



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 06:06 pm BST

PDB ID : 6TJV / pdb_00006tjv
EMDB ID : EMD-10513
Title : Structure of the NDH-1MS complex from *Thermosynechococcus elongatus*
Authors : Schuller, J.M.; Saura, P.; Thiemann, J.; Schuller, S.K.; Gamiz-Hernandez, A.P.; Kurisu, G.; Nowaczyk, M.M.; Kaila, V.R.I.
Deposited on : 2019-11-27
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

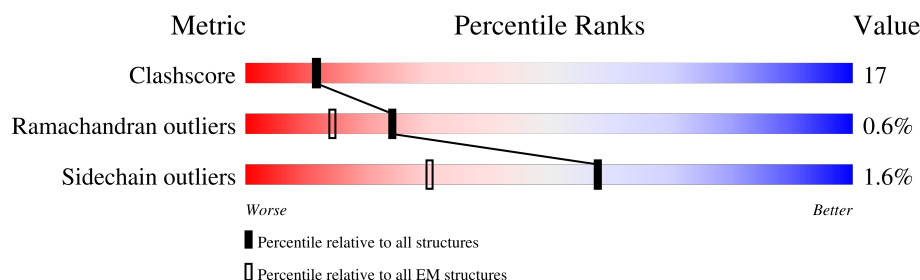
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	372	<div> <div>12%</div> <div>61%</div> <div>34%</div> <div>..</div> </div>
2	B	515	<div> <div>10%</div> <div>70%</div> <div>21%</div> <div>8%</div> </div>
3	C	132	<div> <div>11%</div> <div>62%</div> <div>21%</div> <div>14%</div> </div>
4	D	501	<div> <div>8%</div> <div>64%</div> <div>30%</div> <div>.. 5%</div> </div>
5	E	101	<div> <div>16%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
6	F	611	<div> <div>12%</div> <div>66%</div> <div>28%</div> <div>..</div> </div>
7	G	200	<div> <div>12%</div> <div>64%</div> <div>20%</div> <div>16%</div> </div>
8	H	394	<div> <div>12%</div> <div>64%</div> <div>33%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	196	
10	J	168	
11	K	237	
12	L	76	
13	M	111	
14	N	150	
15	O	70	
16	P	437	
17	Q	149	
18	S	110	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	DGD	A	501	-	-	X	-
19	DGD	L	401	-	-	X	-
21	SQD	F	701	-	-	X	-
21	SQD	F	703	-	-	X	-
21	SQD	K	502	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 33838 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 NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2780	1871	431	468	10		

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	475	Total	C	N	O	S	0	0
			3541	2360	548	617	16		

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	114	Total	C	N	O	S	0	0
			914	629	138	143	4		

- Molecule 4 is a protein called NADH dehydrogenase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	478	Total	C	N	O	S	0	0
			3615	2423	573	605	14		

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	100	Total	C	N	O	S	0	0
			769	506	126	133	4		

- Molecule 6 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	600	Total	C	N	O	S	0	0
			4587	3070	718	776	23		

- Molecule 7 is a protein called NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	168	Total	C	N	O	S	0	0
			1262	844	196	218	4		

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	393	Total	C	N	O	S	0	0
			3153	2035	540	559	19		

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	193	Total	C	N	O	S	0	0
			1520	970	260	277	13		

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	156	Total	C	N	O	S	0	0
			1278	817	218	238	5		

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1594	1024	276	281	13		

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	76	Total	C	N	O	S	0	0
			609	417	93	97	2		

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	110	Total	C	N	O	S	0	0
			879	548	160	169	2		

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	147	Total	C	N	O	S	0	0
			1160	755	200	204	1		

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	68	Total	C	N	O	0	0
			538	349	91	98		

- Molecule 16 is a protein called Tlr0906 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	426	Total	C	N	O	S	0	0
			3496	2294	583	599	20		

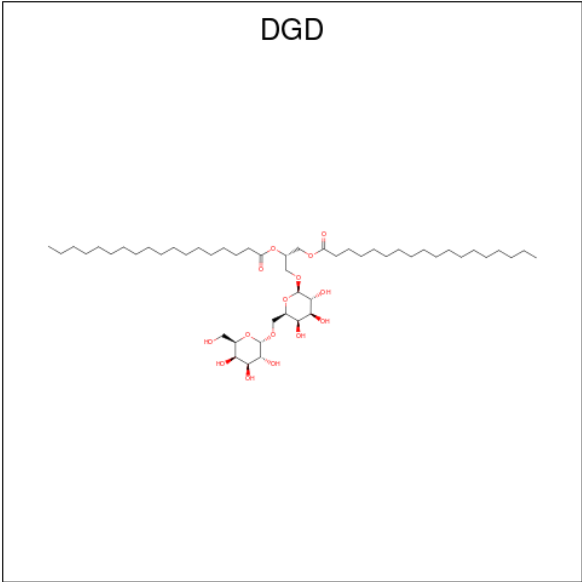
- Molecule 17 is a protein called Tll0220 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	148	Total	C	N	O	S	0	0
			1095	703	179	211	2		

- Molecule 18 is a protein called Tlr0636 protein.

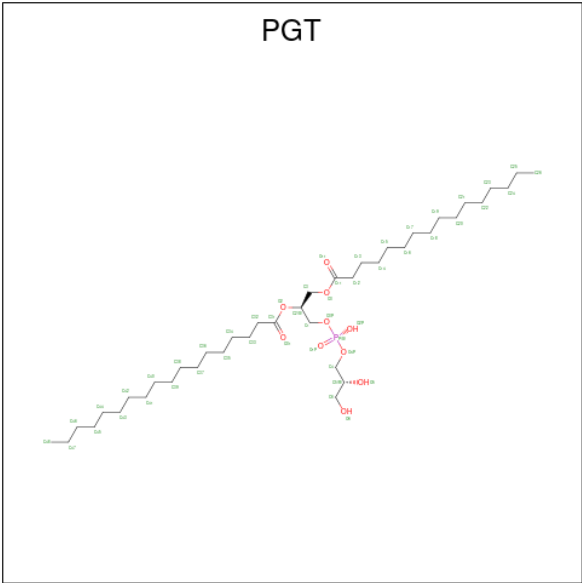
Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	55	Total	C	N	O	S	0	0
			432	280	69	82	1		

- Molecule 19 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			66	51	15	
19	L	1	Total	C	O	0
			66	51	15	

- Molecule 20 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSP HORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



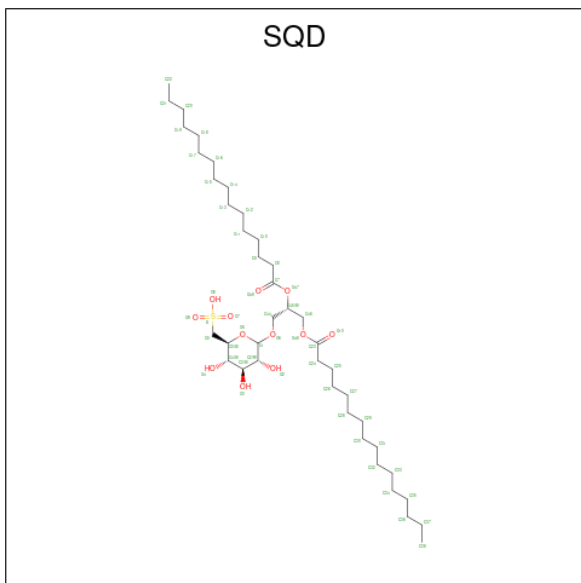
Mol	Chain	Residues	Atoms				AltConf
20	C	1	Total	C	O	P	0
			51	40	10	1	

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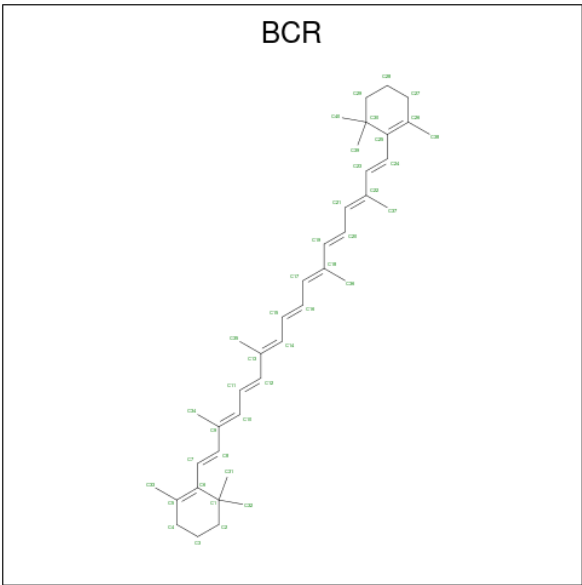
Mol	Chain	Residues	Atoms				AltConf
20	D	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



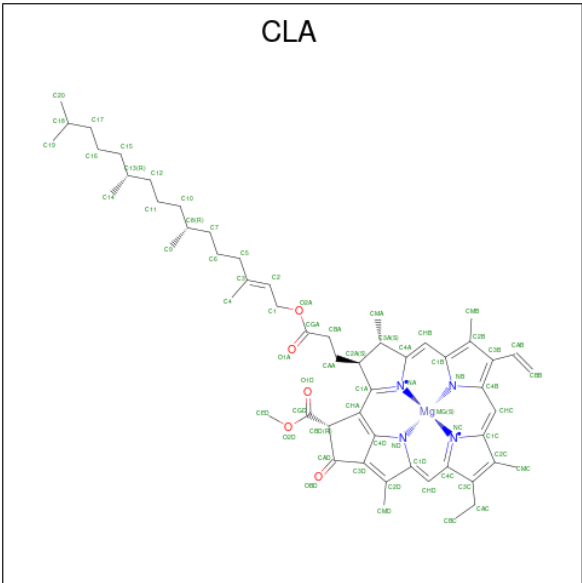
Mol	Chain	Residues	Atoms				AltConf
21	D	1	Total	C	O	S	0
			54	41	12	1	
21	F	1	Total	C	O	S	0
			54	41	12	1	
21	F	1	Total	C	O	S	0
			54	41	12	1	
21	K	1	Total	C	O	S	0
			54	41	12	1	
21	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



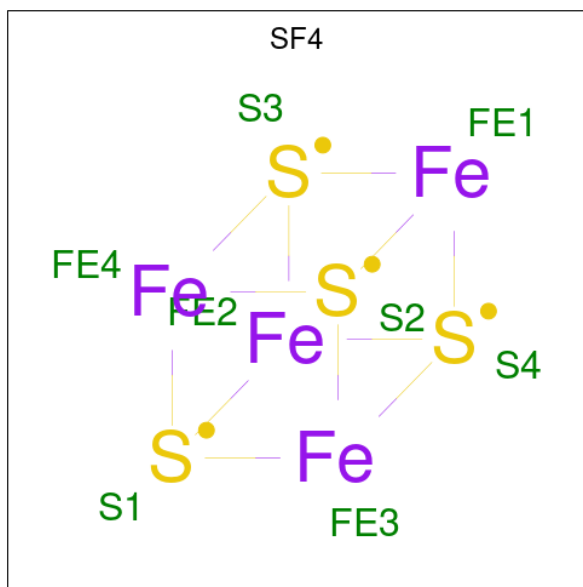
Mol	Chain	Residues	Atoms				AltConf
22	F	1	Total	C			0
			40	40			

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
24	I	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	
24	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	P	1	Total	Zn	0
			1	1	

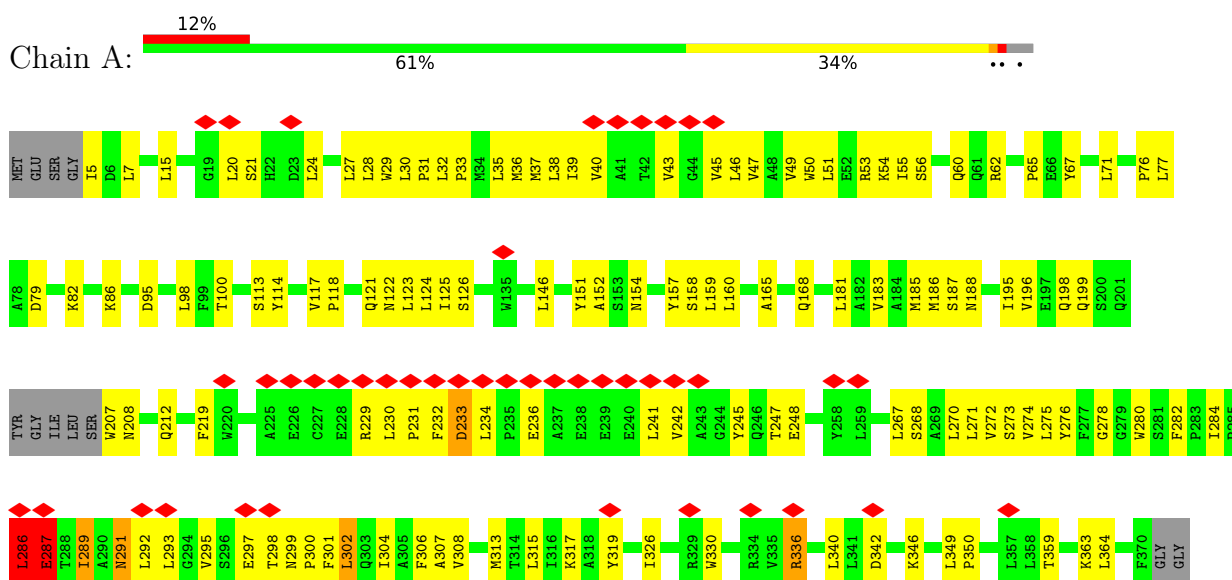
- Molecule 26 is water.

