wwPDB EM Validation Summary Report (i)

Mar 9, 2026 – 02:26 PM UTC

PDB ID	:	8C1R / pdb_00008c1r
EMDB ID	:	EMD-16381
Title	:	Resting state homomeric GluA2 F231A mutant AMPA receptor in complex with TARP gamma-2
Authors	:	Zhang, D.; Ivica, J.; Krieger, J.M.; Ho, H.; Yamashita, K.; Cais, O.; Greger, I.
Deposited on	:	2022-12-21
Resolution	:	3.20 Å(reported)

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

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

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

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

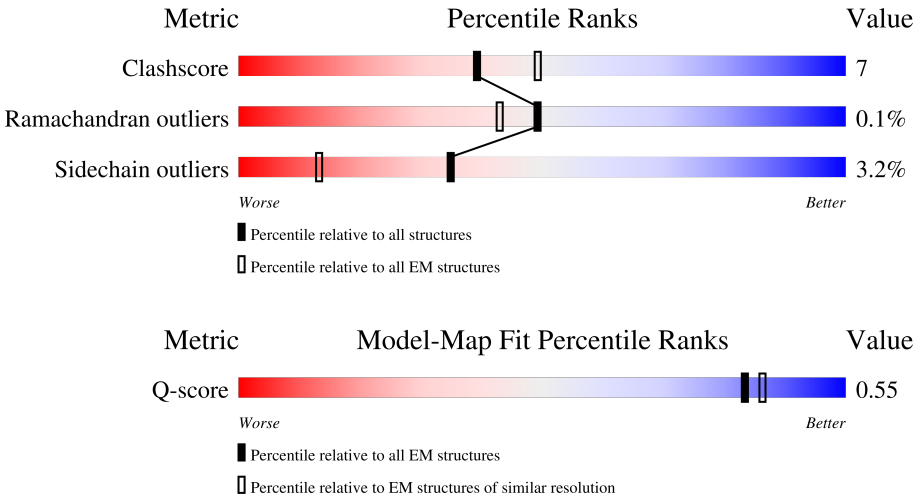
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 (i)

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

The reported resolution of this entry is 3.20 Å.

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



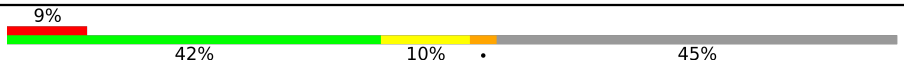
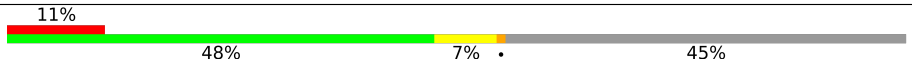
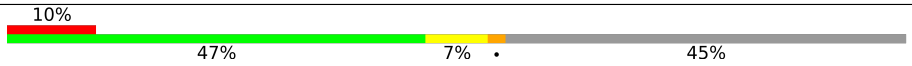
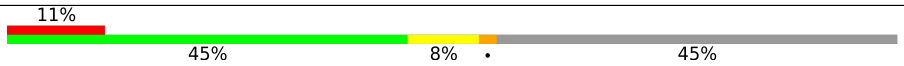
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	891	9% 40% 5% 55%
1	B	891	12% 37% 8% • 54%
1	C	891	12% 38% 7% 55%
1	D	891	10% 37% 8% • 54%

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Mol	Chain	Length	Quality of chain
2	E	322	
2	F	322	
2	G	322	
2	H	322	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18333 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	405	Total	C	N	O	S	2	0
			3105	2022	497	566	20		
1	B	406	Total	C	N	O	S	1	0
			3068	2000	494	554	20		
1	C	405	Total	C	N	O	S	1	0
			3063	1997	490	556	20		
1	D	406	Total	C	N	O	S	1	0
			3076	2005	494	557	20		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	insertion	UNP P19491
A	-6	TYR	-	insertion	UNP P19491
A	-5	LYS	-	insertion	UNP P19491
A	-4	ASP	-	insertion	UNP P19491
A	-3	ASP	-	insertion	UNP P19491
A	-2	ASP	-	insertion	UNP P19491
A	-1	ASP	-	insertion	UNP P19491
A	0	LYS	-	insertion	UNP P19491
A	586	ARG	GLN	variant	UNP P19491
B	-7	ASP	-	insertion	UNP P19491
B	-6	TYR	-	insertion	UNP P19491
B	-5	LYS	-	insertion	UNP P19491
B	-4	ASP	-	insertion	UNP P19491
B	-3	ASP	-	insertion	UNP P19491
B	-2	ASP	-	insertion	UNP P19491
B	-1	ASP	-	insertion	UNP P19491
B	0	LYS	-	insertion	UNP P19491
B	586	ARG	GLN	variant	UNP P19491
C	-7	ASP	-	insertion	UNP P19491
C	-6	TYR	-	insertion	UNP P19491
C	-5	LYS	-	insertion	UNP P19491
C	-4	ASP	-	insertion	UNP P19491

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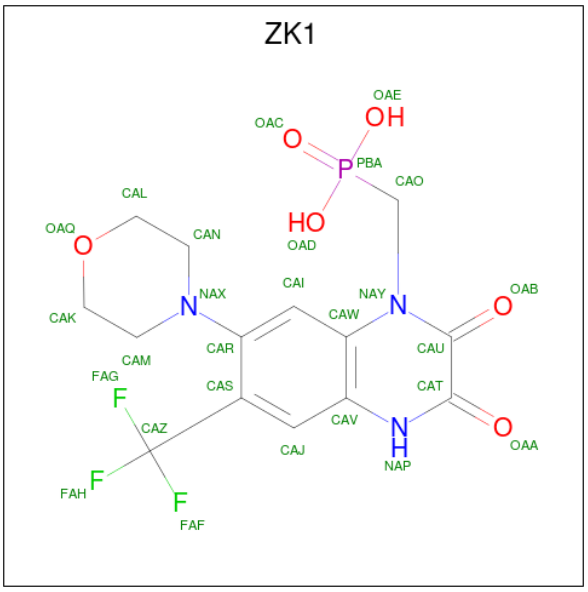
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ASP	-	insertion	UNP P19491
C	-2	ASP	-	insertion	UNP P19491
C	-1	ASP	-	insertion	UNP P19491
C	0	LYS	-	insertion	UNP P19491
C	586	ARG	GLN	variant	UNP P19491
D	-7	ASP	-	insertion	UNP P19491
D	-6	TYR	-	insertion	UNP P19491
D	-5	LYS	-	insertion	UNP P19491
D	-4	ASP	-	insertion	UNP P19491
D	-3	ASP	-	insertion	UNP P19491
D	-2	ASP	-	insertion	UNP P19491
D	-1	ASP	-	insertion	UNP P19491
D	0	LYS	-	insertion	UNP P19491
D	586	ARG	GLN	variant	UNP P19491

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-2 subunit.

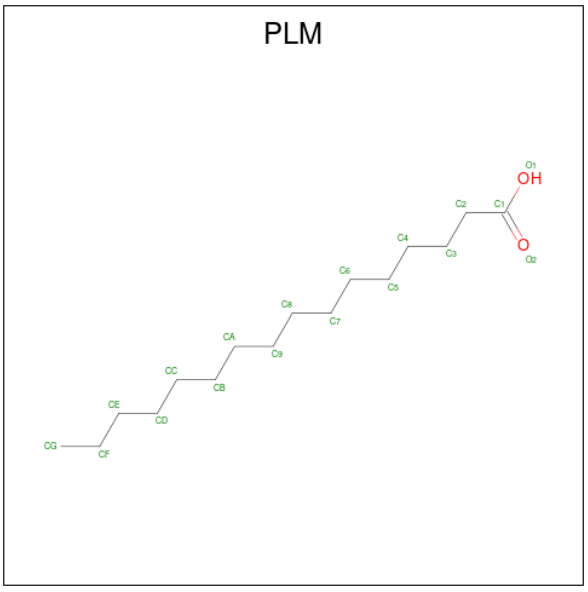
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	177	Total	C	N	O	S	0	0
			1366	897	220	238	11		
2	F	178	Total	C	N	O	S	0	0
			1381	906	225	239	11		
2	G	177	Total	C	N	O	S	0	0
			1372	900	223	238	11		
2	H	177	Total	C	N	O	S	0	0
			1367	899	221	236	11		

- Molecule 3 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (CCD ID: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$) (labeled as "Ligand of Interest" by depositor).



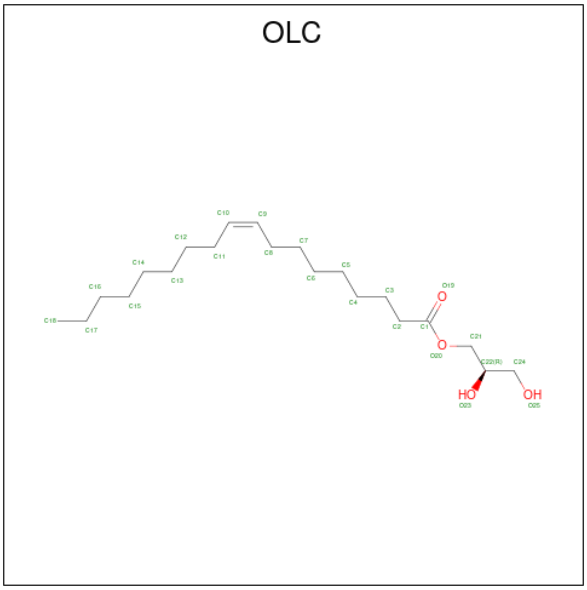
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



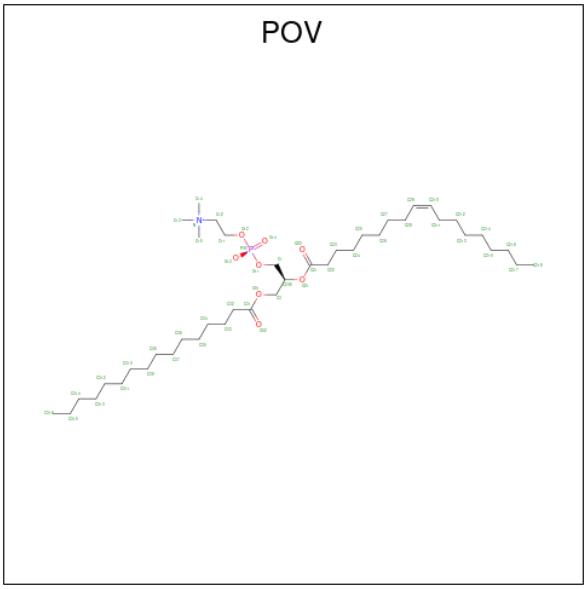
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 18 16 2	0
4	A	1	Total C O 16 14 2	0
4	B	1	Total C O 18 16 2	0
4	C	1	Total C O 18 16 2	0
4	D	1	Total C O 18 16 2	0
4	F	1	Total C O 18 16 2	0
4	G	1	Total C O 18 16 2	0

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



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 25 21 4	0
5	B	1	Total C O 25 21 4	0
5	C	1	Total C O 25 21 4	0
5	D	1	Total C O 25 21 4	0

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C N O P 42 32 1 8 1	0
6	D	1	Total C N O P 40 30 1 8 1	0
6	E	1	Total C N O P 39 29 1 8 1	0
6	G	1	Total C O P 34 25 8 1	0
6	G	1	Total C N O P 42 32 1 8 1	0

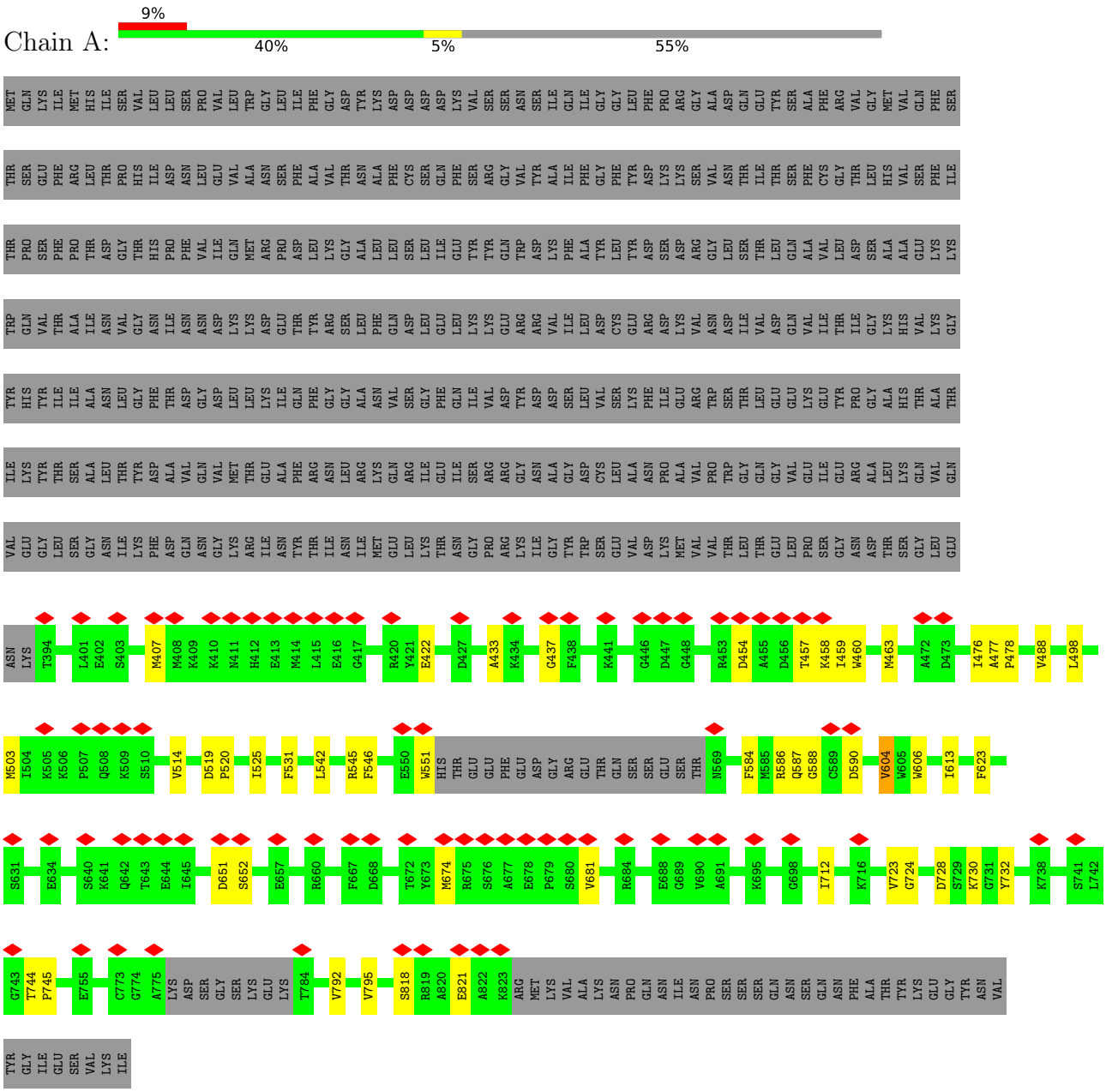
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total O 1 1	0
7	C	3	Total O 3 3	0
7	D	1	Total O 1 1	0
7	G	1	Total O 1 1	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.

