



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 01:50 PM UTC

PDB ID : 8FKT / pdb_00008fkt
EMDB ID : EMD-29256
Title : Human nucleolar pre-60S ribosomal subunit (State C1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.81 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:

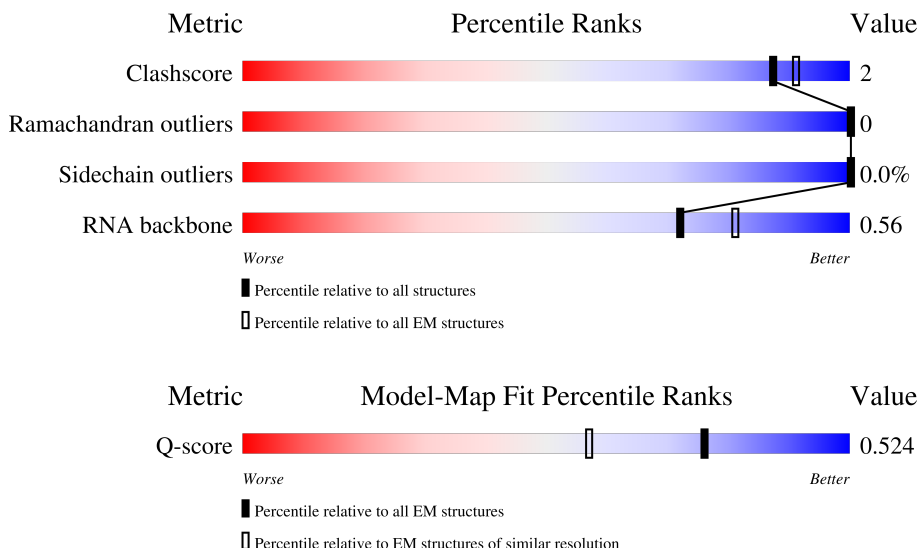
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



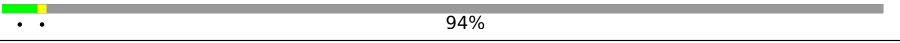
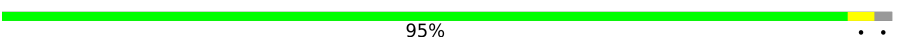
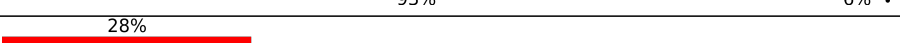
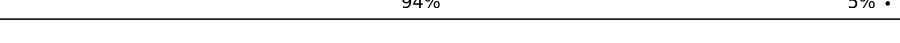
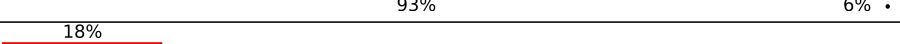
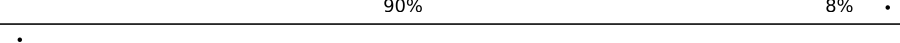
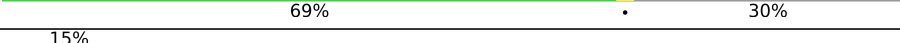
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11740 (2.31 - 3.31)

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	61% 90% 7% •
2	BB	217	74% 98% •
3	L1	157	15% 82% 13% • •

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Mol	Chain	Length	Quality of chain
4	L2	1167	
5	L3	5070	
6	L6	211	
7	L7	203	
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	LQ	135	
20	LS	123	
21	LT	110	
22	LU	105	
23	LW	97	
24	NB	549	
25	NF	260	
26	NH	180	
27	NI	881	
28	NK	129	

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Mol	Chain	Length	Quality of chain
29	NM	300	
30	NO	461	
31	NQ	385	
32	NS	349	
33	SA	427	
34	SC	288	
35	SD	248	
36	SE	266	
37	SG	192	
38	SH	293	
39	SI	255	
40	SJ	847	
41	SK	245	
42	SL	490	
43	SM	588	
44	SN	306	
45	SO	353	
46	SQ	239	
47	SR	634	
48	SS	746	
49	ST	365	
50	SV	163	
51	SW	670	
52	SY	812	
53	SZ	178	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 134945 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
1	BA	160	Total	C	N	O	S	0	0
			1208	749	226	229	4		

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

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

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

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

- Molecule 4 is a RNA chain called ITS2 rRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L3	2125	Total	C	N	O	P	0	0
			45561	20291	8341	14804	2125		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	113	Total	C	N	O	S	0	0
			747	461	143	142	1		

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

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

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

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

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

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

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

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

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

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

- Molecule 19 is a protein called 60S ribosomal protein L32.

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

- Molecule 20 is a protein called 60S ribosomal protein L35.

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

- Molecule 21 is a protein called 60S ribosomal protein L35a.

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

- Molecule 22 is a protein called 60S ribosomal protein L36.

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

- Molecule 23 is a protein called 60S ribosomal protein L37.

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

- Molecule 24 is a protein called Guanine nucleotide-binding protein-like 3.

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

- Molecule 25 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	NF	203	Total	C	N	O	S	0	0
			1661	1058	316	278	9		

- Molecule 26 is a protein called 60S ribosome subunit biogenesis protein NIP7 homolog.

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

- Molecule 27 is a protein called ATP-dependent RNA helicase DDX54.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	NI	598	Total	C	N	O	S	0	0
			3866	2387	736	737	6		

- Molecule 28 is a protein called Protein LLP homolog.

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

- Molecule 29 is a protein called Protein MAK16 homolog.

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

- Molecule 30 is a protein called Ribosomal RNA processing protein 1 homolog A.

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

- Molecule 31 is a protein called WD repeat-containing protein 74.

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

- Molecule 32 is a protein called Ribosome production factor 1.

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

- Molecule 33 is a protein called 60S ribosomal protein L4.

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

- Molecule 34 is a protein called 60S ribosomal protein L6.

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

- Molecule 35 is a protein called 60S ribosomal protein L7.

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

- Molecule 36 is a protein called 60S ribosomal protein L7a.

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

- Molecule 37 is a protein called 60S ribosomal protein L9.

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

- Molecule 38 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

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

- Molecule 39 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SI	228	Total	C	N	O	S	1	0
			1887	1224	352	307	4		

- Molecule 40 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SJ	101	Total	C	N	O	S	0	0
			855	537	165	152	1		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 42 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 43 is a protein called Pescadillo homolog.

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

- Molecule 44 is a protein called Probable rRNA-processing protein EBP2.

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

- Molecule 45 is a protein called Ribosome biogenesis protein BRX1 homolog.

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

- Molecule 46 is a protein called mRNA turnover protein 4 homolog.

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

- Molecule 47 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SR	449	Total	C	N	O	S	0	0
			3695	2352	651	675	17		

- Molecule 48 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SS	256	Total	C	N	O	P S	0	0
			2116	1337	375	394	2 8		

- Molecule 49 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	ST	116	Total	C	N	O	S	0	0
			787	489	152	144	2		

- Molecule 50 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 51 is a protein called ATP-dependent RNA helicase DDX18.

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

- Molecule 52 is a protein called Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase.

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

- Molecule 53 is a protein called Nucleolar protein 16.

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

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	L1	5	Total	Mg	0
			5	5	
54	L2	1	Total	Mg	0
			1	1	
54	L3	52	Total	Mg	0
			52	52	
54	L9	1	Total	Mg	0
			1	1	
54	LQ	1	Total	Mg	0
			1	1	
54	LT	1	Total	Mg	0
			1	1	

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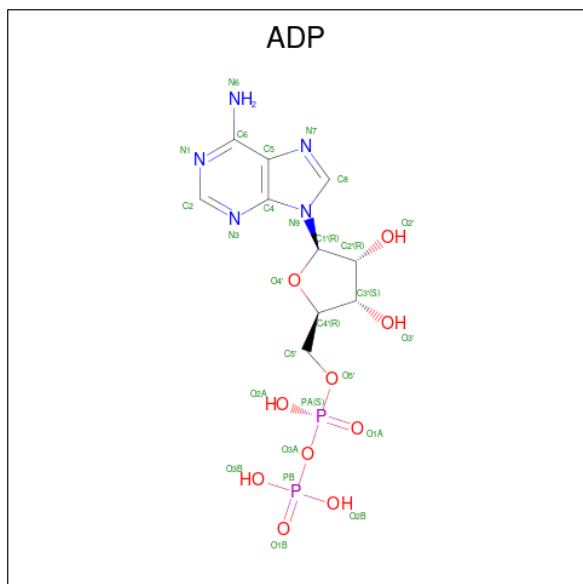
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Mol	Chain	Residues	Atoms		AltConf
54	NI	1	Total	Mg	0
			1	1	
54	SA	1	Total	Mg	0
			1	1	
54	SR	1	Total	Mg	0
			1	1	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

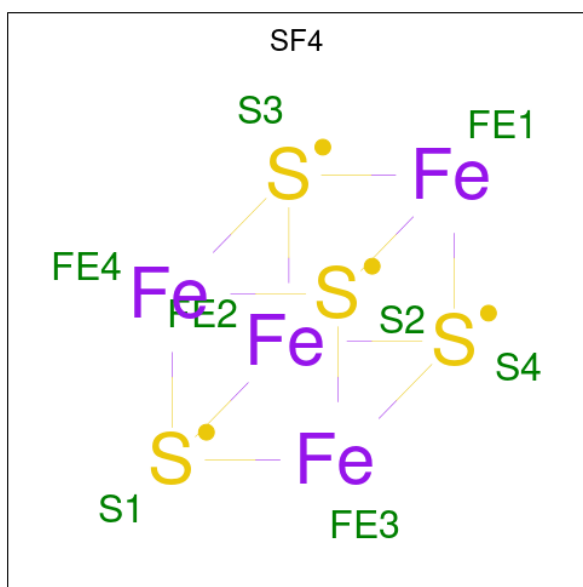
Mol	Chain	Residues	Atoms		AltConf
55	LW	1	Total	Zn	0
			1	1	
55	SV	1	Total	Zn	0
			1	1	

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



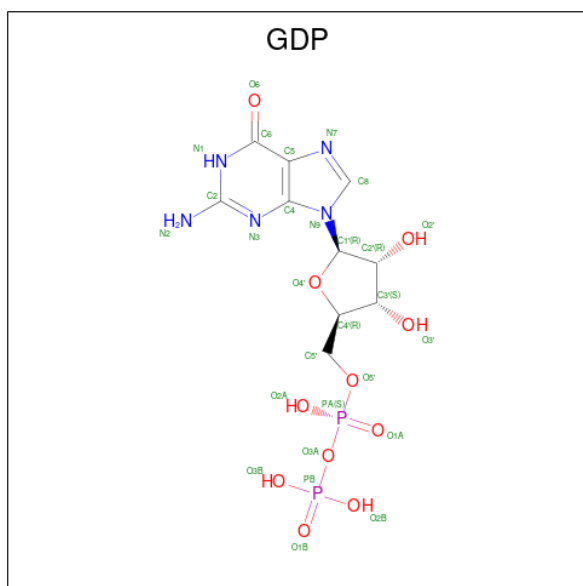
Mol	Chain	Residues	Atoms					AltConf
56	NI	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 58 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

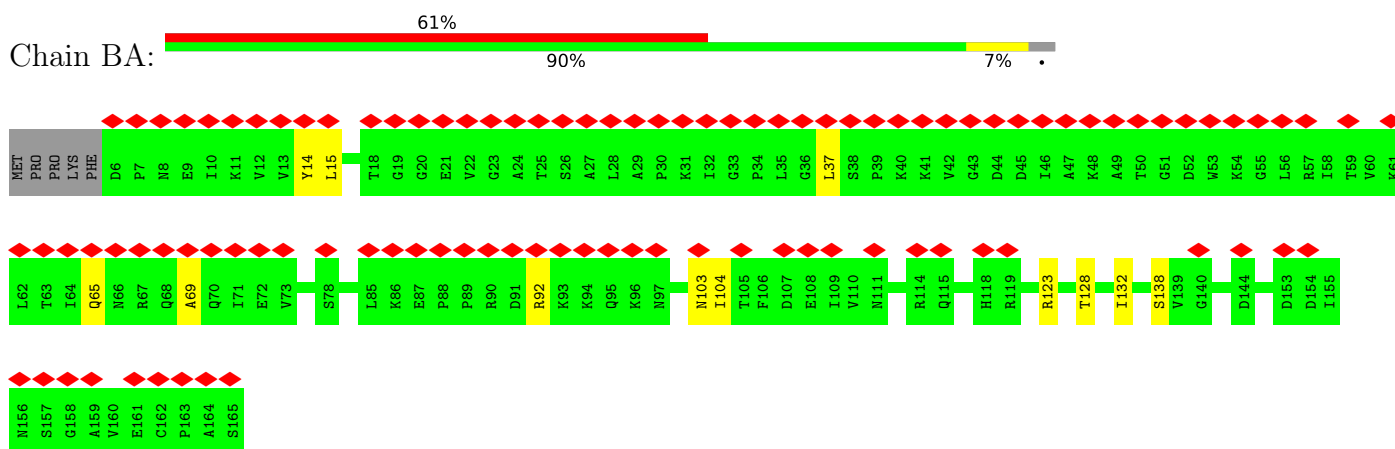
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

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

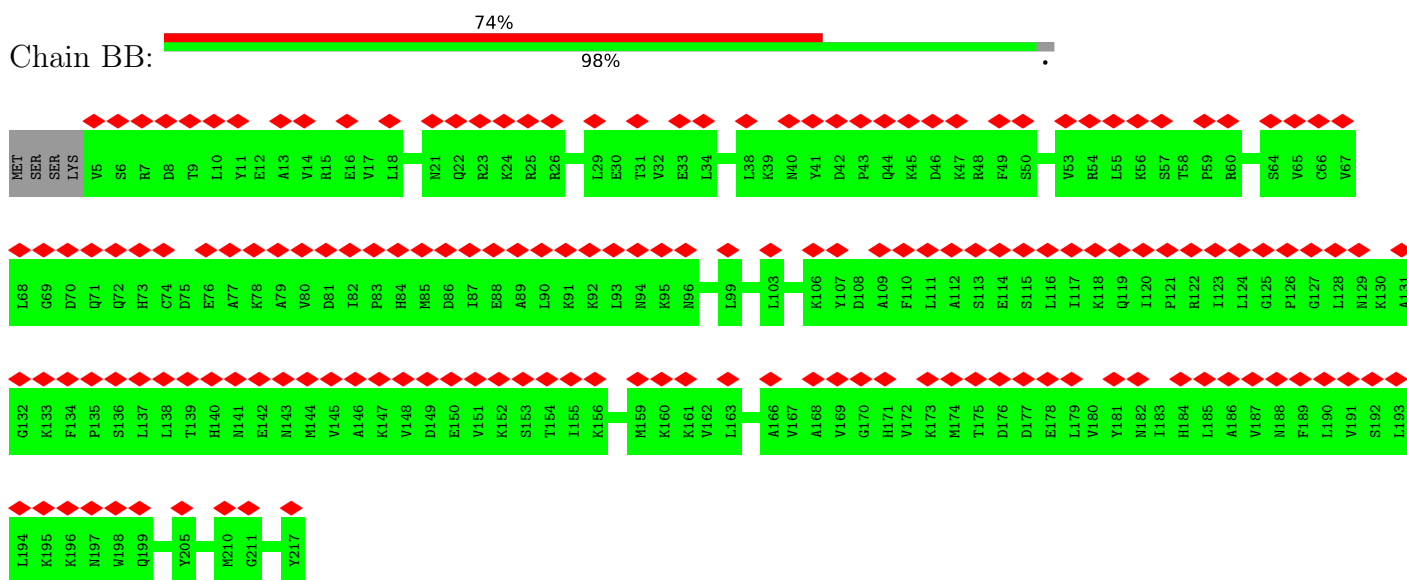
3 Residue-property plots

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

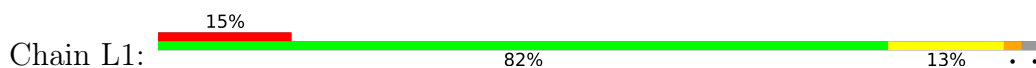
- Molecule 1: 60S ribosomal protein L12

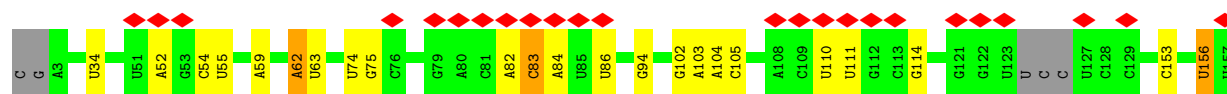


- Molecule 2: 60S ribosomal protein L10a



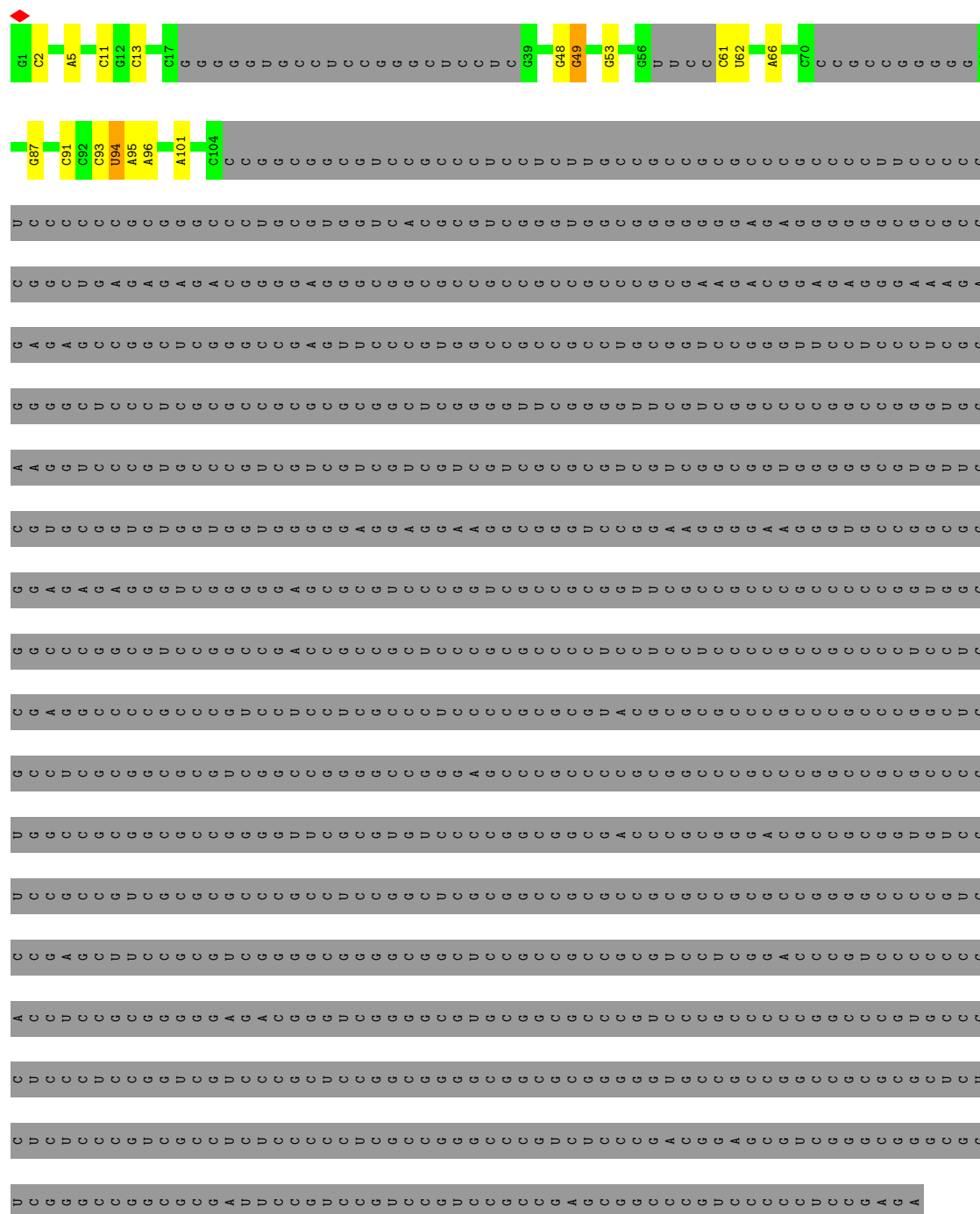
- Molecule 3: 5.8S rRNA





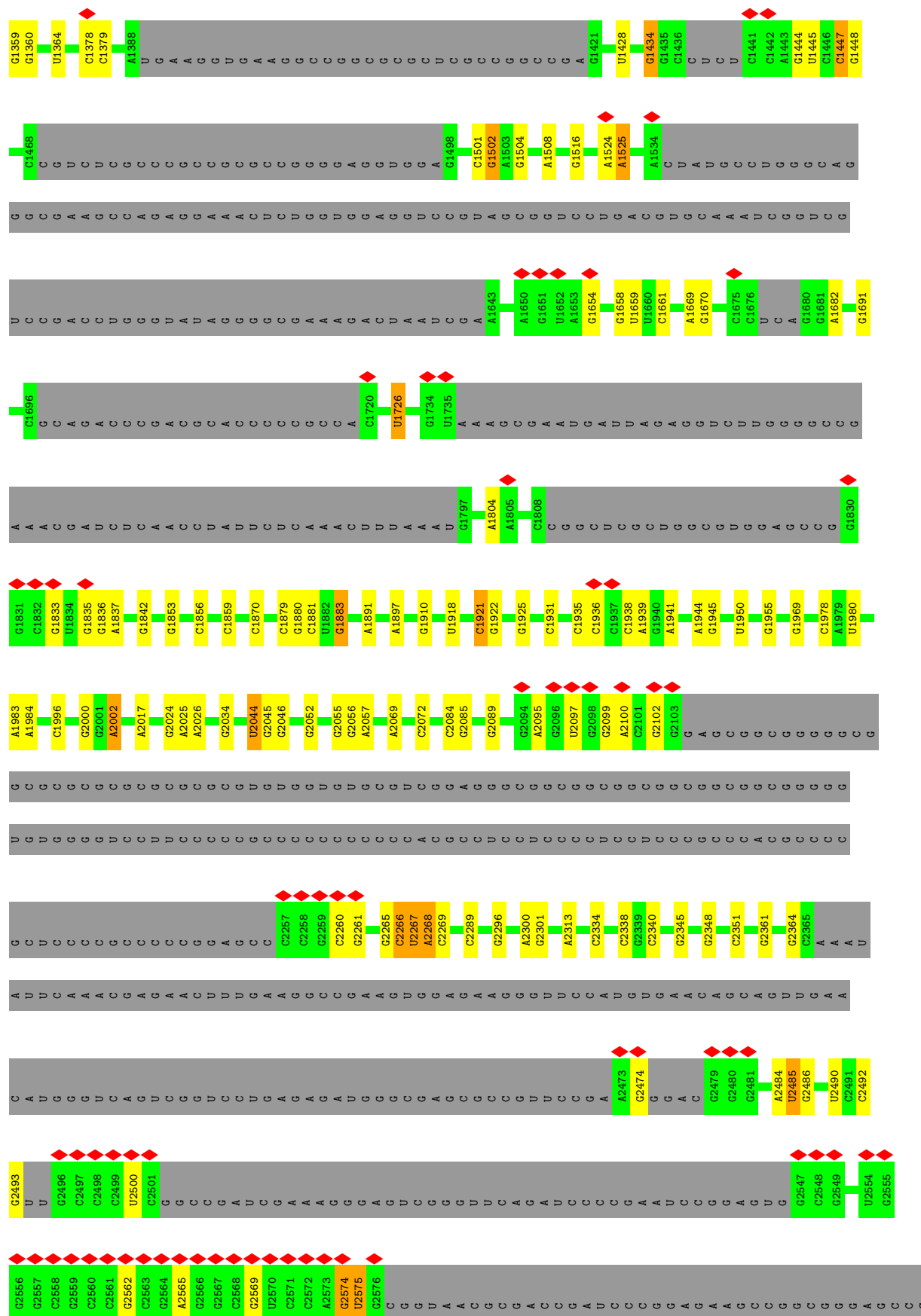
• Molecule 4: ITS2 rRNA

Chain L2: 94%



• Molecule 5: 28S rRNA





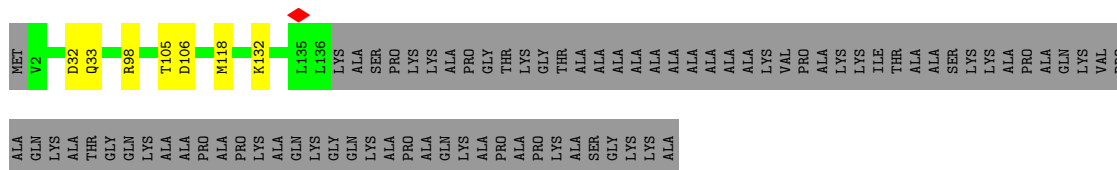




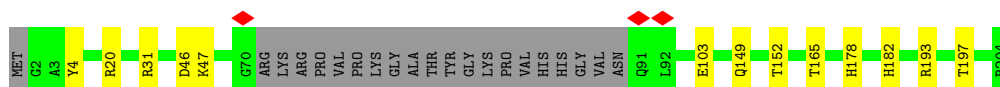
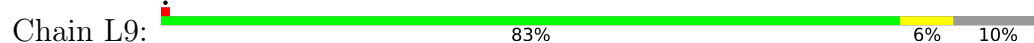
- Molecule 7: 60S ribosomal protein L13a



