



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:28 PM UTC

PDB ID : 6KHI / pdb_00006khi
EMDB ID : EMD-9989
Title : Supercomplex for cyclic electron transport in cyanobacteria
Authors : Pan, X.; Cao, D.; Xie, F.; Zhang, X.; Li, M.
Deposited on : 2019-07-15
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

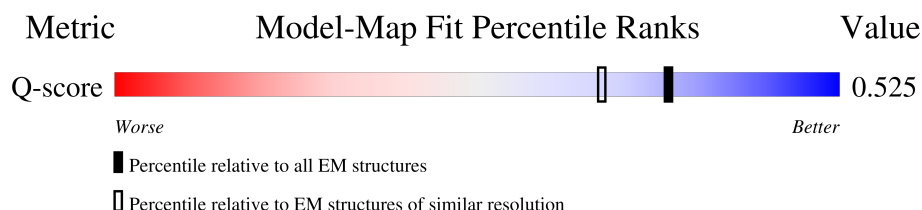
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

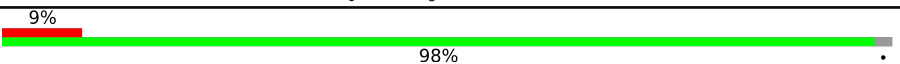
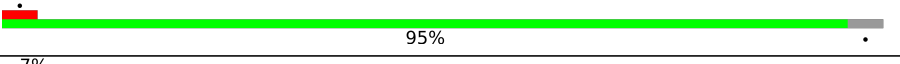
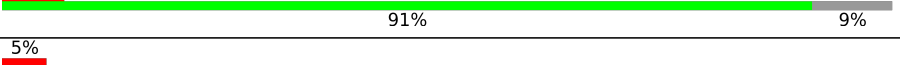
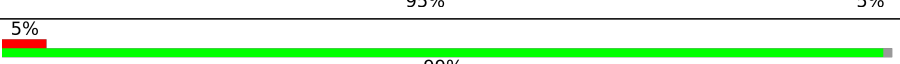
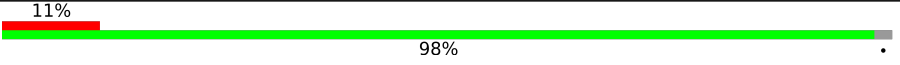
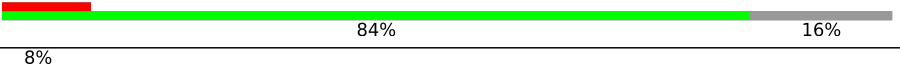
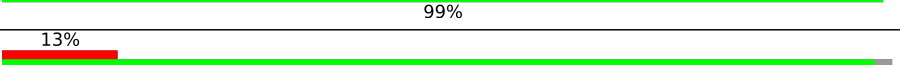
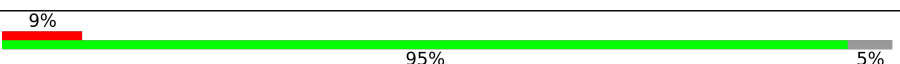
The reported resolution of this entry is 3.00 Å.

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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	
2	B	515	
3	C	132	
4	D	529	
5	E	101	
6	F	656	
7	G	200	
8	H	394	
9	I	196	
10	J	168	

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Mol	Chain	Length	Quality of chain
11	K	237	
12	L	76	
13	M	111	
14	N	150	
15	O	70	
16	P	44	
17	Q	45	
18	S	110	
19	V	146	
20	1	98	

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
24	BCR	D	602	-	X	-	-
24	BCR	D	603	-	X	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 32635 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	366	Total	C	N	O	S	0	0
			2821	1893	439	478	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	492	Total	C	N	O	S	0	0
			3724	2472	578	658	16		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	504	Total	C	N	O	S	0	0
			3897	2614	606	655	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	100	Total	C	N	O	S	0	0
			775	512	127	133	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	641	Total	C	N	O	S	0	0
			4945	3285	778	845	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	169	Total	C	N	O	S	0	0
			1278	855	200	219	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	192	Total	C	N	O	S	0	0
			1537	979	264	281	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	160	Total	C	N	O	S	0	0
			1307	836	222	244	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	205	Total	C	N	O	S	0	0
			1590	1019	275	283	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	74	Total	C	N	O	S	0	0
			595	409	91	94	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1165	758	201	205	1		

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

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

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

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

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

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

- Molecule 18 is a protein called Tlr0636 protein.

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

- Molecule 19 is a protein called Tlr0472 protein.

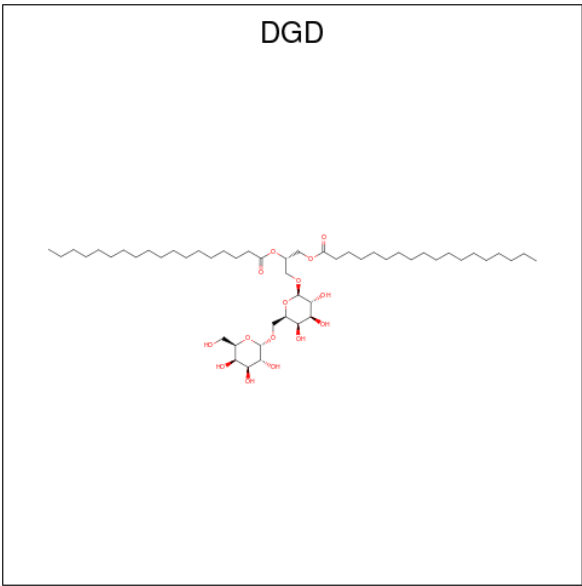
Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	109	Total	C	N	O	S	0	0
			838	545	139	150	4		

- Molecule 20 is a protein called Ferredoxin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1	98	Total	C	N	O	S	0	0
			756	468	117	165	6		

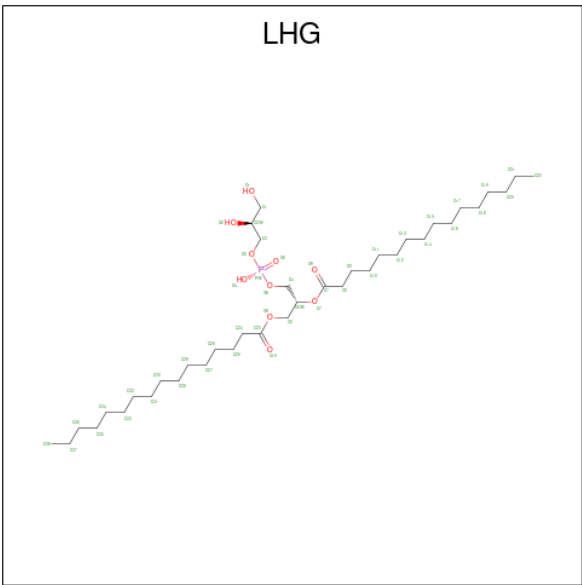
- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



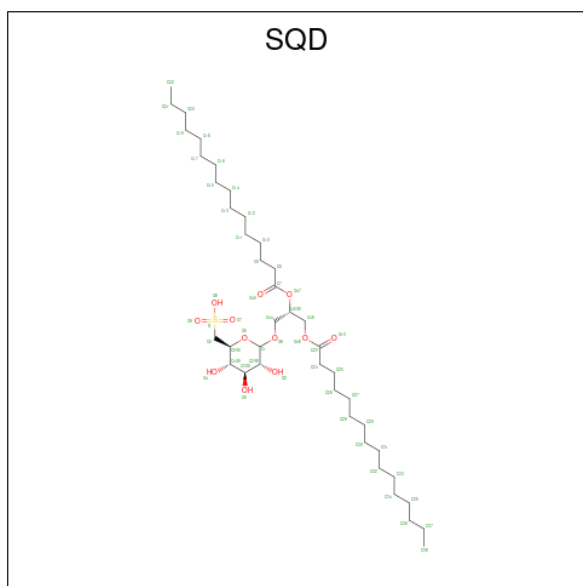
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			62	47	15	
21	A	1	Total	C	O	0
			62	47	15	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



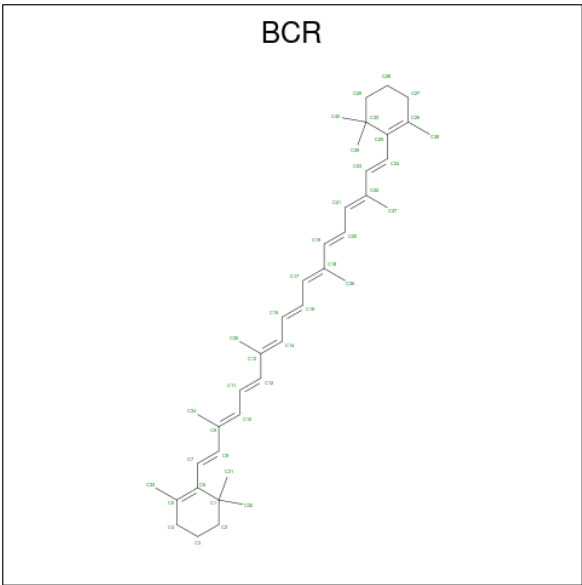
Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total	C	O	P	0
			46	35	10	1	
22	C	1	Total	C	O	P	0
			43	32	10	1	
22	F	1	Total	C	O	P	0
			49	38	10	1	
22	F	1	Total	C	O	P	0
			36	25	10	1	
22	F	1	Total	C	O	P	0
			44	33	10	1	
22	I	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 23 is 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).



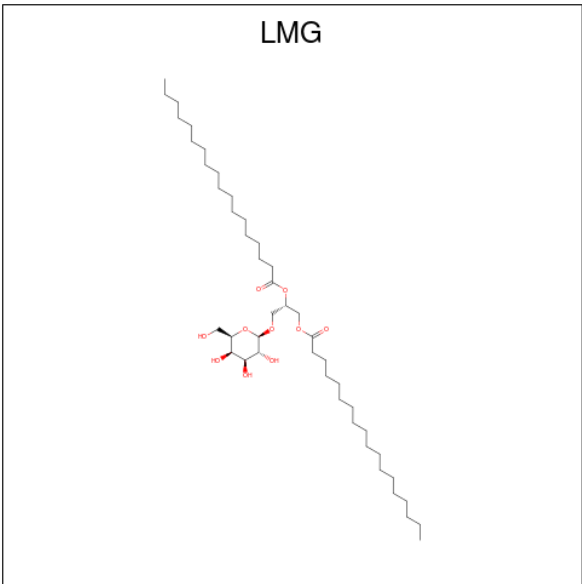
Mol	Chain	Residues	Atoms				AltConf
23	C	1	Total	C	O	S	0
			40	27	12	1	
23	D	1	Total	C	O	S	0
			54	41	12	1	
23	L	1	Total	C	O	S	0
			38	25	12	1	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
24	D	1	Total	C	0
			40	40	
24	D	1	Total	C	0
			40	40	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



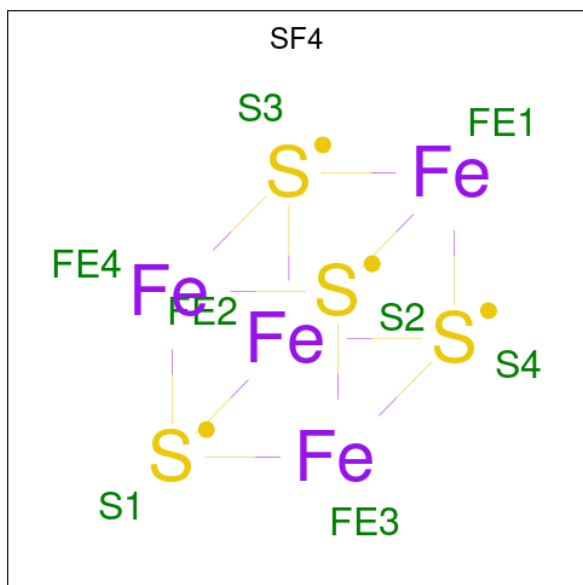
Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	C	O	0
			47	37	10	

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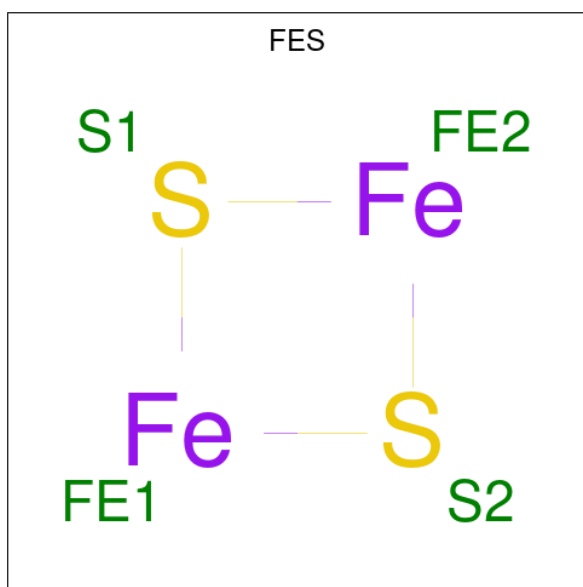
Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	C	O	0
			40	30	10	

- 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
26	I	1	Total	Fe	S	0
			8	4	4	
26	I	1	Total	Fe	S	0
			8	4	4	
26	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

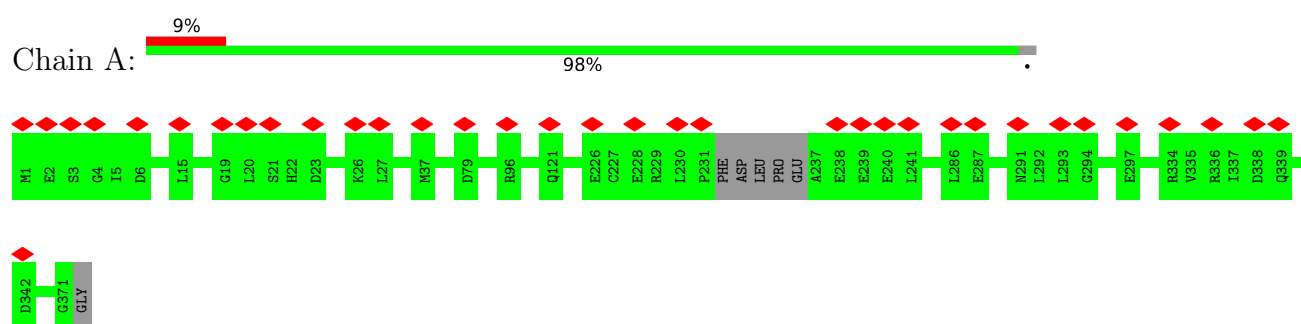


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
27	1	1	4	2	2	0

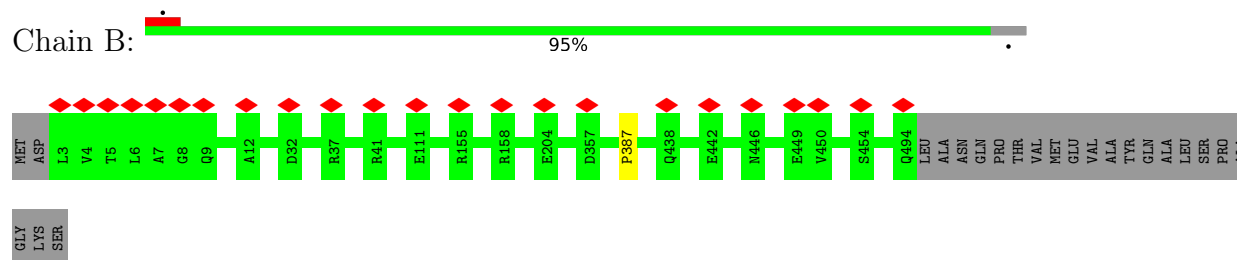
3 Residue-property plots [i](#)

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.

