



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:59 PM UTC

PDB ID : 7OCE / pdb_00007oce
EMDB ID : EMD-12805
Title : Resting state GluA1/A2 AMPA receptor in complex with TARP gamma 8 and CNIH2 (LBD-TMD)
Authors : Zhang, D.; Watson, J.F.; Matthews, P.M.; Cais, O.; Greger, I.H.
Deposited on : 2021-04-26
Resolution : 3.10 Å (reported)
Based on initial models : 6PEQ, 6QKC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

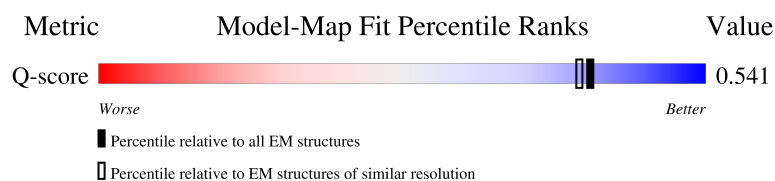
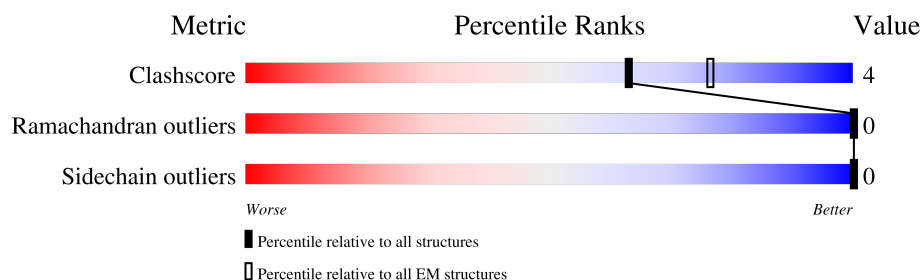
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	915	
1	C	915	
2	B	860	
2	D	860	

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Mol	Chain	Length	Quality of chain
3	E	188	36% 74% 10% 16%
3	G	188	35% 76% 9% 16%
4	I	422	42% 56%
4	J	422	42% 56%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18092 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	410	Total	C	N	O	S	0	0
			3013	1967	497	532	17		
1	C	410	Total	C	N	O	S	0	0
			3013	1967	497	532	17		

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	408	Total	C	N	O	S	0	0
			2975	1941	490	526	18		
2	D	408	Total	C	N	O	S	0	0
			2975	1941	490	526	18		

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 Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	158	Total	C	N	O	S	0	0
			1248	841	193	201	13		
3	E	158	Total	C	N	O	S	0	0
			1248	841	193	201	13		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	161	GLU	-	expression tag	UNP Q5BJU5
G	162	ASN	-	expression tag	UNP Q5BJU5
G	163	LEU	-	expression tag	UNP Q5BJU5
G	164	TYR	-	expression tag	UNP Q5BJU5
G	165	PHE	-	expression tag	UNP Q5BJU5
G	166	GLN	-	expression tag	UNP Q5BJU5
G	167	SER	-	expression tag	UNP Q5BJU5
G	168	GLY	-	expression tag	UNP Q5BJU5
G	169	GLY	-	expression tag	UNP Q5BJU5
G	170	SER	-	expression tag	UNP Q5BJU5
G	171	THR	-	expression tag	UNP Q5BJU5
G	172	GLU	-	expression tag	UNP Q5BJU5
G	173	THR	-	expression tag	UNP Q5BJU5
G	174	SER	-	expression tag	UNP Q5BJU5
G	175	GLN	-	expression tag	UNP Q5BJU5
G	176	VAL	-	expression tag	UNP Q5BJU5
G	177	ALA	-	expression tag	UNP Q5BJU5
G	178	PRO	-	expression tag	UNP Q5BJU5
G	179	ALA	-	expression tag	UNP Q5BJU5
G	180	TYR	-	expression tag	UNP Q5BJU5
G	181	PRO	-	expression tag	UNP Q5BJU5
G	182	TYR	-	expression tag	UNP Q5BJU5
G	183	ASP	-	expression tag	UNP Q5BJU5
G	184	VAL	-	expression tag	UNP Q5BJU5
G	185	PRO	-	expression tag	UNP Q5BJU5
G	186	ASP	-	expression tag	UNP Q5BJU5
G	187	TYR	-	expression tag	UNP Q5BJU5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	188	ALA	-	expression tag	UNP Q5BJU5
E	161	GLU	-	expression tag	UNP Q5BJU5
E	162	ASN	-	expression tag	UNP Q5BJU5
E	163	LEU	-	expression tag	UNP Q5BJU5
E	164	TYR	-	expression tag	UNP Q5BJU5
E	165	PHE	-	expression tag	UNP Q5BJU5
E	166	GLN	-	expression tag	UNP Q5BJU5
E	167	SER	-	expression tag	UNP Q5BJU5
E	168	GLY	-	expression tag	UNP Q5BJU5
E	169	GLY	-	expression tag	UNP Q5BJU5
E	170	SER	-	expression tag	UNP Q5BJU5
E	171	THR	-	expression tag	UNP Q5BJU5
E	172	GLU	-	expression tag	UNP Q5BJU5
E	173	THR	-	expression tag	UNP Q5BJU5
E	174	SER	-	expression tag	UNP Q5BJU5
E	175	GLN	-	expression tag	UNP Q5BJU5
E	176	VAL	-	expression tag	UNP Q5BJU5
E	177	ALA	-	expression tag	UNP Q5BJU5
E	178	PRO	-	expression tag	UNP Q5BJU5
E	179	ALA	-	expression tag	UNP Q5BJU5
E	180	TYR	-	expression tag	UNP Q5BJU5
E	181	PRO	-	expression tag	UNP Q5BJU5
E	182	TYR	-	expression tag	UNP Q5BJU5
E	183	ASP	-	expression tag	UNP Q5BJU5
E	184	VAL	-	expression tag	UNP Q5BJU5
E	185	PRO	-	expression tag	UNP Q5BJU5
E	186	ASP	-	expression tag	UNP Q5BJU5
E	187	TYR	-	expression tag	UNP Q5BJU5
E	188	ALA	-	expression tag	UNP Q5BJU5

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	185	Total	C	N	O	S	0	0
			1284	843	212	222	7		
4	J	185	Total	C	N	O	S	0	0
			1284	843	212	222	7		

There are 12 discrepancies between the modelled and reference sequences:

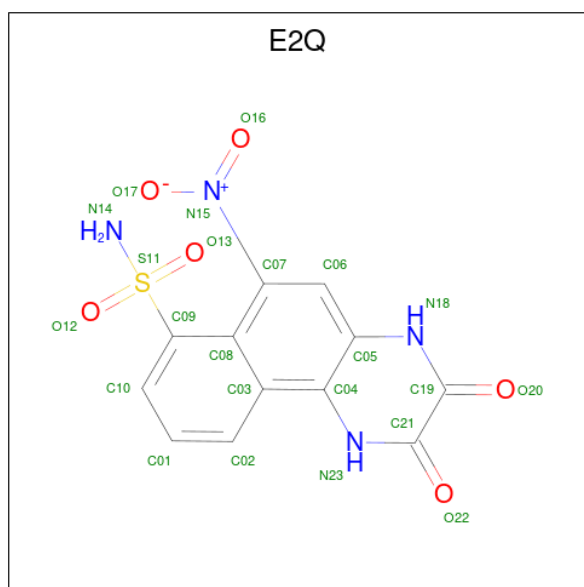
Chain	Residue	Modelled	Actual	Comment	Reference
I	418	LEU	-	expression tag	UNP Q8VHW5

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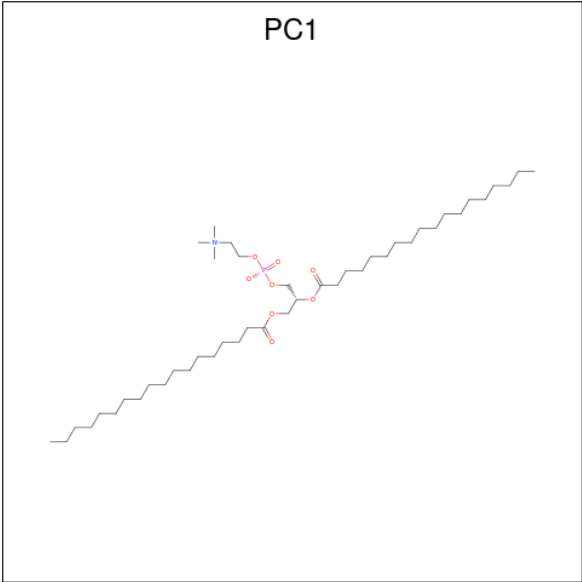
Chain	Residue	Modelled	Actual	Comment	Reference
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	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 5 is 6-nitro-2,3-bis(oxidanylidene)-1,4-dihydrobenzo[f]quinoxaline-7-sulfonamide (CCD ID: E2Q) (formula: C₁₂H₈N₄O₆S).



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

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			20	18	2	
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			20	18	2	
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			25	21	4	
6	A	1	Total	C	O	0
			18	16	2	
6	B	1	Total	C	O	0
			20	18	2	
6	B	1	Total	C	O	0
			16	14	2	
6	B	1	Total	C	O	0
			20	18	2	
6	B	1	Total	C	O	0
			20	18	2	
6	B	1	Total	C	O	0
			20	18	2	
6	B	1	Total	C	O	0
			18	16	2	
6	B	1	Total	C	O	0
			25	21	4	

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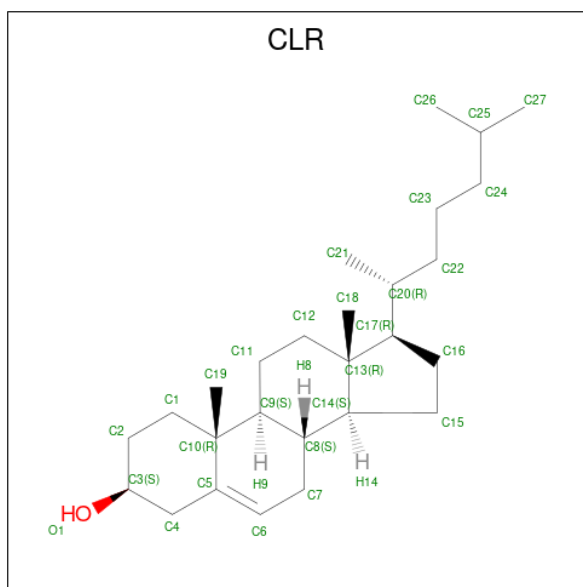
Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			20	18	2	
6	G	1	Total	C	O	0
			20	18	2	
6	G	1	Total	C	O	0
			18	16	2	
6	G	1	Total	C	O	0
			20	18	2	
6	I	1	Total	C	O	0
			18	16	2	
6	I	1	Total	C	O	0
			20	18	2	
6	I	1	Total	C	O	0
			20	18	2	
6	I	1	Total	C	O	0
			20	18	2	
6	I	1	Total	C	O	0
			18	16	2	
6	D	1	Total	C	O	0
			16	14	2	
6	D	1	Total	C	O	0
			20	18	2	
6	D	1	Total	C	O	0
			20	18	2	
6	D	1	Total	C	O	0
			20	18	2	
6	D	1	Total	C	O	0
			18	16	2	
6	D	1	Total	C	O	0
			25	21	4	
6	D	1	Total	C	O	0
			20	18	2	
6	D	1	Total	C	O	0
			20	18	2	
6	J	1	Total	C	O	0
			20	18	2	
6	J	1	Total	C	O	0
			20	18	2	
6	J	1	Total	C	O	0
			20	18	2	

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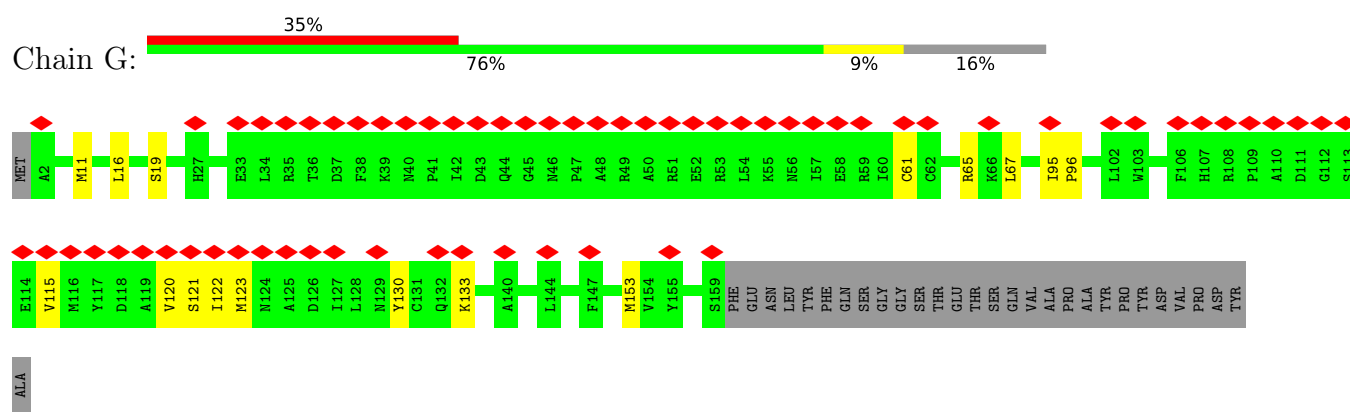
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Mol	Chain	Residues	Atoms			AltConf
6	J	1	Total	C	O	0
			18	16	2	
6	J	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			20	18	2	
6	C	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			20	18	2	
6	C	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			25	21	4	
6	E	1	Total	C	O	0
			18	16	2	
6	E	1	Total	C	O	0
			20	18	2	
6	E	1	Total	C	O	0
			20	18	2	

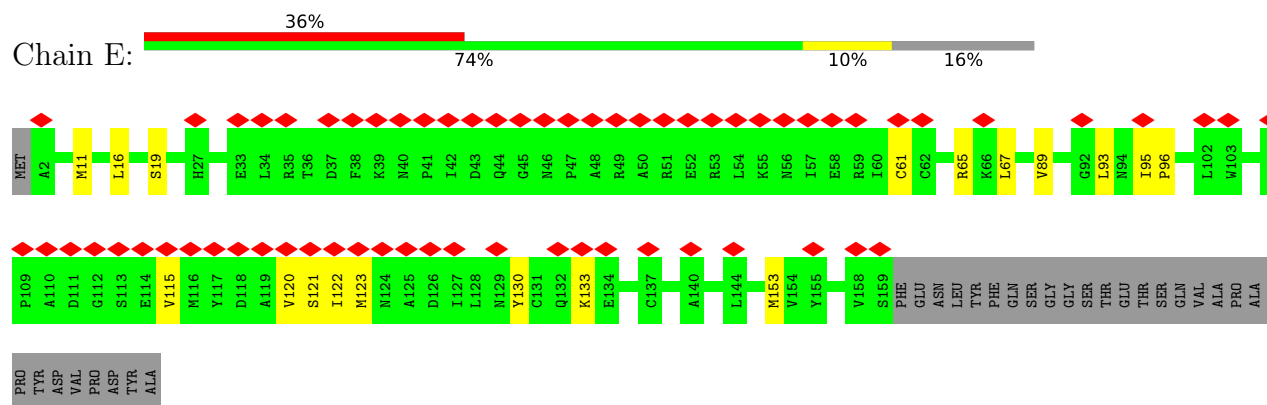
- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



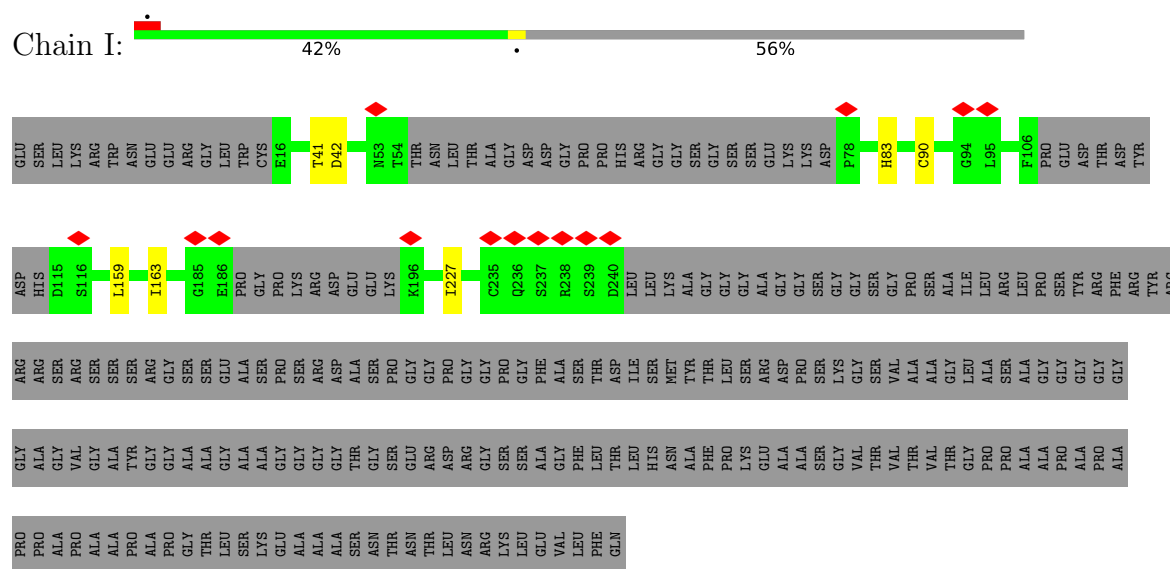
Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total	C	O	0
			28	27	1	
7	E	1	Total	C	O	0
			28	27	1	



- Molecule 3: Protein cornichon homolog 2

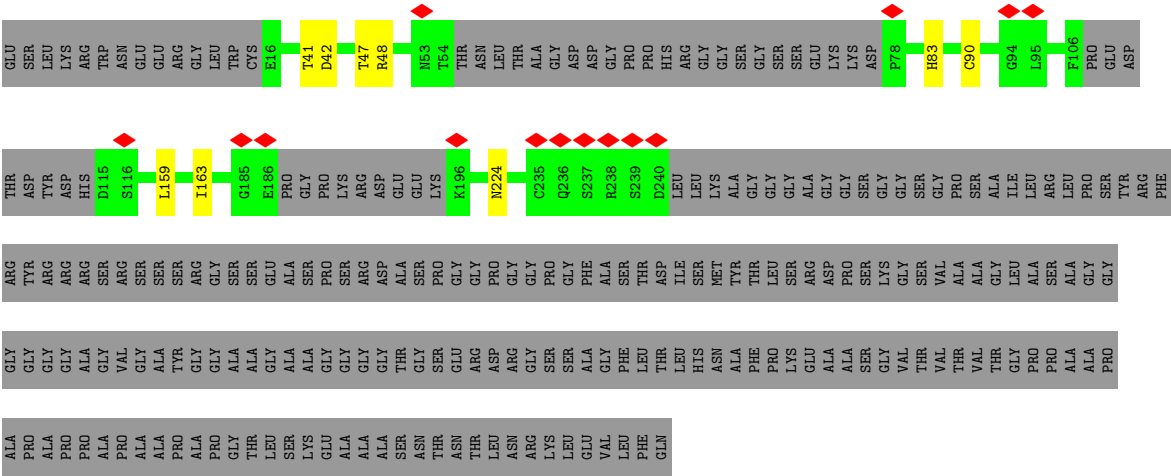


- Molecule 4: Voltage-dependent calcium channel gamma-8 subunit



- Molecule 4: Voltage-dependent calcium channel gamma-8 subunit





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, CLR, 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	0.27	0/3081	0.34	0/4192
1	C	0.27	0/3081	0.34	0/4192
2	B	0.26	0/3043	0.33	0/4141
2	D	0.26	0/3043	0.33	0/4141
3	E	0.15	0/1289	0.29	0/1760
3	G	0.15	0/1289	0.29	0/1760
4	I	0.25	0/1305	0.32	0/1782
4	J	0.25	0/1305	0.32	0/1782
All	All	0.25	0/17436	0.33	0/23750

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3013	0	2868	29	0
1	C	3013	0	2868	31	0
2	B	2975	0	2817	31	0
2	D	2975	0	2817	33	0
3	E	1248	0	1186	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1248	0	1186	12	0
4	I	1284	0	1219	4	0
4	J	1284	0	1219	5	0
5	A	23	0	0	0	0
5	B	23	0	0	1	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
6	A	119	0	194	0	0
6	B	179	0	302	1	0
6	C	119	0	194	0	0
6	D	179	0	302	1	0
6	E	58	0	98	0	0
6	G	58	0	98	0	0
6	I	96	0	161	0	0
6	J	96	0	161	1	0
7	E	28	0	46	3	0
7	G	28	0	46	3	0
All	All	18092	0	17782	152	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 4.