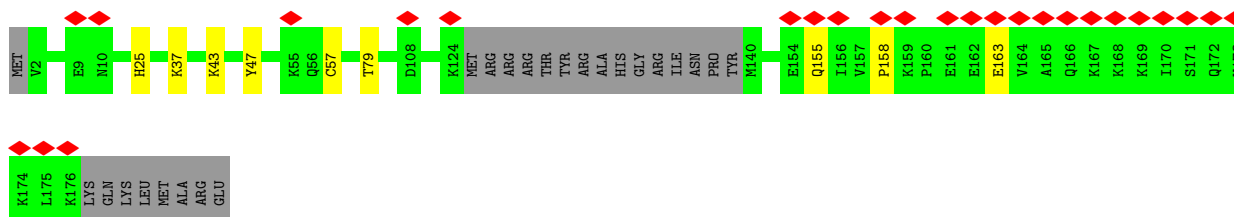
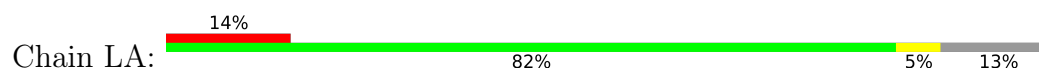
- Molecule 8: 60S ribosomal protein L14



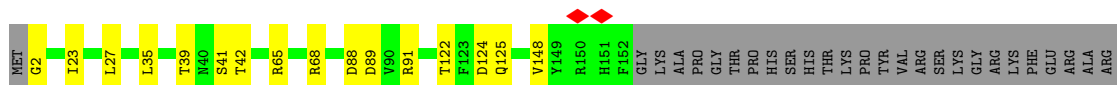
- Molecule 9: 60S ribosomal protein L15



- Molecule 10: 60S ribosomal protein L17



- Molecule 11: 60S ribosomal protein L18



ARG
ARG
ALA
SER
ARG
GLY
TYR
LYS
ASN

- Molecule 12: 60S ribosomal protein L18a

Chain LC:  91% 9%

W L17 L18 T19 C22 H23 E69 K76 W81 P18 L82 R83 Y84 M93 D99 L100 R116 I124 R160 T174 F175 F176

- Molecule 13: 60S ribosomal protein L21

Chain LE:  39% 68% 29%

MET THR ASN THR LYS GLY LYS ARG ARG GLY THR ARG TYR MET PHE SER SER ARG PRO PHE ARG LYS HIS GLY VAL PRO LEU THR TYR MET ARG I33 Y34 K35 K36 G37 D38 I39 K43 K43 MET GLY THR VAL GLN LYS GLY MET PRO HIS K55 C56 Y57 H58 R63 V64 Y65

N66 V67 T68 Q69 H70 A71 V72 G73 I74 N77 K78 Q79 K81 G82 K83 I84 L85 A86 K87 R88 I89 N90 V91 R92 I93 E94 H95 I96 K97 H98 S99 R102 D103 K107 K110 E111 N112 D113 Q114 K115 K116 K117 E118 A119 K120 E121 LYS GLY THR TRP V126 Q127 L128 R136

I154 I157 F158 M159 A160

- Molecule 14: 60S ribosomal protein L23

Chain LG:  16% 83% 13%

MET SER LYS ARG ARG G7 G8 K13 F14 S17 N27 C28 K35 I40 S41 V42 K43 G44 I45 K46 G47 R48 L49 N50 R51 L52 P53 A54 V57 T64 K67 G68 K69 P70 E71 R73 K74 K75 V76 V81 Q84 R85 K86 L96 K109

A140

- Molecule 15: 60S ribosomal protein L23a

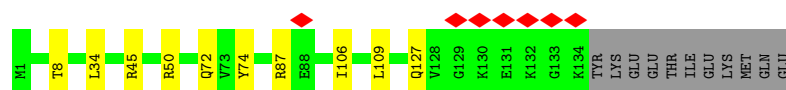
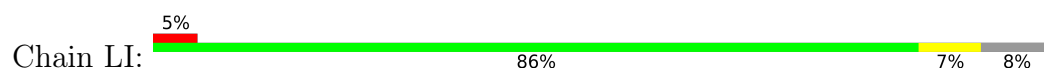
Chain LH:  63% 84% 15%

MET ALA PRO LYS ALA LYS LYS GLY PRO PRO PRO K14 A15 E16 K30 S34 HIS LYS LYS LYS LYS ILE ARG THR SER PRO T45 F46 R47 R48 F49 K50 R55 A65 P66 R67 R68 R69 K70 L71 D72 A75 I76 I77 F78 F79 P80 L81 T82 T83 E84 S85 A86

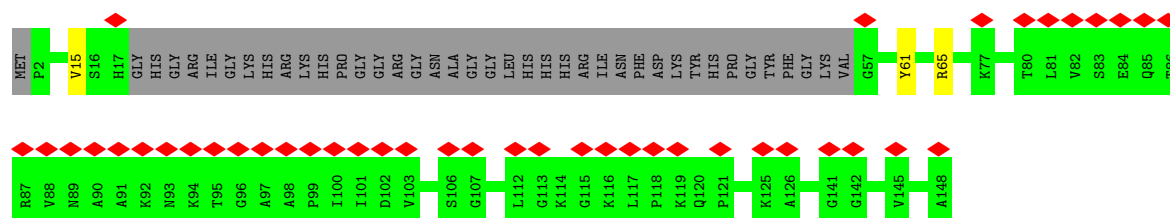
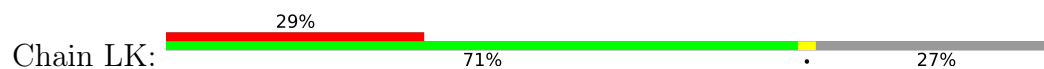
M87 K88 K89 T90 E91 N93 N94 T95 L96 V97 F98 I99 V100 D101 V102 K103 A104 M105 K106 H107 Q108 I109 K110 Q111 A112 V113 K114 K115 L116 Y117 D118 I119 D120 V121 A122 K123 V124 M125 T126 L127 I128 R129 P130 D131 G132 E133 K134 K135 A136 T83 Y137 V138 R139 L140 A141 P142 D143 Y144 D145 A146

L147 D148 V149 A150 M151 K152 I153 G154 I155 I156

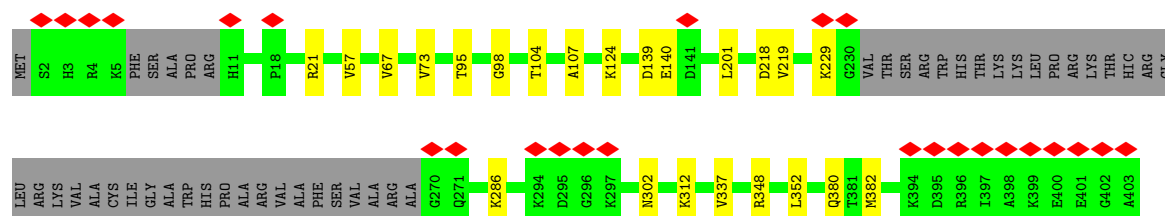
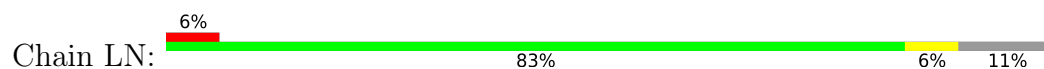
- Molecule 16: 60S ribosomal protein L26



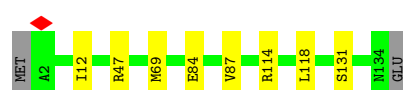
- Molecule 17: 60S ribosomal protein L27a



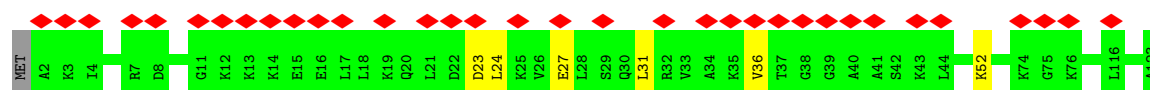
- Molecule 18: 60S ribosomal protein L3



- Molecule 19: 60S ribosomal protein L32



- Molecule 20: 60S ribosomal protein L35

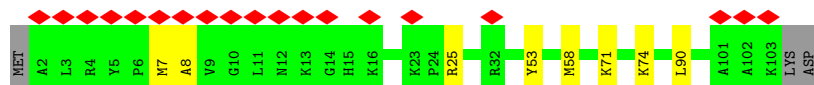
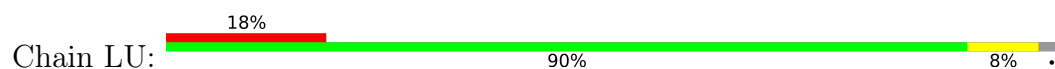


- Molecule 21: 60S ribosomal protein L35a

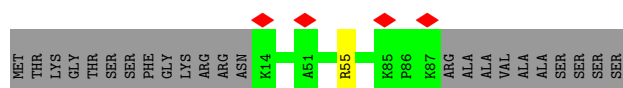
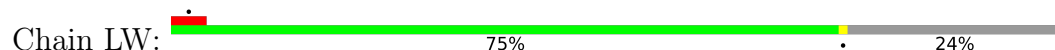




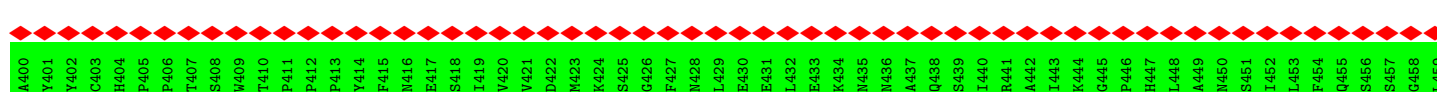
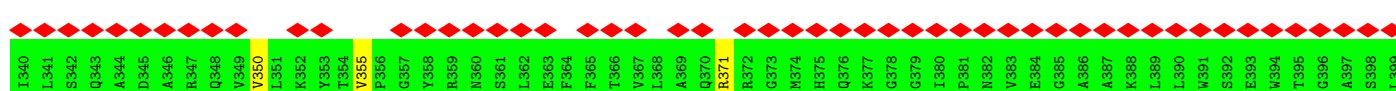
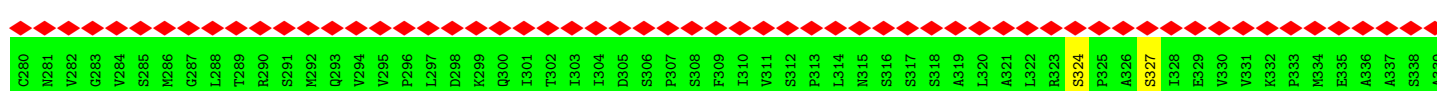
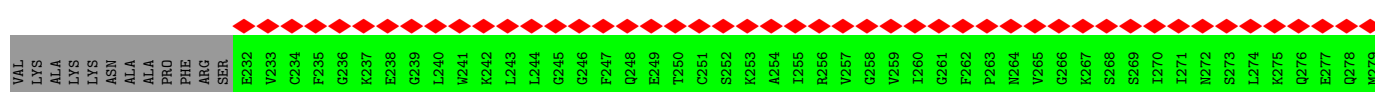
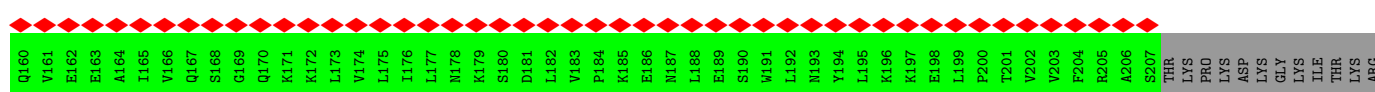
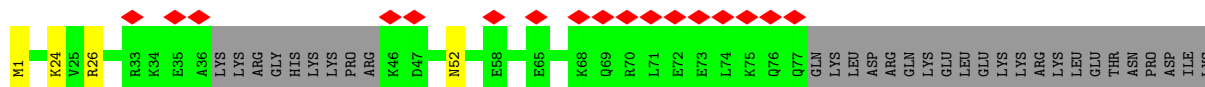
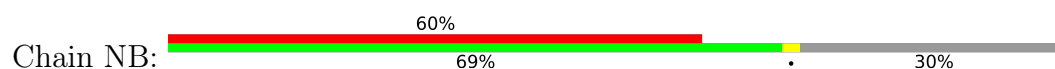
- Molecule 22: 60S ribosomal protein L36



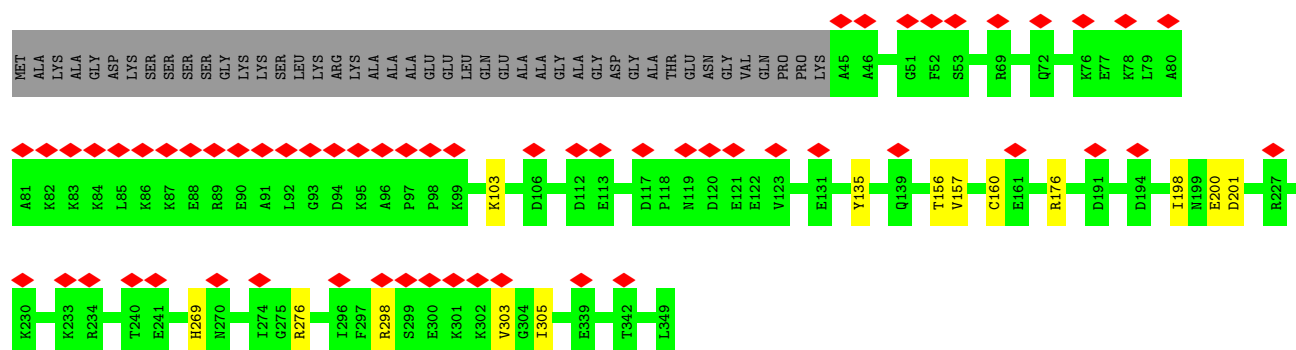
- Molecule 23: 60S ribosomal protein L37



- Molecule 24: Guanine nucleotide-binding protein-like 3

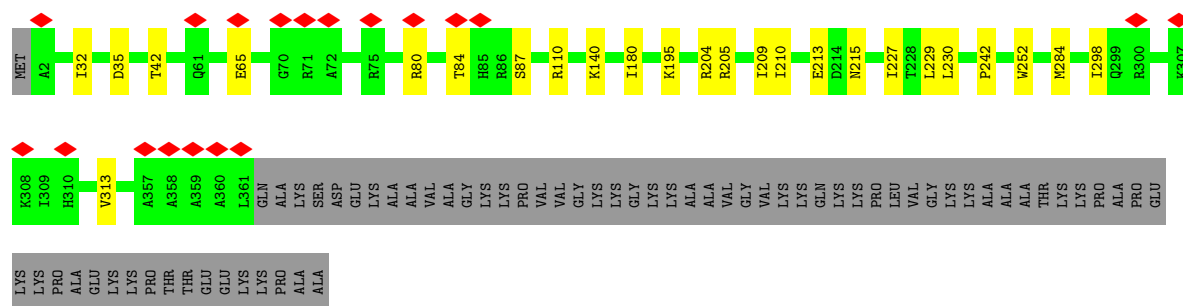


Chain NS: 



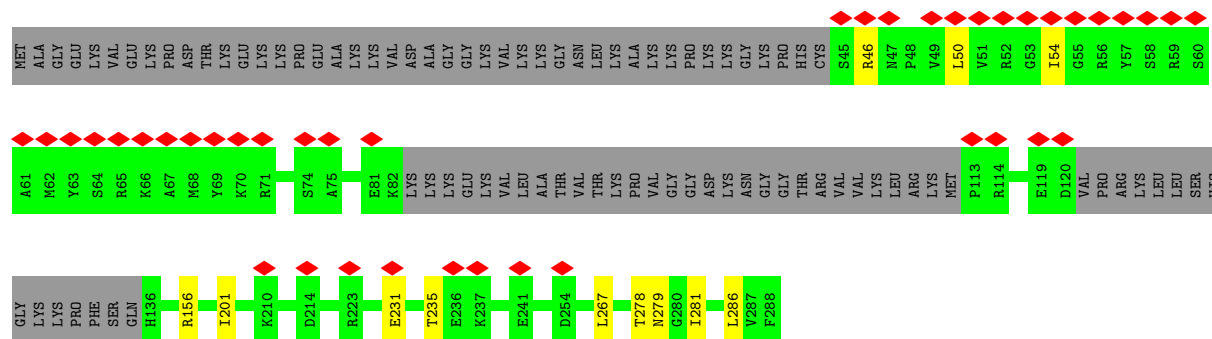
• Molecule 33: 60S ribosomal protein L4

Chain SA: 

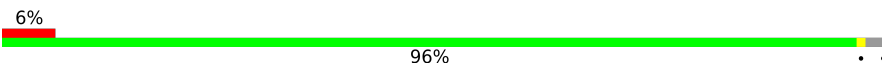


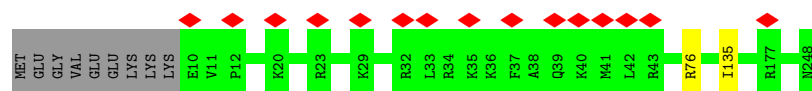
• Molecule 34: 60S ribosomal protein L6

Chain SC: 



• Molecule 35: 60S ribosomal protein L7

Chain SD: 



• Molecule 36: 60S ribosomal protein L7a

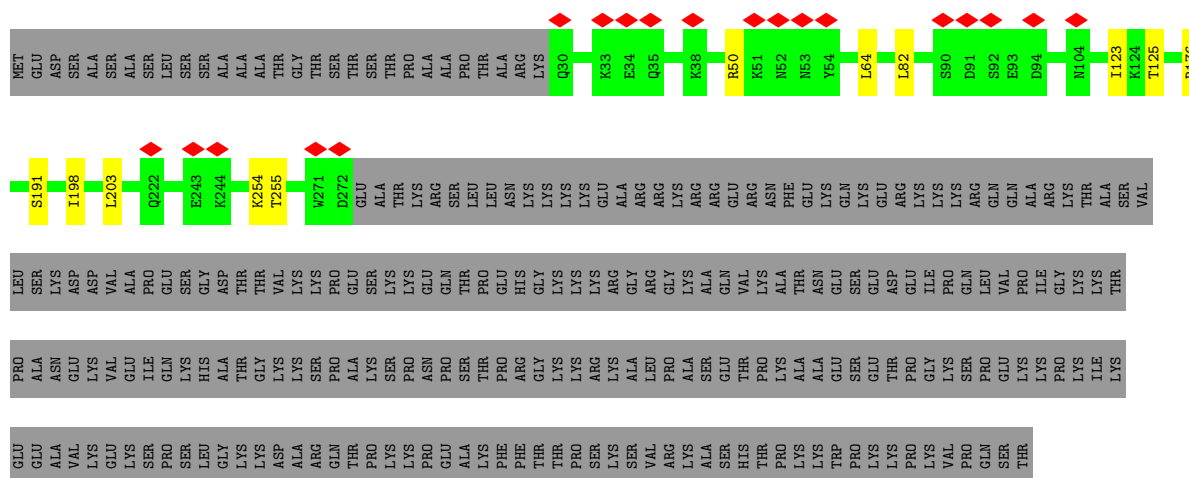
Diagram illustrating a protein structure with various amino acid residues highlighted in yellow and green. The residues are labeled with three-letter codes (e.g., MET, PRO, GLY, LYS, ALA, VAL, ASN, PHE, LEU, ARG, THR, ASP, GLN, ASP, LEU, THR, ARG, PHE, VAL, R56, R57, P58, T61). The diagram is divided into two main sections by a vertical line. The left section shows a sequence of residues from MET to VAL. The right section shows a sequence of residues from R56 to T61. The residues are arranged in a grid-like pattern, with some residues highlighted in yellow and others in green. The background is a light gray color.