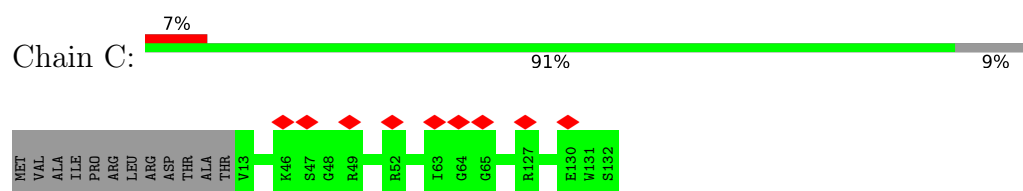
- Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1



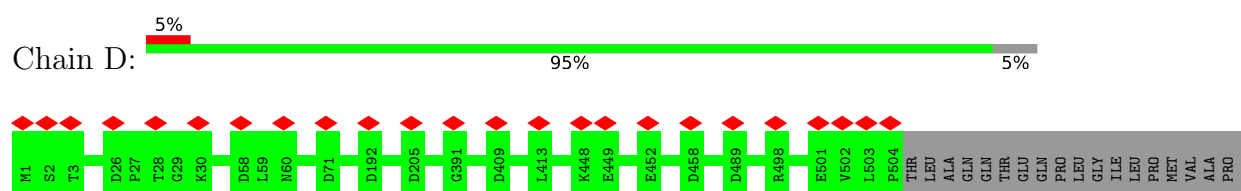
- Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2



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



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



LEU
LYS
ALA
ASN
ALA
GLN

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

Chain E:  5% 99%

MET
Q2
E73
D89
N97
L98
L99
K100
W101

- Molecule 6: NADH dehydrogenase subunit 5

Chain F:  11% 98%

MET
E2
L20
E31
K35
L67
N80
D90
K169
F187
T202
A206
D210
E214
N217
T218
G219
L220
L221
L225
D252
H265
E268
H373
D376
L377
L403
V408
P409
P410
F411
L433
L437
T438
A439
E455

Q456
K457
P462
P463
E464
R465
Q466
GLU
HIS
HIS
ASP
HIS
HIS
SER
SER
HIS
A476
A477
V478
E481
F502
F507
N508
G519
E520
E521
LYS
VAL
ALA
GLU
HIS
A527
V528
D529
L530
L531
T531
E532
F533
L534
I535
G538
S539
S540
M546
K557
G558
T559
P560
S561
A564
I565

A566
K567
A568
D583
E603
V604
D605
D610
T616
E625
Q655
T656

- Molecule 7: NADH-quinone oxidoreductase subunit J

Chain G:  10% 84% 16%

MET
D2
D30
R84
E85
T86
Y87
T88
P91
G92
R93
W94
L95
R96
Q97
G98
S124
D130
R167
E168
L169
V170
LEU
GLU
PRO
GLU
PRO
PRO
ILE
LEU
GLY
GLU
GLU
GLU
VAL
VAL
PRO
PRO
LEU
LEU
PRO
PRO
GLU
ARG
ARG
PRO
PRO
VAL
VAL
ALA
LEU
SER
GLU
LYS

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

Chain H:  8% 99%

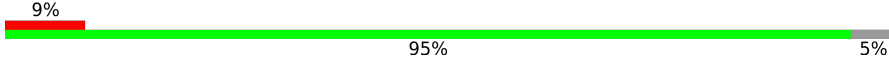
MET
F2
K3
M22
H23
D33
G34
E35
D71
D124
Q128
T129
F130
F131
F132
Y133
D181
D188
E191
R192
L193
I194
T195
F198
R202
D247
W248
D249
E255
D261
G299
A300
R301
K314
K315
L316
D359
K371
D377
R394

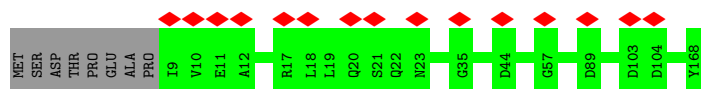
- Molecule 9: NAD(P)H-quinone oxidoreductase subunit I

Chain I:  13% 98%

MET
LYS
F3
L4
M5
Q6
I7
T8
N9
Y10
A11
K12
E13
Q15
K19
Q23
D30
E37
L88
K89
E159
D172
A175
M189
T190
A191
K192
S193
S194
GLU
ASN

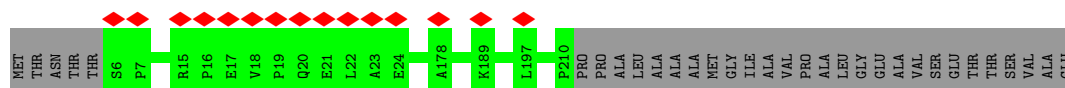
- Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

Chain J: 

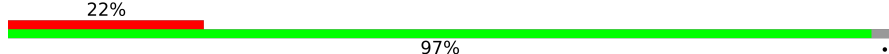


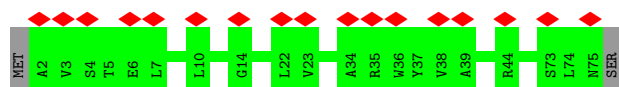
- Molecule 11: NAD(P)H-quinone oxidoreductase subunit K

Chain K: 

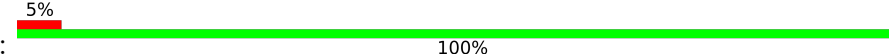


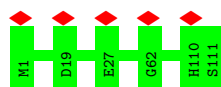
- Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

Chain L: 

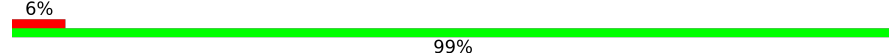


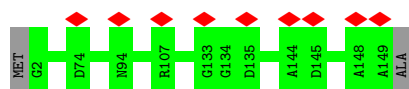
- Molecule 13: NAD(P)H-quinone oxidoreductase subunit M

Chain M: 

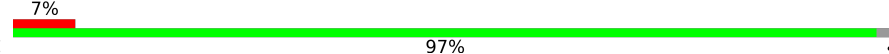


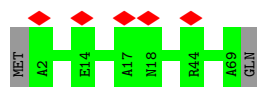
- Molecule 14: NAD(P)H-quinone oxidoreductase subunit N

Chain N: 

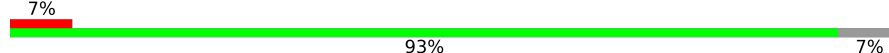


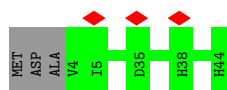
- Molecule 15: NAD(P)H-quinone oxidoreductase subunit O

Chain O: 

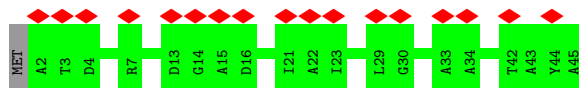
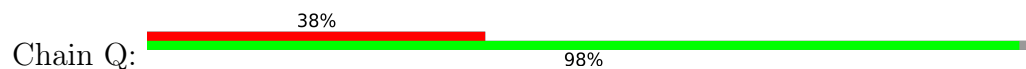


- Molecule 16: proton-translocating NADH-quinone dehydrogenase subunit P

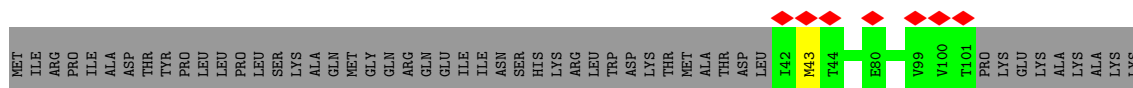
Chain P: 



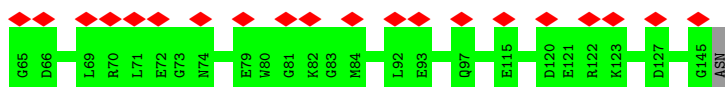
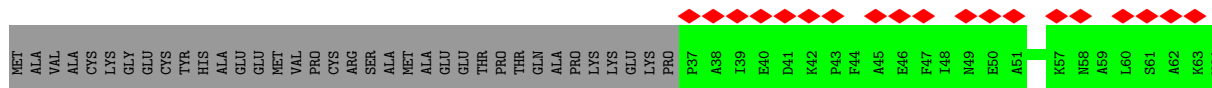
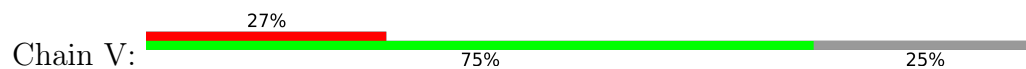
- Molecule 17: proton-translocating NADH-quinone dehydrogenase subunit Q



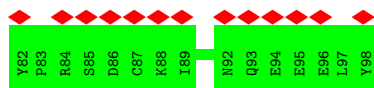
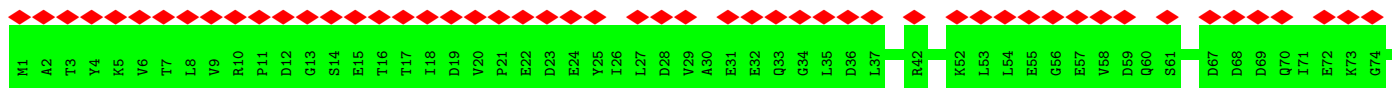
- Molecule 18: Thr0636 protein



- Molecule 19: Thr0472 protein



- Molecule 20: Ferredoxin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152003	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.417	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	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, SQD, SF4, LHG, FES, LMG, BCR

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	0.25	0/2891	0.56	0/3949
2	B	0.25	0/3810	0.52	1/5198 (0.0%)
3	C	0.25	0/1001	0.61	0/1365
4	D	0.25	0/4004	0.49	0/5464
5	E	0.22	0/785	0.45	0/1067
6	F	0.23	0/5087	0.51	0/6930
7	G	0.22	0/1304	0.44	0/1786
8	H	0.28	1/3260 (0.0%)	0.56	0/4417
9	I	0.29	0/1575	0.58	0/2135
10	J	0.22	0/1343	0.52	0/1829
11	K	0.31	0/1630	0.63	0/2218
12	L	0.21	0/615	0.52	0/842
13	M	0.21	0/901	0.54	0/1222
14	N	0.22	0/1197	0.50	0/1628
15	O	0.21	0/550	0.50	0/748
16	P	0.24	0/330	0.51	0/448
17	Q	0.17	0/342	0.38	0/466
18	S	0.22	0/478	0.55	2/652 (0.3%)
19	V	0.24	0/857	0.60	0/1155
20	1	0.20	0/766	0.46	0/1039
All	All	0.25	1/32726 (0.0%)	0.53	3/44558 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	129	THR	C-N	5.79	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
18	S	43	MET	CA-C-N	5.70	132.43	121.54
18	S	43	MET	C-N-CA	5.70	132.43	121.54
2	B	387	PRO	N-CA-C	5.24	117.10	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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
27	FES	1	101	20	0,4,4	-	-	-		
22	LHG	F	702	-	48,48,48	0.91	4 (8%)	51,54,54	1.09	2 (3%)
23	SQD	L	101	-	36,38,54	2.13	9 (25%)	46,49,65	5.43	9 (19%)
22	LHG	F	705	-	43,43,48	0.96	4 (9%)	46,49,54	1.09	2 (4%)
24	BCR	D	603	-	41,41,41	4.21	18 (43%)	56,56,56	5.31	33 (58%)
22	LHG	B	601	-	45,45,48	0.94	4 (8%)	48,51,54	1.10	2 (4%)
25	LMG	F	701	-	47,47,55	0.87	3 (6%)	55,55,63	1.42	7 (12%)
25	LMG	F	703	-	40,40,55	0.92	2 (5%)	48,48,63	1.25	4 (8%)
23	SQD	D	601	-	52,54,54	1.85	10 (19%)	62,65,65	4.69	6 (9%)
22	LHG	I	201	-	43,43,48	0.95	4 (9%)	46,49,54	1.09	2 (4%)
26	SF4	I	203	9	0,12,12	-	-	-		
26	SF4	I	202	9	0,12,12	-	-	-		
22	LHG	F	704	-	35,35,48	1.05	4 (11%)	38,41,54	1.16	2 (5%)
26	SF4	K	301	11	0,12,12	-	-	-		
22	LHG	C	202	-	42,42,48	0.97	4 (9%)	45,48,54	1.10	2 (4%)
24	BCR	D	602	-	41,41,41	4.22	18 (43%)	56,56,56	5.45	36 (64%)
21	DGD	A	401	-	63,63,67	1.23	6 (9%)	77,77,81	1.17	4 (5%)
23	SQD	C	201	-	38,40,54	2.12	10 (26%)	48,51,65	5.31	6 (12%)
21	DGD	A	402	-	63,63,67	1.24	7 (11%)	77,77,81	1.18	4 (5%)

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
27	FES	1	101	20	-	-	0/1/1/1
22	LHG	F	702	-	-	25/53/53/53	-
23	SQD	L	101	-	-	22/33/53/69	0/1/1/1
22	LHG	F	705	-	-	22/48/48/53	-
24	BCR	D	603	-	-	15/29/63/63	0/2/2/2
22	LHG	B	601	-	-	22/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	F	701	-	-	23/42/62/70	0/1/1/1
25	LMG	F	703	-	-	13/35/55/70	0/1/1/1
23	SQD	D	601	-	-	26/49/69/69	0/1/1/1
22	LHG	I	201	-	-	19/48/48/53	-
26	SF4	I	203	9	-	-	0/6/5/5
26	SF4	I	202	9	-	-	0/6/5/5
22	LHG	F	704	-	-	18/40/40/53	-
26	SF4	K	301	11	-	-	0/6/5/5
22	LHG	C	202	-	-	22/47/47/53	-
24	BCR	D	602	-	-	16/29/63/63	0/2/2/2
21	DGD	A	401	-	-	25/51/91/95	0/2/2/2
23	SQD	C	201	-	-	16/35/55/69	0/1/1/1
21	DGD	A	402	-	-	15/51/91/95	0/2/2/2

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	602	BCR	C26-C25	12.93	1.56	1.34
24	D	603	BCR	C26-C25	12.76	1.55	1.34
24	D	602	BCR	C5-C6	12.40	1.55	1.34
24	D	603	BCR	C5-C6	11.61	1.54	1.34
24	D	602	BCR	C10-C9	8.52	1.55	1.35
24	D	603	BCR	C10-C9	8.45	1.55	1.35
24	D	603	BCR	C14-C13	8.32	1.55	1.35
24	D	603	BCR	C17-C18	8.31	1.55	1.35
24	D	602	BCR	C14-C13	7.93	1.54	1.35
24	D	602	BCR	C17-C18	7.90	1.54	1.35
24	D	602	BCR	C21-C22	7.81	1.53	1.35
24	D	603	BCR	C21-C22	7.78	1.53	1.35
23	D	601	SQD	O9-S	7.57	1.66	1.45
23	C	201	SQD	O9-S	7.56	1.66	1.45
23	L	101	SQD	O9-S	7.43	1.66	1.45
23	C	201	SQD	O8-S	5.11	1.66	1.47
23	D	601	SQD	O8-S	5.05	1.66	1.47
23	L	101	SQD	O8-S	4.99	1.66	1.47
24	D	603	BCR	C23-C22	4.38	1.55	1.46
23	C	201	SQD	O5-C5	4.21	1.54	1.44
23	D	601	SQD	O5-C5	4.18	1.54	1.44
24	D	602	BCR	C23-C22	4.12	1.54	1.46
24	D	603	BCR	C15-C14	4.10	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	101	SQD	O5-C5	4.06	1.54	1.44
24	D	602	BCR	C11-C10	4.04	1.55	1.43
24	D	603	BCR	C11-C10	4.02	1.55	1.43
24	D	602	BCR	C15-C14	3.78	1.54	1.43
24	D	602	BCR	C7-C6	3.67	1.57	1.45
21	A	401	DGD	O6E-C1E	3.67	1.51	1.41
24	D	603	BCR	C16-C17	3.59	1.54	1.43
21	A	402	DGD	O6D-C1D	3.56	1.51	1.41
21	A	402	DGD	O6E-C1E	3.52	1.50	1.41
24	D	602	BCR	C16-C17	3.46	1.53	1.43
24	D	603	BCR	C20-C21	3.45	1.53	1.43
24	D	603	BCR	C19-C18	3.43	1.53	1.46
24	D	603	BCR	C12-C13	3.37	1.53	1.46
24	D	602	BCR	C20-C21	3.36	1.53	1.43
24	D	602	BCR	C24-C25	3.30	1.56	1.45
24	D	603	BCR	C7-C6	3.30	1.56	1.45
21	A	401	DGD	O6D-C1D	3.29	1.50	1.41
21	A	401	DGD	O2G-C1B	3.27	1.43	1.34
24	D	603	BCR	C24-C25	3.26	1.56	1.45
24	D	602	BCR	C19-C18	3.25	1.52	1.46
21	A	402	DGD	O2G-C1B	3.24	1.43	1.34
24	D	602	BCR	C12-C13	3.14	1.52	1.46
23	C	201	SQD	O48-C23	3.11	1.42	1.33
23	L	101	SQD	O48-C23	3.08	1.42	1.33
23	C	201	SQD	O47-C45	-2.98	1.39	1.46
23	D	601	SQD	O47-C45	-2.96	1.39	1.46
23	D	601	SQD	O48-C23	2.92	1.41	1.33
22	C	202	LHG	O7-C5	-2.75	1.40	1.46
22	F	705	LHG	O7-C5	-2.73	1.40	1.46
22	B	601	LHG	O7-C5	-2.72	1.40	1.46
22	F	702	LHG	O7-C5	-2.68	1.40	1.46
24	D	603	BCR	C8-C9	2.68	1.51	1.46
23	D	601	SQD	O5-C1	2.62	1.48	1.41
22	F	704	LHG	O7-C5	-2.61	1.40	1.46
22	I	201	LHG	O7-C5	-2.61	1.40	1.46
21	A	402	DGD	O1G-C1A	2.55	1.40	1.33
21	A	402	DGD	O1G-C1G	-2.54	1.39	1.45
25	F	701	LMG	C4-C5	2.52	1.58	1.53
23	C	201	SQD	O47-C7	2.51	1.41	1.34
23	L	101	SQD	O47-C7	2.51	1.41	1.34
21	A	401	DGD	O1G-C1G	-2.50	1.39	1.45
22	C	202	LHG	O8-C23	2.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	201	SQD	O5-C1	2.49	1.48	1.41
22	F	705	LHG	O8-C23	2.49	1.40	1.33
23	L	101	SQD	O47-C45	-2.48	1.40	1.46
22	F	702	LHG	O8-C23	2.47	1.40	1.33
24	D	602	BCR	C8-C9	2.46	1.51	1.46
25	F	703	LMG	C4-C5	2.45	1.58	1.53
21	A	401	DGD	O1G-C1A	2.45	1.40	1.33
23	D	601	SQD	O47-C7	2.43	1.41	1.34
24	D	602	BCR	C30-C25	2.42	1.56	1.53
22	I	201	LHG	O8-C23	2.42	1.40	1.33
22	B	601	LHG	O8-C23	2.41	1.40	1.33
22	F	704	LHG	O8-C23	2.36	1.40	1.33
23	D	601	SQD	O2-C2	2.36	1.48	1.43
23	L	101	SQD	O5-C1	2.31	1.47	1.41
25	F	701	LMG	O6-C1	2.27	1.47	1.41
22	I	201	LHG	O7-C7	2.24	1.40	1.34
22	B	601	LHG	O8-C6	-2.24	1.40	1.45
23	L	101	SQD	O2-C2	2.23	1.48	1.43
22	F	704	LHG	O7-C7	2.21	1.40	1.34
22	F	704	LHG	O8-C6	-2.20	1.40	1.45
22	F	702	LHG	O7-C7	2.20	1.40	1.34
23	C	201	SQD	O3-C3	2.19	1.48	1.43
21	A	402	DGD	O2G-C2G	-2.19	1.41	1.46
22	B	601	LHG	O7-C7	2.18	1.40	1.34
23	C	201	SQD	C3-C2	-2.17	1.46	1.52
23	C	201	SQD	O2-C2	2.17	1.48	1.43
22	F	705	LHG	O8-C6	-2.17	1.40	1.45
23	D	601	SQD	C3-C2	-2.17	1.46	1.52
23	D	601	SQD	O3-C3	2.17	1.48	1.43
23	L	101	SQD	O3-C3	2.16	1.48	1.43
24	D	603	BCR	C38-C26	2.15	1.54	1.50
22	C	202	LHG	O7-C7	2.14	1.40	1.34
22	I	201	LHG	O8-C6	-2.14	1.40	1.45
22	F	702	LHG	O8-C6	-2.13	1.40	1.45
22	F	705	LHG	O7-C7	2.13	1.40	1.34
22	C	202	LHG	O8-C6	-2.09	1.40	1.45
24	D	602	BCR	C38-C26	2.04	1.54	1.50
21	A	401	DGD	O3G-C1D	-2.04	1.36	1.40
24	D	603	BCR	C27-C26	2.04	1.54	1.51
25	F	701	LMG	O1-C7	-2.02	1.40	1.43
21	A	402	DGD	O5D-C1E	-2.01	1.36	1.40
25	F	703	LMG	O7-C8	-2.01	1.41	1.46

