



wwPDB EM Validation Summary Report ⓘ

Feb 24, 2024 – 07:54 PM EST

PDB ID : 7JZ2
EMDB ID : EMD-22528
Title : Succinate: quinone oxidoreductase SQR from E.coli K12
Authors : Lyu, M.; Su, C.-C.; Morgan, C.E.; Bolla, J.R.; Robinson, C.V.; Yu, E.W.
Deposited on : 2020-09-01
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

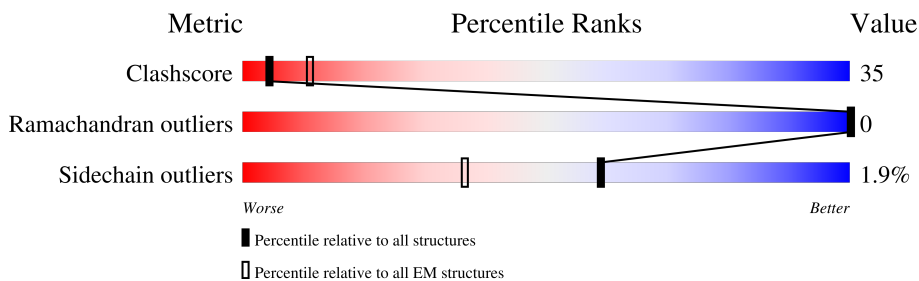
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.50 Å.

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



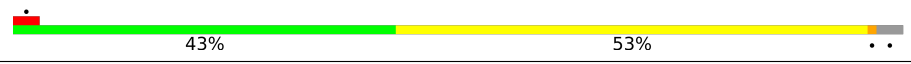
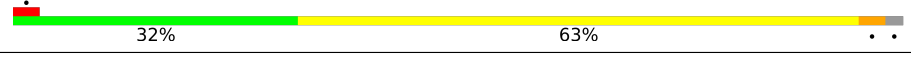

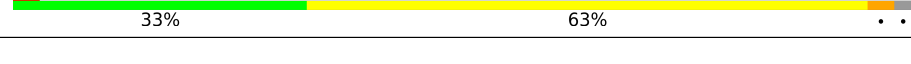
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	588	 35% 46% 18%
1	E	588	 35% 46% 18%
1	I	588	 36% 46% 18%
2	B	238	 50% 48%
2	F	238	 51% 47%
2	J	238	 51% 47%
3	C	129	 5% 44% 52%
3	G	129	 5% 43% 53%

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Mol	Chain	Length	Quality of chain
3	K	129	 43% 53%
4	D	115	 32% 63%
4	H	115	 33% 63%
4	L	115	 33% 63%

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
8	SF4	B	302	-	-	X	-
8	SF4	F	302	-	-	X	-
8	SF4	J	302	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 22866 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	481	3707	2299	670	714	24	0	0
1	E	481	3707	2299	670	714	24	0	0
1	I	481	3707	2299	670	714	24	0	0

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	238	1869	1172	329	348	20	0	0
2	F	238	1869	1172	329	348	20	0	0
2	J	238	1869	1172	329	348	20	0	0

- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b556 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	125	972	647	158	162	5	0	0
3	G	125	972	647	158	162	5	0	0
3	K	125	972	647	158	162	5	0	0

- Molecule 4 is a protein called Succinate dehydrogenase hydrophobic membrane anchor subunit.

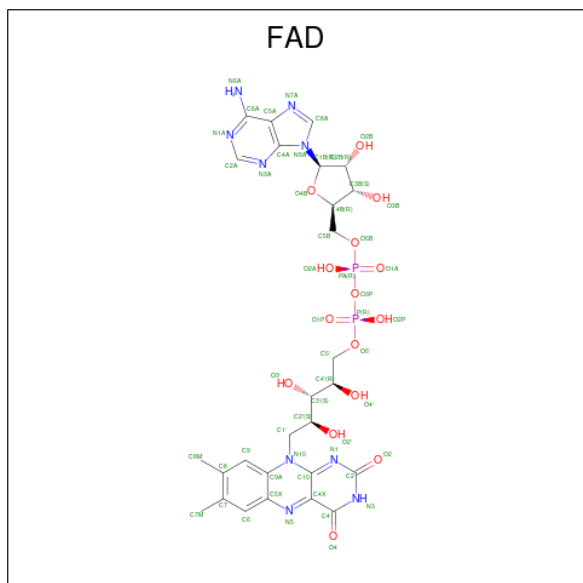
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	113	898	615	136	144	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	113	Total 898	C 615	N 136	O 144	S 3	0	0
4	L	113	Total 898	C 615	N 136	O 144	S 3	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

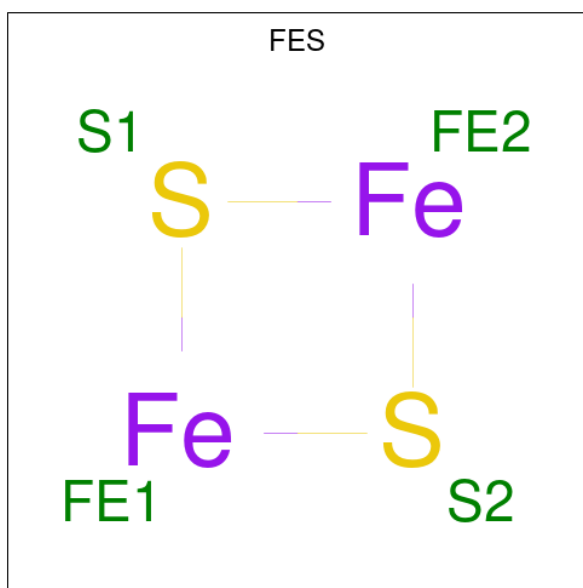


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	Total 53	C 27	N 9	O 15	P 2	0
5	E	1	Total 53	C 27	N 9	O 15	P 2	0
5	I	1	Total 53	C 27	N 9	O 15	P 2	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

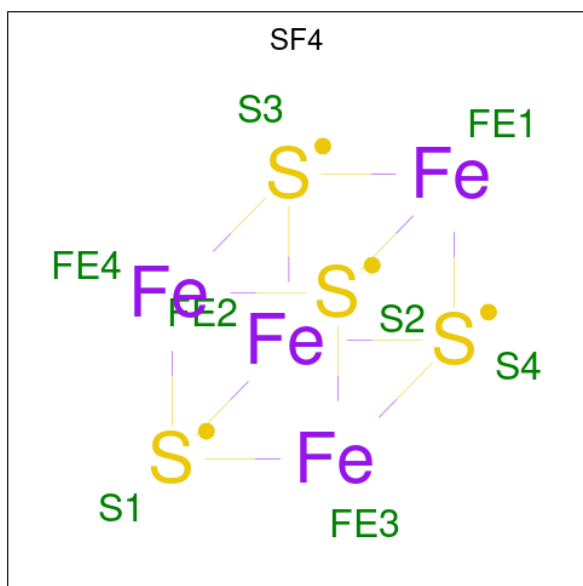
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
6	A	1	Total 1	Na 1	0
6	E	1	Total 1	Na 1	0
6	I	1	Total 1	Na 1	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



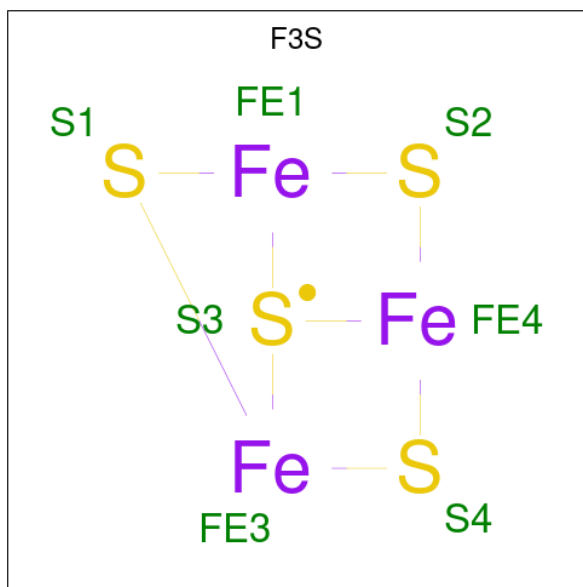
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
7	B	1	4	2	2	0
7	F	1	4	2	2	0
7	J	1	4	2	2	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



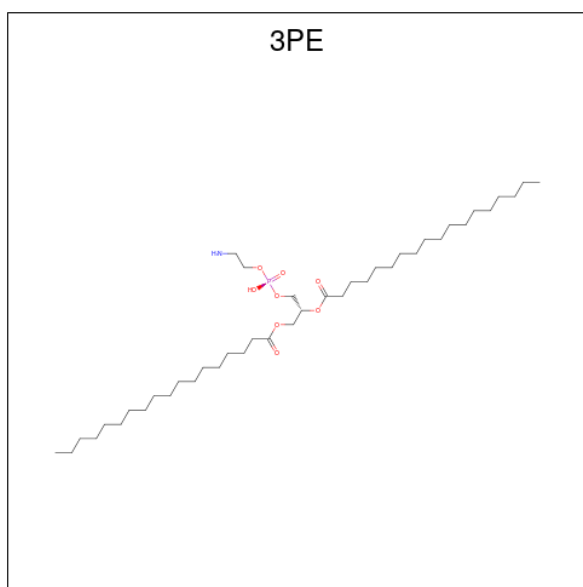
Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	Fe	S	0
			8	4	4	
8	F	1	Total	Fe	S	0
			8	4	4	
8	J	1	Total	Fe	S	0
			8	4	4	

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄) (labeled as "Ligand of Interest" by depositor).



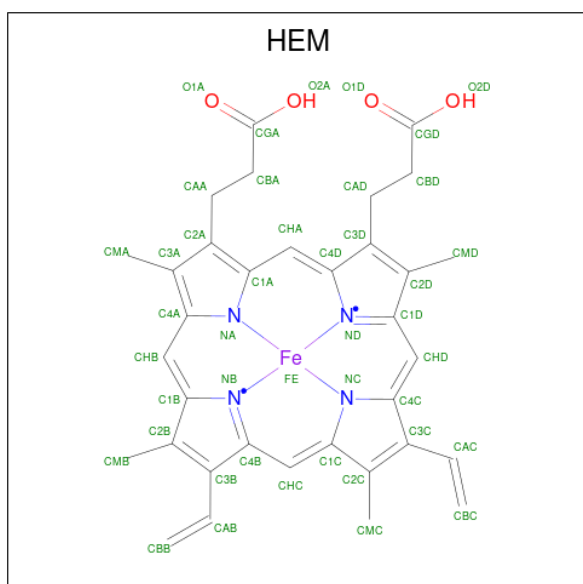
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	Fe	S	0
			7	3	4	
9	F	1	Total	Fe	S	0
			7	3	4	
9	J	1	Total	Fe	S	0
			7	3	4	

- Molecule 10 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



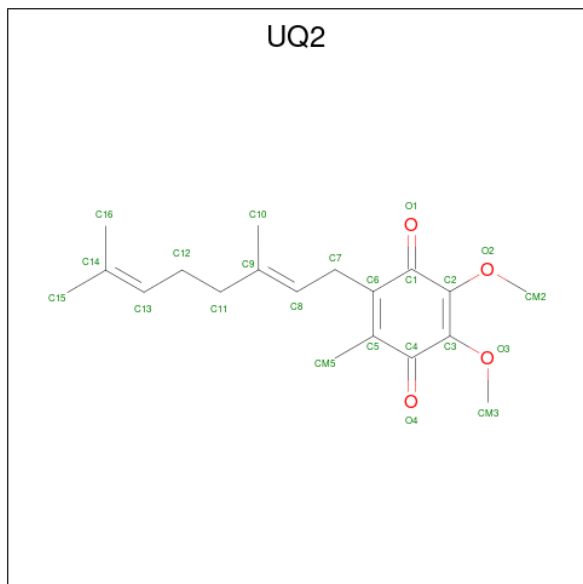
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		
10	C	1	Total	37	27	1	8	1	0
10	G	1	Total	37	27	1	8	1	0
10	K	1	Total	37	27	1	8	1	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				AltConf	
11	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is UBIQUINONE-2 (three-letter code: UQ2) (formula: C₁₉H₂₆O₄).

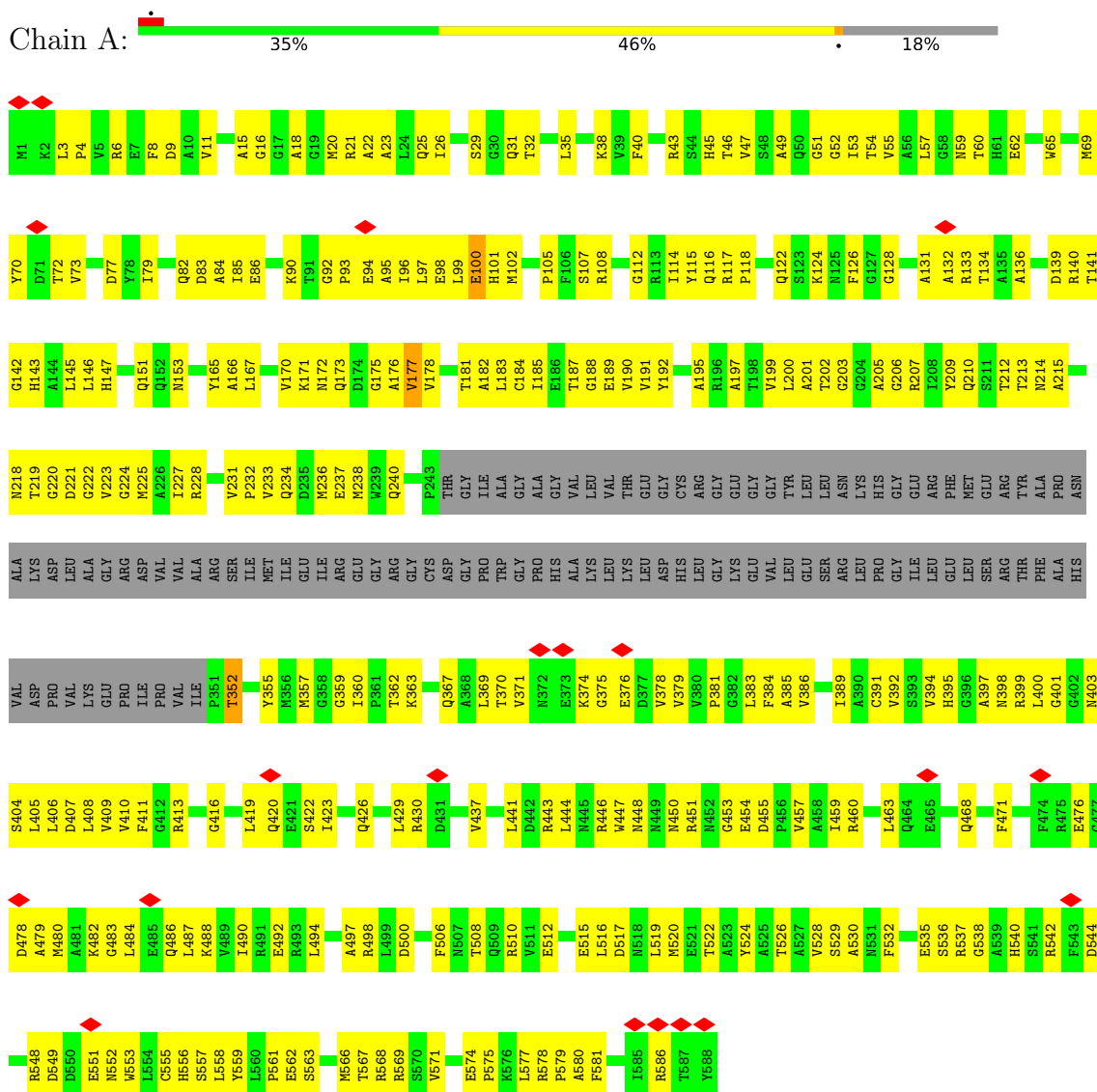


Mol	Chain	Residues	Atoms			AltConf
12	D	1	Total	C	O	0
			23	19	4	
12	H	1	Total	C	O	0
			23	19	4	
12	L	1	Total	C	O	0
			23	19	4	

