



Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 07:36 pm BST

PDB ID : 6QCA / pdb_00006qca
EMDB ID : EMD-4502
Title : Ovine respiratory complex I FRC open class 5
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-27
Resolution : 6.20 Å(reported)
Based on initial model : 5LNK

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

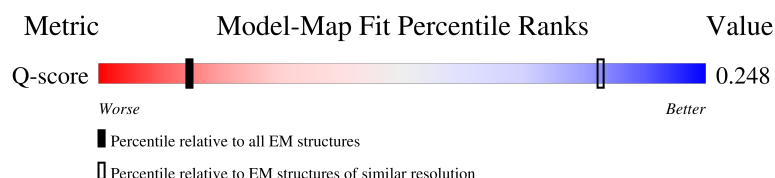
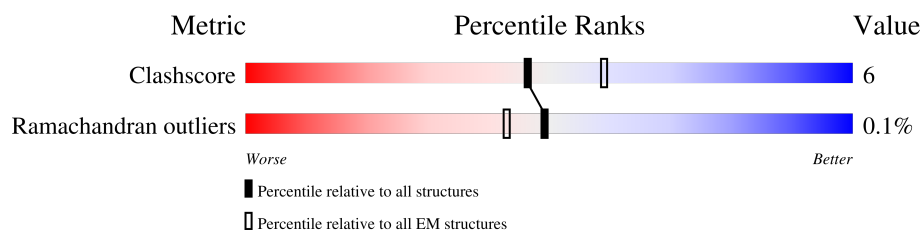
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	-
Q-score	-	25397	537 (5.70 - 6.70)

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	V1	445	11% 90% 6% .
2	V2	217	9% 89% 8% .
3	S1	704	15% 92% 5% .
4	S2	430	24% 93% 5% .
5	S3	228	17% 84% 7% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	S7	179	
7	S8	176	
8	V3	75	
9	S6	96	
10	S4	133	
11	A9	338	
12	A2	98	
13	A5	115	
14	A6	127	
15	A7	112	
16	AL	145	
17	AA	88	
17	AB	88	
18	D3	115	
19	D1	318	
20	D6	175	
21	4L	98	
22	D5	606	
23	D4	459	
24	D2	347	
25	AK	140	
26	B5	143	
27	A8	171	
28	BJ	175	
29	AJ	320	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	S5	105	
31	A3	83	
32	B3	97	
33	C2	120	
34	B4	128	
35	AM	143	
36	B6	127	
37	B7	136	
38	B9	178	
39	B2	72	
40	B8	158	
41	BK	125	
42	C1	49	
43	B1	57	
44	A1	70	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 40144 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 NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	V1	430	Total	C	N	O	0	0
			2099	1239	430	430		

- Molecule 2 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	V2	212	Total	C	N	O	0	0
			1045	621	212	212		

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	S1	688	Total	C	N	O	0	0
			3390	2014	688	688		

- Molecule 4 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	S2	424	Total	C	N	O	0	0
			2090	1242	424	424		

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	S3	208	Total	C	N	O	0	0
			1034	618	208	208		

- Molecule 6 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	S7	156	Total	C	N	O	0	0
			769	457	156	156		

- Molecule 7 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	S8	176	Total	C	N	O	0	0
			871	519	176	176		

- Molecule 8 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	V3	41	Total	C	N	O	0	0
			204	122	41	41		

- Molecule 9 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	S6	95	Total	C	N	O	0	0
			462	272	95	95		

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	S4	126	Total	C	N	O	0	0
			625	373	126	126		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	A9	287	Total	C	N	O	0	0
			1413	839	287	287		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	A2	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 13 is a protein called NDUF5.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	A5	111	Total	C	N	O	0	0
			550	328	111	111		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	A6	114	Total	C	N	O	0	0
			567	339	114	114		

- Molecule 15 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	A7	96	Total	C	N	O	0	0
			476	284	96	96		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	AL	144	Total	C	N	O	0	0
			708	420	144	144		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AA	80	Total	C	N	O	0	0
			397	237	80	80		
17	AB	87	Total	C	N	O	0	0
			432	258	87	87		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	D3	90	Total	C	N	O	0	0
			449	269	90	90		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	D1	303	Total	C	N	O	0	0
			1505	899	303	303		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	D6	171	Total	C	N	O	0	0
			829	487	171	171		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	4L	98	Total	C	N	O	0	0
			486	290	98	98		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	D5	606	Total	C	N	O	0	0
			3001	1789	606	606		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	D4	459	Total	C	N	O	0	0
			2277	1359	459	459		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	D2	347	Total	C	N	O	0	0
			1721	1027	347	347		

- Molecule 25 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	AK	140	Total	C	N	O	0	0
			682	402	140	140		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	B5	139	Total	C	N	O	0	0
			687	409	139	139		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	A8	171	Total	C	N	O	0	0
			847	505	171	171		

- Molecule 28 is a protein called NDUF10.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BJ	171	Total	C	N	O	0	0
			853	511	171	171		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	AJ	319	Total	C	N	O	0	0
			1575	937	319	319		

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	S5	99	Total	C	N	O	0	0
			490	292	99	99		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	A3	74	Total	C	N	O	0	0
			367	219	74	74		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	B3	73	Total	C	N	O	0	0
			356	210	73	73		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	C2	119	Total	C	N	O	0	0
			589	351	119	119		

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	B4	128	Total	C	N	O	0	0
			635	379	128	128		

- Molecule 35 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	AM	139	Total	C	N	O	0	0
			681	403	139	139		

- Molecule 36 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	B6	96	Total	C	N	O	0	0
			477	285	96	96		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	B7	119	Total	C	N	O	0	0
			592	354	119	119		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	B9	176	Total	C	N	O	0	0
			874	522	176	176		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	B2	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	B8	157	Total	C	N	O	0	0
			775	461	157	157		

- Molecule 41 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	BK	102	Total	C	N	O	0	0
			506	302	102	102		

- Molecule 42 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	C1	46	Total	C	N	O	0	0
			227	135	46	46		

- Molecule 43 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	B1	52	Total	C	N	O	0	0
			258	154	52	52		

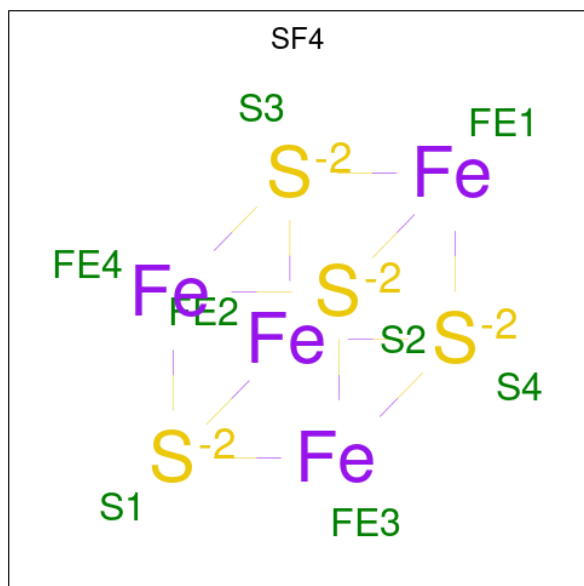
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 44 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	A1	70	Total	C	N	O	0	0
			343	203	70	70		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



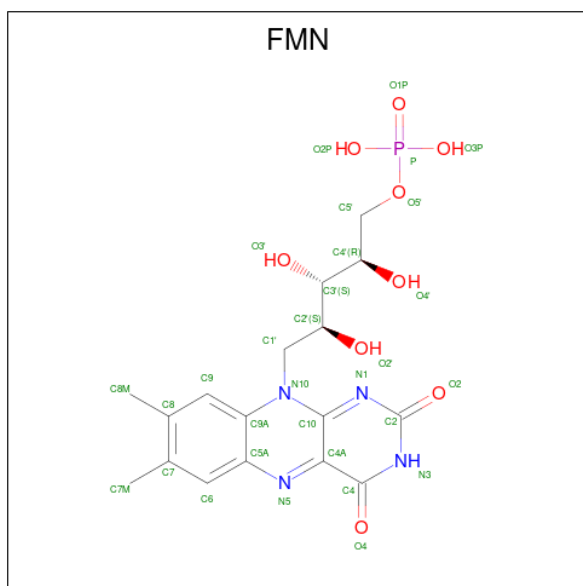
Mol	Chain	Residues	Atoms			AltConf
45	V1	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

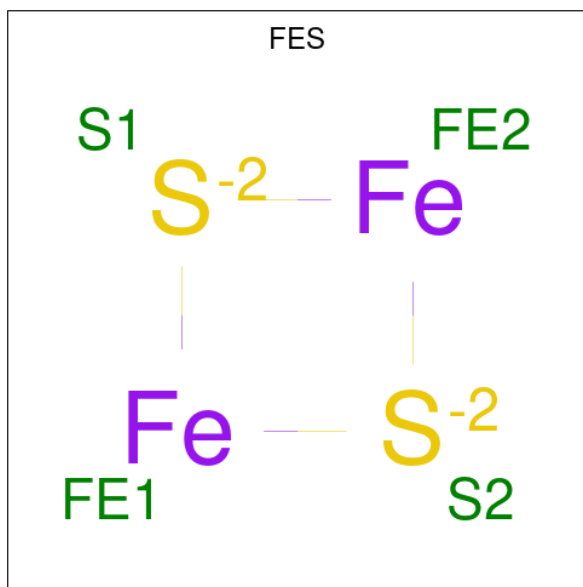
Mol	Chain	Residues	Atoms			AltConf
45	S1	1	Total	Fe	S	0
			8	4	4	
45	S1	1	Total	Fe	S	0
			8	4	4	
45	S7	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
46	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

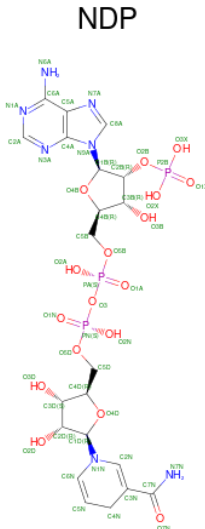


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total	Fe	S	0
			4	2	2	
47	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

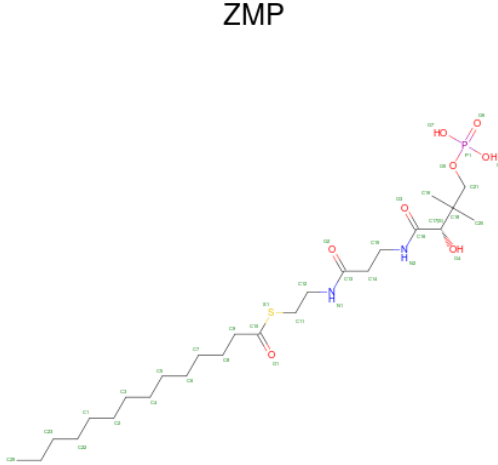
Mol	Chain	Residues	Atoms		AltConf
48	S6	1	Total	Zn	0
			1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					AltConf
49	A9	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 50 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl}]\text{-beta-alanyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

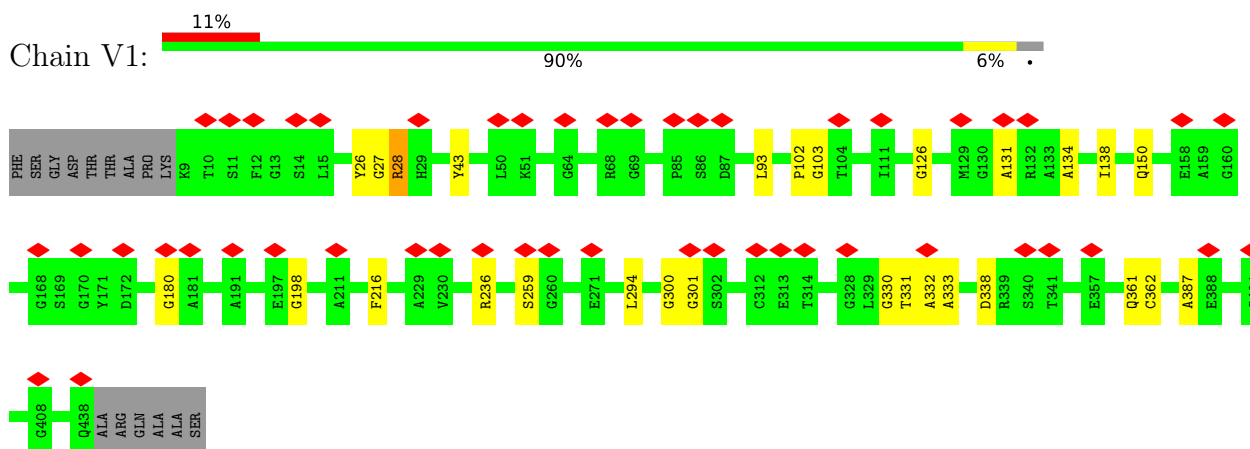


Mol	Chain	Residues	Atoms						AltConf
50	A6	1	Total 34	C 23	N 2	O 7	P 1	S 1	0
50	AB	1	Total 31	C 20	N 2	O 7	P 1	S 1	0

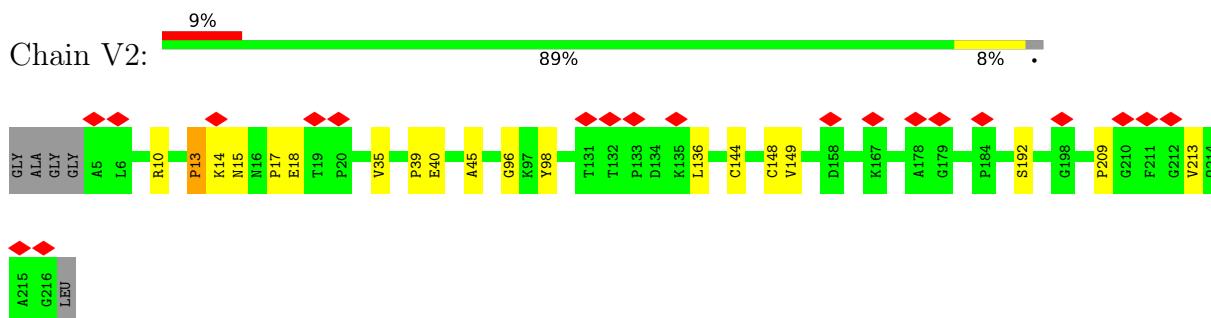
3 Residue-property plots [i](#)

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

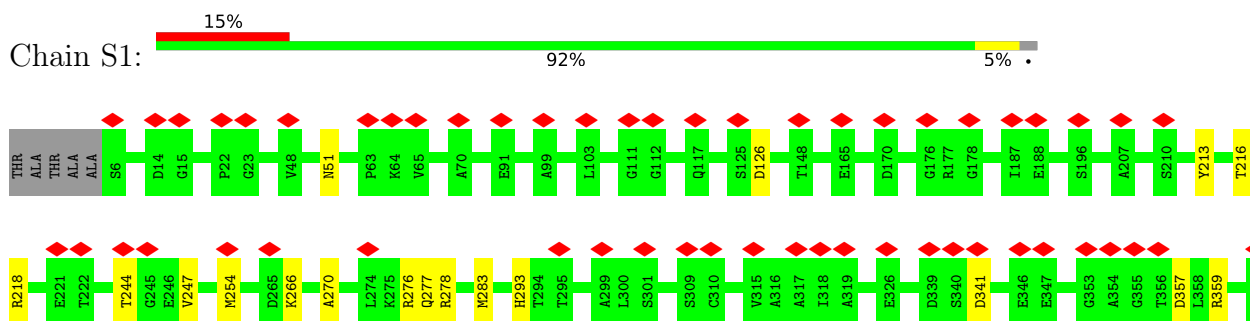
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

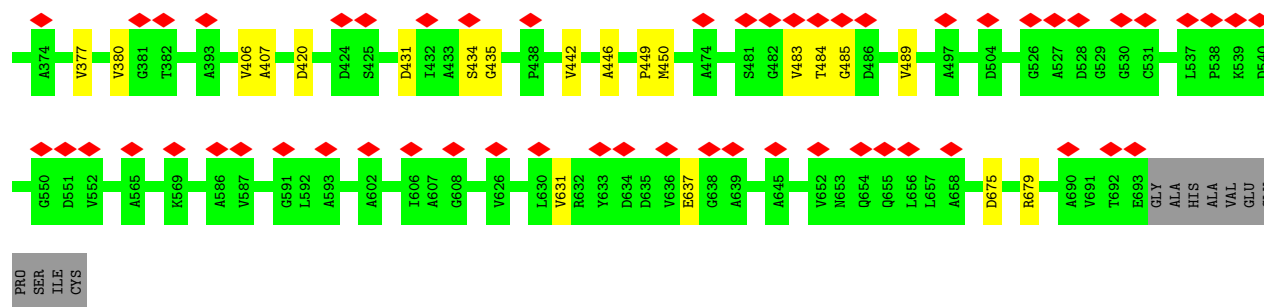


- Molecule 2: NDUFV2

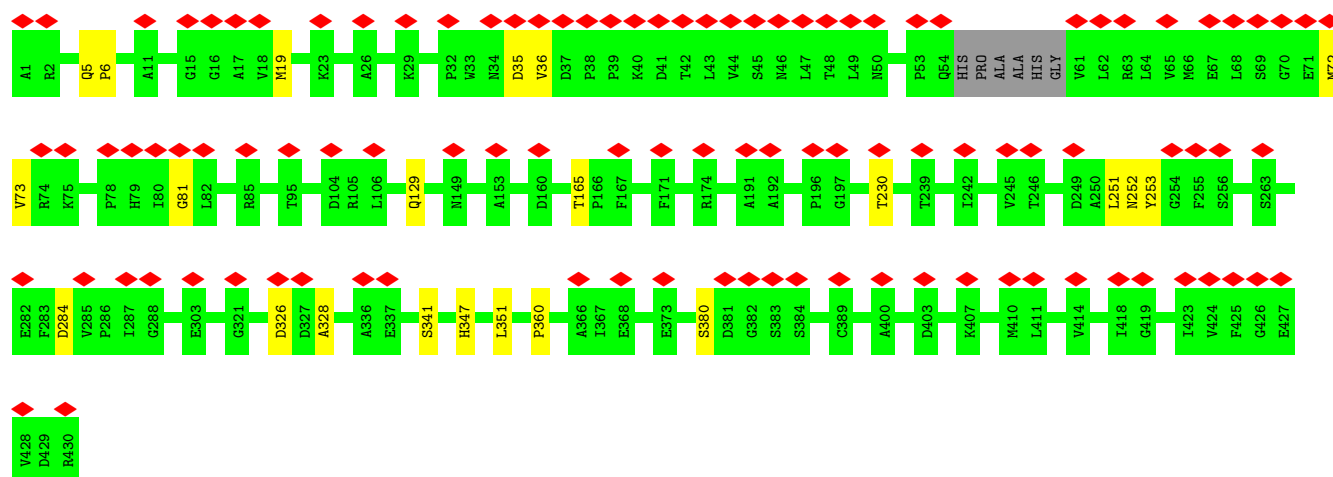


- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

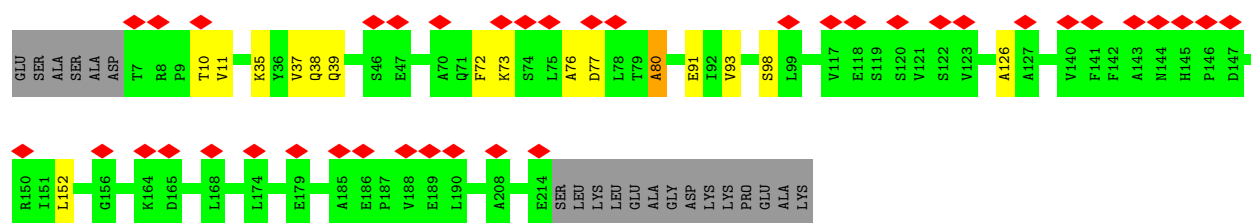
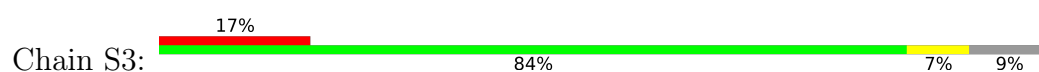