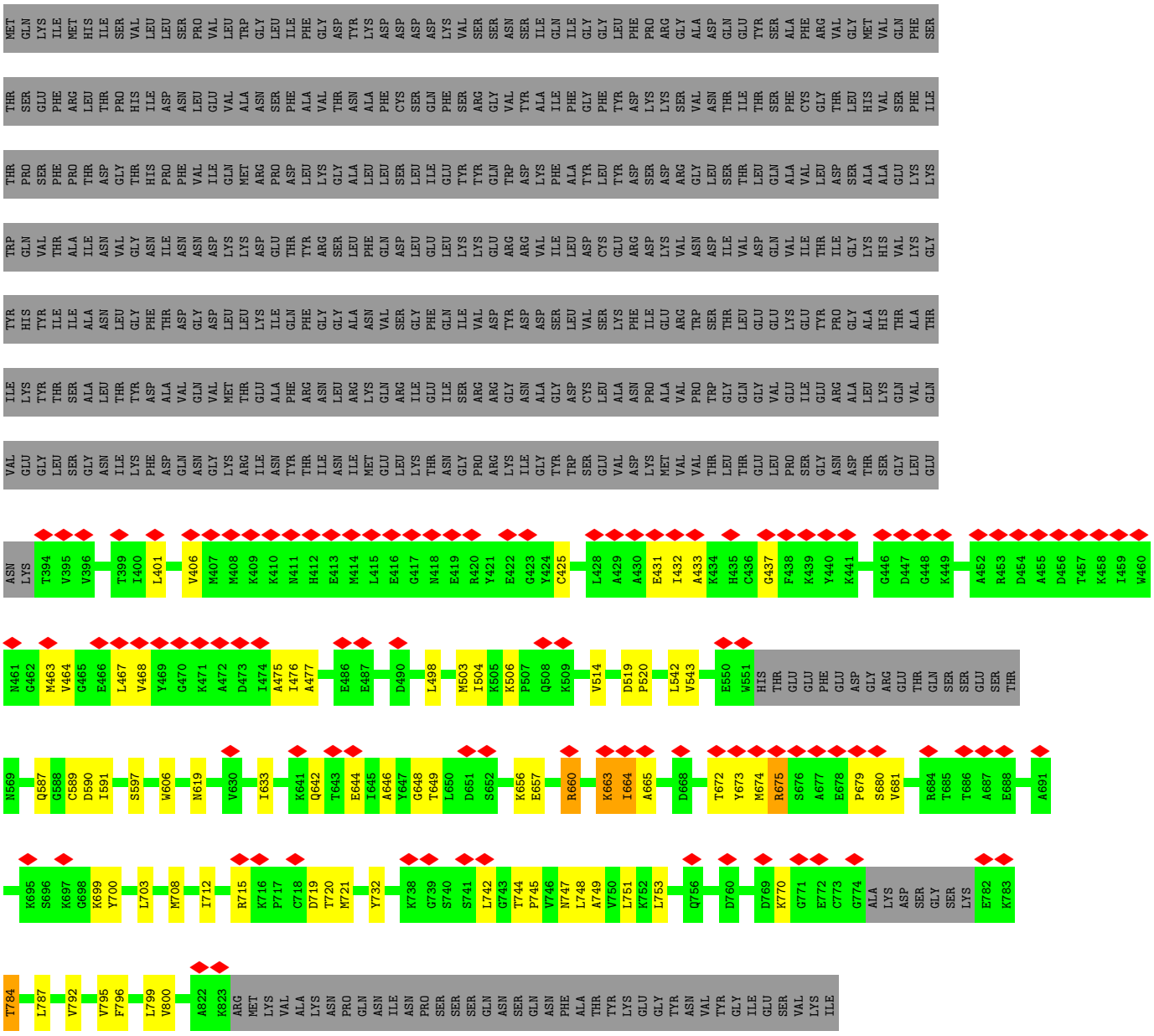
- Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2

Chain B:

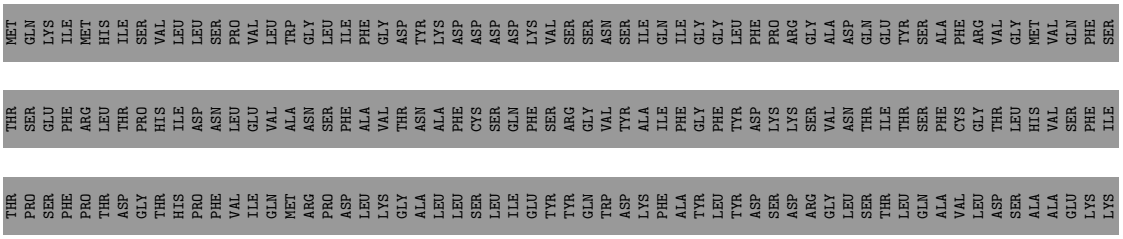


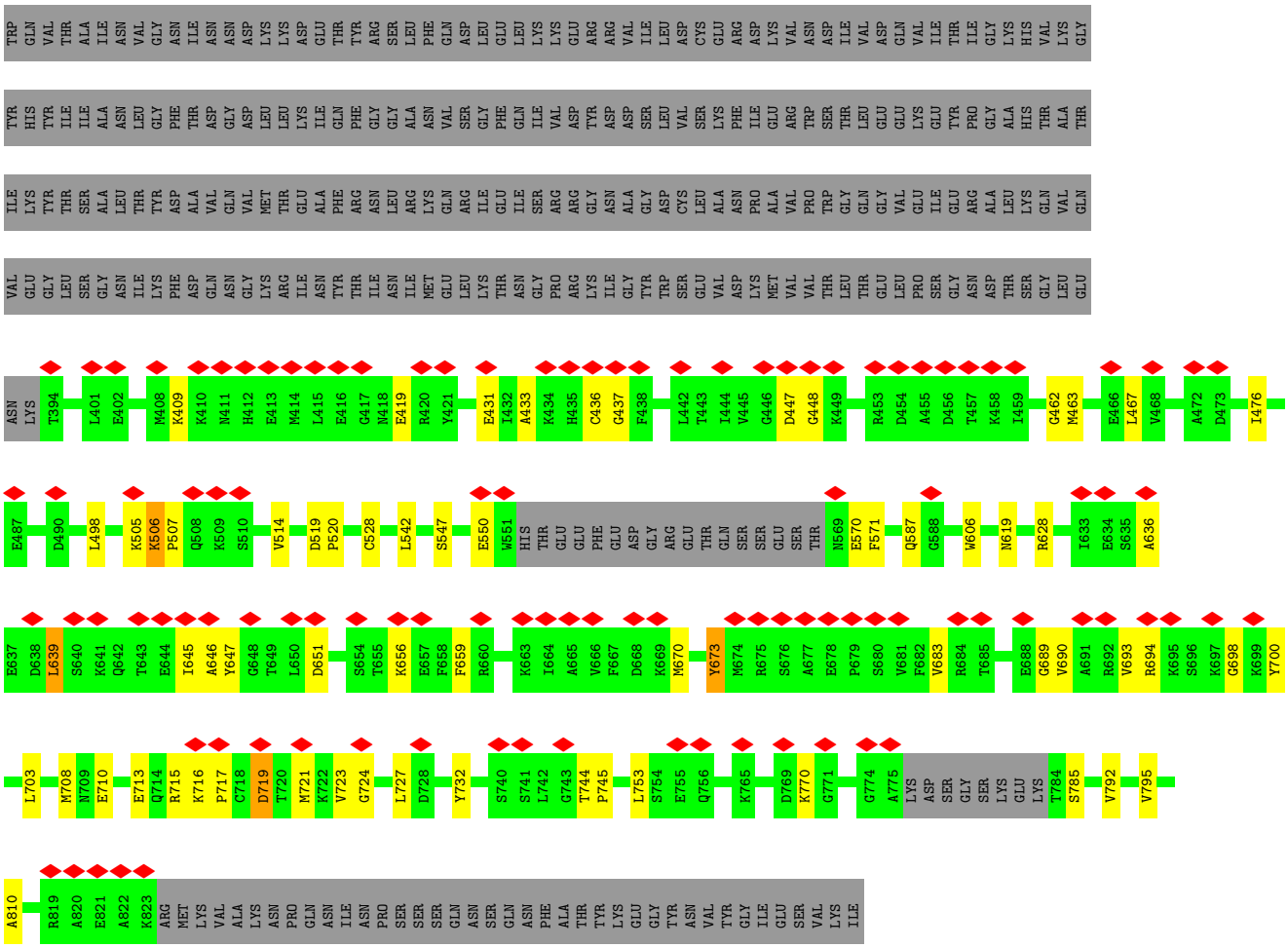


• Molecule 1: Glutamate receptor 2

Chain C:



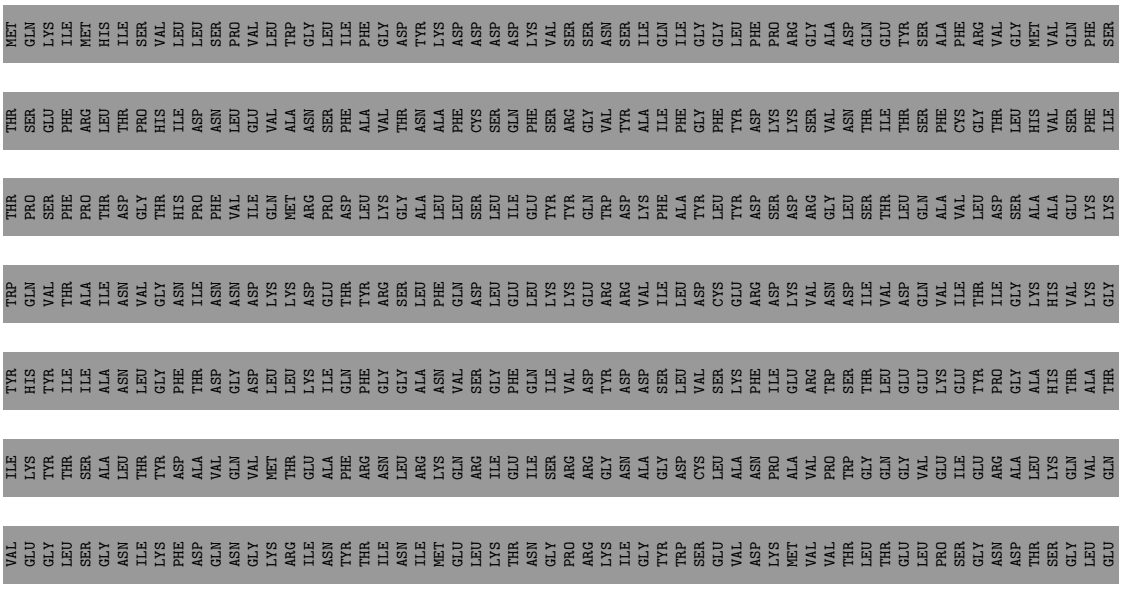


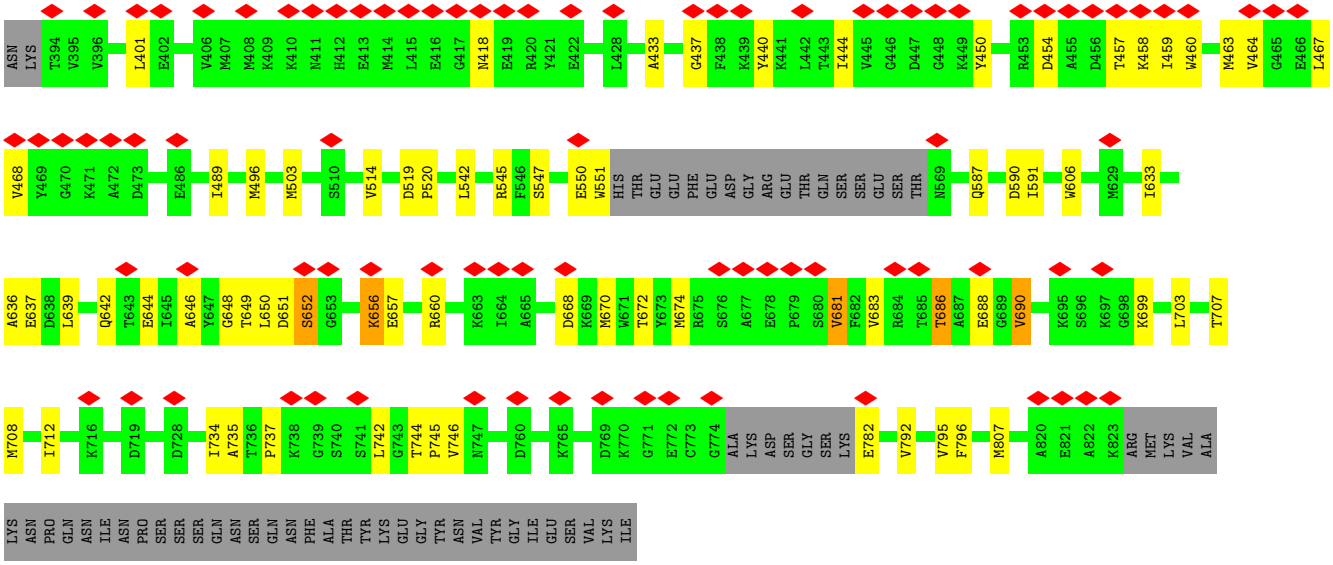


• Molecule 1: Glutamate receptor 2

Chain D:

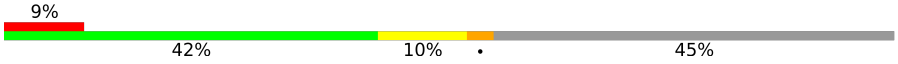


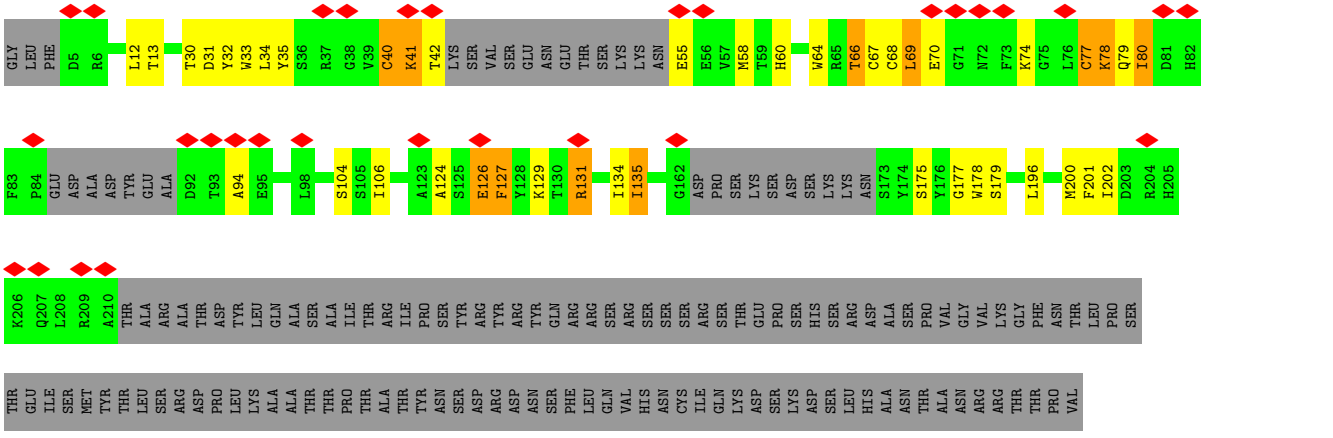




• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit

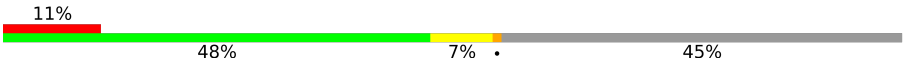
Chain E:

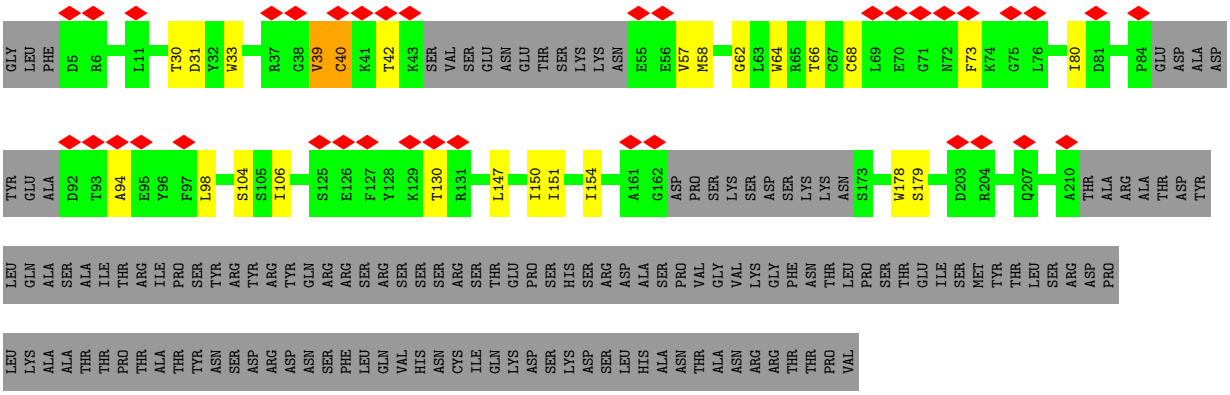




• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit

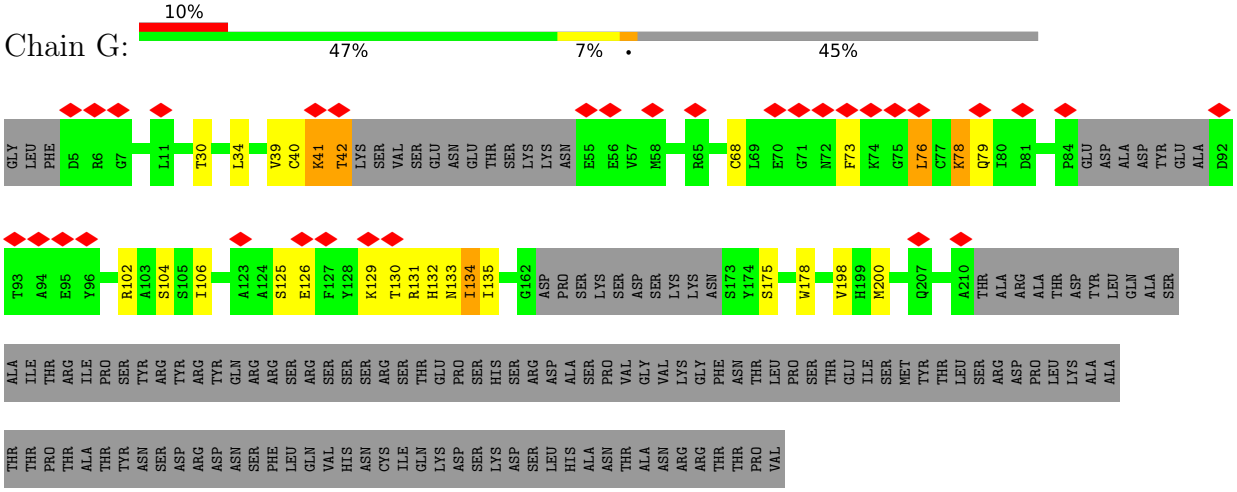
Chain F:





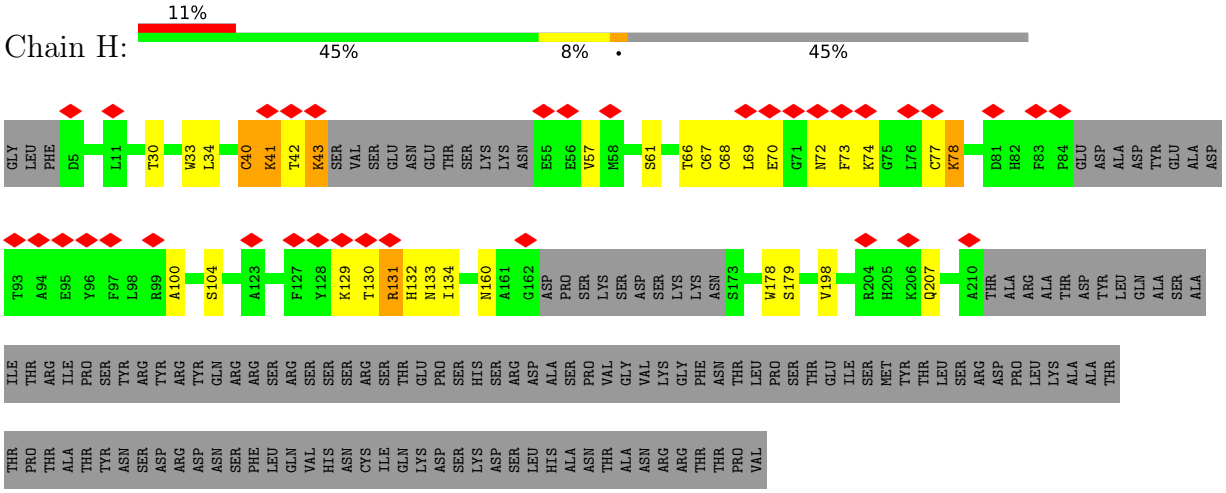
• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit

Chain G:



• Molecule 2: Voltage-dependent calcium channel gamma-2 subunit

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	371741	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	265.972, 265.972, 265.972	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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, ZK1, PLM, POV

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	0.66	0/3177	0.69	0/4309
1	B	0.66	0/3139	0.71	0/4262
1	C	0.65	0/3134	0.71	0/4256
1	D	0.64	0/3147	0.72	0/4271
2	E	0.61	0/1397	0.69	0/1887
2	F	0.58	0/1412	0.64	0/1905
2	G	0.58	0/1403	0.67	0/1894
2	H	0.57	0/1398	0.67	0/1887
All	All	0.63	0/18207	0.70	0/24671

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	3105	0	3040	38	0
1	B	3068	0	2994	61	0
1	C	3063	0	2983	45	0
1	D	3076	0	3007	46	0
2	E	1366	0	1352	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1381	0	1376	19	0
2	G	1372	0	1363	17	0
2	H	1367	0	1361	20	0
3	A	27	0	13	3	0
3	B	27	0	13	1	0
3	C	27	0	13	0	0
3	D	27	0	13	2	0
4	A	34	0	55	0	0
4	B	18	0	31	0	0
4	C	18	0	31	0	0
4	D	18	0	31	0	0
4	F	18	0	31	0	0
4	G	18	0	31	0	0
5	A	25	0	40	0	0
5	B	25	0	40	0	0
5	C	25	0	40	0	0
5	D	25	0	40	0	0
6	B	42	0	56	2	0
6	D	40	0	52	1	0
6	E	39	0	50	3	0
6	G	76	0	96	1	0
7	A	1	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
All	All	18333	0	18152	264	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 264 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)
3:A:901:ZK1:HAMA	3:A:901:ZK1:FAG	1.54	0.96
1:C:506:LYS:HD3	1:C:721:MET:HB2	1.53	0.90
1:A:463:MET:HE1	1:A:477:ALA:HB3	1.55	0.87
1:D:649:THR:HG23	1:D:674:MET:HE1	1.59	0.84
2:E:30:THR:HG21	2:E:178:TRP:CH2	2.18	0.77

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	401/891 (45%)	384 (96%)	16 (4%)	1 (0%)	43 73
1	B	401/891 (45%)	384 (96%)	17 (4%)	0	100 100
1	C	400/891 (45%)	376 (94%)	24 (6%)	0	100 100
1	D	401/891 (45%)	382 (95%)	19 (5%)	0	100 100
2	E	169/322 (52%)	159 (94%)	9 (5%)	1 (1%)	21 56
2	F	170/322 (53%)	164 (96%)	6 (4%)	0	100 100
2	G	169/322 (52%)	164 (97%)	5 (3%)	0	100 100
2	H	169/322 (52%)	157 (93%)	12 (7%)	0	100 100
All	All	2280/4852 (47%)	2170 (95%)	108 (5%)	2 (0%)	49 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	80	ILE
1	A	588	GLY

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	320/765 (42%)	317 (99%)	3 (1%)	70 81
1	B	312/765 (41%)	305 (98%)	7 (2%)	45 71
1	C	311/765 (41%)	307 (99%)	4 (1%)	61 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	314/765 (41%)	306 (98%)	8 (2%)	42 69
2	E	142/274 (52%)	128 (90%)	14 (10%)	7 31
2	F	144/274 (53%)	139 (96%)	5 (4%)	32 64
2	G	143/274 (52%)	133 (93%)	10 (7%)	14 45
2	H	142/274 (52%)	134 (94%)	8 (6%)	19 52
All	All	1828/4156 (44%)	1769 (97%)	59 (3%)	35 65

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	77	CYS
2	H	78	LYS
2	E	135	ILE
2	H	57	VAL
2	G	132	HIS

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

Mol	Chain	Res	Type
2	E	9	GLN
2	F	205	HIS
2	G	132	HIS
2	G	205	HIS
2	H	205	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ZK1	C	901	-	29,29,29	0.95	2 (6%)	45,45,45	0.80	0
4	PLM	B	902	-	17,17,17	0.68	0	17,17,17	0.58	0
4	PLM	A	902	-	17,17,17	0.58	0	17,17,17	0.71	0
6	POV	E	1201	-	38,38,51	0.49	0	44,46,59	0.68	1 (2%)
3	ZK1	D	901	-	29,29,29	0.91	2 (6%)	45,45,45	0.94	2 (4%)
5	OLC	D	903	-	24,24,24	0.36	0	25,25,25	0.51	0
5	OLC	C	902	-	24,24,24	0.57	0	25,25,25	0.36	0
6	POV	G	1103	-	41,41,51	0.41	0	47,49,59	0.94	1 (2%)
6	POV	B	904	-	41,41,51	0.53	0	47,49,59	0.70	1 (2%)
4	PLM	C	903	-	17,17,17	0.66	0	17,17,17	0.67	0
4	PLM	D	902	-	17,17,17	0.68	0	17,17,17	0.66	0
5	OLC	B	903	-	24,24,24	0.48	0	25,25,25	0.67	1 (4%)
5	OLC	A	903	-	24,24,24	0.31	0	25,25,25	0.43	0
6	POV	D	904	-	39,39,51	0.55	0	45,47,59	0.86	1 (2%)
4	PLM	G	1101	-	17,17,17	0.75	0	17,17,17	0.49	0
6	POV	G	1102	-	33,33,51	0.56	0	36,38,59	0.89	2 (5%)
3	ZK1	B	901	-	29,29,29	0.94	2 (6%)	45,45,45	0.75	0
4	PLM	A	904	-	15,15,17	0.76	0	15,15,17	0.82	1 (6%)
3	ZK1	A	901	-	29,29,29	1.19	3 (10%)	45,45,45	0.86	2 (4%)
4	PLM	F	1301	-	17,17,17	0.64	0	17,17,17	0.67	0

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
3	ZK1	C	901	-	-	10/13/23/23	0/3/3/3
4	PLM	B	902	-	-	11/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLM	A	902	-	-	10/15/15/15	-
6	POV	E	1201	-	-	19/42/42/55	-
3	ZK1	D	901	-	-	3/13/23/23	0/3/3/3
5	OLC	D	903	-	-	12/24/24/24	-
5	OLC	C	902	-	-	11/24/24/24	-
6	POV	G	1103	-	-	22/45/45/55	-
6	POV	B	904	-	-	16/45/45/55	-
4	PLM	C	903	-	-	5/15/15/15	-
4	PLM	D	902	-	-	7/15/15/15	-
5	OLC	B	903	-	-	7/24/24/24	-
5	OLC	A	903	-	-	9/24/24/24	-
6	POV	D	904	-	-	16/43/43/55	-
4	PLM	G	1101	-	-	7/15/15/15	-
6	POV	G	1102	-	-	18/35/35/55	-
3	ZK1	B	901	-	-	10/13/23/23	0/3/3/3
4	PLM	A	904	-	-	6/13/13/15	-
3	ZK1	A	901	-	-	6/13/23/23	0/3/3/3
4	PLM	F	1301	-	-	6/15/15/15	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ZK1	PBA-OAE	-2.78	1.48	1.55
3	B	901	ZK1	PBA-OAE	-2.73	1.48	1.55
3	D	901	ZK1	PBA-OAD	-2.67	1.49	1.55
3	C	901	ZK1	PBA-OAD	-2.55	1.49	1.55
3	B	901	ZK1	PBA-OAD	-2.52	1.49	1.55

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	1103	POV	O21-C21-C22	4.72	121.70	111.48
6	D	904	POV	O21-C21-C22	4.49	121.20	111.48
6	B	904	POV	O21-C21-C22	2.85	117.64	111.48
3	D	901	ZK1	CAN-NAX-CAR	2.81	122.85	116.19
3	D	901	ZK1	CAI-CAR-NAX	-2.76	118.57	122.59

There are no chirality outliers.

5 of 211 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	901	ZK1	NAY-CAO-PBA-OAD
3	D	901	ZK1	NAY-CAO-PBA-OAE
5	A	903	OLC	O20-C21-C22-C24
6	E	1201	POV	C1-O11-P-O14
6	E	1201	POV	C11-O12-P-O11

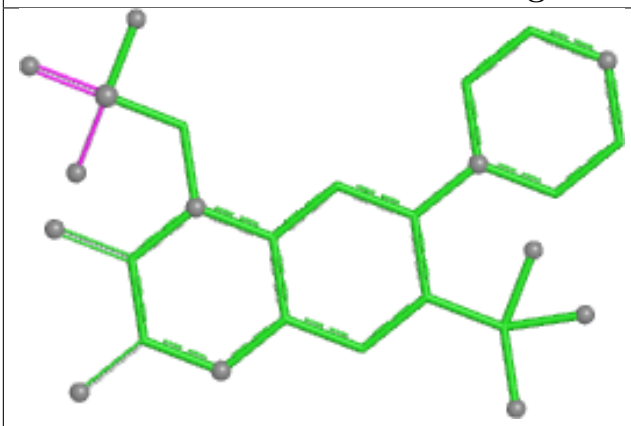
There are no ring outliers.

7 monomers are involved in 13 short contacts:

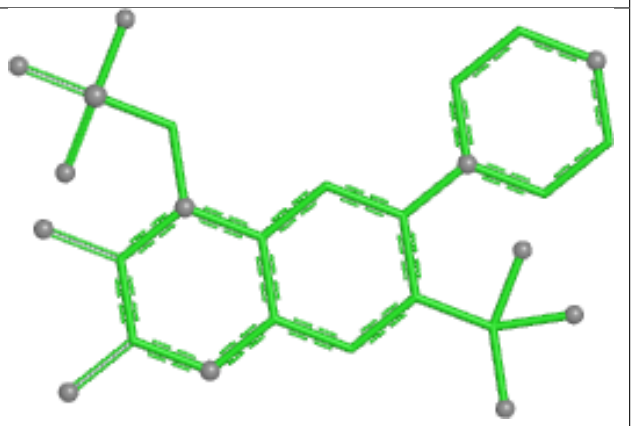
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1201	POV	3	0
3	D	901	ZK1	2	0
6	G	1103	POV	1	0
6	B	904	POV	2	0
6	D	904	POV	1	0
3	B	901	ZK1	1	0
3	A	901	ZK1	3	0

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.

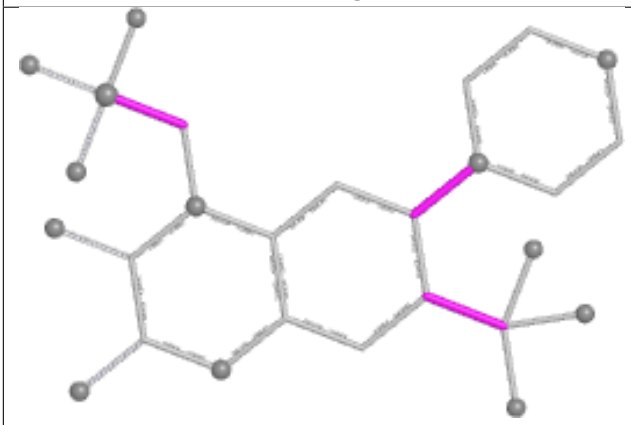
Ligand ZK1 C 901



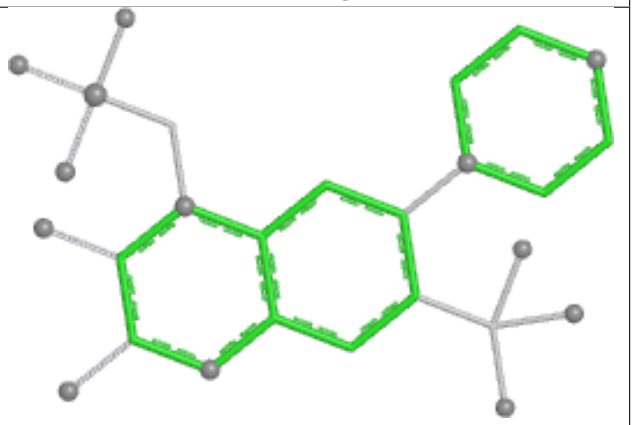
Bond lengths



Bond angles

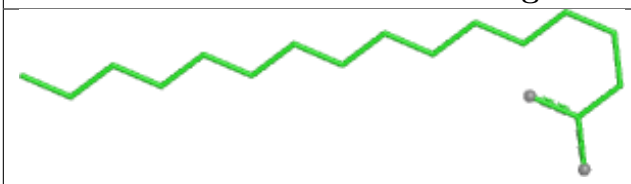


Torsions

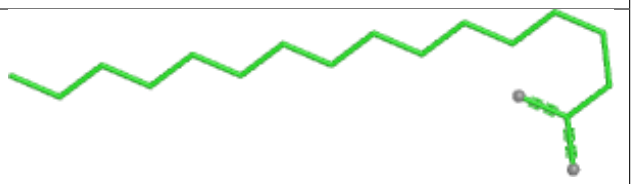


Rings

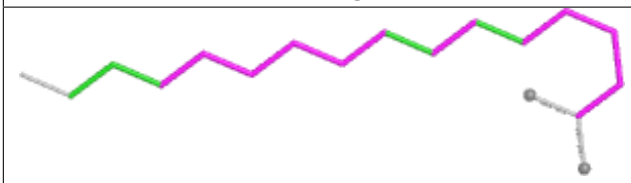
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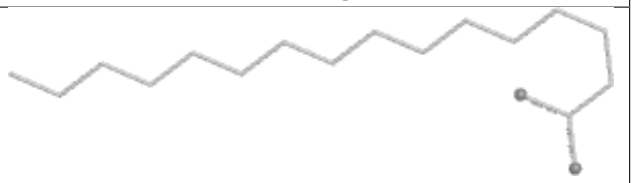
Bond lengths



