Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 06:49 am BST

PDB ID	:	6QKC
EMDB ID	:	EMD-4572
Title	:	GluA1/2 In complex with auxiliary subunit gamma-8
Authors	:	Herguedas, B.; Garcia-Nafria, J.; Greger, I.G.
Deposited on	:	2019-01-28
Resolution	:	4.40 Å(reported)
Based on initial models	:	5WEO, 3UA8, 5KK2

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:

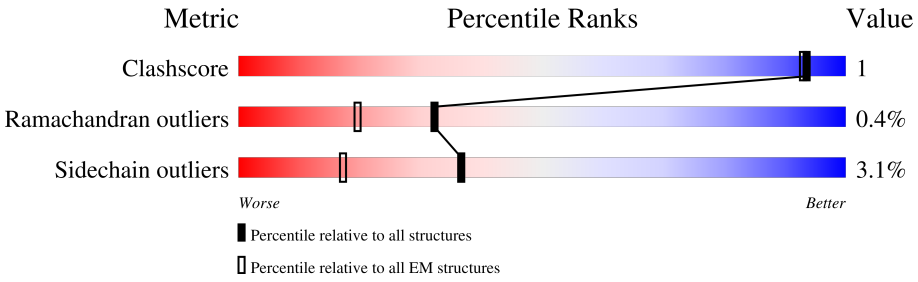
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	915	6% 41% · 57%
1	C	915	5% 40% · 57%
2	B	860	7% 45% · 54%
2	D	860	7% 45% · 54%
3	I	423	6% 36% · 62%
3	J	423	6% 36% · 62%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13794 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 Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	393	Total 2800	C 1835	N 448	O 503	S 14	0	0
1	C	393	Total 2800	C 1835	N 448	O 503	S 14	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490

- Molecule 2 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	396	Total 2769	C 1805	N 455	O 494	S 15	0	0
2	D	396	Total 2769	C 1805	N 455	O 494	S 15	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	conflict	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491

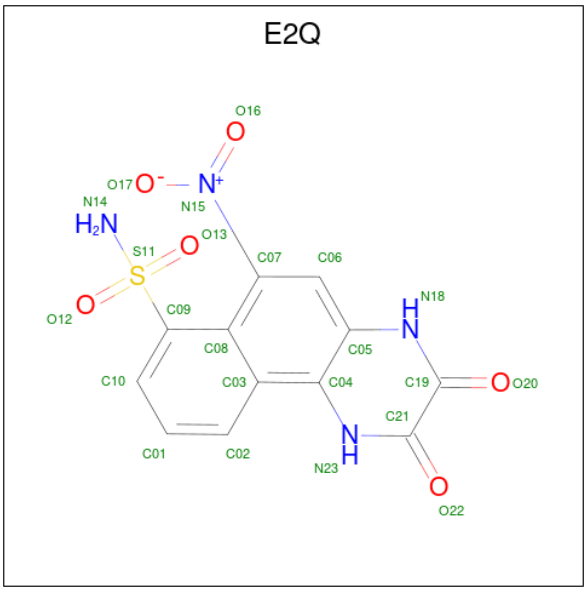
- Molecule 3 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	162	Total	C	N	O	S	0	0
			1132	752	184	191	5		
3	J	162	Total	C	N	O	S	0	0
			1132	752	184	191	5		

There are 14 discrepancies between the modelled and reference sequences:

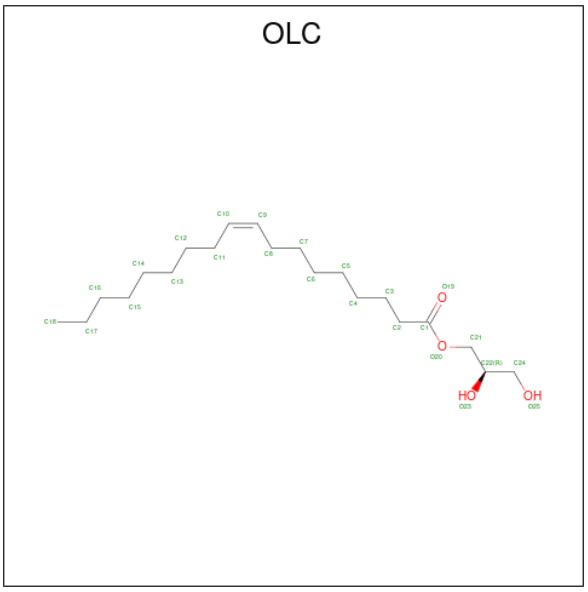
Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	expression tag	UNP Q8VHW5
I	418	LEU	-	expression tag	UNP Q8VHW5
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	1	GLY	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	UNP Q8VHW5
J	420	VAL	-	expression tag	UNP Q8VHW5
J	421	LEU	-	expression tag	UNP Q8VHW5
J	422	PHE	-	expression tag	UNP Q8VHW5
J	423	GLN	-	expression tag	UNP Q8VHW5

- Molecule 4 is 6-nitro-2,3-bis(oxidanylidene)-1,4-dihydrobenzo[f]quinoxaline-7-sulfonamide (three-letter code: E2Q) (formula: $C_{12}H_8N_4O_6S$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			23	12	4	6	1	
4	B	1	Total	C	N	O	S	0
			23	12	4	6	1	
4	C	1	Total	C	N	O	S	0
			23	12	4	6	1	
4	D	1	Total	C	N	O	S	0
			23	12	4	6	1	

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).

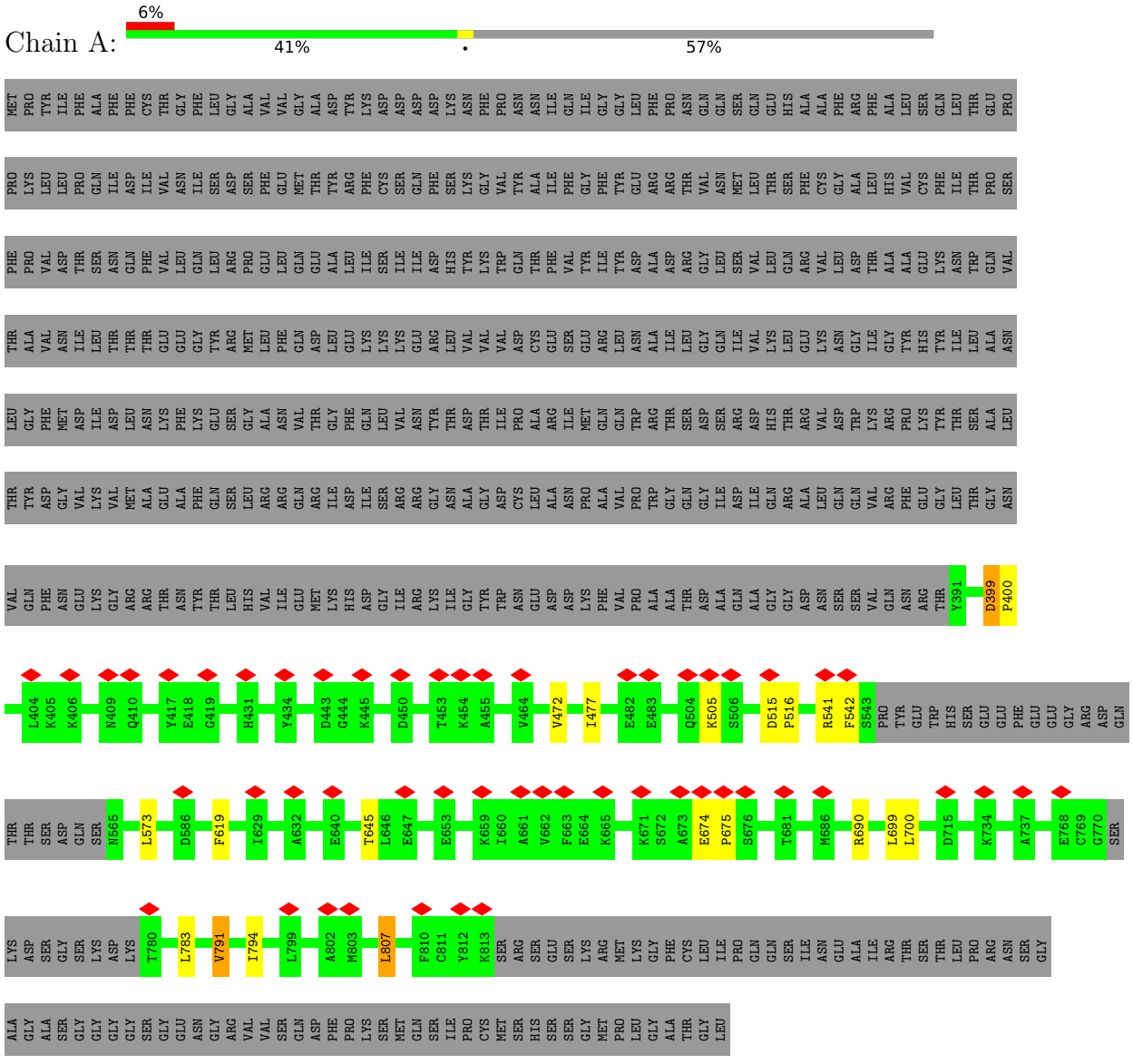


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			25	21	4	
5	A	1	Total	C	O	0
			25	21	4	
5	A	1	Total	C	O	0
			25	21	4	
5	C	1	Total	C	O	0
			25	21	4	
5	C	1	Total	C	O	0
			25	21	4	
5	C	1	Total	C	O	0
			25	21	4	
5	I	1	Total	C	O	0
			25	21	4	
5	I	1	Total	C	O	0
			25	21	4	
5	I	1	Total	C	O	0
			25	21	4	
5	J	1	Total	C	O	0
			25	21	4	
5	J	1	Total	C	O	0
			25	21	4	
5	J	1	Total	C	O	0
			25	21	4	

3 Residue-property plots (i)

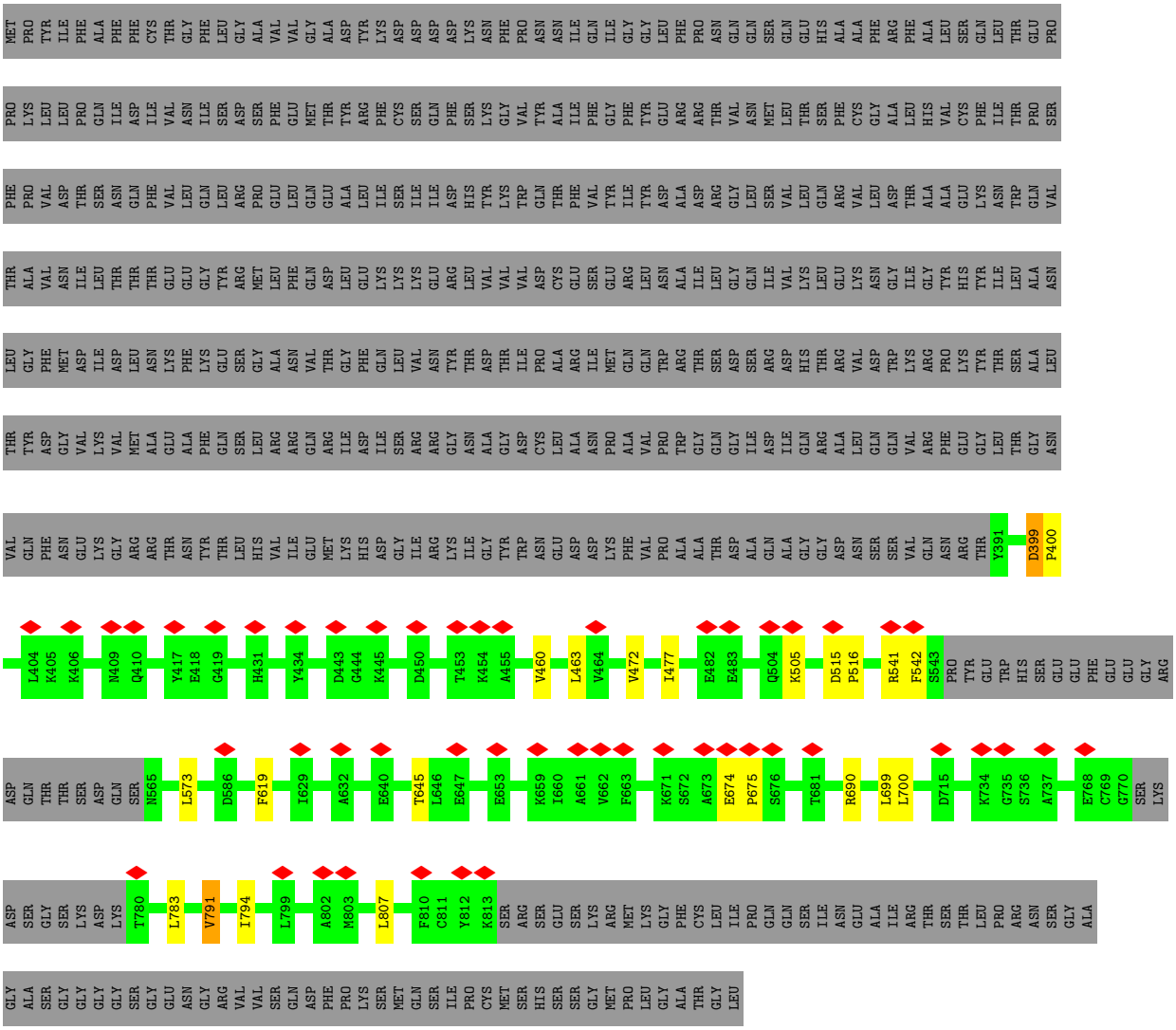
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Glutamate receptor 1