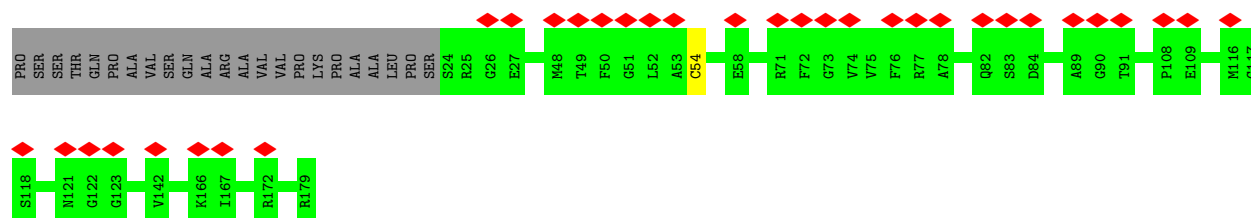
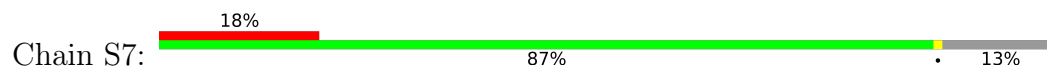
• Molecule 4: NDUFS2



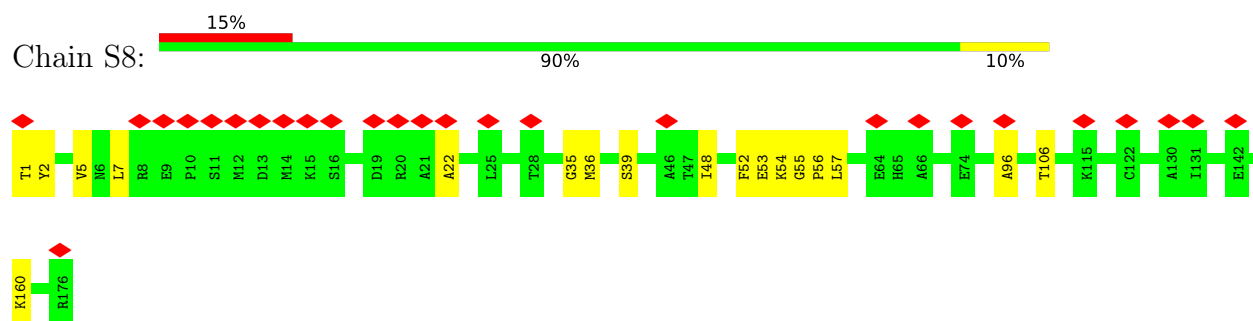
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3



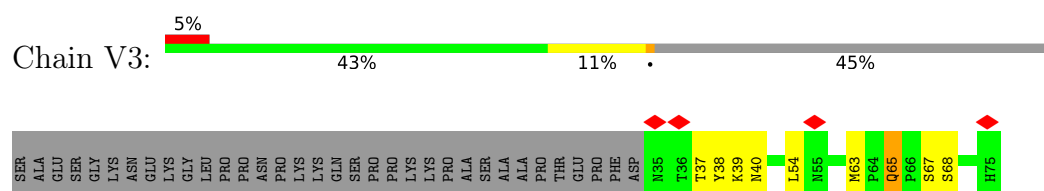
• Molecule 6: NDUFS7



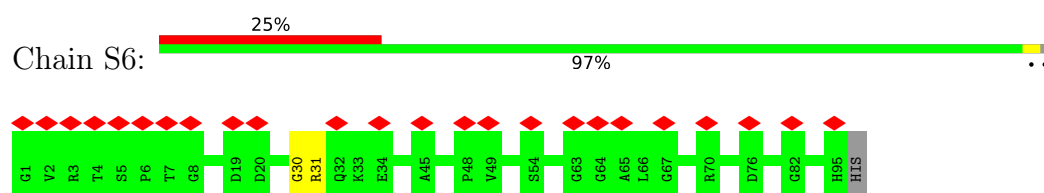
- Molecule 7: NDUFS8



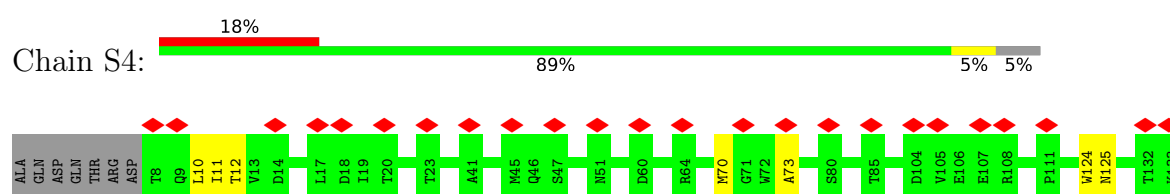
- Molecule 8: NDUFV3



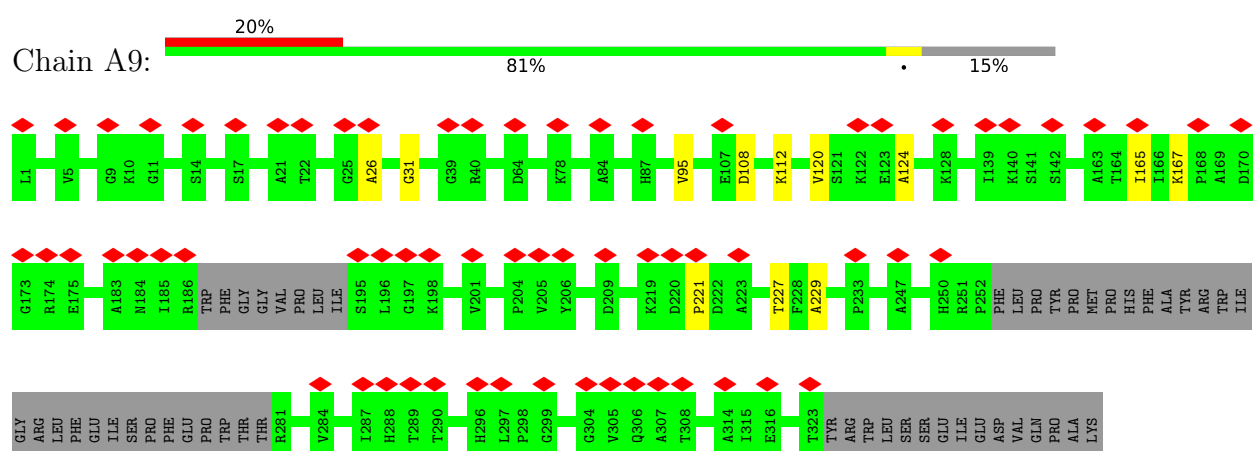
- Molecule 9: NDUFS6



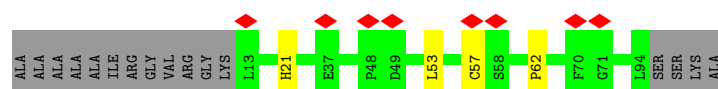
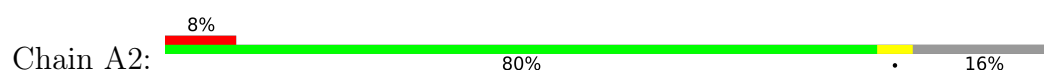
- Molecule 10: NADH:ubiquinone oxidoreductase subunit S4



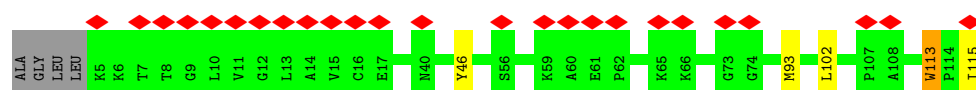
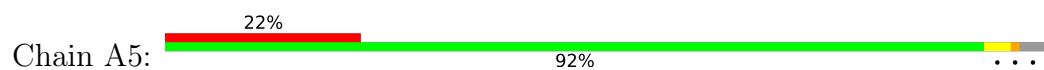
- Molecule 11: NADH:ubiquinone oxidoreductase subunit A9



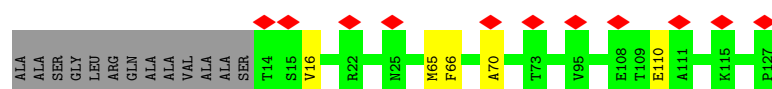
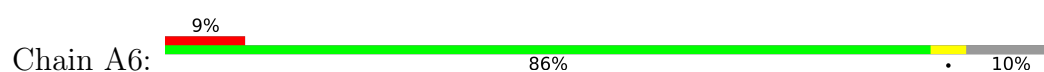
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



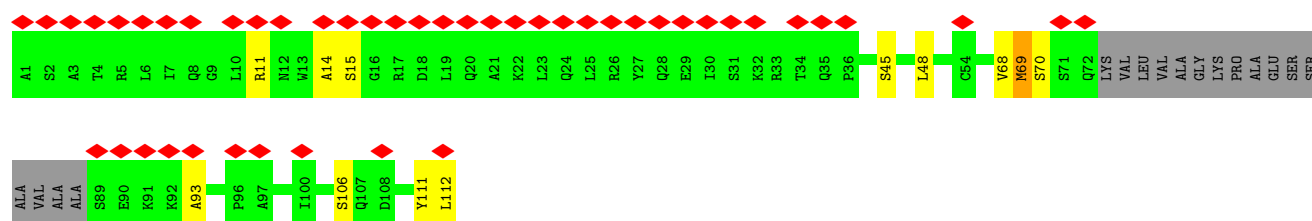
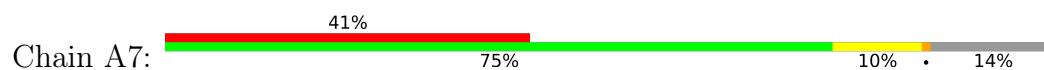
• Molecule 13: NDUFA5



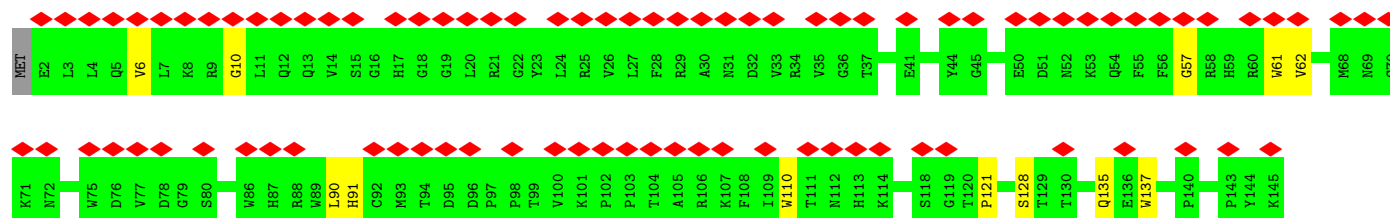
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6



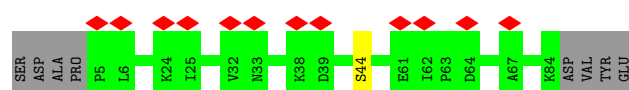
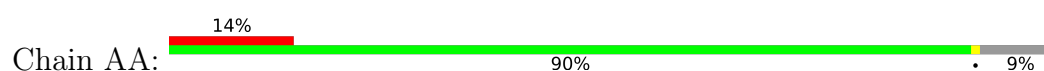
• Molecule 15: NDUFA7



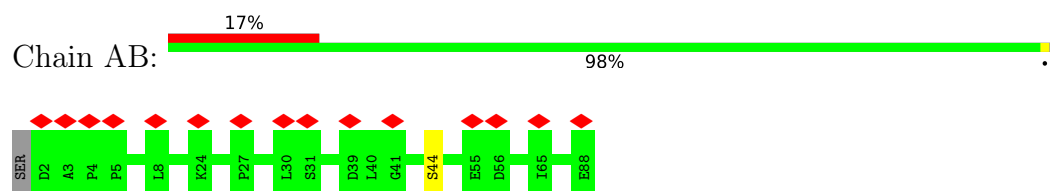
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



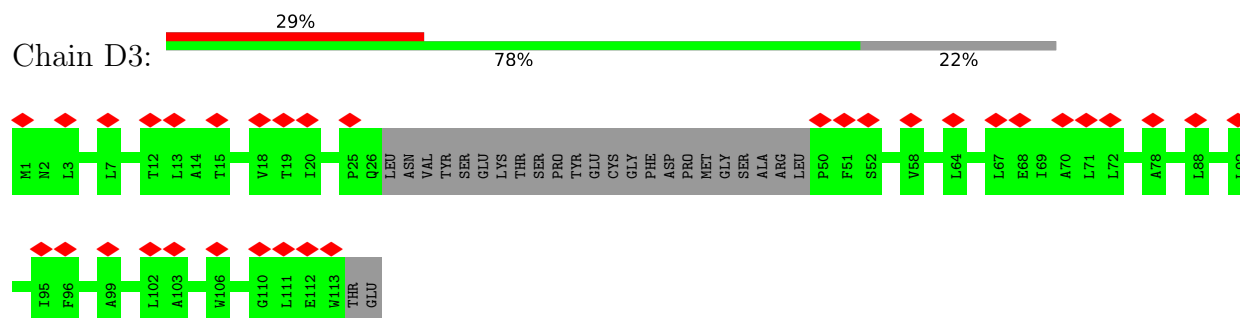
• Molecule 17: Acyl carrier protein



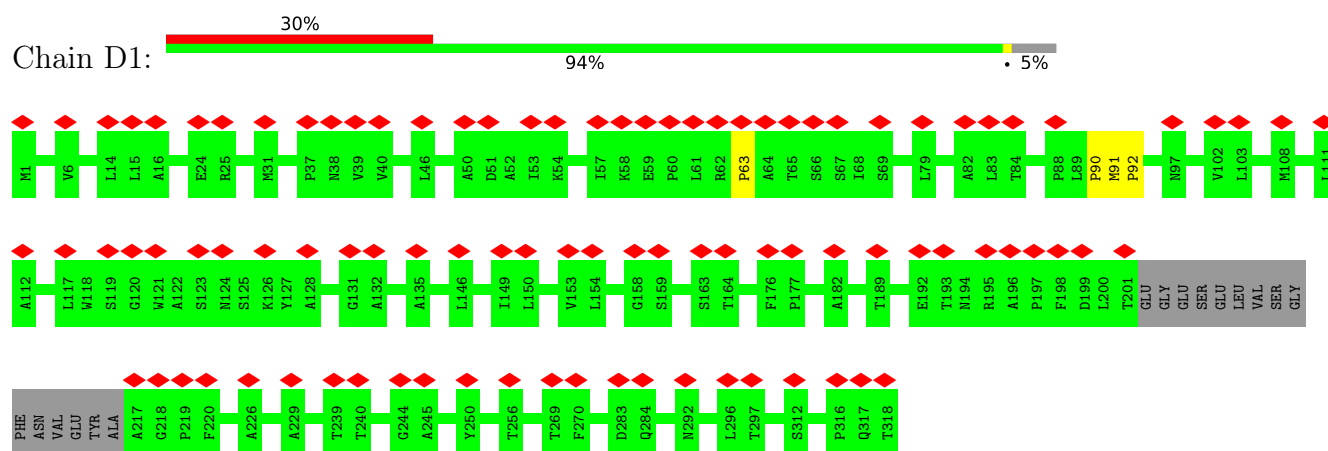
- Molecule 17: Acyl carrier protein



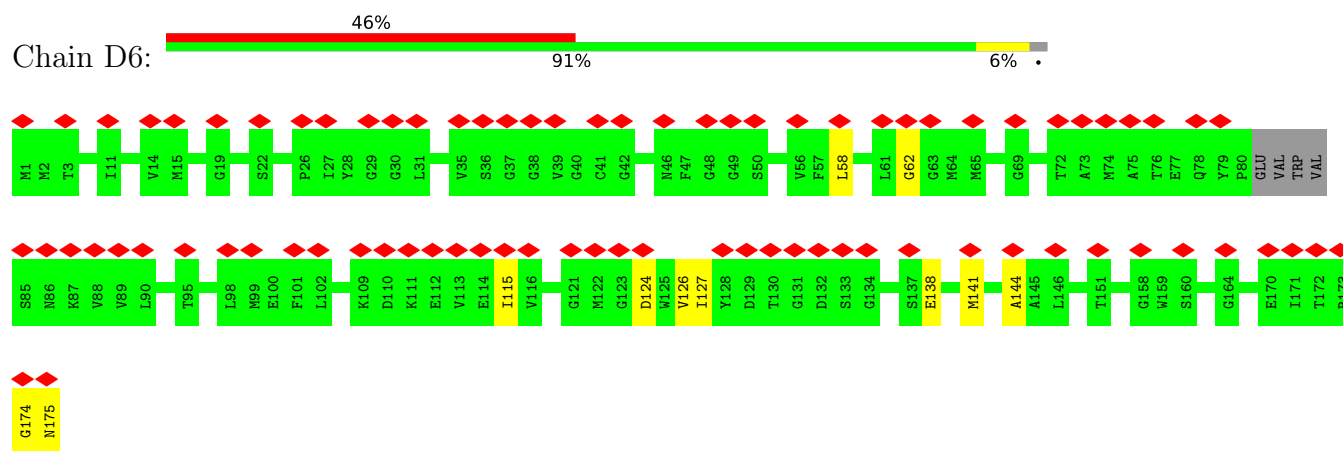
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



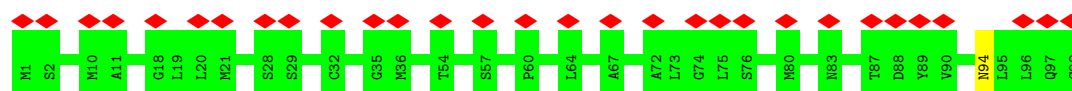
- Molecule 19: NADH-ubiquinone oxidoreductase chain 1



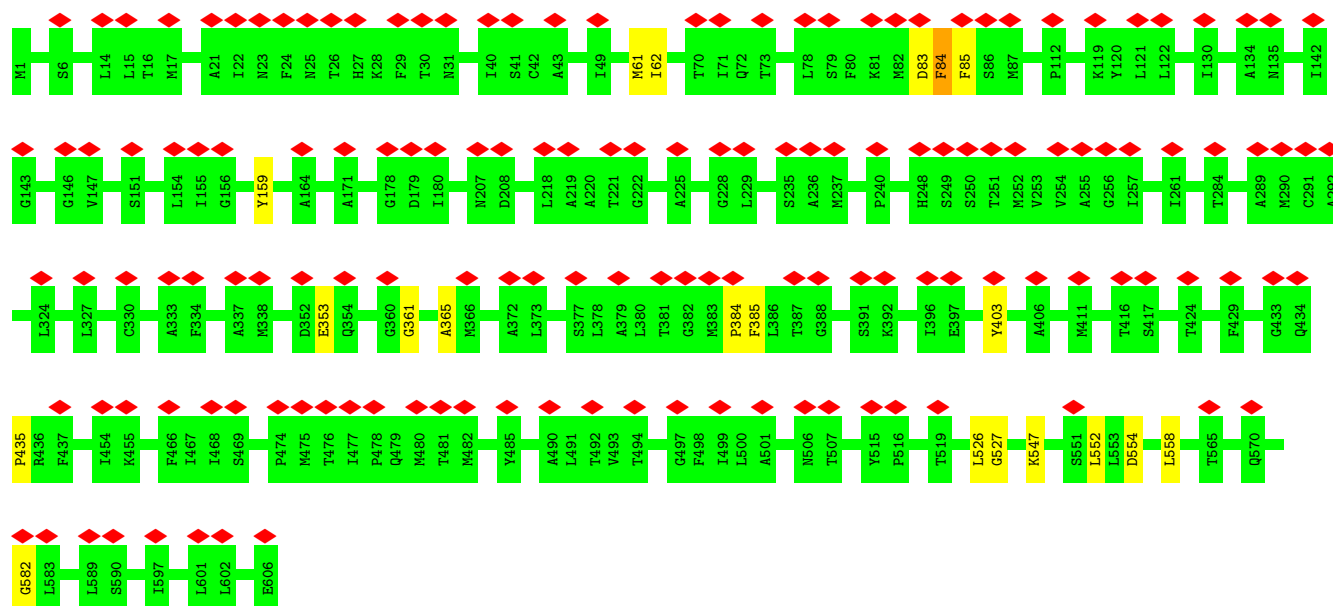
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6



