Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 06:09 AM EST

PDB ID	:	6WEJ
EMDB ID	:	EMD-21649
Title	:	Structure of cGMP-unbound WT TAX-4 reconstituted in lipid nanodiscs
Authors	:	Zheng, X.; Fu, Z.; Su, D.; Zhang, Y.; Li, M.; Pan, Y.; Li, H.; Li, S.; Grassucci, R.A.; Ren, Z.; Hu, Z.; Li, X.; Zhou, M.; Li, G.; Frank, J.; Yang, J.
Deposited on	:	2020-04-02
Resolution	:	2.60 Å(reported)
Based on initial model	:	5H3O

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:

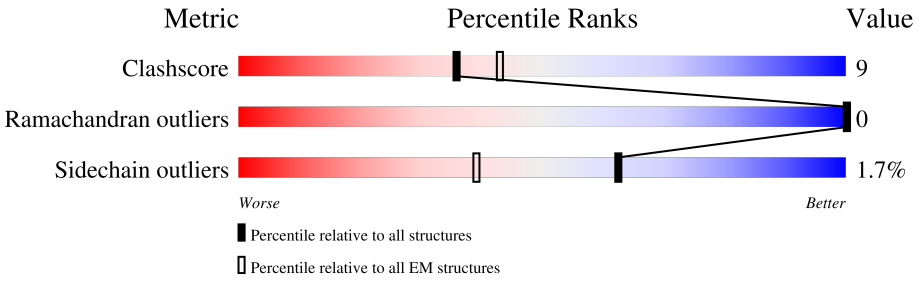
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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	733	54% 15% • 30%
1	B	733	54% 15% • 30%
1	C	733	54% 15% • 30%
1	D	733	54% 14% • 30%

2 Entry composition

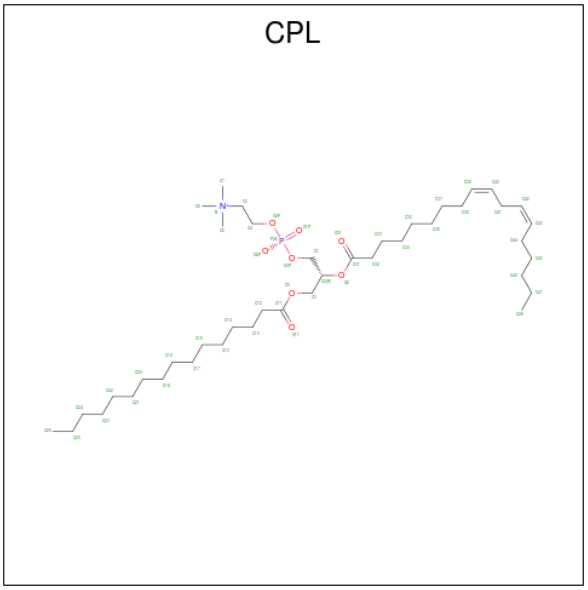
There are 4 unique types of molecules in this entry. The entry contains 17665 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cyclic nucleotide-gated cation channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			4241	2757	715	745	24		
1	B	513	Total	C	N	O	S	0	0
			4241	2757	715	745	24		
1	C	513	Total	C	N	O	S	0	0
			4241	2757	715	745	24		
1	D	513	Total	C	N	O	S	0	0
			4241	2757	715	745	24		

- Molecule 2 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
2	A	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	A	1	Total	C	N	O	P	0
			127	108	1	16	2	

Continued on next page...

Continued from previous page...

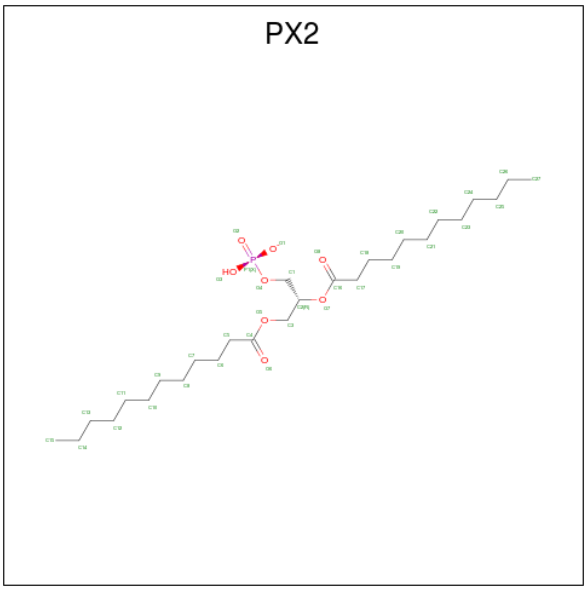
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	A	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	A	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	A	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	B	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	B	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	B	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	B	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	B	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	B	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	C	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	C	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	C	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	C	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	C	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	C	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	D	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	D	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	D	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	D	1	Total	C	N	O	P	0
			127	108	1	16	2	
2	D	1	Total	C	N	O	P	0
			127	108	1	16	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			127	108	1	16	2	

- Molecule 3 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: $C_{27}H_{52}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			48	30	16	2	
3	A	1	Total	C	O	P	0
			48	30	16	2	
3	B	1	Total	C	O	P	0
			48	30	16	2	
3	B	1	Total	C	O	P	0
			48	30	16	2	
3	C	1	Total	C	O	P	0
			48	30	16	2	
3	C	1	Total	C	O	P	0
			48	30	16	2	
3	D	1	Total	C	O	P	0
			48	30	16	2	
3	D	1	Total	C	O	P	0
			48	30	16	2	

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

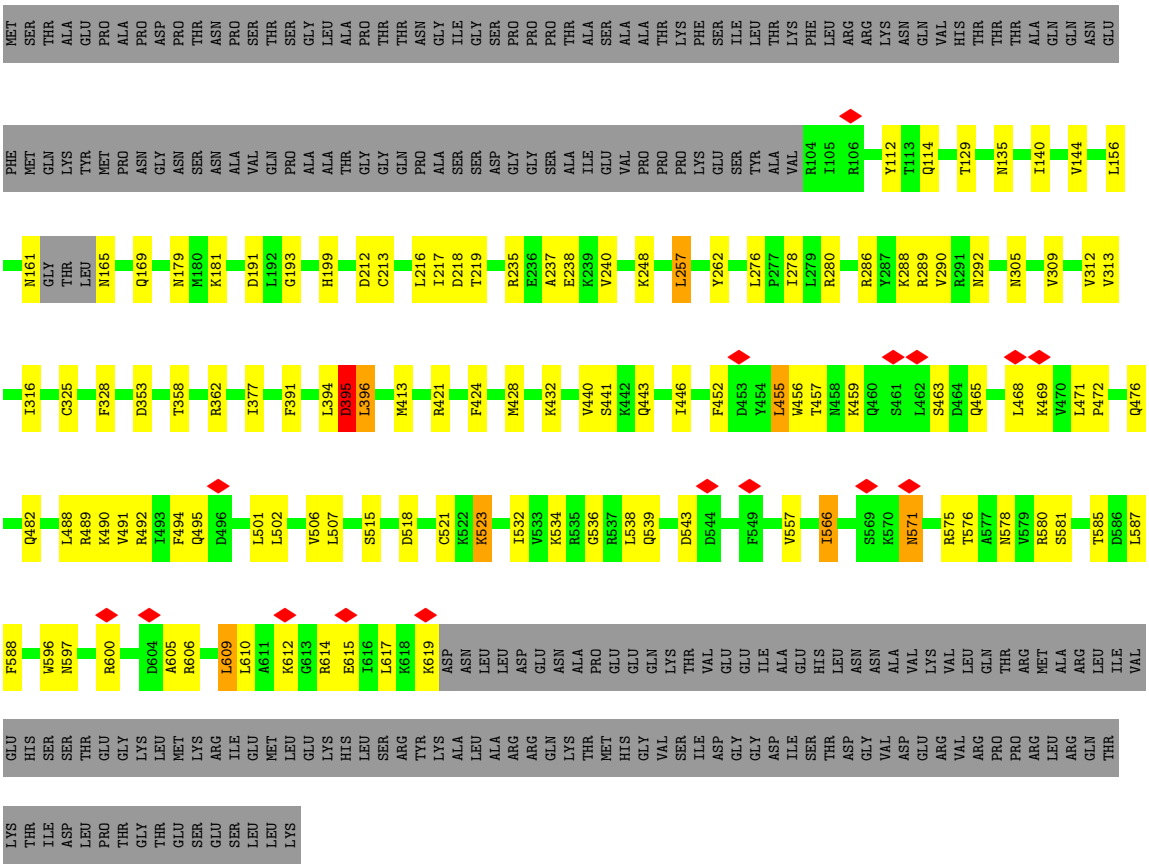
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
4	A	1	1	1	0

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.

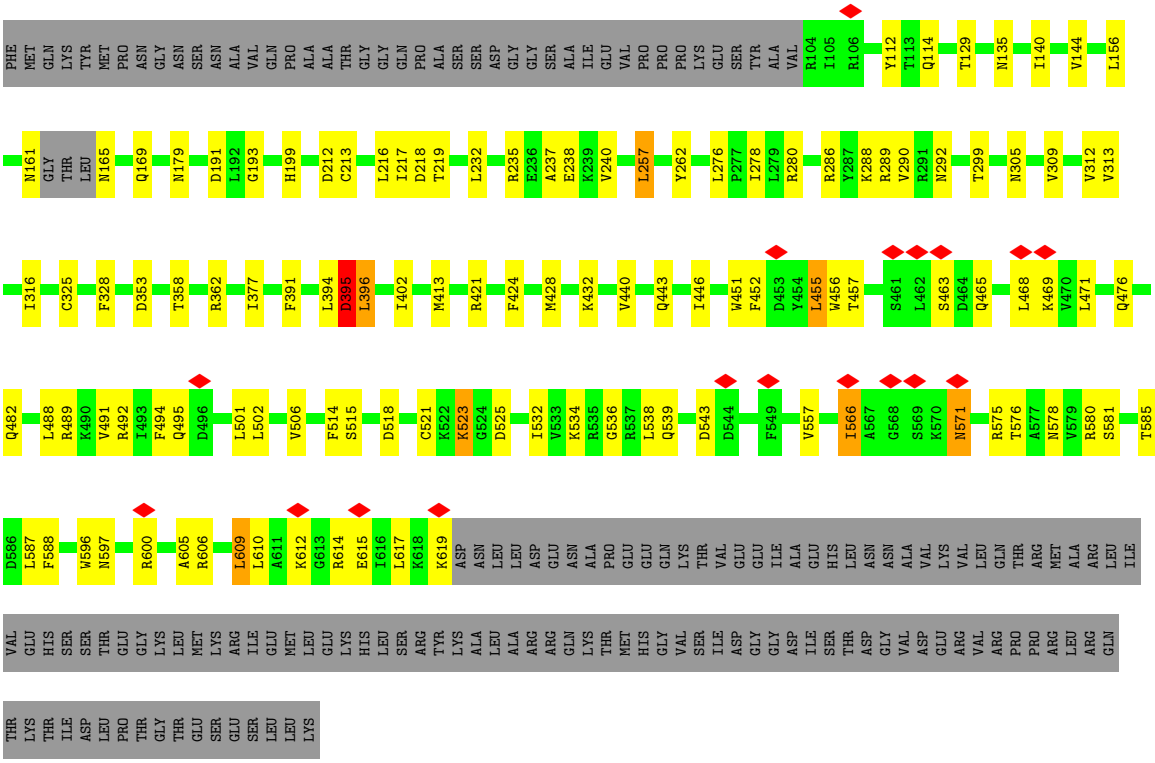
• Molecule 1: Cyclic nucleotide-gated cation channel

Chain A:



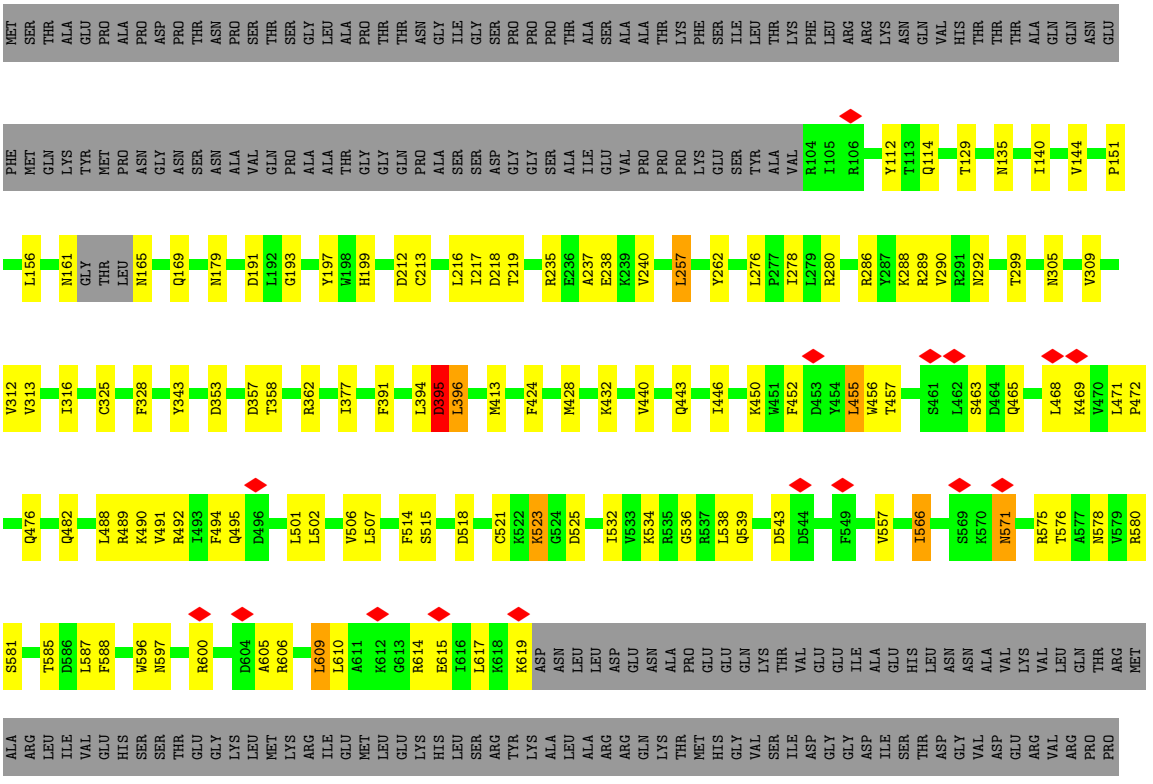
• Molecule 1: Cyclic nucleotide-gated cation channel

Chain B:

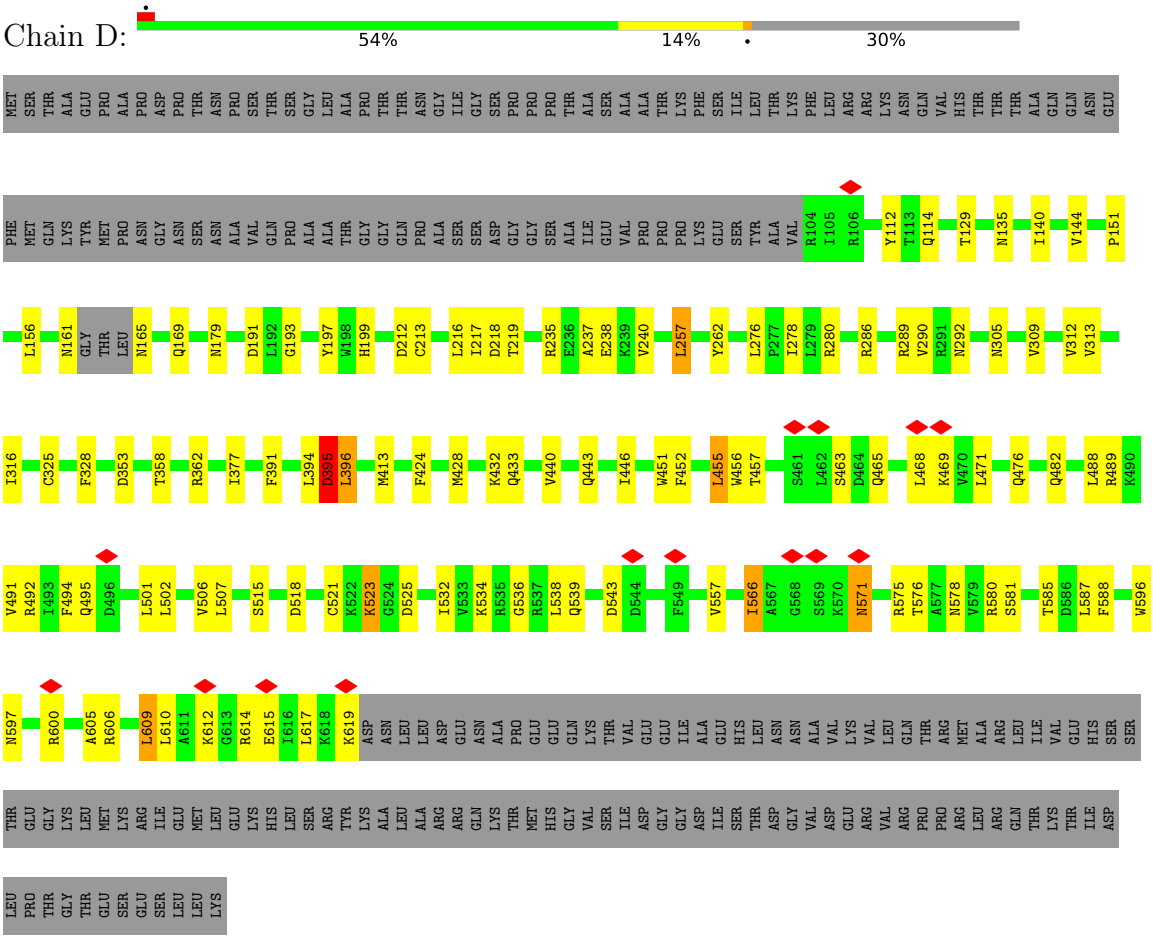


• Molecule 1: Cyclic nucleotide-gated cation channel

Chain C:



• Molecule 1: Cyclic nucleotide-gated cation channel



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	163525	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	66.03	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.851	Depositor
Minimum map value	-4.665	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.574	Depositor
Map size (Å)	316.72, 316.72, 316.72	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PX2, NA, 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	0.64	9/4343 (0.2%)	0.59	8/5889 (0.1%)
1	B	0.64	9/4343 (0.2%)	0.59	8/5889 (0.1%)
1	C	0.64	9/4343 (0.2%)	0.59	8/5889 (0.1%)
1	D	0.64	9/4343 (0.2%)	0.59	8/5889 (0.1%)
All	All	0.64	36/17372 (0.2%)	0.59	32/23556 (0.1%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	395	ASP	CB-CG	-10.77	1.29	1.51
1	D	395	ASP	CB-CG	-10.77	1.29	1.51
1	A	395	ASP	CB-CG	-10.76	1.29	1.51
1	B	395	ASP	CB-CG	-10.75	1.29	1.51
1	A	394	LEU	C-O	-10.06	1.04	1.23
1	B	394	LEU	C-O	-10.05	1.04	1.23
1	D	394	LEU	C-O	-10.05	1.04	1.23
1	C	394	LEU	C-O	-10.04	1.04	1.23
1	D	396	LEU	C-O	-9.13	1.06	1.23
1	A	396	LEU	C-O	-9.12	1.06	1.23
1	B	396	LEU	C-O	-9.09	1.06	1.23
1	C	396	LEU	C-O	-9.08	1.06	1.23
1	B	395	ASP	C-O	-7.57	1.08	1.23
1	A	395	ASP	C-O	-7.54	1.09	1.23
1	D	395	ASP	C-O	-7.54	1.09	1.23
1	C	395	ASP	C-O	-7.51	1.09	1.23
1	B	292	ASN	C-O	-7.04	1.09	1.23
1	A	292	ASN	C-O	-7.03	1.09	1.23
1	C	292	ASN	C-O	-7.03	1.10	1.23
1	D	292	ASN	C-O	-7.02	1.10	1.23
1	C	395	ASP	CG-OD2	-6.88	1.09	1.25
1	D	395	ASP	CG-OD2	-6.85	1.09	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	ASP	CG-OD2	-6.85	1.09	1.25
1	B	395	ASP	CG-OD2	-6.85	1.09	1.25
1	A	395	ASP	CA-CB	-6.12	1.40	1.53
1	D	395	ASP	CA-CB	-6.12	1.40	1.53
1	B	395	ASP	CA-CB	-6.12	1.40	1.53
1	C	395	ASP	CA-CB	-6.10	1.40	1.53
1	B	257	LEU	C-O	-6.03	1.11	1.23
1	A	257	LEU	C-O	-5.78	1.12	1.23
1	D	257	LEU	C-O	-5.67	1.12	1.23
1	C	257	LEU	C-O	-5.57	1.12	1.23
1	D	395	ASP	CG-OD1	-5.53	1.12	1.25
1	C	395	ASP	CG-OD1	-5.53	1.12	1.25
1	A	395	ASP	CG-OD1	-5.52	1.12	1.25
1	B	395	ASP	CG-OD1	-5.51	1.12	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	292	ASN	CB-CA-C	-8.39	93.62	110.40
1	A	292	ASN	CB-CA-C	-8.38	93.65	110.40
1	C	292	ASN	CB-CA-C	-8.37	93.67	110.40
1	D	292	ASN	CB-CA-C	-8.37	93.67	110.40
1	A	395	ASP	CB-CG-OD1	7.81	125.33	118.30
1	D	395	ASP	CB-CG-OD1	7.81	125.33	118.30
1	B	395	ASP	CB-CG-OD1	7.74	125.27	118.30
1	C	395	ASP	CB-CG-OD1	7.74	125.27	118.30
1	B	455	LEU	CA-CB-CG	7.13	131.70	115.30
1	C	455	LEU	CA-CB-CG	7.12	131.69	115.30
1	A	455	LEU	CA-CB-CG	7.11	131.66	115.30
1	D	455	LEU	CA-CB-CG	7.11	131.65	115.30
1	C	394	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	D	394	LEU	CB-CG-CD2	-6.12	100.59	111.00
1	A	394	LEU	CB-CG-CD2	-6.12	100.59	111.00
1	B	394	LEU	CB-CG-CD2	-6.12	100.60	111.00
1	D	257	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	C	566	ILE	O-C-N	5.93	132.19	122.70
1	C	257	LEU	CB-CG-CD1	-5.92	100.93	111.00
1	A	566	ILE	O-C-N	5.92	132.17	122.70
1	D	566	ILE	O-C-N	5.91	132.15	122.70
1	B	566	ILE	O-C-N	5.89	132.13	122.70
1	A	395	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	D	395	ASP	CB-CG-OD2	-5.74	113.13	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	395	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	C	395	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	257	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	B	257	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	C	571	ASN	N-CA-C	5.03	124.59	111.00
1	A	571	ASN	N-CA-C	5.02	124.56	111.00
1	D	571	ASN	N-CA-C	5.02	124.55	111.00
1	B	571	ASN	N-CA-C	5.01	124.54	111.00

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	4241	0	4283	74	0
1	B	4241	0	4283	74	0
1	C	4241	0	4283	73	0
1	D	4241	0	4283	72	0
2	A	127	0	186	6	0
2	B	127	0	186	6	0
2	C	127	0	186	7	0
2	D	127	0	186	6	0
3	A	48	0	43	1	0
3	B	48	0	43	1	0
3	C	48	0	43	2	0
3	D	48	0	43	2	0
4	A	1	0	0	0	0
All	All	17665	0	18048	304	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 9.