-

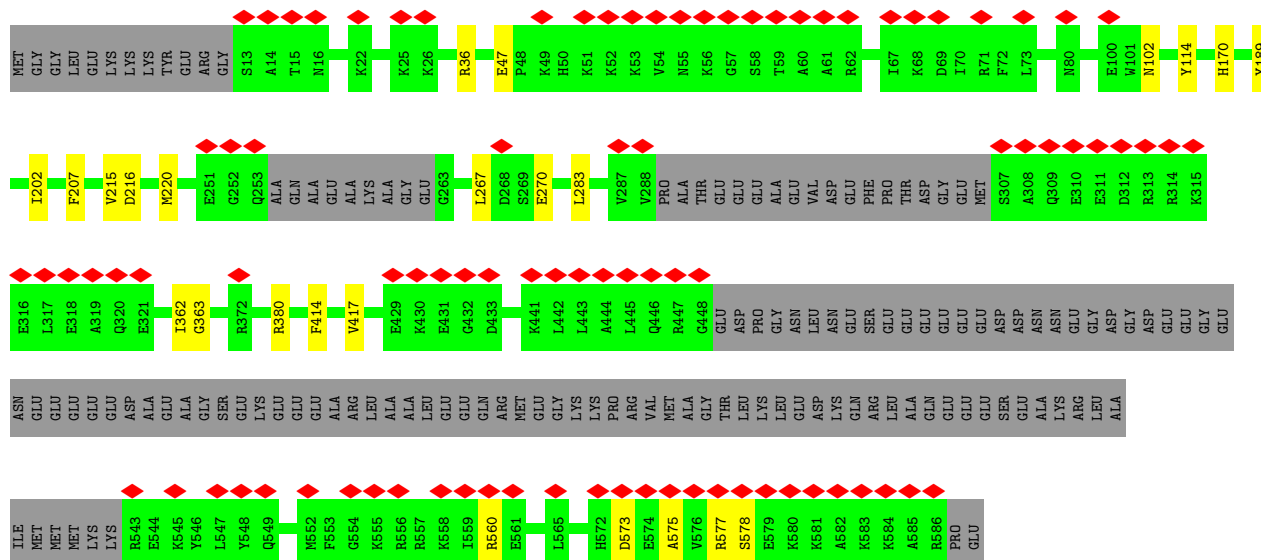
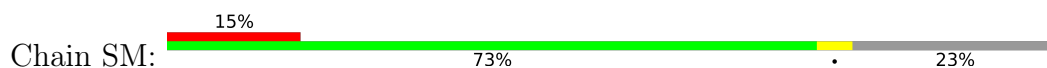
- [illegible]

-
- Sequence logo showing information content (bits) for each residue position (1-100). The y-axis represents information content in bits (0.00 to 0.40). The x-axis shows residue positions. Residues are color-coded: yellow for high information content, green for moderate, and grey for low. Red diamonds indicate specific residues of interest.
- | Residue Position | Residue | Information Content (bits) |
|------------------|---------|----------------------------|
| 1 | Met | 0.00 |
| 2 | Ile | 0.00 |
| 3 | Ser | 0.00 |
| 4 | Ser | 0.00 |
| 5 | Cys | 0.00 |
| 6 | Cys | 0.00 |
| 7 | Thr | 0.00 |
| 8 | Arg | 0.00 |
| 9 | Lys | 0.00 |
| 10 | Met | 0.00 |
| 11 | Ala | 0.00 |
| 12 | Gln | 0.00 |
| 13 | Gln | 0.00 |
| 14 | Gln | 0.00 |
| 15 | Arg | 0.00 |
| 16 | Lys | 0.00 |
| 17 | I18 | 0.00 |
| 18 | P19 | 0.00 |
| 19 | L20 | 0.00 |
| 20 | V21 | 0.00 |
| 21 | K30 | 0.00 |
| 22 | Q33 | 0.00 |
| 23 | K36 | 0.00 |
| 24 | K41 | 0.00 |
| 25 | Q42 | 0.00 |
| 26 | A43 | 0.00 |
| 27 | L44 | 0.00 |
| 28 | L46 | 0.00 |
| 29 | A46 | 0.00 |
| 30 | Lys | 0.00 |
| 31 | Lys | 0.00 |
| 32 | Glu | 0.00 |
| 33 | Gln | 0.00 |
| 34 | Lys | 0.00 |
| 35 | Lys | 0.00 |
| 36 | Gly | 0.00 |
| 37 | Gly | 0.00 |
| 38 | Lys | 0.00 |
| 39 | Lys | 0.00 |
| 40 | Leu | 0.00 |
| 41 | R57 | 0.00 |
| 42 | R70 | 0.00 |
| 43 | V76 | 0.00 |
| 44 | R77 | 0.00 |
| 45 | L78 | 0.00 |
| 46 | R86 | 0.00 |
| 47 | R87 | 0.00 |
| 48 | L88 | 0.00 |
| 49 | E89 | 0.00 |
| 50 | L90 | 0.00 |
| 51 | P91 | 0.00 |
| 52 | D92 | 0.00 |
| 53 | F98 | 0.00 |
| 54 | R101 | 0.00 |
| 55 | D106 | 0.00 |
| 56 | L111 | 0.00 |
| 57 | V112 | 0.00 |
| 58 | I116 | 0.00 |
| 59 | K122 | 0.00 |
| 60 | V143 | 0.00 |
| 61 | V147 | 0.00 |
| 62 | P152 | 0.00 |
| 63 | M153 | 0.00 |
| 64 | K170 | 0.00 |
| 65 | M171 | 0.00 |
| 66 | K172 | 0.00 |
| 67 | T177 | 0.00 |
| 68 | E183 | 0.00 |
| 69 | G187 | 0.00 |
| 70 | I192 | 0.00 |
| 71 | R206 | 0.00 |
| 72 | Y242 | 0.00 |
| 73 | R252 | 0.00 |
| 74 | M255 | 0.00 |

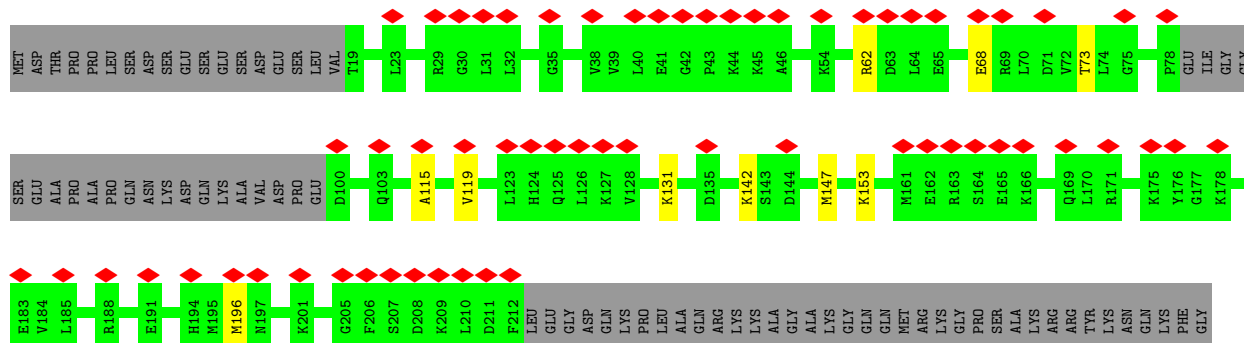
- [illegible]



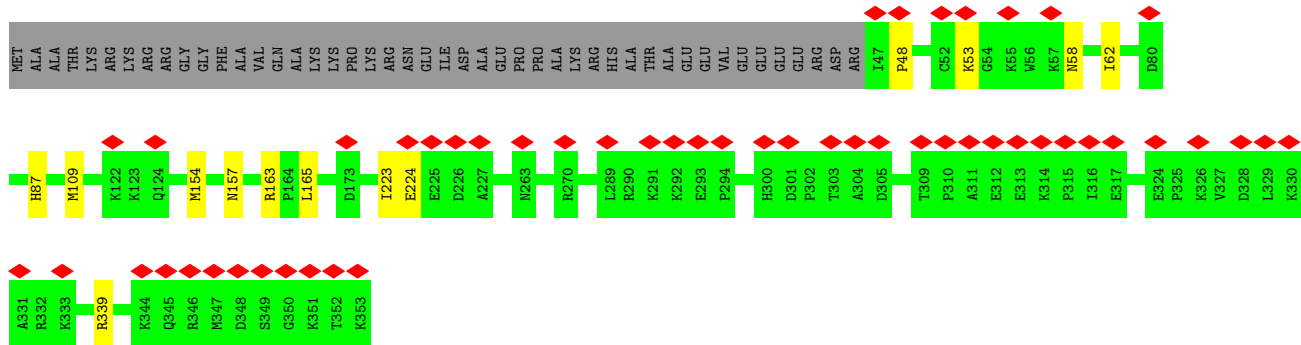
• Molecule 43: Pescadillo homolog



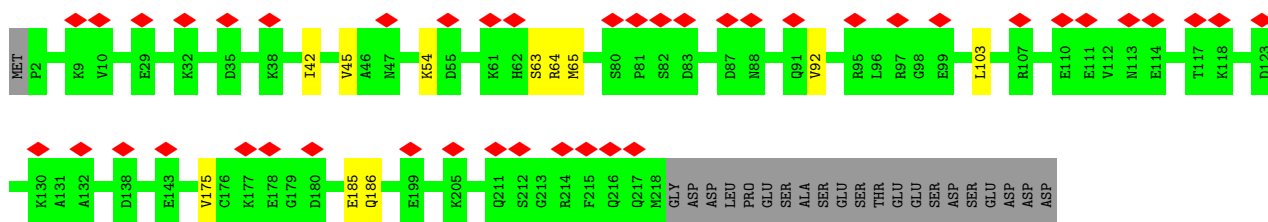
• Molecule 44: Probable rRNA-processing protein EBP2



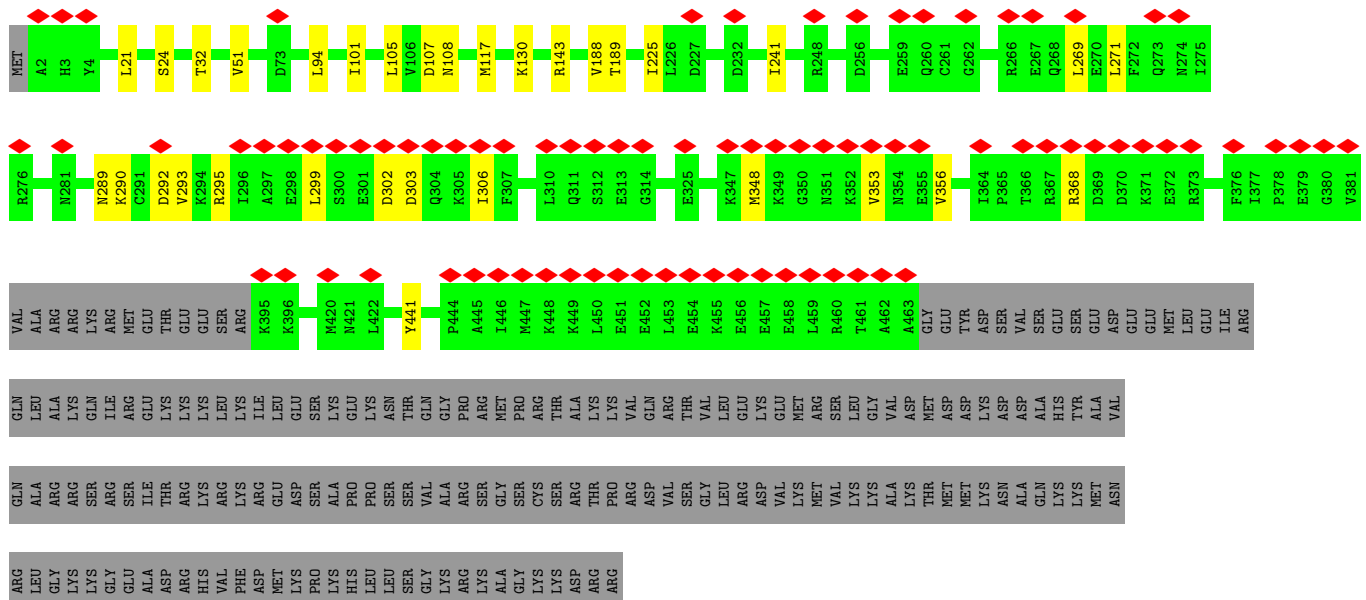
Chain SO:



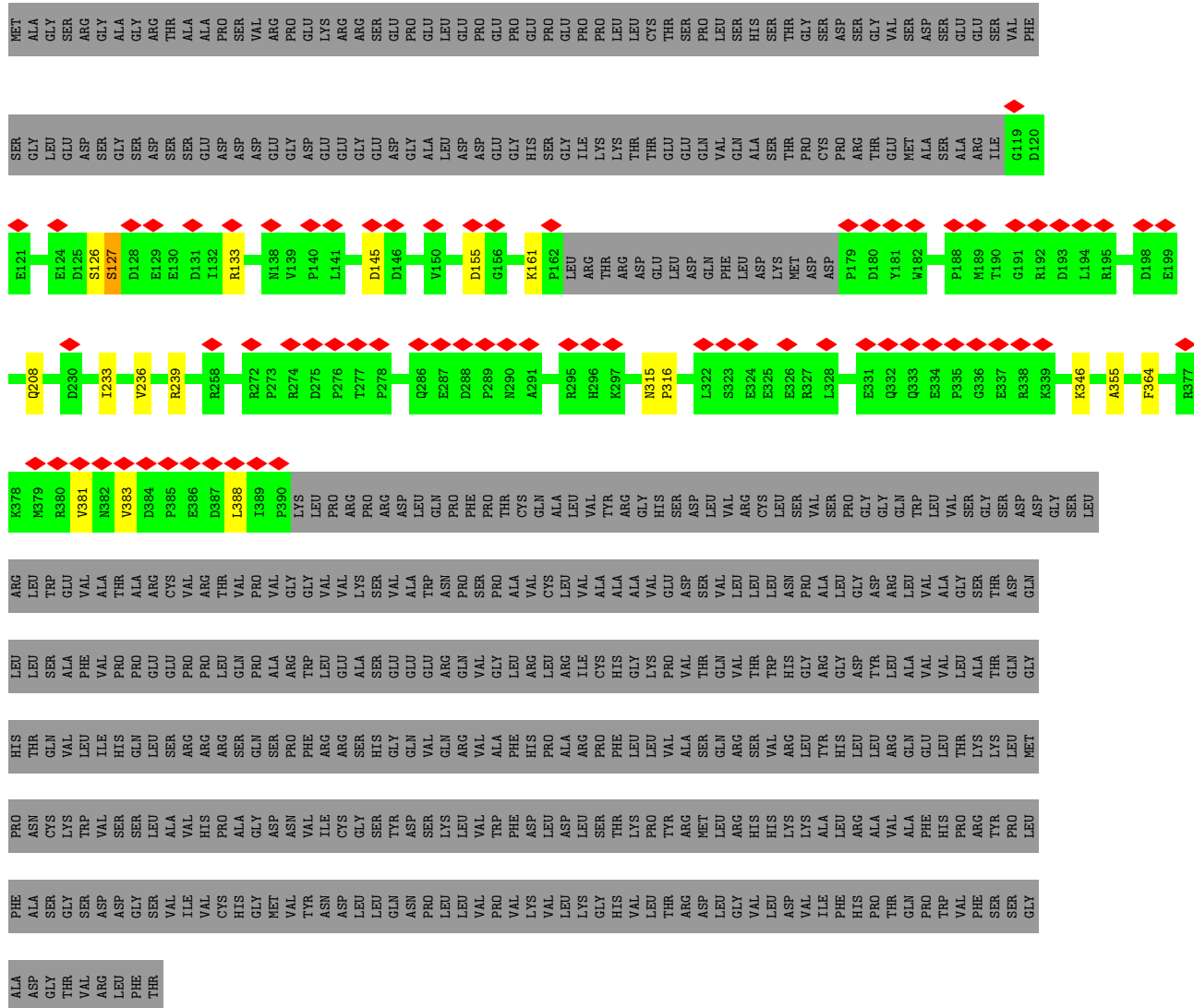
Chain SQ:



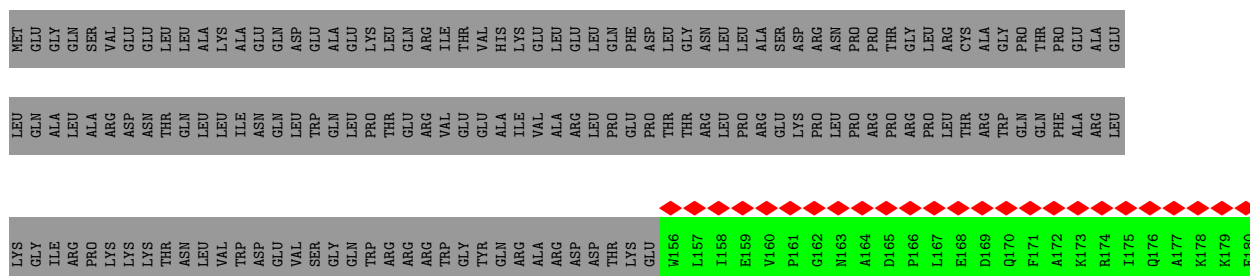
Chain SR:



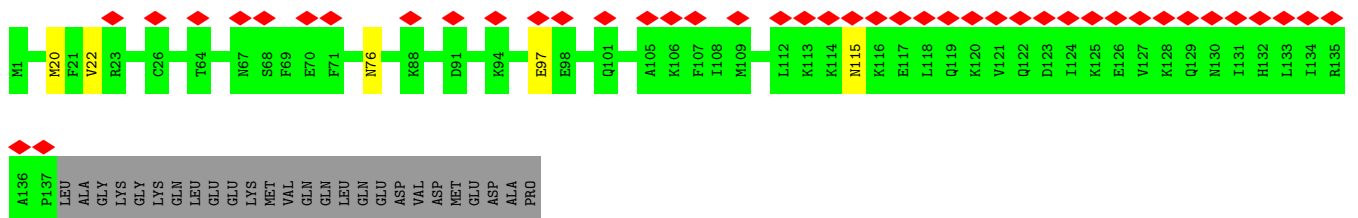
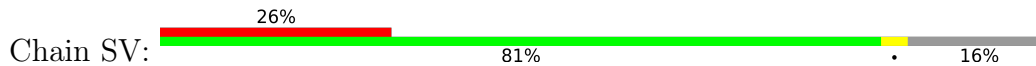
Chain SS:



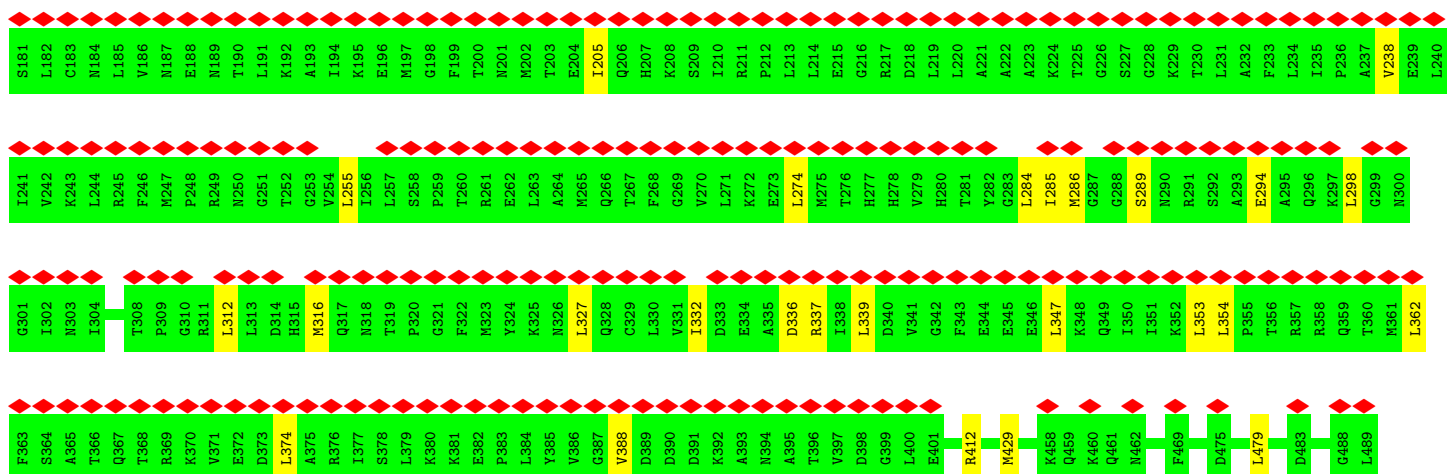
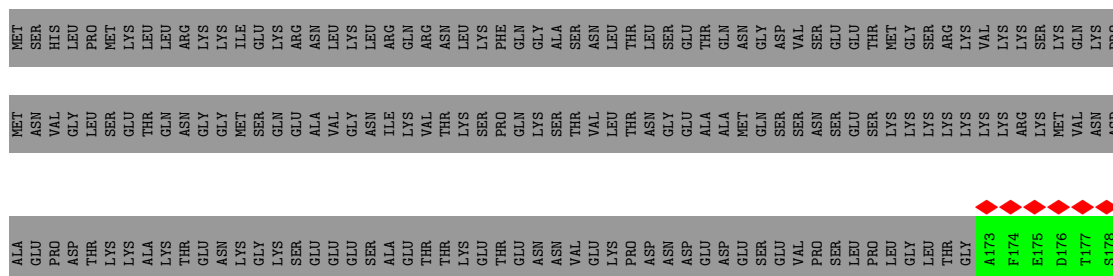
Chain ST:



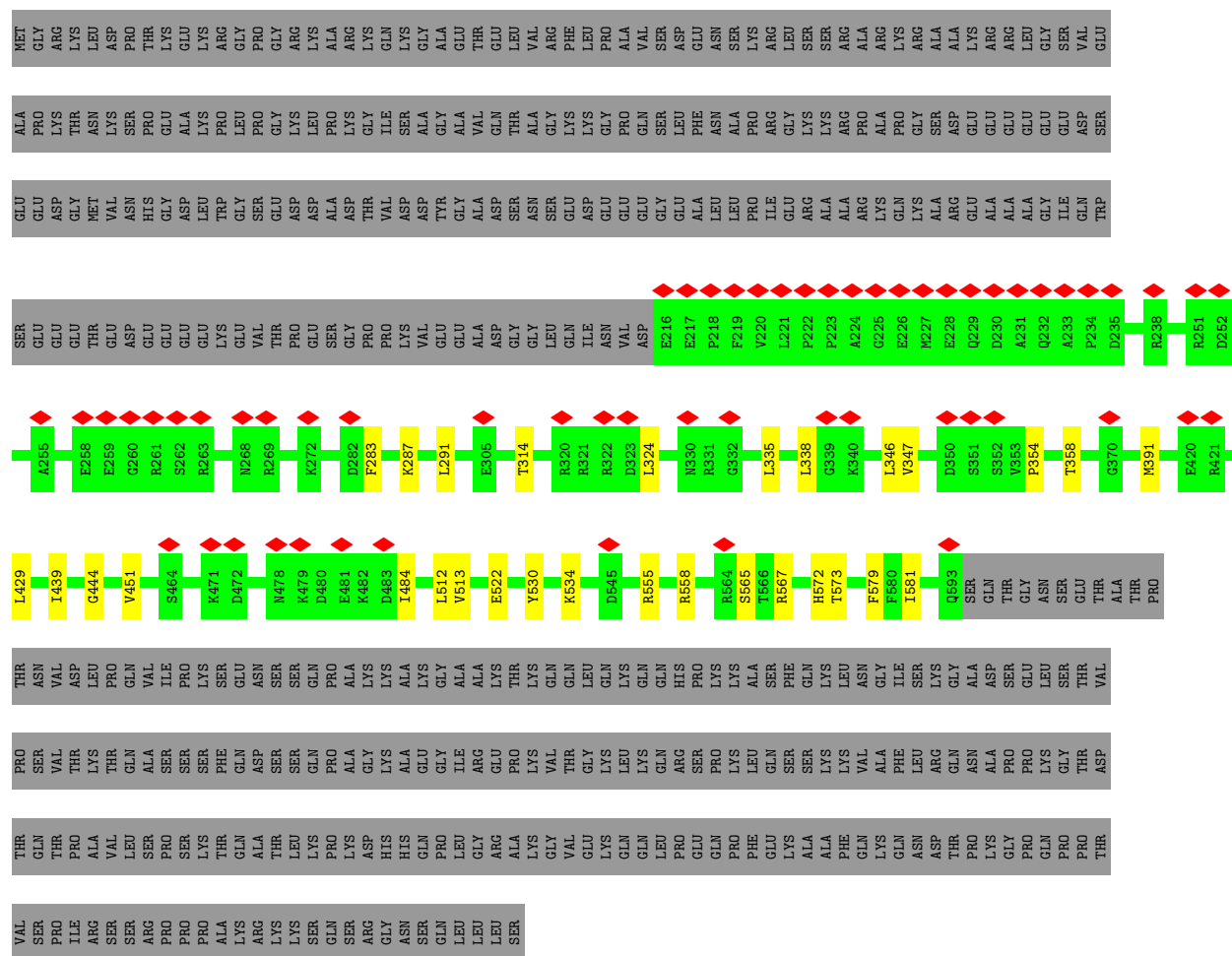
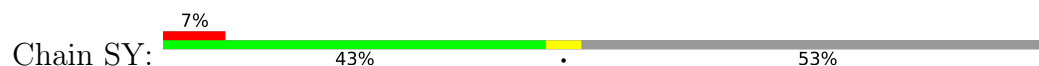
- Molecule 50: Probable ribosome biogenesis protein RLP24



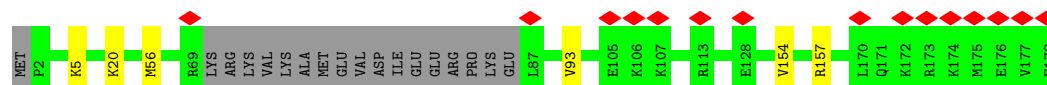
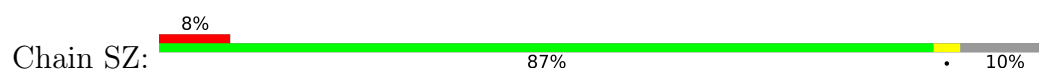
- Molecule 51: ATP-dependent RNA helicase DDX18



- Molecule 52: Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase



- Molecule 53: Nucleolar protein 16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45396	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	6.688	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.170	Depositor
Recommended contour level	1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, SF4, ADP, K, GDP, AME, ZN, MG

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	0.17	0/1224	0.34	0/1651
2	BB	0.15	0/1056	0.34	0/1472
3	L1	0.22	0/3611	0.26	0/5623
4	L2	0.21	0/1634	0.29	0/2538
5	L3	0.23	0/50941	0.29	0/79394
6	L6	0.21	0/1020	0.37	0/1367
7	L7	0.24	0/1666	0.38	0/2228
8	L8	0.23	0/1133	0.38	0/1516
9	L9	0.23	0/1584	0.37	0/2117
10	LA	0.17	0/1309	0.33	0/1752
11	LB	0.21	0/1239	0.32	0/1658
12	LC	0.25	0/1501	0.37	0/2013
13	LE	0.15	0/755	0.37	0/1021
14	LG	0.19	0/1007	0.39	0/1350
15	LH	0.13	0/818	0.32	0/1111
16	LI	0.23	0/1132	0.39	0/1504
17	LK	0.14	0/648	0.34	0/880
18	LN	0.21	0/2938	0.36	0/3923
19	LQ	0.23	0/1114	0.36	0/1486
20	LS	0.16	0/1023	0.29	0/1351
21	LT	0.25	0/895	0.35	0/1198
22	LU	0.20	0/843	0.32	0/1115
23	LW	0.18	0/626	0.34	0/829
24	NB	0.13	0/2449	0.27	0/3335
25	NF	0.17	0/1690	0.31	0/2247
26	NH	0.20	0/1473	0.35	0/1988
27	NI	0.11	0/3906	0.26	0/5329
28	NK	0.17	0/587	0.31	0/767
29	NM	0.20	0/1566	0.32	0/2097
30	NO	0.15	0/2530	0.28	0/3412
31	NQ	0.16	0/2556	0.31	0/3466
32	NS	0.17	0/2592	0.31	0/3487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SA	0.21	0/2918	0.35	0/3920
34	SC	0.16	0/1657	0.33	0/2219
35	SD	0.22	0/2022	0.33	0/2696
36	SE	0.20	0/1517	0.34	0/2046
37	SG	0.22	0/1548	0.34	0/2081
38	SH	0.20	0/1298	0.30	0/1742
39	SI	0.21	0/1930	0.33	0/2595
40	SJ	0.16	0/868	0.29	0/1153
41	SK	0.18	0/1877	0.35	0/2554
42	SL	0.21	0/1994	0.37	0/2684
43	SM	0.18	0/3819	0.29	0/5139
44	SN	0.15	0/1368	0.30	0/1830
45	SO	0.18	0/2608	0.32	0/3506
46	SQ	0.15	0/1817	0.31	0/2435
47	SR	0.18	0/3768	0.32	0/5086
48	SS	0.21	0/2159	0.36	0/2932
49	ST	0.17	0/795	0.33	0/1072
50	SV	0.18	0/1194	0.32	0/1582
51	SW	0.16	0/3620	0.28	0/4886
52	SY	0.20	0/3046	0.32	0/4117
53	SZ	0.17	0/1364	0.30	0/1826
All	All	0.20	0/142253	0.31	0/203326