Mol	Chain	Residues	Atoms		AltConf
26	P	1	Total	O	0
			1	1	

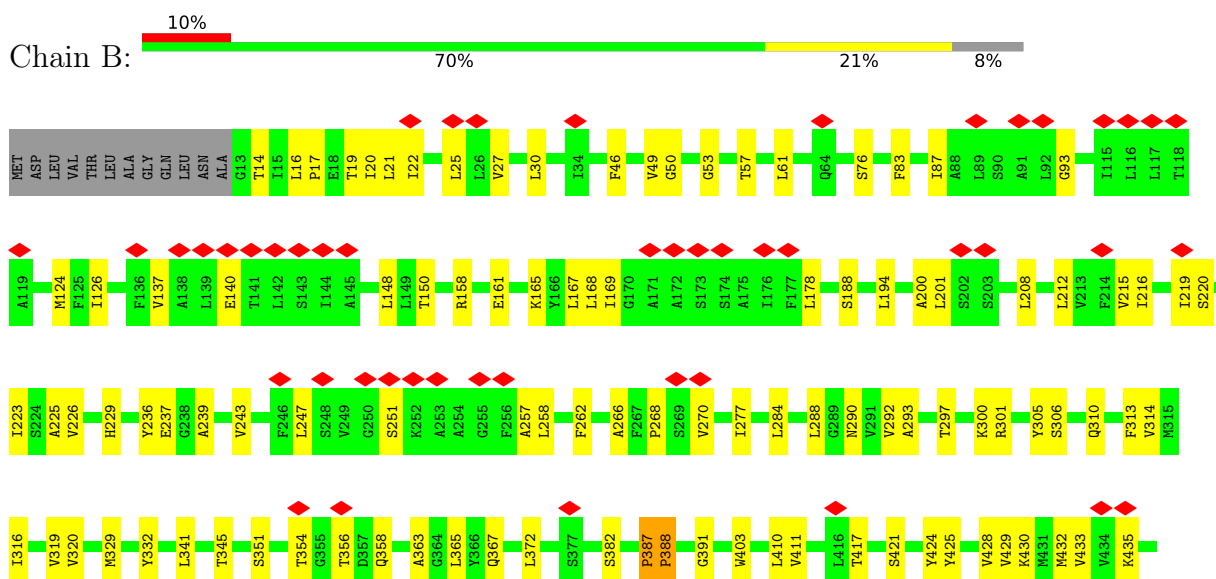
3 Residue-property plots

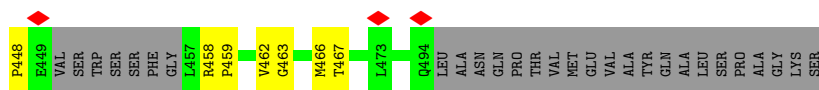
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1

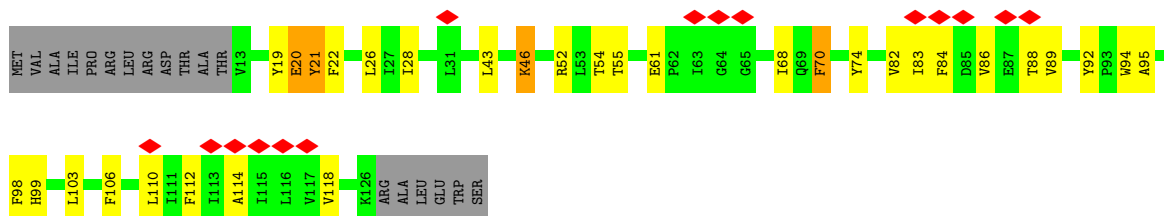


- Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2

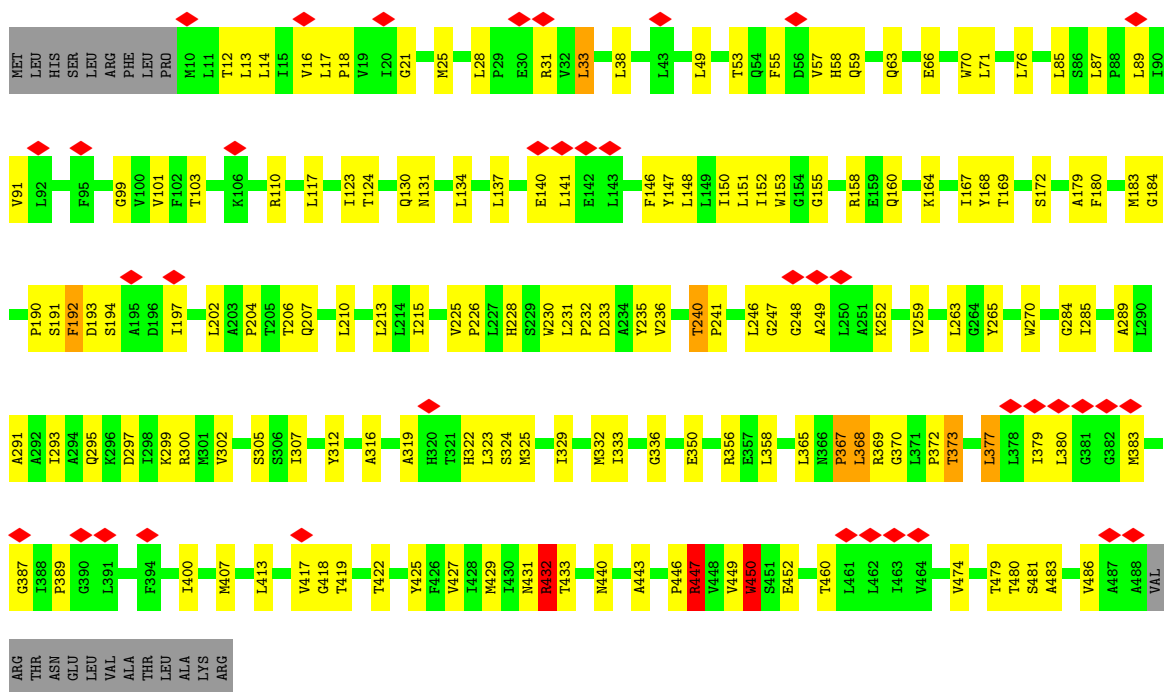




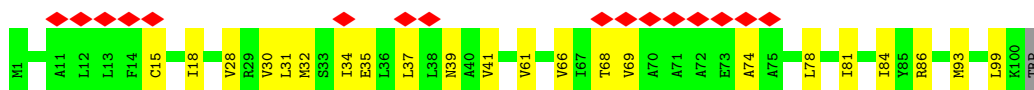
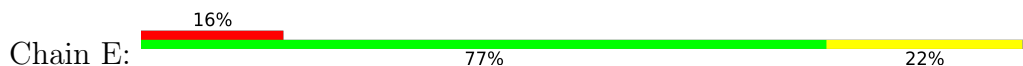
• Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3



• Molecule 4: NADH dehydrogenase subunit 4

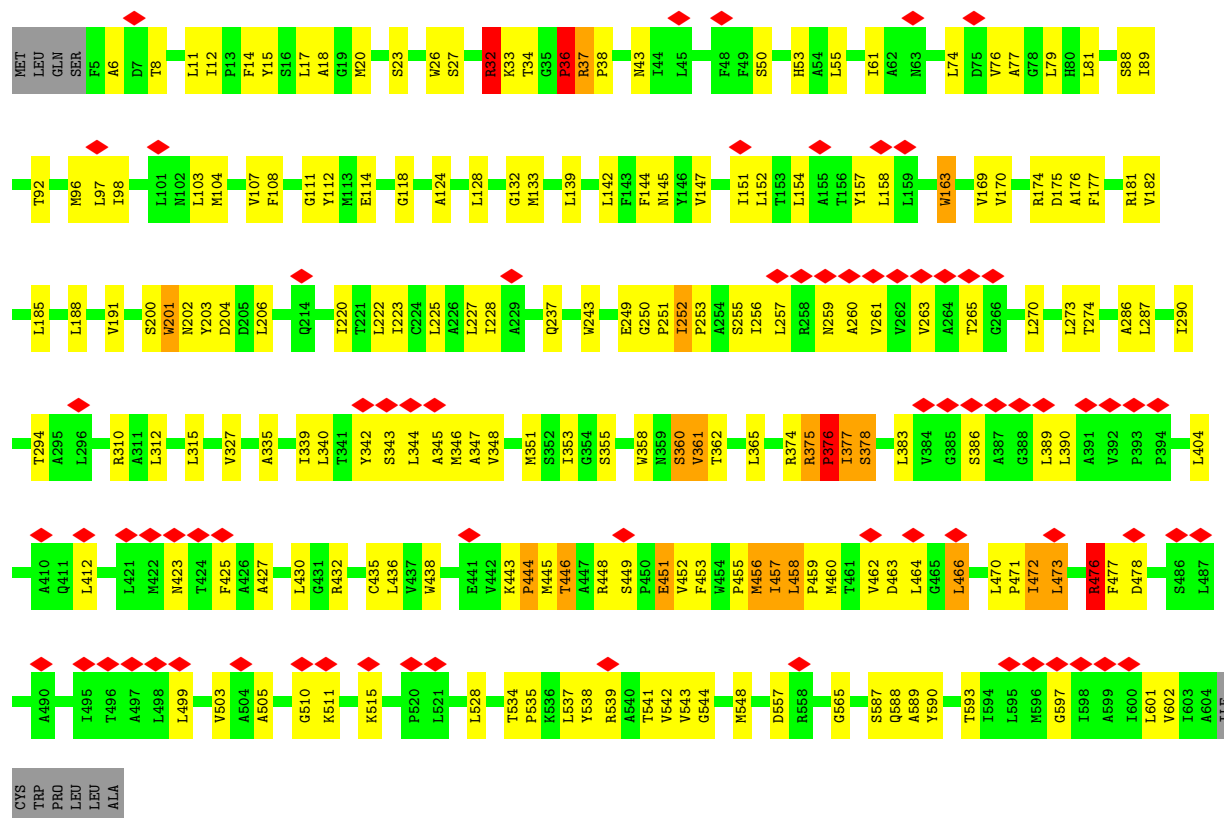


• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L



• Molecule 6: NADH dehydrogenase subunit 5

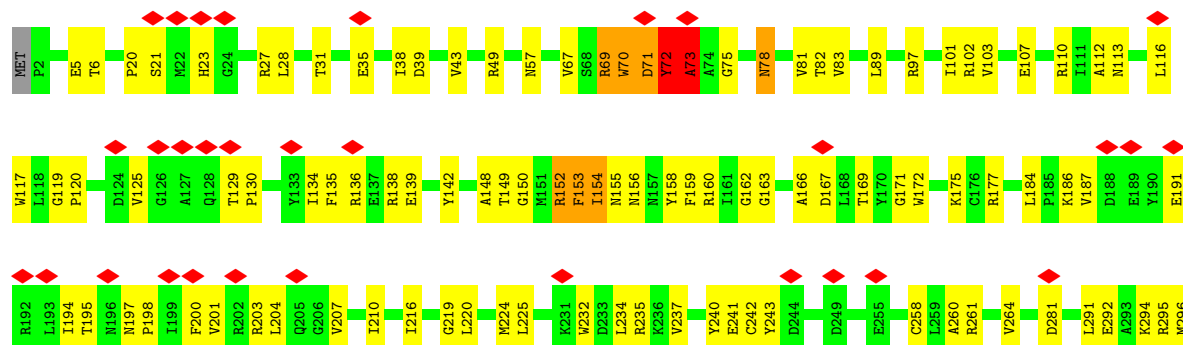




• Molecule 7: NADH dehydrogenase subunit 6

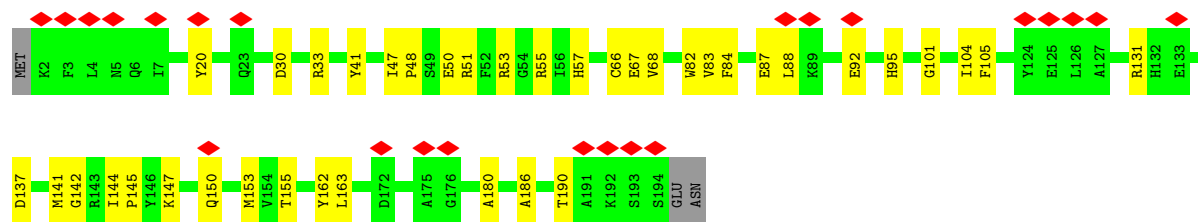
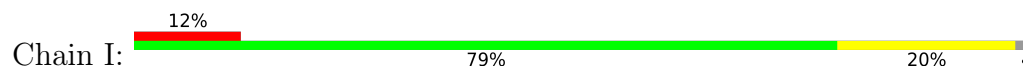