All (152) 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)
2:D:716:LYS:N	2:D:772:GLU:OE2	2.10	0.84
2:B:716:LYS:N	2:B:772:GLU:OE2	2.10	0.83
1:A:624:ARG:NH2	2:B:626:VAL:O	2.12	0.83
2:B:728:ASP:OD2	2:B:729:SER:N	2.14	0.81
2:D:626:VAL:O	1:C:624:ARG:NH2	2.13	0.81
2:D:728:ASP:OD2	2:D:729:SER:N	2.14	0.81
2:B:635:SER:OG	2:B:638:ASP:OD1	2.12	0.66
2:D:635:SER:OG	2:D:638:ASP:OD1	2.12	0.66
2:D:398:THR:OG1	2:D:466:GLU:OE2	2.08	0.65
1:C:711:ARG:NH2	1:C:766:LYS:O	2.34	0.61
1:A:711:ARG:NH2	1:A:766:LYS:O	2.34	0.60
3:E:16:LEU:O	3:E:19:SER:OG	2.19	0.60
7:G:3104:CLR:O1	7:G:3104:CLR:H192	2.02	0.60
1:C:458:GLY:O	1:C:461:GLY:N	2.34	0.59
3:G:16:LEU:O	3:G:19:SER:OG	2.19	0.59
7:E:3104:CLR:H192	7:E:3104:CLR:O1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:GLY:O	1:A:461:GLY:N	2.34	0.59
2:B:814:PHE:HB2	1:C:542:PHE:HE2	1.70	0.57
2:B:398:THR:OG1	2:B:466:GLU:OE2	2.15	0.57
1:A:542:PHE:HE2	2:D:814:PHE:HB2	1.70	0.55
2:D:480:THR:HG1	2:D:732:TYR:HE1	1.55	0.55
3:E:65:ARG:HE	3:E:115:VAL:HB	1.72	0.55
1:C:568:GLY:O	1:C:572:SER:OG	2.19	0.55
3:G:65:ARG:HE	3:G:115:VAL:HB	1.72	0.53
2:D:433:ALA:O	2:D:437:GLY:N	2.34	0.53
1:C:462:GLU:O	1:C:468:ALA:N	2.42	0.53
1:A:462:GLU:O	1:A:468:ALA:N	2.42	0.52
1:A:626:VAL:HG13	1:A:626:VAL:O	2.10	0.52
2:B:433:ALA:O	2:B:437:GLY:N	2.34	0.51
1:C:626:VAL:O	1:C:626:VAL:HG13	2.10	0.51
1:C:499:MET:HE1	1:C:708:ILE:HG21	1.93	0.50
1:A:679:VAL:HG12	1:A:680:ARG:N	2.27	0.50
1:A:568:GLY:O	1:A:572:SER:OG	2.19	0.50
1:A:499:MET:HE1	1:A:708:ILE:HG21	1.93	0.50
2:D:572:GLY:O	2:D:576:SER:OG	2.24	0.49
1:C:747:LEU:O	1:C:751:GLU:HG2	2.12	0.49
2:D:467:LEU:HD11	2:D:475:ALA:HB2	1.95	0.49
3:E:133:LYS:CB	7:E:3104:CLR:H71	2.42	0.49
3:G:61:CYS:SG	3:G:65:ARG:NH2	2.86	0.49
4:I:83:HIS:CE1	4:I:90:CYS:HB2	2.47	0.49
1:C:679:VAL:HG12	1:C:680:ARG:N	2.27	0.49
3:G:133:LYS:CB	7:G:3104:CLR:H71	2.42	0.49
3:E:61:CYS:SG	3:E:65:ARG:NH2	2.86	0.49
1:A:747:LEU:O	1:A:751:GLU:HG2	2.12	0.49
4:J:83:HIS:CE1	4:J:90:CYS:HB2	2.47	0.49
1:A:674:GLU:CB	1:A:677:VAL:HG13	2.43	0.49
1:C:674:GLU:CB	1:C:677:VAL:HG13	2.43	0.48
2:B:467:LEU:HD11	2:B:475:ALA:HB2	1.95	0.48
1:A:462:GLU:OE1	1:A:462:GLU:N	2.47	0.47
2:D:400:ILE:O	2:D:406:VAL:HB	2.15	0.47
1:C:535:VAL:O	1:C:539:VAL:HG22	2.15	0.47
1:A:535:VAL:O	1:A:539:VAL:HG22	2.15	0.47
1:A:714:CYS:HB2	1:A:769:CYS:HB2	1.86	0.47
2:D:443:THR:O	2:D:444:ILE:HD13	2.14	0.47
4:J:224:ASN:ND2	6:J:2502:PC1:O22	2.48	0.47
2:B:443:THR:O	2:B:444:ILE:HD13	2.14	0.46
2:B:467:LEU:HD11	2:B:475:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:809:VAL:HG11	1:C:592:LEU:HD23	1.97	0.46
2:B:400:ILE:O	2:B:406:VAL:HB	2.15	0.46
2:D:467:LEU:HD11	2:D:475:ALA:CB	2.45	0.46
3:E:122:ILE:HG22	3:E:123:MET:N	2.30	0.46
1:A:515:ASP:N	1:A:516:PRO:CD	2.79	0.46
2:B:683:VAL:HG12	2:B:685:THR:H	1.81	0.46
1:C:515:ASP:N	1:C:516:PRO:CD	2.79	0.46
1:C:629:ILE:O	1:C:719:VAL:HG21	2.16	0.46
2:B:460:TRP:CE3	2:B:464:VAL:HG11	2.51	0.46
1:A:629:ILE:O	1:A:719:VAL:HG21	2.16	0.46
3:G:122:ILE:HG22	3:G:123:MET:N	2.30	0.45
2:D:519:ASP:N	2:D:520:PRO:CD	2.79	0.45
1:C:462:GLU:N	1:C:462:GLU:OE1	2.47	0.45
2:B:714:GLN:NE2	2:B:773:CYS:O	2.50	0.45
2:D:460:TRP:CE3	2:D:464:VAL:HG11	2.51	0.45
1:C:492:MET:SD	1:C:703:THR:HG21	2.56	0.45
3:E:95:ILE:N	3:E:96:PRO:HD2	2.32	0.45
1:A:592:LEU:HD23	2:D:809:VAL:HG11	1.98	0.45
2:B:519:ASP:N	2:B:520:PRO:CD	2.79	0.45
2:D:683:VAL:HG12	2:D:685:THR:H	1.80	0.45
2:D:714:GLN:NE2	2:D:773:CYS:O	2.50	0.45
1:C:674:GLU:N	1:C:675:PRO:CA	2.80	0.45
1:A:492:MET:SD	1:A:703:THR:HG21	2.56	0.44
3:G:95:ILE:N	3:G:96:PRO:HD2	2.32	0.44
2:B:464:VAL:O	2:B:468:VAL:HG23	2.18	0.44
2:D:792:VAL:O	2:D:795:VAL:HG22	2.17	0.44
2:B:792:VAL:O	2:B:795:VAL:HG22	2.17	0.44
1:C:494:LEU:HD13	1:C:728:TYR:CZ	2.53	0.44
2:D:464:VAL:O	2:D:468:VAL:HG23	2.18	0.44
1:A:674:GLU:N	1:A:675:PRO:CA	2.80	0.44
4:I:41:THR:HG22	4:I:42:ASP:N	2.32	0.44
3:G:67:LEU:HD23	3:G:67:LEU:O	2.18	0.44
3:E:123:MET:HA	3:E:123:MET:HE3	2.00	0.43
2:D:799:LEU:O	2:D:803:LEU:HG	2.18	0.43
4:J:41:THR:HG22	4:J:42:ASP:N	2.32	0.43
3:E:67:LEU:HD23	3:E:67:LEU:O	2.18	0.43
3:G:123:MET:HE3	3:G:123:MET:HA	2.00	0.43
1:C:541:ARG:NH1	1:C:565:ASN:O	2.44	0.43
2:D:696:SER:OG	2:D:697:LYS:N	2.50	0.43
2:D:702:TYR:CE2	2:D:704:LEU:HB3	2.53	0.43
1:A:494:LEU:HD13	1:A:728:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LEU:O	1:A:803:MET:HG3	2.19	0.43
2:B:799:LEU:O	2:B:803:LEU:HG	2.19	0.43
2:D:650:LEU:HD23	2:D:651:ASP:N	2.34	0.43
2:B:650:LEU:HD23	2:B:651:ASP:N	2.34	0.43
2:B:702:TYR:CE2	2:B:704:LEU:HB3	2.53	0.43
3:G:130:TYR:CE2	7:G:3104:CLR:H152	2.54	0.43
2:D:673:TYR:C	2:D:673:TYR:CD1	2.97	0.43
3:E:120:VAL:HG23	3:E:121:SER:N	2.34	0.43
2:B:696:SER:OG	2:B:697:LYS:N	2.50	0.43
1:C:714:CYS:HB2	1:C:769:CYS:HB2	1.86	0.42
1:A:674:GLU:N	1:A:675:PRO:HA	2.35	0.42
4:I:159:LEU:O	4:I:163:ILE:HG12	2.20	0.42
3:E:130:TYR:CE2	7:E:3104:CLR:H152	2.54	0.42
1:A:542:PHE:CG	1:A:543:SER:N	2.87	0.42
1:C:674:GLU:N	1:C:675:PRO:HA	2.35	0.42
1:C:799:LEU:O	1:C:803:MET:HG3	2.19	0.42
3:E:11:MET:HG3	3:E:153:MET:HG3	2.02	0.42
1:A:676:SER:O	1:A:688:ARG:NH1	2.47	0.42
2:B:673:TYR:C	2:B:673:TYR:CD1	2.97	0.42
3:G:11:MET:HG3	3:G:153:MET:HG3	2.02	0.42
2:B:445:VAL:HG13	2:B:446:GLY:N	2.35	0.42
1:C:542:PHE:CG	1:C:543:SER:N	2.87	0.42
1:A:397:LEU:HD21	1:A:440:ILE:CD1	2.50	0.42
3:G:120:VAL:HG23	3:G:121:SER:N	2.34	0.42
2:D:609:THR:O	2:D:613:ILE:HG12	2.20	0.42
1:C:538:LEU:O	1:C:542:PHE:HD1	2.03	0.42
1:C:397:LEU:HD21	1:C:440:ILE:CD1	2.50	0.41
1:A:541:ARG:NH1	1:A:565:ASN:O	2.44	0.41
2:B:609:THR:O	2:B:613:ILE:HG12	2.20	0.41
2:D:398:THR:HG22	2:D:399:THR:N	2.36	0.41
1:A:538:LEU:O	1:A:542:PHE:HD1	2.03	0.41
4:J:159:LEU:O	4:J:163:ILE:HG12	2.20	0.41
3:E:89:VAL:O	3:E:93:LEU:HD13	2.21	0.41
2:B:683:VAL:HG12	2:B:684:ARG:N	2.35	0.41
2:B:685:THR:HG22	2:B:686:THR:N	2.35	0.41
2:D:445:VAL:HG13	2:D:446:GLY:N	2.35	0.41
2:D:683:VAL:HG12	2:D:684:ARG:N	2.36	0.41
1:C:499:MET:HE2	1:C:716:THR:HG21	2.03	0.41
2:B:426:VAL:HG23	2:B:427:ASP:N	2.36	0.41
2:D:685:THR:HG22	2:D:686:THR:N	2.35	0.41
1:C:759:LYS:O	1:C:763:TRP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:227:ILE:HD11	1:C:541:ARG:O	2.21	0.41
1:A:759:LYS:O	1:A:763:TRP:HB2	2.21	0.40
3:G:122:ILE:CG2	3:G:123:MET:N	2.84	0.40
2:D:611:ILE:HG21	1:C:791:VAL:HG21	2.03	0.40
3:E:122:ILE:CG2	3:E:123:MET:N	2.84	0.40
2:D:426:VAL:HG23	2:D:427:ASP:N	2.36	0.40
2:D:574:PHE:CD2	6:D:908:PC1:H3I1	2.56	0.40
2:B:549:TYR:HE1	6:B:2901:PC1:H221	1.87	0.40
1:A:791:VAL:HG21	2:B:611:ILE:HG21	2.02	0.40
5:B:2902:E2Q:N15	5:B:2902:E2Q:S11	2.95	0.40
1:C:676:SER:O	1:C:688:ARG:NH1	2.47	0.40
2:B:482:THR:HG22	2:B:483:LEU:N	2.36	0.40
4:J:47:THR:OG1	4:J:48:ARG:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	404/915 (44%)	392 (97%)	12 (3%)	0	100	100
1	C	404/915 (44%)	392 (97%)	12 (3%)	0	100	100
2	B	402/860 (47%)	381 (95%)	21 (5%)	0	100	100
2	D	402/860 (47%)	381 (95%)	21 (5%)	0	100	100
3	E	156/188 (83%)	153 (98%)	3 (2%)	0	100	100
3	G	156/188 (83%)	153 (98%)	3 (2%)	0	100	100
4	I	177/422 (42%)	170 (96%)	7 (4%)	0	100	100
4	J	177/422 (42%)	170 (96%)	7 (4%)	0	100	100
All	All	2278/4770 (48%)	2192 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	283/778 (36%)	283 (100%)	0	100	100
1	C	283/778 (36%)	283 (100%)	0	100	100
2	B	278/737 (38%)	278 (100%)	0	100	100
2	D	278/737 (38%)	278 (100%)	0	100	100
3	E	123/166 (74%)	123 (100%)	0	100	100
3	G	123/166 (74%)	123 (100%)	0	100	100
4	I	114/309 (37%)	114 (100%)	0	100	100
4	J	114/309 (37%)	114 (100%)	0	100	100
All	All	1596/3980 (40%)	1596 (100%)	0	100	100

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

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	710	GLN
2	B	714	GLN
2	D	714	GLN
1	C	710	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