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	601	SQD	O9-S-C6	23.77	142.25	106.76
23	C	201	SQD	O9-S-C6	23.75	142.22	106.76
23	L	101	SQD	O9-S-C6	23.72	142.17	106.76
23	C	201	SQD	O7-S-C6	-22.26	73.52	106.76
23	D	601	SQD	O7-S-C6	-22.16	73.66	106.76
23	L	101	SQD	O7-S-C6	-21.94	73.99	106.76
24	D	603	BCR	C33-C5-C6	-14.70	108.44	124.48
24	D	602	BCR	C33-C5-C6	-14.37	108.80	124.48
24	D	602	BCR	C20-C21-C22	-12.86	109.24	127.28
24	D	603	BCR	C38-C26-C25	-11.63	111.79	124.48
24	D	603	BCR	C15-C14-C13	-11.45	111.22	127.28
23	C	201	SQD	O9-S-O7	-11.30	77.07	113.82
23	D	601	SQD	O8-S-O7	11.26	139.58	111.40
23	D	601	SQD	O9-S-O7	-11.26	77.21	113.82
23	L	101	SQD	O9-S-O7	-11.13	77.64	113.82
23	C	201	SQD	O8-S-O7	11.12	139.23	111.40
24	D	602	BCR	C11-C10-C9	-11.03	111.80	127.28
23	L	101	SQD	O8-S-O7	10.87	138.59	111.40
24	D	602	BCR	C15-C14-C13	-10.65	112.35	127.28
24	D	602	BCR	C38-C26-C25	-10.61	112.91	124.48
24	D	603	BCR	C16-C17-C18	-10.51	112.54	127.28
24	D	603	BCR	C11-C10-C9	-10.44	112.64	127.28
24	D	602	BCR	C16-C17-C18	-10.44	112.64	127.28
24	D	603	BCR	C20-C21-C22	-9.18	114.41	127.28
24	D	602	BCR	C36-C18-C17	-8.89	108.41	122.82
24	D	602	BCR	C35-C13-C14	-8.59	108.89	122.82
24	D	602	BCR	C37-C22-C21	-8.38	109.24	122.82
24	D	602	BCR	C34-C9-C10	-8.28	109.41	122.82
24	D	603	BCR	C35-C13-C14	-8.18	109.57	122.82
24	D	603	BCR	C36-C18-C17	-7.90	110.01	122.82
24	D	603	BCR	C37-C22-C21	-7.55	110.58	122.82
24	D	603	BCR	C23-C22-C21	-7.46	107.27	119.01
24	D	603	BCR	C34-C9-C10	-7.17	111.20	122.82
24	D	602	BCR	C37-C22-C23	-6.79	107.71	118.09
24	D	603	BCR	C8-C9-C10	-6.61	108.61	119.01
24	D	603	BCR	C1-C6-C5	-6.43	113.85	122.64
24	D	603	BCR	C35-C13-C12	-6.38	108.34	118.09
24	D	603	BCR	C4-C5-C6	-6.35	114.12	122.70
24	D	602	BCR	C12-C13-C14	-6.12	109.39	119.01
24	D	602	BCR	C27-C26-C25	-6.05	114.52	122.70
24	D	603	BCR	C19-C18-C17	-5.95	109.66	119.01
24	D	602	BCR	C19-C18-C17	-5.92	109.69	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	603	BCR	C7-C6-C5	-5.90	107.96	121.56
24	D	602	BCR	C8-C9-C10	-5.76	109.94	119.01
24	D	602	BCR	C36-C18-C19	-5.74	109.32	118.09
24	D	602	BCR	C34-C9-C8	-5.66	109.44	118.09
24	D	602	BCR	C35-C13-C12	-5.21	110.12	118.09
24	D	603	BCR	C24-C25-C26	-5.14	109.72	121.56
24	D	602	BCR	C30-C25-C26	-5.11	115.65	122.64
24	D	603	BCR	C37-C22-C23	-4.99	110.47	118.09
24	D	603	BCR	C12-C13-C14	-4.89	111.32	119.01
24	D	603	BCR	C30-C25-C26	-4.88	115.96	122.64
24	D	602	BCR	C4-C5-C6	-4.88	116.11	122.70
24	D	603	BCR	C27-C26-C25	-4.88	116.11	122.70
24	D	602	BCR	C23-C22-C21	-4.81	111.45	119.01
24	D	603	BCR	C36-C18-C19	-4.76	110.81	118.09
24	D	603	BCR	C34-C9-C8	-4.75	110.83	118.09
24	D	602	BCR	C1-C6-C5	-4.60	116.35	122.64
24	D	602	BCR	C7-C8-C9	-4.40	119.73	126.23
22	F	702	LHG	O7-C7-C8	4.26	120.70	111.48
23	D	601	SQD	O47-C7-C8	4.25	120.68	111.48
24	D	602	BCR	C29-C30-C25	4.23	116.58	110.44
22	F	704	LHG	O7-C7-C8	4.14	120.43	111.48
24	D	602	BCR	C24-C25-C26	-4.09	112.13	121.56
22	C	202	LHG	O7-C7-C8	4.07	120.29	111.48
24	D	602	BCR	C7-C6-C5	-4.04	112.26	121.56
21	A	402	DGD	O2G-C1B-C2B	4.01	120.15	111.48
24	D	602	BCR	C33-C5-C4	-3.96	105.16	113.60
22	B	601	LHG	O7-C7-C8	3.93	119.99	111.48
22	I	201	LHG	O7-C7-C8	3.92	119.95	111.48
23	L	101	SQD	O47-C7-C8	3.88	119.87	111.48
22	F	705	LHG	O7-C7-C8	3.87	119.86	111.48
24	D	603	BCR	C7-C8-C9	-3.83	120.57	126.23
21	A	401	DGD	O2G-C1B-C2B	3.78	119.66	111.48
24	D	602	BCR	C23-C24-C25	-3.62	117.32	127.00
23	C	201	SQD	O47-C7-C8	3.51	119.08	111.48
24	D	603	BCR	C29-C30-C25	3.31	115.25	110.44
21	A	402	DGD	C4E-C3E-C2E	3.04	116.16	110.83
21	A	401	DGD	C4D-C3D-C2D	3.04	116.16	110.83
23	L	101	SQD	C4-C3-C2	3.04	116.16	110.83
24	D	603	BCR	C11-C12-C13	-3.02	118.09	126.36
25	F	701	LMG	O6-C5-C4	3.02	115.13	109.70
21	A	402	DGD	O1G-C1A-C2A	2.97	120.90	111.83
25	F	703	LMG	O6-C1-O1	-2.85	103.31	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	603	BCR	C38-C26-C27	-2.83	107.57	113.60
22	F	705	LHG	O8-C23-C24	2.81	120.39	111.83
22	F	704	LHG	O8-C23-C24	2.74	120.19	111.83
23	C	201	SQD	O48-C23-C24	2.72	120.12	111.83
22	F	702	LHG	O8-C23-C24	2.71	120.11	111.83
22	C	202	LHG	O8-C23-C24	2.71	120.09	111.83
21	A	401	DGD	O1G-C1A-C2A	2.70	120.08	111.83
24	D	602	BCR	C11-C12-C13	-2.69	118.99	126.36
23	L	101	SQD	O48-C23-C24	2.67	119.99	111.83
24	D	603	BCR	C2-C1-C6	2.67	114.32	110.44
22	B	601	LHG	O8-C23-C24	2.64	119.89	111.83
22	I	201	LHG	O8-C23-C24	2.62	119.82	111.83
25	F	703	LMG	O1-C1-C2	-2.55	104.40	108.27
21	A	401	DGD	O3G-C1D-C2D	2.54	112.13	108.27
25	F	703	LMG	O3-C3-C2	-2.54	104.40	110.38
25	F	701	LMG	O6-C1-C2	2.51	115.52	110.37
24	D	602	BCR	C38-C26-C27	-2.50	108.26	113.60
25	F	701	LMG	C1-O6-C5	2.46	118.53	113.72
24	D	602	BCR	C15-C16-C17	-2.44	118.53	123.52
24	D	603	BCR	C23-C24-C25	-2.42	120.52	127.00
25	F	703	LMG	O1-C7-C8	-2.39	105.01	110.82
25	F	701	LMG	O3-C3-C2	-2.38	104.77	110.38
23	L	101	SQD	C1-O5-C5	-2.37	109.10	113.72
23	D	601	SQD	O48-C23-C24	2.36	119.03	111.83
24	D	602	BCR	C1-C6-C7	-2.36	109.25	115.65
25	F	701	LMG	C38-C37-C36	-2.34	102.55	114.37
24	D	602	BCR	C2-C1-C6	2.32	113.81	110.44
24	D	603	BCR	C1-C6-C7	-2.31	109.39	115.65
25	F	701	LMG	O2-C2-C1	-2.28	104.64	110.08
24	D	602	BCR	C40-C30-C25	-2.27	106.68	110.24
24	D	602	BCR	C28-C27-C26	-2.25	110.05	114.06
21	A	402	DGD	C3E-C4E-C5E	2.23	114.28	110.23
24	D	603	BCR	C33-C5-C4	-2.22	108.87	113.60
23	L	101	SQD	O6-C1-C2	2.21	111.63	108.27
24	D	602	BCR	C20-C19-C18	-2.19	120.35	126.36
24	D	603	BCR	C24-C23-C22	-2.14	123.06	126.23
25	F	701	LMG	O7-C10-O9	-2.12	118.74	123.70

There are no chirality outliers.

All (299) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	601	LHG	C3-O3-P-O5
22	B	601	LHG	C4-O6-P-O3
22	B	601	LHG	C4-O6-P-O4
22	B	601	LHG	C4-O6-P-O5
22	C	202	LHG	O1-C1-C2-O2
22	C	202	LHG	O1-C1-C2-C3
22	C	202	LHG	C1-C2-C3-O3
22	C	202	LHG	O2-C2-C3-O3
22	C	202	LHG	C8-C7-O7-C5
22	F	702	LHG	O1-C1-C2-O2
22	F	702	LHG	O1-C1-C2-C3
22	F	702	LHG	C4-O6-P-O3
22	F	702	LHG	C4-O6-P-O4
22	F	702	LHG	C4-O6-P-O5
22	F	702	LHG	O9-C7-O7-C5
22	F	702	LHG	C8-C7-O7-C5
22	F	704	LHG	C3-O3-P-O5
22	F	704	LHG	O9-C7-O7-C5
22	F	704	LHG	C8-C7-O7-C5
22	F	705	LHG	C3-O3-P-O4
22	F	705	LHG	C3-O3-P-O5
22	F	705	LHG	C3-O3-P-O6
22	F	705	LHG	C5-C4-O6-P
22	I	201	LHG	C1-C2-C3-O3
22	I	201	LHG	C2-C3-O3-P
23	C	201	SQD	C5-C6-S-O7
23	C	201	SQD	C5-C6-S-O8
23	D	601	SQD	O5-C1-O6-C44
23	D	601	SQD	C8-C7-O47-C45
23	D	601	SQD	C5-C6-S-O7
23	D	601	SQD	C5-C6-S-O8
23	L	101	SQD	C46-C45-O47-C7
23	L	101	SQD	C8-C7-O47-C45
23	L	101	SQD	O5-C5-C6-S
23	L	101	SQD	C5-C6-S-O7
23	L	101	SQD	C5-C6-S-O8
24	D	602	BCR	C5-C6-C7-C8
24	D	602	BCR	C7-C8-C9-C34
24	D	602	BCR	C11-C10-C9-C34
24	D	602	BCR	C11-C12-C13-C35
24	D	602	BCR	C12-C13-C14-C15
24	D	602	BCR	C16-C17-C18-C36
24	D	602	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	D	602	BCR	C19-C20-C21-C22
24	D	602	BCR	C20-C21-C22-C37
24	D	602	BCR	C23-C24-C25-C26
24	D	603	BCR	C5-C6-C7-C8
24	D	603	BCR	C11-C10-C9-C34
24	D	603	BCR	C11-C12-C13-C35
24	D	603	BCR	C35-C13-C14-C15
24	D	603	BCR	C13-C14-C15-C16
24	D	603	BCR	C16-C17-C18-C19
24	D	603	BCR	C16-C17-C18-C36
24	D	603	BCR	C20-C21-C22-C37
24	D	603	BCR	C21-C22-C23-C24
24	D	603	BCR	C23-C24-C25-C26
21	A	402	DGD	O1A-C1A-O1G-C1G
21	A	402	DGD	C2A-C1A-O1G-C1G
22	B	601	LHG	O10-C23-O8-C6
21	A	401	DGD	O6E-C5E-C6E-O5E
21	A	401	DGD	O1B-C1B-O2G-C2G
22	C	202	LHG	O9-C7-O7-C5
23	D	601	SQD	O49-C7-O47-C45
23	L	101	SQD	O49-C7-O47-C45
25	F	701	LMG	O9-C10-O7-C8
22	B	601	LHG	C24-C23-O8-C6
22	F	705	LHG	C24-C23-O8-C6
23	D	601	SQD	C24-C23-O48-C46
22	F	702	LHG	O10-C23-O8-C6
23	D	601	SQD	O10-C23-O48-C46
22	F	705	LHG	O2-C2-C3-O3
22	I	201	LHG	O2-C2-C3-O3
23	L	101	SQD	C24-C23-O48-C46
22	F	705	LHG	O10-C23-O8-C6
23	L	101	SQD	O10-C23-O48-C46
25	F	701	LMG	O10-C28-O8-C9
21	A	401	DGD	C4E-C5E-C6E-O5E
21	A	401	DGD	C2B-C1B-O2G-C2G
25	F	701	LMG	C11-C10-O7-C8
22	F	702	LHG	C24-C23-O8-C6
21	A	402	DGD	O6D-C1D-O3G-C3G
24	D	602	BCR	C15-C16-C17-C18
24	D	603	BCR	C9-C10-C11-C12
22	F	705	LHG	C1-C2-C3-O3
25	F	701	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
23	D	601	SQD	C2-C1-O6-C44
21	A	401	DGD	C4D-C5D-C6D-O5D
24	D	602	BCR	C17-C18-C19-C20
24	D	602	BCR	C21-C22-C23-C24
22	F	704	LHG	C7-C8-C9-C10
25	F	703	LMG	C28-C29-C30-C31
22	B	601	LHG	C23-C24-C25-C26
24	D	602	BCR	C35-C13-C14-C15
24	D	603	BCR	C7-C8-C9-C10
24	D	603	BCR	C17-C18-C19-C20
22	F	704	LHG	O1-C1-C2-C3
22	F	705	LHG	O1-C1-C2-C3
24	D	602	BCR	C11-C10-C9-C8
24	D	603	BCR	C11-C10-C9-C8
25	F	703	LMG	C34-C35-C36-C37
21	A	401	DGD	C5A-C6A-C7A-C8A
21	A	402	DGD	C3B-C4B-C5B-C6B
22	I	201	LHG	C14-C15-C16-C17
22	F	702	LHG	C16-C17-C18-C19
25	F	703	LMG	C12-C13-C14-C15
22	C	202	LHG	C34-C35-C36-C37
23	C	201	SQD	C10-C11-C12-C13
23	D	601	SQD	C28-C29-C30-C31
23	D	601	SQD	C14-C15-C16-C17
23	D	601	SQD	C25-C26-C27-C28
22	C	202	LHG	C25-C26-C27-C28
21	A	401	DGD	O6D-C5D-C6D-O5D
21	A	402	DGD	CBB-CCB-CDB-CEB
22	C	202	LHG	C11-C10-C9-C8
23	C	201	SQD	C24-C23-O48-C46
22	B	601	LHG	C25-C26-C27-C28
22	I	201	LHG	C16-C17-C18-C19
22	F	702	LHG	C28-C29-C30-C31
22	F	702	LHG	C15-C16-C17-C18
23	L	101	SQD	C26-C27-C28-C29
25	F	701	LMG	C20-C21-C22-C23
22	F	705	LHG	C8-C7-O7-C5
21	A	401	DGD	C2A-C1A-O1G-C1G
25	F	701	LMG	C34-C35-C36-C37
22	B	601	LHG	C14-C15-C16-C17
25	F	701	LMG	C35-C36-C37-C38
23	D	601	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	A	402	DGD	C2B-C1B-O2G-C2G
22	I	201	LHG	C8-C7-O7-C5
22	F	705	LHG	O9-C7-O7-C5
23	D	601	SQD	C16-C17-C18-C19
24	D	602	BCR	C37-C22-C23-C24
22	C	202	LHG	C12-C13-C14-C15
22	I	201	LHG	C25-C26-C27-C28
23	C	201	SQD	O10-C23-O48-C46
22	I	201	LHG	C26-C27-C28-C29
21	A	401	DGD	C1A-C2A-C3A-C4A
25	F	701	LMG	C33-C34-C35-C36
23	D	601	SQD	O47-C45-C46-O48
22	B	601	LHG	C15-C16-C17-C18
22	F	702	LHG	C14-C15-C16-C17
25	F	703	LMG	O6-C5-C6-O5
25	F	701	LMG	C18-C19-C20-C21
23	D	601	SQD	C26-C27-C28-C29
22	I	201	LHG	C18-C19-C20-C21
21	A	401	DGD	O1A-C1A-O1G-C1G
22	F	704	LHG	O6-C4-C5-C6
22	C	202	LHG	C7-C8-C9-C10
23	L	101	SQD	C11-C10-C9-C8
23	D	601	SQD	C11-C12-C13-C14
21	A	401	DGD	C1B-C2B-C3B-C4B
23	L	101	SQD	C7-C8-C9-C10
23	L	101	SQD	C23-C24-C25-C26
21	A	401	DGD	O1G-C1G-C2G-C3G
22	F	702	LHG	C4-C5-C6-O8
22	F	704	LHG	C4-C5-C6-O8
23	L	101	SQD	C44-C45-C46-O48
25	F	701	LMG	C7-C8-C9-O8
25	F	703	LMG	O1-C7-C8-C9
22	C	202	LHG	C24-C23-O8-C6
25	F	701	LMG	O6-C5-C6-O5
25	F	701	LMG	C16-C17-C18-C19
21	A	402	DGD	C7A-C8A-C9A-CAA
22	I	201	LHG	C11-C10-C9-C8
21	A	401	DGD	C1G-C2G-O2G-C1B
25	F	701	LMG	C7-C8-O7-C10
22	B	601	LHG	C7-C8-C9-C10
22	B	601	LHG	O6-C4-C5-O7
21	A	401	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
23	D	601	SQD	C24-C25-C26-C27
22	F	704	LHG	C29-C30-C31-C32
25	F	703	LMG	C29-C30-C31-C32
22	F	705	LHG	O7-C5-C6-O8
23	C	201	SQD	O47-C45-C46-O48
25	F	701	LMG	O7-C8-C9-O8
23	L	101	SQD	C9-C10-C11-C12
21	A	402	DGD	O1B-C1B-O2G-C2G
23	L	101	SQD	C10-C11-C12-C13
21	A	401	DGD	C2A-C3A-C4A-C5A
22	B	601	LHG	C24-C25-C26-C27
23	C	201	SQD	C9-C10-C11-C12
22	I	201	LHG	O9-C7-O7-C5
21	A	402	DGD	CCB-CDB-CEB-CFB
22	B	601	LHG	O6-C4-C5-C6
22	C	202	LHG	O10-C23-O8-C6
21	A	401	DGD	CFB-CGB-CHB-CIB
23	C	201	SQD	C28-C29-C30-C31
21	A	401	DGD	CCB-CDB-CEB-CFB
22	F	704	LHG	C11-C10-C9-C8
23	L	101	SQD	C25-C26-C27-C28
23	L	101	SQD	C28-C29-C30-C31
25	F	701	LMG	C13-C14-C15-C16
22	F	704	LHG	C9-C10-C11-C12
23	C	201	SQD	C26-C27-C28-C29
22	C	202	LHG	C4-C5-C6-O8
22	F	705	LHG	C4-C5-C6-O8
22	I	201	LHG	C4-C5-C6-O8
23	D	601	SQD	C44-C45-C46-O48
25	F	703	LMG	C32-C33-C34-C35
22	B	601	LHG	C32-C33-C34-C35
22	F	704	LHG	O6-C4-C5-O7
23	D	601	SQD	C11-C10-C9-C8
22	F	702	LHG	O7-C5-C6-O8
22	F	705	LHG	C28-C29-C30-C31
22	F	705	LHG	C7-C8-C9-C10
23	D	601	SQD	C23-C24-C25-C26
25	F	701	LMG	C28-C29-C30-C31
21	A	401	DGD	C2D-C1D-O3G-C3G
21	A	402	DGD	C3A-C4A-C5A-C6A
22	F	705	LHG	O1-C1-C2-O2
22	C	202	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
21	A	402	DGD	C9B-CAB-CBB-CCB
22	C	202	LHG	C13-C14-C15-C16
25	F	701	LMG	C17-C18-C19-C20
22	F	702	LHG	O6-C4-C5-C6
25	F	701	LMG	C29-C30-C31-C32
23	C	201	SQD	C24-C25-C26-C27
22	F	705	LHG	C11-C12-C13-C14
22	C	202	LHG	C24-C25-C26-C27
25	F	701	LMG	C15-C16-C17-C18
21	A	401	DGD	C4B-C5B-C6B-C7B
23	L	101	SQD	C24-C25-C26-C27
21	A	401	DGD	CAA-CBA-CCA-CDA
22	F	702	LHG	O6-C4-C5-O7
23	D	601	SQD	C33-C34-C35-C36
22	B	601	LHG	C27-C28-C29-C30
22	C	202	LHG	O7-C5-C6-O8
22	B	601	LHG	C30-C31-C32-C33
21	A	401	DGD	C8A-C9A-CAA-CBA
21	A	402	DGD	C6A-C7A-C8A-C9A
22	B	601	LHG	C26-C27-C28-C29
22	B	601	LHG	C33-C34-C35-C36
21	A	401	DGD	O6D-C1D-O3G-C3G
22	F	705	LHG	C29-C30-C31-C32
21	A	401	DGD	C3B-C4B-C5B-C6B
22	F	702	LHG	C29-C30-C31-C32
22	F	704	LHG	C24-C23-O8-C6
22	F	702	LHG	C2-C3-O3-P
22	F	705	LHG	C2-C3-O3-P
22	B	601	LHG	C8-C7-O7-C5
25	F	703	LMG	C11-C10-O7-C8
23	C	201	SQD	O5-C5-C6-S
21	A	401	DGD	O1G-C1G-C2G-O2G
22	F	704	LHG	O7-C5-C6-O8
22	I	201	LHG	O7-C5-C6-O8
23	D	601	SQD	O6-C44-C45-O47
25	F	703	LMG	O1-C7-C8-O7
23	C	201	SQD	C44-C45-C46-O48
23	D	601	SQD	O6-C44-C45-C46
25	F	701	LMG	C21-C22-C23-C24
25	F	701	LMG	C31-C32-C33-C34
22	F	702	LHG	C3-O3-P-O5
22	F	704	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
22	F	705	LHG	C4-O6-P-O4
22	I	201	LHG	C3-O3-P-O5
22	I	201	LHG	C4-O6-P-O3
22	I	201	LHG	C4-O6-P-O4
22	F	704	LHG	O10-C23-O8-C6
22	B	601	LHG	O9-C7-O7-C5
23	L	101	SQD	O47-C45-C46-O48
22	F	705	LHG	C27-C28-C29-C30
22	I	201	LHG	C27-C28-C29-C30
25	F	703	LMG	C8-C7-O1-C1
22	F	702	LHG	C12-C13-C14-C15
23	C	201	SQD	C27-C28-C29-C30
22	F	702	LHG	C18-C19-C20-C21
21	A	402	DGD	O1G-C1G-C2G-O2G
23	D	601	SQD	C30-C31-C32-C33
21	A	402	DGD	C8A-C9A-CAA-CBA
22	F	702	LHG	C19-C20-C21-C22
22	C	202	LHG	C26-C27-C28-C29
22	C	202	LHG	C30-C31-C32-C33
23	C	201	SQD	C11-C10-C9-C8
22	F	704	LHG	O1-C1-C2-O2
22	I	201	LHG	C15-C16-C17-C18
22	B	601	LHG	C11-C12-C13-C14
23	D	601	SQD	C12-C13-C14-C15
21	A	401	DGD	C5D-C6D-O5D-C1E
23	L	101	SQD	C45-C44-O6-C1
22	F	702	LHG	C30-C31-C32-C33
25	F	701	LMG	C14-C15-C16-C17
22	F	705	LHG	O6-C4-C5-C6
22	C	202	LHG	C9-C10-C11-C12
25	F	703	LMG	O6-C1-O1-C7
25	F	701	LMG	O7-C10-C11-C12
23	C	201	SQD	C25-C26-C27-C28
21	A	402	DGD	CAA-CBA-CCA-CDA
25	F	703	LMG	C13-C14-C15-C16
24	D	603	BCR	C11-C12-C13-C14
23	L	101	SQD	O48-C23-C24-C25
22	F	704	LHG	O8-C23-C24-C25
22	F	702	LHG	C1-C2-C3-O3
23	C	201	SQD	C5-C6-S-O9
25	F	703	LMG	O9-C10-O7-C8
22	C	202	LHG	C11-C12-C13-C14