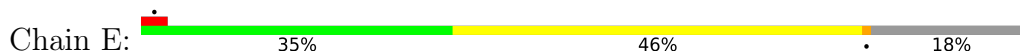
3 Residue-property plots

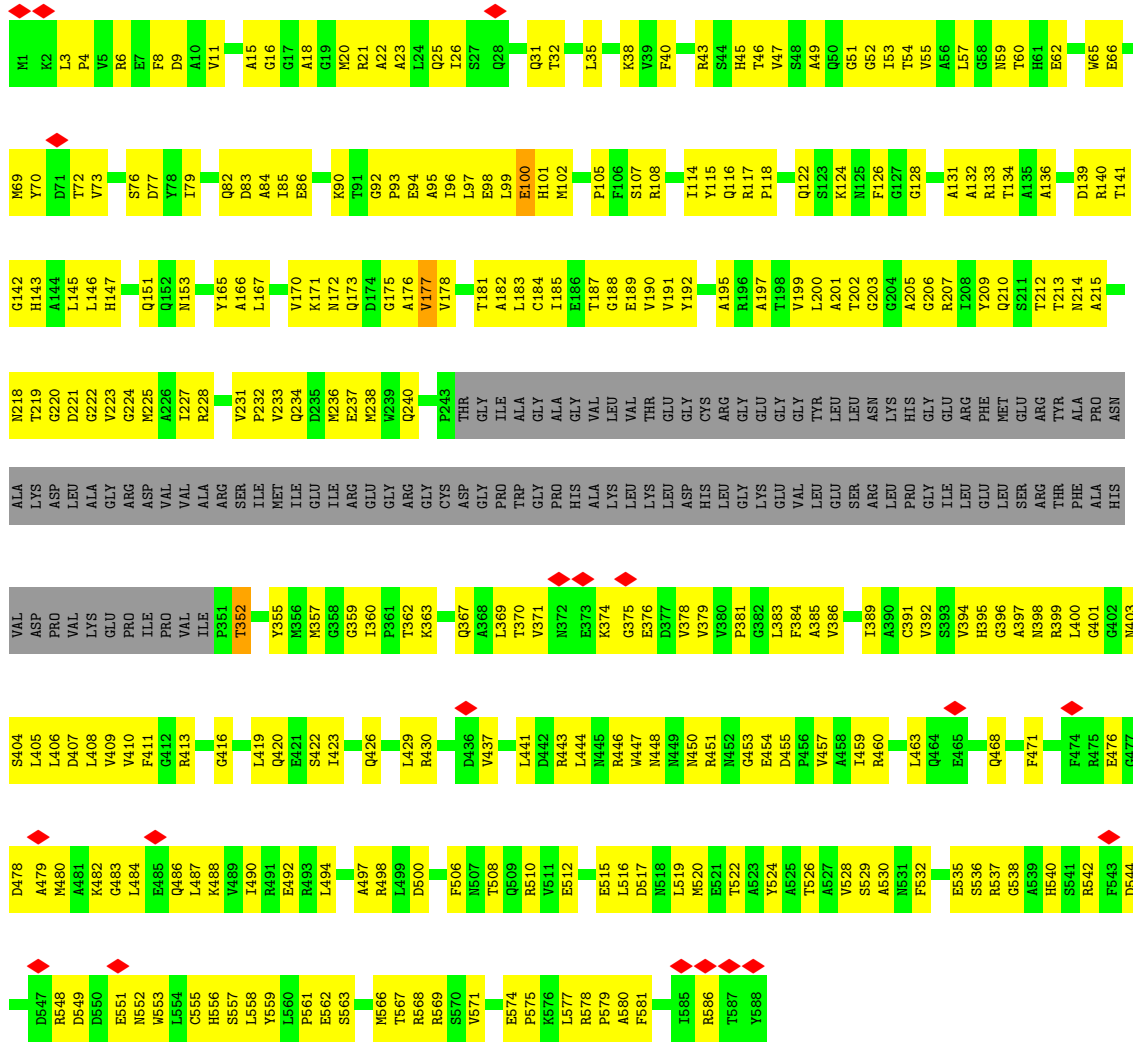
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Succinate dehydrogenase flavoprotein subunit

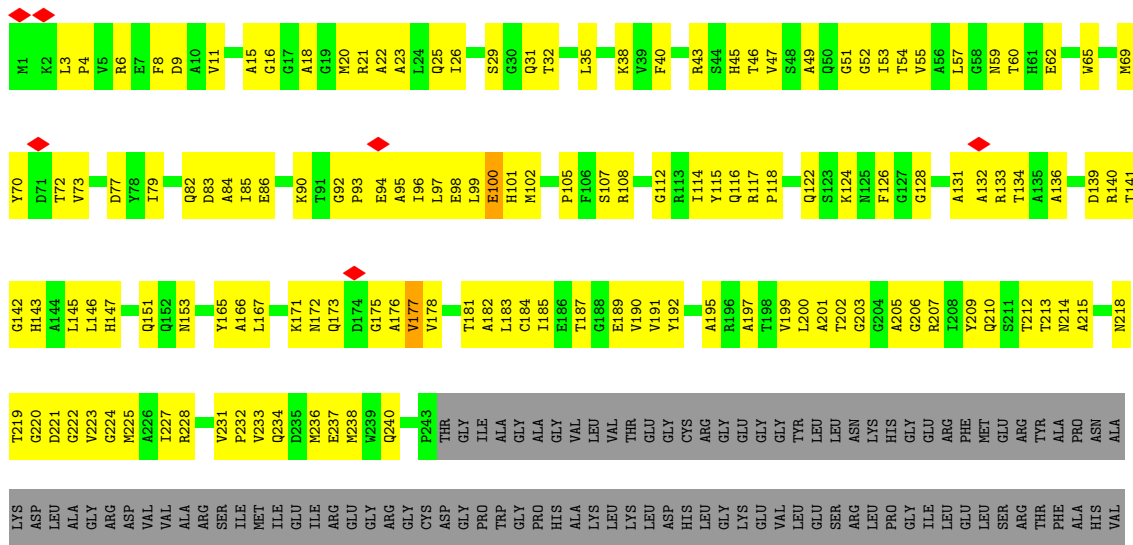
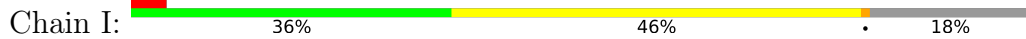


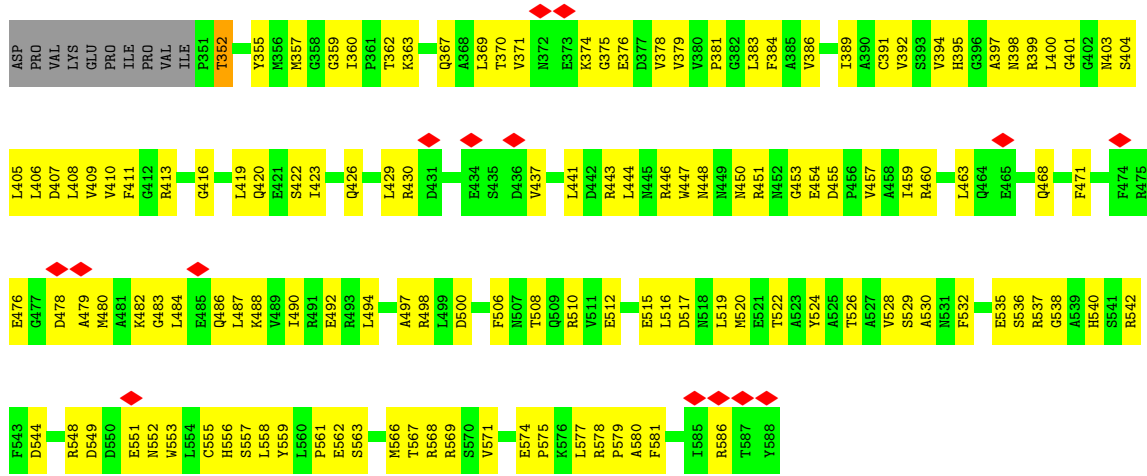
- Molecule 1: Succinate dehydrogenase flavoprotein subunit



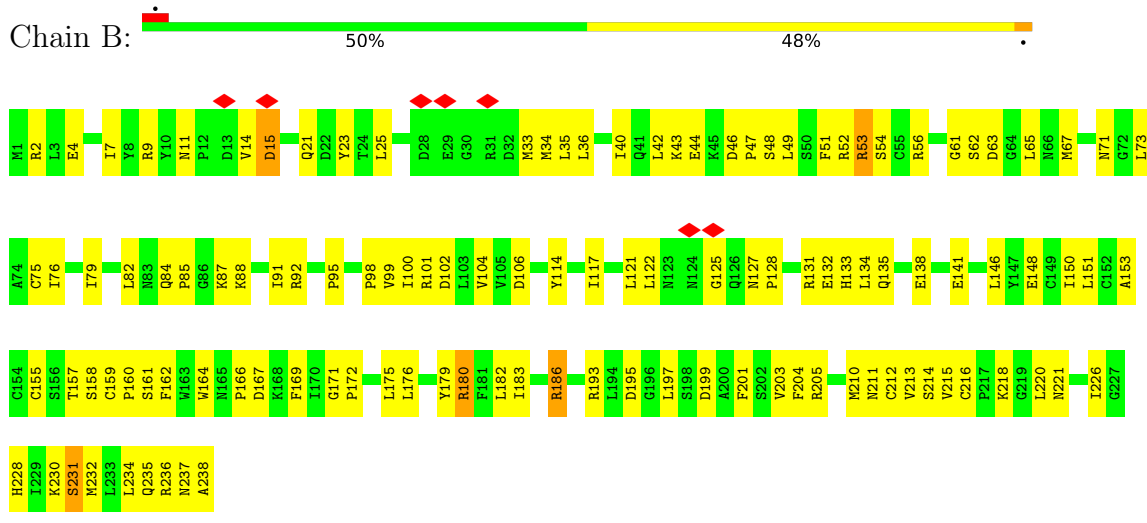


• Molecule 1: Succinate dehydrogenase flavoprotein subunit

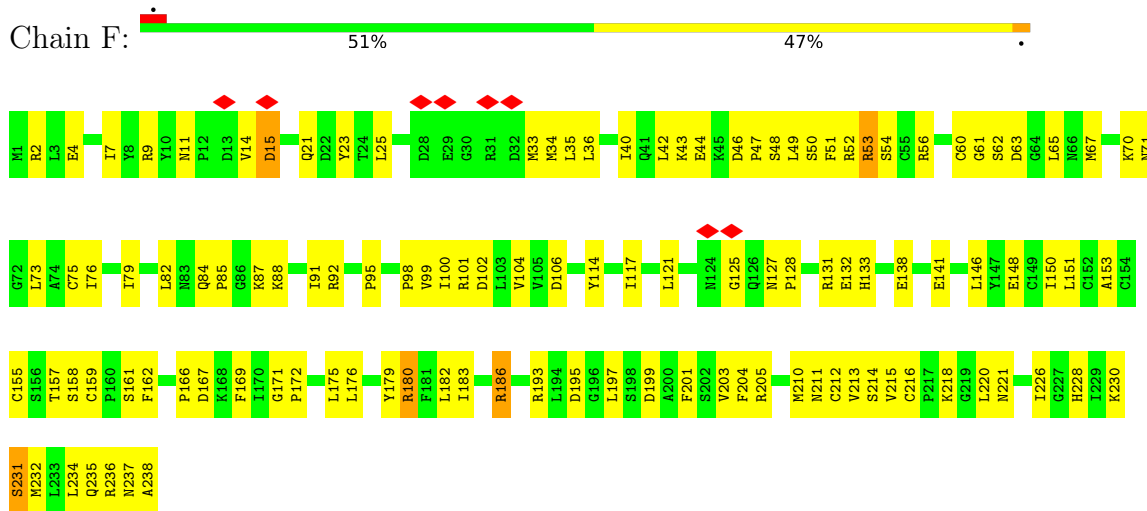




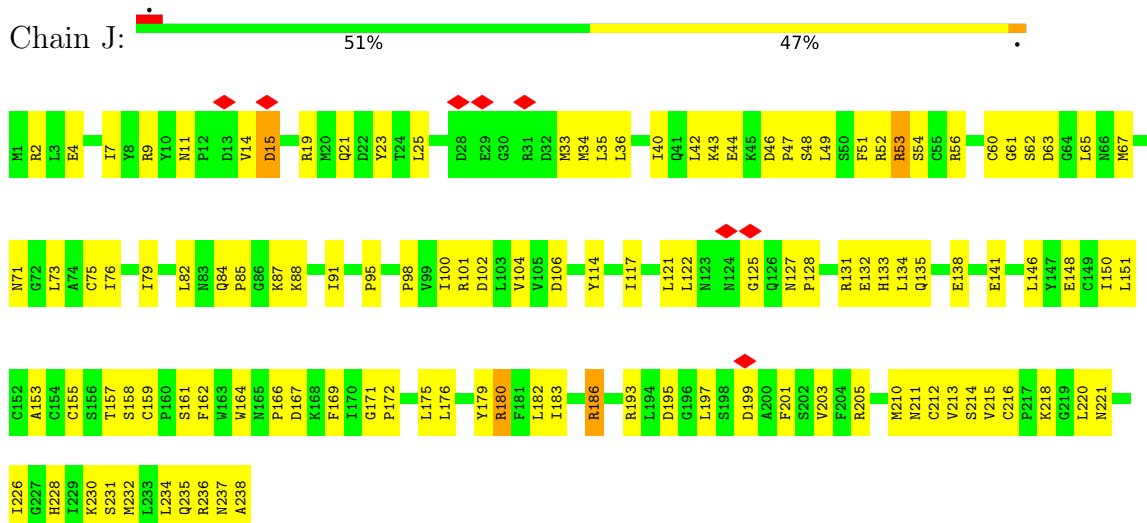
• Molecule 2: Succinate dehydrogenase iron-sulfur subunit