52 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
6	PC1	B	2909	-	24,24,53	0.80	2 (8%)	25,25,61	1.05	1 (4%)
6	PC1	B	2904	-	19,19,53	0.79	1 (5%)	19,19,61	1.05	1 (5%)
6	PC1	D	903	-	19,19,53	0.79	1 (5%)	19,19,61	1.05	1 (5%)
6	PC1	I	3002	-	19,19,53	0.78	1 (5%)	19,19,61	1.10	1 (5%)
6	PC1	C	2701	-	17,17,53	0.83	1 (5%)	17,17,61	0.96	0
6	PC1	D	902	-	15,15,53	0.85	1 (6%)	15,15,61	1.09	0
6	PC1	E	3103	-	19,19,53	0.79	1 (5%)	19,19,61	1.07	0
6	PC1	D	908	-	24,24,53	0.79	2 (8%)	25,25,61	1.05	1 (4%)
6	PC1	C	2707	-	24,24,53	0.81	2 (8%)	25,25,61	1.04	1 (4%)
6	PC1	A	902	-	19,19,53	0.77	1 (5%)	19,19,61	1.03	0
6	PC1	A	904	-	19,19,53	0.78	1 (5%)	19,19,61	1.05	0
5	E2Q	A	901	-	25,25,25	1.77	6 (24%)	32,39,39	2.20	12 (37%)
6	PC1	G	3102	-	17,17,53	0.84	1 (5%)	17,17,61	1.02	0
6	PC1	I	3004	-	19,19,53	0.79	1 (5%)	19,19,61	1.06	0
6	PC1	J	2504	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
6	PC1	C	2705	-	19,19,53	0.78	1 (5%)	19,19,61	1.05	0
6	PC1	E	3101	-	17,17,53	0.85	1 (5%)	17,17,61	1.03	0
7	CLR	G	3104	-	31,31,31	0.31	0	48,48,48	0.63	1 (2%)
6	PC1	J	2503	-	19,19,53	0.79	1 (5%)	19,19,61	1.06	0
6	PC1	D	904	-	19,19,53	0.79	1 (5%)	19,19,61	1.02	0
6	PC1	B	2903	-	15,15,53	0.85	1 (6%)	15,15,61	1.09	0
6	PC1	B	2901	-	19,19,53	0.78	1 (5%)	19,19,61	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PC1	I	3005	-	17,17,53	0.84	1 (5%)	17,17,61	1.07	0
6	PC1	E	3102	-	19,19,53	0.79	1 (5%)	19,19,61	1.04	0
6	PC1	A	907	-	17,17,53	0.84	1 (5%)	17,17,61	0.97	0
6	PC1	A	906	-	24,24,53	0.82	2 (8%)	25,25,61	1.04	1 (4%)
6	PC1	G	3103	-	19,19,53	0.79	1 (5%)	19,19,61	1.07	0
6	PC1	I	3001	-	17,17,53	0.82	1 (5%)	17,17,61	1.11	0
6	PC1	J	2505	-	17,17,53	0.82	1 (5%)	17,17,61	1.11	0
6	PC1	G	3101	-	19,19,53	0.79	1 (5%)	19,19,61	1.04	0
6	PC1	I	3003	-	19,19,53	0.78	1 (5%)	19,19,61	1.02	0
6	PC1	D	907	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
6	PC1	D	909	-	19,19,53	0.78	1 (5%)	19,19,61	1.07	1 (5%)
6	PC1	D	910	-	19,19,53	0.78	1 (5%)	19,19,61	0.93	0
6	PC1	C	2706	-	17,17,53	0.82	1 (5%)	17,17,61	1.05	0
5	E2Q	C	2702	-	25,25,25	1.77	6 (24%)	32,39,39	2.19	12 (37%)
6	PC1	D	905	-	19,19,53	0.77	1 (5%)	19,19,61	1.05	0
6	PC1	C	2704	-	17,17,53	0.81	1 (5%)	17,17,61	1.10	0
5	E2Q	B	2902	-	25,25,25	1.77	6 (24%)	32,39,39	2.18	11 (34%)
6	PC1	C	2703	-	19,19,53	0.77	1 (5%)	19,19,61	1.04	0
6	PC1	J	2502	-	19,19,53	0.78	1 (5%)	19,19,61	1.02	0
6	PC1	A	905	-	17,17,53	0.82	1 (5%)	17,17,61	1.05	0
5	E2Q	D	901	-	25,25,25	1.79	6 (24%)	32,39,39	2.18	11 (34%)
6	PC1	B	2907	-	19,19,53	0.79	1 (5%)	19,19,61	0.96	0
6	PC1	B	2906	-	19,19,53	0.76	1 (5%)	19,19,61	1.05	0
6	PC1	B	2908	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
6	PC1	B	2905	-	19,19,53	0.80	1 (5%)	19,19,61	1.02	0
6	PC1	J	2501	-	19,19,53	0.78	1 (5%)	19,19,61	1.10	1 (5%)
6	PC1	D	906	-	19,19,53	0.80	1 (5%)	19,19,61	0.96	0
7	CLR	E	3104	-	31,31,31	0.31	0	48,48,48	0.63	1 (2%)
6	PC1	A	903	-	17,17,53	0.82	1 (5%)	17,17,61	1.10	0
6	PC1	B	2910	-	19,19,53	0.77	1 (5%)	19,19,61	0.93	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
6	PC1	B	2909	-	-	10/24/24/57	-
6	PC1	B	2904	-	-	8/17/17/57	-
6	PC1	D	903	-	-	8/17/17/57	-
6	PC1	I	3002	-	-	2/17/17/57	-
6	PC1	C	2701	-	-	11/15/15/57	-
6	PC1	D	902	-	-	5/13/13/57	-
6	PC1	E	3103	-	-	6/17/17/57	-
6	PC1	D	908	-	-	10/24/24/57	-
6	PC1	C	2707	-	-	12/24/24/57	-
6	PC1	A	902	-	-	6/17/17/57	-
6	PC1	A	904	-	-	5/17/17/57	-
5	E2Q	A	901	-	-	3/8/10/10	0/3/3/3
6	PC1	G	3102	-	-	2/15/15/57	-
6	PC1	I	3004	-	-	4/17/17/57	-
6	PC1	J	2504	-	-	7/15/15/57	-
6	PC1	C	2705	-	-	5/17/17/57	-
6	PC1	E	3101	-	-	2/15/15/57	-
7	CLR	G	3104	-	-	4/10/68/68	0/4/4/4
6	PC1	J	2503	-	-	4/17/17/57	-
6	PC1	D	904	-	-	3/17/17/57	-
6	PC1	B	2903	-	-	5/13/13/57	-
6	PC1	B	2901	-	-	6/17/17/57	-
6	PC1	I	3005	-	-	7/15/15/57	-
6	PC1	E	3102	-	-	6/17/17/57	-
6	PC1	A	907	-	-	11/15/15/57	-
6	PC1	A	906	-	-	12/24/24/57	-
6	PC1	G	3103	-	-	6/17/17/57	-
6	PC1	I	3001	-	-	5/15/15/57	-
6	PC1	J	2505	-	-	5/15/15/57	-
6	PC1	G	3101	-	-	6/17/17/57	-
6	PC1	I	3003	-	-	6/17/17/57	-
6	PC1	D	907	-	-	5/15/15/57	-
6	PC1	D	909	-	-	6/17/17/57	-
6	PC1	D	910	-	-	9/17/17/57	-
6	PC1	C	2706	-	-	3/15/15/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	E2Q	C	2702	-	-	3/8/10/10	0/3/3/3
6	PC1	D	905	-	-	4/17/17/57	-
6	PC1	C	2704	-	-	8/15/15/57	-
5	E2Q	B	2902	-	-	3/8/10/10	0/3/3/3
6	PC1	C	2703	-	-	6/17/17/57	-
6	PC1	J	2502	-	-	6/17/17/57	-
6	PC1	A	905	-	-	3/15/15/57	-
5	E2Q	D	901	-	-	3/8/10/10	0/3/3/3
6	PC1	B	2907	-	-	5/17/17/57	-
6	PC1	B	2906	-	-	4/17/17/57	-
6	PC1	B	2908	-	-	5/15/15/57	-
6	PC1	B	2905	-	-	3/17/17/57	-
6	PC1	J	2501	-	-	2/17/17/57	-
6	PC1	D	906	-	-	6/17/17/57	-
7	CLR	E	3104	-	-	4/10/68/68	0/4/4/4
6	PC1	A	903	-	-	8/15/15/57	-
6	PC1	B	2910	-	-	9/17/17/57	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	901	E2Q	C09-S11	-5.75	1.69	1.77
5	B	2902	E2Q	C09-S11	-5.72	1.69	1.77
5	A	901	E2Q	C09-S11	-5.72	1.69	1.77
5	C	2702	E2Q	C09-S11	-5.72	1.69	1.77
5	D	901	E2Q	C21-N23	3.21	1.40	1.35
5	A	901	E2Q	C21-N23	3.21	1.40	1.35
5	C	2702	E2Q	C21-N23	3.21	1.40	1.35
5	B	2902	E2Q	C21-N23	3.17	1.40	1.35
6	D	906	PC1	O21-C21	2.90	1.40	1.30
6	I	3004	PC1	O21-C21	2.90	1.40	1.30
6	J	2503	PC1	O21-C21	2.90	1.40	1.30
6	B	2908	PC1	O21-C21	2.90	1.40	1.30
6	D	904	PC1	O21-C21	2.90	1.40	1.30
6	B	2905	PC1	O21-C21	2.90	1.40	1.30
6	E	3102	PC1	O21-C21	2.90	1.40	1.30
6	E	3101	PC1	O21-C21	2.90	1.40	1.30
6	I	3005	PC1	O21-C21	2.89	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	2504	PC1	O21-C21	2.89	1.40	1.30
6	B	2904	PC1	O21-C21	2.89	1.40	1.30
6	D	903	PC1	O21-C21	2.89	1.40	1.30
6	G	3102	PC1	O21-C21	2.89	1.40	1.30
6	D	907	PC1	O21-C21	2.89	1.40	1.30
6	A	907	PC1	O21-C21	2.88	1.40	1.30
6	G	3101	PC1	O21-C21	2.88	1.40	1.30
6	A	903	PC1	O21-C21	2.88	1.40	1.30
6	C	2704	PC1	O21-C21	2.88	1.40	1.30
6	I	3003	PC1	O21-C21	2.88	1.40	1.30
6	B	2901	PC1	O21-C21	2.87	1.40	1.30
6	D	909	PC1	O21-C21	2.87	1.40	1.30
6	E	3103	PC1	O21-C21	2.87	1.40	1.30
6	B	2903	PC1	O21-C21	2.87	1.40	1.30
6	C	2705	PC1	O21-C21	2.87	1.40	1.30
5	A	901	E2Q	C19-N18	2.87	1.39	1.35
5	C	2702	E2Q	C19-N18	2.87	1.39	1.35
6	J	2501	PC1	O21-C21	2.87	1.40	1.30
6	I	3001	PC1	O21-C21	2.87	1.40	1.30
6	J	2505	PC1	O21-C21	2.86	1.40	1.30
6	B	2907	PC1	O21-C21	2.86	1.40	1.30
6	A	904	PC1	O21-C21	2.86	1.40	1.30
6	G	3103	PC1	O21-C21	2.86	1.40	1.30
6	I	3002	PC1	O21-C21	2.86	1.40	1.30
6	J	2502	PC1	O21-C21	2.86	1.40	1.30
6	C	2701	PC1	O21-C21	2.86	1.40	1.30
6	D	902	PC1	O21-C21	2.85	1.40	1.30
6	B	2910	PC1	O21-C21	2.85	1.40	1.30
6	D	910	PC1	O21-C21	2.84	1.40	1.30
6	A	905	PC1	O21-C21	2.84	1.40	1.30
6	C	2706	PC1	O21-C21	2.83	1.40	1.30
6	D	905	PC1	O21-C21	2.83	1.40	1.30
6	A	902	PC1	O21-C21	2.81	1.40	1.30
6	C	2703	PC1	O21-C21	2.81	1.40	1.30
6	B	2906	PC1	O21-C21	2.81	1.40	1.30
5	B	2902	E2Q	C19-N18	2.77	1.39	1.35
5	D	901	E2Q	C19-N18	2.75	1.39	1.35
6	A	906	PC1	O31-C31	2.47	1.40	1.33
6	C	2707	PC1	O31-C31	2.47	1.40	1.33
5	B	2902	E2Q	C07-N15	2.42	1.50	1.45
5	D	901	E2Q	O17-N15	-2.42	1.19	1.35
5	A	901	E2Q	O17-N15	-2.41	1.19	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2702	E2Q	O17-N15	-2.41	1.19	1.35
5	D	901	E2Q	C07-N15	2.41	1.50	1.45
5	B	2902	E2Q	O17-N15	-2.41	1.19	1.35
5	B	2902	E2Q	C06-C07	-2.40	1.36	1.38
5	D	901	E2Q	C06-C07	-2.38	1.36	1.38
5	A	901	E2Q	C07-N15	2.31	1.49	1.45
6	B	2909	PC1	O31-C31	2.30	1.40	1.33
6	B	2909	PC1	O31-C3	-2.29	1.40	1.45
6	D	908	PC1	O31-C31	2.28	1.40	1.33
5	C	2702	E2Q	C07-N15	2.27	1.49	1.45
5	A	901	E2Q	C06-C07	-2.27	1.36	1.38
5	C	2702	E2Q	C06-C07	-2.27	1.36	1.38
6	D	908	PC1	O31-C3	-2.26	1.40	1.45
6	A	906	PC1	O31-C3	-2.14	1.40	1.45
6	C	2707	PC1	O31-C3	-2.10	1.40	1.45

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2902	E2Q	C09-C08-C03	5.43	119.76	116.78
5	A	901	E2Q	C09-C08-C03	5.43	119.76	116.78
5	C	2702	E2Q	C09-C08-C03	5.36	119.72	116.78
5	D	901	E2Q	C09-C08-C03	5.33	119.70	116.78
5	A	901	E2Q	O22-C21-C19	3.78	122.97	119.62
5	C	2702	E2Q	O22-C21-C19	3.78	122.97	119.62
5	D	901	E2Q	O22-C21-C19	3.77	122.96	119.62
5	B	2902	E2Q	O22-C21-C19	3.70	122.90	119.62
5	B	2902	E2Q	O13-S11-O12	3.54	124.24	118.80
5	C	2702	E2Q	O13-S11-O12	3.53	124.23	118.80
5	D	901	E2Q	O13-S11-O12	3.52	124.21	118.80
5	A	901	E2Q	O13-S11-O12	3.51	124.20	118.80
5	D	901	E2Q	C01-C10-C09	3.50	124.26	120.37
5	A	901	E2Q	C01-C10-C09	3.49	124.25	120.37
5	B	2902	E2Q	C01-C10-C09	3.49	124.25	120.37
5	C	2702	E2Q	C01-C10-C09	3.49	124.25	120.37
5	D	901	E2Q	C02-C03-C04	-3.47	118.46	124.70
5	B	2902	E2Q	C02-C03-C04	-3.45	118.49	124.70
5	C	2702	E2Q	C04-C05-N18	3.40	121.84	118.59
5	A	901	E2Q	C02-C03-C04	-3.39	118.59	124.70
5	C	2702	E2Q	C02-C03-C04	-3.39	118.60	124.70
5	A	901	E2Q	C04-C05-N18	3.36	121.81	118.59
5	B	2902	E2Q	C04-C05-N18	3.31	121.76	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	901	E2Q	C04-C05-N18	3.25	121.70	118.59
6	A	906	PC1	O31-C31-C32	3.00	120.97	111.83
6	C	2707	PC1	O31-C31-C32	3.00	120.97	111.83
5	A	901	E2Q	C08-C09-S11	2.96	125.42	121.74
5	C	2702	E2Q	C08-C09-S11	2.92	125.36	121.74
5	C	2702	E2Q	O20-C19-C21	2.91	122.20	119.62
5	B	2902	E2Q	O20-C19-C21	2.89	122.18	119.62
5	D	901	E2Q	O20-C19-C21	2.87	122.17	119.62
5	A	901	E2Q	O20-C19-C21	2.87	122.16	119.62
5	A	901	E2Q	C10-C09-C08	-2.74	116.01	120.18
6	B	2909	PC1	O31-C31-C32	2.73	120.15	111.83
5	D	901	E2Q	C10-C09-C08	-2.72	116.04	120.18
6	D	908	PC1	O31-C31-C32	2.72	120.13	111.83
5	B	2902	E2Q	C10-C09-C08	-2.72	116.05	120.18
5	C	2702	E2Q	C10-C09-C08	-2.71	116.06	120.18
5	A	901	E2Q	O16-N15-C07	-2.62	114.55	119.03
5	C	2702	E2Q	O16-N15-C07	-2.61	114.57	119.03
5	D	901	E2Q	O16-N15-C07	-2.59	114.60	119.03
5	B	2902	E2Q	O16-N15-C07	-2.55	114.66	119.03
5	B	2902	E2Q	C08-C09-S11	2.51	124.85	121.74
5	D	901	E2Q	C08-C09-S11	2.50	124.84	121.74
5	C	2702	E2Q	C05-N18-C19	-2.48	121.34	124.82
5	A	901	E2Q	C05-N18-C19	-2.46	121.38	124.82
5	B	2902	E2Q	C05-N18-C19	-2.43	121.41	124.82
5	D	901	E2Q	C05-N18-C19	-2.43	121.42	124.82
7	E	3104	CLR	C1-C2-C3	2.38	113.64	110.48
7	G	3104	CLR	C1-C2-C3	2.37	113.62	110.48
6	I	3002	PC1	C23-C22-C21	-2.10	109.03	114.51
6	J	2501	PC1	C23-C22-C21	-2.09	109.04	114.51
5	C	2702	E2Q	O13-S11-N14	-2.03	104.43	107.35
6	D	903	PC1	O21-C21-C22	2.02	120.37	114.00
5	A	901	E2Q	O13-S11-N14	-2.01	104.45	107.35
6	D	909	PC1	O21-C21-C22	2.01	120.35	114.00
6	B	2904	PC1	O21-C21-C22	2.01	120.34	114.00

There are no chirality outliers.

All (297) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	E2Q	C06-C07-N15-O16
5	A	901	E2Q	C08-C07-N15-O16
5	B	2902	E2Q	C06-C07-N15-O16

