wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 02:14 AM JST

PDB ID	:	6KHJ / pdb_00006khj
EMDB ID	:	EMD-9990
Title	:	Supercomplex for electron transfer
Authors	:	Pan, X.; Cao, D.; Xie, F.; Zhang, X.; Li, M.
Deposited on	:	2019-07-15
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

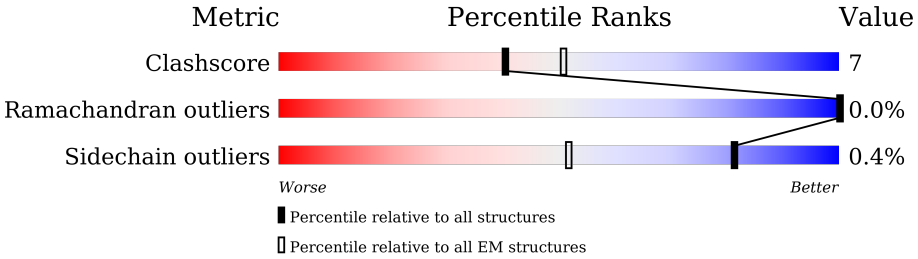
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

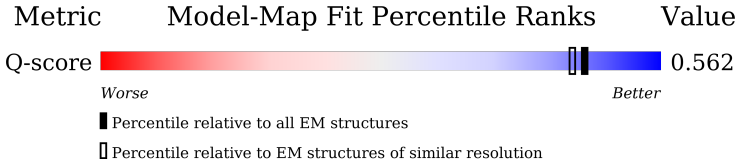
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	372	6% 84% 15% ••
2	B	515	• 80% 14% 5%
3	C	132	8% 71% 20% 9%
4	D	529	• 78% 17% 5%

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Mol	Chain	Length	Quality of chain
5	E	101	85% 15%
6	F	656	82% 16%
7	G	200	8% 72% 13% 15%
8	H	394	5% 78% 22%
9	I	196	17% 71% 24%
10	J	168	7% 79% 14% 6%
11	K	237	11% 63% 23% 14%
12	L	76	11% 87% 9%
13	M	111	7% 82% 18%
14	N	150	74% 23%
15	O	70	7% 86% 11%
16	P	44	82% 11% 7%
17	Q	45	11% 89% 9%
18	S	110	54% 47% 7% 45%

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
23	BCR	D	602	-	X	-	-
23	BCR	F	701	-	X	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 31027 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
			Total	C	N	O	S		
1	A	369	2843	1908	441	483	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	488	3697	2454	574	653	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	120	971	665	149	153	4	0	0

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	504	3896	2614	605	655	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	101	783	517	128	134	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	639	4933	3278	778	840	37	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	170	1286	860	201	220	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	393	3177	2048	545	565	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	189	1516	967	260	276	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	158	1292	825	220	242	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	204	1584	1016	274	281	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	73	590	406	90	93	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	111	885	551	161	171	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	145	1148	747	198	202	1	0	0

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

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

- Molecule 16 is a protein called proton-translocating NADH-quinone dehydrogenase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	41	321	212	52	55	2	0	0

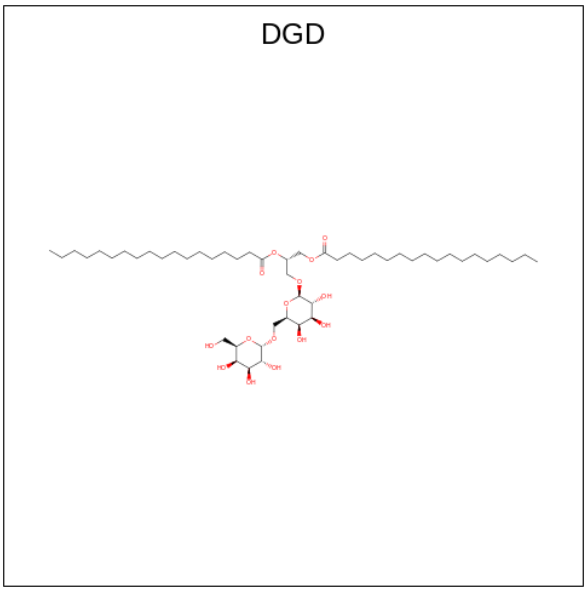
- Molecule 17 is a protein called proton-translocating NADH-quinone dehydrogenase subunit Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	44	333	222	53	56	2	0	0

- Molecule 18 is a protein called Tlr0636 protein.

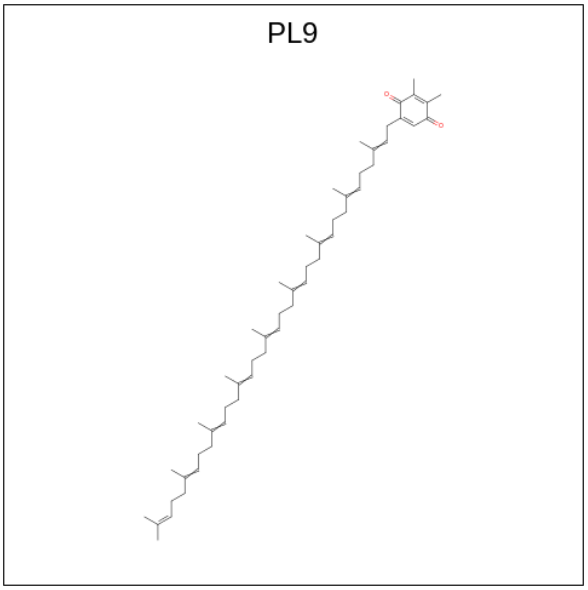
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	60	469	304	74	89	2	0	0

- Molecule 19 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



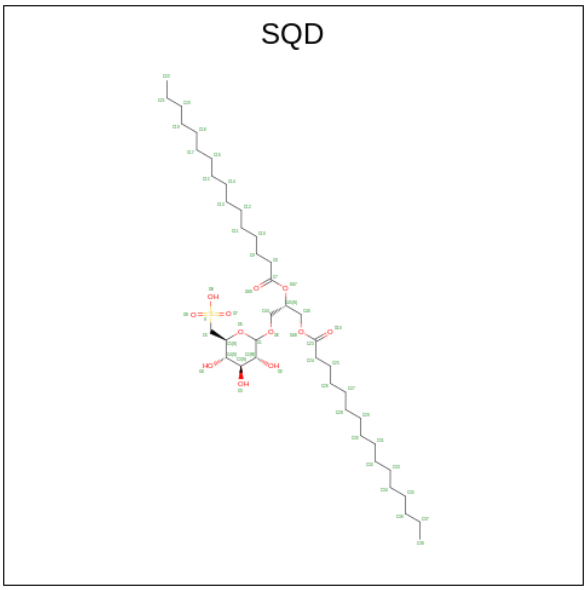
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
19	A	1	55	40	15	0
			Total	C	O	
19	A	1	62	47	15	0

- Molecule 20 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



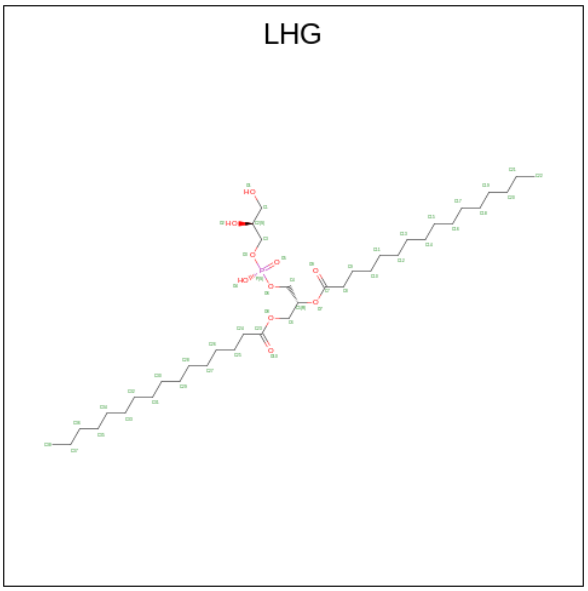
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	A	1	19	17	2	0

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



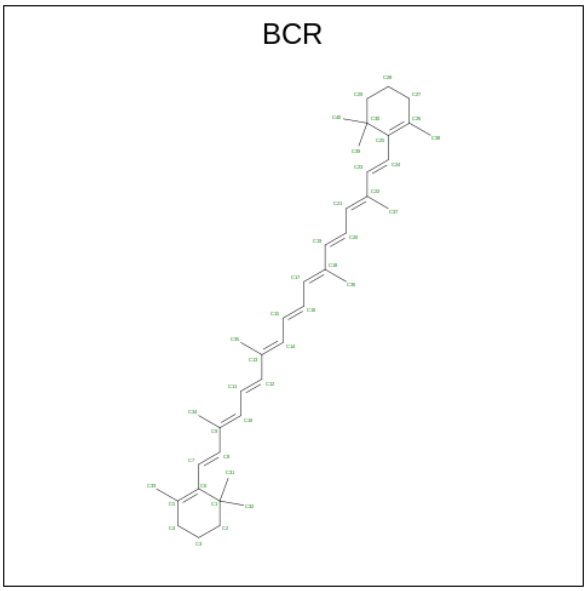
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
21	B	1	54	41	12	1	0
			Total	C	O	S	
21	C	1	40	27	12	1	0
			Total	C	O	S	
21	N	1	38	25	12	1	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



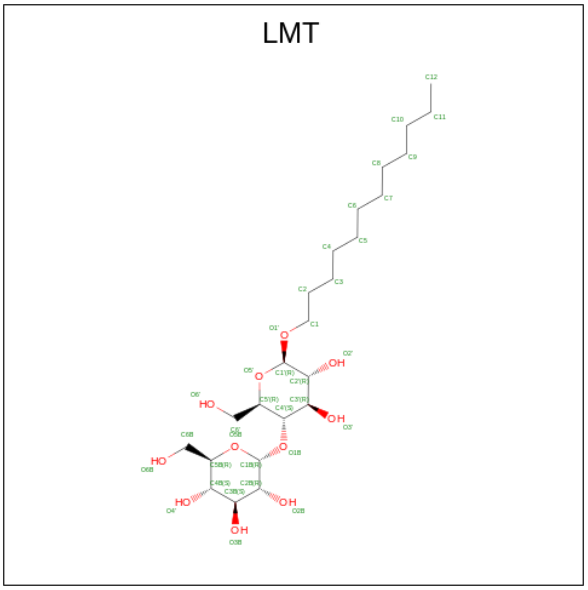
Mol	Chain	Residues	Atoms				AltConf
22	C	1	Total	C	O	P	0
			43	32	10	1	
22	D	1	Total	C	O	P	0
			46	35	10	1	
22	F	1	Total	C	O	P	0
			49	38	10	1	
22	F	1	Total	C	O	P	0
			45	34	10	1	
22	F	1	Total	C	O	P	0
			44	33	10	1	
22	I	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C		
23	D	1	40	40		0
			Total	C		
23	F	1	40	40		0

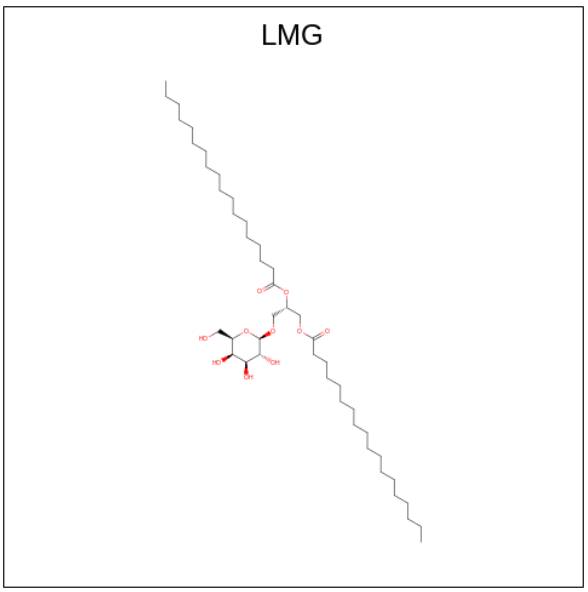
- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	D	1	35	24	11	0

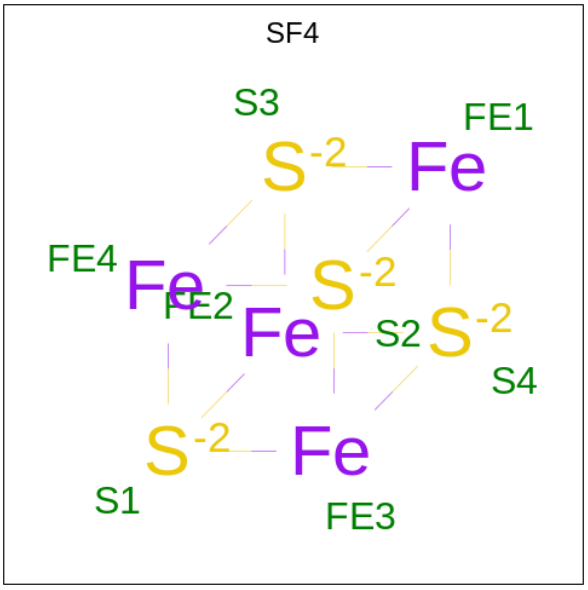
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	F	1	47	37	10	0
			Total	C	O	
25	F	1	40	30	10	0

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



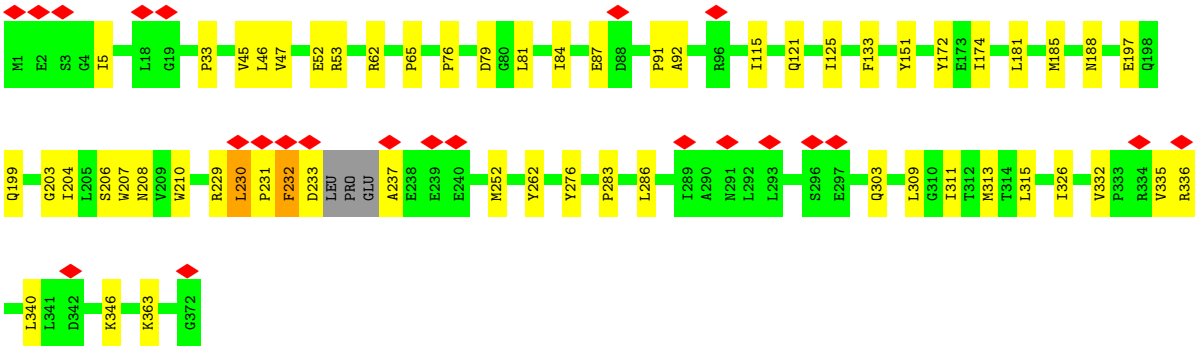
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
26	I	1	8	4	4	0
			Total	Fe	S	
26	I	1	8	4	4	0
			Total	Fe	S	
26	K	1	8	4	4	0

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.

