Full wwPDB EM Validation Report (i)

Feb 24, 2024 – 02:24 PM EST

PDB ID	:	7LFT
EMDB ID	:	EMD-23306
Title	:	Cryo-EM structure of human Apo CNGA1 channel in K+/Ca2+
Authors	:	Xue, J.; Han, Y.; Jiang, Y.
Deposited on	:	2021-01-18
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

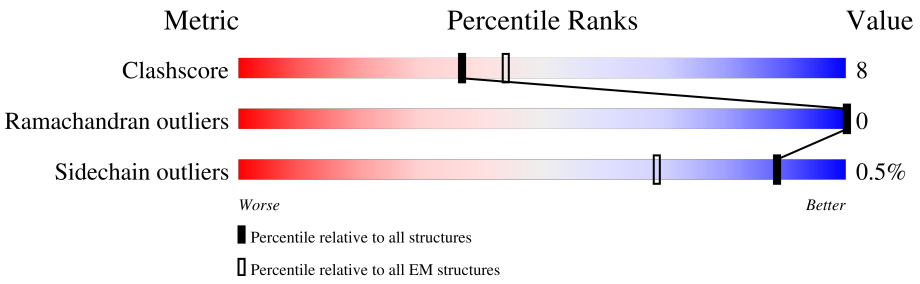
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	560	63% 18% 20%
1	B	560	63% 17% 20%
1	C	560	63% 18% 20%
1	D	560	63% 18% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16595 atoms, of which 1116 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 cGMP-gated cation channel alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	450	3689	2411	595	664	19	0	0
1	B	450	3689	2411	595	664	19	0	0
1	C	450	3689	2411	595	664	19	0	0
1	D	450	3689	2411	595	664	19	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	MET	-	initiating methionine	UNP P29973
A	132	ASP	-	expression tag	UNP P29973
A	133	TYR	-	expression tag	UNP P29973
A	134	LYS	-	expression tag	UNP P29973
A	135	ASP	-	expression tag	UNP P29973
A	136	ASP	-	expression tag	UNP P29973
A	137	ASP	-	expression tag	UNP P29973
A	138	ASP	-	expression tag	UNP P29973
A	139	LYS	-	expression tag	UNP P29973
A	140	GLY	-	expression tag	UNP P29973
A	141	GLY	-	expression tag	UNP P29973
A	142	SER	-	expression tag	UNP P29973
A	143	ALA	-	expression tag	UNP P29973
B	131	MET	-	initiating methionine	UNP P29973
B	132	ASP	-	expression tag	UNP P29973
B	133	TYR	-	expression tag	UNP P29973
B	134	LYS	-	expression tag	UNP P29973
B	135	ASP	-	expression tag	UNP P29973
B	136	ASP	-	expression tag	UNP P29973
B	137	ASP	-	expression tag	UNP P29973
B	138	ASP	-	expression tag	UNP P29973
B	139	LYS	-	expression tag	UNP P29973

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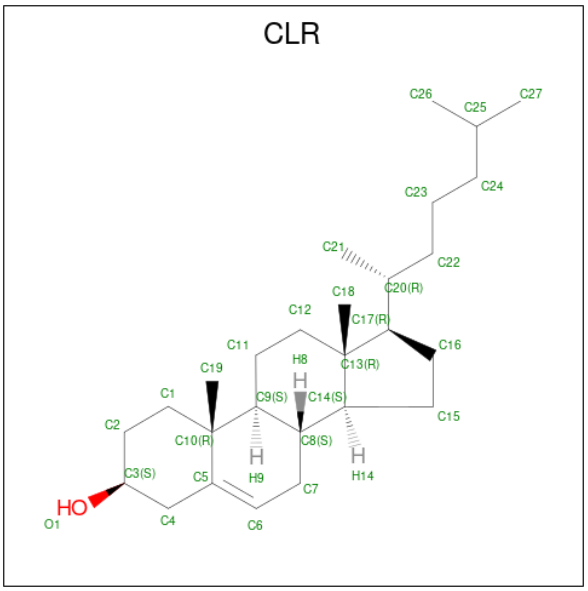
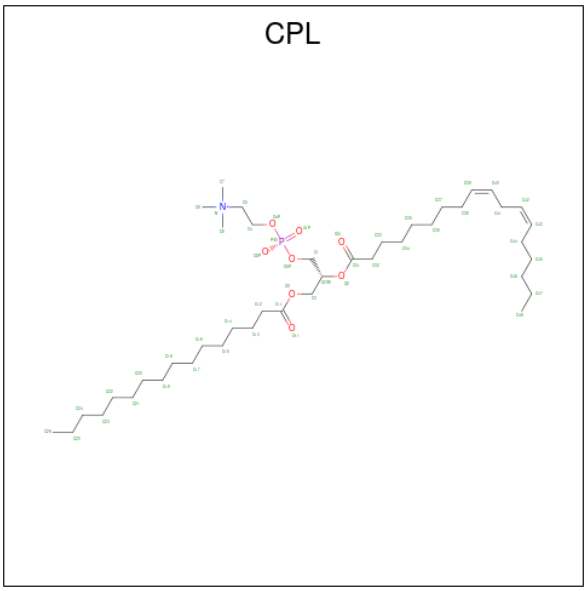
Chain	Residue	Modelled	Actual	Comment	Reference
B	140	GLY	-	expression tag	UNP P29973
B	141	GLY	-	expression tag	UNP P29973
B	142	SER	-	expression tag	UNP P29973
B	143	ALA	-	expression tag	UNP P29973
C	131	MET	-	initiating methionine	UNP P29973
C	132	ASP	-	expression tag	UNP P29973
C	133	TYR	-	expression tag	UNP P29973
C	134	LYS	-	expression tag	UNP P29973
C	135	ASP	-	expression tag	UNP P29973
C	136	ASP	-	expression tag	UNP P29973
C	137	ASP	-	expression tag	UNP P29973
C	138	ASP	-	expression tag	UNP P29973
C	139	LYS	-	expression tag	UNP P29973
C	140	GLY	-	expression tag	UNP P29973
C	141	GLY	-	expression tag	UNP P29973
C	142	SER	-	expression tag	UNP P29973
C	143	ALA	-	expression tag	UNP P29973
D	131	MET	-	initiating methionine	UNP P29973
D	132	ASP	-	expression tag	UNP P29973
D	133	TYR	-	expression tag	UNP P29973
D	134	LYS	-	expression tag	UNP P29973
D	135	ASP	-	expression tag	UNP P29973
D	136	ASP	-	expression tag	UNP P29973
D	137	ASP	-	expression tag	UNP P29973
D	138	ASP	-	expression tag	UNP P29973
D	139	LYS	-	expression tag	UNP P29973
D	140	GLY	-	expression tag	UNP P29973
D	141	GLY	-	expression tag	UNP P29973
D	142	SER	-	expression tag	UNP P29973
D	143	ALA	-	expression tag	UNP P29973

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			74	27	46	1	
2	A	1	Total	C	H	O	0
			74	27	46	1	
2	B	1	Total	C	H	O	0
			74	27	46	1	
2	B	1	Total	C	H	O	0
			74	27	46	1	
2	C	1	Total	C	H	O	0
			74	27	46	1	
2	C	1	Total	C	H	O	0
			74	27	46	1	
2	D	1	Total	C	H	O	0
			74	27	46	1	
2	D	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 3 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H 47 16 31	0
3	A	1	Total C H 29 10 19	0
3	A	1	Total C H 41 14 27	0
3	A	1	Total C H O P 58 20 29 8 1	0
3	A	1	Total C H O P 88 29 50 8 1	0
3	A	1	Total C H 47 16 31	0
3	B	1	Total C H 47 16 31	0
3	B	1	Total C H 29 10 19	0
3	B	1	Total C H 41 14 27	0
3	B	1	Total C H O P 58 20 29 8 1	0
3	B	1	Total C H O P 88 29 50 8 1	0
3	B	1	Total C H 47 16 31	0
3	C	1	Total C H 47 16 31	0
3	C	1	Total C H 29 10 19	0

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Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C H 41 14 27	0
3	C	1	Total C H O P 58 20 29 8 1	0
3	C	1	Total C H O P 88 29 50 8 1	0
3	C	1	Total C H 47 16 31	0
3	D	1	Total C H 47 16 31	0
3	D	1	Total C H 29 10 19	0
3	D	1	Total C H 41 14 27	0
3	D	1	Total C H O P 58 20 29 8 1	0
3	D	1	Total C H O P 88 29 50 8 1	0
3	D	1	Total C H 47 16 31	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	3	Total K 3 3	0

- Molecule 5 is water.

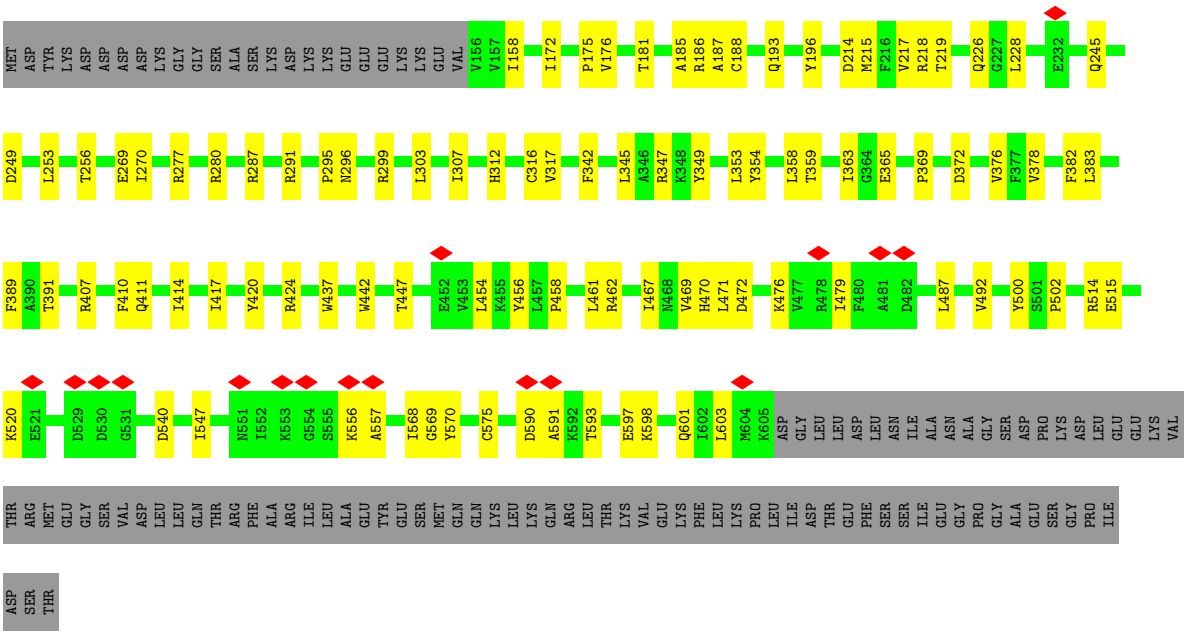
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total O 1 1	0
5	B	1	Total O 1 1	0
5	C	1	Total O 1 1	0
5	D	1	Total O 1 1	0

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.

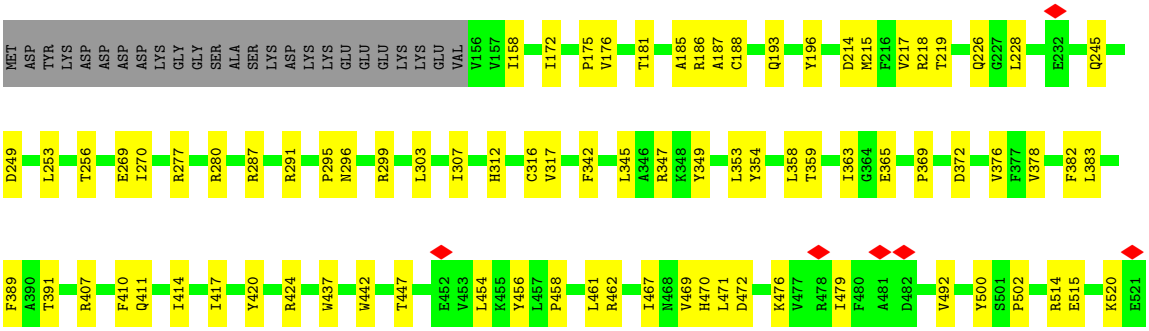
• Molecule 1: cGMP-gated cation channel alpha-1

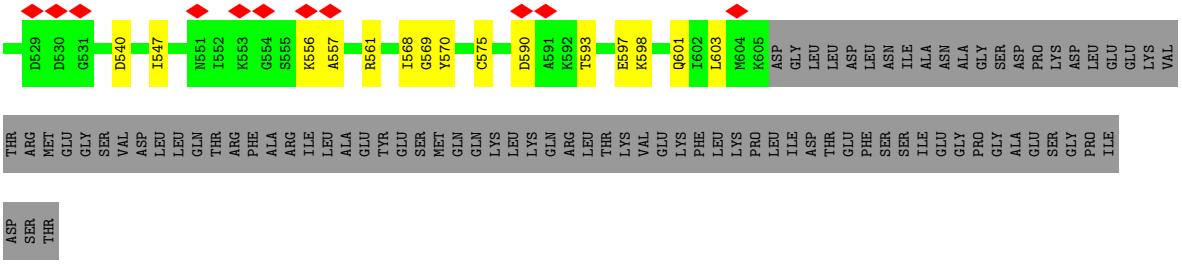
Chain A: 63% 18% 20%



• Molecule 1: cGMP-gated cation channel alpha-1

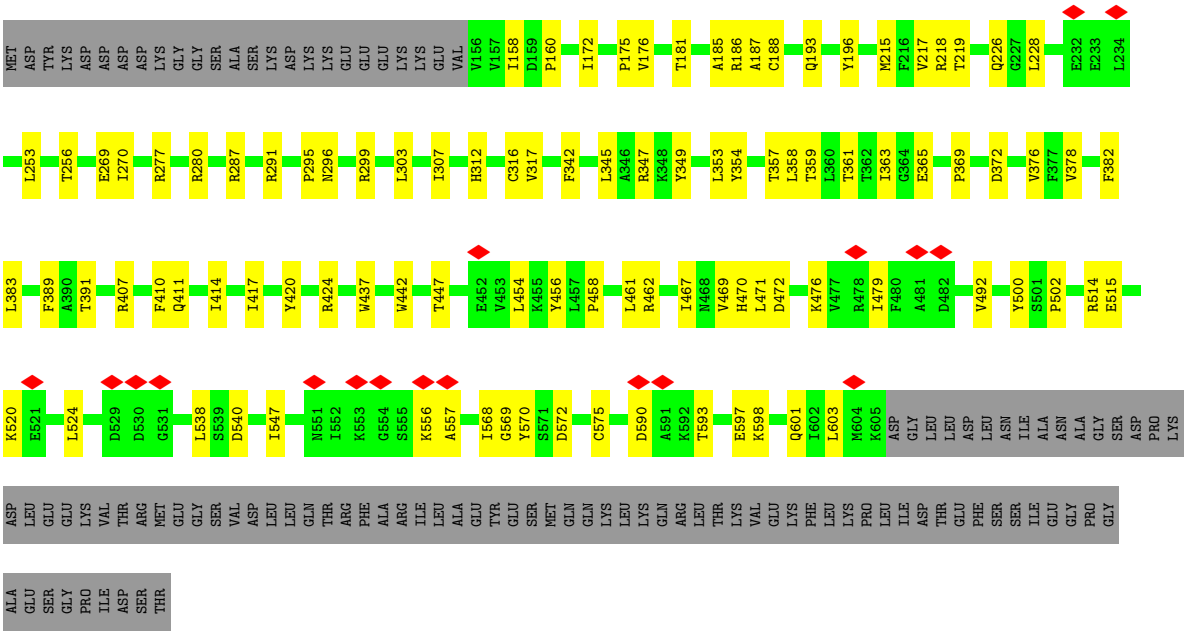
Chain B: 63% 17% 20%





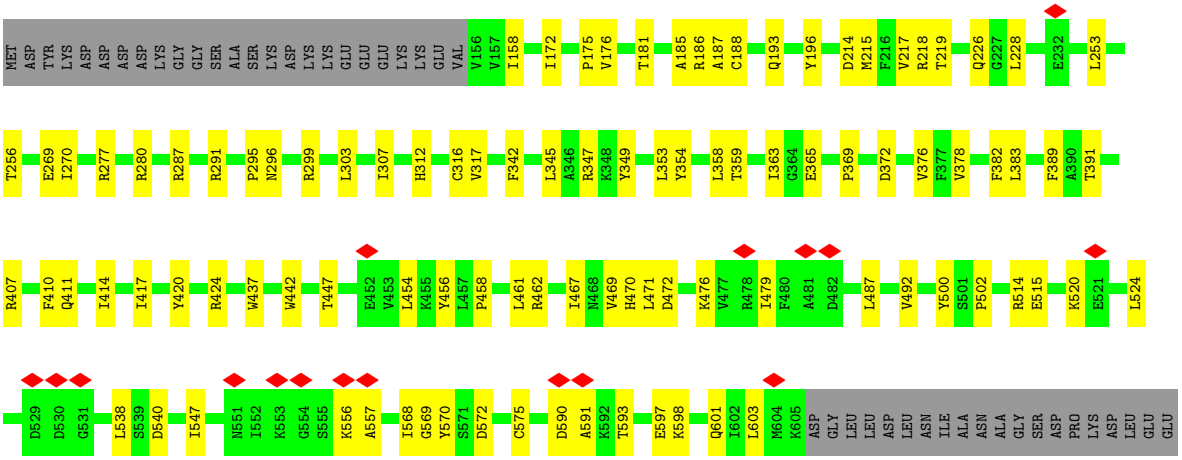
• Molecule 1: cGMP-gated cation channel alpha-1

Chain C:



• Molecule 1: cGMP-gated cation channel alpha-1

Chain D:



LYS VAL THR ARG MET GLU GLY SER VAL ASP LEU LEU GLN THR ARG PHE ALA ARG ILE LEU ALA GLU TYR GLU SER MET GLN GLN LYS LEU LYS GLN ARG LEU THR LYS VAL GLU LYS PHE LEU LYS PRO LEU ILE ASP THR GLU PHE SER SER ILE GLU GLY PRO GLY ALA GLU SER GLY

PRO ILE ASP SER THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	274333	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	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	0.138	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	243.07199, 243.07199, 243.07199	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.844, 0.844, 0.844	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: K, CLR, CPL

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	0.39	0/3774	0.44	0/5113
1	B	0.39	0/3774	0.44	0/5113
1	C	0.39	0/3774	0.44	0/5113
1	D	0.39	0/3774	0.44	0/5113
All	All	0.39	0/15096	0.44	0/20452

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	3689	0	3738	64	0
1	B	3689	0	3738	64	0
1	C	3689	0	3738	67	0
1	D	3689	0	3738	63	0
2	A	56	92	92	8	0
2	B	56	92	92	9	0
2	C	56	92	92	8	0
2	D	56	92	92	7	0
3	A	123	187	187	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	123	187	187	8	0
3	C	123	187	187	8	0
3	D	123	187	187	8	0
4	A	3	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	15479	1116	16068	262	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 8.

