Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 01:33 AM JST

PDB ID	:	7WFF
EMDB ID	:	EMD-32464
Title	:	Subcomplexes B,M and L in the Cylic electron transfer supercomplex NDH-PSI from Arabidopsis
Authors	:	Pan, X.W.; Li, M.
Deposited on	:	2021-12-26
Resolution	:	3.59 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

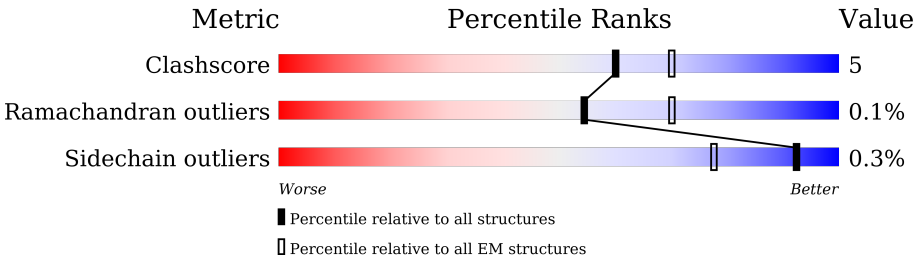
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.59 Å.

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



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

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 <=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	360	28% 75% 9% 15%
2	B	512	6% 82% 13% 5%
3	C	120	18% 73% 5% 22%
4	D	506	86% 12%
5	E	101	5% 72% 16% 12%
6	F	746	81% 9% 9%
7	G	176	8% 84% 11% 5%
8	a	461	74% 26%

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Mol	Chain	Length	Quality of chain
9	b	348	88% 12%
10	c	204	63% 37%
11	d	161	57% 42%
12	e	212	71% 29%
13	f	238	64% 36%
14	g	190	61% 39%
15	h	220	66% 34%
16	i	217	67% 33%
17	j	255	67% 32%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32124 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, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	305	2372	1593	366	409	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	486	3780	2495	577	679	29	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	94	776	544	109	121	2	0	0

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	497	3950	2658	599	668	25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	89	695	458	112	119	6	0	0

- Molecule 6 is a protein called NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	677	5330	3558	829	915	28	0	0

- Molecule 7 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	167	Total	C	N	O	S	0	0
			1281	858	194	224	5		

- Molecule 8 is a protein called Photosynthetic NDH subunit of subcomplex B 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	341	Total	C	N	O	S	0	0
			2655	1692	450	500	13		

- Molecule 9 is a protein called Photosynthetic NDH subunit of subcomplex B 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	307	Total	C	N	O	S	0	0
			2367	1508	392	452	15		

- Molecule 10 is a protein called Photosynthetic NDH subunit of subcomplex B 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	128	Total	C	N	O	S	0	0
			1005	636	180	183	6		

- Molecule 11 is a protein called NDH dependent flow 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	93	Total	C	N	O	S	0	0
			762	497	119	138	8		

- Molecule 12 is a protein called Photosynthetic NDH subunit of subcomplex B 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	e	150	Total	C	N	O	S	0	0
			1206	780	183	236	7		

- Molecule 13 is a protein called Photosynthetic NDH subunit of lumenal location 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	f	153	Total	C	N	O	S	0	0
			1277	823	219	233	2		

- Molecule 14 is a protein called Photosynthetic NDH subunit of lumenal location 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g	115	Total	C	N	O	S	0	0
			965	620	159	180	6		

- Molecule 15 is a protein called Photosynthetic NDH subunit of lumenal location 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	h	145	Total	C	N	O	S	0	0
			1170	753	191	221	5		

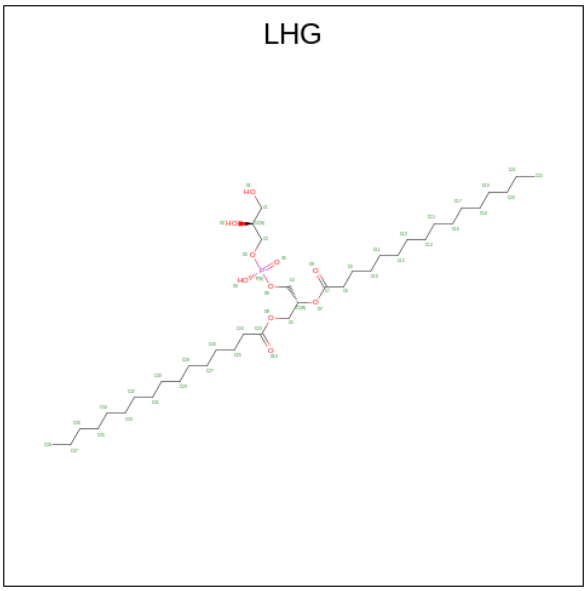
- Molecule 16 is a protein called Photosynthetic NDH subunit of lumenal location 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	i	145	Total	C	N	O	S	0	0
			1098	698	190	204	6		

- Molecule 17 is a protein called Isoform 2 of Photosynthetic NDH subunit of lumenal location 5, chloroplastic.

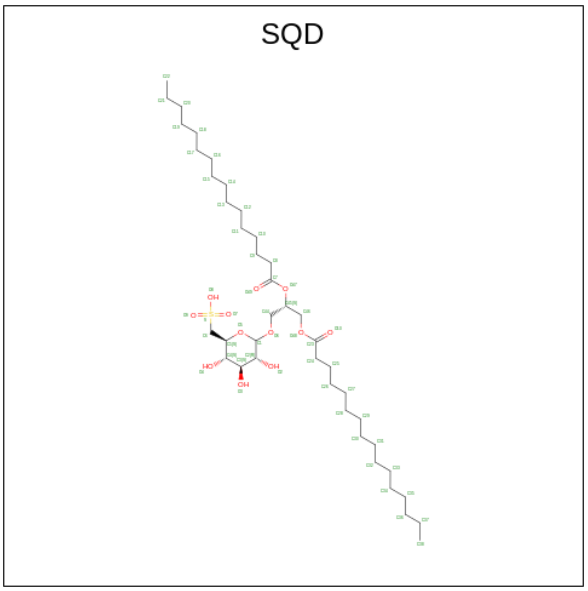
Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	173	Total	C	N	O	S	0	0
			1331	840	236	248	7		

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



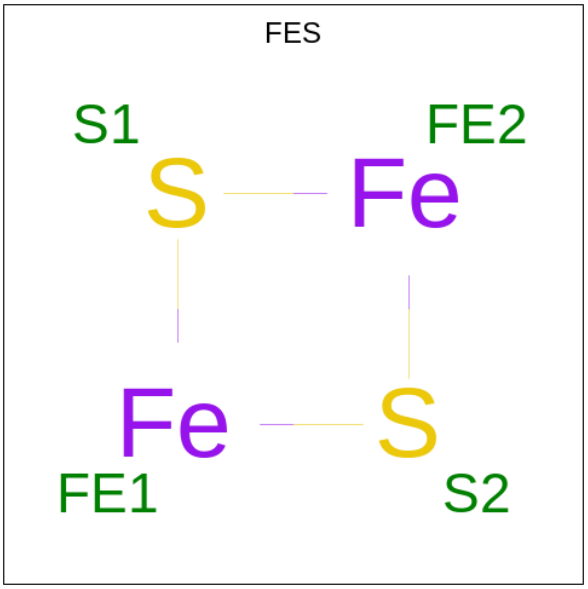
Mol	Chain	Residues	Atoms				AltConf
18	D	1	Total	C	O	P	0
			29	18	10	1	
18	F	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
19	F	1	Total	C	O	S	0
			34	21	12	1	

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



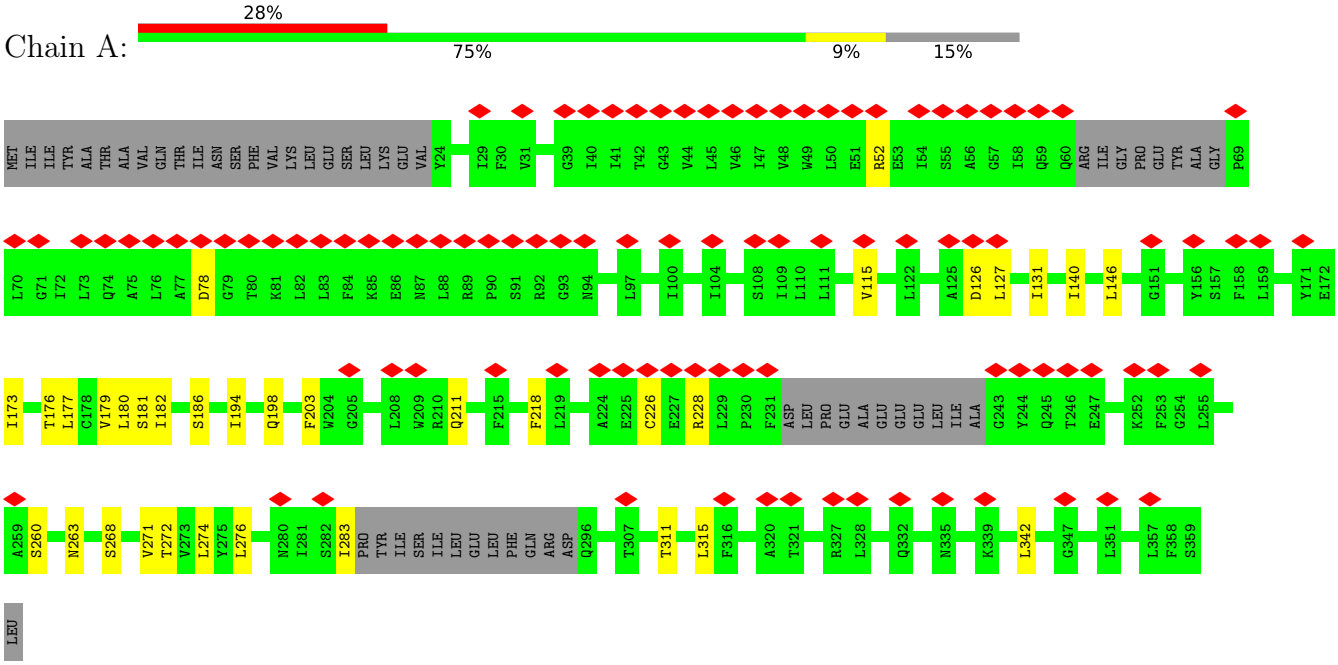
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
20	c	1	4	2	2	0

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.

