SO:48:PRO:O	50:SS:133:ARG:NH1	2.18	0.76
42:SJ:37:ARG:NH2	52:SU:476:ARG:O	2.18	0.76
5:L3:1524:A:O2'	5:L3:1525:A:O5'	2.03	0.76
29:NI:719:GLU:OE1	29:NI:722:ASN:ND2	2.19	0.76
14:LG:111:GLU:OE2	14:LG:131:ARG:NH1	2.19	0.75
25:NA:255:GLY:O	25:NA:259:GLN:NE2	2.20	0.75
5:L3:2343:G:OP2	35:SA:109:ARG:NH2	2.20	0.75
27:NF:17:ARG:NH1	39:SG:180:TYR:OH	2.19	0.74
49:SR:441:TYR:OH	53:SV:97:GLU:OE2	2.04	0.74
28:NH:138:ASP:OD2	52:SU:619:SER:OG	2.05	0.74
5:L3:2102:G:OP2	37:SD:36:LYS:NZ	2.15	0.74
5:L3:4672:A:OP1	14:LG:17:SER:OG	2.03	0.74
53:SV:62:GLU:OE2	53:SV:104:GLN:NE2	2.21	0.73
13:LE:68:THR:OG1	13:LE:71:ALA:O	2.04	0.73
5:L3:2054:U:OP2	7:L7:44:SER:OG	2.04	0.73
49:SR:161:LEU:HD12	49:SR:162:PRO:HD2	1.70	0.73
4:L2:10:U:OP2	44:SL:163:ARG:NH2	2.21	0.72
25:NA:490:ARG:NH1	25:NA:491:LYS:O	2.21	0.72
5:L3:3849:A:OP1	29:NI:834:ARG:NH1	2.22	0.72
3:L1:111:U:OP2	24:LW:20:ARG:NH1	2.23	0.72
5:L3:3835:C:O2'	5:L3:3836:A:OP1	2.08	0.72
18:LN:364:ASP:OD2	49:SR:428:LYS:NZ	2.20	0.72
53:SV:95:ARG:NH1	53:SV:98:GLU:OE1	2.23	0.71
5:L3:470:A:H61	5:L3:685:C:HO2'	1.36	0.71
5:L3:1883:G:OP1	20:LQ:47:ARG:NH1	2.22	0.71
20:LQ:84:GLU:O	20:LQ:87:VAL:HG22	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:NB:52:ASN:OD1	26:NB:57:LYS:NZ	2.21	0.71
5:L3:409:G:O6	31:NM:146:LYS:NZ	2.24	0.71
31:NM:132:ARG:NH1	34:NS:199:ASN:OD1	2.24	0.70
18:LN:213:GLN:O	30:NK:28:ARG:NH2	2.24	0.70
47:SO:61:ARG:NH1	50:SS:128:ASP:OD2	2.24	0.70
5:L3:144:G:OP1	50:SS:271:ARG:NH2	2.25	0.70
13:LE:57:TYR:OH	51:ST:159:GLU:OE2	2.10	0.69
5:L3:4441:A:N6	29:NI:445:ASP:O	2.25	0.69
28:NH:90:ALA:O	28:NH:134:TYR:OH	2.10	0.69
5:L3:369:G:N2	5:L3:372:A:OP2	2.22	0.69
31:NM:20:LYS:NZ	31:NM:39:CYS:SG	2.65	0.69
5:L3:4511:A:N6	18:LN:2:SER:OG	2.25	0.69
22:LT:54:LYS:O	22:LT:66:LYS:NZ	2.26	0.69
36:SC:245:GLN:NE2	36:SC:249:ASP:OD2	2.26	0.69
39:SG:186:THR:O	39:SG:189:GLN:NE2	2.26	0.68
41:SI:70:ARG:NH1	41:SI:106:ASP:O	2.26	0.68
41:SI:29:ARG:HH12	50:SS:368:LEU:HD13	1.59	0.68
49:SR:261:CYS:SG	49:SR:263:HIS:ND1	2.63	0.68
54:SW:285:ILE:HD12	54:SW:305:ILE:HD11	1.74	0.67
5:L3:2102:G:O2'	5:L3:2103:G:OP1	2.12	0.67
5:L3:62:A:N3	5:L3:77:U:O2'	2.27	0.67
5:L3:45:U:O2'	6:L6:14:PHE:O	2.11	0.67
41:SI:177:THR:HG23	50:SS:355:ALA:HB3	1.77	0.67
5:L3:2574:G:O2'	5:L3:2575:U:OP1	2.10	0.67
27:NF:163:LYS:NZ	27:NF:167:TYR:O	2.28	0.67
28:NH:76:THR:OG1	28:NH:78:LYS:NZ	2.27	0.67
18:LN:57:VAL:HG12	18:LN:73:VAL:HG22	1.77	0.67
26:NB:371:ARG:NH1	32:NO:318:SER:OG	2.28	0.67
4:L2:5:A:N6	4:L2:95:A:O2'	2.29	0.66
5:L3:3907:G:O2'	5:L3:3908:A:OP1	2.12	0.66
7:L7:190:ASP:OD1	7:L7:191:LYS:N	2.28	0.66
25:NA:326:ASP:OD2	25:NA:327:THR:N	2.29	0.66
25:NA:319:ARG:O	25:NA:323:HIS:ND1	2.24	0.66
10:LA:158:PRO:O	34:NS:276:ARG:NH2	2.29	0.65
49:SR:301:GLU:OE2	49:SR:304:GLN:NE2	2.30	0.65
5:L3:1444:G:HO2'	5:L3:1448:G:HO2'	1.45	0.65
4:L2:13:C:OP1	41:SI:86:HIS:NE2	2.27	0.64
5:L3:937:U:OP1	8:L8:46:ARG:NH1	2.31	0.64
25:NA:482:MET:HE2	25:NA:526:LEU:HD21	1.79	0.64
5:L3:4940:C:OP1	36:SC:156:ARG:NH1	2.31	0.63
9:L9:31:ARG:NE	42:SJ:708:GLU:OE2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:SD:14:VAL:O	37:SD:19:LYS:NZ	2.31	0.63
47:SO:226:ASP:OD1	51:ST:200:GLN:NE2	2.31	0.63
27:NF:8:GLU:OE2	29:NI:581:SER:OG	2.16	0.62
28:NH:120:ARG:NH1	52:SU:617:GLN:O	2.32	0.62
5:L3:244:G:O6	56:SZ:20:LYS:NZ	2.32	0.62
6:L6:62:PRO:O	6:L6:63:THR:OG1	2.15	0.62
43:SK:98:GLU:OE2	53:SV:76:ASN:ND2	2.33	0.62
5:L3:1369:C:OP2	5:L3:1370:G:O2'	2.05	0.62
5:L3:1833:G:N2	5:L3:1835:G:O4'	2.32	0.62
5:L3:67:C:OP2	5:L3:312:G:N2	2.33	0.62
5:L3:253:G:OP2	47:SO:338:LYS:NZ	2.31	0.62
6:L6:60:ARG:NH2	6:L6:67:HIS:O	2.33	0.62
41:SI:101:ARG:NH1	41:SI:122:LYS:O	2.32	0.62
46:SN:119:VAL:HG11	47:SO:165:LEU:HD22	1.80	0.62
5:L3:1355:G:OP1	11:LB:108:ARG:NH1	2.33	0.62
8:L8:106:ASP:OD2	36:SC:161:ARG:NH2	2.32	0.61
29:NI:559:ARG:NE	49:SR:278:LEU:O	2.33	0.61
5:L3:4910:G:N2	7:L7:106:ASP:O	2.33	0.61
5:L3:1444:G:O2'	5:L3:1448:G:O2'	2.17	0.61
3:L1:87:G:OP2	21:LS:7:ARG:NH2	2.34	0.61
5:L3:2361:G:O6	10:LA:25:HIS:ND1	2.34	0.60
5:L3:5066:U:OP1	10:LA:43:LYS:NZ	2.35	0.60
1:BA:123:ARG:NH2	48:SQ:63:SER:O	2.34	0.60
5:L3:1859:C:OP1	26:NB:26:ARG:NH1	2.35	0.60
5:L3:3961:G:O2'	5:L3:4043:G:N2	2.34	0.60
11:LB:76:GLU:OE1	11:LB:77:ASN:ND2	2.34	0.60
5:L3:404:U:O3'	16:LI:87:ARG:NH2	2.34	0.60
9:L9:126:THR:HG21	42:SJ:712:HIS:HD2	1.66	0.60
1:BA:138:SER:OG	5:L3:2002:A:N6	2.35	0.59
45:SM:170:HIS:HB3	45:SM:283:LEU:HD11	1.84	0.59
52:SU:607:LEU:HD13	52:SU:630:LEU:HD21	1.84	0.59
5:L3:4739:C:OP1	30:NK:109:ARG:NH2	2.36	0.59
54:SW:338:ILE:HG21	54:SW:347:LEU:HD11	1.84	0.59
1:BA:128:THR:O	1:BA:132:ILE:HD12	2.02	0.59
5:L3:306:A:OP1	23:LU:53:TYR:OH	2.20	0.59
10:LA:163:GLU:OE1	34:NS:276:ARG:NH1	2.36	0.59
52:SU:416:VAL:HG22	52:SU:420:MET:CE	2.33	0.59
5:L3:4691:A:OP1	39:SG:75:SER:OG	2.20	0.58
18:LN:160:ILE:HD11	18:LN:193:LYS:HB3	1.85	0.58
5:L3:4678:G:N7	30:NK:11:ARG:NH2	2.51	0.58
20:LQ:26:ASP:OD1	20:LQ:27:ARG:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SR:176:TYR:CE1	49:SR:271:LEU:HD22	2.38	0.58
5:L3:2562:G:O2'	5:L3:2565:A:N6	2.35	0.58
45:SM:189:TYR:CZ	45:SM:202:ILE:HD12	2.37	0.58
12:LC:41:LYS:NZ	37:SD:237:GLU:OE2	2.18	0.58
20:LQ:114:ARG:NH1	31:NM:119:TYR:OH	2.37	0.58
25:NA:311:VAL:HG21	52:SU:775:LEU:CD2	2.33	0.58
42:SJ:165:GLN:NE2	52:SU:226:LEU:HD13	2.19	0.58
54:SW:402:GLN:HE22	54:SW:513:VAL:HG11	1.68	0.57
5:L3:233:U:HO2'	5:L3:234:G:H8	1.49	0.57
5:L3:261:G:H21	50:SS:265:MET:CE	2.17	0.57
5:L3:375:G:OP2	24:LW:52:LYS:NZ	2.31	0.57
5:L3:2275:G:OP2	35:SA:312:ARG:NH1	2.38	0.57
5:L3:4437:U:OP2	27:NF:107:LYS:NZ	2.27	0.57
5:L3:4493:U:O2'	5:L3:4494:G:O4'	2.19	0.57
14:LG:49:LEU:HD23	14:LG:49:LEU:O	2.05	0.57
52:SU:416:VAL:HG12	52:SU:514:LEU:HD11	1.84	0.57
18:LN:95:THR:OG1	18:LN:98:GLY:O	2.18	0.57
9:L9:20:ARG:NH2	42:SJ:693:THR:O	2.37	0.57
5:L3:4347:G:O2'	5:L3:4348:A:O5'	2.19	0.56
15:LH:68:ARG:NH1	21:LS:58:LEU:HD22	2.19	0.56
47:SO:263:ASN:OD1	47:SO:264:MET:N	2.38	0.56
5:L3:1284:G:O2'	5:L3:1285:U:OP2	2.22	0.56
5:L3:4393:G:OP1	46:SN:174:ARG:NH1	2.38	0.56
5:L3:4734:A:OP2	10:LA:173:LYS:NZ	2.25	0.56
13:LE:79:GLN:NE2	13:LE:80:VAL:O	2.38	0.56
36:SC:153:LEU:HD11	36:SC:195:ILE:HG13	1.87	0.56
39:SG:86:LEU:HD22	39:SG:188:GLN:O	2.05	0.56
49:SR:176:TYR:HE1	49:SR:271:LEU:HD22	1.70	0.56
43:SK:123:ARG:NH1	43:SK:126:GLU:OE1	2.39	0.55
52:SU:477:GLU:N	52:SU:477:GLU:OE1	2.38	0.55
5:L3:1524:A:HO2'	5:L3:1525:A:P	2.29	0.55
49:SR:188:VAL:HG23	49:SR:189:THR:HG23	1.89	0.55
5:L3:3835:C:HO2'	5:L3:3836:A:P	2.30	0.55
29:NI:575:ILE:HD12	29:NI:578:ILE:HD11	1.88	0.55
20:LQ:89:LEU:HD13	20:LQ:118:LEU:HD22	1.89	0.55
25:NA:341:VAL:HG21	29:NI:48:ILE:HD11	1.88	0.55
5:L3:47:A:OP2	6:L6:20:ARG:NH1	2.40	0.54
5:L3:1925:G:OP1	8:L8:33:GLN:NE2	2.40	0.54
14:LG:96:LEU:HD13	53:SV:20:MET:HE3	1.89	0.54
33:NQ:65:ARG:O	33:NQ:82:HIS:ND1	2.41	0.54
5:L3:1447:C:OP2	32:NO:215:ARG:NE	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:65:GLN:OE1	1:BA:66:ASN:ND2	2.40	0.54
42:SJ:538:ILE:HG21	52:SU:257:LEU:HD23	1.88	0.54
49:SR:176:TYR:O	49:SR:181:LYS:NZ	2.40	0.54
52:SU:416:VAL:HG22	52:SU:420:MET:HE3	1.89	0.54
9:L9:103:GLU:OE1	9:L9:165:THR:HG21	2.08	0.54
14:LG:39:ILE:HG23	14:LG:61:VAL:CG1	2.38	0.54
43:SK:175:SER:O	43:SK:178:GLN:NE2	2.41	0.53
5:L3:2396:A:O2'	5:L3:2397:G:OP2	2.21	0.53
5:L3:2812:A:C6	42:SJ:78:VAL:HG11	2.43	0.53
53:SV:66:ASP:OD1	53:SV:103:ARG:NH1	2.42	0.53
5:L3:265:C:N4	56:SZ:154:VAL:HG21	2.23	0.53
54:SW:213:LEU:HD22	54:SW:361:MET:HE2	1.91	0.53
5:L3:2334:C:OP2	35:SA:195:LYS:NZ	2.37	0.53
37:SD:203:GLU:OE2	37:SD:203:GLU:N	2.42	0.53
5:L3:122:U:O4	38:SE:107:LYS:NZ	2.41	0.53
32:NO:352:LEU:HD13	36:SC:71:ARG:HH22	1.74	0.53
55:SY:480:ASP:OD1	55:SY:481:GLU:N	2.40	0.53
5:L3:2816:G:N2	5:L3:4645:C:O3'	2.42	0.52
9:L9:165:THR:HG23	9:L9:168:GLY:H	1.74	0.52
5:L3:4493:U:O2'	5:L3:4494:G:O5'	2.27	0.52
25:NA:333:LEU:HD21	25:NA:366:LEU:HD21	1.91	0.52
42:SJ:162:ARG:NH2	52:SU:227:SER:OG	2.41	0.52
52:SU:591:LEU:HD11	52:SU:603:VAL:HG21	1.91	0.52
5:L3:121:A:OP1	38:SE:110:LYS:NZ	2.40	0.52
14:LG:96:LEU:HD13	53:SV:20:MET:CE	2.39	0.52
5:L3:1364:U:OP2	6:L6:36:ARG:NH1	2.42	0.52
12:LC:99:ASP:OD1	12:LC:108:GLN:NE2	2.42	0.52
5:L3:107:G:OP2	6:L6:42:LYS:NZ	2.43	0.52
33:NQ:8:TRP:O	33:NQ:322:ARG:NH2	2.42	0.52
35:SA:204:ARG:NH1	35:SA:205:ARG:O	2.42	0.52
43:SK:4:ARG:HB3	43:SK:208:LEU:HD23	1.91	0.52
33:NQ:192:LEU:HD12	33:NQ:197:LYS:HB2	1.91	0.51
49:SR:174:CYS:SG	49:SR:244:LEU:HD21	2.50	0.51
25:NA:400:TYR:CZ	25:NA:446:ILE:HD12	2.44	0.51
29:NI:101:MET:O	52:SU:729:ARG:NH2	2.42	0.51
49:SR:279:PHE:CE2	49:SR:284:LEU:HD13	2.45	0.51
25:NA:400:TYR:CE1	25:NA:446:ILE:HD12	2.44	0.51
38:SE:164:ILE:O	38:SE:168:VAL:HG13	2.09	0.51
3:L1:74:U:O4	16:LI:72:GLN:NE2	2.43	0.51