All (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ASN:O	1:B:571:ASN:ND2	2.10	0.85
1:C:571:ASN:ND2	1:C:571:ASN:O	2.10	0.85
1:A:571:ASN:O	1:A:571:ASN:ND2	2.10	0.84
1:D:571:ASN:O	1:D:571:ASN:ND2	2.10	0.84
1:A:305:ASN:HB3	1:A:413:MET:HG3	1.61	0.81
1:C:566:ILE:HD13	1:C:617:LEU:HD12	1.61	0.81
1:B:305:ASN:HB3	1:B:413:MET:HG3	1.61	0.81
1:B:566:ILE:HD13	1:B:617:LEU:HD12	1.61	0.81
2:D:801:CPL:H42	2:D:801:CPL:H382	1.63	0.81
1:D:305:ASN:HB3	1:D:413:MET:HG3	1.61	0.81
1:A:566:ILE:HD13	1:A:617:LEU:HD12	1.61	0.80
2:C:801:CPL:H382	2:C:801:CPL:H42	1.63	0.80
1:C:305:ASN:HB3	1:C:413:MET:HG3	1.61	0.80
1:D:135:ASN:OD1	1:D:280:ARG:NH1	2.15	0.80
1:C:135:ASN:OD1	1:C:280:ARG:NH1	2.15	0.80
1:A:135:ASN:OD1	1:A:280:ARG:NH1	2.15	0.80
1:B:135:ASN:OD1	1:B:280:ARG:NH1	2.15	0.80
1:D:566:ILE:HD13	1:D:617:LEU:HD12	1.61	0.80
2:A:801:CPL:H42	2:A:801:CPL:H382	1.63	0.79
2:B:801:CPL:H42	2:B:801:CPL:H382	1.62	0.78
1:C:179:ASN:ND2	1:C:353:ASP:O	2.16	0.78
1:D:179:ASN:ND2	1:D:353:ASP:O	2.17	0.78
1:B:179:ASN:ND2	1:B:353:ASP:O	2.17	0.77
1:A:179:ASN:ND2	1:A:353:ASP:O	2.17	0.77
1:A:112:TYR:OH	1:A:114:GLN:NE2	2.25	0.70
1:B:112:TYR:OH	1:B:114:GLN:NE2	2.24	0.70
1:D:112:TYR:OH	1:D:114:GLN:NE2	2.24	0.70
1:C:112:TYR:OH	1:C:114:GLN:NE2	2.24	0.68
1:A:521:CYS:HB2	1:A:575:ARG:HG3	1.76	0.68
1:C:521:CYS:HB2	1:C:575:ARG:HG3	1.76	0.67
1:D:521:CYS:HB2	1:D:575:ARG:HG3	1.76	0.67
1:B:521:CYS:HB2	1:B:575:ARG:HG3	1.76	0.66
1:B:596:TRP:HH2	1:B:610:LEU:HD21	1.62	0.64
1:C:596:TRP:HH2	1:C:610:LEU:HD21	1.62	0.64
1:A:596:TRP:HH2	1:A:610:LEU:HD21	1.62	0.63
1:C:428:MET:SD	1:C:432:LYS:NZ	2.72	0.63
1:D:428:MET:SD	1:D:432:LYS:NZ	2.72	0.63
1:A:428:MET:SD	1:A:432:LYS:NZ	2.71	0.63
1:B:428:MET:SD	1:B:432:LYS:NZ	2.71	0.63
1:B:440:VAL:HG13	1:C:482:GLN:NE2	2.12	0.63
1:D:596:TRP:HH2	1:D:610:LEU:HD21	1.62	0.63
1:B:191:ASP:O	1:B:193:GLY:N	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ASP:O	1:D:193:GLY:N	2.31	0.63
1:A:191:ASP:O	1:A:193:GLY:N	2.31	0.62
1:B:216:LEU:HD23	1:B:257:LEU:HD11	1.81	0.62
1:C:191:ASP:O	1:C:193:GLY:N	2.32	0.62
1:D:212:ASP:OD2	1:D:262:TYR:OH	2.11	0.61
2:B:801:CPL:H42	2:B:801:CPL:C38	2.32	0.60
1:D:218:ASP:OD1	1:D:289:ARG:NH1	2.35	0.60
1:B:539:GLN:HE21	1:B:580:ARG:HE	1.51	0.59
1:A:218:ASP:OD1	1:A:289:ARG:NH1	2.35	0.59
1:A:600:ARG:HA	1:A:606:ARG:HH12	1.68	0.59
1:C:539:GLN:HE21	1:C:580:ARG:HE	1.51	0.59
1:B:218:ASP:OD1	1:B:289:ARG:NH1	2.35	0.59
1:C:600:ARG:HA	1:C:606:ARG:HH12	1.68	0.59
1:D:539:GLN:HE21	1:D:580:ARG:HE	1.51	0.59
1:A:539:GLN:HE21	1:A:580:ARG:HE	1.50	0.59
1:D:161:ASN:O	1:D:165:ASN:N	2.36	0.58
1:A:161:ASN:O	1:A:165:ASN:N	2.36	0.58
1:B:600:ARG:HA	1:B:606:ARG:HH12	1.68	0.58
1:B:161:ASN:O	1:B:165:ASN:N	2.36	0.58
1:C:161:ASN:O	1:C:165:ASN:N	2.36	0.58
1:C:212:ASP:OD2	1:C:262:TYR:OH	2.11	0.58
1:A:472:PRO:HD3	1:D:451:TRP:CH2	2.39	0.58
1:D:600:ARG:HA	1:D:606:ARG:HH12	1.68	0.58
1:C:218:ASP:OD1	1:C:289:ARG:NH1	2.35	0.58
1:B:463:SER:HB3	1:B:465:GLN:HG2	1.86	0.58
1:D:488:LEU:HD12	1:D:506:VAL:HG12	1.85	0.57
1:C:463:SER:HB3	1:C:465:GLN:HG2	1.86	0.57
1:C:488:LEU:HD12	1:C:506:VAL:HG12	1.85	0.57
1:B:488:LEU:HD12	1:B:506:VAL:HG12	1.85	0.57
2:D:801:CPL:H42	2:D:801:CPL:C38	2.32	0.57
1:A:488:LEU:HD12	1:A:506:VAL:HG12	1.85	0.57
1:A:377:ILE:HD13	1:B:396:LEU:HD22	1.87	0.57
2:A:801:CPL:C32	2:A:801:CPL:HC12	2.35	0.57
2:B:801:CPL:C32	2:B:801:CPL:HC12	2.35	0.56
2:C:801:CPL:H42	2:C:801:CPL:C38	2.32	0.56
1:A:463:SER:HB3	1:A:465:GLN:HG2	1.86	0.56
2:C:801:CPL:C32	2:C:801:CPL:HC12	2.35	0.56
2:D:801:CPL:C32	2:D:801:CPL:HC12	2.35	0.56
1:D:463:SER:HB3	1:D:465:GLN:HG2	1.86	0.56
1:A:212:ASP:OD2	1:A:262:TYR:OH	2.11	0.55
1:A:523:LYS:NZ	1:A:578:ASN:HD21	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:LYS:NZ	1:C:578:ASN:HD21	2.04	0.55
1:B:523:LYS:NZ	1:B:578:ASN:HD21	2.04	0.55
1:C:494:PHE:HE1	1:C:609:LEU:HD21	1.72	0.55
1:D:532:ILE:HG12	1:D:557:VAL:HG12	1.89	0.55
1:B:494:PHE:HE1	1:B:609:LEU:HD21	1.72	0.55
1:A:532:ILE:HG12	1:A:557:VAL:HG12	1.89	0.54
2:A:801:CPL:C42	2:A:801:CPL:C38	2.85	0.54
1:D:523:LYS:NZ	1:D:578:ASN:HD21	2.04	0.54
2:B:801:CPL:C38	2:B:801:CPL:C42	2.85	0.54
1:B:421:ARG:HH22	1:C:299:THR:HG22	1.73	0.54
2:C:801:CPL:C38	2:C:801:CPL:C42	2.85	0.54
2:D:801:CPL:C38	2:D:801:CPL:C42	2.85	0.54
1:A:494:PHE:HE1	1:A:609:LEU:HD21	1.72	0.54
2:A:801:CPL:H42	2:A:801:CPL:C38	2.32	0.53
1:D:216:LEU:HD23	1:D:257:LEU:HD11	1.89	0.53
1:D:494:PHE:HE1	1:D:609:LEU:HD21	1.72	0.53
1:B:532:ILE:HG12	1:B:557:VAL:HG12	1.89	0.53
1:C:532:ILE:HG12	1:C:557:VAL:HG12	1.89	0.53
2:D:801:CPL:H382	2:D:801:CPL:C42	2.38	0.53
1:C:515:SER:OG	1:C:518:ASP:OD2	2.26	0.53
1:B:212:ASP:OD2	1:B:262:TYR:OH	2.11	0.52
1:B:377:ILE:HD13	1:C:396:LEU:HD22	1.91	0.52
1:B:219:THR:HB	1:B:286:ARG:HH22	1.75	0.52
1:D:199:HIS:H	1:D:199:HIS:CD2	2.28	0.51
1:B:515:SER:OG	1:B:518:ASP:OD2	2.26	0.51
1:C:140:ILE:HD11	2:C:806:CPL:H212	1.92	0.51
1:A:515:SER:OG	1:A:518:ASP:OD2	2.26	0.51
1:D:219:THR:HB	1:D:286:ARG:HH22	1.75	0.51
1:A:216:LEU:HD23	1:A:257:LEU:HD11	1.93	0.51
1:B:566:ILE:HD13	1:B:617:LEU:CD1	2.38	0.51
1:A:566:ILE:HD13	1:A:617:LEU:CD1	2.38	0.51
1:D:140:ILE:HD11	2:D:806:CPL:H212	1.92	0.51
1:C:219:THR:HB	1:C:286:ARG:HH22	1.75	0.51
1:C:199:HIS:CD2	1:C:199:HIS:H	2.28	0.50
1:A:140:ILE:HD11	2:A:806:CPL:H212	1.92	0.50
1:A:219:THR:HB	1:A:286:ARG:HH22	1.75	0.50
1:A:534:LYS:HD2	1:A:588:PHE:HE2	1.77	0.50
1:B:140:ILE:HD11	2:B:806:CPL:H212	1.92	0.50
1:D:534:LYS:HD2	1:D:588:PHE:HE2	1.77	0.50
1:D:276:LEU:HG	1:D:278:ILE:HG22	1.94	0.50
1:A:199:HIS:CD2	1:A:199:HIS:H	2.28	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:HG	1:C:278:ILE:HG22	1.94	0.50
1:D:489:ARG:NH1	1:D:494:PHE:O	2.45	0.50
1:A:538:LEU:HD21	1:A:587:LEU:HD11	1.94	0.49
1:C:489:ARG:NH1	1:C:494:PHE:O	2.45	0.49
1:D:538:LEU:HD21	1:D:587:LEU:HD11	1.94	0.49
1:A:276:LEU:HG	1:A:278:ILE:HG22	1.94	0.49
1:B:534:LYS:HD2	1:B:588:PHE:HE2	1.77	0.49
1:A:482:GLN:NE2	1:D:440:VAL:HG13	2.27	0.49
1:B:276:LEU:HG	1:B:278:ILE:HG22	1.94	0.49
1:A:488:LEU:HD23	1:A:491:VAL:HG21	1.94	0.49
1:B:199:HIS:H	1:B:199:HIS:CD2	2.28	0.49
1:B:489:ARG:NH1	1:B:494:PHE:O	2.45	0.49
1:C:468:LEU:O	1:C:476:GLN:NE2	2.45	0.49
1:C:488:LEU:HD23	1:C:491:VAL:HG21	1.94	0.49
1:C:566:ILE:HD13	1:C:617:LEU:CD1	2.38	0.49
1:A:237:ALA:O	1:A:238:GLU:C	2.51	0.49
1:C:538:LEU:HD21	1:C:587:LEU:HD11	1.94	0.49
1:A:468:LEU:O	1:A:476:GLN:NE2	2.46	0.49
1:A:489:ARG:NH1	1:A:494:PHE:O	2.45	0.49
1:D:515:SER:OG	1:D:518:ASP:OD2	2.26	0.49
1:B:534:LYS:HD2	1:B:588:PHE:CE2	2.48	0.49
3:B:803:PX2:O8	3:B:803:PX2:H5	2.13	0.49
1:C:534:LYS:HD2	1:C:588:PHE:HE2	1.77	0.49
1:D:237:ALA:O	1:D:238:GLU:C	2.51	0.49
3:D:803:PX2:O8	3:D:803:PX2:H5	2.13	0.49
1:C:534:LYS:HD2	1:C:588:PHE:CE2	2.48	0.48
1:D:468:LEU:O	1:D:476:GLN:NE2	2.46	0.48
1:D:492:ARG:HA	1:D:495:GLN:HG3	1.95	0.48
3:A:803:PX2:H5	3:A:803:PX2:O8	2.13	0.48
1:B:488:LEU:HD23	1:B:491:VAL:HG21	1.94	0.48
3:C:803:PX2:H5	3:C:803:PX2:O8	2.13	0.48
1:D:488:LEU:HD23	1:D:491:VAL:HG21	1.94	0.48
1:B:468:LEU:O	1:B:476:GLN:NE2	2.45	0.48
1:B:538:LEU:HD21	1:B:587:LEU:HD11	1.94	0.48
1:A:534:LYS:HD2	1:A:588:PHE:CE2	2.48	0.48
1:A:502:LEU:O	1:A:506:VAL:HG13	2.14	0.48
1:C:492:ARG:HA	1:C:495:GLN:HG3	1.95	0.48
1:C:502:LEU:O	1:C:506:VAL:HG13	2.14	0.48
1:D:502:LEU:O	1:D:506:VAL:HG13	2.14	0.48
1:B:502:LEU:O	1:B:506:VAL:HG13	2.14	0.47
1:C:237:ALA:O	1:C:238:GLU:C	2.51	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ARG:HA	1:A:495:GLN:HG3	1.95	0.47
1:D:501:LEU:HD22	1:D:605:ALA:HB1	1.96	0.47
1:D:534:LYS:HD2	1:D:588:PHE:CE2	2.48	0.47
1:A:391:PHE:O	1:A:395:ASP:HB2	2.15	0.47
1:C:213:CYS:O	1:C:217:ILE:HG12	2.15	0.47
1:D:391:PHE:O	1:D:395:ASP:HB2	2.15	0.47
1:B:312:VAL:O	1:B:316:ILE:HG12	2.15	0.47
1:B:391:PHE:O	1:B:395:ASP:HB2	2.15	0.47
1:B:492:ARG:HA	1:B:495:GLN:HG3	1.95	0.47
1:B:501:LEU:HD22	1:B:605:ALA:HB1	1.96	0.47
1:B:288:LYS:HE3	1:B:288:LYS:HB3	1.75	0.47
2:B:801:CPL:H382	2:B:801:CPL:C42	2.38	0.47
1:A:213:CYS:O	1:A:217:ILE:HG12	2.15	0.47
1:D:312:VAL:O	1:D:316:ILE:HG12	2.15	0.47
2:C:801:CPL:H382	2:C:801:CPL:C42	2.38	0.47
1:A:482:GLN:HE21	1:D:440:VAL:HG13	1.79	0.46
1:C:391:PHE:O	1:C:395:ASP:HB2	2.15	0.46
1:A:358:THR:O	1:A:362:ARG:HG3	2.15	0.46
1:C:536:GLY:HA3	1:C:585:THR:HG23	1.98	0.46
1:D:566:ILE:HD13	1:D:617:LEU:CD1	2.38	0.46
1:B:536:GLY:HA3	1:B:585:THR:HG23	1.98	0.46
1:B:213:CYS:O	1:B:217:ILE:HG12	2.15	0.46
1:C:312:VAL:O	1:C:316:ILE:HG12	2.15	0.46
1:C:501:LEU:HD22	1:C:605:ALA:HB1	1.97	0.46
1:D:213:CYS:O	1:D:217:ILE:HG12	2.15	0.46
1:D:536:GLY:HA3	1:D:585:THR:HG23	1.98	0.46
1:A:536:GLY:HA3	1:A:585:THR:HG23	1.98	0.46
1:D:575:ARG:HA	1:D:575:ARG:HD3	1.61	0.46
1:A:312:VAL:O	1:A:316:ILE:HG12	2.15	0.46
1:C:237:ALA:HA	1:C:240:VAL:HG22	1.97	0.46
1:C:575:ARG:HA	1:C:575:ARG:HD3	1.61	0.46
1:B:237:ALA:HA	1:B:240:VAL:HG22	1.97	0.46
1:C:216:LEU:HD23	1:C:257:LEU:HD11	1.96	0.46
1:D:358:THR:O	1:D:362:ARG:HG3	2.15	0.46
1:B:440:VAL:HG13	1:C:482:GLN:HE21	1.77	0.45
1:A:575:ARG:HA	1:A:575:ARG:HD3	1.61	0.45
1:B:443:GLN:O	1:B:446:ILE:HG12	2.17	0.45
1:C:156:LEU:HB3	1:C:169:GLN:HG2	1.98	0.45
1:A:440:VAL:HG13	1:B:482:GLN:NE2	2.31	0.45
1:A:597:ASN:O	1:A:600:ARG:HG2	2.17	0.45
1:B:358:THR:O	1:B:362:ARG:HG3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ALA:HA	1:D:240:VAL:HG22	1.97	0.45
1:D:597:ASN:O	1:D:600:ARG:HG2	2.17	0.45
1:B:144:VAL:HG21	1:B:325:CYS:HB3	1.99	0.45
1:B:523:LYS:HB2	1:B:523:LYS:HE2	1.84	0.45
1:C:358:THR:O	1:C:362:ARG:HG3	2.15	0.45
1:A:144:VAL:HG21	1:A:325:CYS:HB3	1.99	0.45
1:C:597:ASN:O	1:C:600:ARG:HG2	2.17	0.45
1:A:501:LEU:HD22	1:A:605:ALA:HB1	1.97	0.45
1:D:443:GLN:O	1:D:446:ILE:HG12	2.17	0.45
1:C:144:VAL:HG21	1:C:325:CYS:HB3	1.99	0.45
1:A:237:ALA:HA	1:A:240:VAL:HG22	1.97	0.45
1:B:237:ALA:O	1:B:238:GLU:C	2.51	0.45
1:C:443:GLN:O	1:C:446:ILE:HG12	2.17	0.45
1:A:156:LEU:HB3	1:A:169:GLN:HG2	1.98	0.45
1:C:288:LYS:HB3	1:C:288:LYS:HE3	1.75	0.45
1:A:490:LYS:HE3	1:A:490:LYS:HB2	1.83	0.45
1:A:441:SER:H	1:B:482:GLN:NE2	2.15	0.44
1:C:615:GLU:OE2	1:C:619:LYS:HE2	2.18	0.44
1:B:597:ASN:O	1:B:600:ARG:HG2	2.17	0.44
1:C:129:THR:HG23	1:C:290:VAL:HG13	1.99	0.44
1:D:144:VAL:HG21	1:D:325:CYS:HB3	1.99	0.44
1:B:615:GLU:OE2	1:B:619:LYS:HE2	2.18	0.44
1:A:129:THR:HG23	1:A:290:VAL:HG13	1.99	0.44
1:A:523:LYS:HZ1	1:A:578:ASN:HD21	1.66	0.44
1:D:129:THR:HG23	1:D:290:VAL:HG13	1.99	0.44
1:D:156:LEU:HB3	1:D:169:GLN:HG2	1.98	0.44
1:A:443:GLN:O	1:A:446:ILE:HG12	2.17	0.44
1:A:615:GLU:OE2	1:A:619:LYS:HE2	2.18	0.44
1:B:129:THR:HG23	1:B:290:VAL:HG13	1.99	0.44
1:D:507:LEU:HD23	1:D:507:LEU:HA	1.87	0.44
1:B:156:LEU:HB3	1:B:169:GLN:HG2	1.98	0.44
1:B:575:ARG:HD3	1:B:575:ARG:HA	1.61	0.44
1:D:615:GLU:OE2	1:D:619:LYS:HE2	2.18	0.43
1:C:328:PHE:CZ	1:C:362:ARG:HD3	2.54	0.43
1:D:328:PHE:CZ	1:D:362:ARG:HD3	2.54	0.43
1:D:566:ILE:HD12	1:D:614:ARG:HG2	2.01	0.43
1:A:328:PHE:CZ	1:A:362:ARG:HD3	2.54	0.43
1:C:440:VAL:HG13	1:D:482:GLN:NE2	2.34	0.43
1:B:328:PHE:CZ	1:B:362:ARG:HD3	2.54	0.43
1:D:465:GLN:OE1	1:D:469:LYS:NZ	2.52	0.43
1:B:465:GLN:OE1	1:B:469:LYS:NZ	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:566:ILE:HD12	1:C:614:ARG:HG2	2.01	0.43
1:C:465:GLN:OE1	1:C:469:LYS:NZ	2.52	0.42
1:D:581:SER:HB2	1:D:585:THR:OG1	2.19	0.42
1:A:465:GLN:OE1	1:A:469:LYS:NZ	2.52	0.42
1:A:288:LYS:HB3	1:A:288:LYS:HE3	1.75	0.42
1:C:343:TYR:OH	1:C:357:ASP:OD1	2.27	0.42
1:B:581:SER:HB2	1:B:585:THR:OG1	2.19	0.42
1:C:581:SER:HB2	1:C:585:THR:OG1	2.19	0.42
1:A:309:VAL:O	1:A:313:VAL:HG13	2.20	0.42
1:A:581:SER:HB2	1:A:585:THR:OG1	2.19	0.42
1:B:566:ILE:HD12	1:B:614:ARG:HG2	2.01	0.42
1:C:507:LEU:HD23	1:C:507:LEU:HA	1.87	0.42
1:D:523:LYS:HB2	1:D:523:LYS:HE2	1.84	0.42
1:C:377:ILE:HD13	1:D:396:LEU:HD22	2.01	0.42
2:A:801:CPL:H382	2:A:801:CPL:C42	2.38	0.42
1:B:451:TRP:CH2	1:C:472:PRO:HD3	2.55	0.42
1:C:523:LYS:CE	1:C:543:ASP:OD1	2.68	0.41
1:A:181:LYS:HA	1:A:181:LYS:HD3	1.92	0.41
1:D:515:SER:H	1:D:515:SER:HG	1.64	0.41
1:D:523:LYS:CE	1:D:543:ASP:OD1	2.69	0.41
1:A:523:LYS:CE	1:A:543:ASP:OD1	2.68	0.41
1:A:612:LYS:HB2	1:A:612:LYS:NZ	2.36	0.41
1:C:514:PHE:CD1	1:C:587:LEU:HD23	2.56	0.41
1:C:525:ASP:O	1:C:575:ARG:HG2	2.21	0.41
1:C:450:LYS:HE2	1:C:450:LYS:HB3	1.85	0.41
1:A:396:LEU:HD22	1:D:377:ILE:HD13	2.03	0.41
1:D:309:VAL:O	1:D:313:VAL:HG13	2.20	0.41
1:A:566:ILE:HD12	1:A:614:ARG:HG2	2.01	0.41
1:B:309:VAL:O	1:B:313:VAL:HG13	2.20	0.41
1:B:612:LYS:NZ	1:B:612:LYS:HB2	2.36	0.41
1:C:309:VAL:O	1:C:313:VAL:HG13	2.20	0.41
1:D:525:ASP:O	1:D:575:ARG:HG2	2.21	0.41
1:A:421:ARG:HH22	1:B:299:THR:HG22	1.86	0.41
1:A:471:LEU:O	1:A:476:GLN:NE2	2.54	0.41
1:B:471:LEU:O	1:B:476:GLN:NE2	2.54	0.41
1:B:523:LYS:CE	1:B:543:ASP:OD1	2.68	0.41
1:B:525:ASP:O	1:B:575:ARG:HG2	2.21	0.41
1:A:424:PHE:CE1	1:A:456:TRP:HB2	2.56	0.41
1:B:514:PHE:CD1	1:B:587:LEU:HD23	2.56	0.41
1:C:471:LEU:O	1:C:476:GLN:NE2	2.54	0.41
1:D:612:LYS:HB2	1:D:612:LYS:NZ	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LYS:HB3	1:D:433:GLN:NE2	2.36	0.40
1:C:424:PHE:CE1	1:C:456:TRP:HB2	2.57	0.40
1:D:424:PHE:CE1	1:D:456:TRP:HB2	2.56	0.40
1:D:471:LEU:O	1:D:476:GLN:NE2	2.54	0.40
1:A:248:LYS:HA	1:A:248:LYS:HD3	1.83	0.40
1:A:507:LEU:HA	1:A:507:LEU:HD23	1.87	0.40
1:B:232:LEU:HD23	1:B:232:LEU:HA	1.93	0.40
1:B:424:PHE:CE1	1:B:456:TRP:HB2	2.56	0.40
1:C:151:PRO:HD2	1:C:197:TYR:CZ	2.56	0.40
1:C:490:LYS:HE3	1:C:490:LYS:HB2	1.83	0.40
3:D:803:PX2:O8	3:D:803:PX2:C20	2.70	0.40
1:B:316:ILE:HD12	1:B:402:ILE:HG23	2.04	0.40
2:C:801:CPL:H141	2:C:801:CPL:H171	1.88	0.40
3:C:803:PX2:O8	3:C:803:PX2:C20	2.70	0.40
1:D:151:PRO:HD2	1:D:197:TYR:CZ	2.56	0.40
1:D:523:LYS:HZ1	1:D:578:ASN:HD21	1.70	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	509/733 (69%)	487 (96%)	22 (4%)	0	100	100
1	B	509/733 (69%)	487 (96%)	22 (4%)	0	100	100
1	C	509/733 (69%)	487 (96%)	22 (4%)	0	100	100
1	D	509/733 (69%)	487 (96%)	22 (4%)	0	100	100
All	All	2036/2932 (69%)	1948 (96%)	88 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	465/651 (71%)	457 (98%)	8 (2%)	60	81
1	B	465/651 (71%)	457 (98%)	8 (2%)	60	81
1	C	465/651 (71%)	457 (98%)	8 (2%)	60	81
1	D	465/651 (71%)	457 (98%)	8 (2%)	60	81
All	All	1860/2604 (71%)	1828 (98%)	32 (2%)	62	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ARG
1	A	395	ASP
1	A	452	PHE
1	A	455	LEU
1	A	457	THR
1	A	523	LYS
1	A	576	THR
1	A	609	LEU
1	B	235	ARG
1	B	395	ASP
1	B	452	PHE
1	B	455	LEU
1	B	457	THR
1	B	523	LYS
1	B	576	THR
1	B	609	LEU
1	C	235	ARG
1	C	395	ASP
1	C	452	PHE
1	C	455	LEU
1	C	457	THR
1	C	523	LYS
1	C	576	THR
1	C	609	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	235	ARG
1	D	395	ASP
1	D	452	PHE
1	D	455	LEU
1	D	457	THR
1	D	523	LYS
1	D	576	THR
1	D	609	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	154	GLN
1	A	179	ASN
1	A	199	HIS
1	A	386	ASN
1	A	416	ASN
1	A	425	GLN
1	A	482	GLN
1	A	512	GLN
1	A	539	GLN
1	A	578	ASN
1	B	114	GLN
1	B	154	GLN
1	B	179	ASN
1	B	199	HIS
1	B	386	ASN
1	B	416	ASN
1	B	425	GLN
1	B	482	GLN
1	B	512	GLN
1	B	539	GLN
1	B	578	ASN
1	C	114	GLN
1	C	154	GLN
1	C	179	ASN
1	C	199	HIS
1	C	386	ASN
1	C	416	ASN
1	C	425	GLN
1	C	482	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	512	GLN
1	C	539	GLN
1	C	578	ASN
1	D	114	GLN
1	D	154	GLN
1	D	179	ASN
1	D	199	HIS
1	D	386	ASN
1	D	416	ASN
1	D	425	GLN
1	D	433	GLN
1	D	482	GLN
1	D	512	GLN
1	D	539	GLN
1	D	578	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 33 ligands modelled in this entry, 1 is 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	$\#\|Z\|>2$
2	CPL	D	801	-	46,46,51	1.37	7 (15%)	52,54,59	2.27	13 (25%)
2	CPL	C	804	-	8,8,51	0.28	0	7,7,59	0.77	0
2	CPL	D	805	-	8,8,51	0.18	0	7,7,59	0.45	0
2	CPL	B	801	-	46,46,51	1.36	7 (15%)	52,54,59	2.27	13 (25%)
3	PX2	D	808	-	24,24,35	1.17	4 (16%)	28,29,40	1.24	2 (7%)
2	CPL	D	802	-	37,37,51	1.63	4 (10%)	40,42,59	2.13	12 (30%)
2	CPL	A	801	-	46,46,51	1.37	7 (15%)	52,54,59	2.27	13 (25%)
2	CPL	A	806	-	11,11,51	0.58	0	10,10,59	0.64	0
3	PX2	D	803	-	22,22,35	1.57	4 (18%)	26,27,40	2.57	8 (30%)
2	CPL	C	806	-	11,11,51	0.58	0	10,10,59	0.64	0
2	CPL	A	805	-	8,8,51	0.18	0	7,7,59	0.44	0
2	CPL	D	804	-	8,8,51	0.28	0	7,7,59	0.77	0
3	PX2	A	803	-	22,22,35	1.58	4 (18%)	26,27,40	2.58	8 (30%)
2	CPL	B	804	-	8,8,51	0.28	0	7,7,59	0.77	0
2	CPL	C	807	-	11,11,51	0.15	0	10,10,59	0.75	0
3	PX2	A	808	-	24,24,35	1.17	4 (16%)	28,29,40	1.24	2 (7%)
2	CPL	B	805	-	8,8,51	0.17	0	7,7,59	0.44	0
2	CPL	C	805	-	8,8,51	0.17	0	7,7,59	0.45	0
2	CPL	B	802	-	37,37,51	1.63	4 (10%)	40,42,59	2.13	12 (30%)
2	CPL	C	801	-	46,46,51	1.37	7 (15%)	52,54,59	2.27	13 (25%)
2	CPL	A	804	-	8,8,51	0.28	0	7,7,59	0.77	0
2	CPL	B	807	-	11,11,51	0.15	0	10,10,59	0.76	0
3	PX2	C	803	-	22,22,35	1.58	4 (18%)	26,27,40	2.57	8 (30%)
3	PX2	C	808	-	24,24,35	1.16	4 (16%)	28,29,40	1.24	2 (7%)
2	CPL	D	806	-	11,11,51	0.58	0	10,10,59	0.64	0
2	CPL	B	806	-	11,11,51	0.58	0	10,10,59	0.64	0
2	CPL	C	802	-	37,37,51	1.63	4 (10%)	40,42,59	2.13	12 (30%)
2	CPL	D	807	-	11,11,51	0.15	0	10,10,59	0.75	0
2	CPL	A	802	-	37,37,51	1.63	4 (10%)	40,42,59	2.13	12 (30%)
3	PX2	B	803	-	22,22,35	1.57	4 (18%)	26,27,40	2.57	8 (30%)
3	PX2	B	808	-	24,24,35	1.17	4 (16%)	28,29,40	1.24	2 (7%)
2	CPL	A	807	-	11,11,51	0.15	0	10,10,59	0.76	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
2	CPL	D	801	-	-	32/50/50/55	-
2	CPL	C	804	-	-	3/6/6/55	-
2	CPL	D	805	-	-	4/6/6/55	-
2	CPL	B	801	-	-	32/50/50/55	-
3	PX2	D	808	-	-	16/26/26/37	-
2	CPL	D	802	-	-	20/41/41/55	-
2	CPL	A	801	-	-	32/50/50/55	-
2	CPL	A	806	-	-	4/9/9/55	-
3	PX2	D	803	-	-	8/24/24/37	-
2	CPL	C	806	-	-	4/9/9/55	-
2	CPL	A	805	-	-	4/6/6/55	-
2	CPL	D	804	-	-	3/6/6/55	-
3	PX2	A	803	-	-	8/24/24/37	-
2	CPL	B	804	-	-	3/6/6/55	-
2	CPL	C	807	-	-	5/9/9/55	-
3	PX2	A	808	-	-	16/26/26/37	-
2	CPL	B	805	-	-	4/6/6/55	-
2	CPL	C	805	-	-	4/6/6/55	-
2	CPL	B	802	-	-	20/41/41/55	-
2	CPL	C	801	-	-	32/50/50/55	-
2	CPL	A	804	-	-	3/6/6/55	-
2	CPL	B	807	-	-	5/9/9/55	-
3	PX2	C	803	-	-	8/24/24/37	-
3	PX2	C	808	-	-	16/26/26/37	-
2	CPL	D	806	-	-	4/9/9/55	-
2	CPL	B	806	-	-	4/9/9/55	-
2	CPL	C	802	-	-	20/41/41/55	-
2	CPL	D	807	-	-	5/9/9/55	-
2	CPL	A	802	-	-	20/41/41/55	-
3	PX2	B	803	-	-	8/24/24/37	-
3	PX2	B	808	-	-	16/26/26/37	-
2	CPL	A	807	-	-	5/9/9/55	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	CPL	O2-C31	6.96	1.53	1.34
2	C	802	CPL	O2-C31	6.94	1.53	1.34
2	D	802	CPL	O2-C31	6.94	1.53	1.34
2	A	802	CPL	O2-C31	6.94	1.53	1.34
2	C	801	CPL	O2-C31	4.65	1.47	1.34
2	A	801	CPL	O2-C31	4.64	1.47	1.34
2	D	801	CPL	O2-C31	4.63	1.47	1.34
2	B	801	CPL	O2-C31	4.60	1.47	1.34
2	A	802	CPL	O3-C11	4.52	1.46	1.33
2	C	802	CPL	O3-C11	4.51	1.46	1.33
2	D	802	CPL	O3-C11	4.51	1.46	1.33
2	B	802	CPL	O3-C11	4.49	1.46	1.33
2	C	801	CPL	O11-C11	-3.48	1.12	1.22
2	D	801	CPL	O11-C11	-3.47	1.12	1.22
2	A	801	CPL	O11-C11	-3.47	1.12	1.22
2	B	801	CPL	O11-C11	-3.47	1.12	1.22
3	A	803	PX2	O5-C4	3.20	1.42	1.33
3	B	803	PX2	O6-C4	-3.19	1.13	1.22
3	A	803	PX2	O6-C4	-3.19	1.13	1.22
3	C	803	PX2	O6-C4	-3.19	1.13	1.22
3	D	803	PX2	O6-C4	-3.19	1.13	1.22
3	C	803	PX2	O5-C4	3.19	1.42	1.33
3	D	803	PX2	O5-C4	3.18	1.42	1.33
3	B	803	PX2	O5-C4	3.16	1.42	1.33
2	D	801	CPL	C6-N	-2.76	1.41	1.50
3	B	803	PX2	O7-C16	2.75	1.42	1.34
3	C	803	PX2	O7-C16	2.74	1.42	1.34
3	D	803	PX2	O7-C16	2.74	1.42	1.34
2	B	801	CPL	C6-N	-2.74	1.42	1.50
2	A	801	CPL	C6-N	-2.74	1.42	1.50
2	C	801	CPL	C6-N	-2.73	1.42	1.50
3	A	803	PX2	O7-C16	2.73	1.42	1.34
2	C	801	CPL	O2-C2	-2.61	1.40	1.46
2	D	801	CPL	O2-C2	-2.60	1.40	1.46
2	A	801	CPL	O2-C2	-2.58	1.40	1.46
2	B	801	CPL	O2-C2	-2.56	1.40	1.46
2	C	801	CPL	O3-C11	2.45	1.40	1.33
2	D	801	CPL	O3-C11	2.45	1.40	1.33
2	A	801	CPL	O3-C11	2.44	1.40	1.33
2	C	802	CPL	O11-C11	-2.44	1.15	1.22
2	B	801	CPL	O3-C11	2.44	1.40	1.33
2	D	802	CPL	O11-C11	-2.43	1.15	1.22
2	A	802	CPL	O11-C11	-2.42	1.15	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	CPL	O11-C11	-2.42	1.15	1.22
2	B	801	CPL	C8-N	-2.41	1.43	1.50
2	D	801	CPL	C8-N	-2.40	1.43	1.50
2	A	801	CPL	C8-N	-2.40	1.43	1.50
2	C	801	CPL	C8-N	-2.39	1.43	1.50
3	B	808	PX2	O5-C4	2.31	1.40	1.33
2	A	801	CPL	C7-N	-2.30	1.43	1.50
2	B	801	CPL	C7-N	-2.30	1.43	1.50
3	A	808	PX2	O7-C2	-2.30	1.40	1.46
3	B	808	PX2	O7-C2	-2.30	1.40	1.46
3	D	808	PX2	O7-C2	-2.29	1.40	1.46
3	A	808	PX2	O5-C4	2.29	1.40	1.33
2	C	801	CPL	C7-N	-2.28	1.43	1.50
2	D	801	CPL	C7-N	-2.28	1.43	1.50
3	C	808	PX2	O7-C2	-2.28	1.40	1.46
3	C	808	PX2	O5-C4	2.28	1.40	1.33
3	D	808	PX2	O5-C4	2.28	1.40	1.33
3	D	808	PX2	O7-C16	2.27	1.40	1.34
3	B	808	PX2	O7-C16	2.27	1.40	1.34
3	A	808	PX2	O7-C16	2.26	1.40	1.34
3	C	808	PX2	O7-C16	2.25	1.40	1.34
2	D	802	CPL	C13-C12	-2.17	1.44	1.52
3	D	808	PX2	O5-C3	-2.17	1.40	1.45
2	B	802	CPL	C13-C12	-2.17	1.44	1.52
2	A	802	CPL	C13-C12	-2.17	1.44	1.52
2	C	802	CPL	C13-C12	-2.16	1.44	1.52
3	B	808	PX2	O5-C3	-2.15	1.40	1.45
3	A	808	PX2	O5-C3	-2.14	1.40	1.45
3	C	808	PX2	O5-C3	-2.13	1.40	1.45
3	B	803	PX2	P1-O3	-2.07	1.46	1.54
3	C	803	PX2	P1-O3	-2.04	1.47	1.54
3	A	803	PX2	P1-O3	-2.04	1.47	1.54
3	D	803	PX2	P1-O3	-2.04	1.47	1.54