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Mol	Chain	Res	Type	Atoms
5	B	2902	E2Q	C08-C07-N15-O16
5	D	901	E2Q	C06-C07-N15-O16
5	D	901	E2Q	C08-C07-N15-O16
5	C	2702	E2Q	C06-C07-N15-O16
5	C	2702	E2Q	C08-C07-N15-O16
6	A	906	PC1	C1-C2-C3-O31
6	B	2909	PC1	C1-C2-C3-O31
6	B	2909	PC1	O21-C2-C3-O31
6	D	908	PC1	C1-C2-C3-O31
6	D	908	PC1	O21-C2-C3-O31
6	C	2707	PC1	C1-C2-C3-O31
6	A	906	PC1	O32-C31-O31-C3
6	C	2707	PC1	O32-C31-O31-C3
6	A	906	PC1	C32-C31-O31-C3
6	B	2909	PC1	C32-C31-O31-C3
6	D	908	PC1	C32-C31-O31-C3
6	C	2707	PC1	C32-C31-O31-C3
6	B	2909	PC1	O32-C31-O31-C3
6	D	908	PC1	O32-C31-O31-C3
6	A	906	PC1	O21-C2-C3-O31
6	C	2707	PC1	O21-C2-C3-O31
7	G	3104	CLR	C17-C20-C22-C23
7	E	3104	CLR	C17-C20-C22-C23
6	B	2904	PC1	C21-C22-C23-C24
6	D	903	PC1	C21-C22-C23-C24
7	G	3104	CLR	C21-C20-C22-C23
7	E	3104	CLR	C21-C20-C22-C23
6	A	907	PC1	C21-C22-C23-C24
6	C	2701	PC1	C21-C22-C23-C24
6	B	2909	PC1	C31-C32-C33-C34
6	D	908	PC1	C31-C32-C33-C34
6	I	3004	PC1	C22-C23-C24-C25
6	J	2503	PC1	C22-C23-C24-C25
7	G	3104	CLR	C20-C22-C23-C24
7	E	3104	CLR	C20-C22-C23-C24
6	A	907	PC1	C27-C28-C29-C2A
6	C	2701	PC1	C27-C28-C29-C2A
6	B	2904	PC1	C2C-C2D-C2E-C2F
6	D	903	PC1	C2C-C2D-C2E-C2F
6	A	904	PC1	C24-C25-C26-C27
6	C	2705	PC1	C24-C25-C26-C27
6	B	2903	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	D	902	PC1	C23-C24-C25-C26
6	B	2910	PC1	C23-C24-C25-C26
6	D	910	PC1	C23-C24-C25-C26
6	B	2906	PC1	C21-C22-C23-C24
6	D	905	PC1	C21-C22-C23-C24
6	A	903	PC1	C22-C23-C24-C25
6	C	2704	PC1	C22-C23-C24-C25
6	B	2904	PC1	C23-C24-C25-C26
6	B	2909	PC1	C37-C38-C39-C3A
6	D	903	PC1	C23-C24-C25-C26
6	D	908	PC1	C37-C38-C39-C3A
6	B	2901	PC1	C27-C28-C29-C2A
6	D	909	PC1	C27-C28-C29-C2A
6	A	904	PC1	C25-C26-C27-C28
6	C	2705	PC1	C25-C26-C27-C28
6	A	906	PC1	C39-C3A-C3B-C3C
6	A	907	PC1	C29-C2A-C2B-C2C
6	I	3004	PC1	C26-C27-C28-C29
6	J	2503	PC1	C26-C27-C28-C29
6	C	2707	PC1	C39-C3A-C3B-C3C
6	C	2701	PC1	C29-C2A-C2B-C2C
6	J	2502	PC1	C28-C29-C2A-C2B
6	A	906	PC1	C38-C39-C3A-C3B
6	I	3003	PC1	C28-C29-C2A-C2B
6	C	2707	PC1	C38-C39-C3A-C3B
6	B	2909	PC1	C36-C37-C38-C39
6	D	908	PC1	C36-C37-C38-C39
6	A	906	PC1	C3C-C3D-C3E-C3F
6	C	2707	PC1	C3C-C3D-C3E-C3F
6	B	2908	PC1	C22-C23-C24-C25
6	D	907	PC1	C22-C23-C24-C25
6	D	904	PC1	C23-C24-C25-C26
6	B	2910	PC1	C27-C28-C29-C2A
6	D	910	PC1	C27-C28-C29-C2A
6	B	2905	PC1	C23-C24-C25-C26
6	A	903	PC1	C23-C24-C25-C26
6	C	2704	PC1	C23-C24-C25-C26
6	I	3003	PC1	C24-C25-C26-C27
6	J	2502	PC1	C24-C25-C26-C27
6	A	902	PC1	C2D-C2E-C2F-C2G
6	C	2703	PC1	C2D-C2E-C2F-C2G
6	J	2504	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
6	I	3005	PC1	C25-C26-C27-C28
6	A	907	PC1	C26-C27-C28-C29
6	C	2701	PC1	C26-C27-C28-C29
6	A	902	PC1	C28-C29-C2A-C2B
6	A	905	PC1	C26-C27-C28-C29
6	C	2703	PC1	C28-C29-C2A-C2B
6	C	2706	PC1	C26-C27-C28-C29
6	A	907	PC1	C2B-C2C-C2D-C2E
6	C	2701	PC1	C2B-C2C-C2D-C2E
6	D	904	PC1	C27-C28-C29-C2A
6	B	2905	PC1	C27-C28-C29-C2A
6	B	2910	PC1	C2C-C2D-C2E-C2F
6	D	910	PC1	C2C-C2D-C2E-C2F
6	B	2910	PC1	C29-C2A-C2B-C2C
6	D	910	PC1	C29-C2A-C2B-C2C
6	E	3103	PC1	C2B-C2C-C2D-C2E
6	G	3103	PC1	C2B-C2C-C2D-C2E
6	A	906	PC1	C3E-C3F-C3G-C3H
6	C	2707	PC1	C3E-C3F-C3G-C3H
6	G	3101	PC1	C28-C29-C2A-C2B
6	E	3102	PC1	C28-C29-C2A-C2B
6	B	2904	PC1	C29-C2A-C2B-C2C
6	D	903	PC1	C29-C2A-C2B-C2C
6	B	2906	PC1	C25-C26-C27-C28
6	D	905	PC1	C25-C26-C27-C28
5	A	901	E2Q	C08-C09-S11-O12
5	B	2902	E2Q	C08-C09-S11-O13
5	D	901	E2Q	C08-C09-S11-O13
5	C	2702	E2Q	C08-C09-S11-O12
6	G	3103	PC1	C25-C26-C27-C28
6	E	3103	PC1	C25-C26-C27-C28
6	I	3003	PC1	C23-C24-C25-C26
6	J	2502	PC1	C23-C24-C25-C26
6	B	2908	PC1	C2C-C2D-C2E-C2F
6	A	906	PC1	C3A-C3B-C3C-C3D
6	B	2901	PC1	C2D-C2E-C2F-C2G
6	D	909	PC1	C2D-C2E-C2F-C2G
6	C	2707	PC1	C3A-C3B-C3C-C3D
6	D	907	PC1	C27-C28-C29-C2A
6	B	2908	PC1	C27-C28-C29-C2A
6	B	2903	PC1	C26-C27-C28-C29
6	D	909	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	B	2901	PC1	C23-C24-C25-C26
6	D	902	PC1	C26-C27-C28-C29
6	D	906	PC1	C26-C27-C28-C29
6	D	907	PC1	C2C-C2D-C2E-C2F
6	B	2907	PC1	C26-C27-C28-C29
6	I	3005	PC1	C21-C22-C23-C24
6	J	2504	PC1	C21-C22-C23-C24
6	I	3005	PC1	C29-C2A-C2B-C2C
6	J	2504	PC1	C29-C2A-C2B-C2C
6	C	2701	PC1	C23-C24-C25-C26
6	A	907	PC1	C23-C24-C25-C26
6	B	2910	PC1	C2A-C2B-C2C-C2D
6	G	3103	PC1	C22-C23-C24-C25
6	D	910	PC1	C2A-C2B-C2C-C2D
6	B	2903	PC1	C25-C26-C27-C28
6	D	902	PC1	C25-C26-C27-C28
6	E	3103	PC1	C22-C23-C24-C25
6	I	3005	PC1	C23-C24-C25-C26
6	J	2504	PC1	C23-C24-C25-C26
6	A	907	PC1	C28-C29-C2A-C2B
6	C	2701	PC1	C28-C29-C2A-C2B
6	D	910	PC1	C28-C29-C2A-C2B
6	B	2910	PC1	C28-C29-C2A-C2B
6	C	2706	PC1	C28-C29-C2A-C2B
6	A	905	PC1	C28-C29-C2A-C2B
6	B	2907	PC1	C2B-C2C-C2D-C2E
6	D	906	PC1	C2B-C2C-C2D-C2E
6	D	903	PC1	C2F-C2G-C2H-C2I
6	D	908	PC1	C32-C33-C34-C35
6	B	2909	PC1	C32-C33-C34-C35
6	D	903	PC1	C27-C28-C29-C2A
6	B	2904	PC1	C27-C28-C29-C2A
6	B	2904	PC1	C2F-C2G-C2H-C2I
6	E	3101	PC1	C27-C28-C29-C2A
6	G	3102	PC1	C27-C28-C29-C2A
6	J	2505	PC1	C24-C25-C26-C27
6	I	3001	PC1	C26-C27-C28-C29
6	B	2903	PC1	C29-C2A-C2B-C2C
6	D	902	PC1	C29-C2A-C2B-C2C
6	J	2505	PC1	C26-C27-C28-C29
6	I	3001	PC1	C24-C25-C26-C27
6	E	3103	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
6	A	903	PC1	C2D-C2E-C2F-C2G
6	C	2704	PC1	C2D-C2E-C2F-C2G
6	G	3103	PC1	C2C-C2D-C2E-C2F
6	G	3101	PC1	C27-C28-C29-C2A
6	E	3102	PC1	C27-C28-C29-C2A
6	J	2502	PC1	C2C-C2D-C2E-C2F
6	I	3003	PC1	C2C-C2D-C2E-C2F
6	B	2903	PC1	C2B-C2C-C2D-C2E
6	B	2910	PC1	C22-C23-C24-C25
6	D	910	PC1	C22-C23-C24-C25
6	D	902	PC1	C2B-C2C-C2D-C2E
6	G	3101	PC1	C2E-C2F-C2G-C2H
6	I	3001	PC1	C22-C23-C24-C25
6	E	3102	PC1	C2E-C2F-C2G-C2H
6	B	2907	PC1	C23-C24-C25-C26
6	D	906	PC1	C23-C24-C25-C26
6	J	2502	PC1	C29-C2A-C2B-C2C
6	I	3003	PC1	C29-C2A-C2B-C2C
6	A	902	PC1	C29-C2A-C2B-C2C
6	C	2703	PC1	C29-C2A-C2B-C2C
6	B	2907	PC1	C28-C29-C2A-C2B
6	D	906	PC1	C28-C29-C2A-C2B
6	J	2505	PC1	C22-C23-C24-C25
6	A	903	PC1	C25-C26-C27-C28
6	C	2704	PC1	C25-C26-C27-C28
6	A	902	PC1	C2A-C2B-C2C-C2D
6	C	2703	PC1	C2A-C2B-C2C-C2D
6	I	3004	PC1	C2B-C2C-C2D-C2E
6	J	2503	PC1	C2B-C2C-C2D-C2E
6	I	3001	PC1	O22-C21-C22-C23
6	J	2505	PC1	O22-C21-C22-C23
6	A	903	PC1	C29-C2A-C2B-C2C
6	C	2704	PC1	C29-C2A-C2B-C2C
6	B	2909	PC1	C39-C3A-C3B-C3C
6	A	904	PC1	O21-C21-C22-C23
6	C	2705	PC1	O21-C21-C22-C23
6	B	2904	PC1	C2A-C2B-C2C-C2D
6	J	2501	PC1	O22-C21-C22-C23
6	A	905	PC1	C2B-C2C-C2D-C2E
6	D	908	PC1	C39-C3A-C3B-C3C
6	D	903	PC1	C2A-C2B-C2C-C2D
6	A	904	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
6	I	3002	PC1	O22-C21-C22-C23
6	C	2705	PC1	O22-C21-C22-C23
6	C	2706	PC1	C2B-C2C-C2D-C2E
6	A	903	PC1	O21-C21-C22-C23
6	C	2704	PC1	O21-C21-C22-C23
6	A	907	PC1	C25-C26-C27-C28
6	A	902	PC1	C2E-C2F-C2G-C2H
6	C	2701	PC1	C25-C26-C27-C28
6	C	2703	PC1	C2E-C2F-C2G-C2H
6	I	3001	PC1	O21-C21-C22-C23
6	J	2505	PC1	O21-C21-C22-C23
6	D	908	PC1	C38-C39-C3A-C3B
6	B	2909	PC1	C38-C39-C3A-C3B
6	I	3002	PC1	O21-C21-C22-C23
6	J	2501	PC1	O21-C21-C22-C23
6	A	902	PC1	C2B-C2C-C2D-C2E
6	C	2703	PC1	C2B-C2C-C2D-C2E
6	B	2904	PC1	C2E-C2F-C2G-C2H
6	D	903	PC1	C2E-C2F-C2G-C2H
6	I	3005	PC1	O21-C21-C22-C23
6	J	2504	PC1	O21-C21-C22-C23
6	B	2905	PC1	C28-C29-C2A-C2B
6	A	907	PC1	C2A-C2B-C2C-C2D
6	A	903	PC1	O22-C21-C22-C23
6	C	2704	PC1	O22-C21-C22-C23
6	C	2701	PC1	C2A-C2B-C2C-C2D
6	A	906	PC1	C32-C33-C34-C35
6	C	2707	PC1	C32-C33-C34-C35
6	D	904	PC1	C28-C29-C2A-C2B
6	J	2504	PC1	C28-C29-C2A-C2B
6	I	3005	PC1	C28-C29-C2A-C2B
6	A	906	PC1	O11-C1-C2-O21
6	C	2707	PC1	O11-C1-C2-O21
6	I	3005	PC1	O22-C21-C22-C23
6	J	2504	PC1	O22-C21-C22-C23
6	G	3102	PC1	C25-C26-C27-C28
6	E	3101	PC1	C25-C26-C27-C28
6	D	905	PC1	O22-C21-C22-C23
6	B	2906	PC1	O22-C21-C22-C23
6	A	904	PC1	C22-C23-C24-C25
6	C	2705	PC1	C22-C23-C24-C25
6	A	907	PC1	O21-C21-C22-C23

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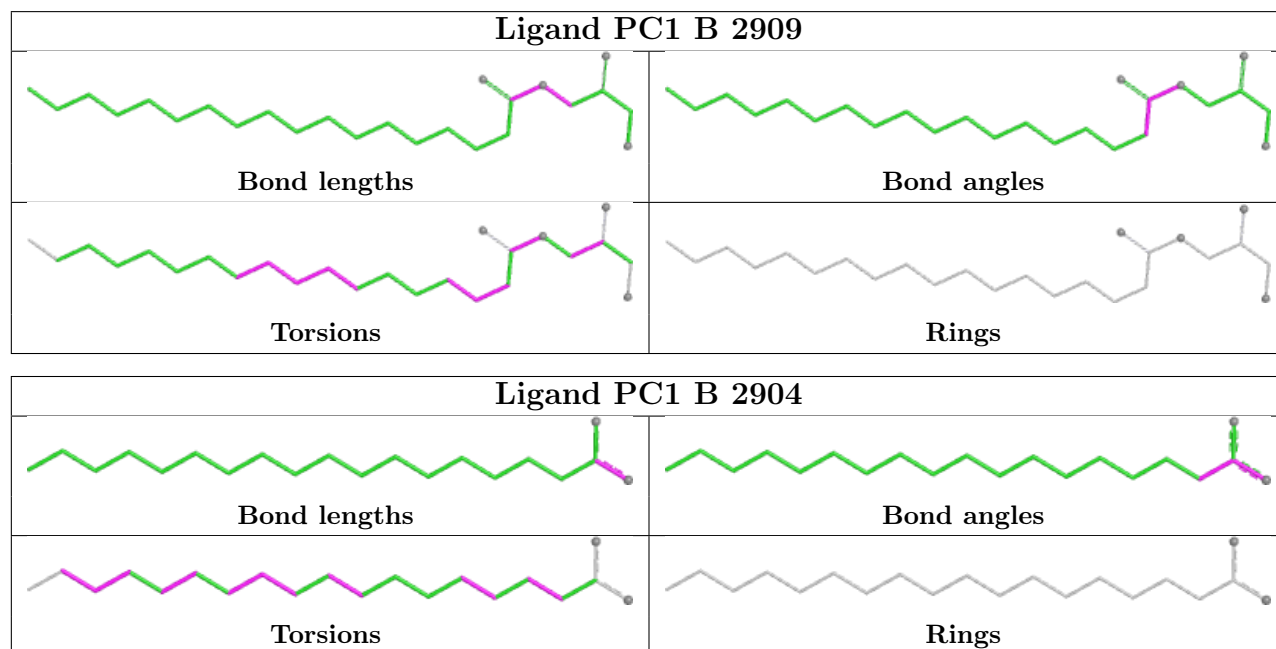
Mol	Chain	Res	Type	Atoms
6	A	907	PC1	O22-C21-C22-C23
6	C	2701	PC1	O21-C21-C22-C23
6	C	2701	PC1	O22-C21-C22-C23
6	G	3103	PC1	O22-C21-C22-C23
6	E	3103	PC1	O22-C21-C22-C23
6	G	3103	PC1	O21-C21-C22-C23
6	E	3103	PC1	O21-C21-C22-C23
6	G	3101	PC1	C24-C25-C26-C27
6	E	3102	PC1	C24-C25-C26-C27
6	B	2910	PC1	O21-C21-C22-C23
6	D	910	PC1	O21-C21-C22-C23
6	C	2704	PC1	C24-C25-C26-C27
6	A	903	PC1	C24-C25-C26-C27
6	B	2908	PC1	C23-C24-C25-C26
6	D	905	PC1	O21-C21-C22-C23
6	D	909	PC1	C25-C26-C27-C28
6	D	907	PC1	C23-C24-C25-C26
6	B	2901	PC1	C25-C26-C27-C28
6	B	2906	PC1	O21-C21-C22-C23
6	G	3101	PC1	O21-C21-C22-C23
6	G	3101	PC1	O22-C21-C22-C23
6	E	3102	PC1	O22-C21-C22-C23
6	E	3102	PC1	O21-C21-C22-C23
6	I	3003	PC1	C25-C26-C27-C28
6	J	2502	PC1	C25-C26-C27-C28
6	D	910	PC1	O22-C21-C22-C23
7	G	3104	CLR	C22-C23-C24-C25
7	E	3104	CLR	C22-C23-C24-C25
6	B	2910	PC1	O22-C21-C22-C23
6	A	906	PC1	C35-C36-C37-C38
6	I	3004	PC1	C25-C26-C27-C28
6	J	2503	PC1	C25-C26-C27-C28
6	C	2707	PC1	C35-C36-C37-C38
6	B	2907	PC1	C25-C26-C27-C28
6	D	906	PC1	C25-C26-C27-C28
6	B	2901	PC1	C22-C23-C24-C25
6	D	909	PC1	C22-C23-C24-C25
6	D	909	PC1	O21-C21-C22-C23
6	B	2901	PC1	O21-C21-C22-C23
6	B	2908	PC1	O21-C21-C22-C23
6	D	907	PC1	O21-C21-C22-C23
6	D	906	PC1	C2D-C2E-C2F-C2G

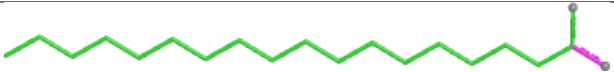
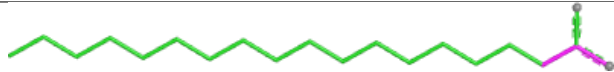
There are no ring outliers.