All (262) 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)
4:A:710:K:K	4:A:711:K:K	1.83	0.82
1:B:345:LEU:HD23	2:B:700:CLR:H11	1.73	0.71
1:C:345:LEU:HD23	2:C:700:CLR:H11	1.73	0.71
1:A:345:LEU:HD23	2:A:701:CLR:H11	1.73	0.71
1:D:345:LEU:HD23	2:D:700:CLR:H11	1.73	0.70
3:A:706:CPL:O31	3:A:706:CPL:H342	1.93	0.68
3:B:705:CPL:O31	3:B:705:CPL:H342	1.94	0.67
3:D:705:CPL:O31	3:D:705:CPL:H342	1.93	0.67
3:C:705:CPL:O31	3:C:705:CPL:H342	1.93	0.66
1:B:186:ARG:HB3	1:B:193:GLN:HB2	1.83	0.61
1:C:186:ARG:HB3	1:C:193:GLN:HB2	1.83	0.60
1:C:442:TRP:HE3	1:C:447:THR:HG21	1.67	0.60
1:A:186:ARG:HB3	1:A:193:GLN:HB2	1.83	0.60
1:D:186:ARG:HB3	1:D:193:GLN:HB2	1.83	0.60
1:D:442:TRP:HE3	1:D:447:THR:HG21	1.67	0.60
1:B:442:TRP:HE3	1:B:447:THR:HG21	1.67	0.59
1:C:383:LEU:HD12	3:C:706:CPL:H222	1.85	0.59
1:A:383:LEU:HD12	3:A:707:CPL:H222	1.85	0.59
1:B:383:LEU:HD12	3:B:706:CPL:H222	1.85	0.59
1:D:383:LEU:HD12	3:D:706:CPL:H222	1.85	0.59
1:B:363:ILE:HG22	1:B:365:GLU:HG2	1.85	0.59
1:A:470:HIS:HB2	1:A:492:VAL:HG13	1.85	0.58
1:C:363:ILE:HG22	1:C:365:GLU:HG2	1.85	0.58
1:A:442:TRP:HE3	1:A:447:THR:HG21	1.67	0.58
1:D:470:HIS:HB2	1:D:492:VAL:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:HG22	1:A:365:GLU:HG2	1.85	0.57
1:D:363:ILE:HG22	1:D:365:GLU:HG2	1.85	0.57
1:B:470:HIS:HB2	1:B:492:VAL:HG13	1.85	0.57
1:C:470:HIS:HB2	1:C:492:VAL:HG13	1.85	0.57
1:B:317:VAL:HG22	3:B:705:CPL:H132	1.88	0.56
1:B:442:TRP:CE3	1:B:447:THR:HG21	2.40	0.56
1:C:317:VAL:HG22	3:C:705:CPL:H132	1.88	0.56
1:C:442:TRP:CE3	1:C:447:THR:HG21	2.40	0.56
1:A:442:TRP:CE3	1:A:447:THR:HG21	2.40	0.55
1:D:442:TRP:CE3	1:D:447:THR:HG21	2.40	0.55
1:A:317:VAL:HG22	3:A:706:CPL:H132	1.88	0.55
1:D:317:VAL:HG22	3:D:705:CPL:H132	1.88	0.55
2:B:700:CLR:H162	2:B:700:CLR:H232	1.89	0.55
2:C:700:CLR:H232	2:C:700:CLR:H162	1.89	0.55
2:D:700:CLR:H162	2:D:700:CLR:H232	1.89	0.54
2:A:701:CLR:H162	2:A:701:CLR:H232	1.89	0.54
1:D:196:TYR:CD1	2:D:701:CLR:H42	2.43	0.54
1:A:515:GLU:HB3	1:A:575:CYS:SG	2.49	0.53
1:B:196:TYR:CD1	2:B:701:CLR:H42	2.43	0.53
1:C:196:TYR:CD1	2:C:701:CLR:H42	2.43	0.53
1:A:547:ILE:HG21	1:A:603:LEU:HD21	1.91	0.53
1:B:515:GLU:HB3	1:B:575:CYS:SG	2.49	0.53
1:B:547:ILE:HG21	1:B:603:LEU:HD21	1.91	0.53
1:A:196:TYR:CD1	2:A:702:CLR:H42	2.43	0.53
1:C:547:ILE:HG21	1:C:603:LEU:HD21	1.91	0.53
1:A:456:TYR:HB2	1:D:417:ILE:HD11	1.91	0.53
1:D:181:THR:O	1:D:312:HIS:NE2	2.42	0.53
1:C:417:ILE:HD11	1:D:456:TYR:HB2	1.92	0.52
1:C:515:GLU:HB3	1:C:575:CYS:SG	2.49	0.52
1:D:547:ILE:HG21	1:D:603:LEU:HD21	1.91	0.52
1:D:515:GLU:HB3	1:D:575:CYS:SG	2.49	0.52
1:D:185:ALA:HB2	1:D:312:HIS:CE1	2.45	0.51
1:A:417:ILE:HD11	1:B:456:TYR:HB2	1.92	0.51
1:C:181:THR:O	1:C:312:HIS:NE2	2.42	0.51
1:A:185:ALA:HB2	1:A:312:HIS:CE1	2.45	0.51
1:B:417:ILE:HD11	1:C:456:TYR:HB2	1.92	0.51
1:C:185:ALA:HB2	1:C:312:HIS:CE1	2.45	0.51
1:B:185:ALA:HB2	1:B:312:HIS:CE1	2.45	0.51
1:A:303:LEU:O	1:A:307:ILE:HG12	2.12	0.50
1:B:181:THR:O	1:B:312:HIS:NE2	2.42	0.50
1:D:342:PHE:HA	1:D:347:ARG:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:O	1:B:307:ILE:HG12	2.12	0.49
1:D:303:LEU:O	1:D:307:ILE:HG12	2.12	0.49
1:A:181:THR:O	1:A:312:HIS:NE2	2.42	0.49
1:C:303:LEU:O	1:C:307:ILE:HG12	2.11	0.49
2:A:702:CLR:C23	2:A:702:CLR:H162	2.43	0.49
2:C:701:CLR:H162	2:C:701:CLR:C23	2.43	0.49
1:A:376:VAL:HG11	3:A:707:CPL:H351	1.95	0.49
1:C:376:VAL:HG11	3:C:706:CPL:H351	1.95	0.49
1:B:376:VAL:HG11	3:B:706:CPL:H351	1.95	0.49
1:C:357:THR:O	1:C:361:THR:OG1	2.27	0.49
1:B:215:MET:O	1:B:219:THR:HG23	2.13	0.48
1:C:342:PHE:HA	1:C:347:ARG:HG2	1.94	0.48
1:D:376:VAL:HG11	3:D:706:CPL:H351	1.95	0.48
1:A:215:MET:O	1:A:219:THR:HG23	2.13	0.48
1:C:215:MET:O	1:C:219:THR:HG23	2.13	0.48
1:D:215:MET:O	1:D:219:THR:HG23	2.13	0.48
1:B:342:PHE:HA	1:B:347:ARG:HG2	1.94	0.48
1:A:342:PHE:HA	1:A:347:ARG:HG2	1.94	0.48
2:D:701:CLR:C23	2:D:701:CLR:H162	2.43	0.48
1:A:296:ASN:OD1	1:A:299:ARG:NH1	2.47	0.47
1:B:472:ASP:O	1:B:476:LYS:HG2	2.14	0.47
2:B:701:CLR:C23	2:B:701:CLR:H162	2.43	0.47
1:C:296:ASN:OD1	1:C:299:ARG:NH1	2.47	0.47
1:D:597:GLU:OE2	1:D:601:GLN:NE2	2.44	0.47
1:D:296:ASN:OD1	1:D:299:ARG:NH1	2.47	0.47
1:B:296:ASN:OD1	1:B:299:ARG:NH1	2.47	0.47
1:B:540:ASP:HB3	1:C:226:GLN:HE22	1.79	0.47
1:C:472:ASP:O	1:C:476:LYS:HG2	2.14	0.47
1:A:353:LEU:HD21	3:B:706:CPL:H191	1.96	0.47
3:A:707:CPL:H191	1:D:353:LEU:HD21	1.96	0.47
1:A:467:ILE:HG23	1:A:471:LEU:HD13	1.96	0.47
1:A:568:ILE:HG22	1:B:228:LEU:HD21	1.97	0.47
1:B:353:LEU:HD21	3:C:706:CPL:H191	1.95	0.47
1:D:472:ASP:O	1:D:476:LYS:HG2	2.14	0.47
1:C:467:ILE:HG23	1:C:471:LEU:HD13	1.96	0.47
1:A:226:GLN:HE22	1:D:540:ASP:HB3	1.80	0.47
1:B:369:PRO:HG3	1:B:378:VAL:HG21	1.98	0.46
1:A:228:LEU:HD21	1:D:568:ILE:HG22	1.97	0.46
1:A:472:ASP:O	1:A:476:LYS:HG2	2.14	0.46
1:A:540:ASP:HB3	1:B:226:GLN:HE22	1.79	0.46
1:B:568:ILE:HG22	1:C:228:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ALA:HB1	1:D:269:GLU:HG3	1.98	0.46
1:C:568:ILE:HG22	1:D:228:LEU:HD21	1.97	0.46
1:B:467:ILE:HG23	1:B:471:LEU:HD13	1.96	0.46
1:C:369:PRO:HG3	1:C:378:VAL:HG21	1.98	0.46
1:D:514:ARG:HG3	1:D:515:GLU:HG3	1.98	0.46
1:B:514:ARG:HG3	1:B:515:GLU:HG3	1.98	0.46
1:C:353:LEU:HD21	3:D:706:CPL:H191	1.96	0.46
1:C:514:ARG:HG3	1:C:515:GLU:HG3	1.98	0.46
1:A:187:ALA:HB1	1:A:269:GLU:HG3	1.98	0.46
1:A:514:ARG:HG3	1:A:515:GLU:HG3	1.98	0.46
1:C:187:ALA:HB1	1:C:269:GLU:HG3	1.98	0.46
1:D:369:PRO:HG3	1:D:378:VAL:HG21	1.98	0.45
1:A:369:PRO:HG3	1:A:378:VAL:HG21	1.98	0.45
1:C:540:ASP:HB3	1:D:226:GLN:HE22	1.80	0.45
1:B:312:HIS:CG	2:B:700:CLR:H263	2.52	0.45
1:B:188:CYS:SG	1:B:316:CYS:HB3	2.57	0.45
2:B:700:CLR:H232	2:B:700:CLR:C16	2.46	0.45
1:D:188:CYS:SG	1:D:316:CYS:HB3	2.57	0.45
1:D:467:ILE:HG23	1:D:471:LEU:HD13	1.96	0.45
1:B:187:ALA:HB1	1:B:269:GLU:HG3	1.98	0.45
2:D:700:CLR:H232	2:D:700:CLR:C16	2.46	0.45
1:A:597:GLU:OE2	1:A:601:GLN:NE2	2.44	0.45
1:C:312:HIS:CG	2:C:700:CLR:H263	2.52	0.45
1:D:287:ARG:O	1:D:291:ARG:HB2	2.17	0.45
1:A:188:CYS:SG	1:A:316:CYS:HB3	2.57	0.45
1:C:188:CYS:SG	1:C:316:CYS:HB3	2.57	0.45
1:A:287:ARG:O	1:A:291:ARG:HB2	2.17	0.45
2:A:701:CLR:H232	2:A:701:CLR:C16	2.47	0.45
1:B:354:TYR:CZ	1:B:358:LEU:HD11	2.52	0.45
1:A:359:THR:HG23	1:A:382:PHE:CE1	2.53	0.44
1:C:354:TYR:CZ	1:C:358:LEU:HD11	2.52	0.44
1:C:597:GLU:OE2	1:C:601:GLN:NE2	2.44	0.44
1:D:312:HIS:CG	2:D:700:CLR:H263	2.52	0.44
1:A:312:HIS:CG	2:A:701:CLR:H263	2.52	0.44
1:C:287:ARG:O	1:C:291:ARG:HB2	2.17	0.44
1:C:359:THR:HG23	1:C:382:PHE:CE1	2.53	0.44
1:A:590:ASP:HA	1:A:593:THR:HG22	2.00	0.44
1:B:287:ARG:O	1:B:291:ARG:HB2	2.17	0.44
1:B:410:PHE:CE2	1:B:414:ILE:HD11	2.53	0.44
1:C:590:ASP:HA	1:C:593:THR:HG22	2.00	0.44
2:C:700:CLR:H232	2:C:700:CLR:C16	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ASP:HA	1:B:593:THR:HG22	2.00	0.44
1:D:354:TYR:CZ	1:D:358:LEU:HD11	2.53	0.44
1:D:359:THR:HG23	1:D:382:PHE:CE1	2.53	0.44
1:A:214:ASP:OD1	1:A:280:ARG:NE	2.43	0.44
1:D:172:ILE:O	1:D:175:PRO:HD2	2.18	0.44
1:D:590:ASP:HA	1:D:593:THR:HG22	2.00	0.44
1:A:410:PHE:CE2	1:A:414:ILE:HD11	2.53	0.44
2:B:700:CLR:H162	2:B:700:CLR:C23	2.46	0.44
1:D:469:VAL:HG13	1:D:520:LYS:HE2	2.00	0.44
1:A:469:VAL:HG13	1:A:520:LYS:HE2	2.00	0.44
1:B:172:ILE:O	1:B:175:PRO:HD2	2.18	0.44
1:C:410:PHE:CE2	1:C:414:ILE:HD11	2.53	0.44
1:A:354:TYR:CZ	1:A:358:LEU:HD11	2.53	0.43
1:A:479:ILE:HA	1:A:598:LYS:HD2	2.00	0.43
1:B:359:THR:HG23	1:B:382:PHE:CE1	2.53	0.43
1:C:172:ILE:O	1:C:175:PRO:HD2	2.18	0.43
1:C:372:ASP:H	3:C:706:CPL:C5	2.31	0.43
1:B:372:ASP:H	3:B:706:CPL:C5	2.31	0.43
1:C:469:VAL:HG13	1:C:520:LYS:HE2	2.00	0.43
1:A:500:TYR:O	1:A:570:TYR:HA	2.19	0.43
1:C:424:ARG:NH1	1:D:572:ASP:OD2	2.51	0.43
1:B:500:TYR:O	1:B:570:TYR:HA	2.19	0.43
1:D:500:TYR:O	1:D:570:TYR:HA	2.19	0.43
1:A:345:LEU:CD2	2:A:701:CLR:H11	2.47	0.43
1:B:469:VAL:HG13	1:B:520:LYS:HE2	2.00	0.43
1:B:479:ILE:HA	1:B:598:LYS:HD2	2.00	0.43
1:D:372:ASP:H	3:D:706:CPL:C5	2.31	0.43
1:D:410:PHE:CE2	1:D:414:ILE:HD11	2.53	0.43
1:B:515:GLU:O	1:B:561:ARG:NH2	2.35	0.43
1:D:479:ILE:HA	1:D:598:LYS:HD2	2.00	0.43
1:B:424:ARG:NH1	1:C:572:ASP:OD2	2.51	0.43
1:B:556:LYS:HG3	1:B:557:ALA:H	1.84	0.43
1:C:407:ARG:NH1	1:C:411:GLN:OE1	2.52	0.43
1:C:556:LYS:HG3	1:C:557:ALA:H	1.84	0.42
1:D:407:ARG:NH1	1:D:411:GLN:OE1	2.52	0.42
1:D:556:LYS:HG3	1:D:557:ALA:H	1.84	0.42
1:A:172:ILE:O	1:A:175:PRO:HD2	2.18	0.42
1:A:372:ASP:H	3:A:707:CPL:C5	2.31	0.42
1:C:349:TYR:CE1	2:C:700:CLR:H213	2.54	0.42
1:A:420:TYR:CZ	1:A:424:ARG:HG3	2.54	0.42
3:A:706:CPL:H122	3:A:706:CPL:H341	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:TYR:CZ	1:C:424:ARG:HG3	2.54	0.42
3:C:705:CPL:H341	3:C:705:CPL:H122	2.02	0.42
1:D:158:ILE:HD12	1:D:217:VAL:HG13	2.01	0.42
1:A:407:ARG:NH1	1:A:411:GLN:OE1	2.52	0.42
1:A:437:TRP:CZ2	1:B:458:PRO:HG3	2.55	0.42
1:B:158:ILE:HD12	1:B:217:VAL:HG13	2.01	0.42
3:B:705:CPL:H122	3:B:705:CPL:H341	2.02	0.42
1:C:437:TRP:CZ2	1:D:458:PRO:HG3	2.54	0.42
1:A:158:ILE:HD12	1:A:217:VAL:HG13	2.01	0.42
1:B:345:LEU:CD2	2:B:700:CLR:H11	2.47	0.42
1:B:597:GLU:OE2	1:B:601:GLN:NE2	2.44	0.42
1:A:349:TYR:CE1	2:A:701:CLR:H213	2.54	0.42
1:B:437:TRP:CZ2	1:C:458:PRO:HG3	2.54	0.42
1:A:458:PRO:HG3	1:D:437:TRP:CZ2	2.55	0.42
1:B:218:ARG:HH11	1:B:280:ARG:HD3	1.85	0.42
1:B:407:ARG:NH1	1:B:411:GLN:OE1	2.52	0.42
3:D:705:CPL:H341	3:D:705:CPL:H122	2.02	0.42
1:C:158:ILE:HD12	1:C:217:VAL:HG13	2.01	0.42
1:D:176:VAL:HG22	1:D:277:ARG:HB3	2.02	0.42
1:A:556:LYS:HG3	1:A:557:ALA:H	1.84	0.42
1:C:391:THR:HG21	3:C:702:CPL:H121	2.02	0.42
1:C:479:ILE:HA	1:C:598:LYS:HD2	2.00	0.42
1:D:349:TYR:CE1	2:D:700:CLR:H213	2.54	0.42
1:D:420:TYR:CZ	1:D:424:ARG:HG3	2.54	0.42
1:C:500:TYR:O	1:C:570:TYR:HA	2.19	0.42
1:C:524:LEU:O	1:C:538:LEU:N	2.50	0.42
1:A:295:PRO:O	1:A:299:ARG:HB2	2.20	0.41
1:B:420:TYR:CZ	1:B:424:ARG:HG3	2.54	0.41
1:D:214:ASP:OD1	1:D:280:ARG:NE	2.43	0.41
1:A:176:VAL:HG22	1:A:277:ARG:HB3	2.01	0.41
1:A:218:ARG:HH11	1:A:280:ARG:HD3	1.85	0.41
1:B:176:VAL:HG22	1:B:277:ARG:HB3	2.01	0.41
1:B:295:PRO:O	1:B:299:ARG:HB2	2.20	0.41
1:B:349:TYR:CE1	2:B:700:CLR:H213	2.54	0.41
1:D:218:ARG:HH11	1:D:280:ARG:HD3	1.85	0.41
1:A:556:LYS:HG3	1:A:557:ALA:N	2.36	0.41
1:D:556:LYS:HG3	1:D:557:ALA:N	2.36	0.41
1:D:256:THR:O	1:D:270:ILE:HD12	2.21	0.41
1:A:391:THR:HG21	3:A:703:CPL:H121	2.02	0.41
1:A:458:PRO:HD2	1:A:461:LEU:HB3	2.02	0.41
1:C:185:ALA:HB2	1:C:312:HIS:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:PRO:O	1:D:299:ARG:HB2	2.20	0.41
1:D:454:LEU:HB3	1:D:462:ARG:HG3	2.03	0.41
1:B:458:PRO:HD2	1:B:461:LEU:HB3	2.02	0.41
1:B:556:LYS:HG3	1:B:557:ALA:N	2.36	0.41
1:C:295:PRO:O	1:C:299:ARG:HB2	2.20	0.41
1:A:454:LEU:HB3	1:A:462:ARG:HG3	2.03	0.41
1:B:245:GLN:NE2	1:B:249:ASP:OD1	2.52	0.41
1:B:454:LEU:HB3	1:B:462:ARG:HG3	2.03	0.41
1:C:176:VAL:HG22	1:C:277:ARG:HB3	2.01	0.41
1:C:454:LEU:HB3	1:C:462:ARG:HG3	2.03	0.41
1:C:556:LYS:HG3	1:C:557:ALA:N	2.36	0.41
1:D:391:THR:HG21	3:D:702:CPL:H121	2.02	0.41
1:D:458:PRO:HD2	1:D:461:LEU:HB3	2.02	0.41
1:B:256:THR:O	1:B:270:ILE:HD12	2.21	0.41
1:C:256:THR:O	1:C:270:ILE:HD12	2.21	0.41
1:C:502:PRO:CA	1:C:569:GLY:HA2	2.51	0.41
1:D:524:LEU:O	1:D:538:LEU:N	2.50	0.41
1:A:245:GLN:NE2	1:A:249:ASP:OD1	2.52	0.40
1:A:487:LEU:HD22	1:A:591:ALA:HB1	2.03	0.40
1:C:218:ARG:HH11	1:C:280:ARG:HD3	1.85	0.40
1:C:277:ARG:HD3	1:C:277:ARG:HA	1.91	0.40
1:A:277:ARG:HD3	1:A:277:ARG:HA	1.92	0.40
1:B:391:THR:HG21	3:B:702:CPL:H121	2.02	0.40
1:B:502:PRO:CA	1:B:569:GLY:HA2	2.52	0.40
1:C:458:PRO:HD2	1:C:461:LEU:HB3	2.02	0.40
1:D:487:LEU:HD22	1:D:591:ALA:HB1	2.04	0.40
1:C:345:LEU:CD2	2:C:700:CLR:H11	2.47	0.40
1:D:502:PRO:CA	1:D:569:GLY:HA2	2.51	0.40
1:A:256:THR:O	1:A:270:ILE:HD12	2.21	0.40
1:B:214:ASP:OD1	1:B:280:ARG:NE	2.43	0.40
1:C:160:PRO:O	1:C:287:ARG:NH2	2.55	0.40
1:A:502:PRO:CA	1:A:569:GLY:HA2	2.52	0.40