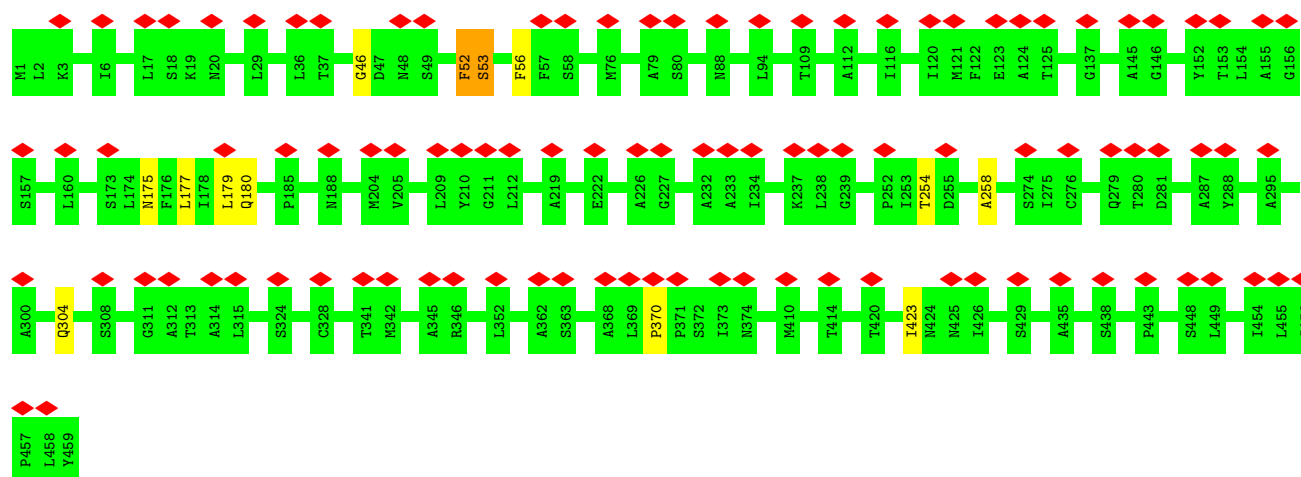
- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L



• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

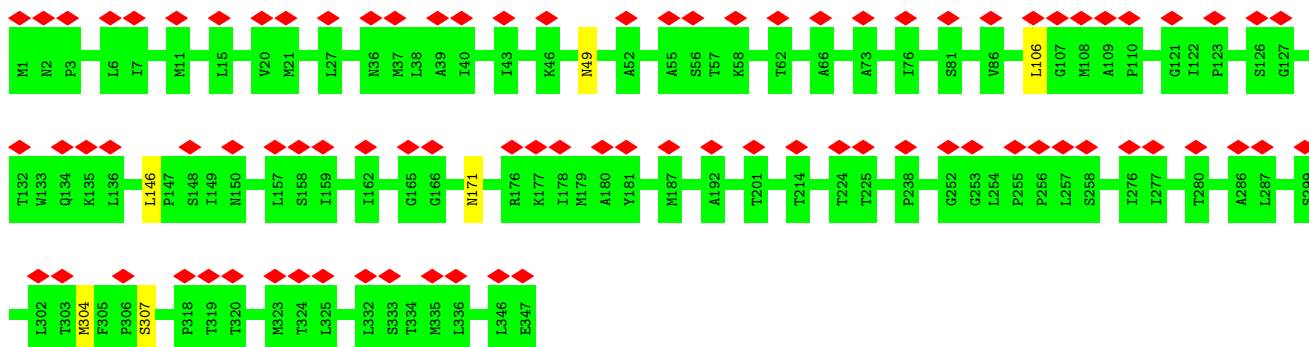


• Molecule 23: NADH-ubiquinone oxidoreductase chain 4



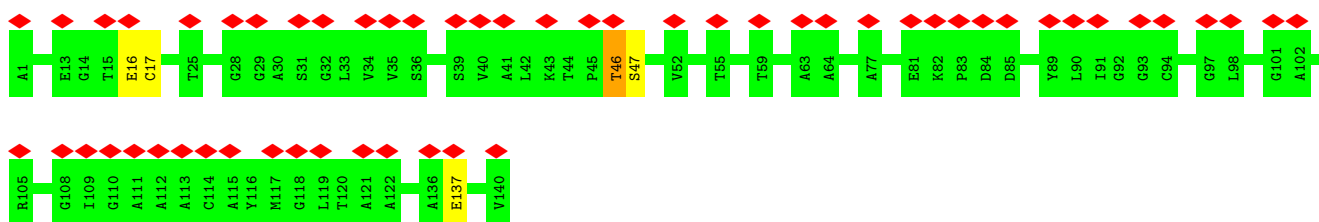
• Molecule 24: NADH-ubiquinone oxidoreductase chain 2





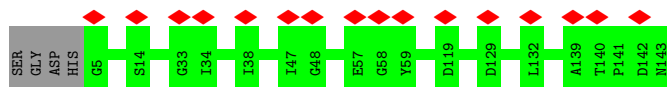
• Molecule 25: NDUFA11

Chain AK:



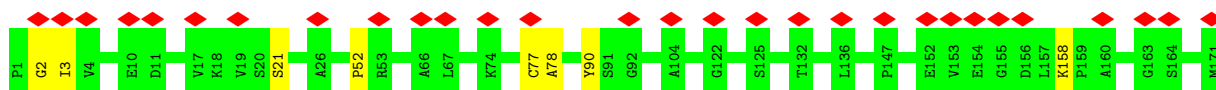
• Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

Chain B5:



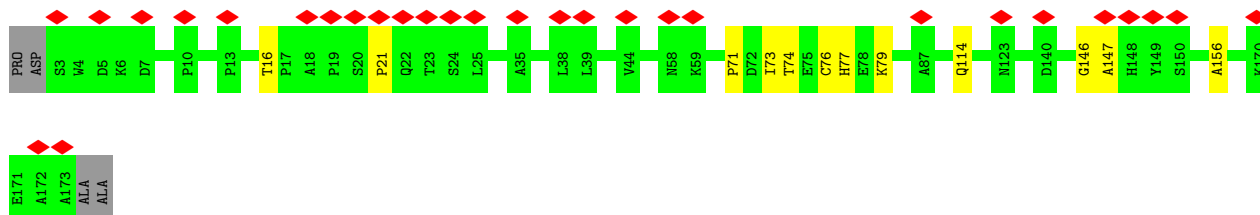
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:

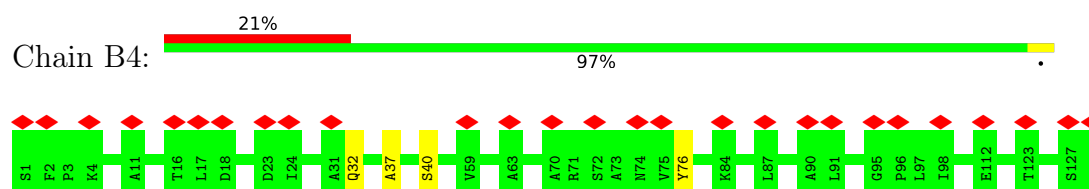


• Molecule 28: NDUF B10

Chain BJ:



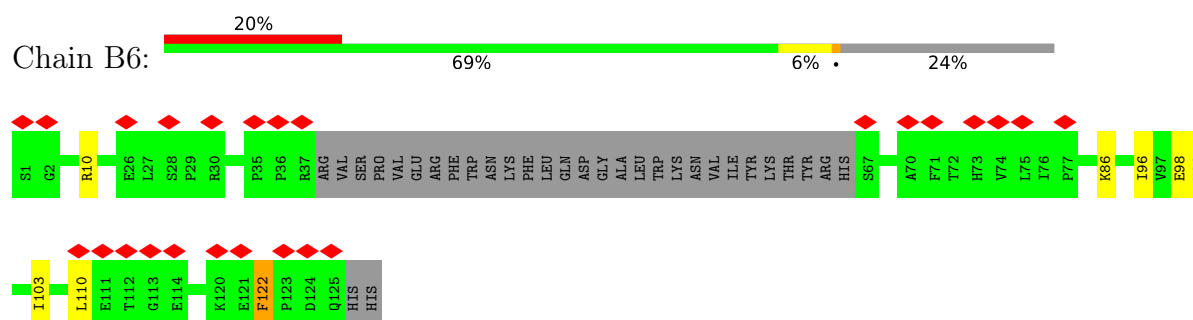
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



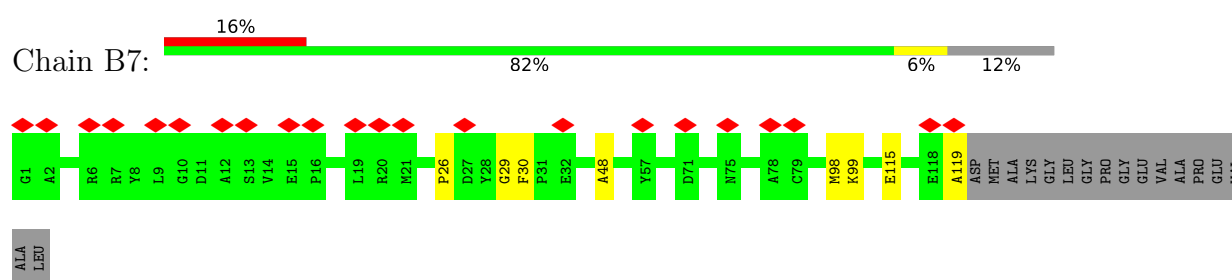
- Molecule 35: NDUFA13



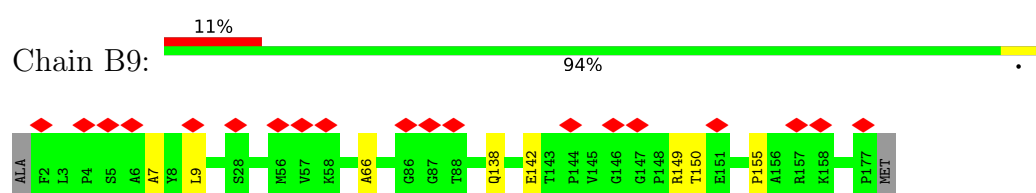
- Molecule 36: NDUF6



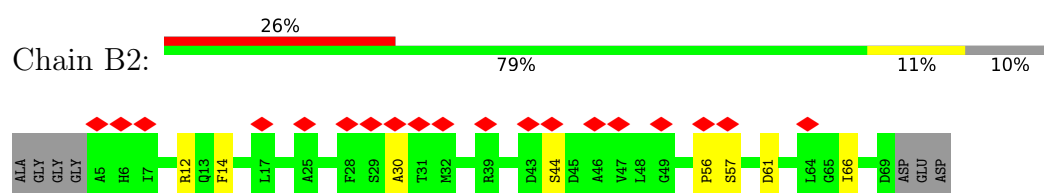
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7



- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

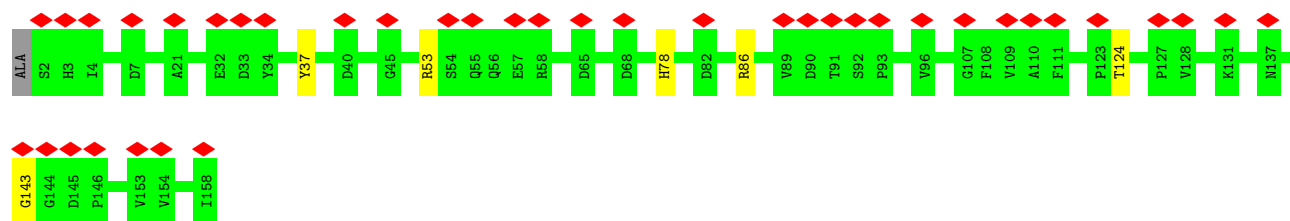


- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

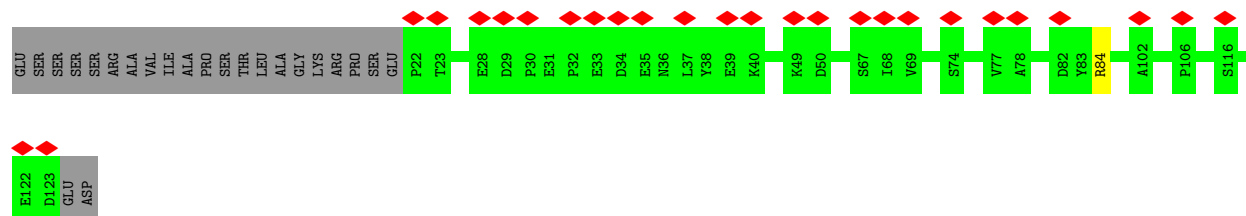
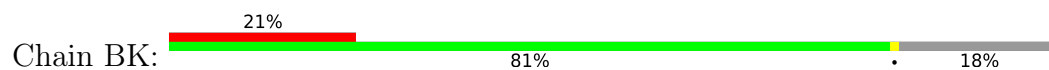


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

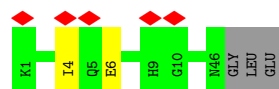
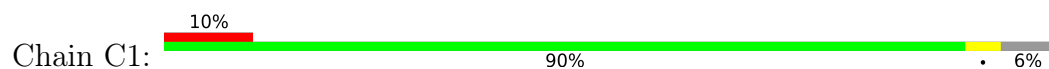




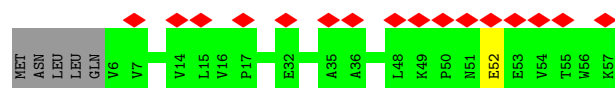
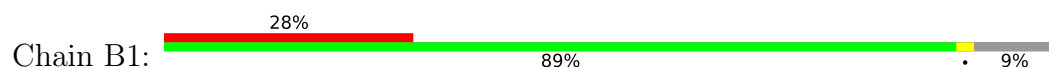
• Molecule 41: NDUFB1



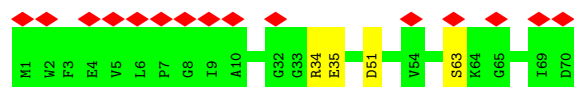
• Molecule 42: NDUF C1



• Molecule 43: NDUF B1



• Molecule 44: NDUFA1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12244	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.574	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, FMN, ZN, SF4, FES, NDP

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	V1	0.27	0/2098	0.69	1/2905 (0.0%)
2	V2	0.32	0/1044	0.86	2/1451 (0.1%)
3	S1	0.27	0/3389	0.69	3/4713 (0.1%)
4	S2	0.32	0/2088	0.69	4/2902 (0.1%)
5	S3	0.31	0/1033	0.79	2/1441 (0.1%)
6	S7	0.32	0/768	0.71	0/1067
7	S8	0.34	0/870	0.67	0/1211
8	V3	0.31	0/203	0.76	0/282
9	S6	0.22	0/461	0.53	0/636
10	S4	0.24	0/624	0.68	2/869 (0.2%)
11	A9	0.27	0/1410	0.68	2/1956 (0.1%)
12	A2	0.25	0/405	0.67	0/563
13	A5	0.26	0/549	0.72	0/764
14	A6	0.27	0/566	0.73	2/789 (0.3%)
15	A7	0.27	0/474	0.74	0/658
16	AL	0.26	0/707	0.71	0/981
17	AA	0.26	0/396	0.74	0/551
17	AB	0.24	0/431	0.59	0/600
18	D3	0.28	0/447	0.63	0/622
19	D1	0.34	0/1503	0.79	2/2095 (0.1%)
20	D6	0.27	0/827	0.74	0/1139
21	4L	0.33	0/485	0.71	0/675
22	D5	0.32	0/3000	0.79	0/4181
23	D4	0.34	0/2276	0.80	3/3174 (0.1%)
24	D2	0.34	1/1720 (0.1%)	0.97	2/2398 (0.1%)
25	AK	0.29	0/681	0.76	4/941 (0.4%)
26	B5	0.26	0/686	0.56	0/954
27	A8	0.27	0/846	0.71	0/1178
28	BJ	0.29	0/852	0.72	2/1190 (0.2%)
29	AJ	0.29	0/1574	0.75	2/2190 (0.1%)
30	S5	0.40	1/489 (0.2%)	0.75	0/680
31	A3	0.28	0/366	0.75	0/509

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	B3	0.33	0/355	0.93	1/490 (0.2%)
33	C2	0.32	0/588	0.81	4/818 (0.5%)
34	B4	0.25	0/634	0.62	0/883
35	AM	0.28	0/680	0.68	0/942
36	B6	0.31	0/475	0.83	1/660 (0.2%)
37	B7	0.27	0/591	0.73	2/824 (0.2%)
38	B9	0.28	0/873	0.70	2/1217 (0.2%)
39	B2	0.33	0/322	0.93	4/448 (0.9%)
40	B8	0.30	0/774	0.95	4/1076 (0.4%)
41	BK	0.26	0/505	0.74	0/703
42	C1	0.27	0/226	0.75	2/313 (0.6%)
43	B1	0.24	0/257	0.68	0/357
44	A1	0.27	0/342	0.63	0/473
All	All	0.30	2/39890 (0.0%)	0.75	53/55469 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	V1	0	2
2	V2	0	3
3	S1	0	6
4	S2	0	2
5	S3	0	2
7	S8	0	1
8	V3	0	2
10	S4	0	1
13	A5	0	2
15	A7	0	2
19	D1	0	2
20	D6	0	2
22	D5	0	5
23	D4	0	2
25	AK	0	2
27	A8	0	1
28	BJ	0	1
29	AJ	0	2
30	S5	0	1
31	A3	0	1
32	B3	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	C2	0	1
34	B4	0	1
36	B6	0	2
37	B7	0	1
39	B2	0	1
40	B8	0	2
42	C1	0	1
43	B1	0	1
44	A1	0	1
All	All	0	56

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S5	94	PRO	C-N	6.54	1.39	1.33
24	D2	146	LEU	C-N	6.08	1.39	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D2	106	LEU	N-CA-C	29.20	146.01	112.72
24	D2	106	LEU	CB-CA-C	-15.76	84.94	110.94
28	BJ	21	PRO	CA-C-N	7.65	135.47	121.70
28	BJ	21	PRO	C-N-CA	7.65	135.47	121.70
29	AJ	229	GLU	CA-C-N	7.60	135.38	121.70
29	AJ	229	GLU	C-N-CA	7.60	135.38	121.70
19	D1	63	PRO	CA-C-N	7.23	134.72	121.70
19	D1	63	PRO	C-N-CA	7.23	134.72	121.70
14	A6	110	GLU	CA-C-N	7.04	134.37	121.70
14	A6	110	GLU	C-N-CA	7.04	134.37	121.70
39	B2	44	SER	CA-C-N	6.98	134.26	121.70
39	B2	44	SER	C-N-CA	6.98	134.26	121.70
33	C2	8	ARG	CA-C-N	6.81	133.96	121.70
33	C2	8	ARG	C-N-CA	6.81	133.96	121.70
3	S1	434	SER	CA-C-N	6.70	133.75	121.70
3	S1	434	SER	C-N-CA	6.70	133.75	121.70
25	AK	17	CYS	CA-C-N	6.66	134.26	121.54
25	AK	17	CYS	C-N-CA	6.66	134.26	121.54
40	B8	78	HIS	CA-C-N	6.41	129.16	120.38
40	B8	78	HIS	C-N-CA	6.41	129.16	120.38
4	S2	230	THR	CA-C-N	6.30	133.58	121.54
4	S2	230	THR	C-N-CA	6.30	133.58	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	S4	10	LEU	CA-C-N	6.01	130.47	120.62
10	S4	10	LEU	C-N-CA	6.01	130.47	120.62
32	B3	45	GLY	N-CA-C	5.97	117.42	111.21
33	C2	4	GLY	CA-C-N	5.92	132.35	121.70
33	C2	4	GLY	C-N-CA	5.92	132.35	121.70
39	B2	61	ASP	CA-C-N	5.87	132.75	121.54
39	B2	61	ASP	C-N-CA	5.87	132.75	121.54
1	V1	332	ALA	N-CA-CB	-5.79	107.57	114.17
5	S3	37	VAL	CA-C-N	5.70	132.71	122.46
5	S3	37	VAL	C-N-CA	5.70	132.71	122.46
38	B9	9	LEU	CA-C-N	5.58	132.20	121.54
38	B9	9	LEU	C-N-CA	5.58	132.20	121.54
2	V2	14	LYS	CA-C-N	5.49	132.03	121.54
2	V2	14	LYS	C-N-CA	5.49	132.03	121.54
3	S1	631	VAL	N-CA-C	-5.45	108.19	113.53
40	B8	37	TYR	CA-C-N	5.37	139.88	127.00
40	B8	37	TYR	C-N-CA	5.37	139.88	127.00
37	B7	26	PRO	CA-C-N	5.26	131.59	121.54
37	B7	26	PRO	C-N-CA	5.26	131.59	121.54
25	AK	137	GLU	CA-C-N	5.22	139.53	127.00
25	AK	137	GLU	C-N-CA	5.22	139.53	127.00
11	A9	221	PRO	CA-C-N	5.21	135.31	125.66
11	A9	221	PRO	C-N-CA	5.21	135.31	125.66
4	S2	72	MET	N-CA-C	-5.20	99.73	110.80
4	S2	165	THR	N-CA-C	5.13	121.15	109.81
42	C1	4	ILE	CA-C-N	5.12	131.32	121.54
42	C1	4	ILE	C-N-CA	5.12	131.32	121.54
23	D4	370	PRO	N-CA-C	5.12	116.94	110.70
23	D4	423	ILE	CA-C-N	5.11	131.31	121.54
23	D4	423	ILE	C-N-CA	5.11	131.31	121.54
36	B6	122	PHE	N-CA-C	5.05	120.98	109.81