Bond angles

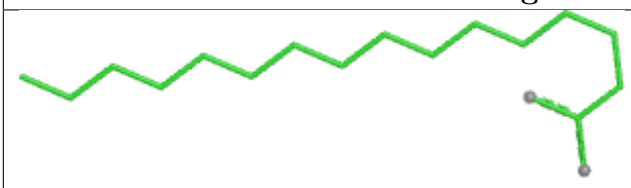


Torsions

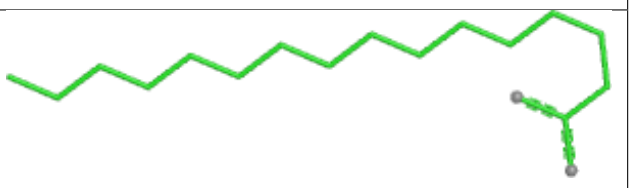


Rings

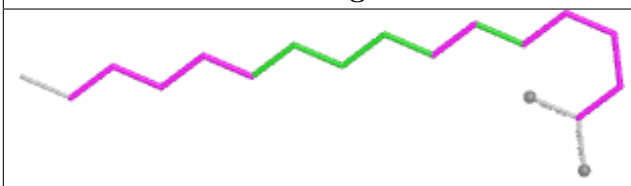
Ligand PLM A 902



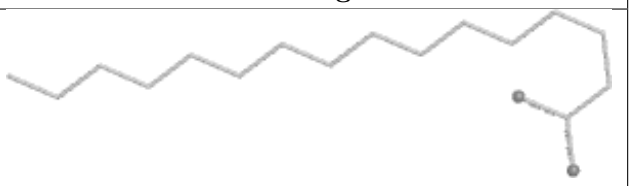
Bond lengths



Bond angles

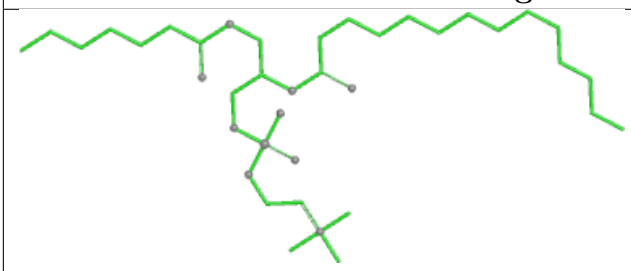


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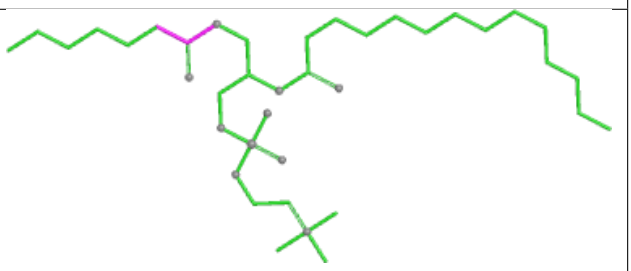


Rings

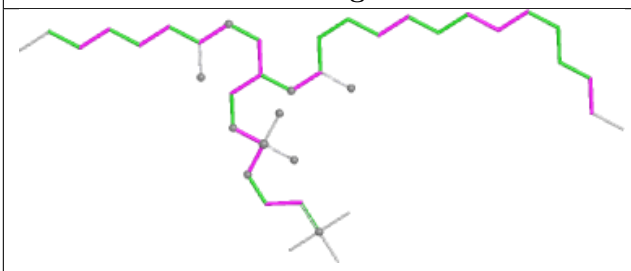
Ligand POV E 1201



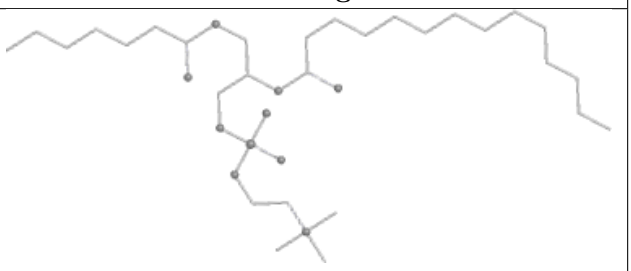
Bond lengths



Bond angles

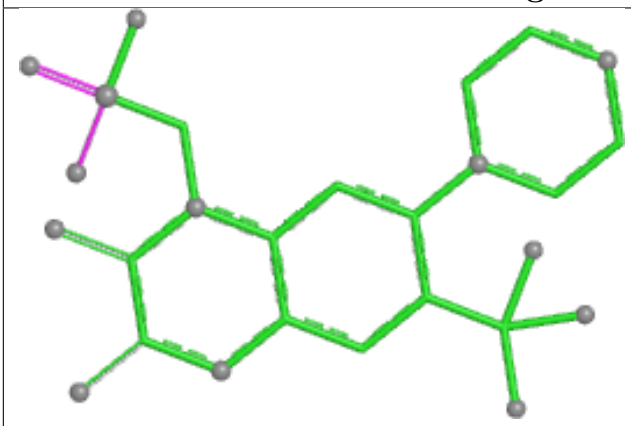


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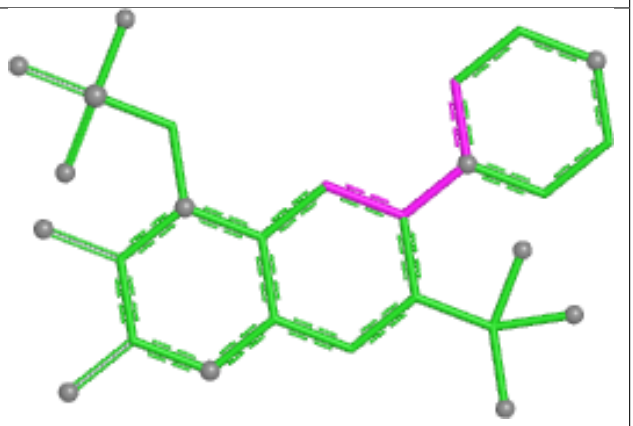


Rings

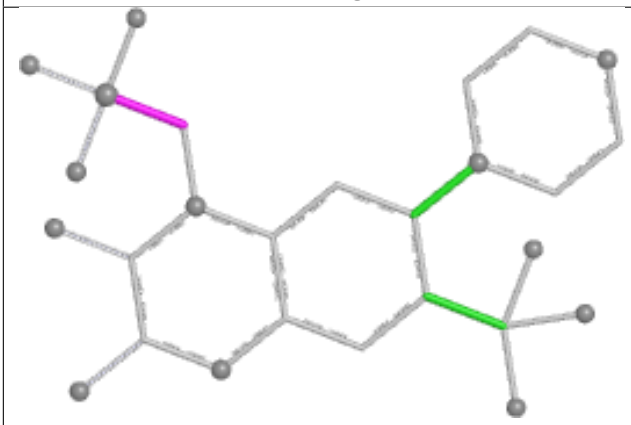
Ligand ZK1 D 901



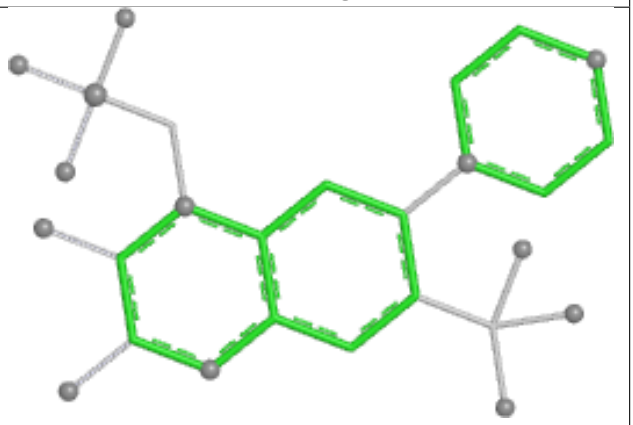
Bond lengths



Bond angles



Torsions

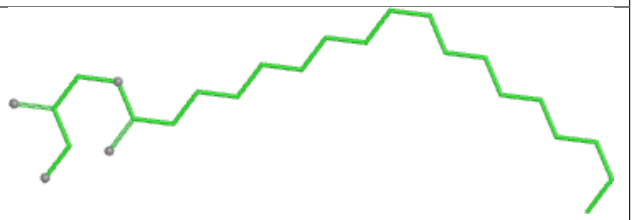


Rings

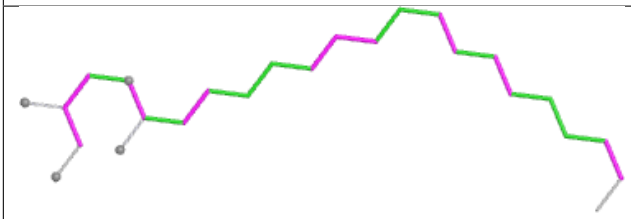
Ligand OLC D 903



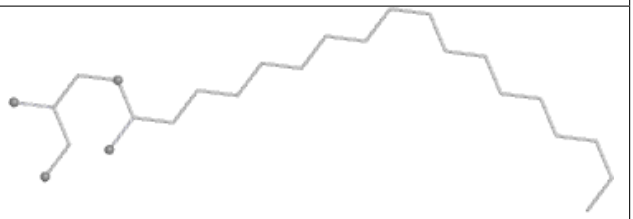
Bond lengths



Bond angles

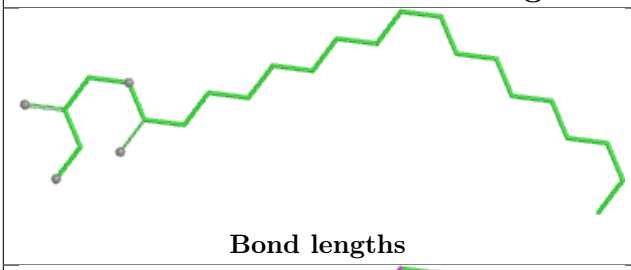


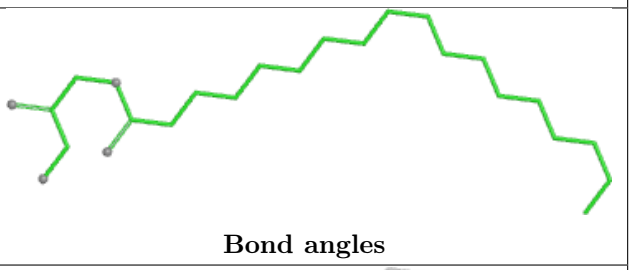
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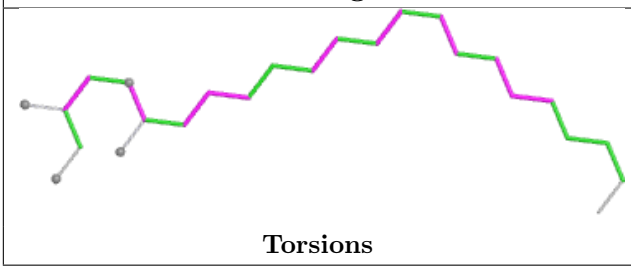


Rings

Ligand OLC C 902

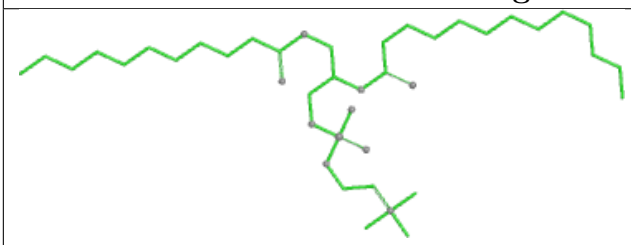

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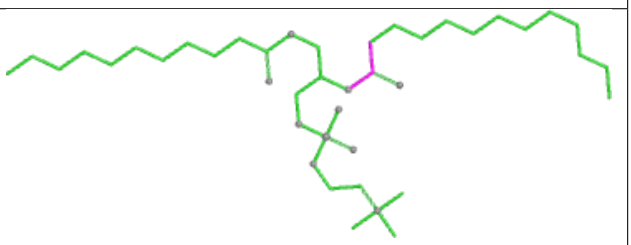

Bond angles

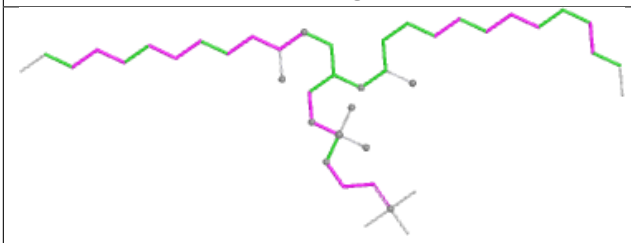

Torsions

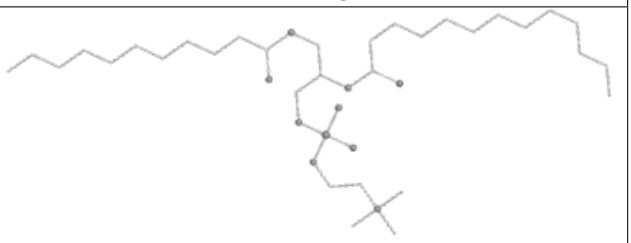

Rings

Ligand POV G 1103

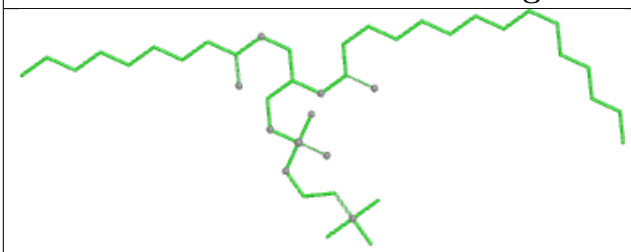

Bond lengths

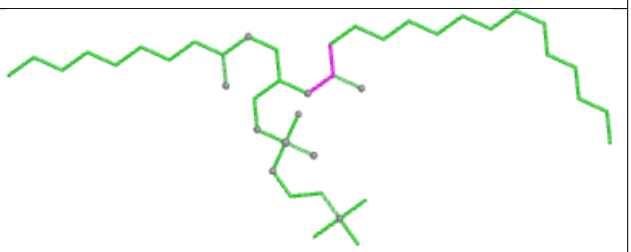

Bond angles

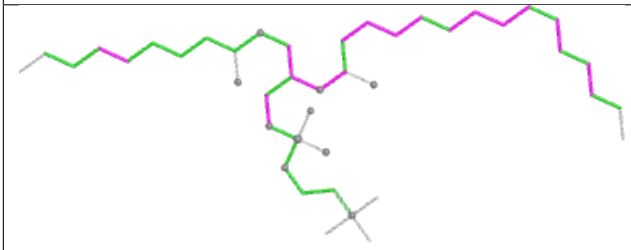

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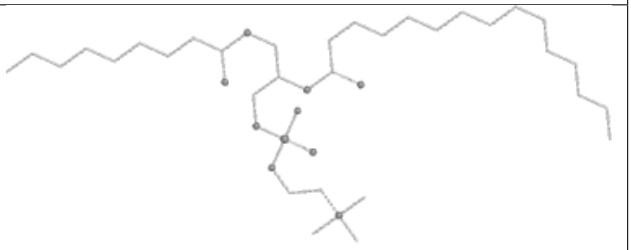