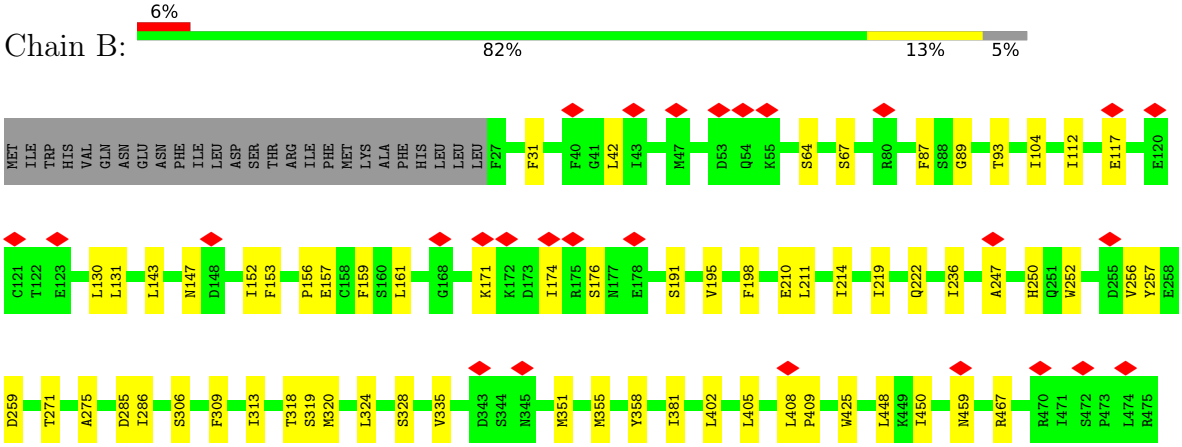
• Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic

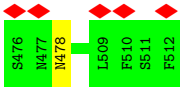
Chain A:



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

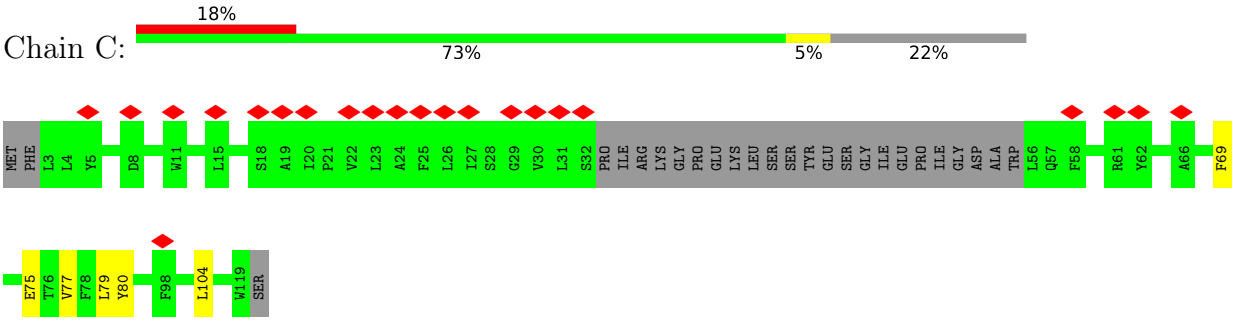
Chain B:





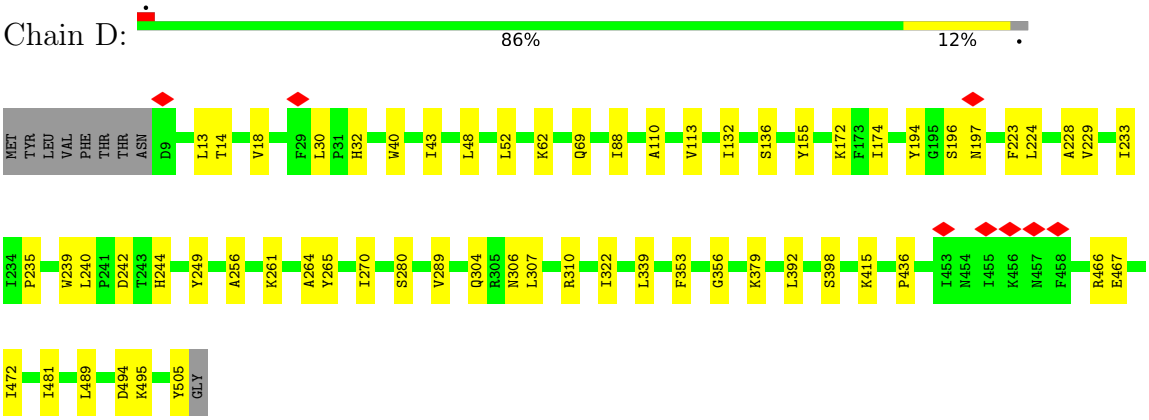
• Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic

Chain C:



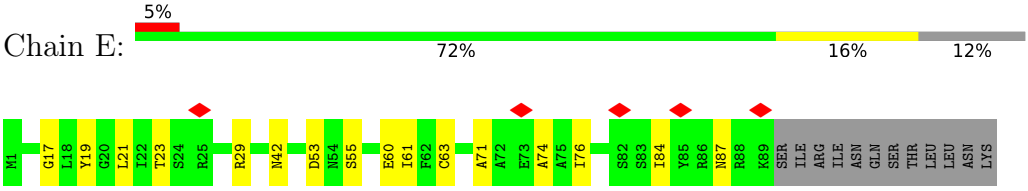
• Molecule 4: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic

Chain D:



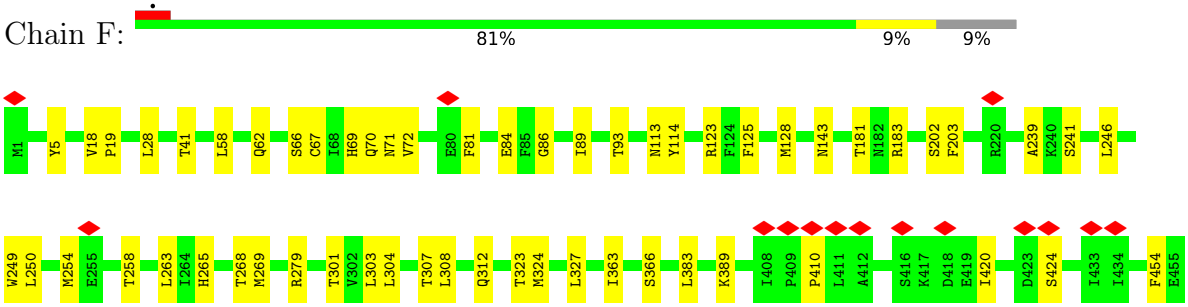
• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic

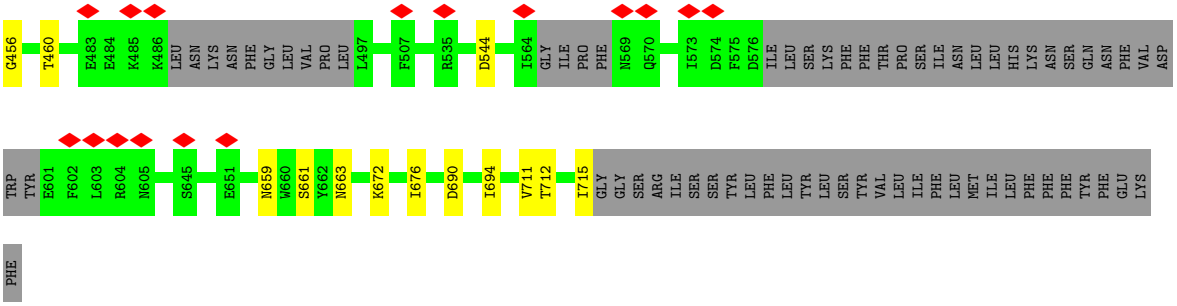
Chain E:



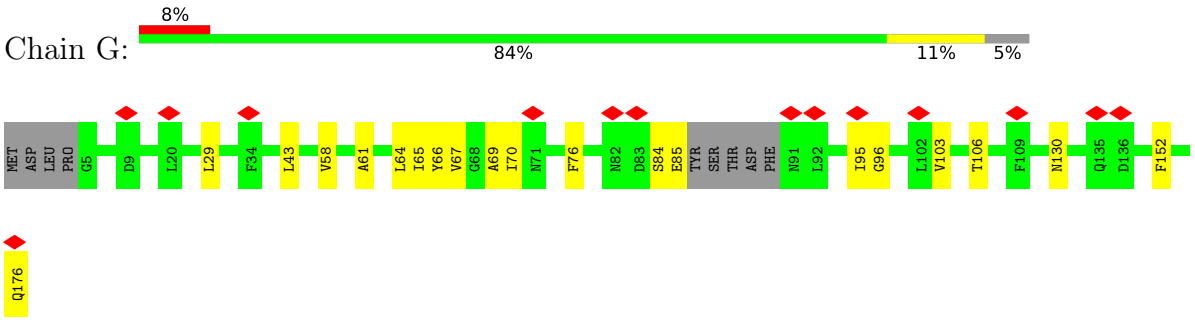
• Molecule 6: NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic

Chain F:

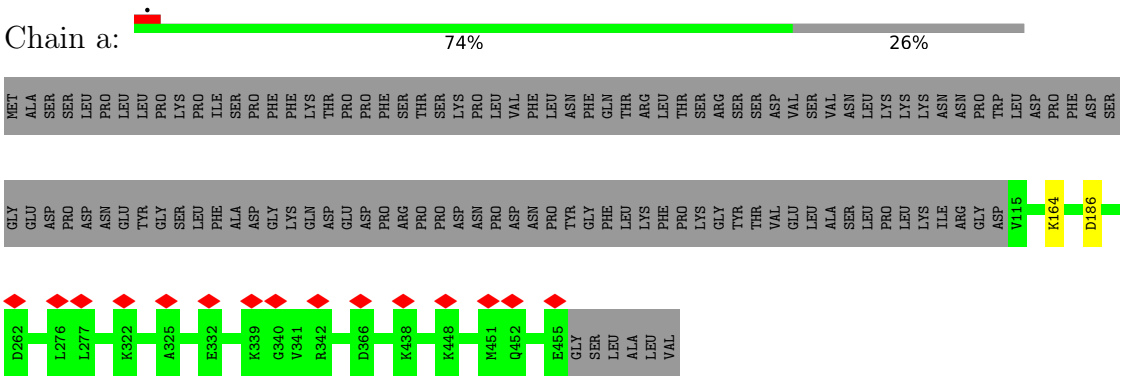




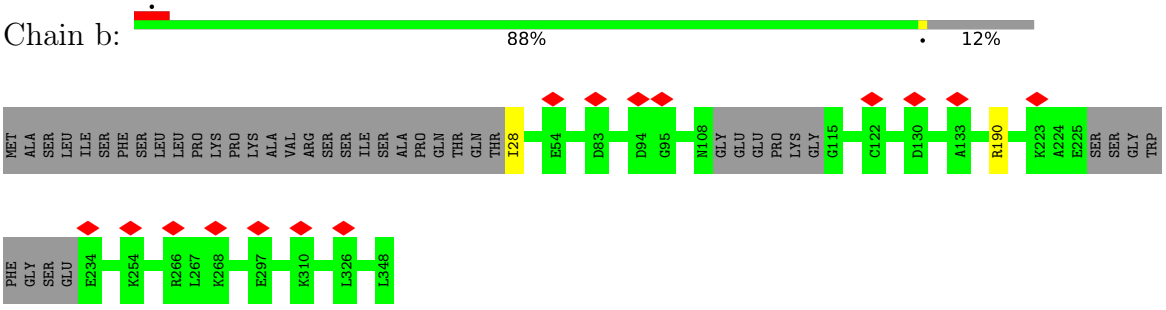
• Molecule 7: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic



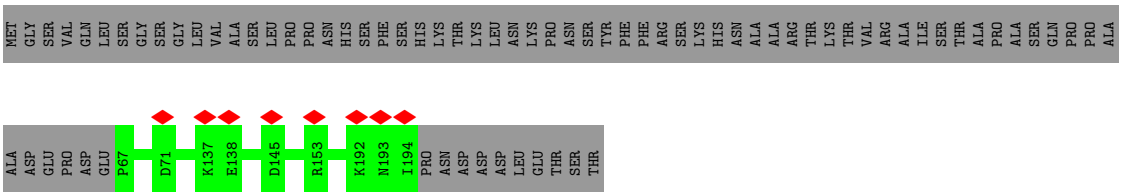
• Molecule 8: Photosynthetic NDH subunit of subcomplex B 1, chloroplastic



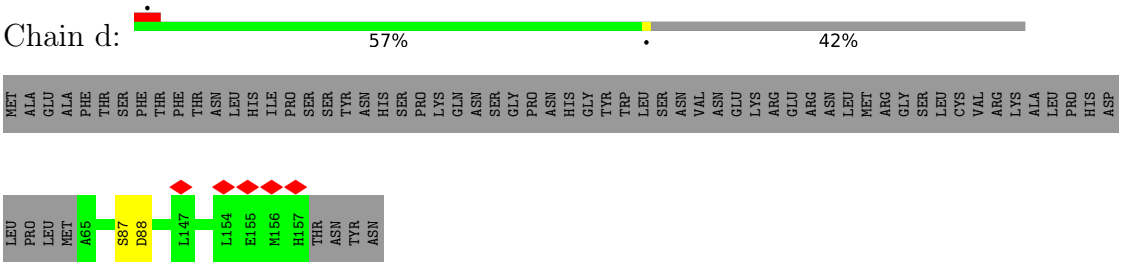
• Molecule 9: Photosynthetic NDH subunit of subcomplex B 2, chloroplastic



