



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:41 PM UTC

PDB ID : 8QRK / pdb_00008qrk
EMDB ID : EMD-18438
Title : mt-SSU assembly intermediate in GTPBP8 knock-out cells, state 1
Authors : Valentin Gese, G.; Cipullo, M.; Rorbach, J.; Hallberg, B.M.
Deposited on : 2023-10-09
Resolution : 6.69 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:

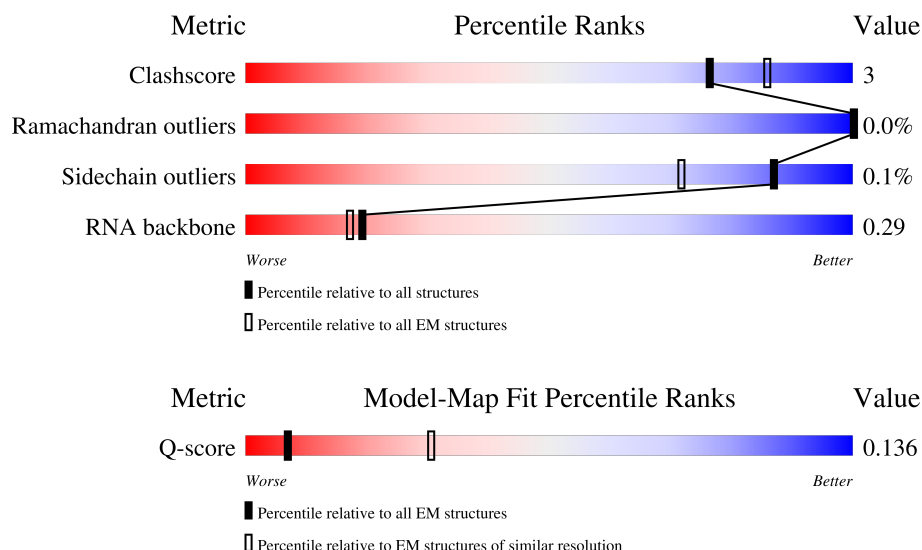
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 6.69 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	480 (6.25 - 7.25)

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	0	218	18% 89% 9% .
2	1	323	29% 80% 6% 15%
3	3	199	8% 34% . 65%

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Mol	Chain	Length	Quality of chain
4	A	955	
5	B	296	
6	C	167	
7	E	125	
8	F	242	
9	H	201	
10	I	194	
11	J	138	
12	K	128	
13	L	257	
14	M	137	
15	N	130	
16	O	258	
17	P	142	
18	Q	86	
19	R	360	
20	S	190	
21	T	173	
22	U	205	
23	W	187	
24	X	398	
25	Y	395	
26	Z	106	
27	D	430	
28	G	396	

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Mol	Chain	Length	Quality of chain
29	V	414	35% 83% 5% 13%
30	4	689	61% 79% 6% 15%

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 66224 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 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

- Molecule 2 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	276	Total	C	N	O	S	0	0
			2238	1419	381	427	11		

- Molecule 3 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 4 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	955	Total	C	N	O	P	0	0
			20282	9098	3652	6577	955		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	709	G	A	conflict	GB OM714795.1

- Molecule 5 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 6 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 7 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 8 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 9 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 10 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	137	Total	C	N	O	S	0	0
			1019	641	193	181	4		

- Molecule 11 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 12 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 13 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 14 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 15 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 16 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	194	Total	C	N	O	S	0	0
			1599	1019	295	278	7		

- Molecule 17 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 18 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	86	Total	C	N	O	S	0	0
			744	460	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 19 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 20 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 21 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 22 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 27 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	339	Total	C	N	O	S	0	0
			2695	1690	509	483	13		

- Molecule 28 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	322	Total	C	N	O	S	0	0
			2655	1688	473	480	14		

- Molecule 29 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 30 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

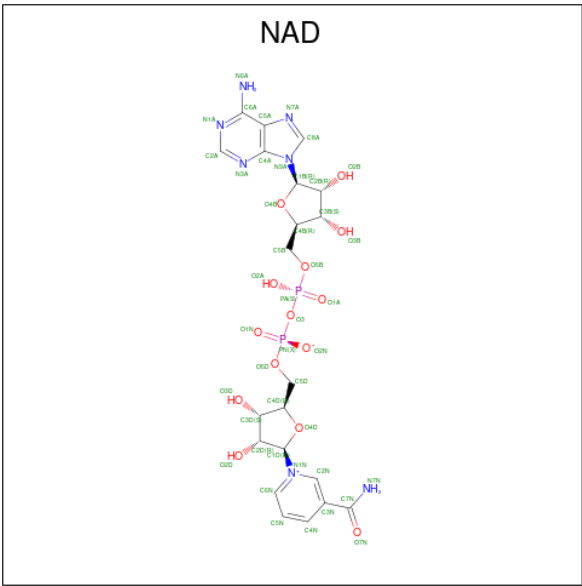
Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	3	1	Total	Mg	0
			1	1	
31	A	45	Total	Mg	0
			45	45	
31	B	1	Total	Mg	0
			1	1	
31	J	1	Total	Mg	0
			1	1	
31	X	1	Total	Mg	0
			1	1	

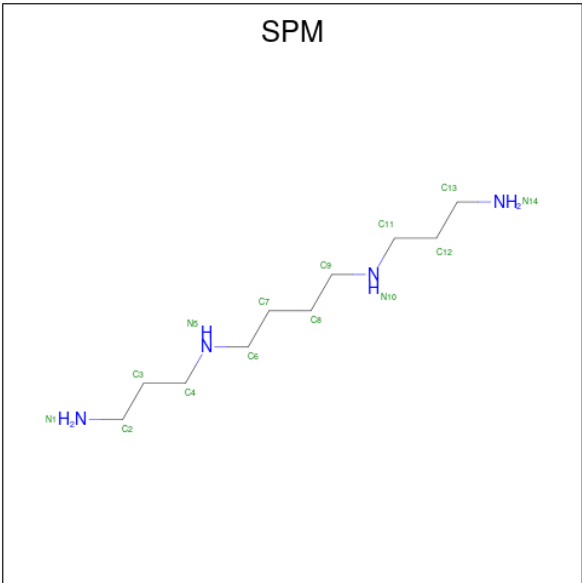
- Molecule 32 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:

C₂₁H₂₇N₇O₁₄P₂).



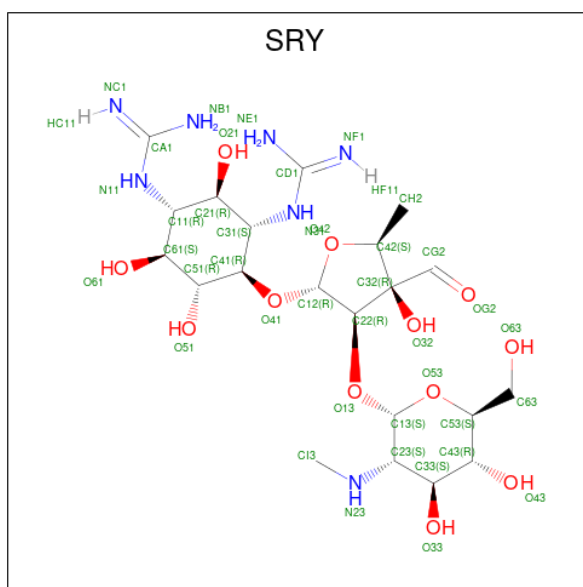
Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 33 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N		0
			14	10	4		

- Molecule 34 is STREPTOMYCIN (CCD ID: SRY) (formula: C₂₁H₃₉N₇O₁₂).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	N	O	0
			40	21	7	12	

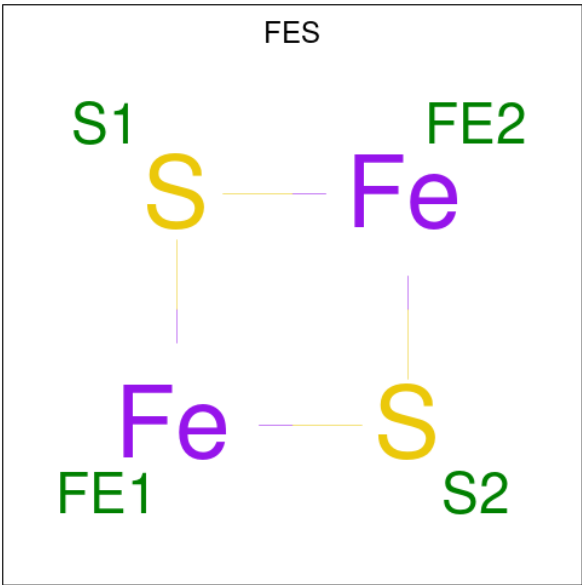
- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
35	A	17	Total	K	0
			17	17	

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

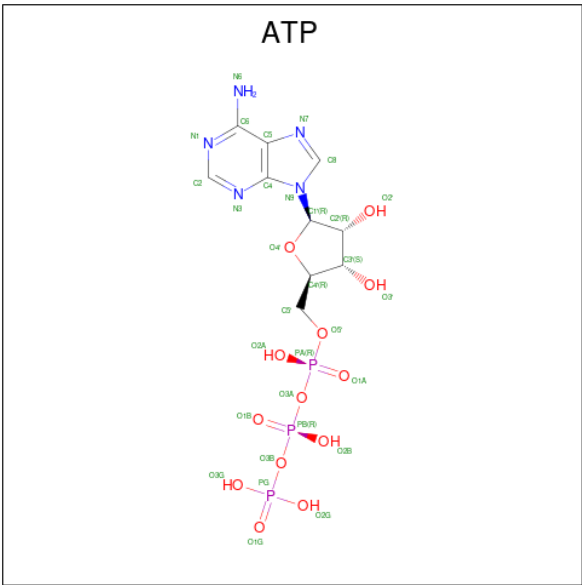
Mol	Chain	Residues	Atoms		AltConf
36	O	1	Total	Zn	0
			1	1	

- Molecule 37 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
37	P	1	Total	Fe	S	0
			4	2	2	
37	T	1	Total	Fe	S	0
			4	2	2	

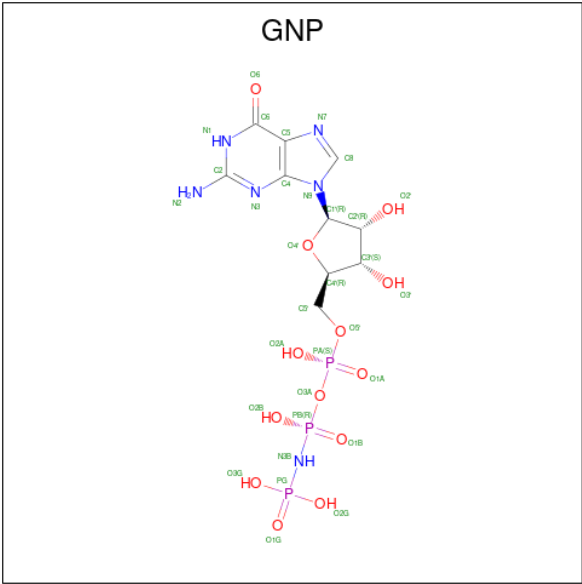
- Molecule 38 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID:

GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

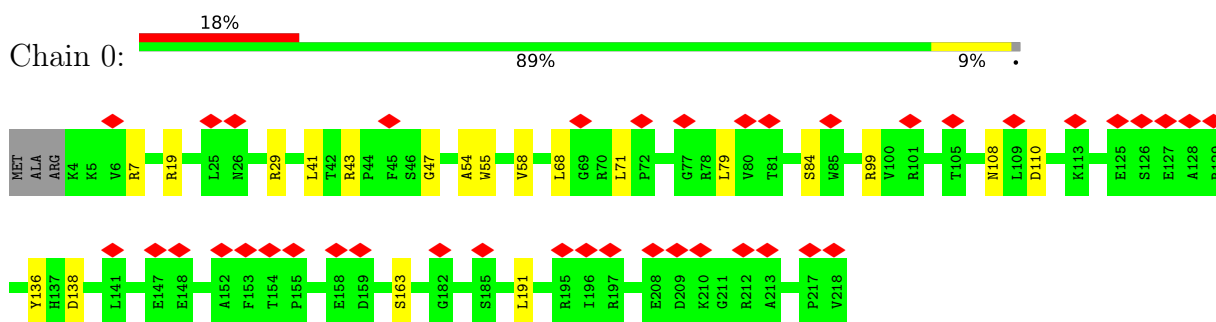


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
39	X	1	32	10	6	13	3	0

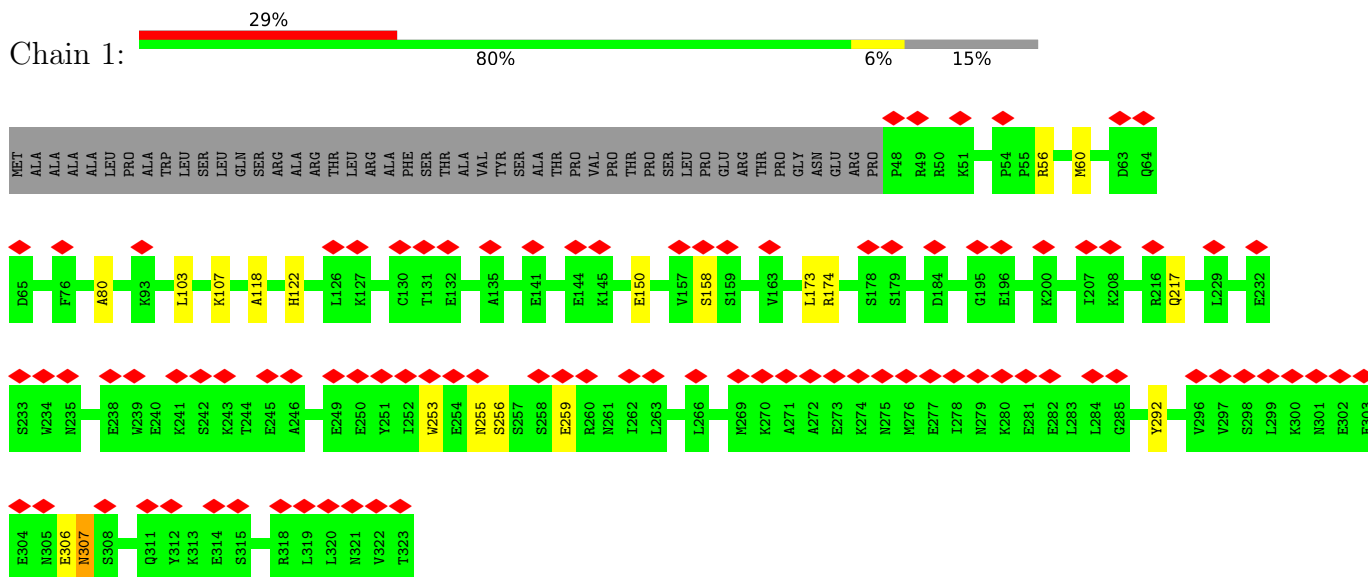
3 Residue-property plots [i](#)

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.

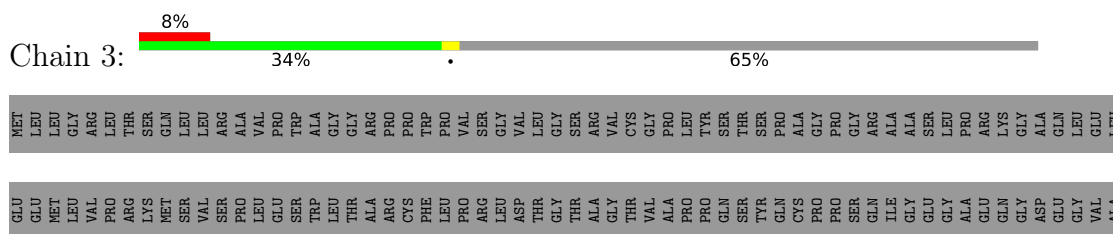
- Molecule 1: 28S ribosomal protein S34, mitochondrial

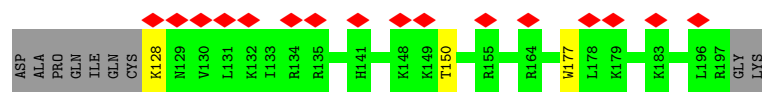


- Molecule 2: 28S ribosomal protein S35, mitochondrial

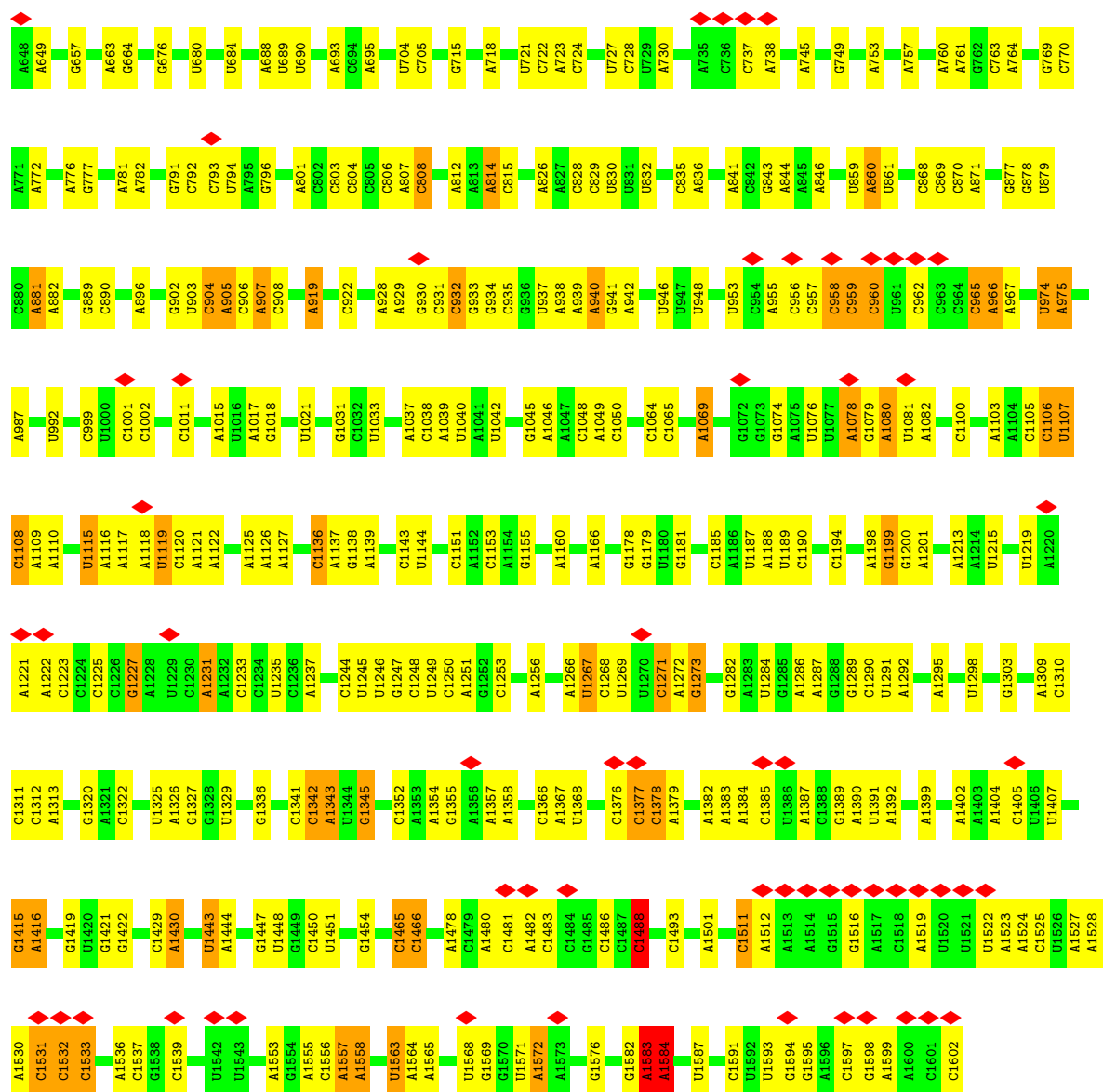


- Molecule 3: Aurora kinase A-interacting protein

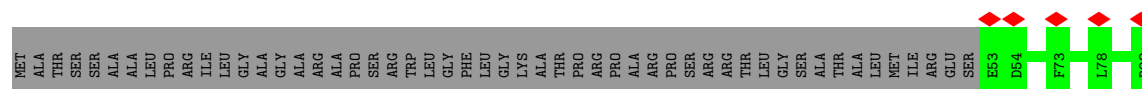
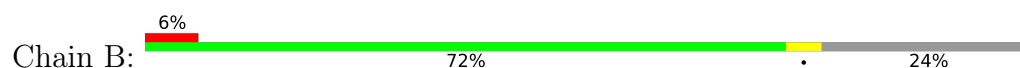