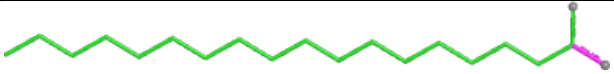
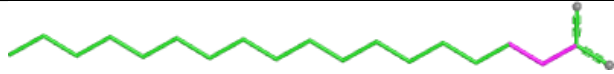
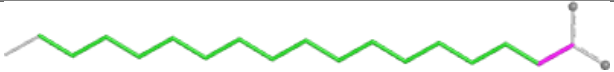
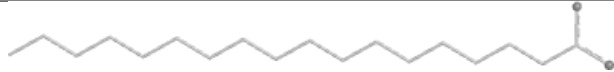
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	908	PC1	1	0
7	G	3104	CLR	3	0
6	B	2901	PC1	1	0
5	B	2902	E2Q	1	0
6	J	2502	PC1	1	0
7	E	3104	CLR	3	0

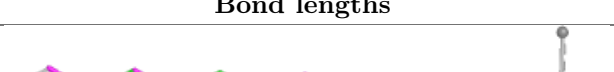
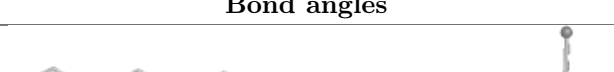
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

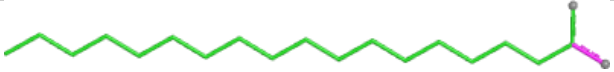
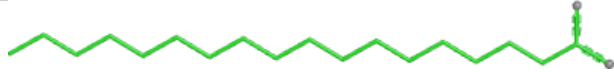
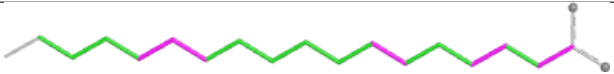
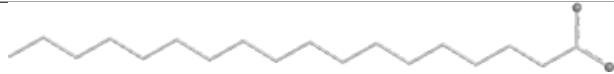


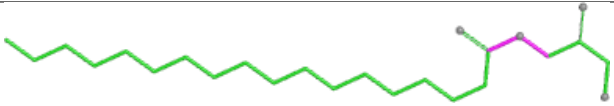
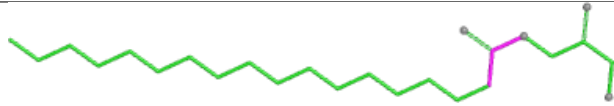
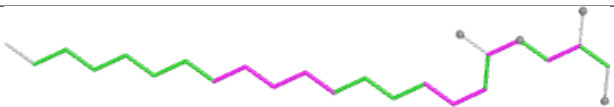
Ligand PC1 D 903			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

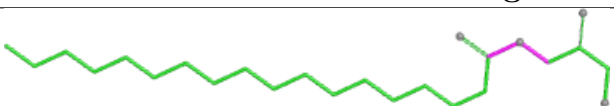
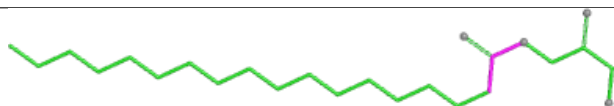
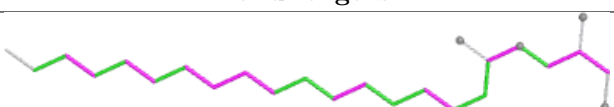
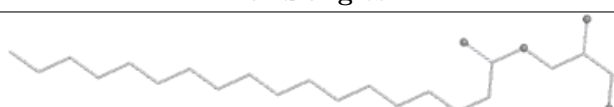
Ligand PC1 I 3002			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

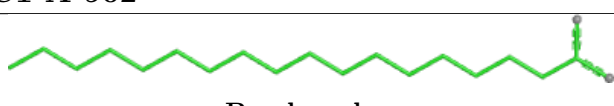
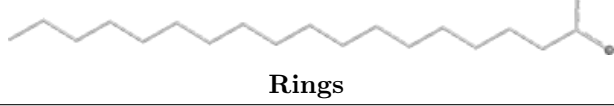
Ligand PC1 C 2701			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

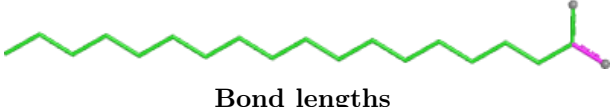
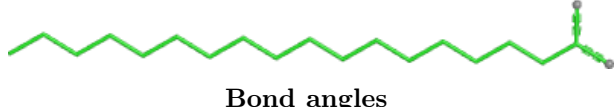
Ligand PC1 D 902			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

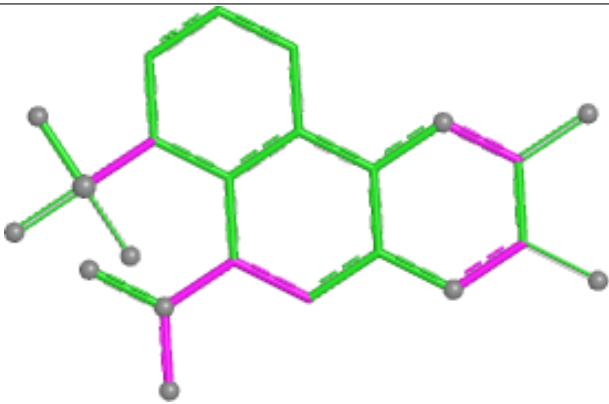
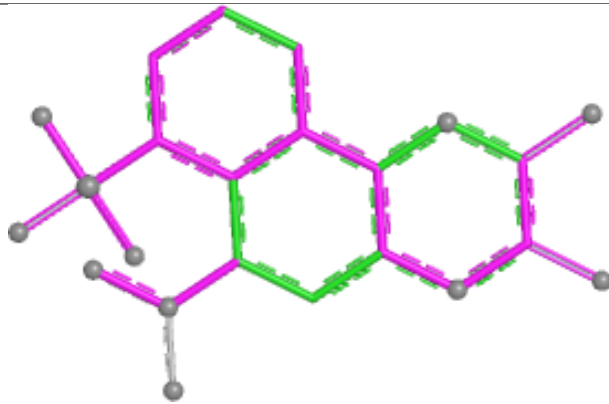
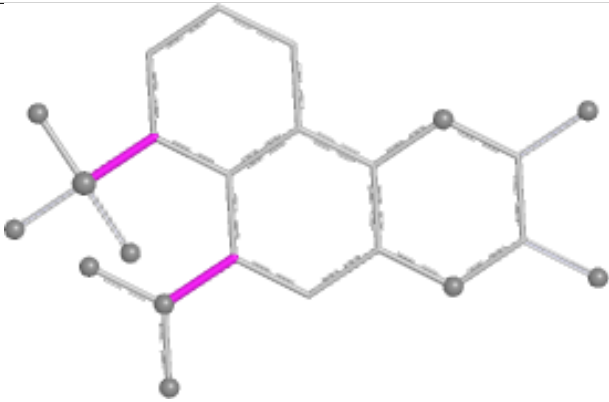
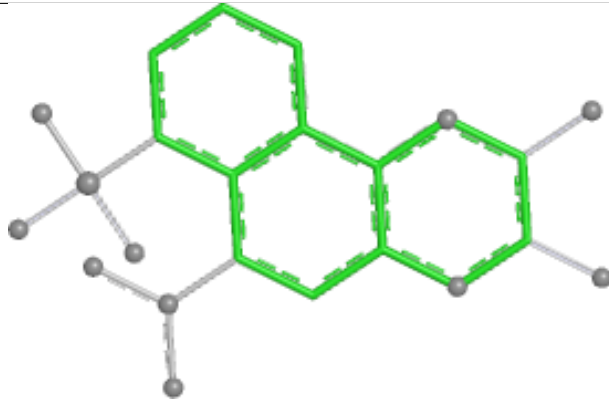
Ligand PC1 E 3103			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

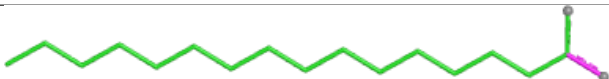
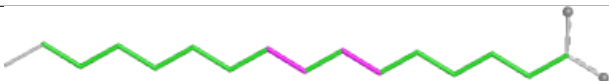
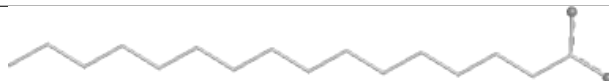
Ligand PC1 D 908	
 Bond lengths	 Bond angles
 Torsions	 Rings

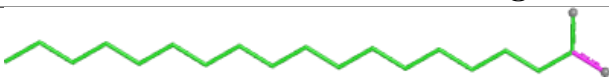
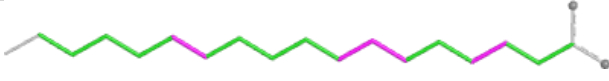
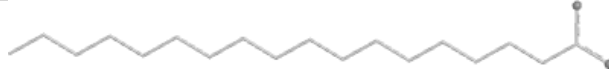
Ligand PC1 C 2707	
 Bond lengths	 Bond angles
 Torsions	 Rings

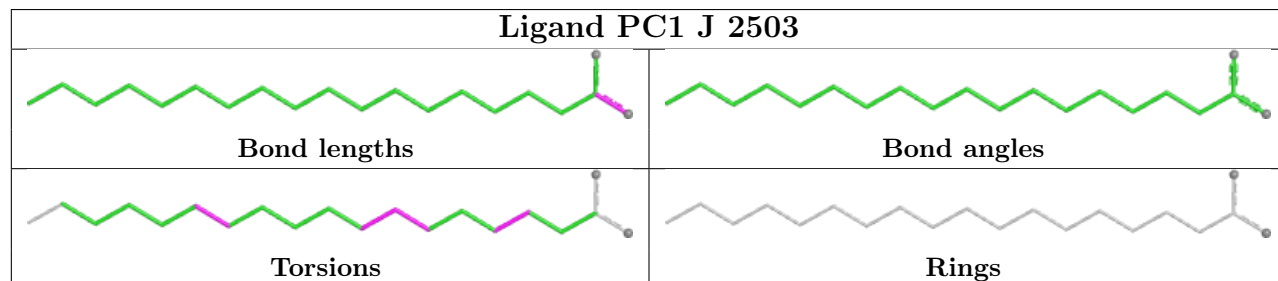
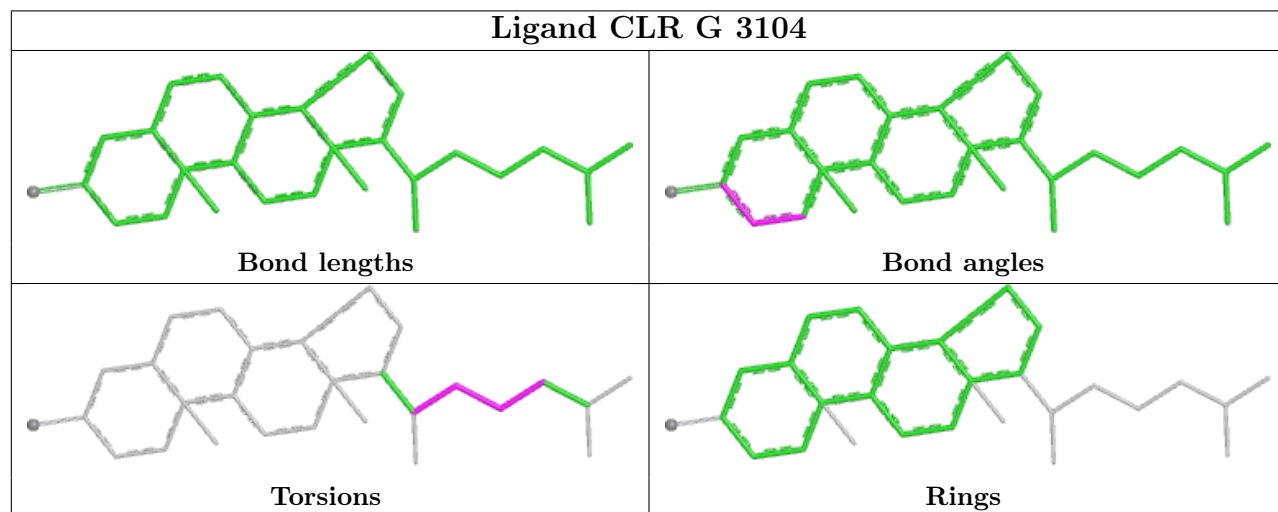
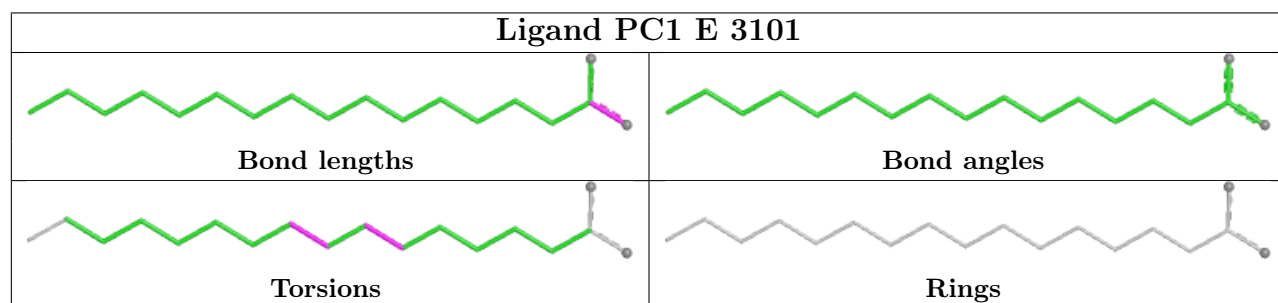
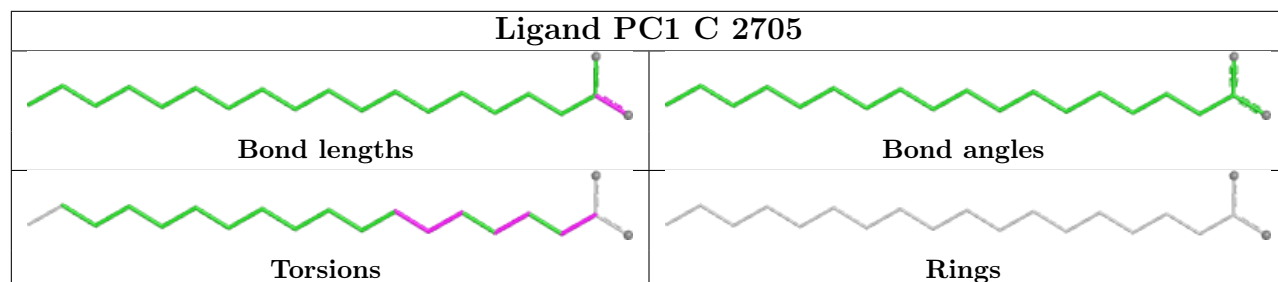
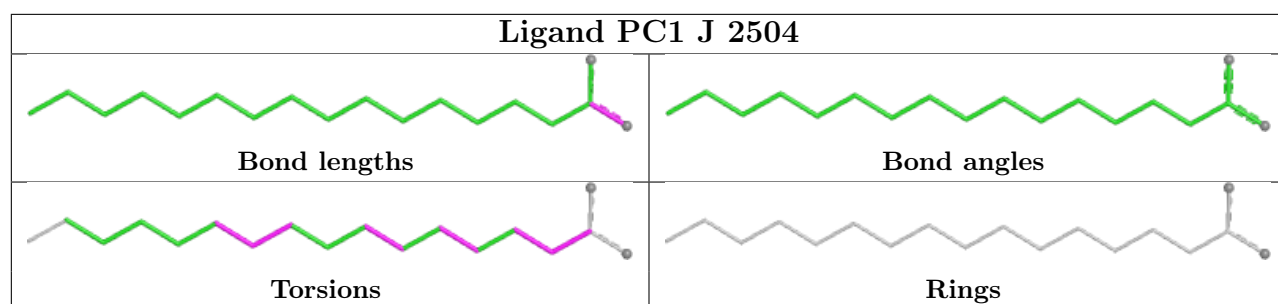
Ligand PC1 A 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

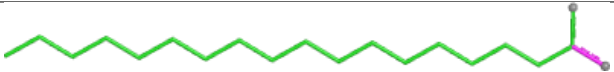
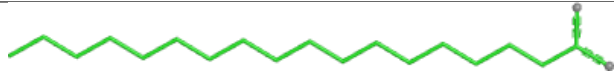
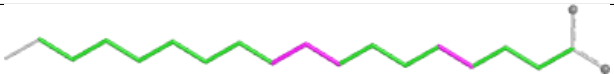
Ligand PC1 A 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand E2Q A 901	
	
Bond lengths	Bond angles
	
Torsions	Rings

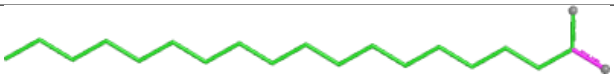
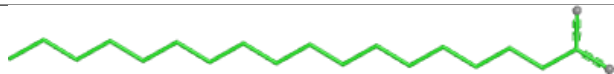
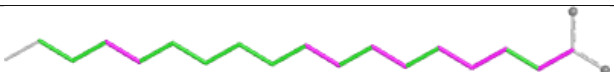
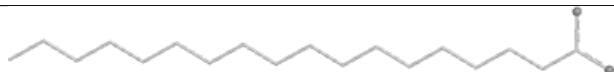
Ligand PC1 G 3102	
	
Bond lengths	Bond angles
	
Torsions	Rings

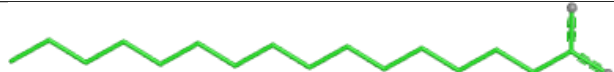
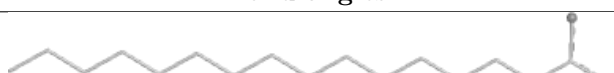
Ligand PC1 I 3004	
	
Bond lengths	Bond angles
	
Torsions	Rings

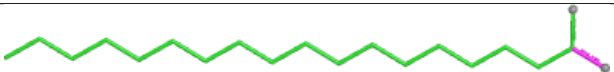
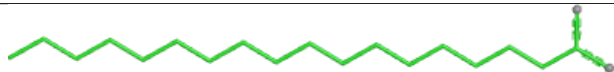
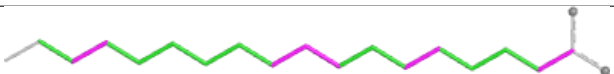
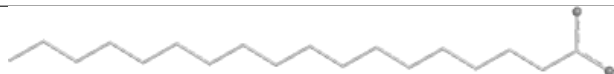


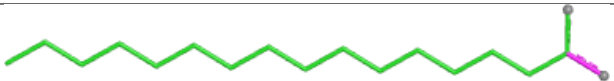
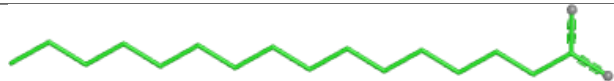
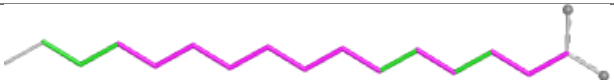
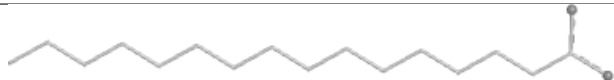
Ligand PC1 D 904			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

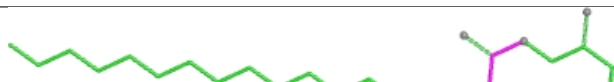
Ligand PC1 B 2903			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

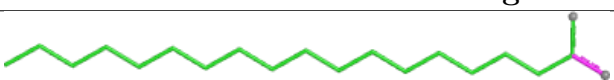
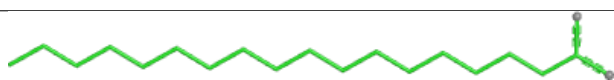
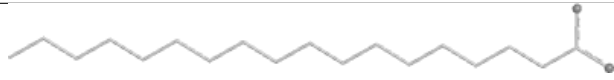
Ligand PC1 B 2901			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

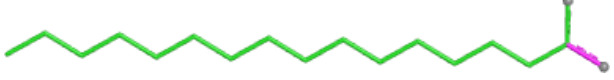
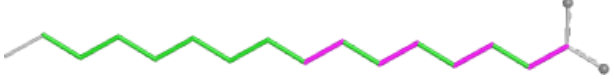
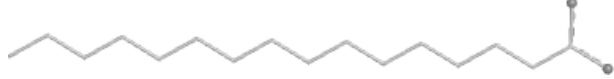
Ligand PC1 I 3005			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

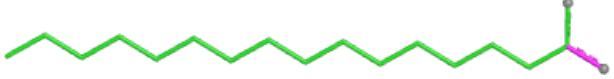
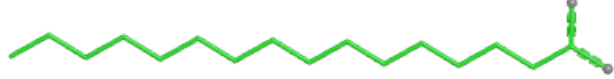
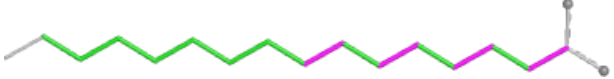
Ligand PC1 E 3102			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

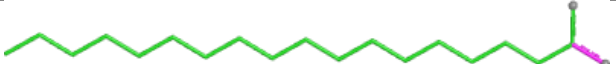
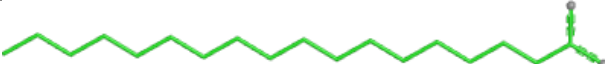
Ligand PC1 A 907	
 Bond lengths	 Bond angles
 Torsions	 Rings

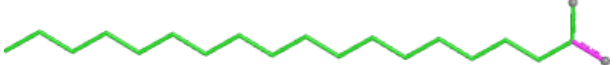
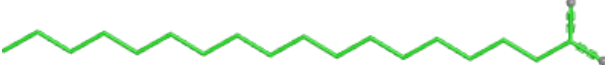
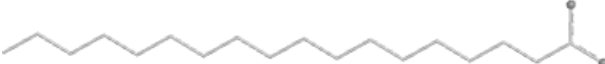
Ligand PC1 A 906	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 G 3103	
 Bond lengths	 Bond angles
 Torsions	 Rings