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	CPL	O2-C31-C32	7.94	128.62	111.50
2	B	801	CPL	O2-C31-C32	7.93	128.60	111.50
2	A	801	CPL	O2-C31-C32	7.93	128.60	111.50
2	D	801	CPL	O2-C31-C32	7.93	128.60	111.50
2	B	801	CPL	O3-C11-C12	6.51	132.34	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	CPL	O3-C11-C12	6.50	132.31	111.91
2	A	801	CPL	O3-C11-C12	6.50	132.30	111.91
2	C	801	CPL	O3-C11-C12	6.50	132.30	111.91
3	B	803	PX2	O7-C16-C17	6.44	125.39	111.50
3	A	803	PX2	O7-C16-C17	6.43	125.36	111.50
3	C	803	PX2	O7-C16-C17	6.42	125.34	111.50
3	D	803	PX2	O7-C16-C17	6.42	125.33	111.50
3	A	803	PX2	O5-C4-O6	-6.04	108.36	123.59
3	B	803	PX2	O5-C4-O6	-6.00	108.44	123.59
3	C	803	PX2	O5-C4-O6	-6.00	108.45	123.59
3	D	803	PX2	O5-C4-O6	-5.99	108.46	123.59
2	D	802	CPL	O2-C31-C32	5.92	124.26	111.50
2	A	802	CPL	O2-C31-C32	5.92	124.25	111.50
2	B	802	CPL	O2-C31-C32	5.91	124.24	111.50
3	B	803	PX2	O5-C4-C5	5.90	130.42	111.91
2	C	802	CPL	O2-C31-C32	5.90	124.21	111.50
3	A	803	PX2	O5-C4-C5	5.90	130.42	111.91
3	D	803	PX2	O5-C4-C5	5.89	130.38	111.91
3	C	803	PX2	O5-C4-C5	5.88	130.36	111.91
2	B	801	CPL	O3-C11-O11	-5.48	109.77	123.59
2	C	801	CPL	O3-C11-O11	-5.48	109.77	123.59
2	D	801	CPL	O3-C11-O11	-5.48	109.77	123.59
2	A	801	CPL	O3-C11-O11	-5.48	109.77	123.59
2	C	802	CPL	O3-C3-C2	4.77	122.33	108.43
2	D	802	CPL	O3-C3-C2	4.77	122.32	108.43
2	A	802	CPL	O3-C3-C2	4.77	122.30	108.43
2	B	802	CPL	O3-C3-C2	4.76	122.28	108.43
2	B	801	CPL	O3-C3-C2	4.60	121.83	108.43
2	A	801	CPL	O3-C3-C2	4.59	121.80	108.43
2	C	801	CPL	O3-C3-C2	4.59	121.79	108.43
2	D	801	CPL	O3-C3-C2	4.58	121.78	108.43
2	D	802	CPL	O3-C11-C12	4.52	126.09	111.91
2	B	802	CPL	O3-C11-C12	4.51	126.08	111.91
2	A	802	CPL	O3-C11-C12	4.51	126.07	111.91
2	C	802	CPL	O3-C11-C12	4.51	126.06	111.91
2	B	801	CPL	C7-N-C6	-4.48	97.46	108.97
2	C	801	CPL	C7-N-C6	-4.47	97.48	108.97
2	A	801	CPL	C7-N-C6	-4.46	97.50	108.97
2	D	801	CPL	C7-N-C6	-4.45	97.53	108.97
2	D	802	CPL	C20-C19-C18	-4.37	92.22	114.42
2	C	802	CPL	C20-C19-C18	-4.37	92.25	114.42
2	B	802	CPL	C20-C19-C18	-4.37	92.25	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	802	CPL	C20-C19-C18	-4.37	92.25	114.42
3	C	808	PX2	O7-C16-C17	3.97	120.07	111.50
3	A	808	PX2	O7-C16-C17	3.97	120.05	111.50
3	D	808	PX2	O7-C16-C17	3.97	120.05	111.50
3	B	808	PX2	O7-C16-C17	3.96	120.04	111.50
2	B	801	CPL	C8-N-C7	3.54	118.08	108.97
2	A	801	CPL	C8-N-C7	3.53	118.05	108.97
2	C	801	CPL	C8-N-C7	3.52	118.01	108.97
2	D	801	CPL	C8-N-C7	3.51	118.00	108.97
2	A	801	CPL	C19-C18-C17	-3.28	97.77	114.42
2	C	801	CPL	C19-C18-C17	-3.28	97.78	114.42
2	B	801	CPL	C19-C18-C17	-3.28	97.78	114.42
2	D	801	CPL	C19-C18-C17	-3.27	97.81	114.42
3	B	803	PX2	O7-C16-O8	-3.17	116.03	123.70
3	D	803	PX2	O7-C16-O8	-3.16	116.06	123.70
3	C	803	PX2	O7-C16-O8	-3.16	116.07	123.70
3	A	803	PX2	O7-C16-O8	-3.16	116.08	123.70
3	C	803	PX2	C2-O7-C16	-3.15	110.05	117.79
3	D	803	PX2	C2-O7-C16	-3.15	110.05	117.79
3	A	803	PX2	C2-O7-C16	-3.13	110.10	117.79
3	B	803	PX2	C2-O7-C16	-3.12	110.10	117.79
3	D	803	PX2	O5-C3-C2	3.07	117.36	108.43
3	A	803	PX2	O5-C3-C2	3.06	117.35	108.43
3	B	803	PX2	O5-C3-C2	3.06	117.33	108.43
3	C	803	PX2	O5-C3-C2	3.06	117.33	108.43
2	B	802	CPL	C3-O3-C11	2.96	128.08	117.12
2	B	802	CPL	O11-C11-C12	-2.95	112.21	123.73
2	D	802	CPL	C3-O3-C11	2.95	128.06	117.12
2	C	802	CPL	O11-C11-C12	-2.95	112.22	123.73
2	A	802	CPL	C3-O3-C11	2.95	128.03	117.12
2	C	802	CPL	C3-O3-C11	2.94	128.03	117.12
2	A	802	CPL	O11-C11-C12	-2.94	112.25	123.73
2	D	802	CPL	O11-C11-C12	-2.94	112.25	123.73
3	C	808	PX2	O5-C4-C5	2.82	120.76	111.91
3	B	808	PX2	O5-C4-C5	2.81	120.73	111.91
3	D	808	PX2	O5-C4-C5	2.81	120.73	111.91
3	A	808	PX2	O5-C4-C5	2.81	120.73	111.91
2	B	802	CPL	C22-C21-C20	-2.76	100.40	114.42
2	C	802	CPL	C14-C13-C12	-2.76	103.26	113.19
2	A	802	CPL	C14-C13-C12	-2.76	103.28	113.19
2	C	802	CPL	C22-C21-C20	-2.75	100.45	114.42
2	D	802	CPL	C14-C13-C12	-2.75	103.29	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	CPL	C14-C13-C12	-2.75	103.30	113.19
2	D	802	CPL	C22-C21-C20	-2.75	100.45	114.42
2	A	802	CPL	C22-C21-C20	-2.75	100.45	114.42
2	D	801	CPL	O31-C31-C32	-2.74	113.03	123.73
2	B	801	CPL	O31-C31-C32	-2.74	113.04	123.73
2	C	801	CPL	O31-C31-C32	-2.73	113.08	123.73
2	A	801	CPL	O31-C31-C32	-2.73	113.08	123.73
2	B	801	CPL	C23-C22-C21	-2.53	101.56	114.42
2	A	801	CPL	C23-C22-C21	-2.53	101.56	114.42
2	C	801	CPL	C23-C22-C21	-2.53	101.57	114.42
2	D	801	CPL	C23-C22-C21	-2.53	101.58	114.42
2	D	802	CPL	C2-O2-C31	2.52	123.99	117.79
2	C	802	CPL	C2-O2-C31	2.52	123.99	117.79
2	A	802	CPL	C2-O2-C31	2.51	123.98	117.79
2	B	802	CPL	C2-O2-C31	2.50	123.96	117.79
3	A	803	PX2	C3-O5-C4	2.49	126.35	117.12
3	D	803	PX2	C3-O5-C4	2.49	126.34	117.12
3	B	803	PX2	C3-O5-C4	2.49	126.34	117.12
3	C	803	PX2	C3-O5-C4	2.48	126.32	117.12
2	B	802	CPL	P-O3P-C1	2.36	135.54	121.68
2	C	802	CPL	P-O3P-C1	2.36	135.53	121.68
2	A	802	CPL	P-O3P-C1	2.36	135.51	121.68
2	D	802	CPL	P-O3P-C1	2.36	135.50	121.68
2	D	802	CPL	O31-C31-C32	-2.27	114.86	123.73
2	A	802	CPL	O31-C31-C32	-2.27	114.88	123.73
2	B	802	CPL	O31-C31-C32	-2.27	114.88	123.73
2	C	802	CPL	O31-C31-C32	-2.27	114.88	123.73
2	C	801	CPL	O2-C31-O31	-2.26	118.25	123.70
2	A	801	CPL	O2-C31-O31	-2.25	118.26	123.70
2	B	801	CPL	O2-C31-O31	-2.23	118.30	123.70
2	D	801	CPL	O2-C31-O31	-2.23	118.31	123.70
2	D	801	CPL	C8-N-C6	-2.18	103.37	108.97
2	C	801	CPL	C8-N-C6	-2.18	103.37	108.97
2	C	801	CPL	C21-C20-C19	-2.18	103.37	114.42
2	B	801	CPL	C8-N-C6	-2.18	103.38	108.97
2	A	801	CPL	C8-N-C6	-2.17	103.38	108.97
2	A	801	CPL	C21-C20-C19	-2.17	103.39	114.42
2	D	801	CPL	C21-C20-C19	-2.17	103.39	114.42
2	B	801	CPL	C21-C20-C19	-2.17	103.42	114.42
2	A	802	CPL	C36-C35-C34	-2.12	103.67	114.42
2	B	802	CPL	C36-C35-C34	-2.12	103.68	114.42
2	C	802	CPL	C36-C35-C34	-2.12	103.68	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	802	CPL	C36-C35-C34	-2.12	103.68	114.42
2	B	801	CPL	C3-O3-C11	2.09	124.87	117.12
2	D	801	CPL	C3-O3-C11	2.09	124.86	117.12
2	A	801	CPL	C3-O3-C11	2.09	124.85	117.12
2	C	801	CPL	C3-O3-C11	2.08	124.83	117.12
3	C	803	PX2	O7-C2-C3	2.02	115.70	108.40
3	A	803	PX2	O7-C2-C3	2.01	115.69	108.40
3	D	803	PX2	O7-C2-C3	2.01	115.68	108.40
3	B	803	PX2	O7-C2-C3	2.01	115.67	108.40