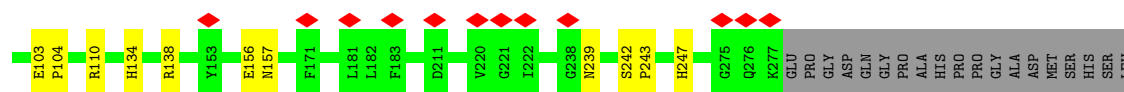


• Molecule 4: 12S mitochondrial rRNA

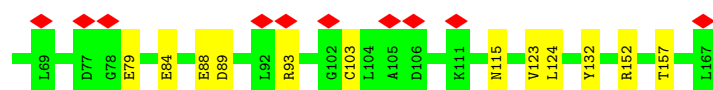
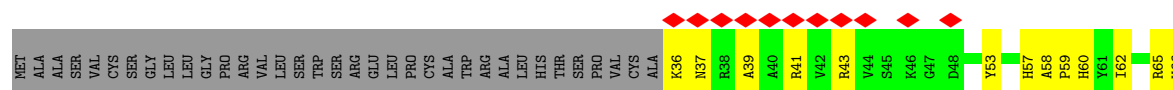


• Molecule 5: 28S ribosomal protein S2, mitochondrial

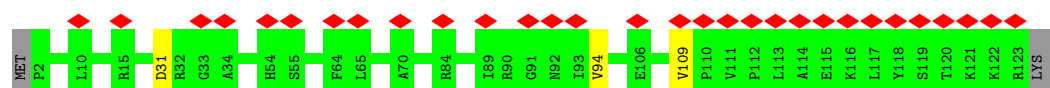




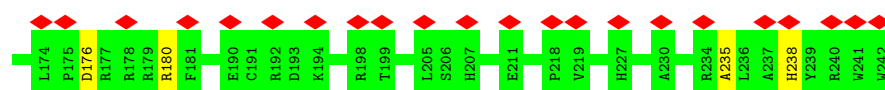
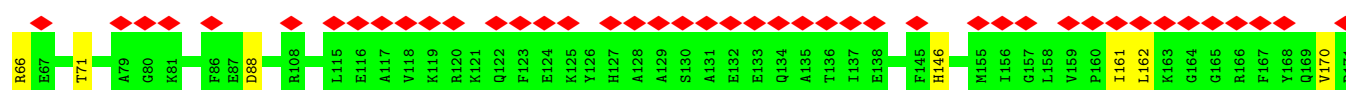
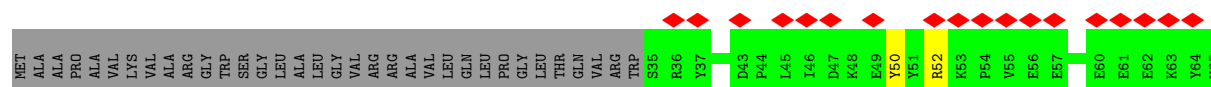
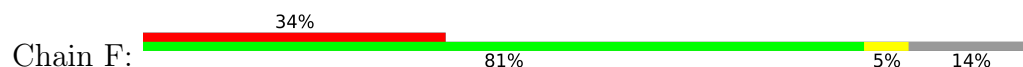
- Molecule 6: 28S ribosomal protein S24, mitochondrial



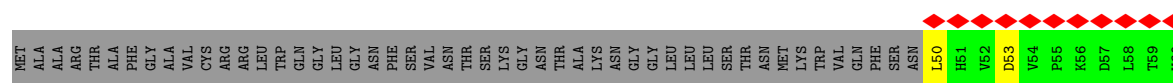
- Molecule 7: 28S ribosomal protein S6, mitochondrial



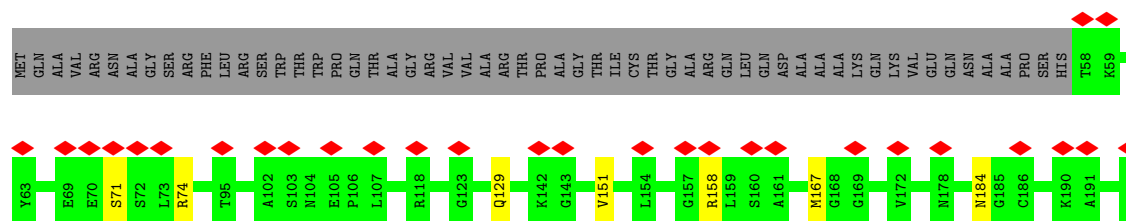
- Molecule 8: 28S ribosomal protein S7, mitochondrial



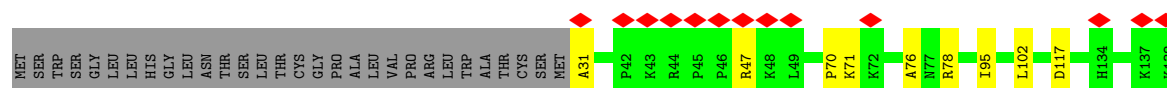
- Molecule 9: 28S ribosomal protein S10, mitochondrial



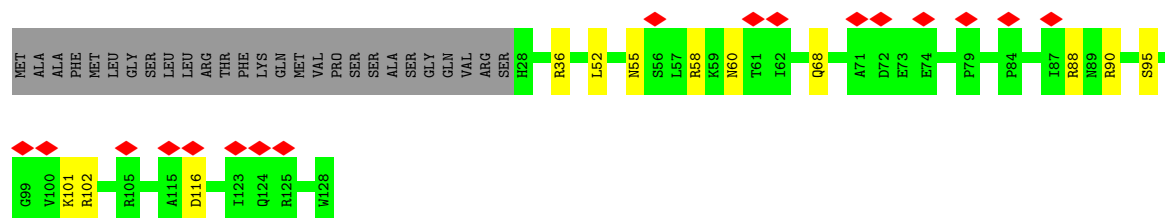
- Molecule 10: 28S ribosomal protein S11, mitochondrial



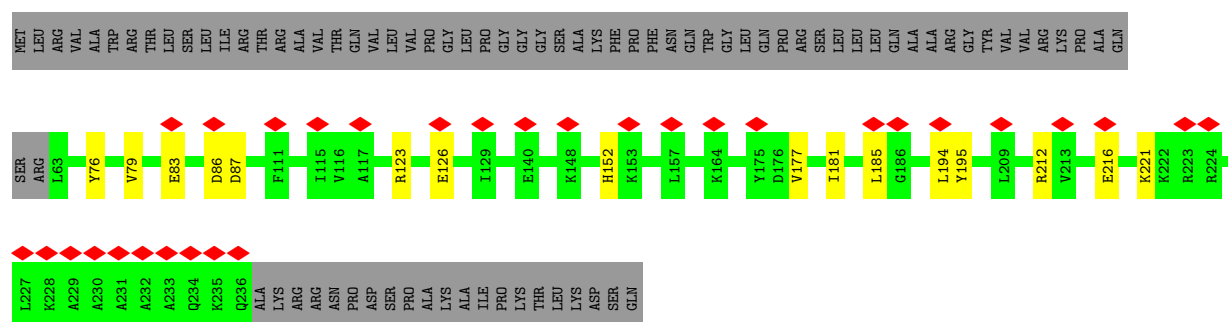
- Molecule 11: 28S ribosomal protein S12, mitochondrial



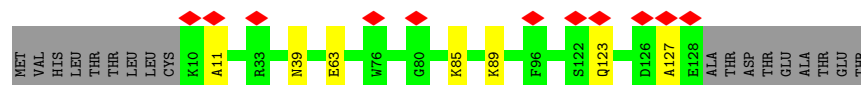
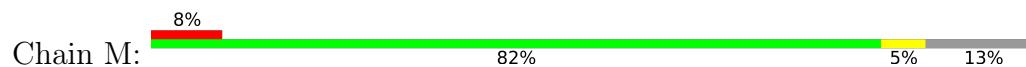
- Molecule 12: 28S ribosomal protein S14, mitochondrial



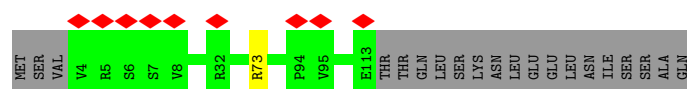
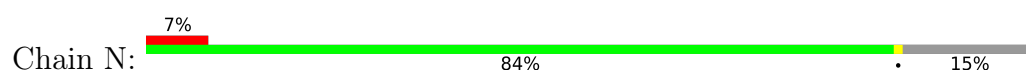
- Molecule 13: 28S ribosomal protein S15, mitochondrial



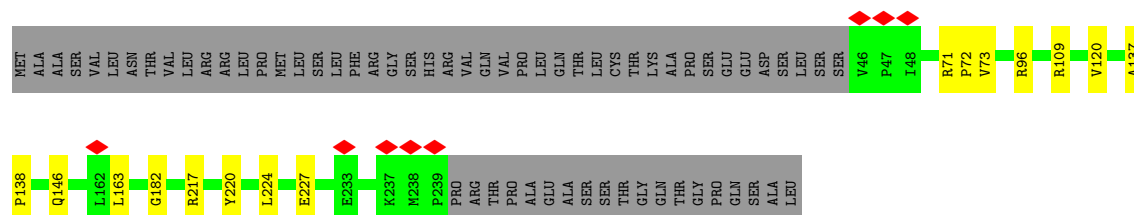
- Molecule 14: 28S ribosomal protein S16, mitochondrial



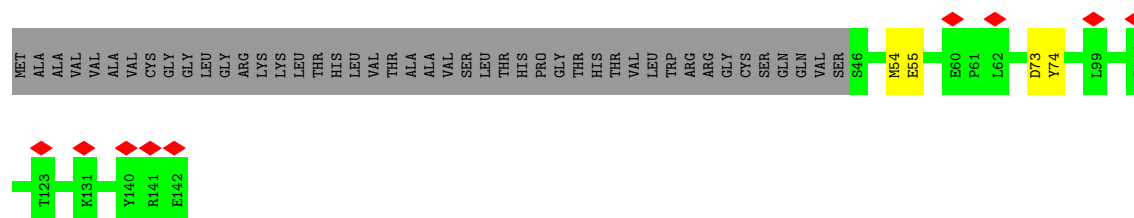
- Molecule 15: 28S ribosomal protein S17, mitochondrial



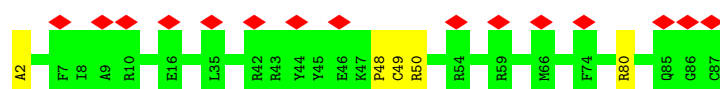
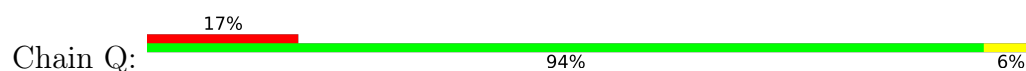
- Molecule 16: 28S ribosomal protein S18b, mitochondrial



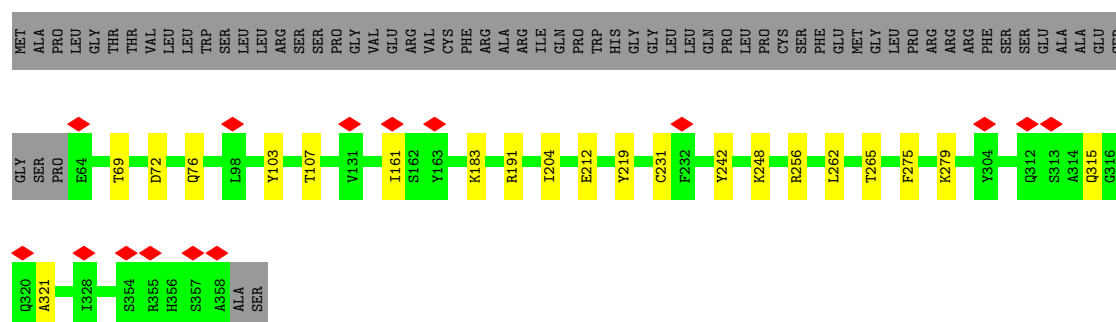
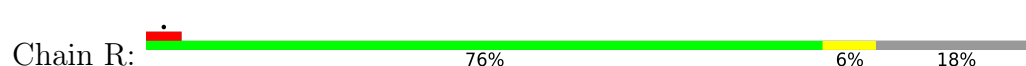
- Molecule 17: 28S ribosomal protein S18c, mitochondrial



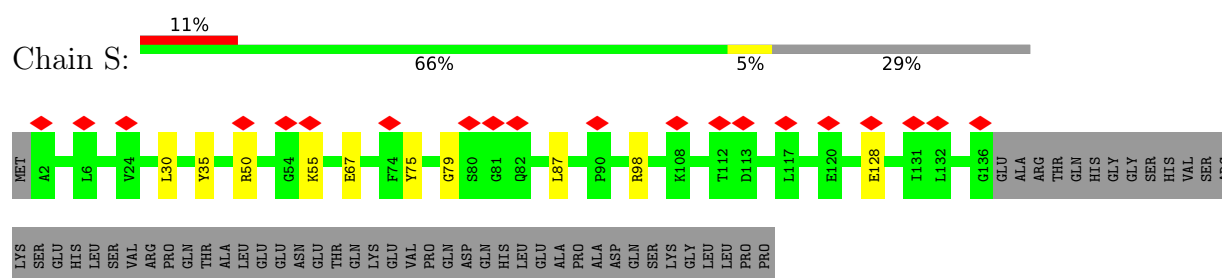
- Molecule 18: 28S ribosomal protein S21, mitochondrial



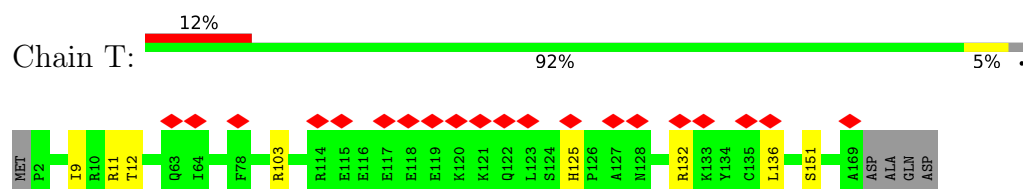
- Molecule 19: 28S ribosomal protein S22, mitochondrial



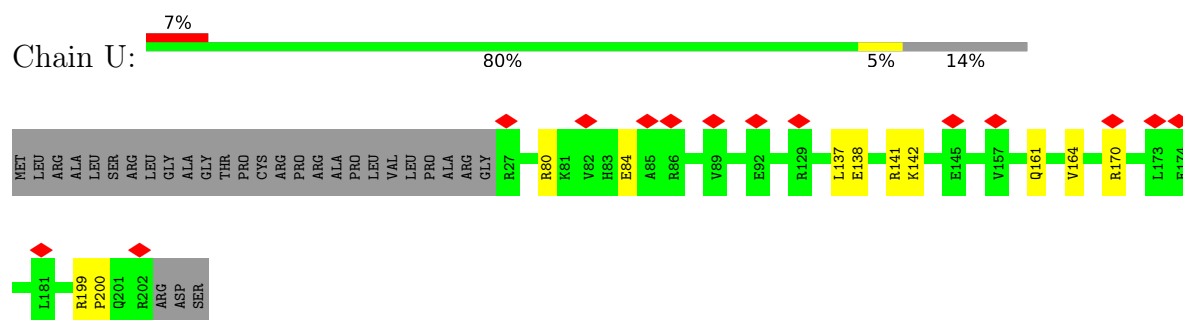
- Molecule 20: 28S ribosomal protein S23, mitochondrial



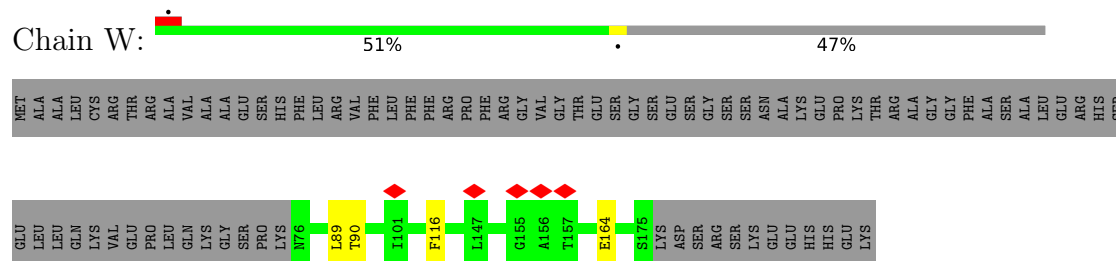
- Molecule 21: 28S ribosomal protein S25, mitochondrial



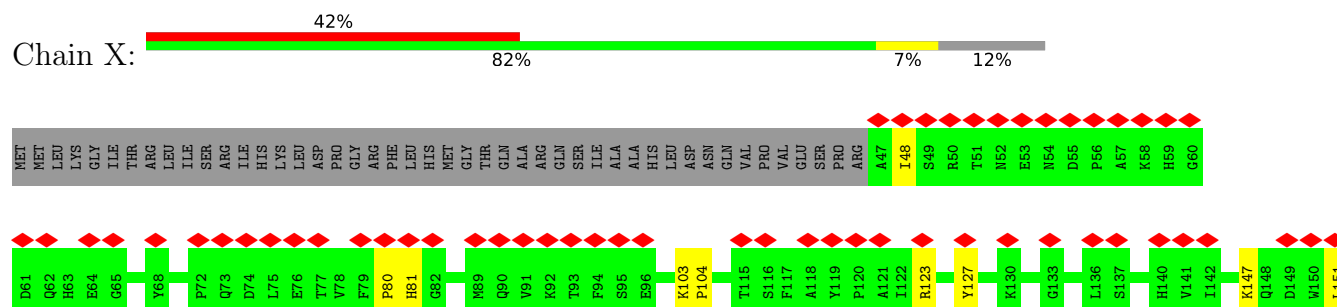
- Molecule 22: 28S ribosomal protein S26, mitochondrial