5:L3:4724:A:O2'	18:LN:104:THR:HG22	2.10	0.51
23:LU:21:VAL:HG21	54:SW:321:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:419:A:N3	5:L3:1332:C:O2'	2.39	0.51
49:SR:285:ILE:HG21	49:SR:331:VAL:HG23	1.92	0.51
49:SR:287:VAL:HG11	49:SR:331:VAL:HG21	1.92	0.51
52:SU:350:LEU:HD12	52:SU:359:HIS:CE1	2.46	0.51
52:SU:617:GLN:N	52:SU:617:GLN:OE1	2.44	0.51
25:NA:487:ASP:O	25:NA:519:ARG:NH1	2.43	0.50
9:L9:126:THR:HG23	9:L9:127:TYR:CD1	2.46	0.50
12:LC:99:ASP:OD2	12:LC:100:LEU:N	2.44	0.50
45:SM:47:GLU:OE1	45:SM:47:GLU:N	2.42	0.50
38:SE:109:GLU:OE2	45:SM:102:ASN:ND2	2.44	0.50
52:SU:493:GLU:O	52:SU:497:ILE:HD12	2.12	0.50
5:L3:261:G:H21	50:SS:265:MET:HE3	1.75	0.50
5:L3:1952:G:OP1	12:LC:139:ARG:NE	2.45	0.50
5:L3:3855:C:O2'	10:LA:54:GLN:NE2	2.43	0.50
10:LA:168:LYS:O	10:LA:171:SER:OG	2.22	0.50
45:SM:215:VAL:HG23	50:SS:364:PHE:CG	2.47	0.50
42:SJ:13:ASP:OD1	42:SJ:14:LYS:N	2.44	0.50
52:SU:534:PHE:CE2	52:SU:538:LEU:HD11	2.47	0.50
49:SR:73:ASP:OD1	49:SR:74:ASP:N	2.44	0.50
5:L3:4493:U:HO2'	5:L3:4494:G:C4'	2.24	0.49
42:SJ:36:ASN:O	42:SJ:40:GLN:N	2.44	0.49
5:L3:2812:A:C5	42:SJ:78:VAL:HG11	2.46	0.49
29:NI:396:ASP:OD1	29:NI:397:LEU:N	2.43	0.49
35:SA:144:ILE:HD12	35:SA:150:LEU:HD11	1.93	0.49
38:SE:157:ILE:HB	38:SE:183:ILE:HD13	1.94	0.49
55:SY:474:ALA:HB1	55:SY:478:ASN:OD1	2.10	0.49
5:L3:1508:A:OP1	35:SA:110:ARG:NH2	2.42	0.49
36:SC:278:THR:HG22	36:SC:279:ASN:H	1.77	0.49
5:L3:4580:U:O2'	18:LN:182:GLU:OE2	2.26	0.49
5:L3:5002:U:OP2	18:LN:385:LYS:NZ	2.45	0.49
49:SR:354:ASN:HA	49:SR:357:LEU:HD23	1.93	0.49
5:L3:455:C:OP1	31:NM:125:LYS:NZ	2.42	0.49
5:L3:1294:A:O2'	34:NS:152:PRO:O	2.28	0.49
5:L3:1669:A:N3	5:L3:1852:U:O2'	2.40	0.49
28:NH:92:TYR:HA	52:SU:682:TYR:HE1	1.78	0.48
39:SG:41:ILE:HG22	39:SG:43:VAL:HG13	1.94	0.48
5:L3:296:A:N3	47:SO:68:ARG:NH1	2.60	0.48
37:SD:147:LEU:O	37:SD:151:ASN:ND2	2.46	0.48
5:L3:182:G:N7	47:SO:339:ARG:NH1	2.62	0.48
27:NF:125:ARG:HE	27:NF:126:ALA:H	1.61	0.48
43:SK:74:ASN:OD1	53:SV:74:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SS:364:PHE:CE2	50:SS:368:LEU:HD11	2.48	0.48
5:L3:2796:G:H22	42:SJ:37:ARG:HH12	1.61	0.48
49:SR:225:ILE:HG13	49:SR:271:LEU:HD21	1.96	0.48
29:NI:765:ARG:NH2	29:NI:767:LEU:HD21	2.29	0.48
54:SW:397:VAL:HG12	54:SW:514:GLY:O	2.14	0.48
5:L3:1693:U:OP2	11:LB:49:LYS:NZ	2.46	0.48
5:L3:4872:G:OP2	8:L8:94:LYS:NZ	2.39	0.48
34:NS:135:TYR:O	34:NS:269:HIS:NE2	2.46	0.48
21:LS:27:GLU:O	21:LS:31:LEU:HD13	2.13	0.48
3:L1:62:A:OP1	21:LS:52:LYS:NZ	2.46	0.47
5:L3:4475:G:OP1	29:NI:583:ARG:NH1	2.47	0.47
25:NA:404:TYR:CD2	25:NA:454:LEU:HD13	2.49	0.47
52:SU:664:ASP:OD2	55:SY:320:ARG:NH1	2.47	0.47
29:NI:294:THR:HG23	29:NI:294:THR:O	2.14	0.47
28:NH:57:ASN:HD22	55:SY:451:VAL:HG22	1.78	0.47
48:SQ:45:VAL:HG23	48:SQ:45:VAL:O	2.14	0.47
9:L9:126:THR:HG21	42:SJ:712:HIS:CD2	2.49	0.47
42:SJ:547:GLU:OE1	52:SU:207:ARG:NH2	2.46	0.47
18:LN:312:LYS:NZ	18:LN:380:GLN:OE1	2.45	0.47
29:NI:708:ALA:O	29:NI:712:VAL:HG23	2.15	0.47
42:SJ:46:ARG:NH2	42:SJ:69:SER:OG	2.47	0.47
42:SJ:825:ASP:OD1	42:SJ:826:SER:N	2.46	0.47
43:SK:101:LEU:HB3	43:SK:107:VAL:HG21	1.97	0.47
51:ST:168:GLU:OE1	51:ST:170:GLN:NE2	2.48	0.47
25:NA:308:SER:O	25:NA:312:LEU:HD23	2.15	0.47
5:L3:203:U:OP1	33:NQ:302:ARG:NH2	2.46	0.46
32:NO:349:CYS:HA	32:NO:352:LEU:HD12	1.96	0.46
5:L3:2258:C:HO2'	5:L3:2260:C:HO2'	1.63	0.46
5:L3:2562:G:N2	5:L3:2565:A:OP2	2.48	0.46
29:NI:553:GLU:O	29:NI:557:LEU:HD23	2.15	0.46
5:L3:2043:A:N1	5:L3:4515:G:O2'	2.40	0.46
5:L3:2836:A:O5'	5:L3:4656:A:N6	2.49	0.46
20:LQ:118:LEU:HD23	31:NM:119:TYR:CE1	2.51	0.46
25:NA:277:ILE:HG21	25:NA:294:LEU:HD11	1.98	0.46
44:SL:108:GLU:OE2	44:SL:112:GLN:NE2	2.48	0.46
17:LK:15:VAL:O	17:LK:15:VAL:HG12	2.16	0.46
25:NA:494:ARG:HA	25:NA:494:ARG:NE	2.30	0.46
39:SG:118:LEU:HD11	39:SG:167:VAL:HG22	1.97	0.46
53:SV:47:ARG:HH11	53:SV:58:ALA:HB2	1.80	0.46
34:NS:155:ARG:NH1	34:NS:231:GLU:OE2	2.43	0.46
48:SQ:25:ASN:O	48:SQ:28:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:NQ:64:ASP:O	33:NQ:66:THR:N	2.49	0.46
5:L3:423:G:N3	10:LA:118:GLN:NE2	2.65	0.45
5:L3:1946:G:O2'	27:NF:36:SER:OG	2.33	0.45
53:SV:127:VAL:HG23	53:SV:128:LYS:HD2	1.97	0.45
5:L3:4475:G:N1	27:NF:5:GLU:OE1	2.50	0.45
15:LH:55:ARG:HH12	45:SM:74:LEU:HD13	1.81	0.45
35:SA:214:ASP:OD2	35:SA:218:ILE:HD12	2.16	0.45
5:L3:4180:G:N2	28:NH:57:ASN:OD1	2.50	0.45
5:L3:4988:U:OP2	18:LN:123:HIS:ND1	2.48	0.45
48:SQ:88:ASN:ND2	48:SQ:213:GLY:O	2.45	0.45
3:L1:75:G:OP2	16:LI:74:TYR:OH	2.35	0.45
5:L3:2569:G:OP1	45:SM:560:ARG:NH1	2.50	0.45
5:L3:4401:G:OP1	26:NB:24:LYS:NZ	2.43	0.45
45:SM:36:ARG:NH2	45:SM:114:TYR:OH	2.48	0.45
5:L3:4883:C:N4	36:SC:181:LEU:O	2.48	0.45
14:LG:61:VAL:O	14:LG:79:ALA:N	2.46	0.45
18:LN:139:ASP:OD2	30:NK:96:TRP:NE1	2.49	0.45
28:NH:123:GLU:HG3	52:SU:575:ILE:HG22	1.99	0.45
49:SR:257:LEU:HD22	49:SR:288:ALA:HB1	1.98	0.45
50:SS:322:LEU:HD13	50:SS:344:PRO:HD2	1.97	0.45
51:ST:232:VAL:O	51:ST:232:VAL:HG12	2.16	0.45
5:L3:2268:A:OP1	31:NM:8:TRP:NE1	2.47	0.45
27:NF:231:THR:HG22	27:NF:232:GLN:N	2.32	0.45
18:LN:286:LYS:NZ	18:LN:302:ASN:O	2.32	0.45
52:SU:640:ASN:OD1	52:SU:641:SER:N	2.50	0.45
1:BA:131:GLU:OE2	5:L3:1972:G:N2	2.50	0.44
11:LB:88:ASP:OD1	11:LB:89:ASP:N	2.50	0.44
31:NM:71:ALA:HA	31:NM:77:LEU:HD13	1.98	0.44
37:SD:114:LEU:HD11	37:SD:121:THR:OG1	2.17	0.44
5:L3:2296:G:O2'	35:SA:242:PRO:O	2.30	0.44
28:NH:87:ASP:OD2	28:NH:88:TYR:N	2.50	0.44
29:NI:342:VAL:HG23	29:NI:407:LEU:HD22	1.99	0.44
5:L3:307:A:N3	5:L3:310:G:O2'	2.46	0.44
18:LN:160:ILE:HD11	18:LN:193:LYS:CB	2.46	0.44
54:SW:203:THR:HG22	54:SW:204:GLU:N	2.33	0.44
5:L3:171:U:O4	56:SZ:157:ARG:NH1	2.51	0.44
26:NB:1:MET:CE	27:NF:43:ILE:HD12	2.48	0.44
42:SJ:134:ALA:O	42:SJ:137:THR:OG1	2.30	0.44
37:SD:220:MET:O	37:SD:220:MET:HG2	2.18	0.44
46:SN:68:GLU:O	47:SO:163:ARG:NH2	2.51	0.44
50:SS:262:ALA:HB3	50:SS:268:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:2045:G:O6	5:L3:3870:C:O2'	2.28	0.44
46:SN:146:GLN:NE2	47:SO:149:LEU:O	2.50	0.44
55:SY:545:ASP:OD1	55:SY:545:ASP:N	2.51	0.44
56:SZ:150:SER:O	56:SZ:154:VAL:HG23	2.18	0.44
1:BA:123:ARG:NE	48:SQ:61:LYS:O	2.51	0.44
28:NH:147:ALA:N	28:NH:162:VAL:O	2.49	0.44
35:SA:134:PRO:HG3	35:SA:150:LEU:HD12	2.00	0.44
25:NA:262:SER:HA	25:NA:297:ARG:HE	1.84	0.43
28:NH:51:ILE:HG22	28:NH:66:LEU:HD11	2.00	0.43
5:L3:4433:G:N3	27:NF:191:THR:HG21	2.33	0.43
35:SA:297:GLU:OE1	35:SA:297:GLU:N	2.50	0.43
3:L1:102:G:OP2	3:L1:104:A:O2'	2.32	0.43
5:L3:4347:G:HO2'	5:L3:4348:A:P	2.41	0.43
28:NH:70:PHE:HA	28:NH:85:ALA:HB2	2.00	0.43
34:NS:235:ARG:HD2	34:NS:236:GLY:N	2.32	0.43
42:SJ:165:GLN:HE22	52:SU:226:LEU:HD13	1.83	0.43
47:SO:230:VAL:HG21	51:ST:207:LEU:HD12	2.00	0.43
45:SM:48:PRO:HB3	45:SM:54:VAL:HG21	2.00	0.43
52:SU:775:LEU:O	52:SU:775:LEU:HD23	2.18	0.43
56:SZ:111:LEU:HD21	56:SZ:115:LEU:HD22	1.99	0.43
5:L3:740:G:H2'	5:L3:741:C:C2	2.54	0.43
34:NS:92:LEU:HD12	34:NS:95:LYS:O	2.19	0.43
48:SQ:40:LEU:HD13	48:SQ:104:PHE:CZ	2.52	0.43
42:SJ:725:GLU:OE1	42:SJ:728:ARG:NH2	2.51	0.43
47:SO:212:ASP:OD1	47:SO:212:ASP:O	2.36	0.43
9:L9:138:PHE:HA	9:L9:143:ARG:HE	1.83	0.43
28:NH:43:ARG:NH2	28:NH:180:THR:OG1	2.46	0.43
28:NH:121:ILE:O	52:SU:575:ILE:HG23	2.19	0.43
42:SJ:670:LEU:HD11	42:SJ:717:LEU:HD13	2.01	0.43
5:L3:740:G:H2'	5:L3:741:C:N1	2.34	0.43
7:L7:16:LEU:HD21	7:L7:83:THR:HG21	2.01	0.43
8:L8:85:LYS:O	8:L8:89:THR:HG23	2.19	0.43
14:LG:18:LEU:HD11	18:LN:4:ARG:HH11	1.83	0.43
5:L3:1886:G:OP1	22:LT:19:ARG:NH1	2.49	0.43
28:NH:85:ALA:HB1	28:NH:89:LEU:HD13	2.01	0.43
54:SW:211:ARG:HB3	54:SW:212:PRO:HD3	2.01	0.43
4:L2:44:G:HO2'	4:L2:45:C:H6	1.66	0.43
5:L3:730:G:OP2	37:SD:76:ARG:NE	2.52	0.43
54:SW:504:ASP:OD1	54:SW:505:ASP:N	2.52	0.43
5:L3:2802:C:O4'	52:SU:286:LYS:NZ	2.52	0.42
49:SR:171:LEU:HD23	49:SR:252:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SW:402:GLN:NE2	54:SW:513:VAL:HG11	2.33	0.42
55:SY:429:LEU:HD12	55:SY:439:ILE:HD11	2.01	0.42
6:L6:80:GLU:HG3	6:L6:110:LEU:HD12	2.01	0.42
29:NI:307:LEU:HD11	29:NI:311:LEU:HD23	2.00	0.42
5:L3:2340:C:H4'	35:SA:42:THR:HG23	2.01	0.42
55:SY:393:CYS:O	55:SY:396:GLY:N	2.52	0.42
36:SC:278:THR:HG22	36:SC:279:ASN:N	2.34	0.42
47:SO:340:GLN:N	47:SO:340:GLN:OE1	2.53	0.42
5:L3:4371:G:H1'	5:L3:4372:U:O4'	2.19	0.42
20:LQ:118:LEU:HD23	31:NM:119:TYR:CD1	2.54	0.42
29:NI:822:GLU:OE1	42:SJ:60:GLN:NE2	2.53	0.42
30:NK:89:GLN:OE1	30:NK:89:GLN:N	2.52	0.42
1:BA:50:THR:HG22	1:BA:58:ILE:HD11	2.02	0.42
1:BA:98:ILE:HD12	1:BA:98:ILE:H	1.85	0.42
5:L3:49:U:O2'	6:L6:20:ARG:NH2	2.53	0.42
5:L3:935:A:O2'	8:L8:46:ARG:NH1	2.53	0.42
5:L3:4493:U:C2'	5:L3:4494:G:O5'	2.67	0.42
29:NI:130:ILE:HD11	29:NI:243:TYR:OH	2.19	0.42
29:NI:250:ASP:OD1	29:NI:251:ARG:N	2.52	0.42
4:L2:93:C:O2'	4:L2:94:U:O5'	2.38	0.42