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	448/560 (80%)	437 (98%)	11 (2%)	0	100	100
1	B	448/560 (80%)	437 (98%)	11 (2%)	0	100	100
1	C	448/560 (80%)	437 (98%)	11 (2%)	0	100	100
1	D	448/560 (80%)	437 (98%)	11 (2%)	0	100	100
All	All	1792/2240 (80%)	1748 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/502 (81%)	404 (100%)	2 (0%)	88	96
1	B	406/502 (81%)	404 (100%)	2 (0%)	88	96
1	C	406/502 (81%)	404 (100%)	2 (0%)	88	96
1	D	406/502 (81%)	404 (100%)	2 (0%)	88	96
All	All	1624/2008 (81%)	1616 (100%)	8 (0%)	89	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	LEU
1	A	389	PHE
1	B	253	LEU
1	B	389	PHE
1	C	253	LEU
1	C	389	PHE
1	D	253	LEU
1	D	389	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	A	470	HIS
1	A	496	GLN
1	A	534	GLN
1	A	559	ASN
1	B	226	GLN
1	B	470	HIS
1	B	496	GLN
1	B	534	GLN
1	B	559	ASN
1	C	226	GLN
1	C	470	HIS
1	C	496	GLN
1	C	534	GLN
1	C	559	ASN
1	D	226	GLN
1	D	470	HIS
1	D	496	GLN
1	D	534	GLN
1	D	559	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 3 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CPL	C	706	-	37,37,51	1.35	3 (8%)	40,42,59	1.40	5 (12%)
3	CPL	A	706	-	28,28,51	1.50	7 (25%)	31,33,59	1.57	5 (16%)
2	CLR	B	700	-	31,31,31	1.01	2 (6%)	48,48,48	1.68	12 (25%)
2	CLR	C	701	-	31,31,31	1.13	2 (6%)	48,48,48	2.15	20 (41%)
3	CPL	B	705	-	28,28,51	1.51	7 (25%)	31,33,59	1.56	5 (16%)
3	CPL	A	707	-	37,37,51	1.35	3 (8%)	40,42,59	1.40	5 (12%)
3	CPL	D	706	-	37,37,51	1.35	3 (8%)	40,42,59	1.40	5 (12%)
2	CLR	A	701	-	31,31,31	1.01	2 (6%)	48,48,48	1.68	12 (25%)
3	CPL	C	705	-	28,28,51	1.51	7 (25%)	31,33,59	1.57	5 (16%)
3	CPL	A	704	-	9,9,51	0.22	0	8,8,59	0.54	0
2	CLR	A	702	-	31,31,31	1.14	2 (6%)	48,48,48	2.15	20 (41%)
3	CPL	D	704	-	13,13,51	0.23	0	12,12,59	0.59	0
3	CPL	D	703	-	9,9,51	0.22	0	8,8,59	0.54	0
3	CPL	A	703	-	15,15,51	0.85	0	14,14,59	0.80	0
3	CPL	C	707	-	15,15,51	0.23	0	14,14,59	0.61	0
3	CPL	A	705	-	13,13,51	0.23	0	12,12,59	0.59	0
2	CLR	D	700	-	31,31,31	1.01	2 (6%)	48,48,48	1.68	12 (25%)
3	CPL	D	702	-	15,15,51	0.85	0	14,14,59	0.79	0
2	CLR	D	701	-	31,31,31	1.13	2 (6%)	48,48,48	2.15	20 (41%)
3	CPL	A	708	-	15,15,51	0.23	0	14,14,59	0.62	0
3	CPL	B	704	-	13,13,51	0.23	0	12,12,59	0.59	0
3	CPL	C	704	-	13,13,51	0.23	0	12,12,59	0.59	0
3	CPL	D	705	-	28,28,51	1.51	7 (25%)	31,33,59	1.57	5 (16%)
2	CLR	C	700	-	31,31,31	1.01	2 (6%)	48,48,48	1.68	11 (22%)
2	CLR	B	701	-	31,31,31	1.14	2 (6%)	48,48,48	2.15	20 (41%)
3	CPL	B	703	-	9,9,51	0.22	0	8,8,59	0.55	0
3	CPL	B	706	-	37,37,51	1.35	3 (8%)	40,42,59	1.40	5 (12%)
3	CPL	C	703	-	9,9,51	0.22	0	8,8,59	0.55	0
3	CPL	C	702	-	15,15,51	0.85	0	14,14,59	0.79	0
3	CPL	B	707	-	15,15,51	0.22	0	14,14,59	0.61	0
3	CPL	D	707	-	15,15,51	0.23	0	14,14,59	0.61	0
3	CPL	B	702	-	15,15,51	0.85	0	14,14,59	0.80	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	CPL	C	706	-	-	17/41/41/55	-
3	CPL	A	706	-	-	13/32/32/55	-
2	CLR	B	700	-	-	6/10/68/68	0/4/4/4
2	CLR	C	701	-	-	3/10/68/68	0/4/4/4
3	CPL	B	705	-	-	13/32/32/55	-
3	CPL	A	707	-	-	17/41/41/55	-
3	CPL	D	706	-	-	17/41/41/55	-
2	CLR	A	701	-	-	6/10/68/68	0/4/4/4
3	CPL	C	705	-	-	13/32/32/55	-
3	CPL	A	704	-	-	6/7/7/55	-
2	CLR	A	702	-	-	3/10/68/68	0/4/4/4
3	CPL	D	704	-	-	7/11/11/55	-
3	CPL	D	703	-	-	6/7/7/55	-
3	CPL	A	703	-	-	8/13/13/55	-
3	CPL	C	707	-	-	8/13/13/55	-
3	CPL	A	705	-	-	7/11/11/55	-
2	CLR	D	700	-	-	6/10/68/68	0/4/4/4
3	CPL	D	702	-	-	8/13/13/55	-
2	CLR	D	701	-	-	3/10/68/68	0/4/4/4
3	CPL	A	708	-	-	8/13/13/55	-
3	CPL	B	704	-	-	7/11/11/55	-
3	CPL	C	704	-	-	7/11/11/55	-
3	CPL	D	705	-	-	13/32/32/55	-
2	CLR	C	700	-	-	6/10/68/68	0/4/4/4
2	CLR	B	701	-	-	3/10/68/68	0/4/4/4
3	CPL	B	703	-	-	6/7/7/55	-
3	CPL	B	706	-	-	17/41/41/55	-
3	CPL	C	703	-	-	6/7/7/55	-
3	CPL	C	702	-	-	8/13/13/55	-
3	CPL	B	707	-	-	8/13/13/55	-
3	CPL	D	707	-	-	8/13/13/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPL	B	702	-	-	8/13/13/55	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	706	CPL	O2-C31	3.37	1.43	1.34
3	A	707	CPL	O2-C31	3.36	1.43	1.34
3	C	706	CPL	O2-C31	3.35	1.43	1.34
3	B	706	CPL	O2-C31	3.34	1.43	1.34
3	B	706	CPL	O3-C11	3.32	1.43	1.33
3	A	707	CPL	O3-C11	3.31	1.43	1.33
3	C	706	CPL	O3-C11	3.31	1.43	1.33
3	D	706	CPL	O3-C11	3.31	1.43	1.33
3	B	705	CPL	O3-C3	-2.78	1.38	1.45
3	C	705	CPL	O3-C3	-2.78	1.38	1.45
3	D	705	CPL	O3-C3	-2.78	1.38	1.45
2	A	702	CLR	C10-C9	-2.77	1.51	1.56
3	A	706	CPL	O3-C3	-2.75	1.38	1.45
2	B	701	CLR	C10-C9	-2.72	1.51	1.56
2	D	701	CLR	C10-C9	-2.72	1.51	1.56
2	C	701	CLR	C10-C9	-2.71	1.51	1.56
3	C	705	CPL	O31-C31	-2.65	1.14	1.22
3	A	706	CPL	O31-C31	-2.63	1.14	1.22
3	B	705	CPL	O31-C31	-2.63	1.14	1.22
3	D	705	CPL	O31-C31	-2.61	1.14	1.22
3	C	705	CPL	O2-C31	2.52	1.41	1.34
3	D	705	CPL	O2-C31	2.52	1.41	1.34
3	A	706	CPL	O2-C31	2.51	1.41	1.34
3	B	705	CPL	O2-C31	2.51	1.41	1.34
3	B	705	CPL	C32-C31	2.35	1.57	1.50
3	C	705	CPL	O3-C11	2.34	1.40	1.33
3	B	705	CPL	O3-C11	2.34	1.40	1.33
3	D	705	CPL	O3-C11	2.34	1.40	1.33
3	D	705	CPL	O2-C2	-2.33	1.40	1.46
3	C	705	CPL	C32-C31	2.32	1.57	1.50
3	D	705	CPL	C32-C31	2.32	1.57	1.50
3	A	706	CPL	O3-C11	2.32	1.40	1.33
3	A	706	CPL	O2-C2	-2.32	1.40	1.46
3	B	705	CPL	O2-C2	-2.32	1.40	1.46
3	C	705	CPL	O2-C2	-2.32	1.40	1.46
3	A	706	CPL	C32-C31	2.31	1.57	1.50
2	A	701	CLR	C15-C14	-2.27	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	CLR	C15-C14	-2.27	1.49	1.54
2	D	700	CLR	C15-C14	-2.27	1.49	1.54
2	C	700	CLR	C15-C14	-2.24	1.49	1.54
2	A	702	CLR	C6-C5	-2.20	1.28	1.33
2	B	701	CLR	C6-C5	-2.17	1.28	1.33
2	C	701	CLR	C6-C5	-2.17	1.28	1.33
2	D	701	CLR	C6-C5	-2.17	1.28	1.33
3	B	705	CPL	P-O2P	-2.11	1.45	1.55
3	C	705	CPL	P-O2P	-2.10	1.45	1.55
3	B	706	CPL	O2-C2	-2.10	1.41	1.46
3	C	706	CPL	O2-C2	-2.10	1.41	1.46
3	A	706	CPL	P-O2P	-2.09	1.45	1.55
3	D	705	CPL	P-O2P	-2.09	1.45	1.55
3	A	707	CPL	O2-C2	-2.08	1.41	1.46
3	D	706	CPL	O2-C2	-2.08	1.41	1.46
2	A	701	CLR	C10-C5	-2.05	1.48	1.52
2	B	700	CLR	C10-C5	-2.02	1.48	1.52
2	C	700	CLR	C10-C5	-2.02	1.48	1.52
2	D	700	CLR	C10-C5	-2.02	1.48	1.52

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	706	CPL	O2-C31-C32	5.06	122.40	111.50
3	C	706	CPL	O2-C31-C32	5.05	122.39	111.50
2	C	701	CLR	C19-C10-C9	-5.05	105.66	111.68
3	B	706	CPL	O2-C31-C32	5.04	122.37	111.50
3	A	707	CPL	O2-C31-C32	5.04	122.35	111.50
2	A	702	CLR	C19-C10-C9	-5.03	105.69	111.68
2	B	701	CLR	C19-C10-C9	-5.02	105.70	111.68
2	D	701	CLR	C19-C10-C9	-5.02	105.70	111.68
2	A	702	CLR	C16-C17-C20	-4.71	104.86	112.15
2	B	701	CLR	C16-C17-C20	-4.70	104.86	112.15
2	C	701	CLR	C16-C17-C20	-4.70	104.88	112.15
2	D	701	CLR	C16-C17-C20	-4.70	104.88	112.15
3	C	705	CPL	O2-C31-C32	4.69	121.61	111.50
3	D	705	CPL	O2-C31-C32	4.69	121.61	111.50
3	A	706	CPL	O2-C31-C32	4.68	121.59	111.50
3	B	705	CPL	O2-C31-C32	4.67	121.56	111.50
2	B	700	CLR	C19-C10-C5	-4.32	101.34	108.34
2	C	700	CLR	C19-C10-C5	-4.32	101.34	108.34
2	D	700	CLR	C19-C10-C5	-4.32	101.34	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	CLR	C19-C10-C5	-4.29	101.40	108.34
2	A	702	CLR	C8-C7-C6	-4.02	106.96	112.73
2	D	701	CLR	C8-C7-C6	-4.01	106.97	112.73
2	B	701	CLR	C8-C7-C6	-4.00	106.98	112.73
2	C	701	CLR	C8-C7-C6	-3.99	107.00	112.73
3	D	705	CPL	C3-C2-C1	-3.55	103.38	111.79
3	C	705	CPL	C3-C2-C1	-3.54	103.42	111.79
3	A	706	CPL	C3-C2-C1	-3.53	103.44	111.79
3	B	705	CPL	C3-C2-C1	-3.52	103.46	111.79
2	A	701	CLR	C19-C10-C1	3.51	114.97	109.43
2	B	700	CLR	C19-C10-C1	3.49	114.94	109.43
2	C	700	CLR	C19-C10-C1	3.49	114.94	109.43
2	B	701	CLR	C4-C5-C10	3.47	121.03	116.42
2	D	700	CLR	C19-C10-C1	3.47	114.91	109.43
2	A	702	CLR	C4-C5-C10	3.45	121.00	116.42
2	D	701	CLR	C4-C5-C10	3.45	121.00	116.42
2	A	702	CLR	C15-C14-C13	-3.44	99.70	103.84
2	C	701	CLR	C4-C5-C10	3.43	120.97	116.42
2	D	701	CLR	C15-C14-C13	-3.41	99.73	103.84
2	B	701	CLR	C15-C14-C13	-3.40	99.74	103.84
2	C	701	CLR	C15-C14-C13	-3.40	99.74	103.84
2	D	701	CLR	C4-C5-C6	-3.18	116.03	120.61
2	B	701	CLR	C4-C5-C6	-3.16	116.05	120.61
2	A	702	CLR	C4-C5-C6	-3.16	116.05	120.61
2	A	702	CLR	C23-C22-C20	-3.16	105.96	115.03
2	C	701	CLR	C4-C5-C6	-3.16	116.06	120.61
2	C	701	CLR	C23-C22-C20	-3.15	105.98	115.03
2	D	701	CLR	C23-C22-C20	-3.15	105.98	115.03
2	B	701	CLR	C23-C22-C20	-3.14	105.99	115.03
3	C	706	CPL	O3-C11-C12	3.14	121.77	111.91
3	B	706	CPL	O3-C11-C12	3.13	121.74	111.91
3	A	707	CPL	O3-C11-C12	3.13	121.74	111.91
3	D	706	CPL	O3-C11-C12	3.13	121.74	111.91
3	C	705	CPL	O2-C31-O31	-3.13	116.13	123.70
3	A	706	CPL	O2-C31-O31	-3.13	116.14	123.70
3	B	705	CPL	O2-C31-O31	-3.12	116.16	123.70
3	D	705	CPL	O2-C31-O31	-3.12	116.16	123.70
2	A	702	CLR	C15-C14-C8	-2.98	114.17	119.08
2	D	701	CLR	C15-C14-C8	-2.97	114.19	119.08
2	C	701	CLR	C15-C14-C8	-2.96	114.21	119.08
2	B	701	CLR	C15-C14-C8	-2.95	114.22	119.08
2	A	702	CLR	C21-C20-C22	-2.88	105.85	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	CLR	C21-C20-C22	-2.86	105.88	110.36
2	D	701	CLR	C21-C20-C22	-2.85	105.90	110.36
2	B	700	CLR	C16-C15-C14	-2.84	99.50	105.13
2	A	701	CLR	C16-C15-C14	-2.83	99.51	105.13
2	D	700	CLR	C16-C15-C14	-2.83	99.51	105.13
2	C	701	CLR	C7-C6-C5	-2.83	119.83	125.06
2	D	701	CLR	C7-C6-C5	-2.83	119.84	125.06
2	C	700	CLR	C16-C15-C14	-2.83	99.53	105.13
2	C	701	CLR	C21-C20-C22	-2.83	105.93	110.36
2	B	701	CLR	C12-C13-C17	2.82	120.79	116.57
2	A	702	CLR	C7-C6-C5	-2.82	119.86	125.06
2	D	700	CLR	C18-C13-C14	-2.82	106.46	111.71
2	C	700	CLR	C18-C13-C14	-2.81	106.47	111.71
2	B	700	CLR	C18-C13-C14	-2.81	106.47	111.71
2	B	701	CLR	C7-C6-C5	-2.80	119.89	125.06
2	D	701	CLR	C12-C13-C17	2.80	120.76	116.57
2	C	701	CLR	C12-C13-C17	2.80	120.75	116.57
2	A	701	CLR	C18-C13-C14	-2.79	106.51	111.71
2	A	702	CLR	C12-C13-C17	2.77	120.72	116.57
2	A	701	CLR	C10-C9-C8	-2.73	108.64	112.73
2	A	702	CLR	C10-C9-C8	-2.73	108.65	112.73
2	B	701	CLR	C10-C9-C8	-2.72	108.65	112.73
2	D	701	CLR	C10-C9-C8	-2.72	108.65	112.73
2	C	701	CLR	C10-C9-C8	-2.72	108.66	112.73
2	C	700	CLR	C10-C9-C8	-2.72	108.66	112.73
2	D	700	CLR	C10-C9-C8	-2.72	108.66	112.73
2	B	700	CLR	C10-C9-C8	-2.69	108.69	112.73
2	C	700	CLR	C1-C2-C3	2.69	113.92	110.47
2	B	701	CLR	C16-C17-C13	2.69	107.08	103.84
2	A	701	CLR	C3-C4-C5	-2.67	107.49	112.03
2	A	701	CLR	C1-C2-C3	2.66	113.88	110.47
2	D	700	CLR	C1-C2-C3	2.66	113.88	110.47
2	C	700	CLR	C3-C4-C5	-2.66	107.51	112.03
2	B	700	CLR	C3-C4-C5	-2.66	107.52	112.03
2	B	700	CLR	C1-C2-C3	2.65	113.87	110.47
2	C	701	CLR	C16-C17-C13	2.65	107.03	103.84
2	C	701	CLR	C22-C20-C17	-2.64	104.82	110.28
2	D	701	CLR	C22-C20-C17	-2.64	104.83	110.28
2	A	702	CLR	C22-C20-C17	-2.64	104.83	110.28
2	D	701	CLR	C16-C17-C13	2.64	107.02	103.84
2	D	700	CLR	C3-C4-C5	-2.64	107.55	112.03
2	C	700	CLR	C22-C20-C17	2.63	115.71	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	CLR	C22-C20-C17	-2.62	104.86	110.28
2	A	702	CLR	C16-C17-C13	2.62	107.00	103.84
2	B	700	CLR	C22-C20-C17	2.61	115.68	110.28
2	A	701	CLR	C22-C20-C17	2.61	115.68	110.28
2	D	700	CLR	C22-C20-C17	2.61	115.68	110.28
2	D	700	CLR	C2-C1-C10	2.61	118.39	112.74
2	A	701	CLR	C2-C1-C10	2.59	118.36	112.74
2	C	700	CLR	C2-C1-C10	2.59	118.34	112.74
2	B	700	CLR	C2-C1-C10	2.58	118.34	112.74
2	A	702	CLR	C13-C17-C20	-2.48	115.60	119.49
3	A	707	CPL	C2-O2-C31	-2.48	111.68	117.79
2	C	701	CLR	C11-C12-C13	-2.48	108.53	112.78
2	A	702	CLR	C11-C12-C13	-2.48	108.53	112.78
3	C	706	CPL	C2-O2-C31	-2.47	111.71	117.79
2	C	701	CLR	C13-C17-C20	-2.46	115.63	119.49
2	B	701	CLR	C13-C17-C20	-2.46	115.63	119.49
2	B	701	CLR	C11-C12-C13	-2.46	108.56	112.78
2	D	701	CLR	C11-C12-C13	-2.46	108.57	112.78
3	D	706	CPL	C2-O2-C31	-2.45	111.75	117.79
3	B	706	CPL	C2-O2-C31	-2.45	111.75	117.79
2	D	701	CLR	C13-C17-C20	-2.44	115.66	119.49
2	A	701	CLR	C11-C12-C13	-2.40	108.67	112.78
2	D	700	CLR	C11-C12-C13	-2.40	108.67	112.78
2	C	700	CLR	C11-C12-C13	-2.38	108.69	112.78
2	B	700	CLR	C11-C12-C13	-2.38	108.70	112.78
3	C	705	CPL	O3-C11-C12	2.37	119.35	111.91
3	D	705	CPL	O3-C11-C12	2.37	119.34	111.91
3	B	705	CPL	O3-C11-C12	2.37	119.34	111.91
3	A	706	CPL	O3-C11-C12	2.36	119.31	111.91
2	B	701	CLR	C2-C3-C4	-2.35	107.09	110.31
3	A	706	CPL	C13-C12-C11	-2.33	105.14	113.62
3	B	705	CPL	C13-C12-C11	-2.33	105.14	113.62
3	D	705	CPL	C13-C12-C11	-2.33	105.14	113.62
3	C	705	CPL	C13-C12-C11	-2.33	105.15	113.62
2	A	702	CLR	C2-C3-C4	-2.32	107.12	110.31
2	C	701	CLR	C2-C3-C4	-2.32	107.12	110.31
2	D	701	CLR	C2-C3-C4	-2.32	107.12	110.31
2	B	701	CLR	C16-C15-C14	-2.25	100.68	105.13
2	D	701	CLR	C16-C15-C14	-2.24	100.70	105.13
2	B	700	CLR	C17-C13-C14	2.24	102.72	100.07
2	C	700	CLR	C17-C13-C14	2.24	102.72	100.07
2	C	701	CLR	C16-C15-C14	-2.23	100.71	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	702	CLR	C16-C15-C14	-2.22	100.72	105.13
2	A	701	CLR	C17-C13-C14	2.22	102.71	100.07
2	D	700	CLR	C17-C13-C14	2.21	102.70	100.07
3	A	707	CPL	O2P-P-O1P	-2.21	101.30	112.24
3	C	706	CPL	O2P-P-O1P	-2.21	101.33	112.24
3	D	706	CPL	O2P-P-O1P	-2.21	101.33	112.24
3	B	706	CPL	O2P-P-O1P	-2.20	101.36	112.24
3	A	707	CPL	C33-C32-C31	-2.18	105.68	113.62
3	B	706	CPL	C33-C32-C31	-2.18	105.68	113.62
3	C	706	CPL	C33-C32-C31	-2.18	105.68	113.62
3	D	706	CPL	C33-C32-C31	-2.18	105.68	113.62
2	A	702	CLR	C7-C8-C14	-2.16	107.77	110.91
2	C	701	CLR	C7-C8-C14	-2.15	107.79	110.91
2	D	701	CLR	C7-C8-C14	-2.15	107.79	110.91
2	B	701	CLR	C7-C8-C14	-2.13	107.82	110.91
2	A	702	CLR	C1-C10-C5	2.07	112.54	108.75
2	B	701	CLR	C1-C10-C5	2.07	112.54	108.75
2	C	701	CLR	C1-C10-C5	2.07	112.54	108.75
2	D	701	CLR	C1-C10-C5	2.07	112.54	108.75
2	A	701	CLR	C15-C14-C8	-2.03	115.73	119.08
2	B	700	CLR	C15-C14-C8	-2.02	115.75	119.08
2	D	700	CLR	C15-C14-C8	-2.00	115.78	119.08

There are no chirality outliers.