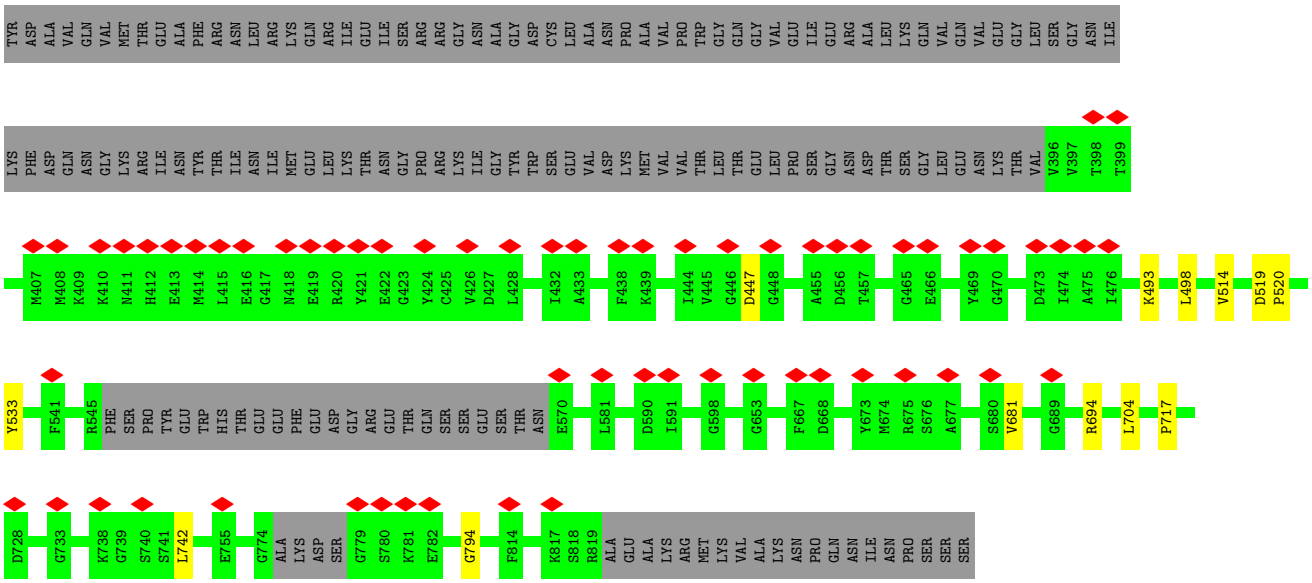
• Molecule 1: Glutamate receptor 1

Chain C:



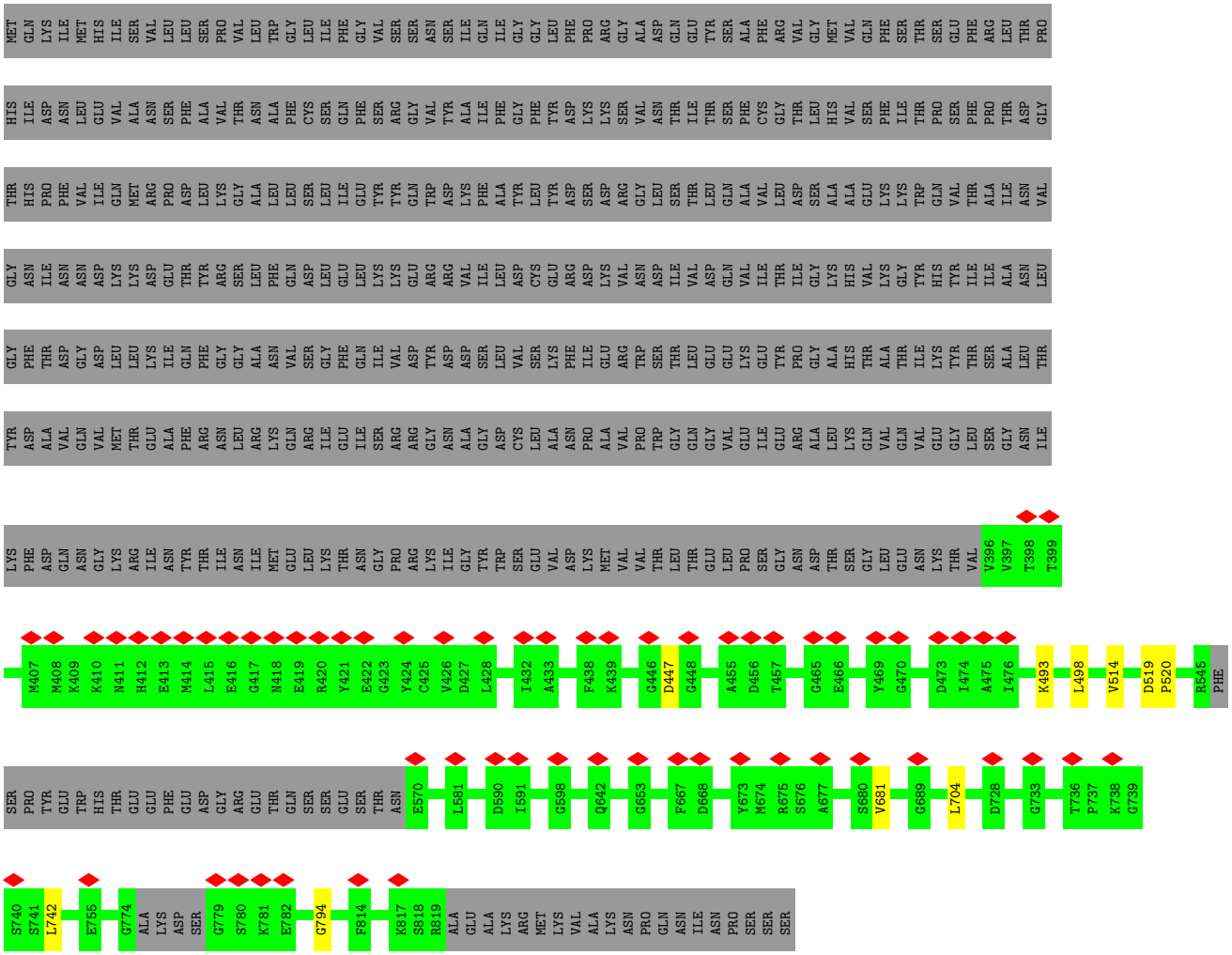
• Molecule 2: Glutamate receptor 2

Chain B:



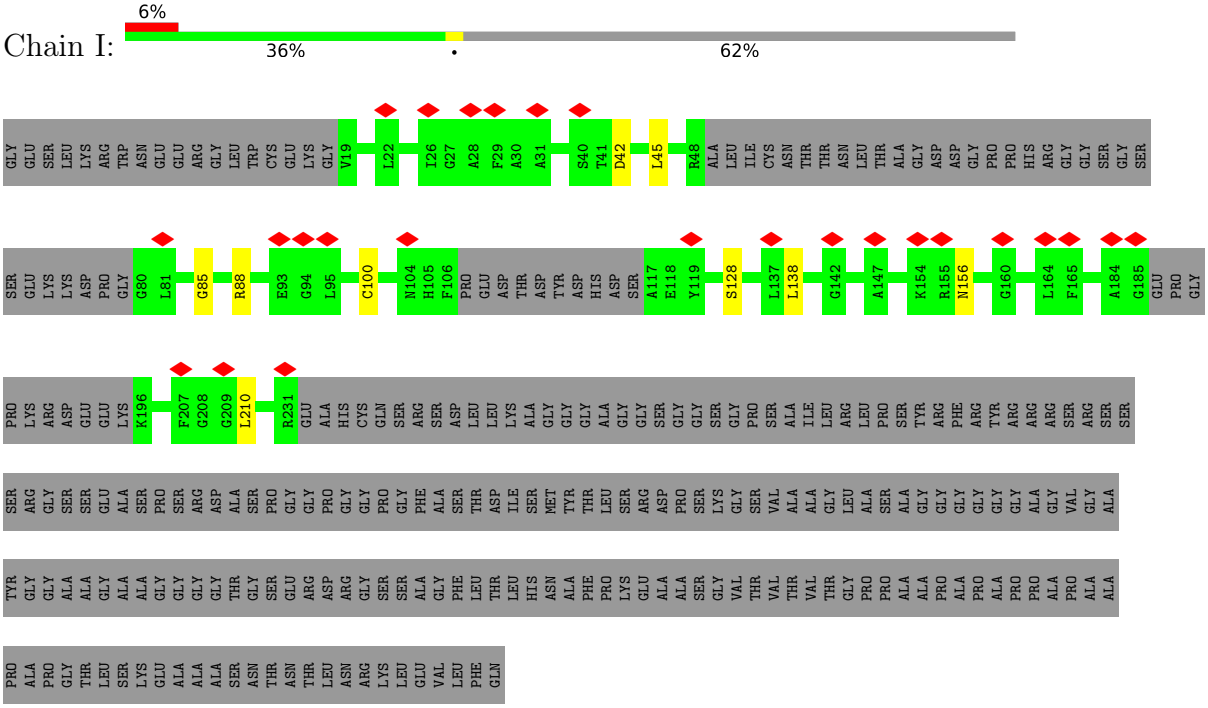
• Molecule 2: Glutamate receptor 2

Chain D:



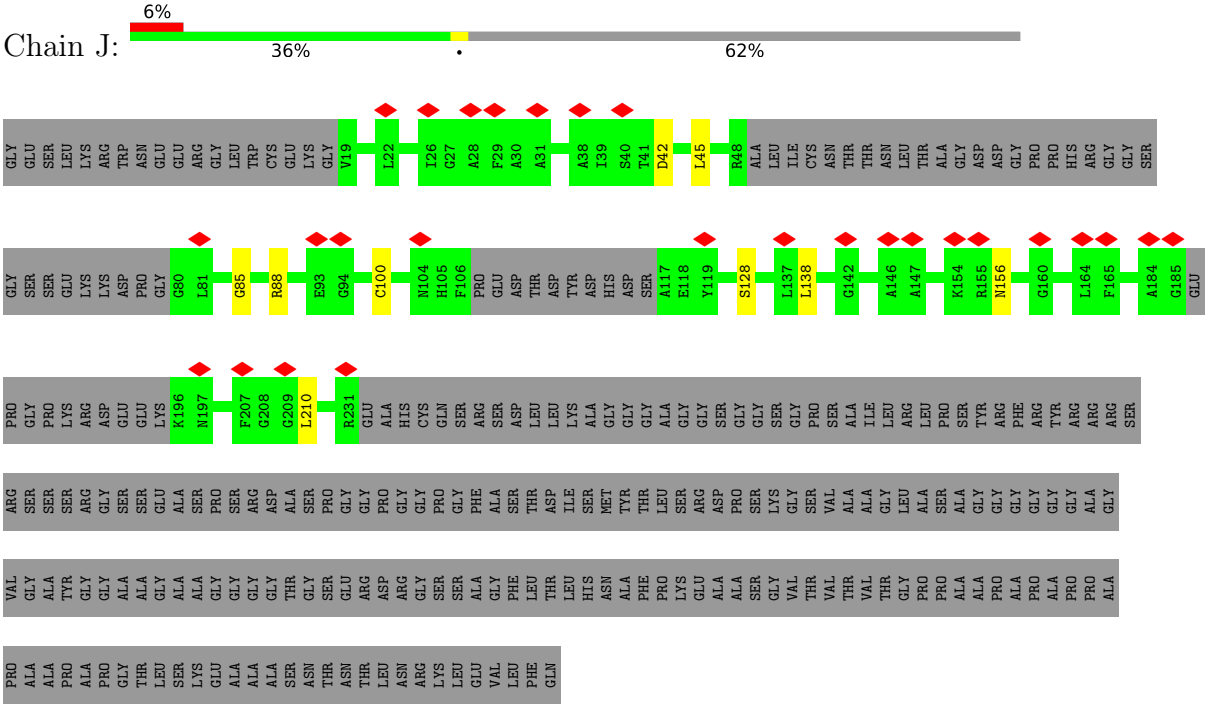
• Molecule 3: Voltage-dependent calcium channel gamma-8 subunit

Chain I:



• Molecule 3: Voltage-dependent calcium channel gamma-8 subunit

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	114730	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	-200	Depositor
Maximum defocus (nm)	-900	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, E2Q

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	0.70	0/2865	0.71	0/3912
1	C	0.70	0/2865	0.71	0/3912
2	B	0.71	0/2830	0.72	0/3869
2	D	0.71	0/2830	0.72	0/3869
3	I	0.72	0/1153	0.73	0/1574
3	J	0.72	0/1153	0.73	0/1574
All	All	0.71	0/13696	0.72	0/18710

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2800	0	2577	8	0
1	C	2800	0	2577	9	0
2	B	2769	0	2547	4	0
2	D	2769	0	2547	4	0
3	I	1132	0	1083	2	0
3	J	1132	0	1083	2	0
4	A	23	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	23	0	0	1	0
4	C	23	0	0	1	0
4	D	23	0	0	1	0
5	A	75	0	120	0	0
5	C	75	0	120	0	0
5	I	75	0	120	0	0
5	J	75	0	120	0	0
All	All	13794	0	12894	31	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 1.

All (31) 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:C:399:ASP:CB	1:C:400:PRO:CD	2.63	0.77
1:A:399:ASP:CB	1:A:400:PRO:CD	2.63	0.76
1:A:399:ASP:CB	1:A:400:PRO:HD3	2.20	0.72
1:C:399:ASP:CB	1:C:400:PRO:HD3	2.20	0.71
2:D:519:ASP:N	2:D:520:PRO:HD2	2.14	0.63
2:B:519:ASP:N	2:B:520:PRO:HD2	2.15	0.61
3:J:42:ASP:HA	3:J:85:GLY:HA3	1.92	0.52
3:I:42:ASP:HA	3:I:85:GLY:HA3	1.94	0.50
1:A:477:ILE:HG21	2:B:493:LYS:HE2	1.97	0.47
3:J:88:ARG:CZ	3:J:100:CYS:HB2	2.46	0.46
4:B:901:E2Q:O13	4:B:901:E2Q:O17	2.35	0.45
1:A:515:ASP:N	1:A:516:PRO:CD	2.80	0.45
1:C:791:VAL:HA	1:C:794:ILE:HD12	1.97	0.45
1:C:477:ILE:HG21	2:D:493:LYS:HE2	1.98	0.45
1:C:515:ASP:N	1:C:516:PRO:CD	2.79	0.45
4:C:901:E2Q:O13	4:C:901:E2Q:O17	2.35	0.45
4:A:901:E2Q:O13	4:A:901:E2Q:O17	2.35	0.44
1:A:645:THR:HG22	1:A:699:LEU:HB2	2.00	0.44
2:D:514:VAL:HG23	2:D:794:GLY:HA2	2.00	0.44
4:D:901:E2Q:O13	4:D:901:E2Q:O17	2.35	0.44
1:A:791:VAL:HA	1:A:794:ILE:HD12	1.98	0.44
3:I:88:ARG:CZ	3:I:100:CYS:HB2	2.49	0.43
1:C:645:THR:HG22	1:C:699:LEU:HB2	2.00	0.43
2:D:519:ASP:N	2:D:520:PRO:CD	2.83	0.41
2:B:514:VAL:HG23	2:B:794:GLY:HA2	2.01	0.41
2:B:694:ARG:HH12	2:B:717:PRO:HD2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:VAL:HA	1:C:463:LEU:HD12	2.03	0.41
1:A:807:LEU:HD22	1:A:807:LEU:HA	1.96	0.41
1:C:674:GLU:CB	1:C:675:PRO:CD	2.99	0.41
1:C:674:GLU:CB	1:C:675:PRO:HD3	2.51	0.41
1:A:674:GLU:CB	1:A:675:PRO:HD3	2.51	0.41