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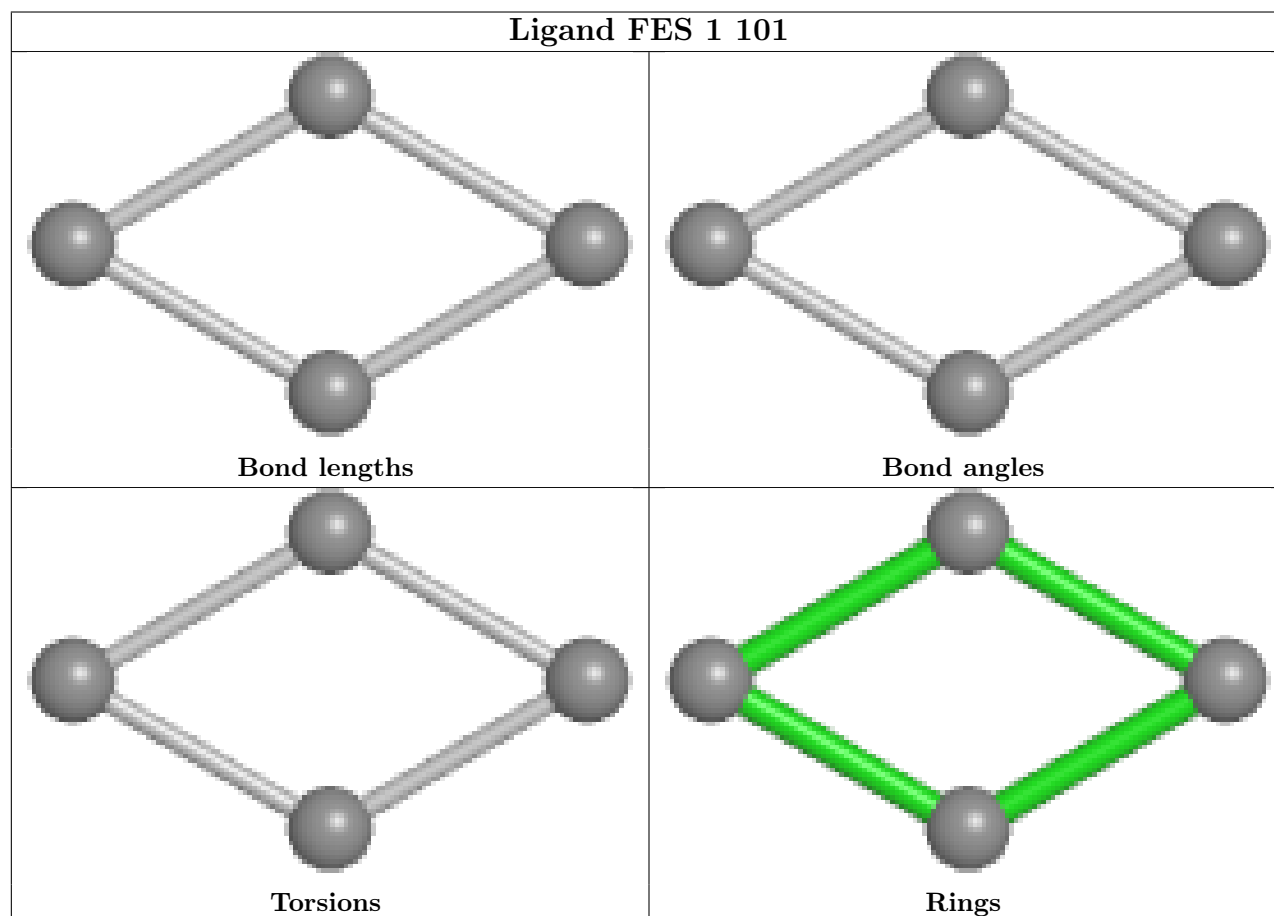
Continued from previous page...

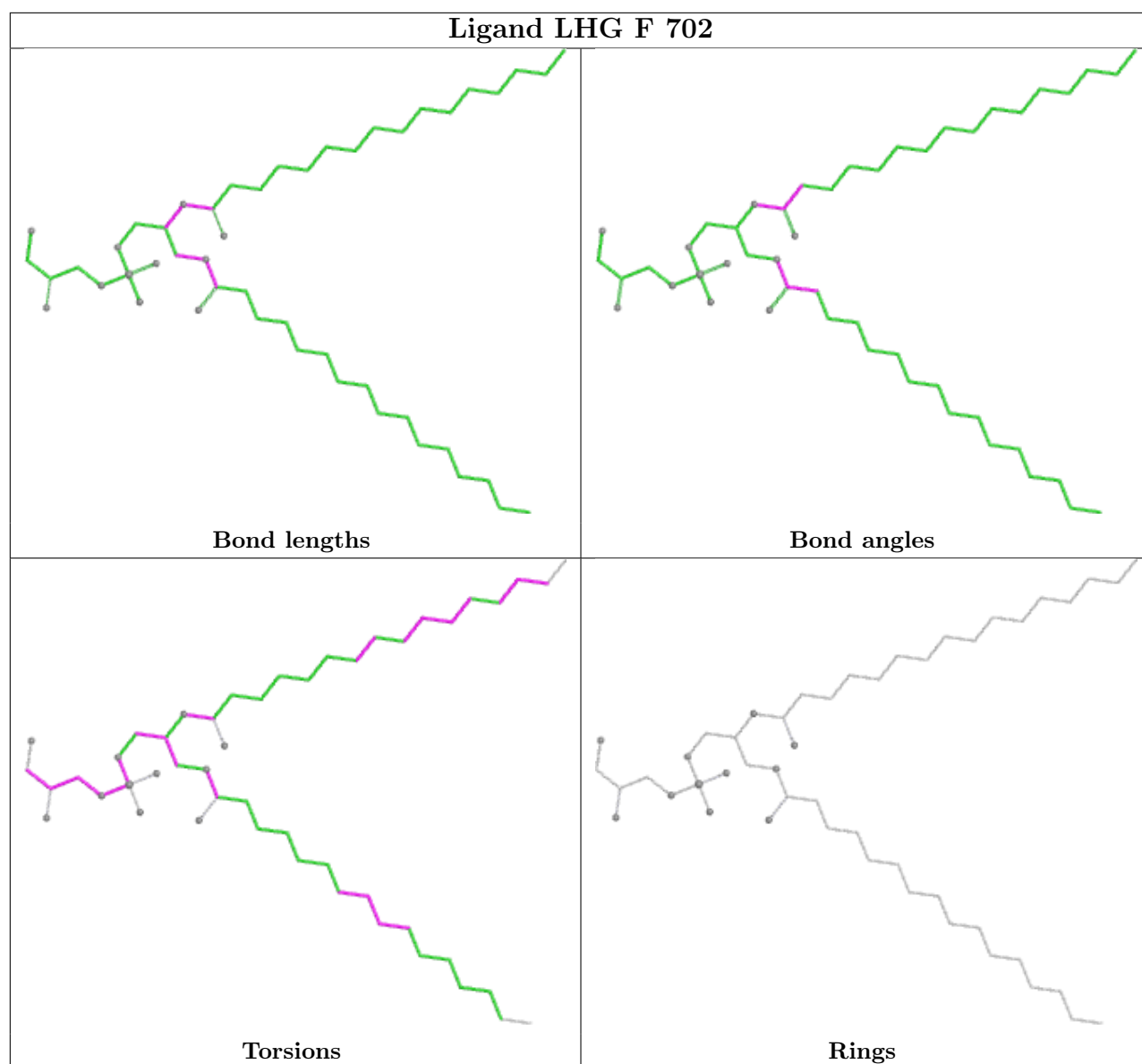
Mol	Chain	Res	Type	Atoms
22	F	704	LHG	O10-C23-C24-C25
22	I	201	LHG	O7-C7-C8-C9
23	D	601	SQD	O48-C23-C24-C25
23	L	101	SQD	O10-C23-C24-C25

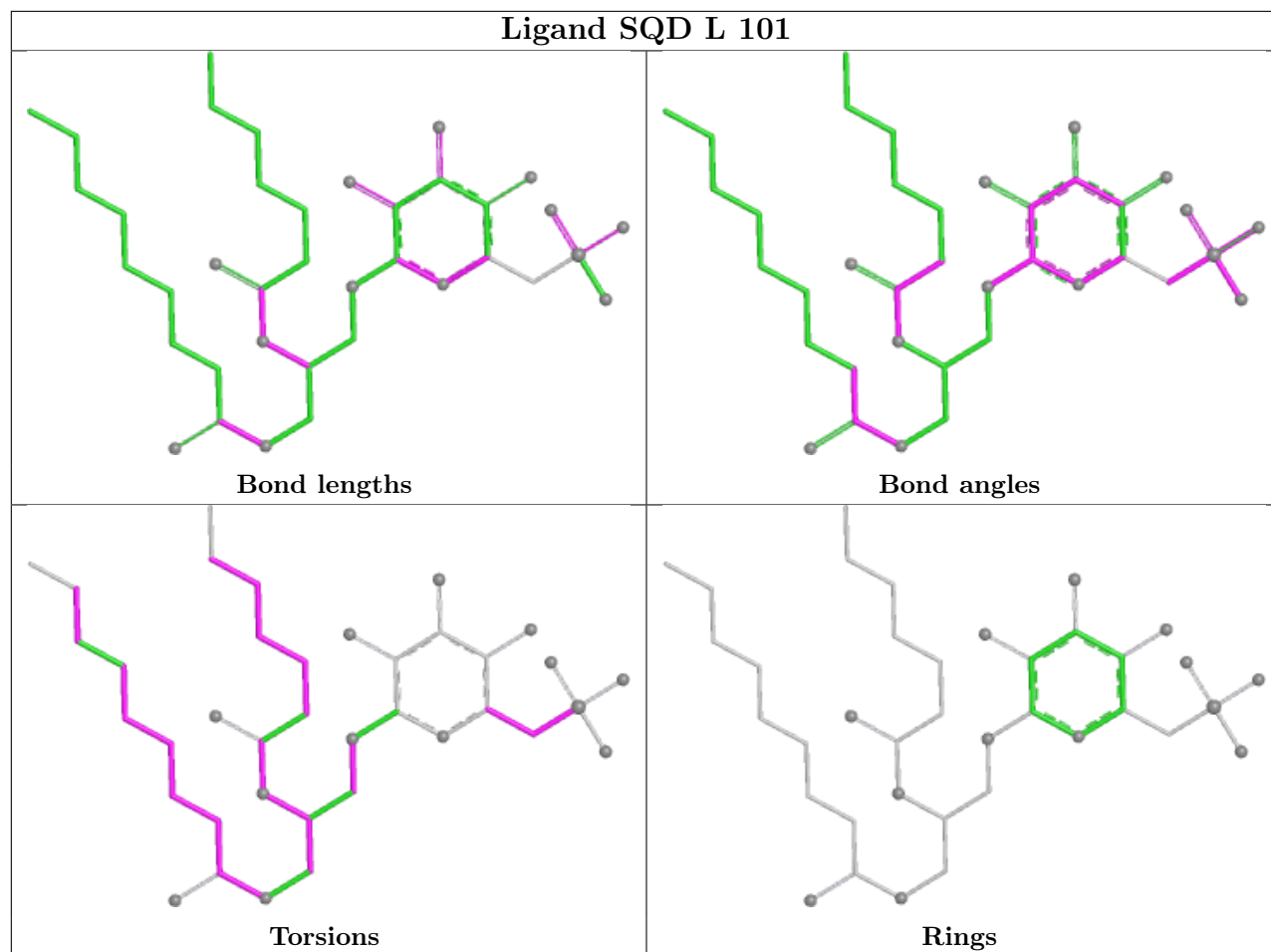
There are no ring outliers.