All (272) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	706	CPL	C4-O4P-P-O1P
3	A	706	CPL	C4-O4P-P-O2P
3	A	707	CPL	C1-O3P-P-O1P
3	A	707	CPL	C4-O4P-P-O1P
3	A	707	CPL	C4-O4P-P-O3P
3	B	705	CPL	C4-O4P-P-O1P
3	B	705	CPL	C4-O4P-P-O2P
3	B	706	CPL	C1-O3P-P-O1P
3	B	706	CPL	C4-O4P-P-O1P
3	B	706	CPL	C4-O4P-P-O3P
3	C	705	CPL	C4-O4P-P-O1P
3	C	705	CPL	C4-O4P-P-O2P
3	C	706	CPL	C1-O3P-P-O1P
3	C	706	CPL	C4-O4P-P-O1P
3	C	706	CPL	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
3	D	705	CPL	C4-O4P-P-O1P
3	D	705	CPL	C4-O4P-P-O2P
3	D	706	CPL	C1-O3P-P-O1P
3	D	706	CPL	C4-O4P-P-O1P
3	D	706	CPL	C4-O4P-P-O3P
2	A	701	CLR	C13-C17-C20-C21
2	B	700	CLR	C13-C17-C20-C21
2	C	700	CLR	C13-C17-C20-C21
2	D	700	CLR	C13-C17-C20-C21
2	A	701	CLR	C16-C17-C20-C21
2	B	700	CLR	C16-C17-C20-C21
2	C	700	CLR	C16-C17-C20-C21
2	D	700	CLR	C16-C17-C20-C21
2	A	701	CLR	C13-C17-C20-C22
2	B	700	CLR	C13-C17-C20-C22
2	C	700	CLR	C13-C17-C20-C22
2	D	700	CLR	C13-C17-C20-C22
2	A	701	CLR	C16-C17-C20-C22
2	B	700	CLR	C16-C17-C20-C22
2	C	700	CLR	C16-C17-C20-C22
2	D	700	CLR	C16-C17-C20-C22
3	A	707	CPL	C12-C13-C14-C15
3	B	706	CPL	C12-C13-C14-C15
3	C	706	CPL	C12-C13-C14-C15
3	D	706	CPL	C12-C13-C14-C15
3	A	705	CPL	C14-C15-C16-C17
3	B	704	CPL	C14-C15-C16-C17
3	C	704	CPL	C14-C15-C16-C17
3	D	704	CPL	C14-C15-C16-C17
3	A	706	CPL	C31-C32-C33-C34
3	B	705	CPL	C31-C32-C33-C34
3	C	705	CPL	C31-C32-C33-C34
3	D	705	CPL	C31-C32-C33-C34
2	A	702	CLR	C17-C20-C22-C23
2	B	701	CLR	C17-C20-C22-C23
2	C	701	CLR	C17-C20-C22-C23
2	D	701	CLR	C17-C20-C22-C23
2	B	701	CLR	C20-C22-C23-C24
2	C	701	CLR	C20-C22-C23-C24
2	D	701	CLR	C20-C22-C23-C24
2	A	702	CLR	C20-C22-C23-C24
2	A	702	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
2	B	701	CLR	C21-C20-C22-C23
2	C	701	CLR	C21-C20-C22-C23
2	D	701	CLR	C21-C20-C22-C23
3	A	706	CPL	C4-O4P-P-O3P
3	A	707	CPL	C1-O3P-P-O4P
3	B	705	CPL	C4-O4P-P-O3P
3	B	706	CPL	C1-O3P-P-O4P
3	C	705	CPL	C4-O4P-P-O3P
3	C	706	CPL	C1-O3P-P-O4P
3	D	705	CPL	C4-O4P-P-O3P
3	D	706	CPL	C1-O3P-P-O4P
3	A	704	CPL	C18-C19-C20-C21
3	A	704	CPL	C19-C20-C21-C22
3	B	703	CPL	C18-C19-C20-C21
3	B	703	CPL	C19-C20-C21-C22
3	C	703	CPL	C18-C19-C20-C21
3	D	703	CPL	C18-C19-C20-C21
3	A	703	CPL	C19-C20-C21-C22
3	B	702	CPL	C19-C20-C21-C22
3	C	702	CPL	C19-C20-C21-C22
3	C	703	CPL	C19-C20-C21-C22
3	D	702	CPL	C19-C20-C21-C22
3	D	703	CPL	C19-C20-C21-C22
3	A	707	CPL	C18-C19-C20-C21
3	B	706	CPL	C18-C19-C20-C21
3	C	706	CPL	C18-C19-C20-C21
3	D	706	CPL	C18-C19-C20-C21
2	A	701	CLR	C23-C24-C25-C27
2	B	700	CLR	C23-C24-C25-C27
2	C	700	CLR	C23-C24-C25-C27
2	D	700	CLR	C23-C24-C25-C27
3	A	705	CPL	C22-C23-C24-C25
3	A	708	CPL	C14-C15-C16-C17
3	A	708	CPL	C18-C19-C20-C21
3	B	704	CPL	C22-C23-C24-C25
3	B	707	CPL	C14-C15-C16-C17
3	B	707	CPL	C18-C19-C20-C21
3	C	704	CPL	C22-C23-C24-C25
3	C	707	CPL	C18-C19-C20-C21
3	D	704	CPL	C22-C23-C24-C25
3	D	707	CPL	C14-C15-C16-C17
3	D	707	CPL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
3	C	707	CPL	C14-C15-C16-C17
3	A	708	CPL	C19-C20-C21-C22
3	B	707	CPL	C19-C20-C21-C22
3	C	707	CPL	C19-C20-C21-C22
3	D	707	CPL	C19-C20-C21-C22
3	A	704	CPL	C22-C23-C24-C25
3	A	708	CPL	C17-C18-C19-C20
3	B	703	CPL	C22-C23-C24-C25
3	B	707	CPL	C17-C18-C19-C20
3	C	703	CPL	C22-C23-C24-C25
3	C	707	CPL	C17-C18-C19-C20
3	D	703	CPL	C22-C23-C24-C25
3	D	707	CPL	C17-C18-C19-C20
3	A	708	CPL	C15-C16-C17-C18
3	B	707	CPL	C15-C16-C17-C18
3	C	707	CPL	C15-C16-C17-C18
3	D	707	CPL	C15-C16-C17-C18
3	A	703	CPL	C17-C18-C19-C20
3	B	702	CPL	C17-C18-C19-C20
3	C	702	CPL	C17-C18-C19-C20
3	D	702	CPL	C17-C18-C19-C20
3	A	705	CPL	C20-C21-C22-C23
3	B	704	CPL	C20-C21-C22-C23
3	C	704	CPL	C20-C21-C22-C23
3	D	704	CPL	C20-C21-C22-C23
3	A	703	CPL	C22-C23-C24-C25
3	B	702	CPL	C22-C23-C24-C25
3	C	702	CPL	C22-C23-C24-C25
3	D	702	CPL	C22-C23-C24-C25
2	A	701	CLR	C23-C24-C25-C26
2	B	700	CLR	C23-C24-C25-C26
2	C	700	CLR	C23-C24-C25-C26
2	D	700	CLR	C23-C24-C25-C26
3	A	706	CPL	C12-C11-O3-C3
3	B	705	CPL	C12-C11-O3-C3
3	C	705	CPL	C12-C11-O3-C3
3	D	705	CPL	C12-C11-O3-C3
3	A	706	CPL	O11-C11-O3-C3
3	B	705	CPL	O11-C11-O3-C3
3	D	705	CPL	O11-C11-O3-C3
3	C	705	CPL	O11-C11-O3-C3
3	C	706	CPL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	A	707	CPL	C21-C22-C23-C24
3	B	706	CPL	C21-C22-C23-C24
3	D	706	CPL	C21-C22-C23-C24
3	A	705	CPL	C19-C20-C21-C22
3	B	704	CPL	C19-C20-C21-C22
3	C	704	CPL	C19-C20-C21-C22
3	D	704	CPL	C19-C20-C21-C22
3	A	707	CPL	C16-C17-C18-C19
3	B	706	CPL	C16-C17-C18-C19
3	C	706	CPL	C16-C17-C18-C19
3	D	706	CPL	C16-C17-C18-C19
3	A	703	CPL	C16-C17-C18-C19
3	B	702	CPL	C16-C17-C18-C19
3	C	702	CPL	C16-C17-C18-C19
3	D	702	CPL	C16-C17-C18-C19
3	A	705	CPL	C21-C22-C23-C24
3	D	704	CPL	C21-C22-C23-C24
3	B	704	CPL	C21-C22-C23-C24
3	C	704	CPL	C21-C22-C23-C24
3	A	706	CPL	C35-C36-C37-C38
3	B	705	CPL	C35-C36-C37-C38
3	C	705	CPL	C35-C36-C37-C38
3	D	705	CPL	C35-C36-C37-C38
3	B	703	CPL	C23-C24-C25-C26
3	C	703	CPL	C23-C24-C25-C26
3	D	703	CPL	C23-C24-C25-C26
3	A	704	CPL	C23-C24-C25-C26
3	A	708	CPL	C22-C23-C24-C25
3	B	707	CPL	C22-C23-C24-C25
3	C	707	CPL	C22-C23-C24-C25
3	D	707	CPL	C22-C23-C24-C25
3	A	706	CPL	C14-C15-C16-C17
3	B	705	CPL	C14-C15-C16-C17
3	D	702	CPL	C13-C14-C15-C16
3	D	705	CPL	C14-C15-C16-C17
3	A	703	CPL	C13-C14-C15-C16
3	B	702	CPL	C13-C14-C15-C16
3	C	702	CPL	C13-C14-C15-C16
3	C	705	CPL	C14-C15-C16-C17
3	A	707	CPL	C1-C2-C3-O3
3	B	706	CPL	C1-C2-C3-O3
3	C	706	CPL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	D	706	CPL	C1-C2-C3-O3
3	A	706	CPL	C12-C13-C14-C15
3	B	705	CPL	C12-C13-C14-C15
3	C	705	CPL	C12-C13-C14-C15
3	D	705	CPL	C12-C13-C14-C15
3	A	703	CPL	C18-C19-C20-C21
3	C	702	CPL	C18-C19-C20-C21
3	D	702	CPL	C18-C19-C20-C21
3	B	702	CPL	C18-C19-C20-C21
3	A	707	CPL	O3P-C1-C2-C3
3	B	706	CPL	O3P-C1-C2-C3
3	C	706	CPL	O3P-C1-C2-C3
3	D	706	CPL	O3P-C1-C2-C3
3	B	706	CPL	C19-C20-C21-C22
3	A	707	CPL	C19-C20-C21-C22
3	C	706	CPL	C19-C20-C21-C22
3	D	706	CPL	C19-C20-C21-C22
3	A	705	CPL	C18-C19-C20-C21
3	B	704	CPL	C18-C19-C20-C21
3	B	705	CPL	C33-C34-C35-C36
3	A	706	CPL	C33-C34-C35-C36
3	A	707	CPL	C22-C23-C24-C25
3	B	706	CPL	C22-C23-C24-C25
3	C	704	CPL	C18-C19-C20-C21
3	C	705	CPL	C33-C34-C35-C36
3	C	706	CPL	C22-C23-C24-C25
3	D	704	CPL	C18-C19-C20-C21
3	D	705	CPL	C33-C34-C35-C36
3	D	706	CPL	C22-C23-C24-C25
3	C	706	CPL	C32-C31-O2-C2
3	A	707	CPL	C1-O3P-P-O2P
3	B	706	CPL	C1-O3P-P-O2P
3	C	706	CPL	C1-O3P-P-O2P
3	D	706	CPL	C1-O3P-P-O2P
3	A	707	CPL	C32-C31-O2-C2
3	B	706	CPL	C32-C31-O2-C2
3	D	706	CPL	C32-C31-O2-C2
3	A	703	CPL	C15-C16-C17-C18
3	B	702	CPL	C15-C16-C17-C18
3	C	702	CPL	C15-C16-C17-C18
3	D	702	CPL	C15-C16-C17-C18
3	A	707	CPL	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
3	B	706	CPL	O31-C31-O2-C2
3	C	706	CPL	O31-C31-O2-C2
3	D	706	CPL	O31-C31-O2-C2
3	B	704	CPL	C17-C18-C19-C20
3	D	704	CPL	C17-C18-C19-C20
3	A	705	CPL	C17-C18-C19-C20
3	C	704	CPL	C17-C18-C19-C20
3	B	703	CPL	C20-C21-C22-C23
3	A	704	CPL	C20-C21-C22-C23
3	C	703	CPL	C20-C21-C22-C23
3	D	703	CPL	C20-C21-C22-C23
3	C	707	CPL	C20-C21-C22-C23
3	D	707	CPL	C20-C21-C22-C23
3	A	708	CPL	C20-C21-C22-C23
3	B	707	CPL	C20-C21-C22-C23
3	B	703	CPL	C17-C18-C19-C20
3	A	704	CPL	C17-C18-C19-C20
3	C	703	CPL	C17-C18-C19-C20
3	D	703	CPL	C17-C18-C19-C20
3	A	707	CPL	O2-C2-C3-O3
3	B	706	CPL	O2-C2-C3-O3
3	C	706	CPL	O2-C2-C3-O3
3	D	706	CPL	O2-C2-C3-O3
3	A	703	CPL	C23-C24-C25-C26
3	B	702	CPL	C23-C24-C25-C26
3	C	702	CPL	C23-C24-C25-C26
3	D	702	CPL	C23-C24-C25-C26
3	C	707	CPL	C21-C22-C23-C24
3	B	707	CPL	C21-C22-C23-C24
3	D	707	CPL	C21-C22-C23-C24
3	A	708	CPL	C21-C22-C23-C24
3	B	705	CPL	O3-C11-C12-C13
3	A	706	CPL	O3-C11-C12-C13
3	C	705	CPL	O3-C11-C12-C13
3	D	705	CPL	O3-C11-C12-C13
3	A	707	CPL	C12-C11-O3-C3
3	B	706	CPL	C12-C11-O3-C3
3	C	706	CPL	C12-C11-O3-C3
3	D	706	CPL	C12-C11-O3-C3
3	A	706	CPL	O31-C31-O2-C2
3	B	705	CPL	O31-C31-O2-C2
3	D	705	CPL	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
3	C	705	CPL	O31-C31-O2-C2
3	A	706	CPL	O11-C11-C12-C13
3	B	705	CPL	O11-C11-C12-C13
3	C	705	CPL	O11-C11-C12-C13
3	D	705	CPL	O11-C11-C12-C13

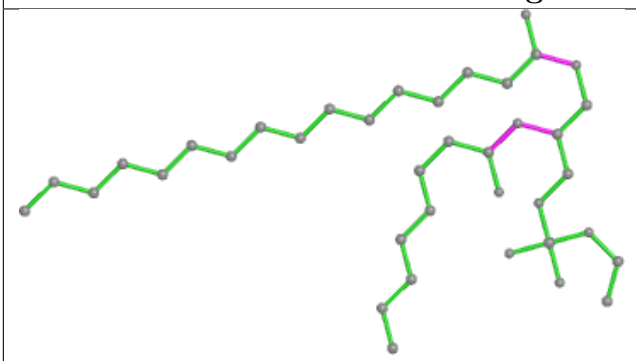
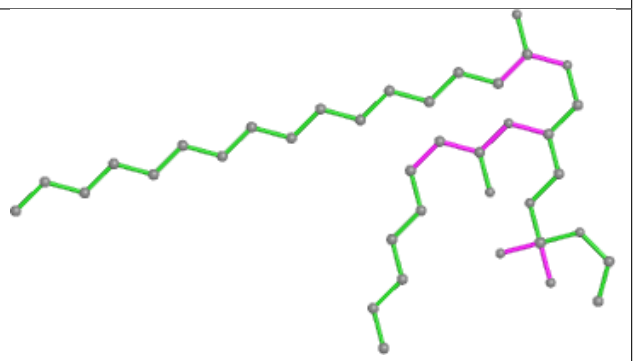
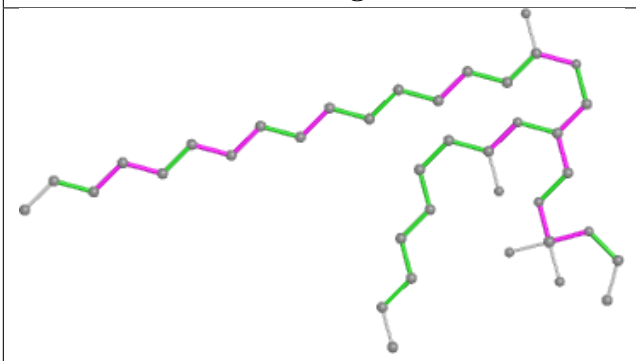
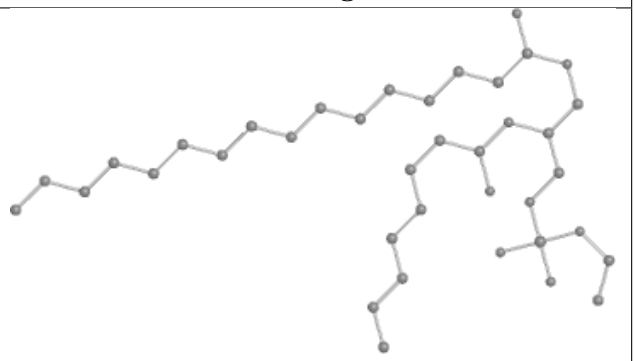
There are no ring outliers.