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	387/915 (42%)	352 (91%)	33 (8%)	2 (0%)	25	63
1	C	387/915 (42%)	352 (91%)	33 (8%)	2 (0%)	25	63
2	B	390/860 (45%)	365 (94%)	25 (6%)	0	100	100
2	D	390/860 (45%)	365 (94%)	25 (6%)	0	100	100
3	I	154/423 (36%)	141 (92%)	11 (7%)	2 (1%)	10	42
3	J	154/423 (36%)	141 (92%)	11 (7%)	2 (1%)	10	42
All	All	1862/4396 (42%)	1716 (92%)	138 (7%)	8 (0%)	32	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	ASP
1	C	399	ASP
1	A	505	LYS
1	C	505	LYS
3	I	156	ASN
3	J	156	ASN
3	I	128	SER
3	J	128	SER

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	252/778 (32%)	242 (96%)	10 (4%)	27	48
1	C	252/778 (32%)	242 (96%)	10 (4%)	27	48
2	B	247/737 (34%)	241 (98%)	6 (2%)	44	63
2	D	247/737 (34%)	242 (98%)	5 (2%)	50	69
3	I	100/309 (32%)	97 (97%)	3 (3%)	36	57
3	J	100/309 (32%)	97 (97%)	3 (3%)	36	57
All	All	1198/3648 (33%)	1161 (97%)	37 (3%)	37	56

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	VAL
1	A	541	ARG
1	A	542	PHE
1	A	573	LEU
1	A	619	PHE
1	A	690	ARG
1	A	700	LEU
1	A	783	LEU
1	A	791	VAL
1	A	807	LEU
2	B	447	ASP
2	B	498	LEU
2	B	533	TYR
2	B	681	VAL
2	B	704	LEU
2	B	742	LEU
1	C	472	VAL
1	C	541	ARG
1	C	542	PHE
1	C	573	LEU
1	C	619	PHE
1	C	690	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	700	LEU
1	C	783	LEU
1	C	791	VAL
1	C	807	LEU
2	D	447	ASP
2	D	498	LEU
2	D	681	VAL
2	D	704	LEU
2	D	742	LEU
3	I	45	LEU
3	I	138	LEU
3	I	210	LEU
3	J	45	LEU
3	J	138	LEU
3	J	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	583	GLN
1	C	583	GLN
3	I	172	ASN
3	J	172	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

16 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	$\#\|Z\| > 2$
4	E2Q	C	901	-	24,25,25	3.47	8 (33%)	32,39,39	2.26	12 (37%)
5	OLC	C	904	-	24,24,24	0.95	1 (4%)	25,25,25	0.83	1 (4%)
5	OLC	J	502	-	24,24,24	0.94	1 (4%)	25,25,25	0.78	1 (4%)
5	OLC	I	501	-	24,24,24	0.95	1 (4%)	25,25,25	0.81	1 (4%)
4	E2Q	D	901	-	24,25,25	3.47	8 (33%)	32,39,39	2.20	11 (34%)
4	E2Q	A	901	-	24,25,25	3.46	8 (33%)	32,39,39	2.25	12 (37%)
4	E2Q	B	901	-	24,25,25	3.47	8 (33%)	32,39,39	2.21	11 (34%)
5	OLC	A	904	-	24,24,24	0.95	1 (4%)	25,25,25	0.83	1 (4%)
5	OLC	I	503	-	24,24,24	0.94	1 (4%)	25,25,25	0.82	1 (4%)
5	OLC	J	503	-	24,24,24	0.95	1 (4%)	25,25,25	0.82	1 (4%)
5	OLC	C	902	-	24,24,24	0.96	1 (4%)	25,25,25	0.77	1 (4%)
5	OLC	I	502	-	24,24,24	0.94	1 (4%)	25,25,25	0.78	1 (4%)
5	OLC	C	903	-	24,24,24	0.95	1 (4%)	25,25,25	0.78	1 (4%)
5	OLC	A	902	-	24,24,24	0.95	1 (4%)	25,25,25	0.77	1 (4%)
5	OLC	J	501	-	24,24,24	0.95	1 (4%)	25,25,25	0.81	1 (4%)
5	OLC	A	903	-	24,24,24	0.95	1 (4%)	25,25,25	0.78	1 (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
4	E2Q	C	901	-	-	2/8/10/10	0/3/3/3
5	OLC	C	904	-	-	15/24/24/24	-
5	OLC	J	502	-	-	11/24/24/24	-
5	OLC	I	501	-	-	13/24/24/24	-
4	E2Q	D	901	-	-	2/8/10/10	0/3/3/3
4	E2Q	A	901	-	-	2/8/10/10	0/3/3/3
4	E2Q	B	901	-	-	2/8/10/10	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	904	-	-	15/24/24/24	-
5	OLC	I	503	-	-	13/24/24/24	-
5	OLC	J	503	-	-	13/24/24/24	-
5	OLC	C	902	-	-	15/24/24/24	-
5	OLC	I	502	-	-	11/24/24/24	-
5	OLC	C	903	-	-	15/24/24/24	-
5	OLC	A	902	-	-	15/24/24/24	-
5	OLC	J	501	-	-	13/24/24/24	-
5	OLC	A	903	-	-	15/24/24/24	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	E2Q	C09-S11	-11.27	1.61	1.77
4	C	901	E2Q	C09-S11	-11.26	1.61	1.77
4	D	901	E2Q	C09-S11	-11.25	1.61	1.77
4	A	901	E2Q	C09-S11	-11.20	1.61	1.77
4	C	901	E2Q	O16-N15	9.96	1.39	1.22
4	A	901	E2Q	O16-N15	9.94	1.39	1.22
4	B	901	E2Q	O16-N15	9.93	1.39	1.22
4	D	901	E2Q	O16-N15	9.92	1.39	1.22
5	C	903	OLC	O20-C1	4.40	1.46	1.33
5	A	903	OLC	O20-C1	4.39	1.46	1.33
5	I	501	OLC	O20-C1	4.38	1.46	1.33
5	J	501	OLC	O20-C1	4.38	1.46	1.33
5	C	902	OLC	O20-C1	4.37	1.46	1.33
5	A	902	OLC	O20-C1	4.36	1.46	1.33
5	A	904	OLC	O20-C1	4.33	1.46	1.33
5	J	503	OLC	O20-C1	4.33	1.46	1.33
5	J	502	OLC	O20-C1	4.32	1.46	1.33
5	I	502	OLC	O20-C1	4.32	1.46	1.33
5	I	503	OLC	O20-C1	4.31	1.45	1.33
5	C	904	OLC	O20-C1	4.30	1.45	1.33
4	B	901	E2Q	S11-N14	-3.99	1.52	1.60
4	A	901	E2Q	S11-N14	-3.98	1.52	1.60
4	D	901	E2Q	S11-N14	-3.98	1.52	1.60
4	C	901	E2Q	S11-N14	-3.93	1.52	1.60
4	B	901	E2Q	C07-N15	-2.91	1.40	1.45
4	D	901	E2Q	C07-N15	-2.90	1.40	1.45
4	C	901	E2Q	C07-N15	-2.88	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	E2Q	C07-N15	-2.82	1.40	1.45
4	D	901	E2Q	O12-S11	2.62	1.48	1.43
4	B	901	E2Q	O12-S11	2.60	1.48	1.43
4	B	901	E2Q	O13-S11	2.58	1.48	1.43
4	A	901	E2Q	O12-S11	2.57	1.48	1.43
4	C	901	E2Q	O12-S11	2.56	1.48	1.43
4	C	901	E2Q	O13-S11	2.56	1.48	1.43
4	C	901	E2Q	C10-C09	2.55	1.40	1.37
4	A	901	E2Q	C10-C09	2.55	1.40	1.37
4	D	901	E2Q	C10-C09	2.54	1.40	1.37
4	A	901	E2Q	O13-S11	2.53	1.48	1.43
4	D	901	E2Q	O13-S11	2.49	1.48	1.43
4	B	901	E2Q	C10-C09	2.47	1.40	1.37
4	A	901	E2Q	C05-N18	-2.30	1.35	1.39
4	D	901	E2Q	C05-N18	-2.26	1.36	1.39
4	C	901	E2Q	C05-N18	-2.23	1.36	1.39
4	B	901	E2Q	C05-N18	-2.22	1.36	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	E2Q	O13-S11-O12	-7.45	106.51	118.76
4	C	901	E2Q	O13-S11-O12	-7.44	106.53	118.76
4	B	901	E2Q	O13-S11-O12	-7.25	106.85	118.76
4	D	901	E2Q	O13-S11-O12	-7.20	106.92	118.76
4	B	901	E2Q	C02-C03-C04	-4.14	117.33	124.78
4	C	901	E2Q	C02-C03-C04	-4.11	117.37	124.78
4	D	901	E2Q	C02-C03-C04	-4.11	117.38	124.78
4	A	901	E2Q	C02-C03-C04	-4.09	117.42	124.78
4	B	901	E2Q	C05-N18-C19	-3.51	120.33	124.80
4	C	901	E2Q	C05-N18-C19	-3.51	120.34	124.80
4	A	901	E2Q	C05-N18-C19	-3.50	120.34	124.80
4	D	901	E2Q	C05-N18-C19	-3.49	120.36	124.80
4	C	901	E2Q	C08-C09-S11	3.24	125.80	121.67
4	A	901	E2Q	C08-C09-S11	3.20	125.75	121.67
4	D	901	E2Q	C08-C09-S11	3.12	125.65	121.67
4	B	901	E2Q	C08-C09-S11	3.11	125.64	121.67
5	A	904	OLC	O20-C1-C2	3.00	121.33	111.91
5	C	904	OLC	O20-C1-C2	3.00	121.33	111.91
4	A	901	E2Q	O13-S11-C09	2.86	111.47	107.28
4	A	901	E2Q	C04-C05-N18	2.84	121.53	118.63
4	C	901	E2Q	O13-S11-C09	2.84	111.44	107.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	503	OLC	O20-C1-C2	2.83	120.78	111.91
5	I	503	OLC	O20-C1-C2	2.82	120.75	111.91
4	C	901	E2Q	C04-C05-N18	2.78	121.46	118.63
4	D	901	E2Q	C04-C05-N18	2.77	121.45	118.63
4	B	901	E2Q	C04-C05-N18	2.75	121.43	118.63
4	A	901	E2Q	O13-S11-N14	2.63	111.27	107.36
4	C	901	E2Q	O13-S11-N14	2.61	111.24	107.36
5	C	902	OLC	O20-C1-C2	2.61	120.10	111.91
5	A	902	OLC	O20-C1-C2	2.59	120.05	111.91
4	D	901	E2Q	C21-C19-N18	2.58	118.65	116.82
4	C	901	E2Q	C21-C19-N18	2.57	118.64	116.82
4	B	901	E2Q	C21-C19-N18	2.55	118.63	116.82
5	I	501	OLC	O20-C1-C2	2.55	119.92	111.91
5	J	501	OLC	O20-C1-C2	2.55	119.90	111.91
4	A	901	E2Q	C21-C19-N18	2.53	118.62	116.82
4	B	901	E2Q	O12-S11-C09	2.52	110.97	107.28
4	D	901	E2Q	O13-S11-N14	2.51	111.09	107.36
5	A	903	OLC	O20-C1-C2	2.50	119.76	111.91
4	B	901	E2Q	O13-S11-N14	2.50	111.07	107.36
4	D	901	E2Q	O12-S11-C09	2.50	110.94	107.28
4	C	901	E2Q	C19-C21-N23	2.50	118.59	116.82
4	A	901	E2Q	C19-C21-N23	2.50	118.59	116.82
4	B	901	E2Q	C19-C21-N23	2.49	118.59	116.82
5	C	903	OLC	O20-C1-C2	2.49	119.72	111.91
5	I	502	OLC	O20-C1-C2	2.47	119.66	111.91
5	J	502	OLC	O20-C1-C2	2.45	119.59	111.91
4	D	901	E2Q	C19-C21-N23	2.41	118.53	116.82
4	D	901	E2Q	O13-S11-C09	2.40	110.79	107.28
4	B	901	E2Q	O13-S11-C09	2.39	110.79	107.28
4	C	901	E2Q	O12-S11-C09	2.33	110.69	107.28
4	A	901	E2Q	O12-S11-C09	2.30	110.65	107.28
4	D	901	E2Q	C04-C03-C08	2.05	121.68	117.08
4	B	901	E2Q	C04-C03-C08	2.04	121.66	117.08
4	C	901	E2Q	C10-C09-S11	-2.04	114.72	117.53
4	A	901	E2Q	C10-C09-S11	-2.04	114.73	117.53
4	A	901	E2Q	C04-C03-C08	2.02	121.62	117.08
4	C	901	E2Q	C04-C03-C08	2.02	121.61	117.08

There are no chirality outliers.