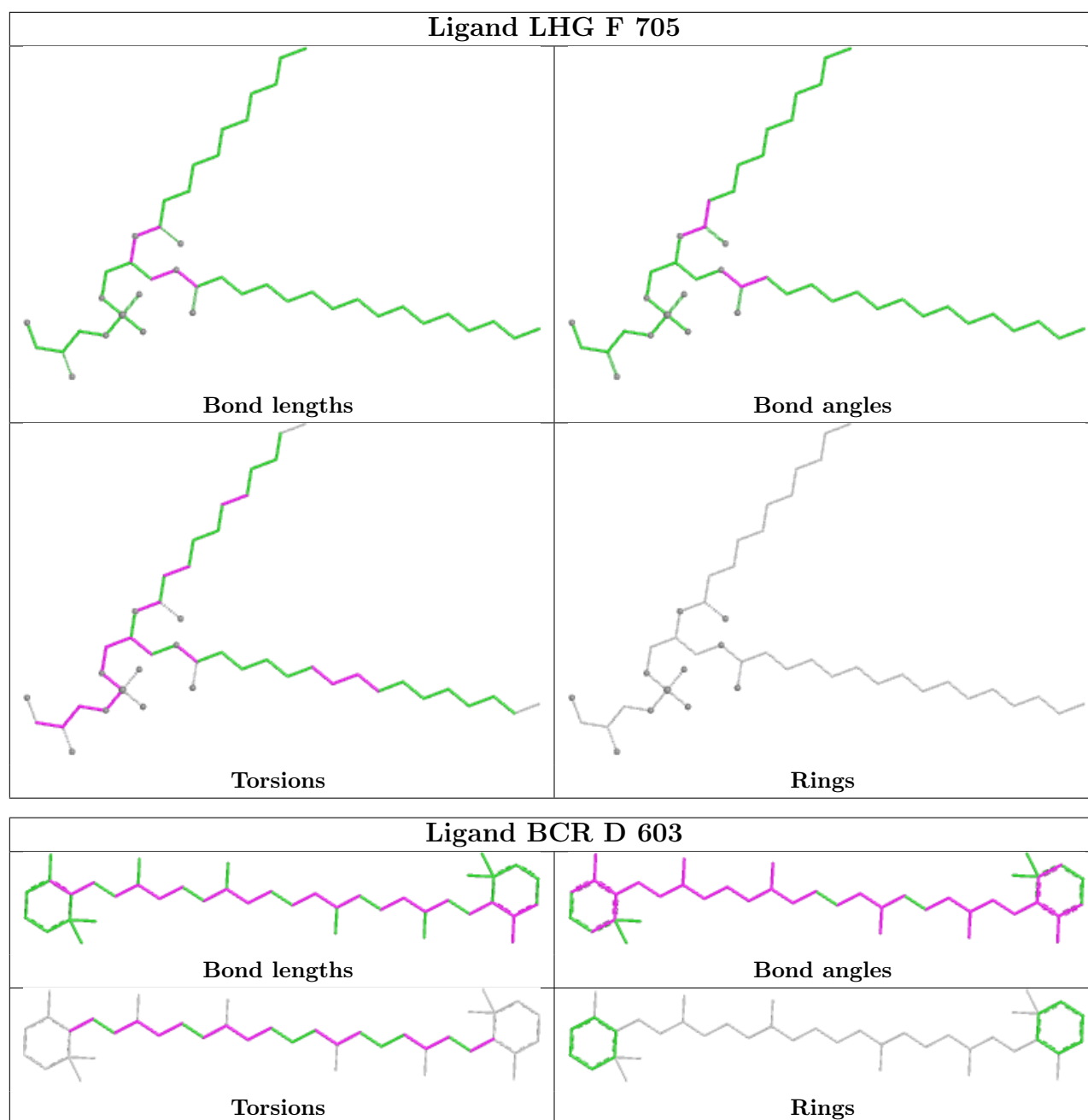
No monomer is involved in short contacts.

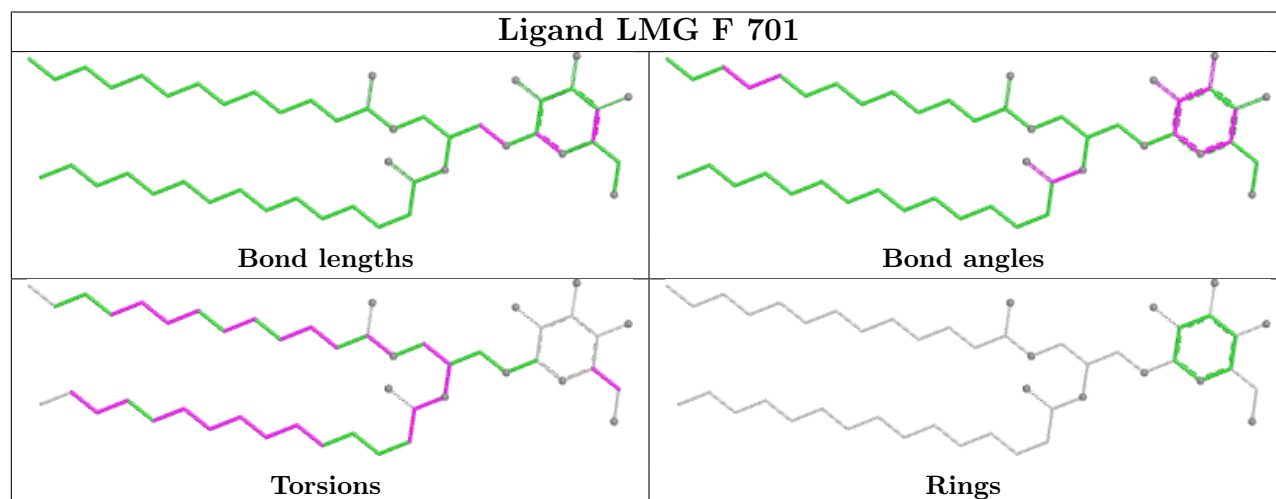
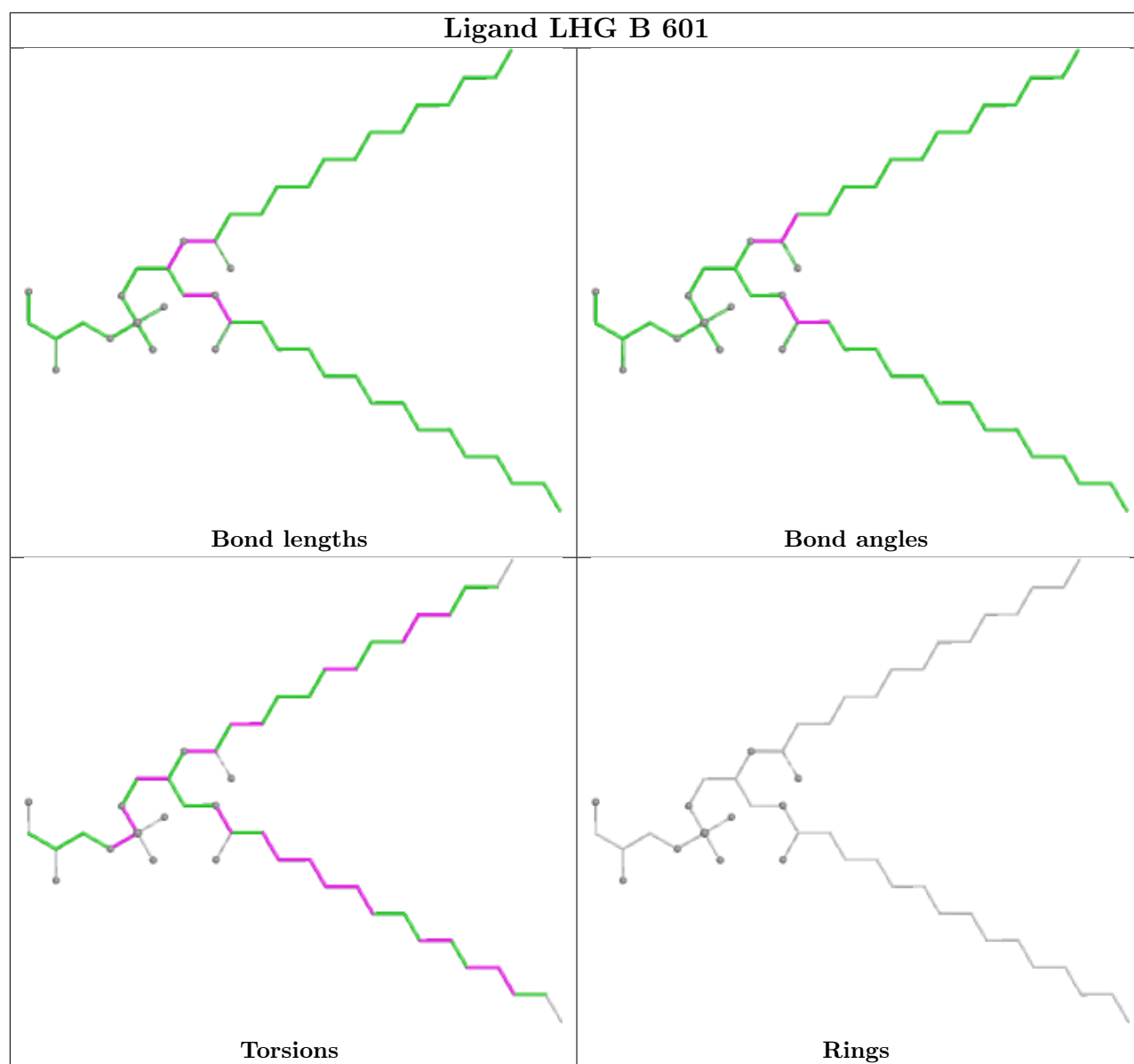
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

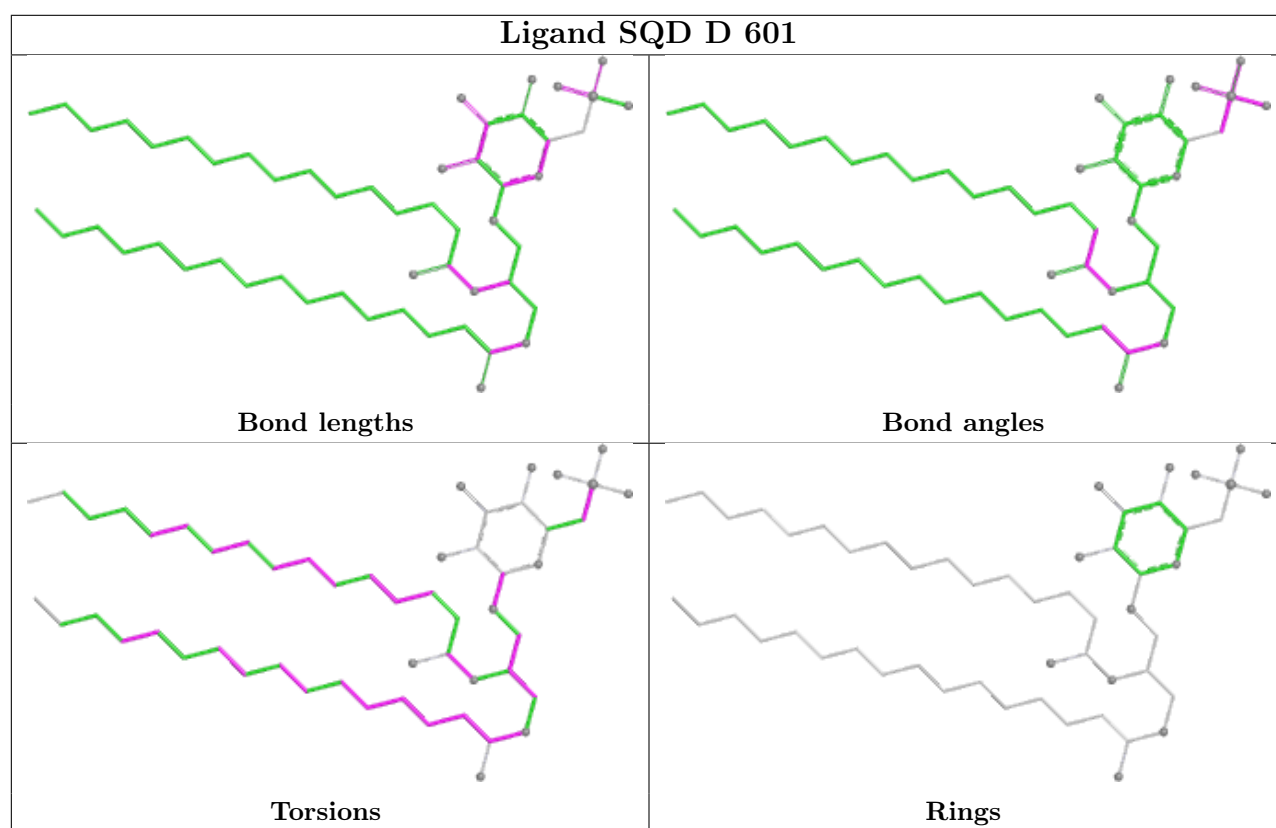
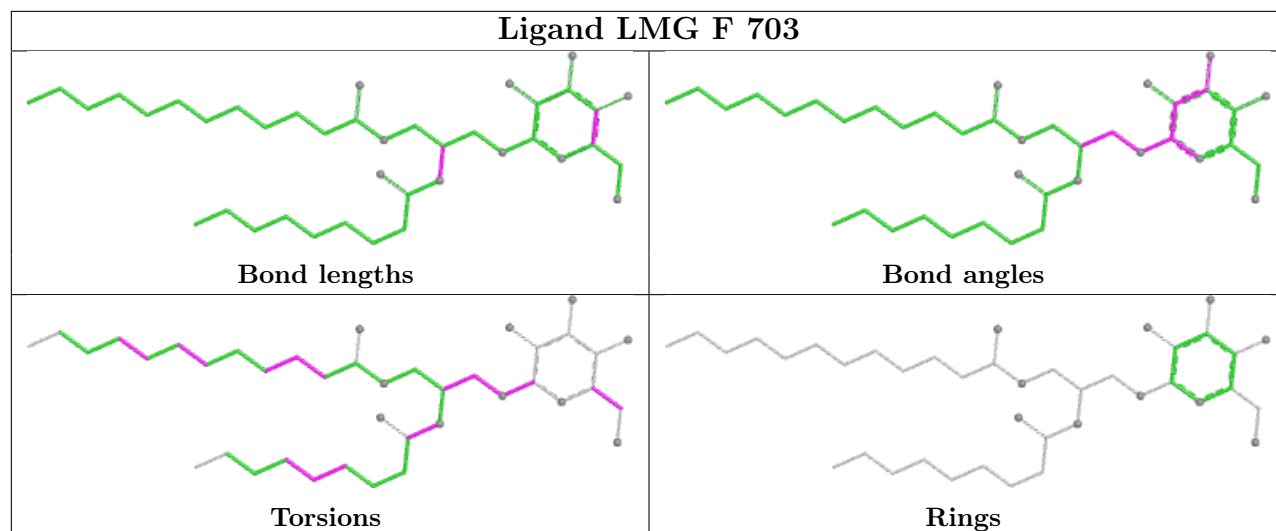