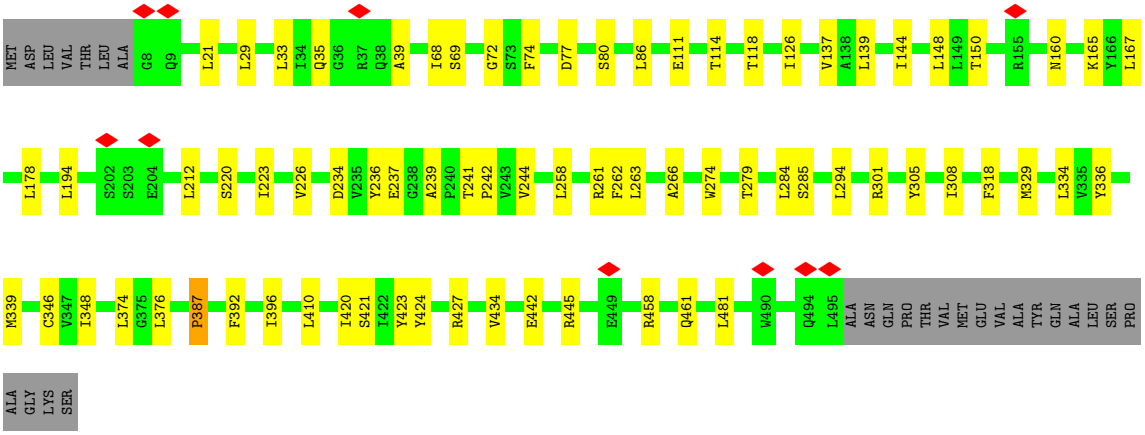
- Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1

Chain A:



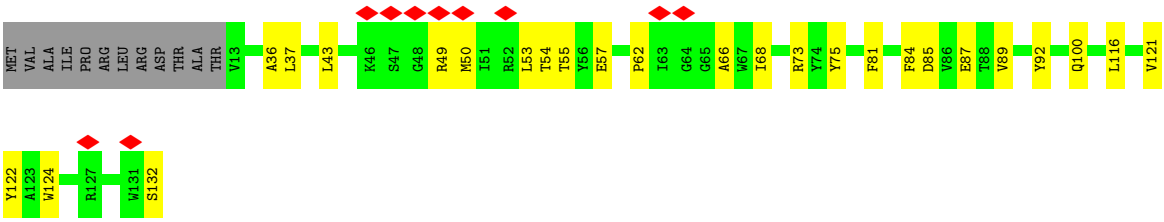
- Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2

Chain B:



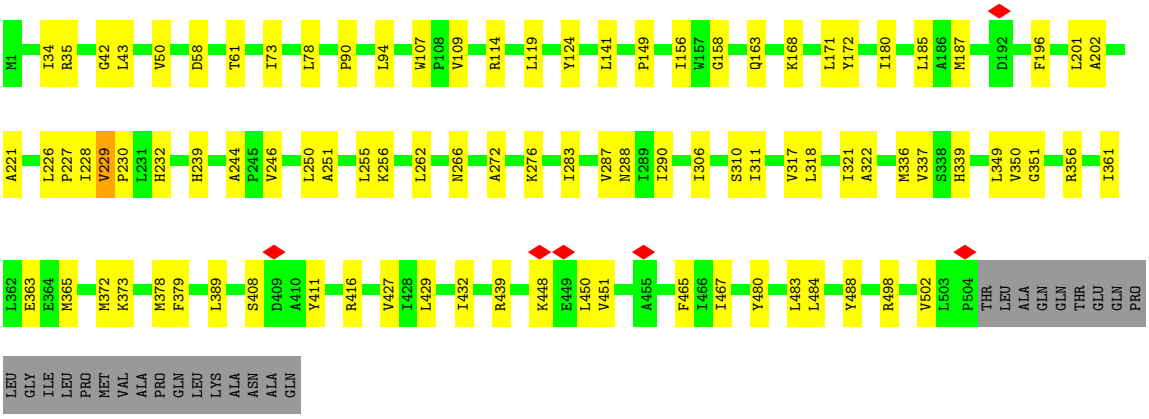
- Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3

Chain C:



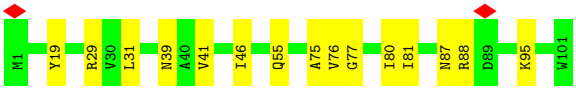
• Molecule 4: NAD(P)H-quinone oxidoreductase chain 4 1

Chain D:



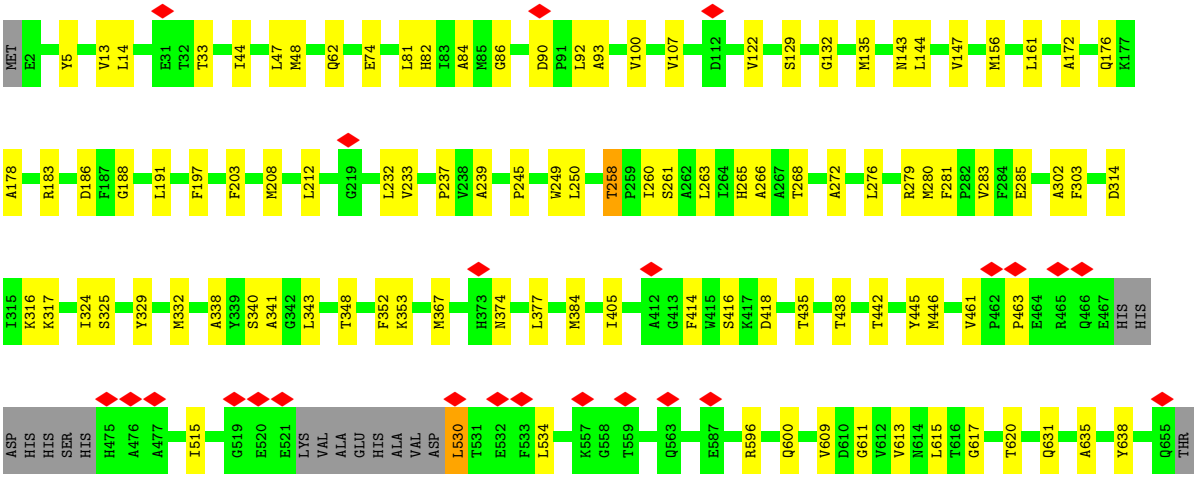
• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L

Chain E:



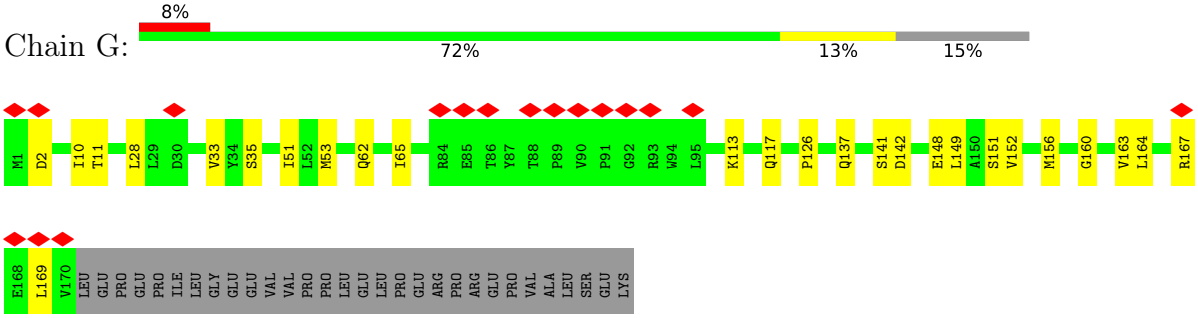
• Molecule 6: NADH dehydrogenase subunit 5

Chain F:



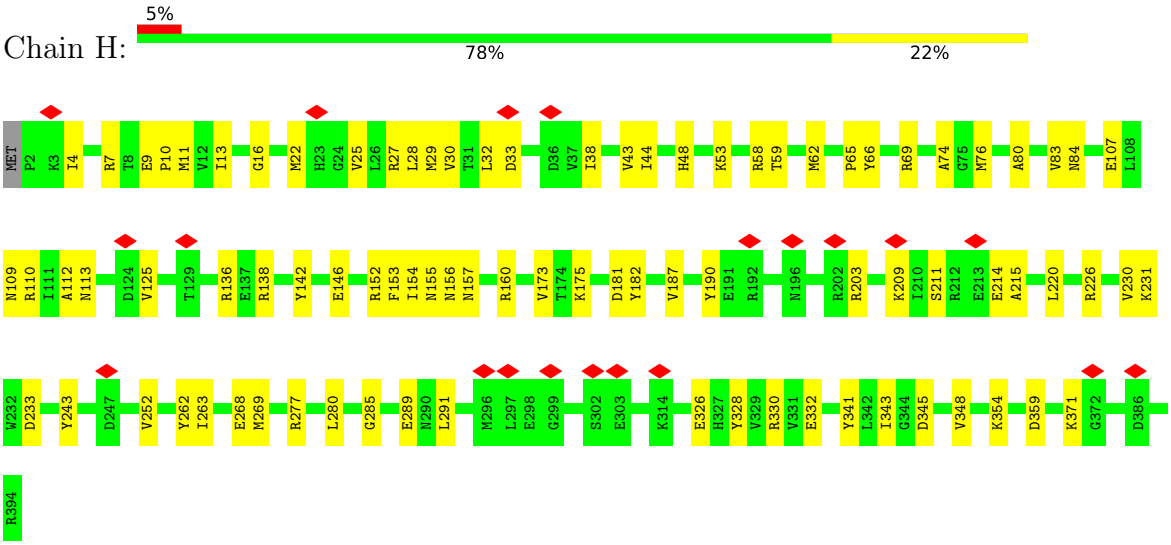
- Molecule 7: NADH-quinone oxidoreductase subunit J

Chain G:



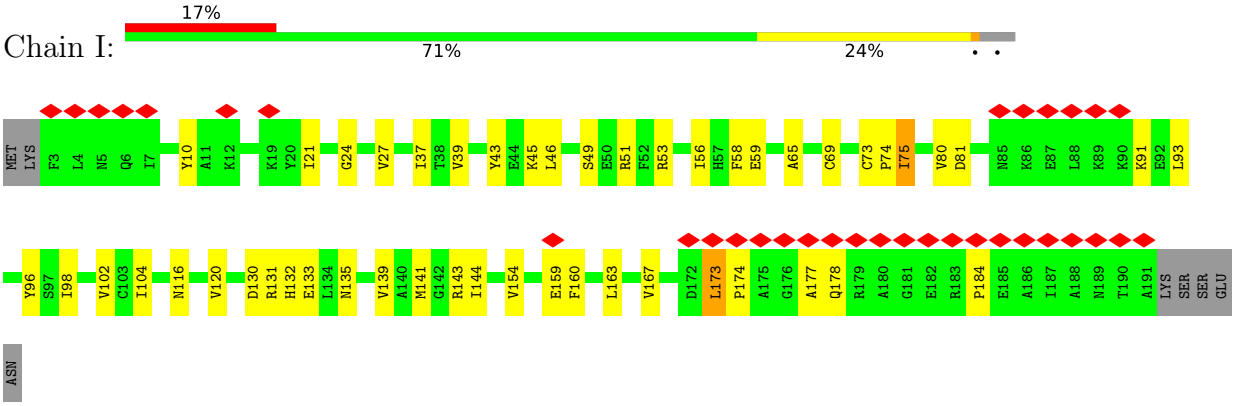
- Molecule 8: NAD(P)H-quinone oxidoreductase subunit H

Chain H:



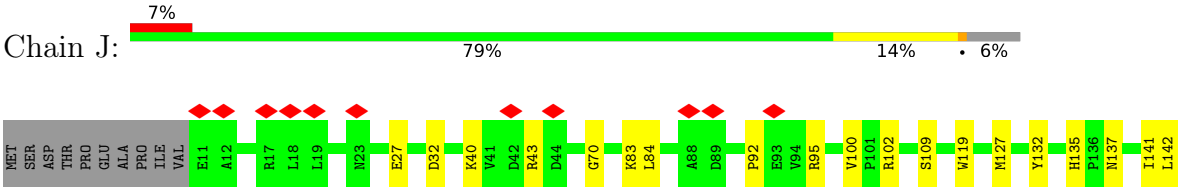
- Molecule 9: NAD(P)H-quinone oxidoreductase subunit I

Chain I:

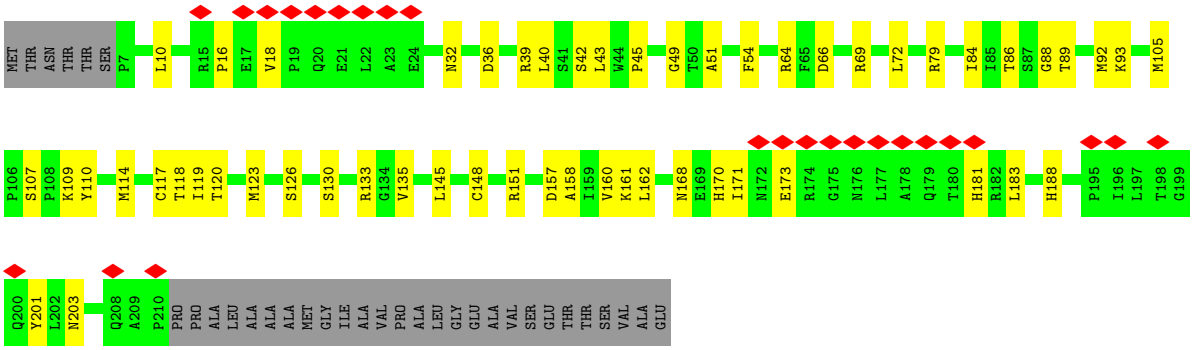


- Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

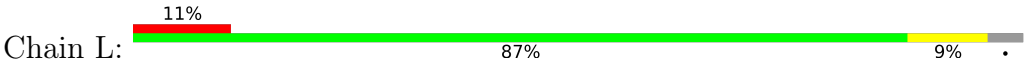
Chain J:

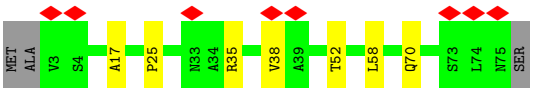


• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K

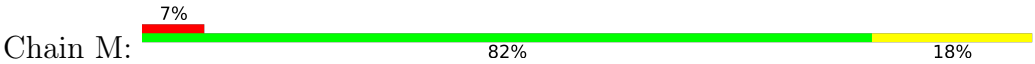


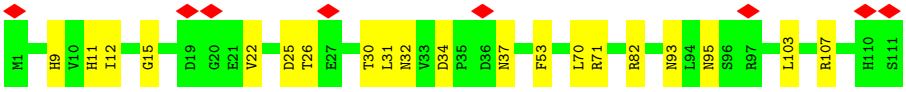
• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L



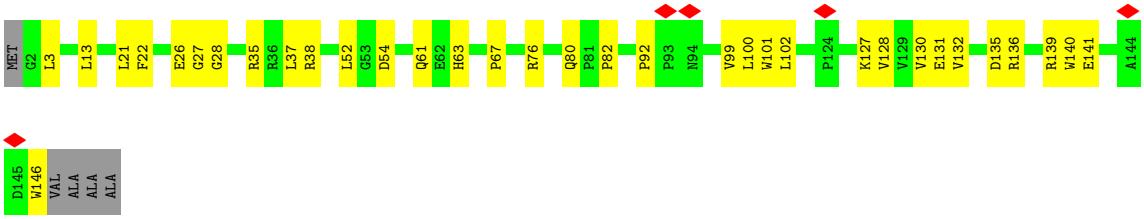


• Molecule 13: NAD(P)H-quinone oxidoreductase subunit M

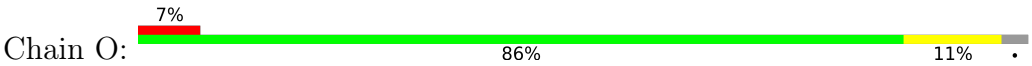


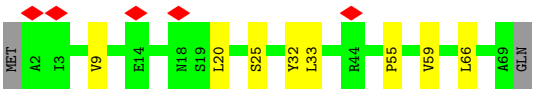


• Molecule 14: NAD(P)H-quinone oxidoreductase subunit N



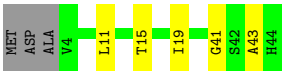
• Molecule 15: NAD(P)H-quinone oxidoreductase subunit O





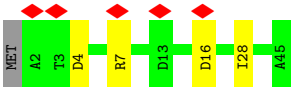
• Molecule 16: proton-translocating NADH-quinone dehydrogenase subunit P

Chain P: 82% 11% 7%



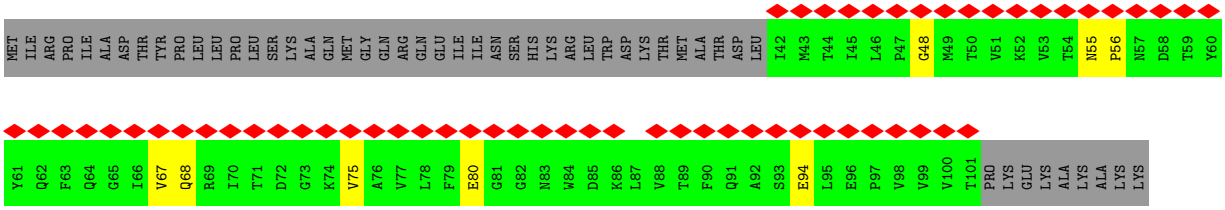
• Molecule 17: proton-translocating NADH-quinone dehydrogenase subunit Q

Chain Q: 11% 89% 9%



• Molecule 18: Tlr0636 protein

Chain S: 54% 47% 7% 45%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	187788	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.383	Depositor
Minimum map value	-0.138	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.06	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LMG, SQD, PL9, BCR, SF4, LMT, LHG

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	0.32	0/2914	0.61	0/3979
2	B	0.29	0/3783	0.57	1/5160 (0.0%)
3	C	0.27	0/1001	0.56	0/1365
4	D	0.30	0/4003	0.53	0/5462
5	E	0.26	0/793	0.50	0/1077
6	F	0.27	0/5076	0.55	2/6914 (0.0%)
7	G	0.25	0/1312	0.50	0/1796
8	H	0.29	0/3260	0.55	1/4417 (0.0%)
9	I	0.35	1/1554 (0.1%)	0.59	2/2108 (0.1%)
10	J	0.26	0/1328	0.50	0/1808
11	K	0.33	0/1624	0.66	2/2209 (0.1%)
12	L	0.25	0/610	0.61	0/835
13	M	0.26	0/901	0.57	0/1222
14	N	0.26	0/1180	0.59	0/1604
15	O	0.24	0/550	0.52	0/748
16	P	0.35	0/330	0.53	0/448
17	Q	0.23	0/342	0.44	0/466
18	S	0.17	0/478	0.48	0/652
All	All	0.29	1/31039 (0.0%)	0.56	8/42270 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	174	PRO	C-N	-8.12	1.23	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	530	LEU	CA-C-N	6.03	133.05	121.54
6	F	530	LEU	C-N-CA	6.03	133.05	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	49	GLY	CA-C-N	5.64	136.43	126.45
11	K	49	GLY	C-N-CA	5.64	136.43	126.45
2	B	387	PRO	N-CA-C	5.57	117.49	110.70

There are no chirality outliers.