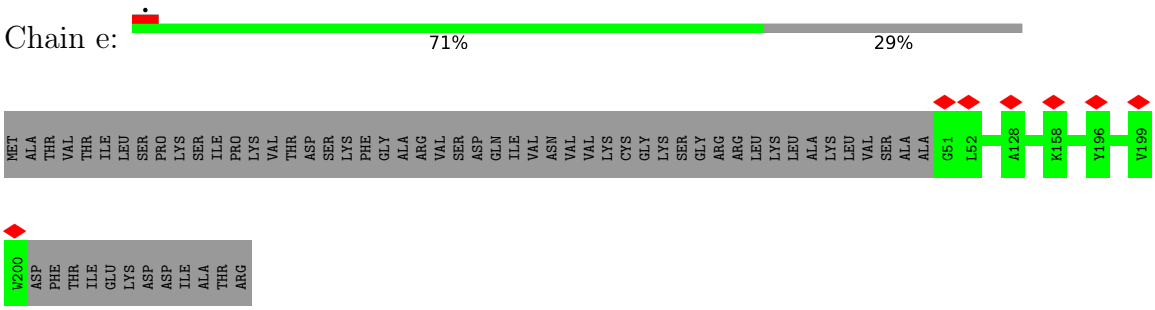
• Molecule 10: Photosynthetic NDH subunit of subcomplex B 3, chloroplastic



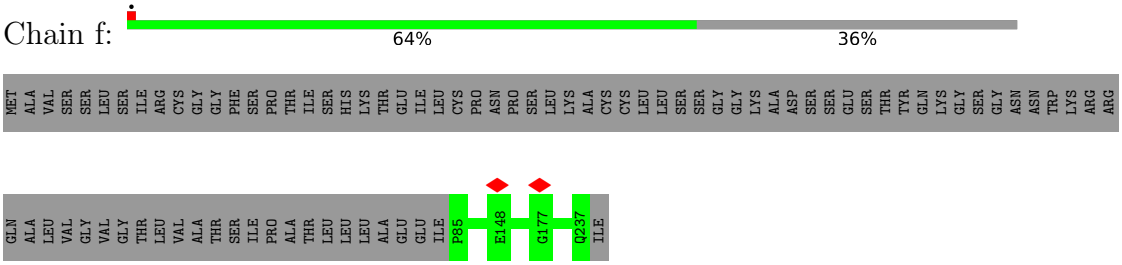
• Molecule 11: NDH dependent flow 6



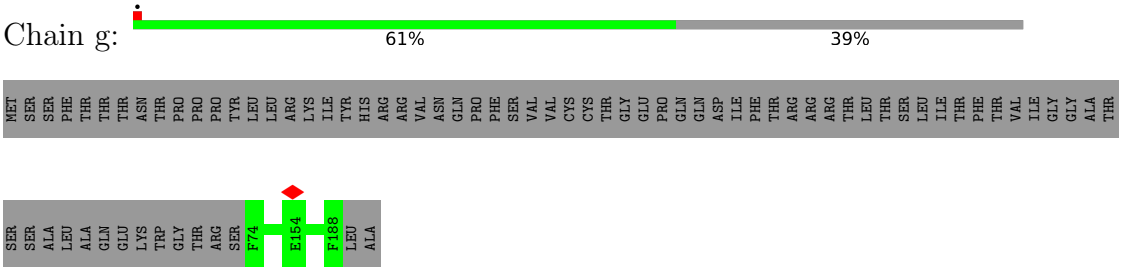
• Molecule 12: Photosynthetic NDH subunit of subcomplex B 5, chloroplastic



• Molecule 13: Photosynthetic NDH subunit of lumenal location 1, chloroplastic

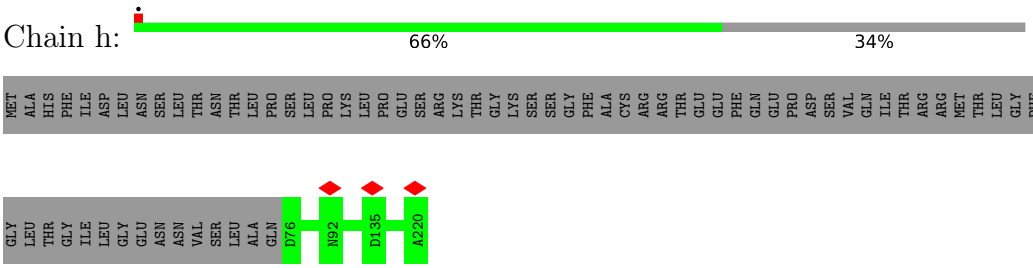


• Molecule 14: Photosynthetic NDH subunit of lumenal location 2, chloroplastic



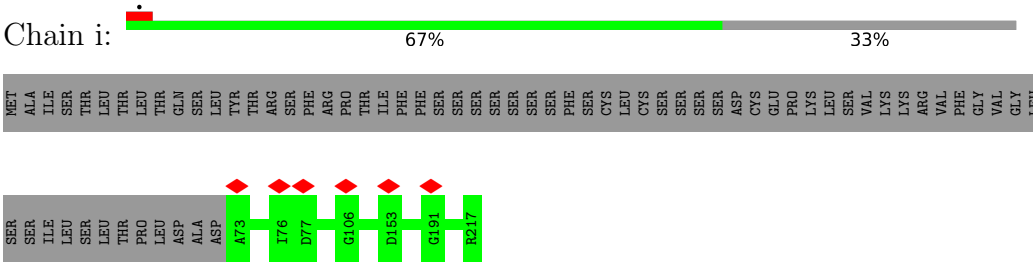
• Molecule 15: Photosynthetic NDH subunit of lumenal location 3, chloroplastic

Chain h:



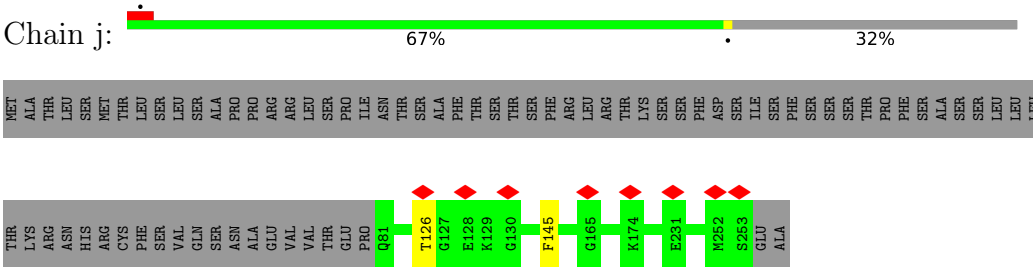
• Molecule 16: Photosynthetic NDH subunit of lumenal location 4, chloroplastic

Chain i:



• Molecule 17: Isoform 2 of Photosynthetic NDH subunit of lumenal location 5, chloroplastic

Chain j:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136022	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 ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.168	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, LHG, SQD

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	0.29	0/2430	0.55	0/3312
2	B	0.34	0/3872	0.58	0/5263
3	C	0.35	0/802	0.51	0/1094
4	D	0.38	0/4062	0.57	0/5514
5	E	0.35	0/705	0.56	0/952
6	F	0.36	0/5478	0.56	0/7446
7	G	0.32	0/1307	0.57	0/1785
8	a	0.34	0/2708	0.59	0/3668
9	b	0.31	0/2417	0.57	0/3265
10	c	0.34	0/1030	0.63	0/1401
11	d	0.40	0/784	0.55	0/1057
12	e	0.34	0/1241	0.55	0/1685
13	f	0.33	0/1312	0.62	0/1777
14	g	0.29	0/986	0.53	0/1329
15	h	0.36	0/1193	0.61	0/1610
16	i	0.34	0/1124	0.58	0/1523
17	j	0.35	0/1357	0.56	0/1823
All	All	0.34	0/32808	0.57	0/44504