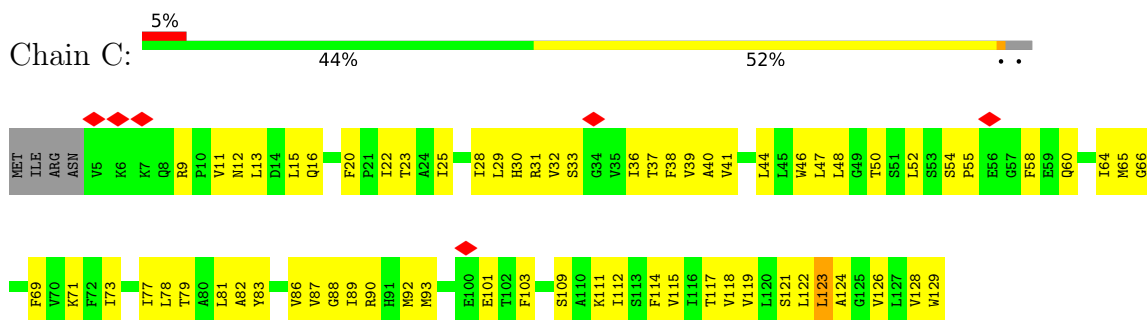
• Molecule 2: Succinate dehydrogenase iron-sulfur subunit



• Molecule 2: Succinate dehydrogenase iron-sulfur subunit



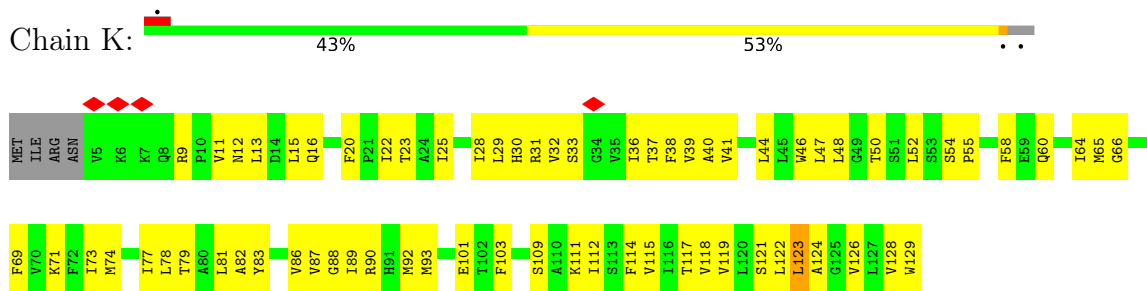
• Molecule 3: Succinate dehydrogenase cytochrome b556 subunit



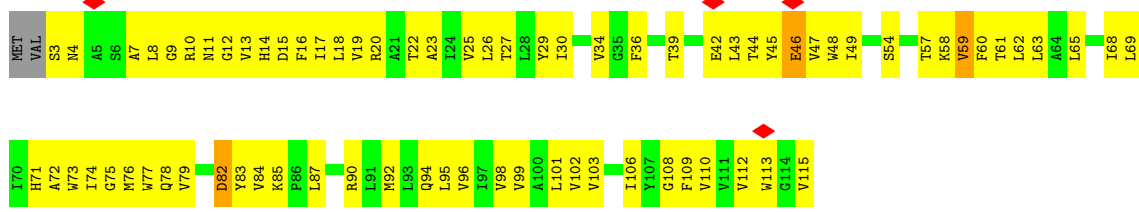
• Molecule 3: Succinate dehydrogenase cytochrome b556 subunit



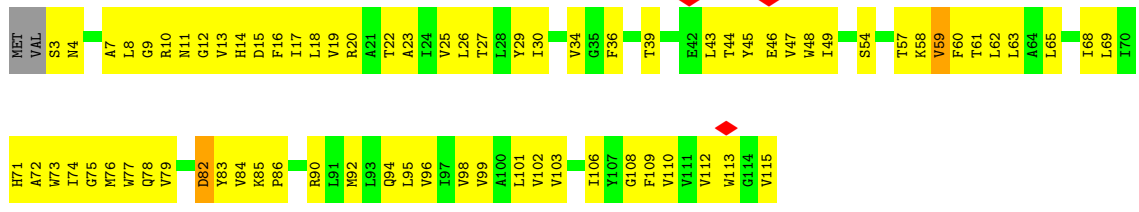
• Molecule 3: Succinate dehydrogenase cytochrome b556 subunit



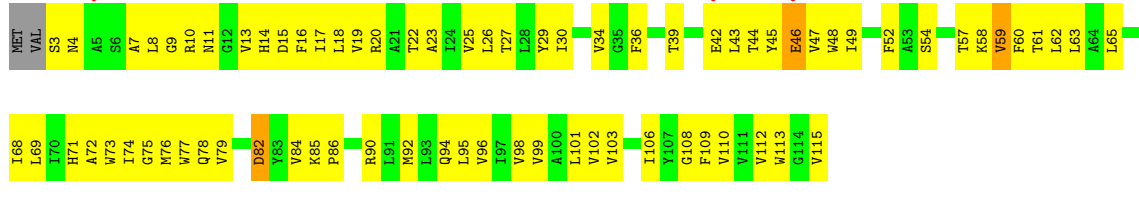
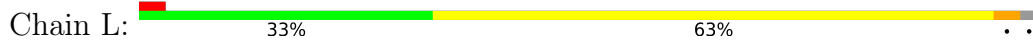
• Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor subunit



● Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor subunit



● Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.666	Depositor
Minimum map value	-1.544	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.172	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	151.20001, 151.20001, 147.96	wwPDB
Map dimensions	137, 140, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: NA, 3PE, UQ2, F3S, FAD, SF4, HEM, FES

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	0.23	0/3778	0.41	0/5110
1	E	0.23	0/3778	0.40	0/5110
1	I	0.23	0/3778	0.40	0/5110
2	B	0.24	0/1908	0.38	0/2578
2	F	0.24	0/1908	0.38	0/2578
2	J	0.24	0/1908	0.38	0/2578
3	C	0.24	0/994	0.35	0/1348
3	G	0.24	0/994	0.35	0/1348
3	K	0.24	0/994	0.35	0/1348
4	D	0.25	0/923	0.36	0/1262
4	H	0.25	0/923	0.36	0/1262
4	L	0.25	0/923	0.36	0/1262
All	All	0.24	0/22809	0.39	0/30894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3707	0	3597	300	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3707	0	3597	302	0
1	I	3707	0	3597	300	0
2	B	1869	0	1859	119	0
2	F	1869	0	1859	121	0
2	J	1869	0	1859	116	0
3	C	972	0	1024	65	0
3	G	972	0	1024	67	0
3	K	972	0	1024	64	0
4	D	898	0	936	81	0
4	H	898	0	936	81	0
4	L	898	0	936	77	0
5	A	53	0	29	5	0
5	E	53	0	29	7	0
5	I	53	0	29	6	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
6	I	1	0	0	0	0
7	B	4	0	0	1	0
7	F	4	0	0	1	0
7	J	4	0	0	1	0
8	B	8	0	0	3	0
8	F	8	0	0	3	0
8	J	8	0	0	3	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
9	J	7	0	0	0	0
10	C	37	0	48	4	0
10	G	37	0	48	4	0
10	K	37	0	48	3	0
11	D	43	0	30	10	0
11	G	43	0	30	9	0
11	K	43	0	30	10	0
12	D	23	0	26	5	0
12	H	23	0	26	3	0
12	L	23	0	26	4	0
All	All	22866	0	22647	1598	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 35.

The worst 5 of 1598 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:E:177:VAL:HG21	1:E:383:LEU:HB2	1.50	0.93
1:I:177:VAL:HG21	1:I:383:LEU:HB2	1.50	0.93
1:A:177:VAL:HG21	1:A:383:LEU:HB2	1.50	0.92
11:D:201:HEM:HBB2	11:D:201:HEM:HHC	1.53	0.91
11:D:201:HEM:HHD	11:D:201:HEM:HBC2	1.55	0.89

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	477/588 (81%)	461 (97%)	16 (3%)	0	100	100
1	E	477/588 (81%)	461 (97%)	16 (3%)	0	100	100
1	I	477/588 (81%)	461 (97%)	16 (3%)	0	100	100
2	B	236/238 (99%)	224 (95%)	12 (5%)	0	100	100
2	F	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
2	J	236/238 (99%)	224 (95%)	12 (5%)	0	100	100
3	C	123/129 (95%)	123 (100%)	0	0	100	100
3	G	123/129 (95%)	123 (100%)	0	0	100	100
3	K	123/129 (95%)	123 (100%)	0	0	100	100
4	D	111/115 (96%)	105 (95%)	6 (5%)	0	100	100
4	H	111/115 (96%)	105 (95%)	6 (5%)	0	100	100
4	L	111/115 (96%)	105 (95%)	6 (5%)	0	100	100
All	All	2841/3210 (88%)	2740 (96%)	101 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	389/473 (82%)	385 (99%)	4 (1%)	76	90
1	E	389/473 (82%)	385 (99%)	4 (1%)	76	90
1	I	389/473 (82%)	385 (99%)	4 (1%)	76	90
2	B	208/208 (100%)	201 (97%)	7 (3%)	37	63
2	F	208/208 (100%)	201 (97%)	7 (3%)	37	63
2	J	208/208 (100%)	201 (97%)	7 (3%)	37	63
3	C	105/109 (96%)	104 (99%)	1 (1%)	76	90
3	G	105/109 (96%)	104 (99%)	1 (1%)	76	90
3	K	105/109 (96%)	104 (99%)	1 (1%)	76	90
4	D	94/96 (98%)	91 (97%)	3 (3%)	39	65
4	H	94/96 (98%)	91 (97%)	3 (3%)	39	65
4	L	94/96 (98%)	91 (97%)	3 (3%)	39	65
All	All	2388/2658 (90%)	2343 (98%)	45 (2%)	59	80

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	59	VAL
2	J	53	ARG
4	H	82	ASP
1	I	352	THR
2	J	180	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	531	ASN
1	I	143	HIS
2	F	113	GLN
1	I	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	153	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	FAD	A	601	-	53,58,58	0.46	0	68,89,89	0.51	2 (2%)
8	SF4	F	302	-	0,12,12	-	-	-	-	-
11	HEM	D	201	4,3	41,50,50	1.50	3 (7%)	45,82,82	1.45	6 (13%)
5	FAD	I	601	-	53,58,58	0.45	0	68,89,89	0.51	2 (2%)
11	HEM	K	201	4,3	41,50,50	1.50	3 (7%)	45,82,82	1.45	6 (13%)
10	3PE	C	1301	-	36,36,50	1.01	4 (11%)	39,41,55	1.11	2 (5%)
11	HEM	G	201	3	41,50,50	1.51	3 (7%)	45,82,82	1.45	6 (13%)
9	F3S	J	303	2	0,9,9	-	-	-	-	-
9	F3S	F	303	2	0,9,9	-	-	-	-	-
9	F3S	B	303	2	0,9,9	-	-	-	-	-
8	SF4	J	302	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SF4	B	302	-	0,12,12	-	-	-	-	-
12	UQ2	L	1201	-	23,23,23	2.67	7 (30%)	28,31,31	1.08	2 (7%)
10	3PE	K	202	-	36,36,50	1.01	4 (11%)	39,41,55	1.11	2 (5%)
12	UQ2	D	202	-	23,23,23	2.68	7 (30%)	28,31,31	1.07	2 (7%)
7	FES	B	301	2	0,4,4	-	-	-	-	-
10	3PE	G	202	-	36,36,50	1.00	4 (11%)	39,41,55	1.11	2 (5%)
12	UQ2	H	1201	-	23,23,23	2.68	7 (30%)	28,31,31	1.08	2 (7%)
7	FES	J	301	2	0,4,4	-	-	-	-	-
5	FAD	E	601	-	53,58,58	0.46	0	68,89,89	0.52	2 (2%)
7	FES	F	301	2	0,4,4	-	-	-	-	-

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
5	FAD	A	601	-	-	11/30/50/50	0/6/6/6
8	SF4	F	302	-	-	-	0/6/5/5
11	HEM	D	201	4,3	-	5/12/54/54	-
5	FAD	I	601	-	-	12/30/50/50	0/6/6/6
11	HEM	K	201	4,3	-	5/12/54/54	-
10	3PE	C	1301	-	-	22/40/40/54	-
11	HEM	G	201	3	-	5/12/54/54	-
9	F3S	J	303	2	-	-	0/3/3/3
9	F3S	F	303	2	-	-	0/3/3/3
9	F3S	B	303	2	-	-	0/3/3/3
8	SF4	J	302	-	-	-	0/6/5/5
8	SF4	B	302	-	-	-	0/6/5/5
12	UQ2	L	1201	-	-	6/15/39/39	0/1/1/1
10	3PE	K	202	-	-	22/40/40/54	-
12	UQ2	D	202	-	-	6/15/39/39	0/1/1/1
7	FES	B	301	2	-	-	0/1/1/1
10	3PE	G	202	-	-	22/40/40/54	-
12	UQ2	H	1201	-	-	6/15/39/39	0/1/1/1
7	FES	J	301	2	-	-	0/1/1/1
5	FAD	E	601	-	-	12/30/50/50	0/6/6/6
7	FES	F	301	2	-	-	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	1201	UQ2	C6-C5	10.15	1.53	1.35
12	D	202	UQ2	C6-C5	10.13	1.53	1.35
12	L	1201	UQ2	C6-C5	10.06	1.53	1.35
11	G	201	HEM	C3C-C2C	-4.65	1.33	1.40
11	D	201	HEM	C3C-C2C	-4.63	1.33	1.40

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	202	3PE	O21-C21-C22	3.89	119.89	111.50
10	C	1301	3PE	O21-C21-C22	3.87	119.85	111.50
10	G	202	3PE	O21-C21-C22	3.85	119.80	111.50
11	K	201	HEM	C1B-NB-C4B	3.08	108.25	105.07
11	G	201	HEM	C1B-NB-C4B	3.06	108.24	105.07

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	FAD	C5B-O5B-PA-O1A
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	C2'-C3'-C4'-O4'
5	A	601	FAD	O3'-C3'-C4'-O4'

There are no ring outliers.