There are no planarity outliers.

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	A	2843	0	2970	58	0
2	B	3697	0	3829	50	0
3	C	971	0	1001	24	0
4	D	3896	0	4042	65	0
5	E	783	0	837	13	0
6	F	4933	0	4981	65	0
7	G	1286	0	1372	22	0
8	H	3177	0	3157	64	0
9	I	1516	0	1482	38	0
10	J	1292	0	1244	19	0
11	K	1584	0	1617	48	0
12	L	590	0	603	5	0
13	M	885	0	865	14	0
14	N	1148	0	1157	26	0
15	O	538	0	549	7	0
16	P	321	0	317	5	0
17	Q	333	0	333	4	0
18	S	469	0	473	5	0
19	A	117	0	156	5	0
20	A	19	0	21	4	0
21	B	54	0	78	6	0
21	C	40	0	44	1	0
21	N	38	0	40	2	0
22	C	43	0	59	2	0
22	D	46	0	62	1	0
22	F	138	0	198	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	I	44	0	61	1	0
23	D	40	0	56	3	0
23	F	40	0	56	4	0
24	D	35	0	45	0	0
25	F	87	0	114	1	0
26	I	16	0	0	2	0
26	K	8	0	0	0	0
All	All	31027	0	31819	439	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 7.

The worst 5 of 439 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:230:LEU:HB3	1:A:231:PRO:CD	1.61	1.30
1:A:230:LEU:CB	1:A:231:PRO:HD2	1.65	1.26
1:A:231:PRO:HD3	1:A:332:VAL:HG21	1.24	1.14
1:A:231:PRO:HD3	1:A:332:VAL:CG2	1.85	1.05
1:A:231:PRO:CD	1:A:332:VAL:HG21	1.99	0.92

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	365/372 (98%)	341 (93%)	23 (6%)	1 (0%)	36 70
2	B	486/515 (94%)	456 (94%)	30 (6%)	0	100 100
3	C	118/132 (89%)	110 (93%)	8 (7%)	0	100 100
4	D	502/529 (95%)	485 (97%)	17 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
6	F	633/656 (96%)	580 (92%)	53 (8%)	0	100	100
7	G	168/200 (84%)	155 (92%)	13 (8%)	0	100	100
8	H	391/394 (99%)	347 (89%)	44 (11%)	0	100	100
9	I	187/196 (95%)	166 (89%)	21 (11%)	0	100	100
10	J	156/168 (93%)	141 (90%)	15 (10%)	0	100	100
11	K	202/237 (85%)	187 (93%)	15 (7%)	0	100	100
12	L	71/76 (93%)	61 (86%)	10 (14%)	0	100	100
13	M	109/111 (98%)	92 (84%)	17 (16%)	0	100	100
14	N	143/150 (95%)	126 (88%)	17 (12%)	0	100	100
15	O	66/70 (94%)	63 (96%)	3 (4%)	0	100	100
16	P	39/44 (89%)	36 (92%)	3 (8%)	0	100	100
17	Q	42/45 (93%)	41 (98%)	1 (2%)	0	100	100
18	S	58/110 (53%)	56 (97%)	2 (3%)	0	100	100
All	All	3835/4106 (93%)	3533 (92%)	301 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	LEU

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	298/302 (99%)	296 (99%)	2 (1%)	76	86
2	B	392/413 (95%)	392 (100%)	0	100	100
3	C	99/109 (91%)	98 (99%)	1 (1%)	68	84
4	D	403/424 (95%)	402 (100%)	1 (0%)	87	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	82/82 (100%)	82 (100%)	0	100	100
6	F	511/527 (97%)	510 (100%)	1 (0%)	87	92
7	G	138/166 (83%)	137 (99%)	1 (1%)	76	86
8	H	337/338 (100%)	335 (99%)	2 (1%)	78	88
9	I	165/172 (96%)	163 (99%)	2 (1%)	63	82
10	J	139/148 (94%)	138 (99%)	1 (1%)	76	86
11	K	173/196 (88%)	173 (100%)	0	100	100
12	L	61/63 (97%)	61 (100%)	0	100	100
13	M	96/96 (100%)	95 (99%)	1 (1%)	68	84
14	N	118/120 (98%)	118 (100%)	0	100	100
15	O	57/59 (97%)	57 (100%)	0	100	100
16	P	35/37 (95%)	35 (100%)	0	100	100
17	Q	31/32 (97%)	31 (100%)	0	100	100
18	S	53/97 (55%)	52 (98%)	1 (2%)	50	76
All	All	3188/3381 (94%)	3175 (100%)	13 (0%)	81	90

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	83	VAL
9	I	75	ILE
18	S	75	VAL
10	J	158	THR
13	M	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	73	GLN
13	M	59	ASN
10	J	120	GLN
11	K	203	ASN
18	S	55	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
21	SQD	N	201	-	37,38,54	2.20	11 (29%)	46,49,65	6.41	7 (15%)
19	DGD	A	402	-	63,63,67	1.22	7 (11%)	77,77,81	1.10	4 (5%)
26	SF4	K	301	11	0,12,12	-	-	-		
23	BCR	D	602	-	41,41,41	5.44	17 (41%)	56,56,56	5.57	32 (57%)
25	LMG	F	702	-	47,47,55	0.85	2 (4%)	55,55,63	1.43	9 (16%)
21	SQD	C	201	-	39,40,54	2.16	11 (28%)	48,51,65	6.13	7 (14%)
22	LHG	F	705	-	44,44,48	0.93	4 (9%)	47,50,54	1.09	2 (4%)
22	LHG	F	706	-	43,43,48	0.94	4 (9%)	46,49,54	1.05	2 (4%)
20	PL9	A	403	-	19,19,55	1.74	5 (26%)	24,25,69	1.70	7 (29%)
21	SQD	B	601	-	53,54,54	1.90	11 (20%)	62,65,65	5.64	6 (9%)
19	DGD	A	401	-	56,56,67	1.29	7 (12%)	70,70,81	1.13	3 (4%)
22	LHG	D	601	-	45,45,48	0.92	4 (8%)	48,51,54	1.08	2 (4%)
22	LHG	C	202	-	42,42,48	0.97	4 (9%)	45,48,54	1.07	2 (4%)
25	LMG	F	704	-	40,40,55	0.86	1 (2%)	48,48,63	1.27	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	LHG	I	201	-	43,43,48	0.93	3 (6%)	46,49,54	1.14	2 (4%)
24	LMT	D	603	-	36,36,36	1.16	5 (13%)	47,47,47	1.06	4 (8%)
23	BCR	F	701	-	41,41,41	5.46	17 (41%)	56,56,56	5.49	35 (62%)
26	SF4	I	202	9	0,12,12	-	-	-		
26	SF4	I	203	9	0,12,12	-	-	-		
22	LHG	F	703	-	48,48,48	0.91	4 (8%)	51,54,54	1.06	2 (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
21	SQD	N	201	-	-	19/33/53/69	0/1/1/1
19	DGD	A	402	-	-	18/51/91/95	0/2/2/2
26	SF4	K	301	11	-	-	0/6/5/5
23	BCR	D	602	-	-	16/29/63/63	0/2/2/2
25	LMG	F	702	-	-	13/42/62/70	0/1/1/1
21	SQD	C	201	-	-	24/35/55/69	0/1/1/1
22	LHG	F	705	-	-	21/49/49/53	-
22	LHG	F	706	-	-	26/48/48/53	-
20	PL9	A	403	-	-	6/10/30/73	0/1/1/1
21	SQD	B	601	-	-	23/49/69/69	0/1/1/1
19	DGD	A	401	-	-	15/44/84/95	0/2/2/2
22	LHG	D	601	-	-	15/50/50/53	-
22	LHG	C	202	-	-	19/47/47/53	-
25	LMG	F	704	-	-	14/35/55/70	0/1/1/1
22	LHG	I	201	-	-	26/48/48/53	-
24	LMT	D	603	-	-	9/21/61/61	0/2/2/2
23	BCR	F	701	-	-	14/29/63/63	0/2/2/2
26	SF4	I	202	9	-	-	0/6/5/5
26	SF4	I	203	9	-	-	0/6/5/5
22	LHG	F	703	-	-	21/53/53/53	-

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	701	BCR	C10-C9	14.86	1.55	1.35
23	D	602	BCR	C10-C9	14.81	1.55	1.35
23	F	701	BCR	C17-C18	14.30	1.54	1.35
23	F	701	BCR	C14-C13	14.27	1.54	1.35
23	D	602	BCR	C17-C18	13.75	1.54	1.35

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	601	SQD	O9-S-C6	29.43	141.92	106.94
21	C	201	SQD	O9-S-C6	29.31	141.77	106.94
21	N	201	SQD	O9-S-C6	29.18	141.61	106.94
21	B	601	SQD	O7-S-C6	-28.40	73.19	106.94
21	N	201	SQD	O7-S-C6	-27.41	74.36	106.94

There are no chirality outliers.

5 of 299 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	402	DGD	C2D-C1D-O3G-C3G
19	A	402	DGD	O6D-C1D-O3G-C3G
20	A	403	PL9	C7-C8-C9-C10
21	B	601	SQD	C2-C1-O6-C44
21	B	601	SQD	O5-C1-O6-C44

There are no ring outliers.

17 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	201	SQD	2	0
19	A	402	DGD	4	0
23	D	602	BCR	3	0
25	F	702	LMG	1	0
21	C	201	SQD	1	0
22	F	705	LHG	1	0
22	F	706	LHG	2	0
20	A	403	PL9	4	0
21	B	601	SQD	6	0
19	A	401	DGD	1	0
22	D	601	LHG	1	0
22	C	202	LHG	2	0
22	I	201	LHG	1	0

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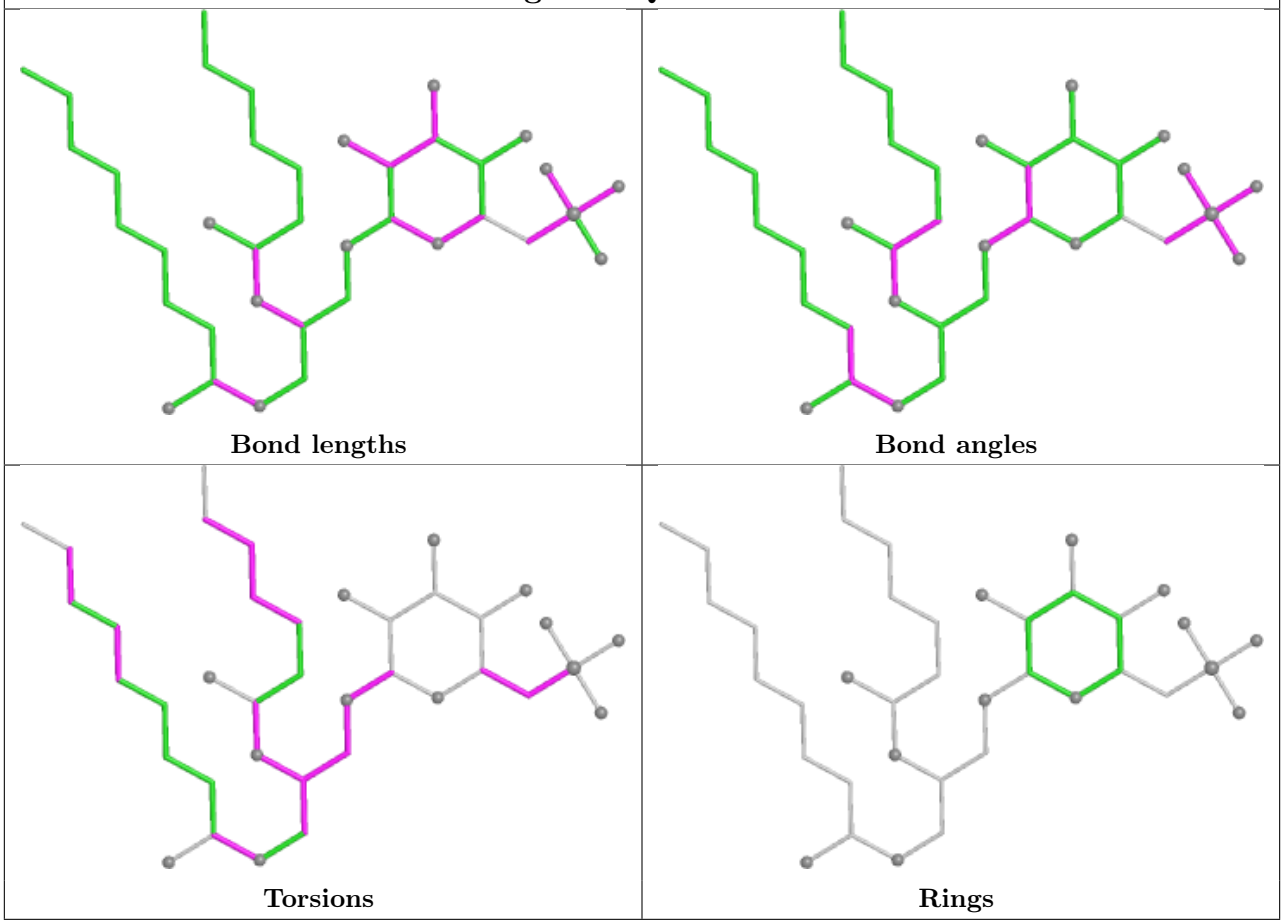
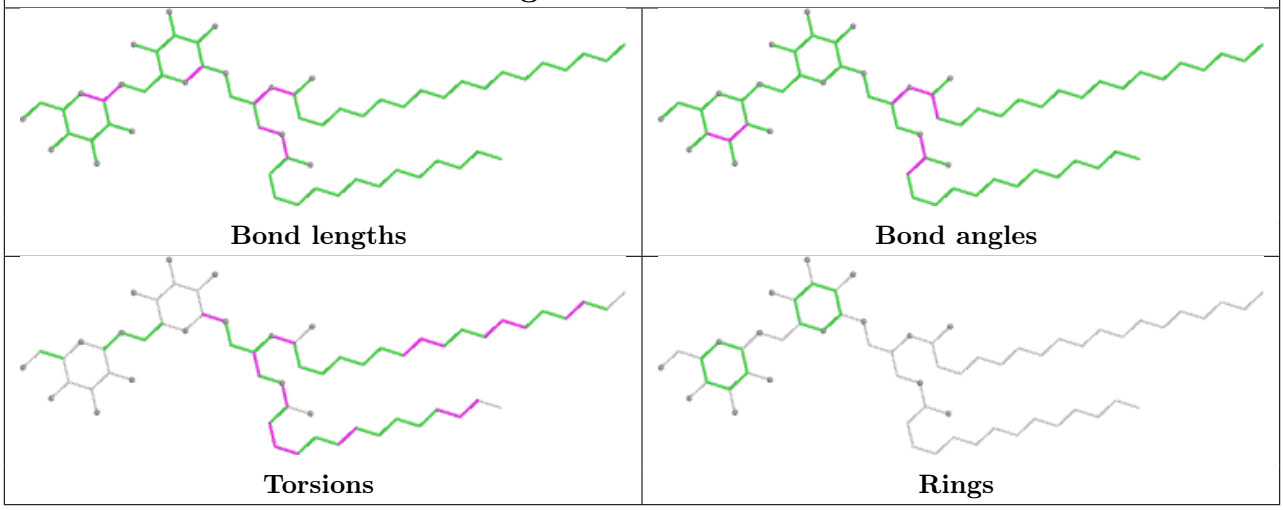
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	F	701	BCR	4	0
26	I	202	SF4	1	0
26	I	203	SF4	1	0
22	F	703	LHG	2	0

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.