There are no chirality outliers.

All (368) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CPL	C5-C4-O4P-P
2	A	801	CPL	O31-C31-O2-C2
2	A	801	CPL	C39-C40-C41-C42
2	A	801	CPL	C1-O3P-P-O1P
2	A	801	CPL	C1-O3P-P-O2P
2	A	801	CPL	C4-O4P-P-O1P
2	A	801	CPL	C4-O4P-P-O2P
2	A	802	CPL	C32-C31-O2-C2
2	A	802	CPL	C4-O4P-P-O1P
2	A	802	CPL	C4-O4P-P-O2P
2	B	801	CPL	C5-C4-O4P-P
2	B	801	CPL	O31-C31-O2-C2
2	B	801	CPL	C39-C40-C41-C42
2	B	801	CPL	C1-O3P-P-O1P
2	B	801	CPL	C1-O3P-P-O2P
2	B	801	CPL	C4-O4P-P-O1P
2	B	801	CPL	C4-O4P-P-O2P
2	B	802	CPL	C32-C31-O2-C2
2	B	802	CPL	C4-O4P-P-O1P
2	B	802	CPL	C4-O4P-P-O2P
2	C	801	CPL	C5-C4-O4P-P
2	C	801	CPL	O31-C31-O2-C2
2	C	801	CPL	C39-C40-C41-C42
2	C	801	CPL	C1-O3P-P-O1P
2	C	801	CPL	C1-O3P-P-O2P
2	C	801	CPL	C4-O4P-P-O1P
2	C	801	CPL	C4-O4P-P-O2P
2	C	802	CPL	C32-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	802	CPL	C4-O4P-P-O1P
2	C	802	CPL	C4-O4P-P-O2P
2	D	801	CPL	C5-C4-O4P-P
2	D	801	CPL	O31-C31-O2-C2
2	D	801	CPL	C39-C40-C41-C42
2	D	801	CPL	C1-O3P-P-O1P
2	D	801	CPL	C1-O3P-P-O2P
2	D	801	CPL	C4-O4P-P-O1P
2	D	801	CPL	C4-O4P-P-O2P
2	D	802	CPL	C32-C31-O2-C2
2	D	802	CPL	C4-O4P-P-O1P
2	D	802	CPL	C4-O4P-P-O2P
3	A	808	PX2	C1-O4-P1-O1
3	A	808	PX2	C1-O4-P1-O3
3	B	808	PX2	C1-O4-P1-O1
3	B	808	PX2	C1-O4-P1-O3
3	C	808	PX2	C1-O4-P1-O1
3	C	808	PX2	C1-O4-P1-O3
3	D	808	PX2	C1-O4-P1-O1
3	D	808	PX2	C1-O4-P1-O3
3	A	803	PX2	O6-C4-O5-C3
3	B	803	PX2	O6-C4-O5-C3
3	C	803	PX2	O6-C4-O5-C3
3	D	803	PX2	O6-C4-O5-C3
3	A	803	PX2	C5-C4-O5-C3
3	B	803	PX2	C5-C4-O5-C3
3	C	803	PX2	C5-C4-O5-C3
3	D	803	PX2	C5-C4-O5-C3
2	A	801	CPL	C32-C31-O2-C2
2	B	801	CPL	C32-C31-O2-C2
2	C	801	CPL	C32-C31-O2-C2
2	D	801	CPL	C32-C31-O2-C2
2	A	802	CPL	O31-C31-O2-C2
2	B	802	CPL	O31-C31-O2-C2
2	C	802	CPL	O31-C31-O2-C2
2	D	802	CPL	O31-C31-O2-C2
2	A	802	CPL	C12-C11-O3-C3
2	B	802	CPL	C12-C11-O3-C3
2	C	802	CPL	C12-C11-O3-C3
2	D	802	CPL	C12-C11-O3-C3
3	A	808	PX2	C5-C4-O5-C3
3	B	808	PX2	C5-C4-O5-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	808	PX2	C5-C4-O5-C3
3	D	808	PX2	C5-C4-O5-C3
2	A	801	CPL	C14-C15-C16-C17
2	B	801	CPL	C14-C15-C16-C17
2	C	801	CPL	C14-C15-C16-C17
2	D	801	CPL	C14-C15-C16-C17
2	A	807	CPL	C14-C15-C16-C17
2	A	807	CPL	C19-C20-C21-C22
2	B	807	CPL	C14-C15-C16-C17
2	B	807	CPL	C19-C20-C21-C22
2	C	807	CPL	C14-C15-C16-C17
2	C	807	CPL	C19-C20-C21-C22
2	D	807	CPL	C14-C15-C16-C17
2	D	807	CPL	C19-C20-C21-C22
2	A	802	CPL	O11-C11-O3-C3
3	A	808	PX2	O6-C4-O5-C3
3	B	808	PX2	O6-C4-O5-C3
3	C	808	PX2	O6-C4-O5-C3
3	D	808	PX2	O6-C4-O5-C3
2	B	802	CPL	O11-C11-O3-C3
2	C	802	CPL	O11-C11-O3-C3
2	D	802	CPL	O11-C11-O3-C3
2	A	801	CPL	C12-C13-C14-C15
2	B	801	CPL	C12-C13-C14-C15
2	C	801	CPL	C12-C13-C14-C15
2	D	801	CPL	C12-C13-C14-C15
2	A	802	CPL	C32-C33-C34-C35
2	B	802	CPL	C32-C33-C34-C35
2	C	802	CPL	C32-C33-C34-C35
2	D	802	CPL	C32-C33-C34-C35
3	A	808	PX2	C17-C16-O7-C2
3	B	808	PX2	C17-C16-O7-C2
3	C	808	PX2	C17-C16-O7-C2
3	D	808	PX2	C17-C16-O7-C2
3	A	808	PX2	C16-C17-C18-C19
3	B	808	PX2	C16-C17-C18-C19
3	C	808	PX2	C16-C17-C18-C19
3	D	808	PX2	C16-C17-C18-C19
2	A	802	CPL	C31-C32-C33-C34
2	B	802	CPL	C31-C32-C33-C34
2	C	802	CPL	C31-C32-C33-C34
2	D	802	CPL	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	808	PX2	O8-C16-O7-C2
3	B	808	PX2	O8-C16-O7-C2
3	C	808	PX2	O8-C16-O7-C2
3	D	808	PX2	O8-C16-O7-C2
3	A	803	PX2	C17-C16-O7-C2
3	B	803	PX2	C17-C16-O7-C2
3	C	803	PX2	C17-C16-O7-C2
3	D	803	PX2	C17-C16-O7-C2
2	A	801	CPL	C1-O3P-P-O4P
2	A	801	CPL	C4-O4P-P-O3P
2	A	802	CPL	C4-O4P-P-O3P
2	B	801	CPL	C1-O3P-P-O4P
2	B	801	CPL	C4-O4P-P-O3P
2	B	802	CPL	C4-O4P-P-O3P
2	C	801	CPL	C1-O3P-P-O4P
2	C	801	CPL	C4-O4P-P-O3P
2	C	802	CPL	C4-O4P-P-O3P
2	D	801	CPL	C1-O3P-P-O4P
2	D	801	CPL	C4-O4P-P-O3P
2	D	802	CPL	C4-O4P-P-O3P
2	A	802	CPL	C11-C12-C13-C14
2	B	802	CPL	C11-C12-C13-C14
2	C	802	CPL	C11-C12-C13-C14
2	D	802	CPL	C11-C12-C13-C14
2	A	801	CPL	C4-C5-N-C7
2	A	801	CPL	C4-C5-N-C8
2	B	801	CPL	C4-C5-N-C7
2	B	801	CPL	C4-C5-N-C8
2	C	801	CPL	C4-C5-N-C7
2	C	801	CPL	C4-C5-N-C8
2	D	801	CPL	C4-C5-N-C7
2	D	801	CPL	C4-C5-N-C8
2	A	807	CPL	C12-C13-C14-C15
2	B	807	CPL	C12-C13-C14-C15
2	C	807	CPL	C12-C13-C14-C15
2	D	807	CPL	C12-C13-C14-C15
3	A	803	PX2	C5-C6-C7-C8
3	B	803	PX2	C5-C6-C7-C8
3	C	803	PX2	C5-C6-C7-C8
3	D	803	PX2	C5-C6-C7-C8
2	A	801	CPL	C1-C2-O2-C31
2	B	801	CPL	C1-C2-O2-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	801	CPL	C1-C2-O2-C31
2	D	801	CPL	C1-C2-O2-C31
3	A	803	PX2	O8-C16-O7-C2
3	B	803	PX2	O8-C16-O7-C2
3	C	803	PX2	O8-C16-O7-C2
3	D	803	PX2	O8-C16-O7-C2
3	A	808	PX2	C4-C5-C6-C7
3	B	808	PX2	C4-C5-C6-C7
3	C	808	PX2	C4-C5-C6-C7
3	D	808	PX2	C4-C5-C6-C7
2	A	801	CPL	C4-C5-N-C6
2	B	801	CPL	C4-C5-N-C6
2	C	801	CPL	C4-C5-N-C6
2	D	801	CPL	C4-C5-N-C6
2	A	807	CPL	C16-C17-C18-C19
2	B	807	CPL	C16-C17-C18-C19
2	C	807	CPL	C16-C17-C18-C19
2	D	807	CPL	C16-C17-C18-C19
2	A	802	CPL	C12-C13-C14-C15
2	D	802	CPL	C12-C13-C14-C15
2	B	802	CPL	C12-C13-C14-C15
2	C	802	CPL	C12-C13-C14-C15
2	A	802	CPL	C15-C16-C17-C18
2	B	801	CPL	C33-C34-C35-C36
2	B	802	CPL	C15-C16-C17-C18
2	B	802	CPL	C19-C20-C21-C22
2	C	802	CPL	C15-C16-C17-C18
2	C	802	CPL	C19-C20-C21-C22
2	D	802	CPL	C15-C16-C17-C18
2	A	801	CPL	C33-C34-C35-C36
2	A	802	CPL	C19-C20-C21-C22
2	C	801	CPL	C33-C34-C35-C36
2	D	801	CPL	C33-C34-C35-C36
2	D	802	CPL	C19-C20-C21-C22
2	A	801	CPL	C18-C19-C20-C21
2	B	801	CPL	C18-C19-C20-C21
2	C	801	CPL	C18-C19-C20-C21
2	D	801	CPL	C18-C19-C20-C21
2	A	806	CPL	C14-C15-C16-C17
2	B	806	CPL	C14-C15-C16-C17
2	C	806	CPL	C14-C15-C16-C17
2	D	806	CPL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	804	CPL	C15-C16-C17-C18
2	B	804	CPL	C15-C16-C17-C18
2	C	804	CPL	C15-C16-C17-C18
2	D	804	CPL	C15-C16-C17-C18
3	A	808	PX2	C17-C18-C19-C20
3	B	808	PX2	C17-C18-C19-C20
3	C	808	PX2	C5-C6-C7-C8
3	D	808	PX2	C5-C6-C7-C8
3	D	808	PX2	C17-C18-C19-C20
2	A	806	CPL	C18-C19-C20-C21
2	B	806	CPL	C18-C19-C20-C21
3	A	808	PX2	C5-C6-C7-C8
3	B	808	PX2	C5-C6-C7-C8
3	C	808	PX2	C17-C18-C19-C20
2	C	806	CPL	C18-C19-C20-C21
2	D	806	CPL	C18-C19-C20-C21
3	A	808	PX2	C1-C2-C3-O5
3	B	808	PX2	C1-C2-C3-O5
3	C	808	PX2	C1-C2-C3-O5
3	D	808	PX2	C1-C2-C3-O5
3	A	808	PX2	C7-C8-C9-C10
3	B	808	PX2	C7-C8-C9-C10
3	C	808	PX2	C7-C8-C9-C10
3	D	808	PX2	C7-C8-C9-C10
2	B	806	CPL	C12-C13-C14-C15
2	D	806	CPL	C12-C13-C14-C15
2	A	806	CPL	C12-C13-C14-C15
2	C	806	CPL	C12-C13-C14-C15
2	B	801	CPL	C22-C23-C24-C25
2	C	801	CPL	C22-C23-C24-C25
2	C	802	CPL	C21-C22-C23-C24
2	D	801	CPL	C22-C23-C24-C25
2	A	801	CPL	C22-C23-C24-C25
2	A	802	CPL	C21-C22-C23-C24
2	B	802	CPL	C21-C22-C23-C24
2	D	802	CPL	C21-C22-C23-C24
2	A	801	CPL	C20-C21-C22-C23
2	B	801	CPL	C20-C21-C22-C23
2	C	801	CPL	C20-C21-C22-C23
2	D	801	CPL	C20-C21-C22-C23
2	D	805	CPL	C14-C15-C16-C17
2	A	805	CPL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	801	CPL	C32-C33-C34-C35
2	B	805	CPL	C14-C15-C16-C17
2	C	801	CPL	C32-C33-C34-C35
2	D	801	CPL	C32-C33-C34-C35
2	A	801	CPL	C32-C33-C34-C35
2	C	805	CPL	C14-C15-C16-C17
2	A	806	CPL	C13-C14-C15-C16
2	B	806	CPL	C13-C14-C15-C16
2	C	806	CPL	C13-C14-C15-C16
2	D	806	CPL	C13-C14-C15-C16
2	A	801	CPL	C23-C24-C25-C26
2	B	801	CPL	C23-C24-C25-C26
2	C	801	CPL	C23-C24-C25-C26
2	D	801	CPL	C23-C24-C25-C26
2	A	802	CPL	O3P-C1-C2-C3
2	B	802	CPL	O3P-C1-C2-C3
2	C	802	CPL	O3P-C1-C2-C3
2	D	802	CPL	O3P-C1-C2-C3
2	A	801	CPL	C31-C32-C33-C34
2	B	801	CPL	C31-C32-C33-C34
2	C	801	CPL	C31-C32-C33-C34
2	D	801	CPL	C31-C32-C33-C34
2	A	802	CPL	C35-C36-C37-C38
2	B	802	CPL	C35-C36-C37-C38
2	C	802	CPL	C35-C36-C37-C38
2	D	802	CPL	C35-C36-C37-C38
2	A	801	CPL	C35-C36-C37-C38
2	B	801	CPL	C35-C36-C37-C38
2	D	801	CPL	C35-C36-C37-C38
2	C	801	CPL	C35-C36-C37-C38
3	A	808	PX2	O7-C2-C3-O5
3	B	808	PX2	O7-C2-C3-O5
3	C	808	PX2	O7-C2-C3-O5
3	D	808	PX2	O7-C2-C3-O5
2	A	805	CPL	C16-C17-C18-C19
2	B	805	CPL	C16-C17-C18-C19
2	C	805	CPL	C16-C17-C18-C19
2	D	805	CPL	C16-C17-C18-C19
3	A	803	PX2	C17-C18-C19-C20
3	B	803	PX2	C17-C18-C19-C20
3	C	803	PX2	C17-C18-C19-C20
3	D	803	PX2	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	808	PX2	C3-C2-O7-C16
3	B	808	PX2	C3-C2-O7-C16
3	C	808	PX2	C3-C2-O7-C16
3	D	808	PX2	C3-C2-O7-C16
2	A	802	CPL	C14-C15-C16-C17
2	B	802	CPL	C14-C15-C16-C17
2	D	802	CPL	C14-C15-C16-C17
2	C	802	CPL	C14-C15-C16-C17
2	A	801	CPL	C40-C41-C42-C43
2	B	801	CPL	C40-C41-C42-C43
2	C	801	CPL	C40-C41-C42-C43
2	D	801	CPL	C40-C41-C42-C43
2	A	801	CPL	O3P-C1-C2-C3
2	B	801	CPL	O3P-C1-C2-C3
2	C	801	CPL	O3P-C1-C2-C3
2	D	801	CPL	O3P-C1-C2-C3
3	A	808	PX2	O4-C1-C2-C3
3	B	808	PX2	O4-C1-C2-C3
3	C	808	PX2	O4-C1-C2-C3
3	D	808	PX2	O4-C1-C2-C3
3	A	808	PX2	O4-C1-C2-O7
3	B	808	PX2	O4-C1-C2-O7
3	C	808	PX2	O4-C1-C2-O7
3	D	808	PX2	O4-C1-C2-O7
2	A	801	CPL	O4P-C4-C5-N
2	B	801	CPL	O4P-C4-C5-N
2	C	801	CPL	O4P-C4-C5-N
2	D	801	CPL	O4P-C4-C5-N
2	A	805	CPL	C15-C16-C17-C18
2	D	805	CPL	C15-C16-C17-C18
2	B	805	CPL	C15-C16-C17-C18
2	C	805	CPL	C15-C16-C17-C18
2	A	801	CPL	C37-C38-C39-C40
2	B	801	CPL	C37-C38-C39-C40
2	C	801	CPL	C37-C38-C39-C40
2	D	801	CPL	C37-C38-C39-C40
2	A	804	CPL	C16-C17-C18-C19
2	C	804	CPL	C16-C17-C18-C19
2	B	804	CPL	C16-C17-C18-C19
2	D	804	CPL	C16-C17-C18-C19
2	A	802	CPL	C1-C2-C3-O3
2	B	802	CPL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	802	CPL	C1-C2-C3-O3
2	D	802	CPL	C1-C2-C3-O3
2	B	805	CPL	C12-C13-C14-C15
2	D	805	CPL	C12-C13-C14-C15
2	A	805	CPL	C12-C13-C14-C15
2	C	805	CPL	C12-C13-C14-C15
2	B	801	CPL	C34-C35-C36-C37
2	A	801	CPL	C34-C35-C36-C37
2	C	801	CPL	C34-C35-C36-C37
2	D	801	CPL	C34-C35-C36-C37
2	A	807	CPL	C20-C21-C22-C23
2	C	807	CPL	C20-C21-C22-C23
2	B	807	CPL	C20-C21-C22-C23
2	D	807	CPL	C20-C21-C22-C23
3	A	803	PX2	C1-O4-P1-O3
3	B	803	PX2	C1-O4-P1-O3
3	C	803	PX2	C1-O4-P1-O3
3	D	803	PX2	C1-O4-P1-O3
2	A	801	CPL	C19-C20-C21-C22
2	D	801	CPL	C19-C20-C21-C22
2	B	801	CPL	C19-C20-C21-C22
2	C	801	CPL	C19-C20-C21-C22
2	A	801	CPL	C36-C37-C38-C39
2	B	801	CPL	C36-C37-C38-C39
2	C	801	CPL	C36-C37-C38-C39
2	D	801	CPL	C36-C37-C38-C39
3	A	803	PX2	C1-C2-C3-O5
3	B	803	PX2	C1-C2-C3-O5
3	C	803	PX2	C1-C2-C3-O5
3	D	803	PX2	C1-C2-C3-O5
2	B	804	CPL	C13-C14-C15-C16
2	C	804	CPL	C13-C14-C15-C16
2	A	804	CPL	C13-C14-C15-C16
2	D	804	CPL	C13-C14-C15-C16
2	A	802	CPL	O3P-C1-C2-O2
2	B	802	CPL	O3P-C1-C2-O2
2	C	802	CPL	O3P-C1-C2-O2
2	D	802	CPL	O3P-C1-C2-O2
2	A	802	CPL	O3-C11-C12-C13
2	B	802	CPL	O3-C11-C12-C13
2	D	802	CPL	O3-C11-C12-C13
2	C	802	CPL	O3-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	801	CPL	O2-C31-C32-C33
2	B	801	CPL	O2-C31-C32-C33
2	C	801	CPL	O2-C31-C32-C33
2	D	801	CPL	O2-C31-C32-C33