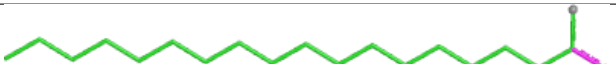
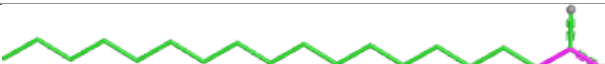
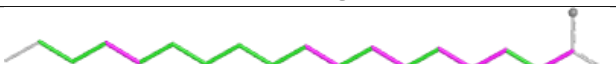
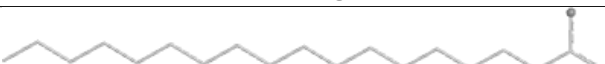
Ligand PC1 I 3001	
 Bond lengths	 Bond angles
 Torsions	 Rings

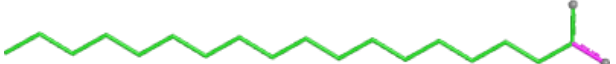
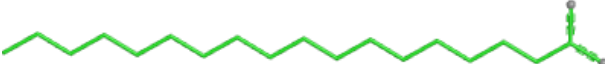
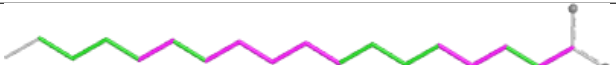
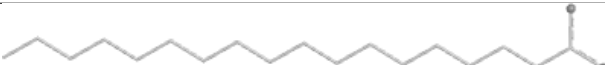
Ligand PC1 J 2505	
 Bond lengths	 Bond angles
 Torsions	 Rings

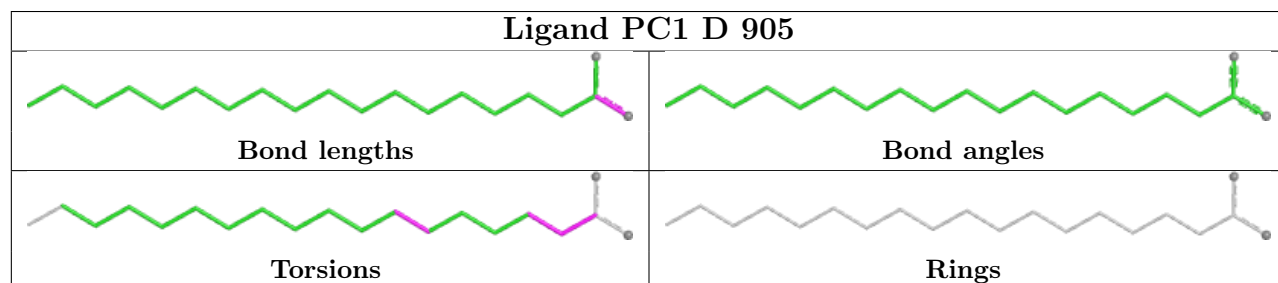
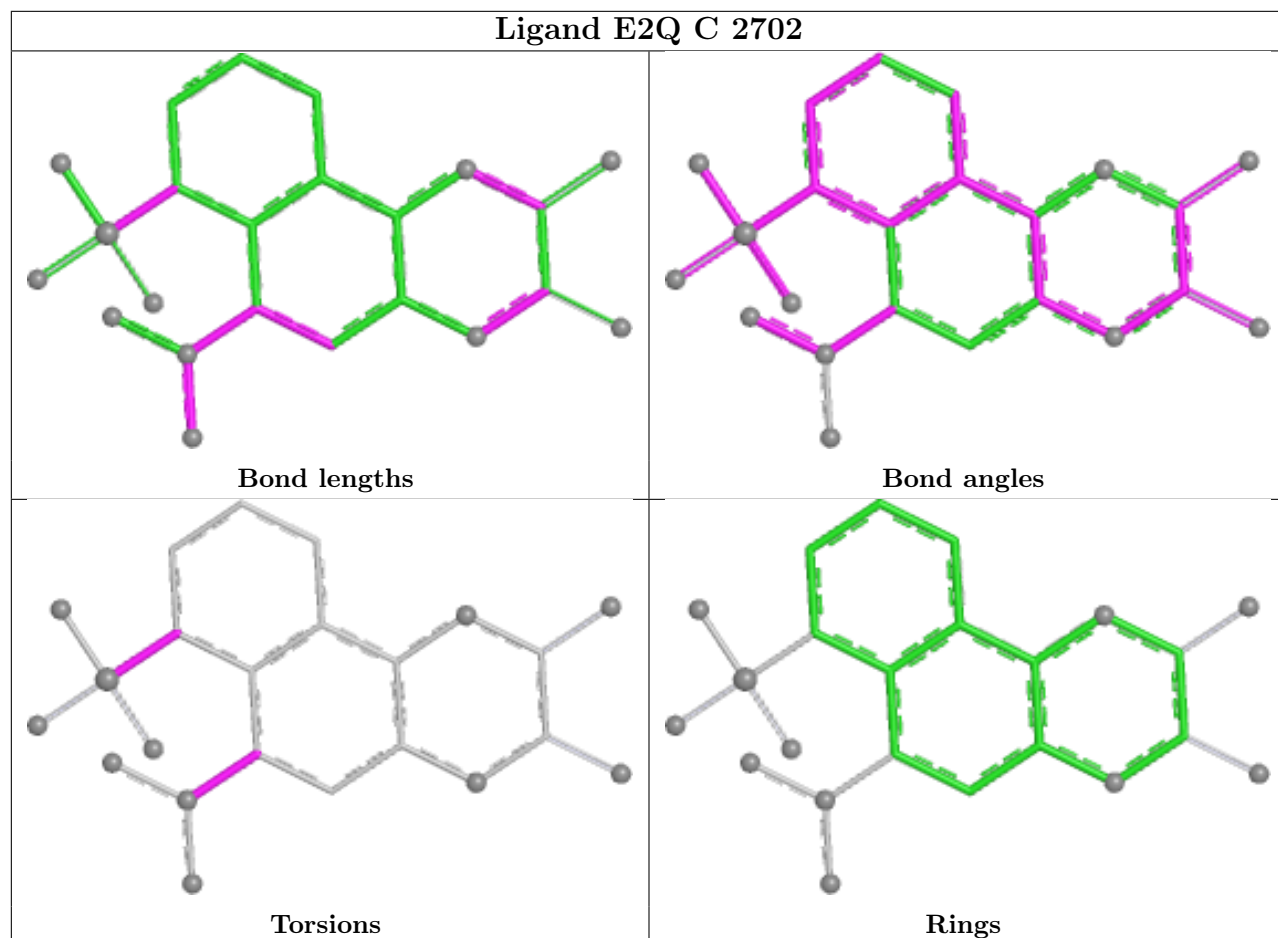
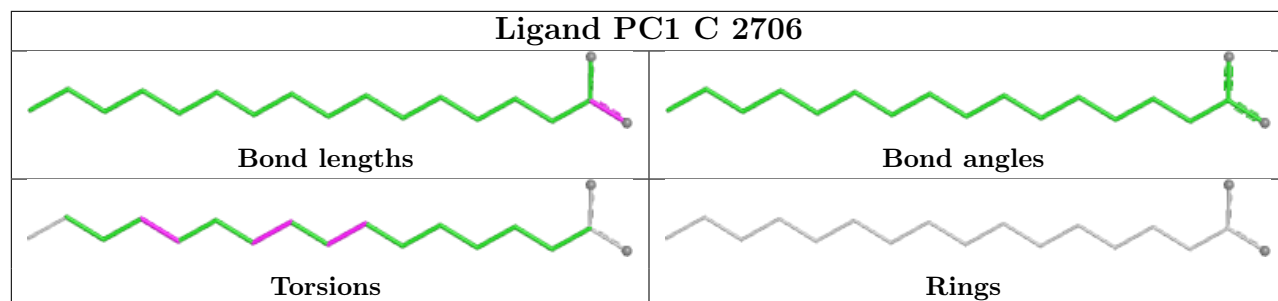
Ligand PC1 G 3101			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

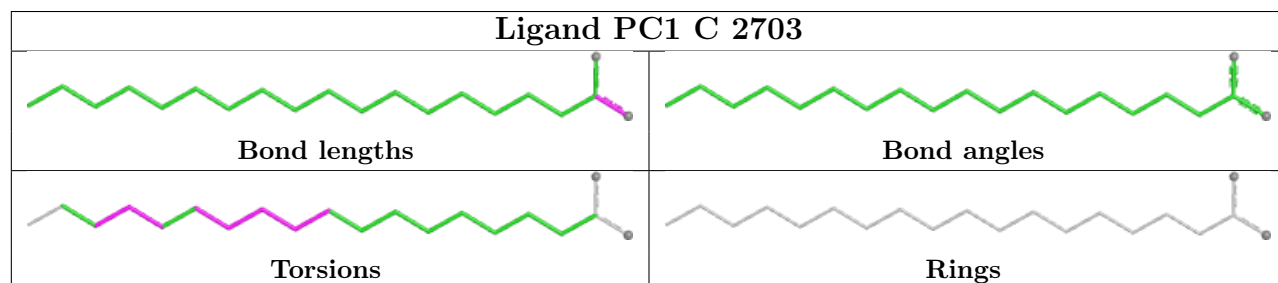
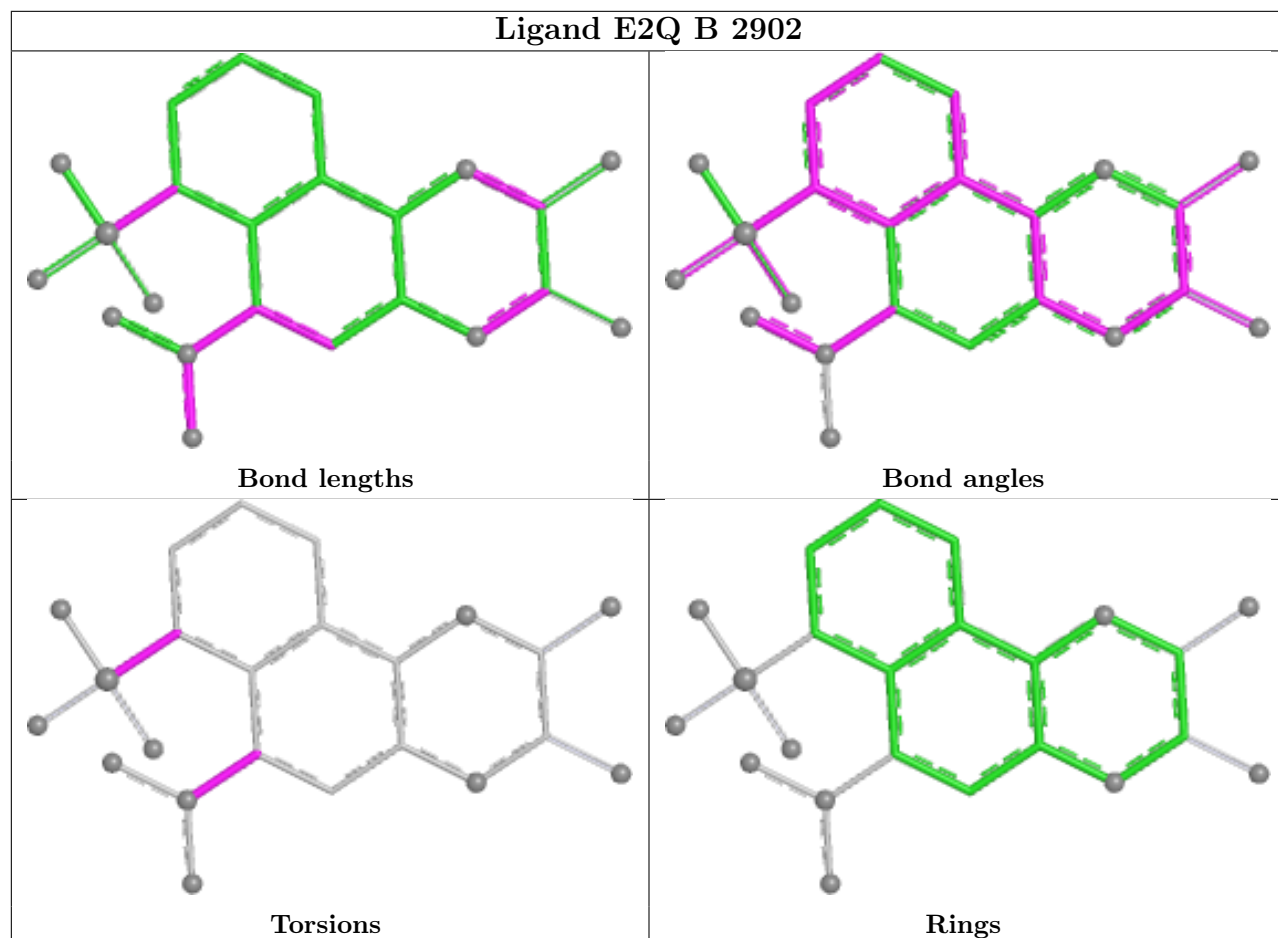
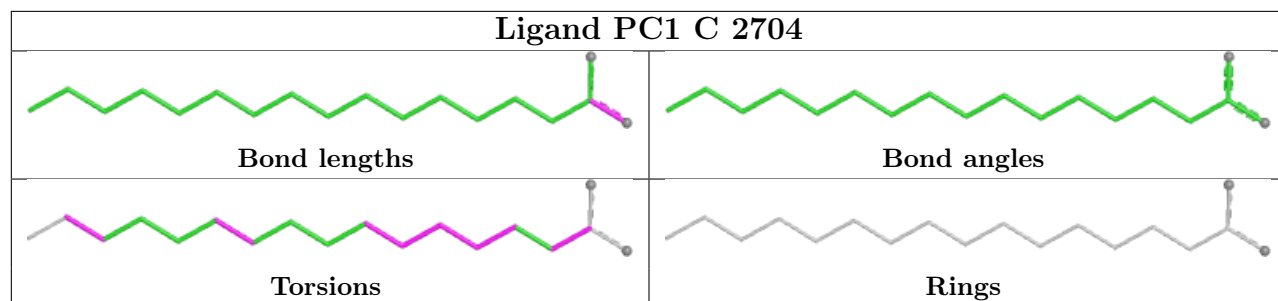
Ligand PC1 I 3003			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

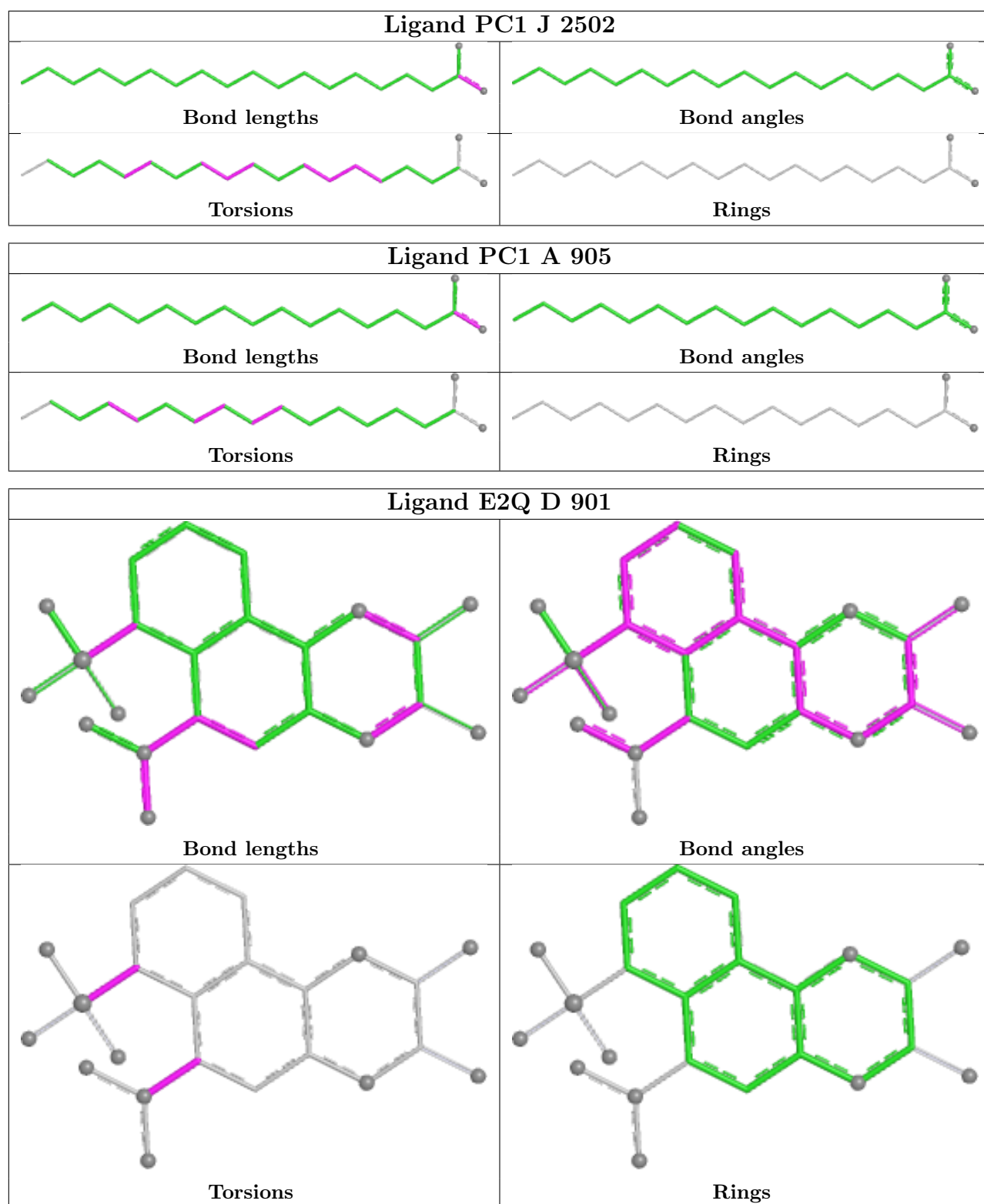
Ligand PC1 D 907			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

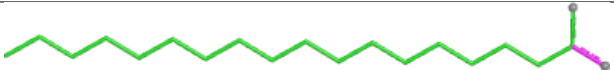
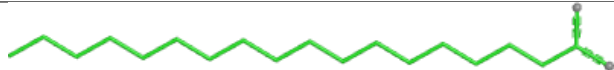
Ligand PC1 D 909			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