20 monomers are involved in 64 short contacts:

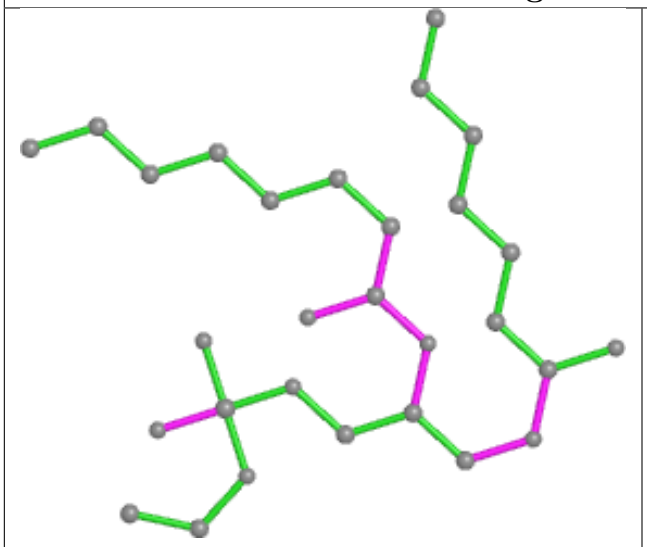
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	706	CPL	4	0
3	A	706	CPL	3	0
2	B	700	CLR	7	0
2	C	701	CLR	2	0
3	B	705	CPL	3	0
3	A	707	CPL	4	0
3	D	706	CPL	4	0
2	A	701	CLR	6	0
3	C	705	CPL	3	0
2	A	702	CLR	2	0
3	A	703	CPL	1	0
2	D	700	CLR	5	0
3	D	702	CPL	1	0
2	D	701	CLR	2	0
3	D	705	CPL	3	0
2	C	700	CLR	6	0
2	B	701	CLR	2	0
3	B	706	CPL	4	0
3	C	702	CPL	1	0
3	B	702	CPL	1	0

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

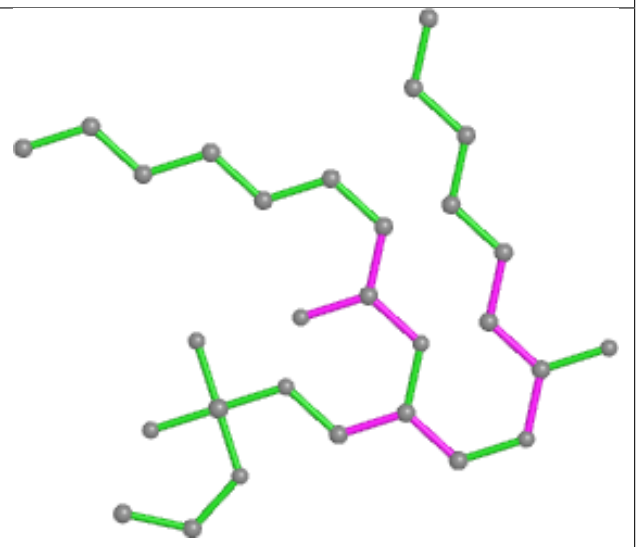
equivalents in the CSD to analyse the geometry.

Ligand CPL C 706	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

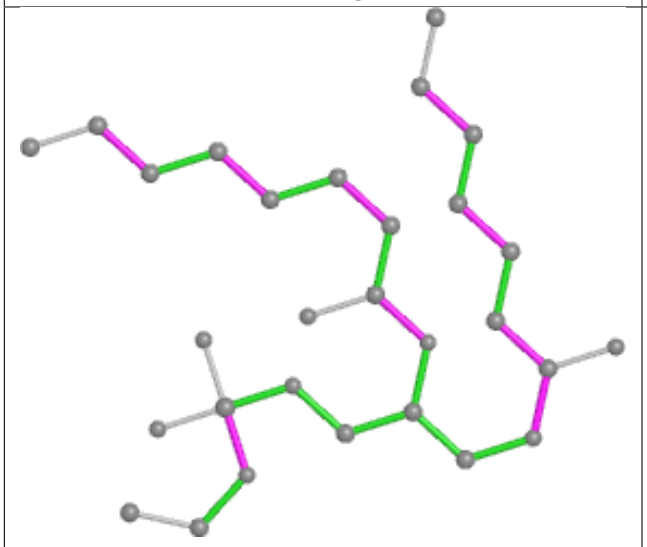
Ligand CPL A 706



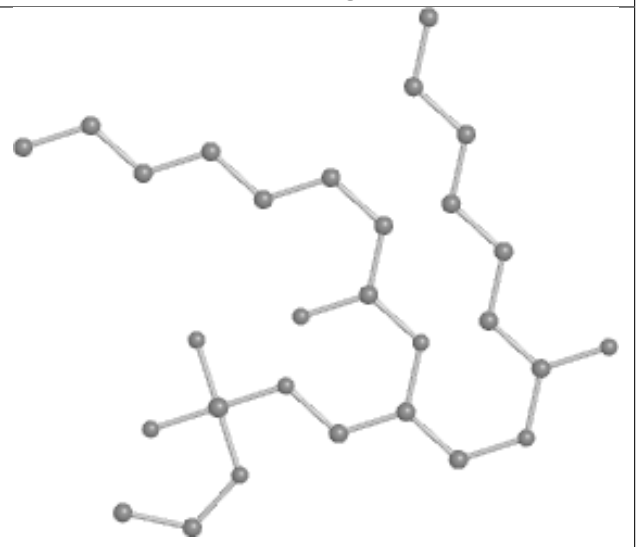
Bond lengths



Bond angles

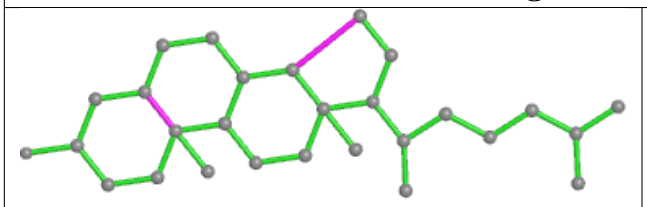


Torsions

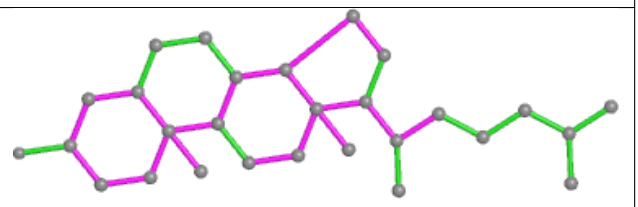


Rings

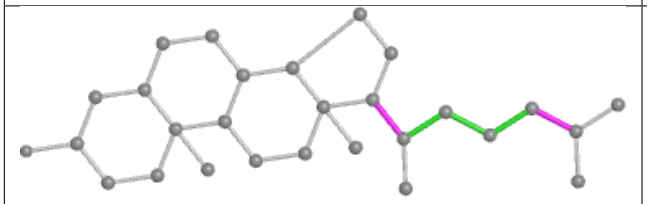
Ligand CLR B 700



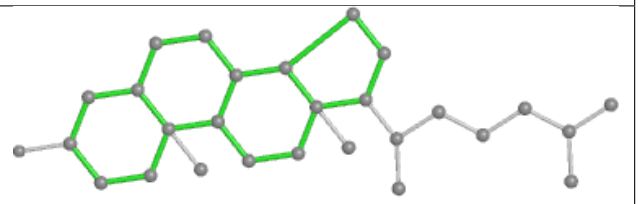
Bond lengths



Bond angles

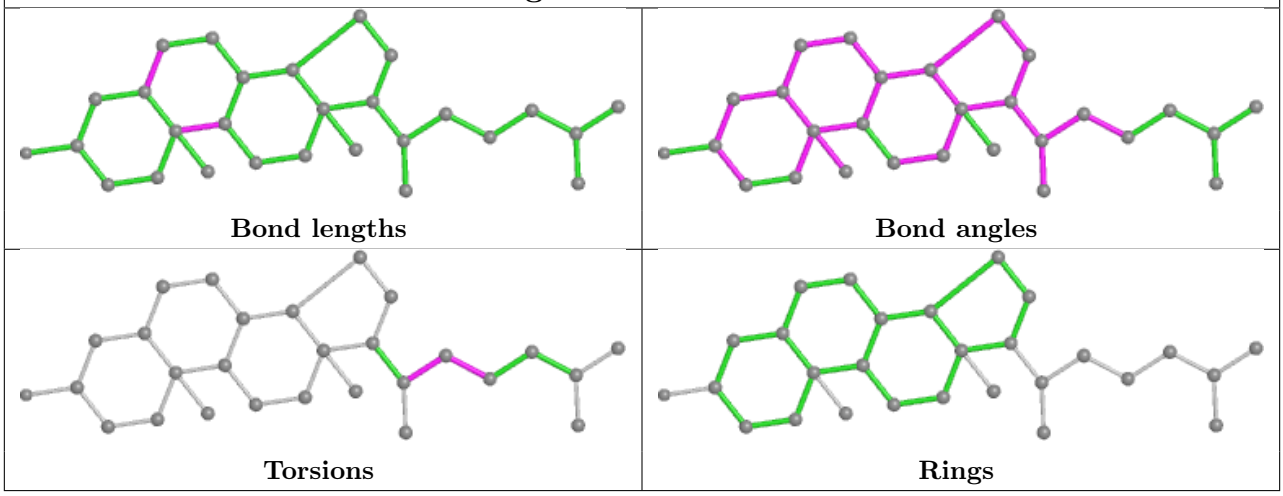


Torsions

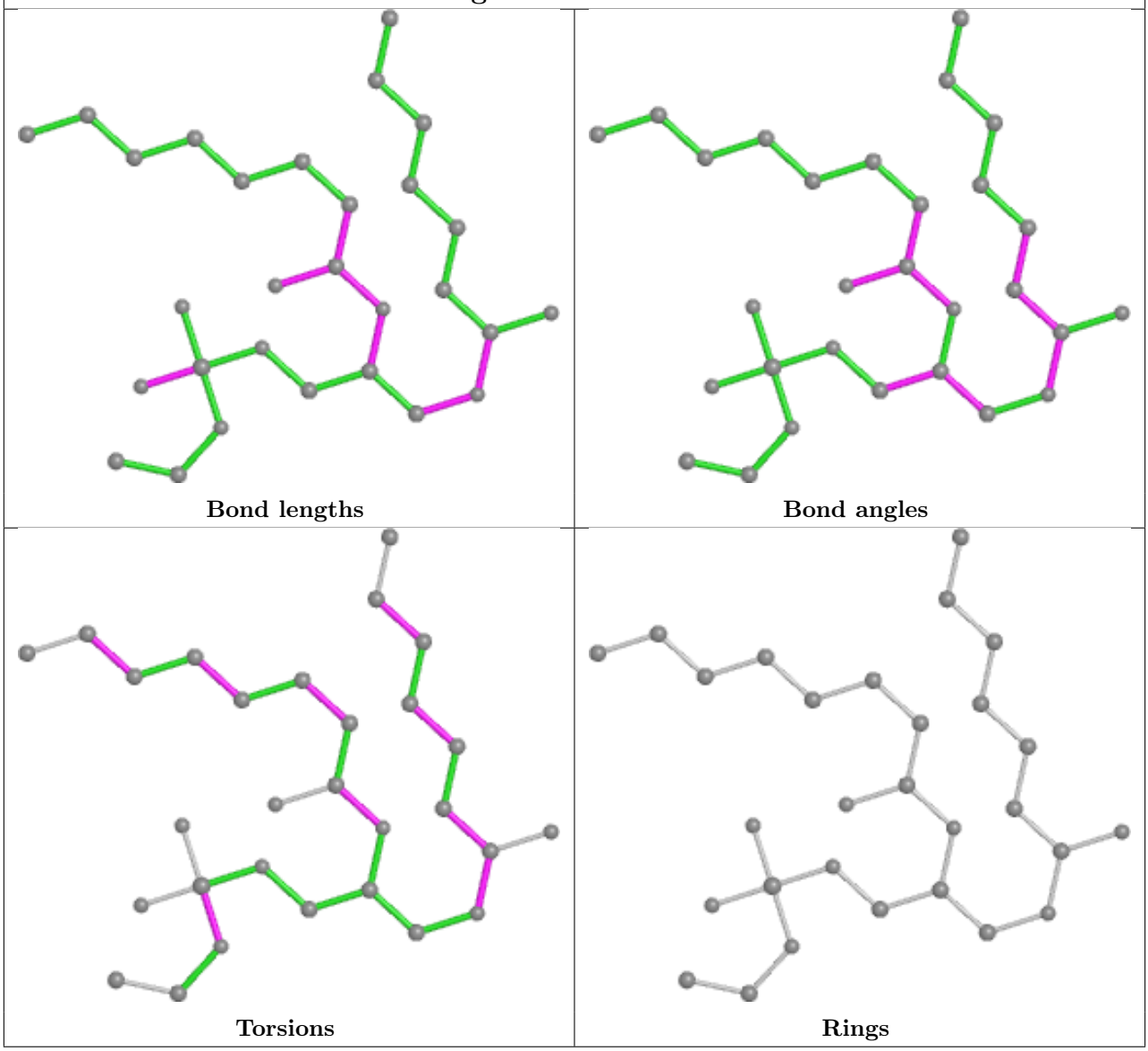


Rings

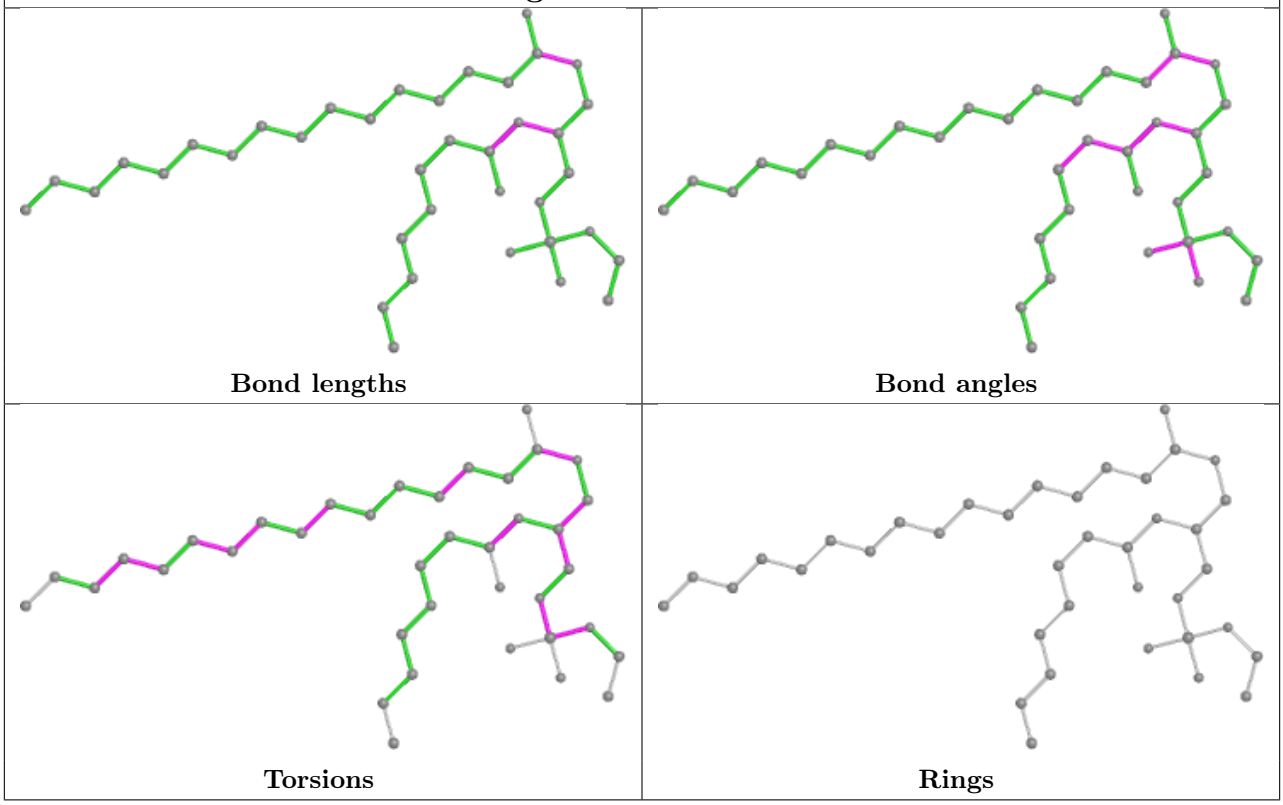
Ligand CLR C 701



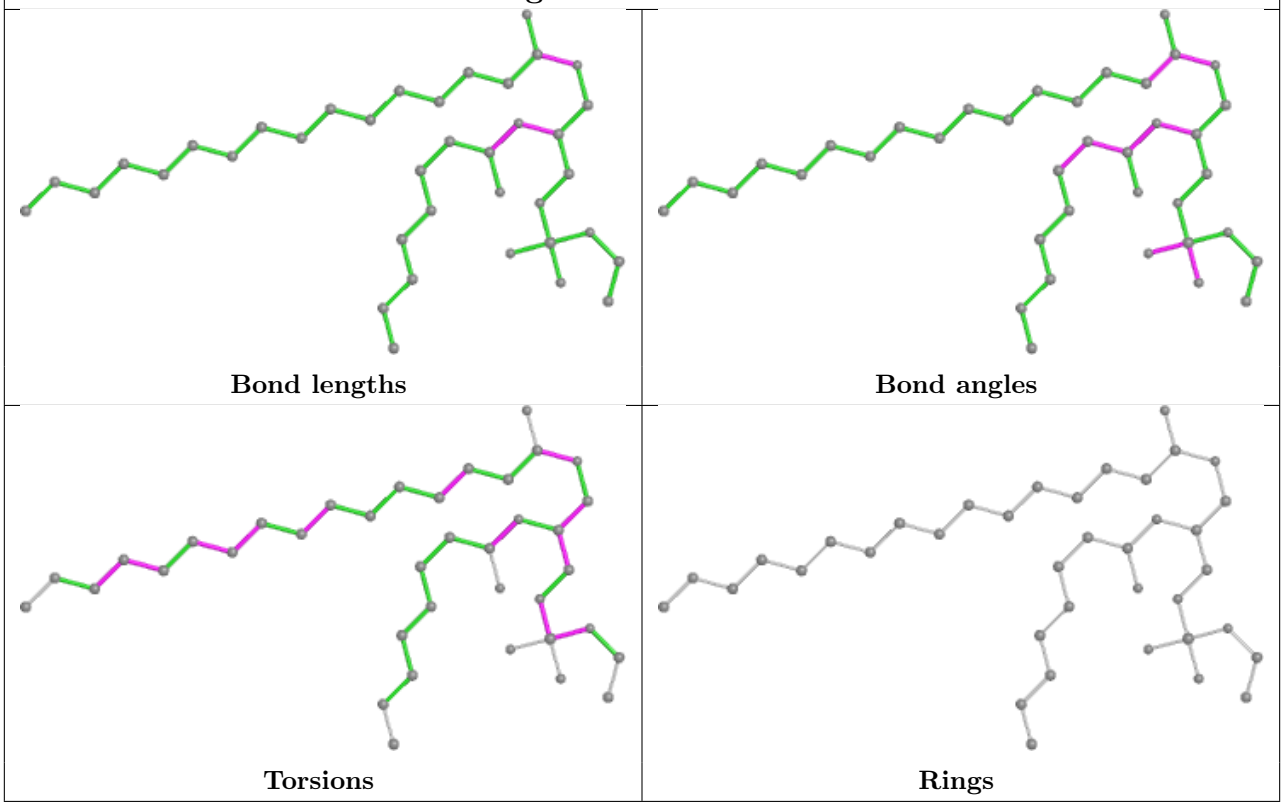
Ligand CPL B 705



Ligand CPL A 707



Ligand CPL D 706



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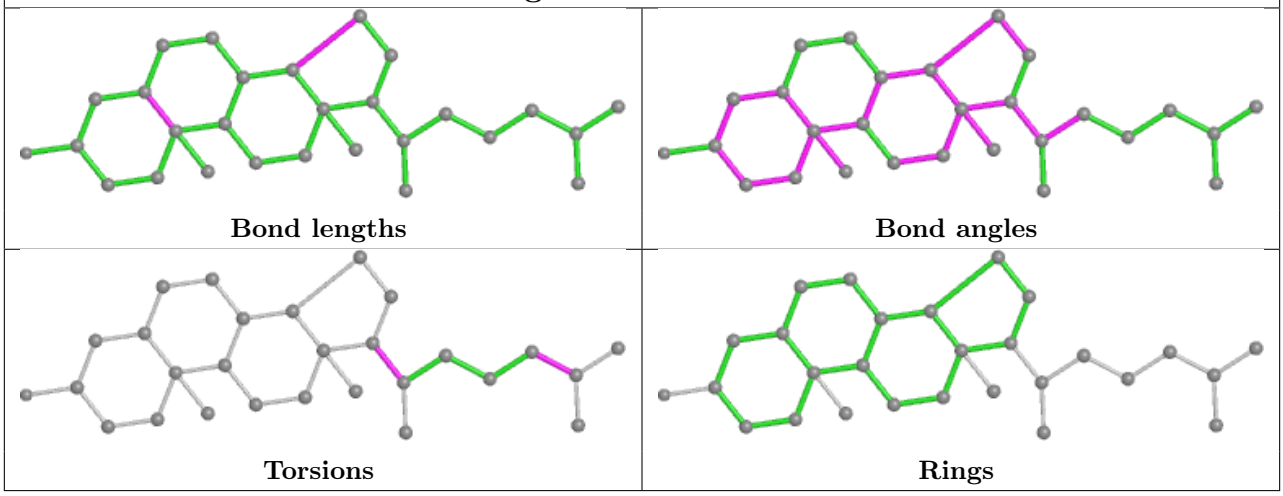