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2372	0	2454	27	0
2	B	3780	0	3840	43	0
3	C	776	0	777	4	0
4	D	3950	0	4072	38	0
5	E	695	0	732	15	0
6	F	5330	0	5289	42	0
7	G	1281	0	1340	20	0
8	a	2655	0	2673	0	0
9	b	2367	0	2371	0	0
10	c	1005	0	1006	0	0
11	d	762	0	730	0	0
12	e	1206	0	1110	0	0
13	f	1277	0	1235	0	0
14	g	965	0	945	0	0
15	h	1170	0	1176	0	0
16	i	1098	0	1084	0	0
17	j	1331	0	1320	0	0
18	D	29	0	28	0	0
18	F	37	0	44	1	0
19	F	34	0	32	1	0
20	c	4	0	0	0	0
All	All	32124	0	32258	165	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 5.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:ARG:NH1	7:G:29:LEU:O	2.22	0.72
5:E:71:ALA:HA	7:G:70:ILE:HD11	1.72	0.69
2:B:247:ALA:O	2:B:250:HIS:ND1	2.25	0.69
6:F:389:LYS:NZ	6:F:456:GLY:O	2.24	0.68
5:E:17:GLY:O	5:E:21:LEU:N	2.29	0.66
4:D:256:ALA:O	4:D:261:LYS:NZ	2.29	0.65
4:D:466:ARG:NH1	4:D:467:GLU:OE2	2.31	0.64
5:E:53:ASP:OD1	7:G:130:ASN:ND2	2.31	0.64
1:A:226:CYS:SG	1:A:263:ASN:OD1	2.57	0.63
1:A:203:PHE:HB3	1:A:283:ILE:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:5:TYR:O	6:F:71:ASN:ND2	2.32	0.62
4:D:280:SER:O	4:D:415:LYS:NZ	2.22	0.61
1:A:182:ILE:HD13	1:A:211:GLN:OE1	2.01	0.61
6:F:58:LEU:O	6:F:62:GLN:HG2	2.00	0.60
4:D:264:ALA:HB1	4:D:322:ILE:HG21	1.82	0.60
4:D:233:ILE:HG22	4:D:235:PRO:HD2	1.84	0.60
4:D:110:ALA:O	4:D:113:VAL:HG12	2.02	0.59
6:F:301:THR:OG1	6:F:324:MET:SD	2.60	0.59
2:B:174:ILE:HD11	5:E:84:ILE:HG23	1.85	0.58
6:F:181:THR:HG23	6:F:246:LEU:HD12	1.85	0.57
6:F:241:SER:HB2	6:F:327:LEU:HD12	1.85	0.57
2:B:147:ASN:ND2	2:B:210:GLU:OE2	2.39	0.56
7:G:65:ILE:O	7:G:69:ALA:HB3	2.04	0.56
2:B:176:SER:HA	2:B:259:ASP:CB	2.35	0.56
4:D:62:LYS:O	4:D:69:GLN:NE2	2.39	0.56
1:A:186:SER:OG	1:A:194:ILE:HG22	2.06	0.56
2:B:448:LEU:HD12	4:D:155:TYR:CE2	2.40	0.55
1:A:228:ARG:NH1	1:A:260:SER:OG	2.40	0.55
1:A:181:SER:HB2	1:A:211:GLN:HE22	1.71	0.55
5:E:87:ASN:ND2	7:G:176:GLN:O	2.40	0.54
2:B:247:ALA:HB2	2:B:306:SER:HA	1.90	0.54
2:B:161:LEU:HD12	5:E:76:ILE:HD12	1.89	0.53
6:F:114:TYR:HH	6:F:258:THR:HG1	1.53	0.53
2:B:42:LEU:CD2	2:B:131:LEU:HD12	2.39	0.53
6:F:113:ASN:ND2	6:F:544:ASP:OD2	2.42	0.53
1:A:115:VAL:HG12	1:A:127:LEU:HD23	1.91	0.52
6:F:202:SER:OG	6:F:203:PHE:N	2.43	0.52
6:F:89:ILE:HD13	6:F:93:THR:HG21	1.91	0.52
1:A:226:CYS:O	1:A:228:ARG:NH1	2.43	0.52
1:A:173:ILE:O	1:A:177:LEU:HD23	2.09	0.52
2:B:31:PHE:HB3	2:B:93:THR:HG21	1.92	0.51
2:B:252:TRP:O	2:B:256:VAL:HG22	2.10	0.51
4:D:249:TYR:HB3	4:D:356:GLY:HA3	1.91	0.51
4:D:392:LEU:O	6:F:183:ARG:NH2	2.39	0.51
6:F:67:CYS:SG	6:F:69:HIS:NE2	2.83	0.51
6:F:254:MET:SD	6:F:254:MET:N	2.83	0.51
2:B:191:SER:O	2:B:195:VAL:HG23	2.11	0.50
6:F:250:LEU:HD11	6:F:265:HIS:CG	2.46	0.50
4:D:472:ILE:CD1	6:F:28:LEU:HD21	2.41	0.50
4:D:249:TYR:HB2	4:D:353:PHE:HA	1.93	0.50
4:D:233:ILE:HG23	4:D:289:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:392:LEU:HD21	4:D:436:PRO:HA	1.93	0.50
2:B:319:SER:OG	2:B:320:MET:N	2.45	0.50
6:F:312:GLN:NE2	6:F:661:SER:O	2.45	0.49
2:B:112:ILE:HD11	2:B:130:LEU:CD1	2.42	0.49
4:D:229:VAL:O	4:D:239:TRP:NE1	2.44	0.49
6:F:420:ILE:O	6:F:424:SER:OG	2.23	0.49
2:B:285:ASP:OD1	2:B:286:ILE:N	2.46	0.49
2:B:219:ILE:O	2:B:222:GLN:NE2	2.46	0.49
2:B:198:PHE:HD1	2:B:236:ILE:HD11	1.78	0.49
1:A:198:GLN:NE2	1:A:274:LEU:O	2.45	0.48
6:F:303:LEU:O	6:F:307:THR:OG1	2.27	0.48
5:E:55:SER:OG	7:G:130:ASN:O	2.32	0.48
4:D:494:ASP:OD1	4:D:495:LYS:N	2.46	0.48
4:D:240:LEU:HD11	4:D:244:HIS:CE1	2.49	0.48
5:E:63:CYS:SG	7:G:58:VAL:HG13	2.54	0.48
6:F:265:HIS:HB2	6:F:323:THR:HG21	1.96	0.48
1:A:176:THR:OG1	3:C:80:TYR:OH	2.20	0.48
7:G:95:ILE:HG22	7:G:96:GLY:H	1.79	0.48
2:B:152:ILE:O	2:B:156:PRO:HG2	2.14	0.47
2:B:320:MET:O	2:B:324:LEU:HD23	2.15	0.47
4:D:13:LEU:HD21	4:D:88:ILE:HD11	1.96	0.47
4:D:48:LEU:O	4:D:52:LEU:HD23	2.14	0.47
4:D:62:LYS:N	4:D:69:GLN:OE1	2.47	0.47
1:A:268:SER:O	1:A:272:THR:HG23	2.14	0.47
1:A:311:THR:O	1:A:315:LEU:HD23	2.14	0.47
4:D:40:TRP:HA	4:D:43:ILE:HG22	1.95	0.47
6:F:70:GLN:O	6:F:72:VAL:N	2.47	0.47
7:G:84:SER:OG	7:G:85:GLU:N	2.47	0.47
6:F:363:ILE:HD11	6:F:454:PHE:CZ	2.49	0.47
1:A:173:ILE:HD12	1:A:173:ILE:H	1.80	0.47
1:A:186:SER:CB	1:A:194:ILE:HG22	2.45	0.47
6:F:268:THR:OG1	6:F:269:MET:N	2.48	0.47
2:B:117:GLU:OE2	2:B:478:ASN:ND2	2.48	0.47
7:G:61:ALA:O	7:G:65:ILE:HG22	2.15	0.47
4:D:379:LYS:NZ	19:F:802:SQD:O2	2.49	0.46
4:D:30:LEU:O	4:D:32:HIS:N	2.48	0.46
6:F:690:ASP:HA	6:F:694:ILE:HG22	1.98	0.46
1:A:140:ILE:HD12	7:G:67:VAL:HG21	1.96	0.46
2:B:171:LYS:HG2	7:G:176:GLN:HB2	1.98	0.46
4:D:14:THR:O	4:D:18:VAL:HG22	2.15	0.46
4:D:339:LEU:HD22	4:D:489:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:ILE:O	4:D:136:SER:OG	2.22	0.46
1:A:180:LEU:HD21	3:C:79:LEU:HB3	1.97	0.46
2:B:87:PHE:O	2:B:89:GLY:N	2.47	0.46
5:E:42:ASN:ND2	5:E:63:CYS:SG	2.86	0.46
5:E:61:ILE:HG21	7:G:152:PHE:CD2	2.50	0.46
4:D:228:ALA:HA	4:D:233:ILE:HD12	1.98	0.46
2:B:42:LEU:HD22	2:B:131:LEU:HD12	1.97	0.45
2:B:157:GLU:O	2:B:161:LEU:HD23	2.16	0.45
4:D:270:ILE:HG22	4:D:270:ILE:O	2.16	0.45
1:A:182:ILE:CD1	1:A:211:GLN:OE1	2.65	0.45
6:F:66:SER:O	6:F:66:SER:OG	2.33	0.45
4:D:172:LYS:NZ	4:D:242:ASP:OD2	2.48	0.45
6:F:72:VAL:HG12	6:F:86:GLY:HA3	1.99	0.45
6:F:711:VAL:O	6:F:715:ILE:HG22	2.17	0.45
5:E:61:ILE:HG21	7:G:152:PHE:HD2	1.81	0.44
6:F:659:ASN:O	6:F:663:ASN:ND2	2.50	0.44
1:A:131:ILE:HD13	1:A:179:VAL:HG13	2.00	0.44
2:B:64:SER:CB	2:B:130:LEU:HD12	2.47	0.44
5:E:74:ALA:HB3	7:G:70:ILE:HD12	1.99	0.44
6:F:123:ARG:NE	18:F:801:LHG:O4	2.48	0.44
3:C:77:VAL:HG22	7:G:64:LEU:HD23	1.99	0.44
6:F:712:THR:HA	6:F:715:ILE:HG22	1.99	0.44
2:B:104:ILE:HD11	2:B:275:ALA:HB2	2.00	0.44
1:A:115:VAL:HG12	1:A:127:LEU:CD2	2.48	0.44
6:F:239:ALA:O	6:F:249:TRP:NE1	2.50	0.44
2:B:328:SER:OG	2:B:358:TYR:OH	2.23	0.43
1:A:173:ILE:HG21	1:A:342:LEU:HD11	2.01	0.43
6:F:672:LYS:HA	6:F:676:ILE:HG22	2.01	0.43
6:F:41:THR:HG1	6:F:125:PHE:HE2	1.65	0.43
1:A:52:ARG:NH2	1:A:78:ASP:OD2	2.51	0.43
2:B:408:LEU:HD11	4:D:174:ILE:HD11	1.99	0.43
6:F:93:THR:OG1	6:F:279:ARG:NH2	2.52	0.43
6:F:363:ILE:O	6:F:366:SER:OG	2.30	0.43
2:B:211:LEU:HA	2:B:214:ILE:HD12	2.00	0.43
2:B:402:LEU:HA	2:B:405:LEU:HD12	2.01	0.43
2:B:335:VAL:HG21	2:B:355:MET:SD	2.59	0.43
6:F:18:VAL:HG13	6:F:19:PRO:HD3	2.01	0.43
5:E:19:TYR:O	5:E:23:THR:OG1	2.34	0.43
1:A:218:PHE:CD2	1:A:271:VAL:HG22	2.54	0.42
2:B:309:PHE:O	2:B:313:ILE:N	2.52	0.42
2:B:64:SER:O	2:B:67:SER:OG	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:ASN:O	2:B:467:ARG:NH2	2.52	0.42
6:F:5:TYR:OH	6:F:62:GLN:NE2	2.51	0.42
3:C:75:GLU:OE1	3:C:104:LEU:HD13	2.19	0.42
5:E:60:GLU:HB3	7:G:58:VAL:HG21	2.01	0.42
2:B:381:ILE:HD11	2:B:450:ILE:HG12	2.01	0.42
4:D:196:SER:OG	4:D:197:ASN:N	2.52	0.42
4:D:304:GLN:O	4:D:310:ARG:NH1	2.52	0.42
6:F:84:GLU:O	6:F:143:ASN:ND2	2.46	0.42
4:D:306:ASN:OD1	4:D:307:LEU:N	2.52	0.42
4:D:398:SER:HB3	4:D:481:ILE:CG2	2.50	0.42
4:D:472:ILE:HD11	6:F:28:LEU:HD21	2.01	0.42
2:B:335:VAL:HG13	2:B:351:MET:HG2	2.01	0.42
2:B:143:LEU:HD13	2:B:156:PRO:HG3	2.02	0.42
1:A:272:THR:HG22	1:A:276:LEU:HD12	2.01	0.41
2:B:256:VAL:HG23	2:B:257:TYR:CD1	2.55	0.41
1:A:126:ASP:N	1:A:126:ASP:OD1	2.53	0.41
1:A:146:LEU:HD11	7:G:76:PHE:CE1	2.55	0.41
2:B:153:PHE:CD1	2:B:195:VAL:HG21	2.55	0.41
2:B:112:ILE:HD11	2:B:130:LEU:HD11	2.01	0.41
2:B:159:PHE:CE2	2:B:271:THR:HG22	2.55	0.41
4:D:224:LEU:O	4:D:228:ALA:HB2	2.19	0.41
6:F:62:GLN:NE2	6:F:89:ILE:HG22	2.35	0.41
2:B:318:THR:O	2:B:381:ILE:HG22	2.21	0.41
2:B:408:LEU:HB2	2:B:409:PRO:HD3	2.03	0.41
7:G:43:LEU:HD13	7:G:66:TYR:CD2	2.56	0.41
1:A:181:SER:HB2	1:A:211:GLN:NE2	2.35	0.41
6:F:304:LEU:O	6:F:308:LEU:HD23	2.21	0.41
6:F:383:LEU:O	6:F:460:THR:OG1	2.37	0.41
6:F:128:MET:CE	6:F:263:LEU:HD22	2.51	0.41
2:B:425:TRP:O	4:D:194:TYR:OH	2.35	0.40
4:D:223:PHE:CZ	4:D:270:ILE:HG21	2.56	0.40
7:G:103:VAL:HA	7:G:106:THR:HG22	2.03	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	A	297/360 (82%)	283 (95%)	14 (5%)	0	100	100
2	B	484/512 (94%)	442 (91%)	42 (9%)	0	100	100
3	C	90/120 (75%)	87 (97%)	3 (3%)	0	100	100
4	D	495/506 (98%)	466 (94%)	29 (6%)	0	100	100
5	E	87/101 (86%)	85 (98%)	2 (2%)	0	100	100
6	F	669/746 (90%)	618 (92%)	49 (7%)	2 (0%)	41	75
7	G	163/176 (93%)	147 (90%)	16 (10%)	0	100	100
8	a	339/461 (74%)	284 (84%)	55 (16%)	0	100	100
9	b	301/348 (86%)	270 (90%)	31 (10%)	0	100	100
10	c	126/204 (62%)	114 (90%)	12 (10%)	0	100	100
11	d	91/161 (56%)	77 (85%)	13 (14%)	1 (1%)	14	53
12	e	148/212 (70%)	126 (85%)	22 (15%)	0	100	100
13	f	151/238 (63%)	126 (83%)	25 (17%)	0	100	100
14	g	113/190 (60%)	113 (100%)	0	0	100	100
15	h	143/220 (65%)	131 (92%)	12 (8%)	0	100	100
16	i	143/217 (66%)	124 (87%)	19 (13%)	0	100	100
17	j	171/255 (67%)	152 (89%)	18 (10%)	1 (1%)	25	64
All	All	4011/5027 (80%)	3645 (91%)	362 (9%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	81	PHE
11	d	87	SER
17	j	145	PHE
6	F	410	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/312 (83%)	258 (100%)	0	100	100
2	B	420/446 (94%)	420 (100%)	0	100	100
3	C	78/103 (76%)	77 (99%)	1 (1%)	69	86
4	D	431/439 (98%)	429 (100%)	2 (0%)	88	95
5	E	75/87 (86%)	75 (100%)	0	100	100
6	F	561/661 (85%)	561 (100%)	0	100	100
7	G	145/154 (94%)	145 (100%)	0	100	100
8	a	288/397 (72%)	286 (99%)	2 (1%)	84	93
9	b	263/297 (89%)	261 (99%)	2 (1%)	81	91
10	c	112/177 (63%)	112 (100%)	0	100	100
11	d	81/143 (57%)	80 (99%)	1 (1%)	71	87
12	e	125/178 (70%)	125 (100%)	0	100	100
13	f	134/207 (65%)	134 (100%)	0	100	100
14	g	104/172 (60%)	104 (100%)	0	100	100
15	h	127/192 (66%)	127 (100%)	0	100	100
16	i	114/180 (63%)	114 (100%)	0	100	100
17	j	143/219 (65%)	142 (99%)	1 (1%)	84	93
All	All	3459/4364 (79%)	3450 (100%)	9 (0%)	92	97