All (172) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	E2Q	C06-C07-N15-O16
4	A	901	E2Q	C08-C07-N15-O16
4	B	901	E2Q	C06-C07-N15-O16
4	B	901	E2Q	C08-C07-N15-O16
4	C	901	E2Q	C06-C07-N15-O16
4	C	901	E2Q	C08-C07-N15-O16
4	D	901	E2Q	C06-C07-N15-O16
4	D	901	E2Q	C08-C07-N15-O16
5	A	902	OLC	O20-C21-C22-C24
5	A	904	OLC	O20-C21-C22-C24
5	C	902	OLC	O20-C21-C22-C24
5	C	904	OLC	O20-C21-C22-C24
5	I	501	OLC	O20-C21-C22-C24
5	J	501	OLC	O20-C21-C22-C24
5	I	503	OLC	C2-C1-O20-C21
5	J	503	OLC	C2-C1-O20-C21
5	A	902	OLC	O20-C21-C22-O23
5	A	904	OLC	O20-C21-C22-O23
5	C	902	OLC	O20-C21-C22-O23
5	C	904	OLC	O20-C21-C22-O23
5	I	501	OLC	O20-C21-C22-O23
5	J	501	OLC	O20-C21-C22-O23
5	I	503	OLC	O19-C1-O20-C21
5	J	503	OLC	O19-C1-O20-C21
5	A	904	OLC	C2-C1-O20-C21
5	C	904	OLC	C2-C1-O20-C21
5	A	904	OLC	O19-C1-O20-C21
5	C	904	OLC	O19-C1-O20-C21
5	C	904	OLC	C3-C4-C5-C6
5	A	904	OLC	C3-C4-C5-C6
5	A	903	OLC	C3-C4-C5-C6
5	C	903	OLC	C3-C4-C5-C6
5	I	502	OLC	C12-C13-C14-C15
5	J	503	OLC	C11-C12-C13-C14
5	A	903	OLC	C2-C3-C4-C5
5	A	904	OLC	C11-C12-C13-C14
5	C	903	OLC	C2-C3-C4-C5
5	I	501	OLC	C3-C4-C5-C6
5	I	502	OLC	C13-C14-C15-C16
5	I	503	OLC	C11-C12-C13-C14
5	J	501	OLC	C3-C4-C5-C6
5	J	502	OLC	C13-C14-C15-C16
5	J	502	OLC	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	902	OLC	C13-C14-C15-C16
5	C	904	OLC	C11-C12-C13-C14
5	I	501	OLC	C12-C13-C14-C15
5	J	501	OLC	C12-C13-C14-C15
5	A	902	OLC	C13-C14-C15-C16
5	A	902	OLC	C12-C13-C14-C15
5	A	902	OLC	C3-C4-C5-C6
5	C	902	OLC	C3-C4-C5-C6
5	C	902	OLC	C12-C13-C14-C15
5	C	904	OLC	C12-C13-C14-C15
5	A	902	OLC	C2-C1-O20-C21
5	C	902	OLC	C2-C1-O20-C21
5	A	902	OLC	C14-C15-C16-C17
5	A	903	OLC	C11-C12-C13-C14
5	A	904	OLC	C12-C13-C14-C15
5	C	902	OLC	C14-C15-C16-C17
5	C	903	OLC	C11-C12-C13-C14
5	C	904	OLC	C5-C6-C7-C8
5	I	501	OLC	C14-C15-C16-C17
5	I	502	OLC	C14-C15-C16-C17
5	J	502	OLC	C14-C15-C16-C17
5	A	904	OLC	C5-C6-C7-C8
5	C	902	OLC	C2-C3-C4-C5
5	I	502	OLC	C5-C6-C7-C8
5	J	502	OLC	C5-C6-C7-C8
5	A	903	OLC	C21-C22-C24-O25
5	A	904	OLC	C21-C22-C24-O25
5	C	903	OLC	C21-C22-C24-O25
5	C	904	OLC	C21-C22-C24-O25
5	I	502	OLC	O20-C21-C22-O23
5	A	902	OLC	C2-C3-C4-C5
5	J	501	OLC	C14-C15-C16-C17
5	A	902	OLC	C4-C5-C6-C7
5	C	902	OLC	C4-C5-C6-C7
5	C	904	OLC	C13-C14-C15-C16
5	A	904	OLC	C13-C14-C15-C16
5	A	902	OLC	O19-C1-O20-C21
5	C	902	OLC	O19-C1-O20-C21
5	C	904	OLC	C14-C15-C16-C17
5	J	503	OLC	C13-C14-C15-C16
5	J	502	OLC	O20-C21-C22-O23
5	I	503	OLC	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	904	OLC	C14-C15-C16-C17
5	J	503	OLC	C3-C4-C5-C6
5	I	503	OLC	C3-C4-C5-C6
5	I	503	OLC	C6-C7-C8-C9
5	J	503	OLC	C6-C7-C8-C9
5	J	503	OLC	C2-C3-C4-C5
5	I	503	OLC	C2-C3-C4-C5
5	A	904	OLC	C1-C2-C3-C4
5	C	904	OLC	C1-C2-C3-C4
5	J	503	OLC	C5-C6-C7-C8
5	A	902	OLC	C11-C12-C13-C14
5	I	503	OLC	C5-C6-C7-C8
5	C	902	OLC	C11-C12-C13-C14
5	A	904	OLC	C15-C16-C17-C18
5	J	502	OLC	C15-C16-C17-C18
5	I	502	OLC	C15-C16-C17-C18
5	C	904	OLC	C15-C16-C17-C18
5	C	903	OLC	C15-C16-C17-C18
5	A	903	OLC	C15-C16-C17-C18
5	I	503	OLC	C4-C5-C6-C7
5	J	503	OLC	C4-C5-C6-C7
5	I	502	OLC	C2-C1-O20-C21
5	J	502	OLC	C2-C1-O20-C21
5	J	501	OLC	C6-C7-C8-C9
5	I	501	OLC	C6-C7-C8-C9
5	A	902	OLC	C5-C6-C7-C8
5	I	501	OLC	C2-C1-O20-C21
5	C	902	OLC	C5-C6-C7-C8
5	J	501	OLC	C5-C6-C7-C8
5	J	501	OLC	C2-C1-O20-C21
5	I	501	OLC	C5-C6-C7-C8
5	J	502	OLC	O19-C1-O20-C21
5	A	903	OLC	C6-C7-C8-C9
5	C	903	OLC	C6-C7-C8-C9
5	I	502	OLC	O19-C1-O20-C21
5	A	903	OLC	C10-C11-C12-C13
5	C	903	OLC	C10-C11-C12-C13
5	I	501	OLC	O19-C1-O20-C21
5	J	501	OLC	O19-C1-O20-C21
5	J	503	OLC	C15-C16-C17-C18
5	I	503	OLC	C1-C2-C3-C4
5	J	503	OLC	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	J	501	OLC	C15-C16-C17-C18
5	I	501	OLC	C15-C16-C17-C18
5	I	503	OLC	C15-C16-C17-C18
5	I	502	OLC	C2-C3-C4-C5
5	J	502	OLC	C2-C3-C4-C5
5	A	903	OLC	O23-C22-C24-O25
5	C	903	OLC	O23-C22-C24-O25
5	A	903	OLC	C4-C5-C6-C7
5	C	903	OLC	C4-C5-C6-C7
5	C	903	OLC	C14-C15-C16-C17
5	A	904	OLC	O20-C1-C2-C3
5	C	904	OLC	O20-C1-C2-C3
5	I	501	OLC	C10-C11-C12-C13
5	J	501	OLC	C10-C11-C12-C13
5	A	903	OLC	C14-C15-C16-C17
5	A	904	OLC	O23-C22-C24-O25
5	C	904	OLC	O23-C22-C24-O25
5	J	501	OLC	O20-C1-C2-C3
5	I	503	OLC	C7-C8-C9-C10
5	J	503	OLC	C7-C8-C9-C10
5	I	501	OLC	O20-C1-C2-C3
5	I	502	OLC	C3-C4-C5-C6
5	J	502	OLC	C3-C4-C5-C6
5	C	903	OLC	O20-C1-C2-C3
5	A	903	OLC	O20-C1-C2-C3
5	A	902	OLC	C10-C11-C12-C13
5	C	902	OLC	C10-C11-C12-C13
5	I	502	OLC	C10-C11-C12-C13
5	J	502	OLC	C10-C11-C12-C13
5	C	902	OLC	O20-C1-C2-C3
5	A	902	OLC	O20-C1-C2-C3
5	A	903	OLC	O19-C1-O20-C21
5	C	903	OLC	O19-C1-O20-C21
5	I	501	OLC	O19-C1-C2-C3
5	J	501	OLC	O19-C1-C2-C3
5	A	903	OLC	C2-C1-O20-C21
5	A	903	OLC	O19-C1-C2-C3
5	C	903	OLC	O19-C1-C2-C3
5	C	902	OLC	O19-C1-C2-C3
5	A	903	OLC	C9-C10-C11-C12
5	C	903	OLC	C9-C10-C11-C12
5	A	902	OLC	O19-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	503	OLC	C10-C11-C12-C13
5	J	503	OLC	C10-C11-C12-C13
5	C	903	OLC	C2-C1-O20-C21

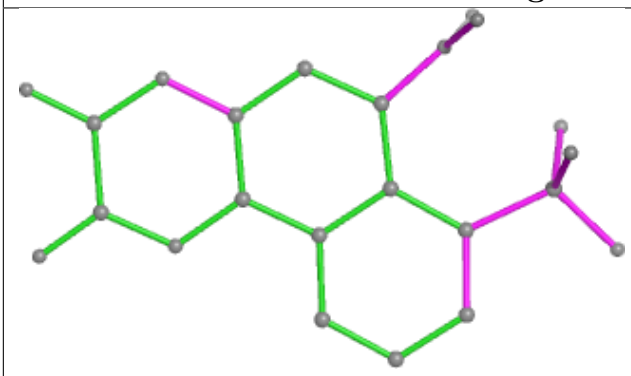
There are no ring outliers.

4 monomers are involved in 4 short contacts:

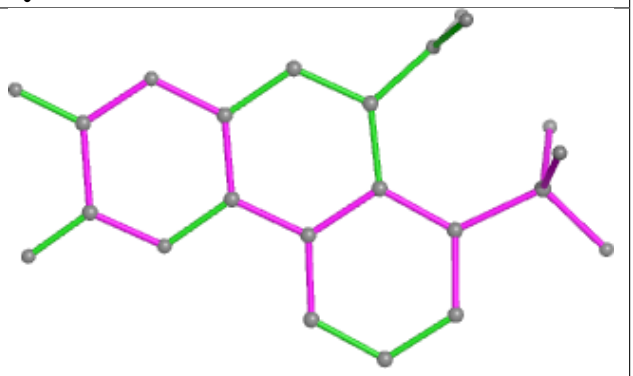
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	901	E2Q	1	0
4	D	901	E2Q	1	0
4	A	901	E2Q	1	0
4	B	901	E2Q	1	0