5:L3:4515:G:OP1	49:SR:49:ARG:NH1	2.48	0.42
29:NI:294:THR:HG21	52:SU:615:ARG:NH1	2.35	0.42
48:SQ:64:ARG:NH1	48:SQ:65:MET:O	2.53	0.42
6:L6:56:ARG:NH1	6:L6:74:ARG:O	2.52	0.42
7:L7:84:VAL:HG11	7:L7:102:LEU:HD22	2.00	0.42
48:SQ:40:LEU:HD11	48:SQ:102:LEU:HB3	2.01	0.42
52:SU:416:VAL:CG2	52:SU:420:MET:HE3	2.50	0.42
28:NH:81:LEU:HD21	28:NH:89:LEU:HD22	2.00	0.42
36:SC:201:ILE:HD11	36:SC:267:LEU:HD21	2.02	0.42
1:BA:52:ASP:OD1	1:BA:52:ASP:N	2.53	0.42
42:SJ:730:ARG:NH2	50:SS:186:GLN:OE1	2.53	0.42
45:SM:244:LEU:HD23	45:SM:285:ARG:HD3	2.02	0.42
54:SW:237:ALA:HB1	54:SW:254:VAL:HG21	2.02	0.42
55:SY:257:ARG:NH2	55:SY:261:ARG:O	2.53	0.42
32:NO:346:GLU:OE1	32:NO:350:ARG:NH2	2.53	0.41
35:SA:209:ILE:HB	35:SA:229:LEU:HD13	2.02	0.41
39:SG:49:GLY:O	39:SG:53:LYS:NZ	2.32	0.41
54:SW:284:LEU:HD21	54:SW:286:MET:CE	2.50	0.41
55:SY:388:ILE:HD12	55:SY:406:MET:SD	2.60	0.41
5:L3:4691:A:O2'	39:SG:68:ALA:O	2.34	0.41
18:LN:219:VAL:HG11	18:LN:337:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SN:62:ARG:NH1	47:SO:58:ASN:OD1	2.53	0.41
49:SR:88:ASP:O	49:SR:91:HIS:N	2.53	0.41
32:NO:232:LEU:HD12	36:SC:50:LEU:HD23	2.03	0.41
34:NS:235:ARG:HD2	34:NS:236:GLY:O	2.21	0.41
42:SJ:94:THR:HG22	42:SJ:139:MET:SD	2.60	0.41
44:SL:255:THR:HG22	44:SL:256:GLU:N	2.35	0.41
5:L3:447:C:H2'	5:L3:448:G:O4'	2.21	0.41
5:L3:2258:C:O2'	5:L3:2260:C:O2'	2.33	0.41
43:SK:85:ARG:NH2	43:SK:89:PRO:O	2.53	0.41
9:L9:43:THR:OG1	9:L9:131:GLU:OE1	2.29	0.41
43:SK:222:PHE:O	43:SK:224:LEU:N	2.54	0.41
49:SR:170:THR:HG23	49:SR:249:ALA:HB2	2.02	0.41
5:L3:425:U:OP1	10:LA:37:LYS:NZ	2.39	0.41
5:L3:2100:A:C2	5:L3:2263:A:C4	3.09	0.41
32:NO:316:THR:O	32:NO:321:ARG:NH1	2.53	0.41
5:L3:4440:G:C2	49:SR:96:LEU:HD13	2.56	0.41
6:L6:63:THR:HG22	6:L6:64:VAL:N	2.36	0.41
18:LN:352:LEU:HD23	18:LN:352:LEU:H	1.86	0.41
27:NF:231:THR:HG22	27:NF:232:GLN:H	1.86	0.41
42:SJ:680:ALA:O	42:SJ:684:LEU:HD13	2.21	0.41
54:SW:203:THR:HG21	54:SW:227:SER:O	2.21	0.41
5:L3:470:A:N6	5:L3:685:C:O2'	2.36	0.41
5:L3:4181:U:H2'	5:L3:4182:G:O4'	2.20	0.41
6:L6:111:GLN:HA	6:L6:114:VAL:HG22	2.03	0.41
38:SE:58:PRO:HG2	38:SE:61:ILE:HD12	2.02	0.41
55:SY:479:LYS:HE2	55:SY:479:LYS:HA	2.03	0.41
5:L3:2088:A:OP2	11:LB:38:ARG:NH1	2.54	0.41
10:LA:12:THR:HG21	31:NM:159:ASP:HB2	2.03	0.41
14:LG:18:LEU:HD11	18:LN:4:ARG:NH1	2.36	0.41
53:SV:66:ASP:OD1	53:SV:67:ASN:N	2.54	0.41
5:L3:431:G:OP2	5:L3:3889:G:N2	2.54	0.41
25:NA:337:TYR:HE1	25:NA:414:LEU:HD23	1.85	0.41
33:NQ:298:ILE:O	33:NQ:298:ILE:HG22	2.21	0.41
36:SC:281:ILE:HG23	36:SC:286:LEU:HD21	2.02	0.41
44:SL:149:LEU:HD21	44:SL:176:ARG:HG3	2.02	0.41
25:NA:493:GLY:O	25:NA:494:ARG:NE	2.52	0.40
35:SA:84:THR:HG22	35:SA:86:ARG:H	1.86	0.40
42:SJ:160:ARG:NH1	42:SJ:190:SER:O	2.54	0.40
52:SU:266:PHE:O	52:SU:270:THR:OG1	2.28	0.40
5:L3:4597:U:O2'	49:SR:399:ARG:NH2	2.53	0.40
5:L3:4910:G:H4'	18:LN:95:THR:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:NQ:91:ARG:NE	33:NQ:105:ASP:OD1	2.54	0.40
50:SS:233:ILE:HD12	54:SW:606:LEU:HD12	2.02	0.40
13:LE:42:ILE:HD11	13:LE:74:ILE:CD1	2.51	0.40
25:NA:554:LEU:HD22	25:NA:570:VAL:HG13	2.04	0.40
29:NI:772:LYS:O	29:NI:776:LYS:N	2.54	0.40
32:NO:214:THR:HG21	32:NO:323:ARG:HH11	1.86	0.40
53:SV:115:ASN:O	53:SV:115:ASN:ND2	2.53	0.40
5:L3:228:C:O2'	16:LI:14:ASN:ND2	2.51	0.40
5:L3:3903:A:H2'	5:L3:3904:G:O4'	2.21	0.40
29:NI:269:PRO:O	29:NI:272:HIS:ND1	2.51	0.40
4:L2:91:C:OP2	44:SL:176:ARG:NH2	2.54	0.40
25:NA:295:LEU:HD13	25:NA:332:VAL:CG2	2.51	0.40
45:SM:129:ASP:OD2	50:SS:293:LEU:HD11	2.22	0.40
46:SN:140:MET:CE	47:SO:159:LEU:HD23	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	158/165 (96%)	158 (100%)	0	0	100	100
2	BB	211/217 (97%)	205 (97%)	6 (3%)	0	100	100
6	L6	118/211 (56%)	116 (98%)	2 (2%)	0	100	100
7	L7	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
8	L8	133/215 (62%)	129 (97%)	4 (3%)	0	100	100
9	L9	179/204 (88%)	179 (100%)	0	0	100	100
10	LA	156/184 (85%)	155 (99%)	1 (1%)	0	100	100
11	LB	149/188 (79%)	149 (100%)	0	0	100	100
12	LC	174/176 (99%)	173 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LE	107/160 (67%)	104 (97%)	3 (3%)	0	100	100
14	LG	132/140 (94%)	129 (98%)	3 (2%)	0	100	100
15	LH	129/156 (83%)	129 (100%)	0	0	100	100
16	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
17	LK	104/148 (70%)	101 (97%)	3 (3%)	0	100	100
18	LN	352/403 (87%)	350 (99%)	2 (1%)	0	100	100
19	LP	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
20	LQ	131/135 (97%)	131 (100%)	0	0	100	100
21	LS	120/123 (98%)	120 (100%)	0	0	100	100
22	LT	107/110 (97%)	107 (100%)	0	0	100	100
23	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
24	LW	72/97 (74%)	72 (100%)	0	0	100	100
25	NA	480/749 (64%)	480 (100%)	0	0	100	100
26	NB	379/549 (69%)	375 (99%)	4 (1%)	0	100	100
27	NF	210/260 (81%)	208 (99%)	2 (1%)	0	100	100
28	NH	178/180 (99%)	176 (99%)	2 (1%)	0	100	100
29	NI	633/881 (72%)	626 (99%)	7 (1%)	0	100	100
30	NK	63/129 (49%)	63 (100%)	0	0	100	100
31	NM	180/300 (60%)	178 (99%)	2 (1%)	0	100	100
32	NO	301/461 (65%)	300 (100%)	1 (0%)	0	100	100
33	NQ	320/385 (83%)	318 (99%)	2 (1%)	0	100	100
34	NS	303/349 (87%)	300 (99%)	3 (1%)	0	100	100
35	SA	358/427 (84%)	352 (98%)	6 (2%)	0	100	100
36	SC	193/288 (67%)	191 (99%)	2 (1%)	0	100	100
37	SD	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
38	SE	183/266 (69%)	181 (99%)	2 (1%)	0	100	100
39	SG	189/192 (98%)	185 (98%)	4 (2%)	0	100	100
40	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
41	SI	222/255 (87%)	217 (98%)	5 (2%)	0	100	100
42	SJ	328/847 (39%)	323 (98%)	5 (2%)	0	100	100
43	SK	242/245 (99%)	237 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	SL	241/490 (49%)	236 (98%)	5 (2%)	0	100	100
45	SM	445/588 (76%)	444 (100%)	1 (0%)	0	100	100
46	SN	169/306 (55%)	169 (100%)	0	0	100	100
47	SO	305/353 (86%)	302 (99%)	3 (1%)	0	100	100
48	SQ	216/239 (90%)	214 (99%)	2 (1%)	0	100	100
49	SR	460/634 (73%)	453 (98%)	7 (2%)	0	100	100
50	SS	237/746 (32%)	233 (98%)	4 (2%)	0	100	100
51	ST	112/365 (31%)	110 (98%)	2 (2%)	0	100	100
52	SU	557/800 (70%)	549 (99%)	8 (1%)	0	100	100
53	SV	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
54	SW	440/670 (66%)	434 (99%)	6 (1%)	0	100	100
55	SY	376/812 (46%)	373 (99%)	3 (1%)	0	100	100
56	SZ	156/178 (88%)	155 (99%)	1 (1%)	0	100	100
All	All	12061/17258 (70%)	11931 (99%)	130 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	BA	132/137 (96%)	132 (100%)	0	100	100
6	L6	104/177 (59%)	104 (100%)	0	100	100
7	L7	171/174 (98%)	171 (100%)	0	100	100
8	L8	115/161 (71%)	115 (100%)	0	100	100
9	L9	155/172 (90%)	155 (100%)	0	100	100
10	LA	142/163 (87%)	142 (100%)	0	100	100
11	LB	136/165 (82%)	136 (100%)	0	100	100
12	LC	157/157 (100%)	157 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	LE	101/140 (72%)	101 (100%)	0	100	100
14	LG	102/107 (95%)	102 (100%)	0	100	100
15	LH	39/133 (29%)	39 (100%)	0	100	100
16	LI	124/135 (92%)	123 (99%)	1 (1%)	81	92
17	LK	29/121 (24%)	29 (100%)	0	100	100
18	LN	313/348 (90%)	313 (100%)	0	100	100
20	LQ	119/121 (98%)	119 (100%)	0	100	100
21	LS	109/110 (99%)	109 (100%)	0	100	100
22	LT	88/89 (99%)	88 (100%)	0	100	100
23	LU	86/89 (97%)	86 (100%)	0	100	100
24	LW	63/80 (79%)	63 (100%)	0	100	100
25	NA	362/656 (55%)	361 (100%)	1 (0%)	92	97
26	NB	142/485 (29%)	142 (100%)	0	100	100
27	NF	193/228 (85%)	192 (100%)	1 (0%)	88	95
28	NH	155/155 (100%)	155 (100%)	0	100	100
29	NI	553/730 (76%)	551 (100%)	2 (0%)	91	96
30	NK	61/115 (53%)	61 (100%)	0	100	100
31	NM	168/272 (62%)	168 (100%)	0	100	100
32	NO	269/392 (69%)	269 (100%)	0	100	100
33	NQ	265/318 (83%)	265 (100%)	0	100	100
34	NS	276/305 (90%)	276 (100%)	0	100	100
35	SA	299/348 (86%)	298 (100%)	1 (0%)	92	97
36	SC	178/252 (71%)	177 (99%)	1 (1%)	86	94
37	SD	207/215 (96%)	207 (100%)	0	100	100
38	SE	158/223 (71%)	158 (100%)	0	100	100
39	SG	170/171 (99%)	170 (100%)	0	100	100
40	SH	140/274 (51%)	140 (100%)	0	100	100
41	SI	202/228 (89%)	202 (100%)	0	100	100
42	SJ	293/733 (40%)	293 (100%)	0	100	100
43	SK	212/213 (100%)	212 (100%)	0	100	100
44	SL	226/437 (52%)	226 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	SM	401/509 (79%)	400 (100%)	1 (0%)	93	97
46	SN	133/260 (51%)	133 (100%)	0	100	100
47	SO	283/319 (89%)	283 (100%)	0	100	100
48	SQ	195/214 (91%)	195 (100%)	0	100	100
49	SR	422/574 (74%)	422 (100%)	0	100	100
50	SS	214/648 (33%)	214 (100%)	0	100	100
51	ST	74/300 (25%)	74 (100%)	0	100	100
52	SU	485/733 (66%)	485 (100%)	0	100	100
53	SV	127/149 (85%)	126 (99%)	1 (1%)	81	92
54	SW	393/591 (66%)	393 (100%)	0	100	100
55	SY	325/685 (47%)	325 (100%)	0	100	100
56	SZ	141/158 (89%)	141 (100%)	0	100	100
All	All	10007/14669 (68%)	9998 (100%)	9 (0%)	93	97