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

Mol	Chain	Res	Type
3	C	69	PHE
4	D	265	TYR
4	D	505	TYR
8	a	164	LYS
8	a	186	ASP
9	b	28	ILE
9	b	190	ARG
11	d	88	ASP
17	j	126	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	248	HIS
4	D	271	ASN
6	F	62	GLN
8	a	177	HIS
9	b	347	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	FES	c	301	10	0,4,4	-	-	-		
18	LHG	F	801	-	36,36,48	0.70	0	39,42,54	1.15	1 (2%)
19	SQD	F	802	-	33,34,54	1.21	4 (12%)	42,45,65	1.81	11 (26%)
18	LHG	D	601	-	28,28,48	0.86	0	31,34,54	1.31	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	FES	c	301	10	-	-	0/1/1/1
18	LHG	F	801	-	-	19/41/41/53	-
19	SQD	F	802	-	-	14/29/49/69	0/1/1/1
18	LHG	D	601	-	-	19/33/33/53	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	802	SQD	O48-C23	3.13	1.42	1.33
19	F	802	SQD	O47-C7	2.91	1.42	1.34
19	F	802	SQD	O4-C4	-2.19	1.37	1.43
19	F	802	SQD	O2-C2	-2.10	1.38	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	F	802	SQD	C44-O6-C1	4.48	122.49	113.74
19	F	802	SQD	O7-S-C6	4.36	112.12	106.94
18	D	601	LHG	O4-P-O5	4.24	133.21	112.24
18	F	801	LHG	O4-P-O5	4.19	132.97	112.24
19	F	802	SQD	O9-S-C6	3.88	111.55	106.94
19	F	802	SQD	O47-C7-C8	3.74	119.56	111.50
19	F	802	SQD	O9-S-O7	-3.72	101.09	113.95
19	F	802	SQD	O8-S-C6	2.80	110.19	105.74
18	D	601	LHG	O8-C23-O10	-2.53	117.22	123.59
19	F	802	SQD	O48-C23-C24	2.50	119.75	111.91
19	F	802	SQD	O5-C5-C4	2.28	113.83	109.69
18	D	601	LHG	O8-C23-C24	2.25	118.98	111.91
19	F	802	SQD	C3-C4-C5	2.23	114.22	110.24
19	F	802	SQD	C1-O5-C5	2.23	118.06	113.69
18	D	601	LHG	C5-O7-C7	-2.15	112.51	117.79
19	F	802	SQD	C4-C3-C2	2.11	114.51	110.82

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	D	601	LHG	O1-C1-C2-C3
18	D	601	LHG	C1-C2-C3-O3
18	D	601	LHG	O2-C2-C3-O3
18	F	801	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
19	F	802	SQD	O5-C1-O6-C44
19	F	802	SQD	C8-C7-O47-C45
19	F	802	SQD	C5-C6-S-O7
19	F	802	SQD	C5-C6-S-O8
19	F	802	SQD	C5-C6-S-O9
19	F	802	SQD	C24-C23-O48-C46
19	F	802	SQD	O49-C7-O47-C45
19	F	802	SQD	O10-C23-O48-C46
18	D	601	LHG	C24-C23-O8-C6
18	D	601	LHG	C23-C24-C25-C26
18	D	601	LHG	O10-C23-O8-C6
18	D	601	LHG	C3-O3-P-O6
19	F	802	SQD	C24-C25-C26-C27
18	F	801	LHG	C30-C31-C32-C33
18	F	801	LHG	C23-C24-C25-C26
18	D	601	LHG	O9-C7-O7-C5
18	D	601	LHG	O1-C1-C2-O2
18	F	801	LHG	C28-C29-C30-C31
18	D	601	LHG	C8-C7-O7-C5
18	F	801	LHG	O6-C4-C5-O7
18	F	801	LHG	O6-C4-C5-C6
18	D	601	LHG	C25-C26-C27-C28
18	F	801	LHG	O9-C7-O7-C5
19	F	802	SQD	C44-C45-C46-O48
18	D	601	LHG	O6-C4-C5-O7
18	F	801	LHG	C33-C34-C35-C36
18	D	601	LHG	C2-C3-O3-P
18	F	801	LHG	C24-C25-C26-C27
18	F	801	LHG	C2-C3-O3-P
18	F	801	LHG	C3-O3-P-O6
18	D	601	LHG	C3-O3-P-O5
18	D	601	LHG	O6-C4-C5-C6
18	F	801	LHG	C32-C33-C34-C35
19	F	802	SQD	O5-C5-C6-S
18	F	801	LHG	C24-C23-O8-C6
18	F	801	LHG	O1-C1-C2-O2
19	F	802	SQD	C2-C1-O6-C44
19	F	802	SQD	O47-C45-C46-O48
18	F	801	LHG	C27-C28-C29-C30
19	F	802	SQD	C46-C45-O47-C7
18	F	801	LHG	C7-C8-C9-C10
18	F	801	LHG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	F	801	LHG	O1-C1-C2-C3
18	D	601	LHG	O7-C7-C8-C9
18	D	601	LHG	O9-C7-C8-C9
18	D	601	LHG	O10-C23-C24-C25
18	D	601	LHG	C4-O6-P-O5
18	F	801	LHG	O10-C23-C24-C25

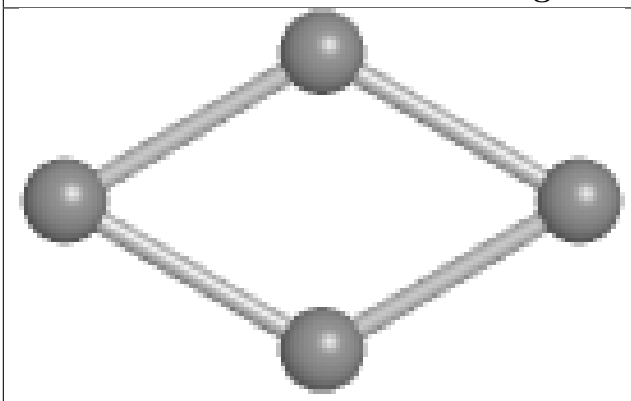
There are no ring outliers.

2 monomers are involved in 2 short contacts:

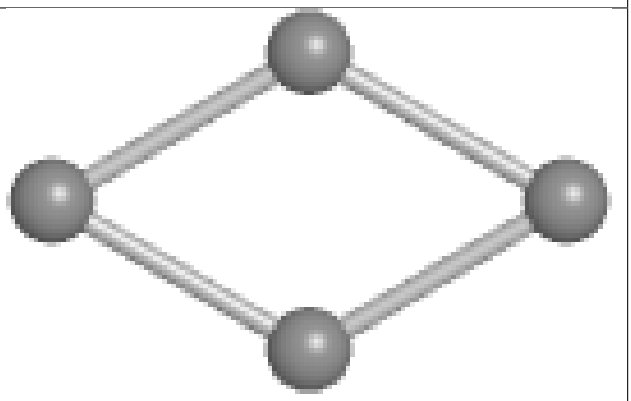
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	F	801	LHG	1	0
19	F	802	SQD	1	0

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 then 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.