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

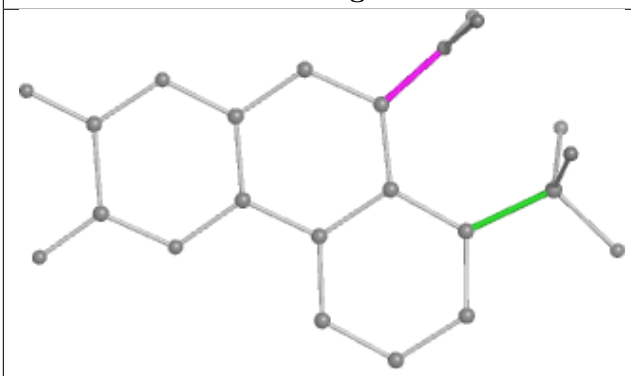
Ligand E2Q C 901



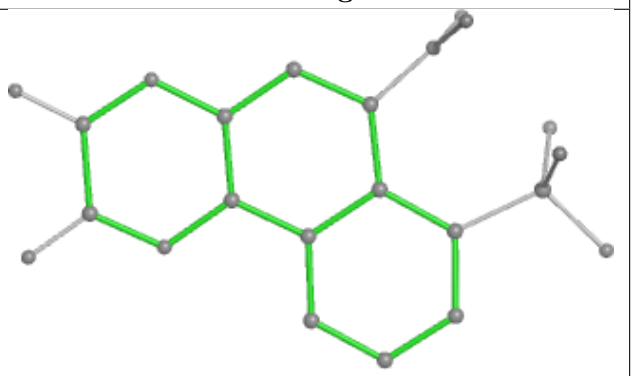
Bond lengths



Bond angles

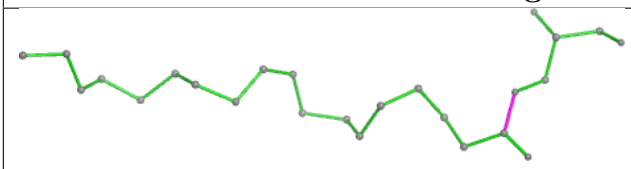


Torsions

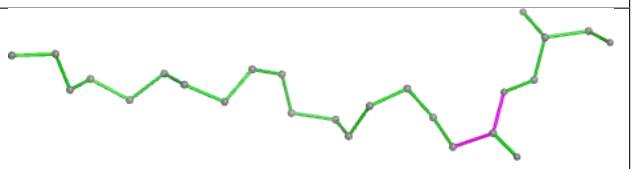


Rings

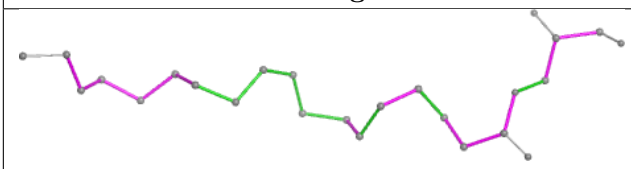
Ligand OLC C 904



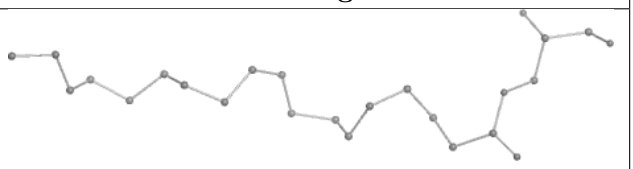
Bond lengths



Bond angles

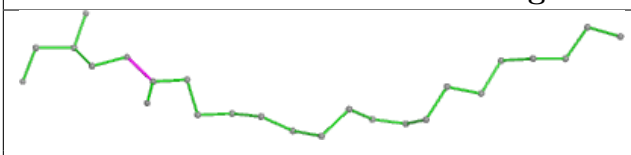


Torsions

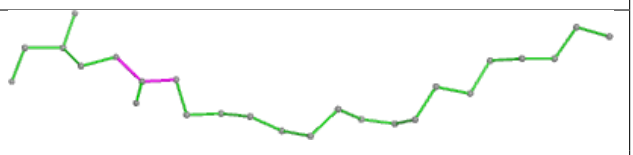


Rings

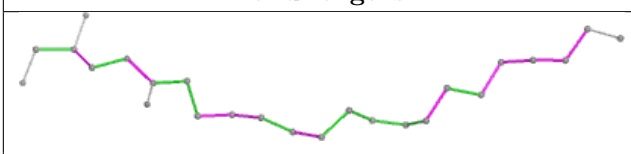
Ligand OLC J 502



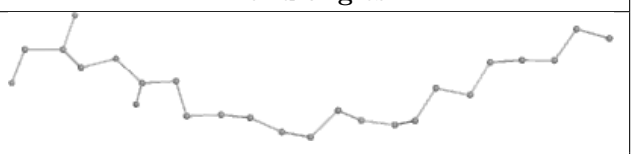
Bond lengths



Bond angles

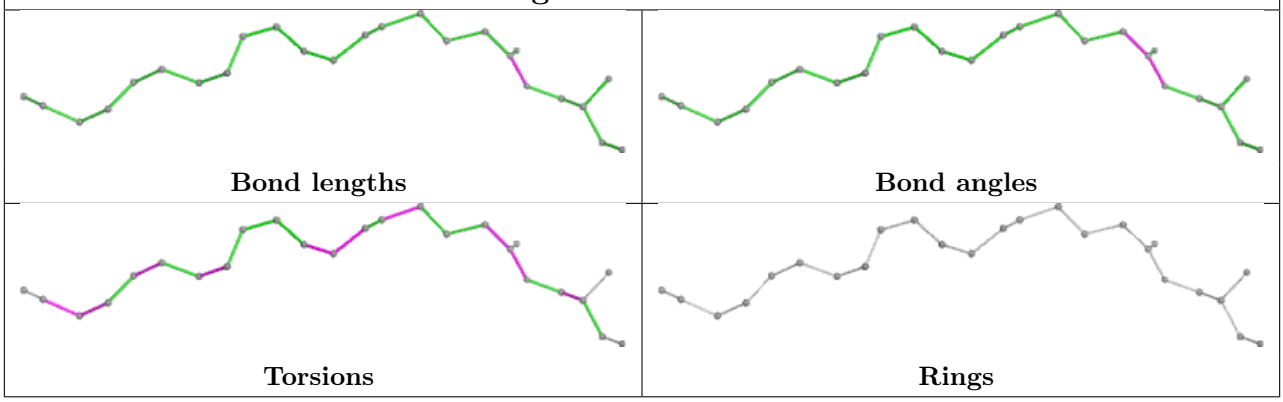


Torsions

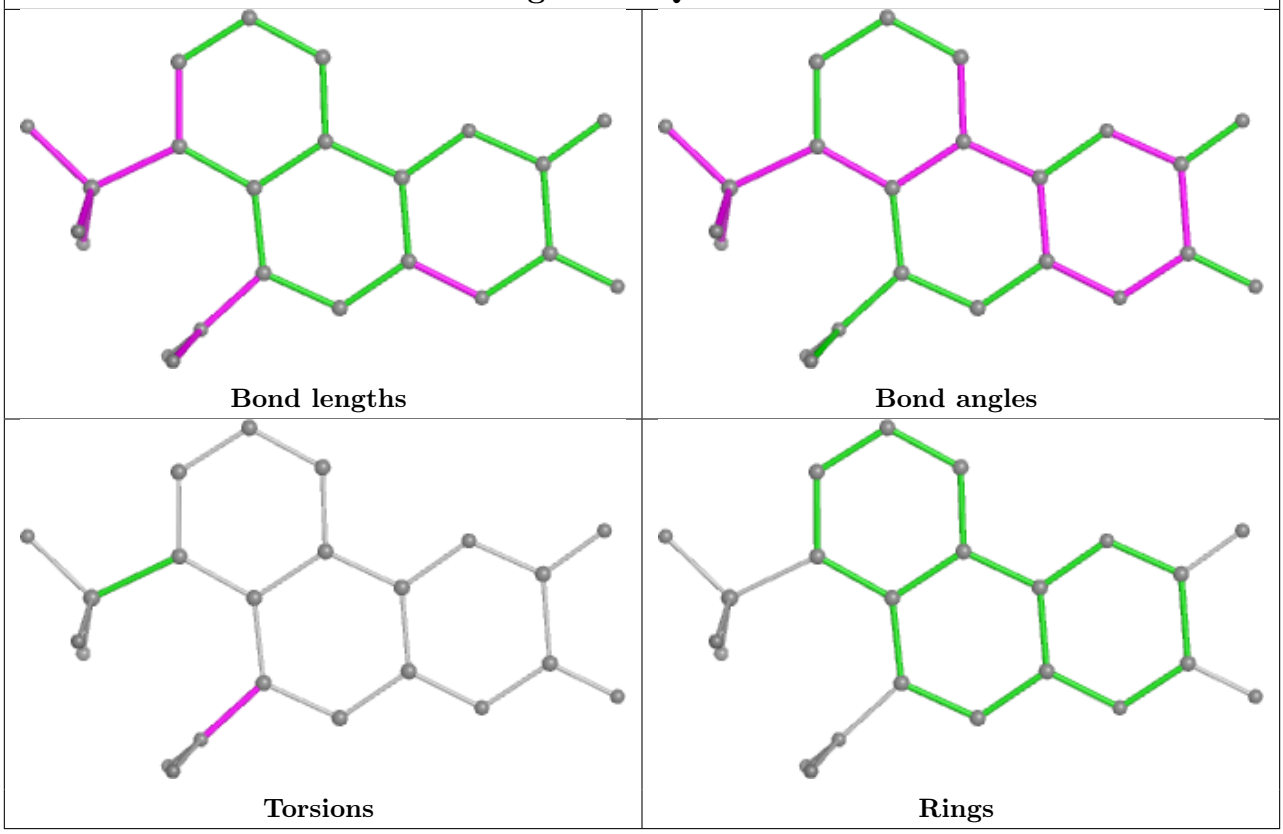


Rings

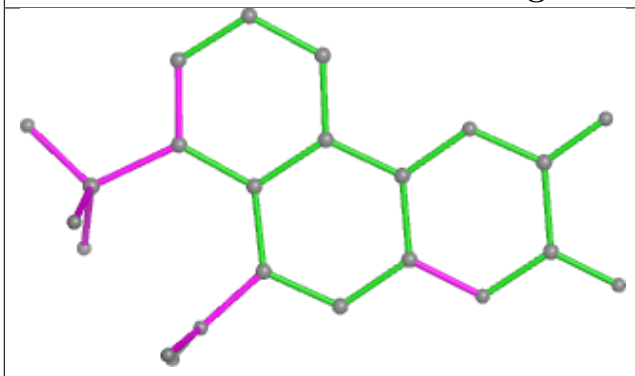
Ligand OLC I 501



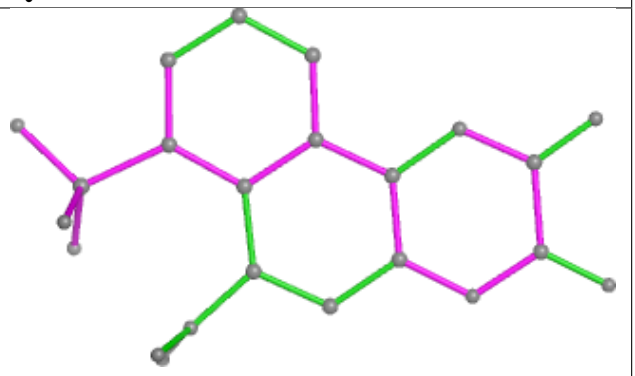
Ligand E2Q D 901



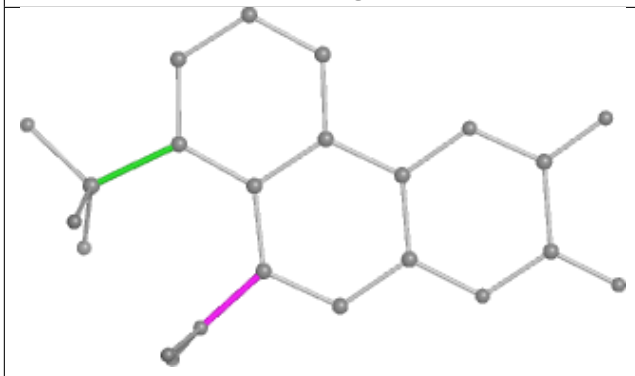
Ligand E2Q A 901



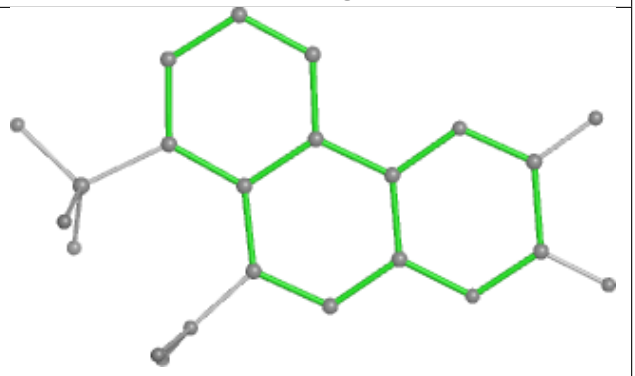
Bond lengths



Bond angles

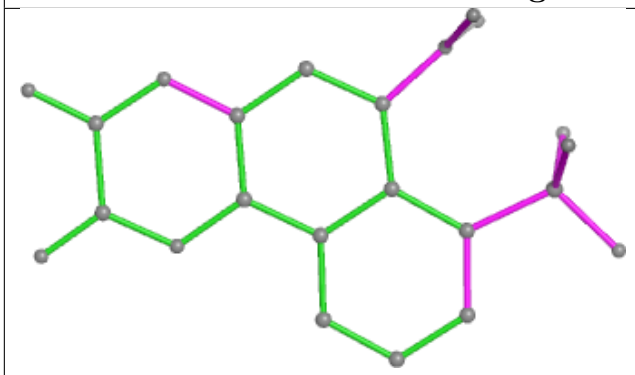


Torsions

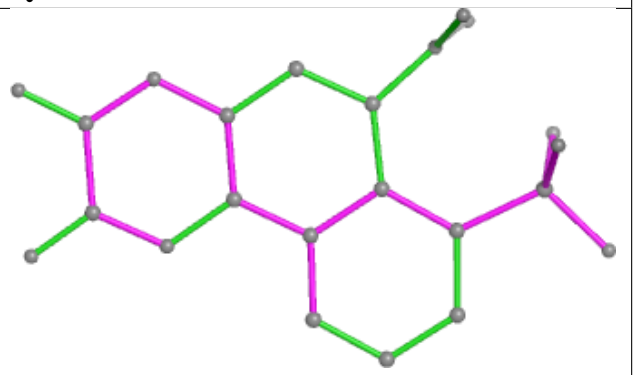


Rings

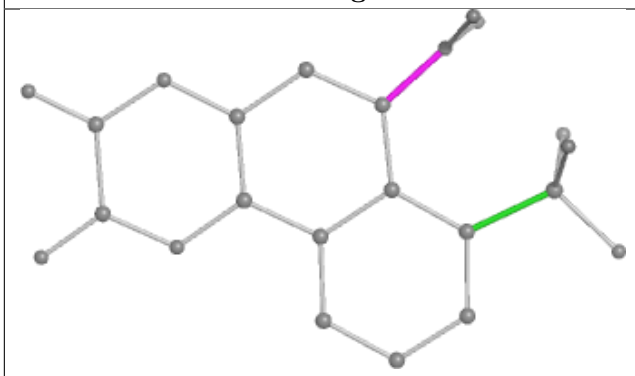