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

Mol	Chain	Res	Type
16	LI	50	ARG
25	NA	490	ARG
27	NF	98	ARG
29	NI	362	ARG
29	NI	572	ARG
35	SA	291	ARG
36	SC	114	ARG
45	SM	218	ARG
53	SV	115	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
9	L9	182	HIS
11	LB	77	ASN
12	LC	37	HIS
25	NA	259	GLN
25	NA	376	HIS
28	NH	175	HIS
35	SA	60	HIS

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Mol	Chain	Res	Type
36	SC	190	HIS
36	SC	227	HIS
36	SC	245	GLN
38	SE	64	GLN
42	SJ	165	GLN
42	SJ	712	HIS
45	SM	211	HIS
49	SR	157	HIS
49	SR	209	HIS
49	SR	304	GLN
50	SS	310	HIS
52	SU	359	HIS
52	SU	592	HIS
52	SU	636	HIS
55	SY	430	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L1	150/157 (95%)	21 (14%)	0
4	L2	65/1167 (5%)	10 (15%)	0
5	L3	2173/5070 (42%)	300 (13%)	7 (0%)
All	All	2388/6394 (37%)	331 (13%)	7 (0%)

All (331) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L1	34	U
3	L1	52	A
3	L1	54	C
3	L1	55	U
3	L1	59	A
3	L1	62	A
3	L1	63	U
3	L1	75	G
3	L1	82	A
3	L1	83	C
3	L1	84	A
3	L1	86	U
3	L1	94	G
3	L1	103	A

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Mol	Chain	Res	Type
3	L1	105	C
3	L1	110	U
3	L1	111	U
3	L1	114	G
3	L1	153	C
3	L1	156	U
3	L1	157	U
4	L2	2	C
4	L2	11	C
4	L2	48	G
4	L2	49	G
4	L2	62	U
4	L2	87	G
4	L2	94	U
4	L2	95	A
4	L2	96	A
4	L2	101	A
5	L3	6	C
5	L3	41	C
5	L3	48	G
5	L3	56	A
5	L3	58	G
5	L3	59	A
5	L3	64	A
5	L3	65	A
5	L3	69	A
5	L3	89	C
5	L3	91	G
5	L3	92	C
5	L3	93	G
5	L3	95	G
5	L3	116	G
5	L3	119	G
5	L3	159	C
5	L3	170	C
5	L3	171	U
5	L3	172	C
5	L3	173	C
5	L3	181	C
5	L3	182	G
5	L3	186	G
5	L3	187	U

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Mol	Chain	Res	Type
5	L3	197	A
5	L3	200	U
5	L3	210	C
5	L3	218	A
5	L3	233	U
5	L3	234	G
5	L3	257	C
5	L3	261	G
5	L3	264	C
5	L3	265	C
5	L3	281	U
5	L3	294	G
5	L3	340	C
5	L3	349	A
5	L3	387	G
5	L3	410	A
5	L3	413	G
5	L3	414	C
5	L3	431	G
5	L3	448	G
5	L3	451	C
5	L3	452	A
5	L3	460	C
5	L3	469	C
5	L3	470	A
5	L3	473	C
5	L3	685	C
5	L3	686	A
5	L3	687	U
5	L3	696	C
5	L3	697	G
5	L3	701	G
5	L3	703	G
5	L3	730	G
5	L3	731	G
5	L3	739	G
5	L3	746	A
5	L3	913	U
5	L3	915	A
5	L3	917	A
5	L3	918	G
5	L3	925	C

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Mol	Chain	Res	Type
5	L3	926	G
5	L3	931	C
5	L3	932	A
5	L3	933	G
5	L3	943	A
5	L3	944	A
5	L3	945	U
5	L3	1287	G
5	L3	1295	C
5	L3	1296	G
5	L3	1297	U
5	L3	1301	C
5	L3	1313	C
5	L3	1314	C
5	L3	1354	A
5	L3	1358	G
5	L3	1359	G
5	L3	1378	C
5	L3	1379	C
5	L3	1445	U
5	L3	1448	G
5	L3	1502	G
5	L3	1525	A
5	L3	1654	G
5	L3	1661	C
5	L3	1670	G
5	L3	1682	A
5	L3	1691	G
5	L3	1726	U
5	L3	1804	A
5	L3	1836	G
5	L3	1837	A
5	L3	1842	G
5	L3	1853	G
5	L3	1870	C
5	L3	1881	C
5	L3	1883	G
5	L3	1891	A
5	L3	1897	A
5	L3	1910	G
5	L3	1918	U
5	L3	1921	C

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Mol	Chain	Res	Type
5	L3	1922	G
5	L3	1925	G
5	L3	1931	C
5	L3	1935	C
5	L3	1938	C
5	L3	1941	A
5	L3	1944	A
5	L3	1945	G
5	L3	1984	A
5	L3	2002	A
5	L3	2004	U
5	L3	2024	G
5	L3	2025	A
5	L3	2026	A
5	L3	2044	U
5	L3	2046	G
5	L3	2055	G
5	L3	2056	G
5	L3	2069	A
5	L3	2084	C
5	L3	2085	G
5	L3	2089	G
5	L3	2095	A
5	L3	2097	U
5	L3	2098	G
5	L3	2099	G
5	L3	2100	A
5	L3	2102	G
5	L3	2103	G
5	L3	2260	C
5	L3	2261	G
5	L3	2265	G
5	L3	2266	C
5	L3	2267	U
5	L3	2268	A
5	L3	2289	C
5	L3	2300	A
5	L3	2301	G
5	L3	2313	A
5	L3	2314	G
5	L3	2348	G
5	L3	2351	C