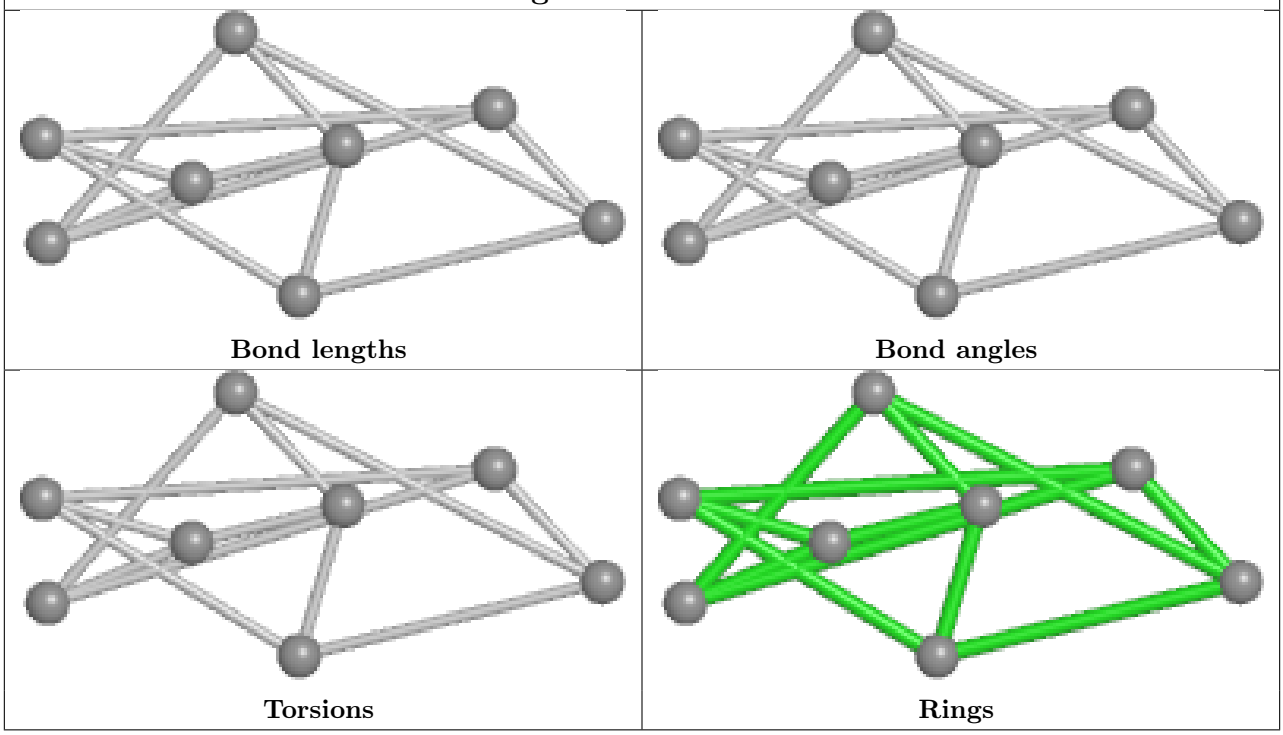
Ligand SQD N 201



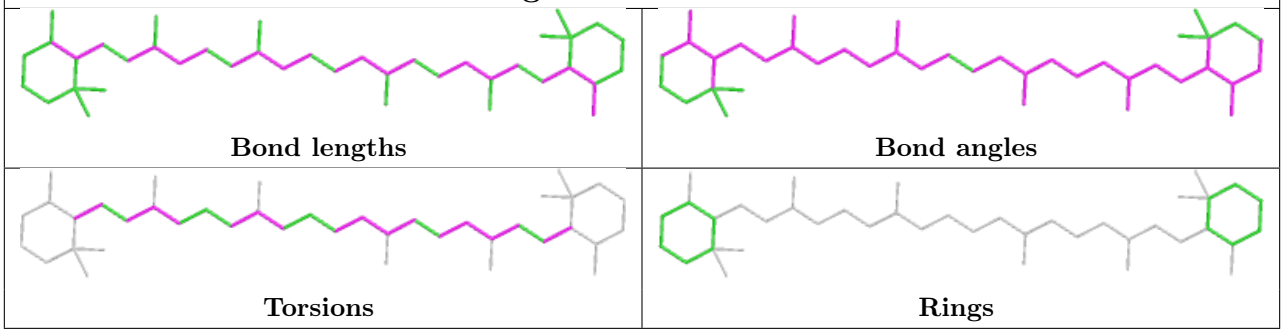
Ligand DGD A 402



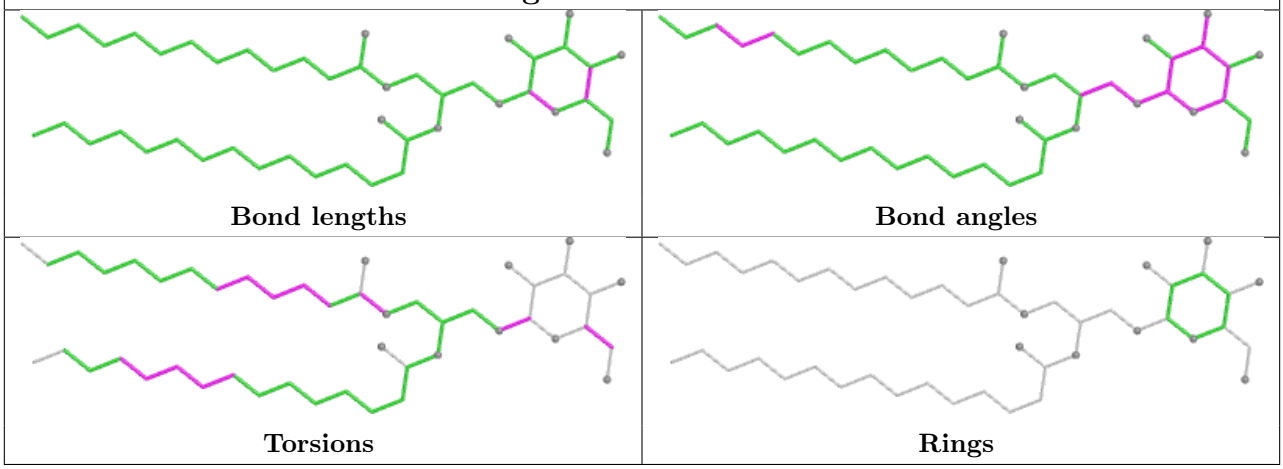
Ligand SF4 K 301



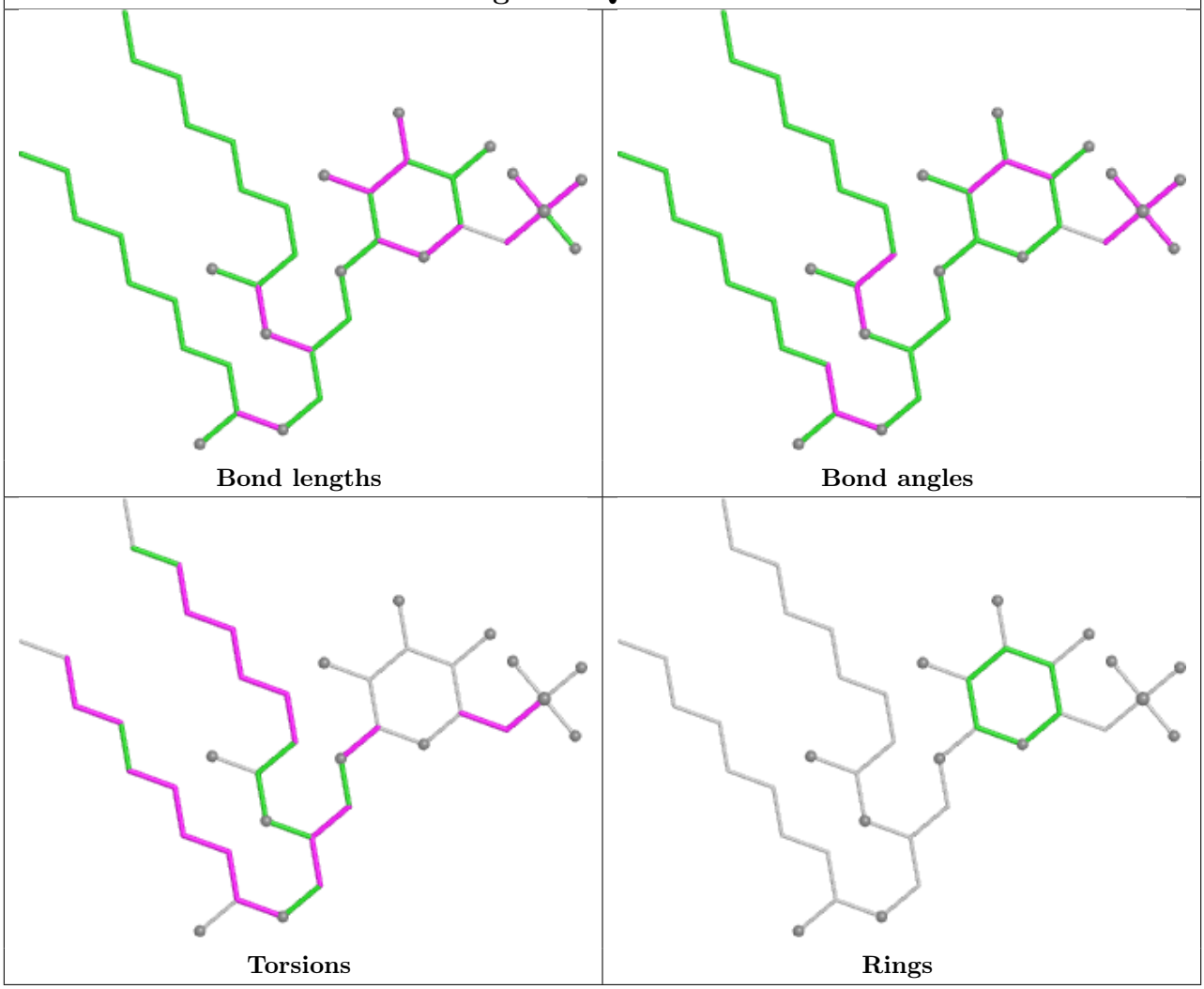
Ligand BCR D 602

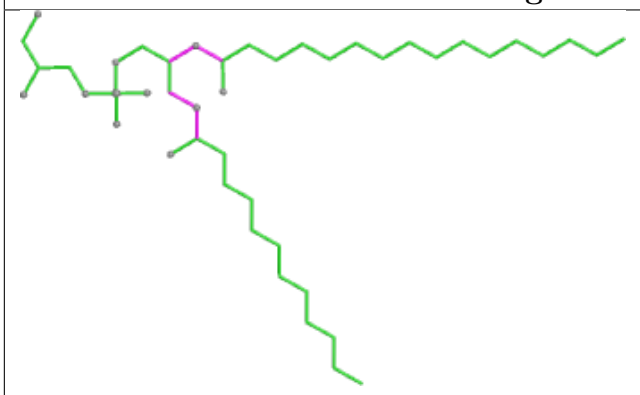
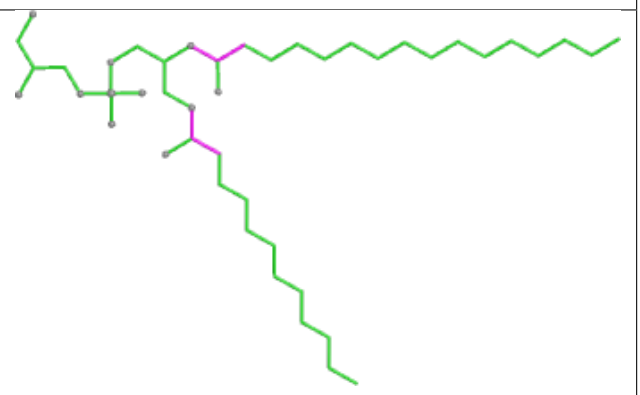
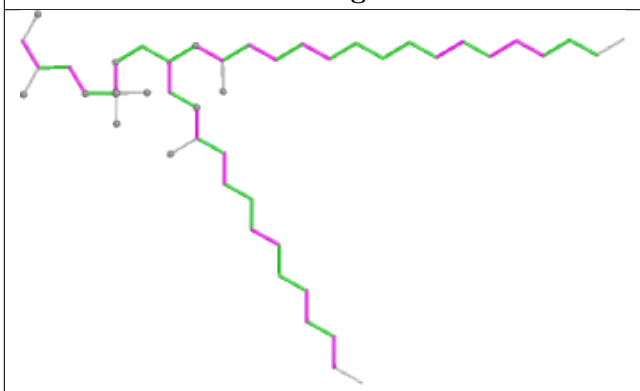
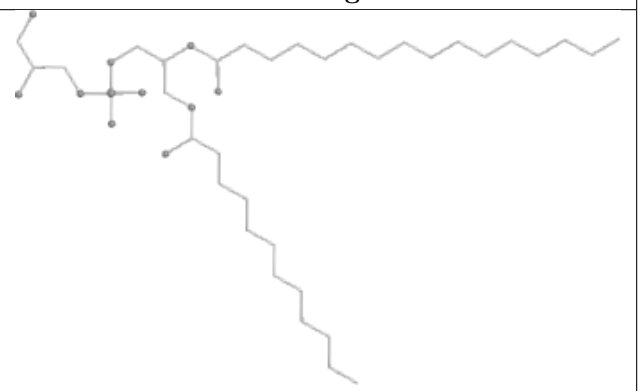