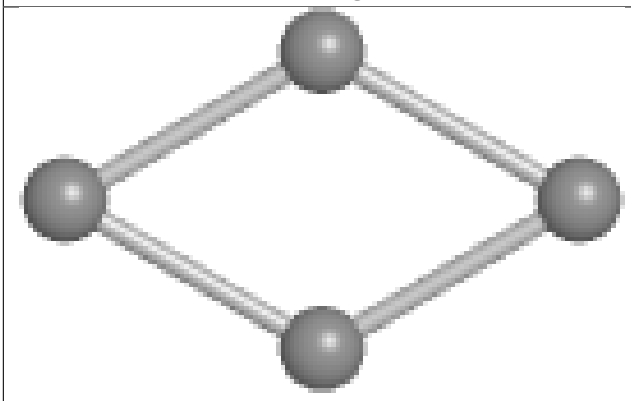
Ligand FES c 301



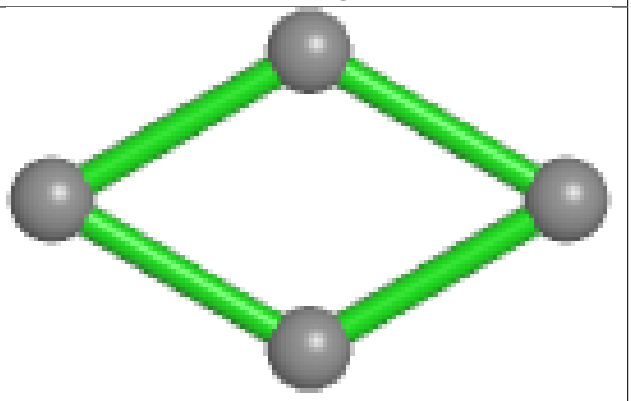
Bond lengths



Bond angles

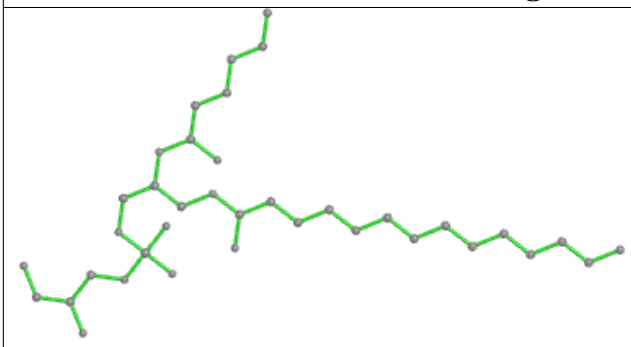


Torsions

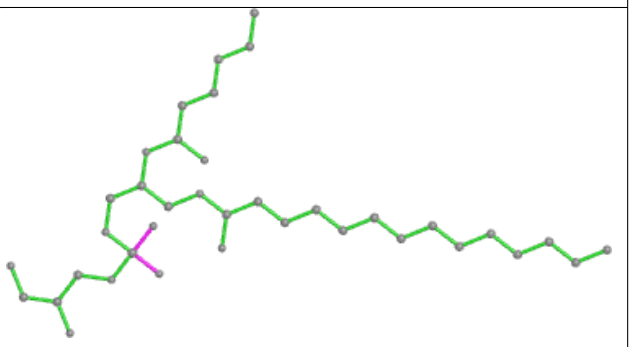


Rings

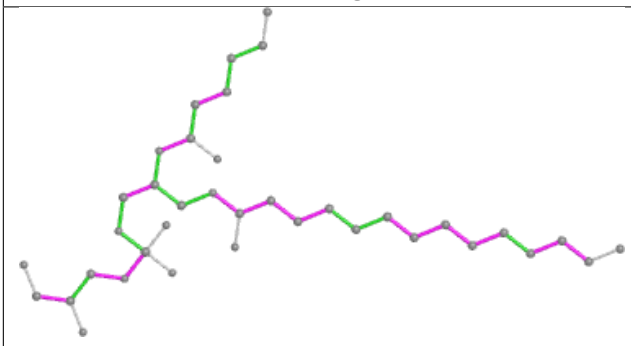
Ligand LHG F 801



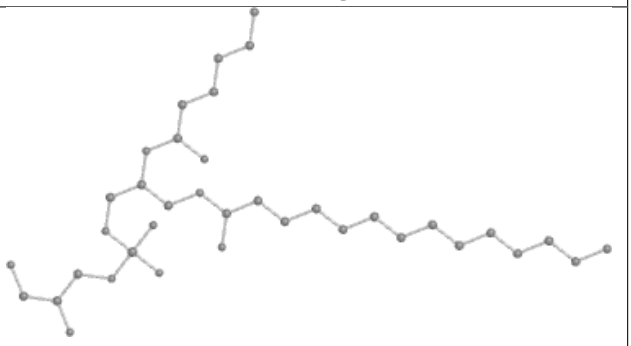
Bond lengths



Bond angles

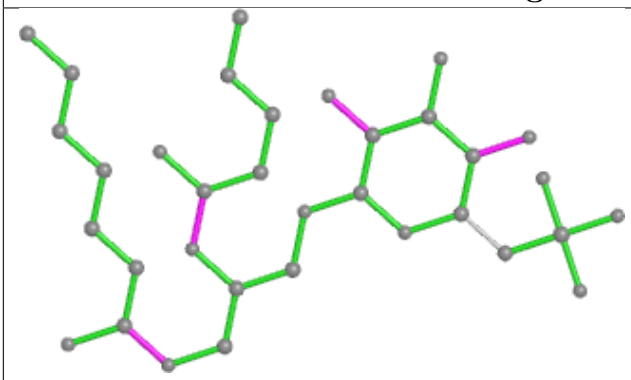


Torsions

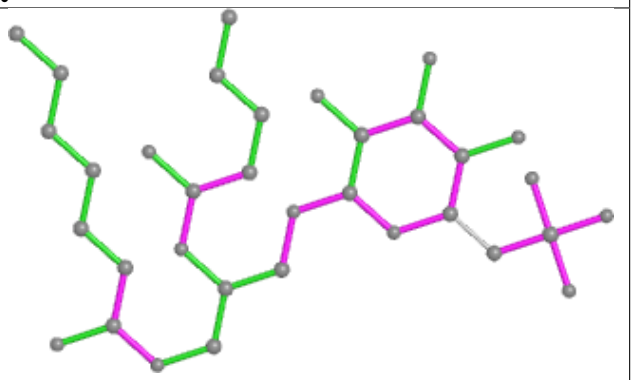


Rings

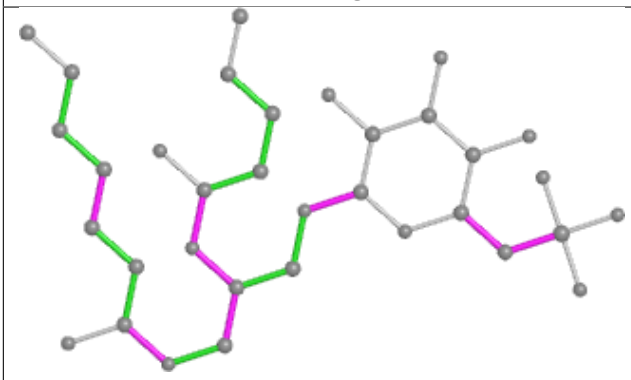
Ligand SQD F 802



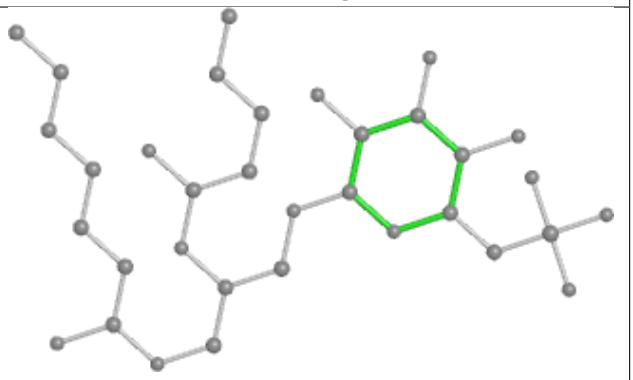
Bond lengths



Bond angles

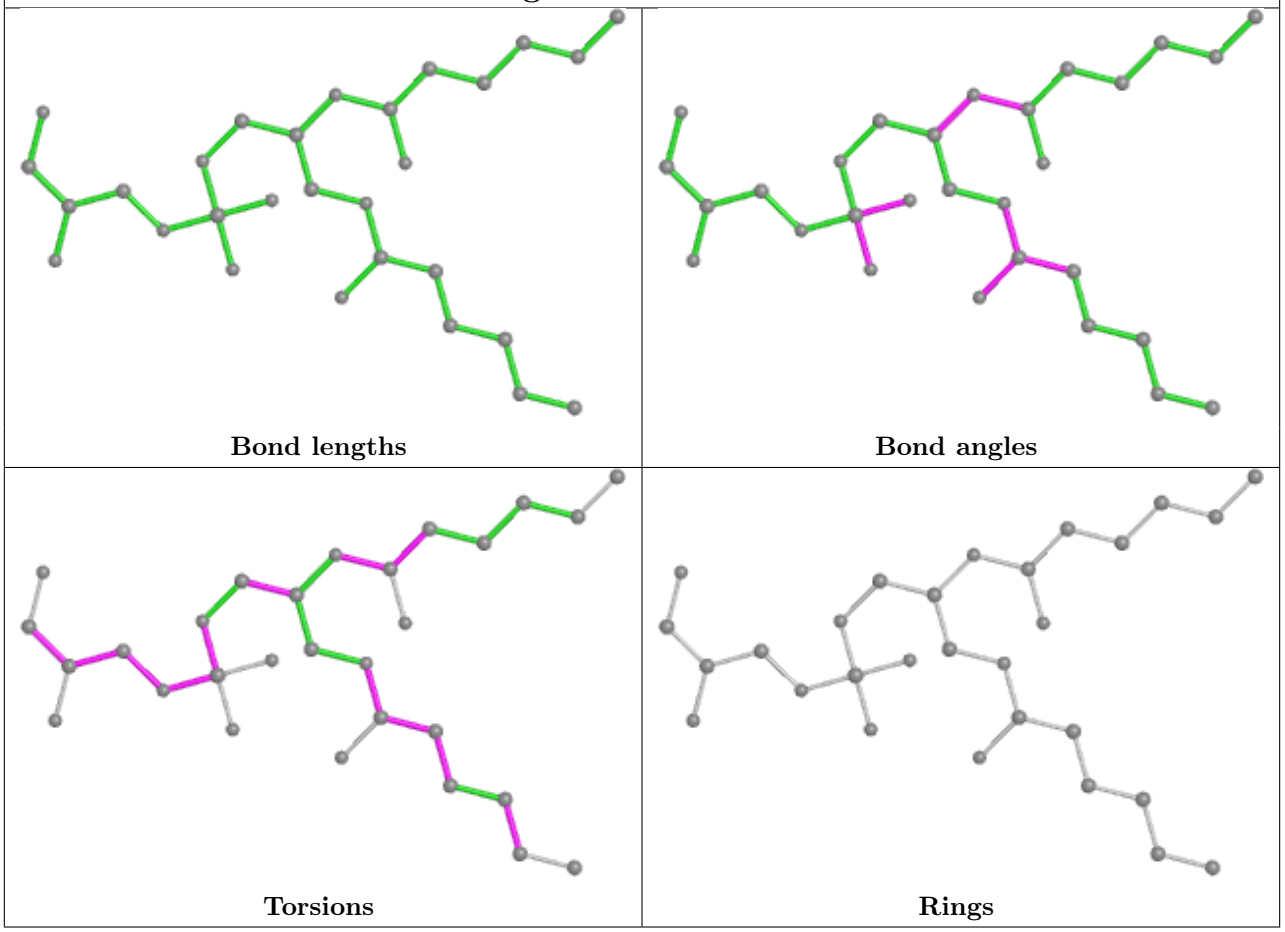


Torsions



Rings

Ligand LHG D 601



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.

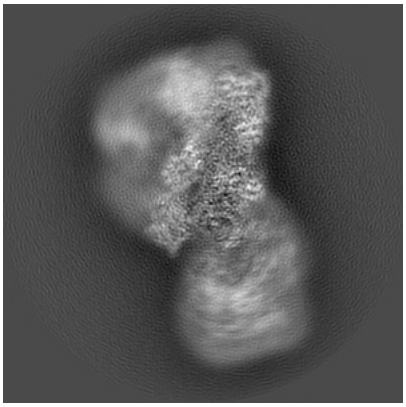
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32464. These allow visual inspection of the internal detail of the map and identification of artifacts.

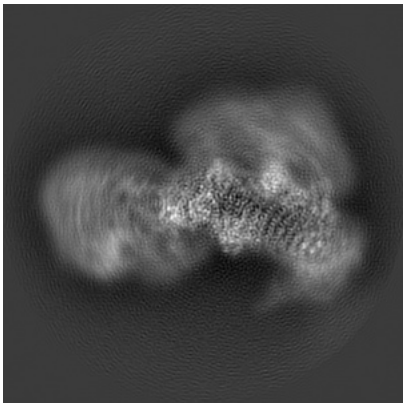
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

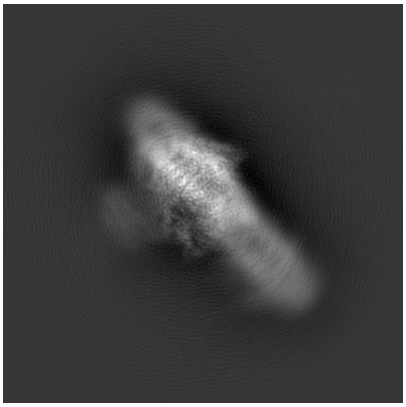
6.1.1 Primary map



X



Y

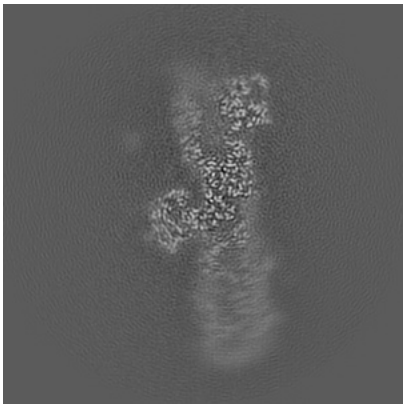


Z

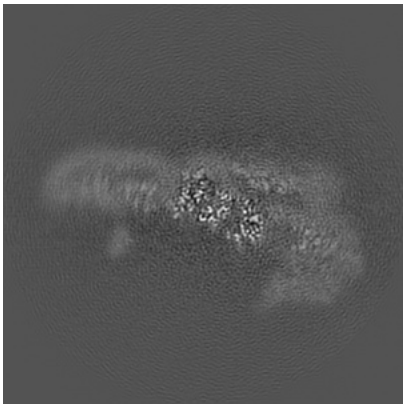
The images above show the map projected in three orthogonal directions.