18 monomers are involved in 82 short contacts:

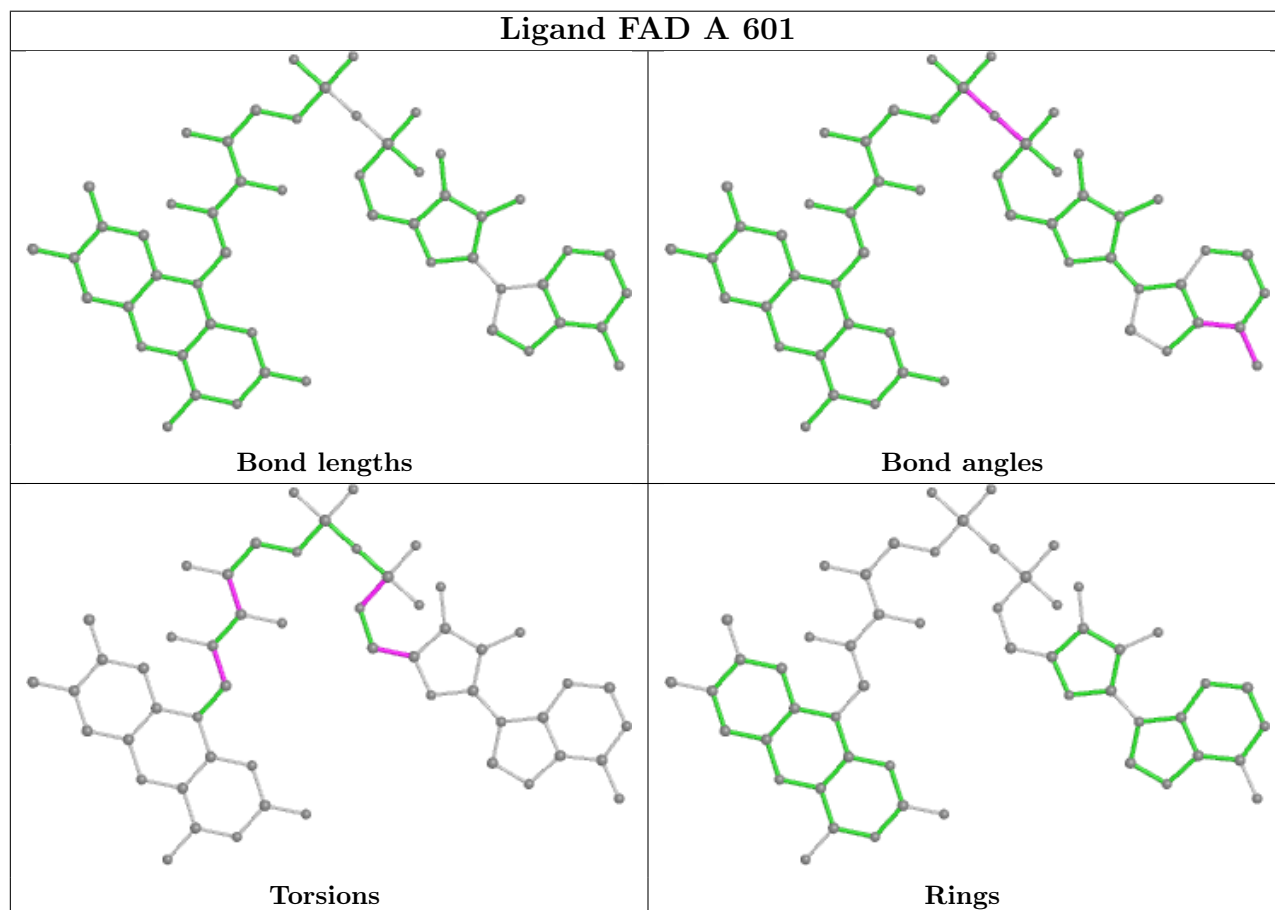
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	FAD	5	0
8	F	302	SF4	3	0
11	D	201	HEM	10	0
5	I	601	FAD	6	0
11	K	201	HEM	10	0
10	C	1301	3PE	4	0
11	G	201	HEM	9	0
8	J	302	SF4	3	0
8	B	302	SF4	3	0
12	L	1201	UQ2	4	0
10	K	202	3PE	3	0

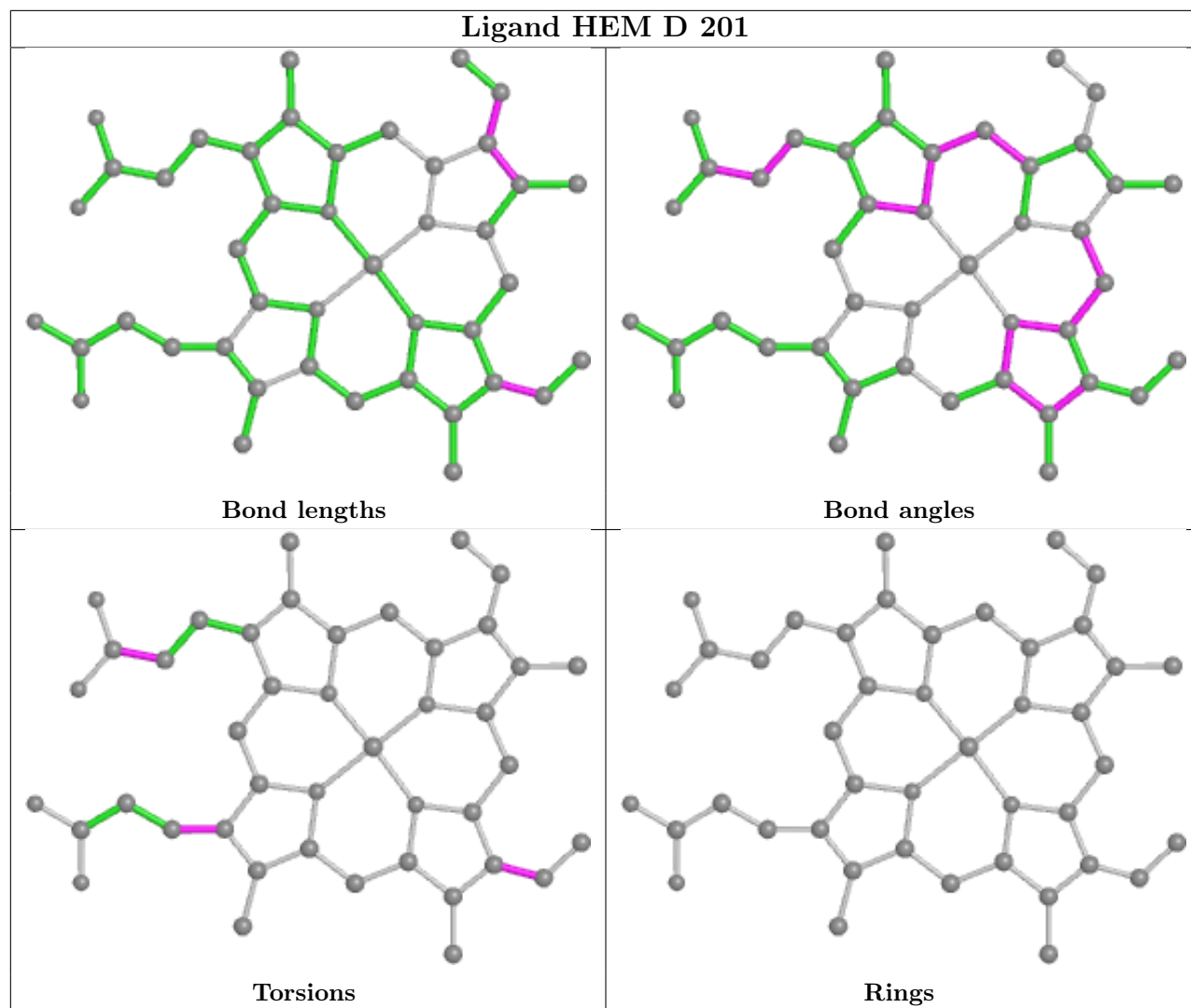
Continued on next page...

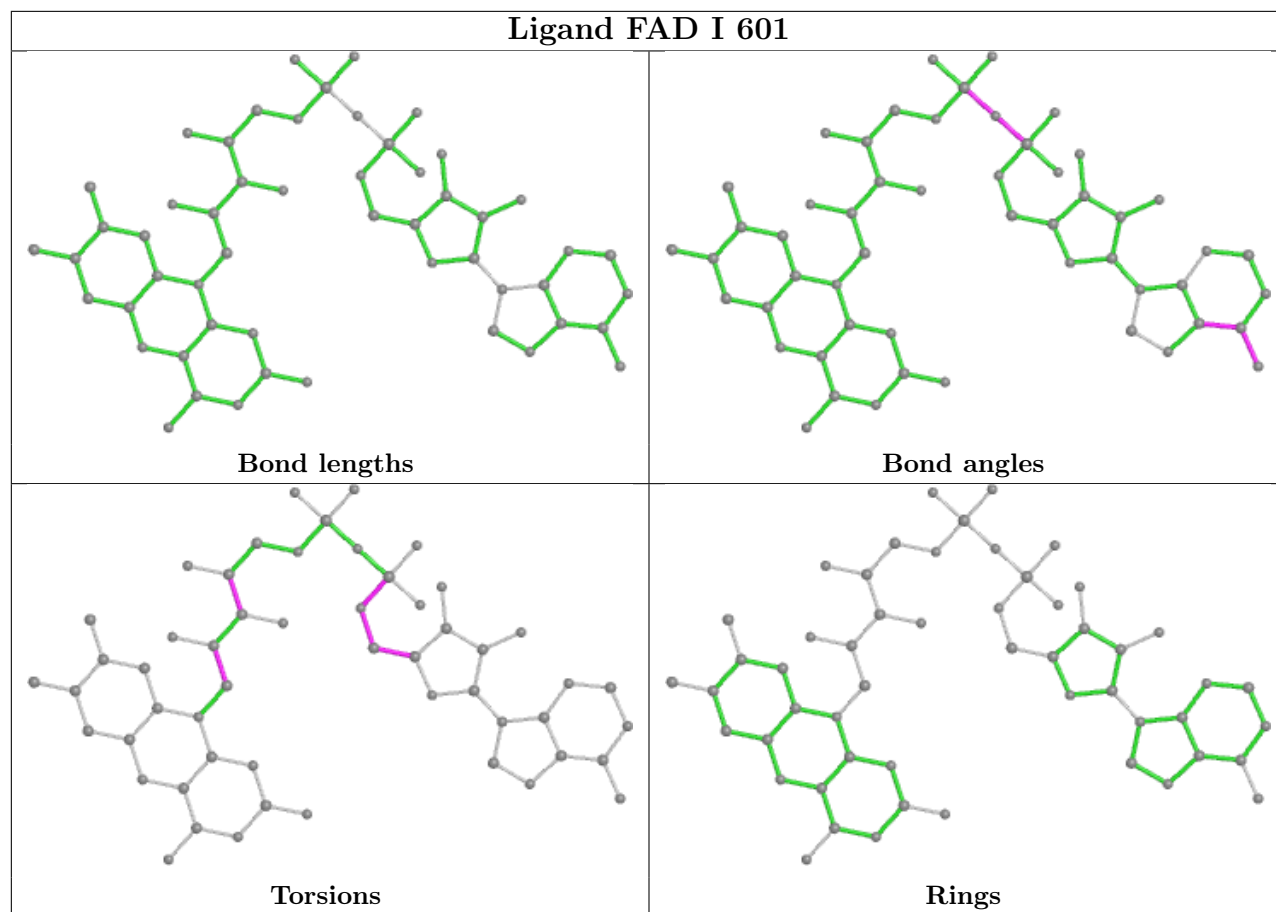
Continued from previous page...

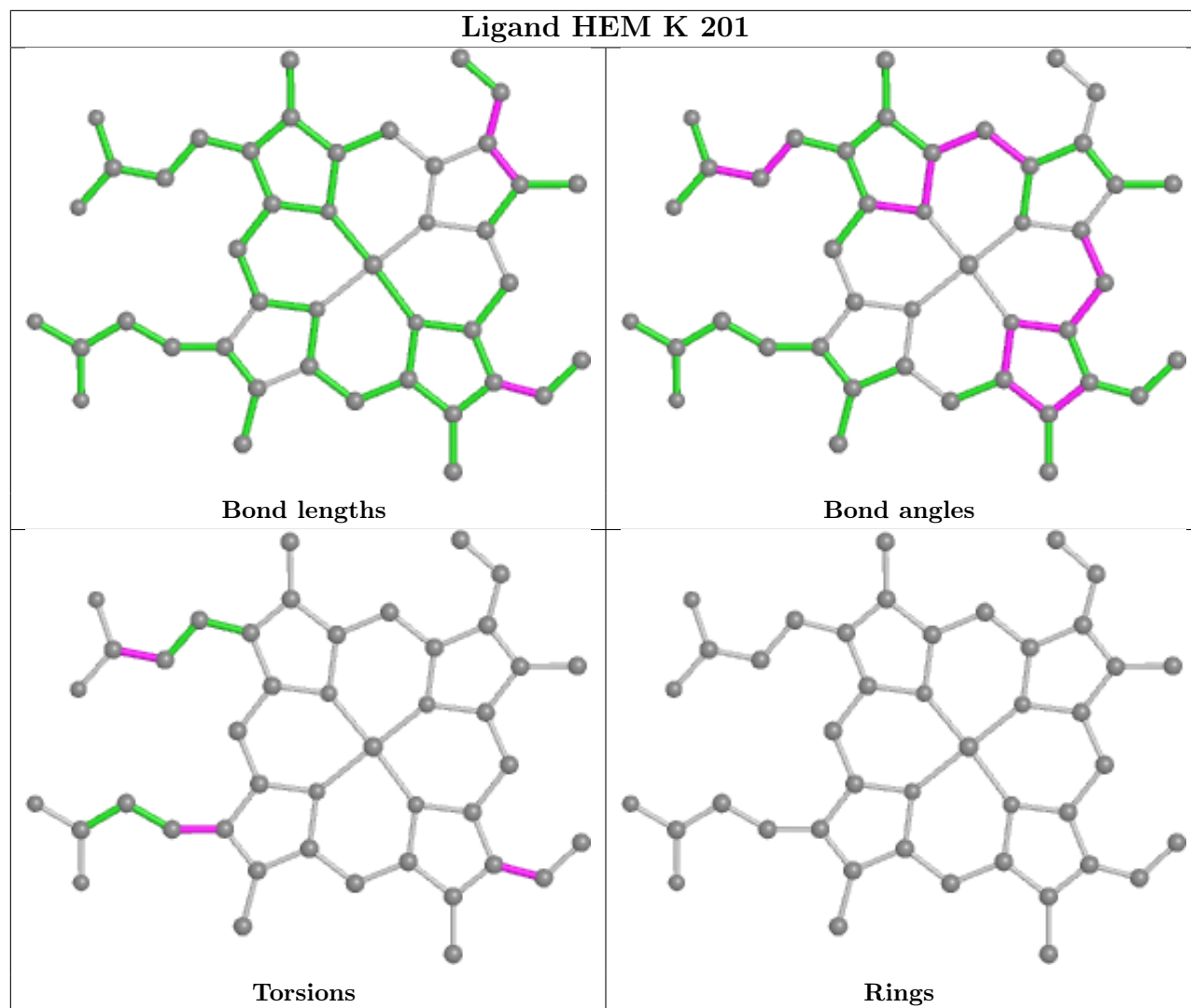
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	202	UQ2	5	0
7	B	301	FES	1	0
10	G	202	3PE	4	0
12	H	1201	UQ2	3	0
7	J	301	FES	1	0
5	E	601	FAD	7	0
7	F	301	FES	1	0