Ligand LMG F 702

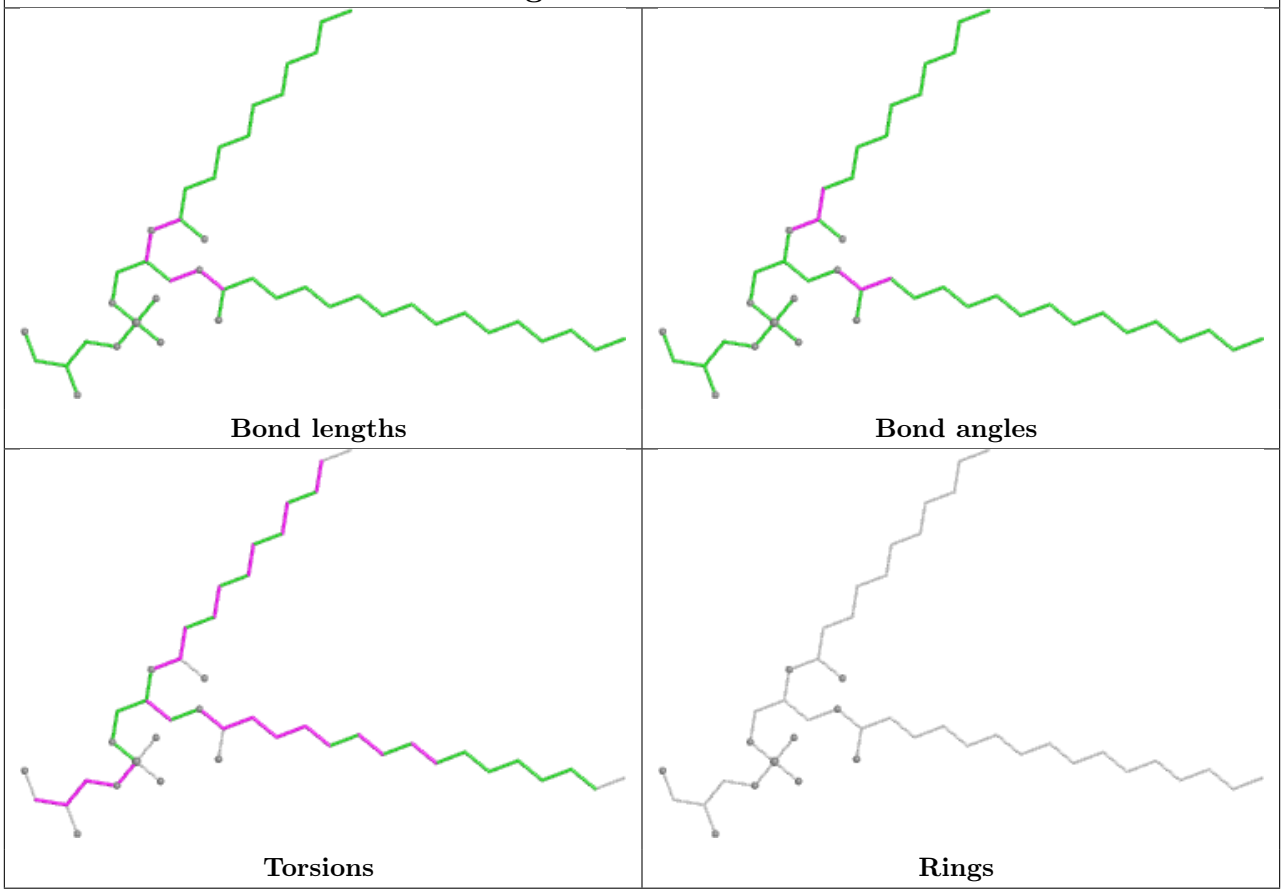


Ligand SQD C 201

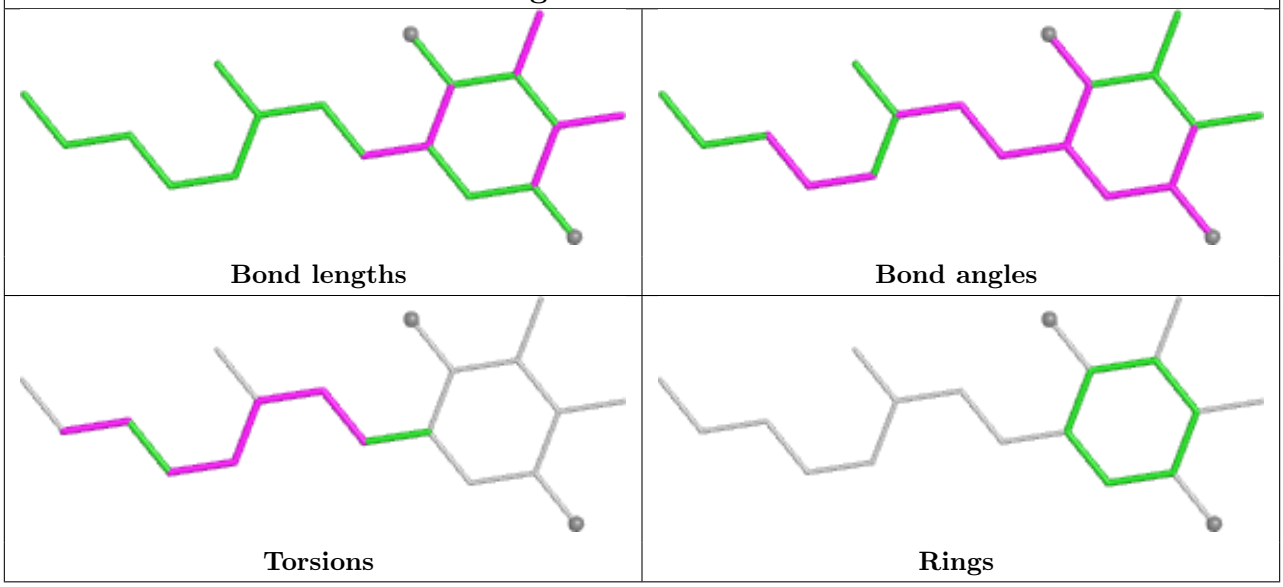


Ligand LHG F 705	
 Bond lengths	 Bond angles
 Torsions	 Rings

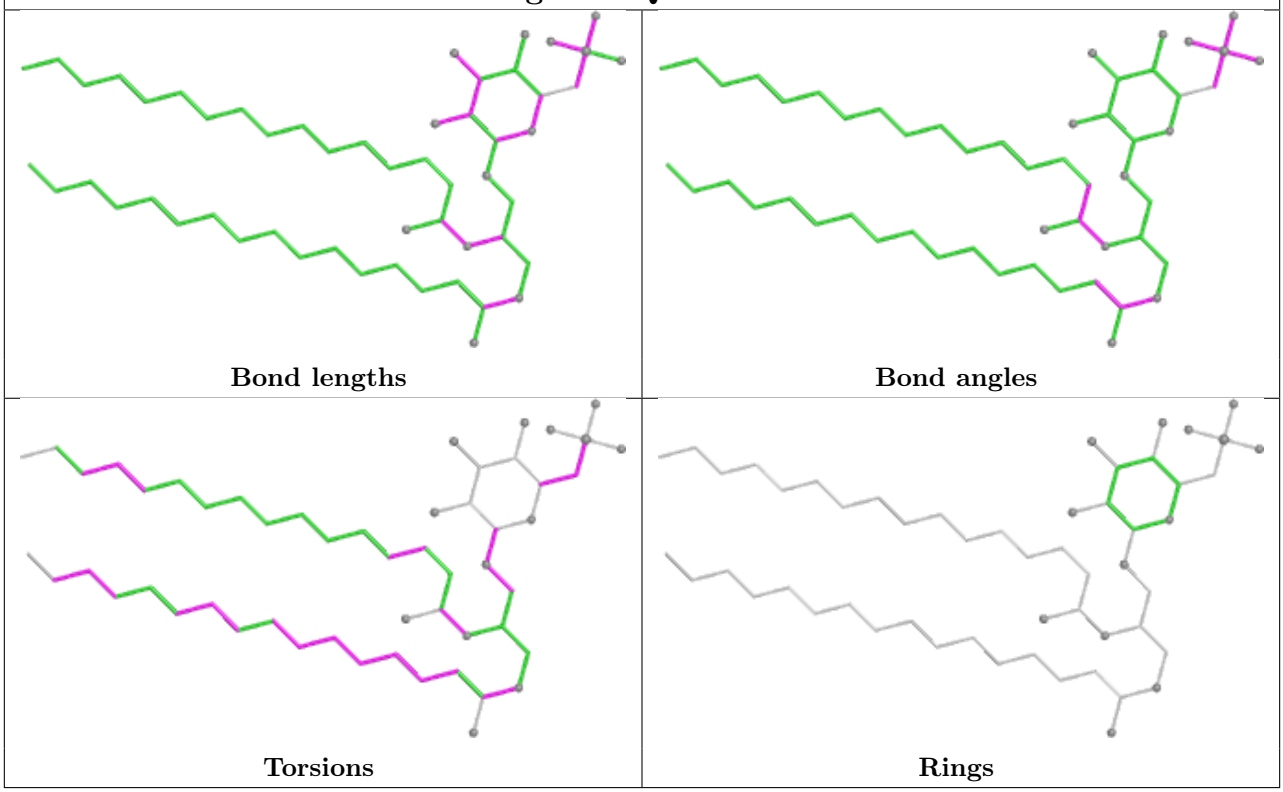
Ligand LHG F 706



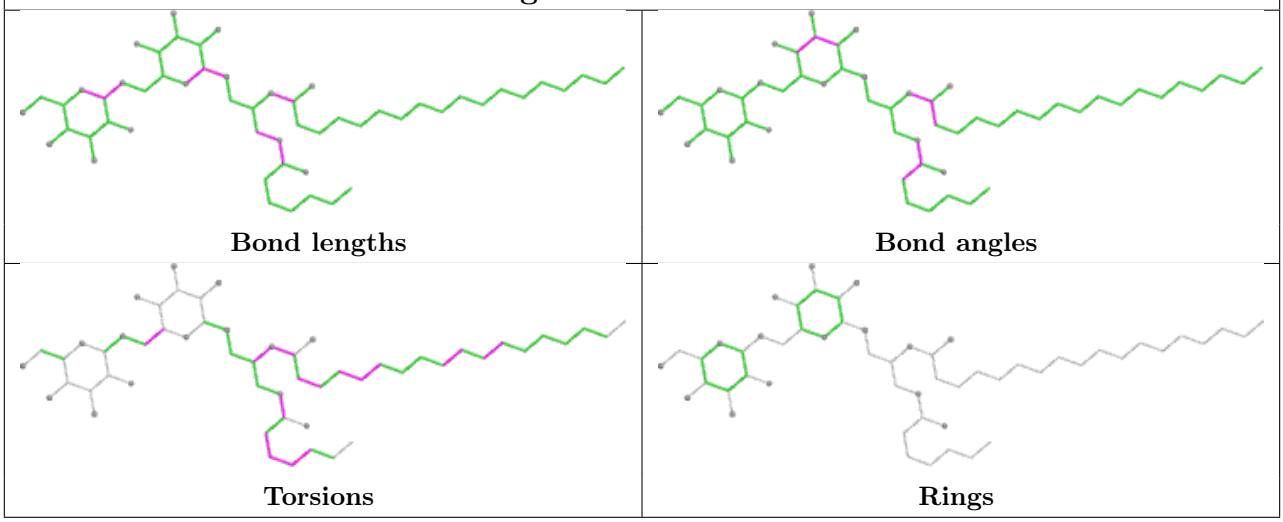
Ligand PL9 A 403



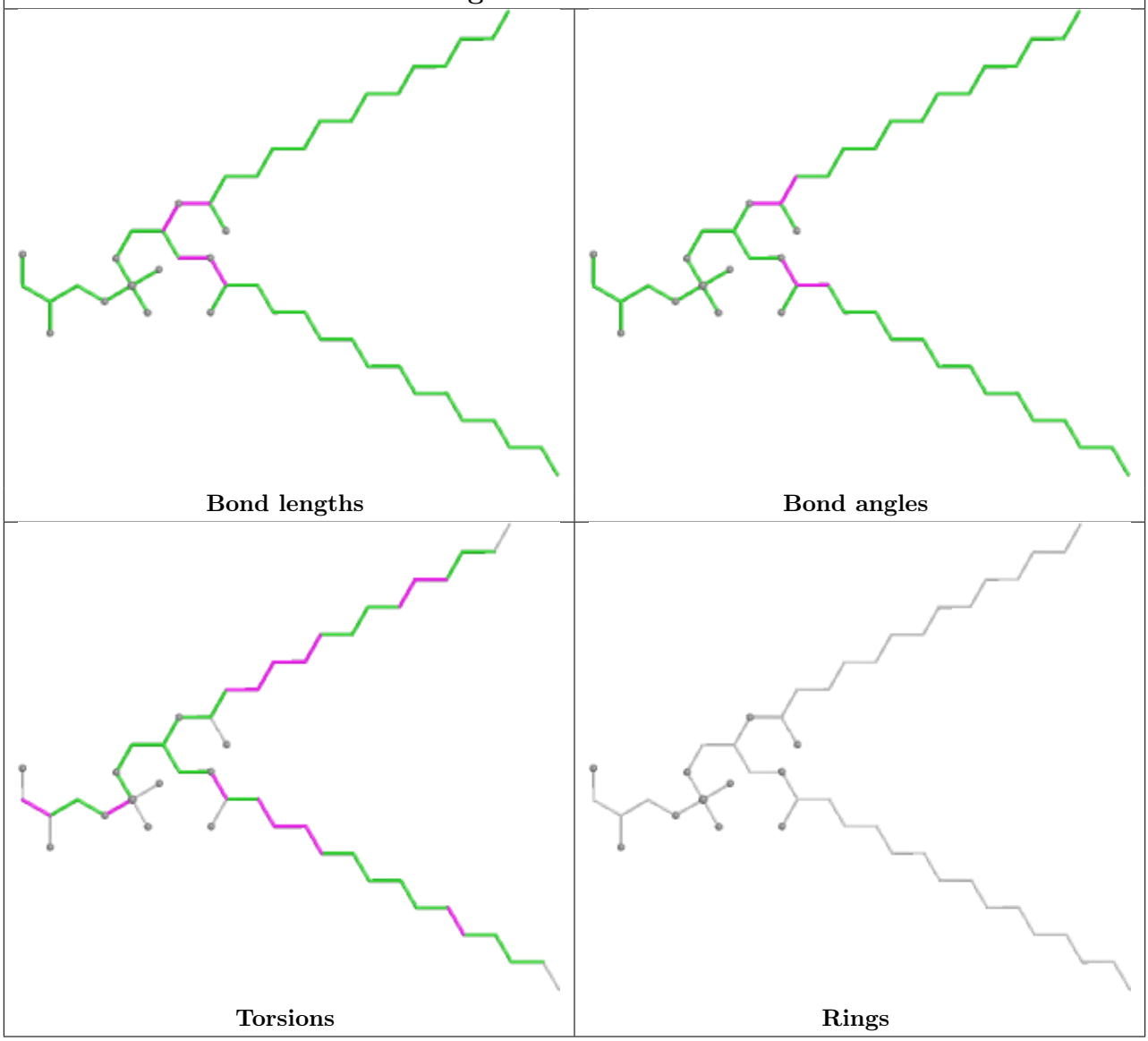
Ligand SQD B 601



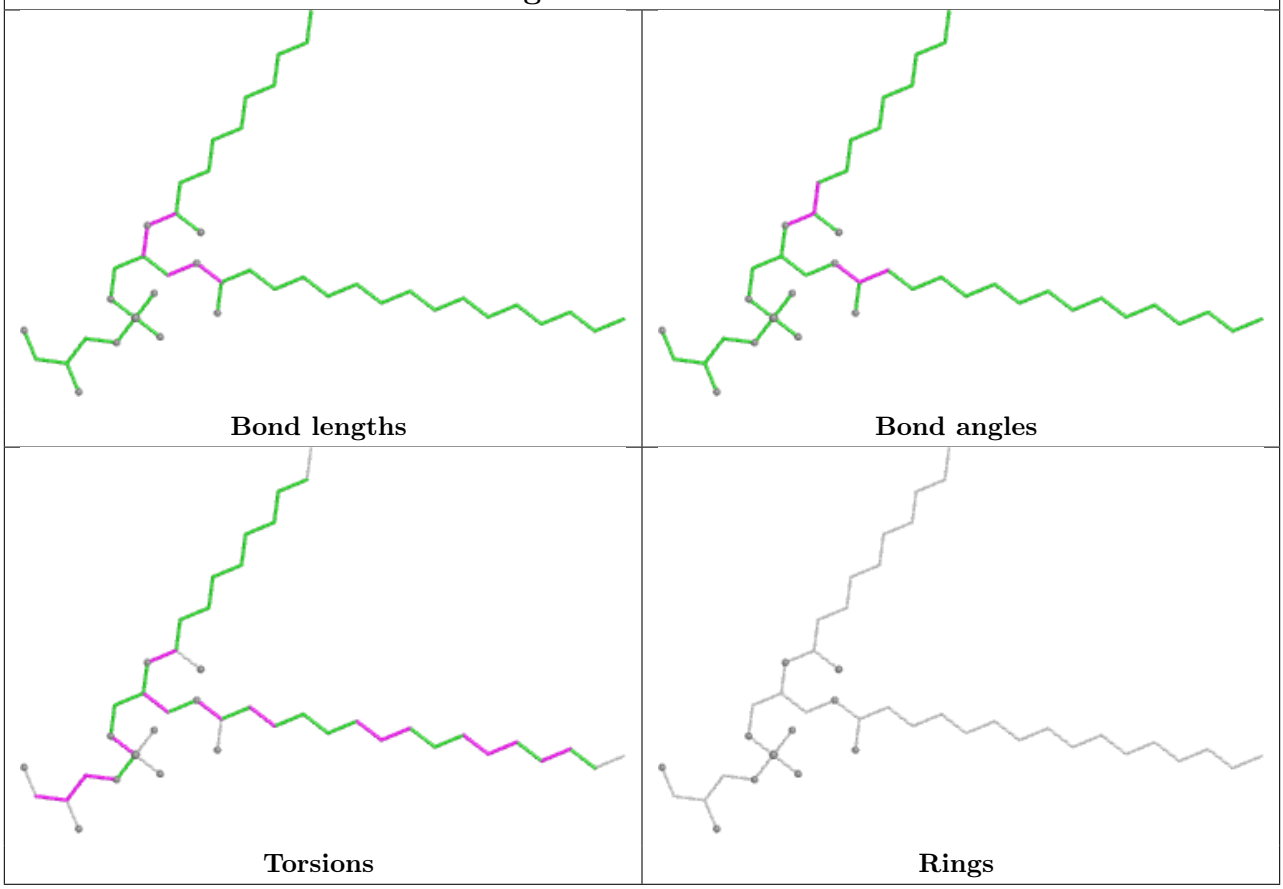
Ligand DGD A 401



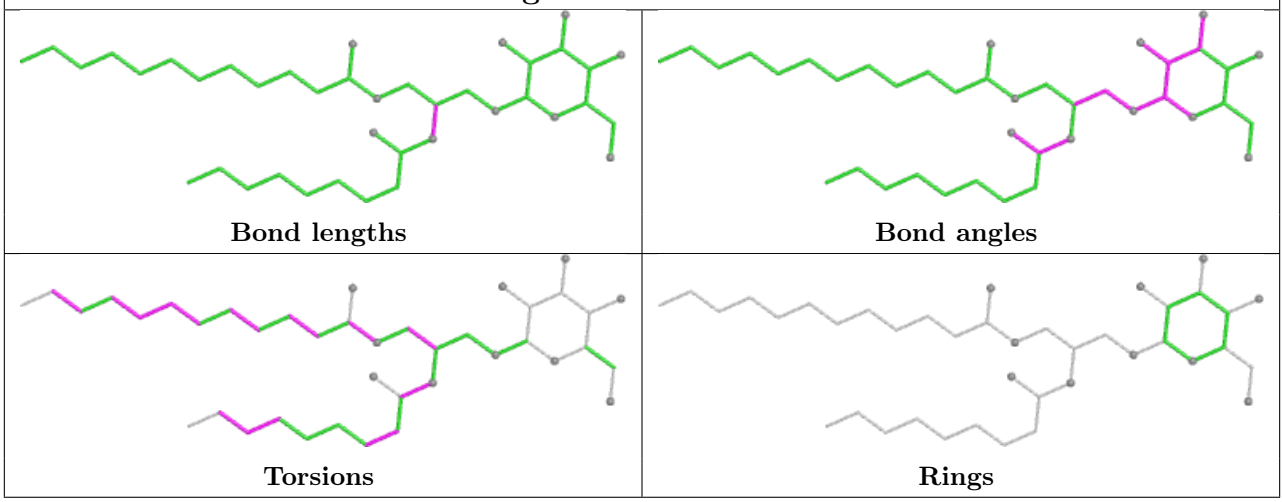
Ligand LHG D 601



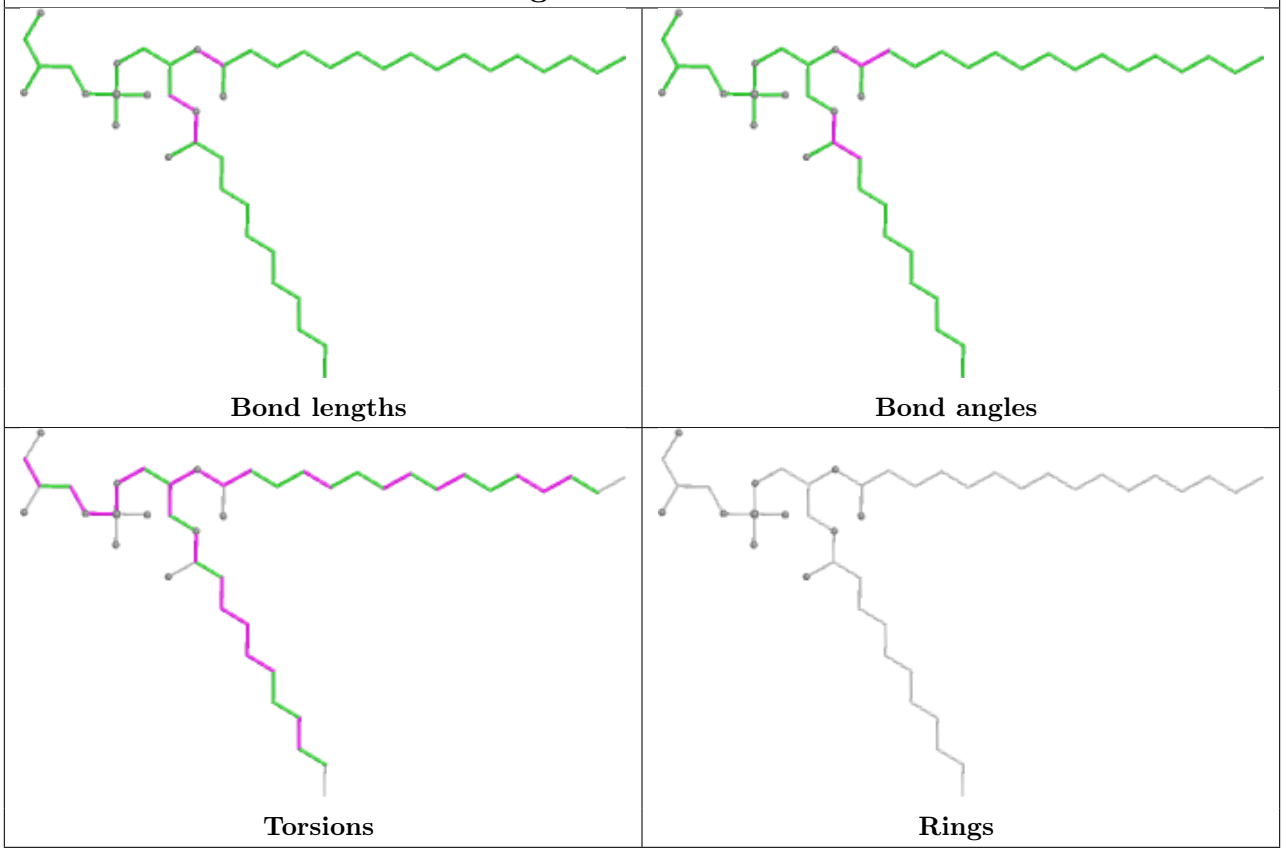
Ligand LHG C 202



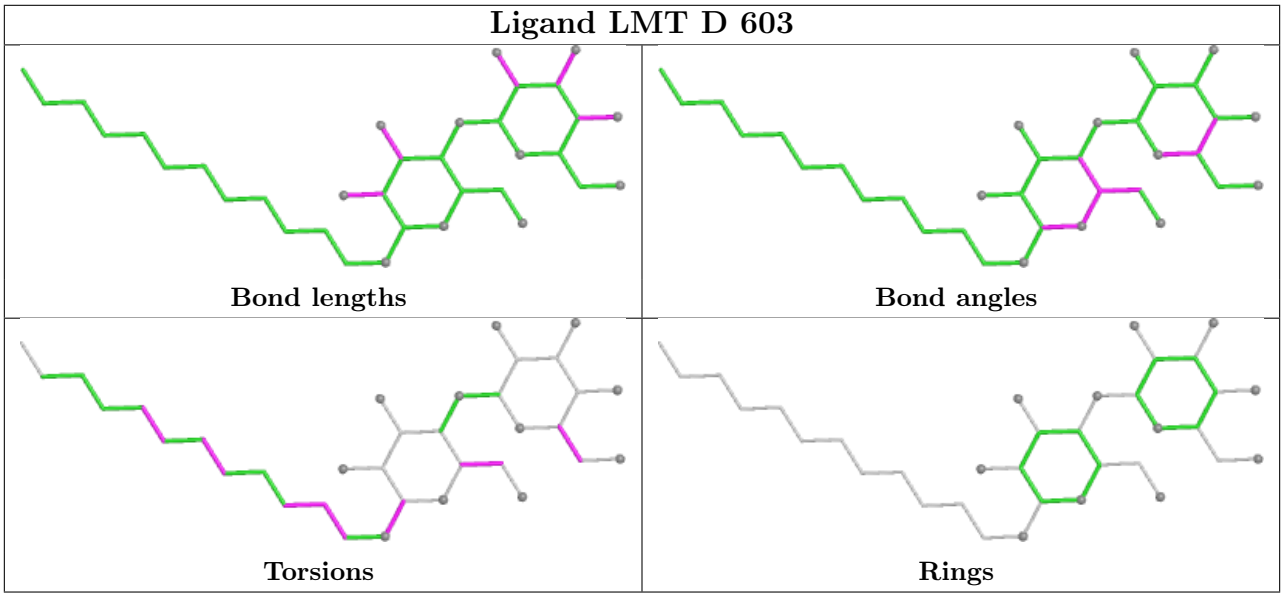
Ligand LMG F 704



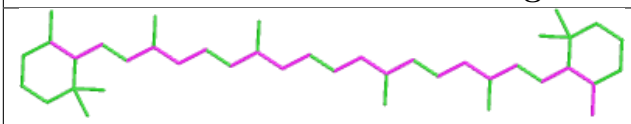
Ligand LHG I 201



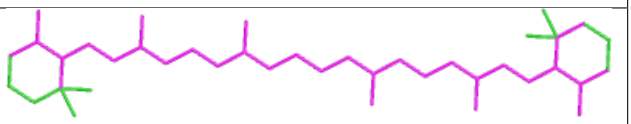
Ligand LMT D 603



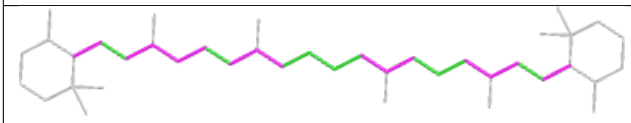
Ligand BCR F 701



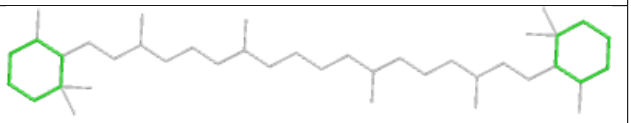
Bond lengths



Bond angles