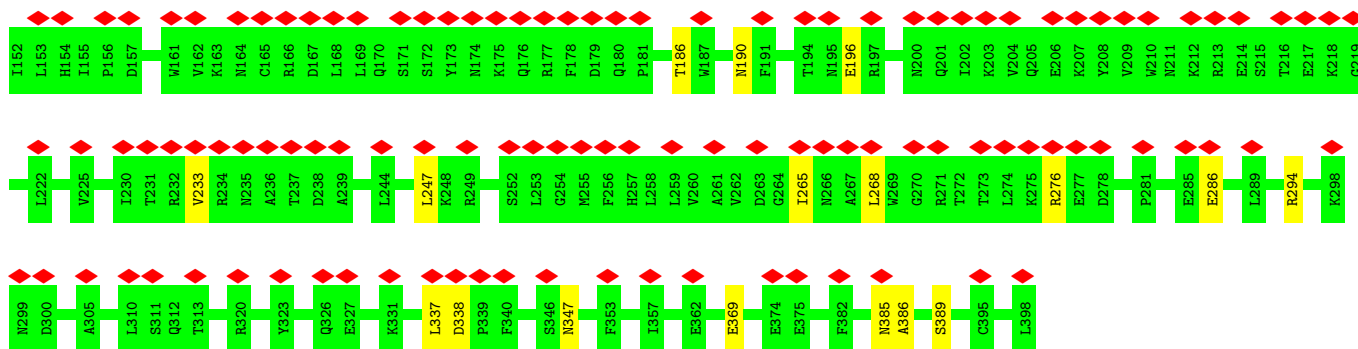


- Molecule 23: 28S ribosomal protein S28, mitochondrial

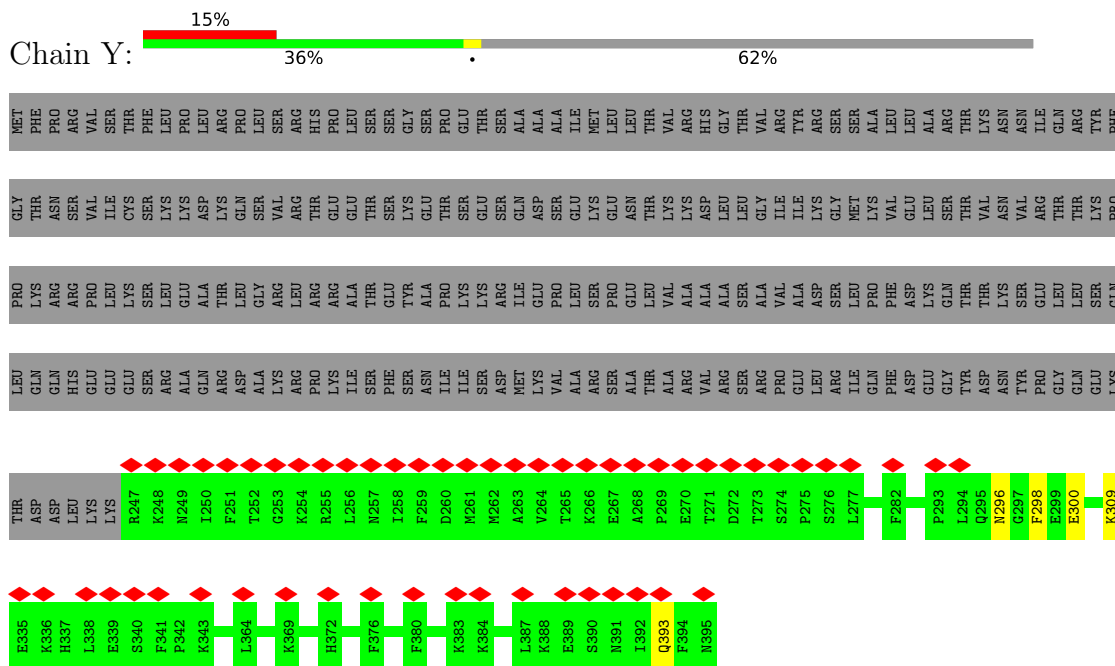


- Molecule 24: 28S ribosomal protein S29, mitochondrial

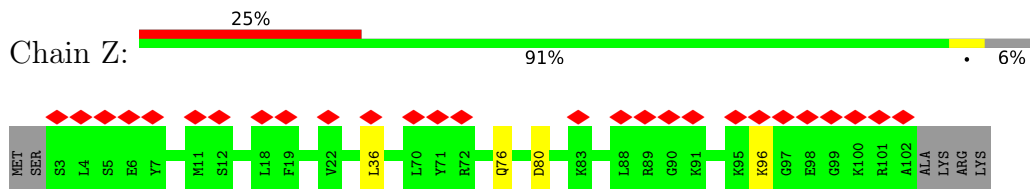




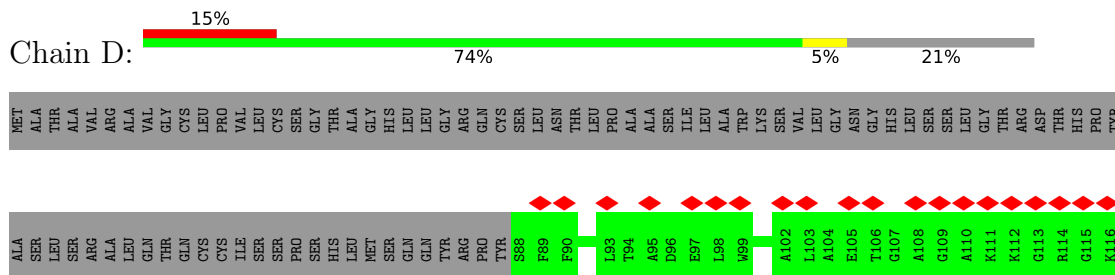
- Molecule 25: 28S ribosomal protein S31, mitochondrial

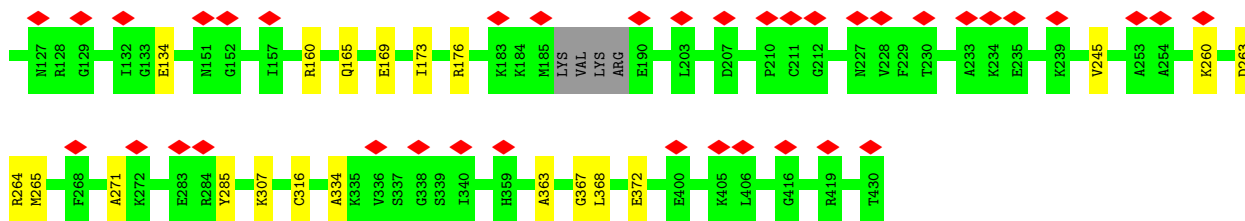


- Molecule 26: 28S ribosomal protein S33, mitochondrial

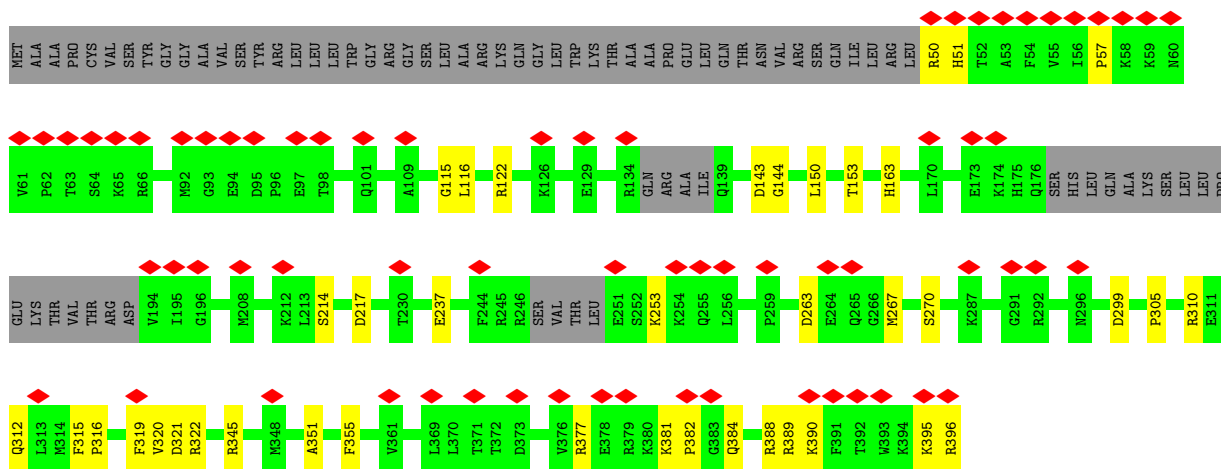


- Molecule 27: 28S ribosomal protein S5, mitochondrial

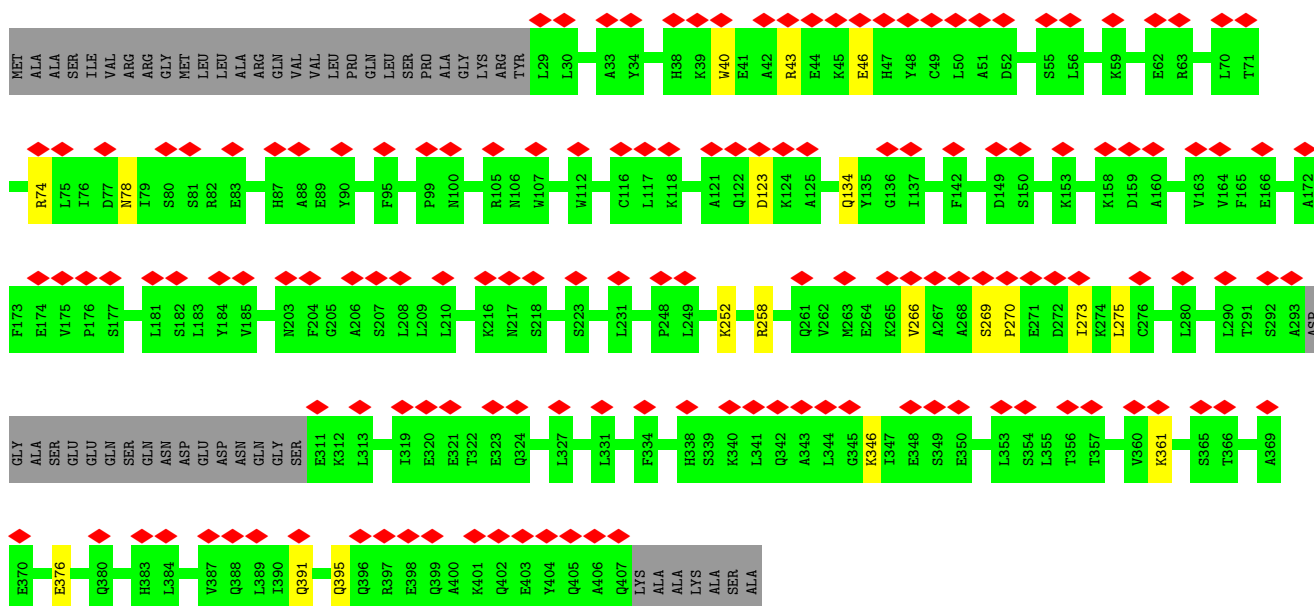
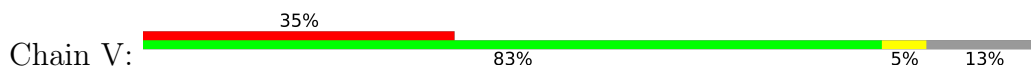




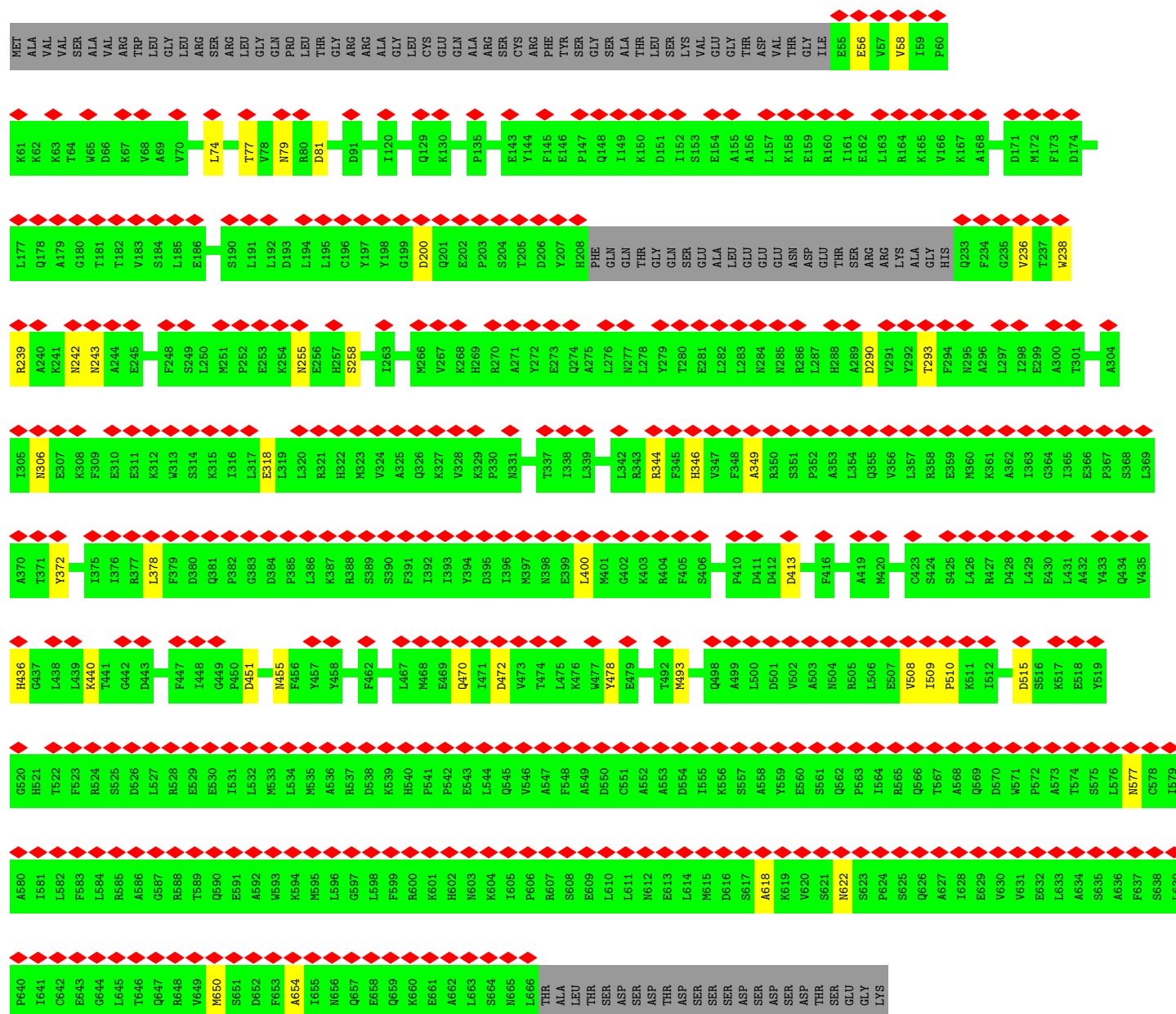
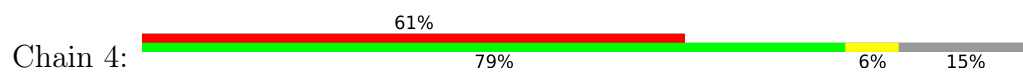
- Molecule 28: 28S ribosomal protein S9, mitochondrial



- Molecule 29: 28S ribosomal protein S27, mitochondrial



- Molecule 30: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.639	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	517.12, 517.12, 517.12	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, SRY, B8T, FES, 5MU, MG, SPM, AYA, NAD, GNP, K, ZN, MA6, 5MC

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	0	0.26	0/1834	0.39	0/2484
2	1	0.30	0/2285	0.35	0/3090
3	3	0.30	0/636	0.45	0/839
4	A	0.29	0/22562	0.35	0/35124
5	B	0.32	0/1871	0.38	0/2531
6	C	0.39	0/1113	0.41	0/1505
7	E	0.27	0/989	0.36	0/1335
8	F	0.26	0/1767	0.35	0/2373
9	H	0.36	0/1178	0.37	0/1598
10	I	0.26	0/1039	0.35	0/1400
11	J	0.34	0/855	0.38	0/1148
12	K	0.40	0/880	0.41	0/1182
13	L	0.30	0/1477	0.36	0/1974
14	M	0.34	0/963	0.41	0/1295
15	N	0.32	0/886	0.33	0/1199
16	O	0.31	0/1655	0.36	0/2254
17	P	0.32	0/798	0.36	0/1070
18	Q	0.33	0/748	0.44	0/994
19	R	0.26	0/2456	0.33	0/3317
20	S	0.26	0/1138	0.33	0/1533
21	T	0.32	0/1402	0.38	0/1883
22	U	0.24	0/1510	0.37	0/2025
23	W	0.27	0/801	0.33	0/1079
24	X	0.26	0/2921	0.35	0/3954
25	Y	0.27	0/1280	0.32	0/1725
26	Z	0.30	0/857	0.36	0/1141
27	D	0.31	0/2746	0.37	0/3675
28	G	0.28	0/2712	0.36	0/3631
29	V	0.19	0/3030	0.32	0/4093
30	4	0.21	0/4877	0.34	0/6598
All	All	0.29	0/69266	0.36	0/98049

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	0	1787	0	1796	13	0
2	1	2238	0	2269	13	0
3	3	625	0	699	3	0
4	A	20282	0	10298	145	0
5	B	1828	0	1815	8	0
6	C	1083	0	1088	16	0
7	E	972	0	1000	3	0
8	F	1725	0	1769	14	0
9	H	1152	0	1183	11	0
10	I	1019	0	1059	3	0
11	J	839	0	887	10	0
12	K	862	0	885	9	0
13	L	1453	0	1540	11	0
14	M	942	0	965	5	0
15	N	868	0	928	1	0
16	O	1599	0	1565	9	0
17	P	781	0	806	2	0
18	Q	744	0	758	3	0
19	R	2409	0	2428	16	0
20	S	1111	0	1115	9	0
21	T	1371	0	1393	7	0
22	U	1488	0	1499	7	0
23	W	789	0	802	4	0
24	X	2849	0	2843	18	0
25	Y	1246	0	1197	5	0
26	Z	839	0	858	3	0
27	D	2695	0	2755	24	0
28	G	2655	0	2643	53	0
29	V	2969	0	2961	13	0
30	4	4768	0	4766	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	3	1	0	0	0	0
31	A	45	0	0	0	0
31	B	1	0	0	0	0
31	J	1	0	0	0	0
31	X	1	0	0	0	0
32	A	44	0	26	8	0
33	A	14	0	26	4	0
34	A	40	0	39	11	0
35	A	17	0	0	0	0
36	O	1	0	0	0	0
37	P	4	0	0	0	0
37	T	4	0	0	0	0
38	X	31	0	12	0	0
39	X	32	0	13	0	0
All	All	66224	0	56686	358	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 3.