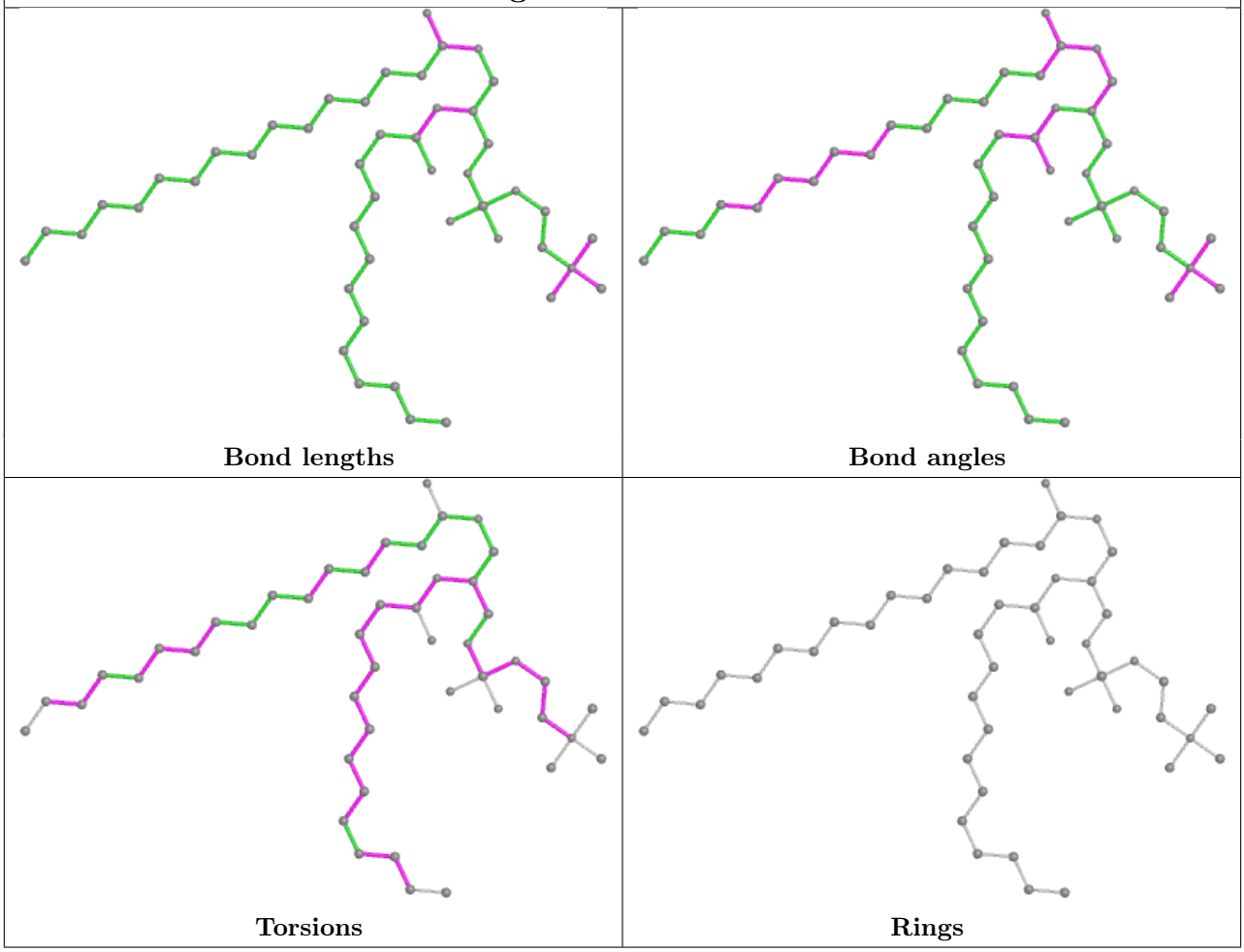
There are no ring outliers.

12 monomers are involved in 31 short contacts:

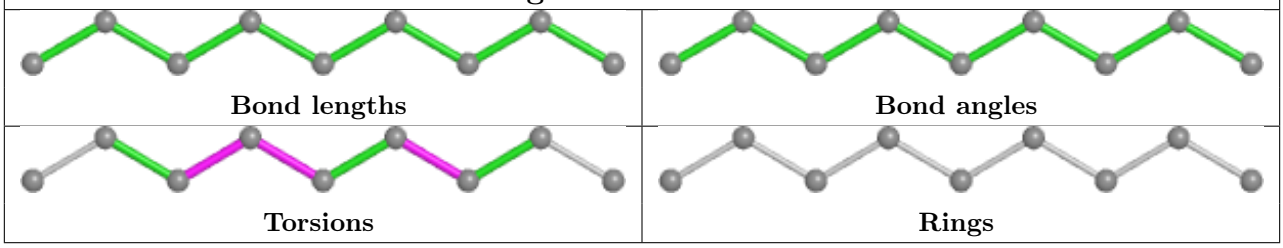
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	CPL	5	0
2	B	801	CPL	5	0
2	A	801	CPL	5	0
2	A	806	CPL	1	0
3	D	803	PX2	2	0
2	C	806	CPL	1	0
3	A	803	PX2	1	0
2	C	801	CPL	6	0
3	C	803	PX2	2	0
2	D	806	CPL	1	0
2	B	806	CPL	1	0
3	B	803	PX2	1	0

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.