Ligand E2Q B 901



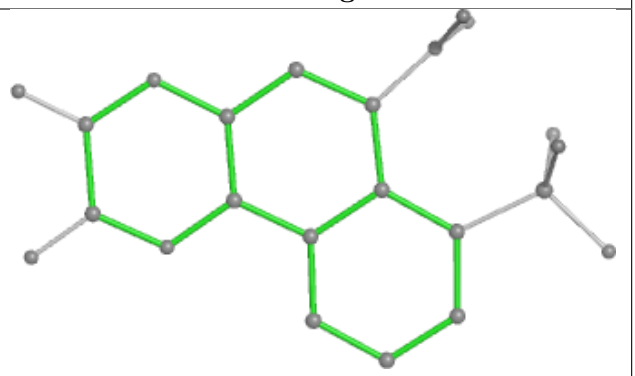
Bond lengths



Bond angles

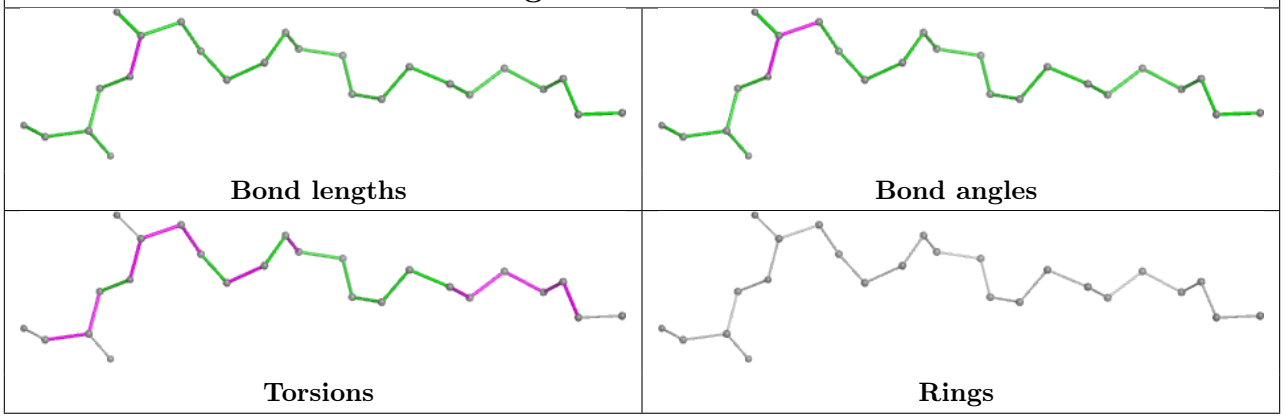


Torsions

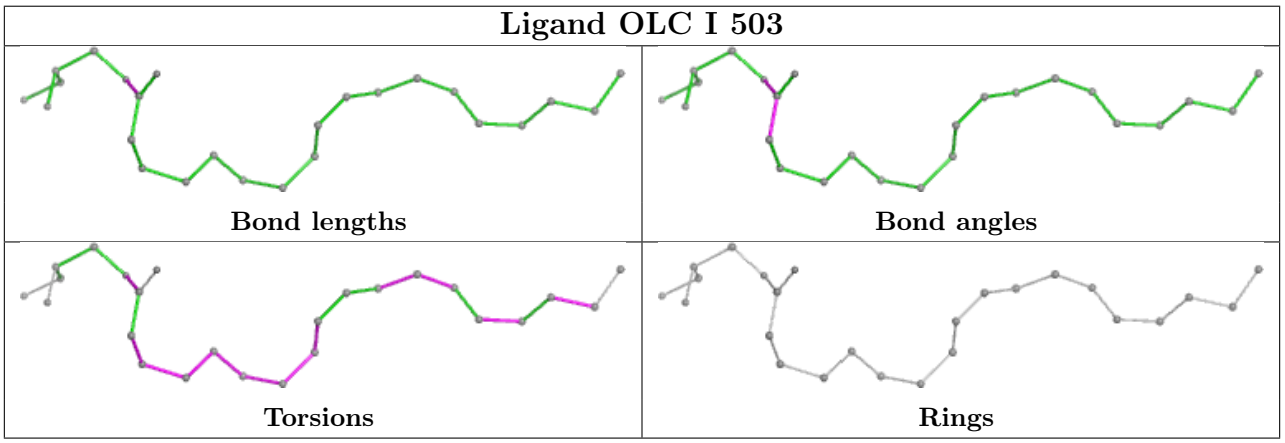


Rings

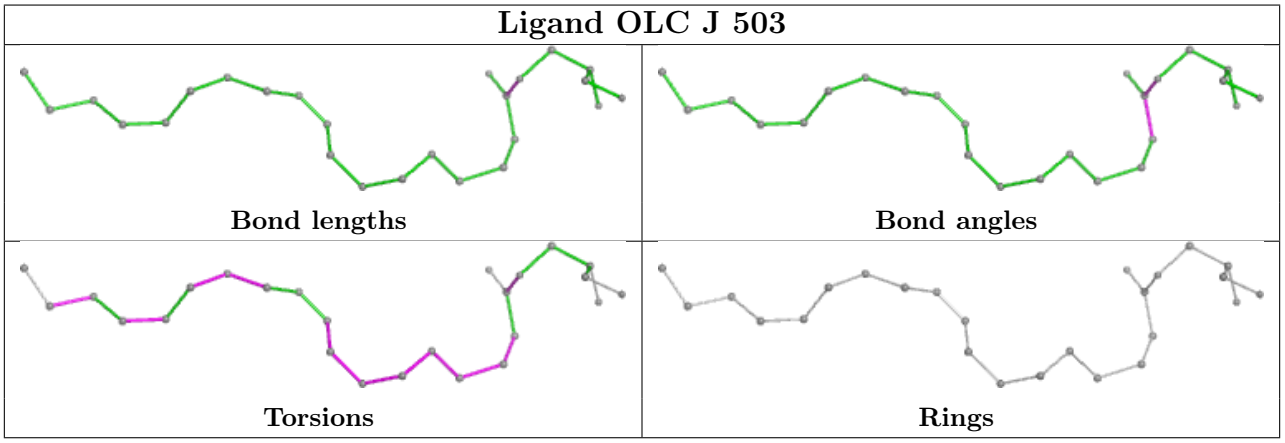
Ligand OLC A 904



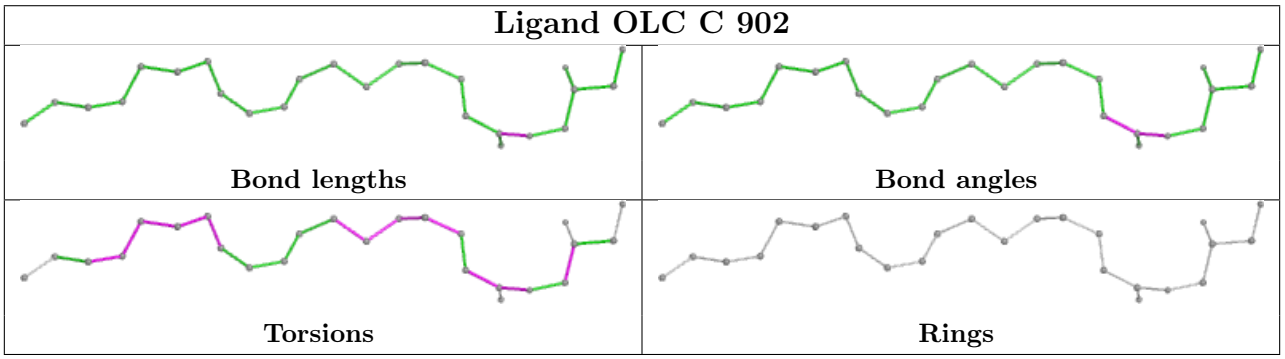
Ligand OLC I 503



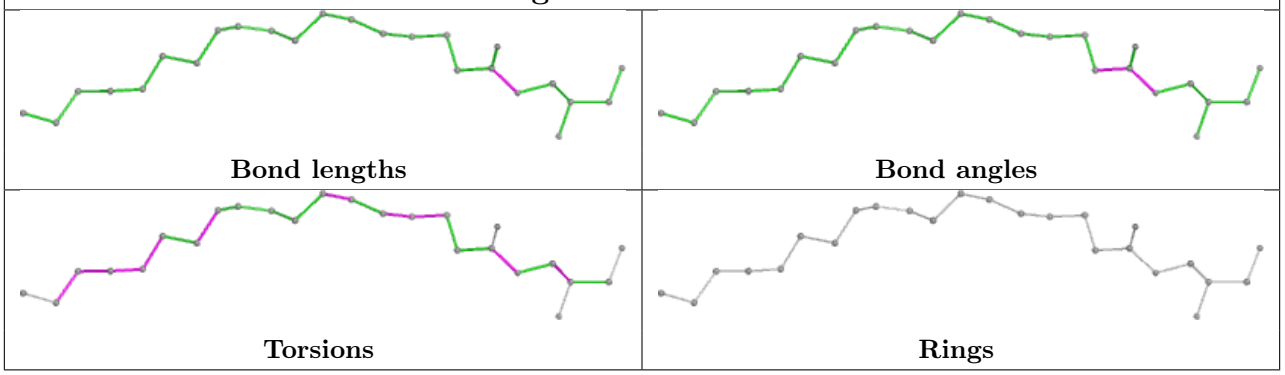
Ligand OLC J 503



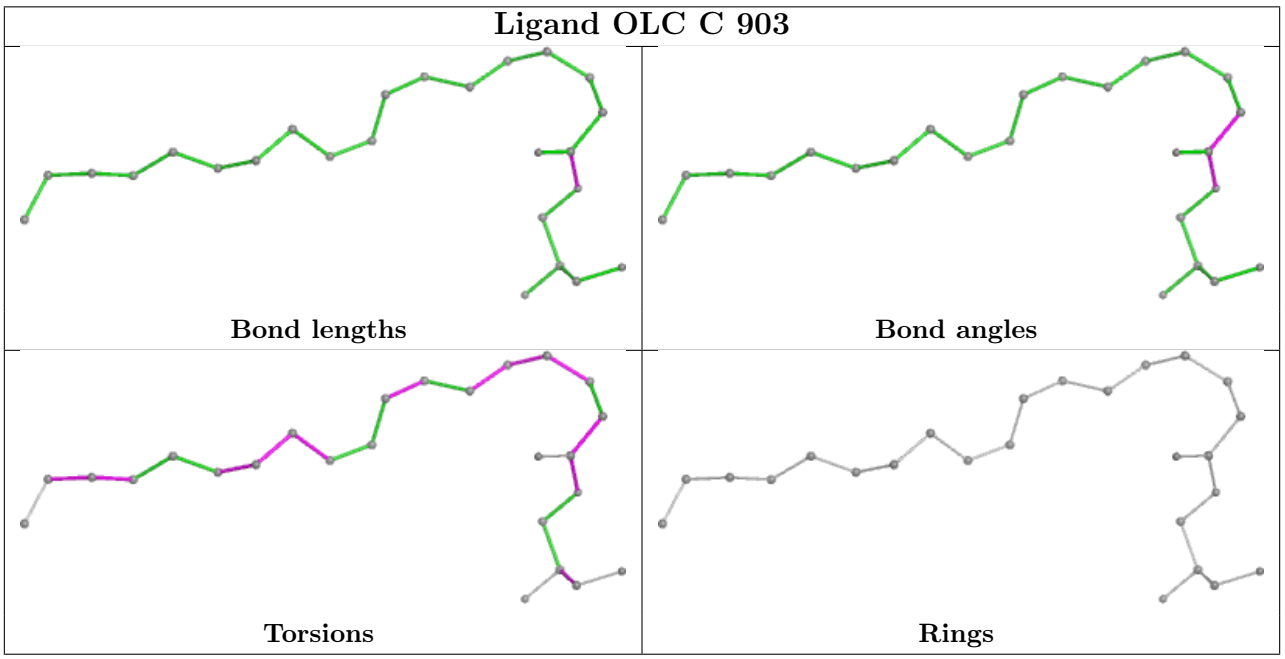
Ligand OLC C 902



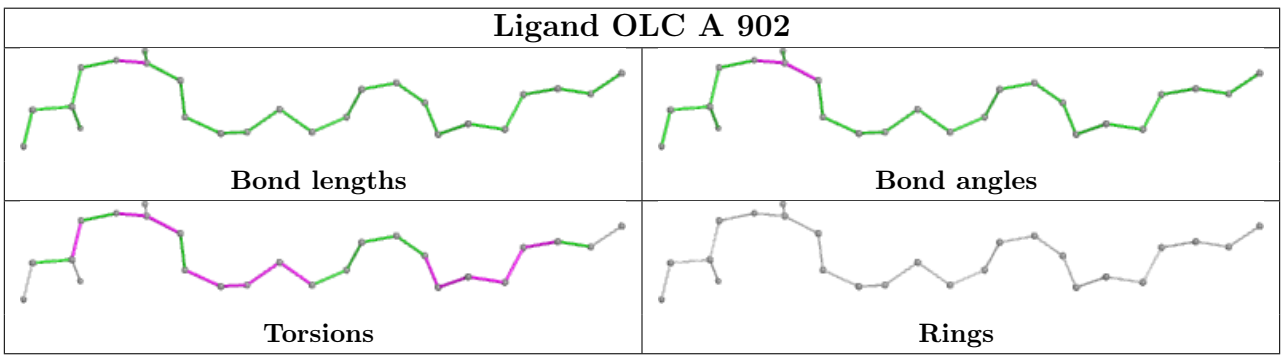
Ligand OLC I 502

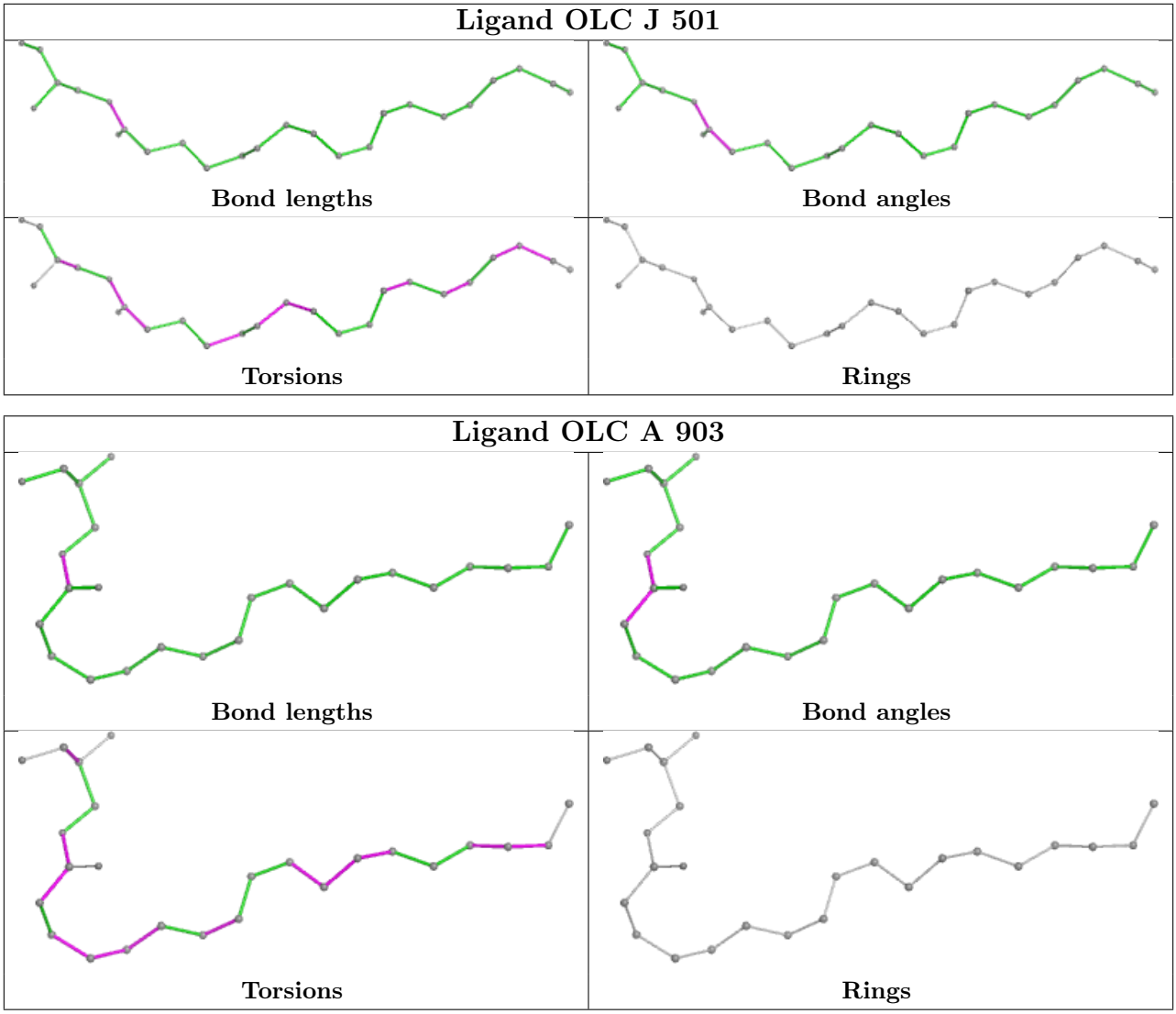


Ligand OLC C 903



Ligand OLC A 902





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

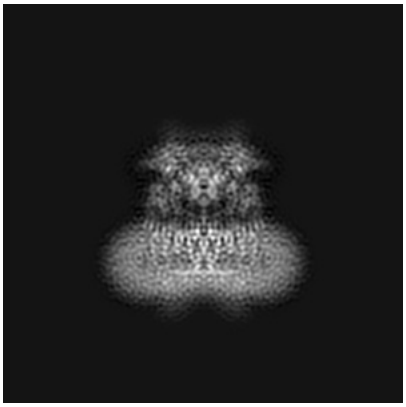
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4572. These allow visual inspection of the internal detail of the map and identification of artifacts.

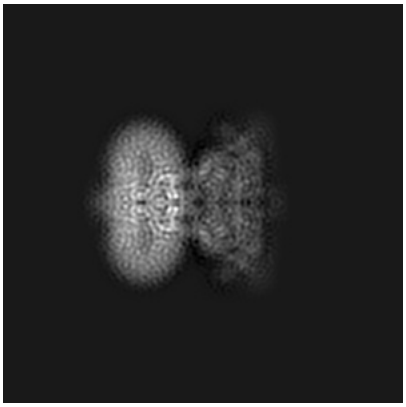
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

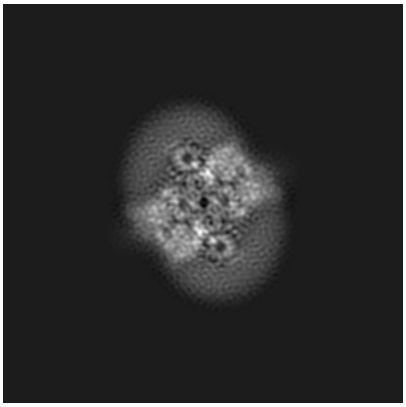
6.1.1 Primary map



X



Y

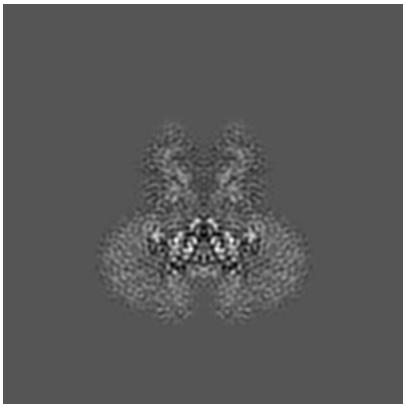


Z

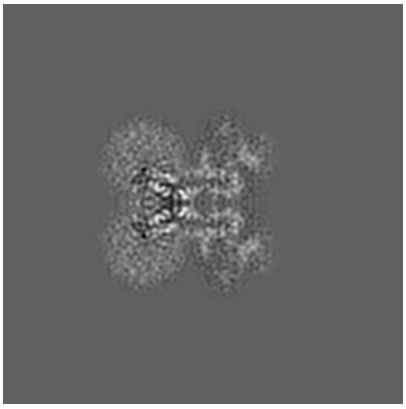
The images above show the map projected in three orthogonal directions.