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8	0
2	BB	1057	0	464	0	0
3	L1	3234	0	1639	6	0
4	L2	1468	0	755	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L3	45561	0	23045	151	0
6	L6	998	0	1067	9	0
7	L7	1634	0	1779	5	0
8	L8	1111	0	1174	6	0
9	L9	1546	0	1585	10	0
10	LA	1286	0	1338	8	0
11	LB	1223	0	1330	15	0
12	LC	1461	0	1502	13	0
13	LE	747	0	599	3	0
14	LG	993	0	1050	16	0
15	LH	813	0	640	2	0
16	LI	1115	0	1205	9	0
17	LK	642	0	455	3	0
18	LN	2884	0	3000	17	0
19	LQ	1096	0	1183	7	0
20	LS	1015	0	1148	4	0
21	LT	876	0	912	6	0
22	LU	832	0	917	6	0
23	LW	612	0	640	1	0
24	NB	2424	0	1868	8	0
25	NF	1661	0	1776	10	0
26	NH	1441	0	1448	12	0
27	NI	3866	0	3171	15	0
28	NK	581	0	656	8	0
29	NM	1550	0	1599	14	0
30	NO	2487	0	2506	10	0
31	NQ	2502	0	2481	13	0
32	NS	2529	0	2563	12	0
33	SA	2864	0	3038	20	0
34	SC	1627	0	1751	8	0
35	SD	1985	0	2128	2	0
36	SE	1491	0	1592	9	0
37	SG	1526	0	1614	6	0
38	SH	1267	0	1291	2	0
39	SI	1887	0	2011	19	0
40	SJ	855	0	876	5	0
41	SK	1852	0	1828	13	0
42	SL	1960	0	2052	8	0
43	SM	3735	0	3830	17	0
44	SN	1350	0	1345	10	0
45	SO	2544	0	2631	13	0
46	SQ	1778	0	1817	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	SR	3695	0	3755	24	0
48	SS	2116	0	2028	16	0
49	ST	787	0	698	3	0
50	SV	1171	0	1232	5	0
51	SW	3549	0	3628	19	0
52	SY	2985	0	3004	20	0
53	SZ	1338	0	1352	5	0
54	L1	5	0	0	0	0
54	L2	1	0	0	0	0
54	L3	52	0	0	0	0
54	L9	1	0	0	0	0
54	LQ	1	0	0	0	0
54	LT	1	0	0	0	0
54	NI	1	0	0	0	0
54	SA	1	0	0	0	0
54	SR	1	0	0	0	0
55	LW	1	0	0	0	0
55	SV	1	0	0	0	0
56	NI	27	0	12	0	0
57	NM	8	0	0	0	0
58	SR	28	0	12	0	0
59	SR	1	0	0	0	0
All	All	134945	0	110277	468	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 (468) 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	0.92
14:LG:40:ILE:HD11	14:LG:64:THR:HG23	1.58	0.86
5:L3:712:C:N3	5:L3:1284:G:N1	2.22	0.85
5:L3:184:U:O2'	5:L3:189:G:OP2	1.95	0.85
51:SW:238:VAL:HG21	51:SW:274:LEU:HD22	1.63	0.81
4:L2:53:G:OP2	38:SH:81:ARG:NH1	2.15	0.80
36:SE:109:GLU:OE2	43:SM:102:ASN:ND2	2.14	0.79
30:NO:346:GLU:OE1	30:NO:350:ARG:NH2	2.15	0.79
46:SQ:64:ARG:NH1	46:SQ:65:MET:O	2.16	0.78
5:L3:1319:U:O2	5:L3:1324:A:N6	2.17	0.78
5:L3:3890:A:OP2	5:L3:4570:G:N2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1444:G:HO2'	5:L3:1448:G:HO2'	1.30	0.77
5:L3:1524:A:O2'	5:L3:1525:A:O5'	2.01	0.76
25:NF:163:LYS:NZ	25:NF:167:TYR:O	2.18	0.76
5:L3:2045:G:O6	5:L3:3870:C:O2'	2.02	0.76
5:L3:1501:C:O2'	11:LB:68:ARG:NH1	2.20	0.75
9:L9:20:ARG:NH2	40:SJ:693:THR:O	2.19	0.75
32:NS:156:THR:OG1	32:NS:200:GLU:OE1	2.01	0.74
3:L1:75:G:OP2	16:LI:74:TYR:OH	2.06	0.74
25:NF:8:GLU:OE2	27:NI:581:SER:OG	2.05	0.74
5:L3:1508:A:OP1	33:SA:110:ARG:NH2	2.19	0.74
5:L3:62:A:N3	5:L3:77:U:O2'	2.21	0.73
5:L3:2574:G:O2'	5:L3:2575:U:OP1	2.06	0.73
5:L3:306:A:OP1	22:LU:53:TYR:OH	2.06	0.72
5:L3:2338:C:OP1	29:NM:22:ARG:NH1	2.23	0.72
5:L3:4354:U:OP1	52:SY:530:TYR:OH	2.05	0.72
5:L3:1983:A:N1	27:NI:579:ASN:ND2	2.37	0.72
51:SW:289:SER:OG	51:SW:294:GLU:OE2	2.07	0.71
5:L3:4678:G:OP1	28:NK:14:ARG:NH1	2.22	0.71
5:L3:2361:G:O6	10:LA:25:HIS:ND1	2.23	0.71
39:SI:92:ASP:OD2	39:SI:242:TYR:OH	2.09	0.71
5:L3:1883:G:OP1	19:LQ:47:ARG:NH1	2.25	0.70
5:L3:304:C:OP2	40:SJ:691:ARG:NH2	2.24	0.70
18:LN:107:ALA:HB2	18:LN:201:LEU:HD22	1.73	0.70
5:L3:1833:G:N2	5:L3:1835:G:O4'	2.25	0.69
5:L3:470:A:H61	5:L3:685:C:HO2'	1.39	0.69
41:SK:119:PRO:O	41:SK:139:ARG:NH2	2.24	0.69
1:BA:138:SER:OG	5:L3:2002:A:N6	2.25	0.69
5:L3:4662:C:O2'	5:L3:5004:C:OP1	2.07	0.69
5:L3:5063:G:O6	18:LN:124:LYS:NZ	2.26	0.69
18:LN:286:LYS:NZ	18:LN:302:ASN:O	2.23	0.69
45:SO:224:GLU:OE2	49:ST:250:LYS:NZ	2.23	0.69
5:L3:4441:A:N6	27:NI:445:ASP:O	2.26	0.68
5:L3:3907:G:O2'	5:L3:3908:A:OP1	2.11	0.67
5:L3:5039:U:O3'	50:SV:115:ASN:ND2	2.27	0.67
24:NB:324:SER:OG	24:NB:327:SER:OG	1.98	0.67
19:LQ:84:GLU:O	19:LQ:87:VAL:HG22	1.94	0.67
5:L3:116:G:O2'	48:SS:239:ARG:NH1	2.27	0.67
26:NH:104:GLU:OE2	26:NH:135:SER:OG	2.10	0.66
33:SA:213:GLU:OE1	33:SA:215:ASN:ND2	2.29	0.66
45:SO:48:PRO:O	48:SS:133:ARG:NH1	2.29	0.66
5:L3:238:C:OP2	16:LI:45:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L1:62:A:OP1	20:LS:52:LYS:NZ	2.29	0.65
39:SI:70:ARG:NH1	39:SI:106:ASP:O	2.29	0.65
4:L2:61:C:N3	42:SL:50:ARG:NH1	2.45	0.65
11:LB:88:ASP:OD1	11:LB:89:ASP:N	2.30	0.65
41:SK:98:GLU:OE2	50:SV:76:ASN:ND2	2.29	0.65
39:SI:177:THR:CG2	48:SS:355:ALA:HB3	2.27	0.65
52:SY:555:ARG:O	52:SY:558:ARG:NH1	2.30	0.64
16:LI:34:LEU:HD21	16:LI:109:LEU:HD21	1.78	0.64
4:L2:13:C:OP1	39:SI:86:HIS:NE2	2.27	0.64
5:L3:4940:C:OP1	34:SC:156:ARG:NH1	2.30	0.64
1:BA:92:ARG:NH2	5:L3:1980:U:OP2	2.30	0.64
30:NO:301:GLU:OE2	30:NO:305:ASN:ND2	2.32	0.63
4:L2:91:C:OP2	42:SL:176:ARG:NH2	2.32	0.63
11:LB:35:LEU:HD21	33:SA:298:ILE:HD11	1.80	0.63
18:LN:57:VAL:HG12	18:LN:73:VAL:HG22	1.81	0.63
5:L3:121:A:OP1	36:SE:110:LYS:NZ	2.32	0.62
3:L1:156:U:OP2	36:SE:89:ARG:NH2	2.32	0.62
14:LG:96:LEU:HD13	50:SV:20:MET:HE3	1.81	0.62
30:NO:120:MET:SD	30:NO:124:MET:HE3	2.39	0.62
39:SI:252:ARG:NH1	43:SM:270:GLU:OE1	2.32	0.62
4:L2:5:A:N6	4:L2:95:A:O2'	2.32	0.62
5:L3:1444:G:O2'	5:L3:1448:G:O2'	2.11	0.62
5:L3:2072:C:OP1	11:LB:2:GLY:N	2.32	0.62
10:LA:158:PRO:O	32:NS:276:ARG:NH2	2.32	0.62
5:L3:1524:A:HO2'	5:L3:1525:A:P	2.22	0.62
5:L3:4929:C:O4'	8:L8:118:MET:HE3	1.99	0.62
6:L6:62:PRO:O	6:L6:63:THR:OG1	2.15	0.62
5:L3:4543:G:N3	26:NH:80:ARG:NH2	2.48	0.62
5:L3:4468:U:HO2'	28:NK:2:ALA:N	1.98	0.62
11:LB:39:THR:HG22	11:LB:41:SER:H	1.65	0.62
12:LC:17:LEU:HD21	13:LE:136:ARG:HH11	1.65	0.61
47:SR:302:ASP:OD2	47:SR:303:ASP:N	2.33	0.61
5:L3:1921:C:O2'	12:LC:160:ARG:NH2	2.33	0.61
11:LB:124:ASP:OD1	11:LB:125:GLN:N	2.34	0.61
5:L3:2044:U:N3	7:L7:63:ASN:OD1	2.33	0.61
10:LA:163:GLU:OE1	32:NS:276:ARG:NH1	2.34	0.61
11:LB:122:THR:OG1	11:LB:124:ASP:OD1	2.16	0.61
39:SI:143:VAL:O	39:SI:147:VAL:HG12	2.00	0.61
5:L3:957:G:N2	5:L3:1283:G:OP2	2.34	0.61
15:LH:79:PHE:CB	20:LS:36:VAL:HG21	2.31	0.60
28:NK:88:ASP:OD1	28:NK:89:GLN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SW:284:LEU:HD21	51:SW:286:MET:HG3	1.82	0.60
12:LC:81:TRP:CZ3	13:LE:154:ILE:HD12	2.37	0.60
43:SM:189:TYR:CZ	43:SM:202:ILE:HD12	2.35	0.60
47:SR:51:VAL:HG21	47:SR:117:MET:HE1	1.84	0.60
48:SS:233:ILE:HD11	51:SW:607:PRO:HD3	1.84	0.60
14:LG:27:ASN:OD1	14:LG:28:CYS:N	2.34	0.60
21:LT:40:GLU:OE2	21:LT:109:ARG:NH2	2.35	0.59
39:SI:177:THR:HG23	48:SS:355:ALA:HB3	1.84	0.59
27:NI:307:LEU:HD21	27:NI:311:LEU:HD23	1.85	0.59
47:SR:188:VAL:HG23	47:SR:189:THR:HG23	1.83	0.59
5:L3:206:U:O2'	5:L3:208:A:N7	2.30	0.59
30:NO:182:ALA:O	34:SC:46:ARG:NH1	2.35	0.59
39:SI:101:ARG:NH1	39:SI:122:LYS:O	2.36	0.59
39:SI:112:VAL:O	39:SI:116:ILE:HD12	2.02	0.59
41:SK:6:SER:OG	41:SK:208:LEU:HD13	2.02	0.59
43:SM:170:HIS:HB3	43:SM:283:LEU:HD11	1.85	0.59
14:LG:68:GLY:O	14:LG:73:ARG:NH1	2.36	0.59
14:LG:40:ILE:CD1	14:LG:64:THR:HG23	2.32	0.58
33:SA:84:THR:OG1	33:SA:87:SER:OG	2.07	0.58
51:SW:285:ILE:HD11	51:SW:298:LEU:HD21	1.85	0.58
5:L3:402:A:O2'	32:NS:103:LYS:O	2.21	0.58
44:SN:147:MET:HE3	45:SO:157:ASN:HB2	1.85	0.58
14:LG:42:VAL:HG13	14:LG:45:ILE:HG22	1.86	0.58
9:L9:103:GLU:OE2	9:L9:165:THR:HG21	2.04	0.58
12:LC:84:TYR:HE1	12:LC:93:MET:HE3	1.67	0.58
5:L3:404:U:O3'	16:LI:87:ARG:NH2	2.37	0.58
21:LT:33:VAL:HG23	21:LT:38:GLU:HB2	1.85	0.58
32:NS:176:ARG:NH2	34:SC:231:GLU:O	2.35	0.58
5:L3:2334:C:OP2	33:SA:195:LYS:NZ	2.33	0.58
29:NM:159:ASP:OD2	32:NS:305:ILE:HD11	2.04	0.58
14:LG:64:THR:HG22	14:LG:76:VAL:HG22	1.86	0.58
5:L3:4437:U:OP2	25:NF:107:LYS:NZ	2.28	0.57
19:LQ:131:SER:N	32:NS:201:ASP:OD2	2.37	0.57
5:L3:1659:U:H2'	17:LK:15:VAL:HG23	1.87	0.57
5:L3:4706:G:OP1	28:NK:12:LYS:NZ	2.37	0.56
19:LQ:118:LEU:HD12	29:NM:119:TYR:HE1	1.69	0.56
5:L3:2851:G:N2	27:NI:754:GLU:O	2.38	0.56
40:SJ:666:GLU:OE1	48:SS:208:GLN:NE2	2.36	0.56
45:SO:53:LYS:NZ	48:SS:155:ASP:OD2	2.37	0.56
5:L3:1950:U:O2'	12:LC:116:ARG:NH1	2.38	0.56
43:SM:207:PHE:CD2	48:SS:355:ALA:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SZ:56:MET:HG2	53:SZ:93:VAL:HG21	1.87	0.56
47:SR:269:LEU:HD12	47:SR:306:ILE:HG23	1.88	0.56
41:SK:2:ALA:HB3	41:SK:215:LEU:HD11	1.87	0.56
43:SM:47:GLU:OE1	43:SM:47:GLU:N	2.38	0.56
26:NH:154:ARG:O	26:NH:154:ARG:NH1	2.39	0.56
29:NM:163:GLU:OE1	32:NS:303:VAL:HG13	2.05	0.56
19:LQ:118:LEU:HD12	29:NM:119:TYR:CE1	2.40	0.55
8:L8:32:ASP:OD2	8:L8:33:GLN:N	2.36	0.55
1:BA:128:THR:O	1:BA:132:ILE:HD12	2.05	0.55
1:BA:138:SER:HG	5:L3:2002:A:N6	2.04	0.55
3:L1:74:U:O4	16:LI:72:GLN:NE2	2.37	0.55
6:L6:21:ARG:NH1	9:L9:197:THR:OG1	2.40	0.55
41:SK:101:LEU:HB3	41:SK:107:VAL:HG21	1.88	0.55
25:NF:115:GLY:O	27:NI:532:LYS:NZ	2.39	0.55
5:L3:5000:G:O3'	18:LN:382:MET:HE1	2.07	0.55
48:SS:383:VAL:HG21	48:SS:388:LEU:HD11	1.88	0.55
5:L3:4478:G:N2	5:L3:4608:G:O2'	2.40	0.55
5:L3:4763:U:HO2'	12:LC:174:THR:HG1	1.51	0.54
9:L9:46:ASP:OD1	9:L9:47:LYS:N	2.40	0.54
10:LA:155:GLN:OE1	32:NS:298:ARG:NH1	2.41	0.54
30:NO:151:MET:HE3	30:NO:196:PRO:HB2	1.89	0.54
33:SA:204:ARG:NH1	33:SA:205:ARG:O	2.40	0.54
37:SG:86:LEU:HD22	37:SG:188:GLN:O	2.07	0.54
4:L2:66:A:OP2	38:SH:168:LYS:NZ	2.40	0.54
5:L3:4437:U:O2'	47:SR:143:ARG:NH2	2.41	0.54
51:SW:412:ARG:NH2	51:SW:501:ASP:OD1	2.40	0.54
34:SC:201:ILE:HD11	34:SC:267:LEU:HD21	1.90	0.53
51:SW:284:LEU:HD23	51:SW:285:ILE:N	2.23	0.53
5:L3:2562:G:O2'	5:L3:2565:A:N6	2.40	0.53
5:L3:4672:A:OP1	14:LG:17:SER:OG	2.11	0.53
44:SN:119:VAL:HG21	45:SO:165:LEU:HD13	1.89	0.53
5:L3:2269:C:O2'	29:NM:13:ASN:ND2	2.42	0.53
24:NB:1:MET:CE	25:NF:43:ILE:HD12	2.38	0.53
26:NH:57:ASN:HD22	52:SY:451:VAL:HG12	1.72	0.53
5:L3:364:G:O6	23:LW:55:ARG:NH2	2.41	0.53
18:LN:139:ASP:OD1	18:LN:140:GLU:N	2.42	0.53
31:NQ:91:ARG:NE	31:NQ:105:ASP:OD2	2.41	0.53
37:SG:128:MET:HA	37:SG:128:MET:HE2	1.90	0.53
52:SY:429:LEU:HD12	52:SY:439:ILE:HD11	1.91	0.53
12:LC:76:LYS:NZ	12:LC:100:LEU:O	2.37	0.53
5:L3:1354:A:HO2'	17:LK:61:TYR:HH	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LC:82:LEU:HD12	12:LC:124:ILE:HG23	1.91	0.53
18:LN:218:ASP:OD2	18:LN:348:ARG:NH2	2.40	0.52
47:SR:441:TYR:OH	50:SV:97:GLU:OE2	2.21	0.52
36:SE:218:LEU:O	36:SE:222:ILE:HD12	2.09	0.52
47:SR:348:MET:HA	47:SR:348:MET:HE3	1.92	0.52
52:SY:579:PHE:HE2	52:SY:581:ILE:HD11	1.73	0.52
5:L3:1447:C:O5'	30:NO:323:ARG:NH2	2.42	0.52
33:SA:180:ILE:HD11	33:SA:227:ILE:HD11	1.92	0.52
31:NQ:52:THR:OG1	31:NQ:95:GLN:OE1	2.23	0.52
39:SI:171:ASN:O	39:SI:171:ASN:ND2	2.35	0.52
46:SQ:45:VAL:HG23	46:SQ:45:VAL:O	2.09	0.52
47:SR:107:ASP:OD1	47:SR:108:ASN:N	2.42	0.52
18:LN:95:THR:OG1	18:LN:98:GLY:O	2.16	0.52
5:L3:1859:C:OP1	24:NB:26:ARG:NH1	2.43	0.51
5:L3:4763:U:O2'	12:LC:174:THR:OG1	2.19	0.51
5:L3:4962:C:O2	28:NK:92:GLN:NE2	2.43	0.51
5:L3:1516:G:O2'	6:L6:17:ASP:OD1	2.21	0.51
5:L3:4567:G:O2'	5:L3:4981:G:N7	2.39	0.51
5:L3:4872:G:O6	8:L8:98:ARG:NH1	2.44	0.51
41:SK:174:SER:O	41:SK:178:GLN:N	2.42	0.51
1:BA:14:TYR:C	1:BA:15:LEU:HD12	2.35	0.51
34:SC:50:LEU:O	34:SC:54:ILE:N	2.44	0.51
25:NF:217:GLY:HA3	44:SN:196:MET:HE1	1.93	0.51
31:NQ:1:MET:SD	31:NQ:2:ALA:N	2.83	0.51
1:BA:123:ARG:NH2	46:SQ:63:SER:O	2.44	0.51
9:L9:149:GLN:O	9:L9:152:THR:OG1	2.26	0.51
20:LS:23:ASP:OD1	20:LS:24:LEU:N	2.44	0.51
31:NQ:27:ARG:O	31:NQ:29:GLN:NE2	2.44	0.50
5:L3:72:C:N3	6:L6:60:ARG:NH2	2.60	0.50
5:L3:2267:U:OP1	29:NM:41:ARG:N	2.45	0.50
31:NQ:64:ASP:O	31:NQ:66:THR:N	2.45	0.50
43:SM:575:ALA:O	43:SM:578:SER:OG	2.23	0.50
26:NH:114:LEU:O	26:NH:117:GLY:N	2.44	0.50
51:SW:205:ILE:HD13	51:SW:388:VAL:HG21	1.93	0.50
44:SN:73:THR:HG23	44:SN:73:THR:O	2.12	0.50
52:SY:287:LYS:NZ	52:SY:522:GLU:OE1	2.26	0.50
52:SY:314:THR:HG22	52:SY:324:LEU:HD23	1.94	0.50
7:L7:14:HIS:CE1	7:L7:119:VAL:HG23	2.47	0.50
33:SA:209:ILE:HB	33:SA:229:LEU:HD13	1.93	0.50
52:SY:338:LEU:HD13	52:SY:347:VAL:HG22	1.94	0.50
5:L3:1283:G:H5'	33:SA:313:VAL:HG13	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LI:106:ILE:HG21	16:LI:109:LEU:HD23	1.93	0.49
27:NI:597:ASP:OD2	47:SR:94:LEU:HD22	2.12	0.49
47:SR:356:VAL:HG12	47:SR:356:VAL:O	2.11	0.49
51:SW:327:LEU:HD23	51:SW:354:LEU:HD23	1.94	0.49
10:LA:47:TYR:OH	10:LA:57:CYS:O	2.26	0.49
19:LQ:12:ILE:HD11	19:LQ:69:MET:HE3	1.94	0.49
30:NO:63:MET:HE3	30:NO:117:LYS:HB2	1.94	0.49
5:L3:709:C:OP1	21:LT:89:ARG:NH2	2.46	0.49
5:L3:4405:G:OP2	47:SR:130:LYS:NZ	2.31	0.49
5:L3:4895:C:O3'	8:L8:132:LYS:NZ	2.46	0.49
22:LU:71:LYS:NZ	48:SS:127:SEP:O3P	2.37	0.49
44:SN:142:LYS:NZ	45:SO:154:MET:O	2.44	0.49
48:SS:315:ASN:OD1	48:SS:346:LYS:NZ	2.23	0.49
4:L2:49:G:H1'	39:SI:76:VAL:HG21	1.95	0.49
29:NM:13:ASN:OD1	29:NM:14:LYS:N	2.45	0.49
20:LS:27:GLU:O	20:LS:31:LEU:HD23	2.13	0.49
33:SA:84:THR:HG1	33:SA:87:SER:HG	1.48	0.49
43:SM:36:ARG:NH2	43:SM:114:TYR:OH	2.41	0.49
4:L2:93:C:HO2'	4:L2:94:U:P	2.36	0.49
12:LC:99:ASP:OD1	12:LC:100:LEU:N	2.45	0.49
52:SY:565:SER:O	52:SY:567:ARG:NH1	2.45	0.49
18:LN:219:VAL:HG11	18:LN:337:VAL:CG2	2.43	0.48
41:SK:175:SER:O	47:SR:368:ARG:NH2	2.45	0.48
47:SR:225:ILE:HD11	47:SR:241:ILE:HD11	1.95	0.48
3:L1:83:C:H42	16:LI:50:ARG:CZ	2.26	0.48
5:L3:4678:G:N7	28:NK:11:ARG:NH2	2.60	0.48
5:L3:5047:C:O2'	5:L3:5050:C:OP2	2.25	0.48
29:NM:23:THR:OG1	29:NM:26:GLN:O	2.24	0.48
37:SG:134:CYS:SG	37:SG:144:LEU:HD11	2.54	0.48
5:L3:369:G:N2	5:L3:372:A:OP2	2.40	0.48
5:L3:1502:G:OP1	11:LB:65:ARG:NH1	2.46	0.48
27:NI:231:ALA:O	27:NI:235:SER:N	2.47	0.48
1:BA:37:LEU:HD11	1:BA:69:ALA:HB2	1.96	0.48
5:L3:1434:G:OP1	24:NB:371:ARG:NH1	2.42	0.48
5:L3:5066:U:OP1	10:LA:43:LYS:NZ	2.45	0.48
47:SR:225:ILE:CD1	47:SR:241:ILE:HD11	2.44	0.48
5:L3:2485:U:O2'	43:SM:216:ASP:OD2	2.30	0.48
5:L3:4483:C:H5''	47:SR:21:LEU:HD13	1.95	0.48
41:SK:2:ALA:CB	41:SK:215:LEU:HD11	2.44	0.48
30:NO:316:THR:O	30:NO:321:ARG:NH1	2.47	0.48
27:NI:462:THR:HB	27:NI:479:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:SA:65:GLU:OE1	33:SA:80:ARG:NH1	2.47	0.47
44:SN:131:LYS:NZ	45:SO:223:ILE:O	2.47	0.47
4:L2:93:C:O2'	4:L2:94:U:O5'	2.23	0.47
26:NH:152:ASP:O	26:NH:156:VAL:HG13	2.14	0.47
41:SK:108:THR:HG21	41:SK:129:LEU:HD11	1.95	0.47
5:L3:4910:G:H4'	18:LN:95:THR:HG22	1.96	0.47
24:NB:1:MET:HE3	25:NF:43:ILE:HD12	1.95	0.47
25:NF:97:SER:OG	25:NF:98:ARG:N	2.48	0.47
51:SW:336:ASP:HA	51:SW:339:LEU:HD12	1.95	0.47
52:SY:335:LEU:HD22	52:SY:346:LEU:HB3	1.97	0.47
13:LE:116:LYS:HG3	13:LE:128:LEU:HD11	1.96	0.47
51:SW:284:LEU:HD23	51:SW:284:LEU:C	2.39	0.47
5:L3:1358:G:O2'	5:L3:1360:G:O6	2.30	0.47
12:LC:19:THR:HG23	12:LC:22:CYS:H	1.80	0.47
26:NH:65:SER:OG	52:SY:439:ILE:HD12	2.15	0.47
5:L3:4726:G:OP2	28:NK:98:ASN:ND2	2.48	0.47
1:BA:103:ASN:OD1	1:BA:104:ILE:N	2.48	0.46
5:L3:40:G:OP2	44:SN:153:LYS:NZ	2.48	0.46
5:L3:4401:G:OP1	24:NB:24:LYS:NZ	2.45	0.46
14:LG:57:VAL:HA	14:LG:81:VAL:HG13	1.97	0.46
47:SR:225:ILE:HG23	47:SR:271:LEU:HD21	1.96	0.46
5:L3:47:A:OP2	6:L6:20:ARG:NH1	2.47	0.46
5:L3:2000:G:O2'	5:L3:2017:A:N1	2.44	0.46
5:L3:4434:C:O4'	25:NF:191:THR:HG23	2.14	0.46
5:L3:4724:A:O2'	18:LN:104:THR:HG22	2.15	0.46
15:LH:30:LYS:O	36:SE:89:ARG:NH1	2.47	0.46
27:NI:475:GLY:O	27:NI:479:MET:HE3	2.15	0.46
5:L3:1726:U:H5'	35:SD:135:ILE:HD11	1.96	0.46
42:SL:123:ILE:HD11	42:SL:191:SER:HA	1.97	0.46
5:L3:4993:G:H22	5:L3:5058:A:H2	1.63	0.46
5:L3:4046:A:N1	52:SY:558:ARG:NH2	2.64	0.46
33:SA:210:ILE:HG21	33:SA:252:TRP:CZ3	2.51	0.46
34:SC:235:THR:O	34:SC:235:THR:HG23	2.15	0.46
5:L3:4910:G:N2	7:L7:106:ASP:O	2.48	0.46
5:L3:4347:G:O2'	5:L3:4348:A:O5'	2.29	0.46
41:SK:222:PHE:O	41:SK:224:LEU:N	2.49	0.46
5:L3:68:U:OP1	9:L9:178:HIS:ND1	2.44	0.46
5:L3:346:G:OP1	16:LI:8:THR:HG23	2.15	0.46
21:LT:43:LEU:O	21:LT:109:ARG:NH1	2.49	0.46
27:NI:422:PHE:O	27:NI:426:VAL:HG22	2.16	0.46
39:SI:183:GLU:O	39:SI:187:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:28:C:OP2	9:L9:193:ARG:NH2	2.49	0.46
5:L3:223:G:O2'	5:L3:225:G:OP2	2.33	0.46
5:L3:4697:U:OP1	25:NF:25:ARG:NH2	2.49	0.46
39:SI:171:ASN:HD22	39:SI:171:ASN:C	2.22	0.46
44:SN:68:GLU:O	45:SO:163:ARG:NH2	2.49	0.46
48:SS:145:ASP:O	48:SS:161:LYS:NZ	2.49	0.45
22:LU:58:MET:HE2	22:LU:90:LEU:HD22	1.98	0.45
43:SM:215:VAL:HG23	48:SS:364:PHE:CG	2.51	0.45
46:SQ:185:GLU:N	46:SQ:185:GLU:OE2	2.49	0.45
21:LT:33:VAL:HG13	21:LT:33:VAL:O	2.16	0.45
43:SM:573:ASP:O	43:SM:577:ARG:NE	2.43	0.45
31:NQ:197:LYS:C	31:NQ:198:LEU:HD12	2.42	0.45
5:L3:4903:G:OP1	28:NK:82:ASN:ND2	2.44	0.45
22:LU:74:LYS:HD3	45:SO:109:MET:HE1	1.98	0.45
44:SN:62:ARG:NH1	45:SO:58:ASN:OD1	2.50	0.45
47:SR:295:ARG:O	47:SR:299:LEU:HD13	2.17	0.45
51:SW:429:MET:SD	51:SW:479:LEU:HD23	2.56	0.45
5:L3:244:G:O6	53:SZ:20:LYS:NZ	2.48	0.45
5:L3:730:G:OP2	35:SD:76:ARG:NE	2.50	0.45
5:L3:2562:G:N2	5:L3:2565:A:OP2	2.49	0.45
47:SR:348:MET:HE3	47:SR:353:VAL:HG11	1.98	0.45
52:SY:287:LYS:O	52:SY:291:LEU:HD23	2.16	0.44
5:L3:182:G:N7	45:SO:339:ARG:NH1	2.65	0.44
5:L3:4768:G:OP1	7:L7:168:TYR:OH	2.27	0.44
11:LB:27:LEU:HB2	33:SA:284:MET:HE1	1.98	0.44
33:SA:140:LYS:O	33:SA:204:ARG:NH2	2.49	0.44
47:SR:289:ASN:OD1	47:SR:290:LYS:N	2.48	0.44
11:LB:27:LEU:CB	33:SA:284:MET:HE1	2.47	0.44
32:NS:160:CYS:SG	32:NS:198:ILE:HD12	2.57	0.44
29:NM:71:ALA:HA	29:NM:77:LEU:HD13	1.98	0.44
37:SG:63:ASN:ND2	37:SG:66:GLU:OE2	2.51	0.44
5:L3:45:U:O2'	6:L6:14:PHE:O	2.20	0.44
5:L3:171:U:O4	53:SZ:157:ARG:NH1	2.49	0.44
5:L3:1295:C:O2'	32:NS:157:VAL:HG11	2.17	0.44
14:LG:109:LYS:HE3	27:NI:503:LEU:HD22	1.98	0.44
36:SE:58:PRO:HG2	36:SE:61:ILE:HD12	1.98	0.44
5:L3:1346:C:OP1	11:LB:148:VAL:HG12	2.17	0.44
5:L3:1364:U:OP2	6:L6:36:ARG:NH1	2.44	0.44
21:LT:37:ASP:OD1	21:LT:38:GLU:N	2.50	0.44
5:L3:740:G:H2'	5:L3:741:C:N1	2.33	0.44
5:L3:958:G:N2	5:L3:1285:U:OP1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:4745:G:H22	5:L3:4955:A:H2	1.66	0.44
5:L3:4479:A:OP1	5:L3:4610:A:O2'	2.35	0.44
24:NB:350:VAL:HG13	24:NB:355:VAL:O	2.17	0.44
8:L8:105:THR:HG22	8:L8:106:ASP:N	2.33	0.43
31:NQ:113:HIS:CD2	31:NQ:124:LEU:HD21	2.53	0.43
47:SR:101:ILE:HG22	47:SR:105:LEU:HD13	2.00	0.43
5:L3:358:C:O2	53:SZ:5:LYS:NZ	2.51	0.43
26:NH:29:ASP:OD1	49:ST:269:LEU:HD11	2.18	0.43
5:L3:265:C:N4	53:SZ:154:VAL:HG21	2.32	0.43
18:LN:312:LYS:NZ	18:LN:380:GLN:OE1	2.50	0.43
30:NO:99:PHE:CD2	30:NO:125:VAL:HG11	2.53	0.43
41:SK:231:THR:O	41:SK:234:THR:OG1	2.30	0.43
45:SO:62:ILE:HD12	45:SO:87:HIS:NE2	2.33	0.43
34:SC:278:THR:HG22	34:SC:279:ASN:N	2.33	0.43
52:SY:512:LEU:HD23	52:SY:513:VAL:N	2.32	0.43
29:NM:42:SER:O	29:NM:48:ASN:ND2	2.51	0.43
5:L3:4569:U:N3	5:L3:4570:G:O6	2.50	0.43
5:L3:1669:A:H2'	5:L3:1670:G:O4'	2.19	0.43
14:LG:96:LEU:HD11	50:SV:22:VAL:HG23	2.01	0.43
33:SA:210:ILE:HD13	33:SA:230:LEU:HB2	1.98	0.43
5:L3:291:U:O2'	9:L9:182:HIS:NE2	2.45	0.43
5:L3:1428:U:OP1	11:LB:42:THR:HG21	2.18	0.43
7:L7:16:LEU:HD21	7:L7:83:THR:HG21	2.00	0.43
46:SQ:65:MET:CG	46:SQ:103:LEU:HD13	2.49	0.43
18:LN:219:VAL:HG11	18:LN:337:VAL:HG21	1.99	0.43
39:SI:153:ASN:ND2	43:SM:267:LEU:HD12	2.34	0.43
5:L3:4180:G:N2	26:NH:57:ASN:OD1	2.52	0.43
18:LN:352:LEU:HD23	18:LN:352:LEU:H	1.83	0.43
27:NI:307:LEU:HD23	27:NI:308:ASN:N	2.33	0.43
44:SN:115:ALA:O	44:SN:119:VAL:HG22	2.19	0.43
46:SQ:42:ILE:HD11	46:SQ:92:VAL:HG13	2.01	0.43
5:L3:911:U:H2'	5:L3:912:G:O4'	2.18	0.42
11:LB:42:THR:O	11:LB:42:THR:HG22	2.18	0.42
48:SS:316:PRO:O	48:SS:346:LYS:NZ	2.49	0.42
51:SW:316:MET:HE3	51:SW:353:LEU:HD12	1.99	0.42
5:L3:85:G:O2'	5:L3:97:G:O6	2.29	0.42
5:L3:2268:A:OP1	29:NM:8:TRP:NE1	2.44	0.42
41:SK:44:ASP:OD1	41:SK:45:THR:N	2.52	0.42
47:SR:348:MET:CE	47:SR:353:VAL:HG11	2.49	0.42
51:SW:347:LEU:HD23	51:SW:374:LEU:HD11	2.01	0.42
5:L3:425:U:OP1	10:LA:37:LYS:NZ	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LN:67:VAL:O	18:LN:67:VAL:HG12	2.20	0.42
27:NI:485:GLN:NE2	27:NI:489:ASP:OD1	2.52	0.42
31:NQ:192:LEU:HD12	31:NQ:197:LYS:HB2	2.00	0.42
39:SI:98:PHE:HB2	39:SI:152:PRO:HG3	2.00	0.42
43:SM:414:PHE:O	43:SM:417:VAL:HG22	2.18	0.42
5:L3:151:G:OP2	9:L9:4:TYR:OH	2.26	0.42
5:L3:4569:U:H4'	10:LA:79:THR:HG21	2.00	0.42
42:SL:64:LEU:HD23	42:SL:255:THR:HG22	2.02	0.42
51:SW:541:LEU:HD13	51:SW:548:LEU:HD21	2.01	0.42
5:L3:2296:G:O2'	33:SA:242:PRO:O	2.36	0.42
5:L3:4543:G:N7	26:NH:15:LYS:NZ	2.61	0.42
29:NM:87:TYR:CZ	29:NM:91:LEU:HD11	2.55	0.42
32:NS:135:TYR:O	32:NS:269:HIS:NE2	2.50	0.42
5:L3:4977:A:O2'	18:LN:21:ARG:NH2	2.52	0.42
5:L3:4978:G:H22	18:LN:229:LYS:HE3	1.85	0.42
14:LG:84:GLN:NE2	14:LG:86:LYS:O	2.53	0.42
33:SA:35:ASP:OD1	33:SA:35:ASP:N	2.52	0.42
41:SK:155:SER:OG	41:SK:156:ASN:N	2.53	0.42
5:L3:1955:G:OP2	24:NB:52:ASN:ND2	2.53	0.42
26:NH:179:LEU:O	26:NH:180:THR:OG1	2.35	0.42
36:SE:207:VAL:HG21	36:SE:215:LEU:HD22	2.02	0.42
3:L1:102:G:OP2	3:L1:104:A:O2'	2.30	0.41
5:L3:4464:A:N7	47:SR:32:THR:OG1	2.45	0.41
12:LC:69:GLU:OE2	12:LC:76:LYS:NZ	2.51	0.41
19:LQ:114:ARG:NH1	29:NM:119:TYR:OH	2.53	0.41
36:SE:165:GLU:OE2	36:SE:165:GLU:N	2.53	0.41
5:L3:447:C:H2'	5:L3:448:G:O4'	2.20	0.41
5:L3:4354:U:OP1	52:SY:534:LYS:NZ	2.45	0.41
8:L8:118:MET:HE2	8:L8:118:MET:HA	2.02	0.41
16:LI:127:GLN:HA	16:LI:127:GLN:OE1	2.21	0.41
31:NQ:298:ILE:O	31:NQ:298:ILE:HG22	2.19	0.41
34:SC:281:ILE:HG23	34:SC:286:LEU:HD21	2.01	0.41
51:SW:255:LEU:HD21	51:SW:312:LEU:HD21	2.02	0.41
4:L2:61:C:C2	42:SL:50:ARG:NH1	2.89	0.41
6:L6:94:ILE:O	6:L6:94:ILE:HG22	2.20	0.41
14:LG:45:ILE:HD13	14:LG:54:ALA:HB2	2.02	0.41
22:LU:7:MET:HE3	22:LU:8:ALA:O	2.20	0.41
36:SE:177:MET:CE	48:SS:236:VAL:HG23	2.50	0.41
12:LC:84:TYR:CE1	12:LC:93:MET:HE3	2.53	0.41
14:LG:67:LYS:HA	14:LG:73:ARG:HD3	2.02	0.41
31:NQ:252:ALA:HB1	31:NQ:261:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SY:391:MET:HE1	52:SY:444:GLY:O	2.21	0.41
11:LB:23:ILE:HD11	33:SA:32:ILE:O	2.21	0.41
42:SL:82:LEU:HB2	42:SL:203:LEU:HD13	2.01	0.41
11:LB:91:ARG:O	17:LK:65:ARG:NH1	2.53	0.41
39:SI:78:LEU:HD13	39:SI:111:LEU:HD23	2.03	0.41
47:SR:292:ASP:OD1	47:SR:293:VAL:N	2.53	0.41
5:L3:2569:G:OP1	43:SM:560:ARG:NH1	2.51	0.41
6:L6:100:PRO:O	22:LU:25:ARG:NH2	2.50	0.41
9:L9:31:ARG:NH1	40:SJ:708:GLU:OE2	2.53	0.41
39:SI:116:ILE:HD12	39:SI:116:ILE:H	1.84	0.41
39:SI:192:ILE:HD11	43:SM:380:ARG:HE	1.86	0.41
46:SQ:175:VAL:O	46:SQ:186:GLN:NE2	2.53	0.41
51:SW:284:LEU:HD21	51:SW:286:MET:HE2	2.03	0.41
51:SW:332:ILE:HB	51:SW:362:LEU:HD12	2.02	0.41
5:L3:180:C:N3	45:SO:339:ARG:NH1	2.69	0.41
5:L3:2340:C:H4'	33:SA:42:THR:HG23	2.03	0.41
26:NH:137:ALA:O	26:NH:139:ILE:N	2.54	0.41
31:NQ:11:VAL:HG22	31:NQ:319:LEU:HD12	2.02	0.41
37:SG:118:LEU:HD11	37:SG:167:VAL:HG22	2.03	0.41
42:SL:125:THR:HG21	42:SL:198:ILE:HD13	2.03	0.41
43:SM:215:VAL:HG22	43:SM:220:MET:HE2	2.03	0.41
52:SY:354:PRO:O	52:SY:358:THR:HG23	2.21	0.41
52:SY:572:HIS:CD2	52:SY:573:THR:HG23	2.56	0.41
5:L3:3903:A:H2'	5:L3:3904:G:O4'	2.21	0.41
5:L3:4405:G:O6	47:SR:24:SER:OG	2.38	0.41
5:L3:1337:A:N1	5:L3:1658:G:O2'	2.47	0.40
52:SY:335:LEU:HD23	52:SY:347:VAL:O	2.20	0.40
30:NO:151:MET:HE1	30:NO:197:PHE:CE1	2.55	0.40
31:NQ:139:ASP:OD2	31:NQ:142:HIS:ND1	2.34	0.40
46:SQ:65:MET:HG2	46:SQ:103:LEU:HD13	2.03	0.40
5:L3:1879:C:H2'	5:L3:1880:G:O4'	2.21	0.40
5:L3:2486:G:OP2	39:SI:36:LYS:NZ	2.50	0.40
5:L3:4691:A:O2'	37:SG:68:ALA:O	2.36	0.40
31:NQ:277:CYS:SG	31:NQ:284:LEU:HD13	2.62	0.40
42:SL:254:LYS:NZ	42:SL:255:THR:O	2.45	0.40
49:ST:231:SER:O	49:ST:232:VAL:HG12	2.21	0.40
5:L3:1325:C:O2	40:SJ:833:ARG:NH1	2.47	0.40
5:L3:2052:G:O2'	5:L3:2057:A:N1	2.43	0.40
5:L3:2266:C:O2	5:L3:2266:C:H2'	2.21	0.40
43:SM:362:ILE:HG22	43:SM:363:GLY:N	2.36	0.40
5:L3:67:C:OP2	5:L3:312:G:N2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1996:C:O2	46:SQ:54:LYS:NZ	2.55	0.40
14:LG:45:ILE:HD13	14:LG:54:ALA:CB	2.52	0.40
14:LG:109:LYS:HG3	27:NI:503:LEU:HD22	2.03	0.40
48:SS:381:VAL:HG12	48:SS:383:VAL:HG13	2.04	0.40
51:SW:336:ASP:OD1	51:SW:337:ARG:N	2.55	0.40
52:SY:283:PHE:CZ	52:SY:484:ILE:HD12	2.56	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%)	157 (99%)	1 (1%)	0	100	100
2	BB	211/217 (97%)	206 (98%)	5 (2%)	0	100	100
6	L6	118/211 (56%)	116 (98%)	2 (2%)	0	100	100
7	L7	197/203 (97%)	195 (99%)	2 (1%)	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%)	156 (100%)	0	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
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%)	126 (98%)	3 (2%)	0	100	100
16	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
17	LK	104/148 (70%)	100 (96%)	4 (4%)	0	100	100
18	LN	352/403 (87%)	347 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	LQ	131/135 (97%)	131 (100%)	0	0	100	100
20	LS	120/123 (98%)	120 (100%)	0	0	100	100
21	LT	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
22	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
23	LW	72/97 (74%)	72 (100%)	0	0	100	100
24	NB	379/549 (69%)	375 (99%)	4 (1%)	0	100	100
25	NF	195/260 (75%)	193 (99%)	2 (1%)	0	100	100
26	NH	178/180 (99%)	176 (99%)	2 (1%)	0	100	100
27	NI	590/881 (67%)	585 (99%)	5 (1%)	0	100	100
28	NK	63/129 (49%)	63 (100%)	0	0	100	100
29	NM	180/300 (60%)	180 (100%)	0	0	100	100
30	NO	301/461 (65%)	300 (100%)	1 (0%)	0	100	100
31	NQ	320/385 (83%)	316 (99%)	4 (1%)	0	100	100
32	NS	303/349 (87%)	297 (98%)	6 (2%)	0	100	100
33	SA	358/427 (84%)	354 (99%)	4 (1%)	0	100	100
34	SC	193/288 (67%)	190 (98%)	3 (2%)	0	100	100
35	SD	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
36	SE	183/266 (69%)	181 (99%)	2 (1%)	0	100	100
37	SG	189/192 (98%)	185 (98%)	4 (2%)	0	100	100
38	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
39	SI	225/255 (88%)	221 (98%)	4 (2%)	0	100	100
40	SJ	95/847 (11%)	95 (100%)	0	0	100	100
41	SK	242/245 (99%)	235 (97%)	7 (3%)	0	100	100
42	SL	241/490 (49%)	233 (97%)	8 (3%)	0	100	100
43	SM	445/588 (76%)	445 (100%)	0	0	100	100
44	SN	169/306 (55%)	169 (100%)	0	0	100	100
45	SO	305/353 (86%)	302 (99%)	3 (1%)	0	100	100
46	SQ	216/239 (90%)	214 (99%)	2 (1%)	0	100	100
47	SR	445/634 (70%)	439 (99%)	6 (1%)	0	100	100
48	SS	250/746 (34%)	241 (96%)	9 (4%)	0	100	100
49	ST	112/365 (31%)	109 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	SV	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
51	SW	440/670 (66%)	433 (98%)	7 (2%)	0	100	100
52	SY	376/812 (46%)	374 (100%)	2 (0%)	0	100	100
53	SZ	156/178 (88%)	154 (99%)	2 (1%)	0	100	100
All	All	10630/15584 (68%)	10496 (99%)	134 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	132/137 (96%)	131 (99%)	1 (1%)	73	90
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
13	LE	51/140 (36%)	51 (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%)	124 (100%)	0	100	100
17	LK	29/121 (24%)	29 (100%)	0	100	100
18	LN	313/348 (90%)	313 (100%)	0	100	100
19	LQ	119/121 (98%)	119 (100%)	0	100	100
20	LS	109/110 (99%)	109 (100%)	0	100	100
21	LT	88/89 (99%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	LU	86/89 (97%)	86 (100%)	0	100	100
23	LW	63/80 (79%)	63 (100%)	0	100	100
24	NB	142/485 (29%)	142 (100%)	0	100	100
25	NF	180/228 (79%)	180 (100%)	0	100	100
26	NH	155/155 (100%)	155 (100%)	0	100	100
27	NI	267/730 (37%)	267 (100%)	0	100	100
28	NK	61/115 (53%)	61 (100%)	0	100	100
29	NM	168/272 (62%)	168 (100%)	0	100	100
30	NO	269/392 (69%)	269 (100%)	0	100	100
31	NQ	265/318 (83%)	265 (100%)	0	100	100
32	NS	276/305 (90%)	276 (100%)	0	100	100
33	SA	299/348 (86%)	299 (100%)	0	100	100
34	SC	178/252 (71%)	178 (100%)	0	100	100
35	SD	207/215 (96%)	207 (100%)	0	100	100
36	SE	158/223 (71%)	158 (100%)	0	100	100
37	SG	170/171 (99%)	170 (100%)	0	100	100
38	SH	140/274 (51%)	140 (100%)	0	100	100
39	SI	205/228 (90%)	204 (100%)	1 (0%)	81	93
40	SJ	91/733 (12%)	91 (100%)	0	100	100
41	SK	212/213 (100%)	212 (100%)	0	100	100
42	SL	226/437 (52%)	226 (100%)	0	100	100
43	SM	401/509 (79%)	401 (100%)	0	100	100
44	SN	133/260 (51%)	133 (100%)	0	100	100
45	SO	283/319 (89%)	283 (100%)	0	100	100
46	SQ	195/214 (91%)	195 (100%)	0	100	100
47	SR	410/574 (71%)	410 (100%)	0	100	100
48	SS	227/648 (35%)	227 (100%)	0	100	100
49	ST	60/300 (20%)	60 (100%)	0	100	100
50	SV	127/149 (85%)	127 (100%)	0	100	100
51	SW	393/591 (66%)	393 (100%)	0	100	100
52	SY	325/685 (47%)	325 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	SZ	141/158 (89%)	141 (100%)	0	100	100
All	All	8599/13280 (65%)	8597 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	65	GLN
39	SI	171	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	65	GLN
1	BA	156	ASN
6	L6	111	GLN
7	L7	26	GLN
7	L7	96	GLN
8	L8	20	HIS
9	L9	109	HIS
9	L9	201	HIS
10	LA	54	GLN
12	LC	37	HIS
12	LC	108	GLN
13	LE	131	GLN
14	LG	101	ASN
16	LI	96	HIS
17	LK	62	HIS
17	LK	66	ASN
21	LT	99	HIS
22	LU	15	HIS
22	LU	26	HIS
22	LU	36	HIS
27	NI	308	ASN
27	NI	349	HIS
28	NK	101	GLN
29	NM	60	GLN
31	NQ	113	HIS
31	NQ	205	HIS
31	NQ	248	HIS
31	NQ	250	GLN
31	NQ	296	HIS