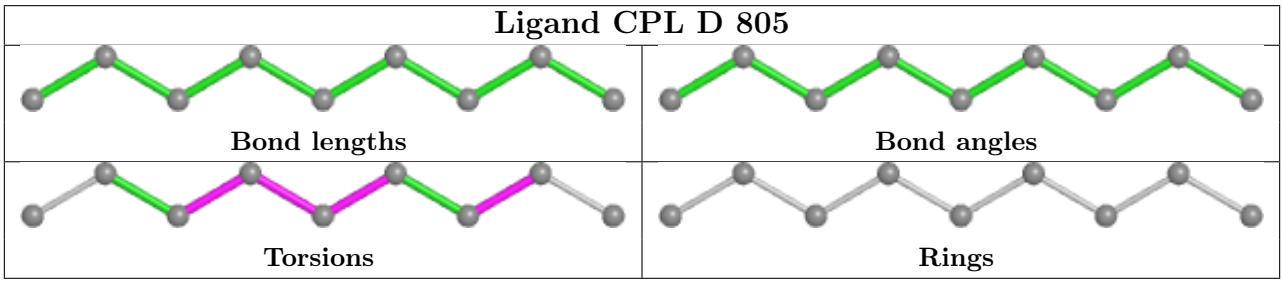
Ligand CPL D 801



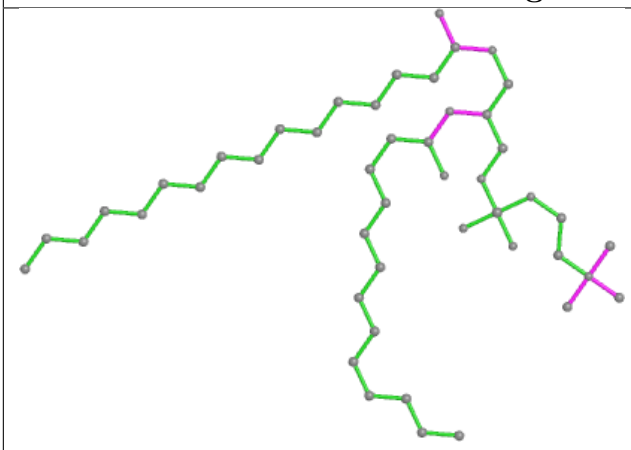
Ligand CPL C 804



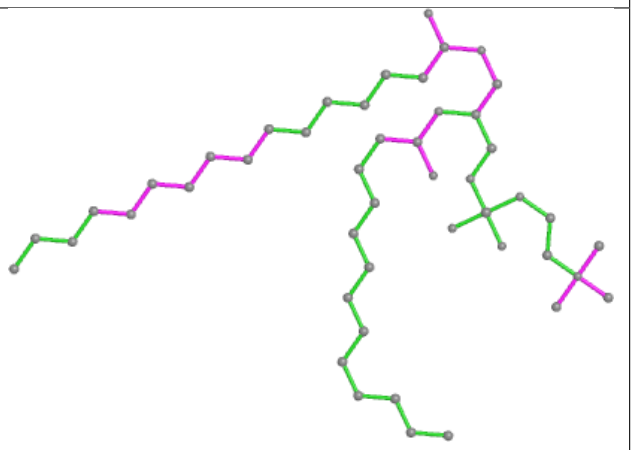
Ligand CPL D 805



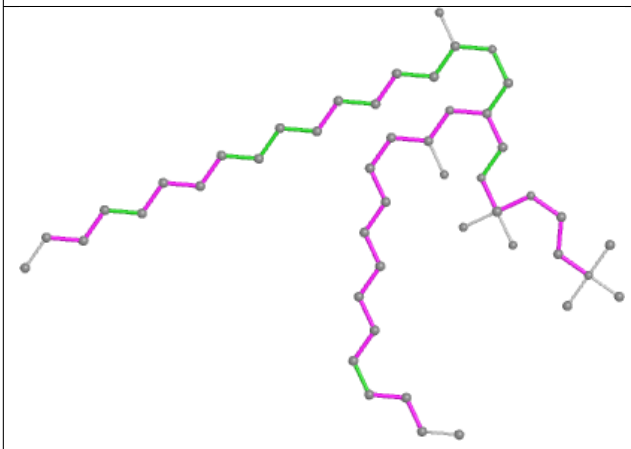
Ligand CPL B 801



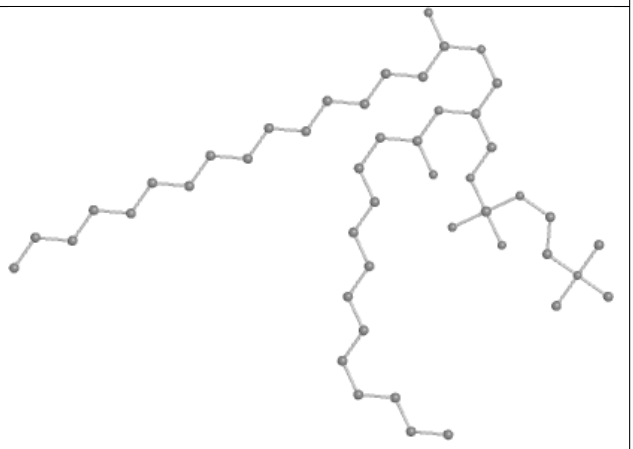
Bond lengths



Bond angles

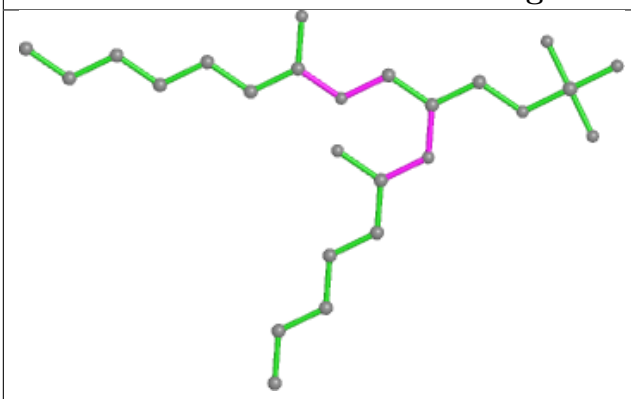


Torsions

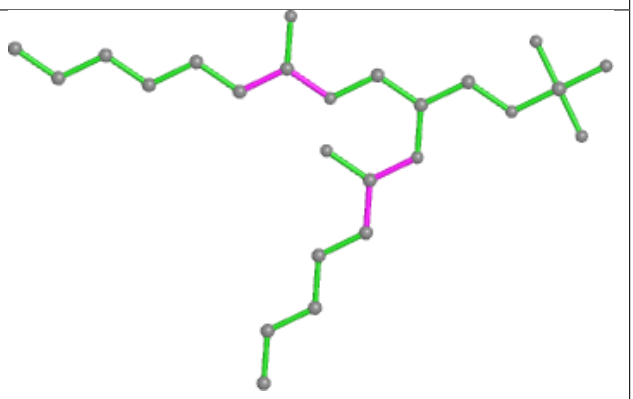


Rings

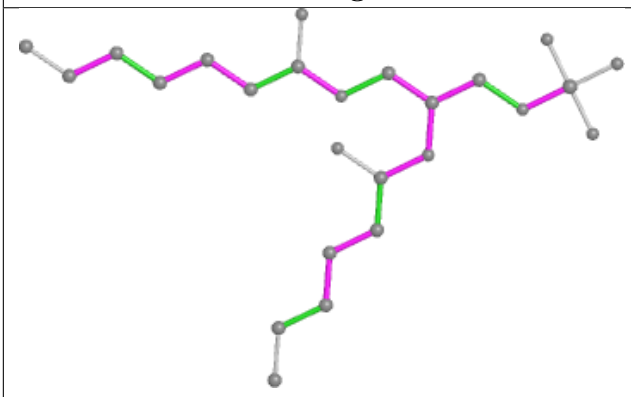
Ligand PX2 D 808



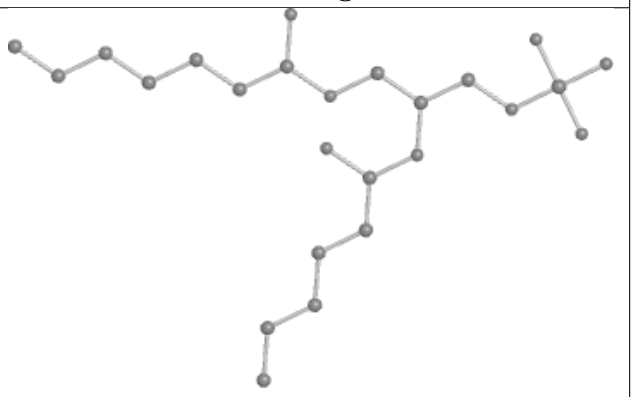
Bond lengths



Bond angles

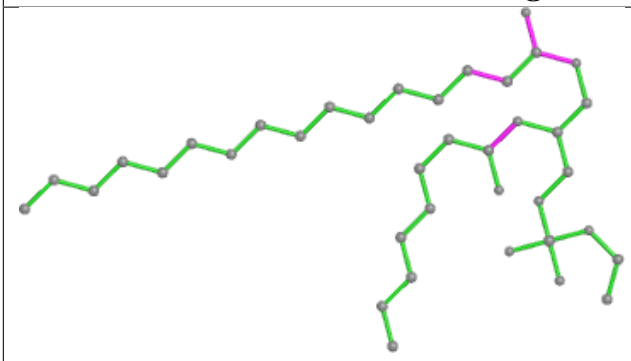


Torsions

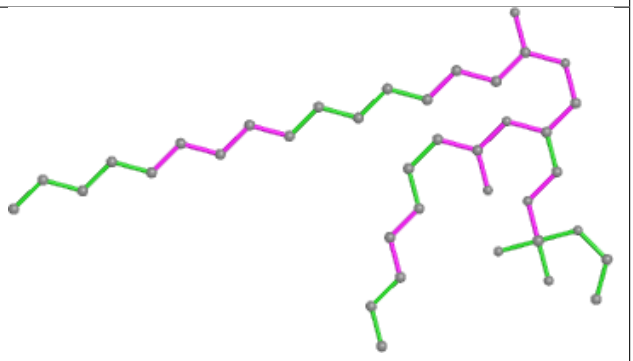


Rings

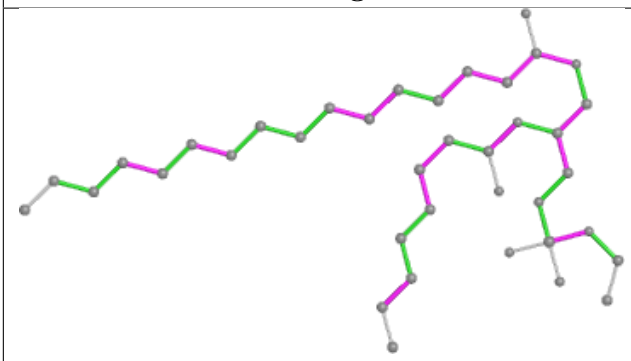
Ligand CPL D 802



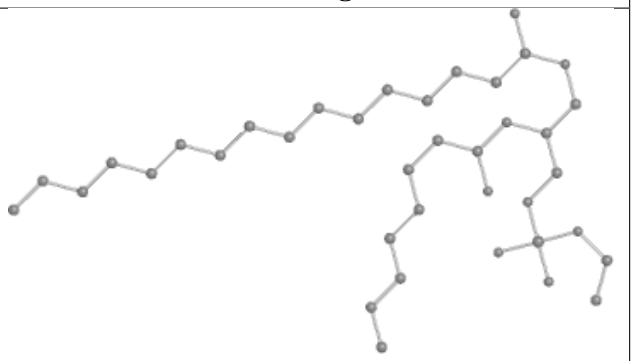
Bond lengths



Bond angles

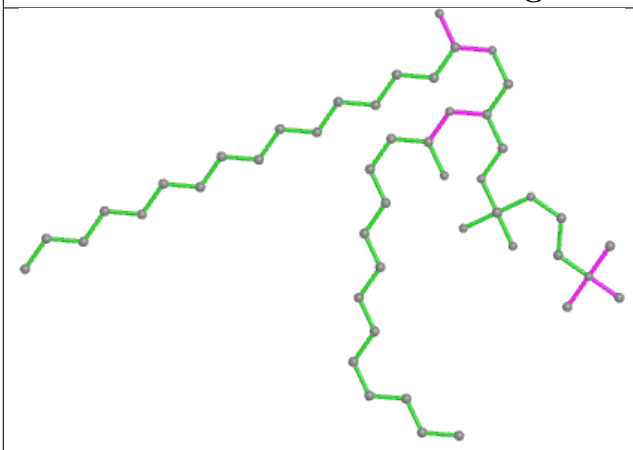


Torsions

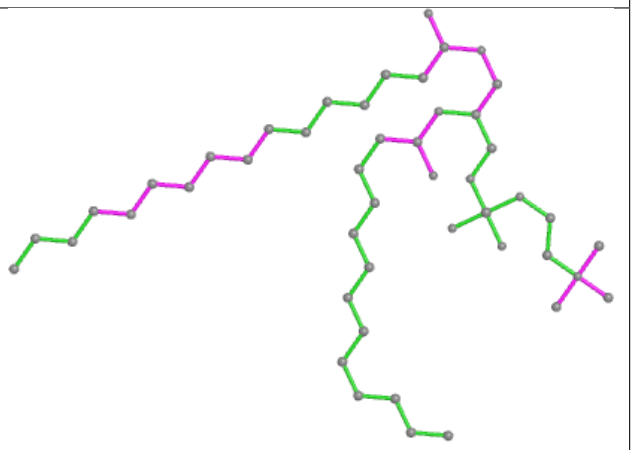


Rings

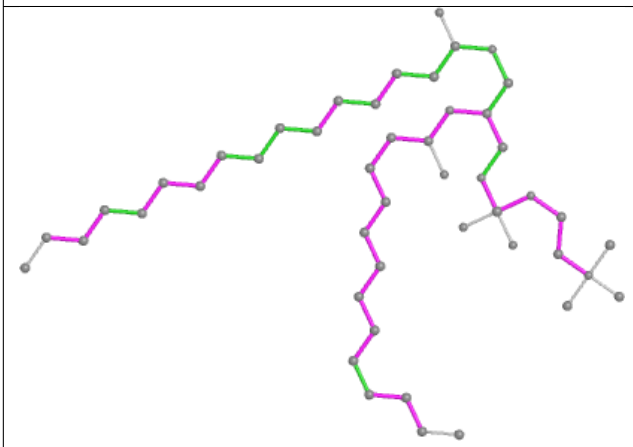
Ligand CPL A 801



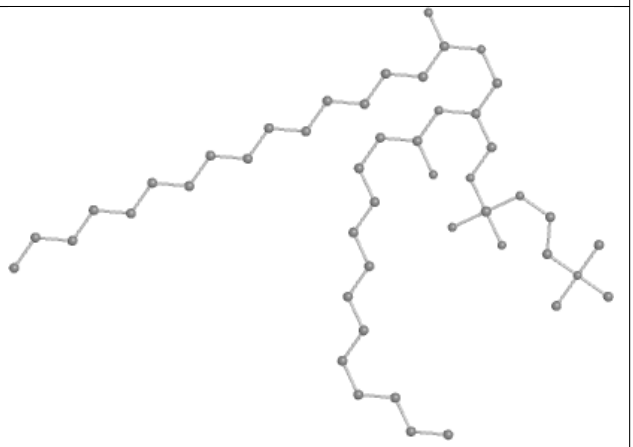
Bond lengths



Bond angles

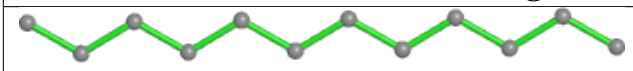


Torsions

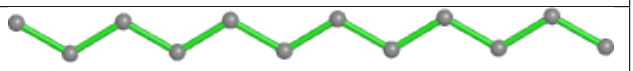


Rings

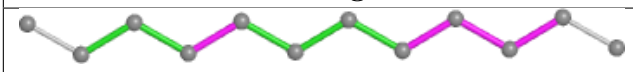
Ligand CPL A 806



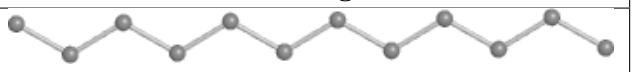
Bond lengths



Bond angles

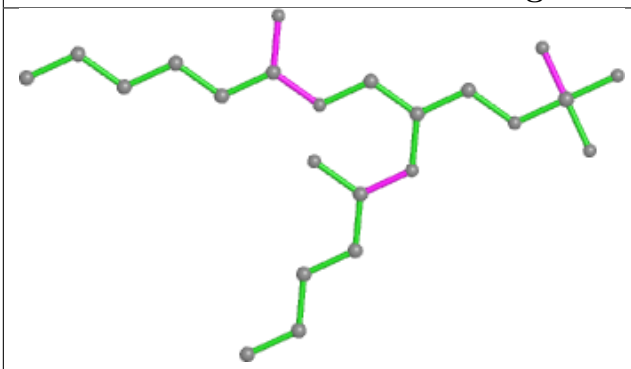


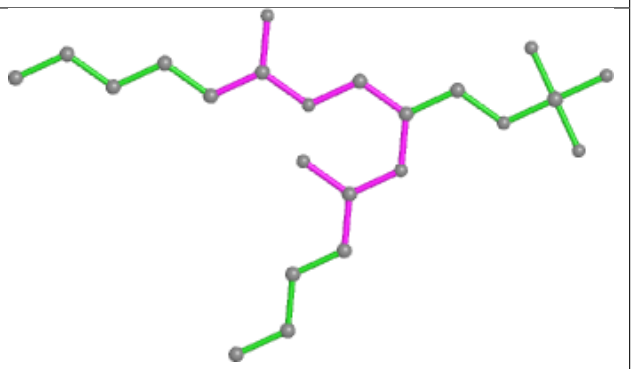
Torsions

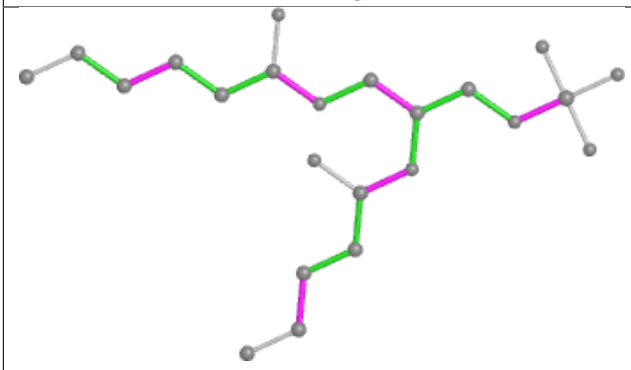


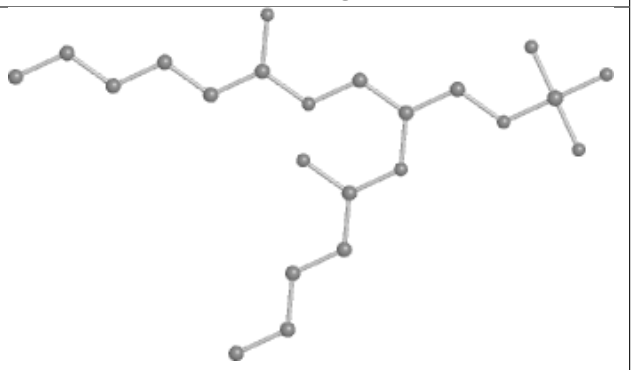
Rings

Ligand PX2 D 803

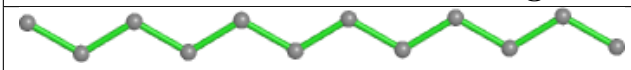

Bond lengths

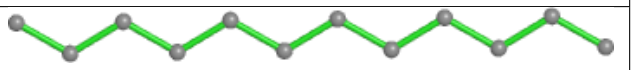

Bond angles

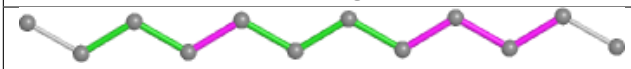

Torsions

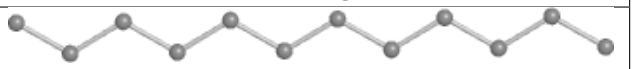

Rings

Ligand CPL C 806

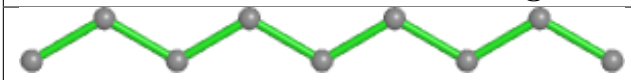

Bond lengths

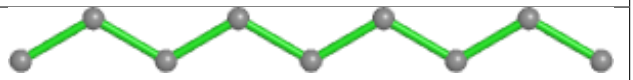

Bond angles

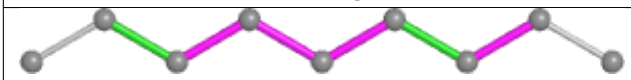

Torsions


Rings

Ligand CPL A 805

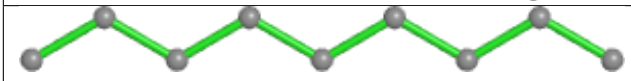

Bond lengths

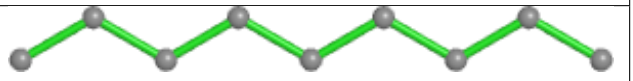

Bond angles

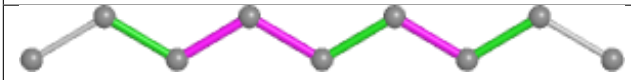

Torsions

Rings

Ligand CPL D 804

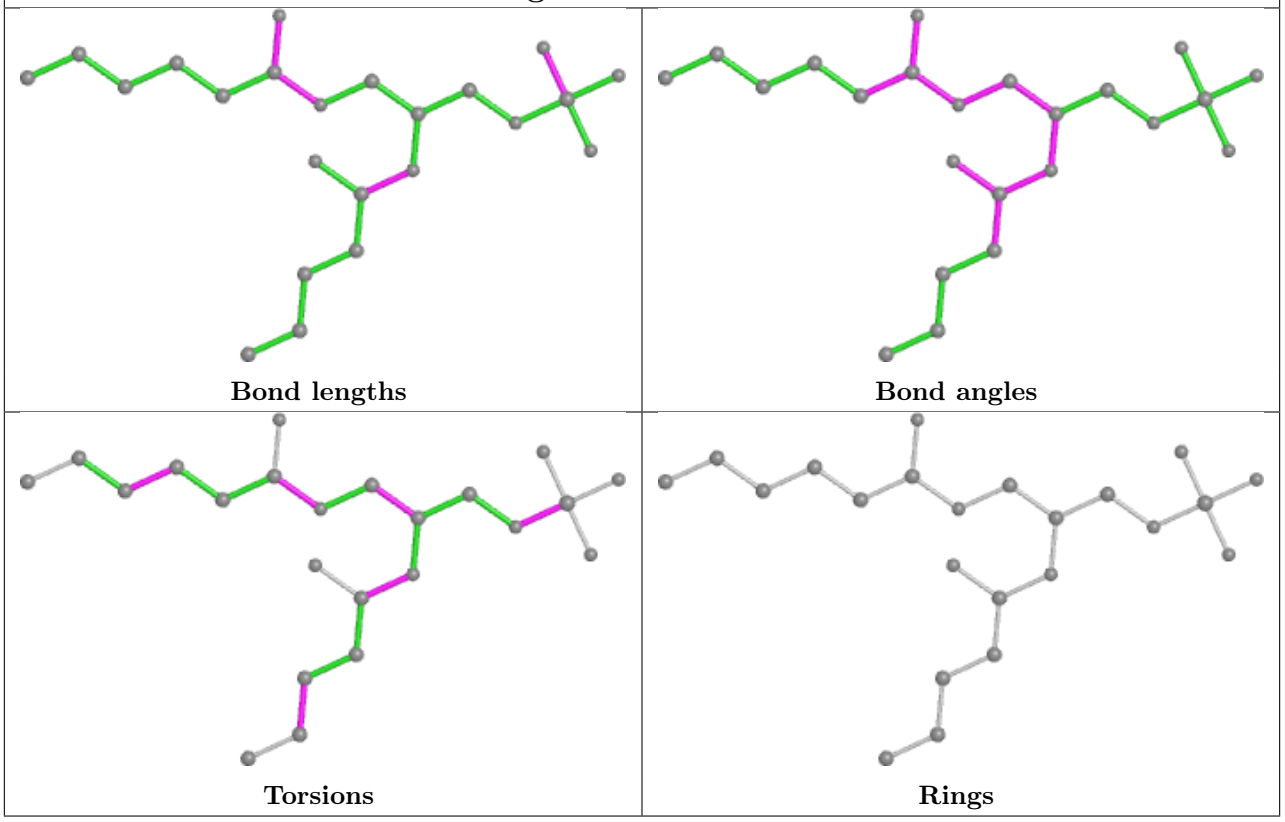

Bond lengths


Bond angles

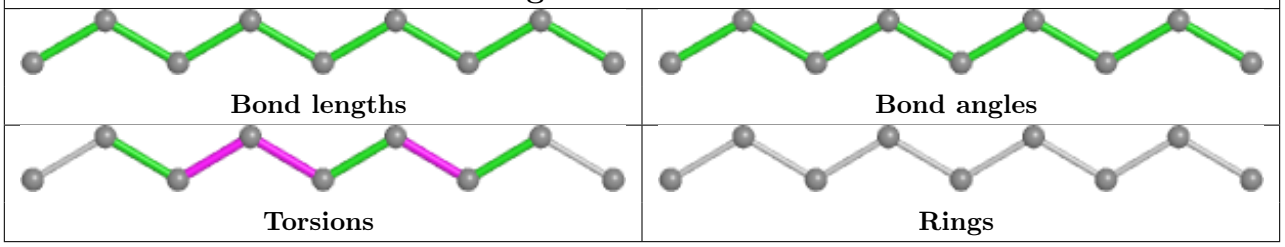

Torsions

Rings

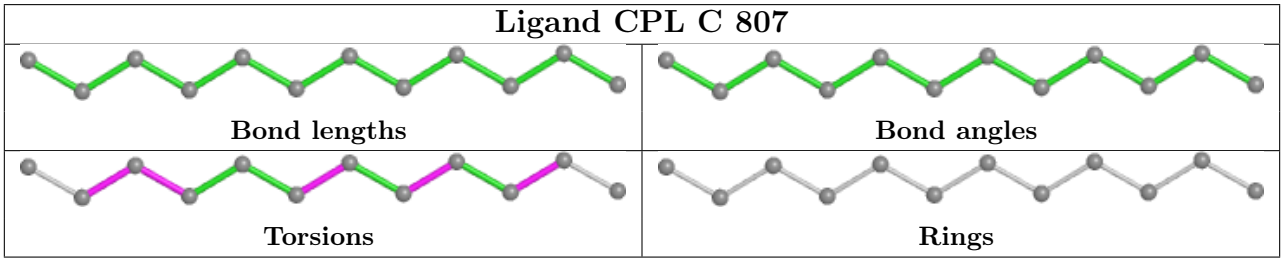
Ligand PX2 A 803



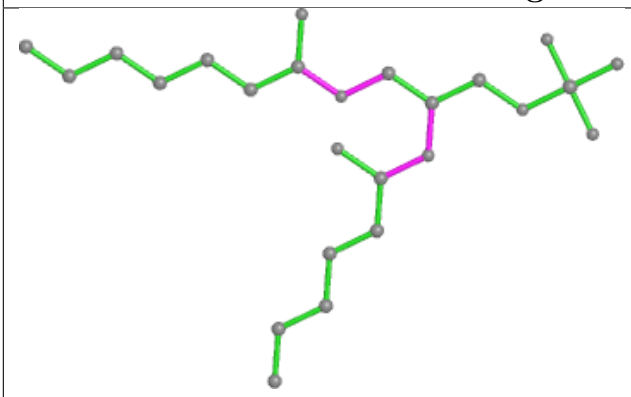
Ligand CPL B 804



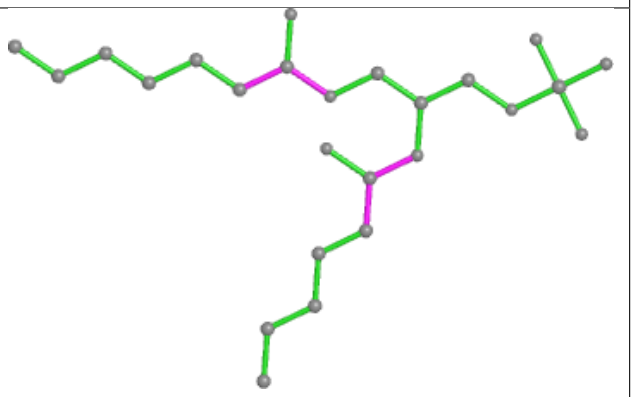
Ligand CPL C 807