• Molecule 8: NAD(P)H-quinone oxidoreductase subunit H

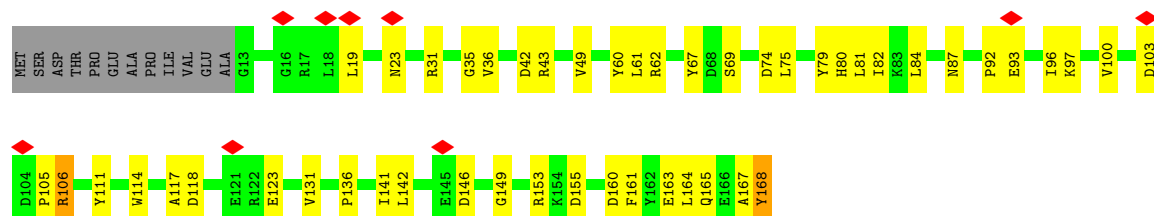




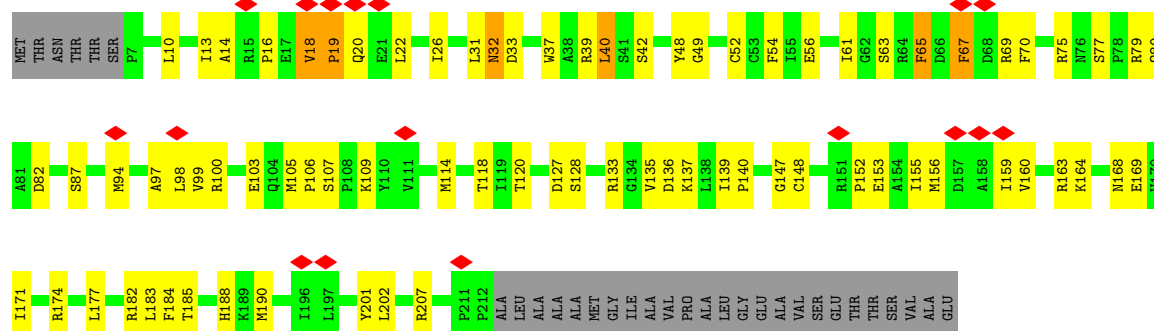
• Molecule 9: NAD(P)H-quinone oxidoreductase subunit I



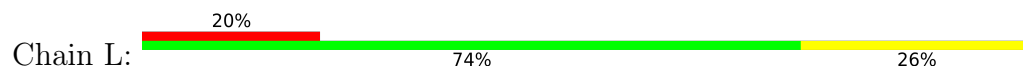
• Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

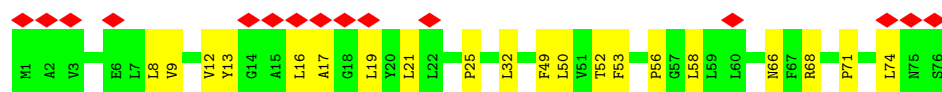


• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K

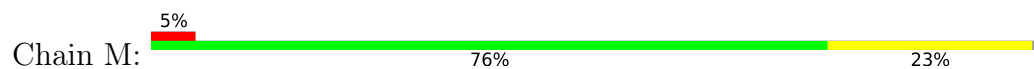


• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

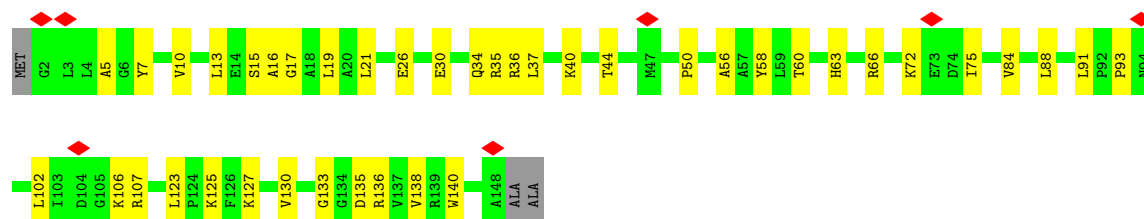




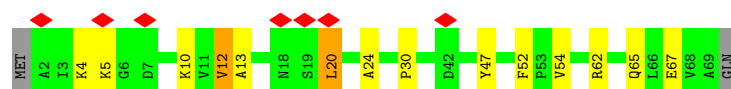
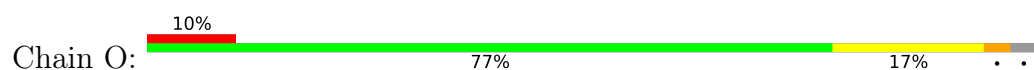
- Molecule 13: NAD(P)H-quinone oxidoreductase subunit M



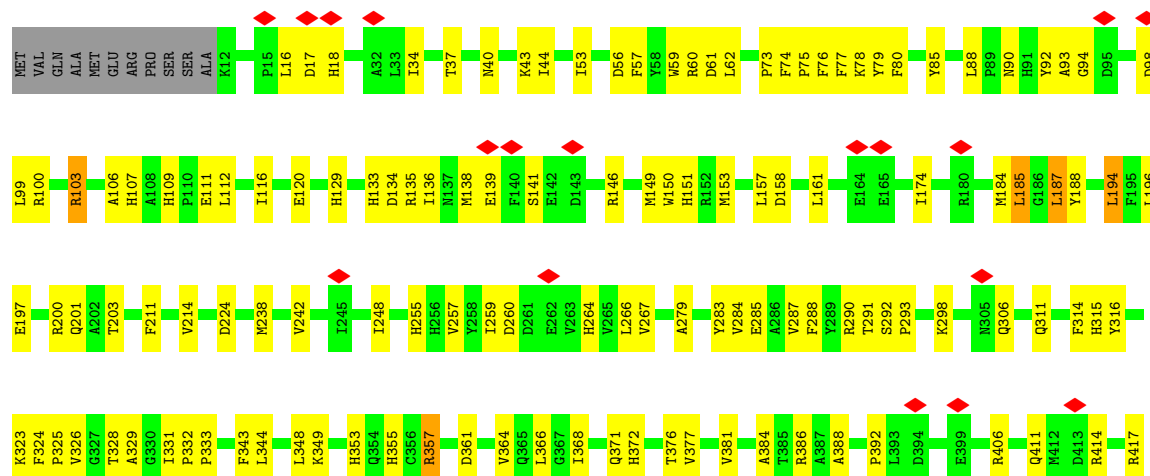
- Molecule 14: NAD(P)H-quinone oxidoreductase subunit N

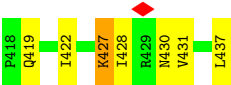


- Molecule 15: NAD(P)H-quinone oxidoreductase subunit O

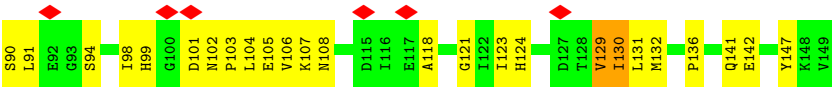
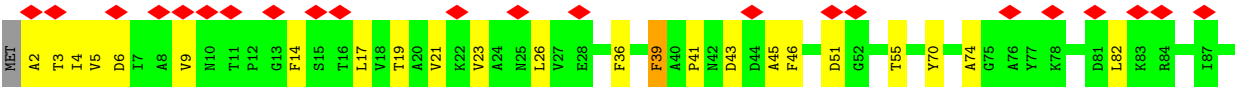


- Molecule 16: Thr0906 protein

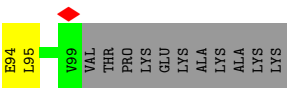
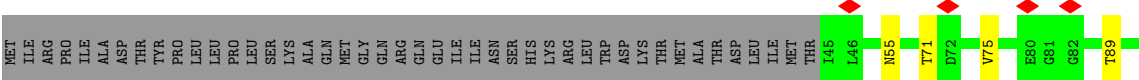




• Molecule 17: Tll0220 protein



• Molecule 18: Tlr0636 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	170151	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 ($e^-/\text{\AA}^2$)	40.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.267	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, CLA, SF4, SQD, ZN, BCR, PGT

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	A	0.37	0/2851	0.55	1/3900 (0.0%)
2	B	0.37	0/3623	0.49	0/4947
3	C	0.41	1/942 (0.1%)	0.62	1/1285 (0.1%)
4	D	0.53	4/3703 (0.1%)	0.59	4/5065 (0.1%)
5	E	0.36	0/777	0.48	0/1054
6	F	0.54	6/4715 (0.1%)	0.58	5/6472 (0.1%)
7	G	0.34	0/1288	0.45	0/1765
8	H	0.36	0/3236	0.58	2/4389 (0.0%)
9	I	0.39	0/1558	0.47	0/2116
10	J	0.35	0/1314	0.51	0/1789
11	K	0.36	0/1636	0.52	0/2228
12	L	0.33	0/629	0.49	0/860
13	M	0.35	0/895	0.54	0/1214
14	N	0.34	0/1192	0.47	0/1621
15	O	0.33	0/550	0.53	1/748 (0.1%)
16	P	0.39	0/3615	0.51	1/4915 (0.0%)
17	Q	0.28	0/1117	0.50	0/1533
18	S	0.33	0/441	0.48	0/601
All	All	0.41	11/34082 (0.0%)	0.54	15/46502 (0.0%)

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
2	B	0	1
4	D	0	3
6	F	1	4
8	H	0	2
11	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	1
All	All	1	13

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	376	PRO	N-CA	13.37	1.70	1.47
6	F	444	PRO	N-CA	13.23	1.69	1.47
4	D	367	PRO	N-CA	11.11	1.66	1.47
6	F	27	SER	C-N	8.37	1.50	1.34
6	F	443	LYS	C-N	6.09	1.45	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	73	ALA	CA-C-N	-13.46	87.58	117.20
8	H	73	ALA	C-N-CA	-12.23	91.11	121.70
6	F	444	PRO	CA-N-CD	-11.36	95.60	111.50
3	C	20	GLU	CB-CA-C	-8.74	92.91	110.40
6	F	376	PRO	CA-N-CD	-7.59	100.87	111.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	F	36	PRO	CA

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	387	PRO	Peptide
4	D	370	GLY	Mainchain
4	D	432	ARG	Sidechain
4	D	447	ARG	Sidechain
6	F	32	ARG	Sidechain

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	A	2780	0	2901	166	0
2	B	3541	0	3650	93	0
3	C	914	0	945	37	0
4	D	3615	0	3819	148	0
5	E	769	0	827	23	0
6	F	4587	0	4763	237	0
7	G	1262	0	1334	39	0
8	H	3153	0	3116	107	0
9	I	1520	0	1474	32	0
10	J	1278	0	1233	42	0
11	K	1594	0	1629	97	0
12	L	609	0	625	38	0
13	M	879	0	860	23	0
14	N	1160	0	1171	31	0
15	O	538	0	549	9	0
16	P	3496	0	3375	107	0
17	Q	1095	0	1109	31	0
18	S	432	0	430	4	0
19	A	66	0	96	64	0
19	L	66	0	93	57	0
20	C	51	0	78	12	0
20	D	51	0	78	13	0
21	D	54	0	77	14	0
21	F	108	0	156	56	0
21	K	54	0	78	46	0
21	L	54	0	78	17	0
22	F	40	0	56	10	0
23	F	46	0	33	18	0
24	I	16	0	0	1	0
24	K	8	0	0	0	0
25	P	1	0	0	0	0
26	P	1	0	0	0	0
All	All	33838	0	34633	1193	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 17.