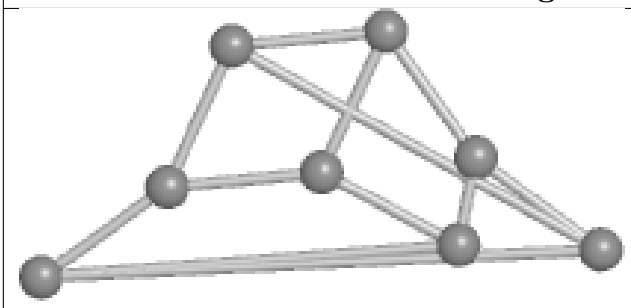


Torsions

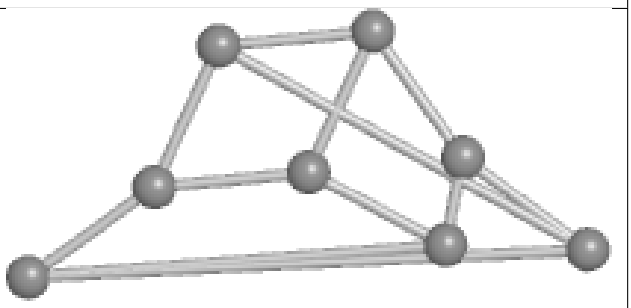


Rings

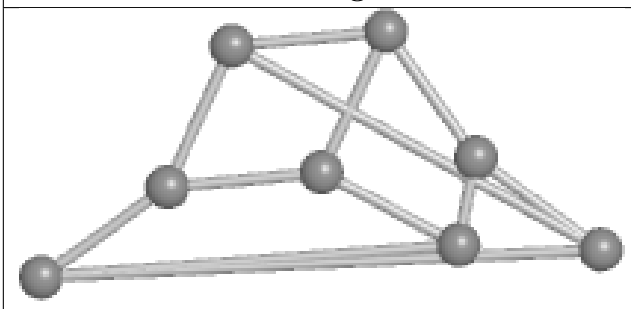
Ligand SF4 I 202



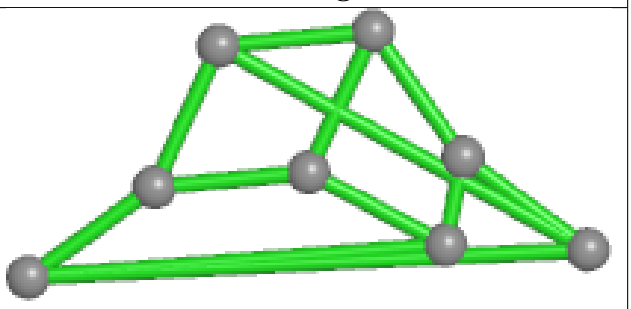
Bond lengths



Bond angles

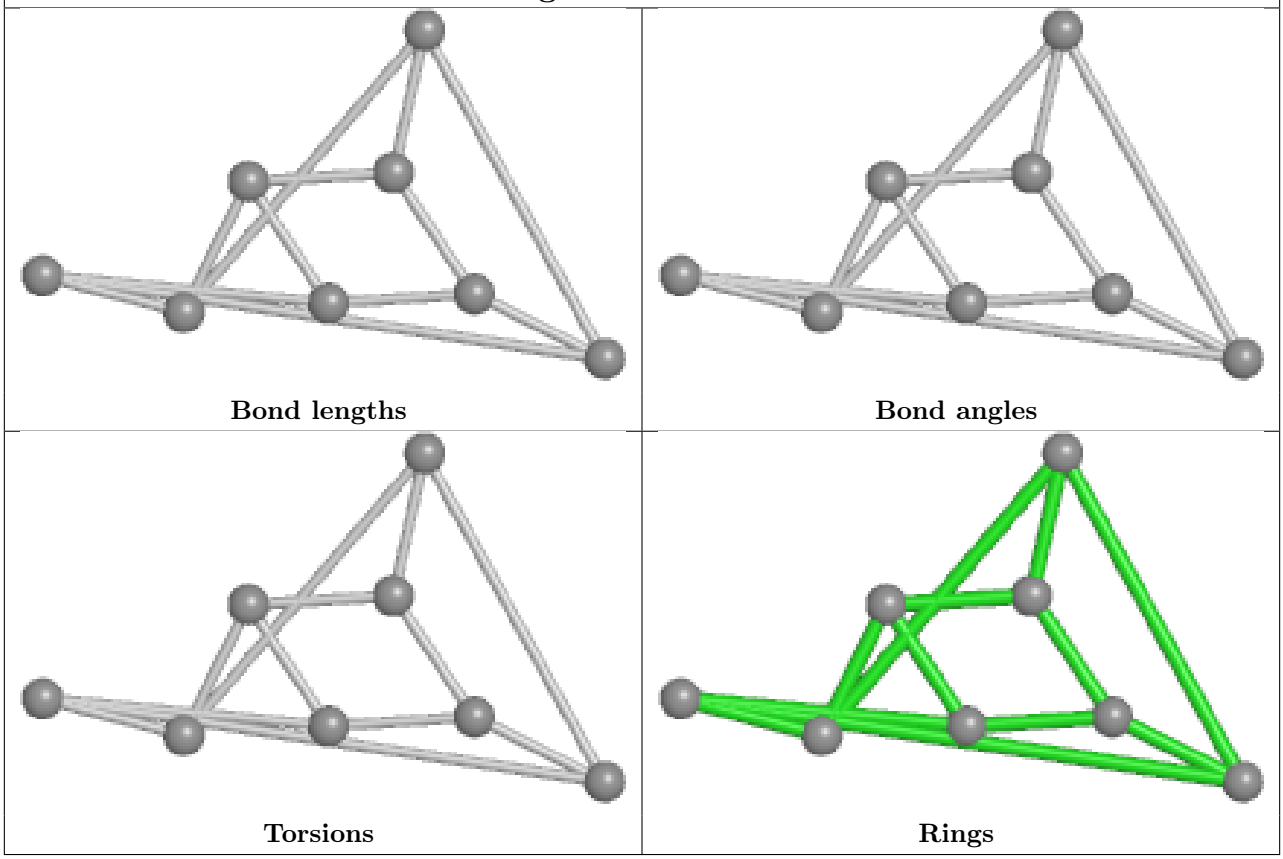


Torsions

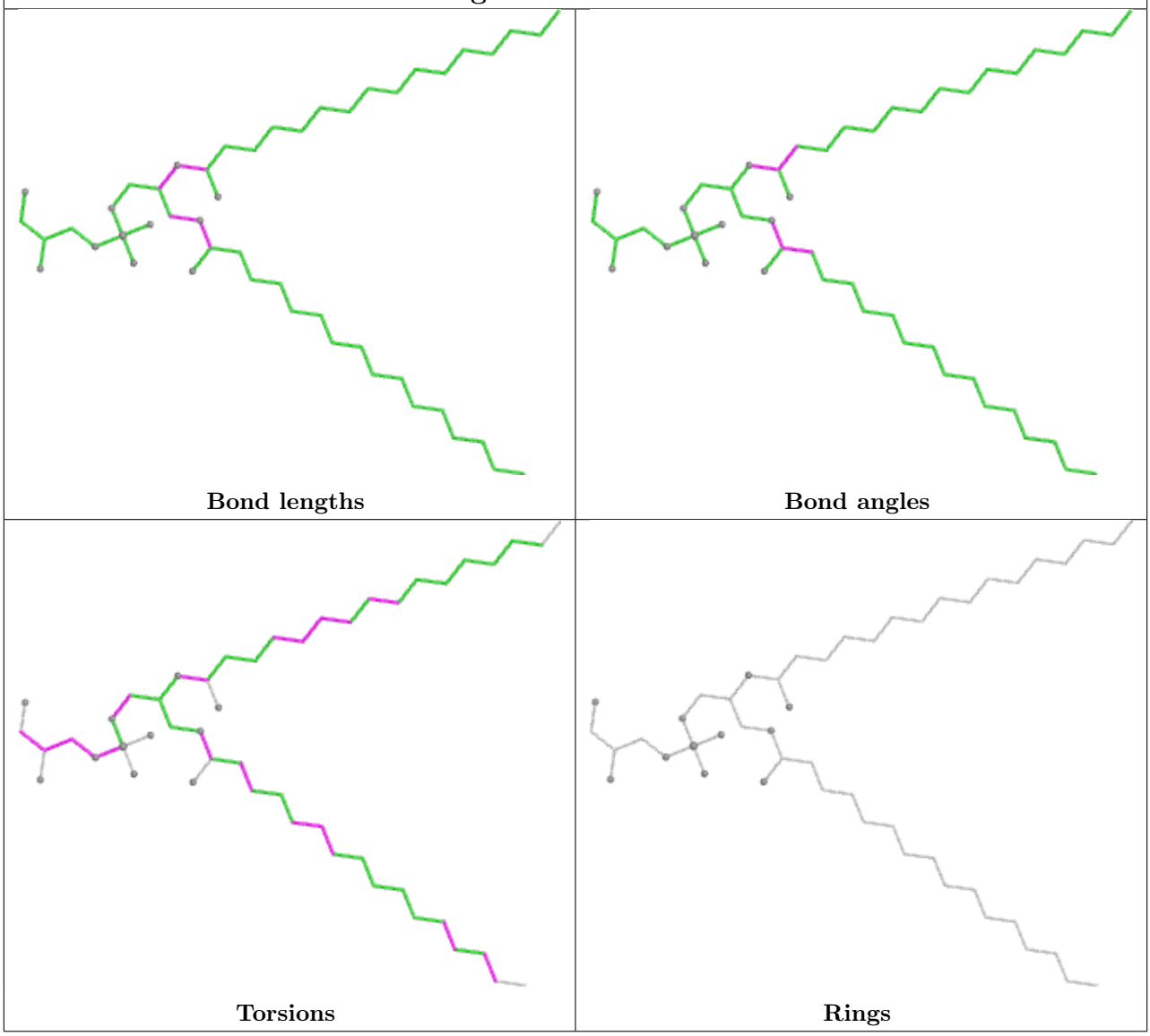


Rings

Ligand SF4 I 203



Ligand LHG F 703



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.

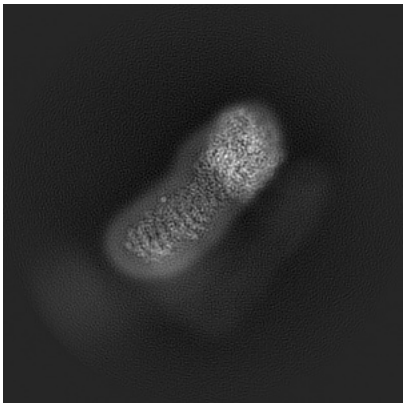
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9990. These allow visual inspection of the internal detail of the map and identification of artifacts.

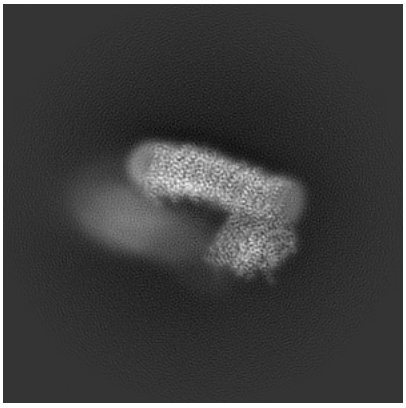
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

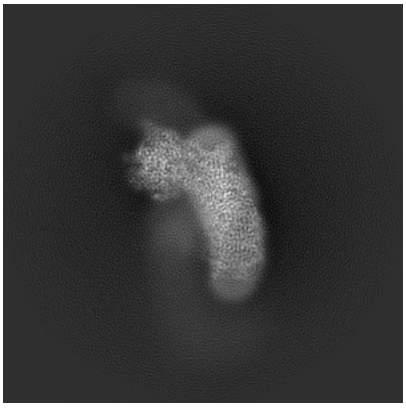
6.1.1 Primary map



X



Y

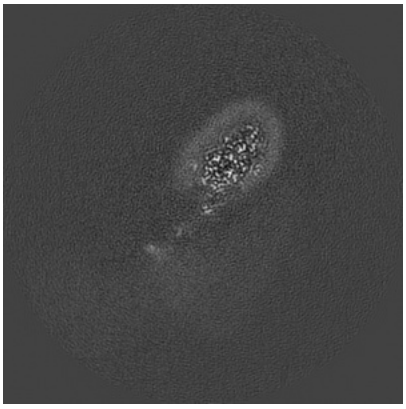


Z

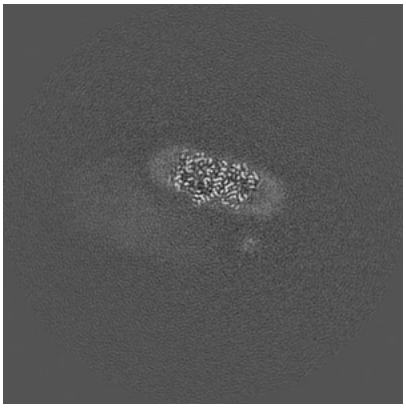