Rings

Ligand POV B 904

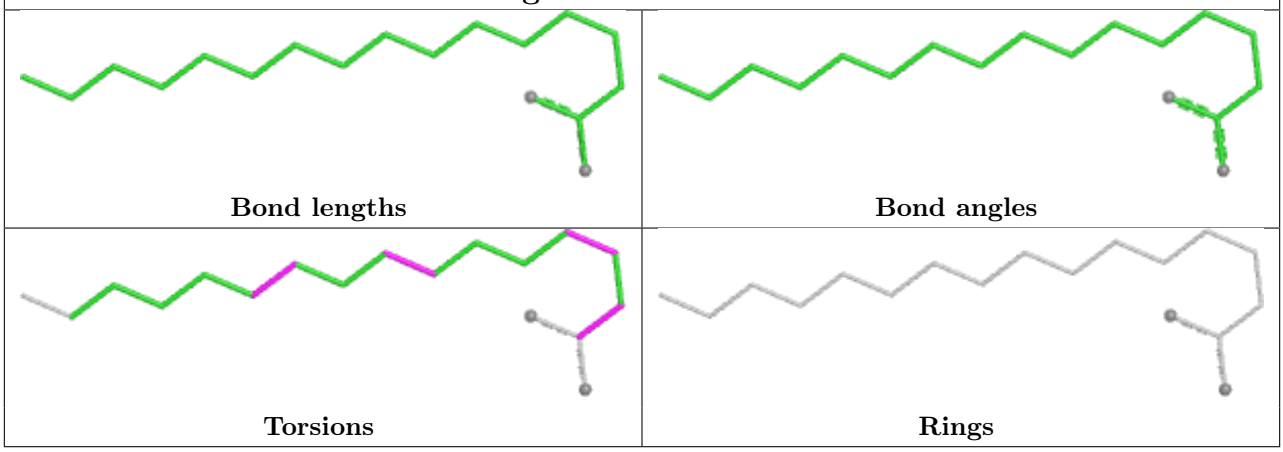

Bond lengths


Bond angles

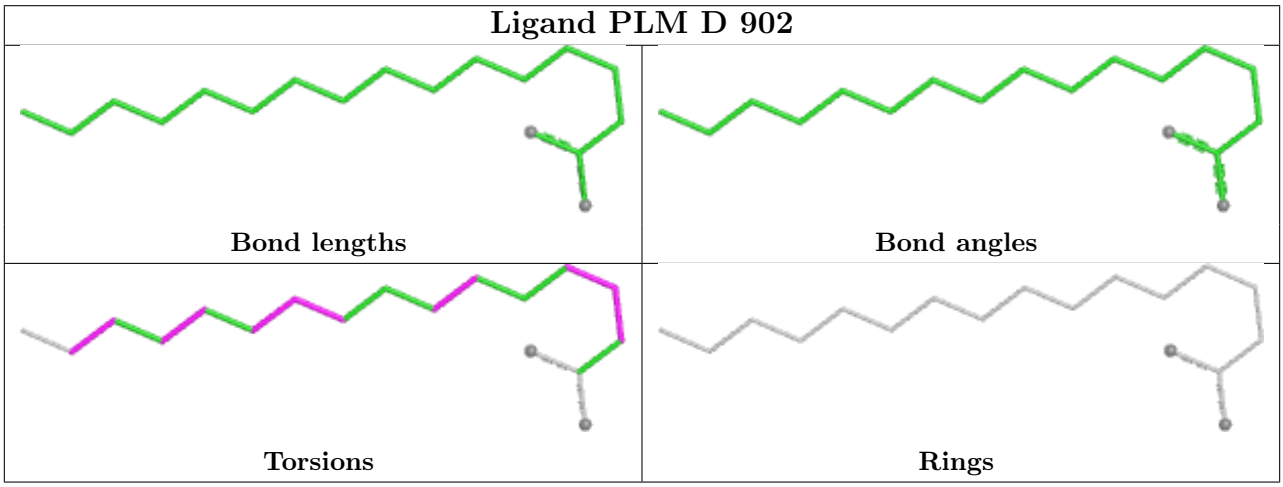

Torsions


Rings

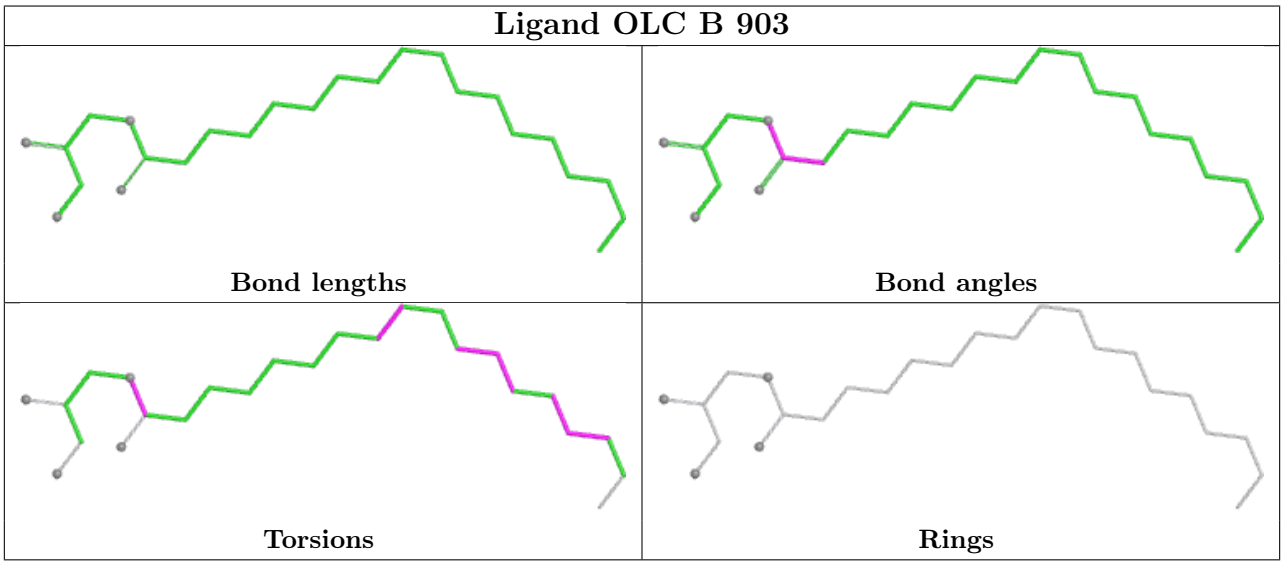
Ligand PLM C 903



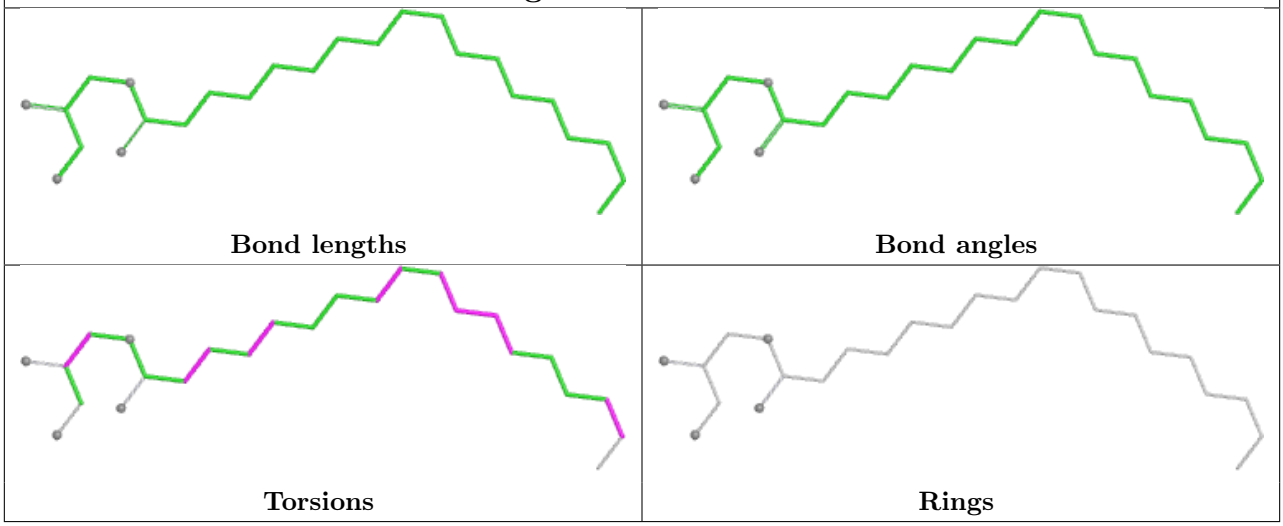
Ligand PLM D 902



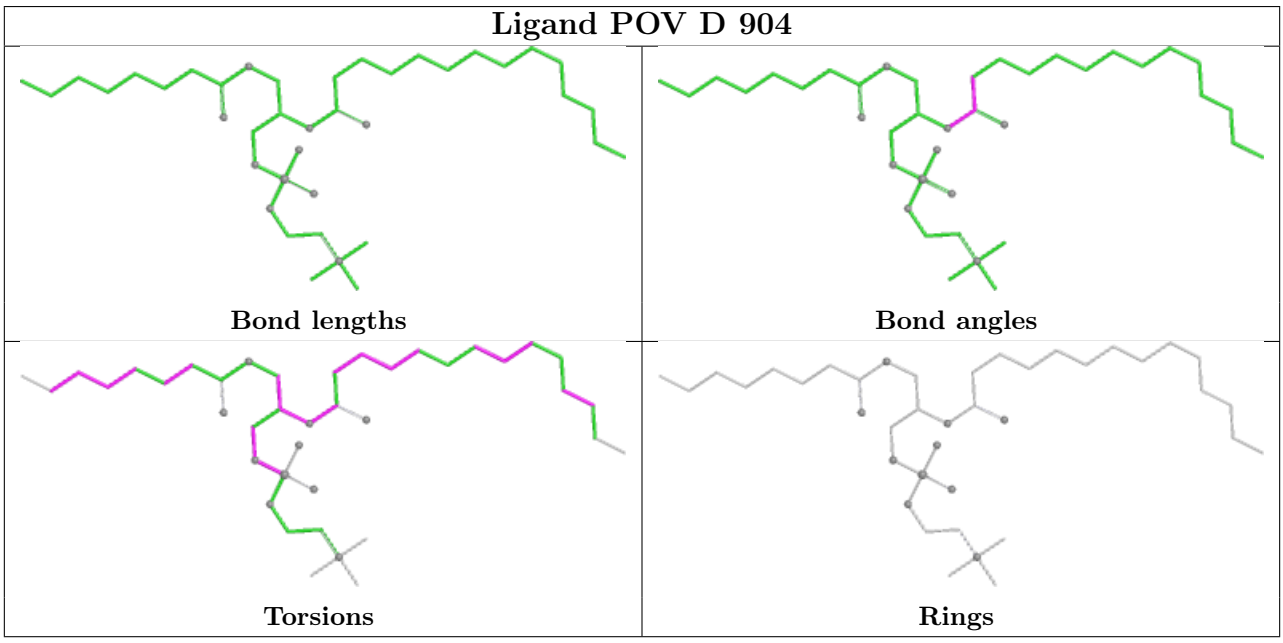
Ligand OLC B 903



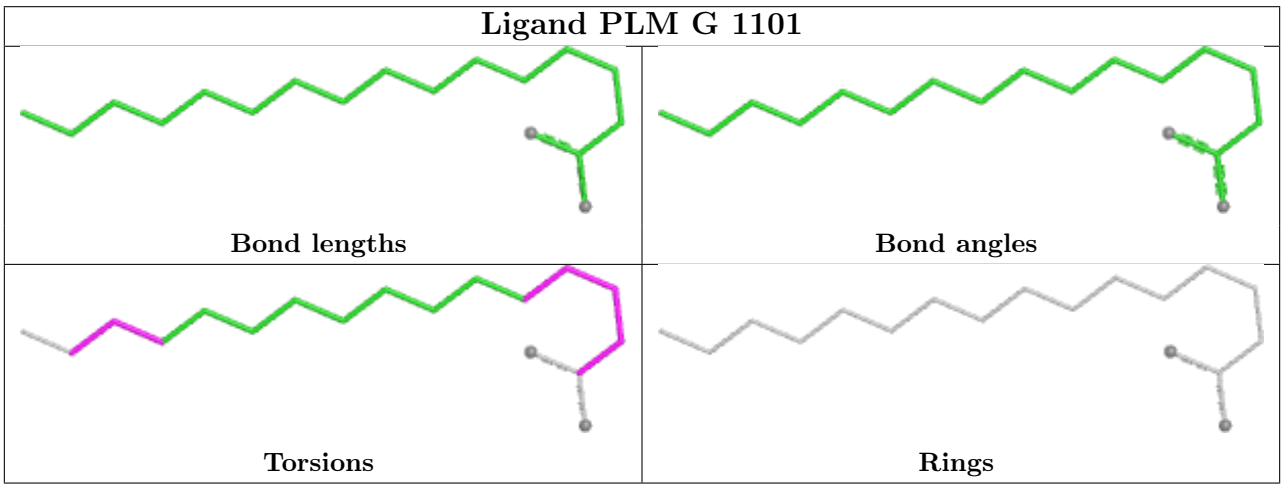
Ligand OLC A 903



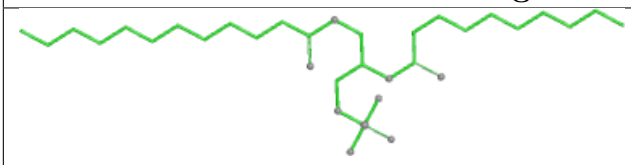
Ligand POV D 904



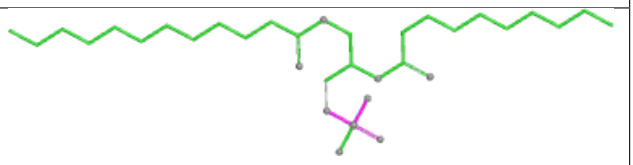
Ligand PLM G 1101



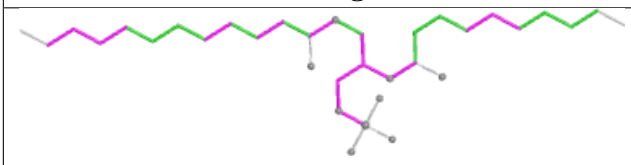
Ligand POV G 1102



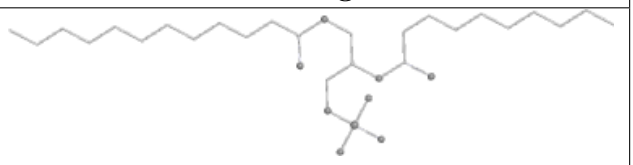
Bond lengths



Bond angles

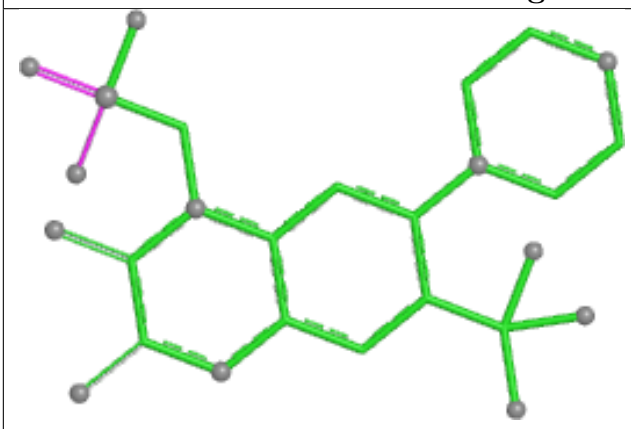


Torsions

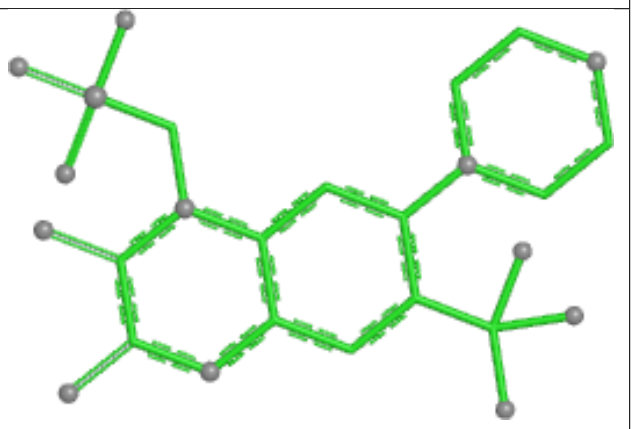


Rings

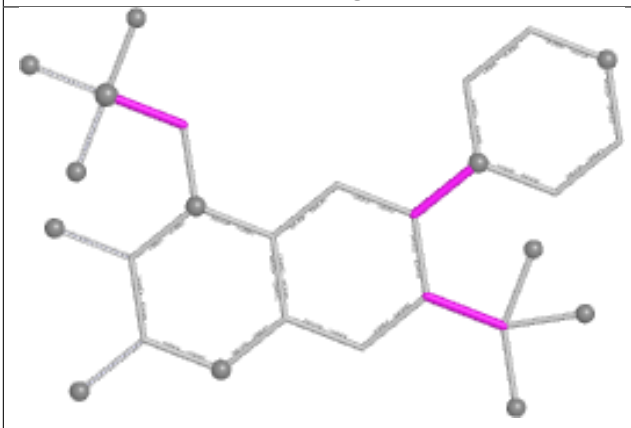
Ligand ZK1 B 901



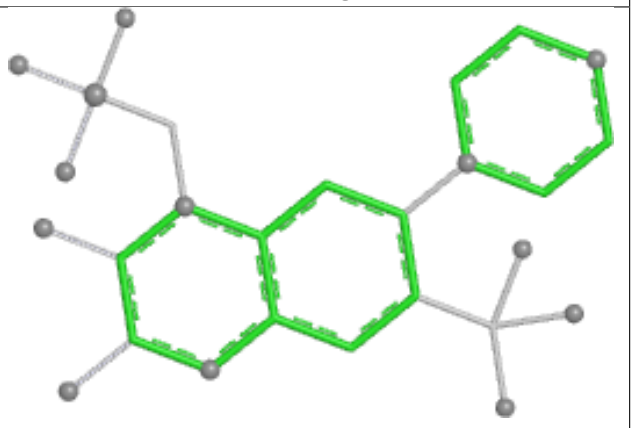
Bond lengths



Bond angles

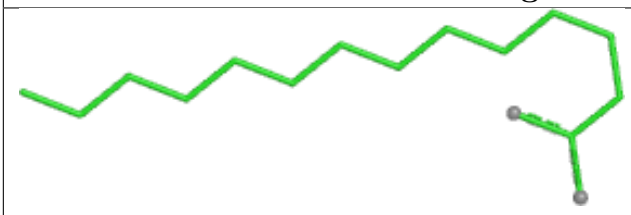


Torsions

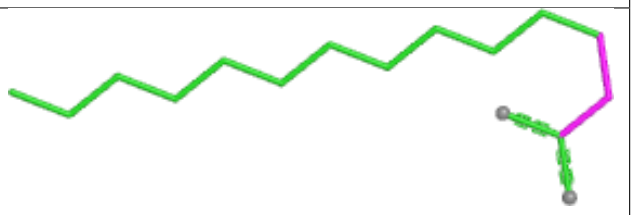


Rings

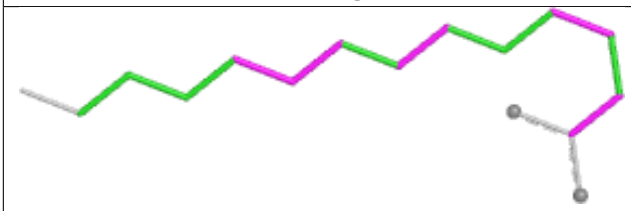
Ligand PLM A 904



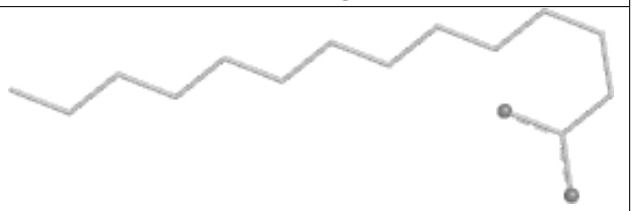
Bond lengths



Bond angles

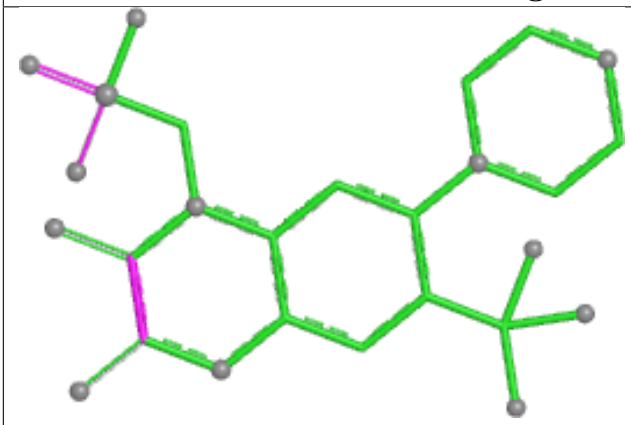


Torsions

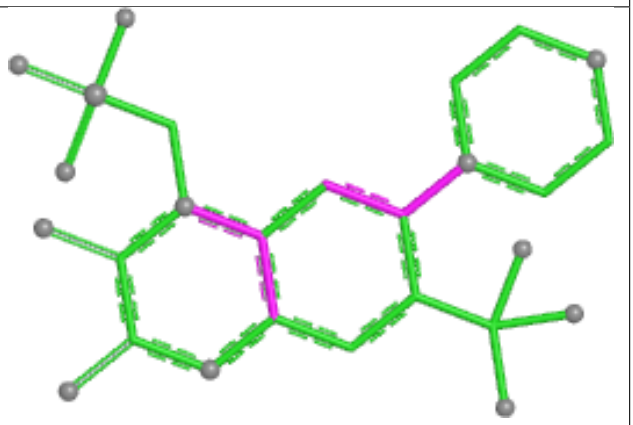


Rings

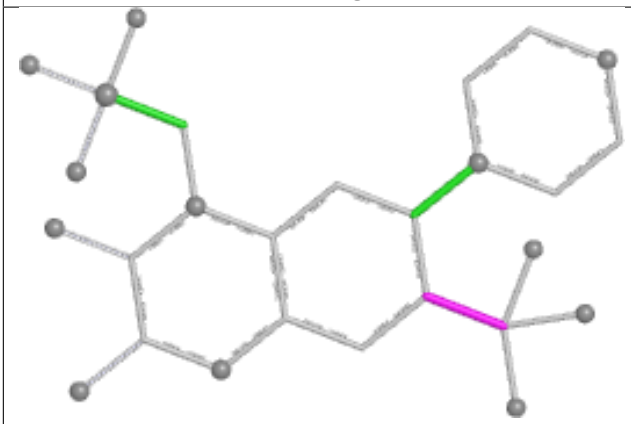
Ligand ZK1 A 901