The worst 5 of 1193 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)
1:A:36:MET:CE	19:A:501:DGD:HA31	1.19	1.64
1:A:35:LEU:HD11	19:A:501:DGD:C6A	1.17	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:19:LEU:CD2	19:L:401:DGD:HBS2	1.30	1.59
19:A:501:DGD:CEB	19:L:401:DGD:HAV2	1.28	1.59
11:K:171:ILE:HD11	21:K:502:SQD:C9	1.36	1.56

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	A	357/372 (96%)	314 (88%)	38 (11%)	5 (1%)	9	40
2	B	471/515 (92%)	428 (91%)	42 (9%)	1 (0%)	44	75
3	C	112/132 (85%)	101 (90%)	10 (9%)	1 (1%)	14	49
4	D	476/501 (95%)	428 (90%)	45 (10%)	3 (1%)	22	57
5	E	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
6	F	598/611 (98%)	539 (90%)	54 (9%)	5 (1%)	16	51
7	G	166/200 (83%)	155 (93%)	11 (7%)	0	100	100
8	H	391/394 (99%)	341 (87%)	45 (12%)	5 (1%)	10	41
9	I	191/196 (97%)	168 (88%)	22 (12%)	1 (0%)	25	60
10	J	154/168 (92%)	128 (83%)	26 (17%)	0	100	100
11	K	204/237 (86%)	174 (85%)	29 (14%)	1 (0%)	25	60
12	L	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
13	M	108/111 (97%)	86 (80%)	22 (20%)	0	100	100
14	N	145/150 (97%)	118 (81%)	27 (19%)	0	100	100
15	O	66/70 (94%)	52 (79%)	13 (20%)	1 (2%)	8	38
16	P	424/437 (97%)	367 (87%)	55 (13%)	2 (0%)	25	60
17	Q	146/149 (98%)	116 (80%)	28 (19%)	2 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	S	53/110 (48%)	49 (92%)	4 (8%)	0	100	100
All	All	4234/4530 (94%)	3725 (88%)	482 (11%)	27 (1%)	24	57

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	GLU
1	A	302	LEU
6	F	36	PRO
6	F	478	ASP
8	H	73	ALA

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	A	291/302 (96%)	286 (98%)	5 (2%)	56	78
2	B	367/413 (89%)	367 (100%)	0	100	100
3	C	93/109 (85%)	90 (97%)	3 (3%)	34	65
4	D	374/397 (94%)	367 (98%)	7 (2%)	52	76
5	E	81/82 (99%)	81 (100%)	0	100	100
6	F	481/492 (98%)	464 (96%)	17 (4%)	31	63
7	G	134/166 (81%)	134 (100%)	0	100	100
8	H	331/338 (98%)	324 (98%)	7 (2%)	48	74
9	I	162/172 (94%)	162 (100%)	0	100	100
10	J	138/148 (93%)	134 (97%)	4 (3%)	37	67
11	K	174/196 (89%)	169 (97%)	5 (3%)	37	67
12	L	63/63 (100%)	63 (100%)	0	100	100
13	M	95/96 (99%)	95 (100%)	0	100	100
14	N	119/120 (99%)	119 (100%)	0	100	100
15	O	57/59 (97%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	358/374 (96%)	352 (98%)	6 (2%)	56	78
17	Q	120/123 (98%)	118 (98%)	2 (2%)	56	78
18	S	48/97 (50%)	48 (100%)	0	100	100
All	All	3486/3747 (93%)	3430 (98%)	56 (2%)	58	79

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	466	LEU
17	Q	108	ASN
8	H	72	TYR
17	Q	39	PHE
16	P	129	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
8	H	19	HIS
16	P	371	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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
20	PGT	D	602	-	50,50,50	0.95	4 (8%)	53,56,56	1.62	6 (11%)
23	CLA	F	704	-	46,54,73	2.57	15 (32%)	53,90,113	3.93	24 (45%)
24	SF4	I	202	-	0,12,12	-	-	-	-	-
24	SF4	K	501	-	0,12,12	-	-	-	-	-
24	SF4	I	201	-	0,12,12	-	-	-	-	-
21	SQD	D	601	-	53,54,54	1.67	13 (24%)	62,65,65	2.84	19 (30%)
20	PGT	C	201	-	50,50,50	0.88	4 (8%)	53,56,56	1.64	7 (13%)
21	SQD	F	703	-	53,54,54	1.18	4 (7%)	62,65,65	1.51	11 (17%)
21	SQD	K	502	-	53,54,54	1.47	11 (20%)	62,65,65	2.10	12 (19%)
19	DGD	L	401	12,1	67,67,67	0.86	2 (2%)	81,81,81	0.95	4 (4%)
19	DGD	A	501	-	67,67,67	1.05	3 (4%)	81,81,81	2.41	25 (30%)
21	SQD	F	701	-	53,54,54	1.17	4 (7%)	62,65,65	1.49	6 (9%)
22	BCR	F	702	-	41,41,41	0.89	2 (4%)	56,56,56	4.77	26 (46%)
21	SQD	L	402	-	53,54,54	1.52	10 (18%)	62,65,65	2.24	15 (24%)

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
20	PGT	D	602	-	-	27/55/55/55	-
23	CLA	F	704	-	-	1/15/93/115	-
24	SF4	I	202	-	-	-	0/6/5/5
24	SF4	K	501	-	-	-	0/6/5/5
24	SF4	I	201	-	-	-	0/6/5/5
21	SQD	D	601	-	-	26/49/69/69	0/1/1/1
20	PGT	C	201	-	-	26/55/55/55	-
21	SQD	F	703	-	-	26/49/69/69	0/1/1/1
21	SQD	K	502	-	-	23/49/69/69	0/1/1/1
19	DGD	L	401	12,1	-	30/55/95/95	0/2/2/2
19	DGD	A	501	-	-	26/55/95/95	0/2/2/2
21	SQD	F	701	-	-	21/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	F	702	-	-	4/29/63/63	0/2/2/2
21	SQD	L	402	-	-	26/49/69/69	0/1/1/1

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	704	CLA	C1D-ND	7.99	1.47	1.37
21	L	402	SQD	C6-S	-5.47	1.57	1.77
23	F	704	CLA	O2D-CGD	5.21	1.45	1.33
23	F	704	CLA	C3C-C2C	5.15	1.47	1.36
23	F	704	CLA	C3B-C2B	5.05	1.47	1.40

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	702	BCR	C2-C1-C6	-17.74	83.17	110.48
22	F	702	BCR	C31-C1-C6	-15.29	85.49	110.30
23	F	704	CLA	C1D-ND-C4D	-13.15	96.99	106.33
21	D	601	SQD	O3-C3-C2	-12.26	82.01	110.35
22	F	702	BCR	C32-C1-C6	11.76	129.38	110.30

There are no chirality outliers.

5 of 236 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	501	DGD	C2D-C1D-O3G-C3G
19	A	501	DGD	O6D-C1D-O3G-C3G
19	L	401	DGD	C2B-C1B-O2G-C2G
19	L	401	DGD	O6E-C1E-O5D-C6D
20	C	201	PGT	C5-C4-O4P-P

There are no ring outliers.

12 monomers are involved in 280 short contacts:

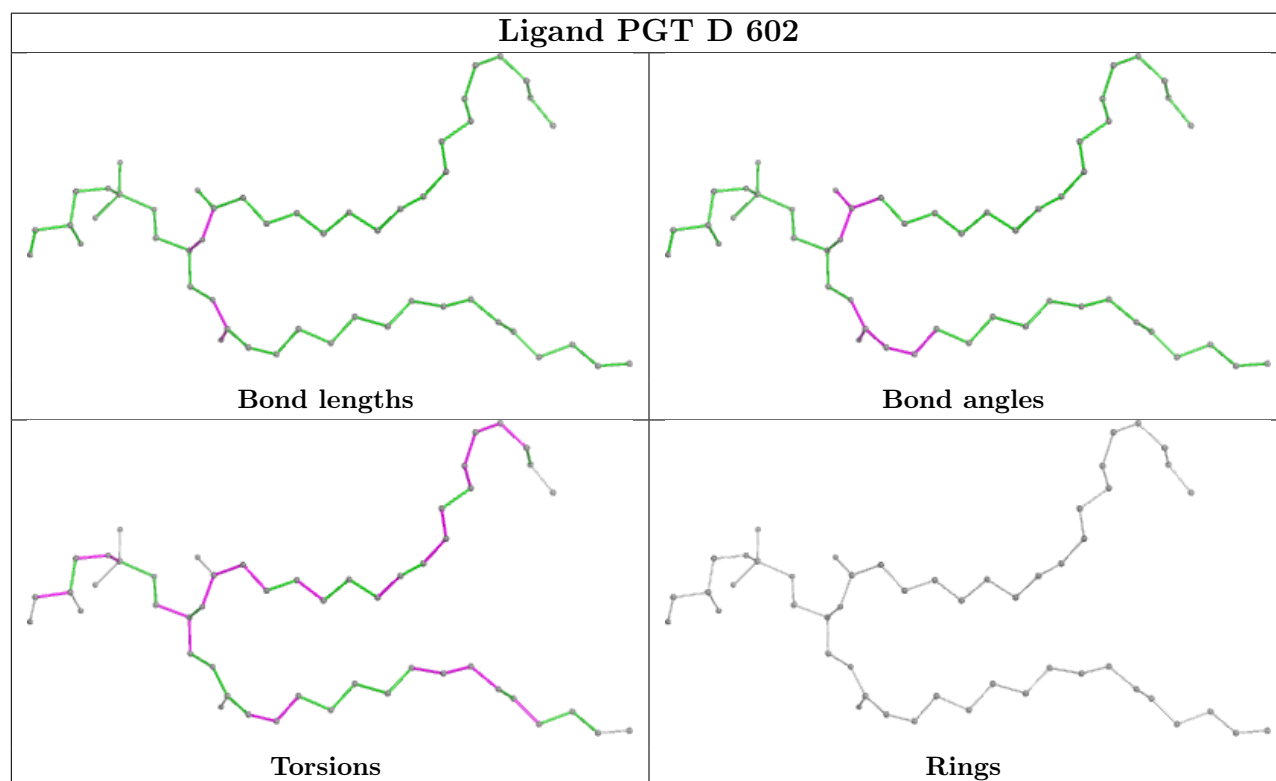
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	602	PGT	13	0
23	F	704	CLA	18	0
24	I	201	SF4	1	0
21	D	601	SQD	14	0
20	C	201	PGT	12	0

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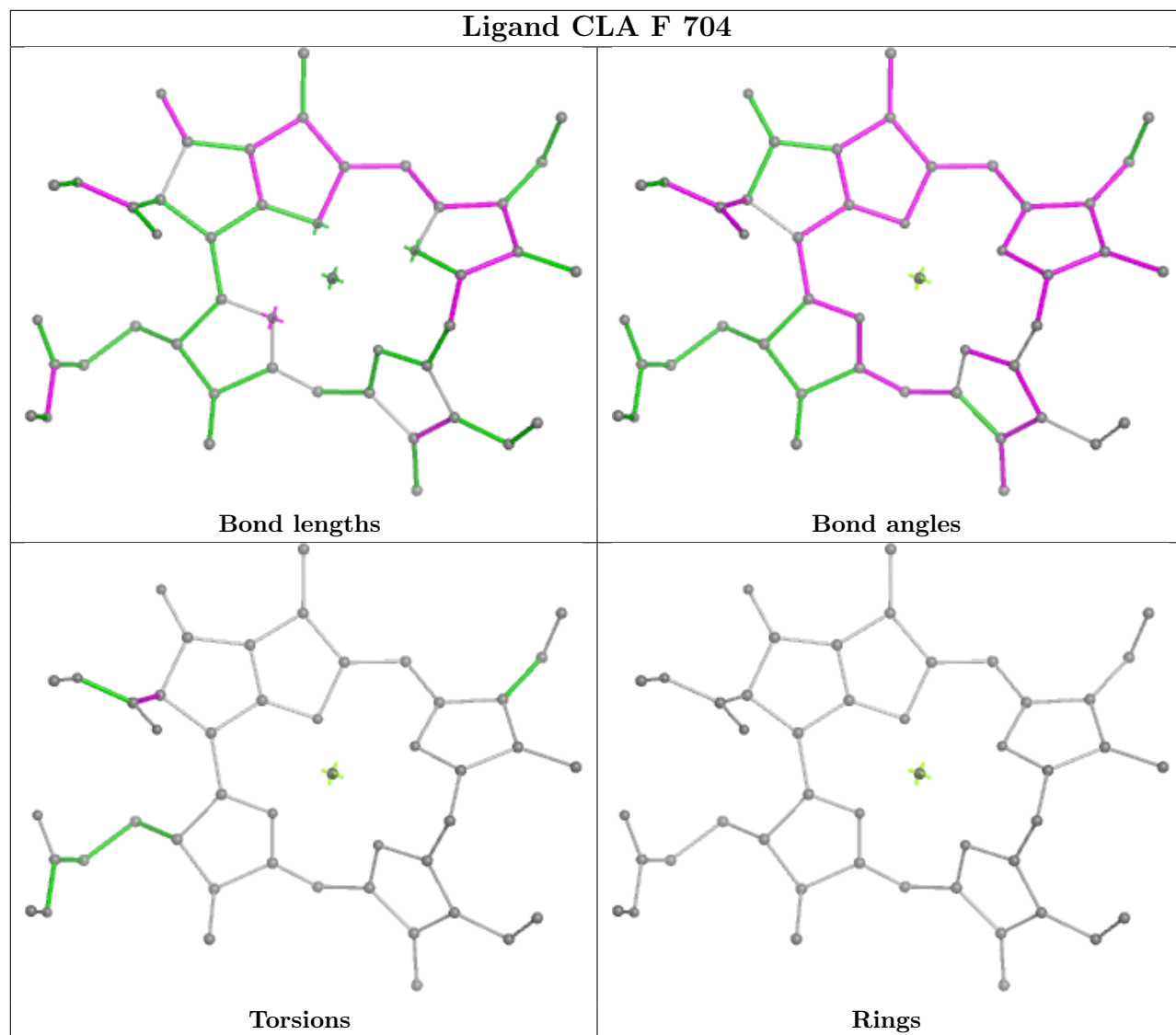
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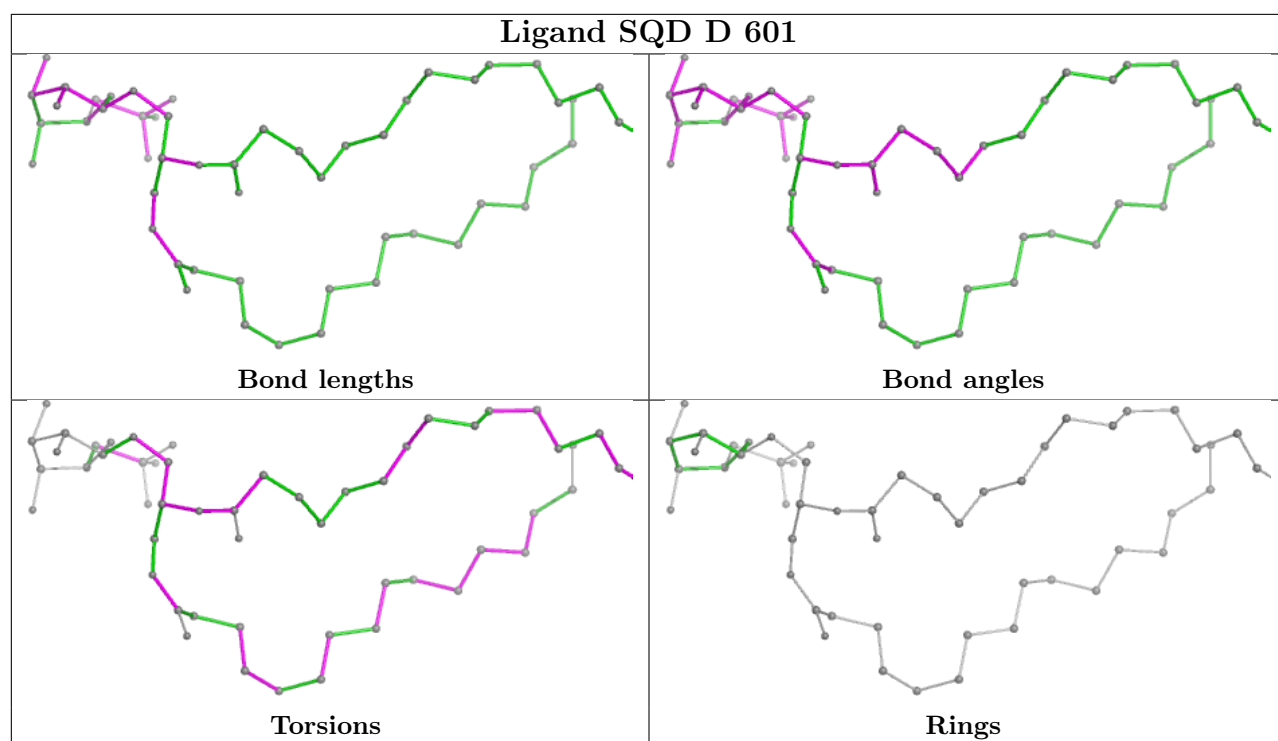
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	703	SQD	26	0
21	K	502	SQD	46	0
19	L	401	DGD	57	0
19	A	501	DGD	64	0
21	F	701	SQD	30	0
22	F	702	BCR	10	0
21	L	402	SQD	17	0