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Mol	Chain	Res	Type
32	NS	206	ASN
32	NS	293	HIS
32	NS	348	HIS
33	SA	89	GLN
33	SA	142	HIS
33	SA	215	ASN
33	SA	329	ASN
34	SC	136	HIS
34	SC	190	HIS
34	SC	227	HIS
35	SD	126	ASN
35	SD	235	ASN
37	SG	163	GLN
39	SI	66	HIS
39	SI	255	ASN
40	SJ	712	HIS
40	SJ	726	HIS
40	SJ	836	GLN
41	SK	162	HIS
42	SL	46	HIS
42	SL	218	HIS
43	SM	154	HIS
43	SM	375	HIS
43	SM	572	HIS
44	SN	113	GLN
44	SN	124	HIS
44	SN	146	GLN
45	SO	258	HIS
46	SQ	186	GLN
47	SR	37	HIS
47	SR	128	GLN
47	SR	157	HIS
47	SR	209	HIS
47	SR	246	HIS
47	SR	436	HIS
48	SS	186	GLN
49	ST	200	GLN
49	ST	213	GLN
50	SV	115	ASN
51	SW	187	ASN
51	SW	278	HIS
51	SW	593	HIS

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Mol	Chain	Res	Type
52	SY	256	GLN
52	SY	446	GLN
52	SY	574	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L1	150/157 (95%)	19 (12%)	0
4	L2	65/1167 (5%)	9 (13%)	0
5	L3	2089/5070 (41%)	288 (13%)	4 (0%)
All	All	2304/6394 (36%)	316 (13%)	4 (0%)

All (316) 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	82	A
3	L1	83	C
3	L1	84	A
3	L1	86	U
3	L1	94	G
3	L1	103	A
3	L1	105	C
3	L1	110	U
3	L1	111	U
3	L1	114	G
3	L1	153	C
3	L1	156	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

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Mol	Chain	Res	Type
4	L2	96	A
4	L2	101	A
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	108	A
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
5	L3	190	G
5	L3	197	A
5	L3	200	U
5	L3	204	U
5	L3	210	C
5	L3	218	A
5	L3	225	G
5	L3	233	U
5	L3	234	G
5	L3	253	G
5	L3	261	G
5	L3	265	C
5	L3	315	G
5	L3	326	C
5	L3	340	C

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Mol	Chain	Res	Type
5	L3	347	A
5	L3	349	A
5	L3	362	A
5	L3	387	G
5	L3	399	G
5	L3	410	A
5	L3	413	G
5	L3	431	G
5	L3	448	G
5	L3	451	C
5	L3	452	A
5	L3	469	C
5	L3	473	C
5	L3	685	C
5	L3	686	A
5	L3	696	C
5	L3	697	G
5	L3	701	G
5	L3	729	G
5	L3	730	G
5	L3	731	G
5	L3	739	G
5	L3	746	A
5	L3	910	G
5	L3	913	U
5	L3	915	A
5	L3	917	A
5	L3	918	G
5	L3	925	C
5	L3	926	G
5	L3	932	A
5	L3	933	G
5	L3	943	A
5	L3	944	A
5	L3	945	U
5	L3	956	A
5	L3	1284	G
5	L3	1287	G
5	L3	1295	C
5	L3	1296	G
5	L3	1297	U
5	L3	1301	C

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Mol	Chain	Res	Type
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	1434	G
5	L3	1445	U
5	L3	1447	C
5	L3	1502	G
5	L3	1504	G
5	L3	1525	A
5	L3	1654	G
5	L3	1661	C
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	1856	C
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
5	L3	1922	G
5	L3	1925	G
5	L3	1931	C
5	L3	1935	C
5	L3	1936	C
5	L3	1938	C
5	L3	1939	A
5	L3	1941	A
5	L3	1944	A
5	L3	1945	G

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Mol	Chain	Res	Type
5	L3	1969	G
5	L3	1978	C
5	L3	1984	A
5	L3	2002	A
5	L3	2024	G
5	L3	2025	A
5	L3	2026	A
5	L3	2034	G
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	2099	G
5	L3	2100	A
5	L3	2102	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	2345	G
5	L3	2348	G
5	L3	2351	C
5	L3	2364	G
5	L3	2474	G
5	L3	2484	A
5	L3	2485	U
5	L3	2490	U
5	L3	2492	C
5	L3	2493	G
5	L3	2500	U

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Mol	Chain	Res	Type
5	L3	2575	U
5	L3	2769	U
5	L3	2844	A
5	L3	2845	A
5	L3	2848	G
5	L3	2852	U
5	L3	3845	A
5	L3	3853	U
5	L3	3868	G
5	L3	3870	C
5	L3	3875	G
5	L3	3877	A
5	L3	3878	C
5	L3	3879	G
5	L3	3881	G
5	L3	3889	G
5	L3	3892	U
5	L3	3894	A
5	L3	3895	G
5	L3	3897	G
5	L3	3906	A
5	L3	3907	G
5	L3	3908	A
5	L3	3926	C
5	L3	3938	G
5	L3	3939	G
5	L3	3940	U
5	L3	3941	G
5	L3	3942	A
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	4374	U
5	L3	4376	A
5	L3	4380	A

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Mol	Chain	Res	Type
5	L3	4385	A
5	L3	4386	C
5	L3	4390	A
5	L3	4392	G
5	L3	4393	G
5	L3	4398	C
5	L3	4401	G
5	L3	4405	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
5	L3	4491	G
5	L3	4493	U
5	L3	4495	G
5	L3	4496	A
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	4540	C
5	L3	4541	G
5	L3	4545	G
5	L3	4546	A
5	L3	4568	A
5	L3	4584	A
5	L3	4590	A
5	L3	4606	G
5	L3	4608	G
5	L3	4652	G
5	L3	4656	A
5	L3	4670	C

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Mol	Chain	Res	Type
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
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	4914	C
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 (4) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
5	L3	2574	G
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	$\# Z > 2$
48	SEP	SS	127	48	8,9,10	1.56	1 (12%)	7,12,14	1.09	1 (14%)
48	SEP	SS	126	48	8,9,10	1.60	1 (12%)	7,12,14	1.72	2 (28%)
29	AME	NM	1	29	9,10,11	1.52	2 (22%)	9,11,13	1.25	1 (11%)

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
48	SEP	SS	127	48	-	1/6/8/10	-
48	SEP	SS	126	48	-	4/6/8/10	-
29	AME	NM	1	29	-	3/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	SS	126	SEP	P-O1P	3.50	1.61	1.50
48	SS	127	SEP	P-O1P	3.44	1.61	1.50
29	NM	1	AME	CT1-N	3.43	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	NM	1	AME	OT-CT1	-2.03	1.18	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	SS	126	SEP	OG-CB-CA	3.63	111.67	108.14
29	NM	1	AME	CT2-CT1-N	2.21	119.78	116.12
48	SS	126	SEP	OG-P-O1P	2.19	112.35	106.44
48	SS	127	SEP	OG-CB-CA	2.04	110.13	108.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	NM	1	AME	C-CA-CB-CG
48	SS	126	SEP	CB-OG-P-O2P
48	SS	126	SEP	CB-OG-P-O3P
29	NM	1	AME	CA-CB-CG-SD
48	SS	126	SEP	CB-OG-P-O1P
29	NM	1	AME	N-CA-CB-CG
48	SS	127	SEP	N-CA-CB-OG
48	SS	126	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	SS	127	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 67 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
56	ADP	NI	1001	54	28,29,29	1.37	4 (14%)	43,45,45	1.87	10 (23%)
57	SF4	NM	401	29	0,12,12	-	-	-	-	-
58	GDP	SR	1001	54,59	29,30,30	3.01	13 (44%)	45,47,47	2.71	17 (37%)

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
56	ADP	NI	1001	54	-	1/16/32/32	0/3/3/3
57	SF4	NM	401	29	-	-	0/6/5/5
58	GDP	SR	1001	54,59	-	0/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	SR	1001	GDP	O6-C6	8.65	1.40	1.23
58	SR	1001	GDP	C5-N7	6.53	1.52	1.39
58	SR	1001	GDP	C2-N2	4.82	1.45	1.34
58	SR	1001	GDP	PA-O3A	4.60	1.64	1.59
56	NI	1001	ADP	C5-C4	4.45	1.47	1.39
58	SR	1001	GDP	C8-N9	-4.22	1.28	1.37
58	SR	1001	GDP	C4-N9	-3.95	1.28	1.38
58	SR	1001	GDP	C5-C4	3.68	1.48	1.38
58	SR	1001	GDP	C4-N3	2.76	1.40	1.34
56	NI	1001	ADP	C5-C6	2.54	1.48	1.41
58	SR	1001	GDP	PB-O3B	-2.39	1.45	1.54
56	NI	1001	ADP	C8-N7	2.39	1.36	1.31
58	SR	1001	GDP	PB-O2B	-2.38	1.46	1.54
56	NI	1001	ADP	C5-N7	-2.38	1.34	1.39
58	SR	1001	GDP	C2'-C3'	-2.22	1.47	1.53
58	SR	1001	GDP	O4'-C1'	2.09	1.46	1.42
58	SR	1001	GDP	PA-O2A	-2.01	1.46	1.55

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	SR	1001	GDP	C8-N9-C4	8.06	121.14	106.03
58	SR	1001	GDP	N9-C4-N3	6.70	139.36	125.95
58	SR	1001	GDP	C5-C4-N3	-6.66	117.79	128.39
56	NI	1001	ADP	C5-C4-N3	-5.74	118.82	126.72
58	SR	1001	GDP	C2-N3-C4	5.33	121.47	112.30
58	SR	1001	GDP	C6-C5-N7	4.97	139.34	130.29
58	SR	1001	GDP	C4-C5-N7	-4.77	103.11	110.67
56	NI	1001	ADP	N3-C4-N9	4.59	134.98	127.17
56	NI	1001	ADP	C2-N3-C4	3.87	121.27	111.83
56	NI	1001	ADP	N3-C2-N1	-3.79	122.84	128.58
56	NI	1001	ADP	C4-C5-N7	-3.41	106.68	110.58
58	SR	1001	GDP	N9-C8-N7	-3.25	107.37	113.40
56	NI	1001	ADP	C4-N9-C8	2.98	108.87	105.74
58	SR	1001	GDP	C2-N1-C6	-2.96	119.73	125.11
58	SR	1001	GDP	O2B-PB-O3A	2.91	114.38	104.64
58	SR	1001	GDP	O3B-PB-O3A	2.77	113.93	104.64
56	NI	1001	ADP	C5-N7-C8	2.70	107.70	103.45
58	SR	1001	GDP	C3'-C2'-C1'	2.66	106.50	101.46
58	SR	1001	GDP	C5-C6-N1	2.61	119.89	113.25
58	SR	1001	GDP	C1'-N9-C4	-2.57	118.90	126.49
58	SR	1001	GDP	C2'-C3'-C4'	2.57	107.57	102.61
58	SR	1001	GDP	C1'-N9-C8	-2.39	119.94	126.73
56	NI	1001	ADP	N9-C8-N7	-2.39	110.55	113.94
58	SR	1001	GDP	O6-C6-C5	-2.35	120.32	126.53
58	SR	1001	GDP	O2A-PA-O1A	-2.34	101.58	112.44
56	NI	1001	ADP	C6-C5-N7	2.19	136.30	132.09
56	NI	1001	ADP	C2-N1-C6	2.04	122.08	118.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

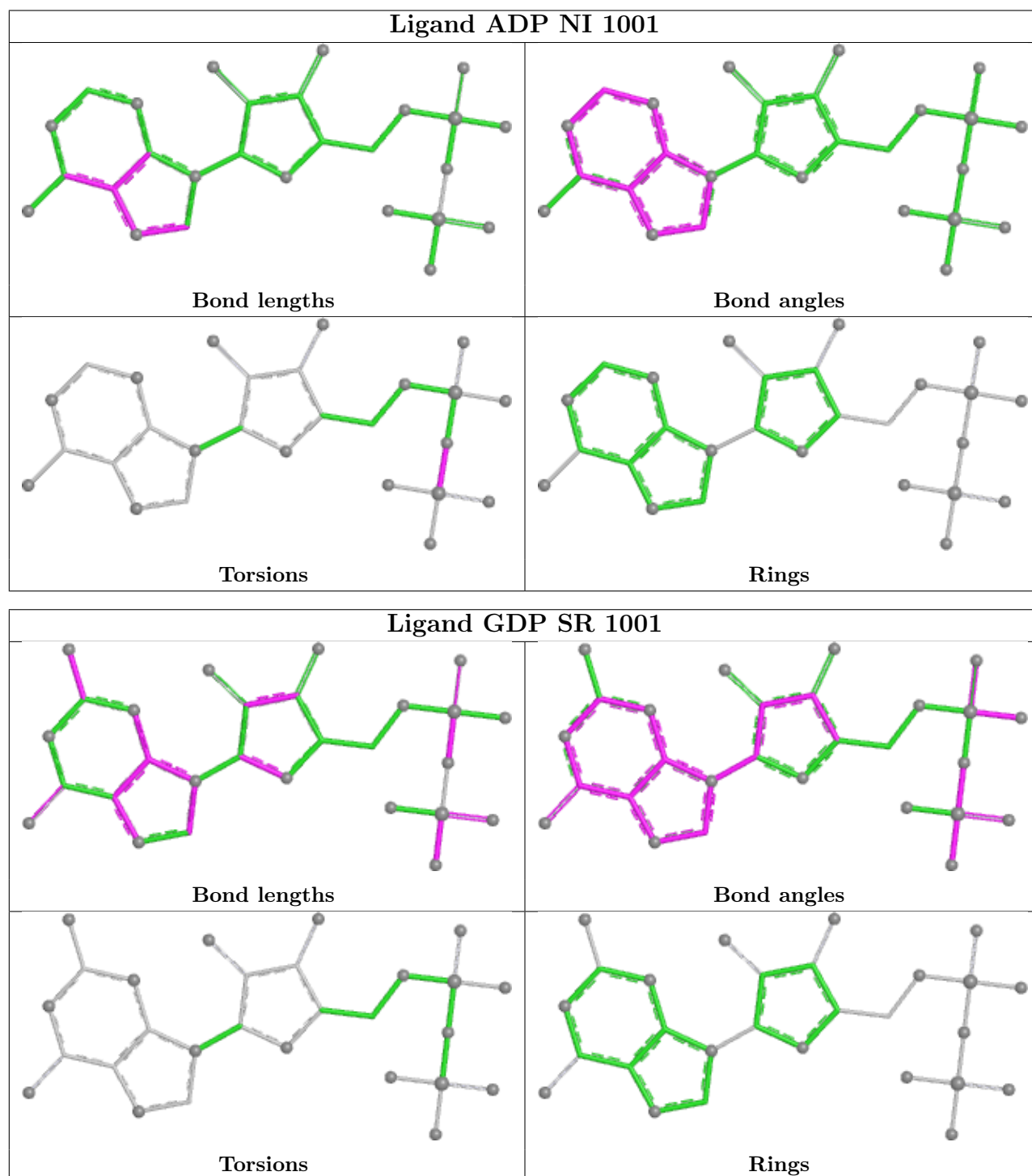
Mol	Chain	Res	Type	Atoms
56	NI	1001	ADP	PA-O3A-PB-O3B

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](#)

There are no chain breaks in this entry.