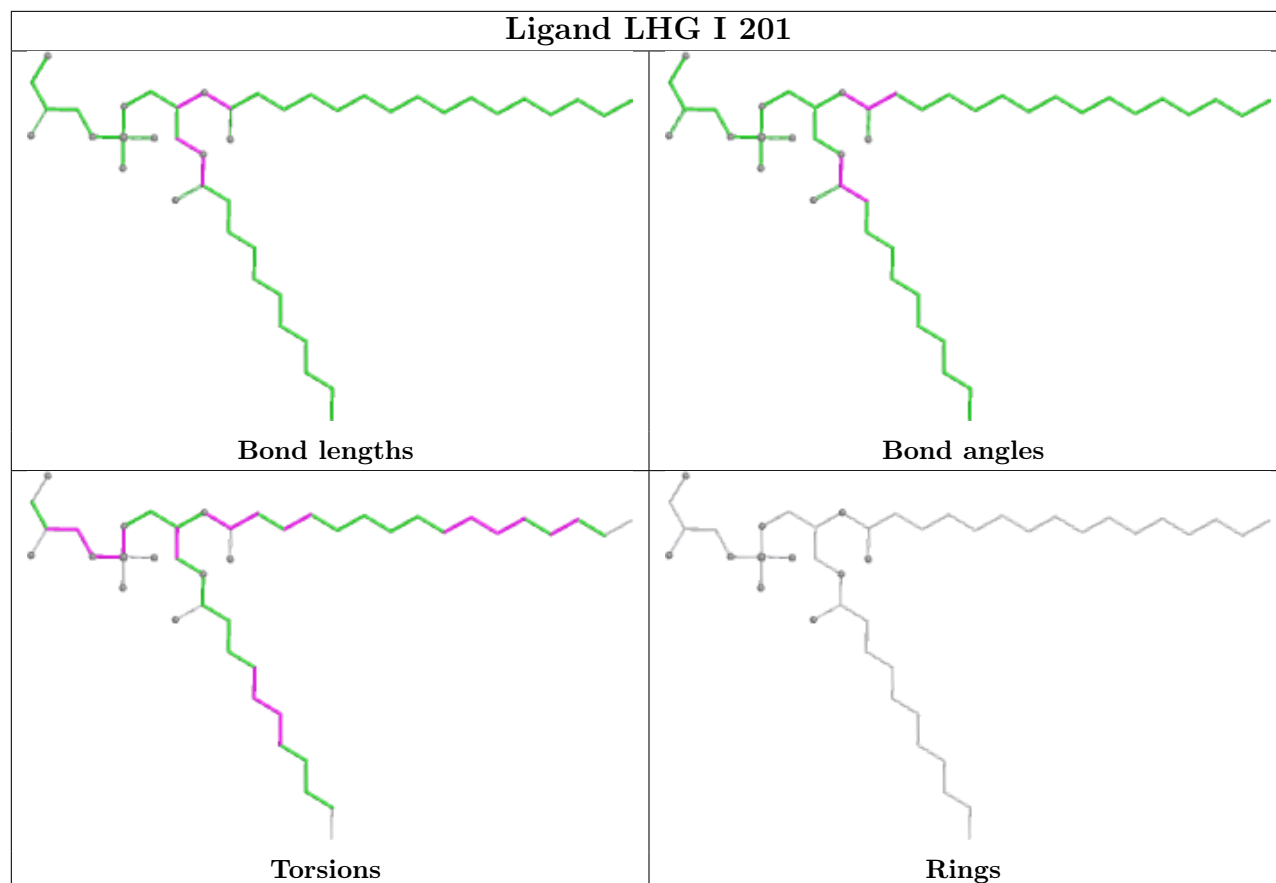




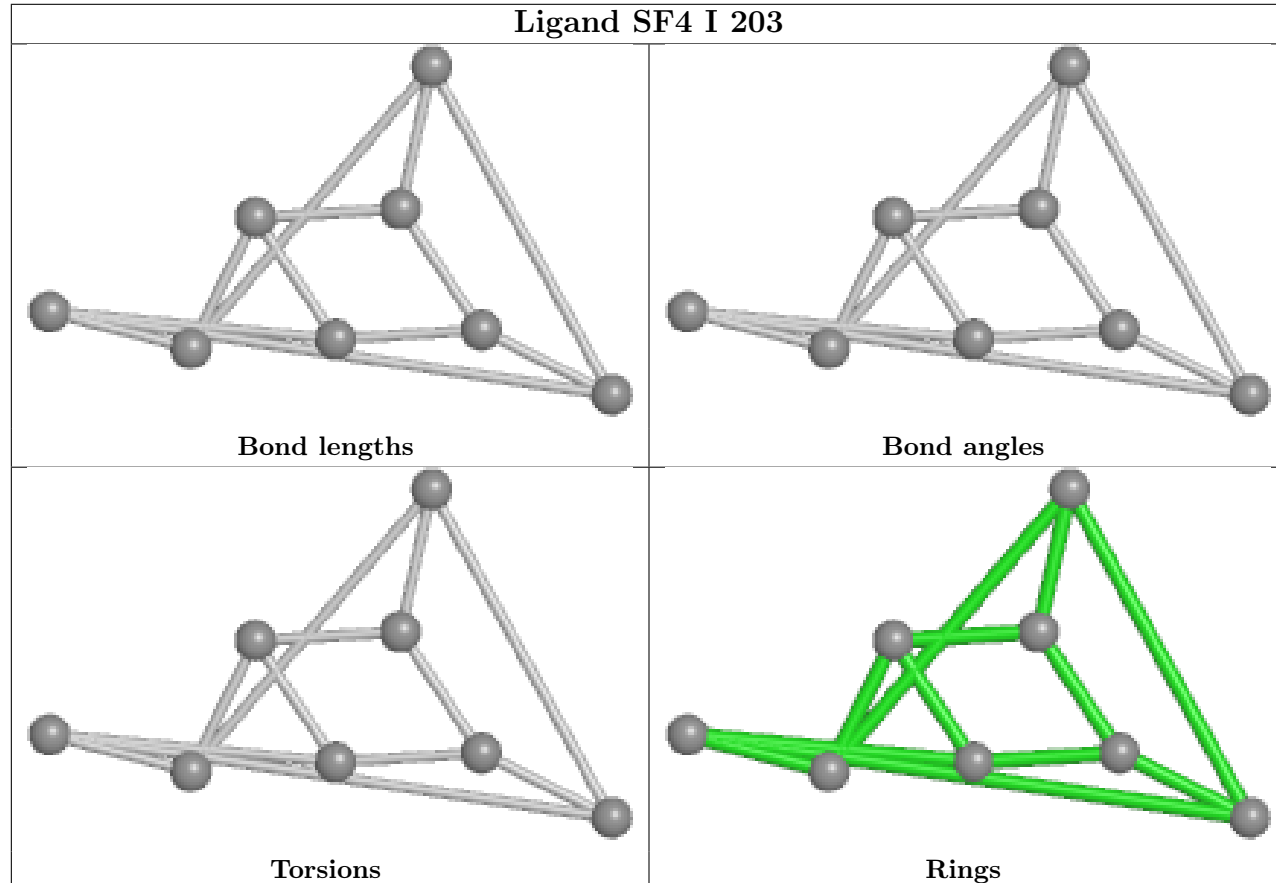


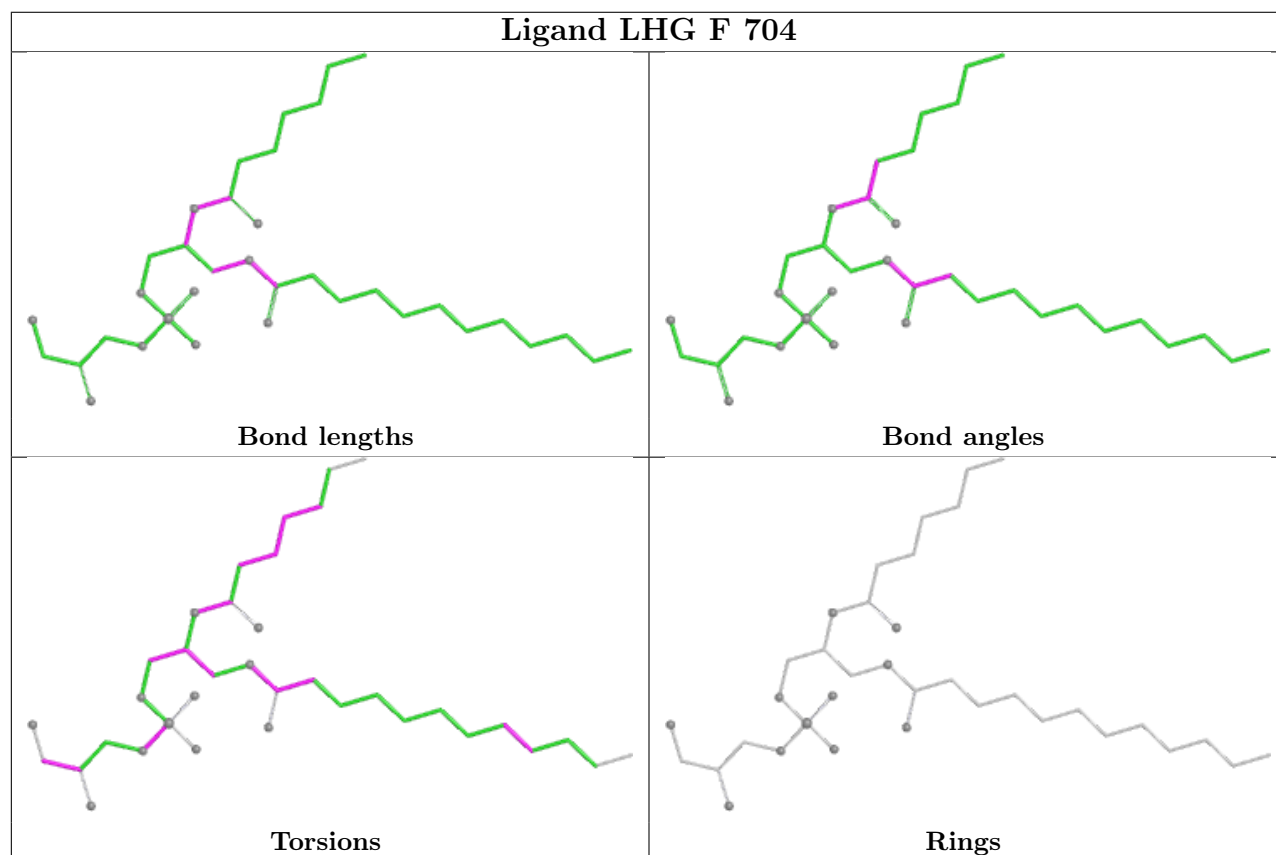
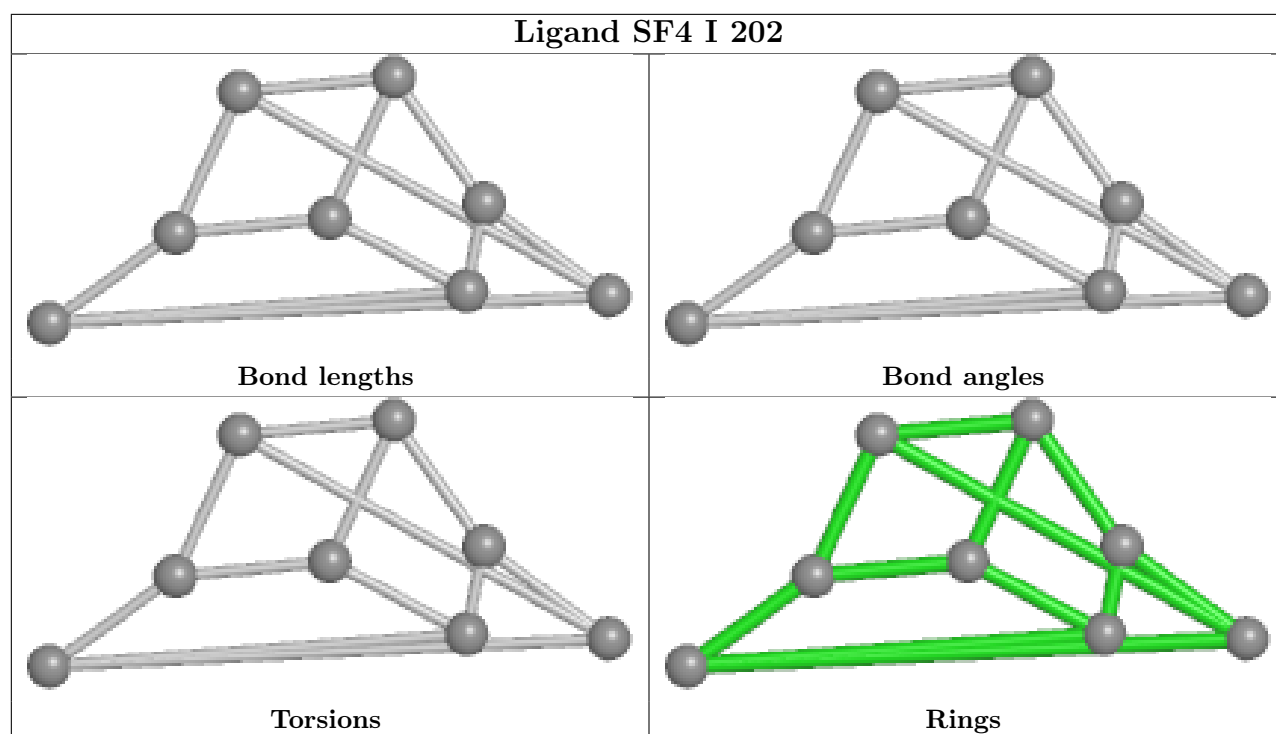


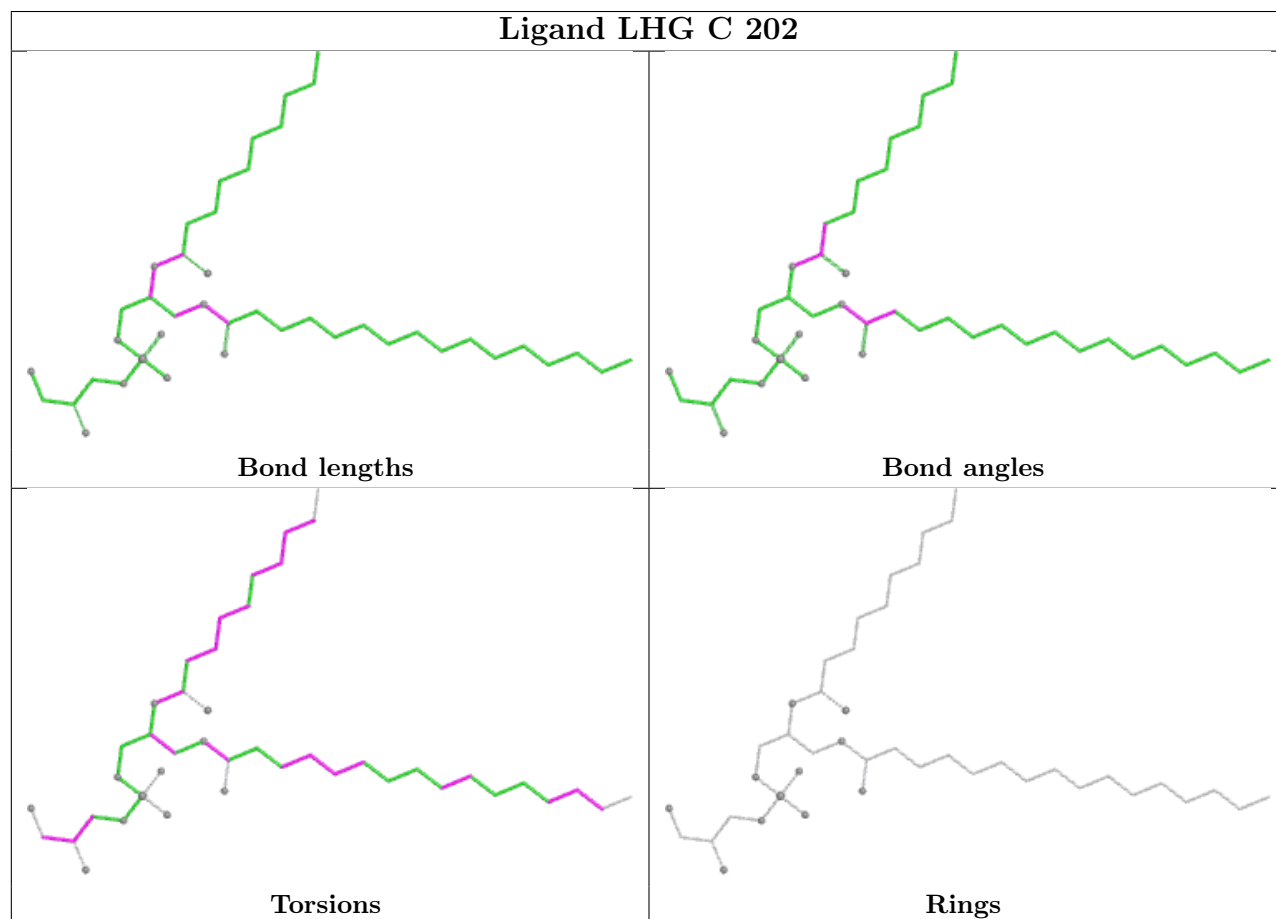
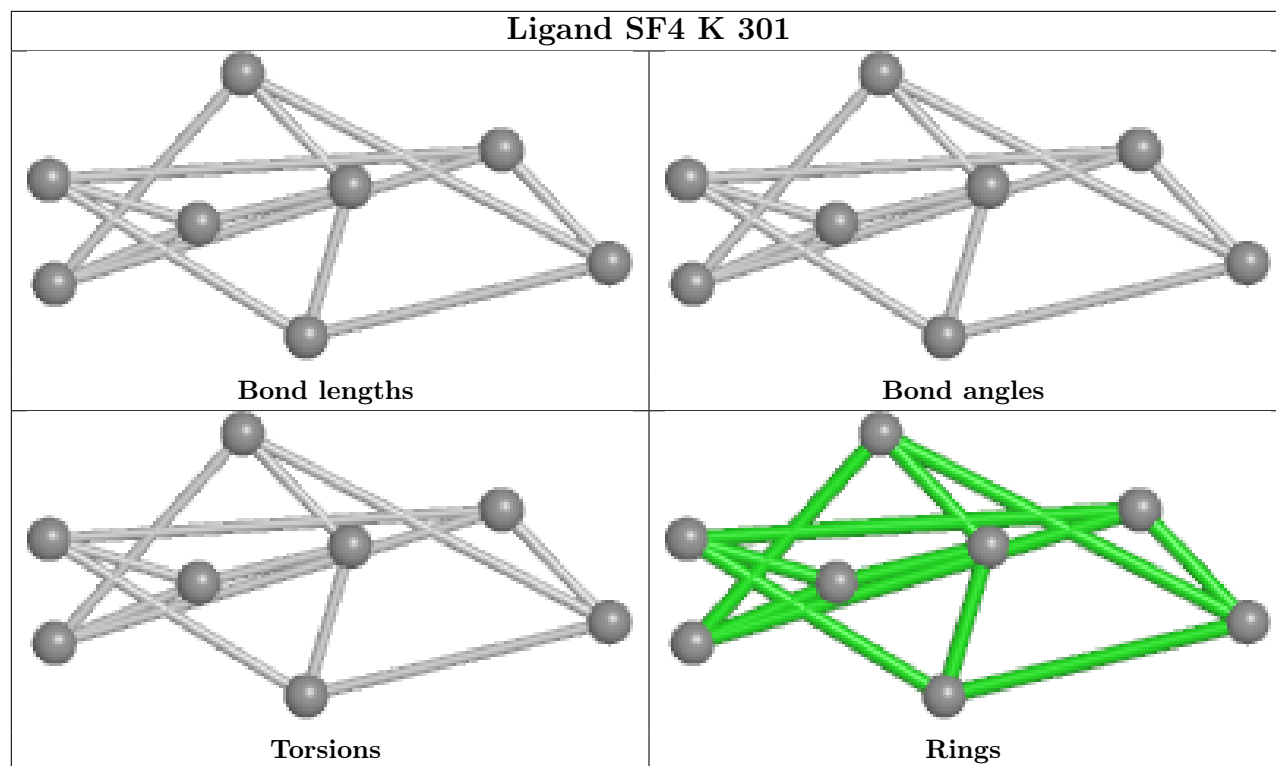
Ligand LHG I 201