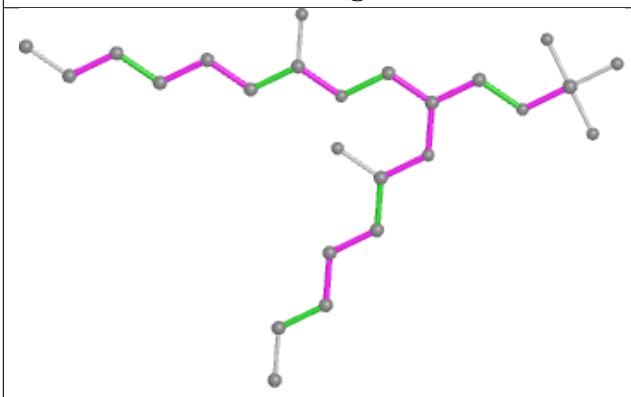
Ligand PX2 A 808



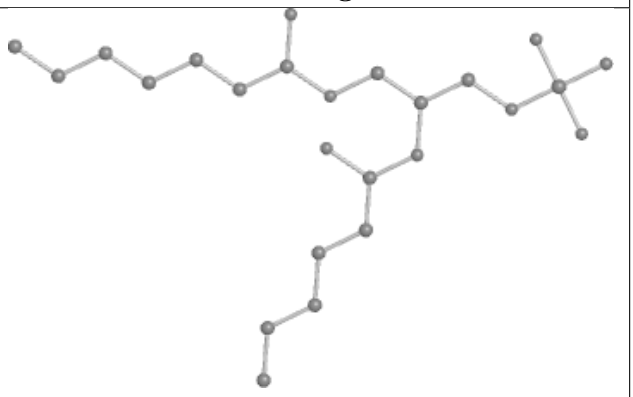
Bond lengths



Bond angles

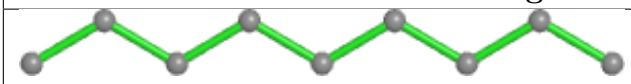


Torsions

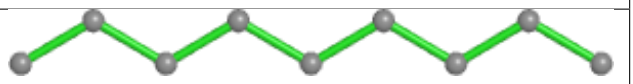


Rings

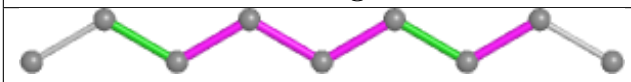
Ligand CPL B 805



Bond lengths



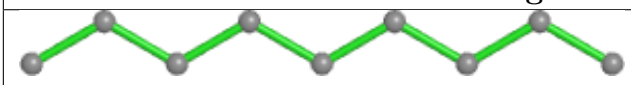
Bond angles



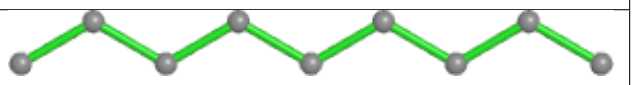
Torsions

Rings

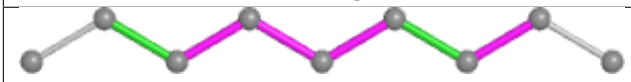
Ligand CPL C 805



Bond lengths



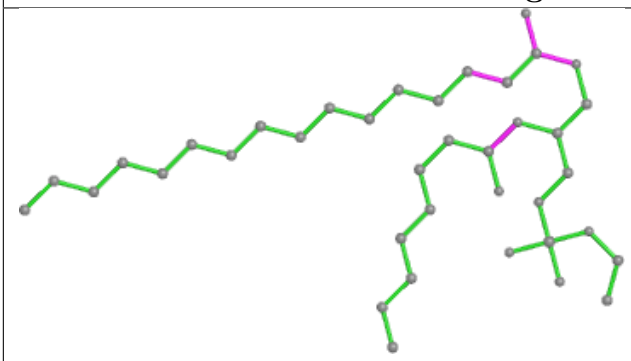
Bond angles



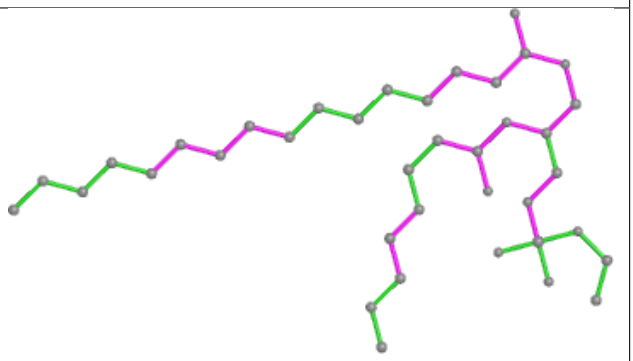
Torsions

Rings

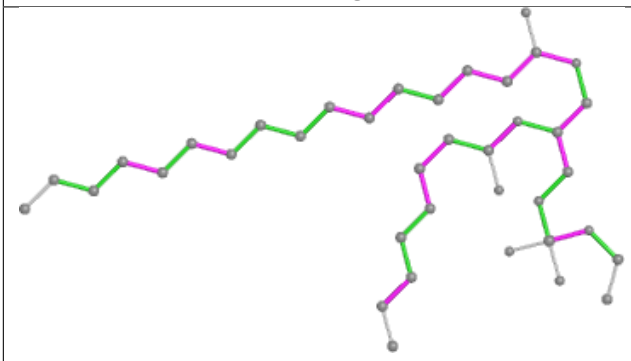
Ligand CPL B 802



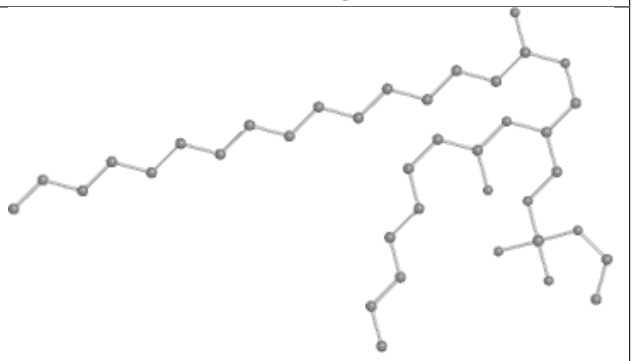
Bond lengths



Bond angles

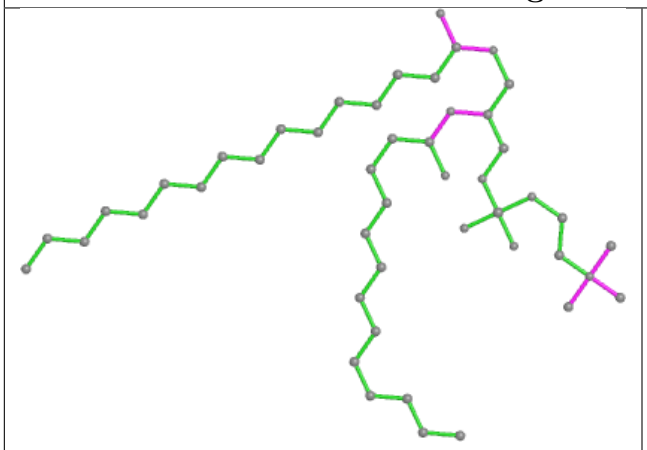


Torsions

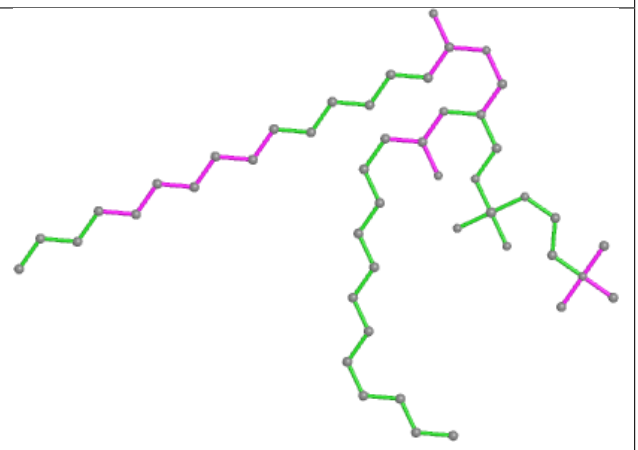


Rings

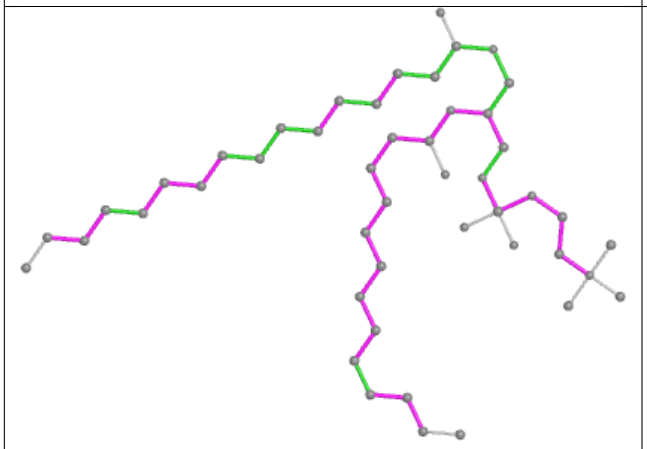
Ligand CPL C 801



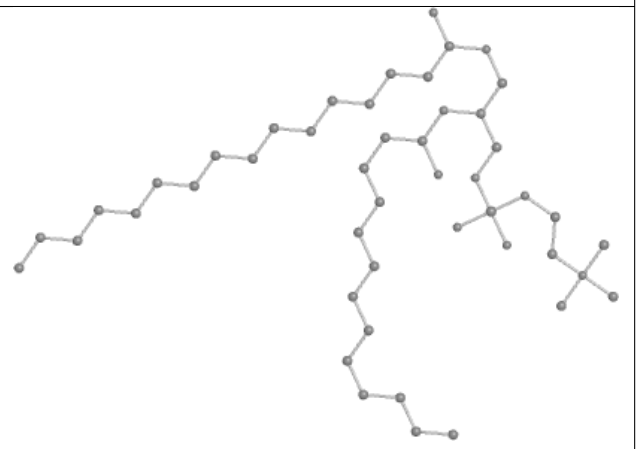
Bond lengths



Bond angles

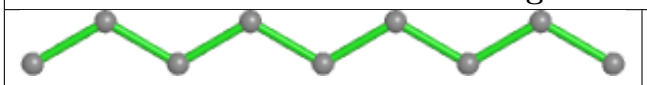


Torsions

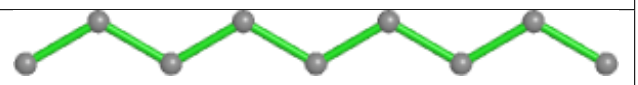


Rings

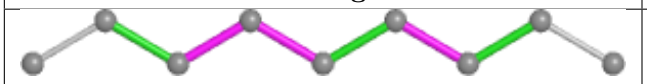
Ligand CPL A 804



Bond lengths



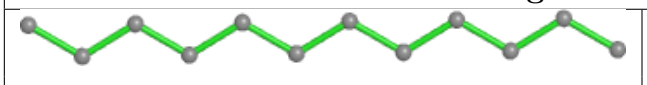
Bond angles



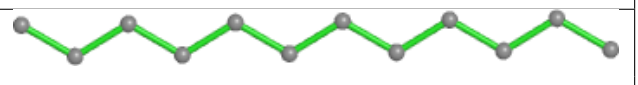
Torsions

Rings

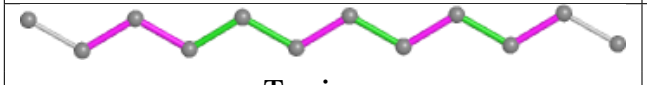
Ligand CPL B 807



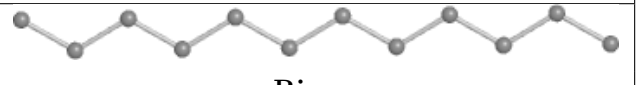
Bond lengths



Bond angles

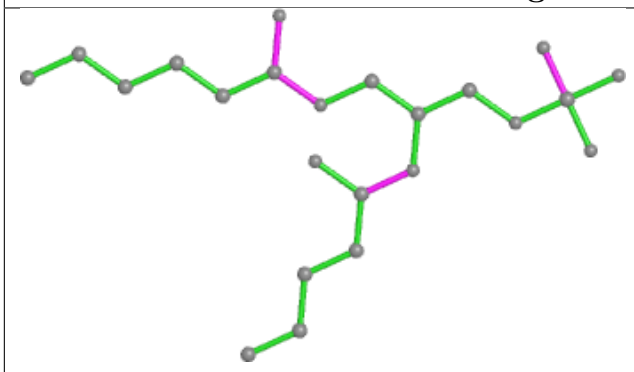


Torsions

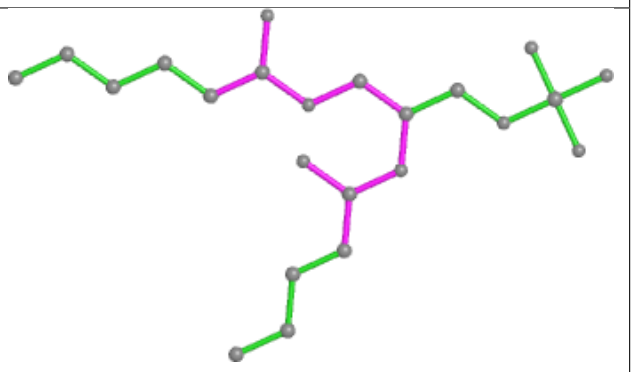


Rings

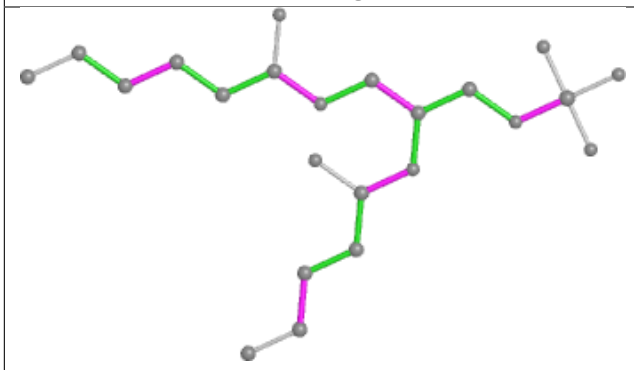
Ligand PX2 C 803



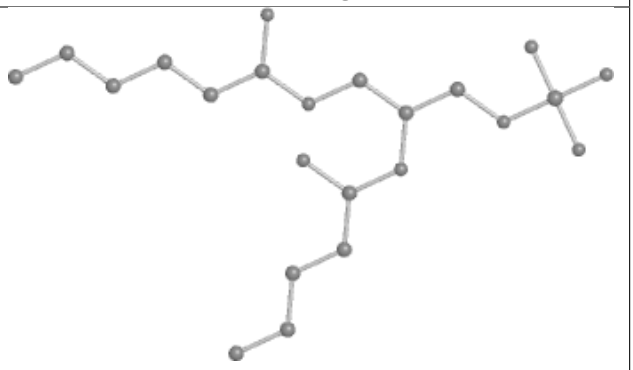
Bond lengths



Bond angles

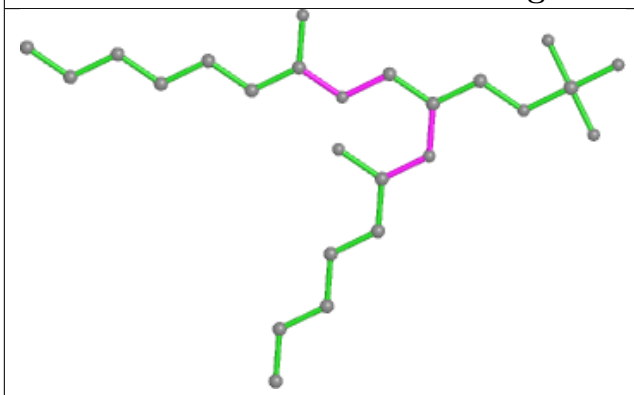


Torsions

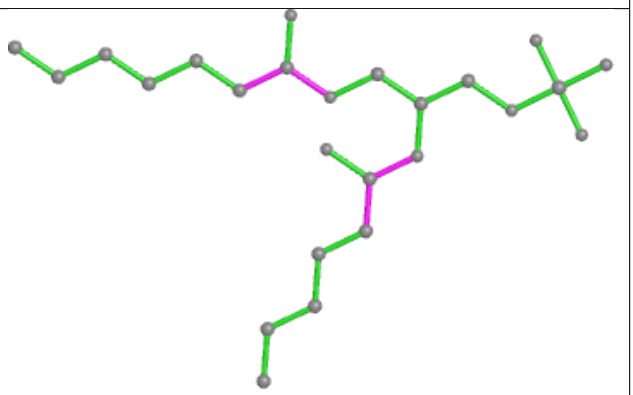


Rings

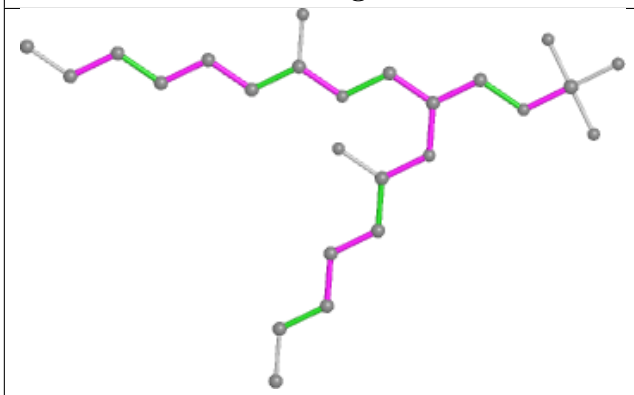
Ligand PX2 C 808



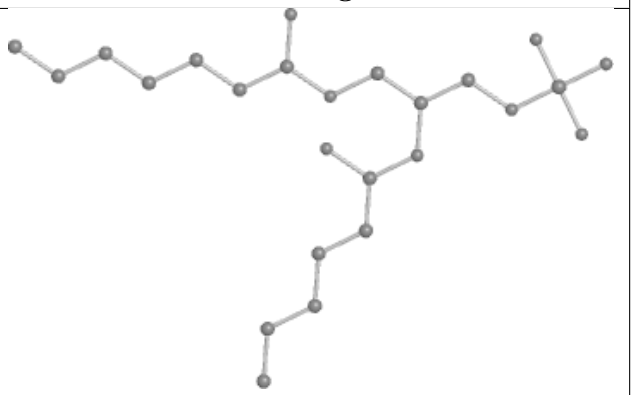
Bond lengths



Bond angles

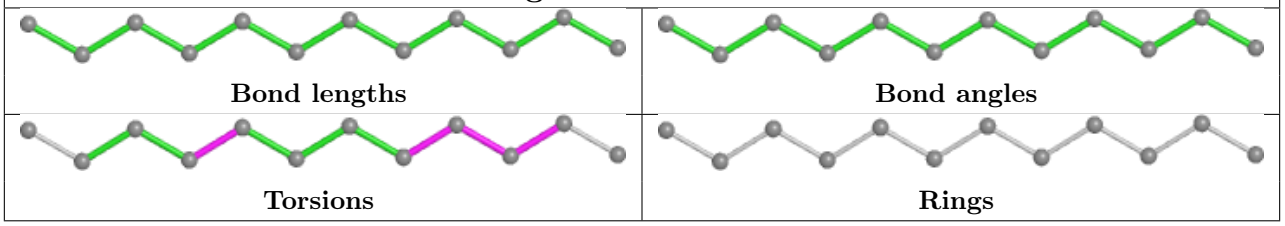


Torsions

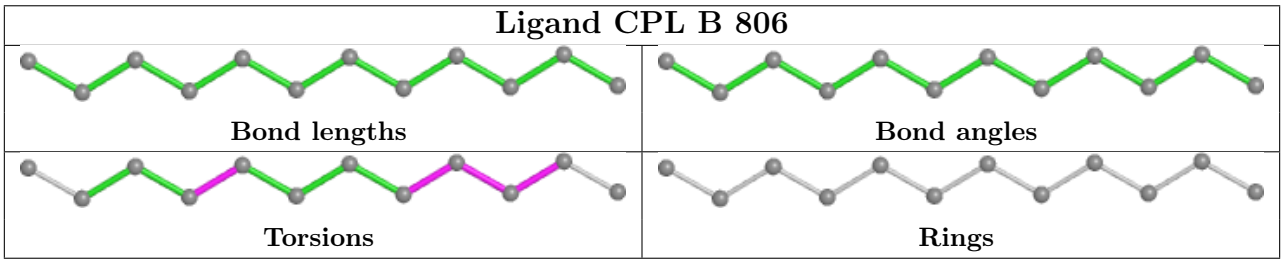


Rings

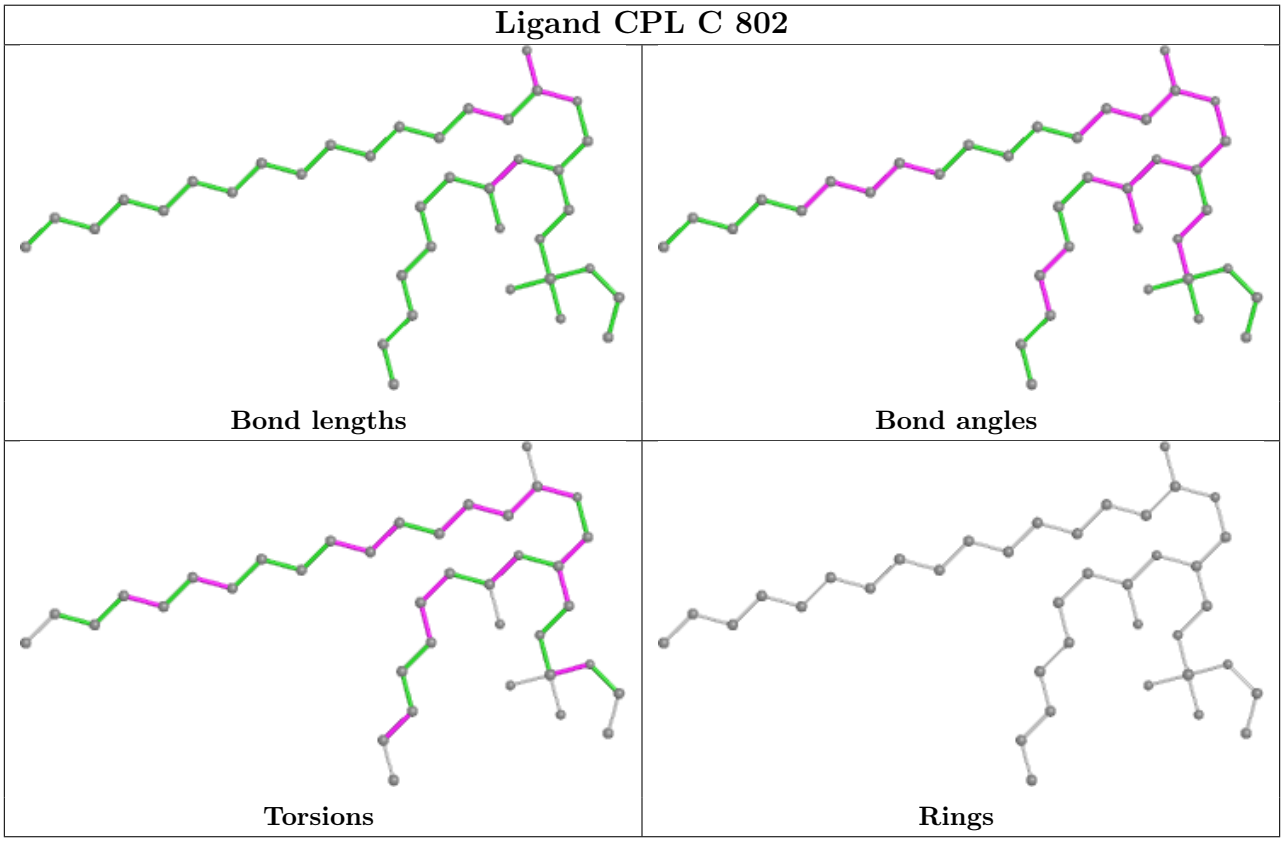
Ligand CPL D 806



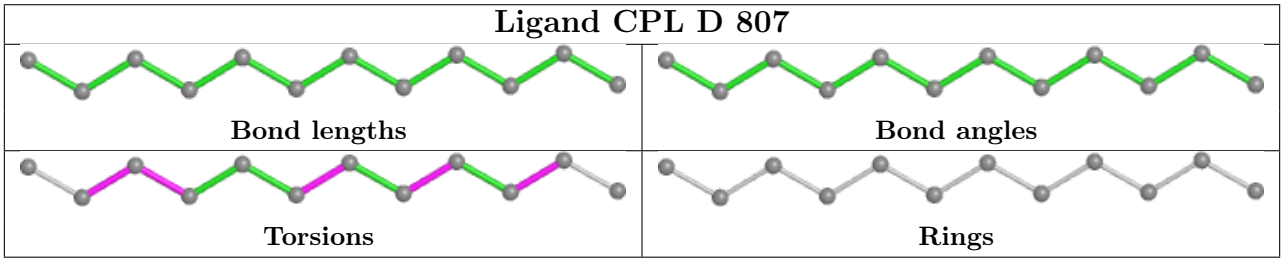
Ligand CPL B 806



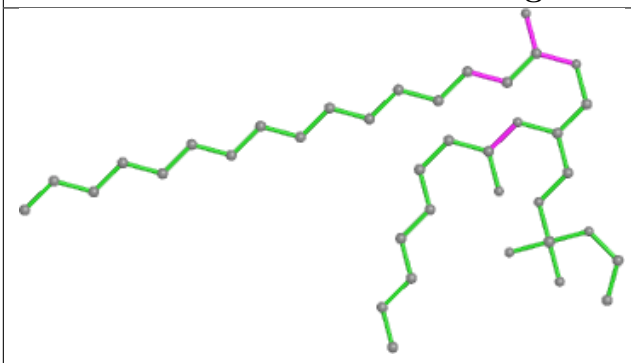
Ligand CPL C 802



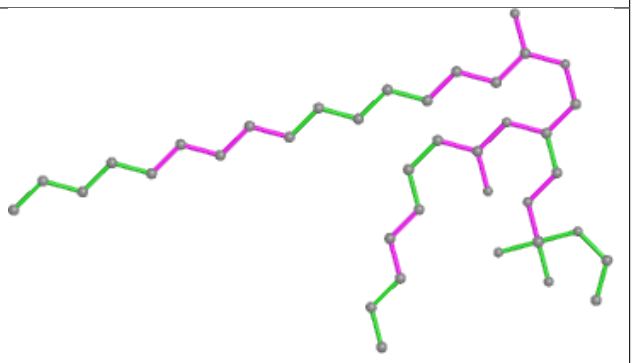
Ligand CPL D 807



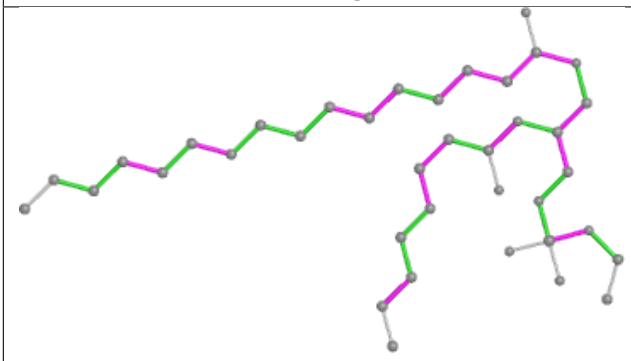
Ligand CPL A 802



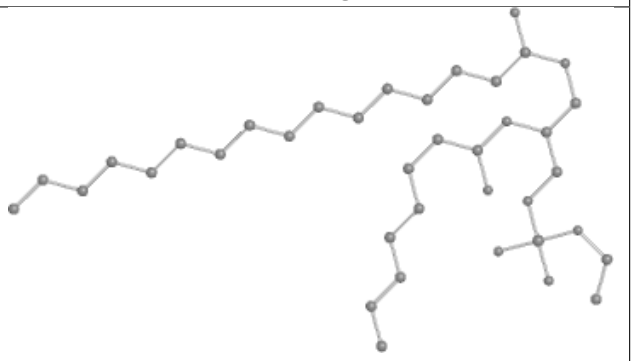
Bond lengths



Bond angles

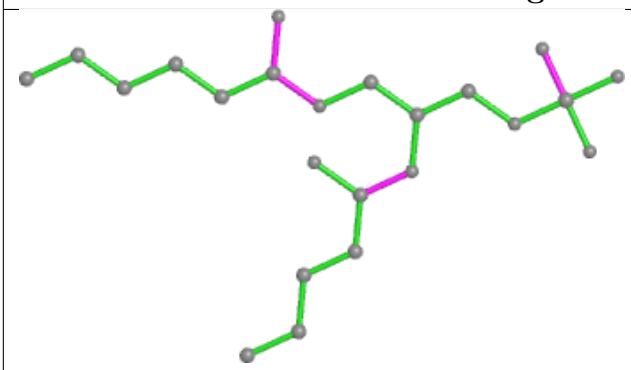