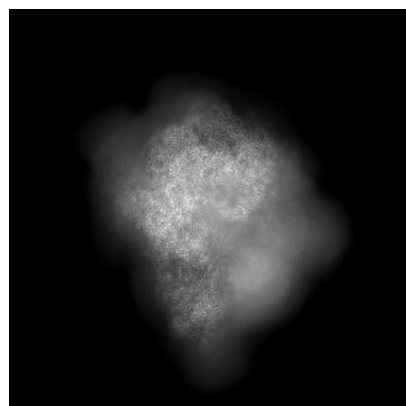
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29256. These allow visual inspection of the internal detail of the map and identification of artifacts.

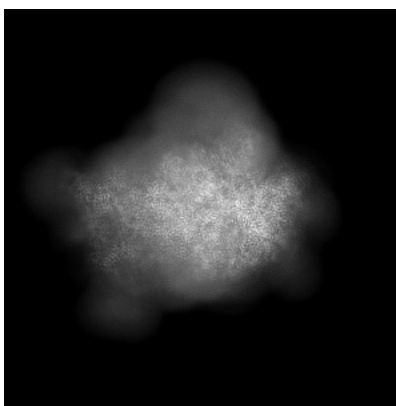
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

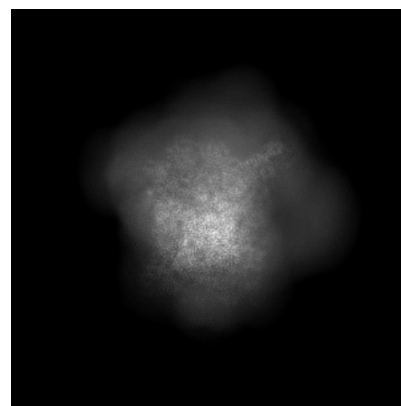
6.1.1 Primary map



X

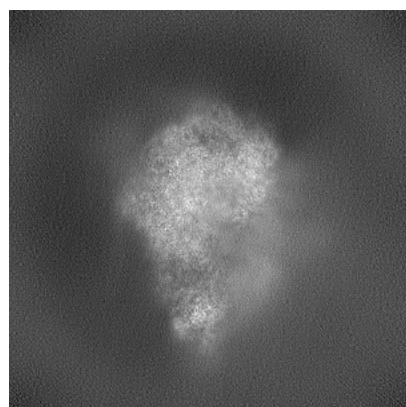


Y

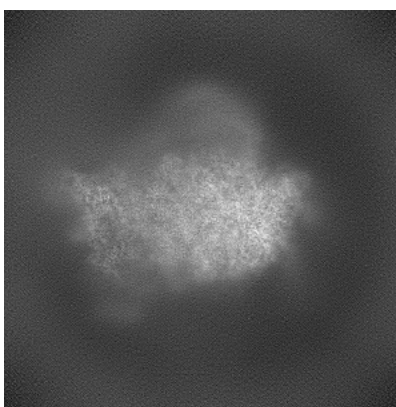


Z

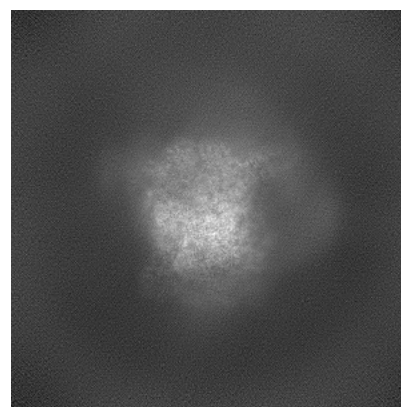
6.1.2 Raw map



X



Y

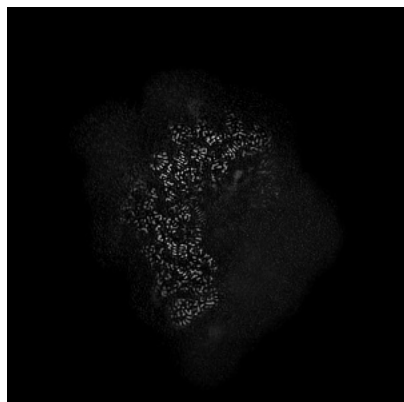


Z

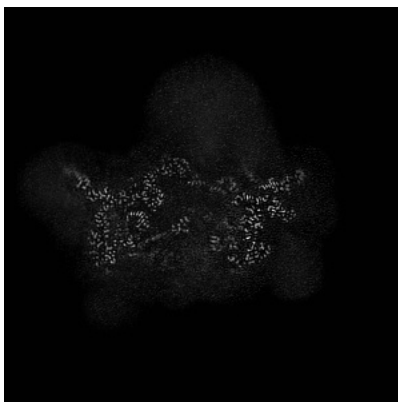
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

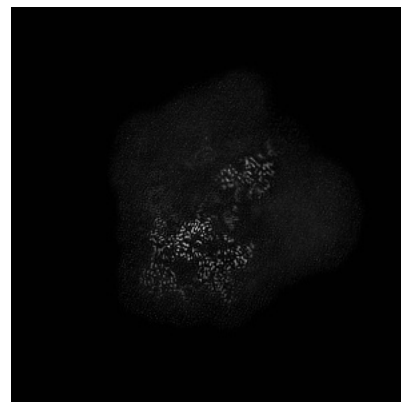
6.2.1 Primary map



X Index: 240

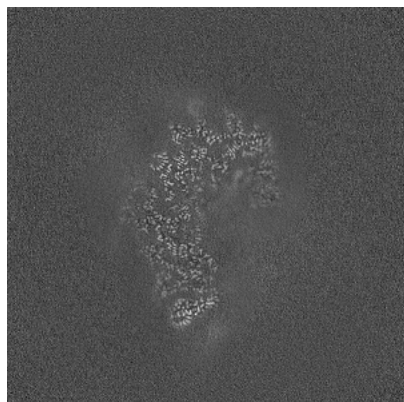


Y Index: 240

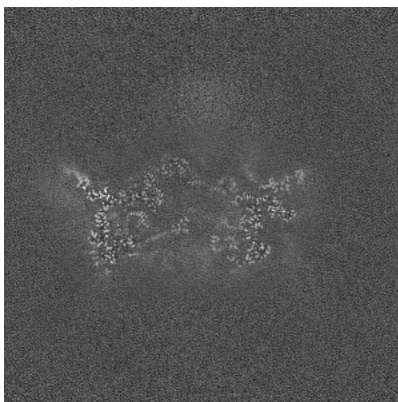


Z Index: 240

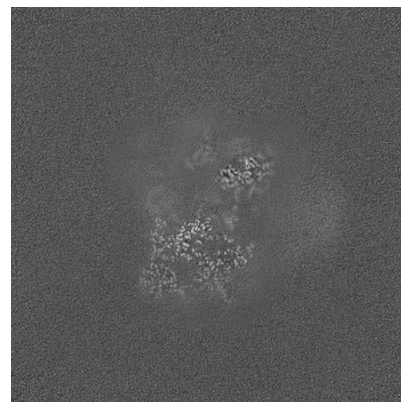
6.2.2 Raw map



X Index: 240



Y Index: 240

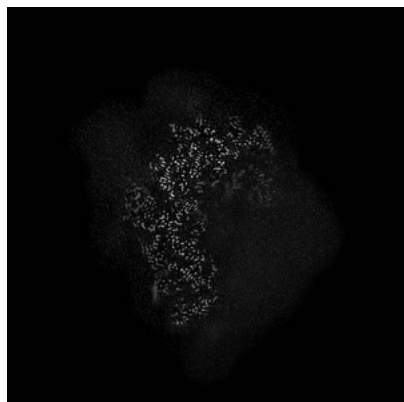


Z Index: 240

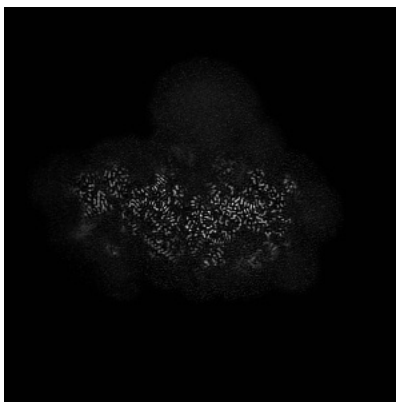
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

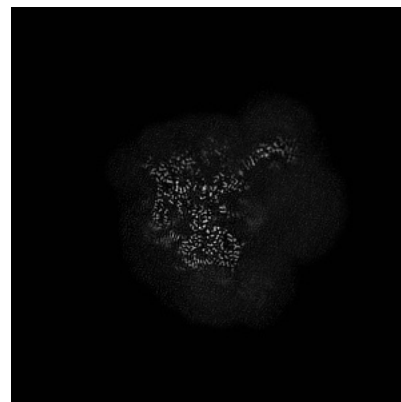
6.3.1 Primary map



X Index: 237

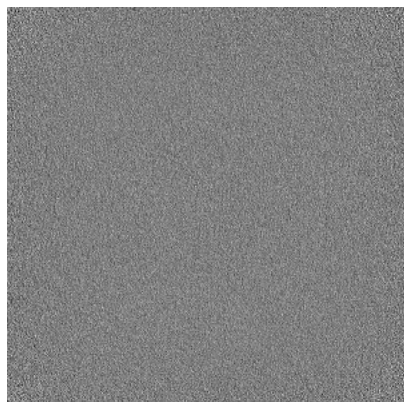


Y Index: 211

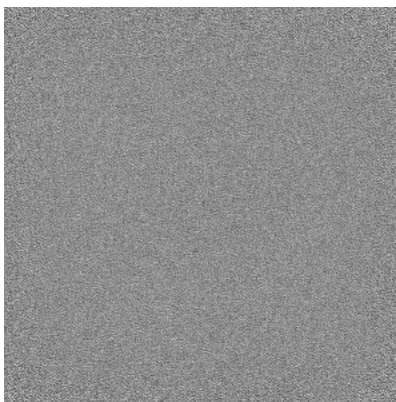


Z Index: 288

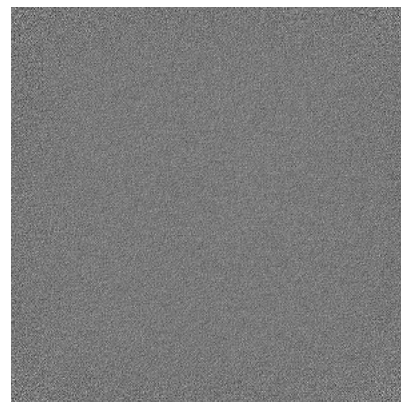
6.3.2 Raw map



X Index: 0



Y Index: 0

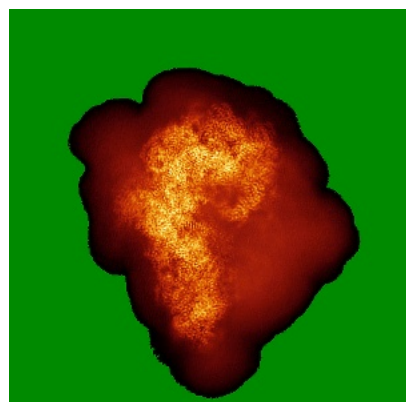


Z Index: 0

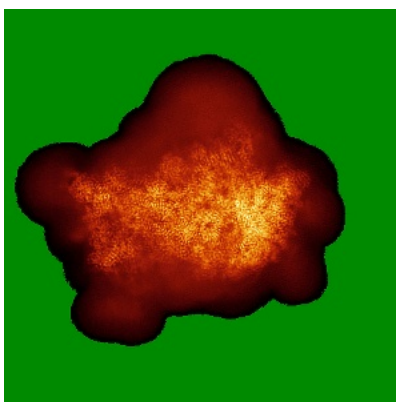
The images above show the largest variance slices of the map in three orthogonal directions.

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

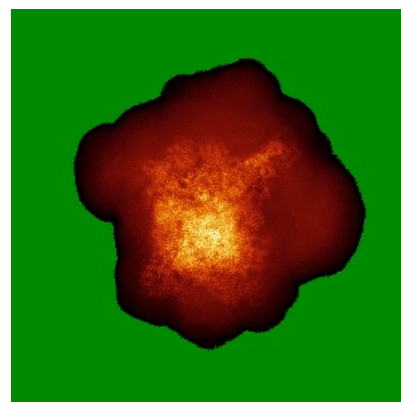
6.4.1 Primary map



X



Y

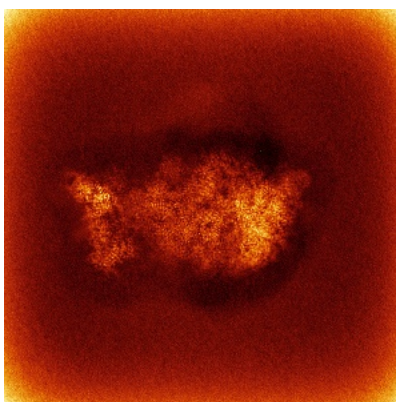


Z

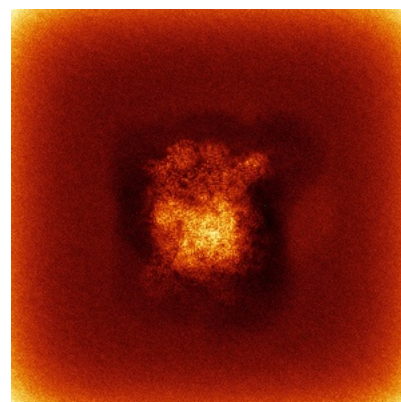
6.4.2 Raw map



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



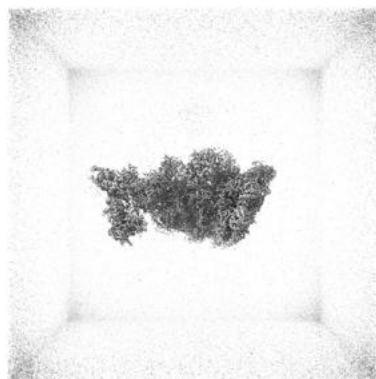
Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

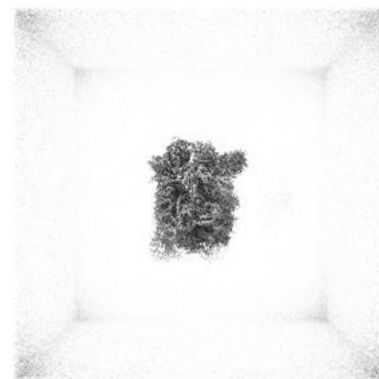
6.5.2 Raw map



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.

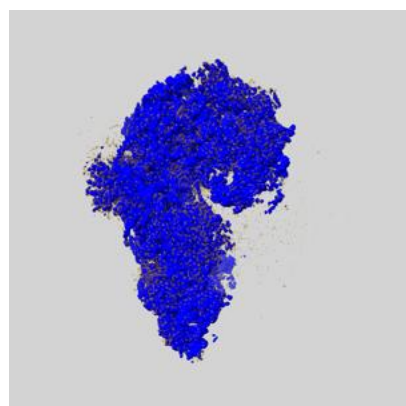
6.6 Mask visualisation [i](#)

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

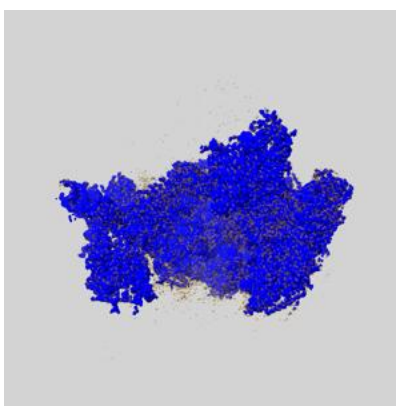
A mask typically either:

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

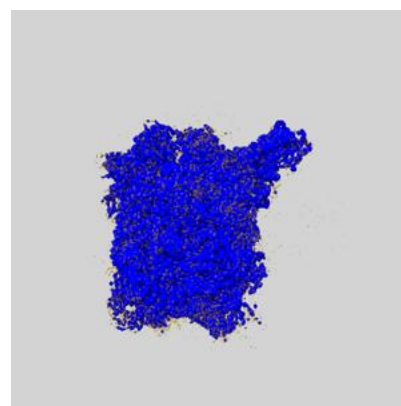
6.6.1 emd_29256_msk_1.map [i](#)