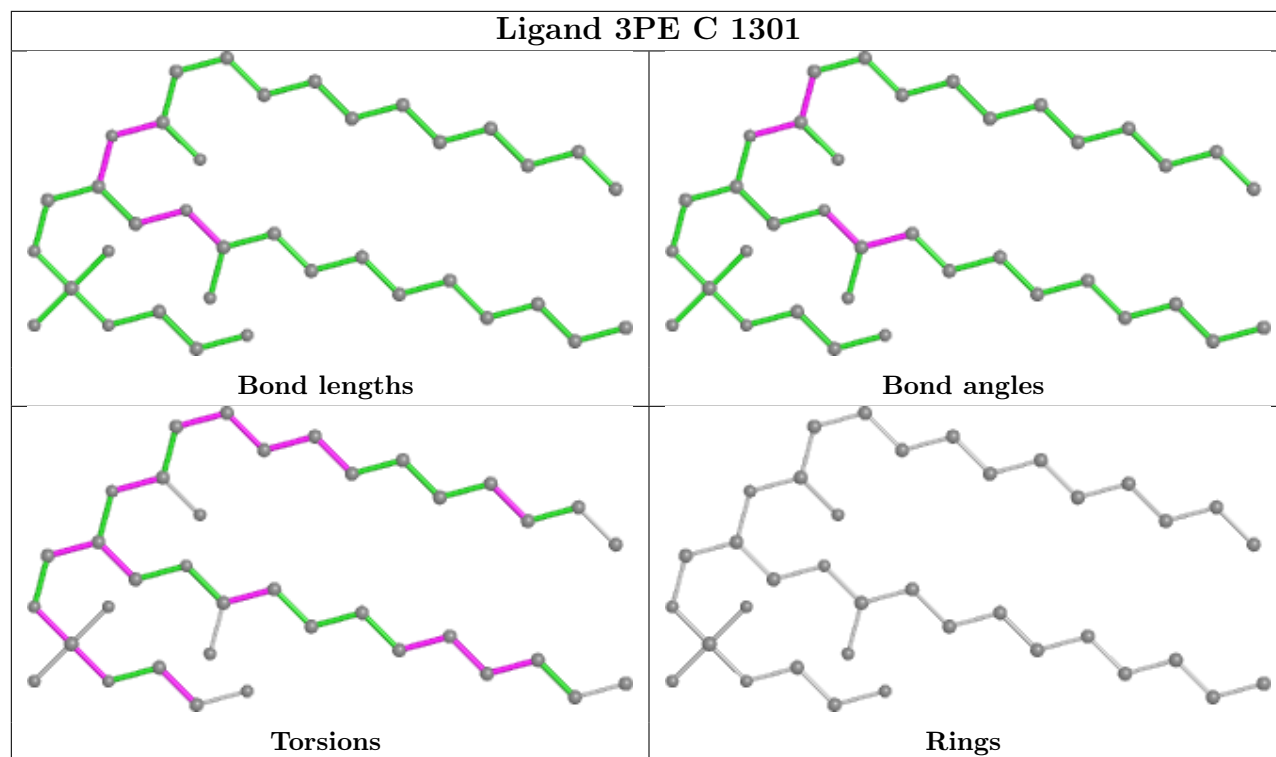
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