All (358) 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)
4:A:882:A:OP2	28:G:51:HIS:CE1	1.63	1.51
4:A:906:C:C2	28:G:50:ARG:HG2	1.56	1.40
4:A:906:C:O2	28:G:50:ARG:HG2	1.19	1.30
4:A:906:C:O4'	28:G:50:ARG:NH1	1.75	1.18
4:A:882:A:OP2	28:G:51:HIS:NE2	1.77	1.17
4:A:782:A:OP1	32:A:1701:NAD:O2D	1.72	1.07
4:A:906:C:O2	28:G:50:ARG:CG	2.05	1.04
4:A:906:C:C1'	28:G:50:ARG:NH1	2.20	1.04
4:A:1466:C:C6	8:F:162:LEU:CD2	2.46	0.99
4:A:1466:C:C6	8:F:162:LEU:HD22	1.98	0.97
4:A:882:A:P	28:G:51:HIS:CE1	2.58	0.97
4:A:1273:G:C6	4:A:1303:G:N1	2.37	0.93
4:A:882:A:OP2	28:G:51:HIS:HE1	1.44	0.93
4:A:906:C:C2	28:G:50:ARG:CG	2.50	0.93
4:A:1466:C:C5	8:F:162:LEU:HD22	2.07	0.87
4:A:1466:C:H6	8:F:162:LEU:HD21	1.41	0.85
4:A:1273:G:C6	4:A:1303:G:C2	2.63	0.85
4:A:904:C:O2	27:D:118:THR:OG1	1.95	0.85
4:A:1556:C:OP1	34:A:1703:SRY:N11	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1466:C:C6	8:F:162:LEU:HD21	2.14	0.82
4:A:878:G:OP1	28:G:51:HIS:HD2	1.64	0.81
9:H:134:TYR:OH	12:K:116:ASP:OD1	2.01	0.78
4:A:1235:U:OP1	12:K:36:ARG:NH2	2.17	0.77
4:A:1466:C:H6	8:F:162:LEU:CD2	1.92	0.76
4:A:904:C:H1'	27:D:119:LYS:CD	2.17	0.75
28:G:214:SER:N	28:G:217:ASP:OD2	2.19	0.75
4:A:906:C:O2	28:G:50:ARG:N	2.22	0.73
27:D:285:TYR:OH	27:D:372:GLU:OE2	2.05	0.73
21:T:132:ARG:NH1	21:T:136:LEU:O	2.22	0.72
13:L:126:GLU:HG2	13:L:177:VAL:HG11	1.71	0.71
14:M:63:GLU:OE1	19:R:191:ARG:NH1	2.24	0.71
4:A:841:A:OP1	14:M:39:ASN:ND2	2.25	0.70
4:A:1322:C:OP2	6:C:36:LYS:NZ	2.23	0.70
4:A:877:G:H5''	28:G:50:ARG:N	2.07	0.70
4:A:882:A:P	28:G:51:HIS:HE1	2.07	0.70
34:A:1703:SRY:O51	11:J:71:LYS:NZ	2.25	0.69
28:G:312:GLN:OE1	28:G:345:ARG:NH2	2.25	0.69
4:A:932:C:N3	21:T:11:ARG:NH1	2.41	0.69
24:X:268:LEU:O	24:X:294:ARG:NH1	2.26	0.68
4:A:769:G:OP2	15:N:73:ARG:NH2	2.25	0.68
4:A:781:A:H1'	32:A:1701:NAD:O1N	1.94	0.67
4:A:1273:G:O6	4:A:1303:G:N1	2.26	0.67
1:O:7:ARG:NH1	4:A:1511:C:OP1	2.26	0.67
6:C:115:ASN:ND2	25:Y:309:LYS:O	2.27	0.67
19:R:212:GLU:OE1	19:R:248:LYS:NZ	2.25	0.67
30:4:306:ASN:OD1	30:4:344:ARG:NH2	2.29	0.66
27:D:363:ALA:O	27:D:367:GLY:N	2.30	0.65
16:O:182:GLY:O	19:R:183:LYS:NZ	2.28	0.65
30:4:200:ASP:OD2	30:4:243:ASN:N	2.30	0.65
4:A:904:C:C2	27:D:119:LYS:HB3	2.33	0.64
4:A:1556:C:P	34:A:1703:SRY:HB11	2.20	0.64
6:C:37:ASN:O	6:C:43:ARG:NH2	2.30	0.64
13:L:86:ASP:OD1	13:L:87:ASP:N	2.30	0.64
1:O:29:ARG:NH2	4:A:1530:A:OP1	2.31	0.63
4:A:1555:A:H5''	34:A:1703:SRY:NB1	2.13	0.63
4:A:906:C:C1'	28:G:50:ARG:HH11	2.11	0.63
3:3:128:LYS:NZ	4:A:1107:U:O4	2.31	0.63
29:V:74:ARG:O	29:V:78:ASN:ND2	2.31	0.63
30:4:470:GLN:NE2	30:4:472:ASP:OD2	2.31	0.63
30:4:74:LEU:O	30:4:77:THR:OG1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:1701:NAD:H4N	13:L:195:TYR:HA	1.79	0.62
4:A:904:C:H1'	27:D:119:LYS:HD3	1.80	0.62
4:A:1273:G:C5	4:A:1303:G:N2	2.67	0.62
19:R:317:ALA:O	19:R:321:ALA:N	2.32	0.62
30:4:349:ALA:HB3	30:4:378:LEU:HD11	1.80	0.62
4:A:1273:G:O6	4:A:1303:G:C6	2.53	0.61
4:A:1287:A:OP2	27:D:260:LYS:NZ	2.30	0.61
6:C:124:LEU:O	6:C:132:TYR:OH	2.17	0.61
4:A:782:A:OP1	32:A:1701:NAD:C2D	2.47	0.61
4:A:1557:A:O2'	4:A:1558:A:O5'	2.18	0.61
12:K:60:ASN:OD1	12:K:68:GLN:NE2	2.33	0.61
4:A:906:C:H1'	28:G:50:ARG:NH1	2.16	0.61
4:A:781:A:C8	32:A:1701:NAD:H51A	2.36	0.60
4:A:1569:G:OP2	4:A:1572:A:O2'	2.18	0.60
1:0:19:ARG:NH1	4:A:808:C:OP1	2.34	0.60
4:A:906:C:C6	28:G:50:ARG:CZ	2.85	0.60
4:A:1555:A:H5''	34:A:1703:SRY:HB12	1.67	0.60
5:B:156:GLU:OE1	28:G:163:HIS:ND1	2.35	0.60
4:A:1199:G:N1	4:A:1422:G:OP2	2.34	0.60
4:A:904:C:C2	27:D:118:THR:OG1	2.54	0.60
2:1:56:ARG:NH2	30:4:81:ASP:OD2	2.34	0.59
34:A:1703:SRY:O61	11:J:71:LYS:NZ	2.33	0.59
28:G:388:ARG:O	28:G:390:LYS:NZ	2.32	0.59
30:4:239:ARG:O	30:4:242:ASN:ND2	2.36	0.59
8:F:50:TYR:O	8:F:66:ARG:NH2	2.36	0.59
18:Q:80:ARG:NH1	23:W:164:GLU:OE1	2.35	0.59
30:4:618:ALA:O	30:4:622:ASN:N	2.35	0.59
4:A:843:G:N2	4:A:846:A:OP2	2.30	0.58
19:R:161:ILE:O	21:T:125:HIS:NE2	2.36	0.58
4:A:1273:G:N1	4:A:1303:G:C2	2.70	0.58
6:C:152:ARG:NH1	25:Y:300:GLU:OE2	2.34	0.58
4:A:1048:C:O2'	32:A:1701:NAD:O2B	2.14	0.58
27:D:265:MET:SD	28:G:57:PRO:HD2	2.43	0.57
1:0:99:ARG:NH2	4:A:1528:A:OP1	2.37	0.57
4:A:1227:G:OP1	9:H:128:LYS:NZ	2.30	0.57
4:A:1583:MA6:H93	4:A:1584:MA6:C9	2.34	0.57
29:V:40:TRP:O	29:V:43:ARG:NH1	2.38	0.57
30:4:372:TYR:CE2	30:4:400:LEU:HD21	2.40	0.57
30:4:346:HIS:HA	30:4:378:LEU:HD12	1.85	0.57
4:A:904:C:O2	27:D:119:LYS:HB3	2.04	0.57
24:X:276:ARG:NH2	24:X:286:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:451:ASP:OD1	30:4:455:ASN:ND2	2.38	0.57
4:A:878:G:OP1	28:G:51:HIS:CD2	2.52	0.56
10:I:71:SER:O	10:I:74:ARG:NH1	2.37	0.56
4:A:906:C:H1'	28:G:50:ARG:HH11	1.70	0.56
4:A:1037:A:O2'	13:L:152:HIS:NE2	2.30	0.56
29:V:270:PRO:O	29:V:346:LYS:NZ	2.38	0.56
32:A:1701:NAD:H4N	13:L:194:LEU:O	2.05	0.56
18:Q:49:CYS:SG	18:Q:50:ARG:NH1	2.78	0.56
4:A:906:C:O2	28:G:50:ARG:CB	2.53	0.56
4:A:1231:A:OP1	12:K:88:ARG:NH2	2.27	0.56
30:4:478:TYR:OH	30:4:515:ASP:OD2	2.18	0.56
4:A:1555:A:C5'	34:A:1703:SRY:HB12	2.19	0.56
4:A:769:G:N2	4:A:772:A:OP2	2.38	0.55
34:A:1703:SRY:O51	11:J:71:LYS:CE	2.54	0.55
2:1:150:GLU:OE1	2:1:174:ARG:NH2	2.38	0.55
16:O:217:ARG:NH2	16:O:227:GLU:OE2	2.39	0.55
9:H:89:ASP:OD1	9:H:141:ARG:NH1	2.35	0.55
4:A:958:C:H4'	4:A:959:C:H5'	1.89	0.55
4:A:1443:U:OP2	12:K:102:ARG:NH2	2.40	0.55
19:R:103:TYR:OH	27:D:307:LYS:NZ	2.39	0.55
4:A:881:A:OP2	28:G:51:HIS:CE1	2.59	0.55
2:1:253:TRP:O	2:1:256:SER:OG	2.24	0.54
2:1:158:SER:OG	6:C:79:GLU:OE1	2.16	0.54
4:A:1271:C:H3'	4:A:1272:A:H8	1.71	0.54
4:A:1429:C:H4'	4:A:1430:A:H5''	1.89	0.54
24:X:147:LYS:HE2	24:X:147:LYS:HA	1.89	0.54
27:D:265:MET:SD	28:G:57:PRO:CD	2.96	0.54
4:A:1273:G:C5	4:A:1303:G:C2	2.96	0.54
4:A:934:G:O6	11:J:31:ALA:N	2.41	0.53
4:A:1556:C:P	34:A:1703:SRY:NB1	2.80	0.53
34:A:1703:SRY:O51	11:J:71:LYS:HE3	2.08	0.53
8:F:88:ASP:OD2	8:F:146:HIS:NE2	2.37	0.53
28:G:322:ARG:NH1	28:G:355:PHE:O	2.41	0.53
4:A:1048:C:P	33:A:1702:SPM:HN12	2.32	0.53
4:A:906:C:N1	28:G:50:ARG:CZ	2.72	0.53
4:A:1376:C:H4'	4:A:1377:C:H5'	1.90	0.53
4:A:684:U:O2'	21:T:151:SER:OG	2.25	0.53
4:A:1532:C:O2'	4:A:1533:C:OP1	2.23	0.53
19:R:219:TYR:O	19:R:256:ARG:NH1	2.42	0.52
4:A:1415:G:OP2	4:A:1415:G:N2	2.37	0.52
30:4:236:VAL:HG12	30:4:238:TRP:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1342:C:OP2	26:Z:96:LYS:NZ	2.36	0.52
4:A:1069:A:O2'	4:A:1587:U:O2	2.25	0.52
30:4:413:ASP:N	30:4:413:ASP:OD1	2.42	0.52
2:1:307:ASN:HD22	2:1:307:ASN:C	2.18	0.52
4:A:906:C:OP1	27:D:118:THR:HG22	2.10	0.51
4:A:1273:G:C6	4:A:1303:G:C6	2.98	0.51
4:A:906:C:C6	28:G:50:ARG:NH2	2.78	0.51
4:A:946:U:OP2	33:A:1702:SPM:N10	2.43	0.51
4:A:905:A:O2'	4:A:907:A:OP1	2.27	0.51
28:G:263:ASP:OD1	28:G:267:MET:N	2.42	0.51
2:1:103:LEU:O	2:1:107:LYS:HG3	2.11	0.51
16:O:73:VAL:O	16:O:109:ARG:NH2	2.43	0.51
4:A:860:A:N7	4:A:919:A:O2'	2.41	0.51
27:D:245:VAL:HG22	27:D:271:ALA:HB1	1.93	0.51
4:A:1488:5MC:O2	4:A:1584:MA6:O2'	2.20	0.50
4:A:1583:MA6:H93	4:A:1584:MA6:H92	1.92	0.50
4:A:906:C:OP1	27:D:118:THR:CG2	2.60	0.50
5:B:138:ARG:NH1	20:S:30:LEU:O	2.44	0.50
4:A:812:A:O2'	4:A:814:A:N1	2.45	0.50
4:A:904:C:H1'	27:D:119:LYS:HD2	1.90	0.50
4:A:1046:A:O2'	33:A:1702:SPM:H21	2.11	0.50
20:S:98:ARG:NH2	20:S:128:GLU:OE1	2.42	0.50
28:G:143:ASP:OD1	28:G:144:GLY:N	2.45	0.50
28:G:320:VAL:HG23	28:G:322:ARG:HG2	1.93	0.50
27:D:134:GLU:OE2	27:D:160:ARG:NH1	2.37	0.50
28:G:381:LYS:N	28:G:381:LYS:HD2	2.27	0.50
4:A:1583:MA6:H93	4:A:1584:MA6:N6	2.27	0.50
24:X:123:ARG:NH2	24:X:337:LEU:O	2.44	0.50
10:I:151:VAL:HG11	10:I:158:ARG:HG3	1.94	0.49
29:V:391:GLN:O	29:V:395:GLN:N	2.40	0.49
21:T:9:ILE:O	21:T:12:THR:OG1	2.24	0.49
27:D:165:GLN:NE2	27:D:169:GLU:OE2	2.46	0.49
1:O:41:LEU:HD13	1:O:55:TRP:CG	2.48	0.49
4:A:1451:U:OP1	28:G:382:PRO:O	2.30	0.49
14:M:123:GLN:O	14:M:127:ALA:N	2.41	0.49
4:A:904:C:O2	27:D:119:LYS:CB	2.61	0.49
2:1:306:GLU:OE2	24:X:127:TYR:OH	2.29	0.49
4:A:1343:A:O2'	4:A:1345:G:N7	2.42	0.49
29:V:266:VAL:HG21	29:V:275:LEU:HG	1.94	0.49
28:G:320:VAL:O	28:G:321:ASP:OD1	2.31	0.49
1:O:108:ASN:OD1	29:V:134:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:123:ASP:OD1	29:V:123:ASP:N	2.46	0.48
5:B:243:PRO:O	5:B:247:HIS:ND1	2.43	0.48
4:A:1046:A:OP2	33:A:1702:SPM:H61	2.13	0.48
1:O:54:ALA:O	1:O:58:VAL:HG23	2.14	0.48
27:D:173:ILE:HG23	27:D:176:ARG:NH2	2.28	0.48
28:G:270:SER:OG	28:G:351:ALA:O	2.28	0.48
20:S:75:TYR:O	20:S:79:GLY:N	2.47	0.48
24:X:347:ASN:HB3	24:X:386:ALA:O	2.14	0.48
4:A:745:A:H5'	14:M:11:ALA:HB2	1.95	0.47
28:G:237:GLU:OE2	28:G:237:GLU:N	2.41	0.47
2:1:217:GLN:NE2	25:Y:326:SER:O	2.42	0.47
4:A:1454:G:OP2	28:G:377:ARG:NH2	2.41	0.47
4:A:1555:A:C5'	34:A:1703:SRY:NB1	2.77	0.47
20:S:87:LEU:HD13	23:W:89:LEU:HD13	1.96	0.47
20:S:87:LEU:HD12	23:W:116:PHE:O	2.14	0.47
28:G:150:LEU:O	28:G:153:THR:OG1	2.31	0.47
2:1:60:MET:HE1	2:1:80:ALA:O	2.15	0.47
4:A:1465:C:H4'	8:F:162:LEU:HD23	1.96	0.47
30:4:436:HIS:O	30:4:440:LYS:HG2	2.15	0.47
1:O:84:SER:N	1:O:138:ASP:OD1	2.39	0.47
19:R:275:PHE:O	19:R:279:LYS:N	2.47	0.47
4:A:1267:U:H2'	4:A:1268:C:C6	2.50	0.47
22:U:137:LEU:O	22:U:141:ARG:N	2.40	0.47
6:C:39:ALA:O	6:C:41:ARG:NH1	2.47	0.47
11:J:78:ARG:NH1	11:J:117:ASP:OD2	2.47	0.47
4:A:1136:C:H2'	4:A:1137:A:H5''	1.96	0.47
4:A:1378:C:O2	24:X:389:SER:OG	2.26	0.47
30:4:493:MET:HA	30:4:493:MET:HE2	1.97	0.47
19:R:191:ARG:HG3	19:R:204:ILE:HG23	1.96	0.46
4:A:906:C:N1	28:G:50:ARG:NH1	2.61	0.46
29:V:361:LYS:O	29:V:361:LYS:HG2	2.15	0.46
22:U:80:ARG:O	22:U:84:GLU:N	2.49	0.46
4:A:1557:A:HO2'	4:A:1558:A:P	2.36	0.46
19:R:231:CYS:SG	19:R:242:TYR:HA	2.56	0.46
22:U:161:GLN:O	22:U:164:VAL:HG12	2.16	0.46
6:C:57:HIS:HB2	6:C:66:LYS:HD2	1.97	0.46
2:1:255:ASN:N	2:1:259:GLU:OE2	2.47	0.46
4:A:1416:A:H5'	4:A:1416:A:H8	1.81	0.46
8:F:176:ASP:OD2	8:F:180:ARG:NH1	2.49	0.46
29:V:46:GLU:OE2	29:V:74:ARG:NE	2.47	0.46
4:A:965:C:H3'	4:A:966:A:H5''	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:103:CYS:O	6:C:123:VAL:HA	2.16	0.46
25:Y:296:ASN:OD1	25:Y:298:PHE:N	2.49	0.46
4:A:974:U:O2'	4:A:975:A:N7	2.48	0.45
4:A:958:C:C4'	4:A:959:C:H5'	2.46	0.45
5:B:134:HIS:O	5:B:138:ARG:HG3	2.17	0.45
4:A:1531:C:O3'	4:A:1532:C:H6	1.98	0.45
16:O:137:ALA:HB3	16:O:138:PRO:HD3	1.99	0.45
1:O:68:LEU:HA	1:O:71:LEU:HD12	1.97	0.45
5:B:110:ARG:NH2	23:W:90:THR:O	2.49	0.45
6:C:58:ALA:HB1	6:C:59:PRO:CD	2.46	0.45
4:A:919:A:OP2	16:O:96:ARG:NH2	2.44	0.45
4:A:948:U:OP2	4:A:1045:G:N1	2.41	0.45
1:O:136:TYR:OH	4:A:705:C:OP2	2.27	0.45
4:A:1046:A:O2'	4:A:1048:C:OP2	2.28	0.45
4:A:1143:C:N4	4:A:1576:G:OP1	2.49	0.45
29:V:269:SER:HB2	29:V:270:PRO:HD2	1.98	0.45
5:B:239:ASN:ND2	5:B:242:SER:OG	2.50	0.44
9:H:121:LEU:HD21	9:H:128:LYS:HD2	1.99	0.44
28:G:384:GLN:HB3	28:G:389:ARG:O	2.17	0.44
4:A:1115:U:OP1	20:S:55:LYS:NZ	2.43	0.44
5:B:103:GLU:N	5:B:104:PRO:CD	2.80	0.44
6:C:89:ASP:O	6:C:93:ARG:HG3	2.18	0.44
28:G:395:LYS:O	28:G:396:ARG:OXT	2.36	0.44
29:V:252:LYS:O	29:V:258:ARG:NH1	2.50	0.44
12:K:90:ARG:NH1	12:K:95:SER:O	2.49	0.44
4:A:940:A:H8	4:A:940:A:H5''	1.83	0.44
4:A:1450:C:O2'	9:H:131:ARG:NH2	2.45	0.44
6:C:123:VAL:HG23	6:C:157:THR:HG22	2.00	0.44
24:X:80:PRO:HB2	24:X:190:ASN:OD1	2.17	0.44
28:G:116:LEU:O	28:G:122:ARG:NH2	2.45	0.44
1:O:110:ASP:OD1	1:O:110:ASP:N	2.40	0.44
22:U:84:GLU:O	22:U:84:GLU:HG2	2.18	0.44
24:X:48:ILE:O	24:X:48:ILE:HG12	2.18	0.44
30:4:58:VAL:HG23	30:4:58:VAL:O	2.17	0.44
25:Y:393:GLN:O	25:Y:393:GLN:HG3	2.19	0.43
4:A:1366:C:H3'	4:A:1367:A:H5'	2.01	0.43
24:X:186:THR:O	24:X:190:ASN:ND2	2.51	0.43
24:X:233:VAL:HG12	24:X:233:VAL:O	2.18	0.43
4:A:1078:A:N6	4:A:1563:U:OP1	2.50	0.43
24:X:369:GLU:CD	24:X:369:GLU:H	2.26	0.43
22:U:138:GLU:O	22:U:142:LYS:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:959:C:H2'	4:A:960:C:H5''	1.99	0.43
4:A:1273:G:C4	4:A:1303:G:N2	2.87	0.43
20:S:67:GLU:OE2	20:S:67:GLU:N	2.52	0.43
24:X:265:ILE:HG12	24:X:265:ILE:O	2.17	0.43
28:G:315:PHE:HB3	28:G:316:PRO:HD3	2.00	0.43
4:A:727:U:H2'	4:A:728:C:O4'	2.17	0.43
13:L:76:TYR:O	13:L:79:VAL:HG22	2.19	0.43
16:O:146:GLN:OE1	16:O:146:GLN:HA	2.18	0.43
26:Z:76:GLN:O	26:Z:80:ASP:N	2.49	0.43
2:1:118:ALA:O	2:1:122:HIS:N	2.45	0.43
4:A:1033:U:H4'	7:E:94:VAL:HG12	2.00	0.43
14:M:85:LYS:O	14:M:89:LYS:HG3	2.19	0.43
9:H:188:ILE:O	9:H:188:ILE:HG13	2.19	0.43
17:P:73:ASP:OD1	17:P:74:TYR:N	2.52	0.43
19:R:76:GLN:HA	19:R:76:GLN:OE1	2.19	0.43
4:A:1430:A:OP1	28:G:388:ARG:NH2	2.47	0.43
24:X:385:ASN:ND2	28:G:299:ASP:OD2	2.51	0.43
4:A:684:U:HO2'	21:T:151:SER:HG	1.57	0.43
13:L:221:LYS:HA	13:L:221:LYS:HE2	1.99	0.43
30:4:509:ILE:N	30:4:510:PRO:CD	2.82	0.43
11:J:70:PRO:HB3	11:J:117:ASP:HB3	1.99	0.42
12:K:55:ASN:OD1	12:K:58:ARG:NH2	2.51	0.42
19:R:262:LEU:O	19:R:265:THR:OG1	2.25	0.42
30:4:255:ASN:O	30:4:258:SER:OG	2.30	0.42
4:A:904:C:H1'	27:D:119:LYS:HB3	2.00	0.42
4:A:1198:A:C2'	4:A:1199:G:H5'	2.49	0.42
19:R:69:THR:OG1	19:R:72:ASP:OD1	2.37	0.42
19:R:107:THR:HG22	27:D:368:LEU:HD22	2.00	0.42
22:U:199:ARG:HG3	22:U:200:PRO:HD2	2.00	0.42
28:G:305:PRO:O	28:G:310:ARG:NH2	2.51	0.42
30:4:318:GLU:OE1	30:4:318:GLU:HA	2.19	0.42
4:A:1481:C:O2	4:A:1481:C:O2'	2.32	0.42
7:E:31:ASP:OD1	22:U:170:ARG:NH2	2.52	0.42
10:I:129:GLN:NE2	10:I:167:MET:SD	2.91	0.42
8:F:161:ILE:HD12	8:F:170:VAL:HG21	2.01	0.42
1:0:43:ARG:O	1:0:47:GLY:N	2.47	0.42
2:1:292:TYR:OH	24:X:338:ASP:OD1	2.36	0.42
4:A:1271:C:O2	4:A:1271:C:H2'	2.18	0.42
8:F:52:ARG:NH2	28:G:319:PHE:O	2.53	0.42
16:O:120:VAL:HG13	16:O:163:LEU:HD13	2.01	0.42
1:0:163:SER:HA	1:0:191:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:181:ILE:HG23	13:L:185:LEU:HD12	2.02	0.42
4:A:906:C:O2	28:G:50:ARG:CA	2.67	0.42
24:X:196:GLU:OE2	24:X:196:GLU:HA	2.20	0.42
4:A:663:A:H2'	4:A:664:G:C8	2.55	0.41
7:E:109:VAL:HG23	7:E:109:VAL:O	2.20	0.41
8:F:235:ALA:O	8:F:238:HIS:NE2	2.53	0.41
4:A:781:A:O2'	32:A:1701:NAD:H2D	2.20	0.41
4:A:928:A:OP2	11:J:47:ARG:NH2	2.53	0.41
4:A:1079:G:C2'	4:A:1080:A:H5'	2.50	0.41
9:H:50:LEU:HD13	9:H:53:ASP:O	2.21	0.41
13:L:123:ARG:O	13:L:123:ARG:HG2	2.21	0.41
21:T:103:ARG:O	21:T:103:ARG:HG2	2.21	0.41
27:D:316:CYS:HB3	27:D:334:ALA:HB3	2.03	0.41
29:V:376:GLU:HA	29:V:376:GLU:OE1	2.20	0.41
9:H:84:ASP:OD1	28:G:115:GLY:HA3	2.21	0.41
17:P:54:MET:HG2	17:P:55:GLU:N	2.35	0.41
24:X:103:LYS:N	24:X:104:PRO:CD	2.84	0.41
2:1:173:LEU:HD23	2:1:173:LEU:C	2.45	0.41
4:A:1119:U:O4'	20:S:50:ARG:NH1	2.51	0.41
4:A:1136:C:C2'	4:A:1137:A:H5''	2.49	0.41
9:H:184:ILE:HG22	9:H:184:ILE:O	2.20	0.41
19:R:315:GLN:HA	19:R:315:GLN:OE1	2.19	0.41
9:H:76:LEU:HB2	9:H:148:LEU:HD13	2.01	0.41
24:X:151:LEU:HD21	24:X:247:LEU:HD22	2.02	0.41
30:4:508:VAL:O	30:4:508:VAL:HG12	2.20	0.41
5:B:157:ASN:OD1	28:G:163:HIS:NE2	2.53	0.41
13:L:212:ARG:NH1	13:L:216:GLU:OE2	2.49	0.41
6:C:53:TYR:OH	6:C:65:ARG:O	2.23	0.41
6:C:84:GLU:O	6:C:88:GLU:HG3	2.21	0.41
11:J:70:PRO:HD3	11:J:76:ALA:O	2.20	0.41
20:S:35:TYR:C	20:S:35:TYR:CD1	2.98	0.41
30:4:650:MET:HA	30:4:654:ALA:HB3	2.03	0.41
6:C:62:ILE:O	6:C:66:LYS:O	2.38	0.41
11:J:95:ILE:HG12	11:J:102:LEU:HD12	2.03	0.41
16:O:220:TYR:O	16:O:224:LEU:HG	2.21	0.41
19:R:242:TYR:CD1	19:R:242:TYR:C	2.99	0.41
30:4:290:ASP:OD1	30:4:293:THR:OG1	2.37	0.41
4:A:1271:C:H3'	4:A:1272:A:C8	2.55	0.41
4:A:1591:C:OP1	18:Q:48:PRO:HB2	2.21	0.41
6:C:58:ALA:HB3	6:C:60:HIS:CE1	2.56	0.41
12:K:52:LEU:HD11	26:Z:36:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:56:GLU:OE1	30:4:56:GLU:HA	2.21	0.40
4:A:1106:C:O2'	4:A:1108:C:OP2	2.19	0.40
27:D:263:ASP:OD1	27:D:264:ARG:N	2.53	0.40
9:H:50:LEU:HD12	30:4:79:ASN:HB3	2.02	0.40
16:O:71:ARG:HB3	16:O:72:PRO:HD2	2.03	0.40
29:V:269:SER:HB2	29:V:273:ILE:HD12	2.03	0.40
8:F:71:THR:O	28:G:253:LYS:NZ	2.50	0.40
12:K:101:LYS:HD3	12:K:101:LYS:HA	1.96	0.40
13:L:83:GLU:HA	13:L:83:GLU:OE1	2.21	0.40
3:3:150:THR:HG22	3:3:150:THR:O	2.22	0.40
3:3:177:TRP:CD1	3:3:177:TRP:C	2.99	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	0	213/218 (98%)	207 (97%)	6 (3%)	0	100	100
2	1	274/323 (85%)	260 (95%)	14 (5%)	0	100	100
3	3	68/199 (34%)	65 (96%)	3 (4%)	0	100	100
5	B	223/296 (75%)	212 (95%)	11 (5%)	0	100	100
6	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
7	E	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
8	F	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
9	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	56
10	I	135/194 (70%)	126 (93%)	8 (6%)	1 (1%)	18	56
11	J	106/138 (77%)	100 (94%)	6 (6%)	0	100	100
12	K	99/128 (77%)	99 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	L	172/257 (67%)	168 (98%)	4 (2%)	0	100	100
14	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
15	N	108/130 (83%)	101 (94%)	7 (6%)	0	100	100
16	O	192/258 (74%)	184 (96%)	8 (4%)	0	100	100
17	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
18	Q	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
19	R	293/360 (81%)	287 (98%)	6 (2%)	0	100	100
20	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
21	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
22	U	174/205 (85%)	171 (98%)	3 (2%)	0	100	100
23	W	98/187 (52%)	93 (95%)	5 (5%)	0	100	100
24	X	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
25	Y	147/395 (37%)	145 (99%)	2 (1%)	0	100	100
26	Z	98/106 (92%)	94 (96%)	4 (4%)	0	100	100
27	D	335/430 (78%)	323 (96%)	12 (4%)	0	100	100
28	G	314/396 (79%)	302 (96%)	12 (4%)	0	100	100
29	V	358/414 (86%)	350 (98%)	8 (2%)	0	100	100
30	4	584/689 (85%)	563 (96%)	21 (4%)	0	100	100
All	All	5530/7184 (77%)	5362 (97%)	166 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	I	184	ASN
9	H	126	ILE