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Mol	Chain	Res	Type
5	L3	2374	A
5	L3	2378	G
5	L3	2382	A
5	L3	2383	C
5	L3	2384	U
5	L3	2395	A
5	L3	2396	A
5	L3	2397	G
5	L3	2398	U
5	L3	2474	G
5	L3	2484	A
5	L3	2490	U
5	L3	2492	C
5	L3	2493	G
5	L3	2500	U
5	L3	2574	G
5	L3	2575	U
5	L3	2769	U
5	L3	2796	G
5	L3	2798	A
5	L3	2799	G
5	L3	2814	C
5	L3	2818	C
5	L3	2844	A
5	L3	2845	A
5	L3	2848	G
5	L3	2852	U
5	L3	2853	C
5	L3	3630	A
5	L3	3835	C
5	L3	3836	A
5	L3	3840	U
5	L3	3845	A
5	L3	3853	U
5	L3	3868	G
5	L3	3877	A
5	L3	3878	C
5	L3	3879	G
5	L3	3881	G
5	L3	3889	G
5	L3	3894	A
5	L3	3895	G

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Mol	Chain	Res	Type
5	L3	3897	G
5	L3	3906	A
5	L3	3907	G
5	L3	3908	A
5	L3	3926	C
5	L3	3930	U
5	L3	3938	G
5	L3	3939	G
5	L3	3940	U
5	L3	3941	G
5	L3	3942	A
5	L3	3967	G
5	L3	4049	U
5	L3	4064	C
5	L3	4183	G
5	L3	4188	U
5	L3	4348	A
5	L3	4349	C
5	L3	4350	C
5	L3	4357	G
5	L3	4372	U
5	L3	4373	G
5	L3	4376	A
5	L3	4380	A
5	L3	4385	A
5	L3	4390	A
5	L3	4392	G
5	L3	4393	G
5	L3	4398	C
5	L3	4401	G
5	L3	4433	G
5	L3	4437	U
5	L3	4438	U
5	L3	4439	U
5	L3	4441	A
5	L3	4442	U
5	L3	4451	G
5	L3	4464	A
5	L3	4466	C
5	L3	4475	G
5	L3	4476	C
5	L3	4480	A

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Mol	Chain	Res	Type
5	L3	4494	G
5	L3	4495	G
5	L3	4496	A
5	L3	4499	G
5	L3	4512	U
5	L3	4513	A
5	L3	4518	A
5	L3	4521	U
5	L3	4522	G
5	L3	4523	A
5	L3	4538	G
5	L3	4540	C
5	L3	4541	G
5	L3	4545	G
5	L3	4546	A
5	L3	4548	A
5	L3	4549	G
5	L3	4550	G
5	L3	4551	U
5	L3	4552	U
5	L3	4568	A
5	L3	4584	A
5	L3	4590	A
5	L3	4608	G
5	L3	4653	C
5	L3	4656	A
5	L3	4670	C
5	L3	4671	C
5	L3	4672	A
5	L3	4678	G
5	L3	4684	A
5	L3	4708	A
5	L3	4709	U
5	L3	4719	G
5	L3	4720	C
5	L3	4737	G
5	L3	4741	C
5	L3	4742	G
5	L3	4745	G
5	L3	4751	G
5	L3	4754	G
5	L3	4757	C

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Mol	Chain	Res	Type
5	L3	4759	C
5	L3	4765	G
5	L3	4772	C
5	L3	4773	C
5	L3	4870	G
5	L3	4871	C
5	L3	4880	C
5	L3	4882	U
5	L3	4883	C
5	L3	4900	C
5	L3	4901	G
5	L3	4910	G
5	L3	4943	A
5	L3	4976	U
5	L3	5006	U
5	L3	5013	C
5	L3	5014	A
5	L3	5020	G
5	L3	5026	U
5	L3	5030	U
5	L3	5041	G
5	L3	5050	C
5	L3	5062	G

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L3	2102	G
5	L3	2574	G
5	L3	2798	A
5	L3	3835	C
5	L3	4347	G
5	L3	4520	G
5	L3	5013	C

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

3 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
50	SEP	SS	127	50	8,9,10	1.53	1 (12%)	8,12,14	1.29	2 (25%)
50	SEP	SS	126	50	8,9,10	1.54	1 (12%)	8,12,14	1.68	2 (25%)
31	AME	NM	1	31	9,10,11	1.46	1 (11%)	9,11,13	1.50	2 (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
50	SEP	SS	127	50	-	1/5/8/10	-
50	SEP	SS	126	50	-	1/5/8/10	-
31	AME	NM	1	31	-	2/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	SS	126	SEP	P-O1P	3.37	1.61	1.50
50	SS	127	SEP	P-O1P	3.35	1.61	1.50
31	NM	1	AME	CT1-N	3.30	1.45	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	SS	126	SEP	OG-CB-CA	3.21	111.26	108.14
50	SS	126	SEP	P-OG-CB	-2.88	110.37	118.30
31	NM	1	AME	CE-SD-CG	2.37	108.55	100.40
31	NM	1	AME	CT2-CT1-N	2.21	119.83	116.10
50	SS	127	SEP	P-OG-CB	-2.17	112.33	118.30
50	SS	127	SEP	OG-CB-CA	2.05	110.14	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	NM	1	AME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
31	NM	1	AME	N-CA-CB-CG
50	SS	127	SEP	N-CA-CB-OG
50	SS	126	SEP	CA-CB-OG-P

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 71 ligands modelled in this entry, 68 are monoatomic - leaving 3 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
61	GDP	SR	1001	62,57	24,30,30	2.55	8 (33%)	30,47,47	1.71	9 (30%)
59	ADP	NI	1001	57	24,29,29	0.92	1 (4%)	29,45,45	1.46	4 (13%)
60	SF4	NM	401	31	0,12,12	-	-	-	-	-

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
61	GDP	SR	1001	62,57	-	0/12/32/32	0/3/3/3
59	ADP	NI	1001	57	-	2/12/32/32	0/3/3/3
60	SF4	NM	401	31	-	-	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	SR	1001	GDP	O6-C6	8.34	1.40	1.23
61	SR	1001	GDP	C2-N2	4.76	1.45	1.34
61	SR	1001	GDP	O4'-C1'	4.35	1.47	1.41
61	SR	1001	GDP	C5-C4	2.36	1.49	1.43
59	NI	1001	ADP	C5-C4	2.31	1.47	1.40
61	SR	1001	GDP	PB-O2B	-2.22	1.46	1.54
61	SR	1001	GDP	PB-O3B	-2.21	1.46	1.54
61	SR	1001	GDP	C2'-C1'	-2.15	1.50	1.53
61	SR	1001	GDP	C2'-C3'	-2.03	1.47	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	SR	1001	GDP	C3'-C2'-C1'	3.85	106.77	100.98
59	NI	1001	ADP	N3-C2-N1	-3.72	122.86	128.68
61	SR	1001	GDP	C5-C6-N1	3.32	119.81	113.95
59	NI	1001	ADP	PA-O3A-PB	-3.30	121.49	132.83
61	SR	1001	GDP	O2B-PB-O3A	2.92	114.41	104.64
61	SR	1001	GDP	C2-N1-C6	-2.86	119.84	125.10
61	SR	1001	GDP	O3B-PB-O3A	2.78	113.95	104.64
59	NI	1001	ADP	C4-C5-N7	-2.75	106.53	109.40
61	SR	1001	GDP	PA-O3A-PB	-2.61	123.86	132.83
59	NI	1001	ADP	C3'-C2'-C1'	2.60	104.89	100.98
61	SR	1001	GDP	C2'-C3'-C4'	2.57	107.64	102.64
61	SR	1001	GDP	O2A-PA-O1A	-2.17	101.49	112.24
61	SR	1001	GDP	O6-C6-C5	-2.13	120.22	124.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

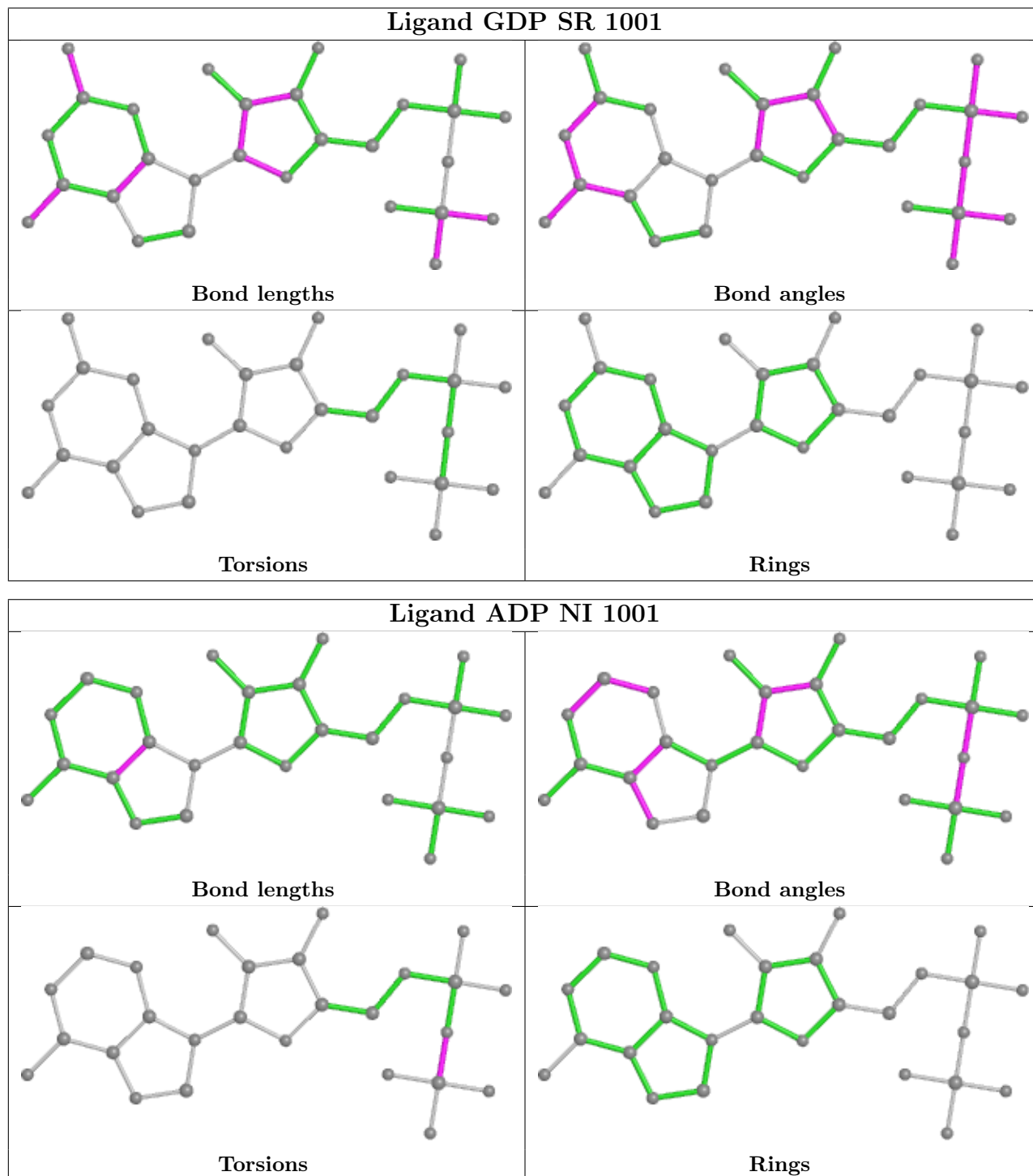
Mol	Chain	Res	Type	Atoms
59	NI	1001	ADP	PA-O3A-PB-O3B
59	NI	1001	ADP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	L3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L3	2403:A	O3'	2473:A	P	61.11

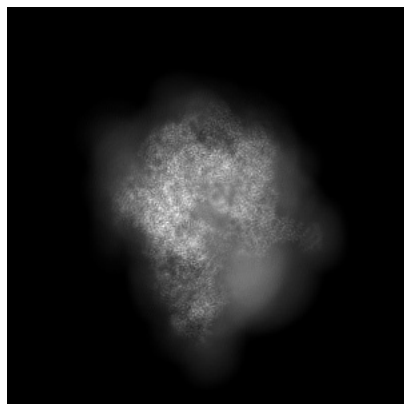
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29258. These allow visual inspection of the internal detail of the map and identification of artifacts.