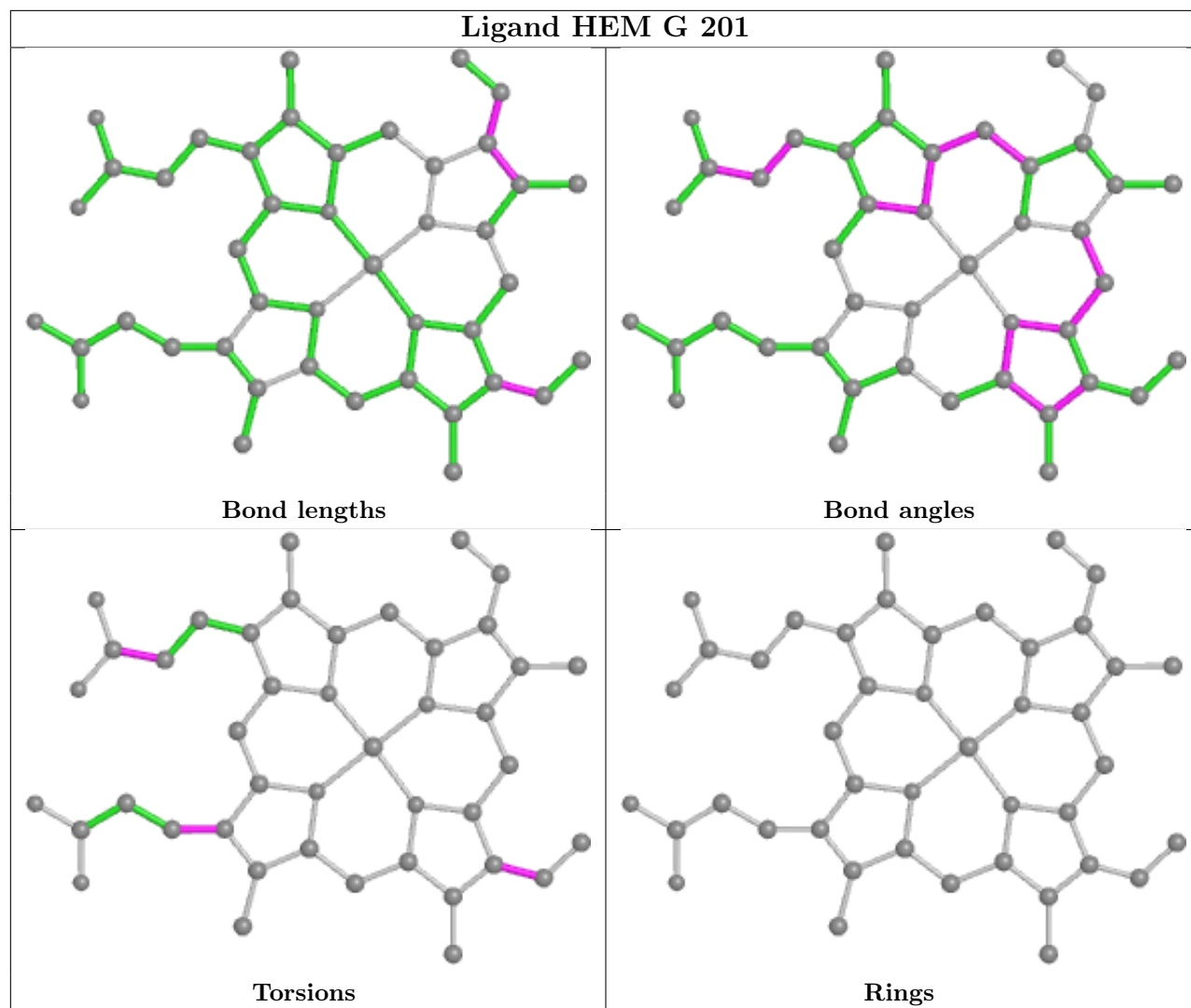


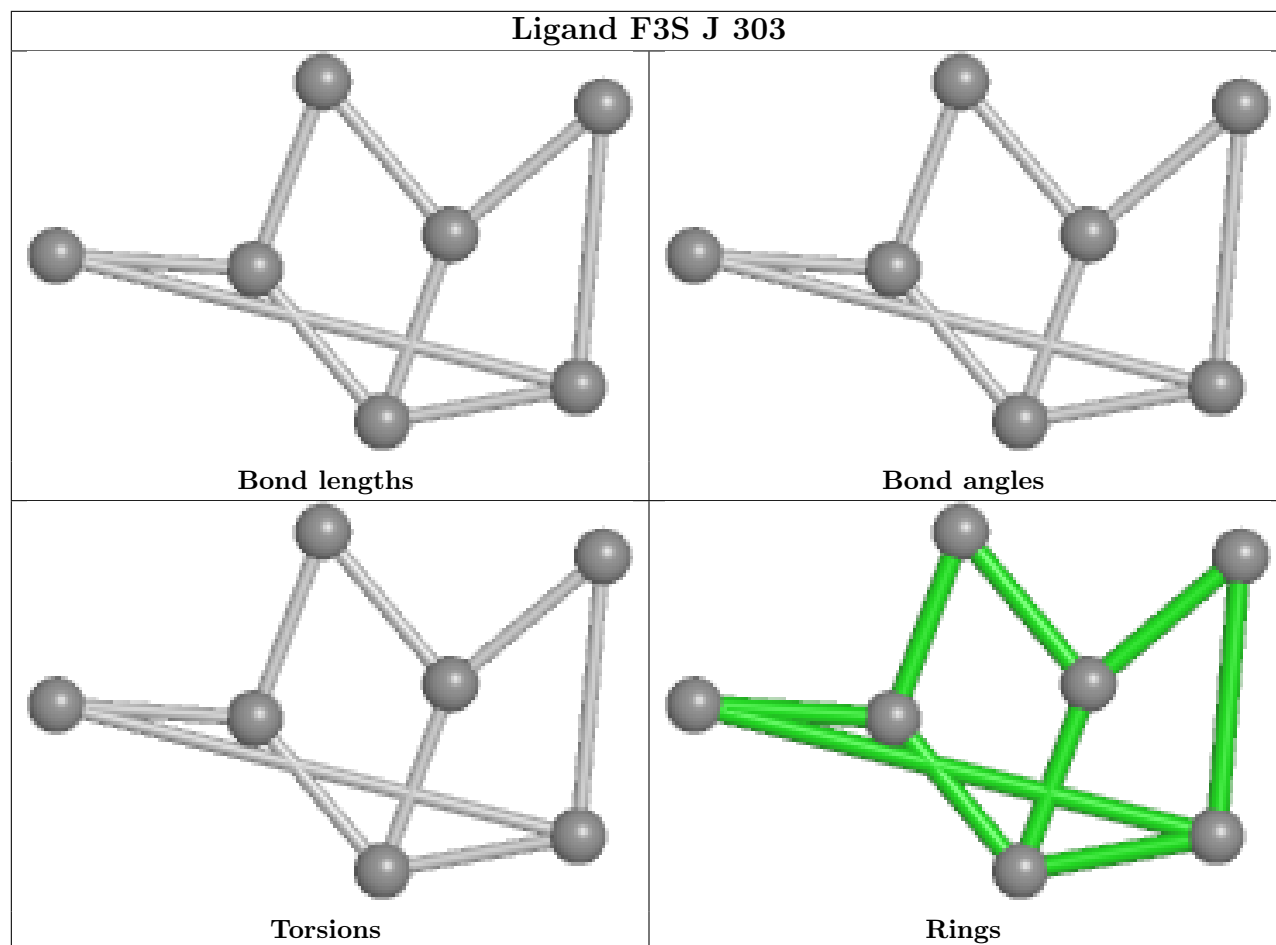


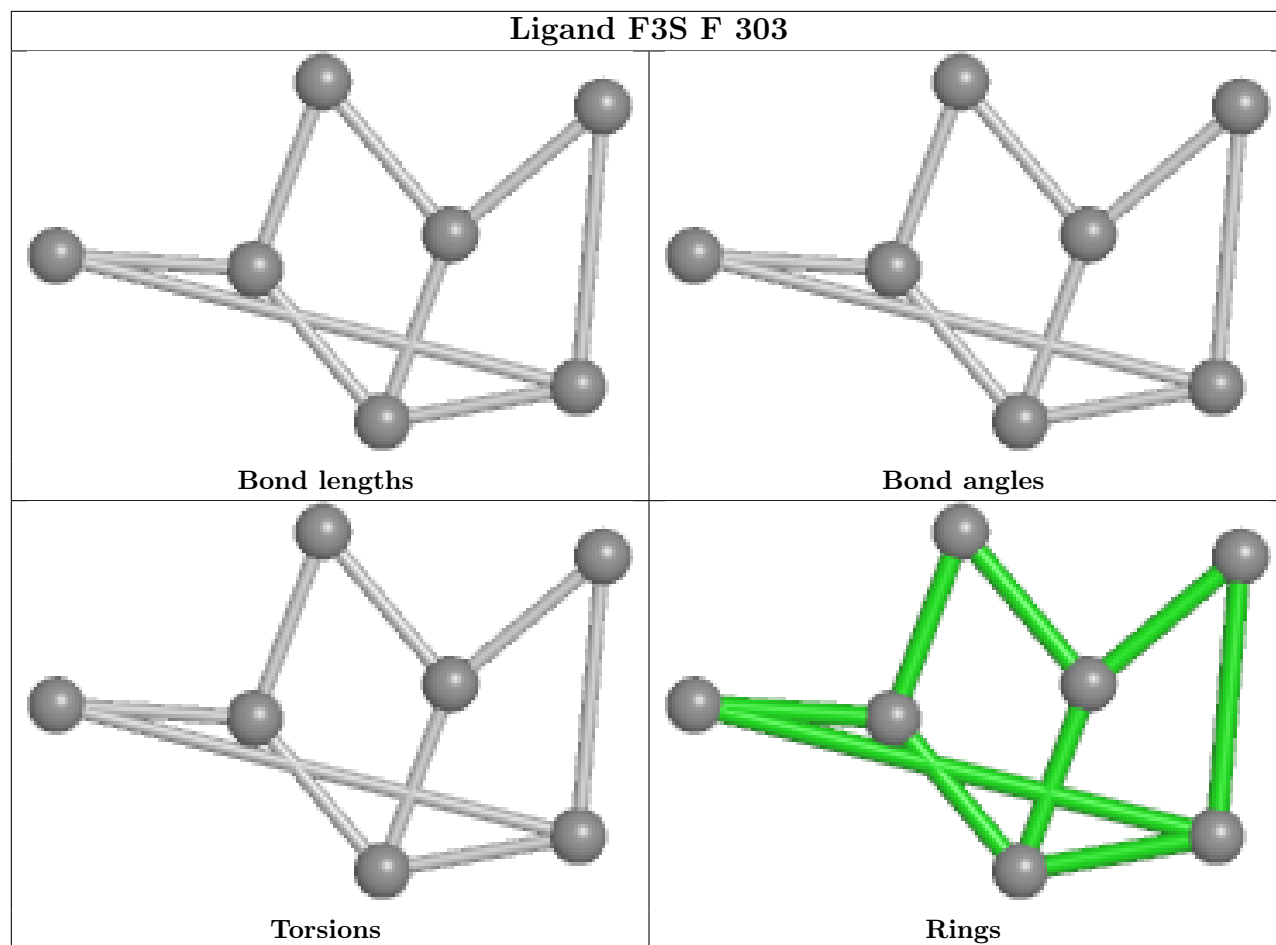


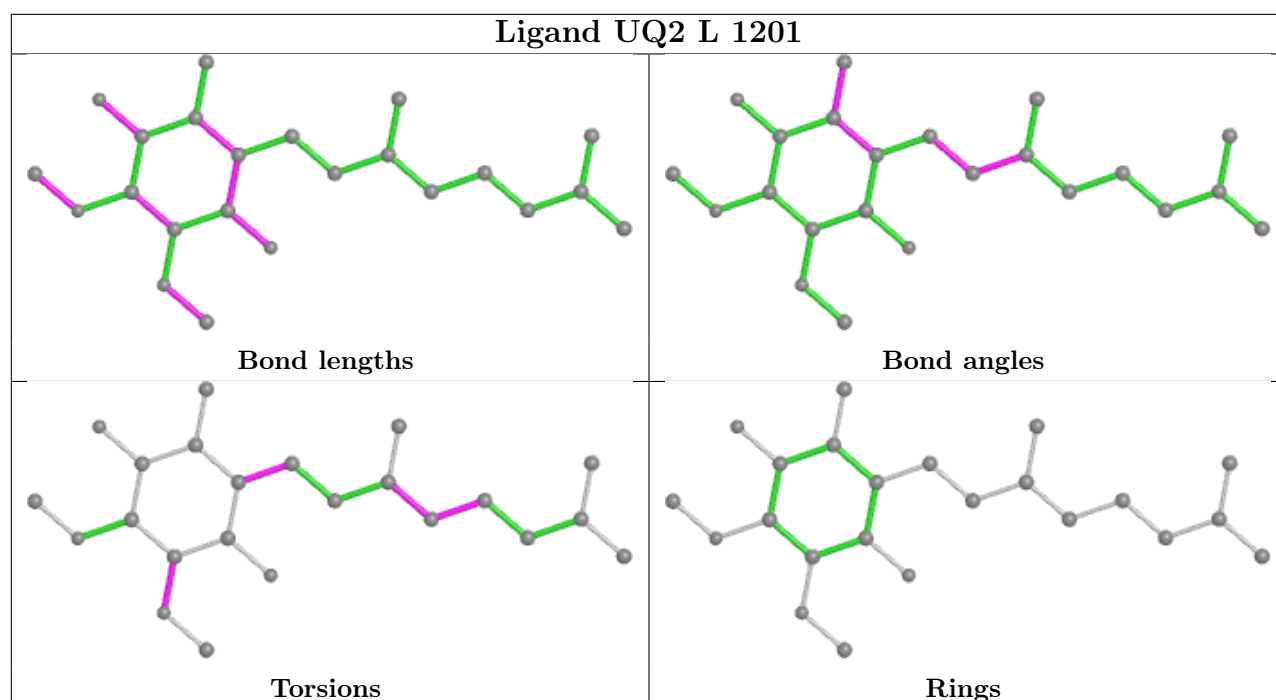
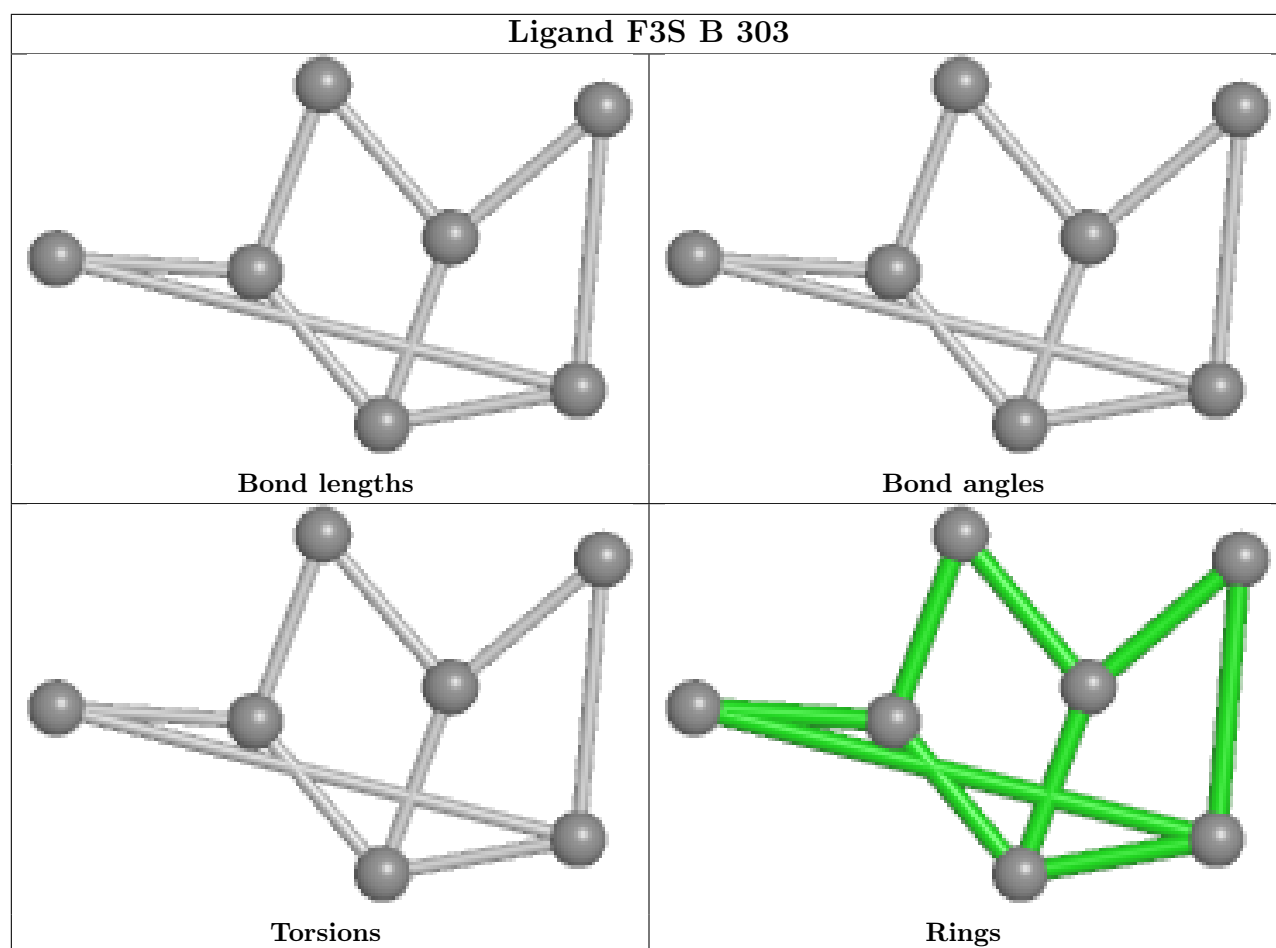


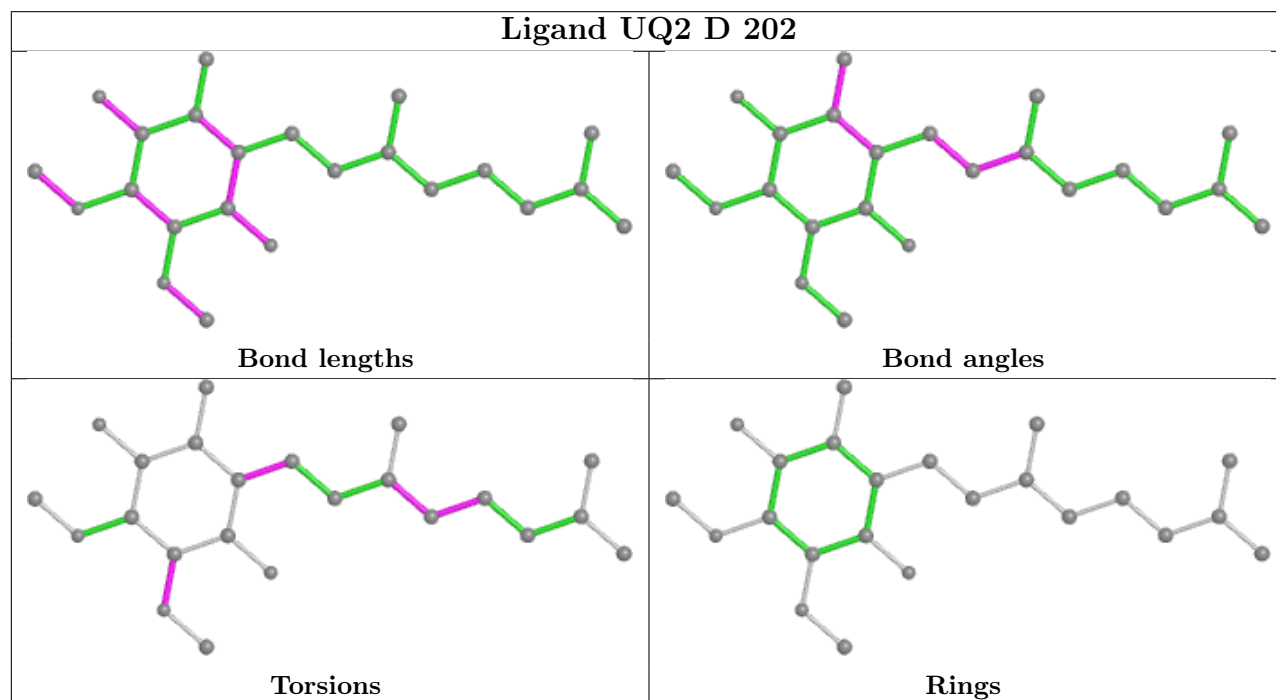
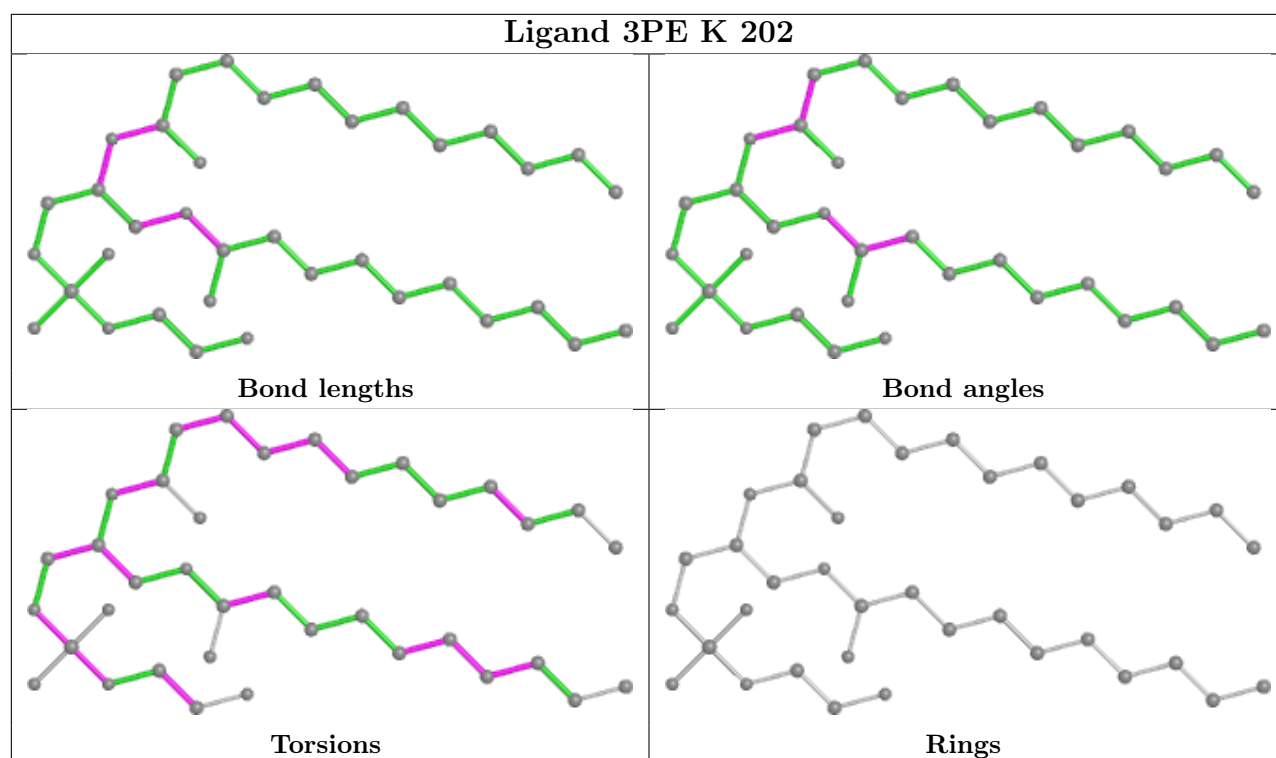


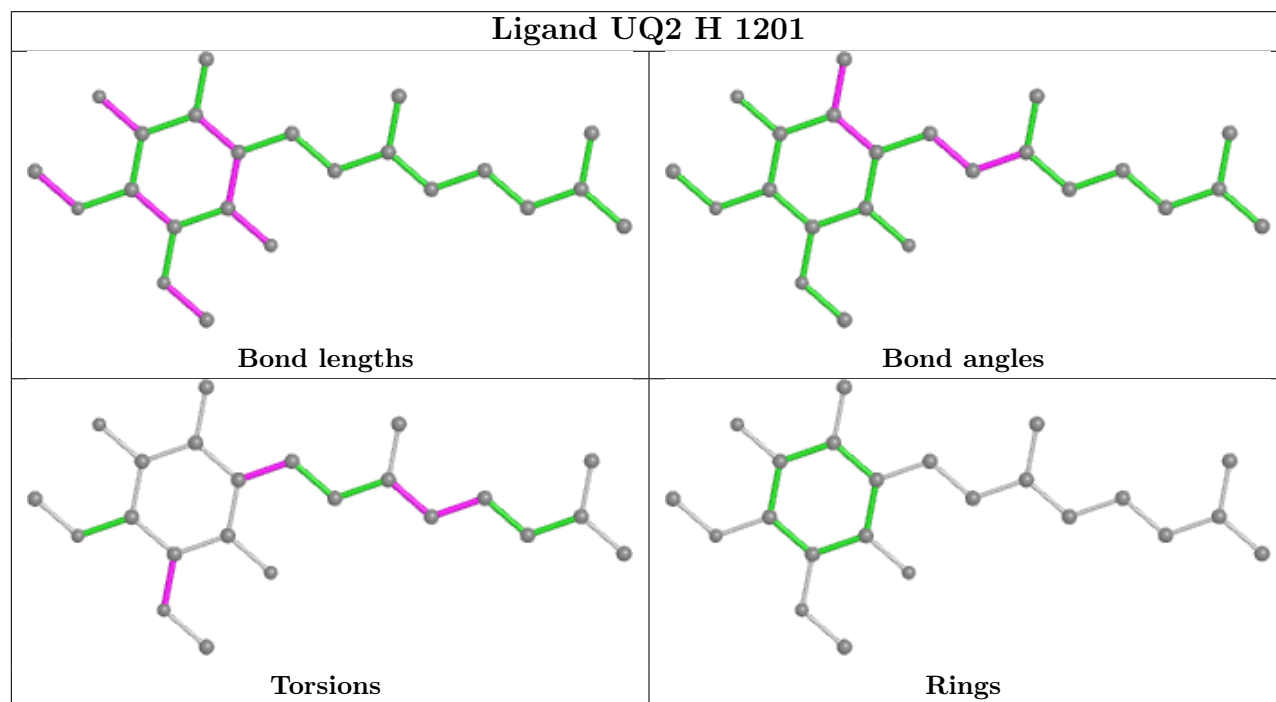
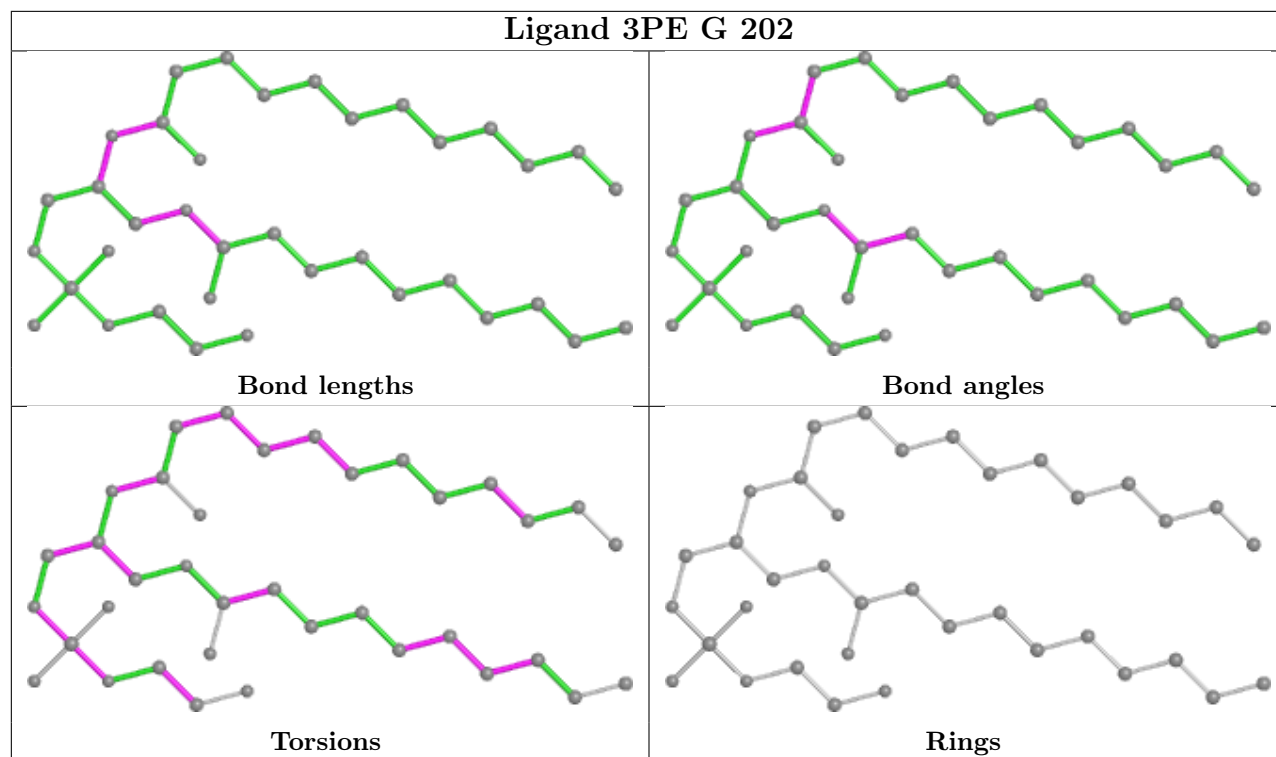