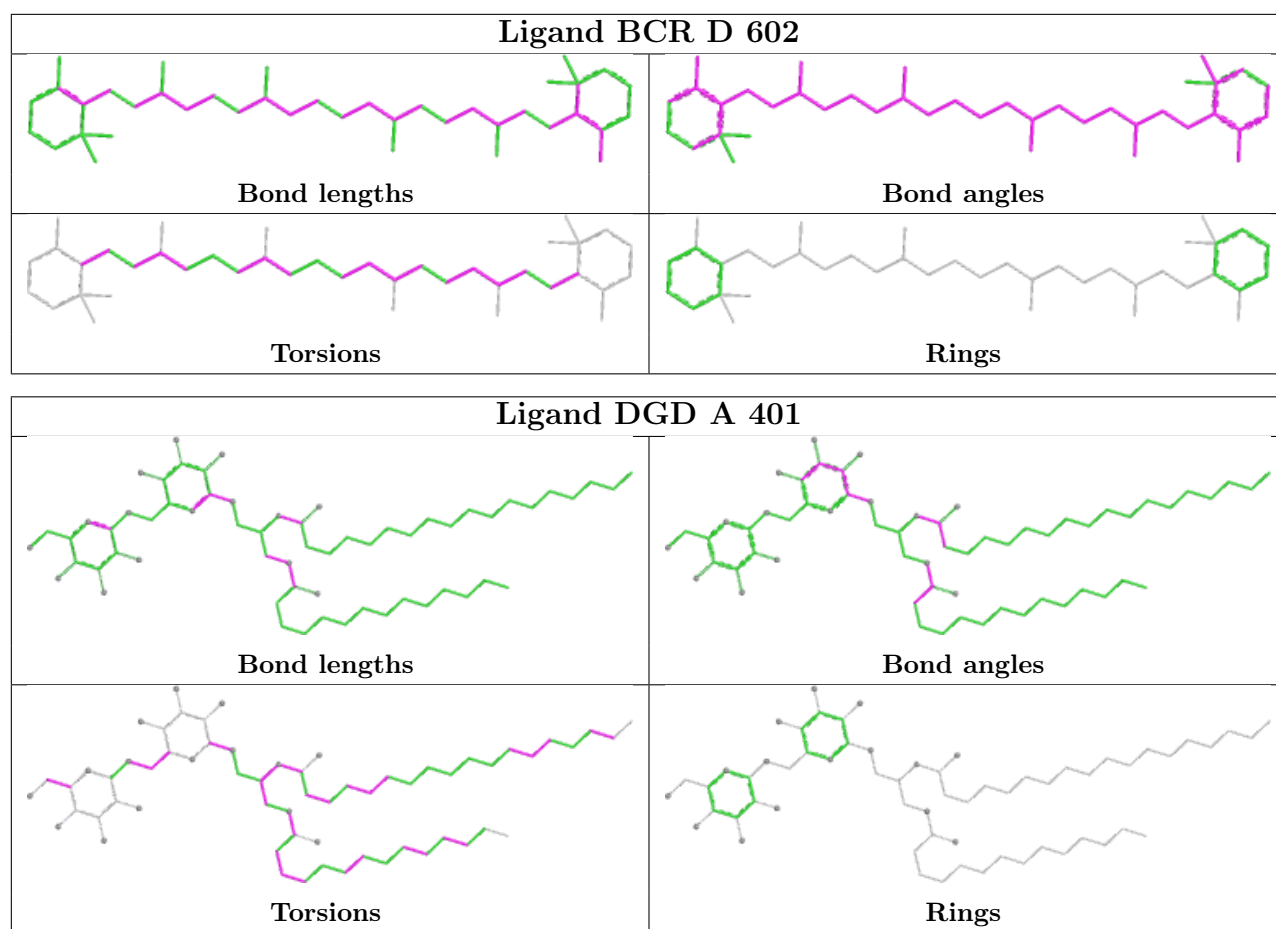


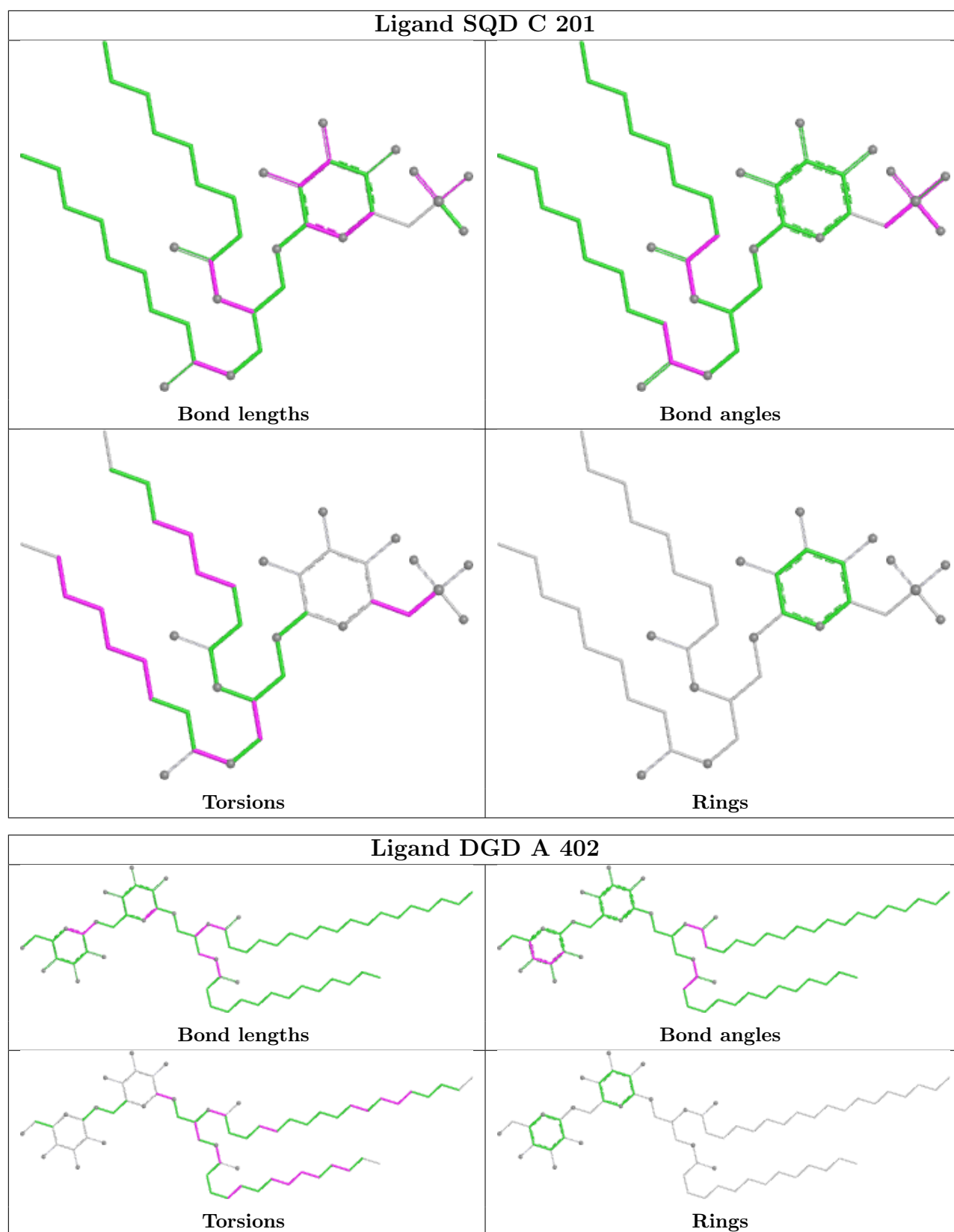
Ligand SF4 I 203











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.

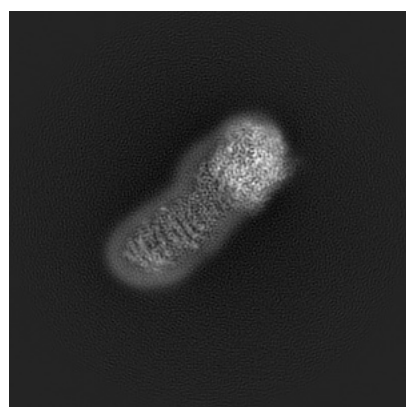
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9989. These allow visual inspection of the internal detail of the map and identification of artifacts.

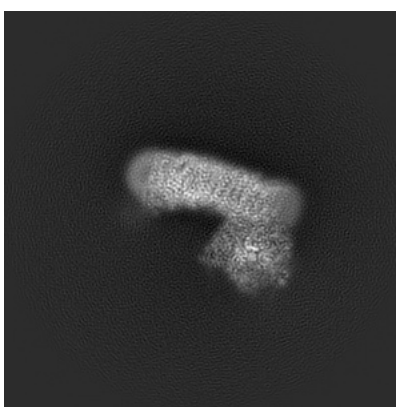
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

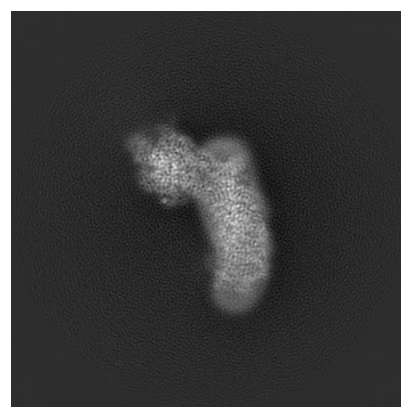
6.1.1 Primary map



X



Y

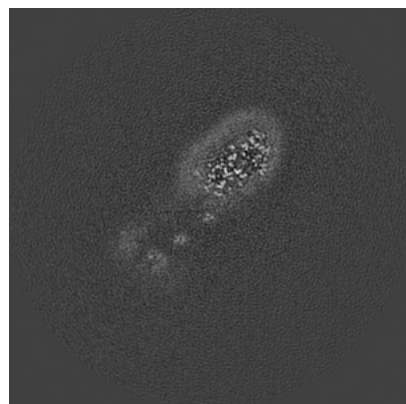


Z

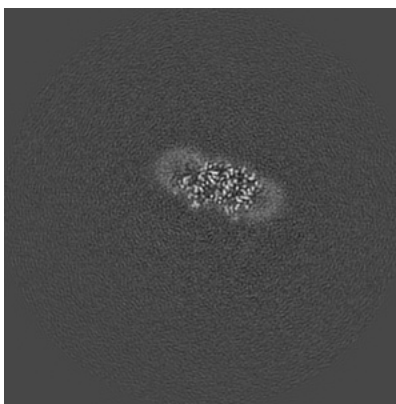
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

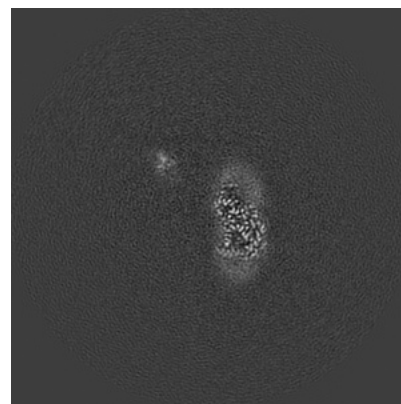
6.2.1 Primary map



X Index: 200



Y Index: 200

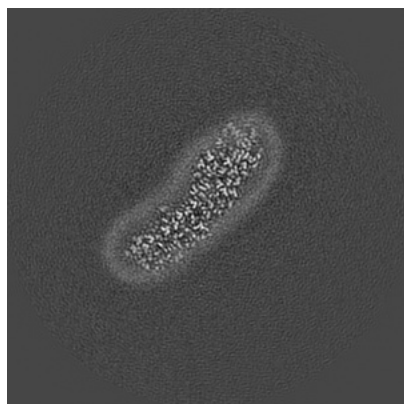


Z Index: 200

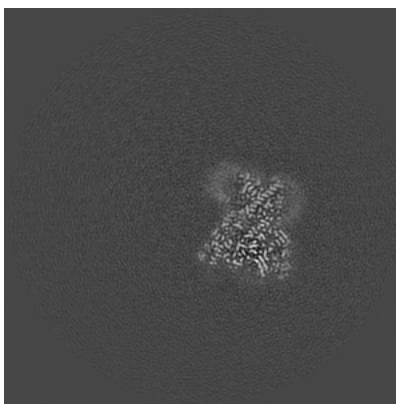
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

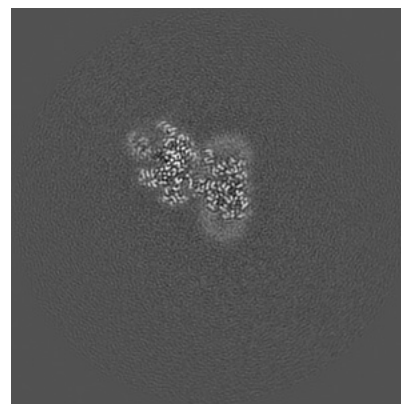
6.3.1 Primary map



X Index: 221



Y Index: 246

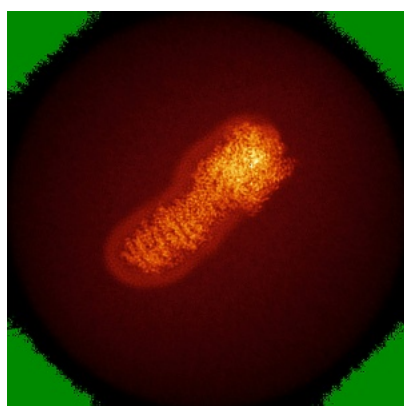


Z Index: 242

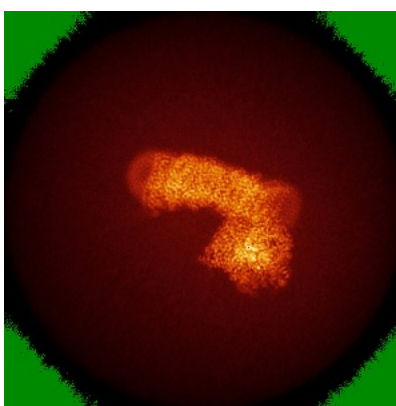
The images above show the largest variance slices of the map in three orthogonal directions.

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

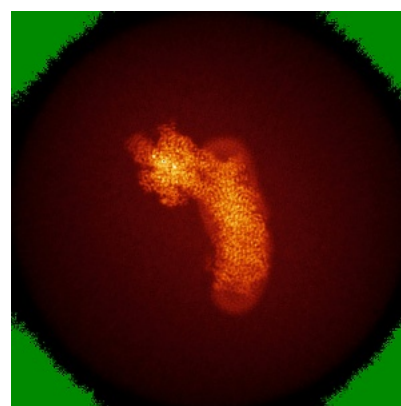
6.4.1 Primary map



X



Y

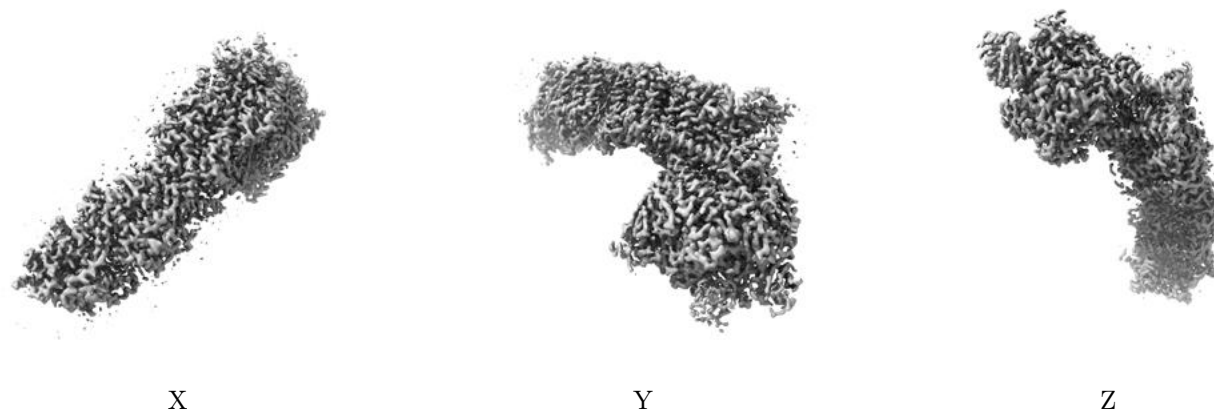


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

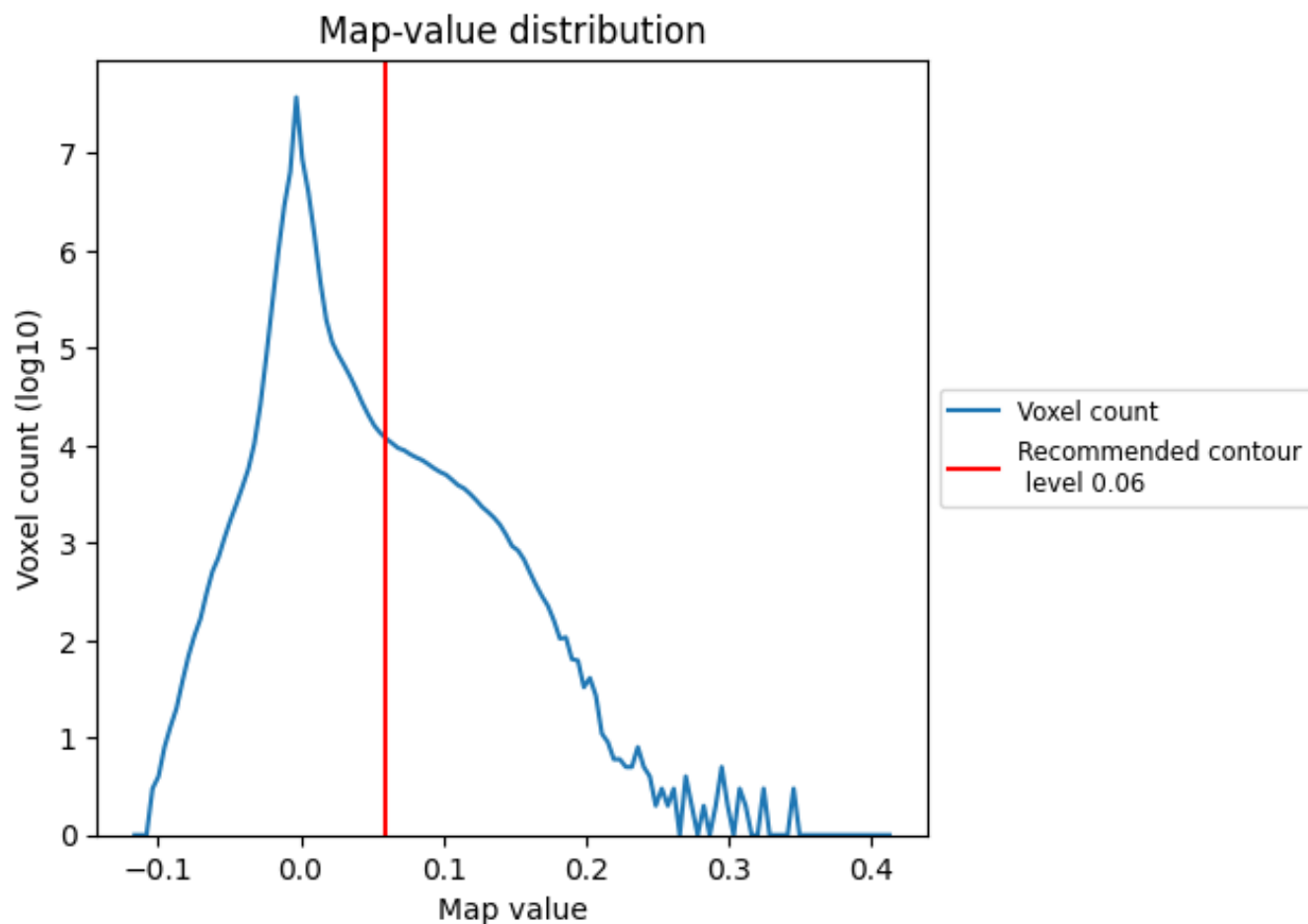
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