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

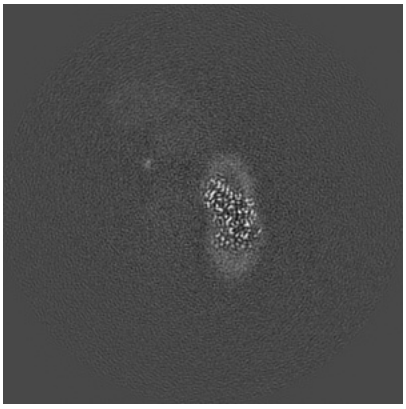
6.2.1 Primary map



X Index: 200



Y Index: 200

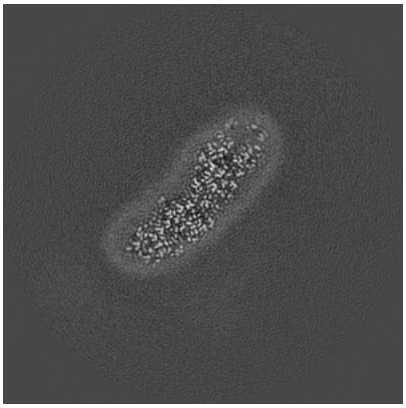


Z Index: 200

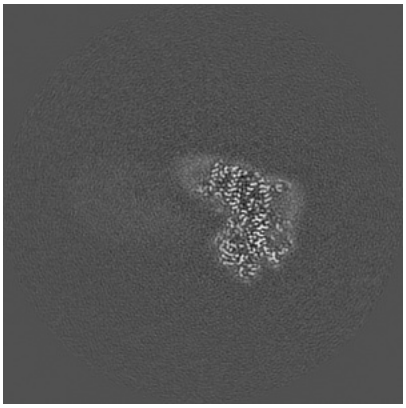
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

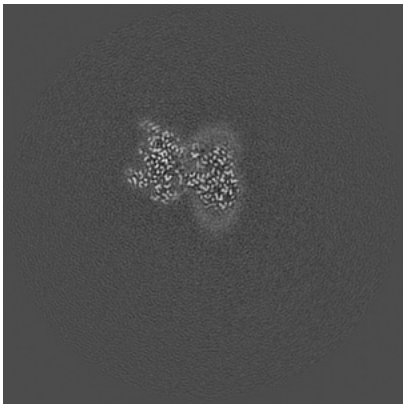
6.3.1 Primary map



X Index: 222



Y Index: 226

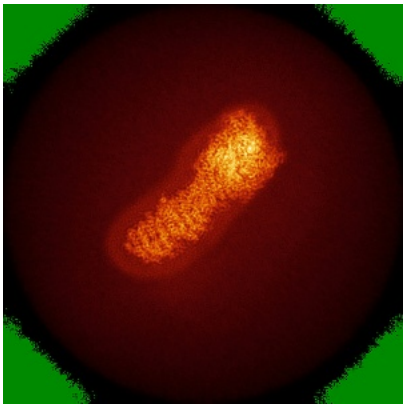


Z Index: 247

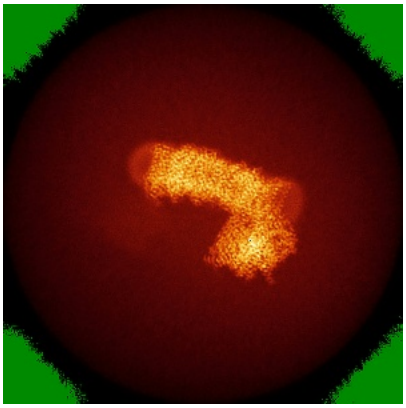
The images above show the largest variance slices of the map in three orthogonal directions.

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

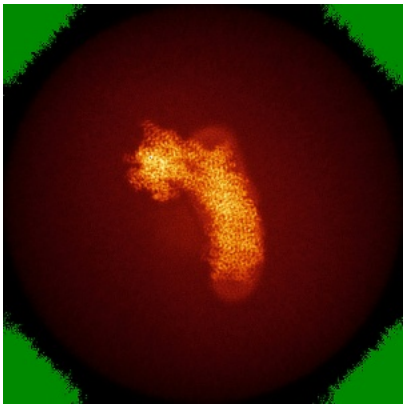
6.4.1 Primary map



X



Y

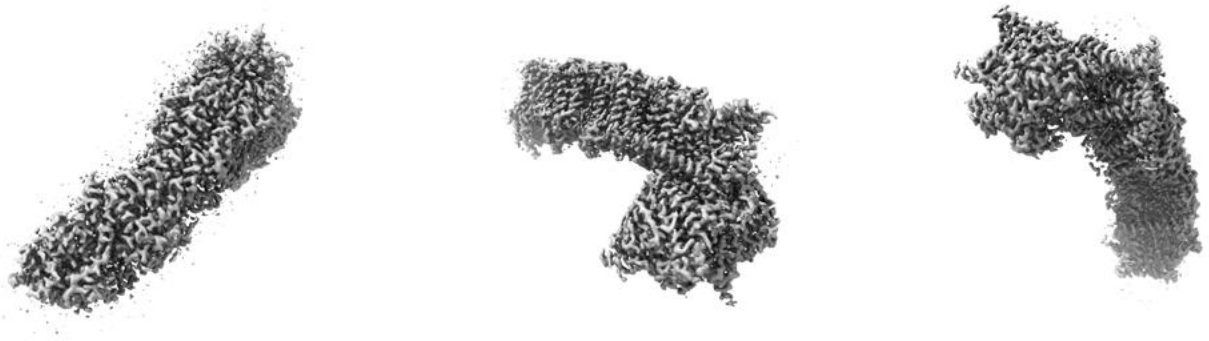


Z

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

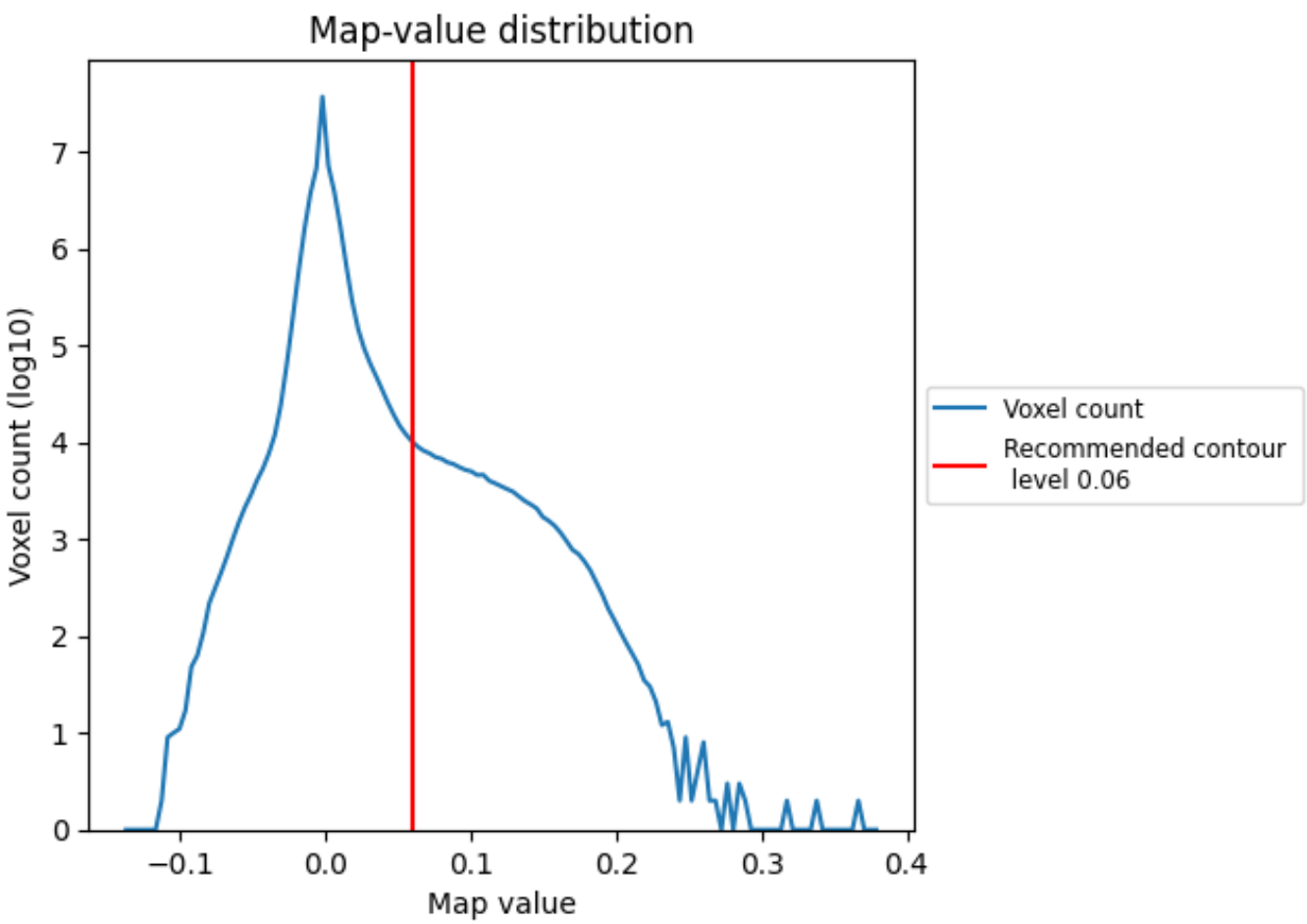
6.6 Mask visualisation (i)