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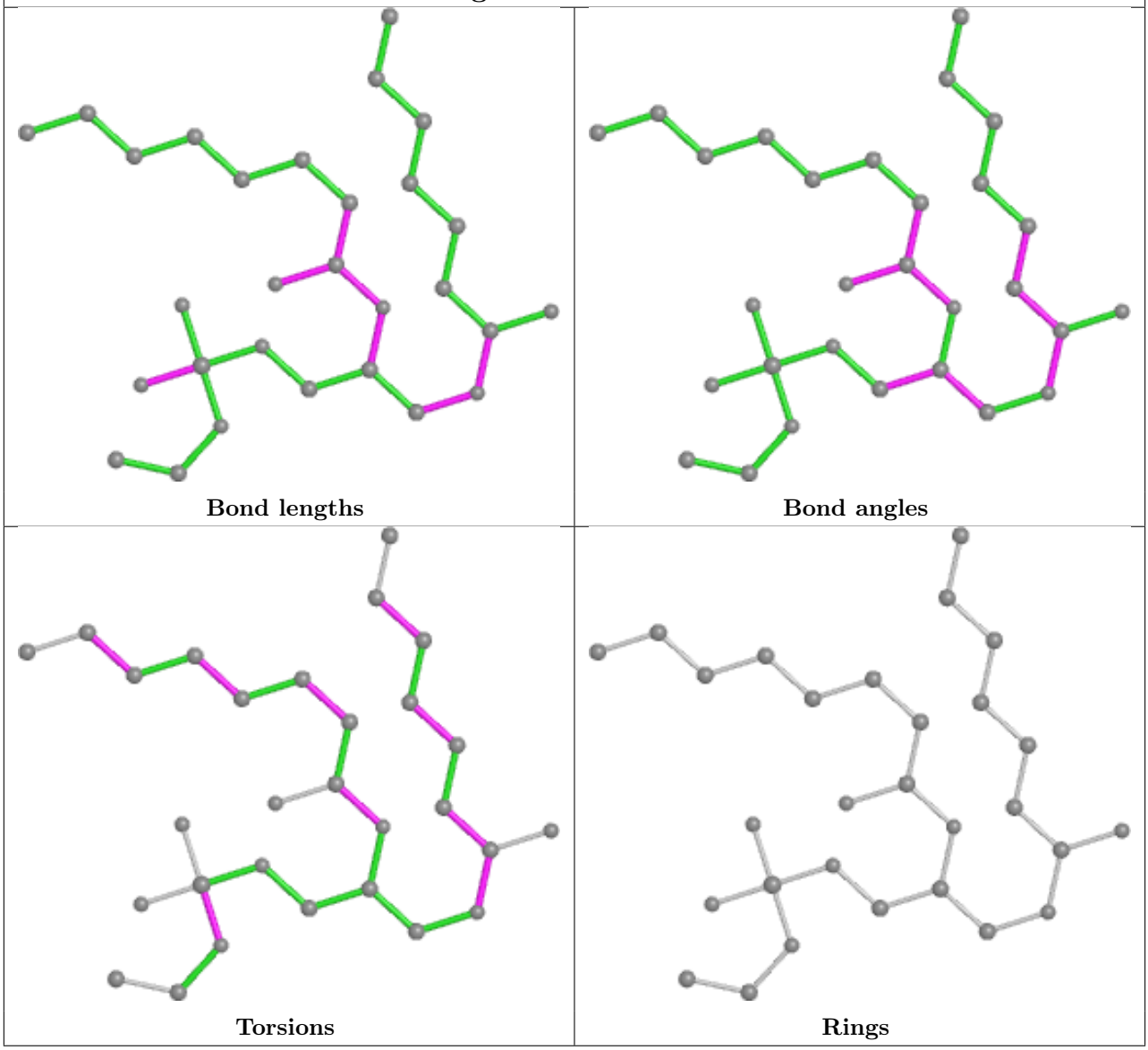

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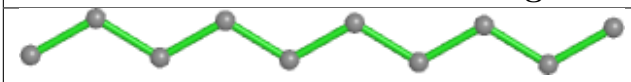
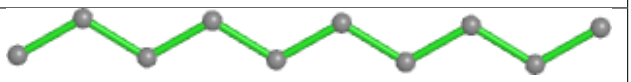
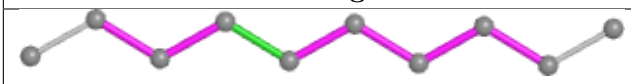


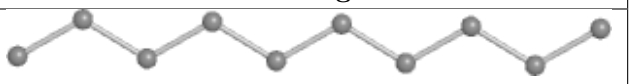
Bond lengths



Bond angles

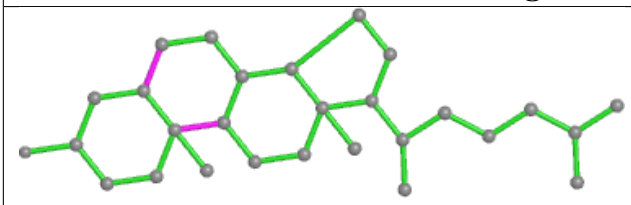


Torsions

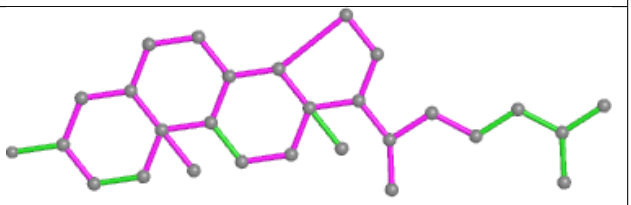


Rings

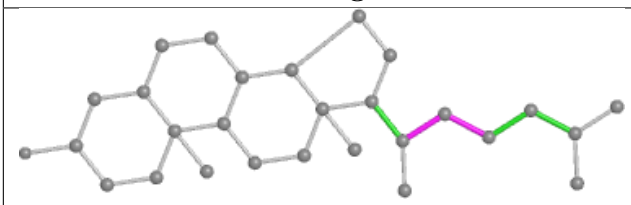
Ligand CLR A 702



Bond lengths



Bond angles



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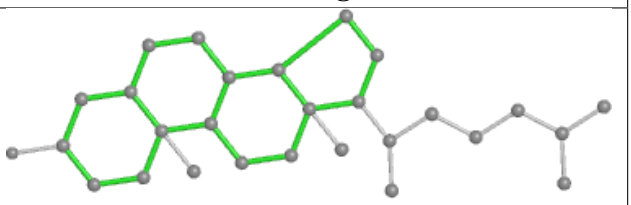
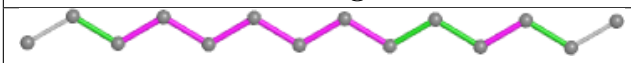


Rings

Ligand CPL D 704

Bond lengths

Bond angles



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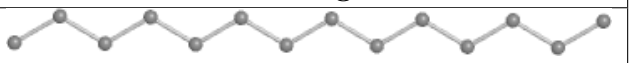


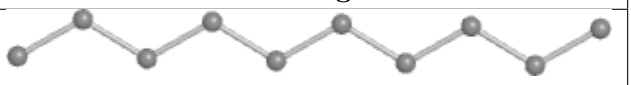
Rings

Ligand CPL D 703

Bond lengths

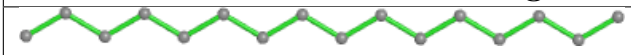
Bond angles

Torsions



Rings

Ligand CPL A 703



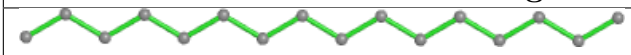
Bond lengths

Bond angles

Torsions

Rings

Ligand CPL C 707



Bond lengths

Bond angles

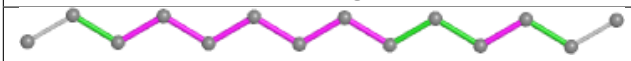
Torsions

Rings

Ligand CPL A 705

Bond lengths

Bond angles



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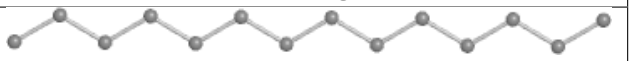
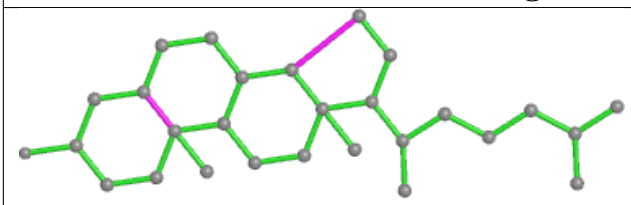
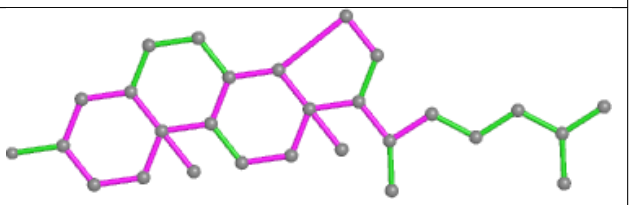


Rings

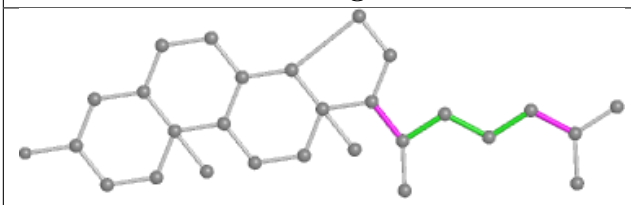
Ligand CLR D 700



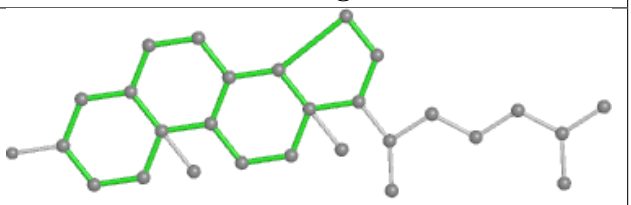
Bond lengths



Bond angles

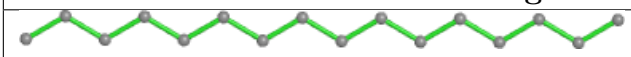


Torsions



Rings

Ligand CPL D 702



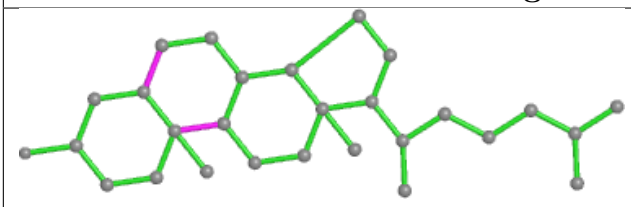
Bond lengths

Bond angles

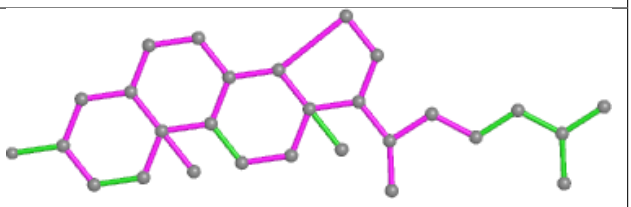
Torsions

Rings

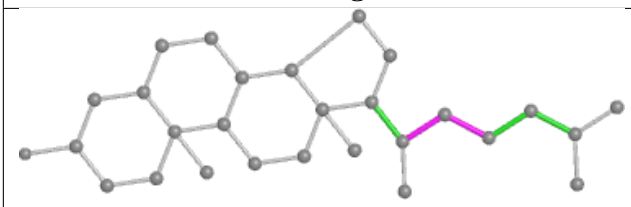
Ligand CLR D 701



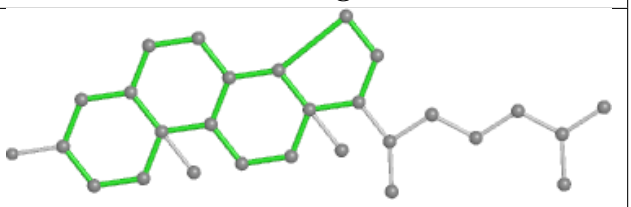
Bond lengths



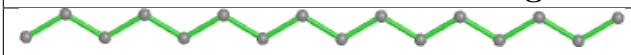
Bond angles

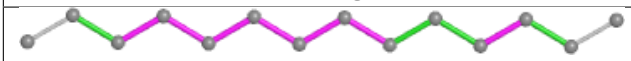
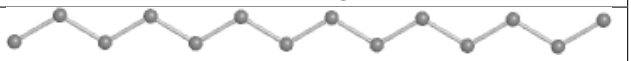


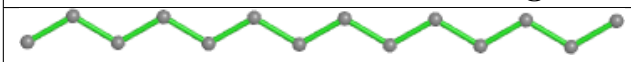
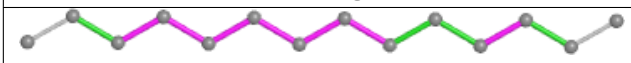
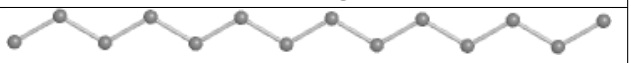
Torsions



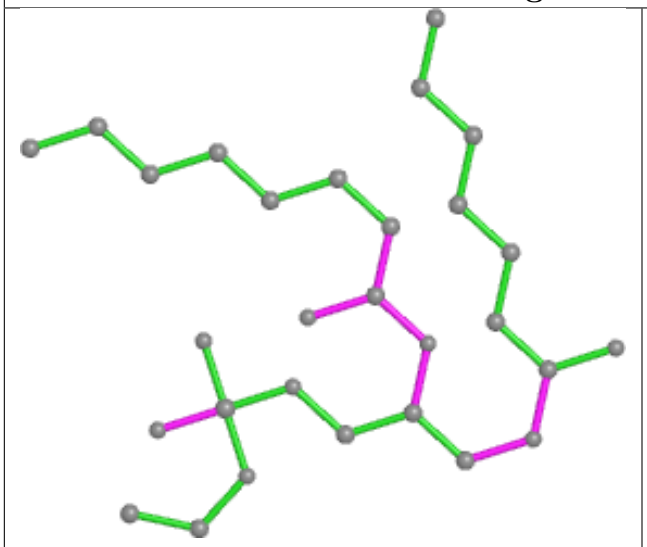
Rings

Ligand CPL A 708	
 Bond lengths	Bond angles
Torsions	Rings

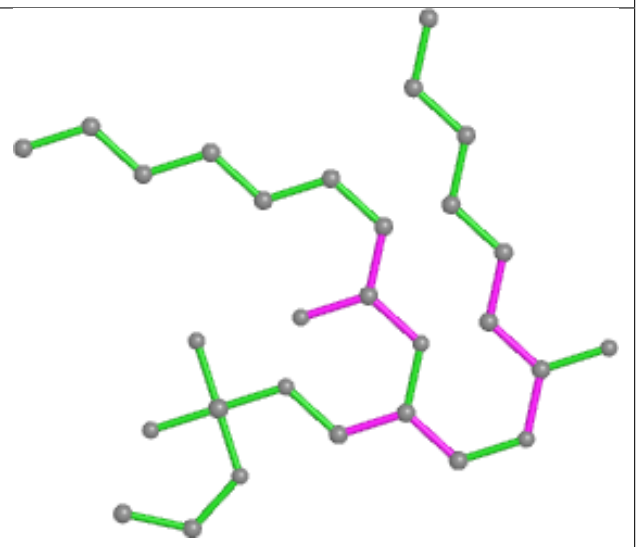
Ligand CPL B 704	
Bond lengths	Bond angles
 Torsions	 Rings