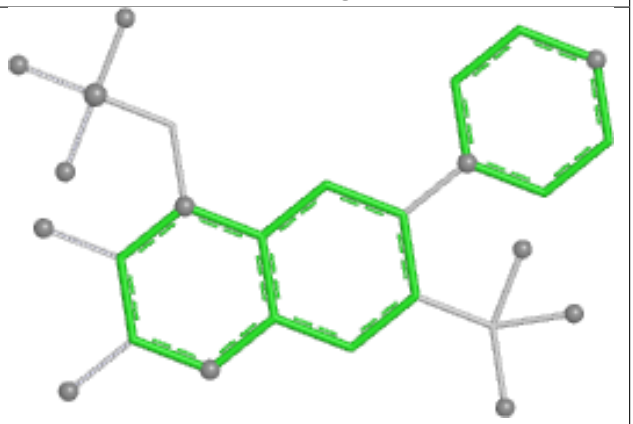
Bond lengths



Bond angles

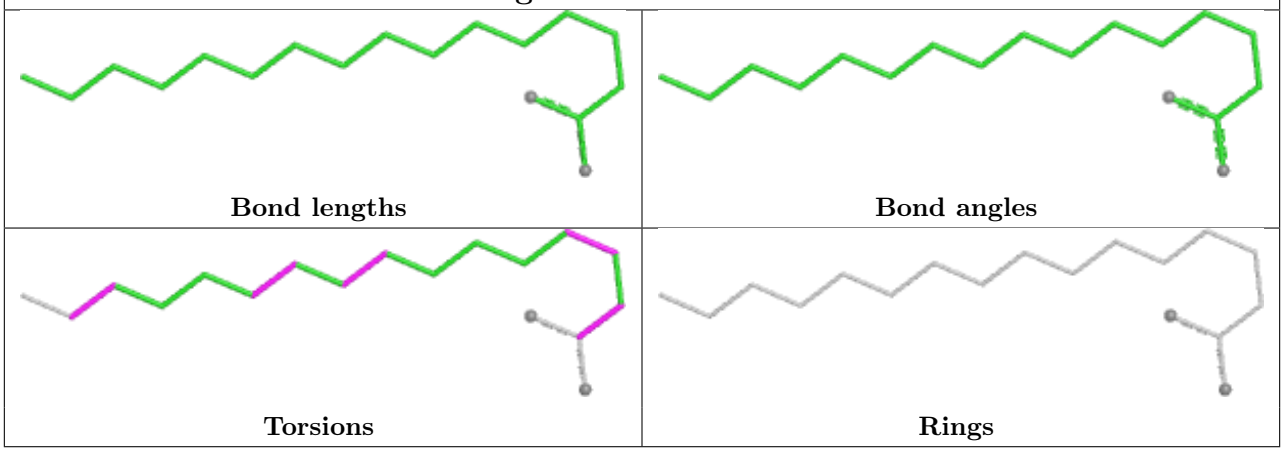


Torsions



Rings

Ligand PLM F 1301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

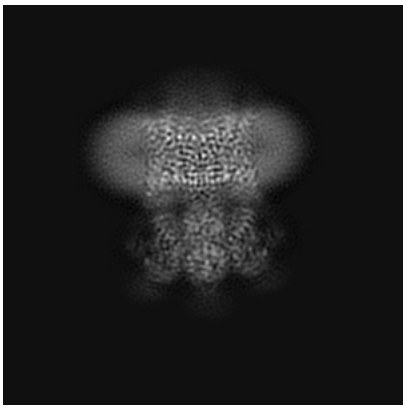
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16381. These allow visual inspection of the internal detail of the map and identification of artifacts.

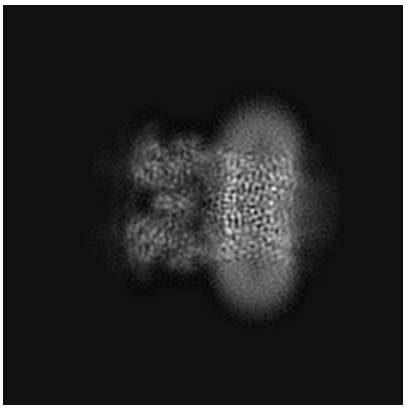
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

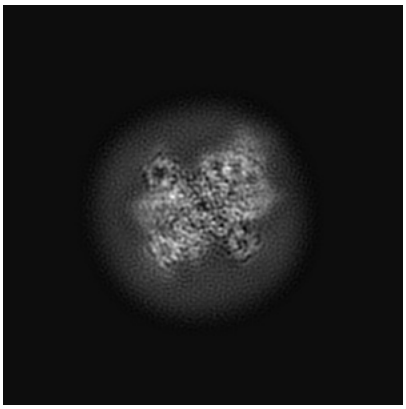
6.1.1 Primary map



X

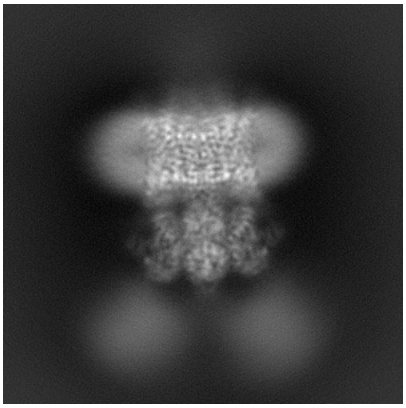


Y

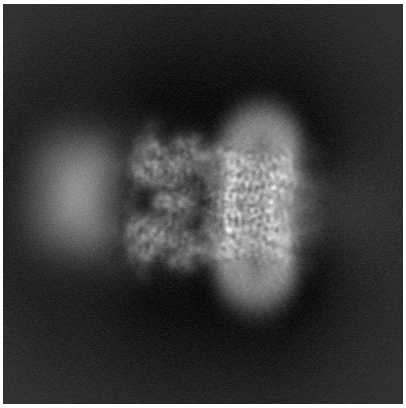


Z

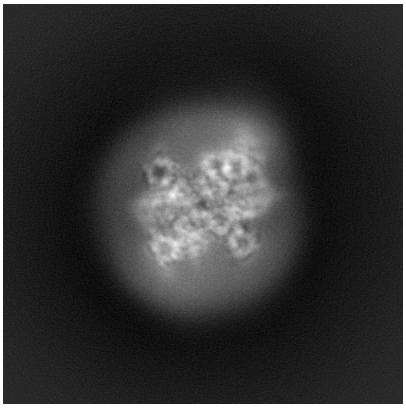
6.1.2 Raw map



X



Y

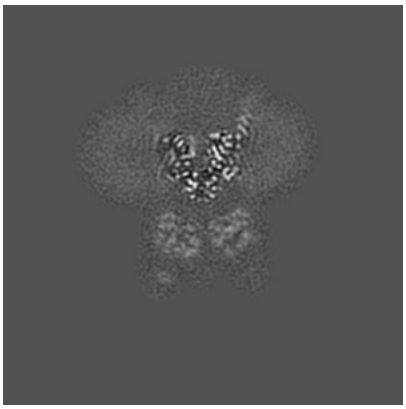


Z

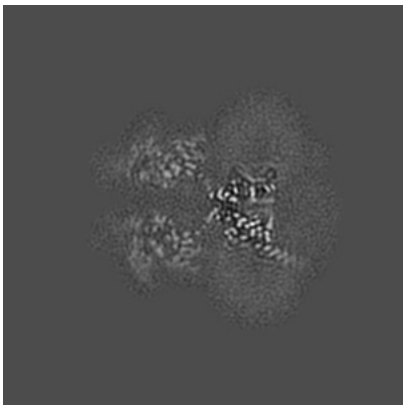
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

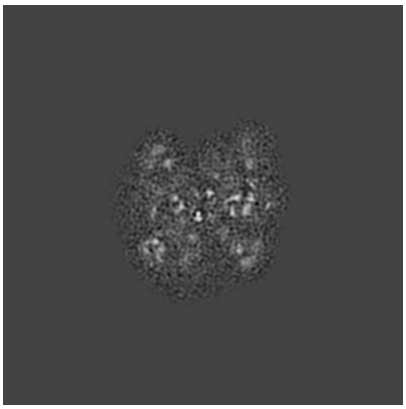
6.2.1 Primary map



X Index: 161

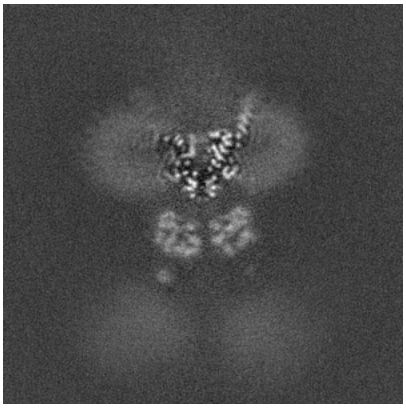


Y Index: 161

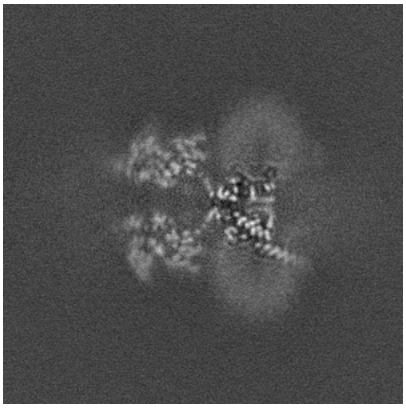


Z Index: 161

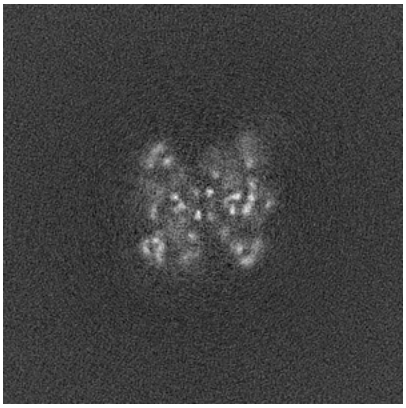
6.2.2 Raw map



X Index: 161



Y Index: 161

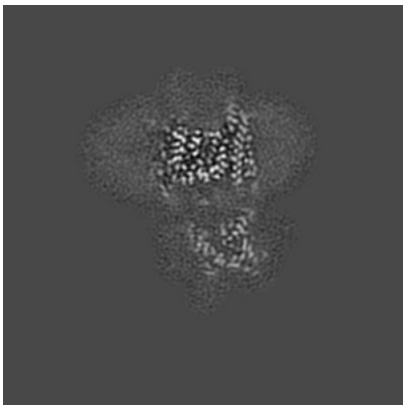


Z Index: 161

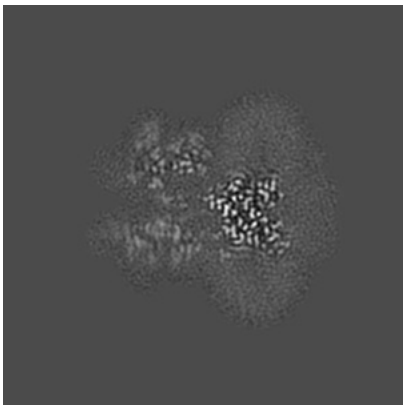
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