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	A1	63	SER	Peptide
31	A3	57	ARG	Peptide
13	A5	113	TRP	Peptide
13	A5	93	MET	Peptide
15	A7	68	VAL	Peptide
15	A7	69	MET	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
27	A8	52	PRO	Peptide
29	AJ	216	GLU	Peptide
29	AJ	278	PHE	Peptide
25	AK	16	GLU	Peptide
25	AK	46	THR	Peptide
43	B1	52	GLU	Peptide
39	B2	56	PRO	Peptide
32	B3	16	PRO	Peptide
32	B3	22	LYS	Peptide
32	B3	58	ASN	Peptide
34	B4	76	TYR	Peptide
36	B6	122	PHE	Peptide
36	B6	86	LYS	Peptide
37	B7	30	PHE	Peptide
40	B8	53	ARG	Peptide
40	B8	86	ARG	Peptide
28	BJ	79	LYS	Peptide
42	C1	6	GLU	Peptide
33	C2	8	ARG	Peptide
19	D1	90	PRO	Peptide
19	D1	91	MET	Peptide
23	D4	52	PHE	Peptide
23	D4	53	SER	Peptide
22	D5	159	TYR	Peptide
22	D5	353	GLU	Peptide
22	D5	365	ALA	Peptide
22	D5	526	LEU	Peptide
22	D5	84	PHE	Mainchain
20	D6	115	ILE	Peptide
20	D6	124	ASP	Peptide
3	S1	213	TYR	Peptide
3	S1	218	ARG	Peptide
3	S1	247	VAL	Peptide
3	S1	254	MET	Peptide
3	S1	341	ASP	Peptide
3	S1	380	VAL	Peptide
4	S2	341	SER	Peptide
4	S2	73	VAL	Peptide
5	S3	76	ALA	Peptide
5	S3	80	ALA	Mainchain
10	S4	11	ILE	Peptide
30	S5	92	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
7	S8	106	THR	Peptide
1	V1	28	ARG	Peptide
1	V1	331	THR	Peptide
2	V2	10	ARG	Peptide
2	V2	13	PRO	Peptide
2	V2	35	VAL	Peptide
8	V3	63	MET	Peptide
8	V3	65	GLN	Peptide

5.2 Too-close contacts [i](#)

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	V1	2099	0	994	30	0
2	V2	1045	0	462	22	0
3	S1	3390	0	1573	25	0
4	S2	2090	0	930	33	0
5	S3	1034	0	445	28	0
6	S7	769	0	351	0	0
7	S8	871	0	401	69	0
8	V3	204	0	78	23	0
9	S6	462	0	211	5	0
10	S4	625	0	274	12	0
11	A9	1413	0	639	6	0
12	A2	406	0	178	3	0
13	A5	550	0	239	4	0
14	A6	567	0	236	13	0
15	A7	476	0	210	54	0
16	AL	708	0	294	26	0
17	AA	397	0	168	2	0
17	AB	432	0	183	2	0
18	D3	449	0	203	0	0
19	D1	1505	0	676	0	0
20	D6	829	0	381	5	0
21	4L	486	0	222	1	0
22	D5	3001	0	1331	9	0
23	D4	2277	0	1004	8	0
24	D2	1721	0	744	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	AK	682	0	358	1	0
26	B5	687	0	302	0	0
27	A8	847	0	364	8	0
28	BJ	853	0	375	27	0
29	AJ	1575	0	694	36	0
30	S5	490	0	215	0	0
31	A3	367	0	157	0	0
32	B3	356	0	178	7	0
33	C2	589	0	254	50	0
34	B4	635	0	281	19	0
35	AM	681	0	302	8	0
36	B6	477	0	187	9	0
37	B7	592	0	260	13	0
38	B9	874	0	374	26	0
39	B2	323	0	136	16	0
40	B8	775	0	318	1	0
41	BK	506	0	214	1	0
42	C1	227	0	97	0	0
43	B1	258	0	109	0	0
44	A1	343	0	159	3	0
45	S1	16	0	0	0	0
45	S7	8	0	0	0	0
45	S8	16	0	0	0	0
45	V1	8	0	0	1	0
46	V1	31	0	19	1	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	1	0
50	A6	34	0	40	10	0
50	AB	31	0	34	8	0
All	All	40144	0	17880	353	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 6.