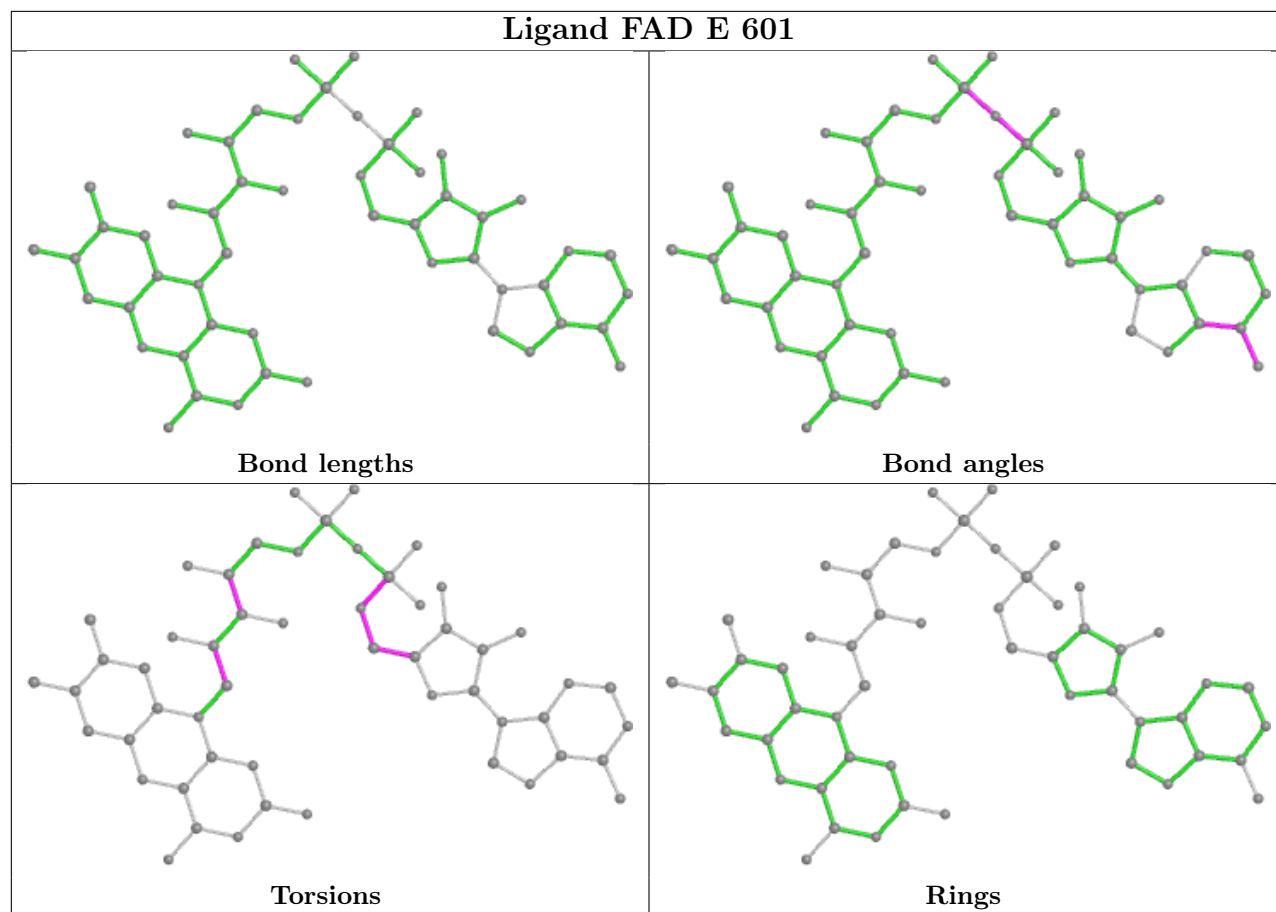












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

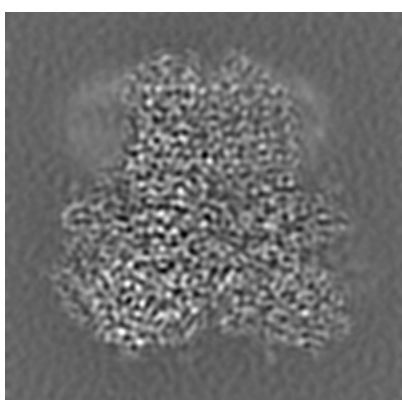
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22528. These allow visual inspection of the internal detail of the map and identification of artifacts.

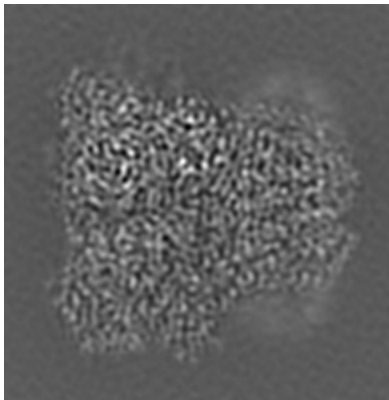
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

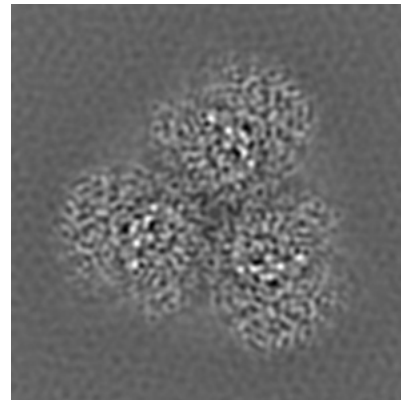
6.1.1 Primary map



X



Y

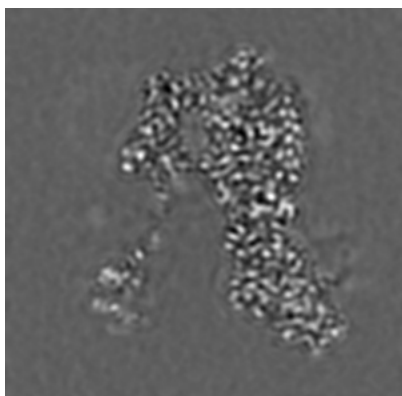


Z

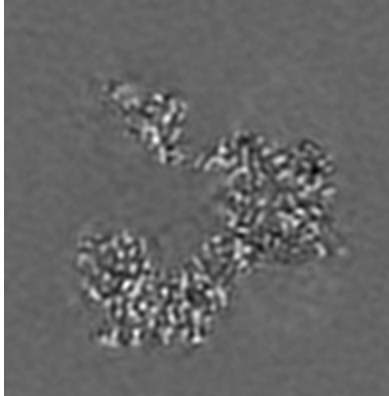
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

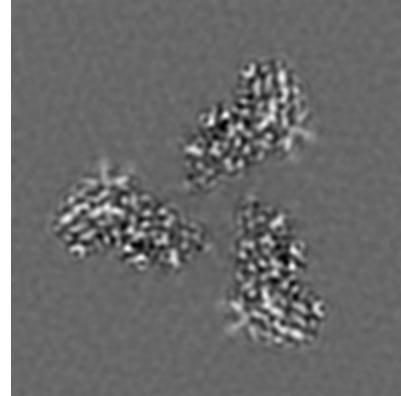
6.2.1 Primary map



X Index: 70



Y Index: 70

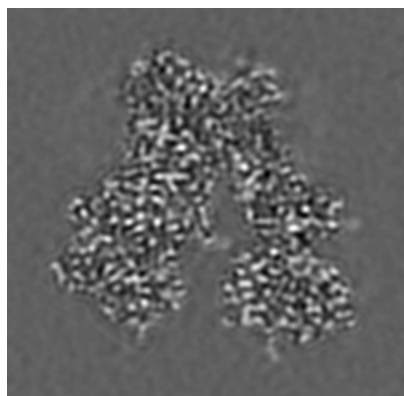


Z Index: 68

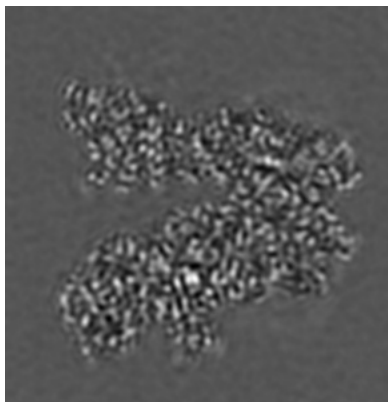
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

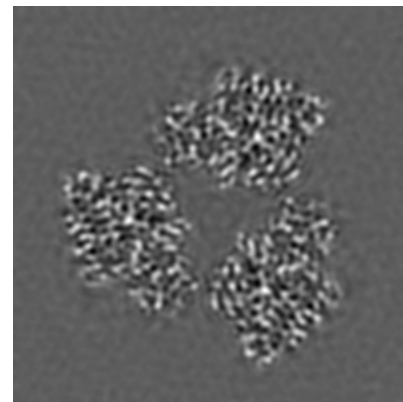
6.3.1 Primary map



X Index: 84



Y Index: 55

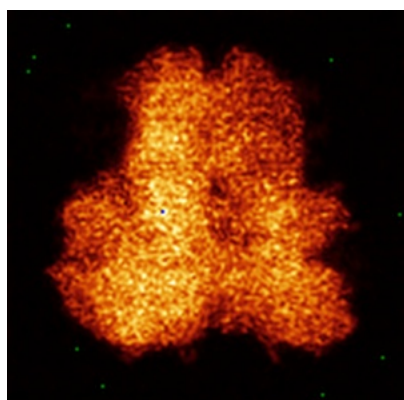


Z Index: 44

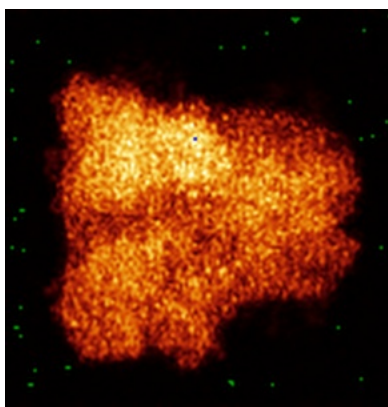
The images above show the largest variance slices of the map in three orthogonal directions.

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

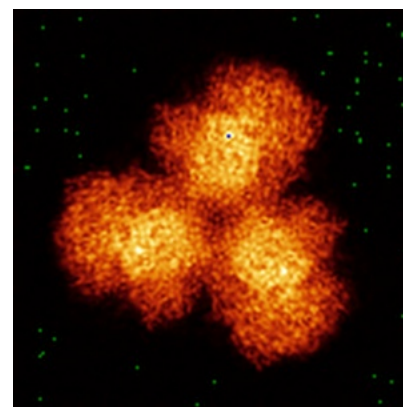
6.4.1 Primary map



X



Y

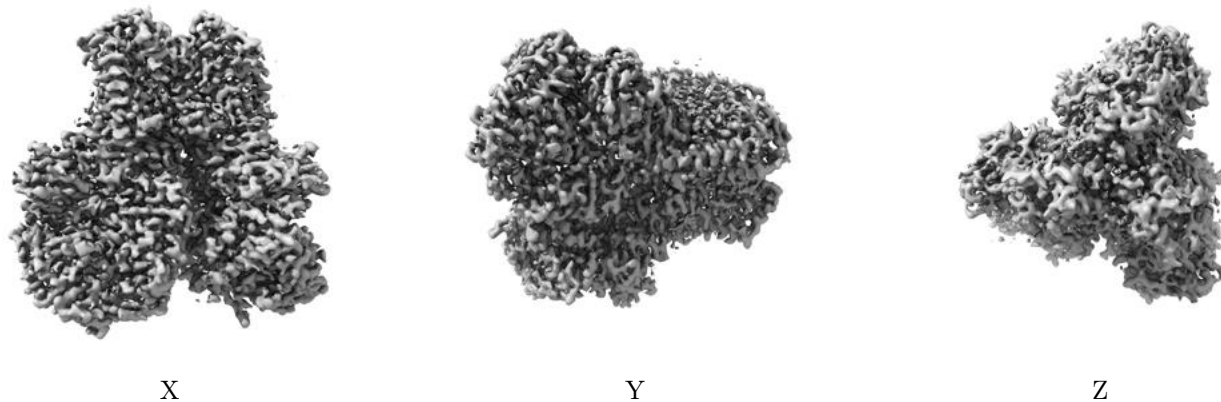


Z

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

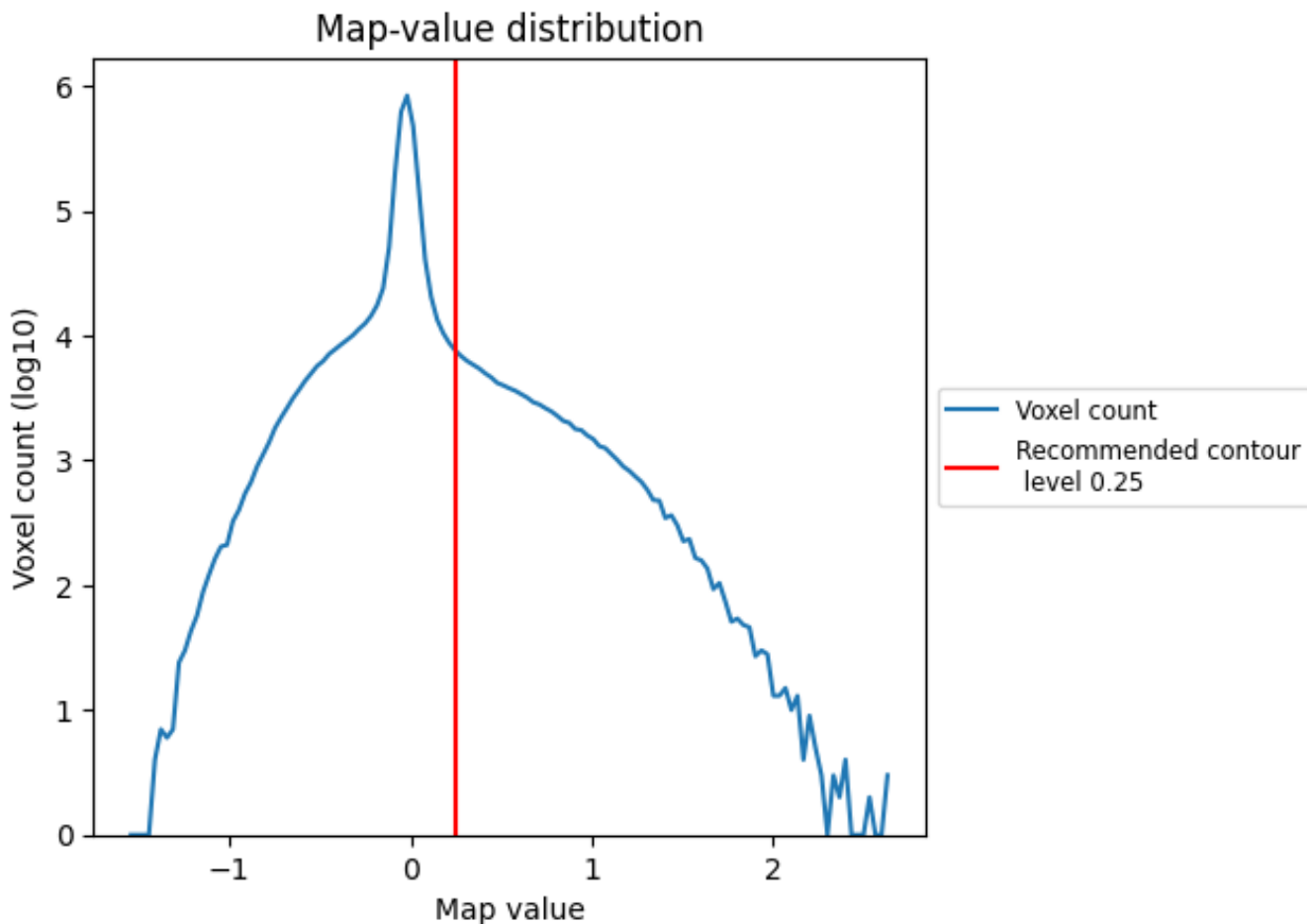
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