Ligand CPL C 704	
 Bond lengths	Bond angles
 Torsions	 Rings

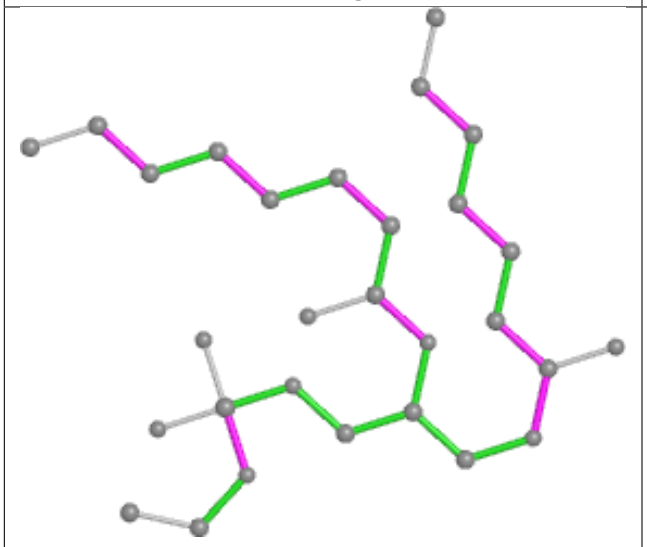
Ligand CPL D 705



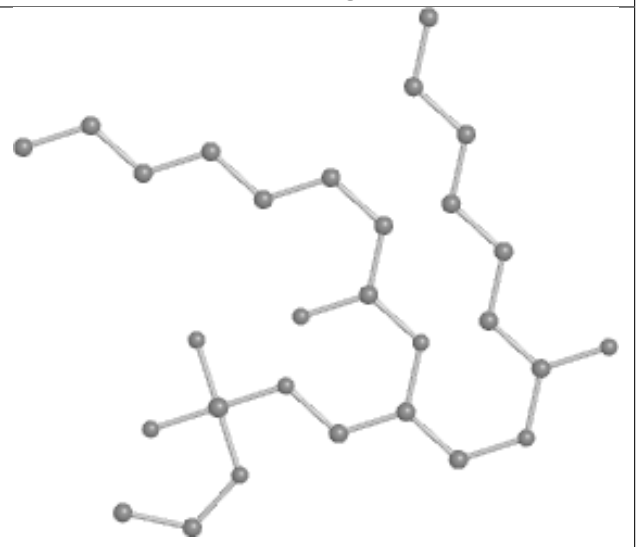
Bond lengths



Bond angles

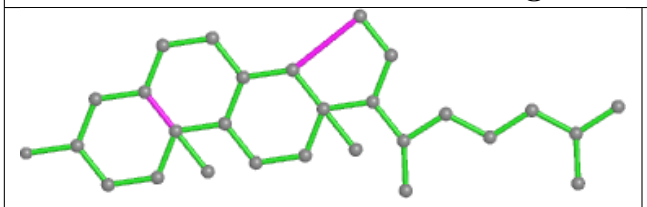


Torsions

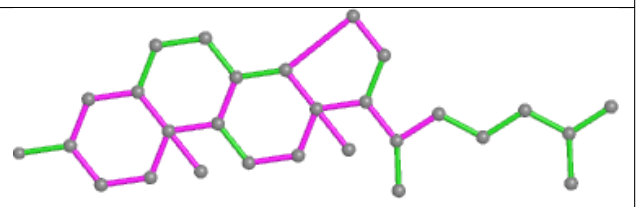


Rings

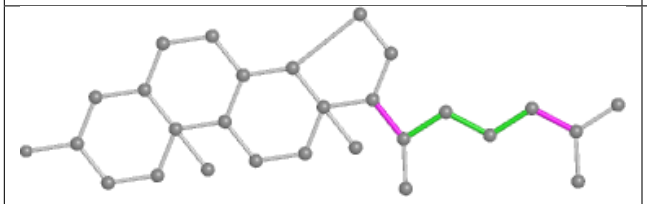
Ligand CLR C 700



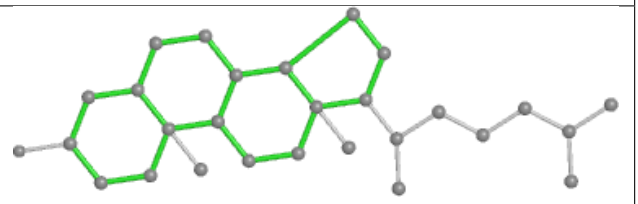
Bond lengths



Bond angles

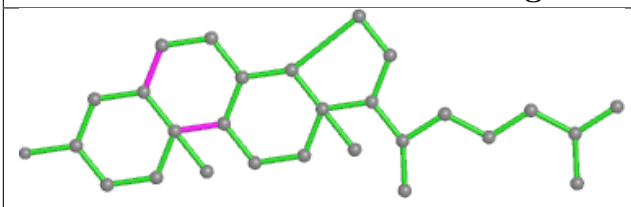


Torsions

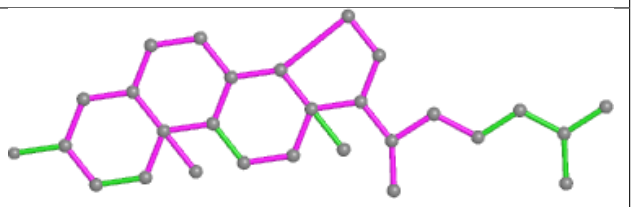


Rings

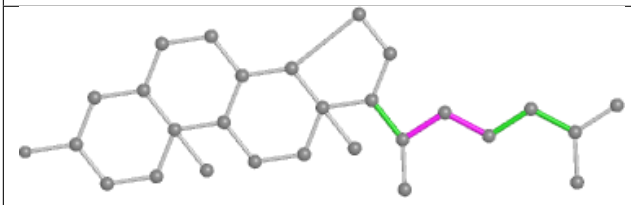
Ligand CLR B 701



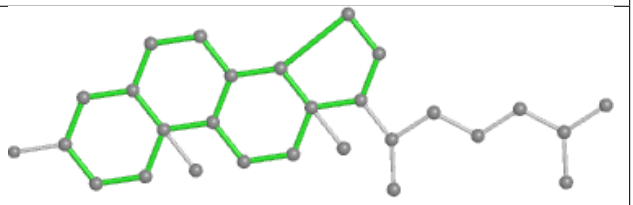
Bond lengths



Bond angles



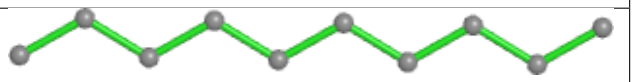
Torsions



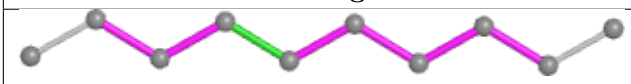
Rings

Ligand CPL B 703

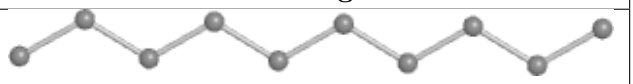
Bond lengths



Bond angles

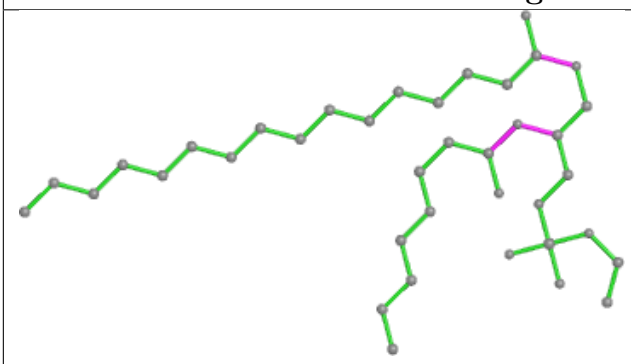


Torsions

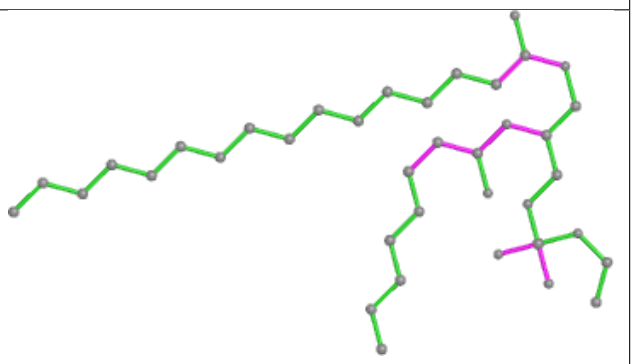


Rings

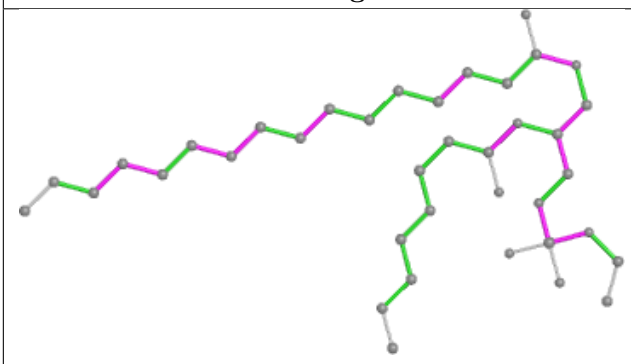
Ligand CPL B 706



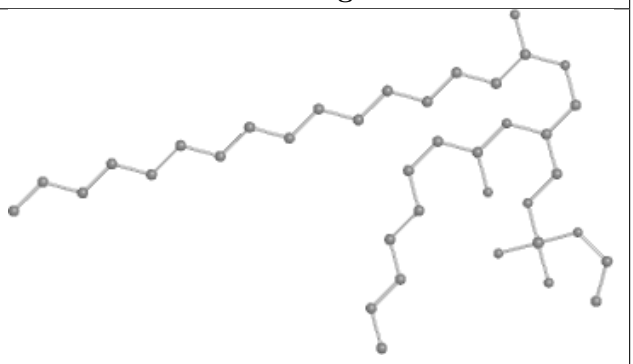
Bond lengths



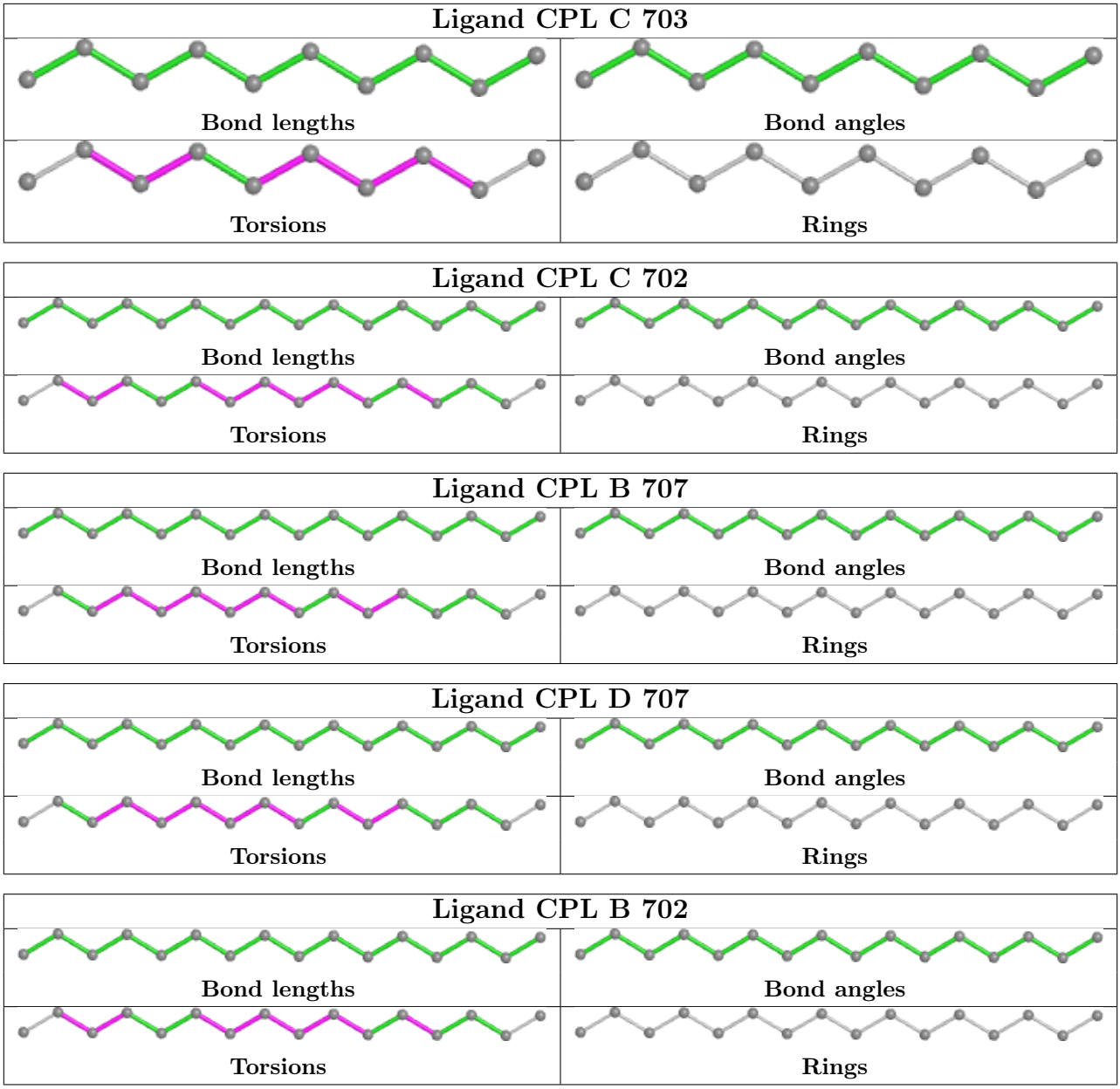
Bond angles



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.

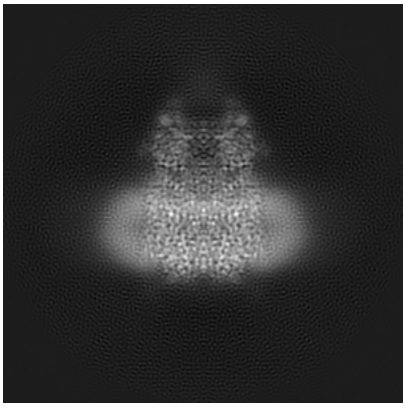
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23306. These allow visual inspection of the internal detail of the map and identification of artifacts.

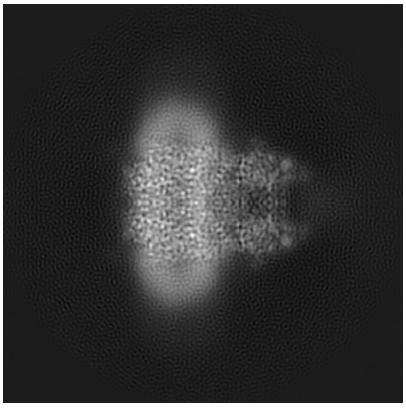
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

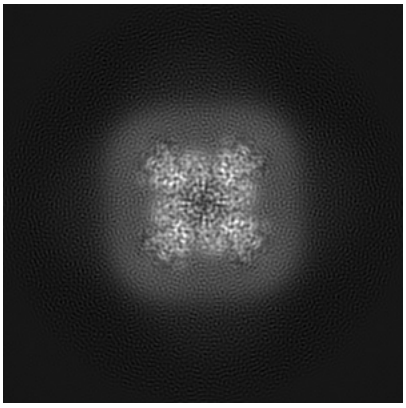
6.1.1 Primary map



X



Y

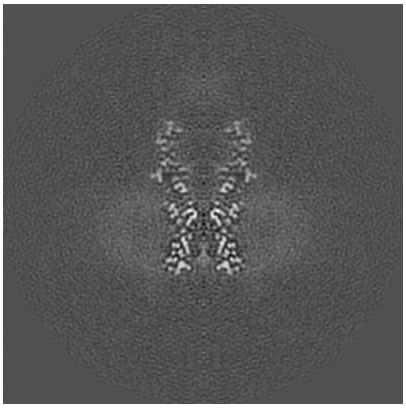


Z

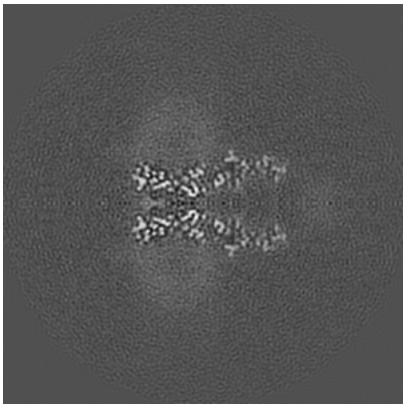
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

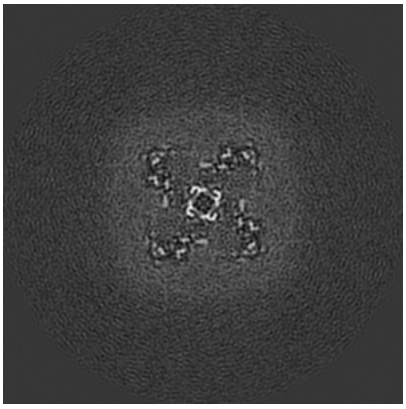
6.2.1 Primary map



X Index: 144



Y Index: 144

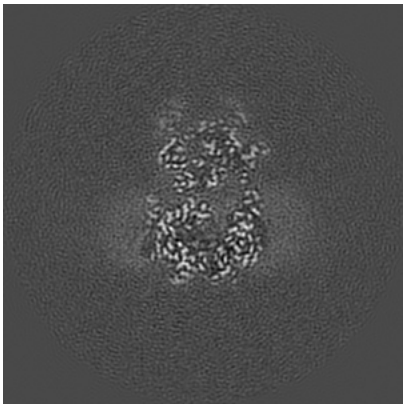


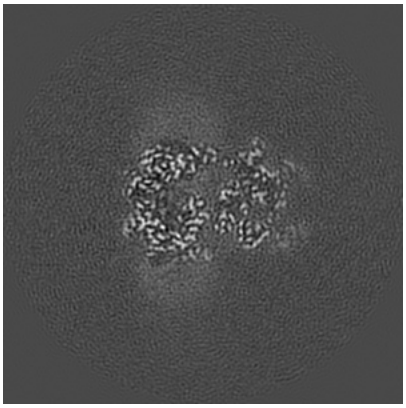
Z Index: 144

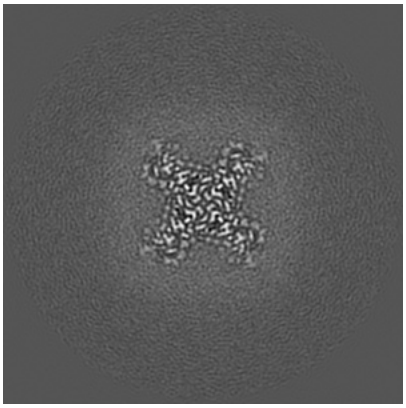
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 167

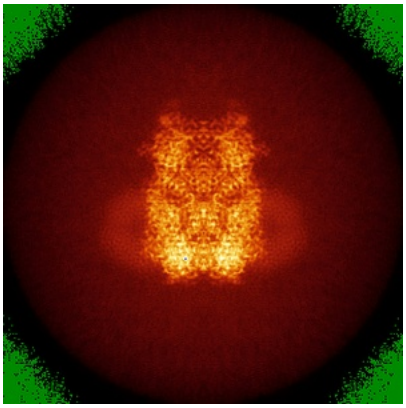

Y Index: 121

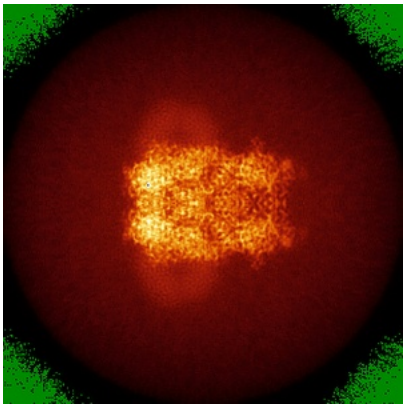

Z Index: 110

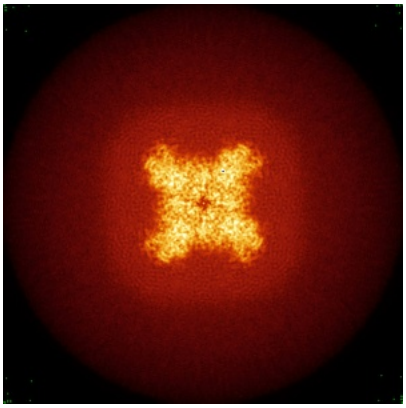
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

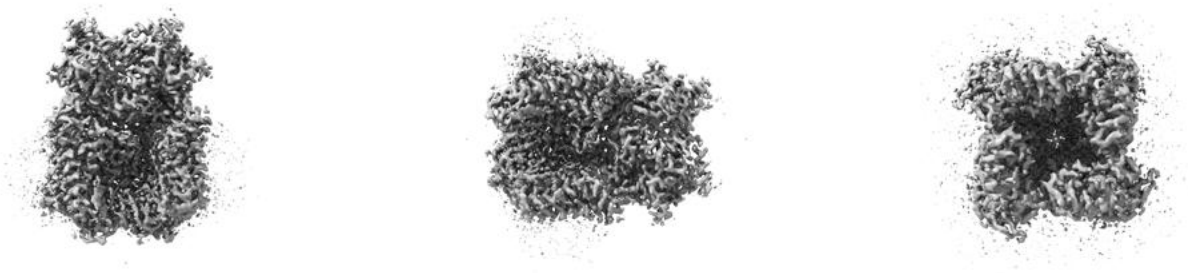

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

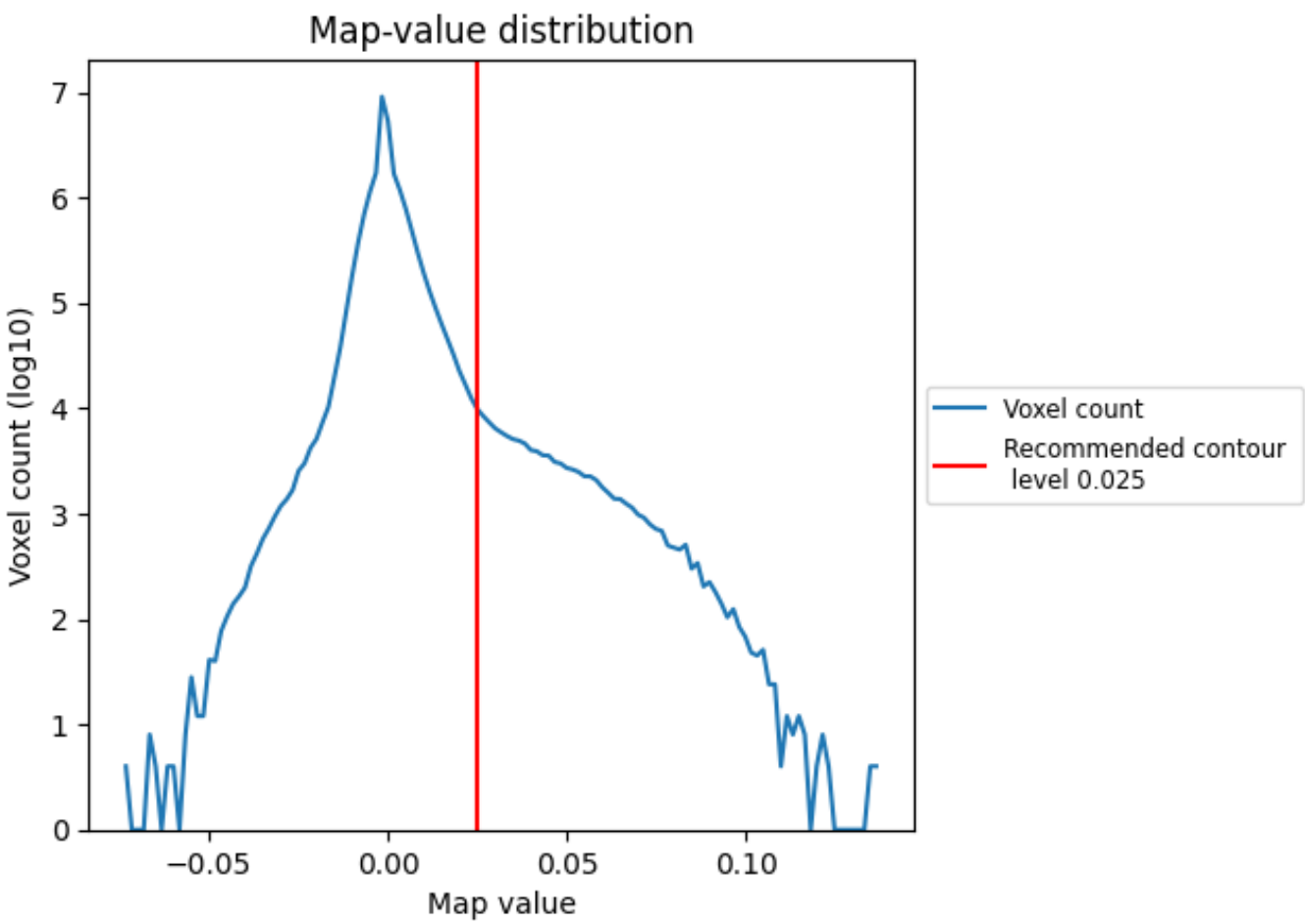
6.6 Mask visualisation (i)