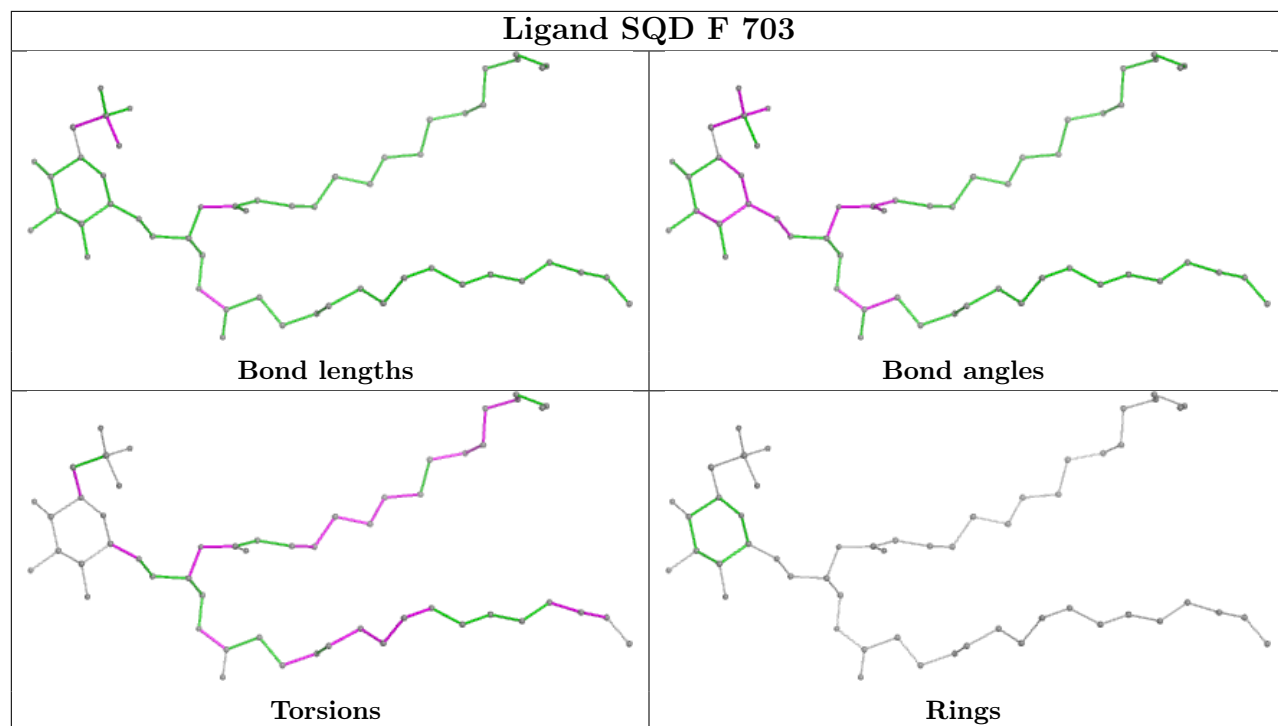
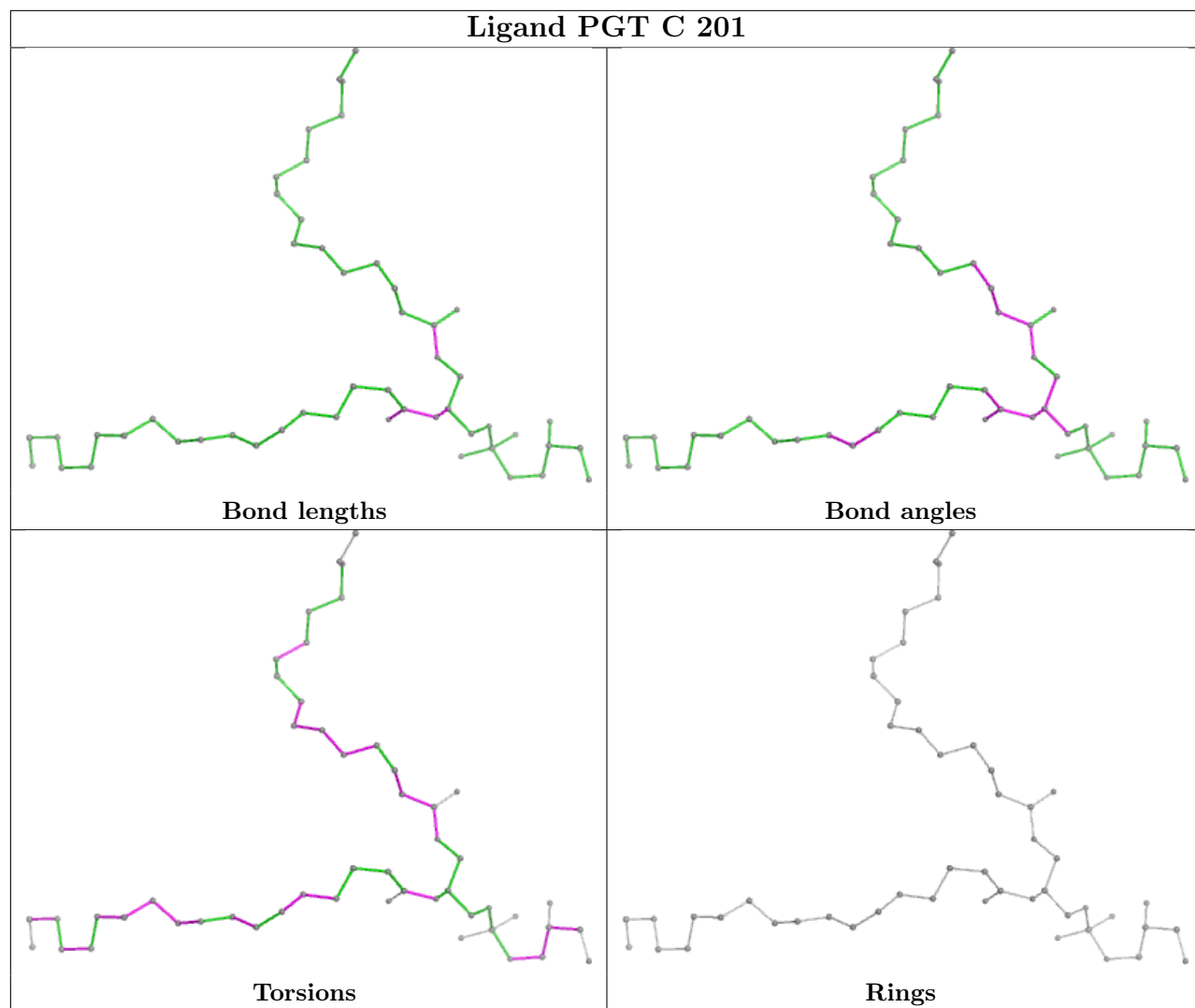
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