6.2 Central slices

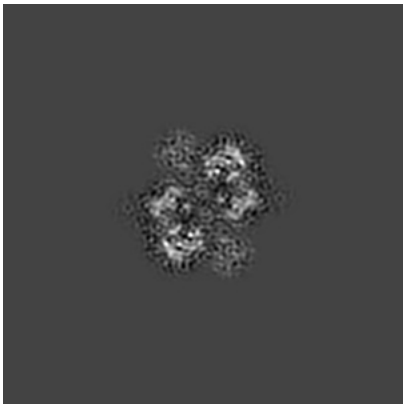
6.2.1 Primary map



X Index: 110



Y Index: 110

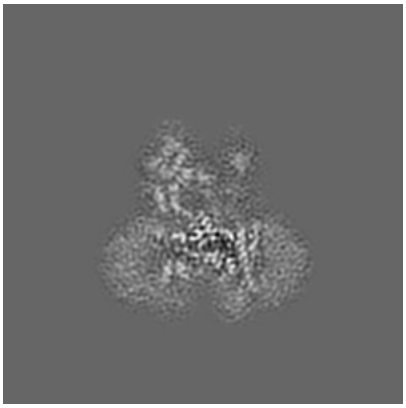


Z Index: 110

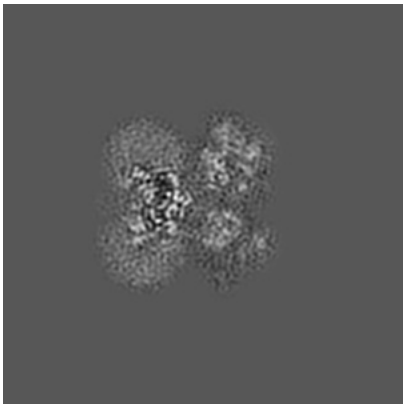
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

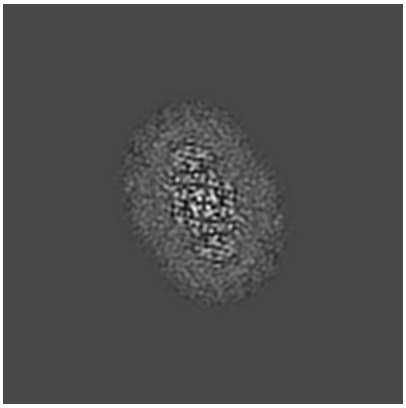
6.3.1 Primary map



X Index: 106



Y Index: 114

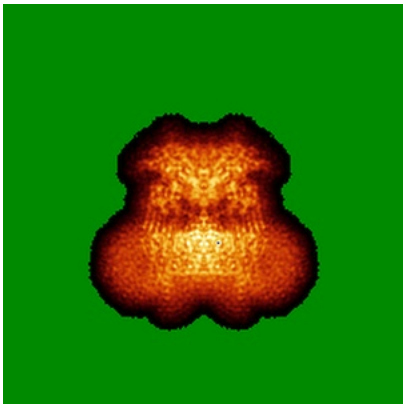


Z Index: 91

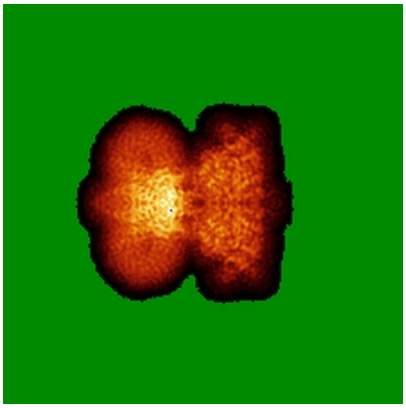
The images above show the largest variance slices of the map in three orthogonal directions.

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

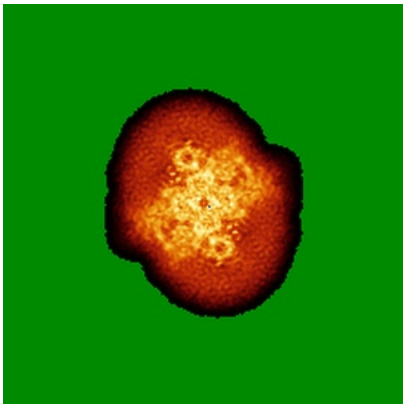
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

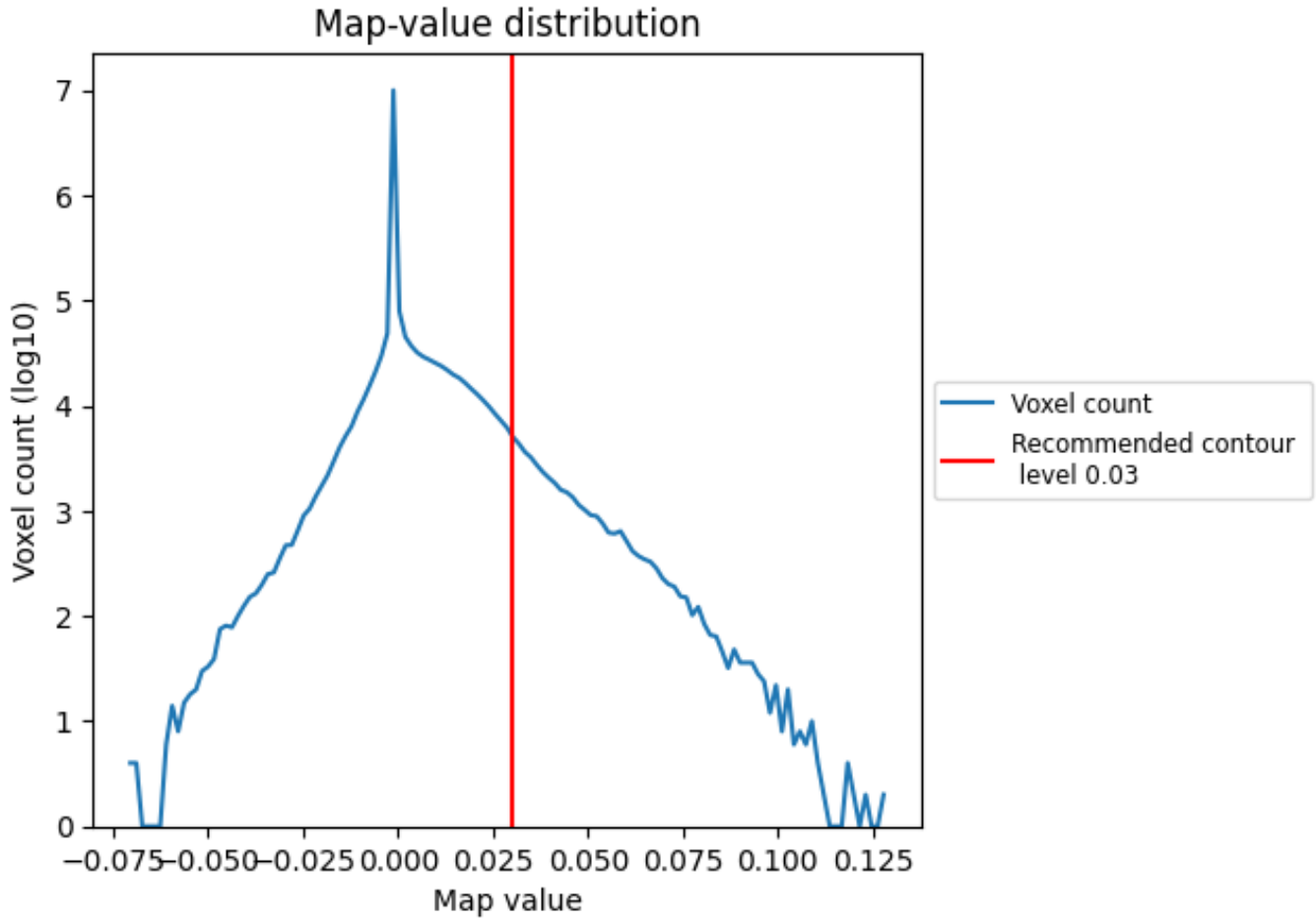
6.6 Mask visualisation (i)

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

7 Map analysis

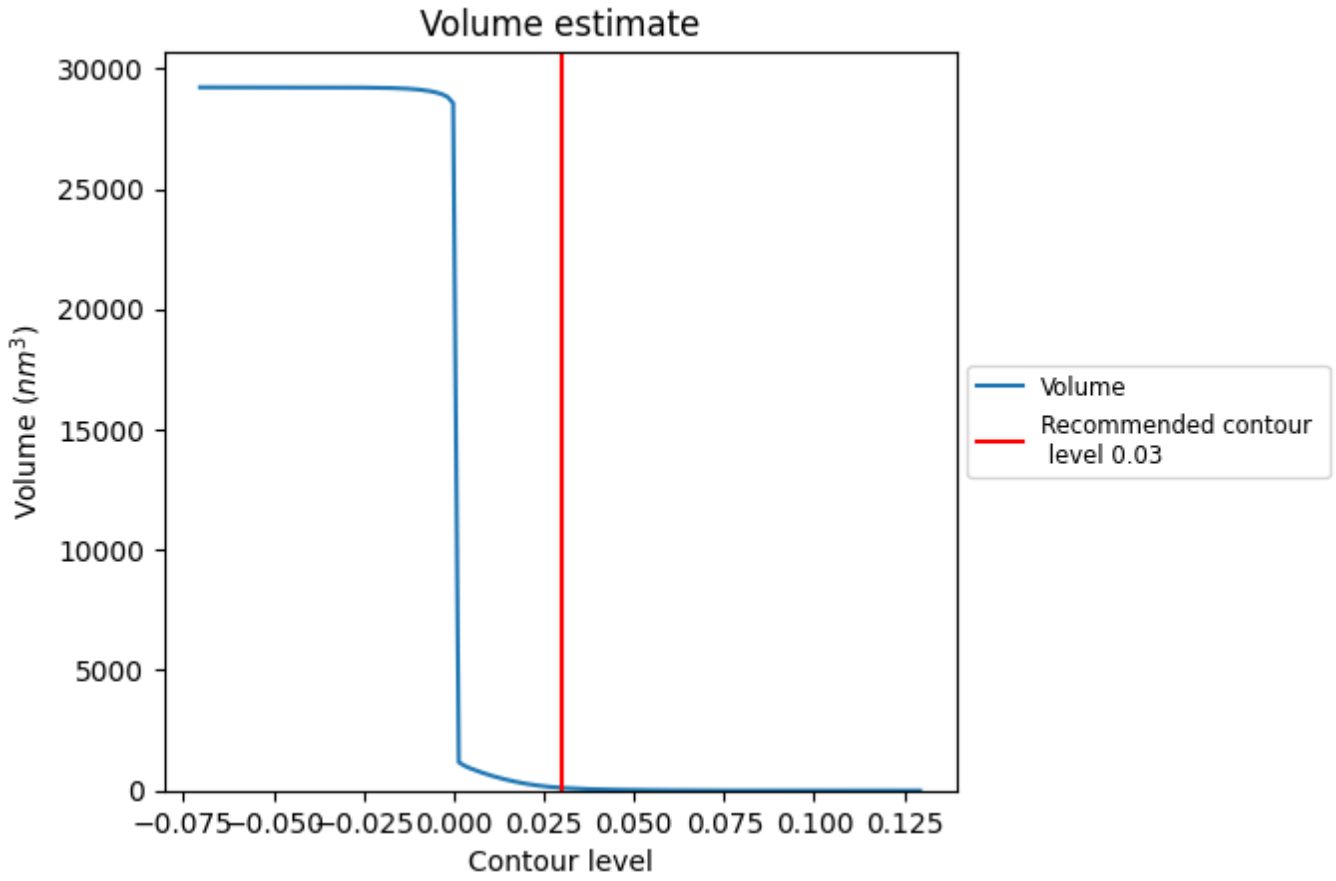
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

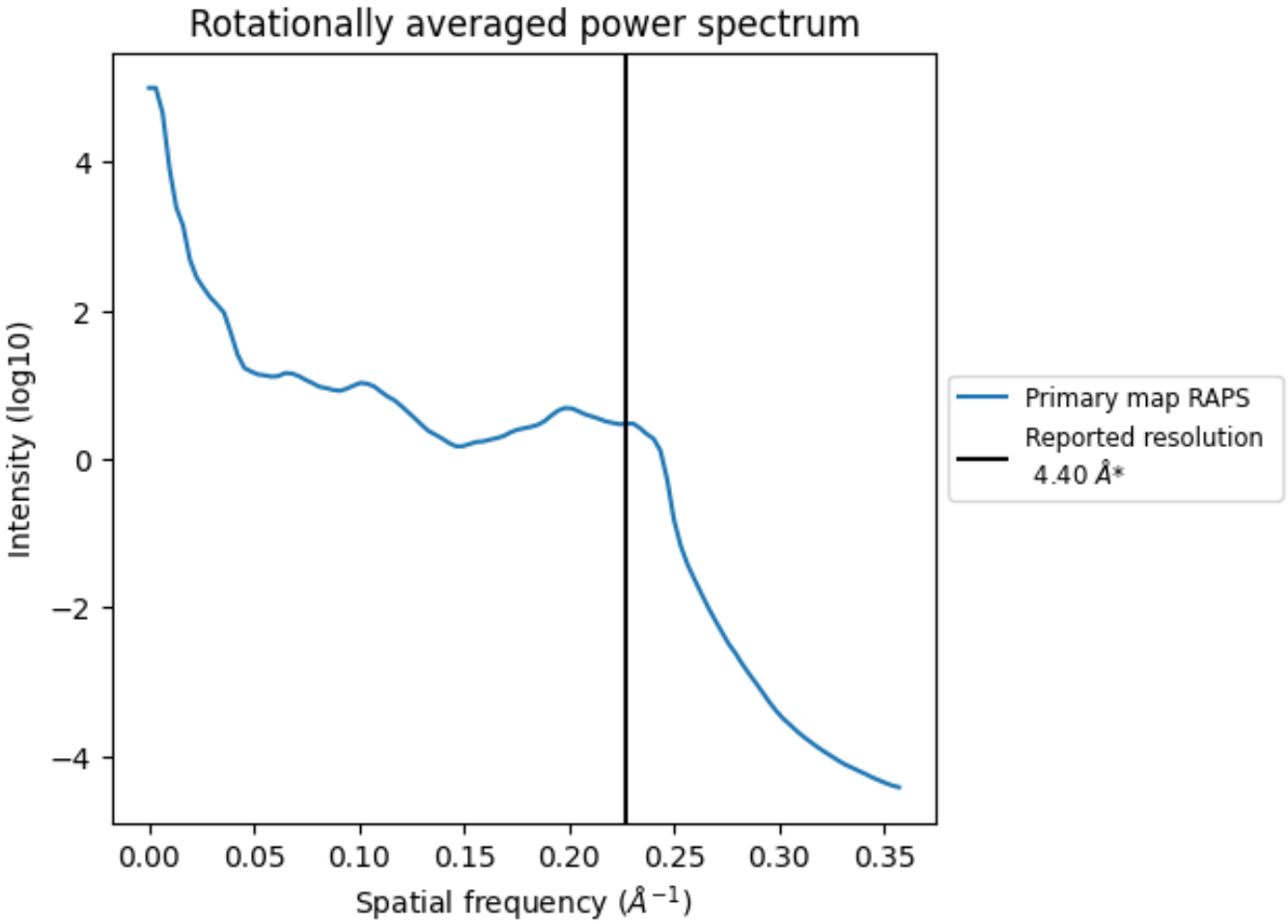
7.2 Volume estimate (i)



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 103 kDa.