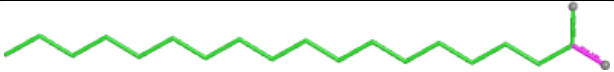
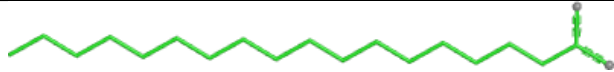
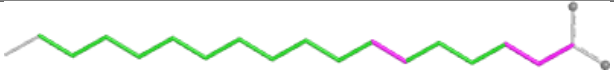
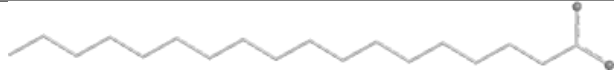
Ligand PC1 D 910			
 Bond lengths		 Bond angles	
 Torsions		 Rings	



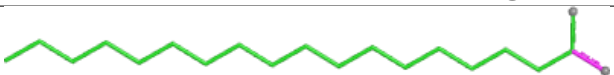
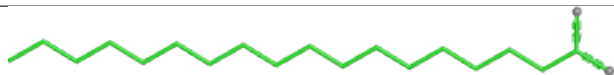
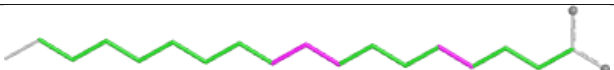
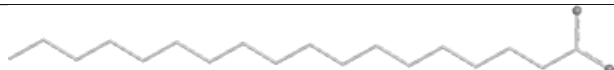


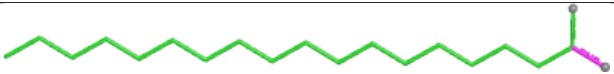
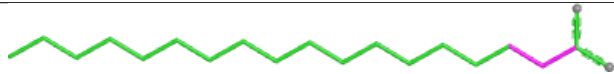
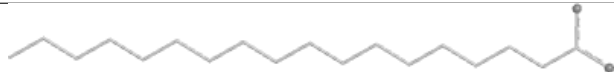


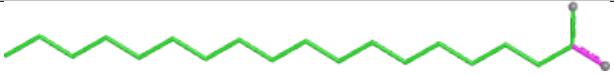
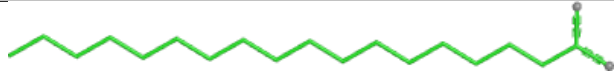
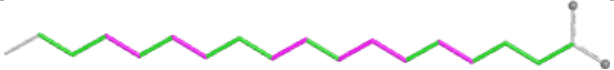
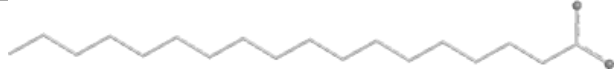
Ligand PC1 B 2907			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

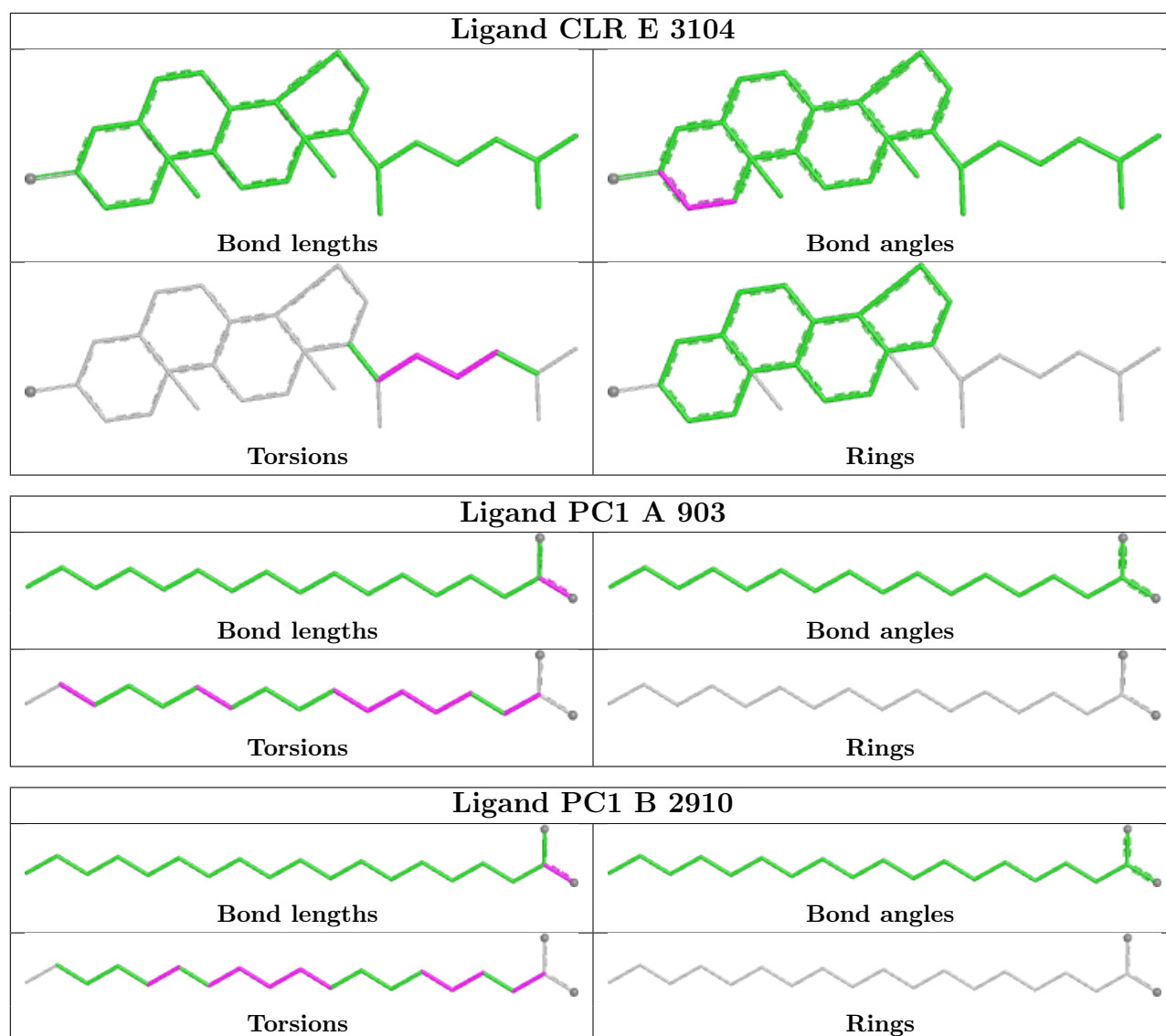
Ligand PC1 B 2906			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 B 2908			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 B 2905			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 J 2501			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 D 906			
 Bond lengths		 Bond angles	
 Torsions		 Rings	



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

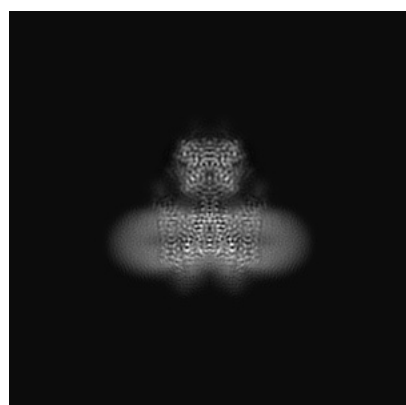
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12805. These allow visual inspection of the internal detail of the map and identification of artifacts.

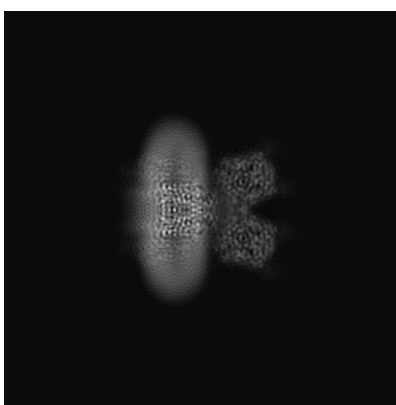
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

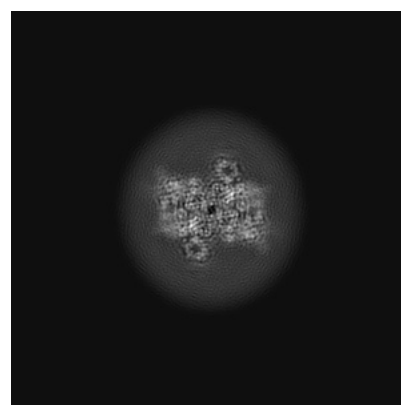
6.1.1 Primary map



X



Y

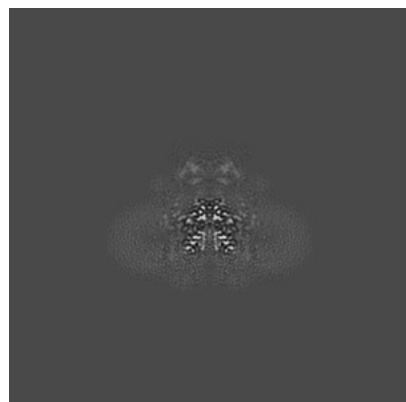


Z

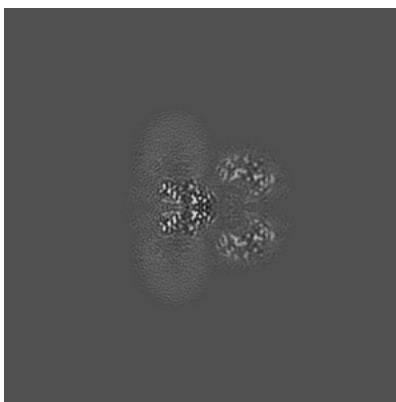
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

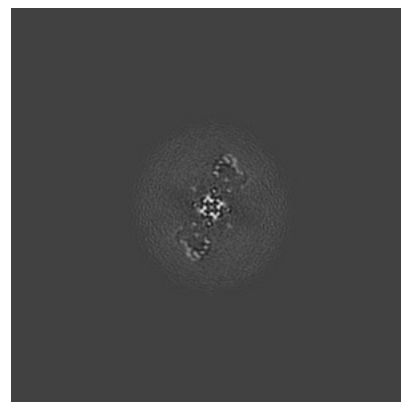
6.2.1 Primary map



X Index: 160



Y Index: 160

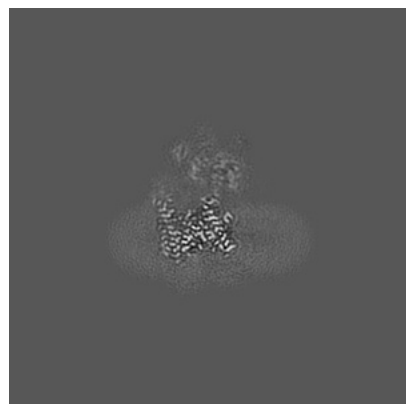


Z Index: 160

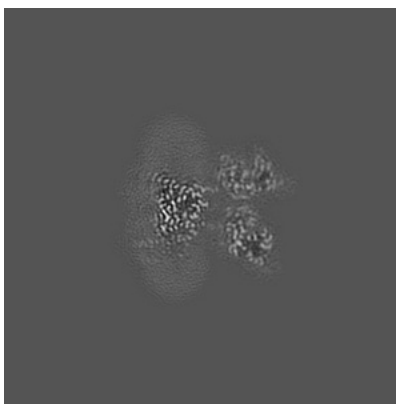
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

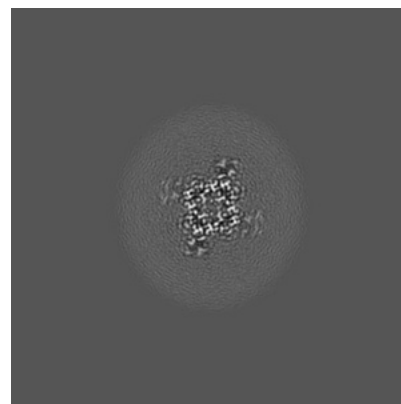
6.3.1 Primary map



X Index: 152



Y Index: 173

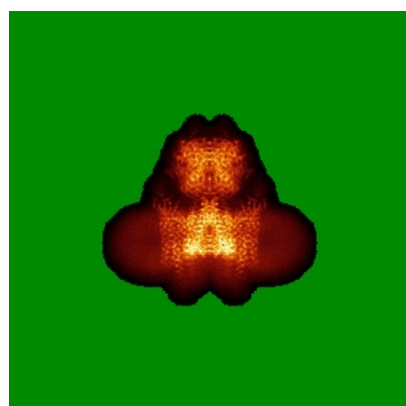


Z Index: 128

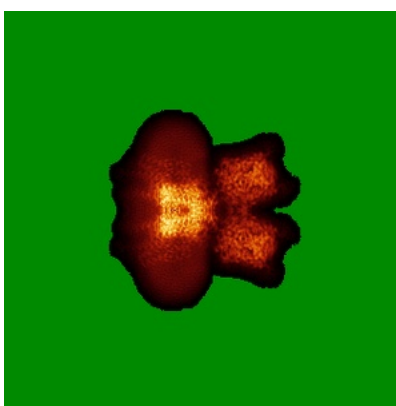
The images above show the largest variance slices of the map in three orthogonal directions.

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

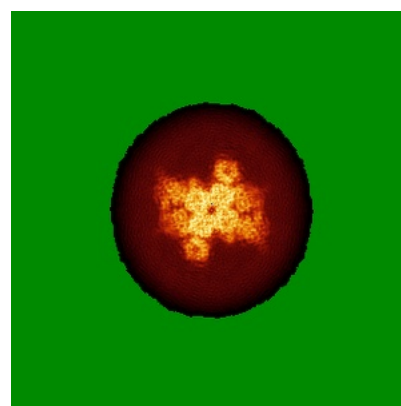
6.4.1 Primary map



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

This section was not generated.

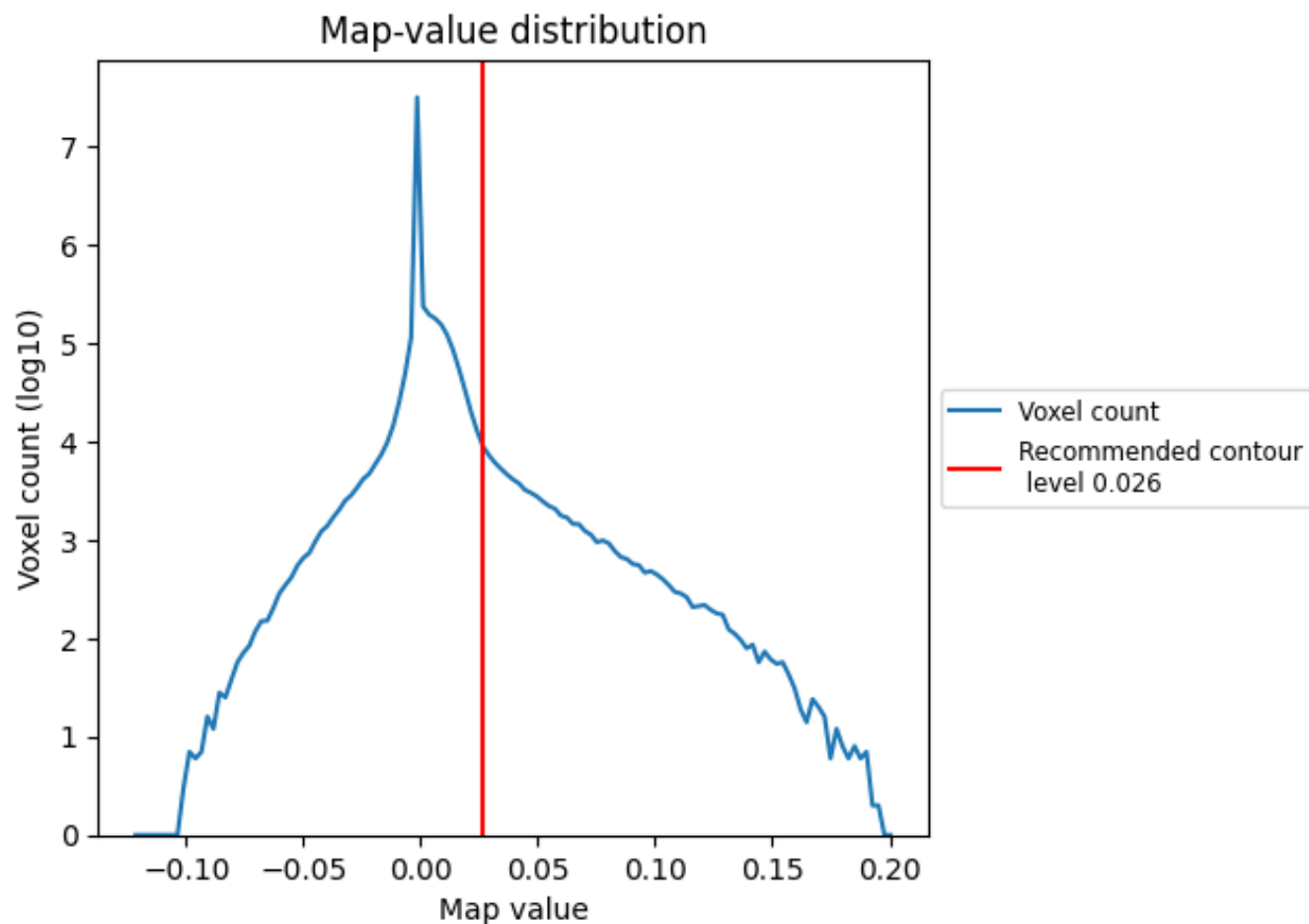
6.6 Mask visualisation

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

7 Map analysis [i](#)

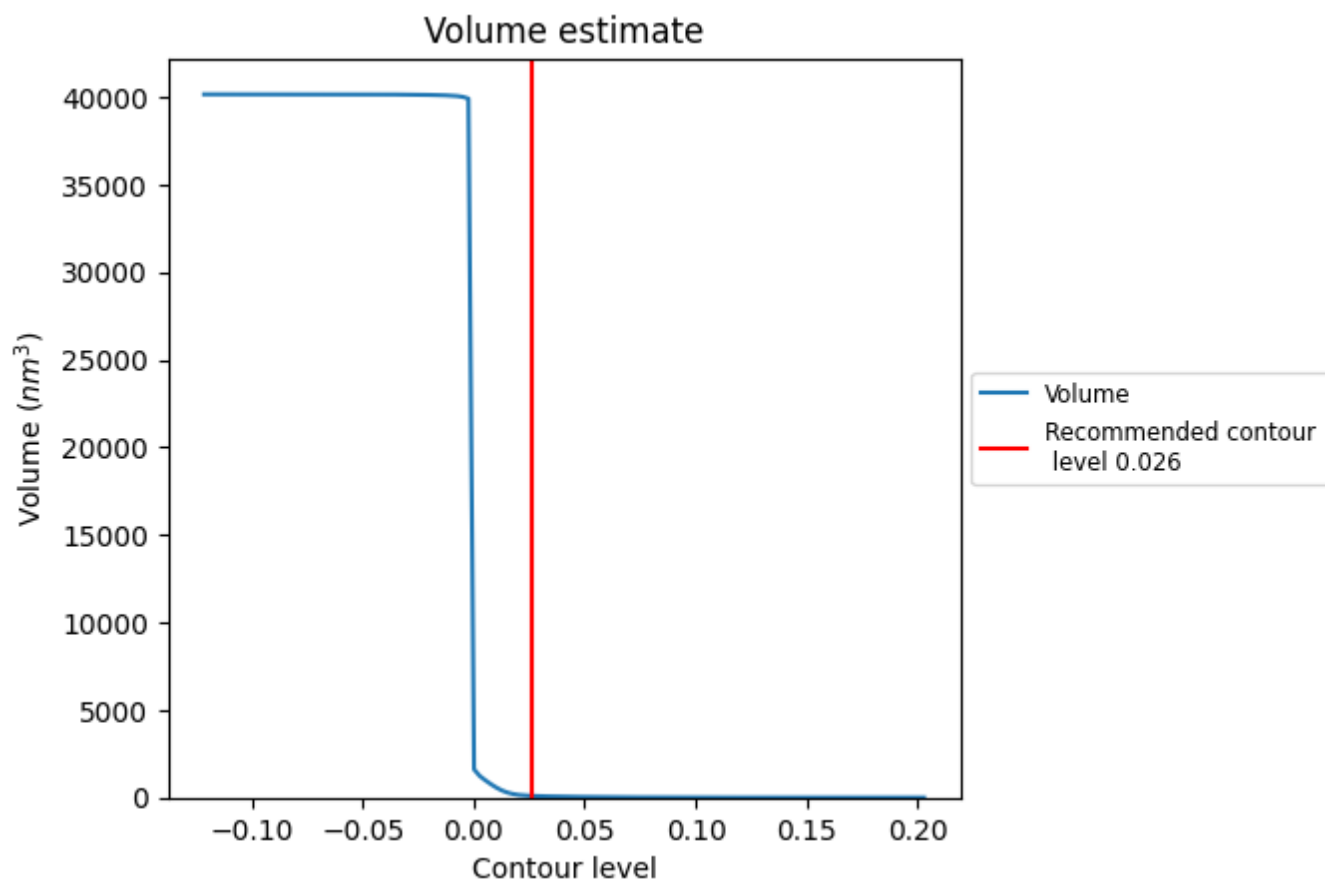
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