6.2 Central slices

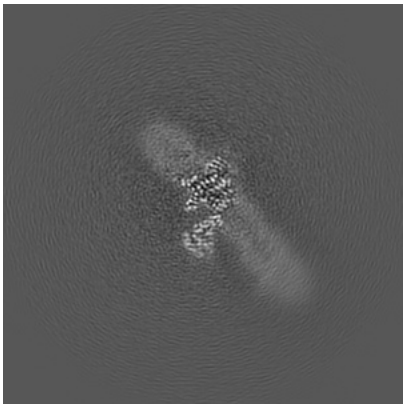
6.2.1 Primary map



X Index: 200



Y Index: 200

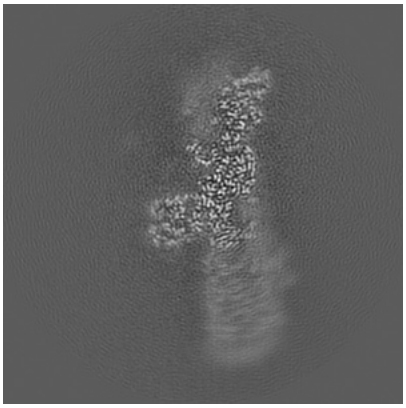


Z Index: 200

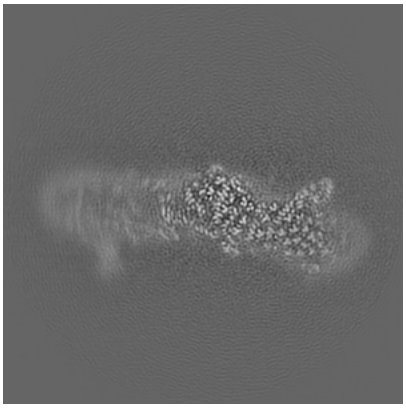
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

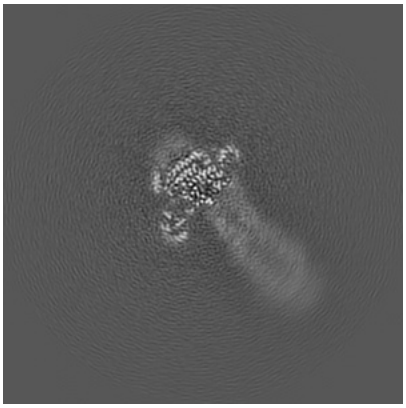
6.3.1 Primary map



X Index: 192



Y Index: 227

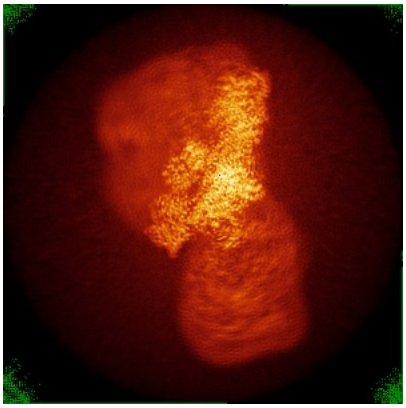


Z Index: 223

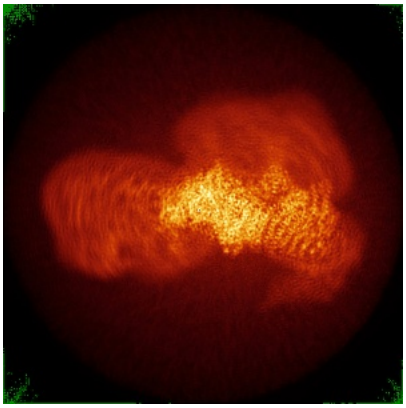
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

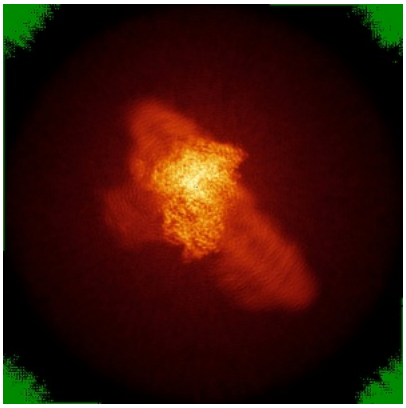
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

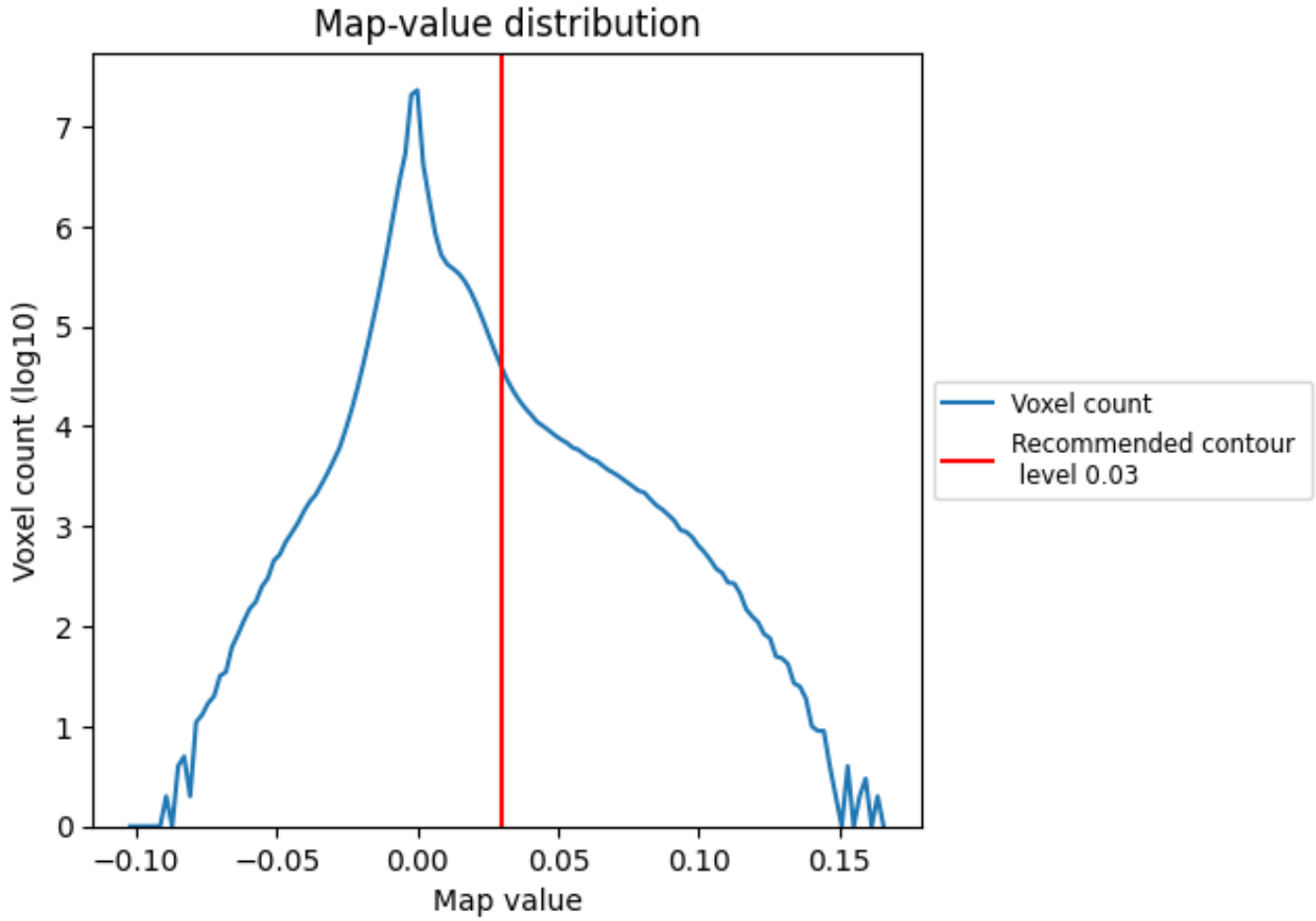
6.6 Mask visualisation (i)

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

7 Map analysis

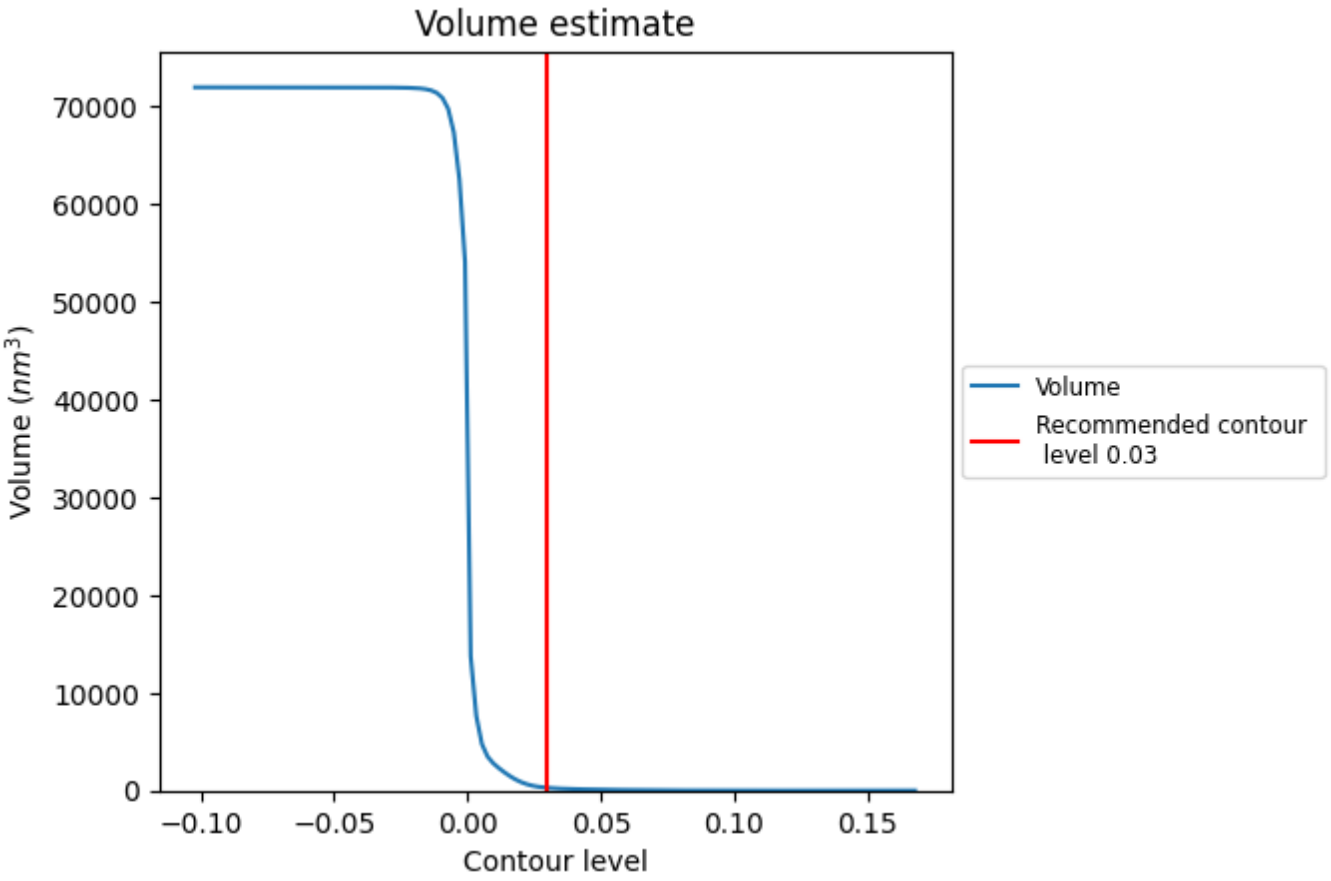
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