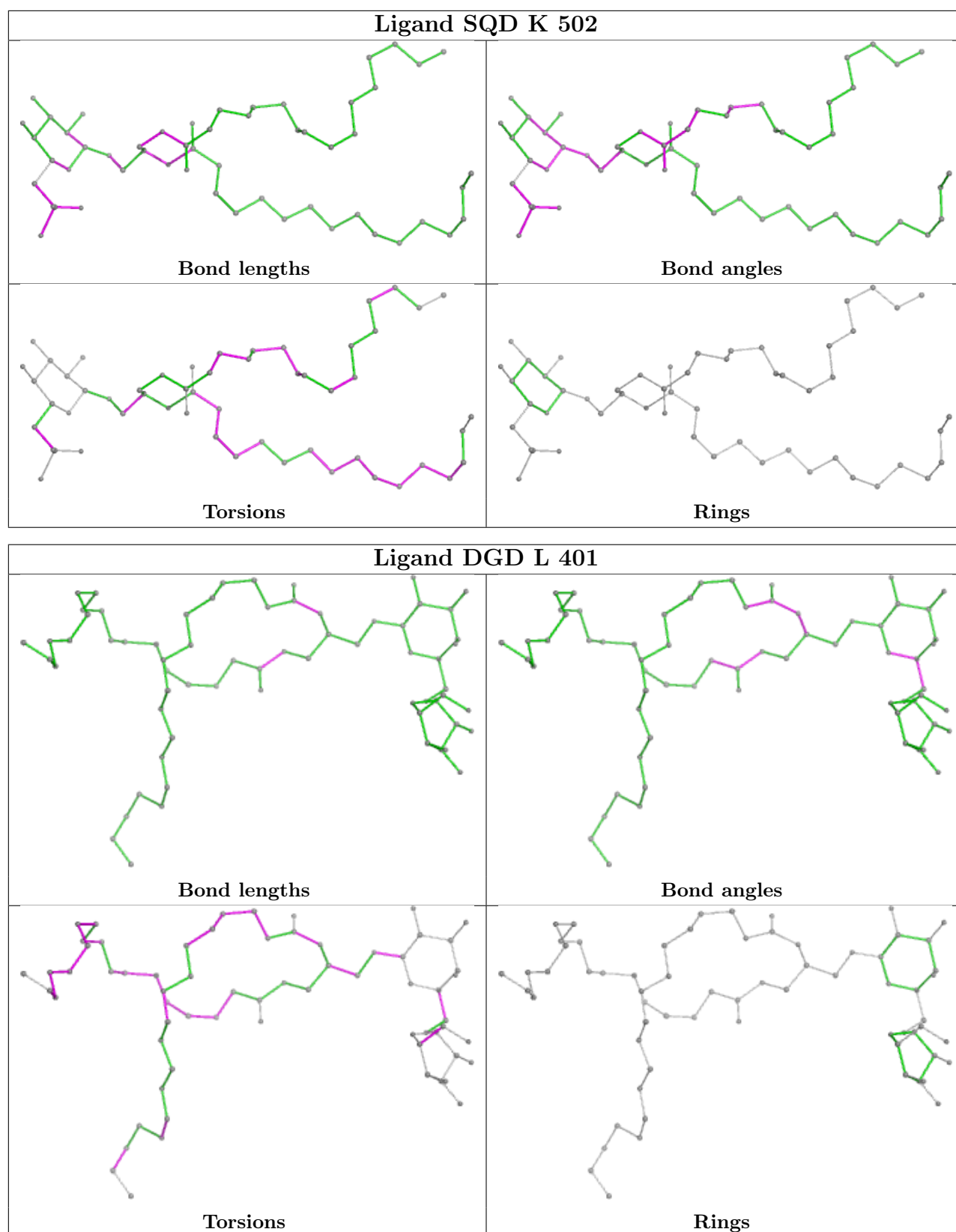


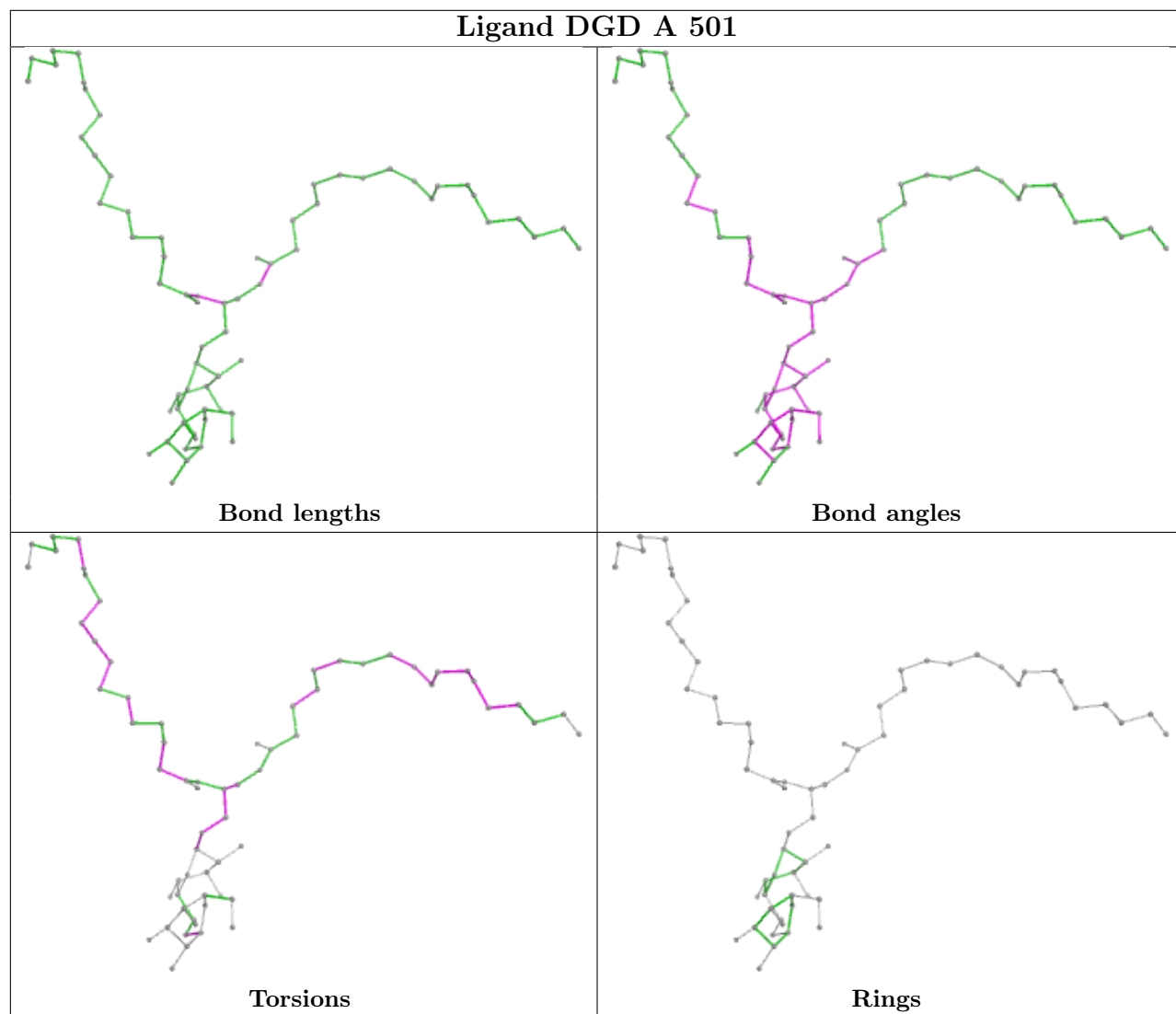
Ligand CLA F 704

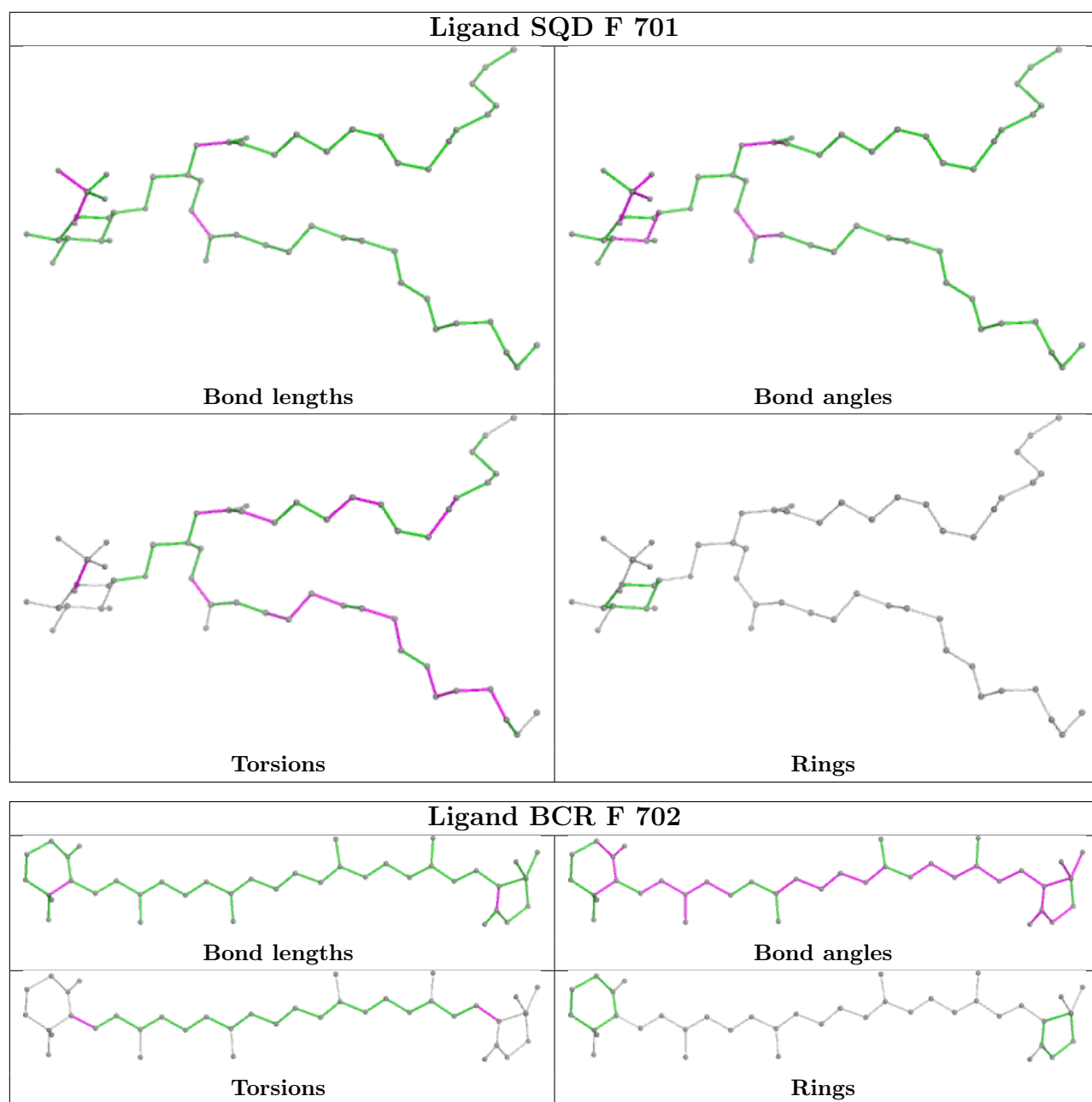


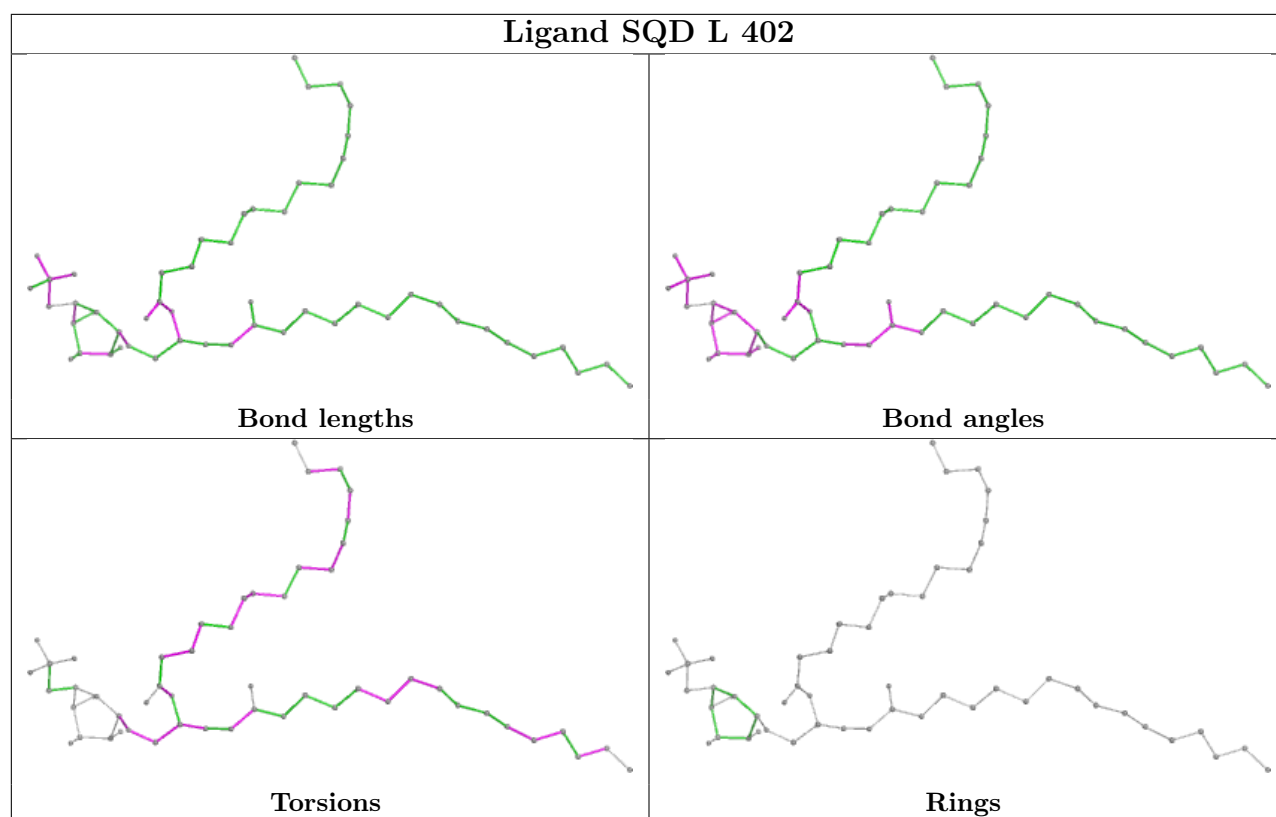












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

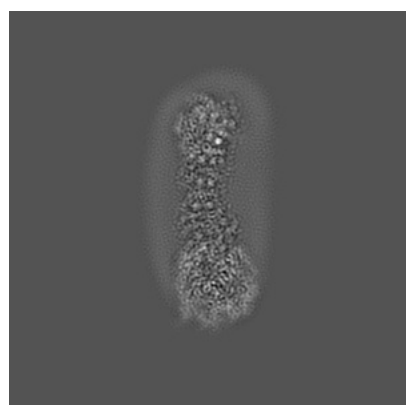
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10513. These allow visual inspection of the internal detail of the map and identification of artifacts.

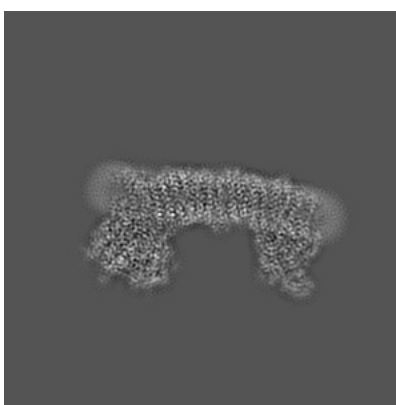
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

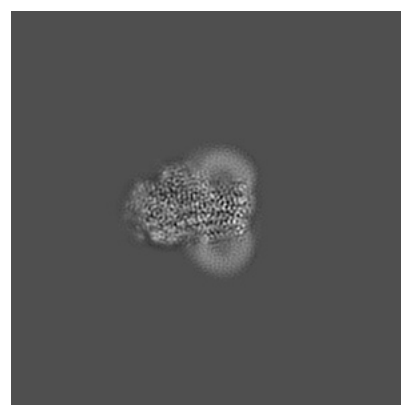
6.1.1 Primary map



X



Y

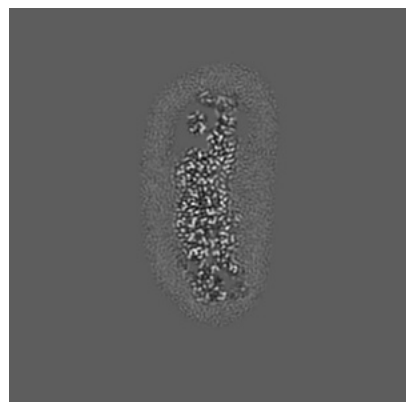


Z

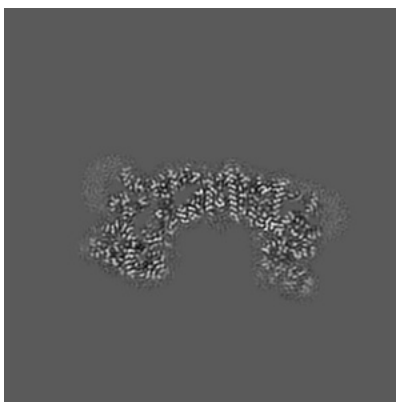
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140