All (353) 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)
37:B7:99:LYS:HA	39:B2:57:SER:CB	1.22	1.60
7:S8:35:GLY:CA	15:A7:14:ALA:HB1	1.29	1.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S8:35:GLY:C	15:A7:14:ALA:HB1	1.30	1.50
7:S8:35:GLY:O	15:A7:14:ALA:CB	1.67	1.39
29:AJ:317:ILE:CA	33:C2:56:ALA:HA	1.54	1.34
7:S8:35:GLY:CA	15:A7:14:ALA:CB	2.06	1.34
5:S3:80:ALA:HA	5:S3:91:GLU:O	1.17	1.32
7:S8:56:PRO:HA	16:AL:91:HIS:O	1.25	1.32
14:A6:70:ALA:HA	50:A6:201:ZMP:O2	1.23	1.31
7:S8:35:GLY:C	15:A7:14:ALA:CB	2.02	1.31
2:V2:39:PRO:HA	8:V3:65:GLN:CB	1.59	1.30
7:S8:56:PRO:HA	16:AL:91:HIS:C	1.57	1.29
3:S1:431:ASP:O	3:S1:435:GLY:HA2	1.31	1.28
3:S1:431:ASP:O	3:S1:435:GLY:CA	1.81	1.28
37:B7:99:LYS:CA	39:B2:57:SER:CB	2.10	1.27
29:AJ:317:ILE:CB	33:C2:56:ALA:HB2	1.65	1.26
10:S4:12:THR:CB	14:A6:16:VAL:H	1.49	1.26
29:AJ:317:ILE:C	33:C2:56:ALA:HA	1.58	1.25
32:B3:55:GLY:HA3	39:B2:14:PHE:CB	1.70	1.22
1:V1:27:GLY:O	8:V3:37:THR:O	1.58	1.20
28:BJ:16:THR:O	36:B6:110:LEU:N	1.75	1.19
29:AJ:317:ILE:CA	33:C2:56:ALA:CA	2.20	1.19
32:B3:55:GLY:N	39:B2:14:PHE:CB	2.06	1.19
2:V2:39:PRO:CA	8:V3:65:GLN:CB	2.22	1.18
37:B7:29:GLY:HA3	39:B2:66:ILE:O	1.40	1.17
21:4L:94:ASN:HA	22:D5:582:GLY:O	1.43	1.17
7:S8:2:TYR:O	15:A7:106:SER:N	1.78	1.17
29:AJ:305:ARG:N	33:C2:50:ARG:CB	2.09	1.16
32:B3:55:GLY:H	39:B2:14:PHE:CB	1.57	1.16
34:B4:37:ALA:HA	38:B9:149:ARG:HA	1.18	1.15
32:B3:55:GLY:CA	39:B2:14:PHE:CB	2.23	1.14
7:S8:35:GLY:O	15:A7:14:ALA:HB3	1.37	1.13
29:AJ:317:ILE:HA	33:C2:56:ALA:CA	1.75	1.13
29:AJ:317:ILE:HA	33:C2:56:ALA:CB	1.79	1.12
34:B4:40:SER:CB	38:B9:150:THR:N	2.13	1.12
7:S8:56:PRO:CA	16:AL:91:HIS:O	1.96	1.12
7:S8:22:ALA:HB2	35:AM:31:GLY:HA3	1.29	1.09
4:S2:284:ASP:HA	7:S8:1:THR:O	1.50	1.09
7:S8:52:PHE:CB	16:AL:62:VAL:O	2.01	1.08
28:BJ:76:CYS:O	33:C2:108:THR:CA	2.01	1.08
28:BJ:76:CYS:O	33:C2:109:TYR:N	1.85	1.08
28:BJ:146:GLY:HA2	33:C2:119:VAL:O	1.50	1.08
10:S4:12:THR:CB	14:A6:16:VAL:N	2.15	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AJ:317:ILE:HA	33:C2:56:ALA:HA	1.24	1.06
7:S8:35:GLY:HA2	15:A7:14:ALA:HB1	1.14	1.06
28:BJ:76:CYS:O	33:C2:108:THR:HA	1.55	1.06
29:AJ:304:TYR:C	33:C2:50:ARG:CB	2.28	1.06
3:S1:357:ASP:CB	12:A2:53:LEU:HA	1.85	1.05
7:S8:35:GLY:HA2	15:A7:14:ALA:CB	1.74	1.04
50:AB:101:ZMP:H6	38:B9:66:ALA:HB1	1.38	1.04
3:S1:126:ASP:CB	4:S2:328:ALA:HB3	1.86	1.03
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.58	1.03
7:S8:7:LEU:CB	15:A7:112:LEU:N	2.22	1.03
28:BJ:156:ALA:HB2	33:C2:114:GLU:O	1.57	1.03
29:AJ:317:ILE:O	33:C2:56:ALA:N	1.90	1.03
14:A6:66:PHE:HA	50:A6:201:ZMP:H11	1.40	1.01
4:S2:284:ASP:CB	7:S8:1:THR:C	2.33	1.00
29:AJ:317:ILE:CB	33:C2:56:ALA:CB	2.38	1.00
1:V1:27:GLY:C	8:V3:37:THR:O	2.04	1.00
2:V2:40:GLU:O	8:V3:67:SER:HA	1.59	0.99
37:B7:29:GLY:HA3	39:B2:66:ILE:C	1.85	0.99
3:S1:431:ASP:O	3:S1:435:GLY:HA3	1.62	0.99
7:S8:57:LEU:N	16:AL:91:HIS:O	1.96	0.99
34:B4:37:ALA:CA	38:B9:149:ARG:HA	1.92	0.99
32:B3:50:TRP:CB	39:B2:12:ARG:CB	2.42	0.97
7:S8:35:GLY:O	15:A7:14:ALA:HB1	1.39	0.97
34:B4:32:GLN:CB	38:B9:7:ALA:HB1	1.95	0.97
1:V1:27:GLY:O	8:V3:37:THR:C	2.07	0.97
4:S2:284:ASP:CA	7:S8:1:THR:O	2.13	0.97
50:A6:201:ZMP:P1	17:AA:44:SER:CB	2.53	0.96
7:S8:36:MET:HA	15:A7:15:SER:CB	1.96	0.96
29:AJ:304:TYR:HA	33:C2:50:ARG:CB	1.95	0.96
7:S8:56:PRO:C	16:AL:91:HIS:O	2.09	0.95
37:B7:29:GLY:CA	39:B2:66:ILE:O	2.13	0.95
4:S2:129:GLN:N	5:S3:10:THR:O	2.00	0.95
34:B4:32:GLN:C	38:B9:7:ALA:HB1	1.91	0.95
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.14	0.95
7:S8:2:TYR:O	15:A7:106:SER:CB	2.15	0.95
34:B4:40:SER:CB	38:B9:150:THR:O	2.14	0.95
28:BJ:77:HIS:HA	33:C2:108:THR:HA	1.47	0.94
34:B4:40:SER:CB	38:B9:150:THR:C	2.40	0.94
7:S8:52:PHE:O	16:AL:62:VAL:N	2.00	0.94
28:BJ:156:ALA:CB	33:C2:114:GLU:O	2.15	0.94
7:S8:35:GLY:CA	15:A7:14:ALA:CA	2.47	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AB:44:SER:CB	50:AB:101:ZMP:P1	2.56	0.93
7:S8:35:GLY:HA3	15:A7:14:ALA:CA	1.98	0.93
34:B4:40:SER:CB	38:B9:150:THR:H	1.81	0.92
1:V1:26:TYR:CB	2:V2:192:SER:CB	2.46	0.92
7:S8:35:GLY:C	15:A7:14:ALA:C	2.37	0.92
7:S8:7:LEU:CB	15:A7:111:TYR:C	2.43	0.92
2:V2:39:PRO:CB	8:V3:65:GLN:CB	2.49	0.90
2:V2:39:PRO:CB	8:V3:65:GLN:C	2.45	0.90
7:S8:22:ALA:CB	35:AM:31:GLY:HA3	2.01	0.90
29:AJ:317:ILE:CA	33:C2:56:ALA:CB	2.45	0.90
4:S2:253:TYR:HA	5:S3:126:ALA:HB2	1.51	0.90
7:S8:52:PHE:C	16:AL:62:VAL:H	1.80	0.89
34:B4:37:ALA:HA	38:B9:149:ARG:CA	2.02	0.89
14:A6:70:ALA:CA	50:A6:201:ZMP:O2	2.15	0.89
10:S4:70:MET:O	16:AL:128:SER:CB	2.21	0.88
2:V2:39:PRO:CB	8:V3:65:GLN:O	2.22	0.88
29:AJ:317:ILE:C	33:C2:56:ALA:CA	2.42	0.88
7:S8:36:MET:N	15:A7:14:ALA:O	2.06	0.88
29:AJ:317:ILE:CB	33:C2:56:ALA:CA	2.52	0.88
29:AJ:304:TYR:CA	33:C2:50:ARG:CB	2.52	0.88
7:S8:35:GLY:C	15:A7:14:ALA:O	2.17	0.87
7:S8:35:GLY:HA3	15:A7:14:ALA:HA	1.56	0.87
10:S4:70:MET:C	16:AL:128:SER:CB	2.48	0.86
4:S2:284:ASP:CB	7:S8:1:THR:O	2.22	0.86
5:S3:38:GLN:O	15:A7:69:MET:O	1.94	0.85
34:B4:32:GLN:C	38:B9:7:ALA:CB	2.48	0.85
14:A6:65:MET:O	50:A6:201:ZMP:O1	1.96	0.83
28:BJ:146:GLY:CA	33:C2:119:VAL:O	2.26	0.83
29:AJ:317:ILE:O	33:C2:56:ALA:CA	2.26	0.83
7:S8:2:TYR:O	15:A7:106:SER:CA	2.26	0.83
1:V1:198:GLY:HA3	2:V2:45:ALA:HA	1.61	0.83
29:AJ:317:ILE:CA	33:C2:56:ALA:HB2	2.09	0.80
28:BJ:76:CYS:O	33:C2:108:THR:C	2.25	0.79
5:S3:80:ALA:HA	5:S3:91:GLU:C	2.06	0.79
36:B6:103:ILE:O	37:B7:48:ALA:HB2	1.81	0.79
3:S1:276:ARG:O	16:AL:135:GLN:CB	2.30	0.79
8:V3:68:SER:CB	10:S4:125:ASN:HA	2.13	0.79
29:AJ:317:ILE:O	33:C2:56:ALA:HA	1.82	0.78
28:BJ:77:HIS:CA	33:C2:108:THR:HA	2.13	0.78
1:V1:28:ARG:N	8:V3:39:LYS:CB	2.45	0.77
29:AJ:317:ILE:CB	33:C2:56:ALA:N	2.47	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S8:7:LEU:O	15:A7:112:LEU:CB	2.33	0.77
1:V1:27:GLY:HA2	8:V3:40:ASN:H	1.49	0.77
4:S2:326:ASP:CB	15:A7:45:SER:CB	2.63	0.76
28:BJ:74:THR:O	33:C2:110:ARG:CB	2.34	0.76
29:AJ:304:TYR:O	33:C2:50:ARG:O	2.02	0.75
34:B4:40:SER:CB	38:B9:150:THR:CA	2.65	0.74
4:S2:81:GLY:HA3	5:S3:152:LEU:HA	1.68	0.74
4:S2:5:GLN:CB	29:AJ:286:ALA:HB3	2.17	0.74
7:S8:35:GLY:C	15:A7:14:ALA:CA	2.59	0.74
28:BJ:77:HIS:HA	33:C2:108:THR:CA	2.18	0.74
9:S6:31:ARG:HA	16:AL:121:PRO:O	1.87	0.74
10:S4:12:THR:CB	14:A6:16:VAL:CB	2.67	0.73
3:S1:278:ARG:O	16:AL:137:TRP:N	2.22	0.73
10:S4:12:THR:CB	14:A6:16:VAL:CA	2.67	0.73
3:S1:216:THR:HA	7:S8:96:ALA:O	1.88	0.72
4:S2:6:PRO:N	24:D2:304:MET:O	2.22	0.72
4:S2:253:TYR:CA	5:S3:126:ALA:HB2	2.19	0.72
27:A8:2:GLY:O	35:AM:107:GLU:HA	1.89	0.71
14:A6:66:PHE:CA	50:A6:201:ZMP:H11	2.19	0.71
3:S1:442:VAL:O	3:S1:446:ALA:HB2	1.89	0.71
5:S3:38:GLN:HA	15:A7:70:SER:O	1.90	0.71
1:V1:28:ARG:HA	8:V3:37:THR:O	1.91	0.70
9:S6:30:GLY:O	16:AL:121:PRO:O	2.09	0.70
4:S2:284:ASP:CB	7:S8:2:TYR:N	2.54	0.70
24:D2:307:SER:O	29:AJ:284:ILE:O	2.10	0.70
28:BJ:16:THR:O	36:B6:110:LEU:CB	2.39	0.70
5:S3:38:GLN:O	15:A7:70:SER:HA	1.91	0.70
23:D4:177:LEU:O	23:D4:180:GLN:C	2.35	0.70
4:S2:129:GLN:H	5:S3:10:THR:C	1.98	0.69
7:S8:5:VAL:C	15:A7:111:TYR:CB	2.66	0.69
9:S6:30:GLY:O	16:AL:121:PRO:HA	1.92	0.69
7:S8:39:SER:HA	15:A7:11:ARG:CB	2.23	0.69
14:A6:66:PHE:HA	50:A6:201:ZMP:C11	2.20	0.69
50:AB:101:ZMP:H7A	38:B9:66:ALA:HB2	1.74	0.69
7:S8:54:LYS:O	16:AL:90:LEU:O	2.11	0.68
7:S8:2:TYR:N	15:A7:106:SER:CB	2.57	0.68
5:S3:38:GLN:O	15:A7:70:SER:CA	2.42	0.68
34:B4:32:GLN:CA	38:B9:7:ALA:HB1	2.24	0.68
7:S8:2:TYR:C	15:A7:106:SER:CB	2.67	0.68
4:S2:129:GLN:CB	5:S3:10:THR:C	2.68	0.67
28:BJ:76:CYS:C	33:C2:108:THR:HA	2.20	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B7:29:GLY:CA	39:B2:66:ILE:C	2.63	0.67
34:B4:32:GLN:O	38:B9:7:ALA:CB	2.42	0.66
27:A8:90:TYR:O	44:A1:35:GLU:CB	2.43	0.66
28:BJ:76:CYS:O	33:C2:108:THR:CB	2.43	0.66
1:V1:150:GLN:CB	8:V3:54:LEU:CB	2.75	0.65
3:S1:637:GLU:CB	12:A2:57:CYS:O	2.45	0.65
23:D4:46:GLY:H	41:BK:84:ARG:HA	1.63	0.65
37:B7:99:LYS:N	39:B2:57:SER:CB	2.60	0.65
1:V1:126:GLY:HA2	1:V1:131:ALA:HB3	1.79	0.64
4:S2:284:ASP:CB	7:S8:2:TYR:CA	2.76	0.64
27:A8:3:ILE:HA	35:AM:107:GLU:HA	1.79	0.64
29:AJ:305:ARG:CB	33:C2:50:ARG:CB	2.76	0.64
50:AB:101:ZMP:C6	38:B9:66:ALA:HB1	2.23	0.64
28:BJ:16:THR:O	36:B6:110:LEU:CA	2.44	0.64
7:S8:2:TYR:H	15:A7:106:SER:CB	2.10	0.64
4:S2:284:ASP:CB	7:S8:2:TYR:HA	2.27	0.64
28:BJ:73:ILE:O	33:C2:109:TYR:CB	2.46	0.63
27:A8:21:SER:CB	44:A1:51:ASP:CB	2.75	0.63
4:S2:129:GLN:O	5:S3:10:THR:CB	2.45	0.63
37:B7:29:GLY:HA3	39:B2:66:ILE:N	2.14	0.63
4:S2:129:GLN:O	5:S3:10:THR:CA	2.46	0.63
29:AJ:304:TYR:C	33:C2:50:ARG:O	2.43	0.62
7:S8:36:MET:CA	15:A7:15:SER:CB	2.76	0.62
20:D6:58:LEU:O	20:D6:62:GLY:HA3	1.98	0.62
7:S8:39:SER:HA	15:A7:11:ARG:HA	1.83	0.61
24:D2:307:SER:O	29:AJ:284:ILE:N	2.24	0.61
1:V1:93:LEU:O	1:V1:134:ALA:HA	2.00	0.61
23:D4:304:GLN:O	28:BJ:147:ALA:HB2	2.00	0.60
50:AB:101:ZMP:H6	38:B9:66:ALA:CB	2.22	0.60
9:S6:30:GLY:O	16:AL:121:PRO:CA	2.50	0.60
34:B4:32:GLN:O	38:B9:7:ALA:HB2	2.02	0.60
4:S2:19:MET:N	24:D2:171:ASN:O	2.28	0.60
12:A2:21:HIS:O	12:A2:62:PRO:HA	2.02	0.59
24:D2:307:SER:N	29:AJ:284:ILE:O	2.34	0.59
5:S3:39:GLN:HA	15:A7:69:MET:O	2.02	0.59
1:V1:361:GLN:O	3:S1:51:ASN:CB	2.50	0.58
22:D5:547:LYS:O	22:D5:552:LEU:CB	2.52	0.58
37:B7:115:GLU:O	37:B7:119:ALA:HB3	2.04	0.58
2:V2:39:PRO:CB	8:V3:65:GLN:CA	2.81	0.58
8:V3:68:SER:CB	10:S4:125:ASN:CB	2.82	0.57
13:A5:46:TYR:CB	15:A7:93:ALA:HB2	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B6:103:ILE:O	37:B7:48:ALA:CB	2.52	0.57
50:AB:101:ZMP:H7A	38:B9:66:ALA:CB	2.35	0.57
1:V1:103:GLY:HA2	2:V2:148:CYS:CB	2.34	0.57
7:S8:35:GLY:CA	15:A7:14:ALA:O	2.53	0.57
36:B6:10:ARG:CB	38:B9:155:PRO:CB	2.82	0.57
8:V3:68:SER:CB	10:S4:125:ASN:CA	2.82	0.57
28:BJ:74:THR:HA	33:C2:109:TYR:C	2.30	0.57
1:V1:300:GLY:HA2	1:V1:330:GLY:H	1.70	0.57
1:V1:294:LEU:HA	1:V1:338:ASP:HA	1.86	0.56
28:BJ:146:GLY:HA3	33:C2:119:VAL:CB	2.35	0.56
5:S3:77:ASP:O	5:S3:93:VAL:O	2.23	0.56
7:S8:55:GLY:O	16:AL:91:HIS:HA	2.06	0.56
23:D4:177:LEU:O	23:D4:180:GLN:O	2.23	0.56
7:S8:5:VAL:CA	15:A7:111:TYR:CB	2.84	0.56
7:S8:56:PRO:CA	16:AL:91:HIS:C	2.53	0.56
3:S1:277:GLN:HA	16:AL:135:GLN:O	2.06	0.55
7:S8:39:SER:CB	15:A7:11:ARG:O	2.55	0.55
1:V1:259:SER:CB	2:V2:149:VAL:HA	2.37	0.55
7:S8:35:GLY:HA2	15:A7:14:ALA:HB2	1.81	0.55
34:B4:32:GLN:CB	38:B9:7:ALA:CB	2.78	0.55
1:V1:301:GLY:HA2	1:V1:333:ALA:HB3	1.89	0.55
4:S2:253:TYR:C	5:S3:126:ALA:HB2	2.32	0.55
22:D5:361:GLY:H	22:D5:435:PRO:HA	1.72	0.55
29:AJ:305:ARG:CA	33:C2:50:ARG:CB	2.84	0.55
1:V1:216:PHE:O	10:S4:124:TRP:HA	2.08	0.54
1:V1:27:GLY:HA2	8:V3:40:ASN:N	2.21	0.54
3:S1:377:VAL:HA	3:S1:450:MET:O	2.07	0.54
13:A5:46:TYR:CB	15:A7:93:ALA:CB	2.85	0.54
34:B4:32:GLN:O	38:B9:7:ALA:HB1	2.05	0.54
2:V2:39:PRO:CA	8:V3:65:GLN:O	2.56	0.53
28:BJ:156:ALA:HB1	33:C2:114:GLU:O	2.04	0.53
34:B4:32:GLN:C	38:B9:7:ALA:HB2	2.32	0.53
7:S8:2:TYR:C	15:A7:106:SER:H	2.07	0.53
23:D4:52:PHE:O	23:D4:56:PHE:CB	2.57	0.53
29:AJ:317:ILE:HA	33:C2:56:ALA:HB1	1.86	0.53
7:S8:22:ALA:HB2	35:AM:31:GLY:CA	2.19	0.53
4:S2:129:GLN:O	5:S3:10:THR:HA	2.08	0.52
22:D5:62:ILE:O	36:B6:96:ILE:HA	2.09	0.52
7:S8:39:SER:HA	15:A7:11:ARG:CA	2.39	0.52
16:AL:6:VAL:O	16:AL:10:GLY:N	2.40	0.52
5:S3:38:GLN:O	15:A7:69:MET:C	2.53	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AJ:25:ILE:O	29:AJ:123:VAL:HA	2.11	0.51
20:D6:141:MET:HA	20:D6:144:ALA:HB3	1.93	0.51
22:D5:83:ASP:O	22:D5:85:PHE:N	2.43	0.51
1:V1:28:ARG:CA	8:V3:37:THR:O	2.57	0.51
4:S2:129:GLN:H	5:S3:11:VAL:HA	1.76	0.50
4:S2:5:GLN:CB	29:AJ:286:ALA:CB	2.87	0.50
4:S2:251:LEU:CB	5:S3:73:LYS:CB	2.89	0.50
7:S8:35:GLY:CA	15:A7:14:ALA:C	2.82	0.50
3:S1:407:ALA:HA	3:S1:420:ASP:O	2.12	0.50
4:S2:36:VAL:HA	24:D2:49:ASN:CB	2.42	0.50
23:D4:254:THR:O	23:D4:258:ALA:HB2	2.11	0.50
28:BJ:74:THR:O	33:C2:110:ARG:N	2.45	0.50
38:B9:138:GLN:O	38:B9:142:GLU:CB	2.60	0.49
37:B7:29:GLY:HA3	39:B2:66:ILE:CA	2.41	0.49
7:S8:35:GLY:HA3	15:A7:14:ALA:C	2.37	0.49
1:V1:198:GLY:CA	2:V2:45:ALA:HA	2.40	0.49
4:S2:252:ASN:O	5:S3:126:ALA:HB2	2.13	0.49
50:AB:101:ZMP:O2	50:AB:101:ZMP:N2	2.45	0.49
3:S1:266:LYS:O	3:S1:270:ALA:HB2	2.12	0.49
3:S1:450:MET:HA	3:S1:489:VAL:O	2.13	0.49
7:S8:35:GLY:HA3	15:A7:14:ALA:O	2.12	0.49
2:V2:40:GLU:N	8:V3:65:GLN:O	2.46	0.48
27:A8:90:TYR:CB	44:A1:34:ARG:HA	2.43	0.48
28:BJ:114:GLN:O	36:B6:99:LYS:HA	2.13	0.48
27:A8:3:ILE:HA	35:AM:106:GLY:O	2.14	0.48
37:B7:98:MET:C	39:B2:57:SER:CB	2.87	0.48
1:V1:103:GLY:CA	2:V2:148:CYS:CB	2.91	0.48
11:A9:167:LYS:O	11:A9:229:ALA:HA	2.14	0.48
2:V2:96:GLY:HA3	2:V2:136:LEU:H	1.77	0.48
4:S2:360:PRO:HA	4:S2:380:SER:O	2.14	0.48
14:A6:65:MET:C	50:A6:201:ZMP:O1	2.57	0.48
20:D6:58:LEU:O	20:D6:62:GLY:CA	2.60	0.48
32:B3:53:MET:HA	32:B3:57:ALA:HB2	1.96	0.47
7:S8:5:VAL:HA	15:A7:111:TYR:CB	2.44	0.47
7:S8:39:SER:CA	15:A7:11:ARG:HA	2.44	0.47
23:D4:254:THR:O	23:D4:258:ALA:CB	2.62	0.47
5:S3:72:PHE:HA	5:S3:98:SER:HA	1.97	0.47
11:A9:120:VAL:O	11:A9:124:ALA:HB2	2.14	0.47
29:AJ:317:ILE:C	33:C2:56:ALA:H	2.14	0.47
7:S8:53:GLU:HA	16:AL:61:TRP:HA	1.97	0.47
14:A6:65:MET:CB	50:A6:201:ZMP:H6	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:384:PRO:HA	22:D5:385:PHE:HA	1.54	0.47
1:V1:236:ARG:O	2:V2:213:VAL:CB	2.63	0.47
46:V1:501:FMN:O5'	46:V1:501:FMN:O3'	2.30	0.47
10:S4:12:THR:CB	14:A6:16:VAL:O	2.63	0.46
32:B3:69:GLY:O	39:B2:30:ALA:HA	2.15	0.46
3:S1:675:ASP:O	3:S1:679:ARG:CB	2.64	0.46
17:AB:44:SER:CB	50:AB:101:ZMP:O7	2.64	0.46
4:S2:347:HIS:O	4:S2:351:LEU:CB	2.64	0.46
15:A7:111:TYR:HA	15:A7:112:LEU:HA	1.63	0.46
28:BJ:76:CYS:C	33:C2:108:THR:CB	2.89	0.46
4:S2:35:ASP:O	24:D2:49:ASN:CB	2.64	0.45
7:S8:7:LEU:CB	15:A7:112:LEU:CA	2.92	0.45
9:S6:30:GLY:O	16:AL:121:PRO:C	2.59	0.45
34:B4:37:ALA:CB	38:B9:149:ARG:HA	2.45	0.45
1:V1:43:TYR:CB	2:V2:209:PRO:CB	2.95	0.45
3:S1:377:VAL:O	3:S1:406:VAL:HA	2.17	0.45
1:V1:28:ARG:N	8:V3:37:THR:O	2.50	0.45
3:S1:442:VAL:O	3:S1:446:ALA:CB	2.63	0.45
7:S8:160:LYS:HA	16:AL:110:TRP:CB	2.47	0.44
3:S1:483:VAL:HA	3:S1:484:THR:HA	1.65	0.44
2:V2:13:PRO:HA	2:V2:15:ASN:H	1.82	0.44
1:V1:387:ALA:HB1	15:A7:48:LEU:CB	2.47	0.44
1:V1:362:CYS:N	45:V1:500:SF4:S2	2.77	0.44
4:S2:129:GLN:N	5:S3:10:THR:C	2.68	0.44
7:S8:55:GLY:O	16:AL:91:HIS:CA	2.66	0.44
3:S1:449:PRO:O	3:S1:489:VAL:CA	2.47	0.44
27:A8:77:CYS:HA	27:A8:78:ALA:HA	1.71	0.44
33:C2:8:ARG:H	33:C2:9:ALA:HB3	1.81	0.44
50:A6:201:ZMP:O6	17:AA:44:SER:CB	2.65	0.44
23:D4:175:ASN:O	23:D4:179:LEU:N	2.38	0.43
28:BJ:156:ALA:HB1	33:C2:115:GLU:HA	2.00	0.43
3:S1:283:MET:HA	3:S1:293:HIS:HA	2.00	0.43
11:A9:108:ASP:O	11:A9:112:LYS:CB	2.66	0.43
1:V1:102:PRO:CB	2:V2:144:CYS:CB	2.97	0.43
1:V1:138:ILE:O	1:V1:180:GLY:N	2.52	0.43
11:A9:26:ALA:HA	11:A9:31:GLY:HA3	2.01	0.43
7:S8:22:ALA:CB	35:AM:31:GLY:CA	2.85	0.43
34:B4:37:ALA:CB	38:B9:149:ARG:CB	2.96	0.43
11:A9:95:VAL:O	49:A9:401:NDP:O3D	2.33	0.42
27:A8:158:LYS:O	33:C2:84:ALA:HB1	2.18	0.42
20:D6:174:GLY:HA2	20:D6:175:ASN:HA	1.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AJ:119:GLY:HA3	29:AJ:120:GLN:HA	1.83	0.42
29:AJ:313:GLY:HA3	29:AJ:314:ASP:HA	1.71	0.42
7:S8:48:ILE:CB	16:AL:57:GLY:O	2.67	0.42
22:D5:554:ASP:O	22:D5:558:LEU:CB	2.68	0.42
2:V2:98:TYR:H	2:V2:136:LEU:HA	1.85	0.42
3:S1:244:THR:C	10:S4:73:ALA:HB2	2.45	0.42
22:D5:403:TYR:HA	40:B8:124:THR:O	2.20	0.42
28:BJ:74:THR:CB	33:C2:110:ARG:HA	2.49	0.41
11:A9:165:ILE:O	11:A9:227:THR:HA	2.21	0.41
29:AJ:75:GLY:HA3	29:AJ:76:ASN:HA	1.73	0.41
3:S1:484:THR:H	3:S1:485:GLY:HA2	1.86	0.41
13:A5:113:TRP:O	13:A5:115:ILE:N	2.54	0.41
22:D5:61:MET:HA	36:B6:98:GLU:HA	2.03	0.41
35:AM:27:ARG:HA	35:AM:28:GLY:HA3	1.71	0.41
2:V2:17:PRO:HA	2:V2:18:GLU:HA	1.77	0.41
4:S2:252:ASN:O	5:S3:126:ALA:CB	2.69	0.41
20:D6:126:VAL:HA	20:D6:127:ILE:HA	1.73	0.41
5:S3:35:LYS:HA	13:A5:102:LEU:HA	2.02	0.40
5:S3:38:GLN:O	15:A7:70:SER:N	2.54	0.40
25:AK:46:THR:HA	25:AK:47:SER:HA	1.86	0.40
4:S2:6:PRO:CB	24:D2:304:MET:O	2.69	0.40
29:AJ:202:ILE:O	29:AJ:206:TYR:CB	2.69	0.40
1:V1:27:GLY:HA3	8:V3:38:TYR:HA	0.72	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	V1	428/445 (96%)	381 (89%)	47 (11%)	0	100	100
2	V2	210/217 (97%)	167 (80%)	43 (20%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S1	686/704 (97%)	614 (90%)	71 (10%)	1 (0%)	48	83
4	S2	420/430 (98%)	379 (90%)	41 (10%)	0	100	100
5	S3	206/228 (90%)	180 (87%)	26 (13%)	0	100	100
6	S7	154/179 (86%)	136 (88%)	17 (11%)	1 (1%)	21	59
7	S8	174/176 (99%)	157 (90%)	17 (10%)	0	100	100
8	V3	39/75 (52%)	32 (82%)	7 (18%)	0	100	100
9	S6	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
10	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
11	A9	281/338 (83%)	244 (87%)	37 (13%)	0	100	100
12	A2	80/98 (82%)	72 (90%)	8 (10%)	0	100	100
13	A5	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
14	A6	112/127 (88%)	105 (94%)	7 (6%)	0	100	100
15	A7	92/112 (82%)	77 (84%)	15 (16%)	0	100	100
16	AL	142/145 (98%)	119 (84%)	23 (16%)	0	100	100
17	AA	78/88 (89%)	67 (86%)	11 (14%)	0	100	100
17	AB	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
18	D3	86/115 (75%)	81 (94%)	5 (6%)	0	100	100
19	D1	299/318 (94%)	273 (91%)	25 (8%)	1 (0%)	36	72
20	D6	167/175 (95%)	145 (87%)	21 (13%)	1 (1%)	21	59
21	4L	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
22	D5	604/606 (100%)	532 (88%)	70 (12%)	2 (0%)	36	72
23	D4	457/459 (100%)	411 (90%)	45 (10%)	1 (0%)	43	78
24	D2	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
25	AK	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
26	B5	137/143 (96%)	124 (90%)	13 (10%)	0	100	100
27	A8	169/171 (99%)	136 (80%)	33 (20%)	0	100	100
28	BJ	169/175 (97%)	151 (89%)	17 (10%)	1 (1%)	21	59
29	AJ	317/320 (99%)	277 (87%)	40 (13%)	0	100	100
30	S5	97/105 (92%)	80 (82%)	17 (18%)	0	100	100
31	A3	72/83 (87%)	60 (83%)	12 (17%)	0	100	100
32	B3	71/97 (73%)	58 (82%)	13 (18%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	C2	117/120 (98%)	104 (89%)	13 (11%)	0	100	100
34	B4	126/128 (98%)	111 (88%)	15 (12%)	0	100	100
35	AM	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
36	B6	92/127 (72%)	79 (86%)	13 (14%)	0	100	100
37	B7	117/136 (86%)	100 (86%)	17 (14%)	0	100	100
38	B9	174/178 (98%)	148 (85%)	26 (15%)	0	100	100
39	B2	63/72 (88%)	54 (86%)	9 (14%)	0	100	100
40	B8	155/158 (98%)	117 (76%)	37 (24%)	1 (1%)	21	59
41	BK	100/125 (80%)	81 (81%)	19 (19%)	0	100	100
42	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
43	B1	50/57 (88%)	46 (92%)	4 (8%)	0	100	100
44	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	7980/8509 (94%)	7032 (88%)	939 (12%)	9 (0%)	49	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	D5	84	PHE
23	D4	53	SER
3	S1	359	ARG
6	S7	54	CYS
22	D5	527	GLY
20	D6	138	GLU
40	B8	143	GLY
28	BJ	71	PRO
19	D1	92	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z > 2$
50	ZMP	AB	101	-	24,30,36	0.76	1 (4%)	29,37,45	1.30	3 (10%)
45	SF4	S1	802	-	0,12,12	-	-	-		
45	SF4	V1	500	-	0,12,12	-	-	-		
46	FMN	V1	501	-	33,33,33	0.27	0	48,50,50	0.42	0
47	FES	V2	300	-	0,4,4	-	-	-		
45	SF4	S1	801	-	0,12,12	-	-	-		
47	FES	S1	803	-	0,4,4	-	-	-		
45	SF4	S7	300	-	0,12,12	-	-	-		
49	NDP	A9	401	-	49,52,52	0.43	1 (2%)	66,80,80	0.44	0
45	SF4	S8	202	-	0,12,12	-	-	-		
45	SF4	S8	201	-	0,12,12	-	-	-		
50	ZMP	A6	201	-	27,33,36	0.66	1 (3%)	32,40,45	1.00	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	ZMP	AB	101	-	-	16/35/37/43	-
45	SF4	S1	802	-	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FMN	V1	501	-	-	7/18/18/18	0/3/3/3
45	SF4	V1	500	-	-	-	0/6/5/5
47	FES	V2	300	-	-	-	0/1/1/1
45	SF4	S1	801	-	-	-	0/6/5/5
47	FES	S1	803	-	-	-	0/1/1/1
45	SF4	S7	300	-	-	-	0/6/5/5
49	NDP	A9	401	-	-	13/34/77/77	0/5/5/5
45	SF4	S8	202	-	-	-	0/6/5/5
45	SF4	S8	201	-	-	-	0/6/5/5
50	ZMP	A6	201	-	-	15/38/40/43	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AB	101	ZMP	C9-C10	2.25	1.53	1.50
49	A9	401	NDP	P2B-O2B	2.24	1.63	1.59
50	A6	201	ZMP	C9-C10	2.14	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	AB	101	ZMP	O1-C10-C9	-3.39	119.98	123.99
50	A6	201	ZMP	O1-C10-C9	-2.59	120.92	123.99
50	AB	101	ZMP	C11-C12-N1	-2.52	107.11	112.42
50	AB	101	ZMP	C15-C14-C13	-2.47	108.24	112.36