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	0	188/190 (99%)	187 (100%)	1 (0%)	81	83
2	1	254/291 (87%)	253 (100%)	1 (0%)	84	84
3	3	65/166 (39%)	65 (100%)	0	100	100
5	B	198/249 (80%)	198 (100%)	0	100	100
6	C	115/143 (80%)	115 (100%)	0	100	100
7	E	104/107 (97%)	104 (100%)	0	100	100
8	F	185/209 (88%)	185 (100%)	0	100	100
9	H	130/180 (72%)	130 (100%)	0	100	100
10	I	105/147 (71%)	105 (100%)	0	100	100
11	J	93/118 (79%)	93 (100%)	0	100	100
12	K	91/113 (80%)	91 (100%)	0	100	100
13	L	158/226 (70%)	158 (100%)	0	100	100
14	M	97/113 (86%)	97 (100%)	0	100	100
15	N	96/115 (84%)	96 (100%)	0	100	100
16	O	175/230 (76%)	175 (100%)	0	100	100
17	P	88/123 (72%)	88 (100%)	0	100	100
18	Q	78/78 (100%)	78 (100%)	0	100	100
19	R	264/318 (83%)	264 (100%)	0	100	100
20	S	116/164 (71%)	116 (100%)	0	100	100
21	T	153/157 (98%)	153 (100%)	0	100	100
22	U	152/174 (87%)	152 (100%)	0	100	100
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	311/351 (89%)	310 (100%)	1 (0%)	86	86
25	Y	137/357 (38%)	137 (100%)	0	100	100
26	Z	90/95 (95%)	90 (100%)	0	100	100
27	D	282/357 (79%)	282 (100%)	0	100	100
28	G	281/342 (82%)	281 (100%)	0	100	100
29	V	325/364 (89%)	325 (100%)	0	100	100
30	4	526/609 (86%)	525 (100%)	1 (0%)	87	87
All	All	4944/6244 (79%)	4940 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	79	LEU
2	1	307	ASN
24	X	81	HIS
30	4	577	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	137	HIS
1	0	145	HIS
7	E	81	HIS
8	F	169	GLN
8	F	207	HIS
8	F	224	HIS
9	H	147	HIS
10	I	87	HIS
11	J	105	HIS
11	J	134	HIS
12	K	28	HIS
13	L	162	GLN
16	O	166	HIS
16	O	223	HIS
19	R	214	ASN
20	S	66	HIS
21	T	51	ASN
23	W	106	HIS
24	X	140	HIS
24	X	291	HIS
27	D	347	GLN
27	D	359	HIS
27	D	369	HIS
27	D	415	GLN
28	G	51	HIS
28	G	87	HIS
28	G	308	GLN
29	V	38	HIS
29	V	87	HIS
29	V	188	HIS
29	V	215	GLN
30	4	489	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	954/955 (99%)	283 (29%)	11 (1%)

All (283) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	649	A
4	A	657	G
4	A	676	G
4	A	680	U
4	A	688	A
4	A	689	U
4	A	690	U
4	A	693	A
4	A	695	A
4	A	704	U
4	A	715	G
4	A	718	A
4	A	721	U
4	A	722	C
4	A	723	A
4	A	724	C
4	A	730	A
4	A	737	C
4	A	738	A
4	A	749	G
4	A	753	A
4	A	757	A
4	A	760	A
4	A	761	A
4	A	763	C
4	A	764	A
4	A	770	C
4	A	776	A
4	A	777	G
4	A	791	G
4	A	792	C
4	A	793	C
4	A	794	U
4	A	796	G
4	A	801	A
4	A	803	C
4	A	804	C
4	A	806	C

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Mol	Chain	Res	Type
4	A	807	A
4	A	808	C
4	A	814	A
4	A	815	C
4	A	826	A
4	A	828	C
4	A	829	C
4	A	830	U
4	A	832	U
4	A	835	C
4	A	836	A
4	A	844	A
4	A	859	U
4	A	860	A
4	A	861	U
4	A	868	C
4	A	869	C
4	A	870	C
4	A	871	A
4	A	879	U
4	A	881	A
4	A	889	G
4	A	890	C
4	A	896	A
4	A	902	G
4	A	903	U
4	A	904	C
4	A	905	A
4	A	907	A
4	A	908	C
4	A	919	A
4	A	922	C
4	A	929	A
4	A	930	G
4	A	931	C
4	A	932	C
4	A	933	G
4	A	935	C
4	A	937	U
4	A	938	A
4	A	939	A
4	A	940	A

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Mol	Chain	Res	Type
4	A	941	G
4	A	942	A
4	A	953	U
4	A	955	A
4	A	956	C
4	A	957	C
4	A	958	C
4	A	959	C
4	A	960	C
4	A	962	C
4	A	965	C
4	A	966	A
4	A	967	A
4	A	974	U
4	A	975	A
4	A	987	A
4	A	992	U
4	A	999	C
4	A	1001	C
4	A	1002	C
4	A	1011	C
4	A	1015	A
4	A	1017	A
4	A	1018	G
4	A	1021	U
4	A	1031	G
4	A	1038	C
4	A	1039	A
4	A	1040	U
4	A	1042	U
4	A	1049	A
4	A	1050	C
4	A	1064	C
4	A	1065	C
4	A	1069	A
4	A	1074	G
4	A	1078	A
4	A	1080	A
4	A	1081	U
4	A	1082	A
4	A	1100	C
4	A	1103	A

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Mol	Chain	Res	Type
4	A	1105	C
4	A	1106	C
4	A	1107	U
4	A	1108	C
4	A	1109	A
4	A	1110	A
4	A	1115	U
4	A	1116	A
4	A	1117	A
4	A	1118	A
4	A	1119	U
4	A	1120	C
4	A	1121	A
4	A	1122	A
4	A	1125	A
4	A	1126	A
4	A	1127	A
4	A	1136	C
4	A	1138	G
4	A	1139	A
4	A	1144	U
4	A	1151	C
4	A	1153	C
4	A	1155	G
4	A	1160	A
4	A	1166	A
4	A	1178	G
4	A	1179	G
4	A	1181	G
4	A	1185	C
4	A	1187	U
4	A	1188	A
4	A	1189	U
4	A	1190	C
4	A	1194	C
4	A	1199	G
4	A	1200	G
4	A	1201	A
4	A	1213	A
4	A	1215	U
4	A	1219	U
4	A	1221	A

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Mol	Chain	Res	Type
4	A	1222	A
4	A	1223	C
4	A	1225	C
4	A	1227	G
4	A	1231	A
4	A	1233	C
4	A	1237	A
4	A	1244	C
4	A	1245	U
4	A	1246	U
4	A	1247	G
4	A	1248	C
4	A	1249	U
4	A	1250	C
4	A	1251	A
4	A	1253	C
4	A	1256	A
4	A	1266	A
4	A	1267	U
4	A	1269	U
4	A	1271	C
4	A	1273	G
4	A	1282	G
4	A	1284	U
4	A	1286	A
4	A	1289	G
4	A	1290	C
4	A	1291	U
4	A	1292	A
4	A	1295	A
4	A	1298	U
4	A	1309	A
4	A	1310	C
4	A	1311	C
4	A	1312	C
4	A	1313	A
4	A	1320	G
4	A	1325	U
4	A	1326	A
4	A	1327	G
4	A	1329	U
4	A	1336	G

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Mol	Chain	Res	Type
4	A	1341	C
4	A	1342	C
4	A	1343	A
4	A	1345	G
4	A	1352	C
4	A	1354	A
4	A	1355	G
4	A	1357	A
4	A	1358	A
4	A	1368	U
4	A	1377	C
4	A	1378	C
4	A	1379	A
4	A	1382	A
4	A	1383	A
4	A	1384	A
4	A	1385	C
4	A	1387	A
4	A	1389	G
4	A	1390	A
4	A	1391	U
4	A	1392	A
4	A	1399	A
4	A	1402	A
4	A	1404	A
4	A	1405	C
4	A	1407	U
4	A	1415	G
4	A	1416	A
4	A	1419	G
4	A	1421	G
4	A	1430	A
4	A	1443	U
4	A	1444	A
4	A	1447	G
4	A	1448	U
4	A	1465	C
4	A	1466	C
4	A	1478	A
4	A	1480	A
4	A	1482	A
4	A	1483	C

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Mol	Chain	Res	Type
4	A	1493	C
4	A	1501	A
4	A	1511	C
4	A	1512	A
4	A	1516	G
4	A	1519	A
4	A	1522	U
4	A	1523	A
4	A	1524	A
4	A	1525	C
4	A	1527	A
4	A	1529	A
4	A	1532	C
4	A	1533	C
4	A	1536	A
4	A	1537	C
4	A	1539	C
4	A	1553	A
4	A	1558	A
4	A	1563	U
4	A	1564	A
4	A	1565	A
4	A	1568	U
4	A	1571	U
4	A	1572	A
4	A	1582	G
4	A	1583	MA6
4	A	1584	MA6
4	A	1593	U
4	A	1594	G
4	A	1595	G
4	A	1597	C
4	A	1598	G
4	A	1599	A
4	A	1602	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	723	A
4	A	930	G
4	A	965	C

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Mol	Chain	Res	Type
4	A	1246	U
4	A	1342	C
4	A	1465	C
4	A	1488	5MC
4	A	1512	A
4	A	1531	C
4	A	1532	C
4	A	1557	A

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

6 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
4	5MC	A	1488	4	19,22,23	1.70	3 (15%)	26,32,35	1.91	8 (30%)
4	MA6	A	1583	4	23,26,27	0.84	1 (4%)	33,38,41	2.09	9 (27%)
4	MA6	A	1584	4	23,26,27	0.84	1 (4%)	33,38,41	2.13	9 (27%)
4	5MU	A	1076	4	19,22,23	1.13	3 (15%)	27,32,35	2.19	8 (29%)
4	B8T	A	1486	4	19,22,23	0.89	2 (10%)	25,31,34	0.99	1 (4%)
18	AYA	Q	2	18	6,7,8	1.39	1 (16%)	6,8,10	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5MC	A	1488	4	-	0/7/25/26	0/2/2/2
4	MA6	A	1583	4	-	0/11/29/30	0/3/3/3
4	MA6	A	1584	4	-	1/11/29/30	0/3/3/3
4	5MU	A	1076	4	-	0/7/25/26	0/2/2/2
4	B8T	A	1486	4	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	AYA	Q	2	18	-	1/5/6/8	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1488	5MC	C5-C4	-5.32	1.40	1.44
18	Q	2	AYA	CA-N	-2.87	1.43	1.46
4	A	1488	5MC	C2-N1	-2.79	1.34	1.40
4	A	1076	5MU	C4-C5	-2.77	1.40	1.44
4	A	1076	5MU	C2-N1	-2.70	1.34	1.38
4	A	1486	B8T	C2-N1	-2.28	1.35	1.40
4	A	1584	MA6	C5-N7	-2.28	1.34	1.39
4	A	1486	B8T	C6-N1	2.22	1.43	1.38
4	A	1583	MA6	C5-N7	-2.11	1.35	1.39
4	A	1488	5MC	C2'-C3'	-2.08	1.47	1.53
4	A	1076	5MU	C4-N3	-2.06	1.35	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1076	5MU	C4-N3-C2	-5.58	120.03	127.34
4	A	1584	MA6	C5-C4-N3	-5.15	119.62	126.72
4	A	1583	MA6	N1-C2-N3	-4.85	121.25	128.58
4	A	1076	5MU	N3-C2-N1	4.75	121.07	114.89
4	A	1584	MA6	N1-C2-N3	-4.73	121.42	128.58
4	A	1583	MA6	C5-C4-N3	-4.54	120.47	126.72
4	A	1583	MA6	C2-N1-C6	4.49	122.80	111.83
4	A	1584	MA6	C2-N1-C6	4.33	122.41	111.83
4	A	1076	5MU	C5-C4-N3	4.30	119.06	115.32
4	A	1076	5MU	O4-C4-C5	-4.27	120.03	124.92
4	A	1488	5MC	O3'-C3'-C4'	4.18	123.10	111.08
4	A	1584	MA6	C5-N7-C8	4.10	109.90	103.45
4	A	1583	MA6	C5-N7-C8	4.01	109.76	103.45
4	A	1584	MA6	N3-C4-N9	3.91	133.82	127.17
4	A	1488	5MC	O3'-C3'-C2'	3.79	123.98	111.82
4	A	1584	MA6	C2-N3-C4	3.72	120.92	111.83
4	A	1583	MA6	N3-C4-N9	3.70	133.45	127.17
4	A	1583	MA6	C2-N3-C4	3.52	120.43	111.83
4	A	1488	5MC	C5-C6-N1	-3.49	119.53	123.31
4	A	1584	MA6	C4-C5-N7	-3.47	106.61	110.58
4	A	1583	MA6	N9-C8-N7	-3.35	109.18	113.94
4	A	1583	MA6	C4-C5-N7	-3.28	106.83	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1488	5MC	O2'-C2'-C3'	3.11	121.79	111.82
4	A	1076	5MU	C5-C6-N1	-3.10	119.94	123.31
4	A	1584	MA6	N9-C8-N7	-3.05	109.61	113.94
4	A	1076	5MU	C5M-C5-C6	-2.62	119.31	122.85
4	A	1076	5MU	O2-C2-N1	-2.61	119.40	122.80
4	A	1488	5MC	O2'-C2'-C1'	2.54	118.84	110.10
4	A	1488	5MC	CM5-C5-C6	-2.51	119.46	122.85
4	A	1583	MA6	C4-N9-C8	2.30	108.15	105.74
4	A	1488	5MC	C1'-N1-C6	-2.23	117.48	121.15
4	A	1584	MA6	C4-C5-C6	2.22	118.21	115.91
4	A	1488	5MC	C5-C4-N3	-2.22	119.48	121.75
4	A	1076	5MU	C6-C5-C4	2.13	119.78	118.02
4	A	1486	B8T	C5-C4-N4	-2.11	117.77	122.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	Q	2	AYA	C-CA-N-CT
4	A	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1488	5MC	1	0
4	A	1583	MA6	3	0
4	A	1584	MA6	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 67 are monoatomic - leaving 7 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	$\# Z > 2$
32	NAD	A	1701	31	46,48,48	1.02	2 (4%)	64,73,73	1.54	9 (14%)
33	SPM	A	1702	-	13,13,13	0.16	0	12,12,12	1.15	0
34	SRY	A	1703	-	40,42,42	0.80	2 (5%)	49,63,63	1.26	5 (10%)
38	ATP	X	402	31	32,33,33	1.31	5 (15%)	48,52,52	1.72	9 (18%)
39	GNP	X	403	-	34,34,34	1.28	5 (14%)	47,54,54	0.91	0
37	FES	P	201	7,17	0,4,4	-	-	-		
37	FES	T	201	14,21	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	NAD	A	1701	31	-	1/30/62/62	0/5/5/5
33	SPM	A	1702	-	-	0/11/11/11	-
34	SRY	A	1703	-	-	1/20/87/87	0/3/3/3
38	ATP	X	402	31	-	0/22/38/38	0/3/3/3
39	GNP	X	403	-	-	4/18/38/38	0/3/3/3
37	FES	P	201	7,17	-	-	0/1/1/1
37	FES	T	201	14,21	-	-	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	X	403	GNP	PB-O3A	4.30	1.64	1.59
38	X	402	ATP	C5-C4	4.23	1.46	1.39
39	X	403	GNP	PB-O1B	3.15	1.50	1.46
34	A	1703	SRY	CD1-N31	2.95	1.38	1.33
39	X	403	GNP	PG-N3B	2.90	1.70	1.63
32	A	1701	NAD	C2N-N1N	-2.82	1.31	1.35
32	A	1701	NAD	O4D-C1D	2.79	1.44	1.40
39	X	403	GNP	PG-O1G	2.75	1.50	1.46
34	A	1703	SRY	CA1-N11	2.72	1.37	1.33
38	X	402	ATP	C5-N7	-2.52	1.34	1.39
38	X	402	ATP	C5-C6	2.38	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	402	ATP	C8-N7	2.29	1.36	1.31
39	X	403	GNP	PB-O2B	-2.22	1.50	1.56
38	X	402	ATP	C4-N9	-2.07	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	X	402	ATP	C5-C4-N3	-5.64	118.95	126.72
32	A	1701	NAD	C5A-C4A-N3A	-5.52	119.12	126.72
34	A	1703	SRY	C12-O42-C42	-4.54	101.14	108.48
38	X	402	ATP	N3-C4-N9	4.50	134.82	127.17
32	A	1701	NAD	N3A-C2A-N1A	-4.26	122.13	128.58
32	A	1701	NAD	N3A-C4A-N9A	4.12	134.18	127.17
38	X	402	ATP	C2-N3-C4	3.85	121.24	111.83
38	X	402	ATP	N3-C2-N1	-3.72	122.95	128.58
32	A	1701	NAD	C2A-N3A-C4A	3.58	120.58	111.83
32	A	1701	NAD	C5A-N7A-C8A	3.57	109.06	103.45
32	A	1701	NAD	C4A-C5A-N7A	-3.26	106.85	110.58
34	A	1703	SRY	O42-C12-C22	-3.24	103.84	107.31
38	X	402	ATP	C4-C5-N7	-3.22	106.90	110.58
38	X	402	ATP	C4-N9-C8	2.82	108.70	105.74
38	X	402	ATP	C5-N7-C8	2.46	107.32	103.45
32	A	1701	NAD	N9A-C8A-N7A	-2.40	110.54	113.94
34	A	1703	SRY	C41-C31-N31	-2.26	107.30	110.91
34	A	1703	SRY	CI3-N23-C23	-2.24	111.34	114.23
38	X	402	ATP	N9-C8-N7	-2.17	110.86	113.94
38	X	402	ATP	C6-C5-N7	2.12	136.17	132.09
34	A	1703	SRY	CH2-C42-C32	-2.10	111.91	116.27
32	A	1701	NAD	O7N-C7N-N7N	-2.09	119.59	122.62
32	A	1701	NAD	C2A-N1A-C6A	2.03	122.07	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