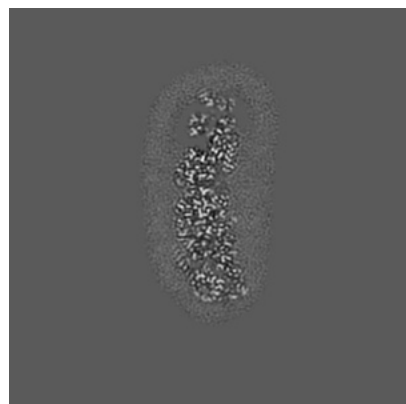


Z Index: 140

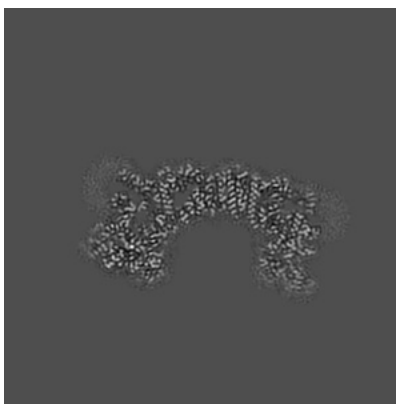
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

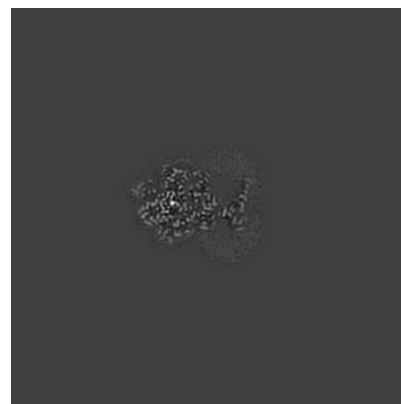
6.3.1 Primary map



X Index: 138



Y Index: 142

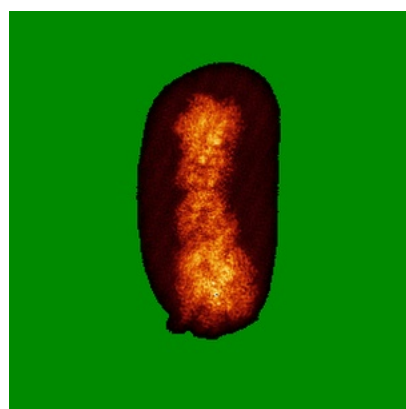


Z Index: 89

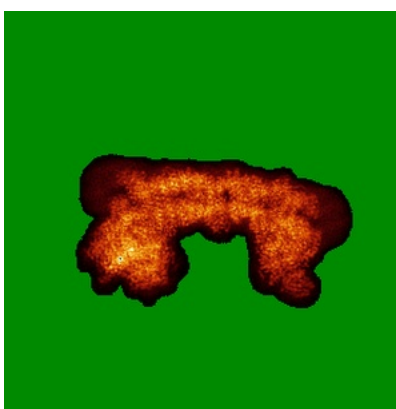
The images above show the largest variance slices of the map in three orthogonal directions.

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

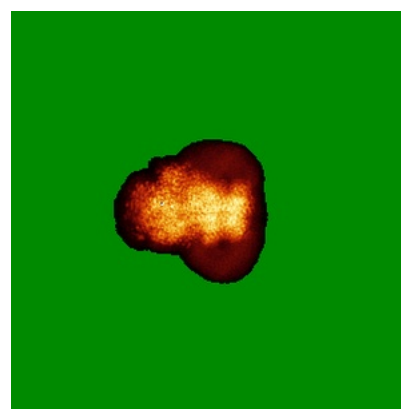
6.4.1 Primary map



X



Y

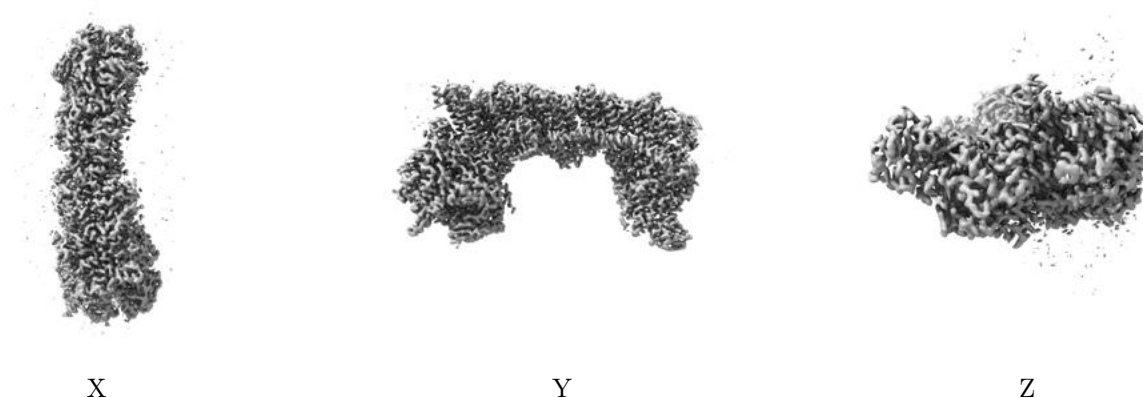


Z

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

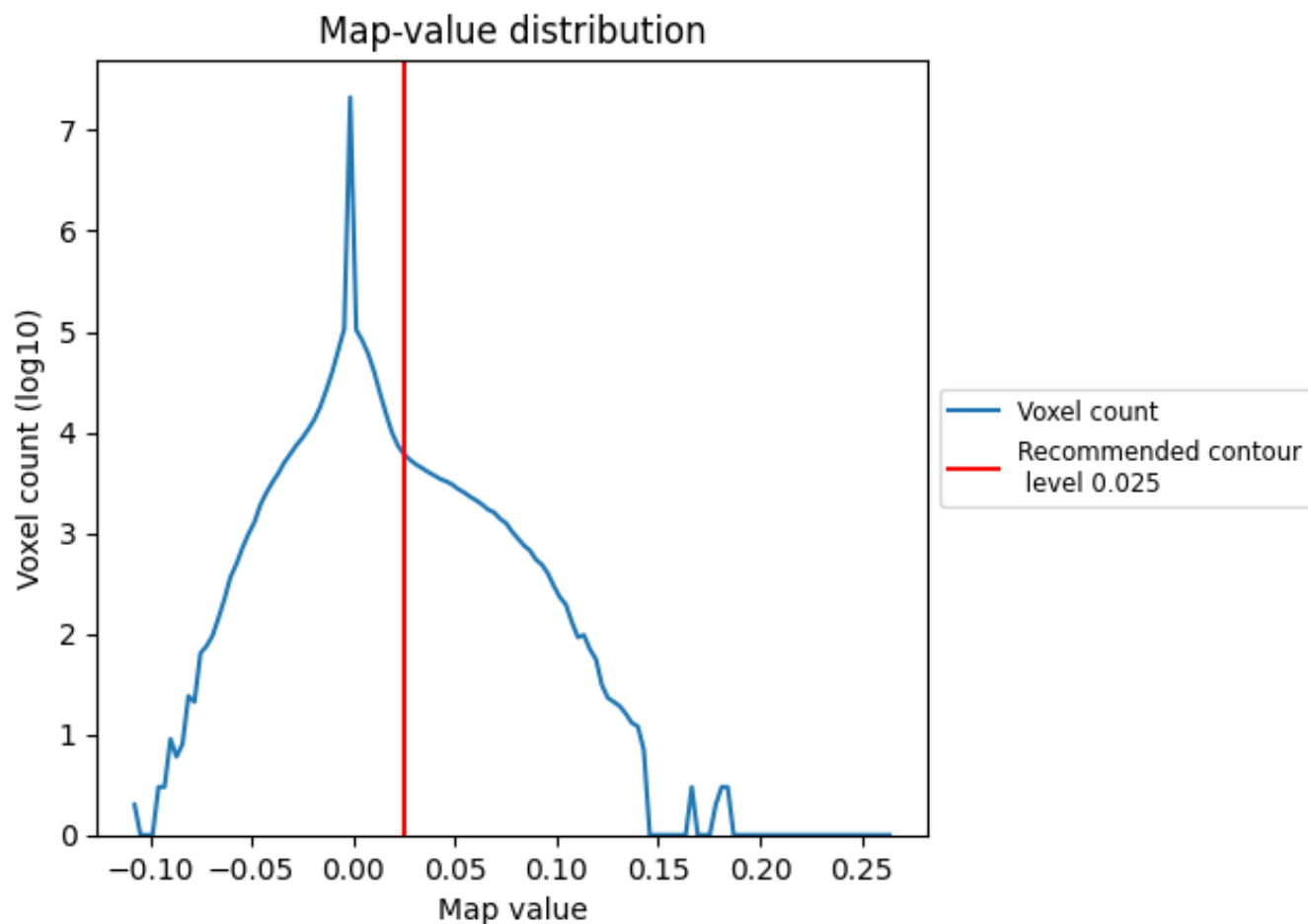
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

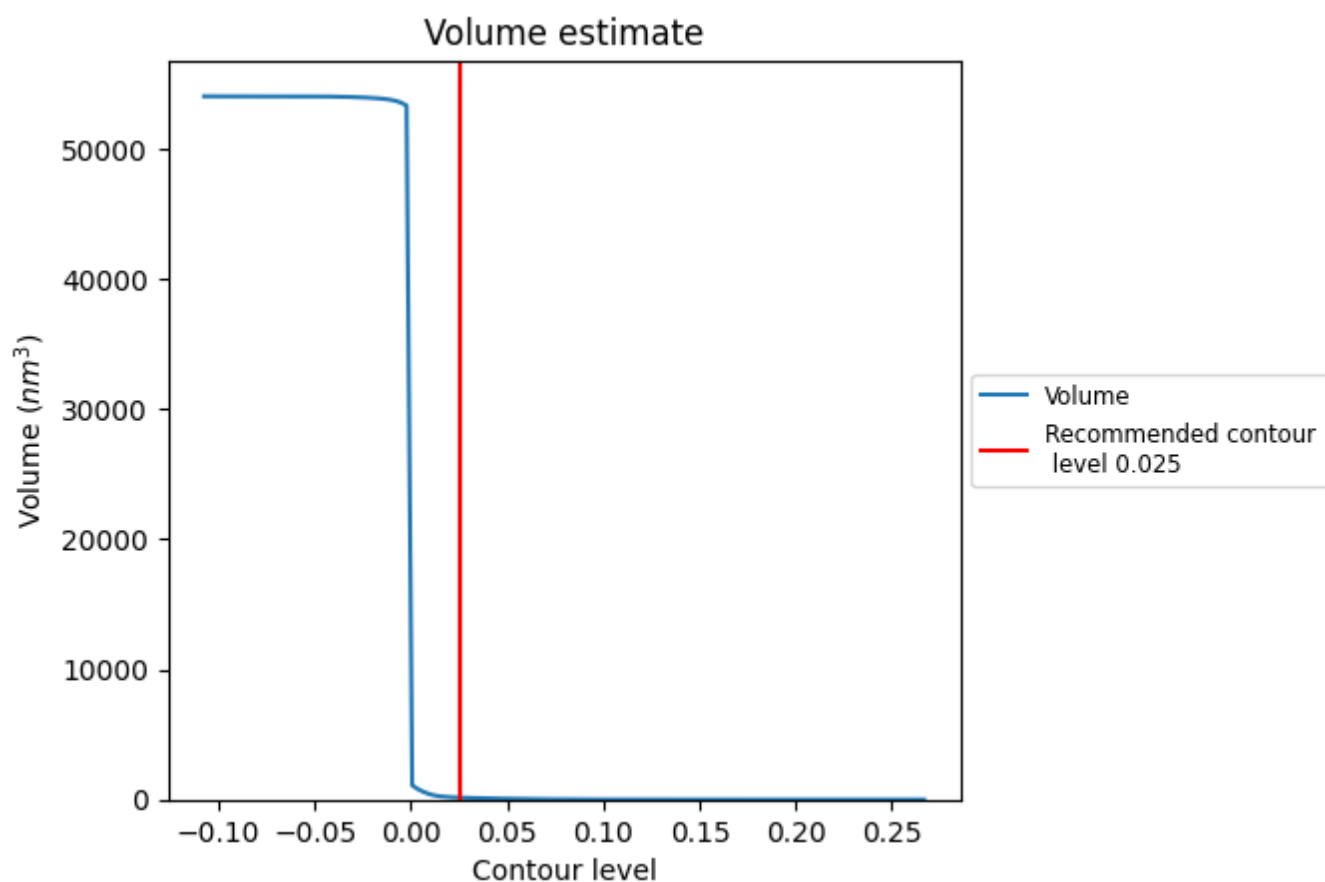
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