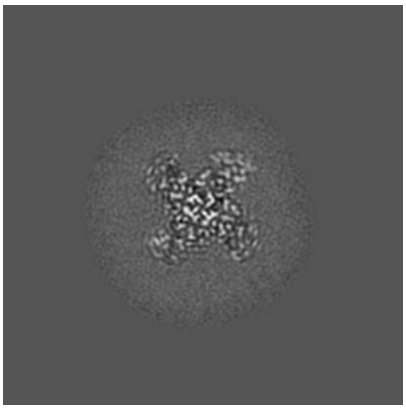
6.3.1 Primary map



X Index: 179

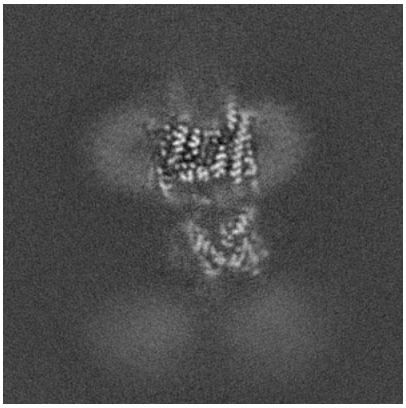


Y Index: 168

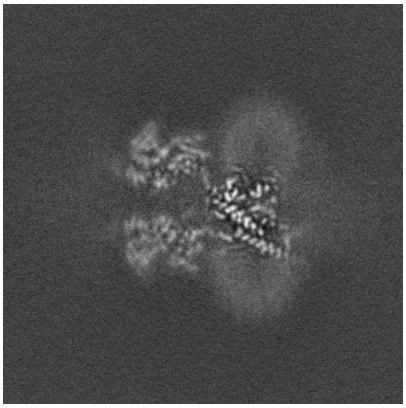


Z Index: 185

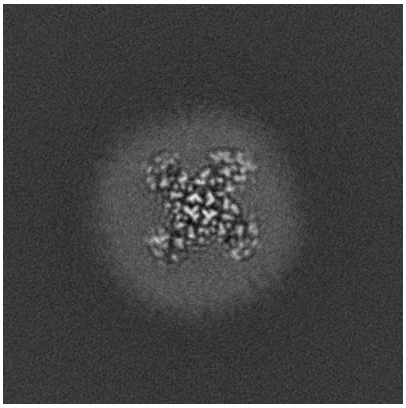
6.3.2 Raw map



X Index: 180



Y Index: 164

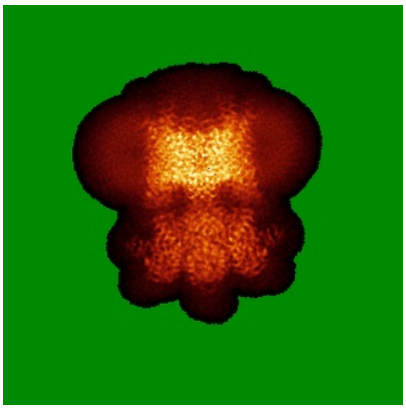


Z Index: 185

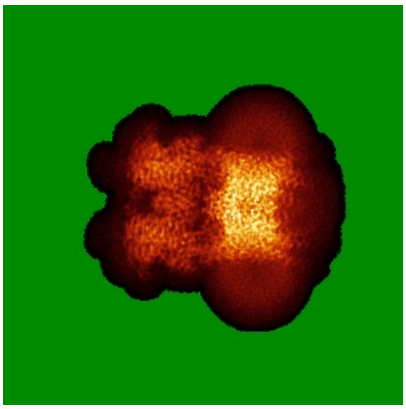
The images above show the largest variance slices of the map in three orthogonal directions.

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

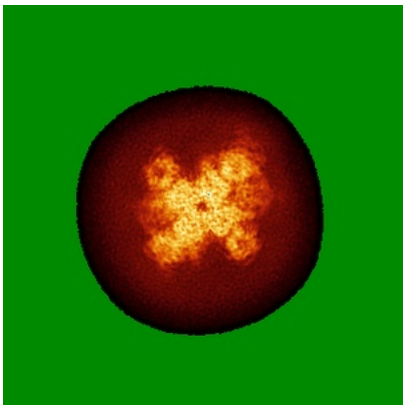
6.4.1 Primary map



X

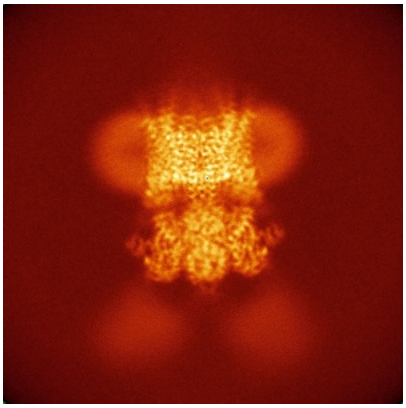


Y

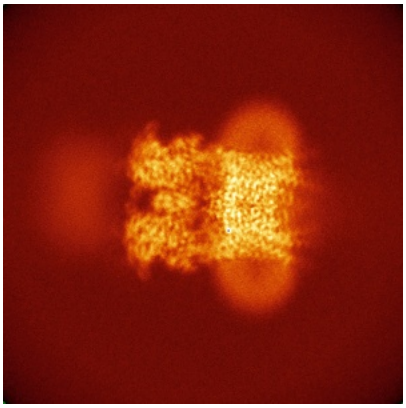


Z

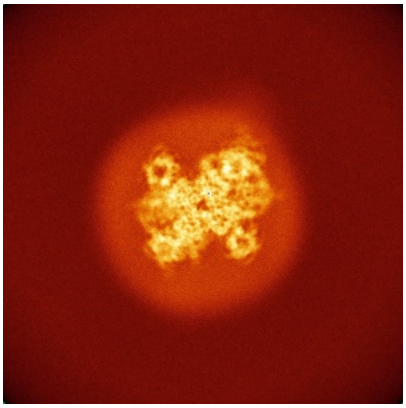
6.4.2 Raw map



X



Y

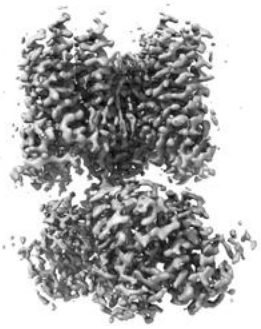


Z

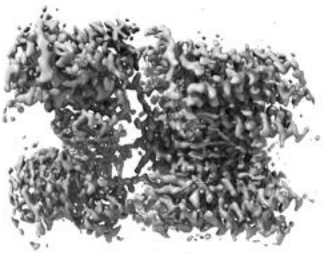
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

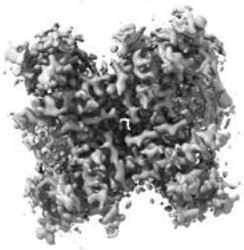
6.5.1 Primary map



X



Y



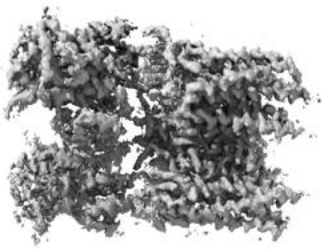
Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

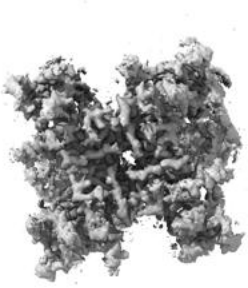
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

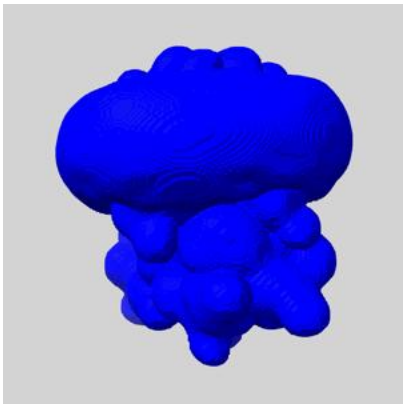
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

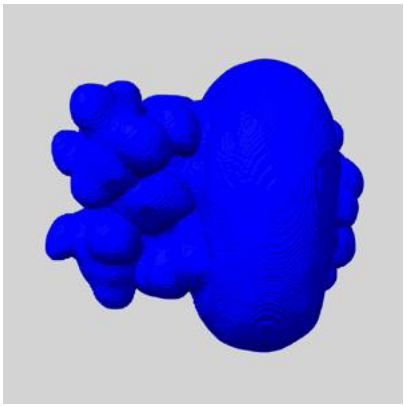
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

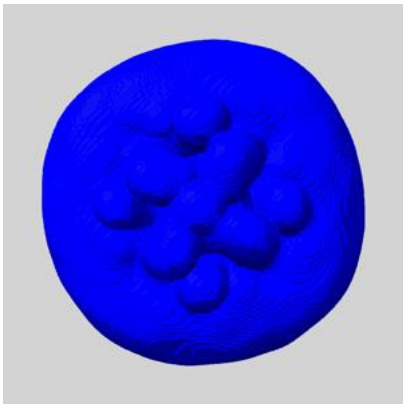
6.6.1 emd_16381_msk_1.map (i)



X



Y

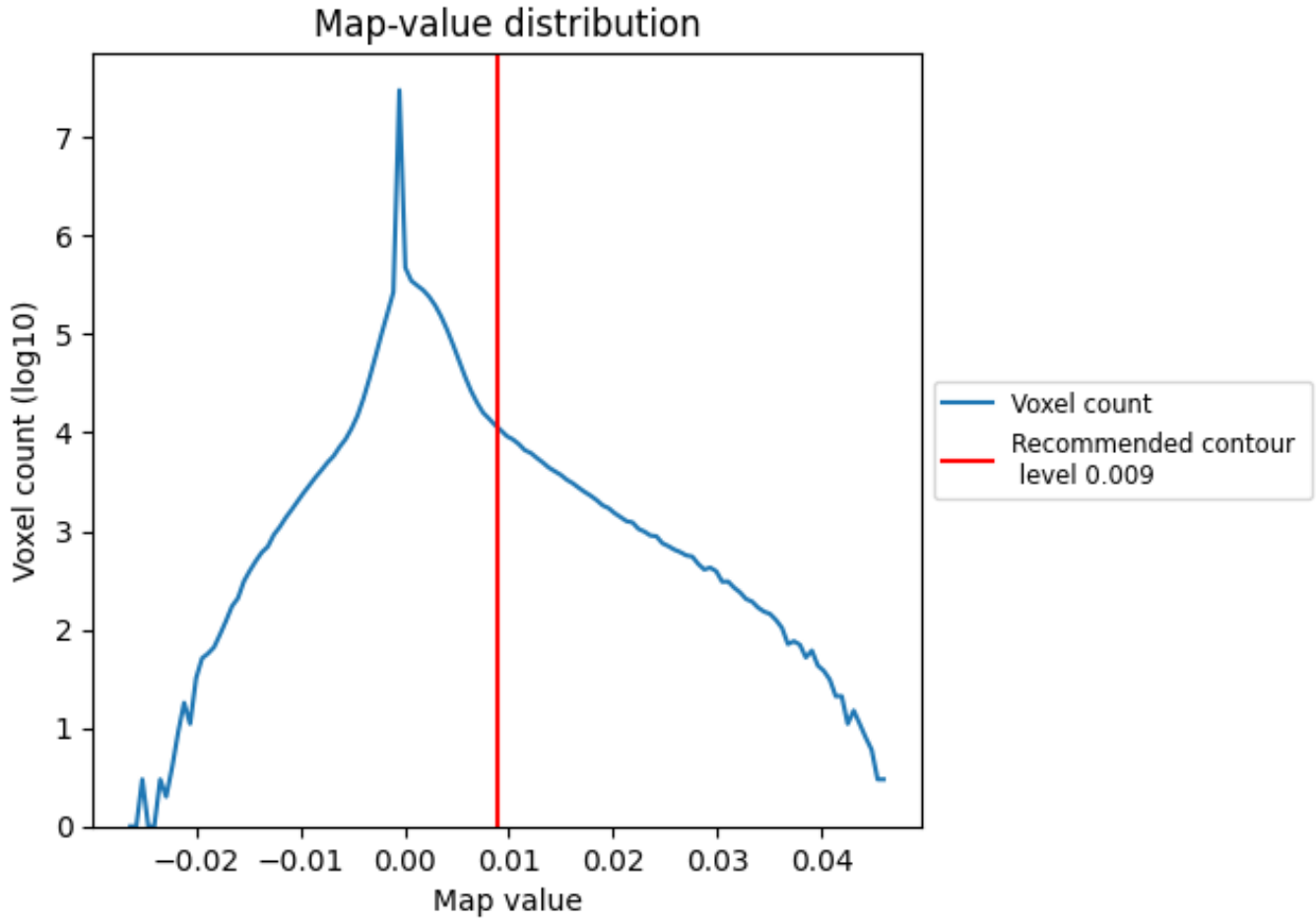


Z

7 Map analysis

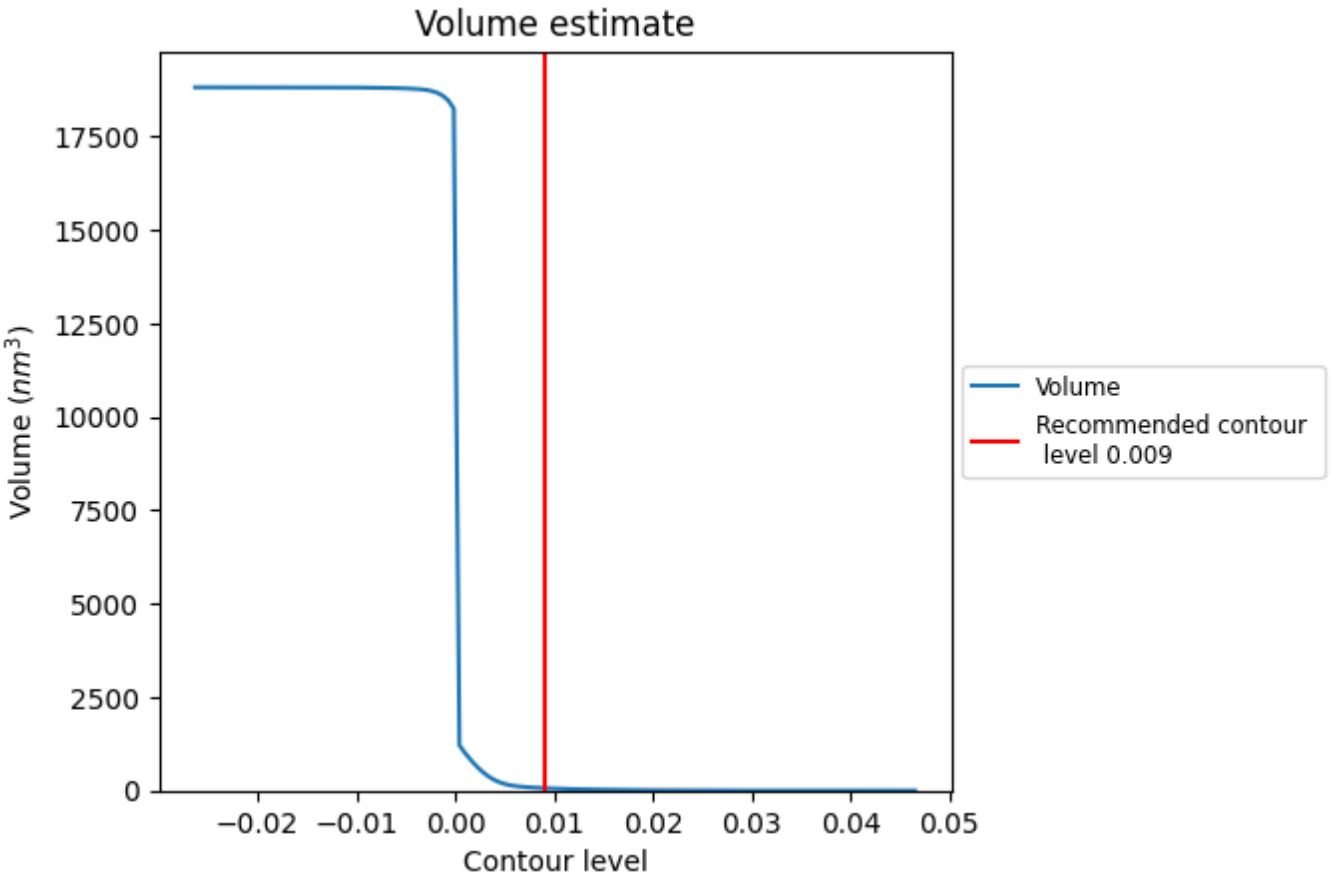
This section contains the results of statistical analysis of the map.