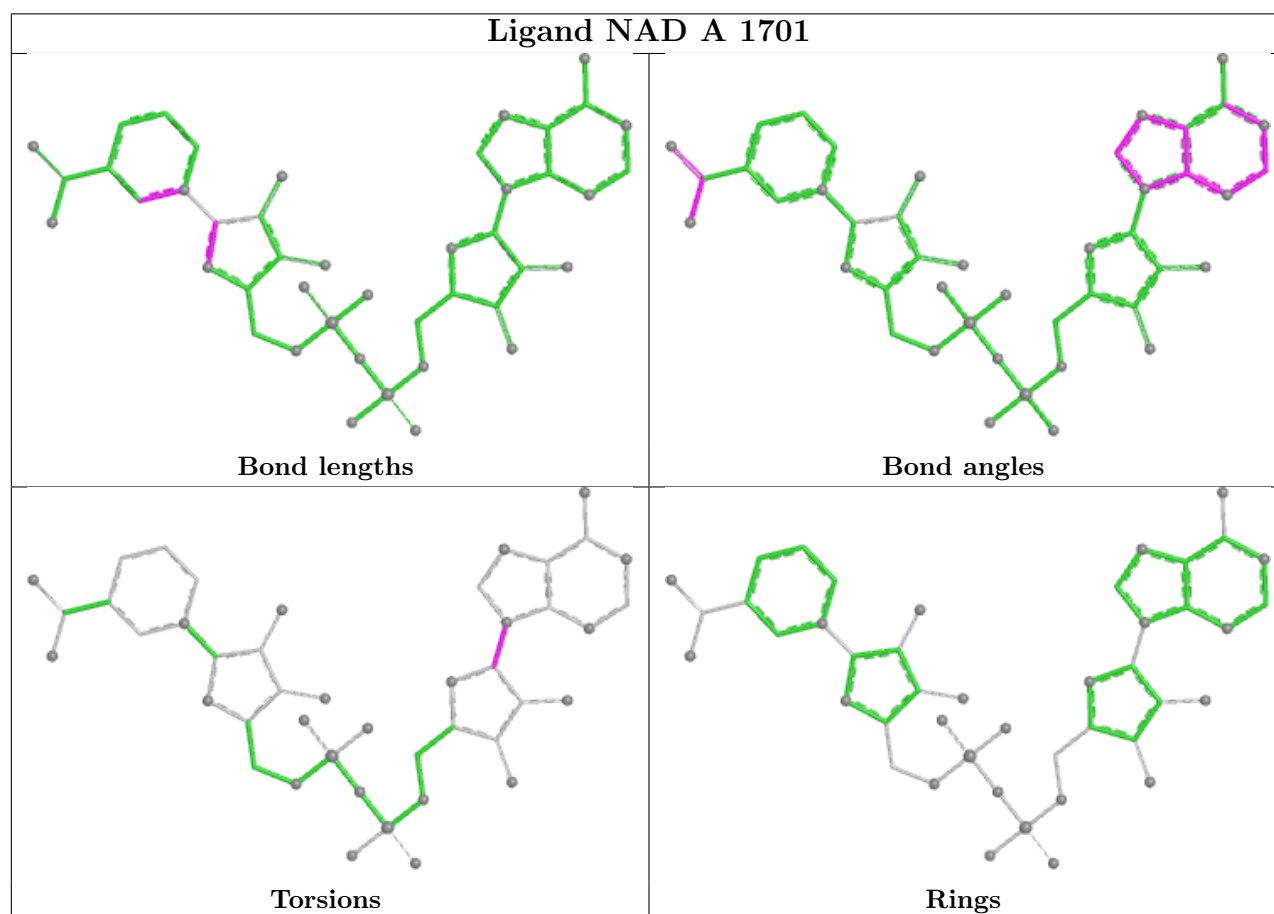
Mol	Chain	Res	Type	Atoms
39	X	403	GNP	PG-N3B-PB-O3A
39	X	403	GNP	PA-O3A-PB-O2B
39	X	403	GNP	C5'-O5'-PA-O1A
34	A	1703	SRY	C13-C23-N23-CI3
39	X	403	GNP	PG-N3B-PB-O1B
32	A	1701	NAD	C2B-C1B-N9A-C8A

There are no ring outliers.

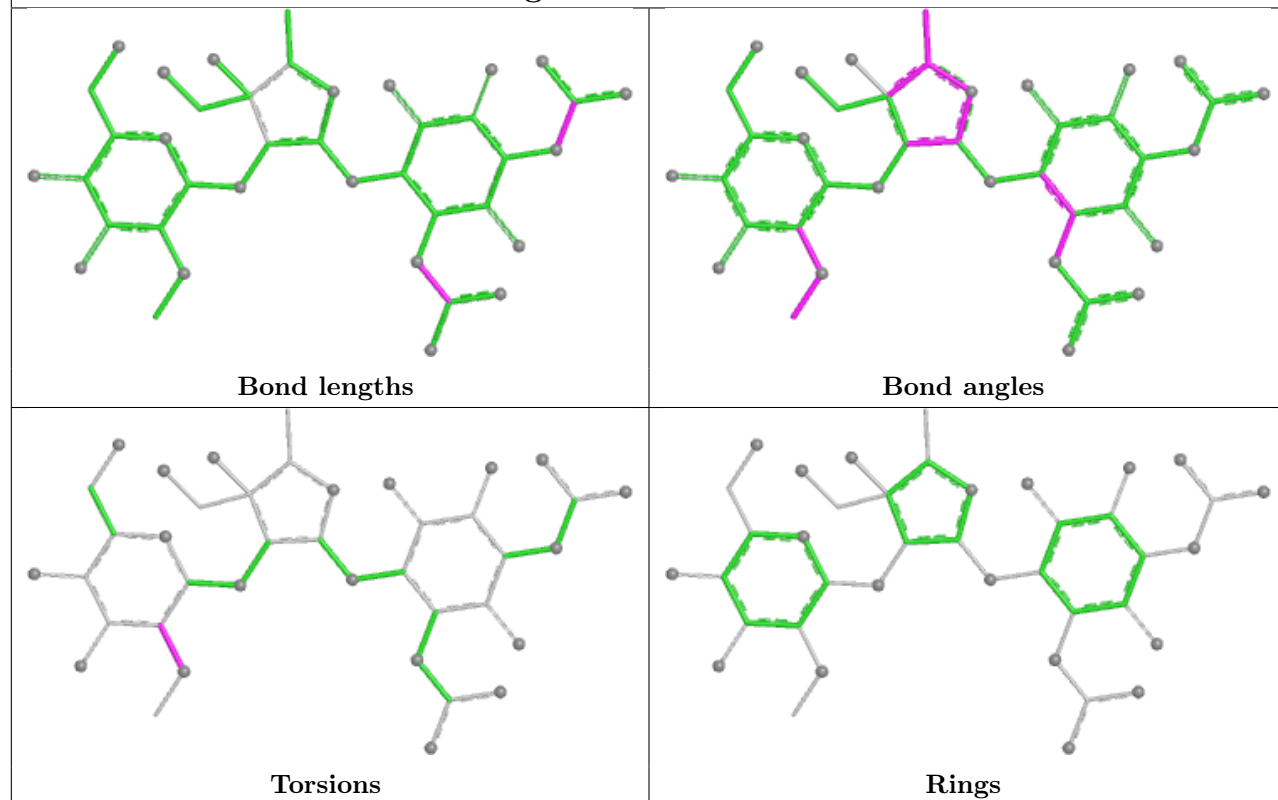
3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	1701	NAD	8	0
33	A	1702	SPM	4	0
34	A	1703	SRY	11	0

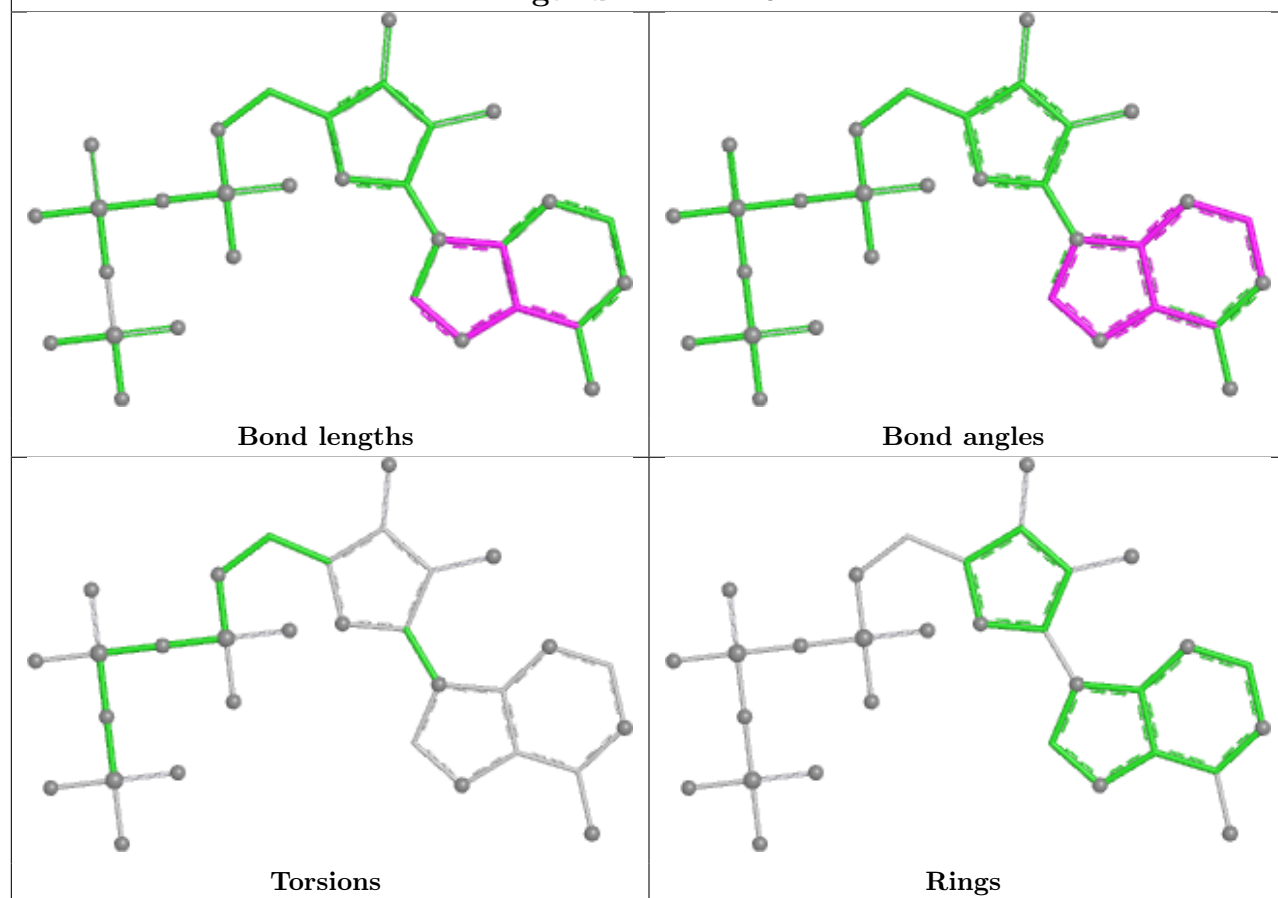
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

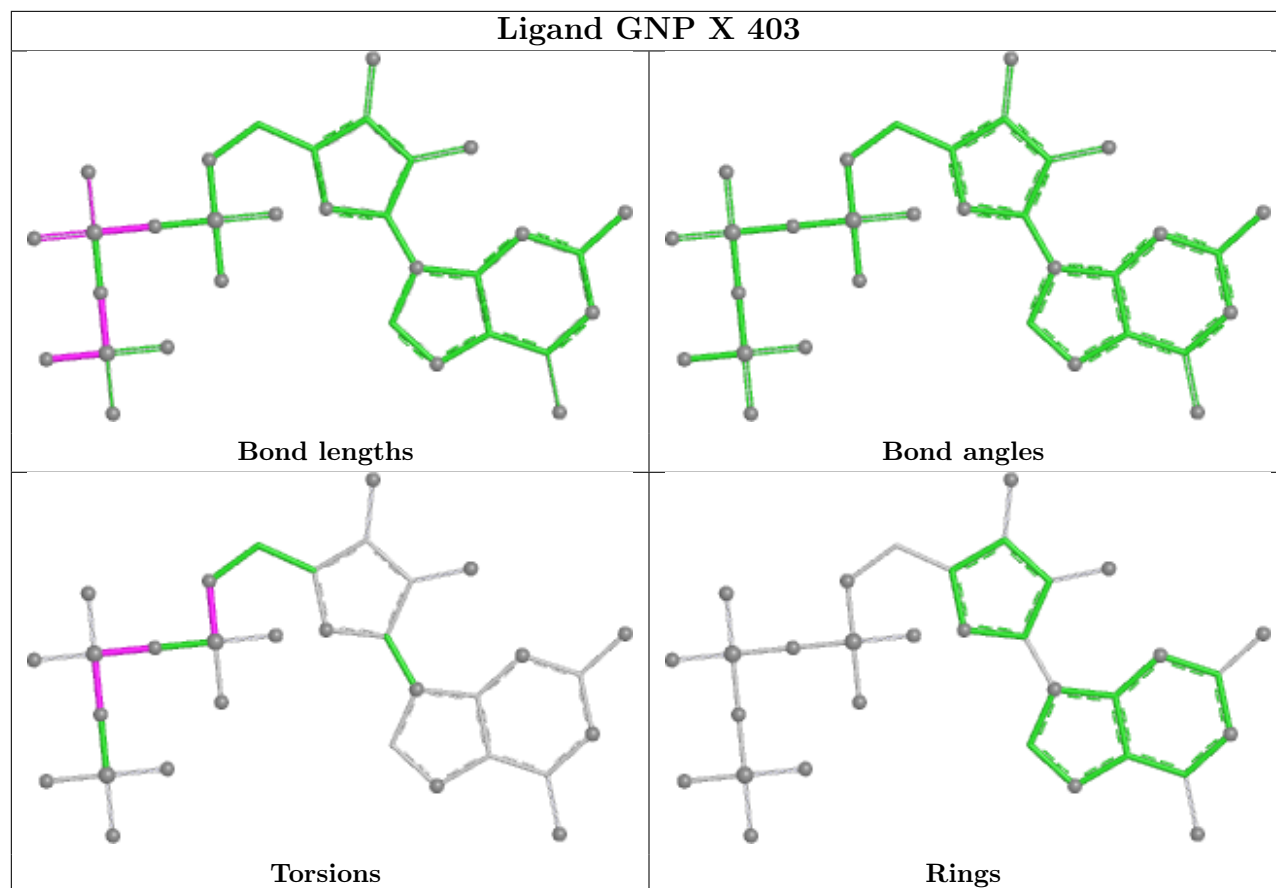


Ligand SRY A 1703



Ligand ATP X 402





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.

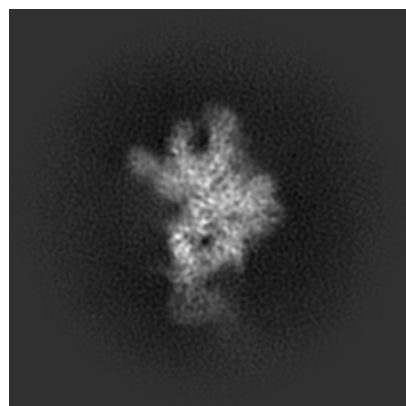
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18438. These allow visual inspection of the internal detail of the map and identification of artifacts.