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C2'-C3'-C4'-O4'
46	V1	501	FMN	C2'-C3'-C4'-C5'
46	V1	501	FMN	O3'-C3'-C4'-C5'
46	V1	501	FMN	C5'-O5'-P-O2P
46	V1	501	FMN	C5'-O5'-P-O3P
49	A9	401	NDP	C5B-O5B-PA-O1A
49	A9	401	NDP	C5B-O5B-PA-O2A
49	A9	401	NDP	C1B-C2B-O2B-P2B
50	A6	201	ZMP	C9-C10-S1-C11
50	A6	201	ZMP	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

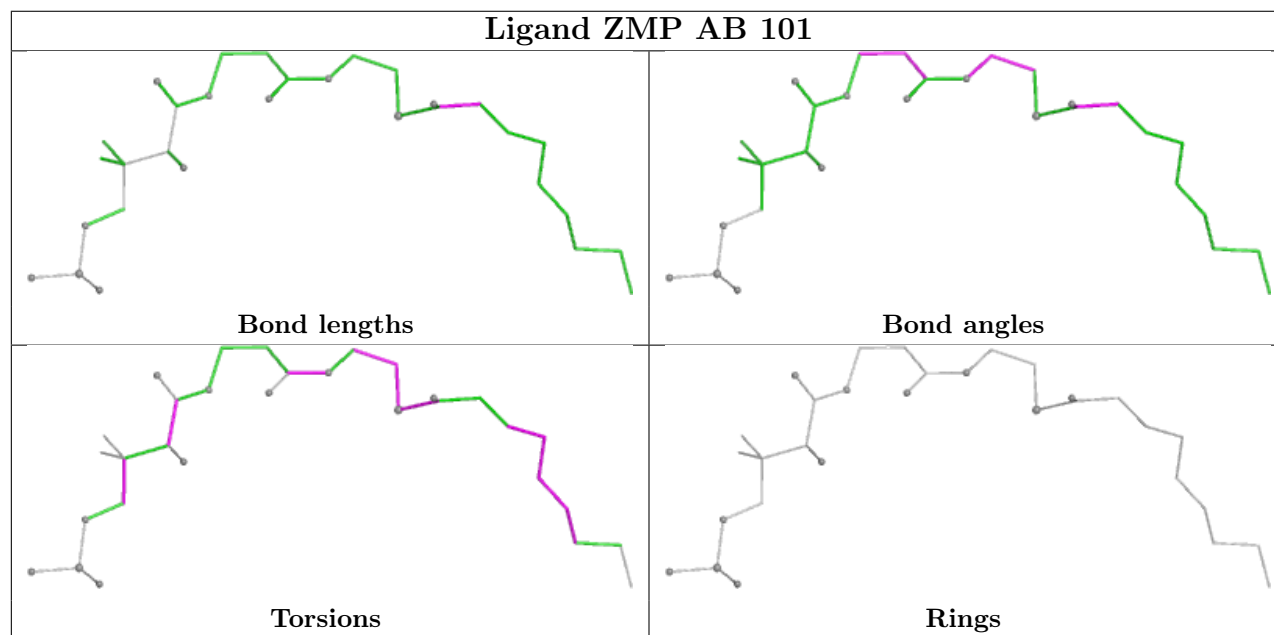
Mol	Chain	Res	Type	Atoms
50	AB	101	ZMP	C17-C18-C21-O5
50	AB	101	ZMP	C12-C11-S1-C10
50	AB	101	ZMP	O1-C10-S1-C11
50	AB	101	ZMP	C9-C10-S1-C11
50	A6	201	ZMP	C14-C13-N1-C12
50	AB	101	ZMP	C14-C13-N1-C12
46	V1	501	FMN	O3'-C3'-C4'-O4'
50	A6	201	ZMP	O2-C13-N1-C12
50	AB	101	ZMP	O2-C13-N1-C12
50	AB	101	ZMP	C5-C6-C7-C8
50	AB	101	ZMP	C3-C4-C5-C6
50	AB	101	ZMP	C6-C7-C8-C9
50	A6	201	ZMP	C2-C1-C22-C23
46	V1	501	FMN	C5'-O5'-P-O1P
50	A6	201	ZMP	O4-C17-C18-C19
50	AB	101	ZMP	S1-C11-C12-N1
50	AB	101	ZMP	N2-C16-C17-C18
50	A6	201	ZMP	O1-C10-S1-C11
49	A9	401	NDP	PN-O3-PA-O5B
49	A9	401	NDP	C2B-O2B-P2B-O3X
50	A6	201	ZMP	O4-C17-C18-C21
50	AB	101	ZMP	O3-C16-C17-O4
50	AB	101	ZMP	C19-C18-C21-O5
50	AB	101	ZMP	C20-C18-C21-O5
49	A9	401	NDP	O4D-C1D-N1N-C6N
49	A9	401	NDP	C2D-C1D-N1N-C6N
50	AB	101	ZMP	O3-C16-C17-C18
50	A6	201	ZMP	C11-C12-N1-C13
50	A6	201	ZMP	C12-C11-S1-C10
50	A6	201	ZMP	C4-C5-C6-C7
49	A9	401	NDP	O4B-C4B-C5B-O5B
50	A6	201	ZMP	C16-C17-C18-C19
50	A6	201	ZMP	C16-C17-C18-C20
49	A9	401	NDP	C5B-O5B-PA-O3
50	A6	201	ZMP	O4-C17-C18-C20
49	A9	401	NDP	C4B-C5B-O5B-PA
49	A9	401	NDP	C2D-C1D-N1N-C2N
49	A9	401	NDP	PA-O3-PN-O2N
50	AB	101	ZMP	C4-C5-C6-C7
49	A9	401	NDP	O4D-C1D-N1N-C2N
50	A6	201	ZMP	C16-C17-C18-C21

There are no ring outliers.

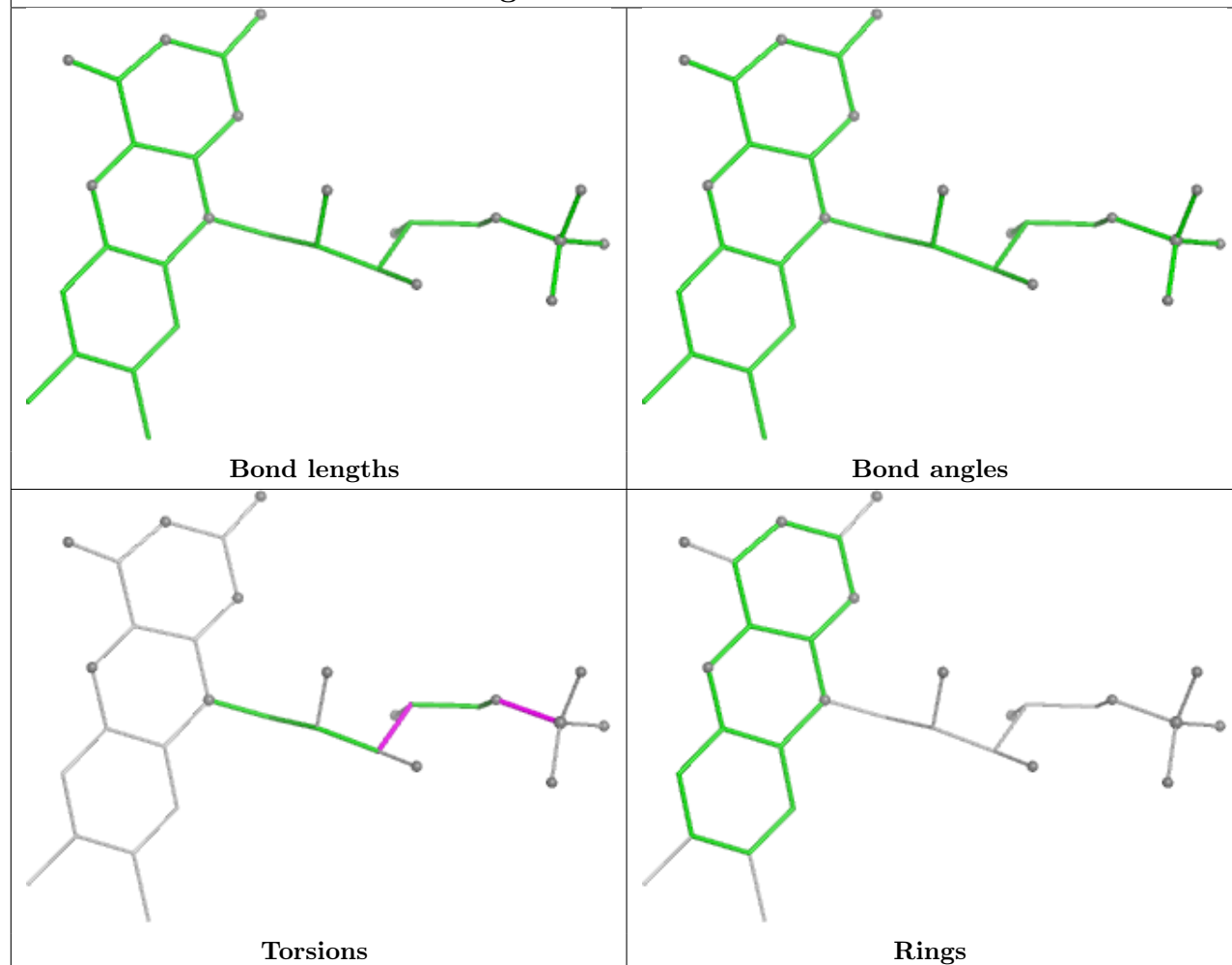
5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	AB	101	ZMP	8	0
45	V1	500	SF4	1	0
46	V1	501	FMN	1	0
49	A9	401	NDP	1	0
50	A6	201	ZMP	10	0

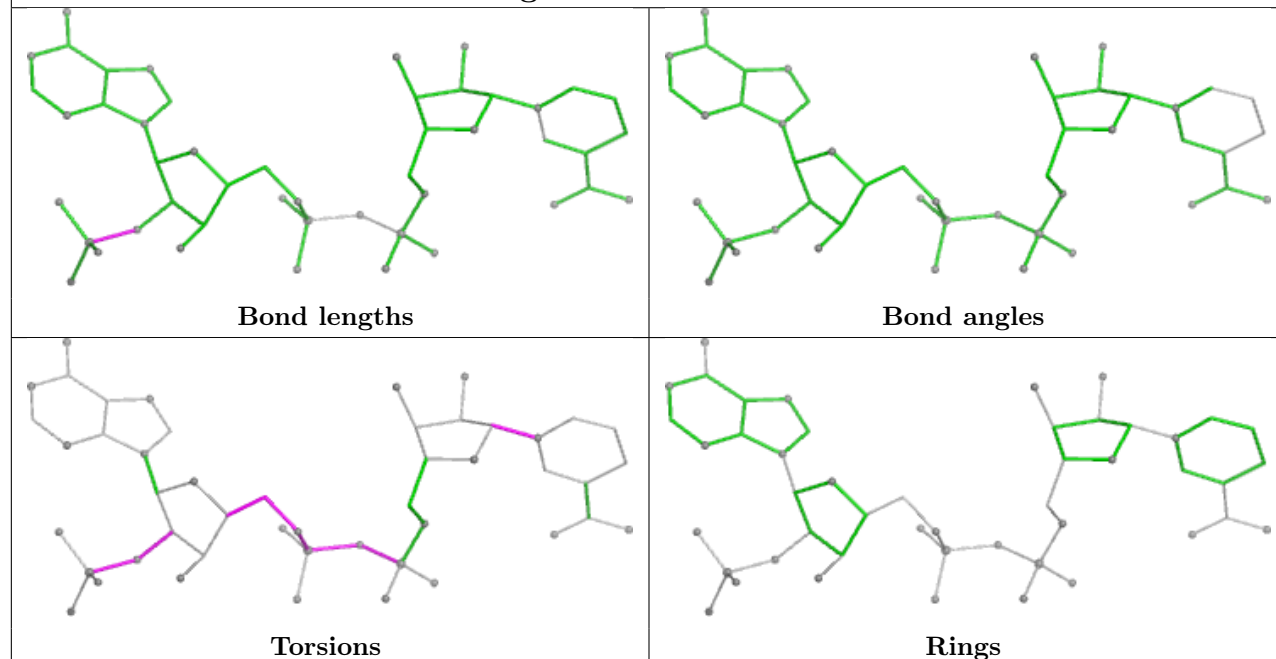
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

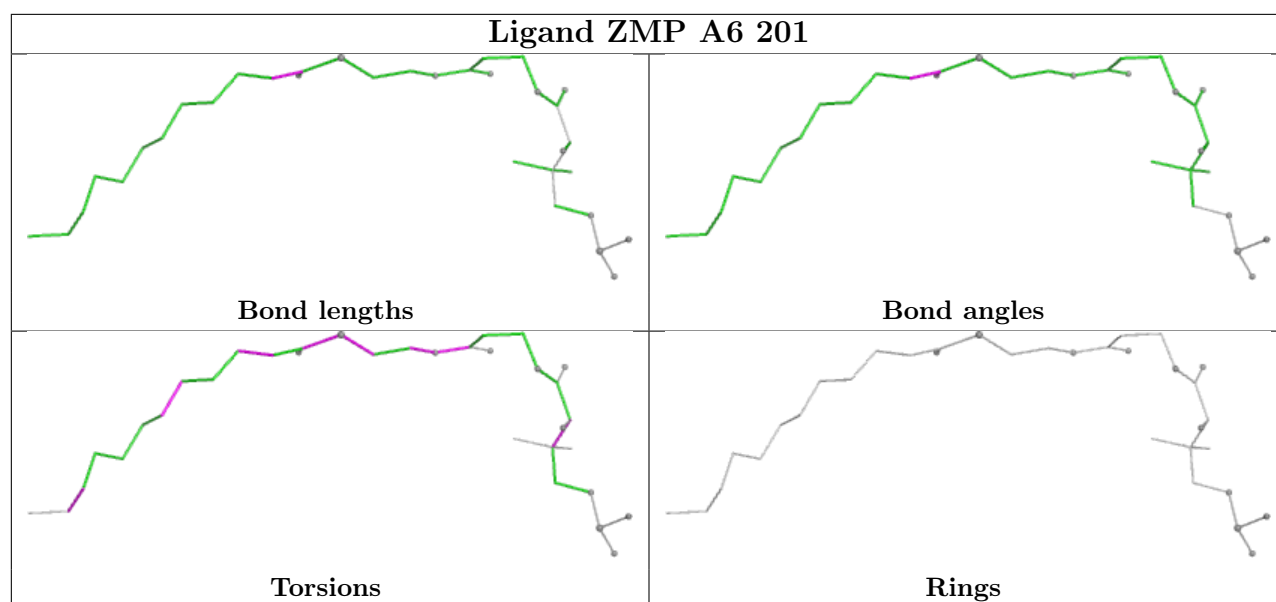


Ligand FMN V1 501



Ligand NDP A9 401





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.

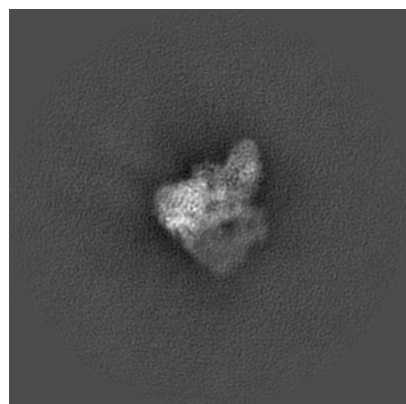
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4502. These allow visual inspection of the internal detail of the map and identification of artifacts.

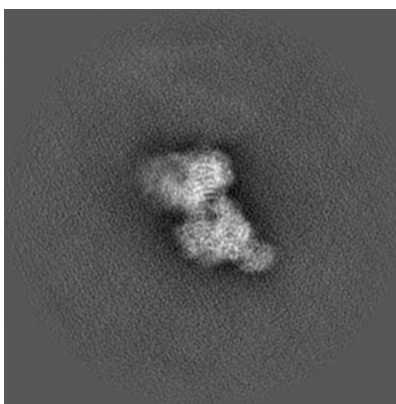
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

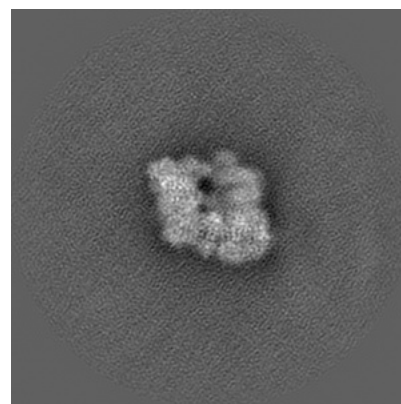
6.1.1 Primary map



X

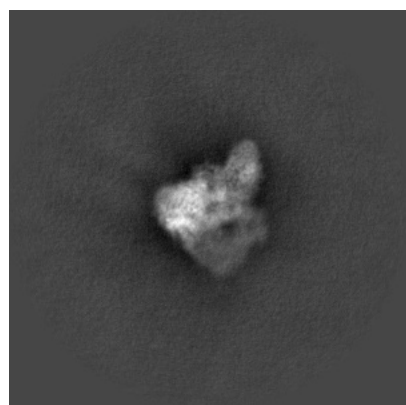


Y

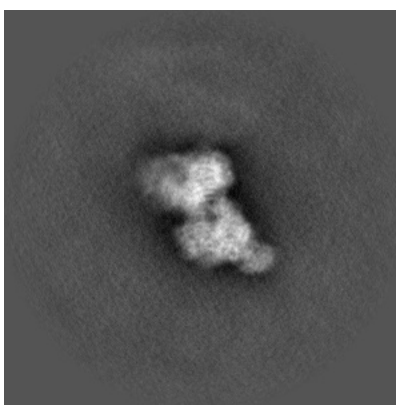


Z

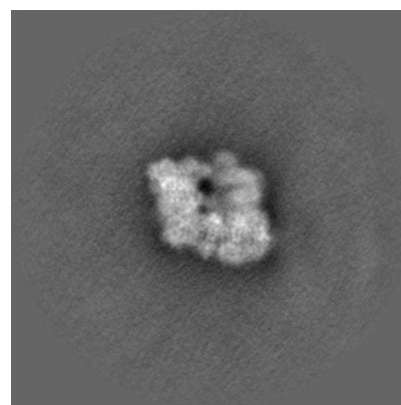
6.1.2 Raw map



X



Y

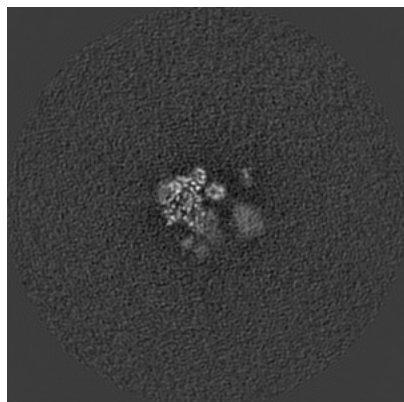


Z

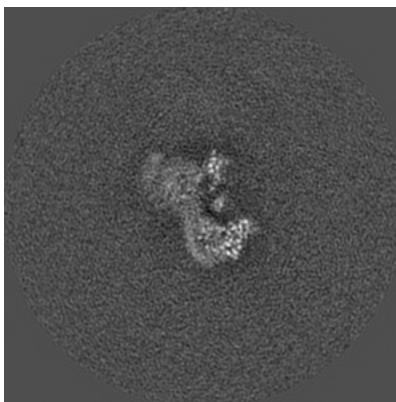
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