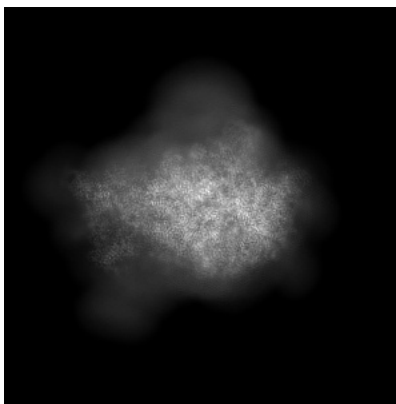
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

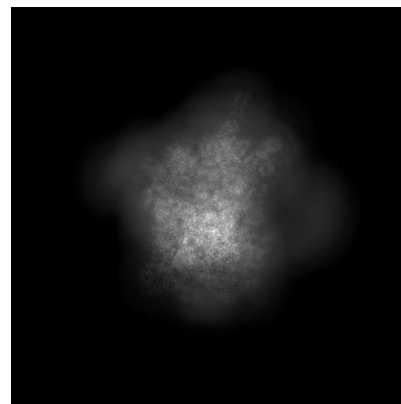
6.1.1 Primary map



X

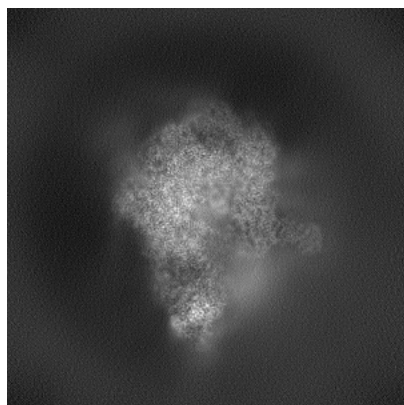


Y

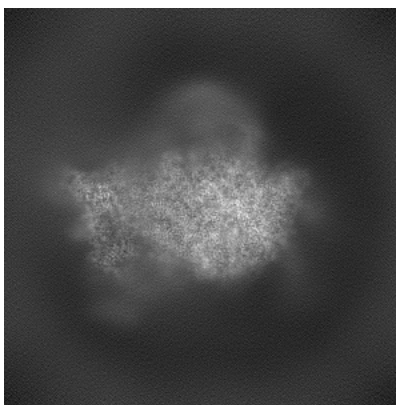


Z

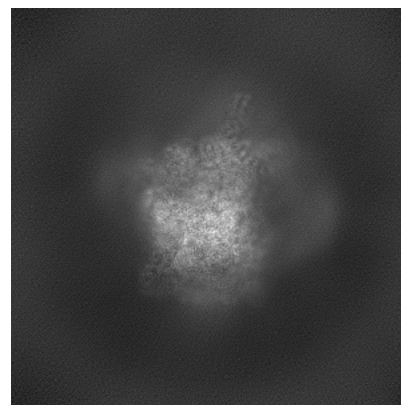
6.1.2 Raw map



X



Y

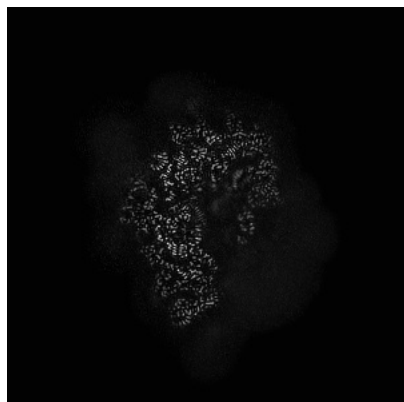


Z

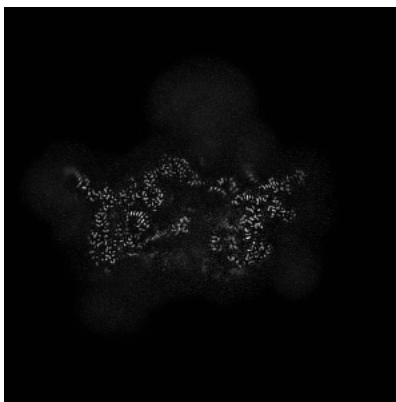
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

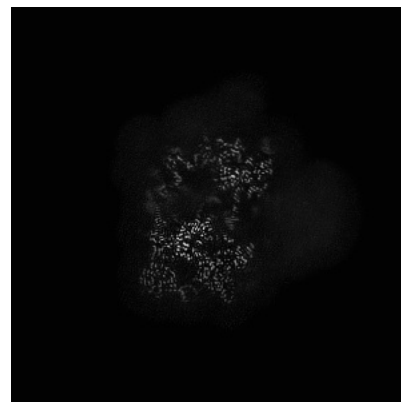
6.2.1 Primary map



X Index: 240

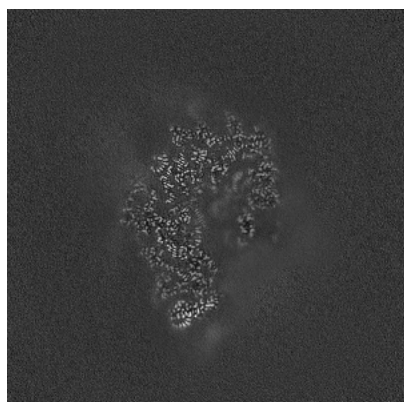


Y Index: 240

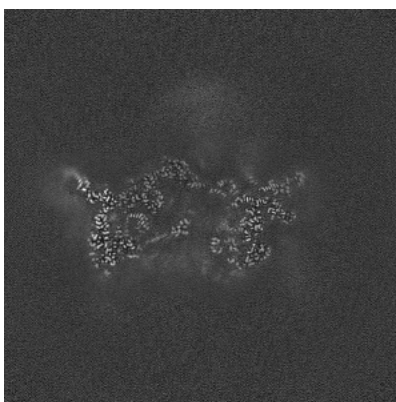


Z Index: 240

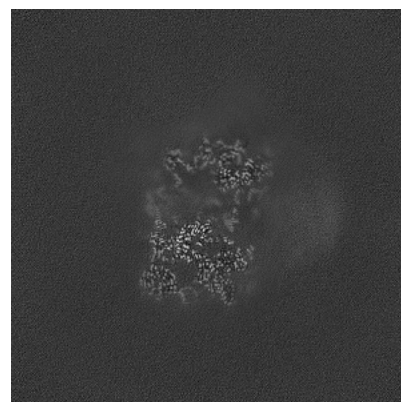
6.2.2 Raw map



X Index: 240



Y Index: 240

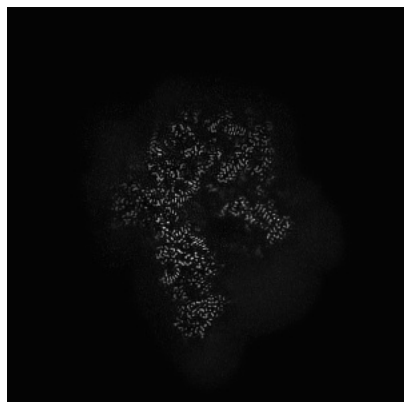


Z Index: 240

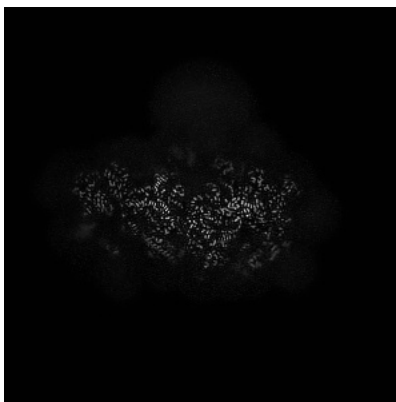
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

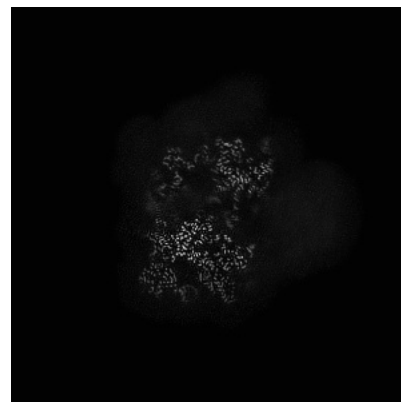
6.3.1 Primary map



X Index: 255

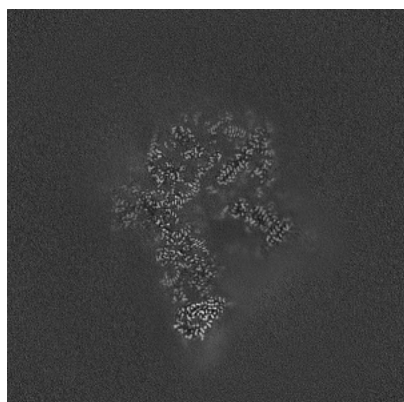


Y Index: 210

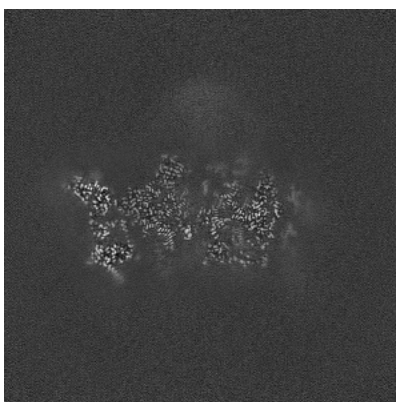


Z Index: 239

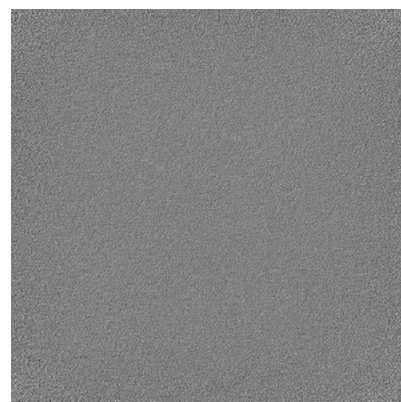
6.3.2 Raw map



X Index: 255



Y Index: 225

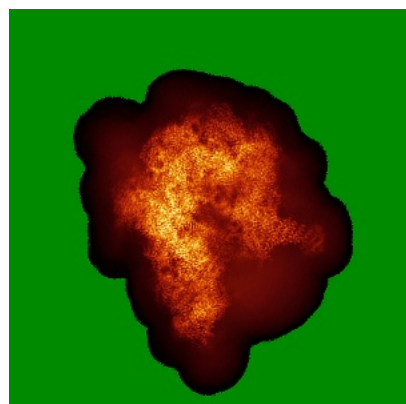


Z Index: 0

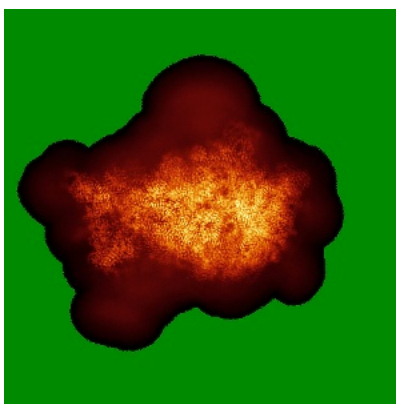
The images above show the largest variance slices of the map in three orthogonal directions.

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

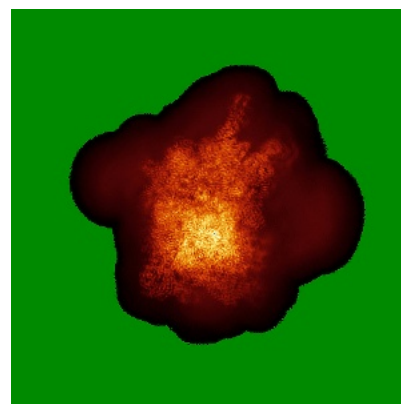
6.4.1 Primary map



X

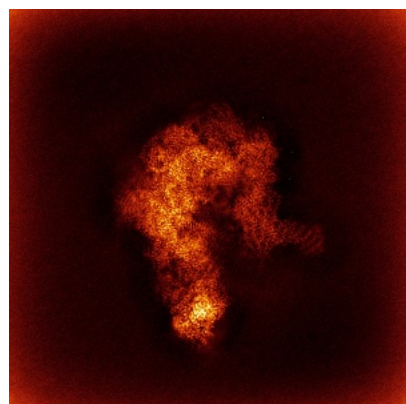


Y

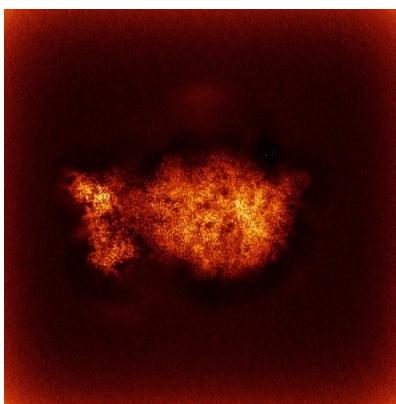


Z

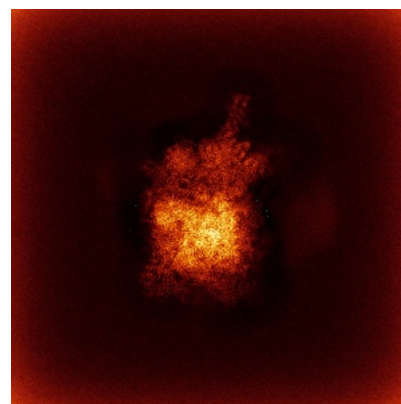
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