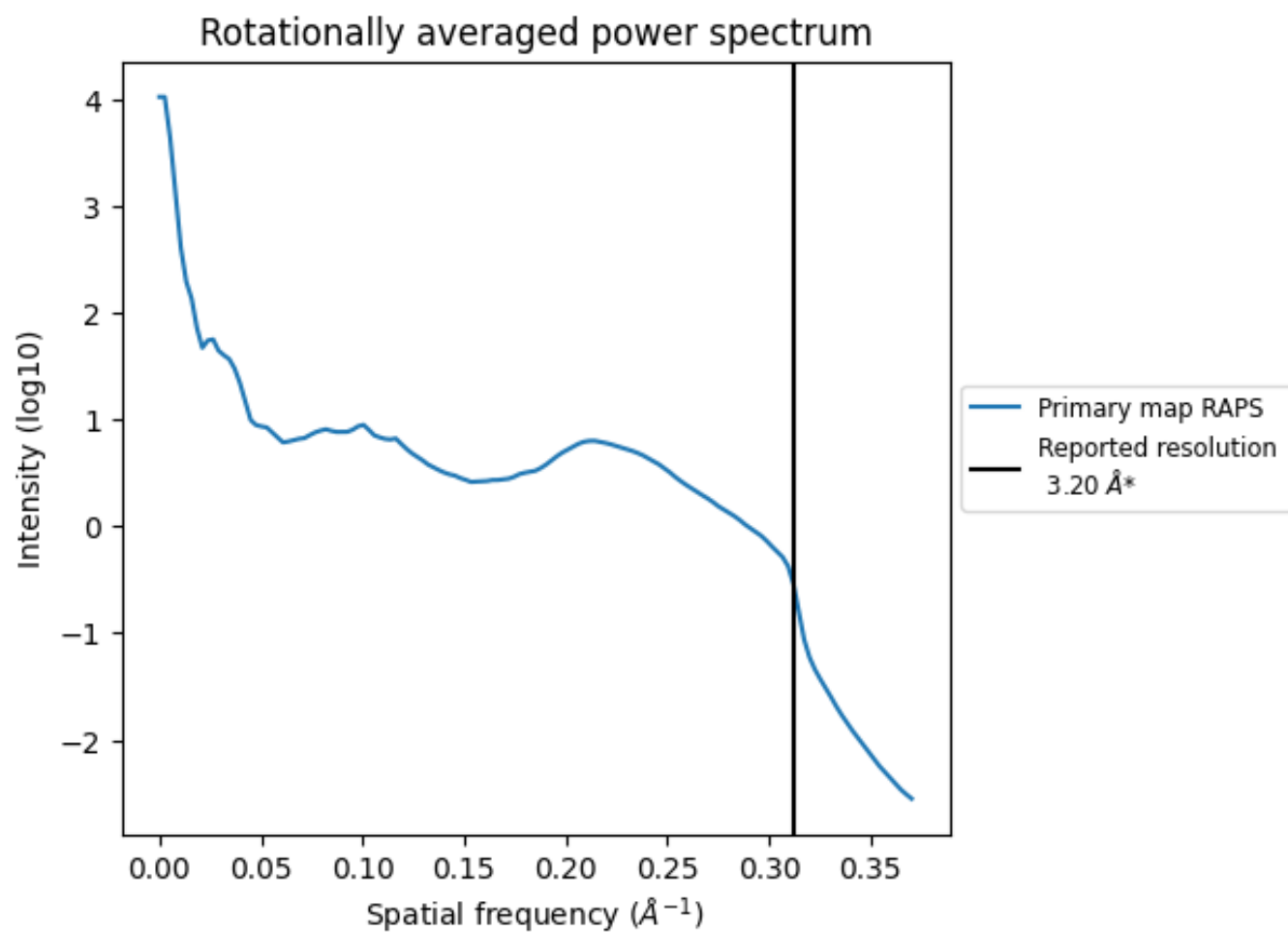
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 138 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 0.312 Å⁻¹

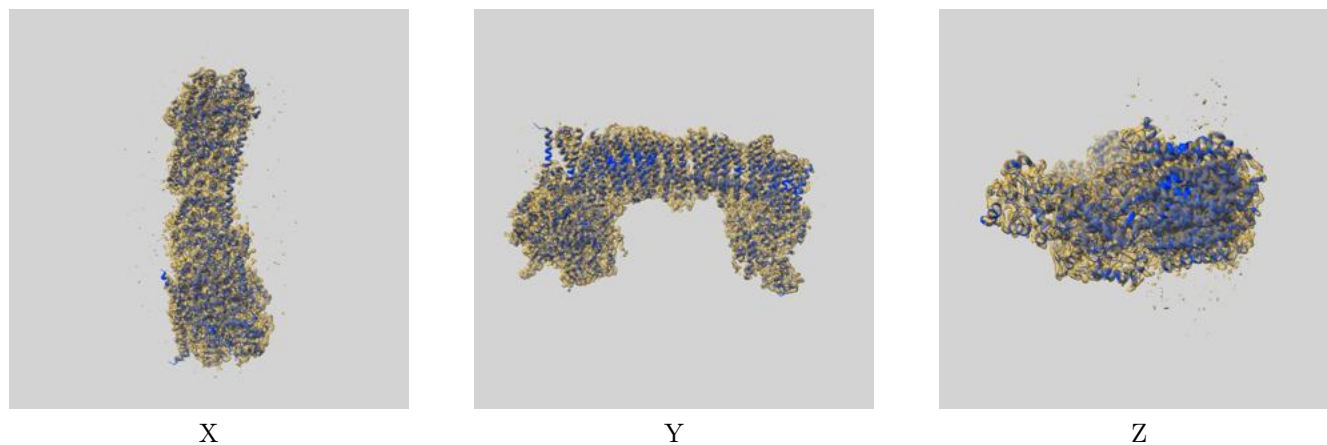
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

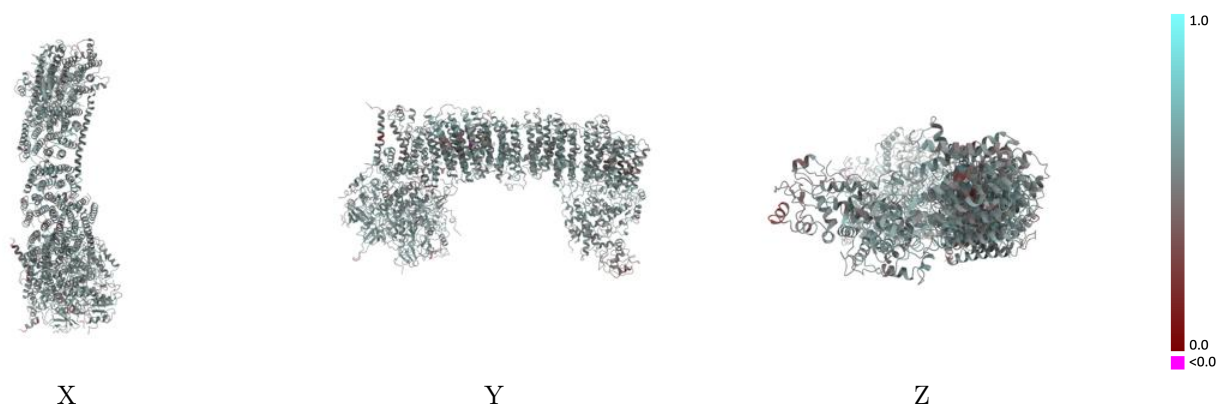
This section contains information regarding the fit between EMDB map EMD-10513 and PDB model 6TJV. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



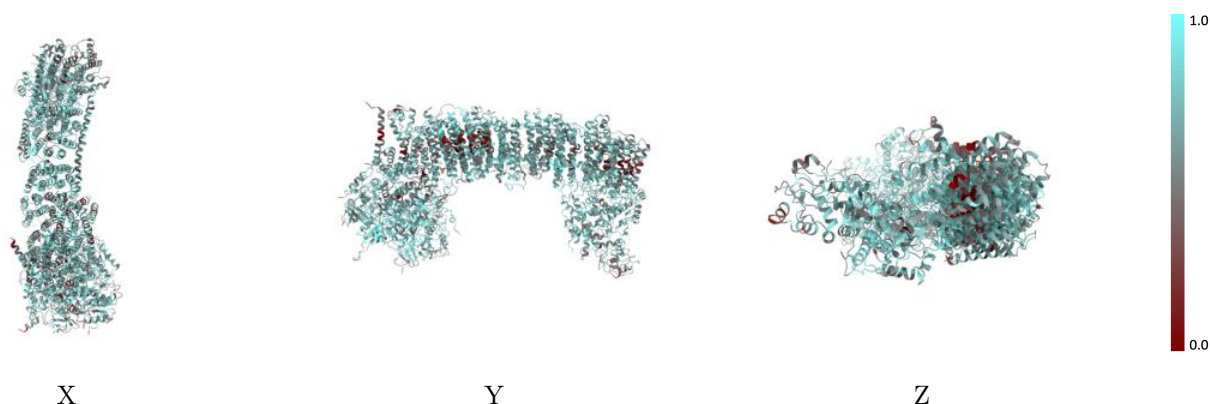
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



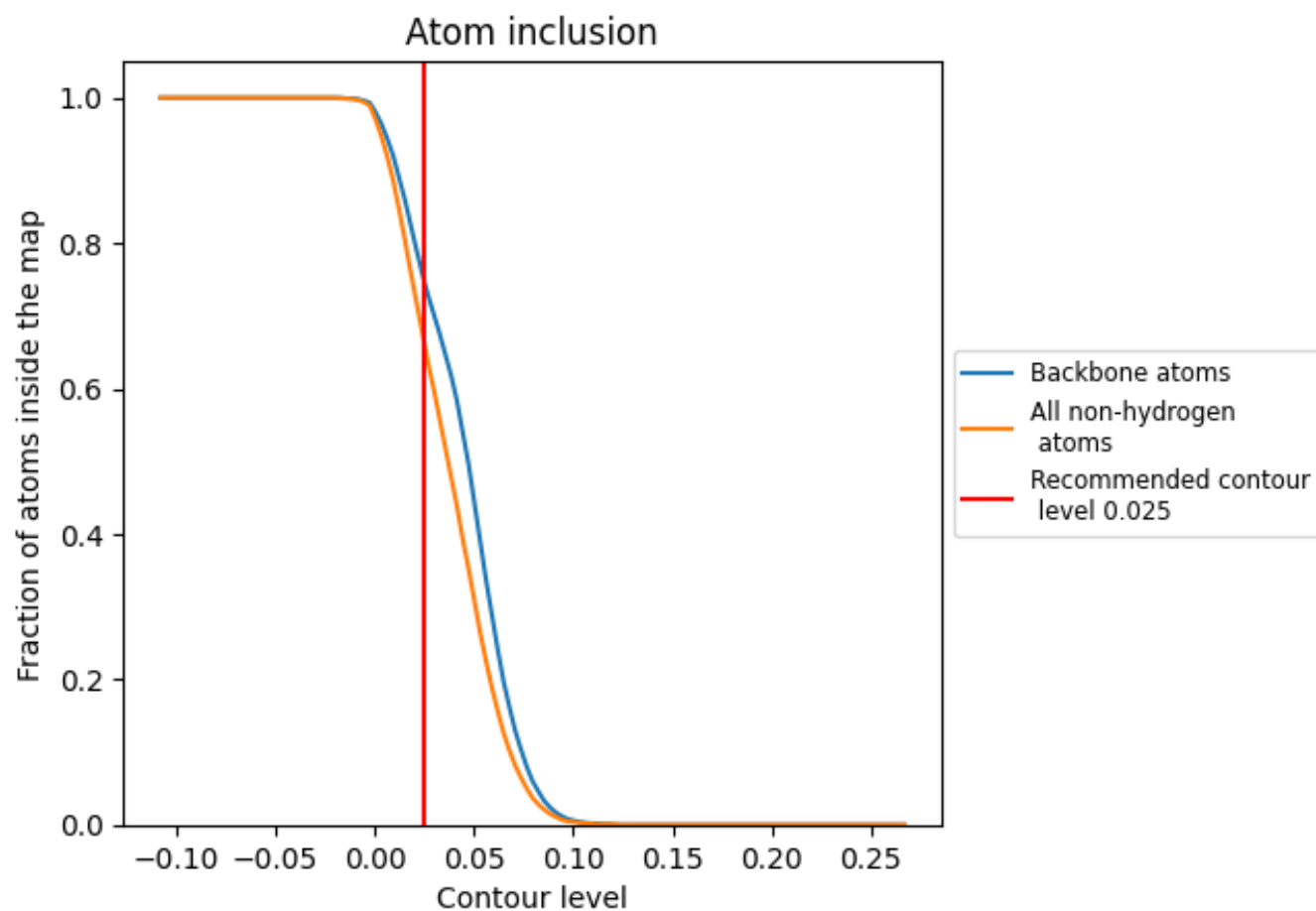
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.5290
A	 0.6310	 0.5260
B	 0.6850	 0.5340
C	 0.6220	 0.5210
D	 0.6890	 0.5430
E	 0.6580	 0.5340
F	 0.6200	 0.5220
G	 0.6380	 0.5280
H	 0.6660	 0.5310
I	 0.6930	 0.5310
J	 0.6850	 0.5240
K	 0.6880	 0.5460
L	 0.5320	 0.5080
M	 0.7180	 0.5320
N	 0.6890	 0.5360
O	 0.6770	 0.5070
P	 0.7200	 0.5390
Q	 0.5670	 0.4690
S	 0.6490	 0.5480