X



Y

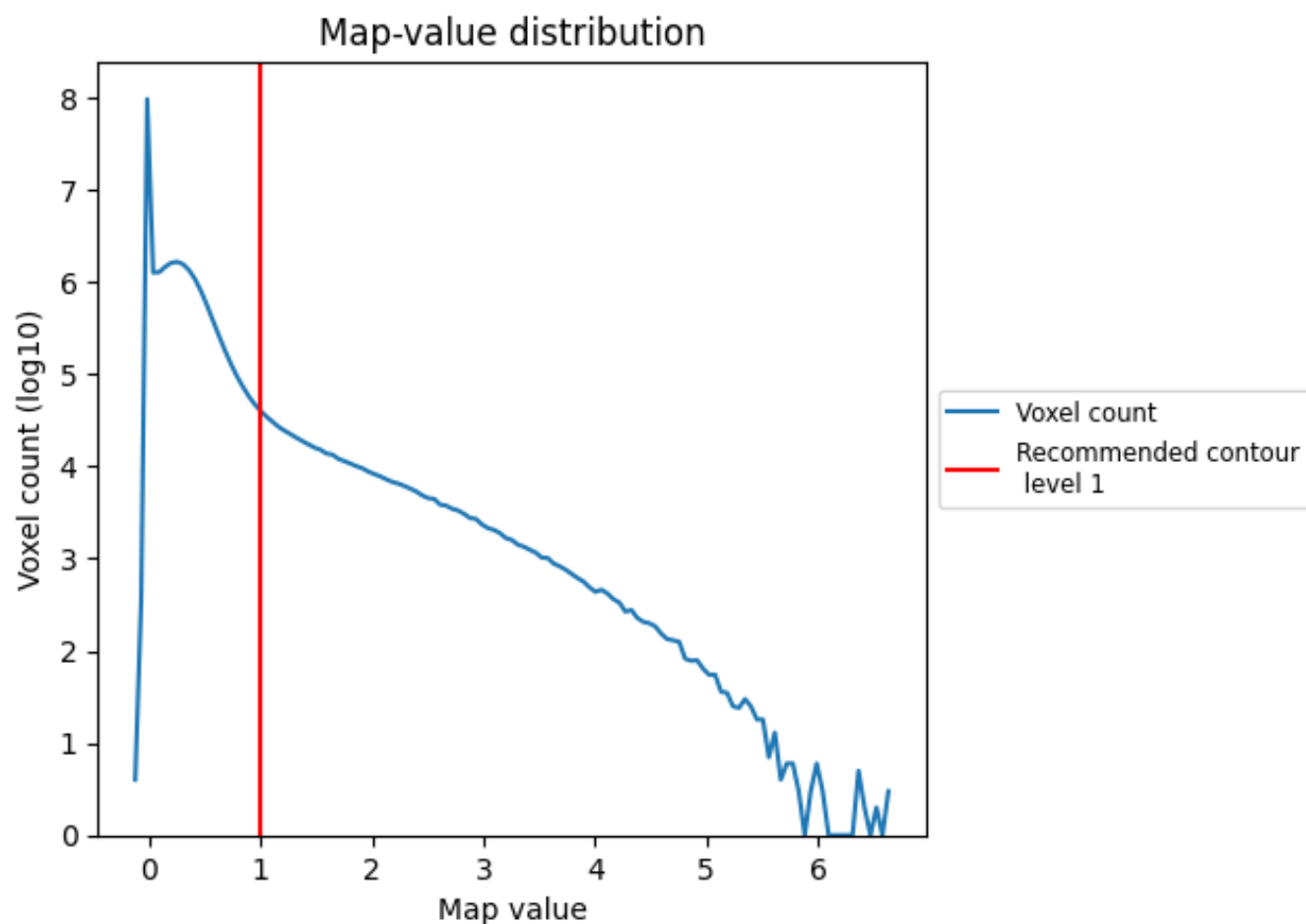


Z

7 Map analysis [i](#)

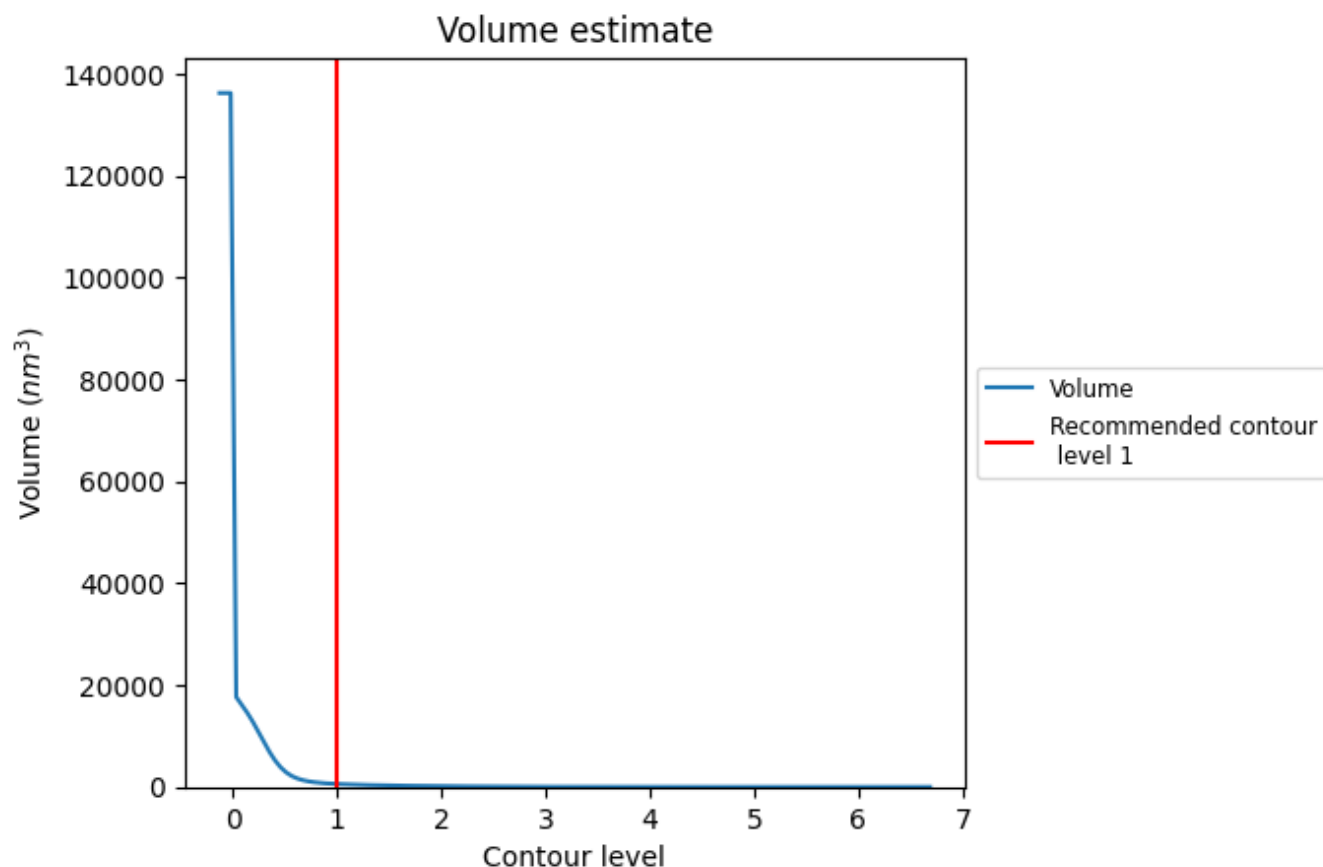
This section contains the results of statistical analysis of the map.

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.

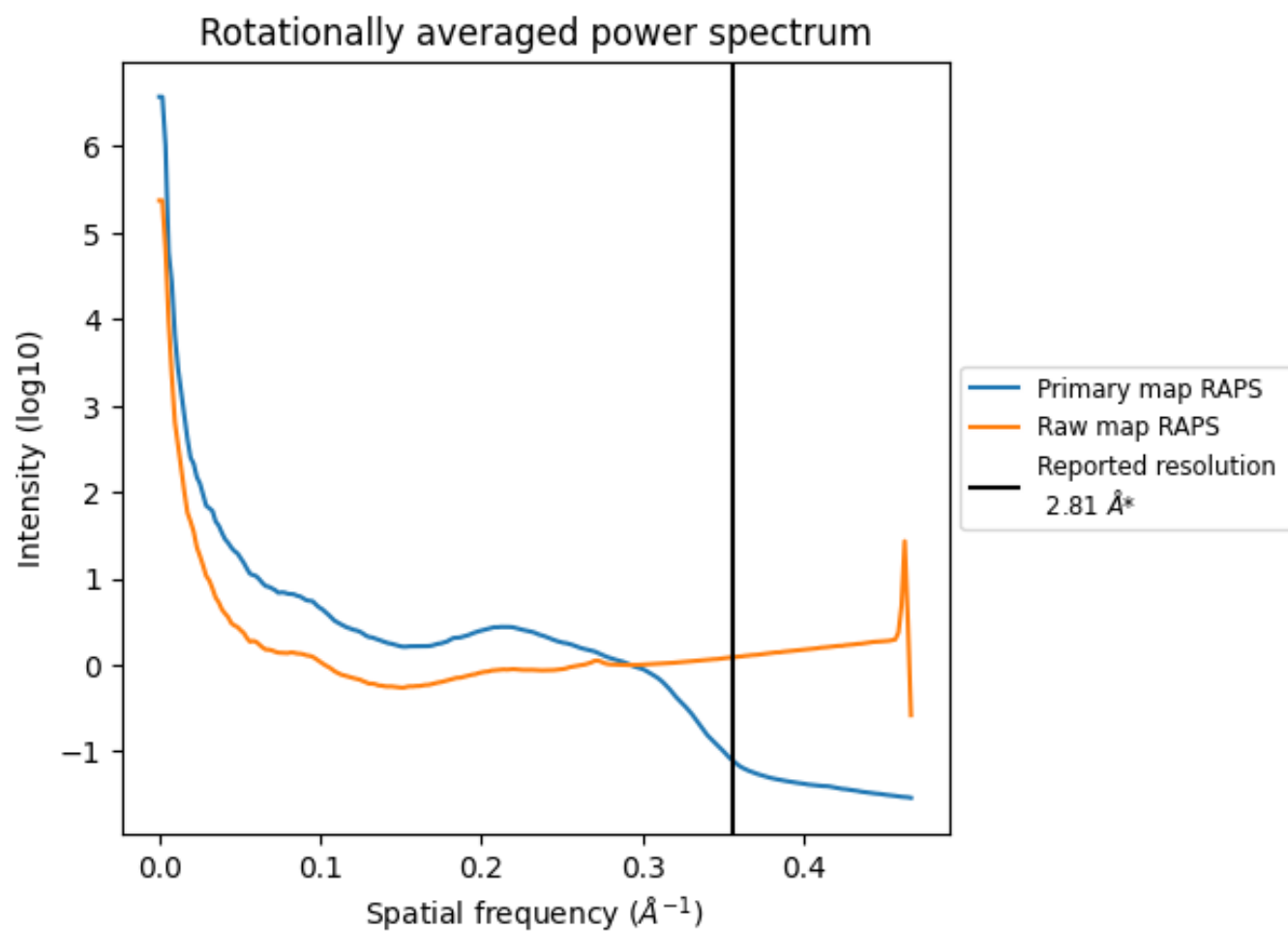
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 588 nm³; this corresponds to an approximate mass of 531 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

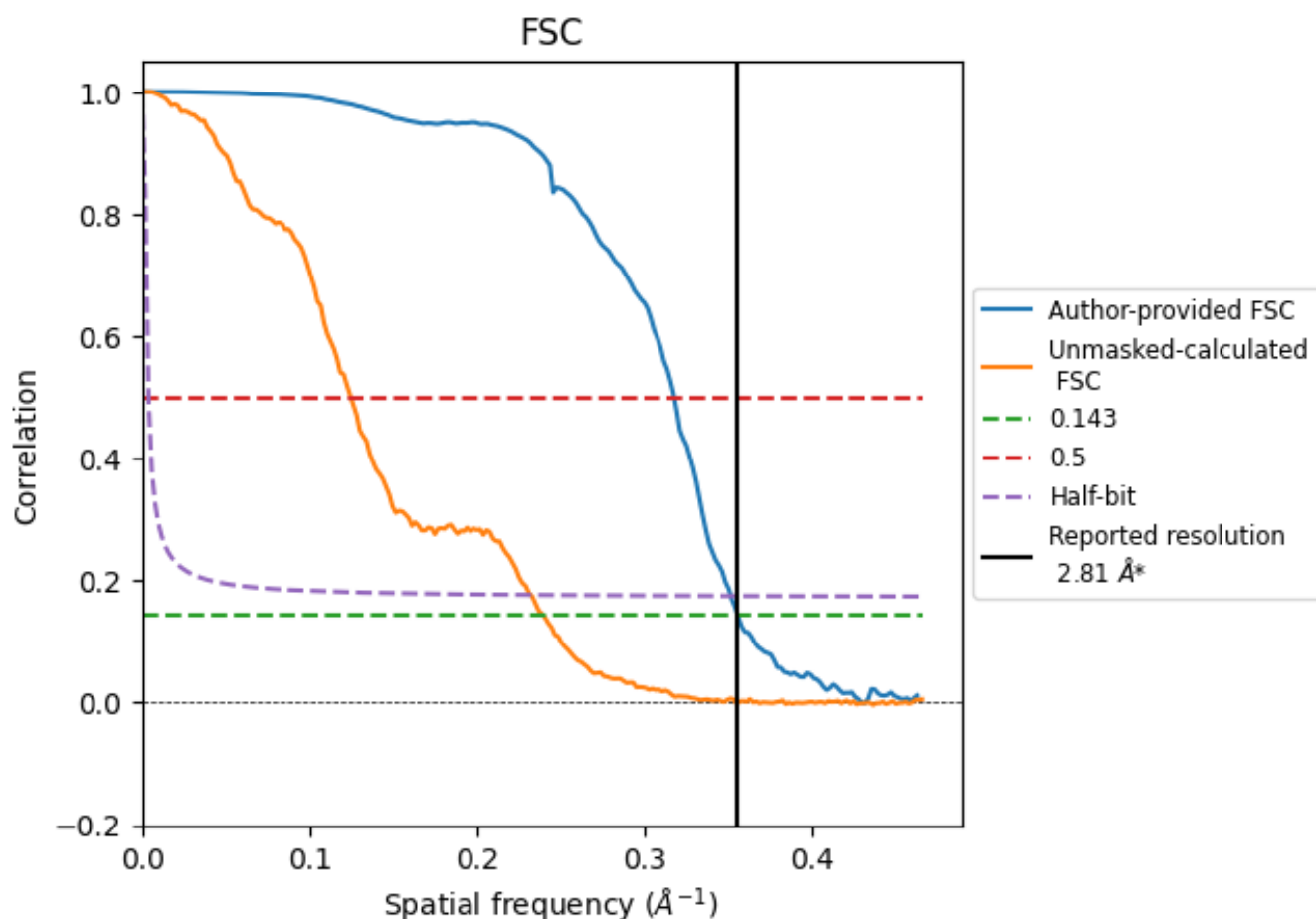


*Reported resolution corresponds to spatial frequency of $0.356 \text{ \AA}^{-1}$

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 0.356 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

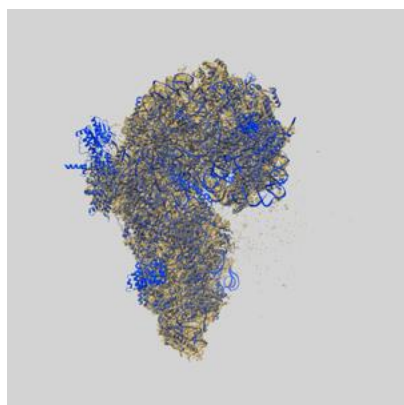
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.14	2.84
Unmasked-calculated*	4.17	8.02	4.30

*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 4.17 differs from the reported value 2.81 by more than 10 %

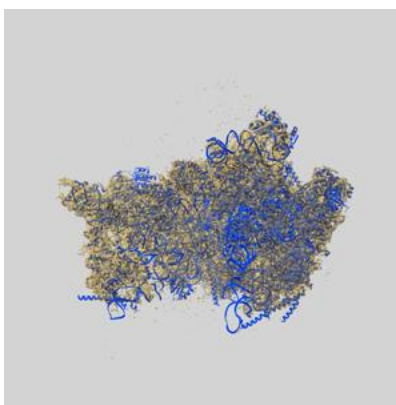
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29256 and PDB model 8FKT. Per-residue inclusion information can be found in section 3 on page 16.

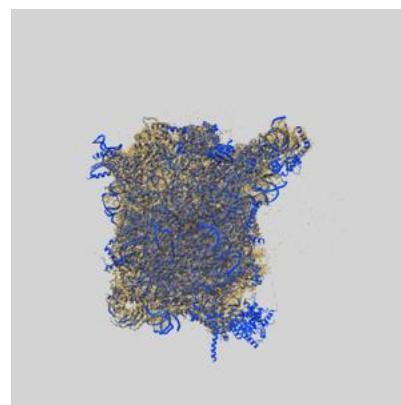
9.1 Map-model overlay [i](#)



X



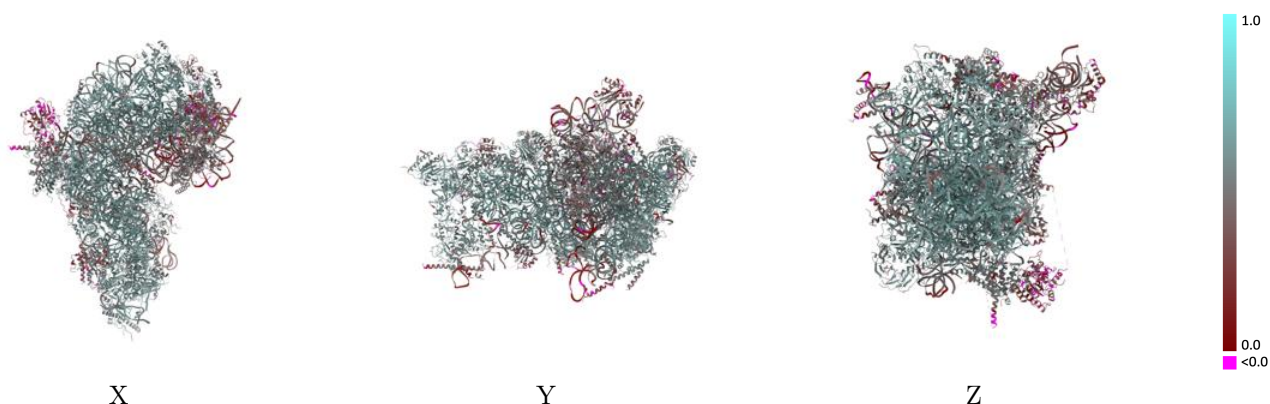
Y



Z

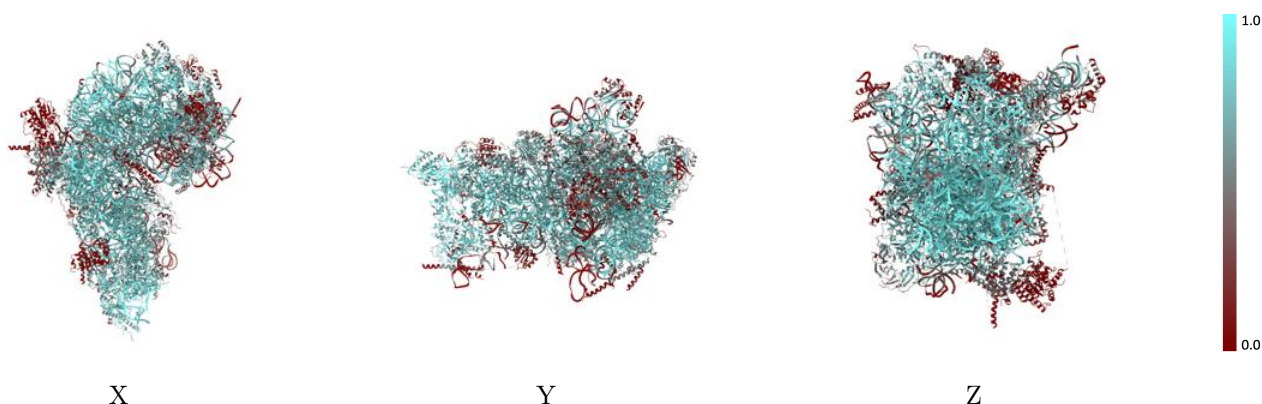
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



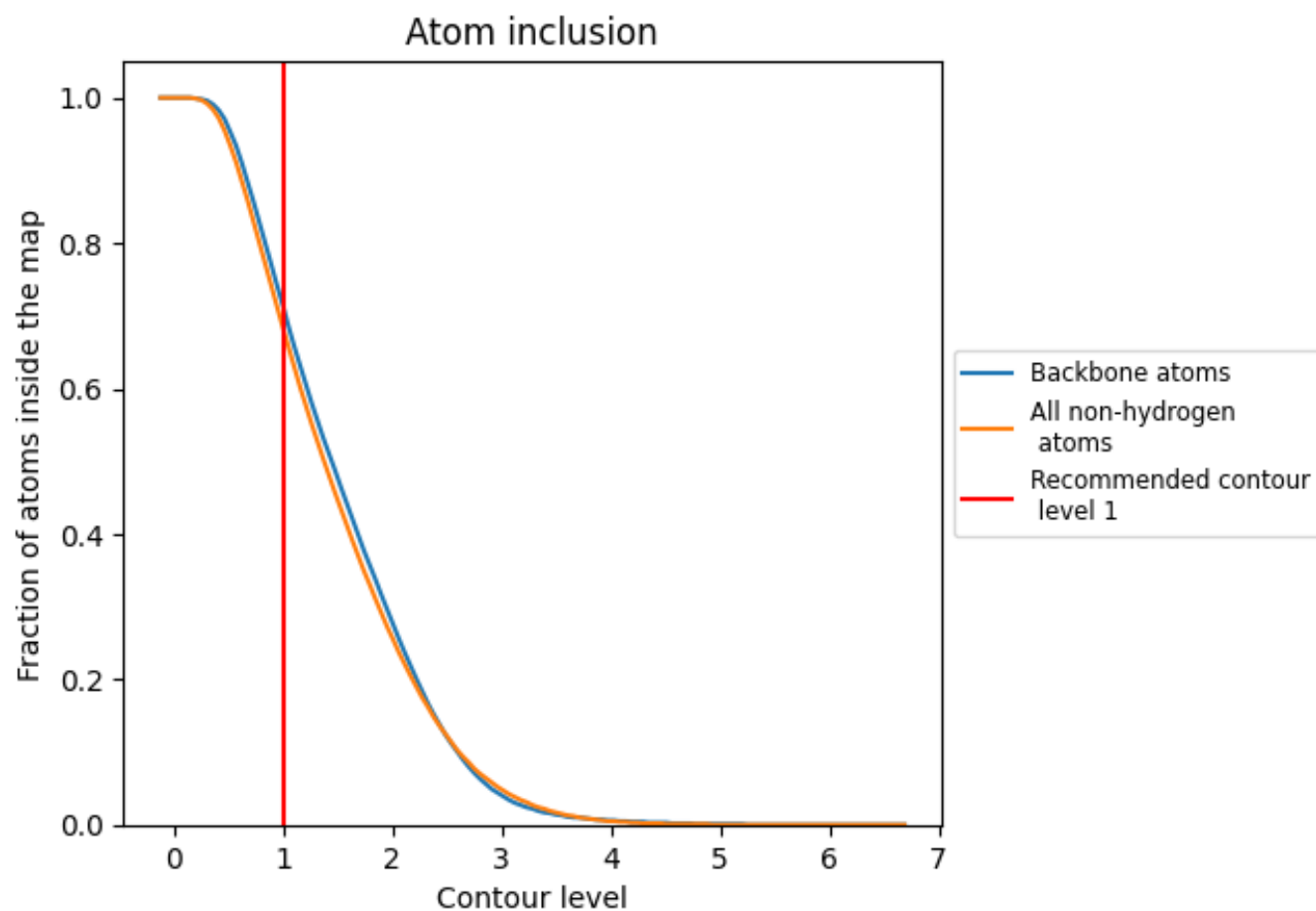
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 68% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6820	 0.5240
BA	 0.3140	 0.4180
BB	 0.2640	 0.2980
L1	 0.7680	 0.5490
L2	 0.8790	 0.5500
L3	 0.7720	 0.5300
L6	 0.8190	 0.5910
L7	 0.8850	 0.6130
L8	 0.8860	 0.6050
L9	 0.8760	 0.6260
LA	 0.6590	 0.5360
LB	 0.8560	 0.6080
LC	 0.8930	 0.6220
LE	 0.4580	 0.4600
LG	 0.6070	 0.5210
LH	 0.2840	 0.4200
LI	 0.8000	 0.5950
LK	 0.5310	 0.4350
LN	 0.7950	 0.5950
LQ	 0.8830	 0.6270
LS	 0.5890	 0.5330
LT	 0.9500	 0.6420
LU	 0.6620	 0.5720
LW	 0.7860	 0.6000
NB	 0.1940	 0.2960
NF	 0.6500	 0.5230
NH	 0.6120	 0.4310
NI	 0.2320	 0.4010
NK	 0.6330	 0.5480
NM	 0.6490	 0.5410
NO	 0.4570	 0.4810
NQ	 0.5600	 0.5260
NS	 0.6150	 0.5430
SA	 0.8170	 0.5970
SC	 0.6810	 0.5550



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Chain	Atom inclusion	Q-score
SD	 0.8220	 0.5940
SE	 0.7940	 0.5940
SG	 0.8130	 0.6100
SH	 0.7830	 0.5660
SI	 0.7220	 0.5410
SJ	 0.3800	 0.4620
SK	 0.6830	 0.5360
SL	 0.7330	 0.5400
SM	 0.6600	 0.5120
SN	 0.4770	 0.4640
SO	 0.6360	 0.5470
SQ	 0.6140	 0.5470
SR	 0.6770	 0.5480
SS	 0.5890	 0.5140
ST	 0.2720	 0.3740
SV	 0.5630	 0.4820
SW	 0.4040	 0.4480
SY	 0.6390	 0.4300
SZ	 0.7020	 0.5550