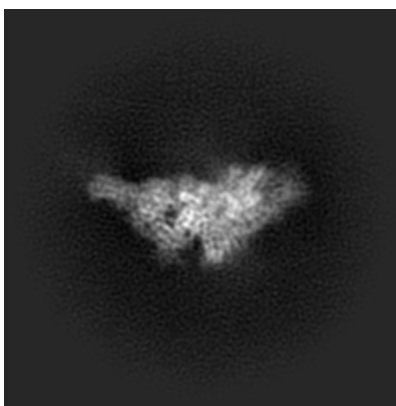
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

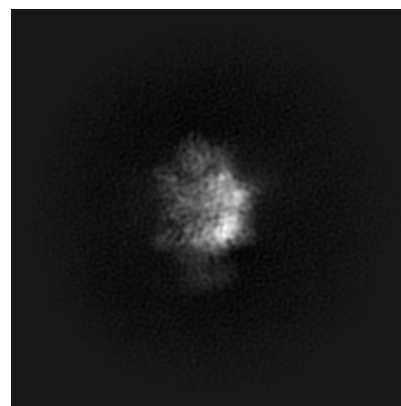
6.1.1 Primary map



X

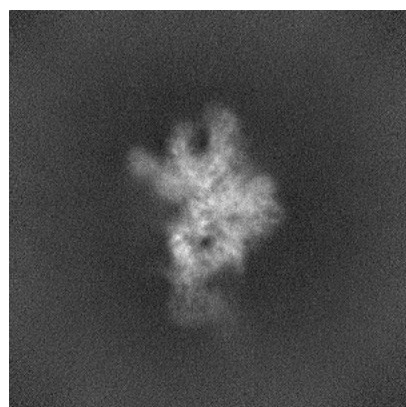


Y

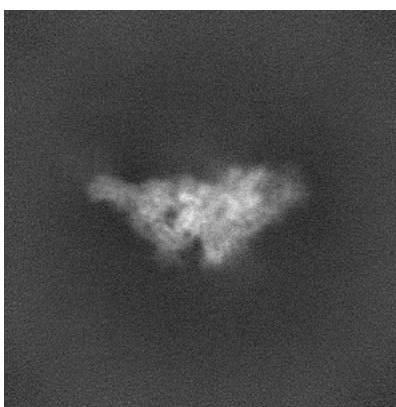


Z

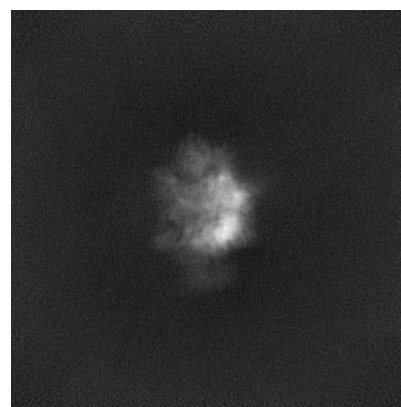
6.1.2 Raw map



X



Y

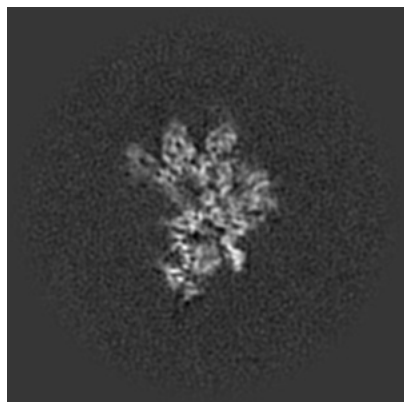


Z

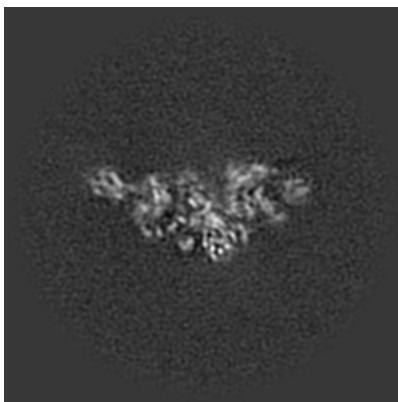
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

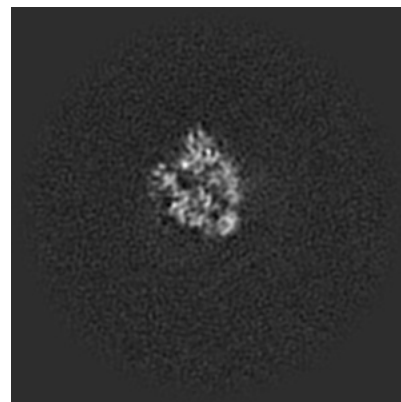
6.2.1 Primary map



X Index: 256

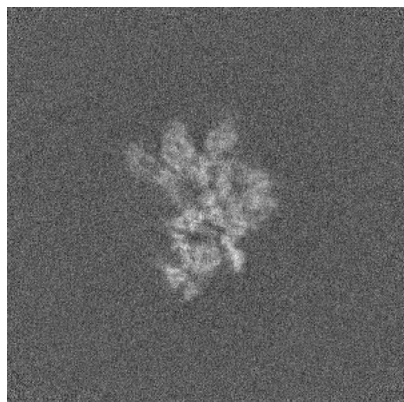


Y Index: 256

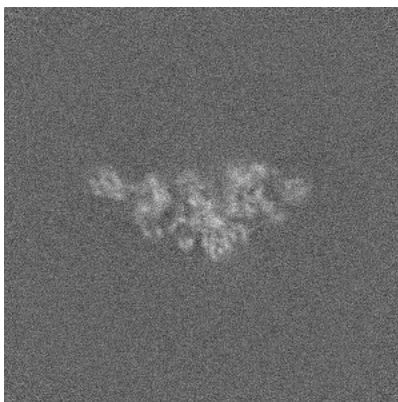


Z Index: 256

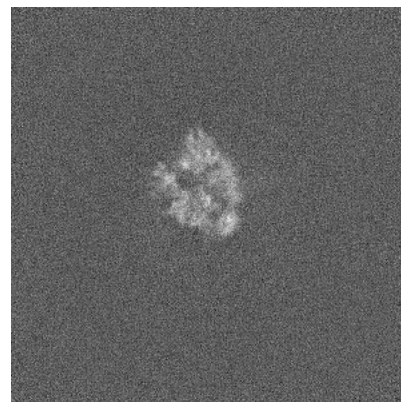
6.2.2 Raw map



X Index: 256



Y Index: 256

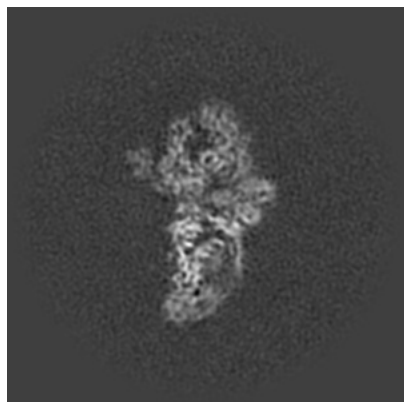


Z Index: 256

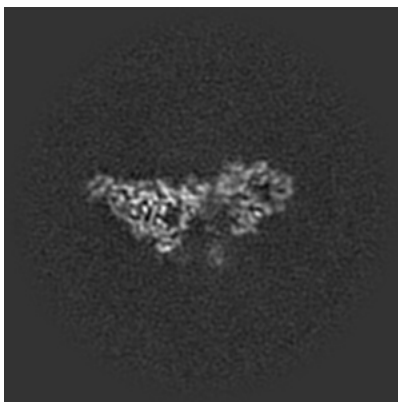
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

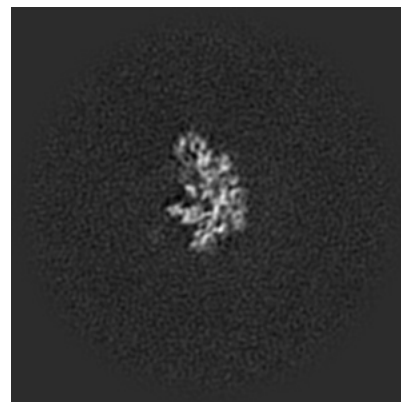
6.3.1 Primary map



X Index: 272

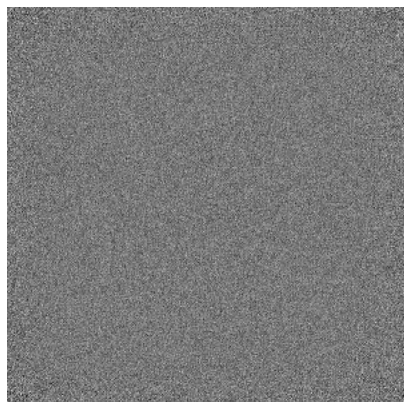


Y Index: 228

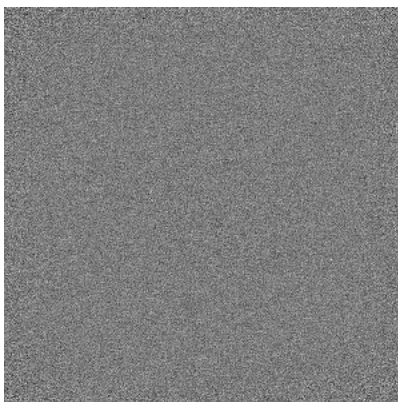


Z Index: 239

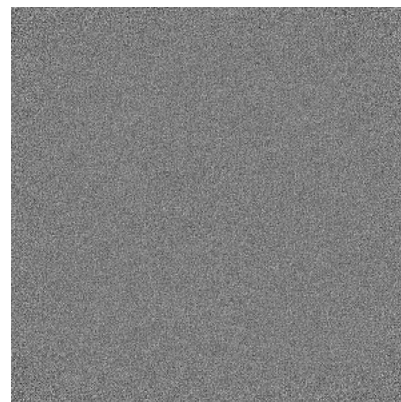
6.3.2 Raw map



X Index: 0



Y Index: 0

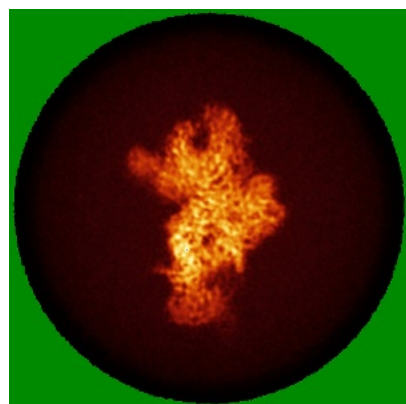


Z Index: 0

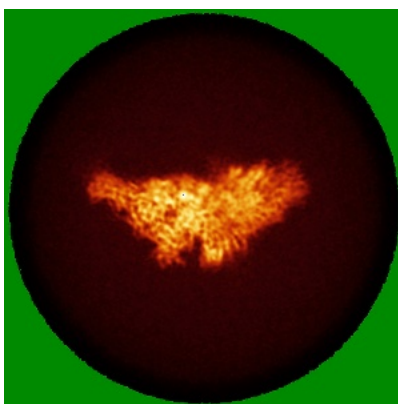
The images above show the largest variance slices of the map in three orthogonal directions.

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

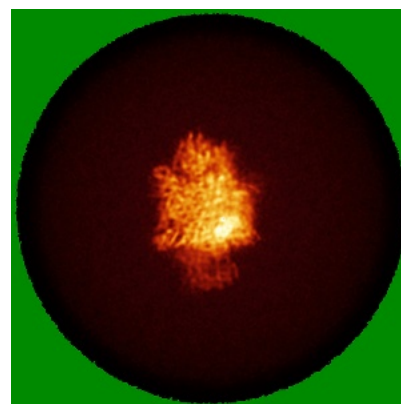
6.4.1 Primary map



X

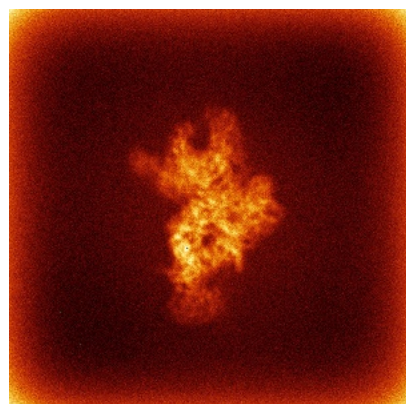


Y

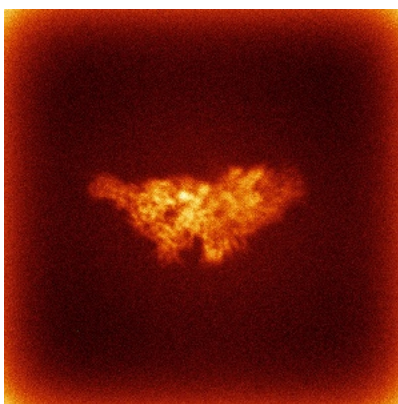


Z

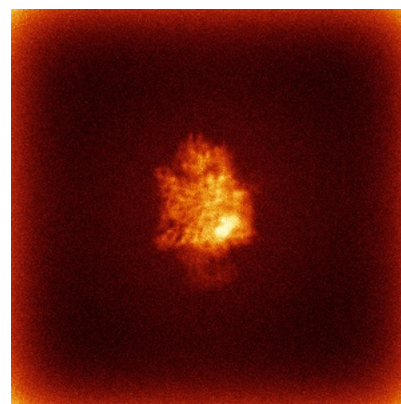
6.4.2 Raw map



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](#)

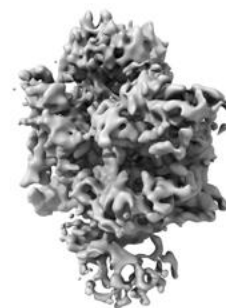
6.5.1 Primary map



X



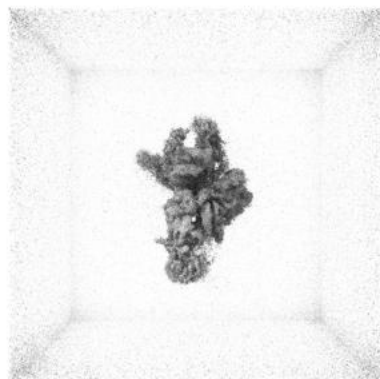
Y



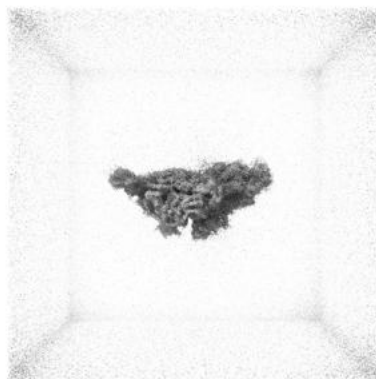
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

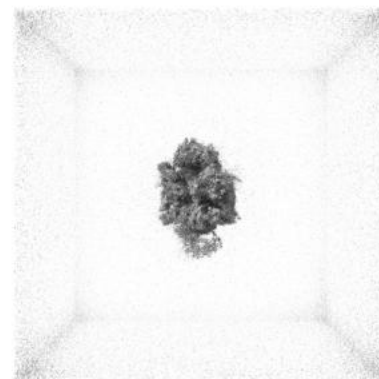
6.5.2 Raw map



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.

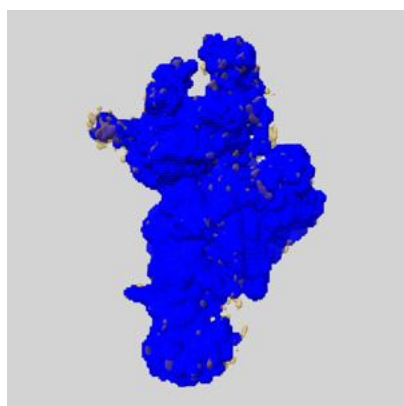
6.6 Mask visualisation [i](#)

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

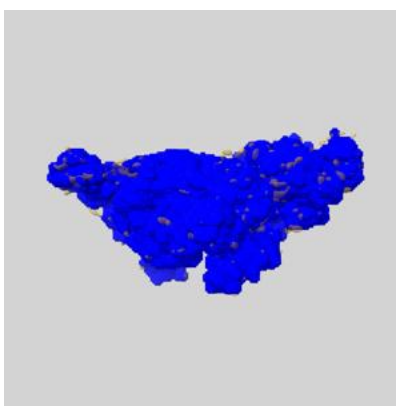
A mask typically either:

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

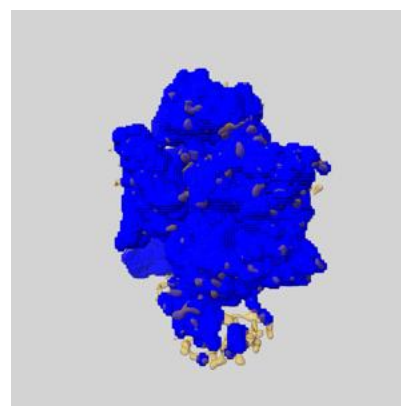
6.6.1 emd_18438_msk_1.map [i](#)



X



Y

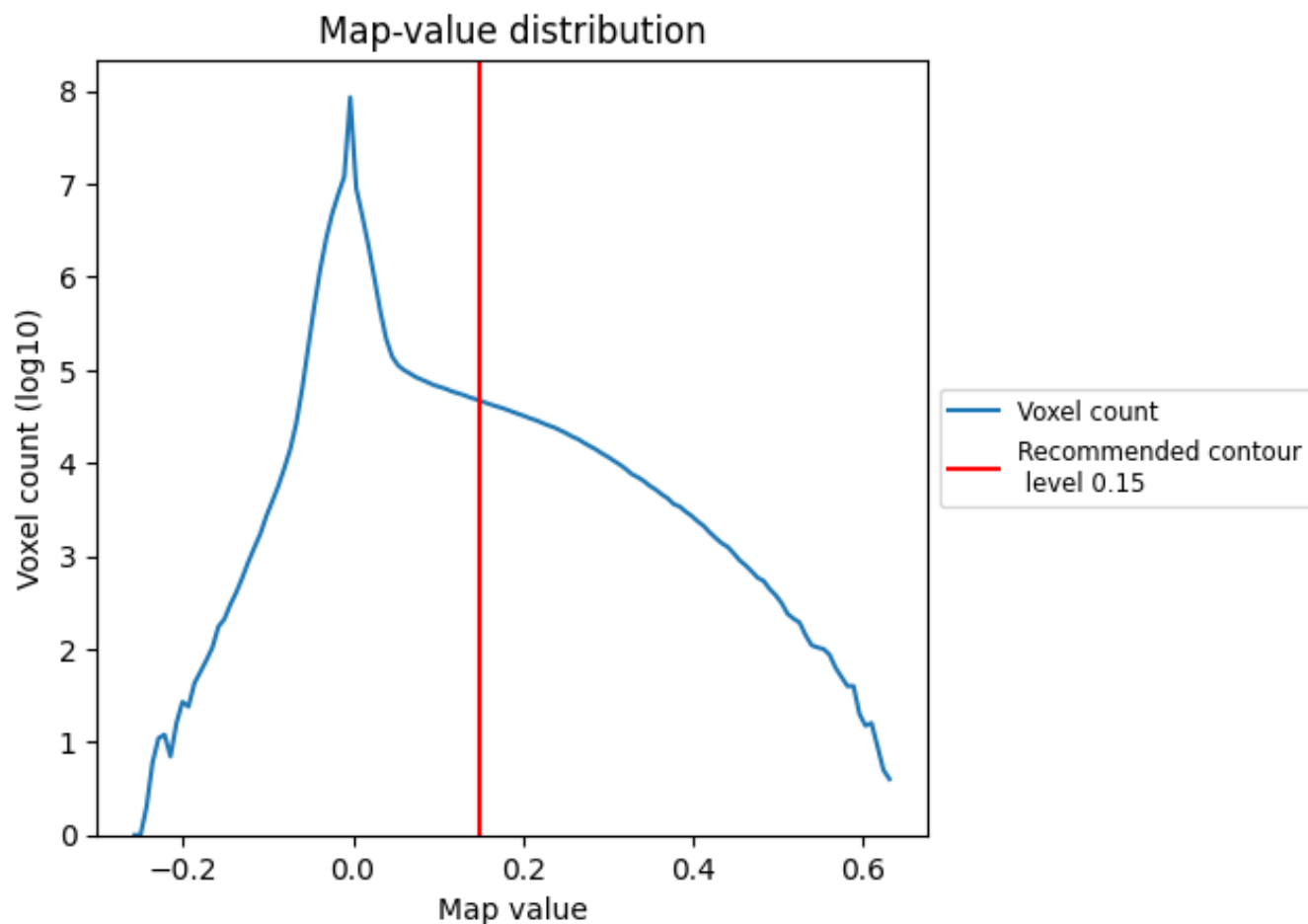


Z

7 Map analysis [i](#)

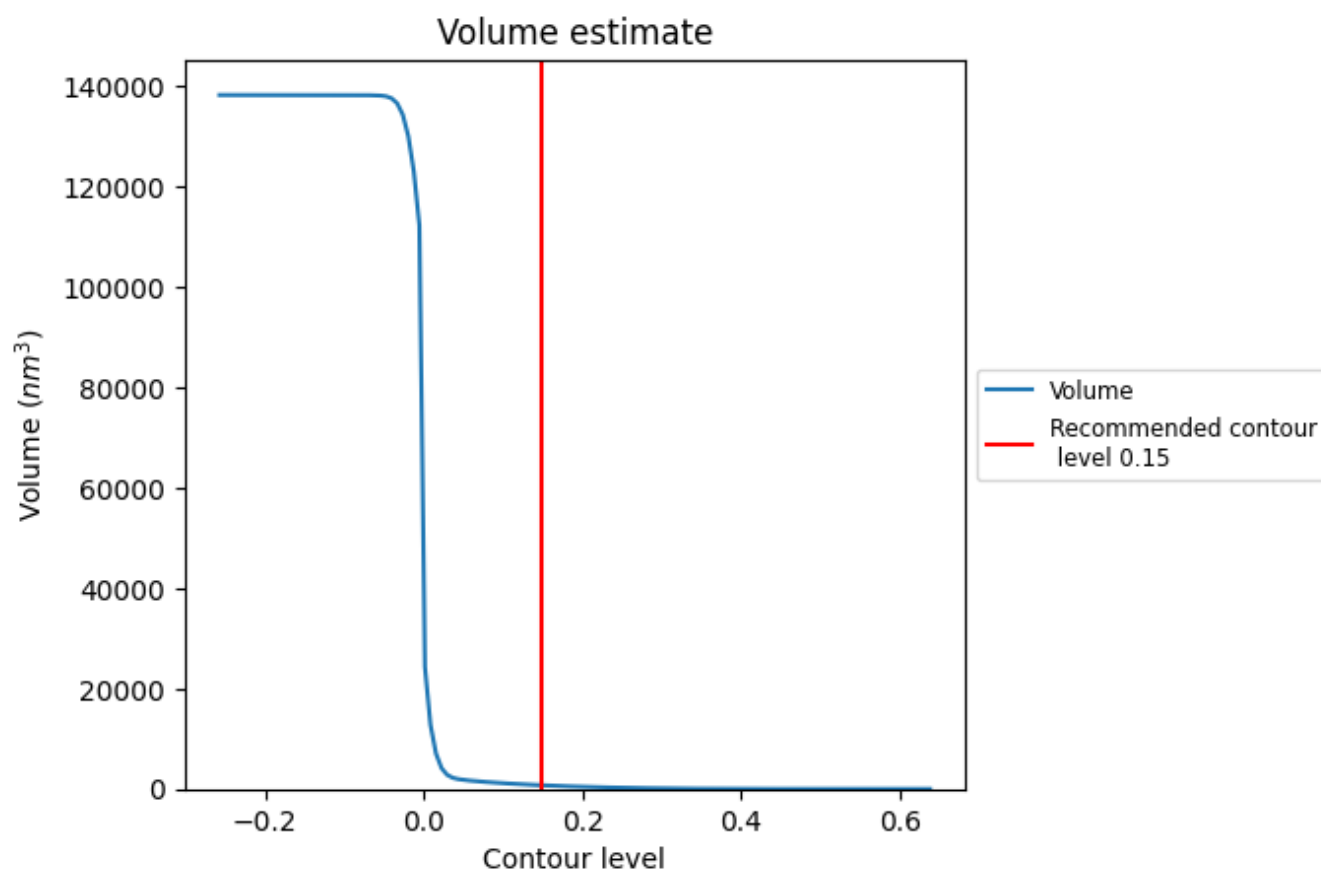
This section contains the results of statistical analysis of the map.