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.

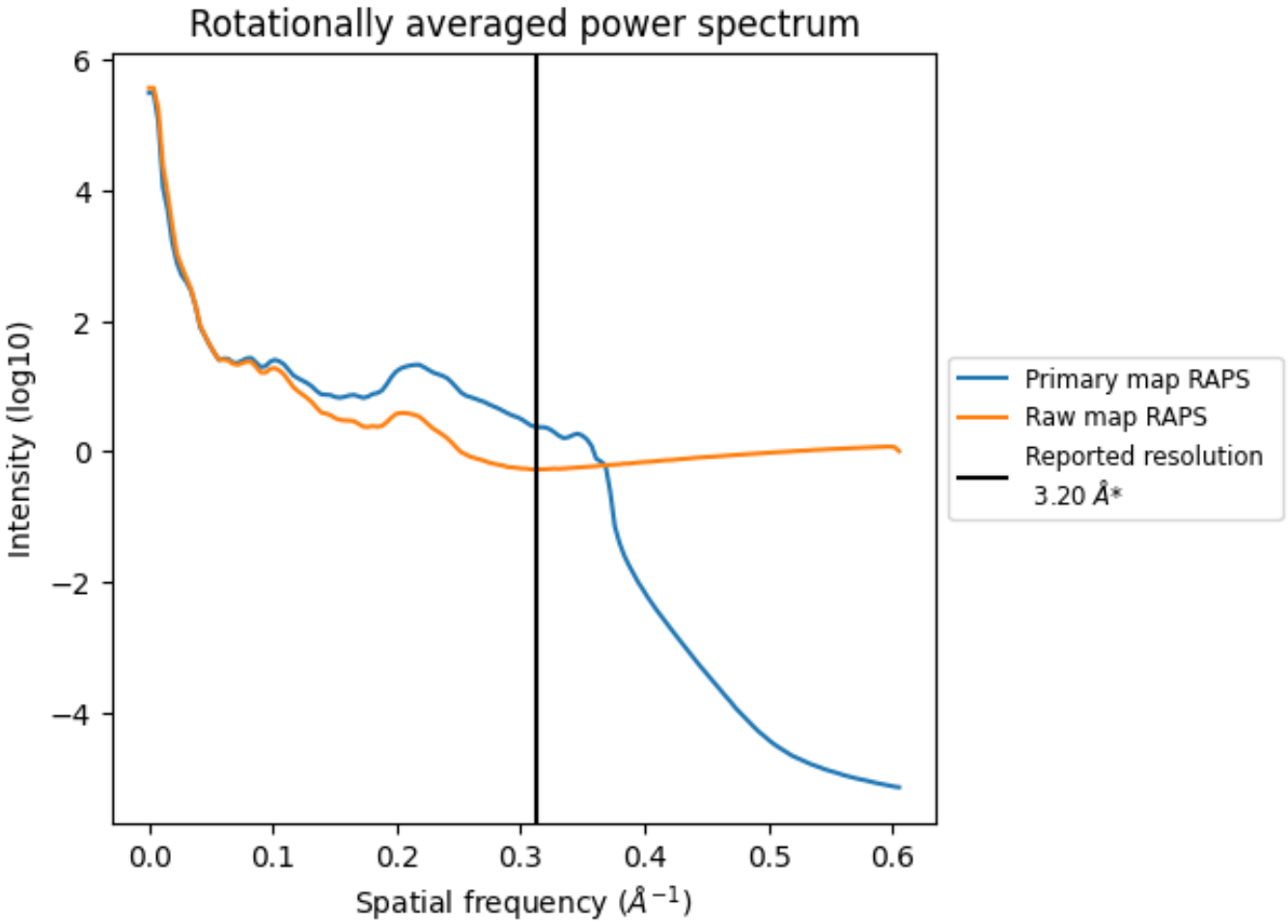
7.2 Volume estimate (i)



The volume at the recommended contour level is 64 nm^3; this corresponds to an approximate mass of 58 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)

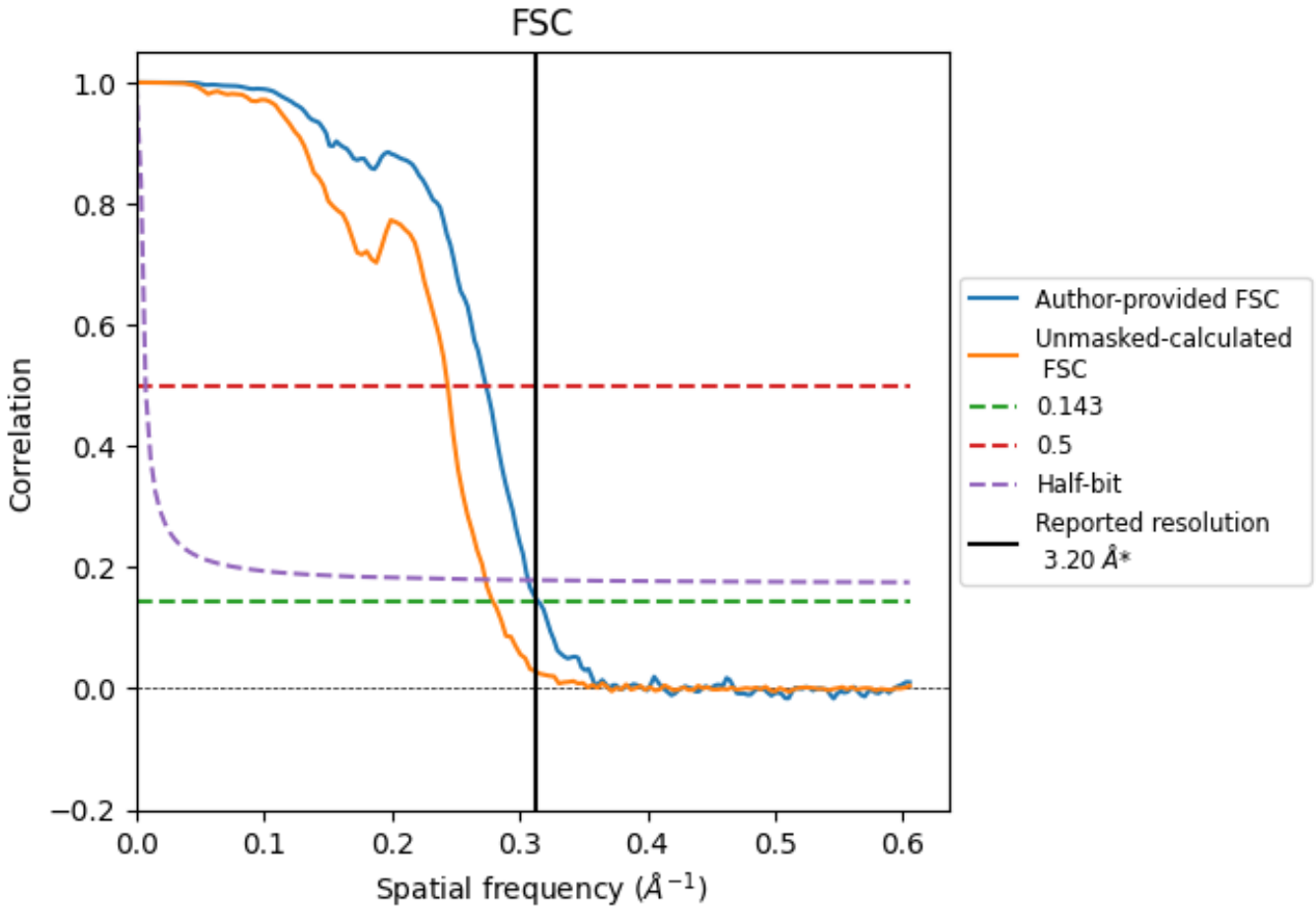


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

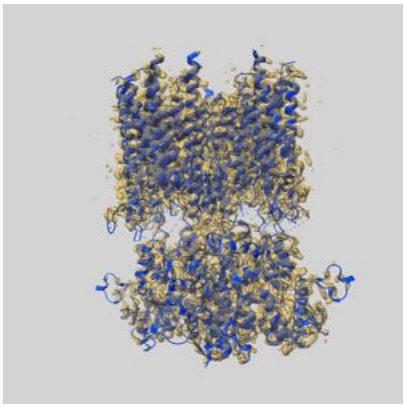
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.65	3.26
Unmasked-calculated*	3.58	4.10	3.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 3.2 by more than 10 %

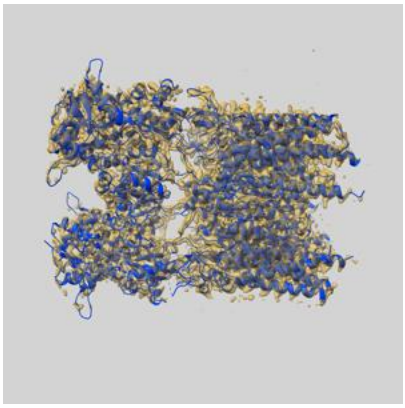
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16381 and PDB model 8C1R. Per-residue inclusion information can be found in section 3 on page 9.

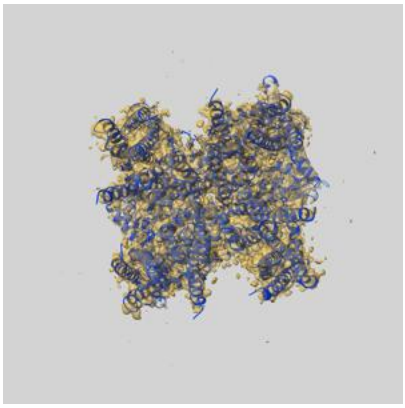
9.1 Map-model overlay



X



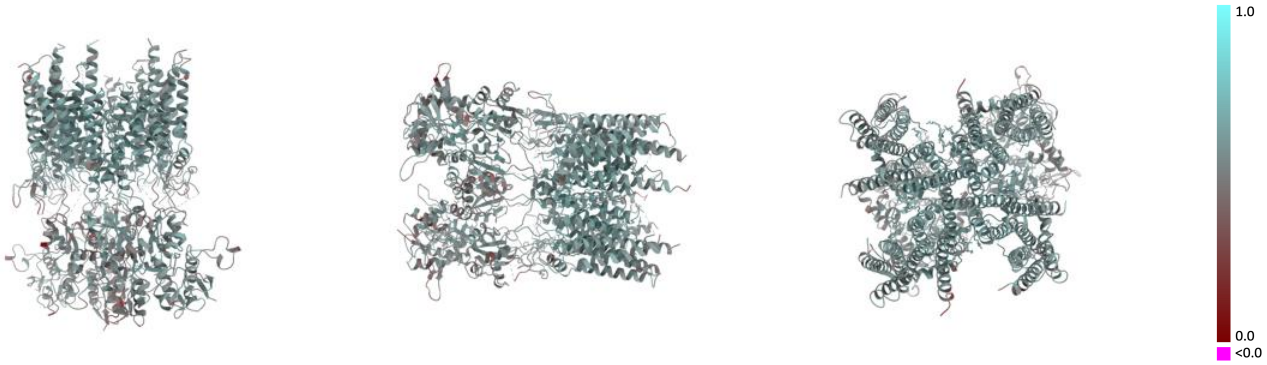
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



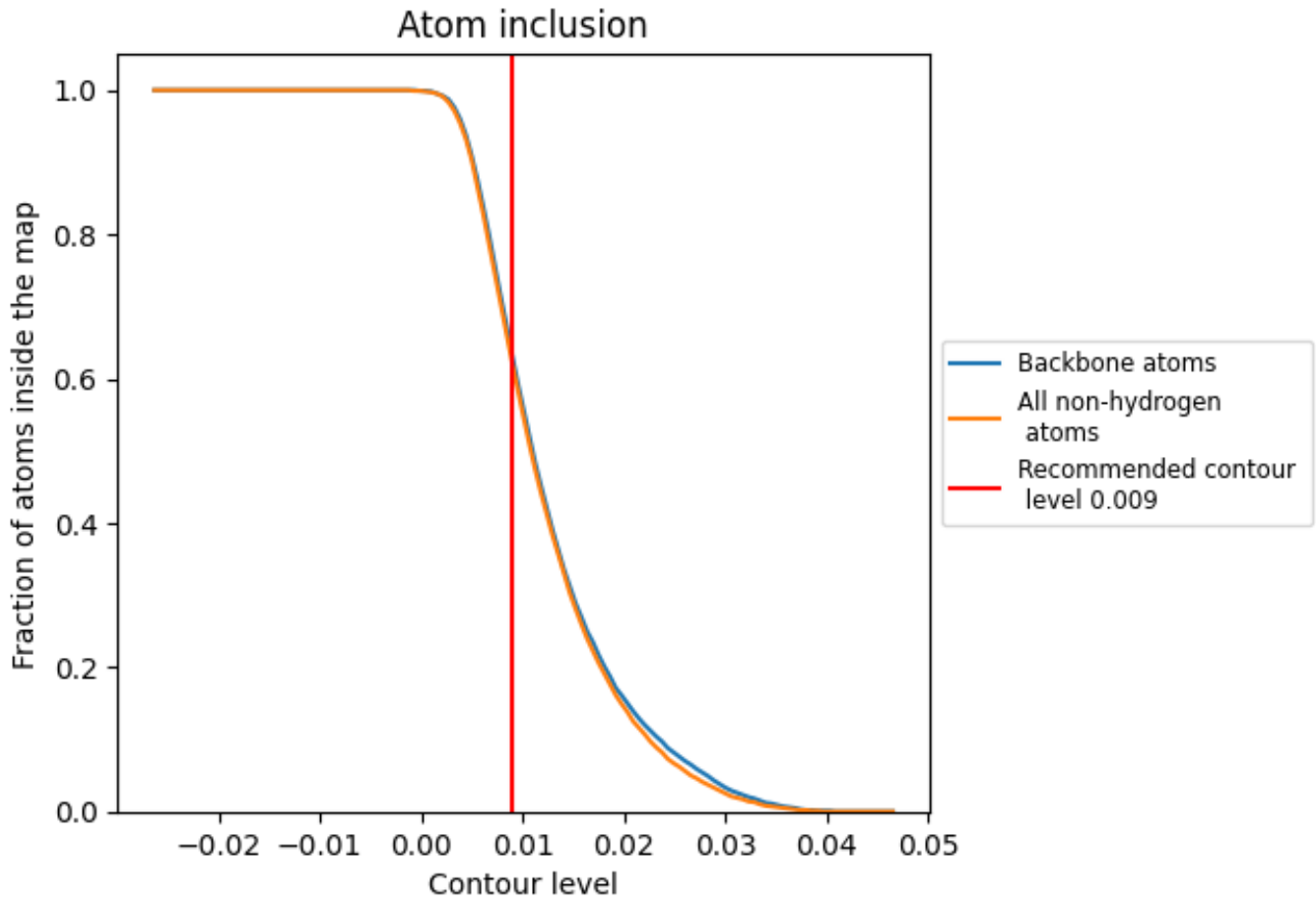
X Y Z

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

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 62% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.5500
A	0.6590	0.5610
B	0.5950	0.5400
C	0.6170	0.5490
D	0.6390	0.5520
E	0.6370	0.5490
F	0.5950	0.5500
G	0.6160	0.5500
H	0.6300	0.5480