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

7.3 Rotationally averaged power spectrum (i)

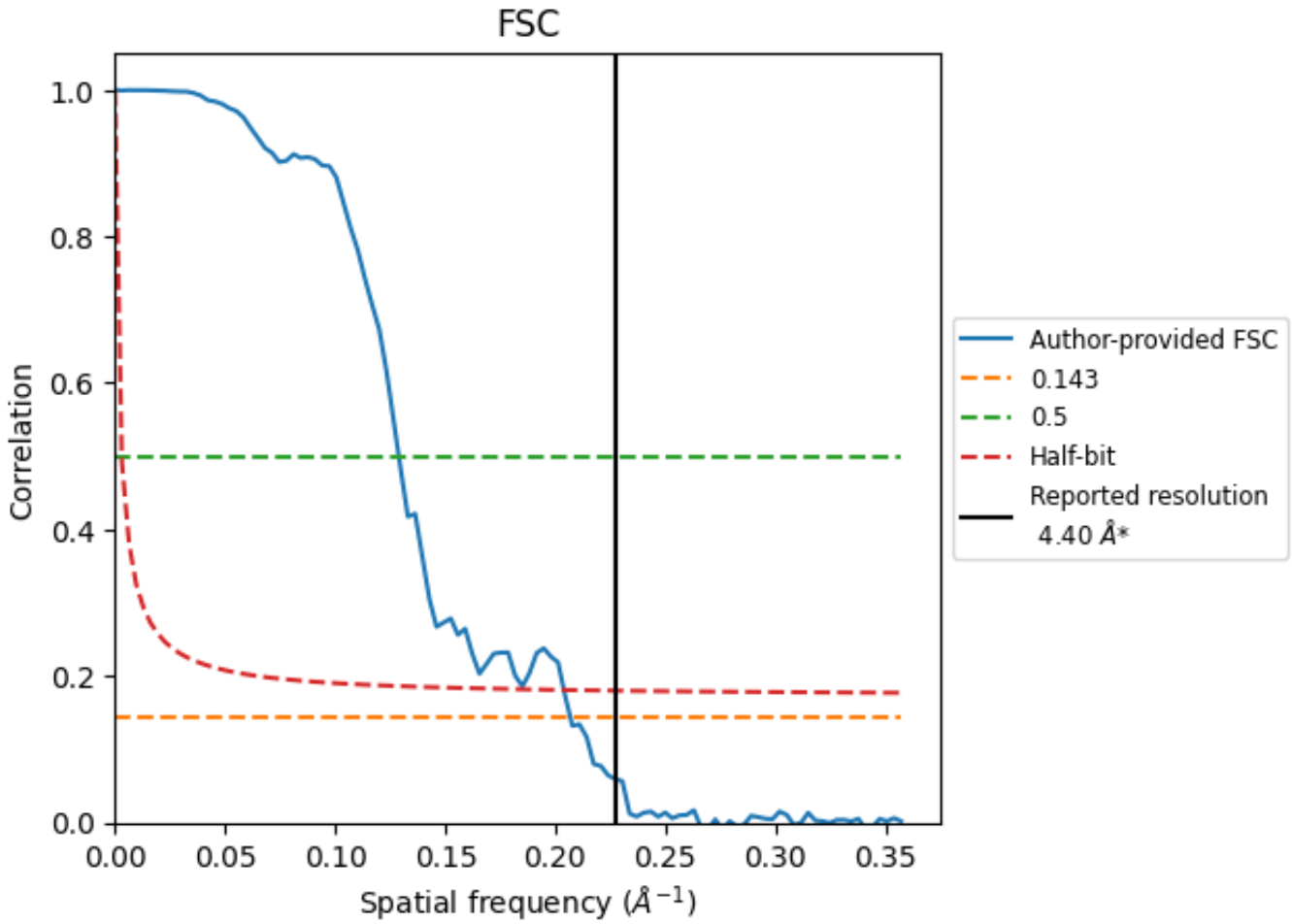


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

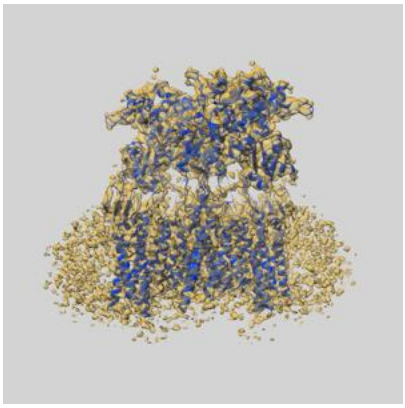
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.83	7.75	4.90
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

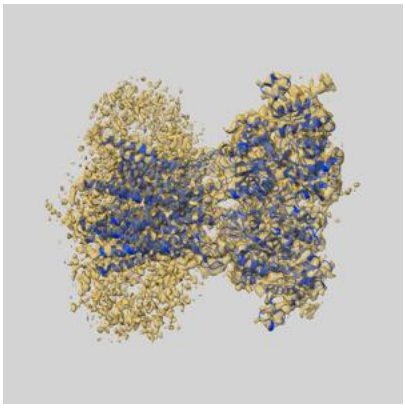
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4572 and PDB model 6QKC. Per-residue inclusion information can be found in section 3 on page 7.

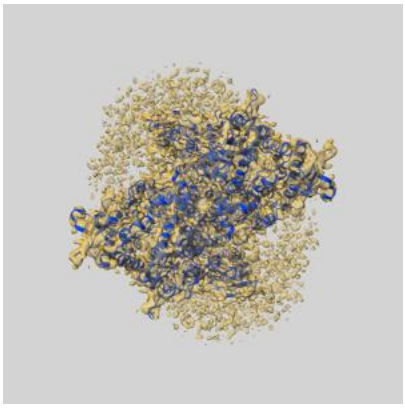
9.1 Map-model overlay



X



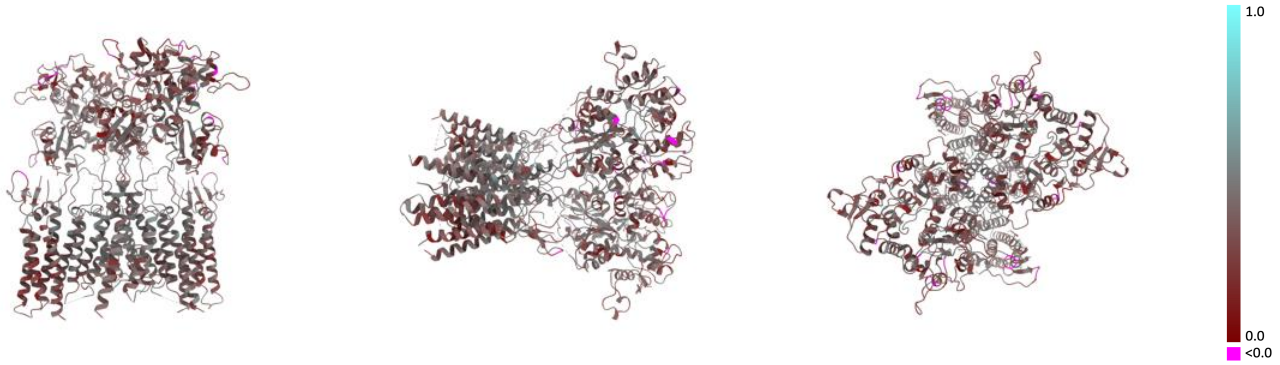
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

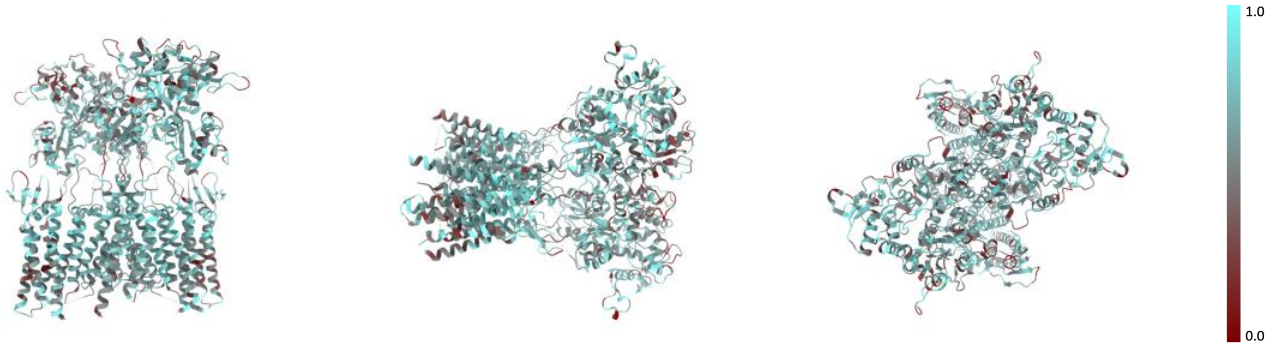
9.2 Q-score mapped to coordinate model



X Y Z

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

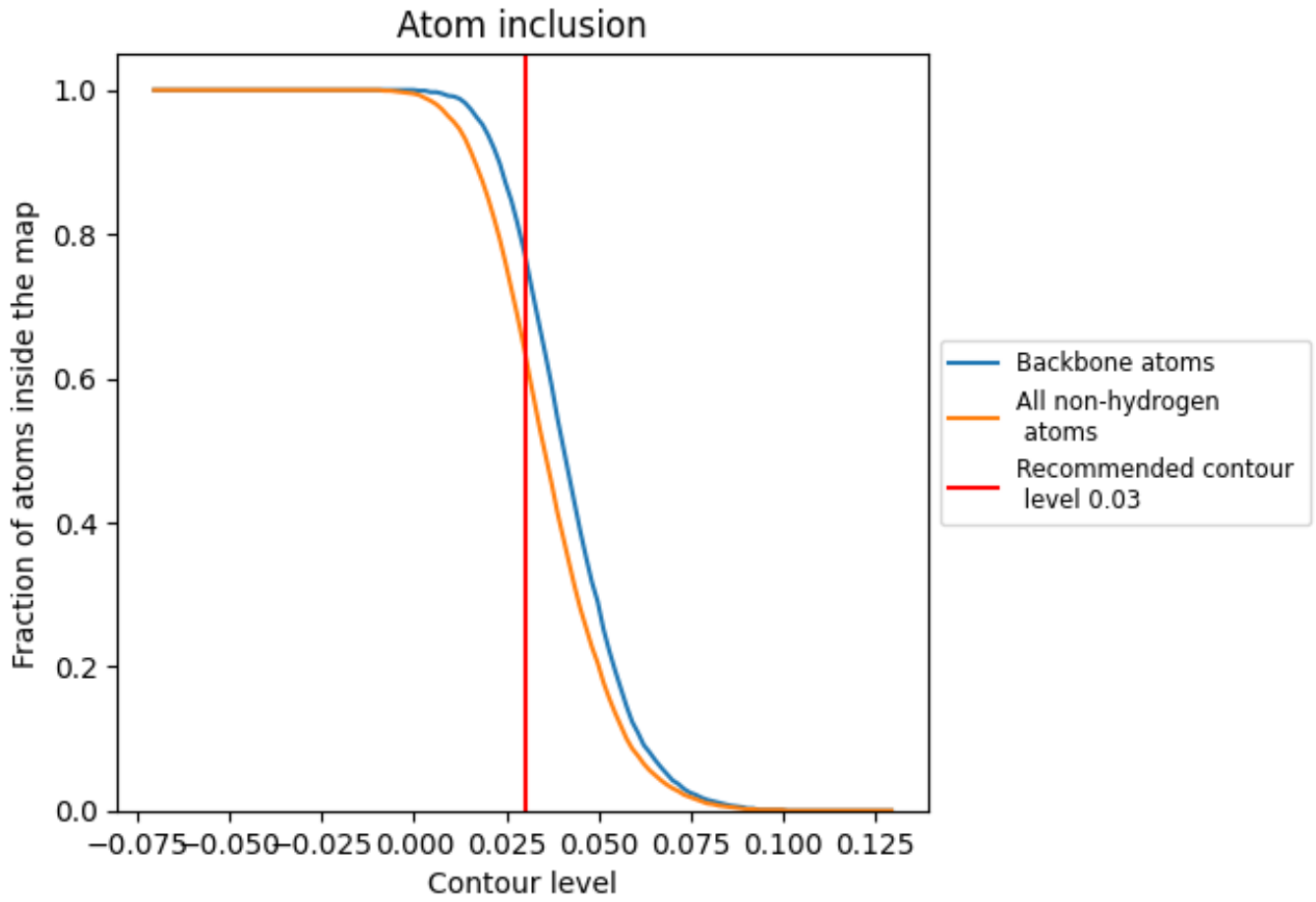
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 77% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6380	0.3760
A	0.6450	0.3780
B	0.6260	0.3820
C	0.6420	0.3790
D	0.6260	0.3790
I	0.6530	0.3620
J	0.6480	0.3610