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.

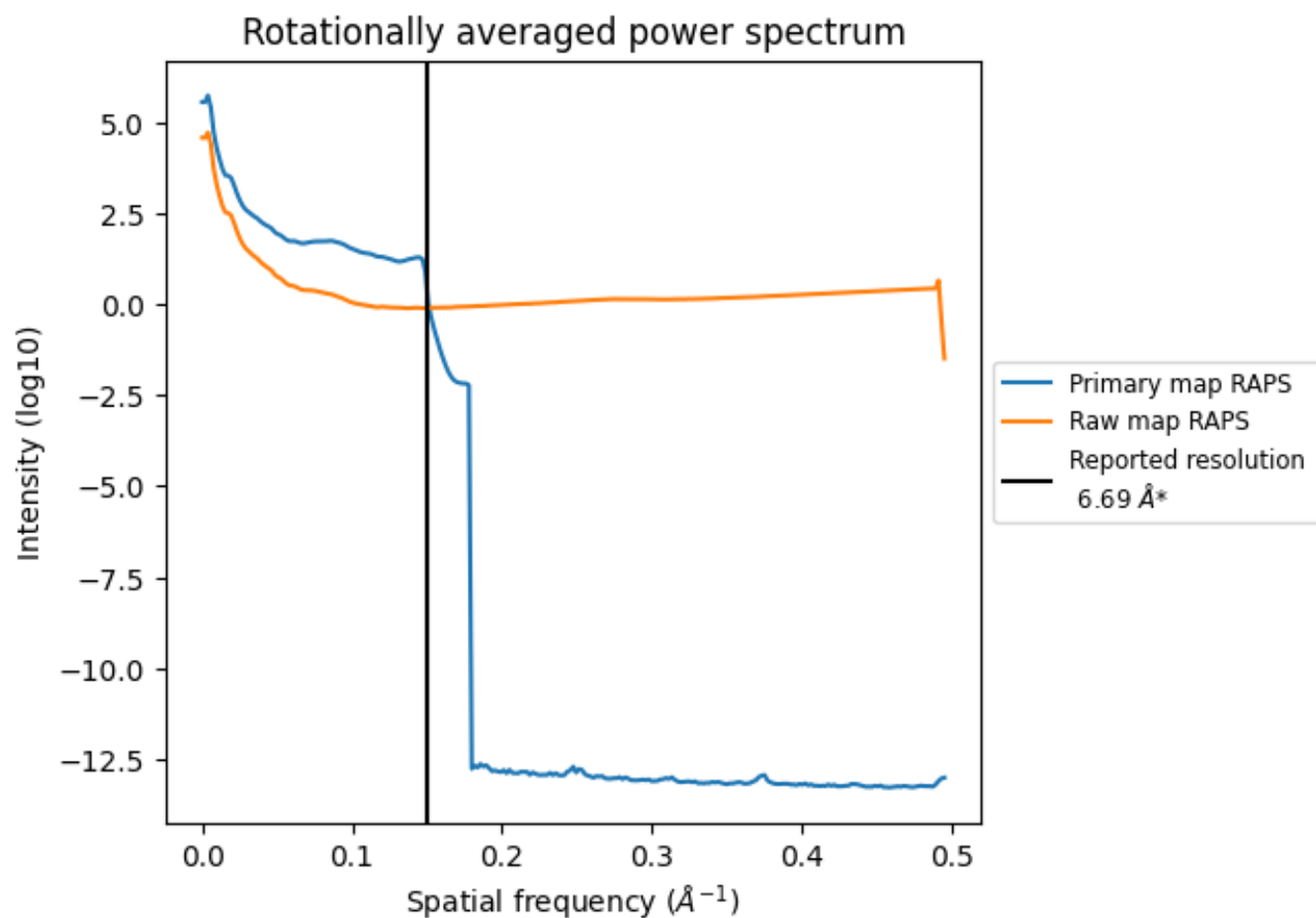
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 732 nm³; this corresponds to an approximate mass of 661 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 ⓘ

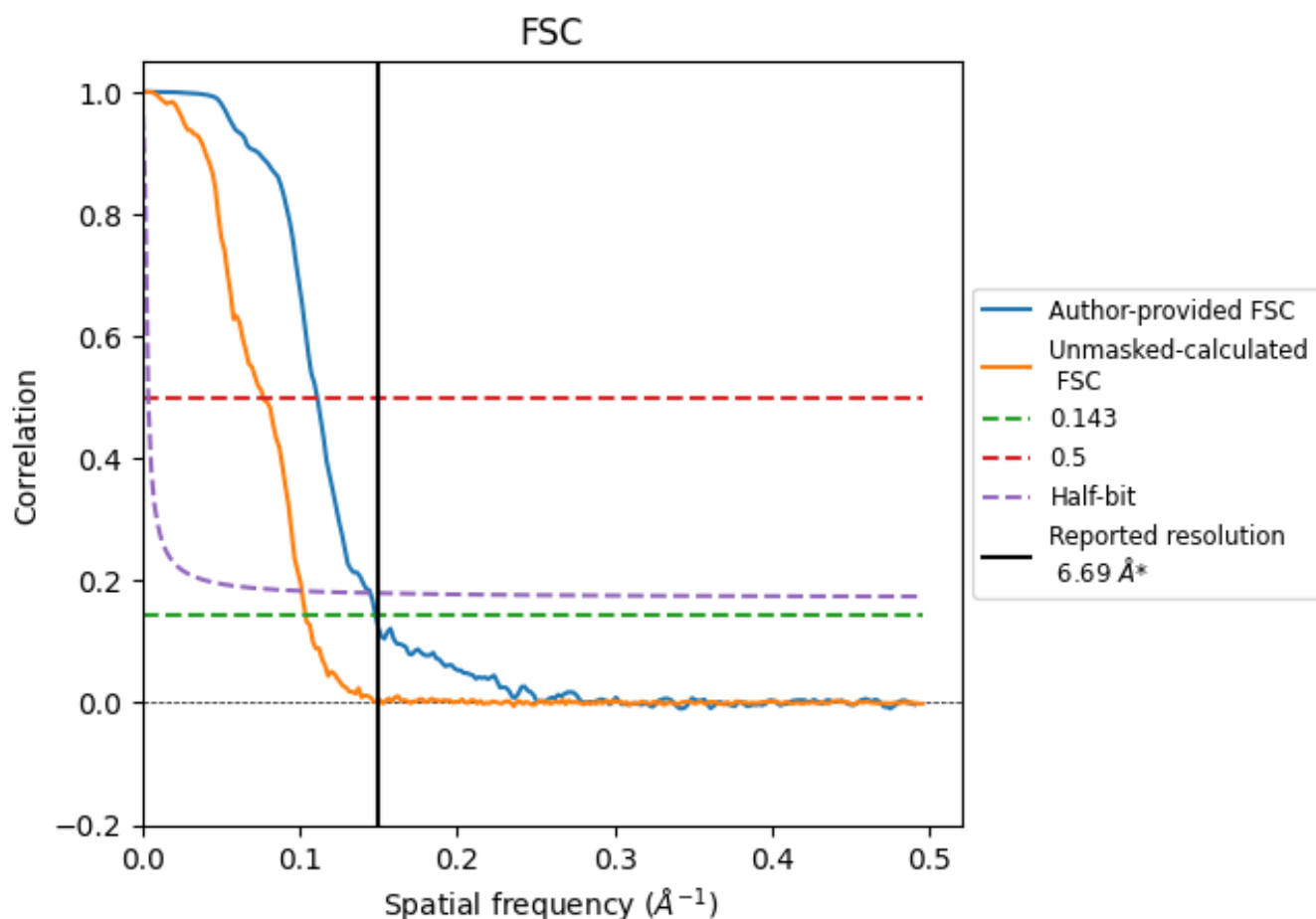


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.149 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

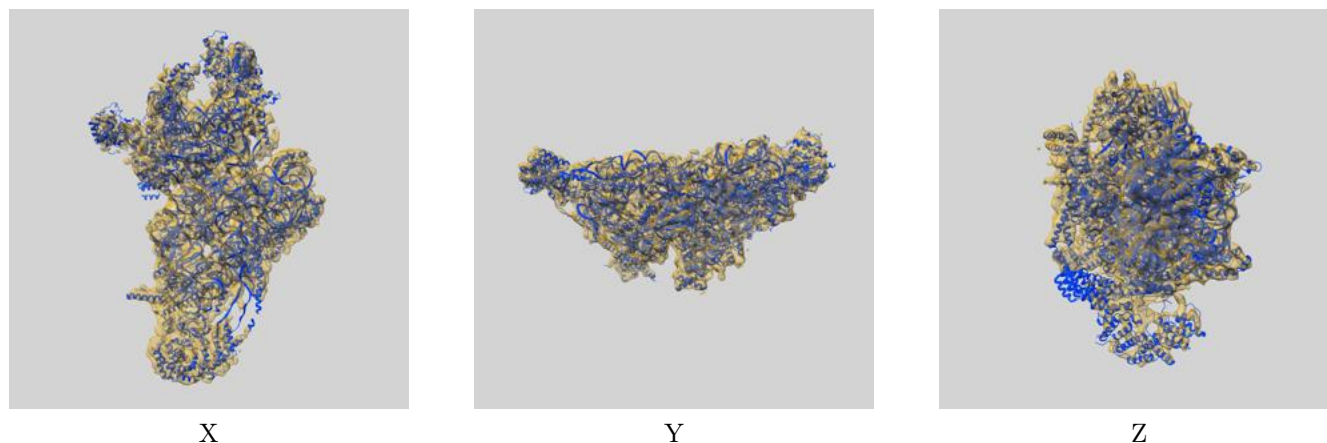
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.69	-	-
Author-provided FSC curve	6.75	9.00	6.91
Unmasked-calculated*	9.64	13.02	9.88

*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 9.64 differs from the reported value 6.69 by more than 10 %

9 Map-model fit [i](#)

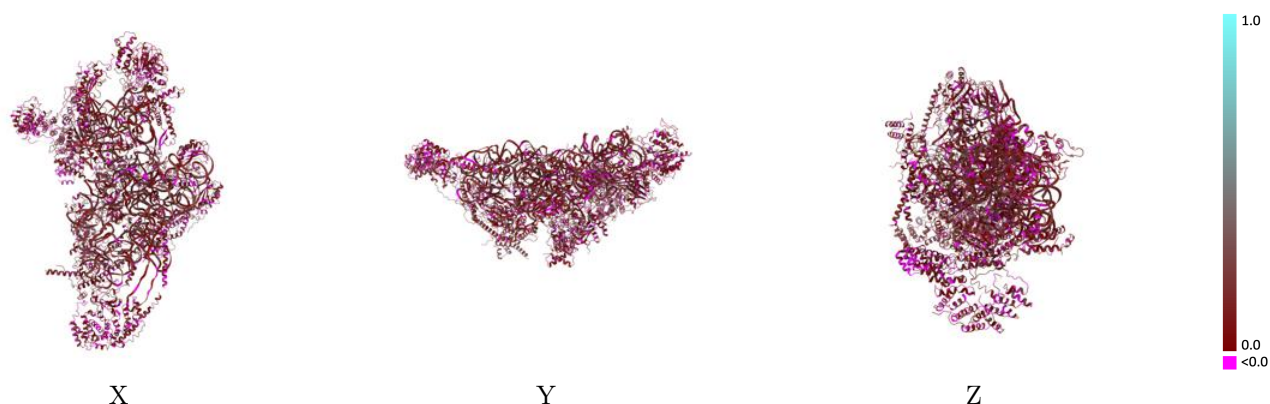
This section contains information regarding the fit between EMDB map EMD-18438 and PDB model 8QRK. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



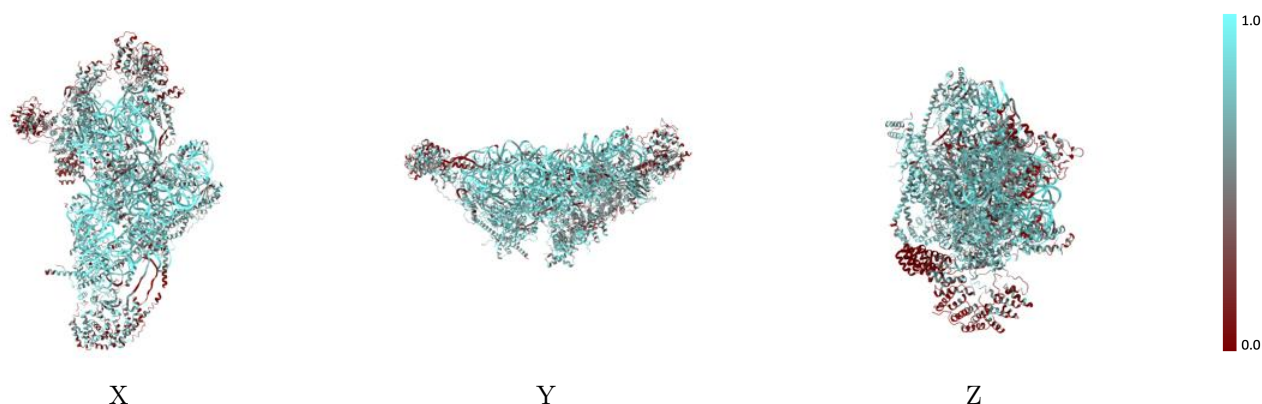
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



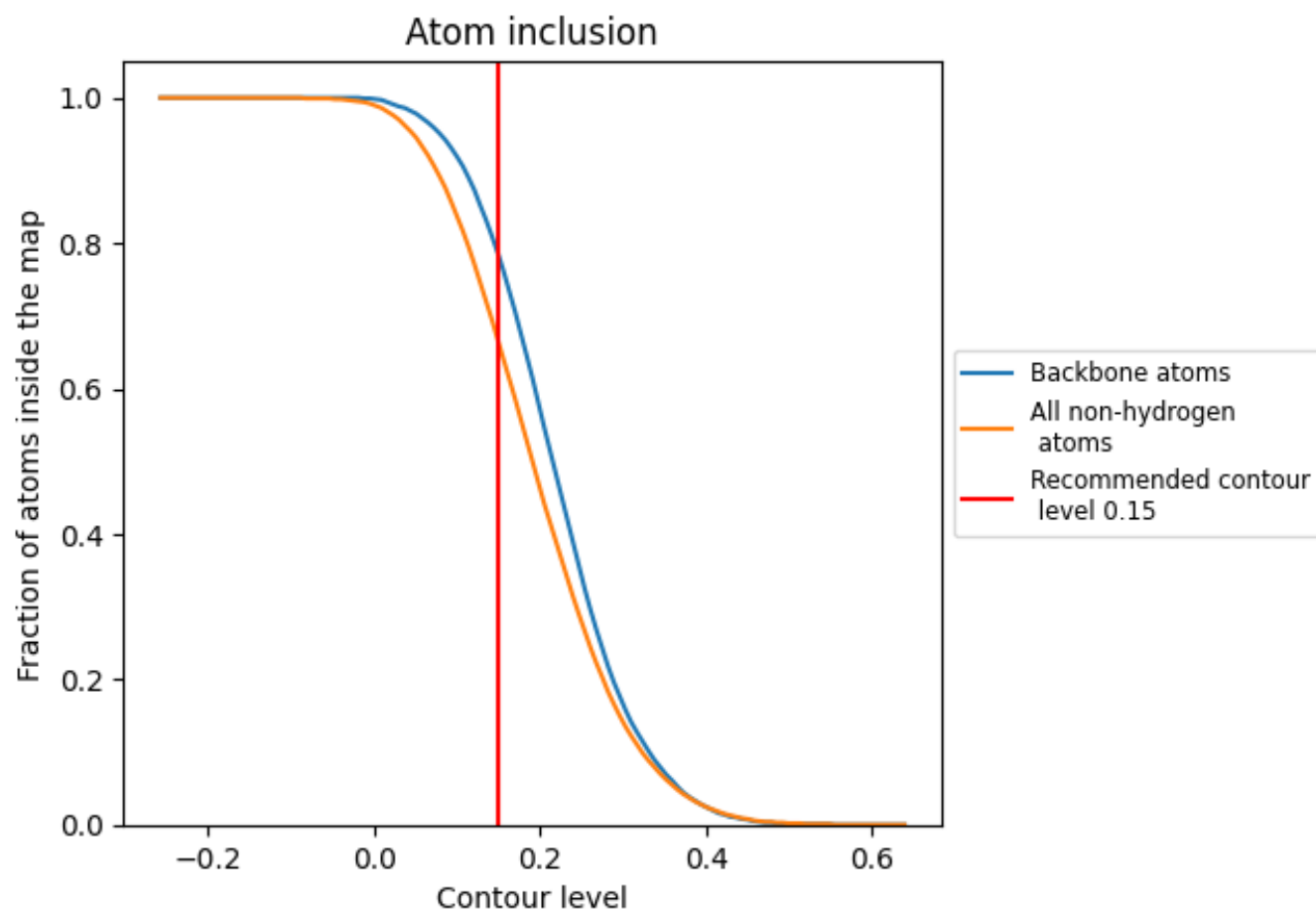
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 66% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.1360
0	 0.6630	 0.1280
1	 0.5120	 0.1300
3	 0.5910	 0.1230
4	 0.2530	 0.0700
A	 0.8470	 0.1700
B	 0.7230	 0.1370
C	 0.6420	 0.1050
D	 0.6290	 0.1410
E	 0.5830	 0.0950
F	 0.4670	 0.1020
G	 0.5920	 0.1230
H	 0.5820	 0.1190
I	 0.6830	 0.1110
J	 0.6920	 0.1420
K	 0.6840	 0.1030
L	 0.6500	 0.1250
M	 0.7590	 0.1380
N	 0.7270	 0.1270
O	 0.7880	 0.1690
P	 0.7100	 0.1110
Q	 0.6360	 0.1360
R	 0.7510	 0.1590
S	 0.6810	 0.1400
T	 0.6770	 0.1560
U	 0.6790	 0.1460
V	 0.4930	 0.0890
W	 0.7550	 0.1570
X	 0.4200	 0.1000
Y	 0.4670	 0.1310
Z	 0.6010	 0.1150