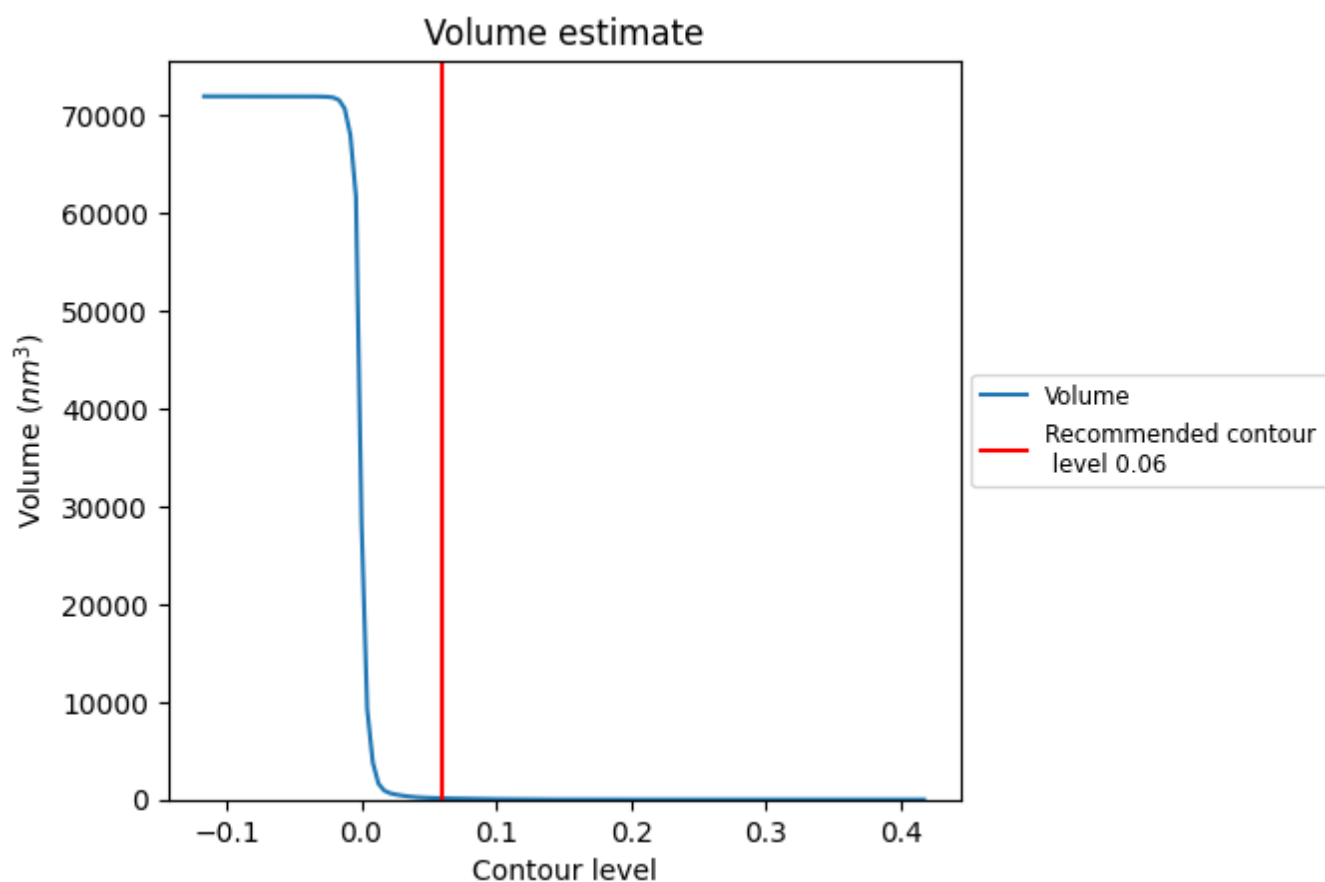
This section contains the results of statistical analysis of the map.

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.

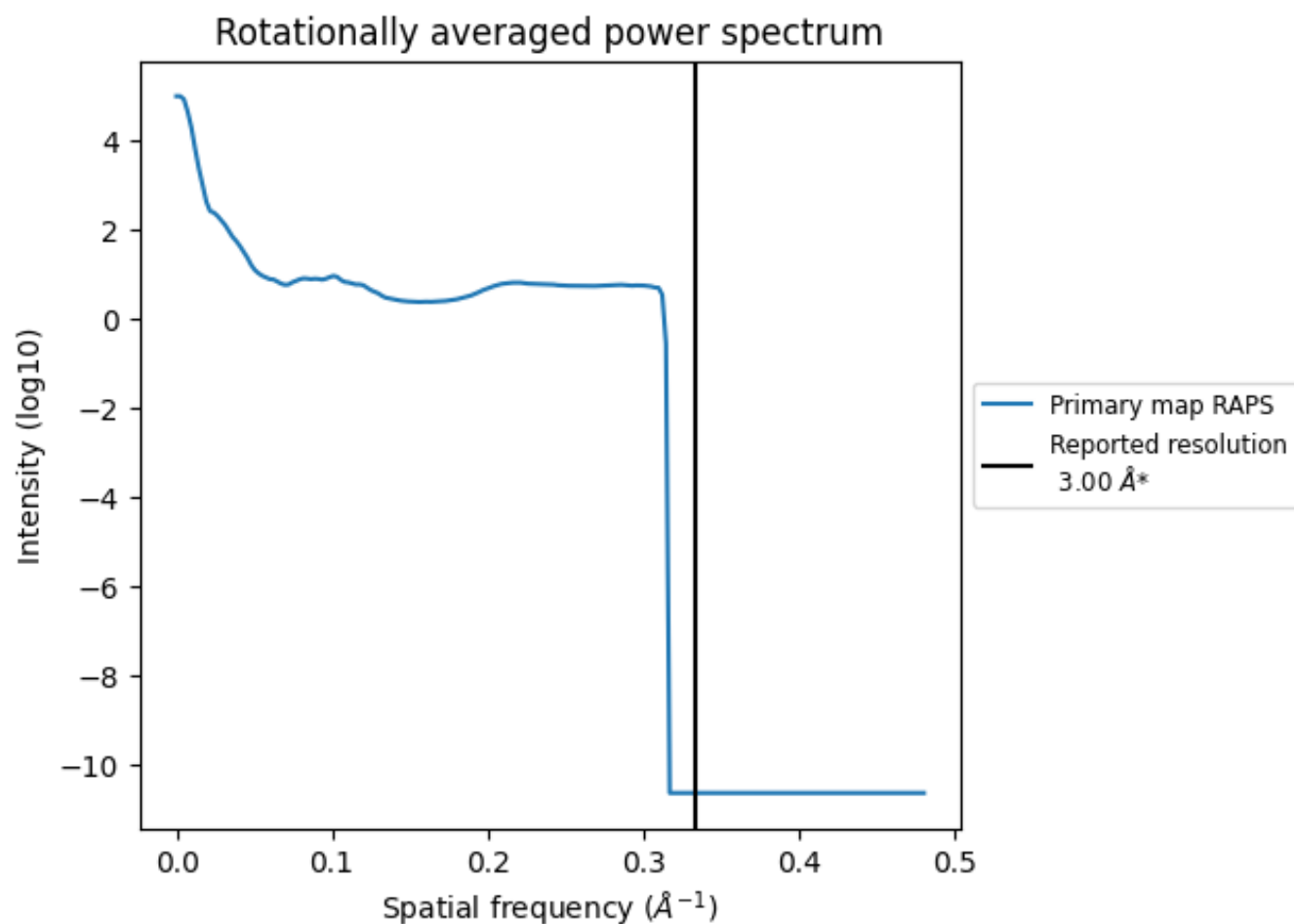
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 120 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

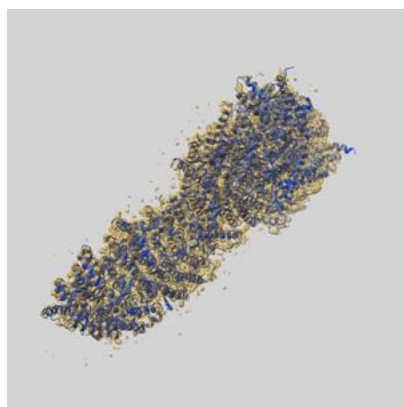
8 Fourier-Shell correlation ⓘ

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

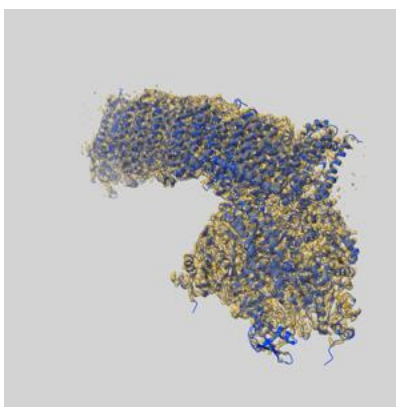
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9989 and PDB model 6KHI. Per-residue inclusion information can be found in section [3](#) on page [12](#).

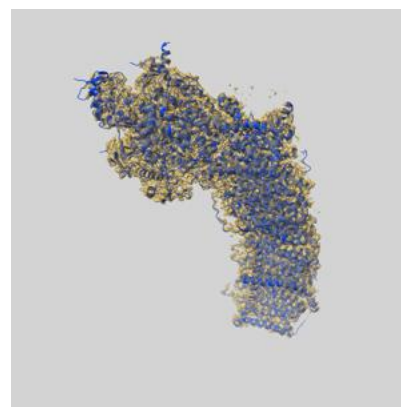
9.1 Map-model overlay [i](#)



X



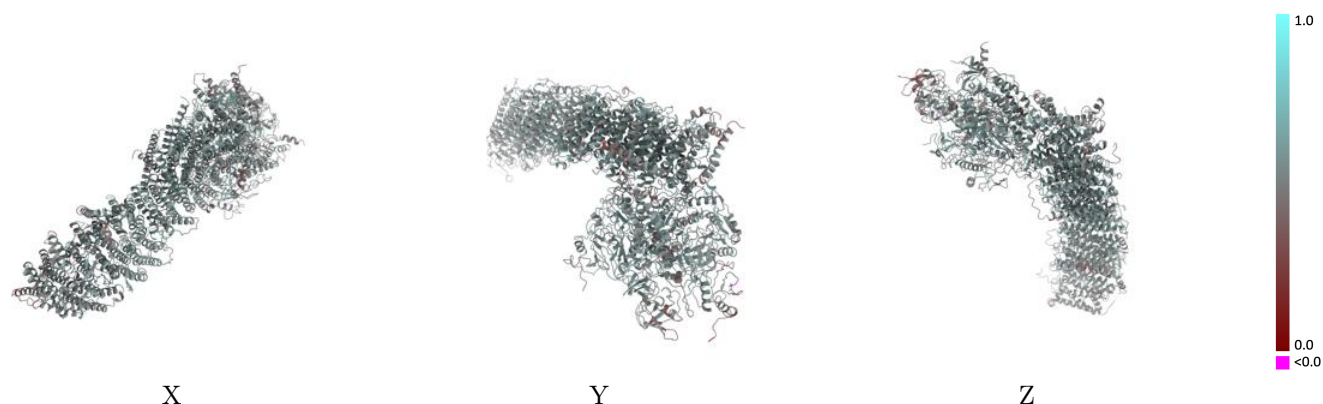
Y



Z

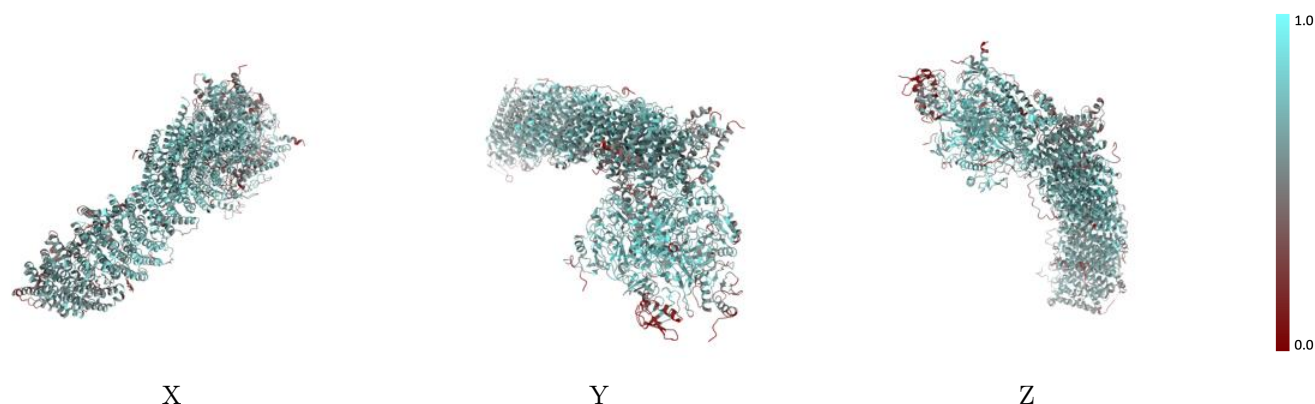
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



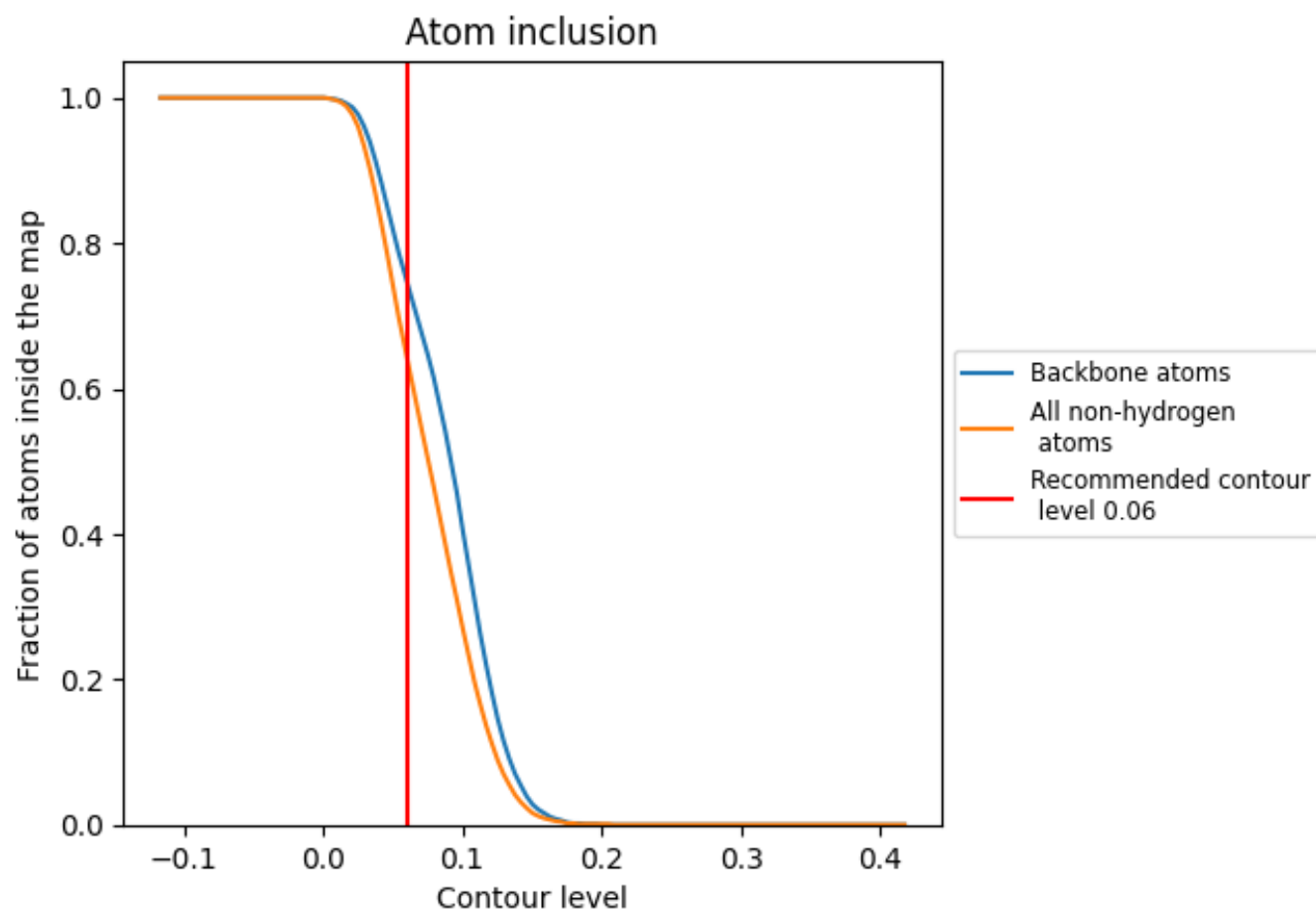
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 64% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.5250
1	 0.2890	 0.4610
A	 0.6410	 0.5260
B	 0.6920	 0.5410
C	 0.6360	 0.5270
D	 0.6890	 0.5390
E	 0.6890	 0.5400
F	 0.5890	 0.5040
G	 0.6340	 0.5320
H	 0.6850	 0.5330
I	 0.6710	 0.5260
J	 0.6840	 0.5260
K	 0.7160	 0.5400
L	 0.5840	 0.5040
M	 0.6970	 0.5330
N	 0.6970	 0.5370
O	 0.6710	 0.5540
P	 0.6810	 0.5310
Q	 0.4480	 0.4860
S	 0.6140	 0.5260
V	 0.4640	 0.4610