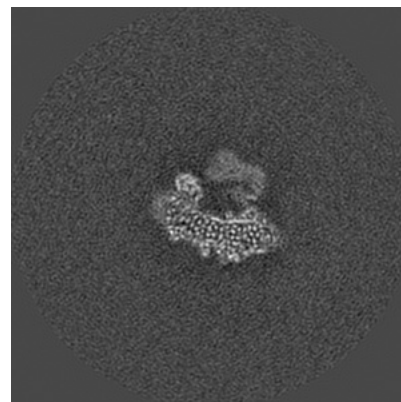
6.2.1 Primary map



X Index: 256

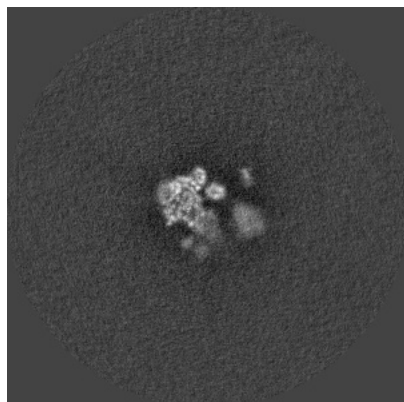


Y Index: 256

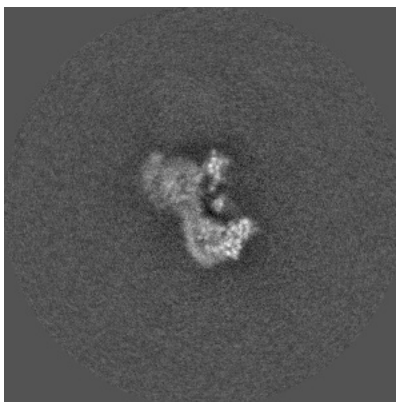


Z Index: 256

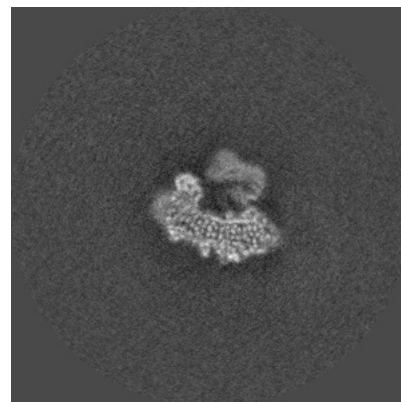
6.2.2 Raw map



X Index: 256



Y Index: 256

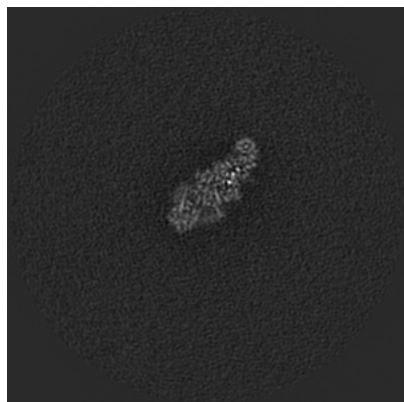


Z Index: 256

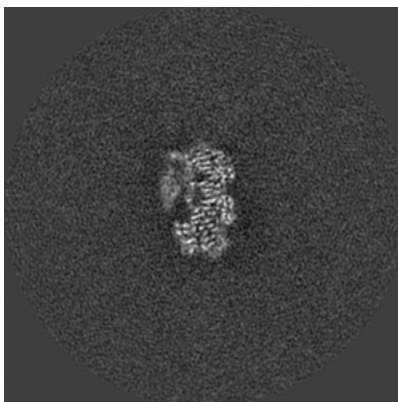
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

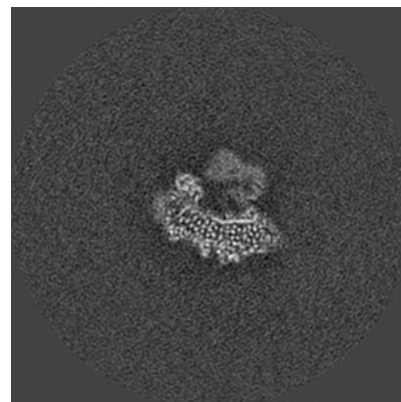
6.3.1 Primary map



X Index: 205

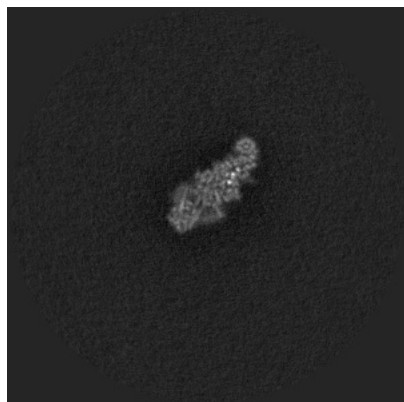


Y Index: 230

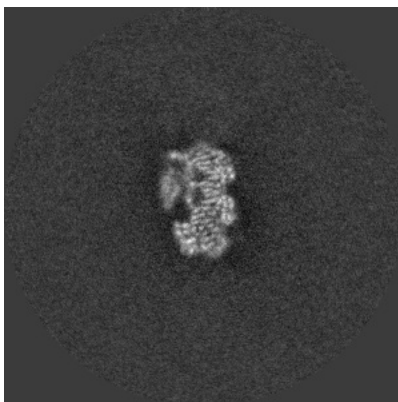


Z Index: 255

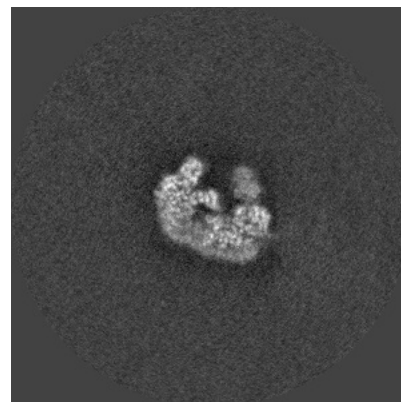
6.3.2 Raw map



X Index: 205



Y Index: 230

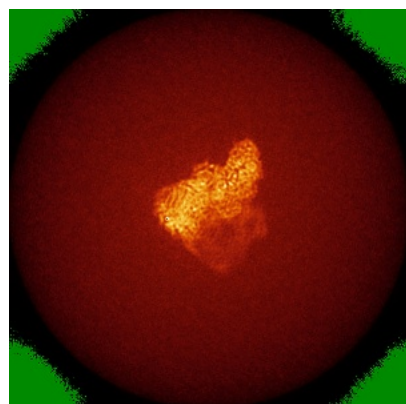


Z Index: 276

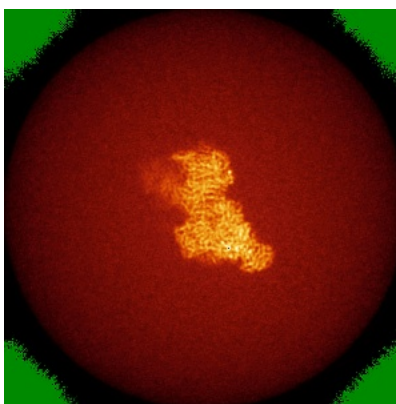
The images above show the largest variance slices of the map in three orthogonal directions.

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

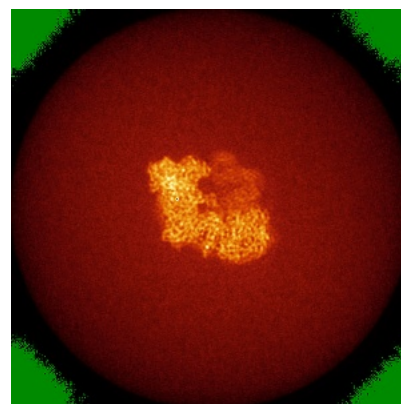
6.4.1 Primary map



X

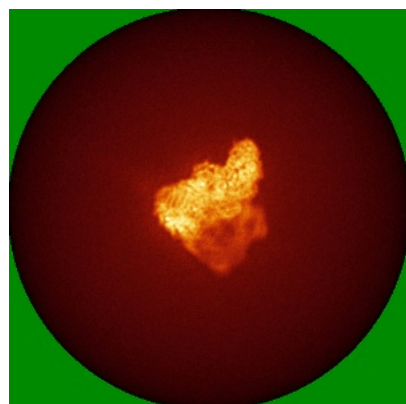


Y

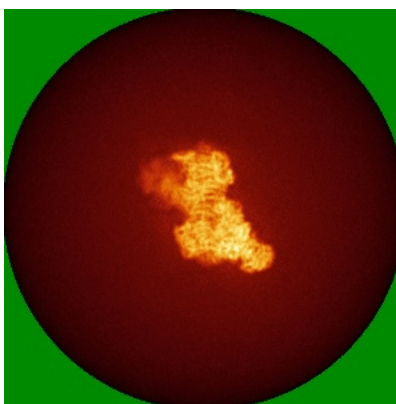


Z

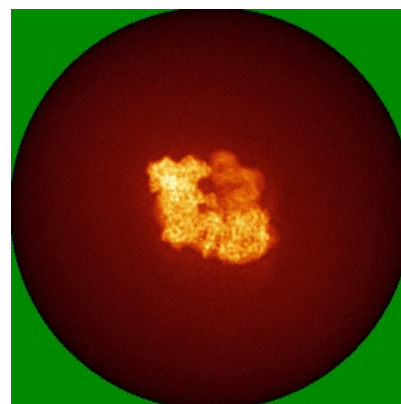
6.4.2 Raw map



X



Y

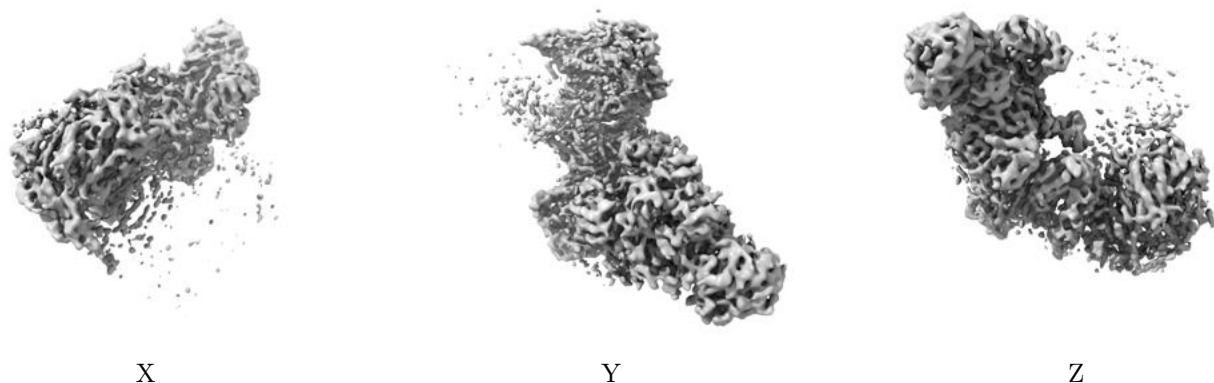


Z

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.

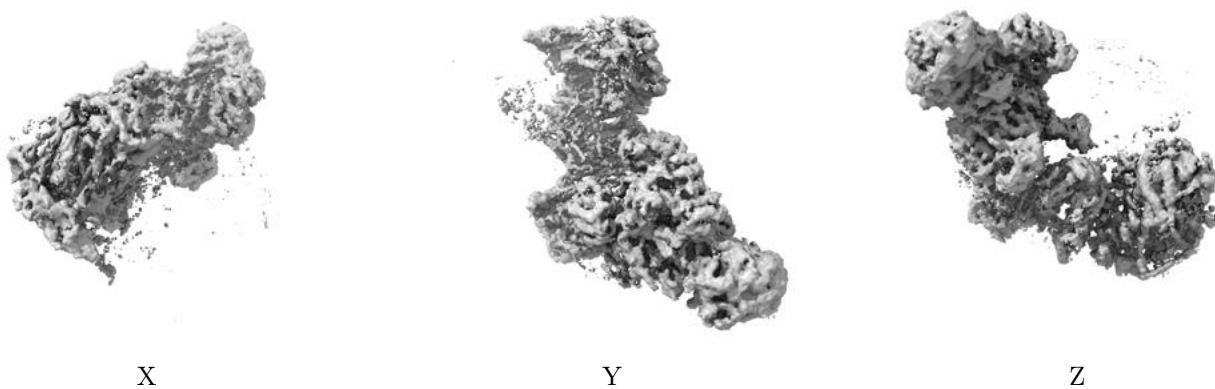
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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.

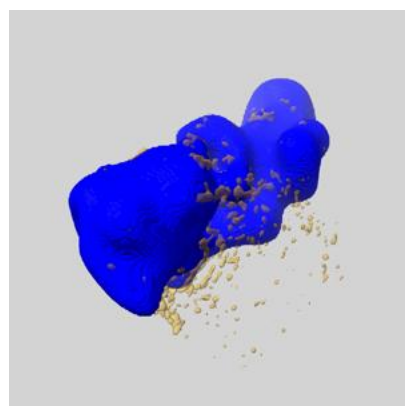
6.6 Mask visualisation [i](#)

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

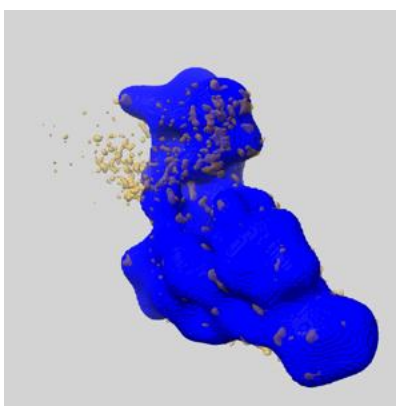
A mask typically either:

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

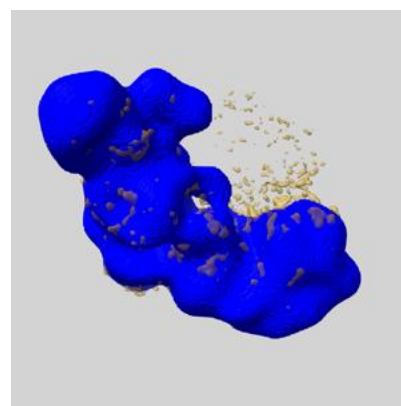
6.6.1 emd_4502_msk_1.map [i](#)



X



Y

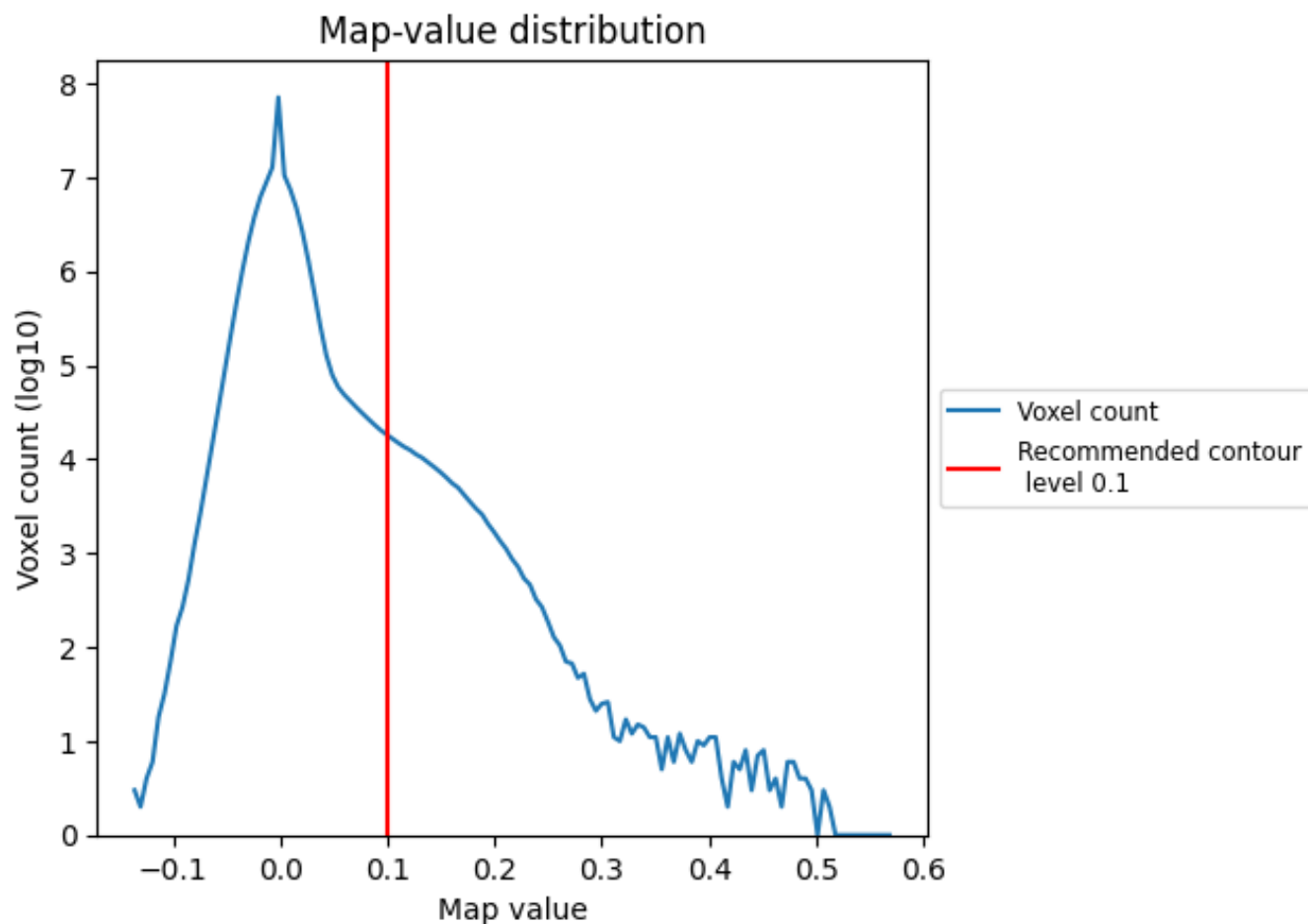


Z

7 Map analysis [i](#)

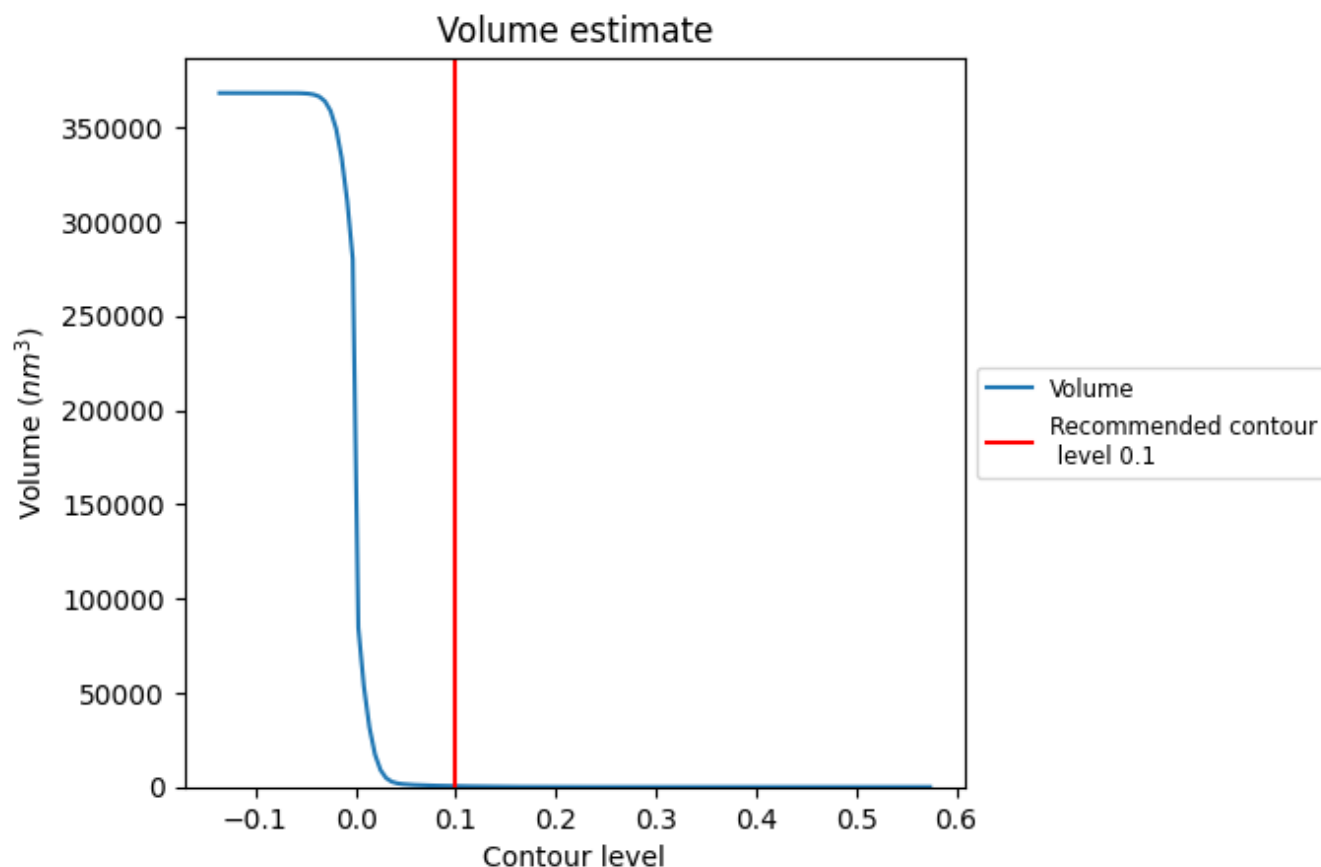
This section contains the results of statistical analysis of the map.