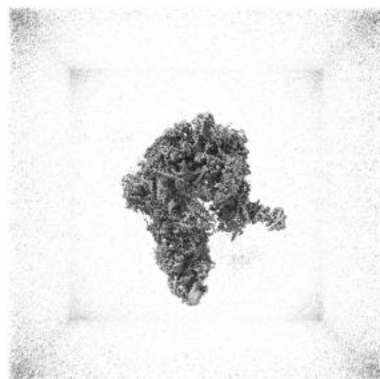
Y



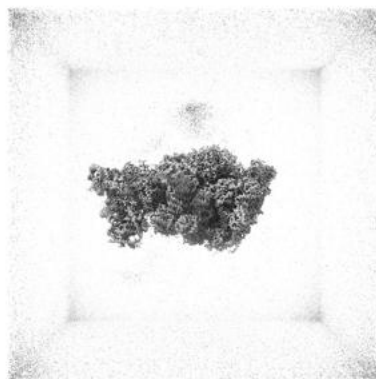
Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

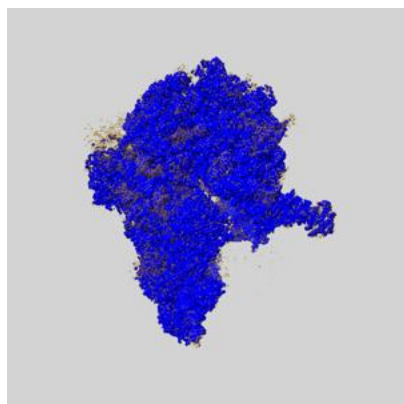
6.6 Mask visualisation [i](#)

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

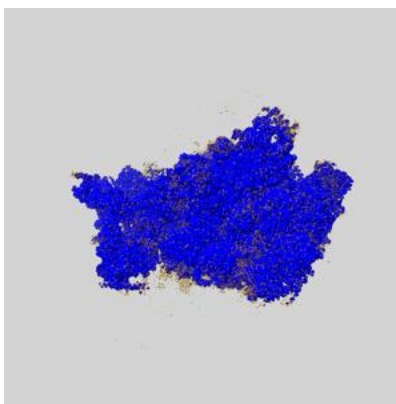
A mask typically either:

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

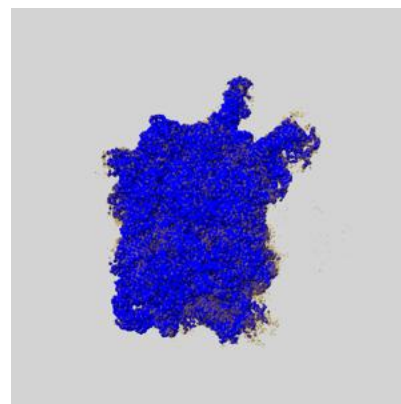
6.6.1 emd_29258_msk_1.map [i](#)



X



Y

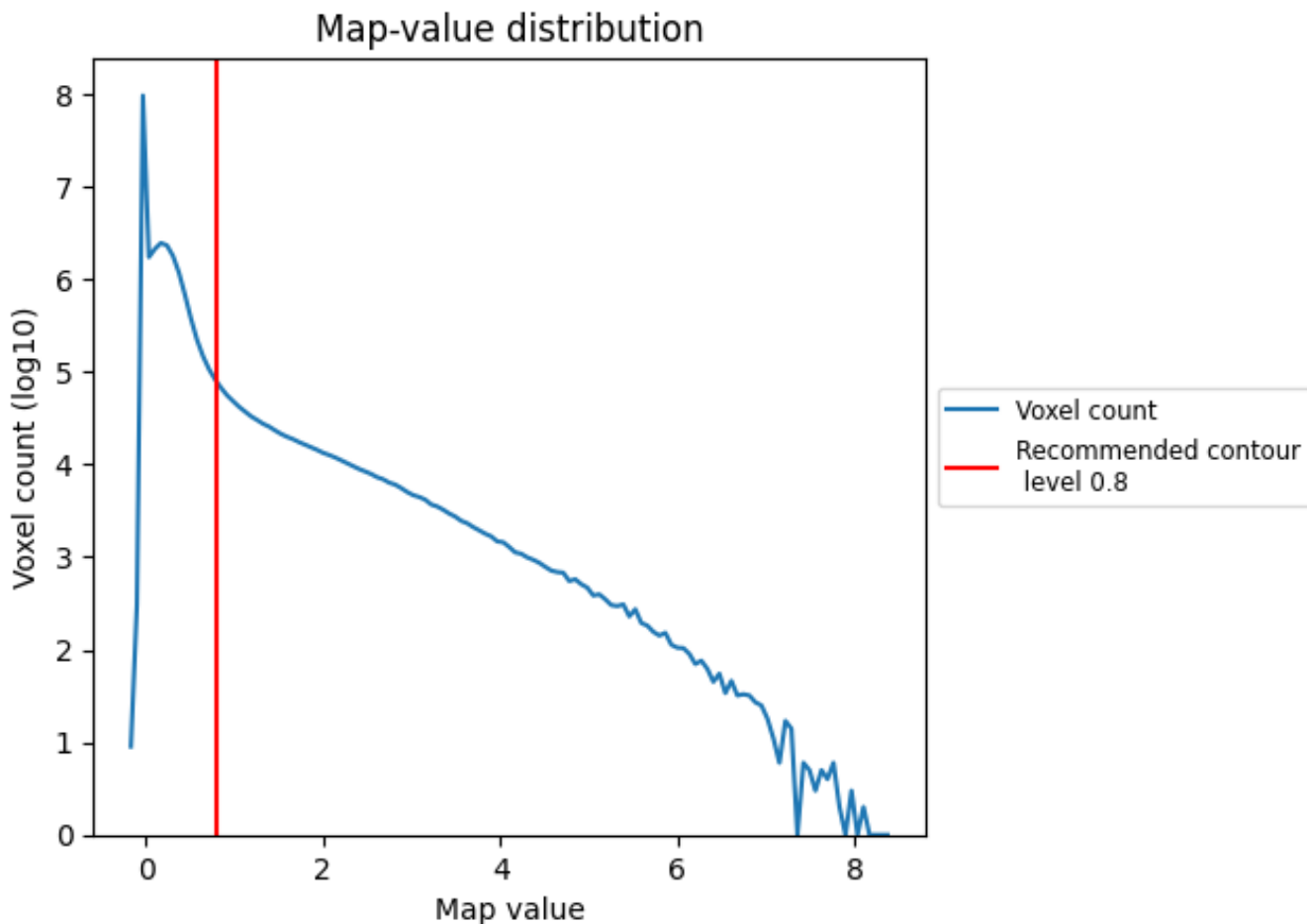


Z

7 Map analysis [i](#)

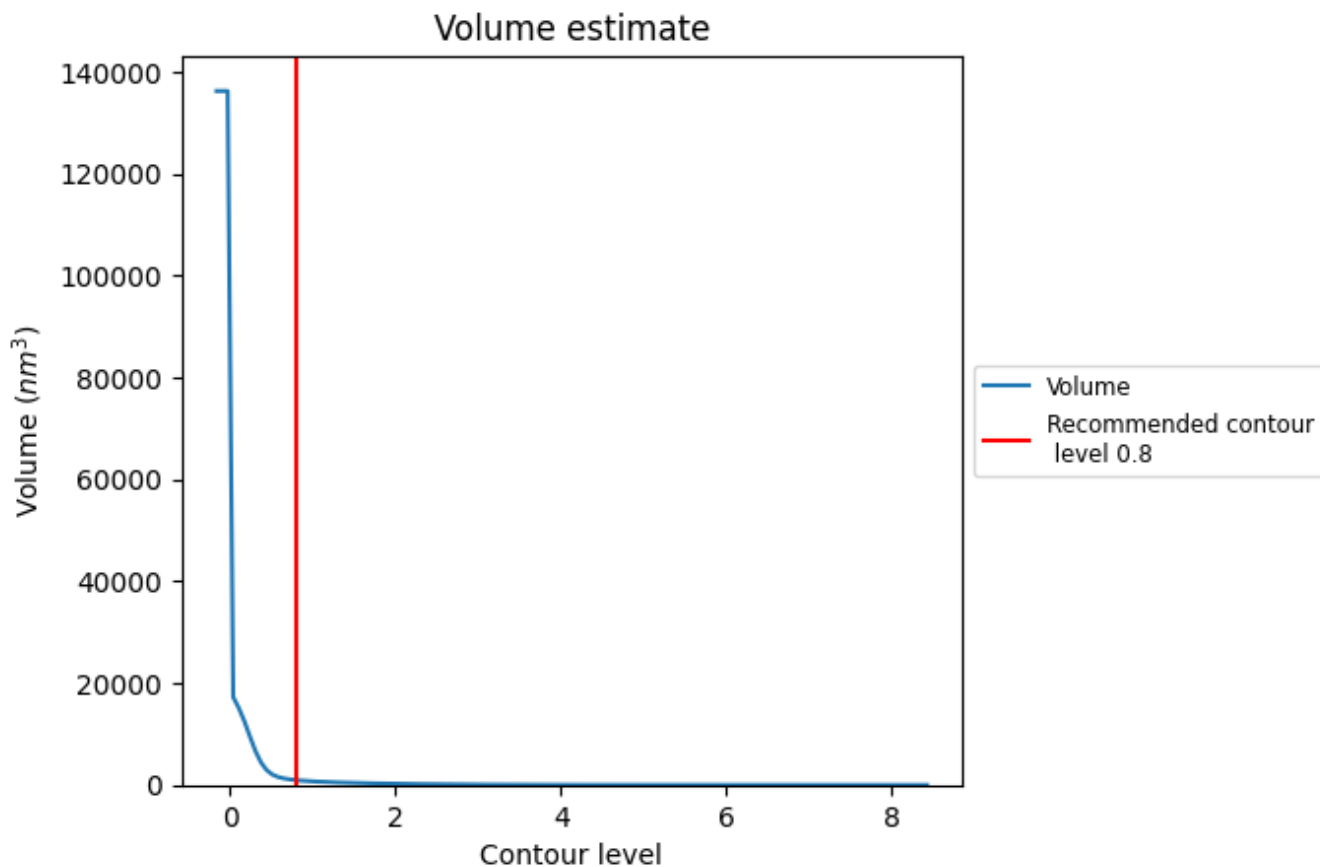
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

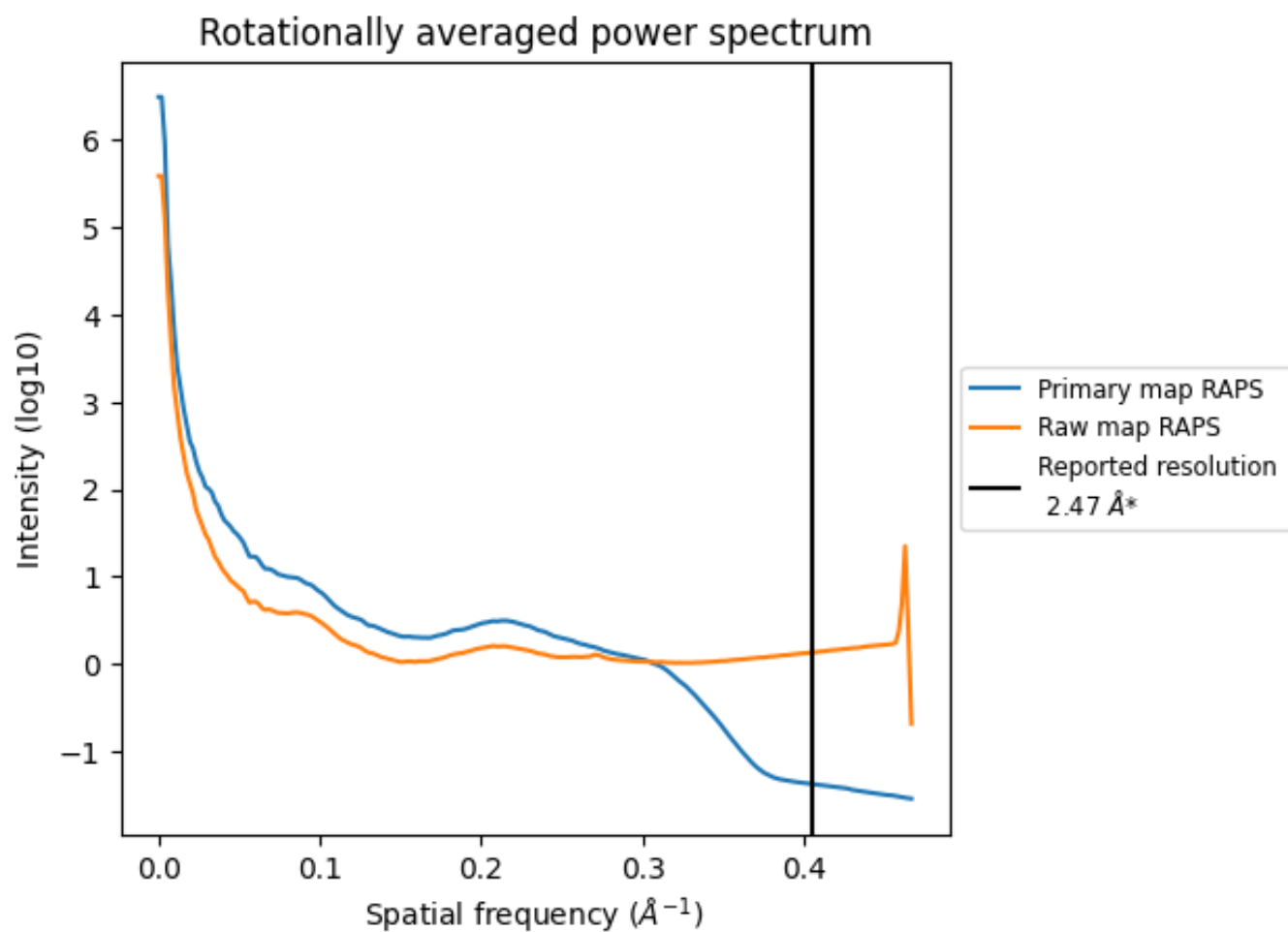
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 950 nm^3 ; this corresponds to an approximate mass of 859 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