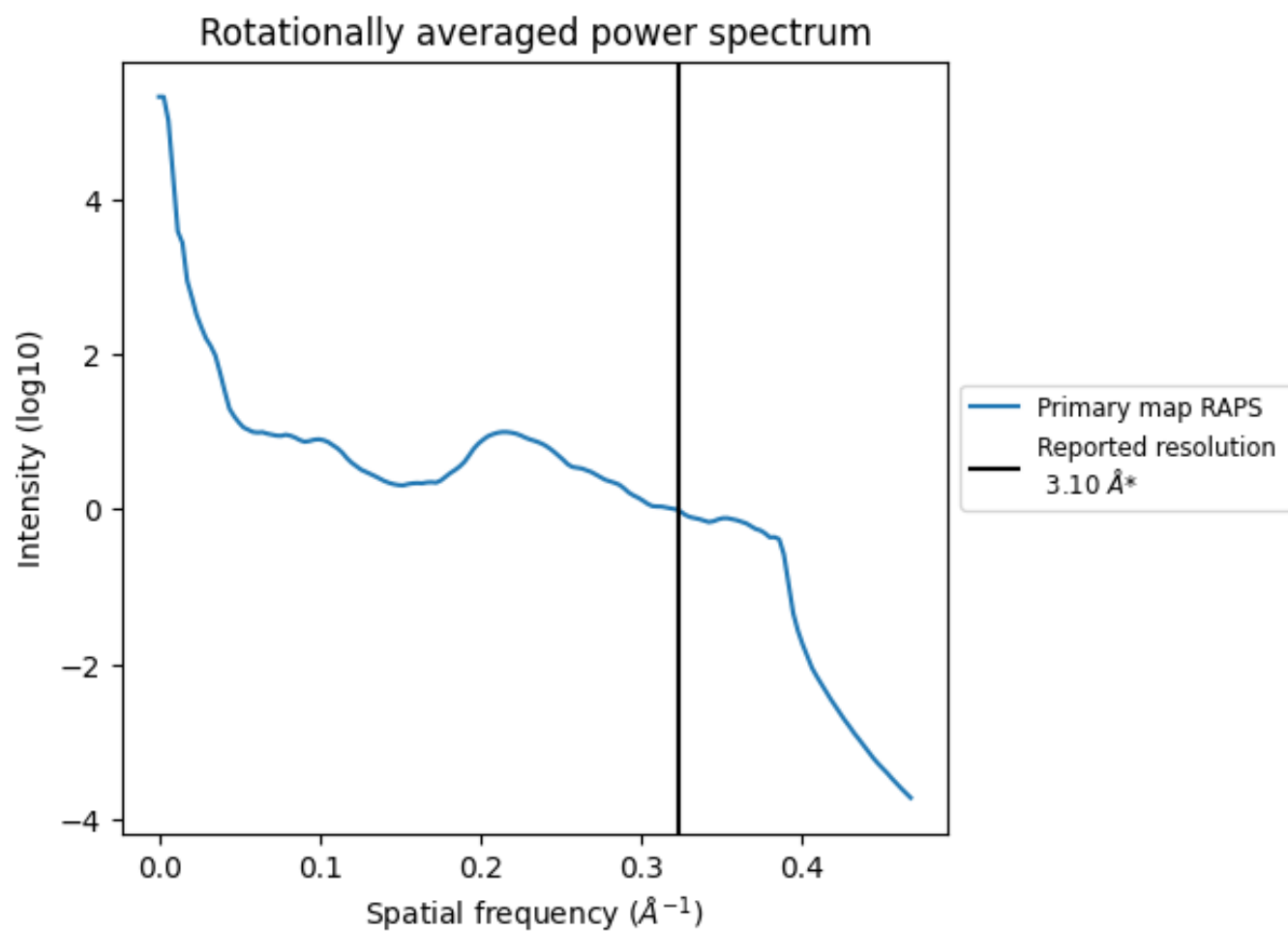
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm^3 ; this corresponds to an approximate mass of 87 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

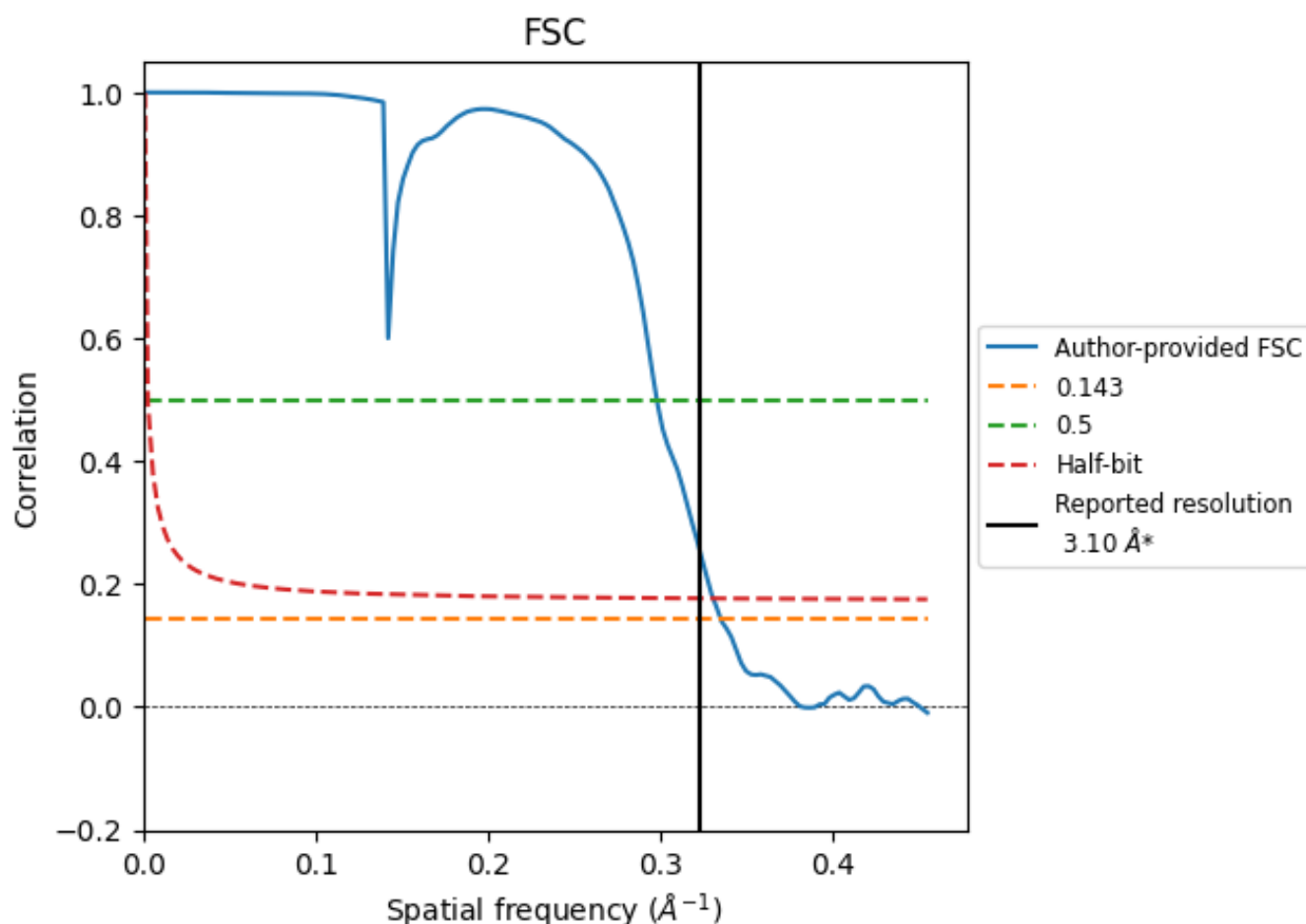


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

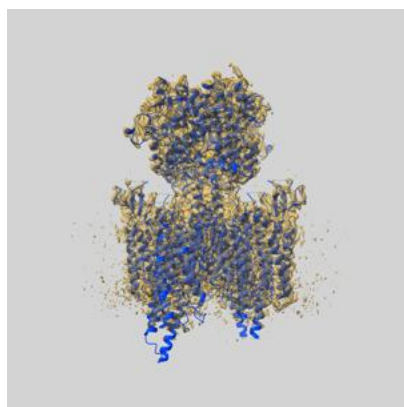
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	2.99	3.36	3.03
Unmasked-calculated*	-	-	-

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

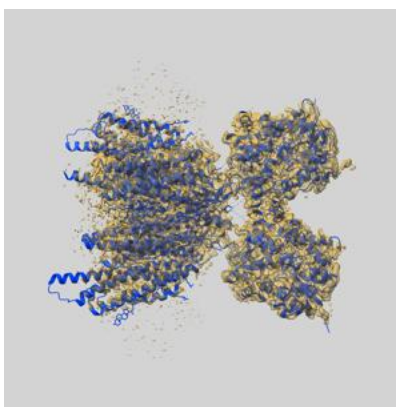
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12805 and PDB model 7OCE. Per-residue inclusion information can be found in section 3 on page 12.

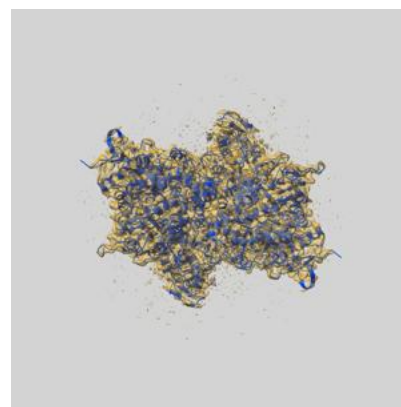
9.1 Map-model overlay [i](#)



X



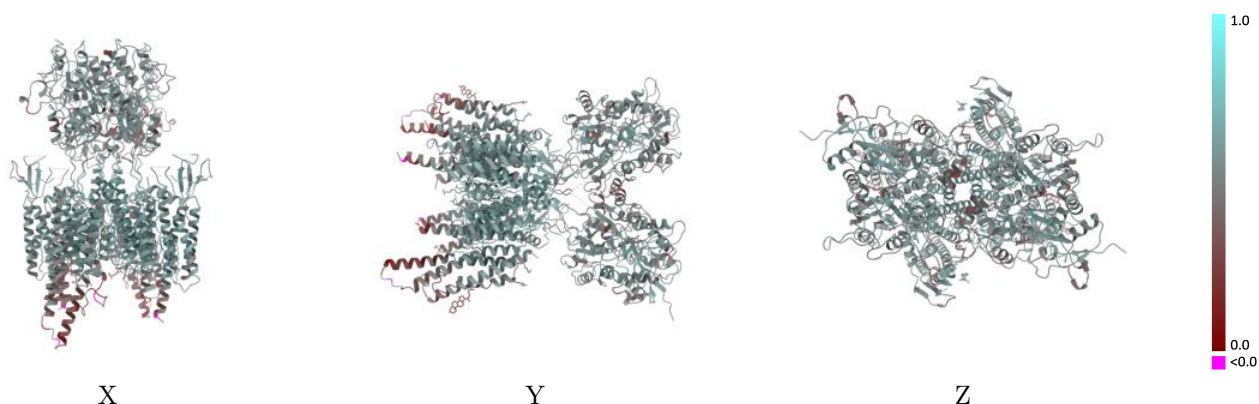
Y



Z

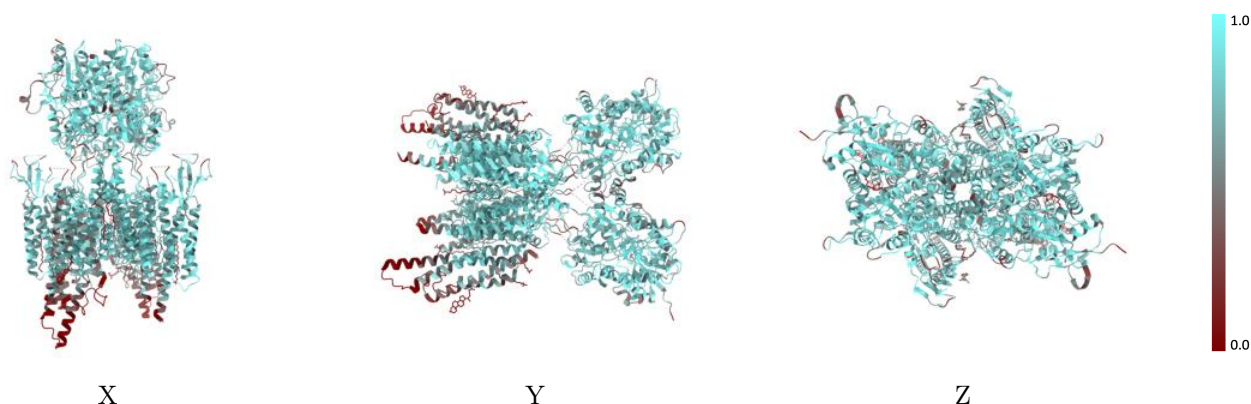
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



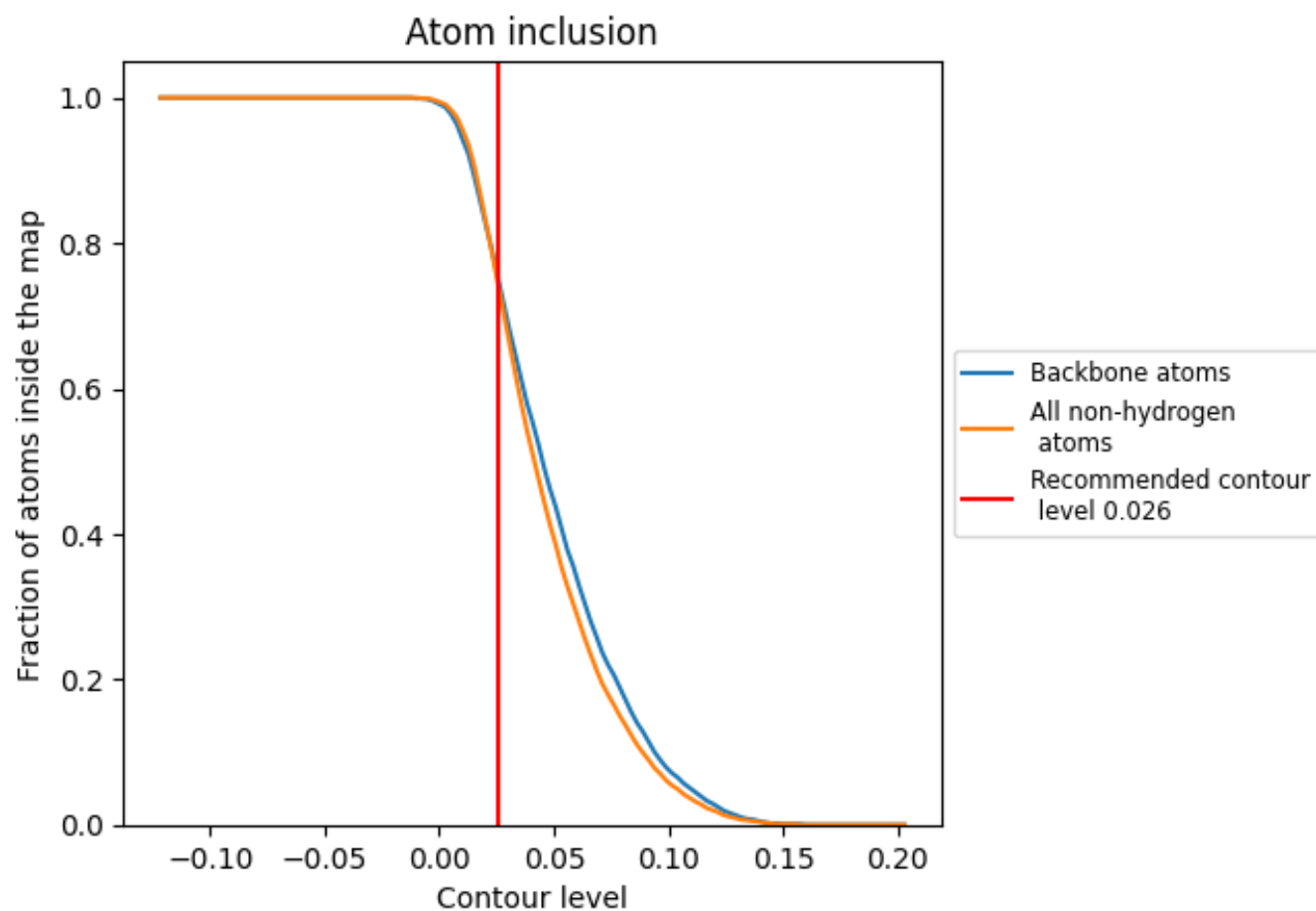
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.5410
A	0.7810	0.5540
B	0.7970	0.5540
C	0.7830	0.5550
D	0.7980	0.5560
E	0.4660	0.4600
G	0.4560	0.4590
I	0.7680	0.5580
J	0.7640	0.5560

1.0

0.0

<0.0