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.

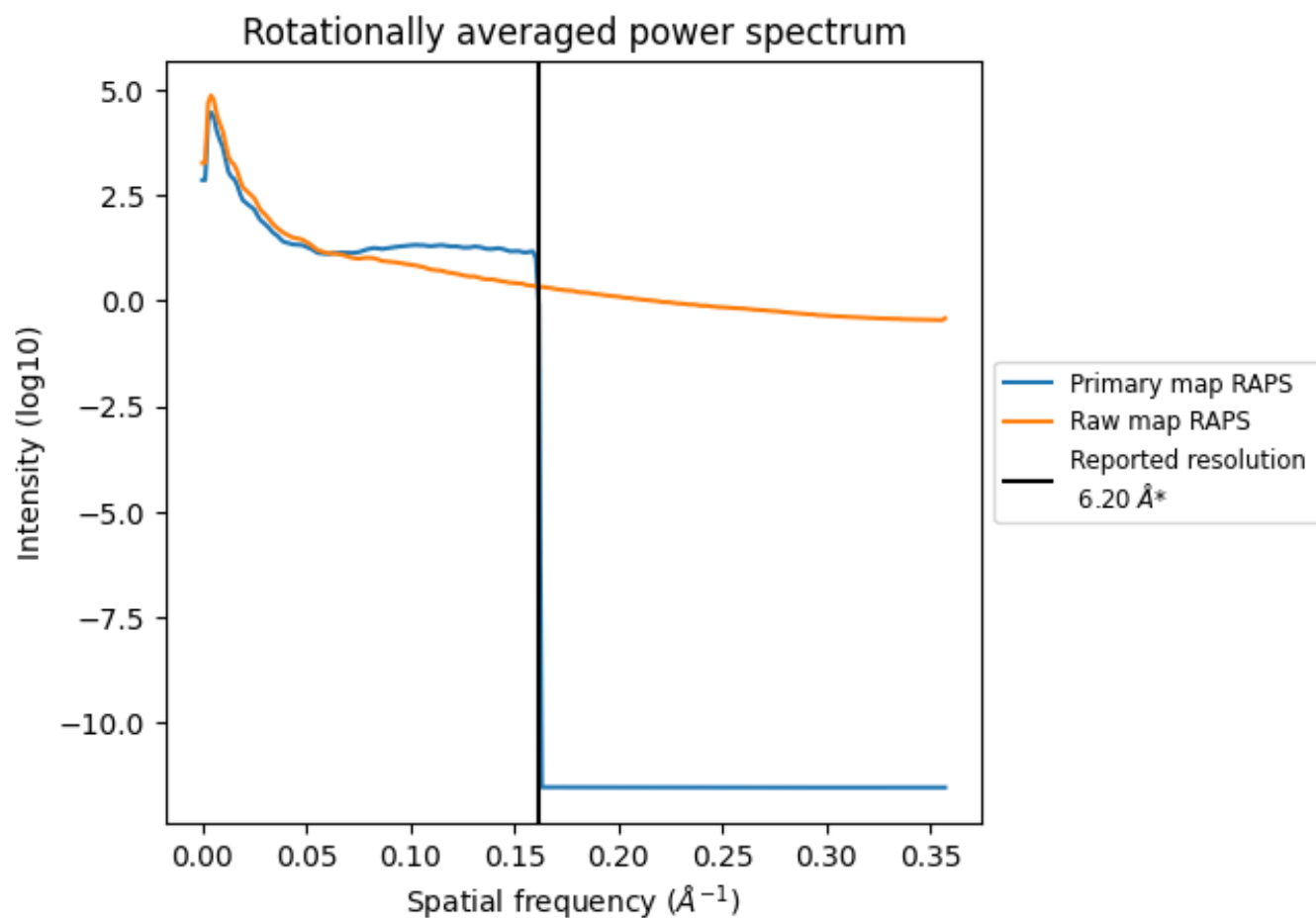
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 436 nm^3 ; this corresponds to an approximate mass of 394 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 ⓘ

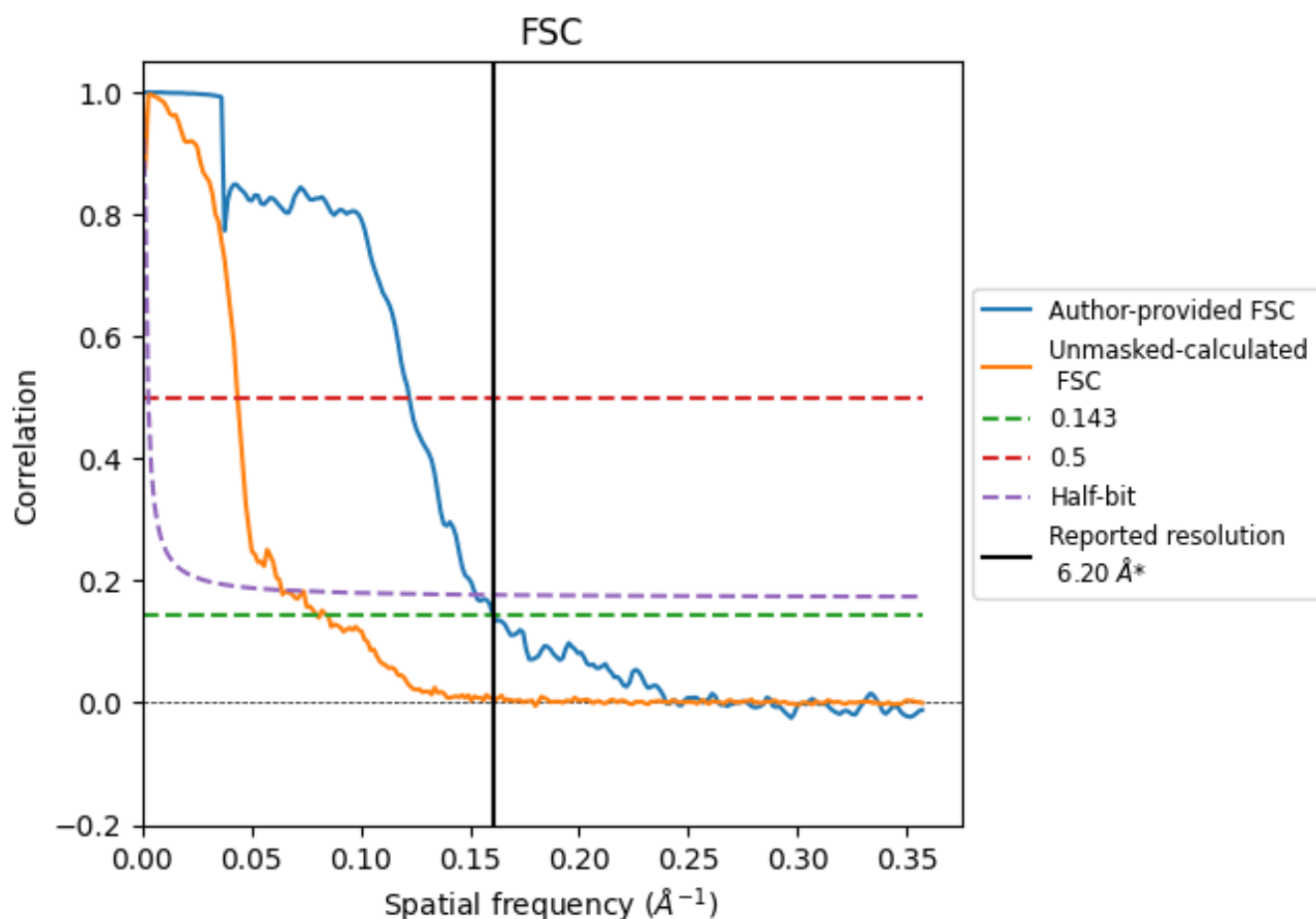


*Reported resolution corresponds to spatial frequency of 0.161 $\text{\AA}^{-1}$

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 0.161 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

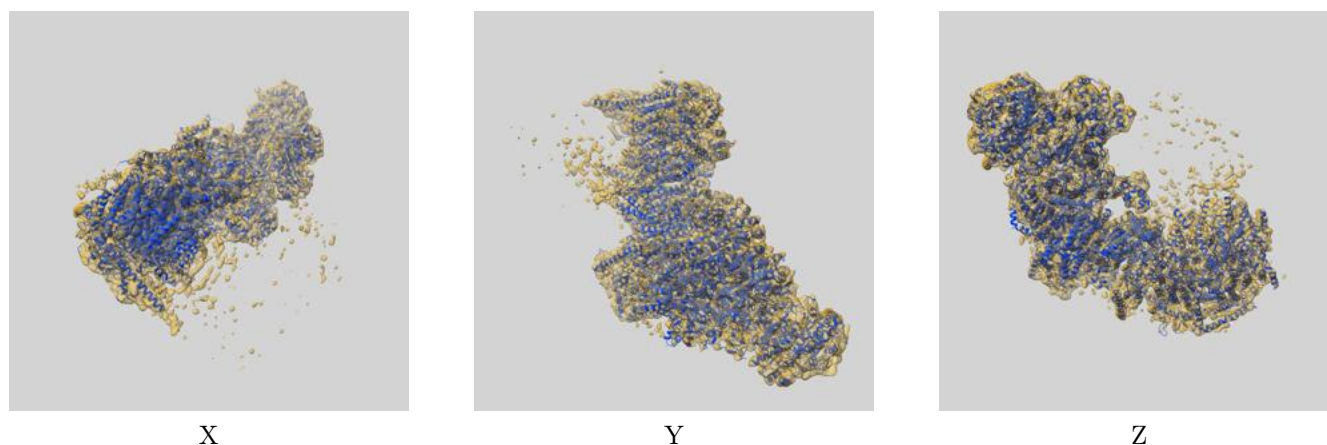
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.22	8.18	6.55
Unmasked-calculated*	12.50	22.88	15.67

*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 12.50 differs from the reported value 6.2 by more than 10 %

9 Map-model fit [i](#)

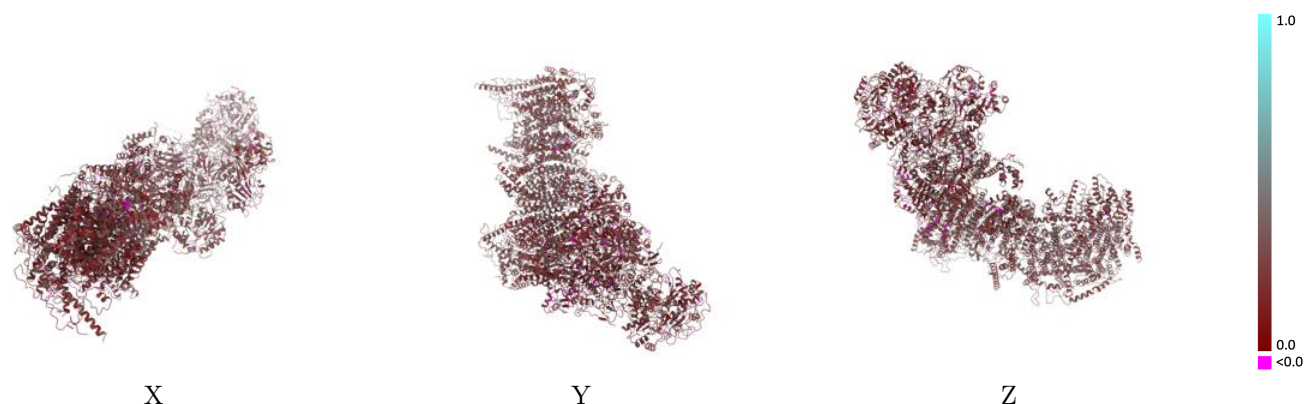
This section contains information regarding the fit between EMDB map EMD-4502 and PDB model 6QCA. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



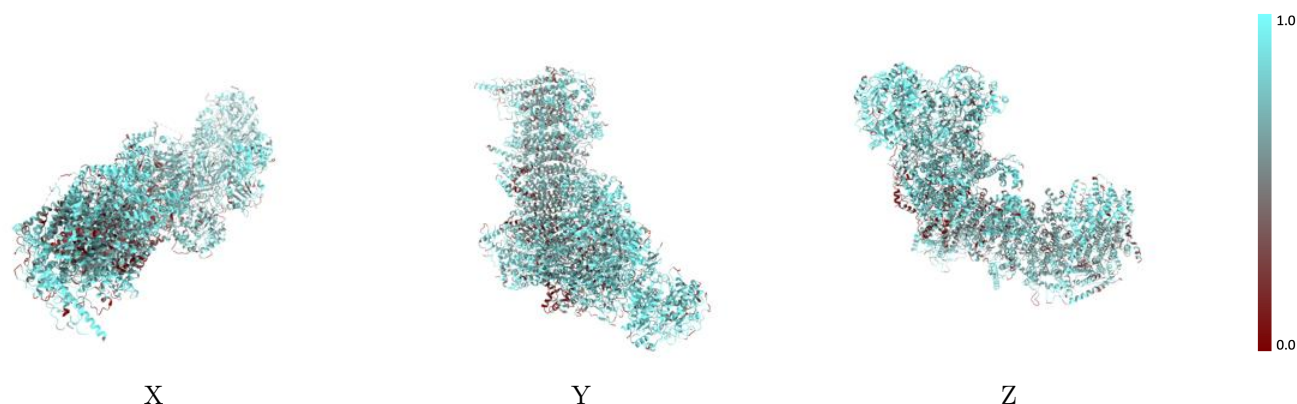
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



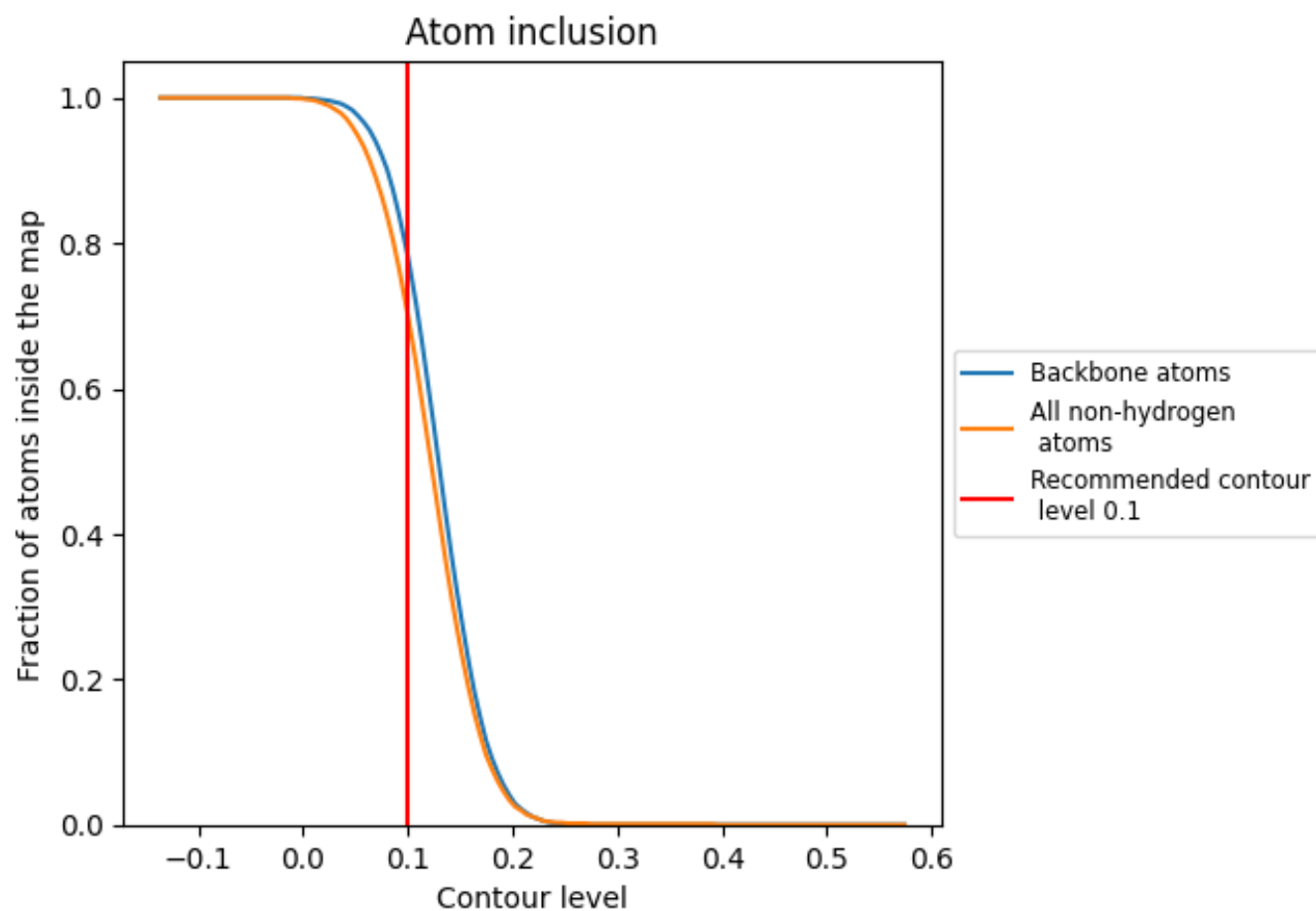
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7010	 0.2480
4L	 0.5970	 0.2520
A1	 0.7230	 0.2520
A2	 0.8280	 0.2330
A3	 0.6480	 0.2540
A5	 0.7110	 0.2560
A6	 0.7540	 0.2660
A7	 0.4710	 0.2030
A8	 0.7760	 0.2750
A9	 0.7070	 0.2440
AA	 0.7730	 0.2390
AB	 0.7240	 0.2450
AJ	 0.7410	 0.2550
AK	 0.5530	 0.2510
AL	 0.3770	 0.2010
AM	 0.7230	 0.2370
B1	 0.6430	 0.2480
B2	 0.6530	 0.2270
B3	 0.5930	 0.2350
B4	 0.7210	 0.2440
B5	 0.7920	 0.2570
B6	 0.7000	 0.2530
B7	 0.7600	 0.2430
B8	 0.6730	 0.2590
B9	 0.8080	 0.2710
BJ	 0.7770	 0.2620
BK	 0.6920	 0.2660
C1	 0.7880	 0.2580
C2	 0.7170	 0.2470
D1	 0.6050	 0.2490
D2	 0.6430	 0.2560
D3	 0.5640	 0.2670
D4	 0.6750	 0.2540
D5	 0.6660	 0.2470
D6	 0.5100	 0.2450



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S1	 0.7640	 0.2410
S2	 0.6720	 0.2430
S3	 0.7280	 0.2560
S4	 0.7260	 0.2630
S5	 0.7490	 0.2430
S6	 0.6980	 0.2600
S7	 0.6920	 0.2490
S8	 0.7380	 0.2300
V1	 0.8140	 0.2360
V2	 0.8300	 0.2480
V3	 0.8190	 0.2580