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

7 Map analysis (i)

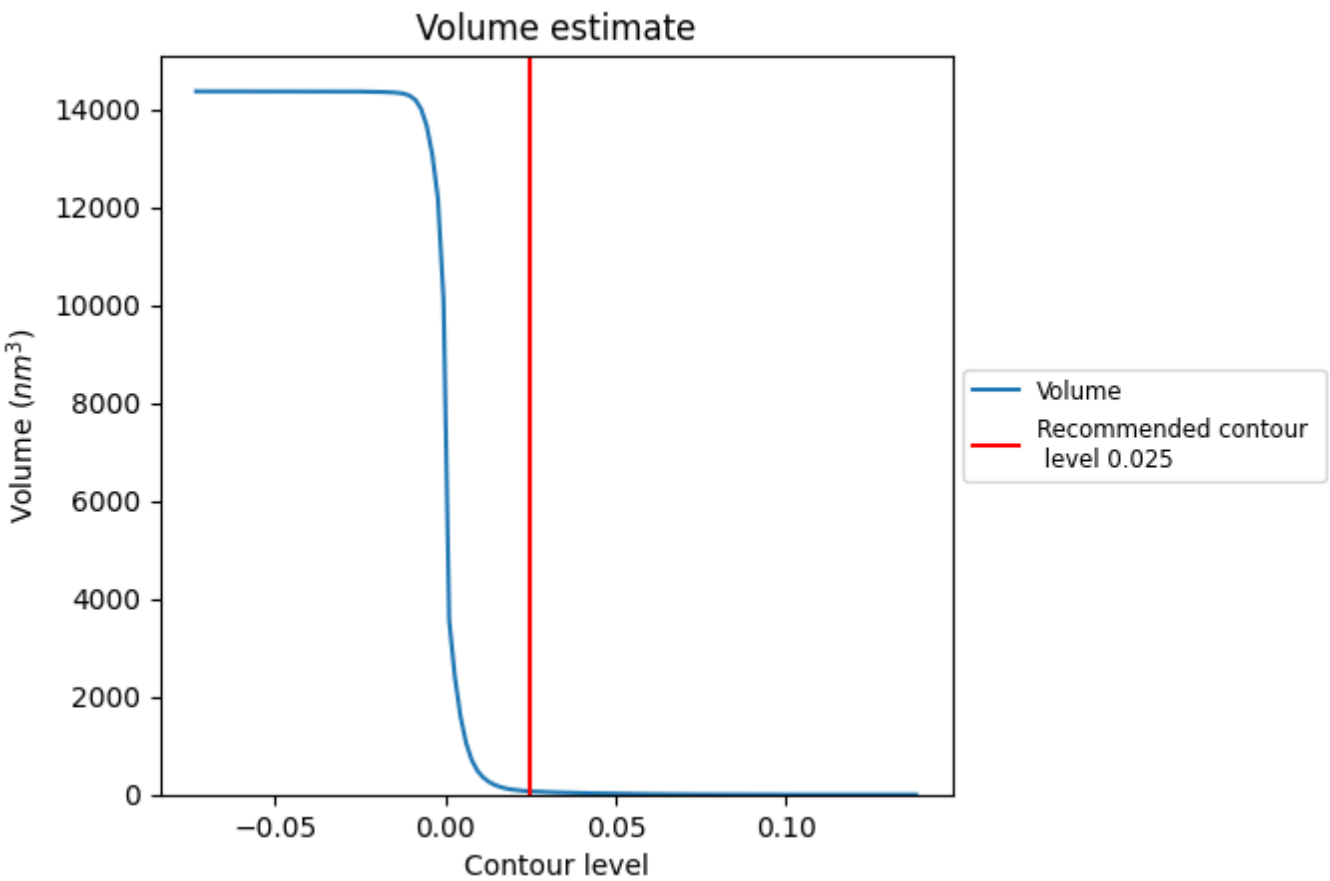
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

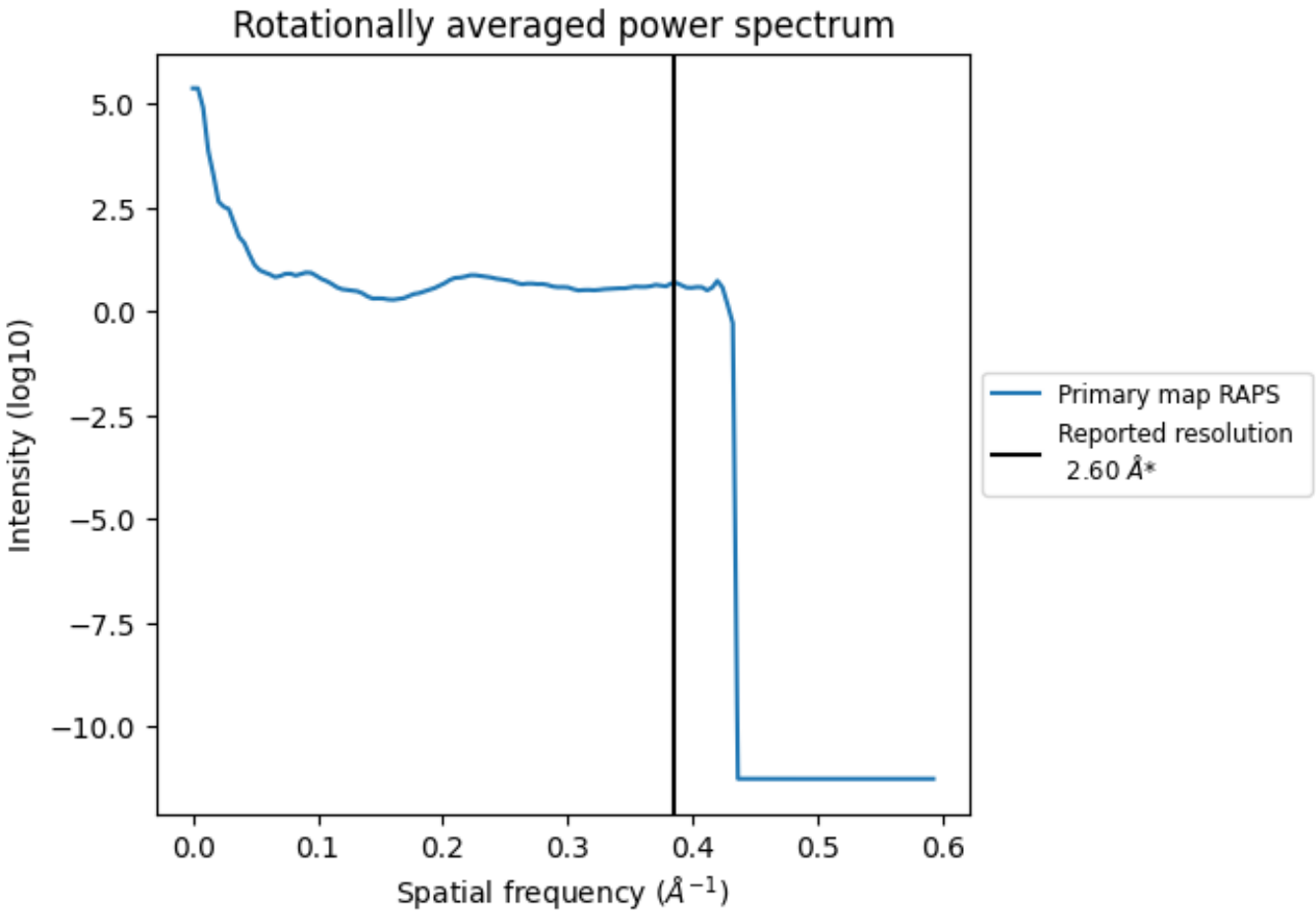
7.2 Volume estimate (i)



The volume at the recommended contour level is 66 nm^3; this corresponds to an approximate mass of 60 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)

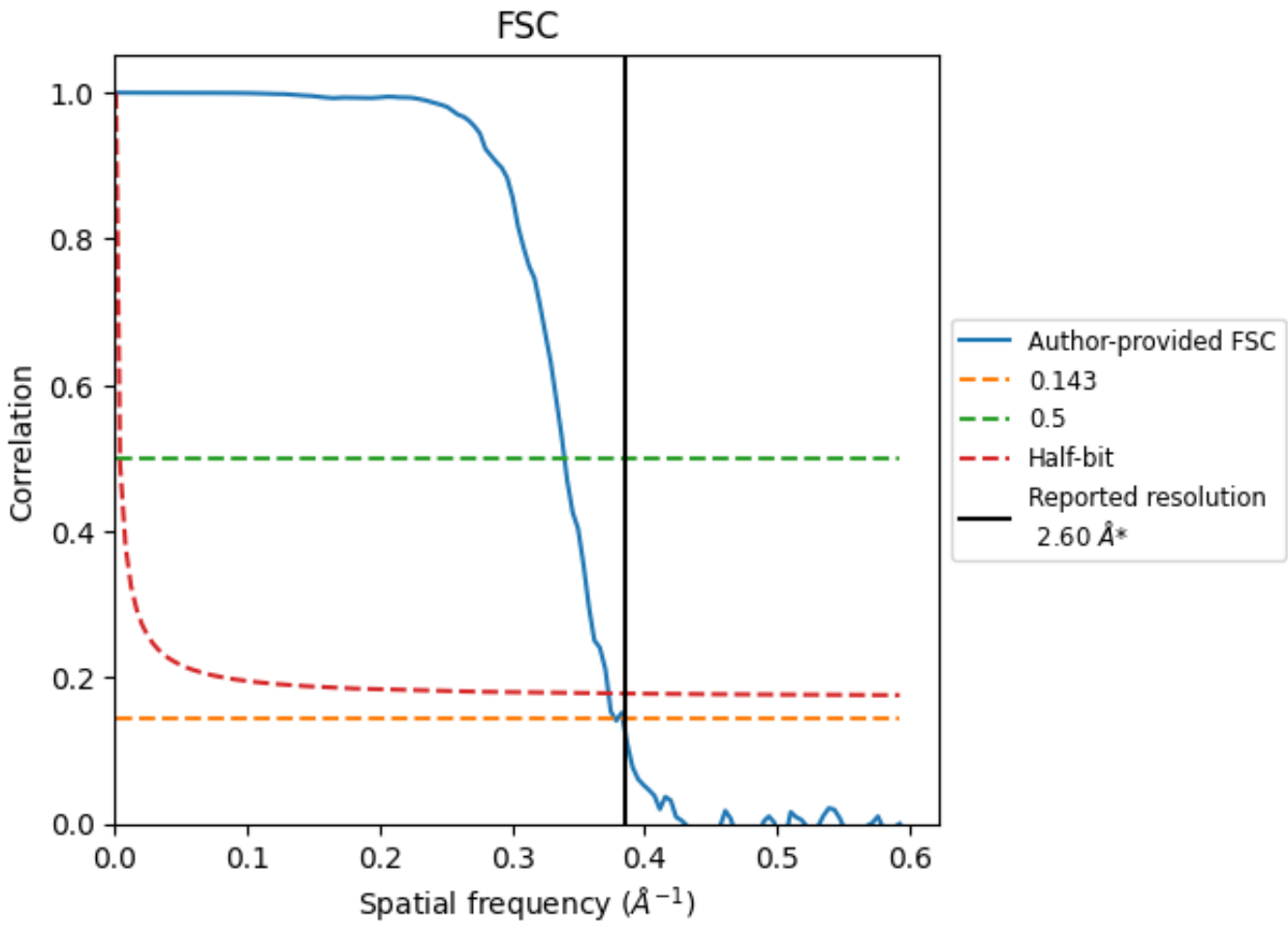


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

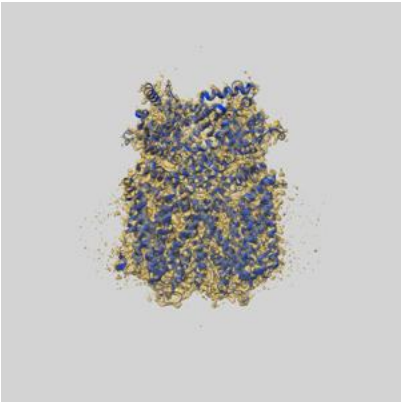
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.65	2.95	2.68
Unmasked-calculated*	-	-	-

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

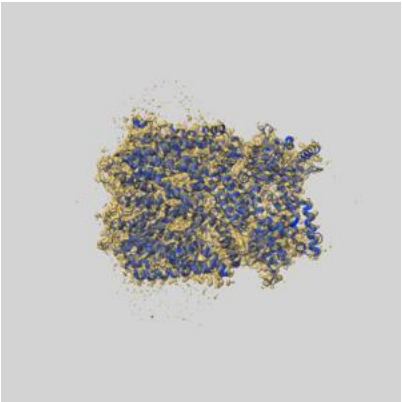
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23306 and PDB model 7LFT. Per-residue inclusion information can be found in section 3 on page 8.

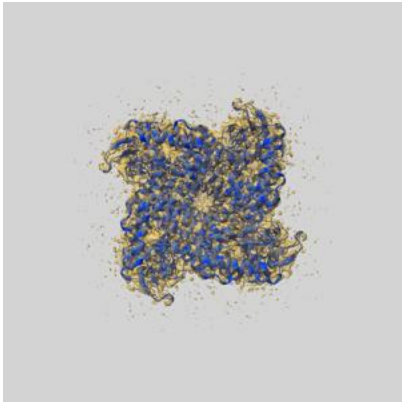
9.1 Map-model overlay (i)



X



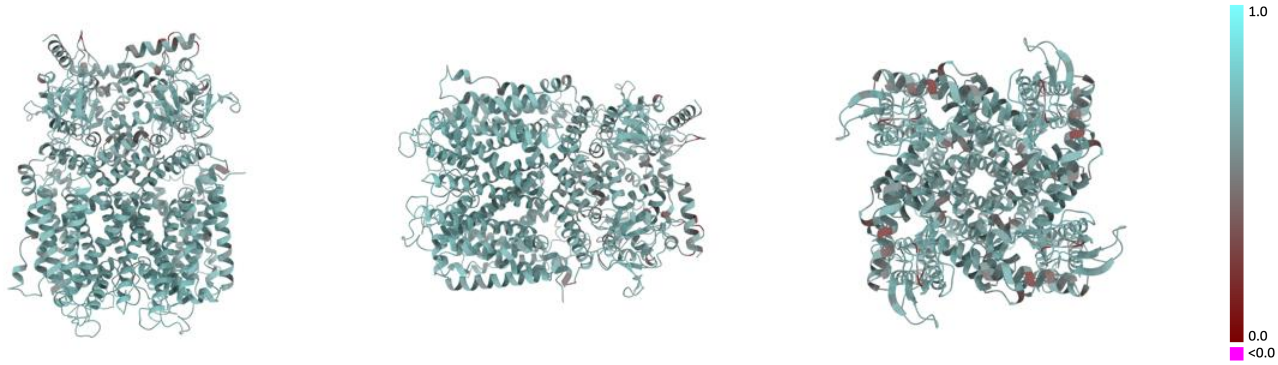
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

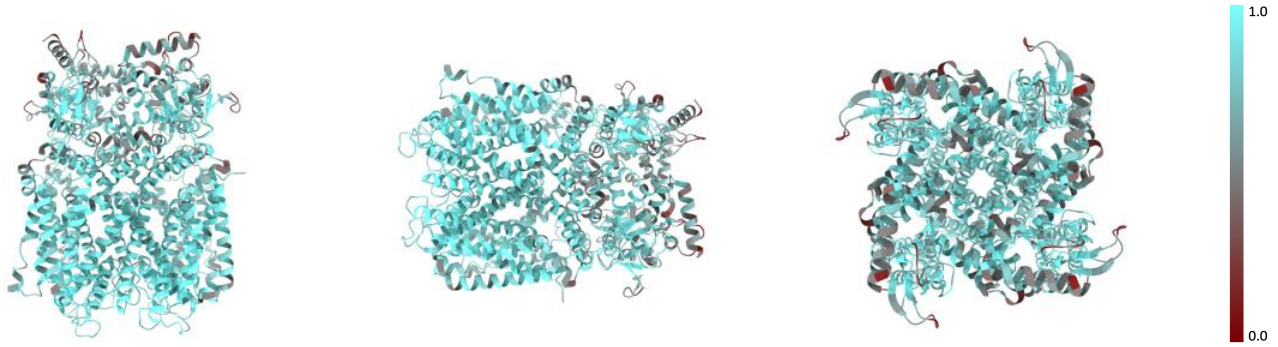
9.2 Q-score mapped to coordinate model (i)



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.

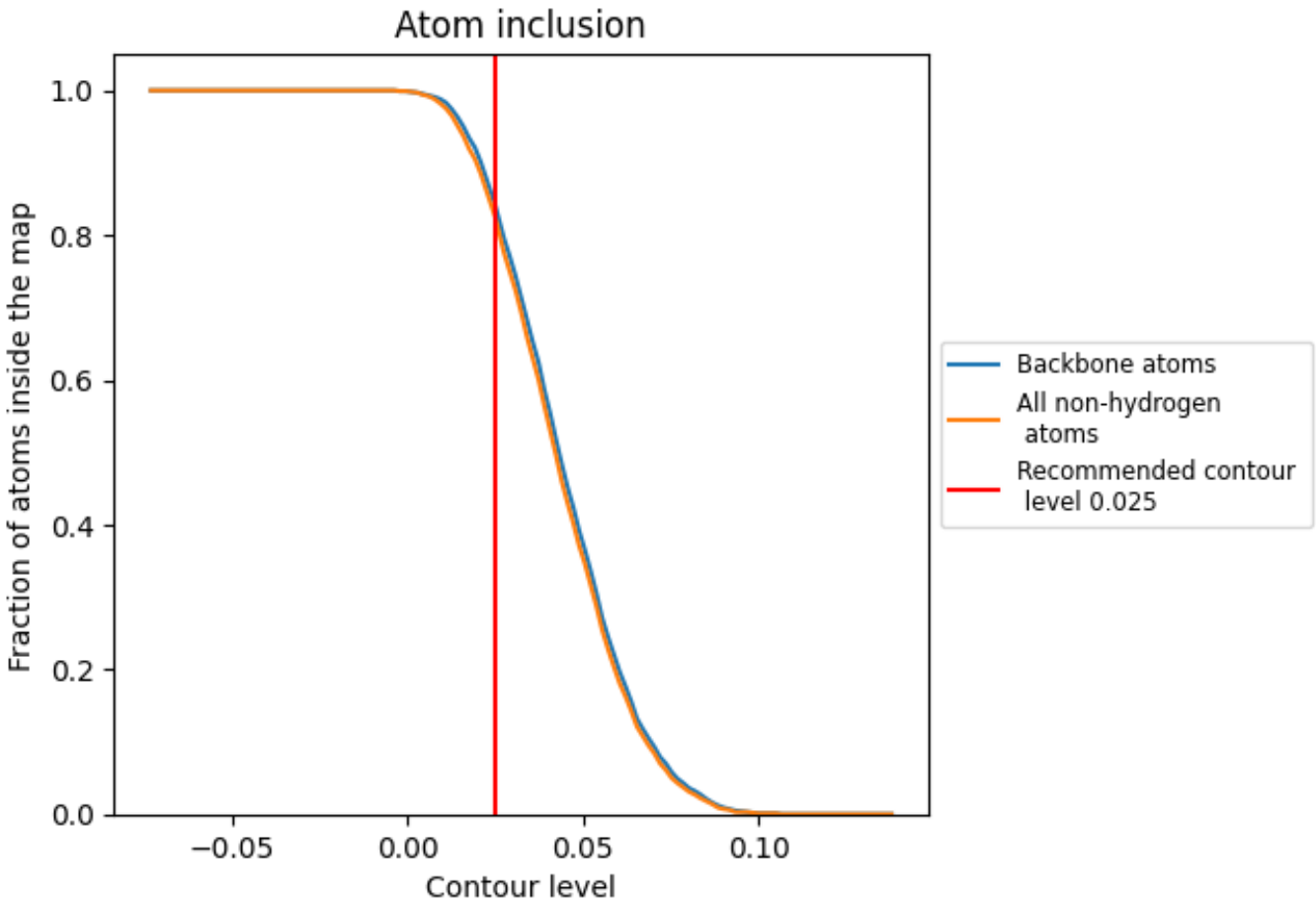
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.6380
A	0.8310	0.6380
B	0.8310	0.6380
C	0.8320	0.6390
D	0.8320	0.6380