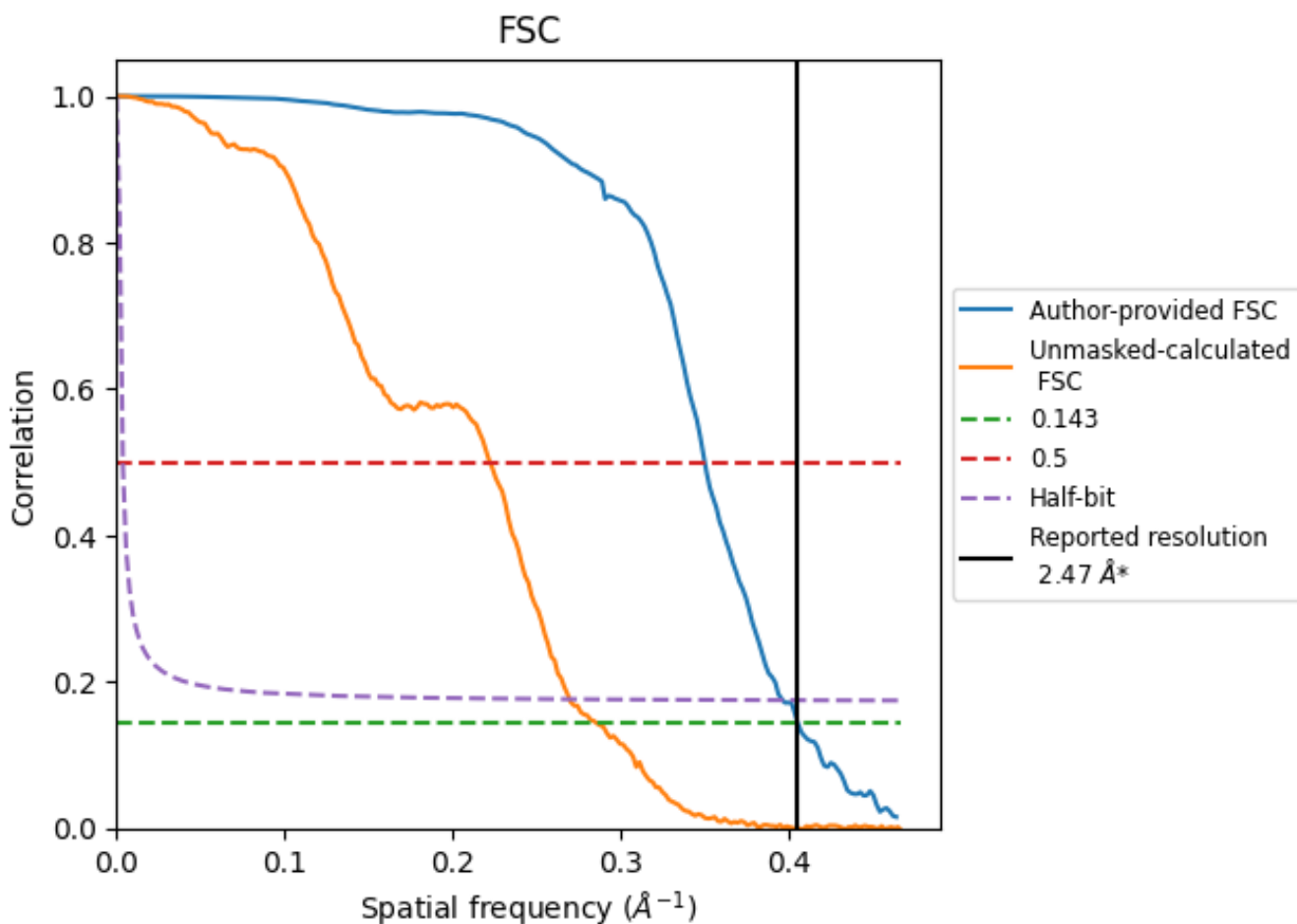


*Reported resolution corresponds to spatial frequency of 0.405 \AA^{-1}

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 0.405 Å⁻¹

8.2 Resolution estimates [i](#)

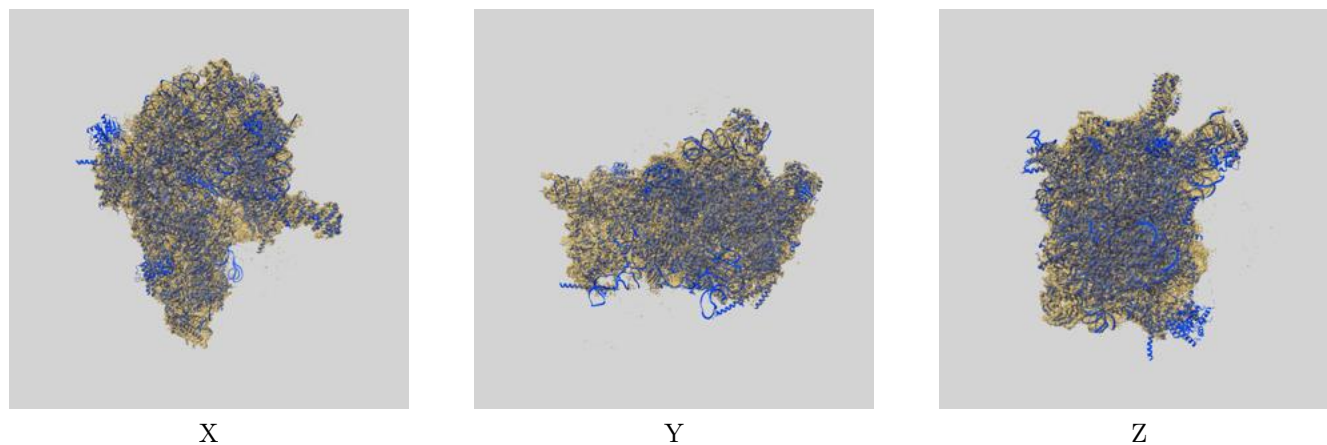
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.47	2.86	2.52
Unmasked-calculated*	3.50	4.50	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.50 differs from the reported value 2.47 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29258 and PDB model 8FKV. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



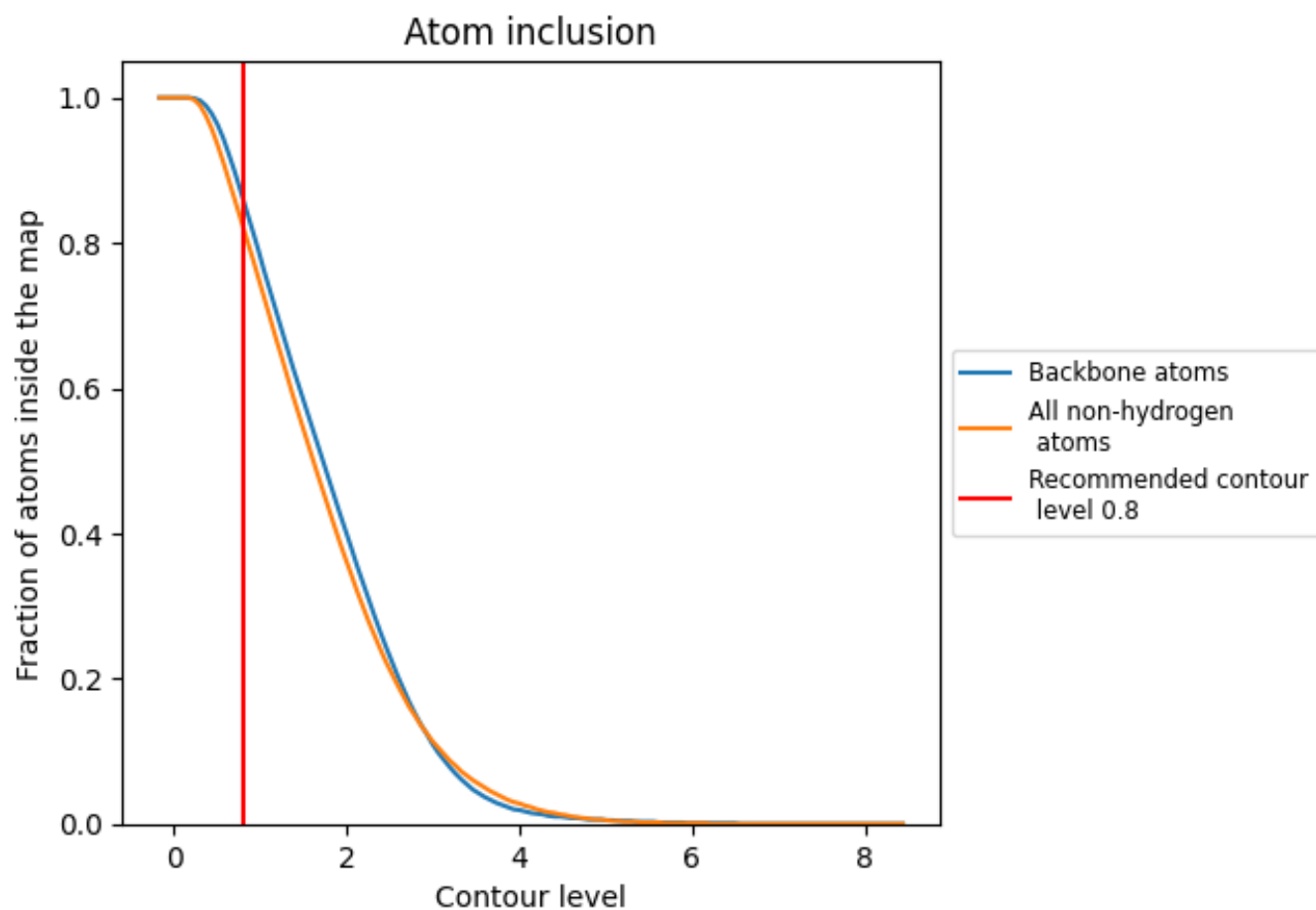
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary













































The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8250	 0.5490
BA	 0.3420	 0.3900
BB	 0.3170	 0.2800
L1	 0.8950	 0.5710
L2	 0.9440	 0.5930
L3	 0.8780	 0.5560
L6	 0.9280	 0.6120
L7	 0.9460	 0.6230
L8	 0.9490	 0.6350
L9	 0.9630	 0.6400
LA	 0.8560	 0.6020
LB	 0.9460	 0.6230
LC	 0.9480	 0.6390
LE	 0.6130	 0.4520
LG	 0.8640	 0.5840
LH	 0.3830	 0.3360
LI	 0.9040	 0.6110
LK	 0.7760	 0.4410
LN	 0.8820	 0.6050
LP	 0.4960	 0.4240
LQ	 0.9630	 0.6420
LS	 0.7710	 0.5290
LT	 0.9740	 0.6540
LU	 0.8520	 0.5980
LW	 0.9250	 0.6130
NA	 0.7360	 0.3980
NB	 0.3350	 0.3380
NF	 0.8700	 0.5850
NH	 0.9160	 0.5640
NI	 0.7950	 0.5260
NK	 0.7950	 0.5500
NM	 0.8670	 0.5850
NO	 0.7370	 0.5350
NQ	 0.8660	 0.5830
NS	 0.8650	 0.5980



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SA	 0.9160	 0.6170
SC	 0.8660	 0.5940
SD	 0.9230	 0.6220
SE	 0.9240	 0.6260
SG	 0.8900	 0.6190
SH	 0.8730	 0.5960
SI	 0.8510	 0.5810
SJ	 0.6940	 0.4780
SK	 0.8750	 0.5810
SL	 0.8340	 0.5850
SM	 0.7800	 0.5440
SN	 0.7540	 0.5210
SO	 0.8450	 0.5780
SQ	 0.6980	 0.5570
SR	 0.8140	 0.5650
SS	 0.8090	 0.5630
ST	 0.5440	 0.4530
SU	 0.7720	 0.4660
SV	 0.6540	 0.5050
SW	 0.5820	 0.4880
SY	 0.8590	 0.5510
SZ	 0.8510	 0.5630