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

7 Map analysis (i)

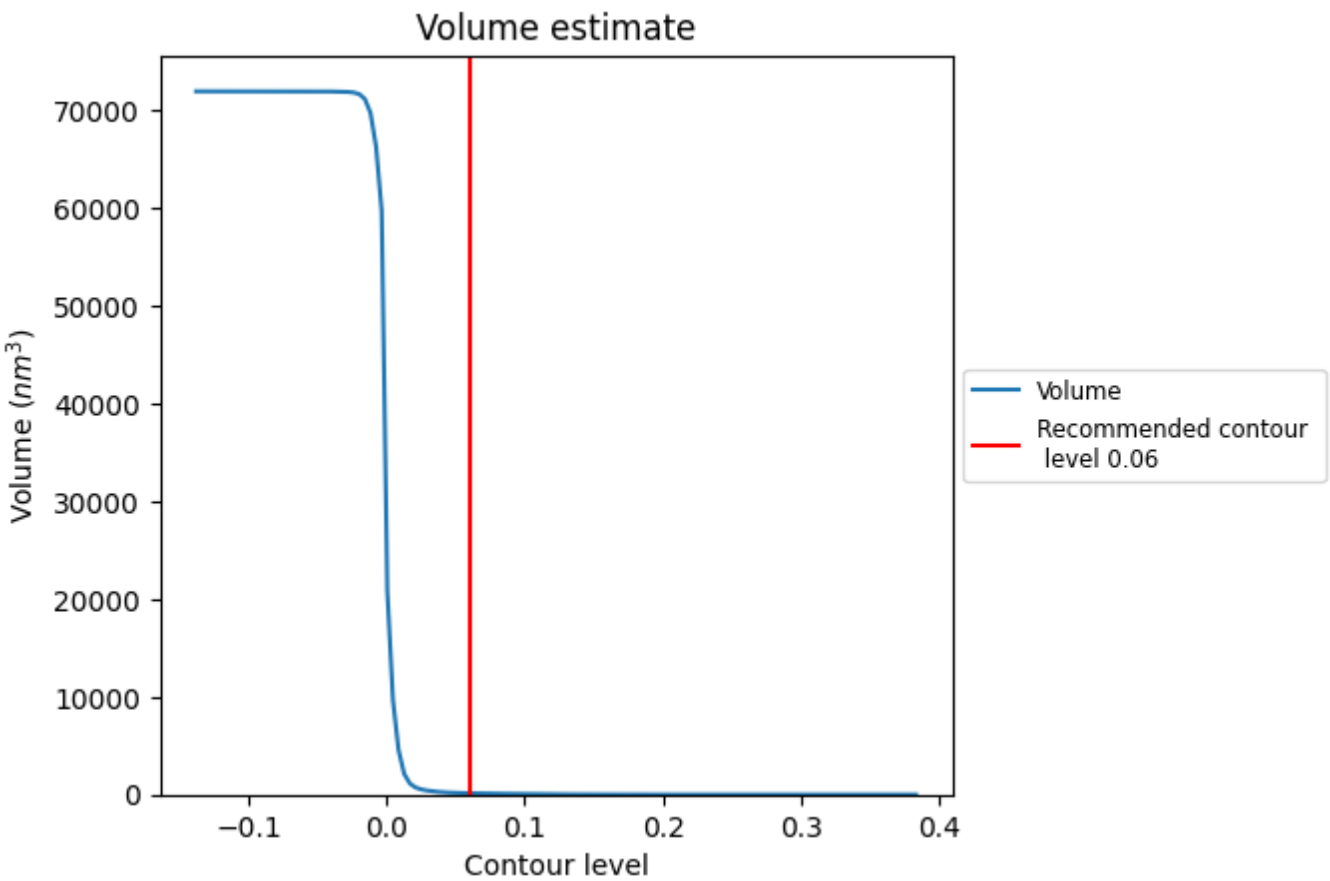
This section contains the results of statistical analysis of the map.

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.

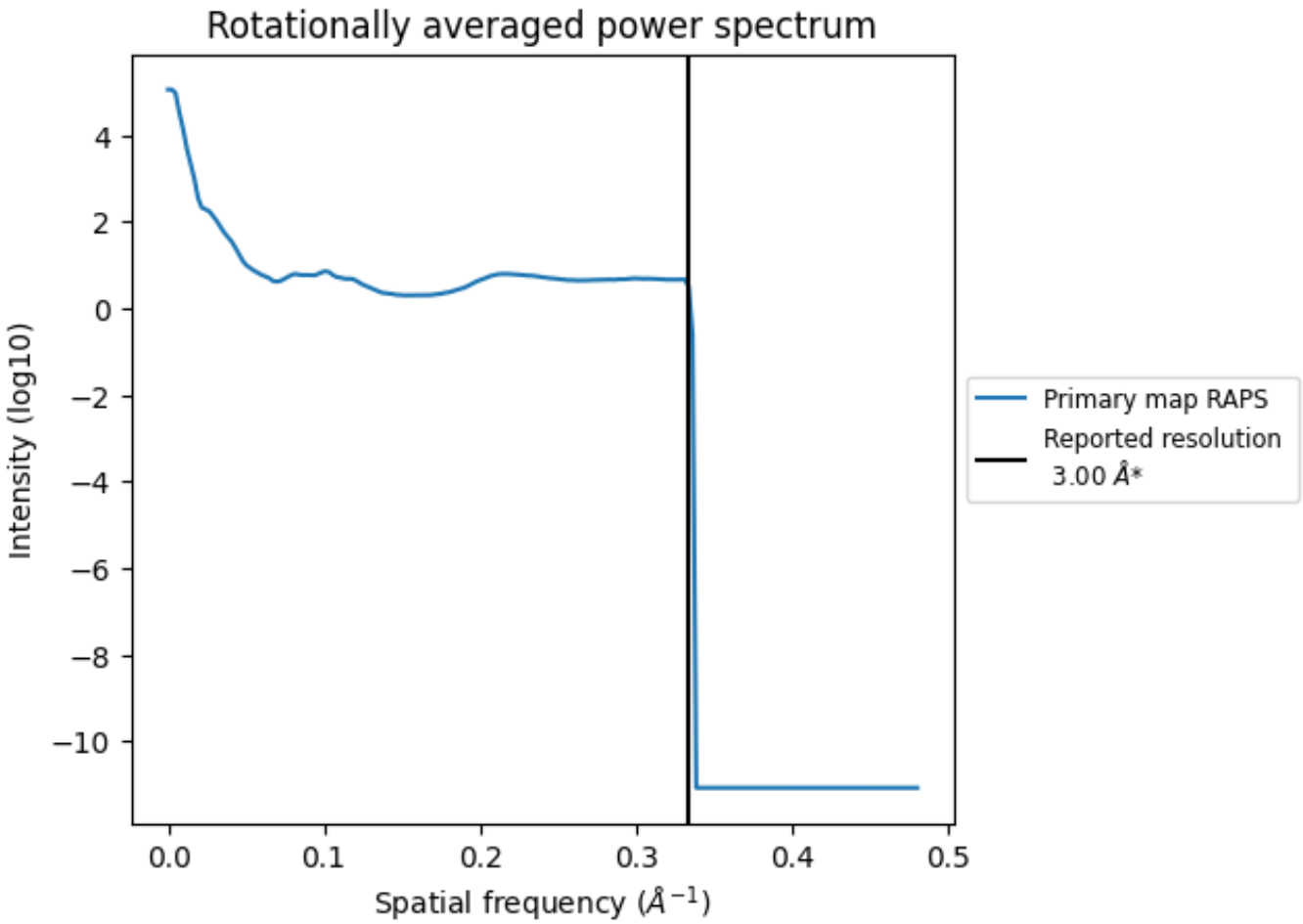
7.2 Volume estimate (i)



The volume at the recommended contour level is 137 nm^3; this corresponds to an approximate mass of 124 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 0.333 Å^{-1}

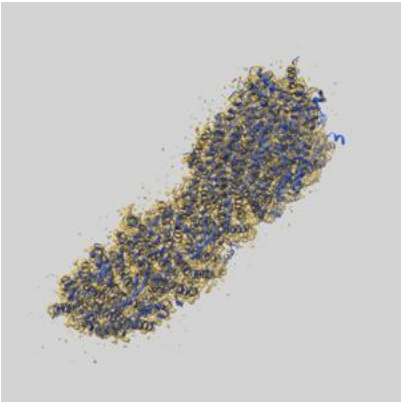
8 Fourier-Shell correlation (i)

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

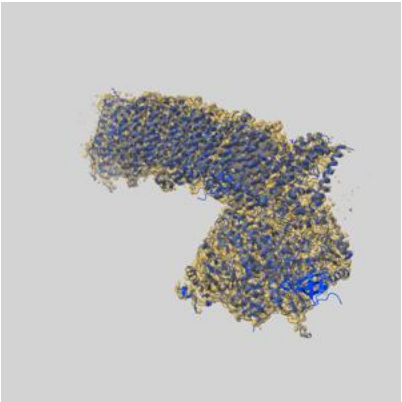
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9990 and PDB model 6KHJ. Per-residue inclusion information can be found in section 3 on page 13.

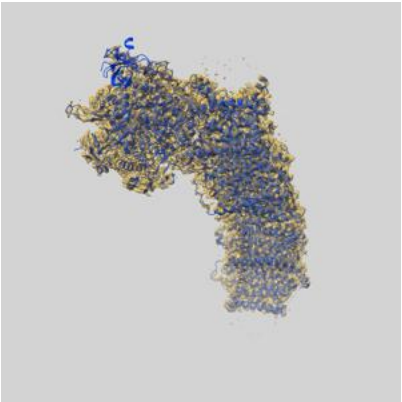
9.1 Map-model overlay (i)



X



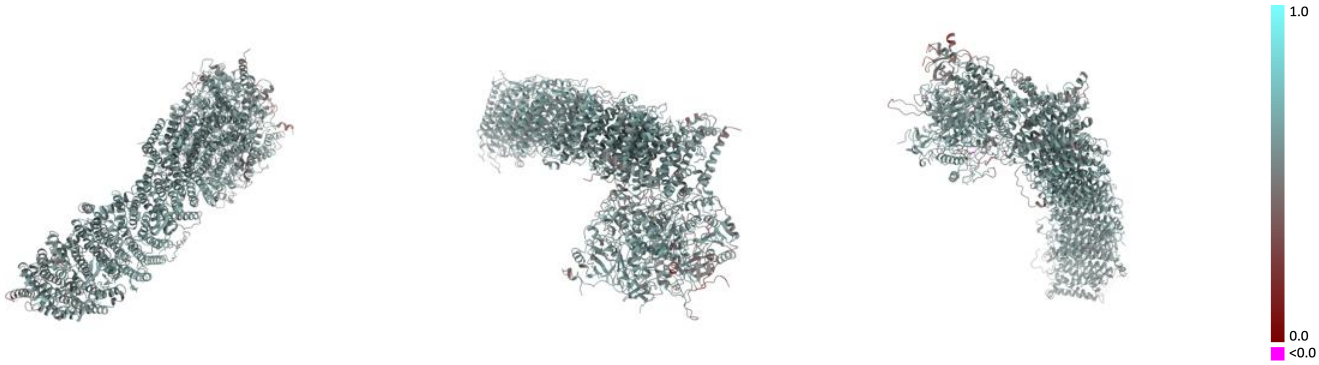
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

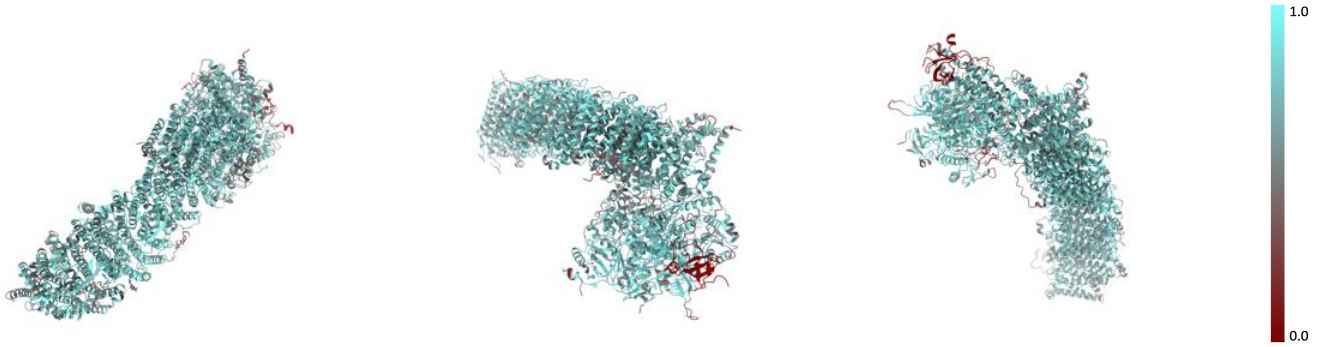
9.2 Q-score mapped to coordinate model (i)



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.

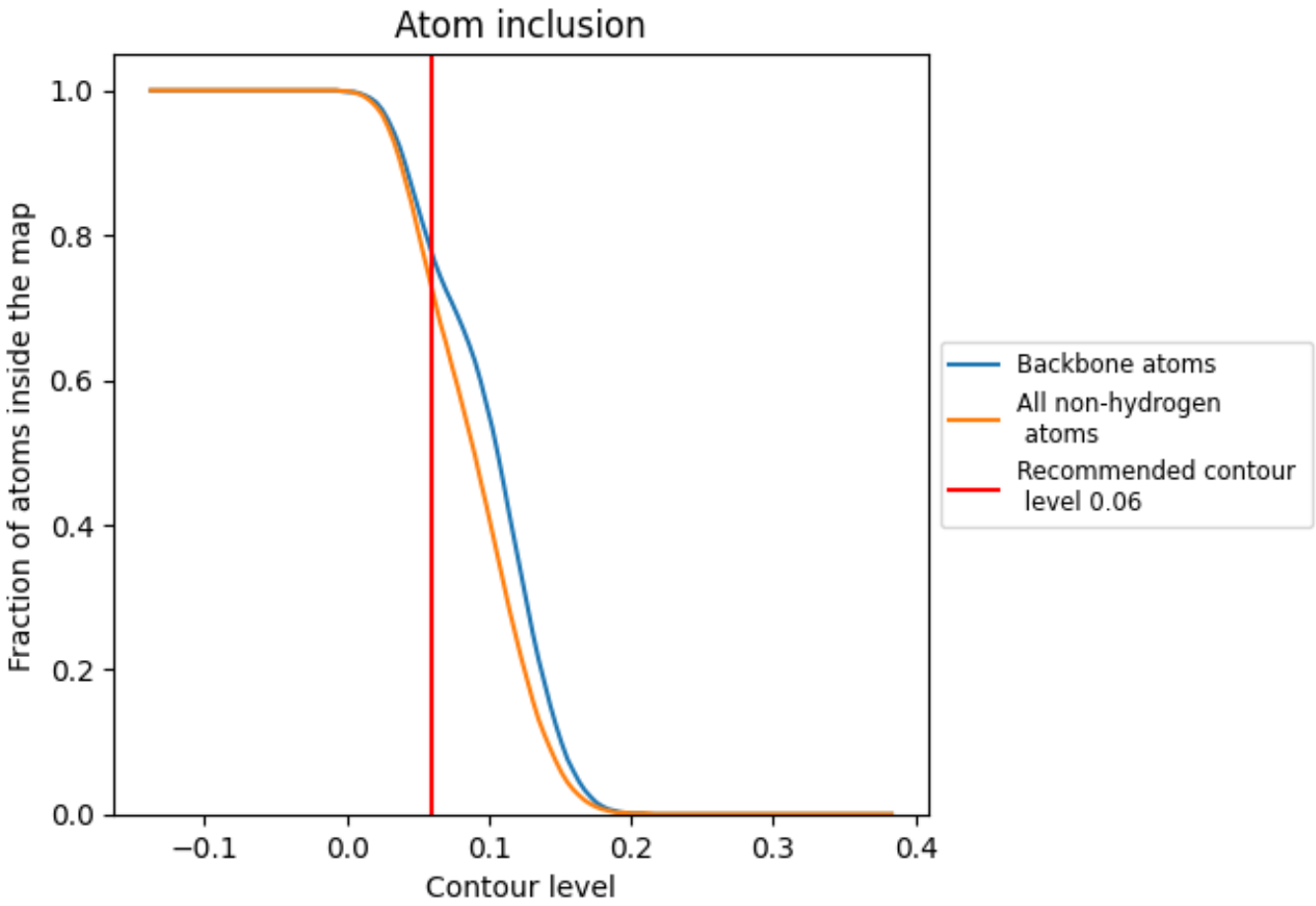
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.5620
A	0.7210	0.5630
B	0.7720	0.5820
C	0.7160	0.5540
D	0.7870	0.5850
E	0.7640	0.5800
F	0.7140	0.5560
G	0.7120	0.5670
H	0.7360	0.5620
I	0.6710	0.5370
J	0.7560	0.5650
K	0.7430	0.5550
L	0.6610	0.5260
M	0.7480	0.5590
N	0.7250	0.5490
O	0.7340	0.5710
P	0.7570	0.5730
Q	0.6310	0.5320
S	0.0260	0.4260