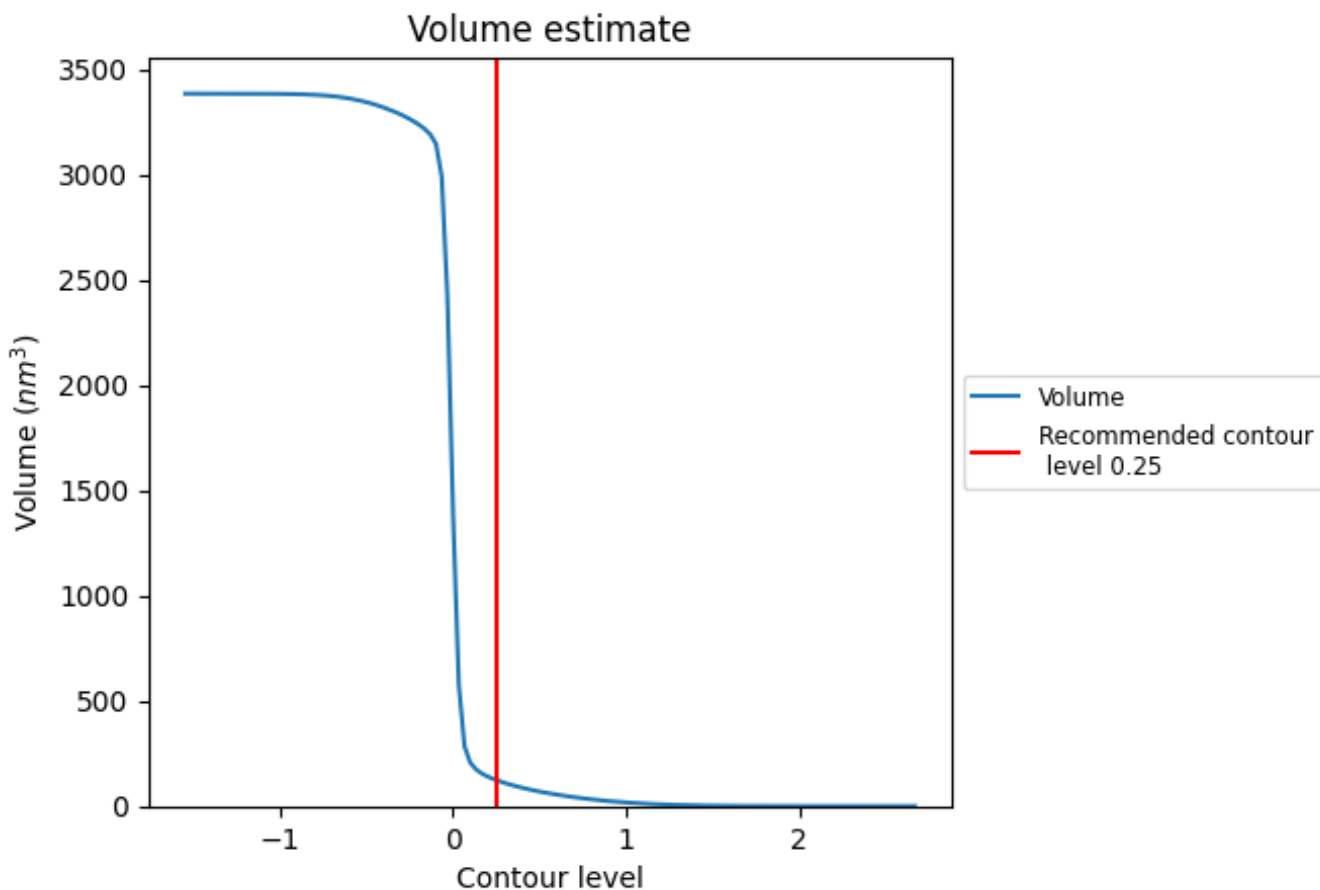
This section contains the results of statistical analysis of the map.

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 124 nm³; this corresponds to an approximate mass of 112 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

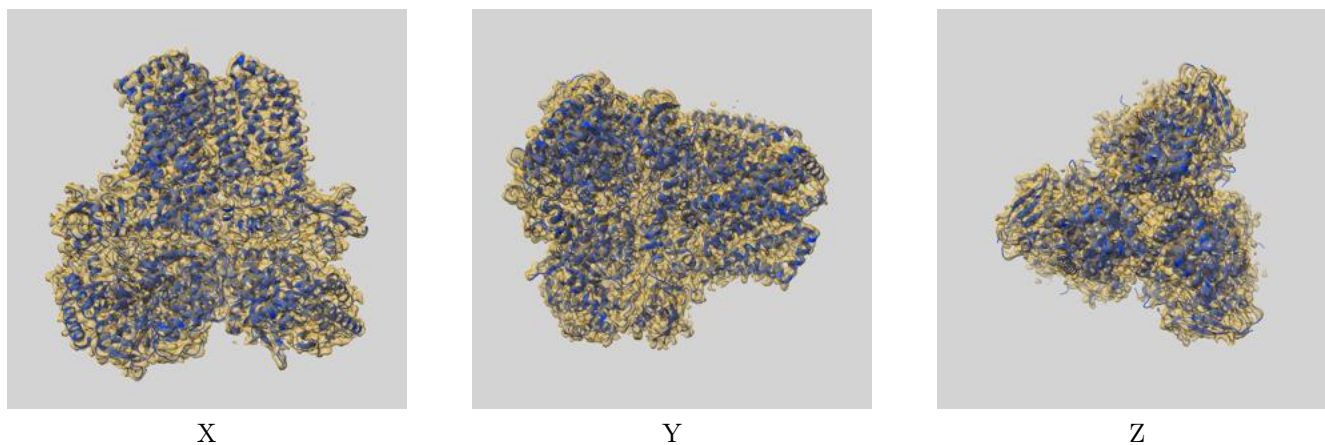
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

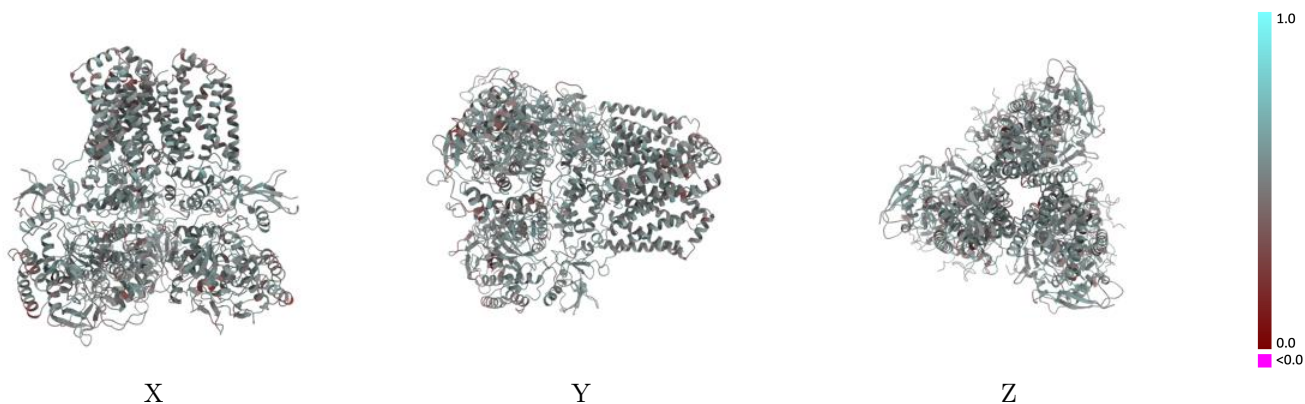
This section contains information regarding the fit between EMDB map EMD-22528 and PDB model 7JZ2. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



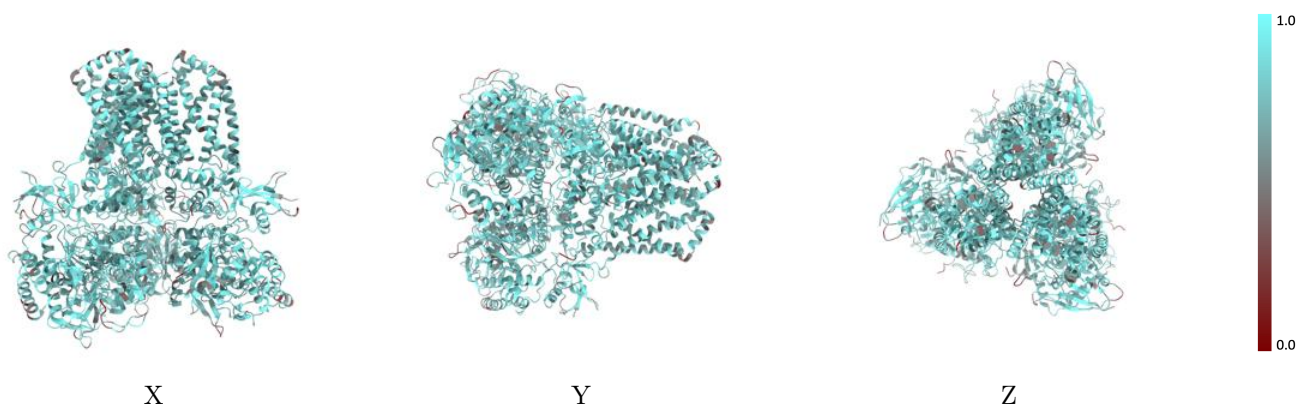
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



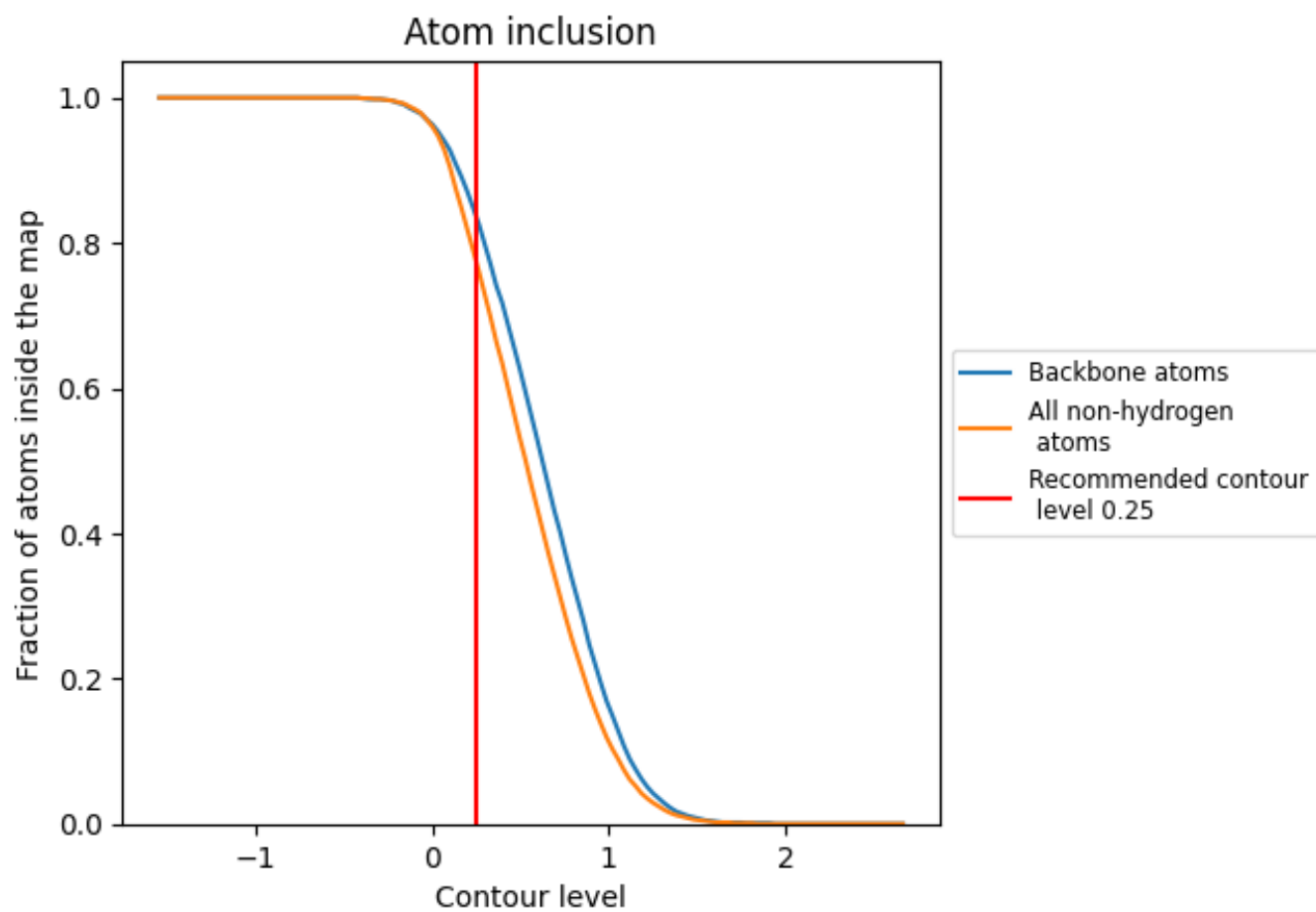
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.5100
A	 0.7670	 0.5040
B	 0.8080	 0.5280
C	 0.7370	 0.5070
D	 0.7760	 0.4980
E	 0.7630	 0.5030
F	 0.8090	 0.5300
G	 0.7560	 0.5120
H	 0.7790	 0.4970
I	 0.7630	 0.5030
J	 0.8050	 0.5300
K	 0.7440	 0.5110
L	 0.7890	 0.5000