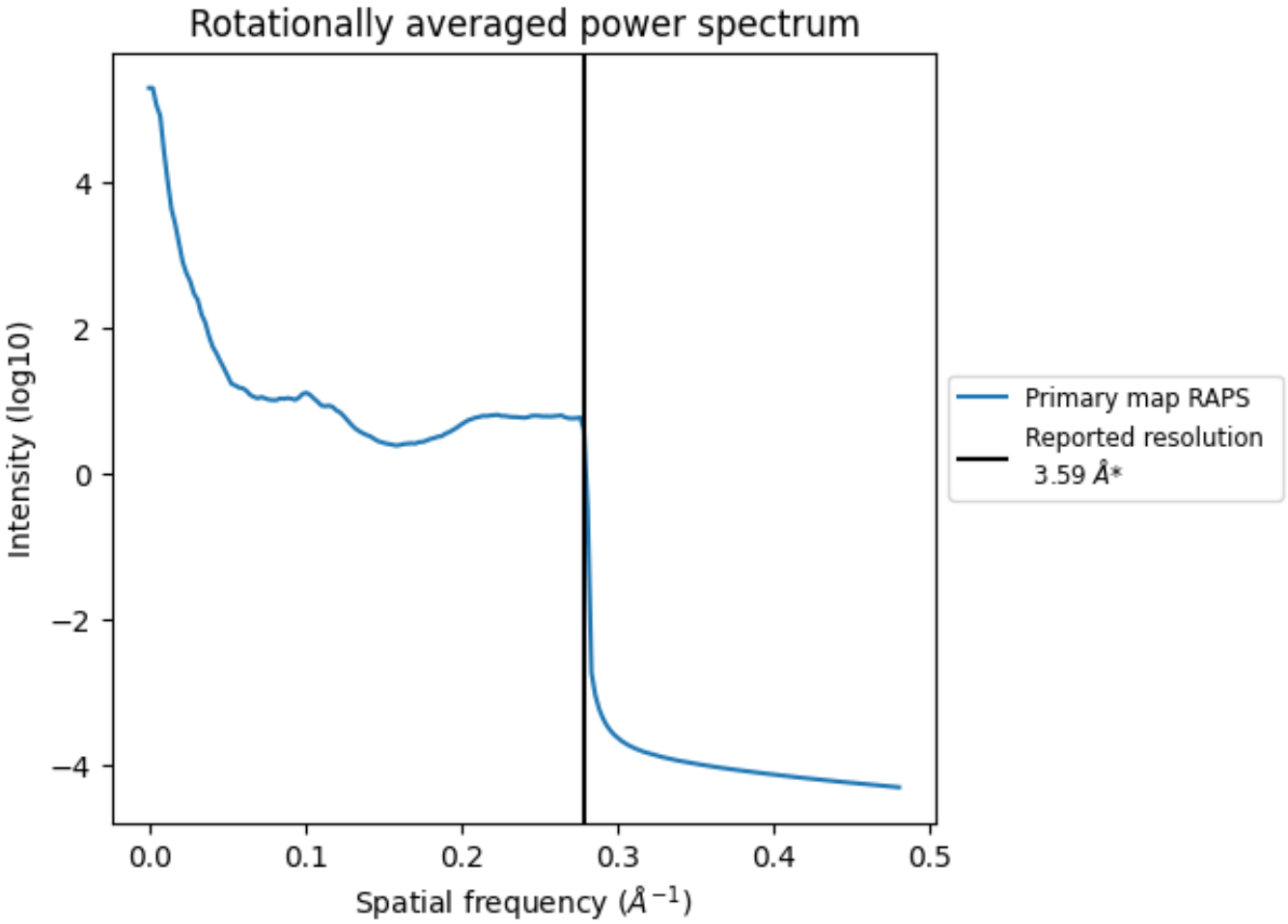
7.2 Volume estimate



The volume at the recommended contour level is 283 nm^3; this corresponds to an approximate mass of 256 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

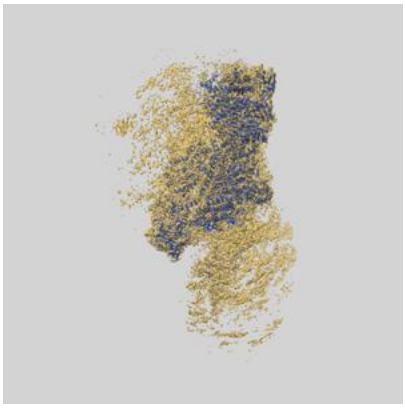
8 Fourier-Shell correlation (i)

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

9 Map-model fit

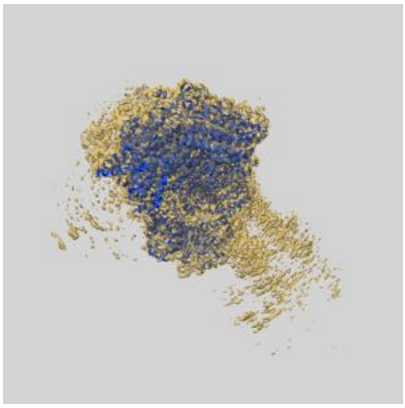
This section contains information regarding the fit between EMDB map EMD-32464 and PDB model 7WFF. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay



X

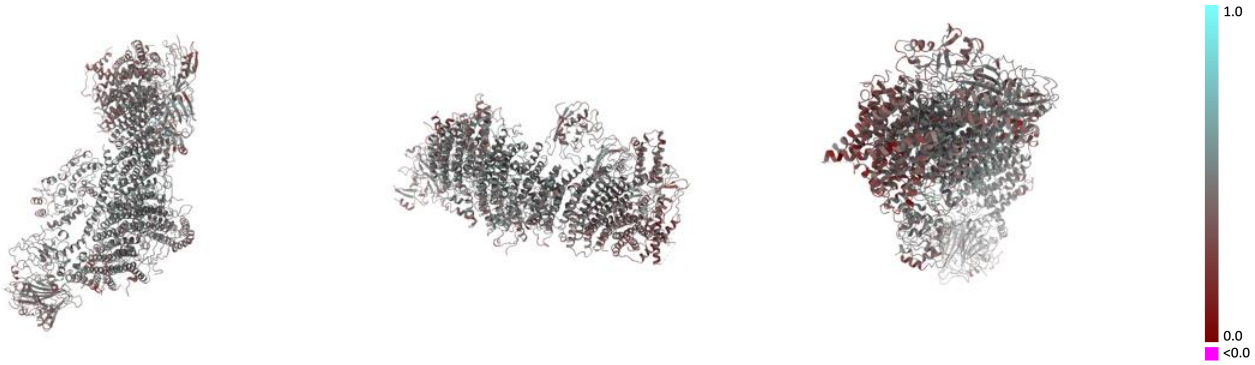
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

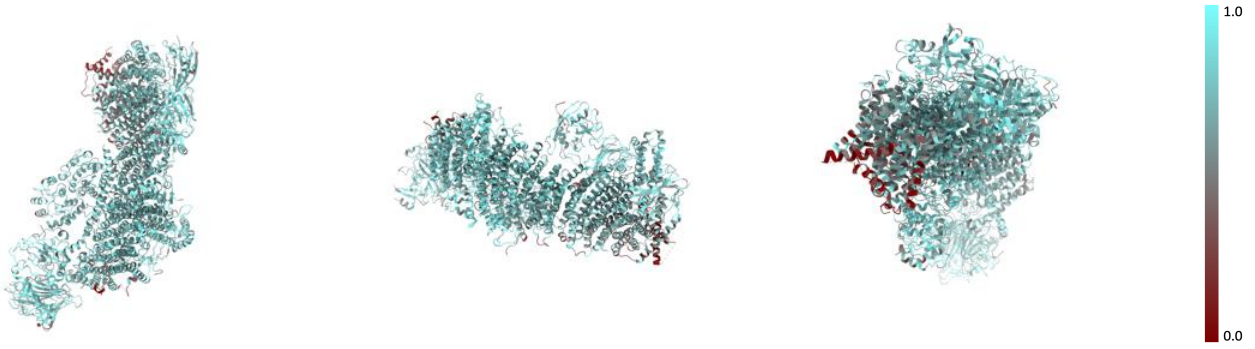
9.2 Q-score mapped to coordinate model



X Y Z

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

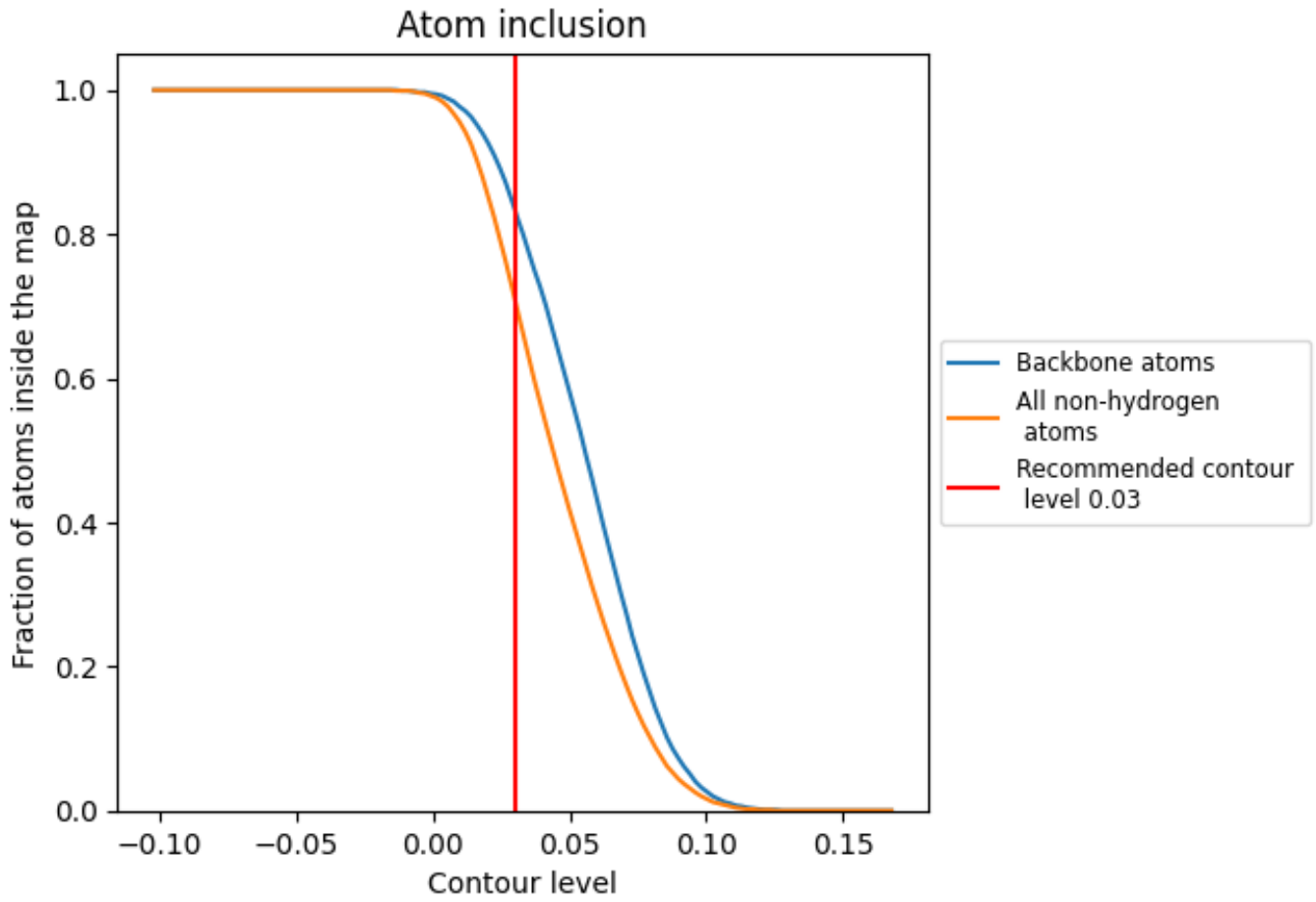
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 71% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.4430
A	0.4970	0.3430
B	0.6970	0.4580
C	0.5580	0.3750
D	0.7700	0.4900
E	0.6520	0.4180
F	0.7370	0.4630
G	0.6350	0.4290
a	0.7430	0.4510
b	0.7220	0.4180
c	0.7460	0.4640
d	0.7340	0.4610
e	0.7430	0.4500
f	0.7180	0.4010
g	0.7410	0.4110
h	0.7770	0.4480
i	0.7640	0.4760
j	0.7100	0.4410