Torsions

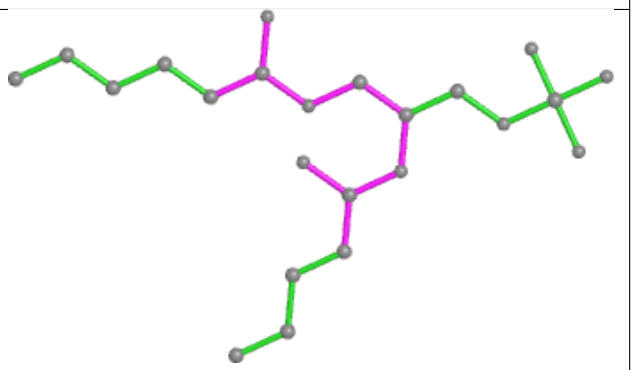


Rings

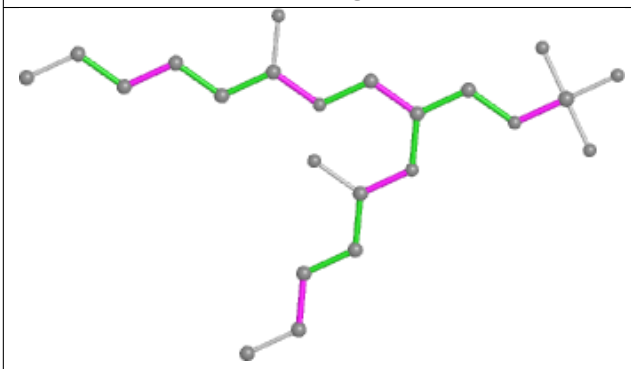
Ligand PX2 B 803



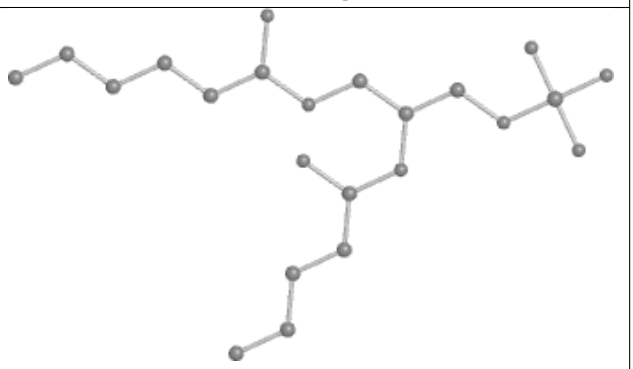
Bond lengths



Bond angles

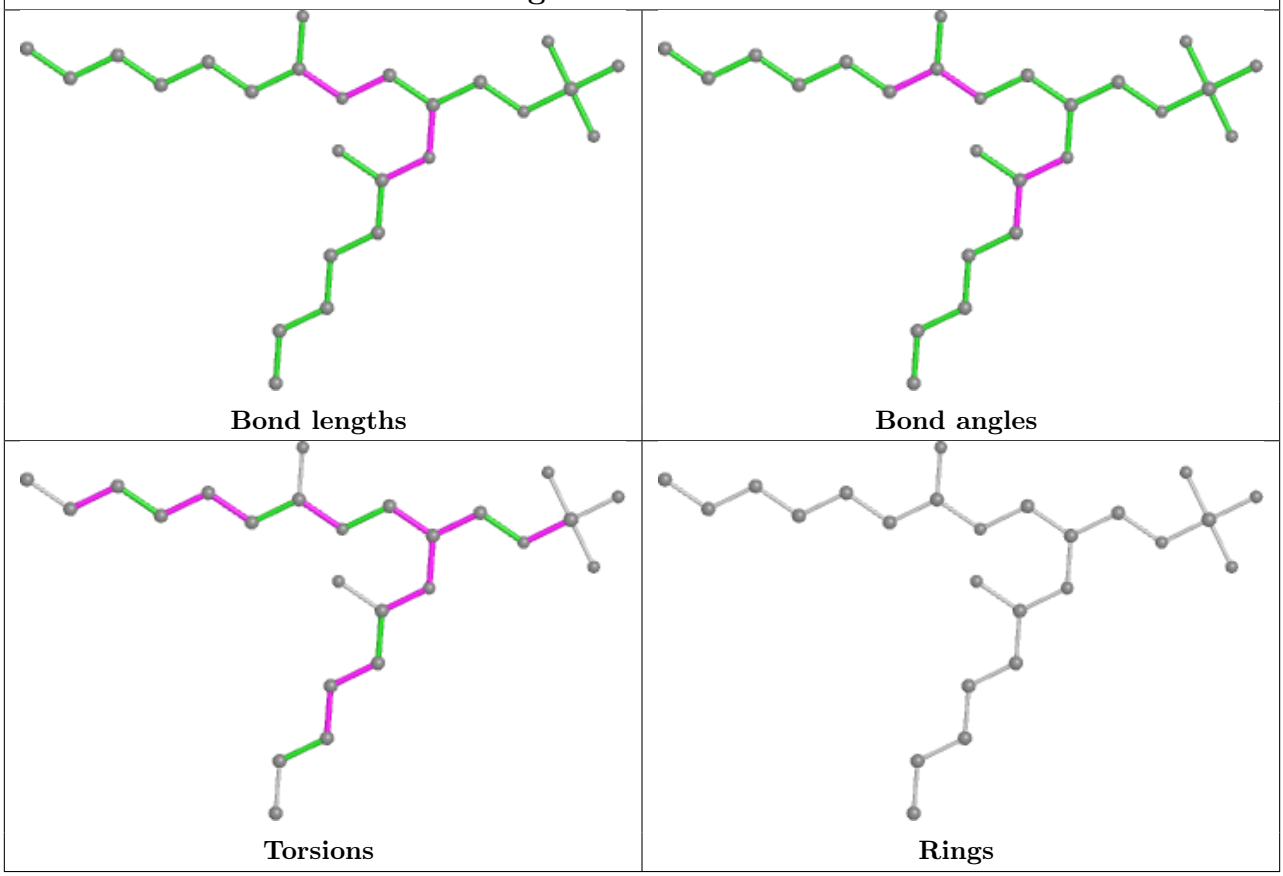


Torsions

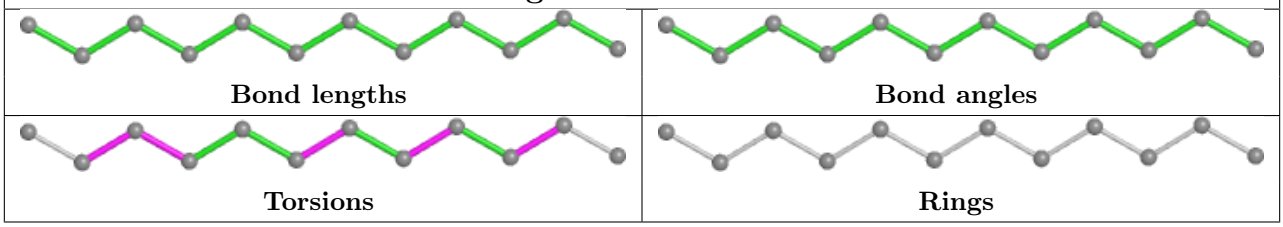


Rings

Ligand PX2 B 808



Ligand CPL A 807



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

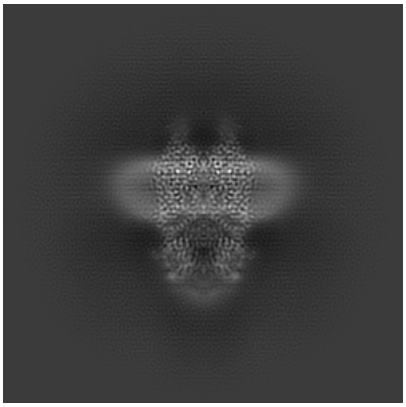
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21649. These allow visual inspection of the internal detail of the map and identification of artifacts.

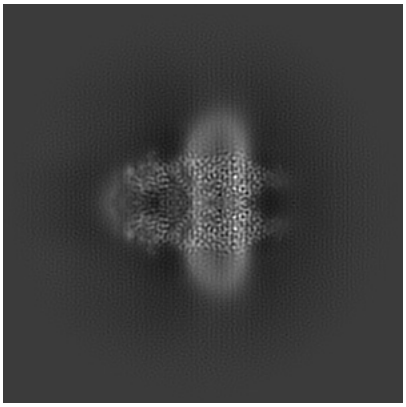
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

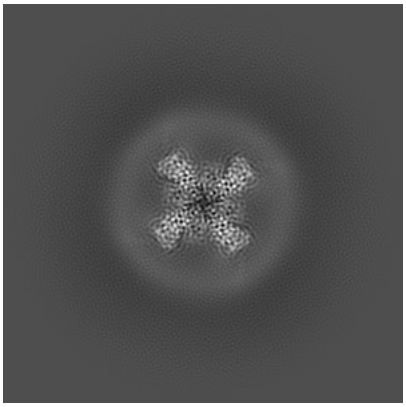
6.1.1 Primary map



X



Y

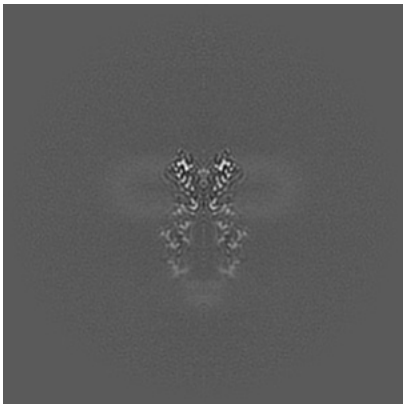


Z

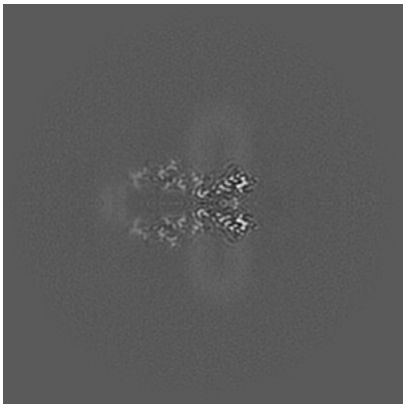
The images above show the map projected in three orthogonal directions.

6.2 Central slices

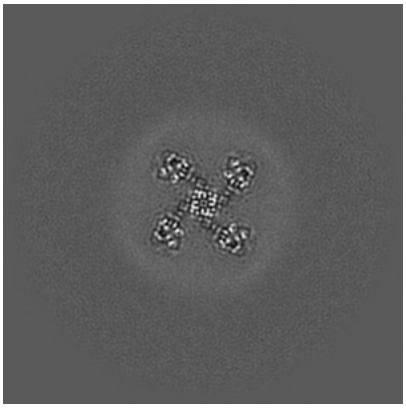
6.2.1 Primary map



X Index: 148



Y Index: 148

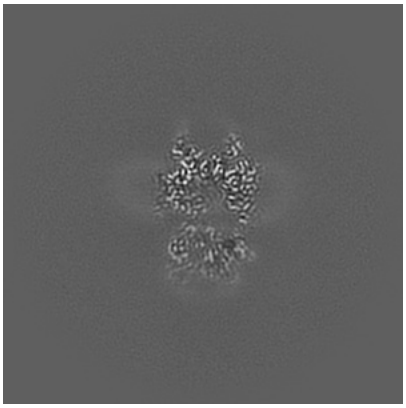


Z Index: 148

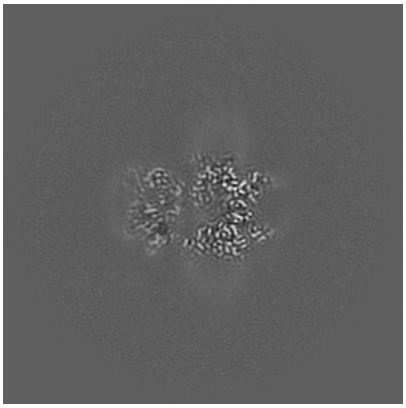
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

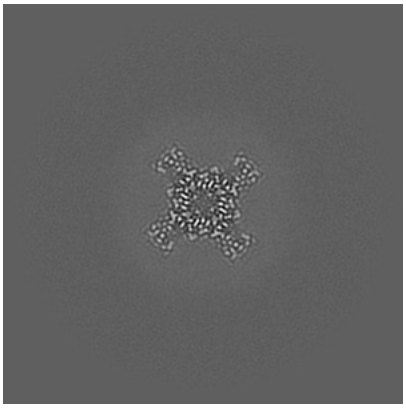
6.3.1 Primary map



X Index: 129



Y Index: 129

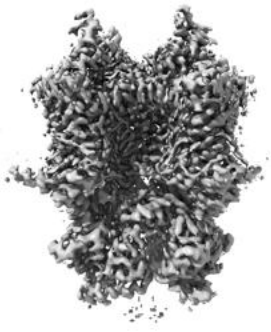


Z Index: 174

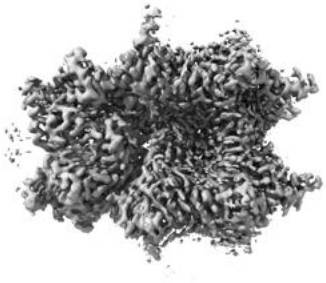
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

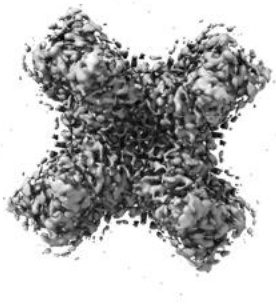
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.574. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

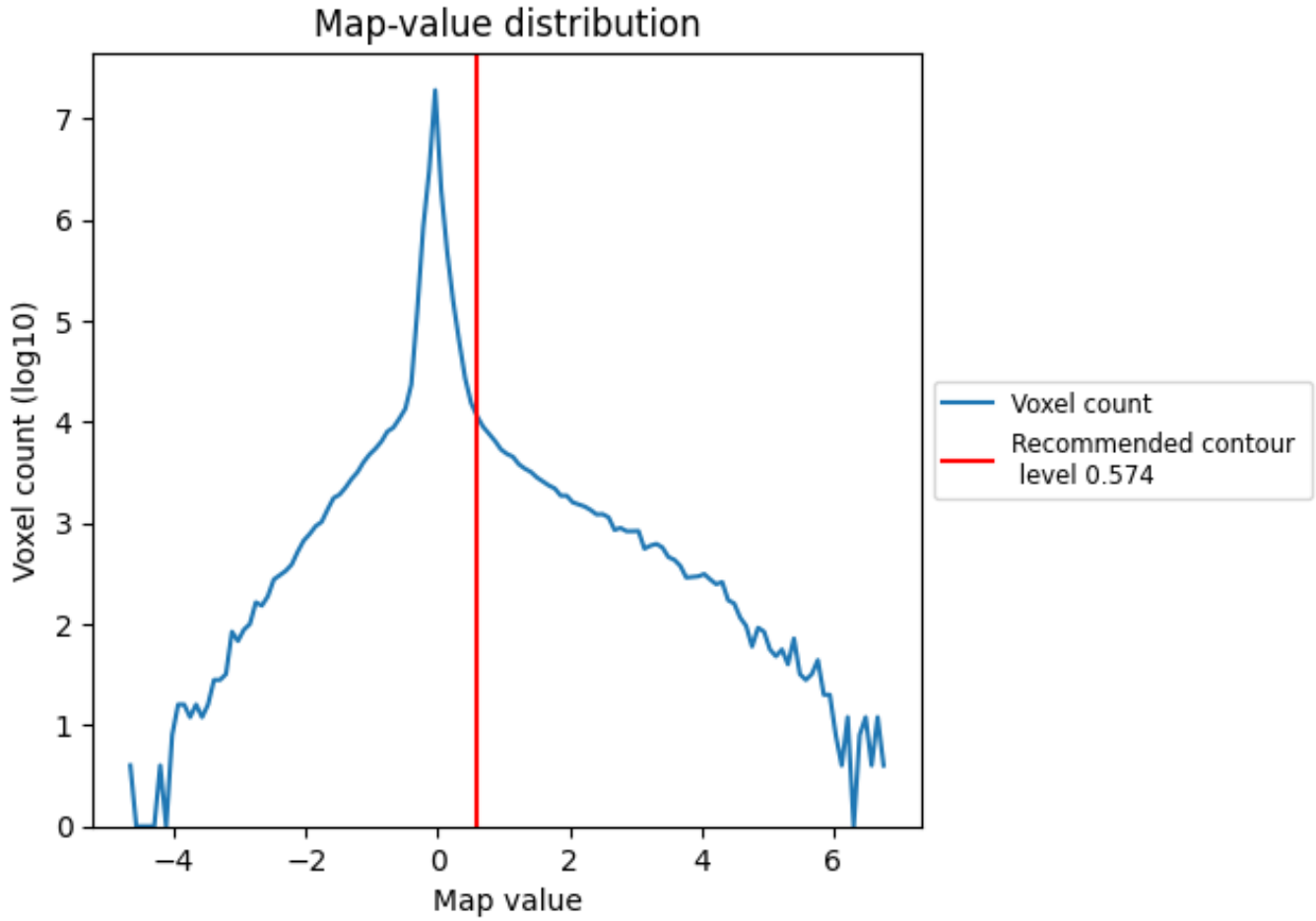
6.5 Mask visualisation (i)

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

7 Map analysis

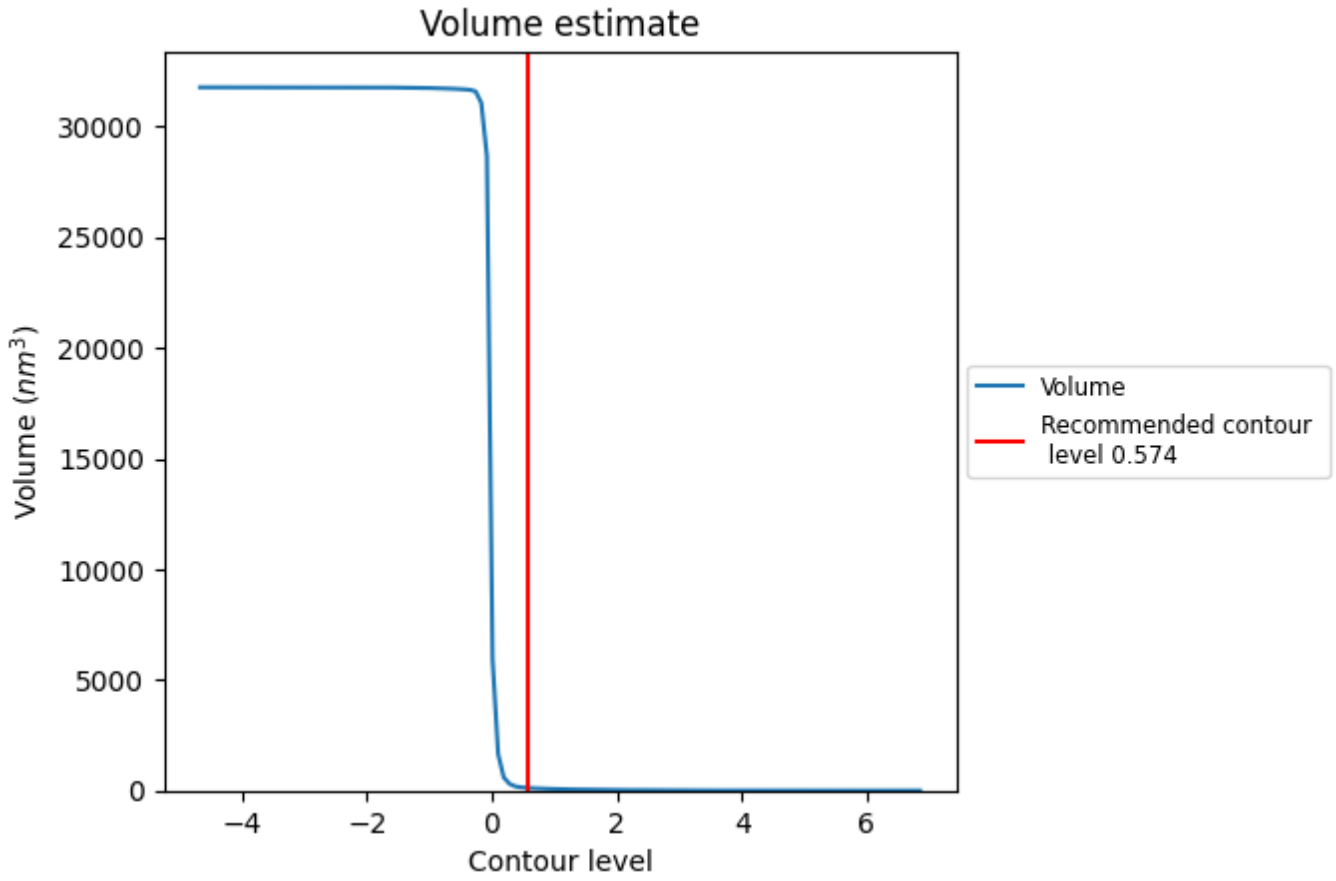
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

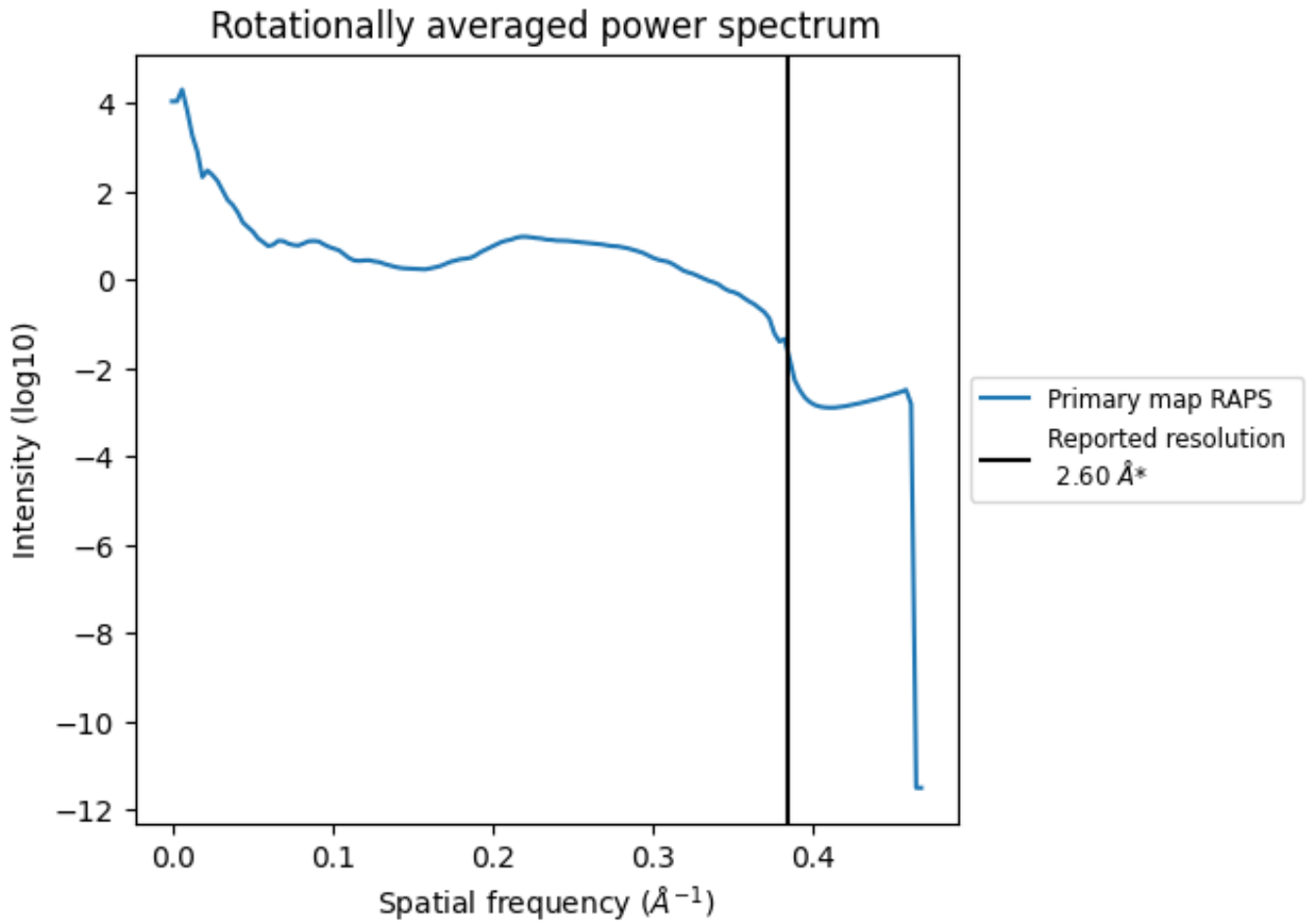
7.2 Volume estimate



The volume at the recommended contour level is 119 nm^3; this corresponds to an approximate mass of 107 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 $Å^{-1}$

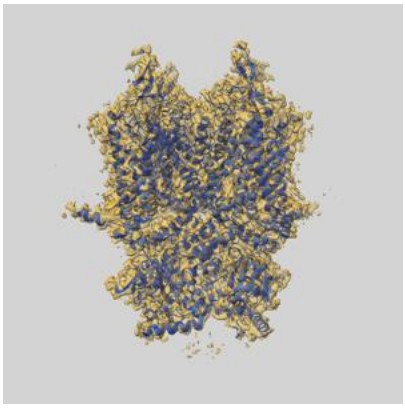
8 Fourier-Shell correlation (i)

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

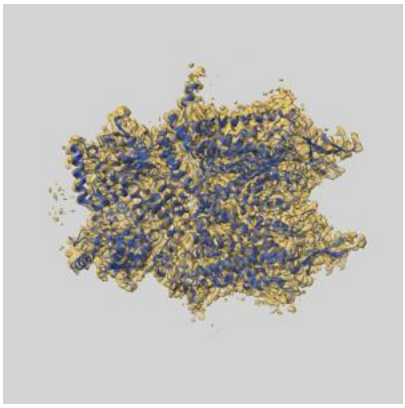
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21649 and PDB model 6WEJ. Per-residue inclusion information can be found in section 3 on page 7.

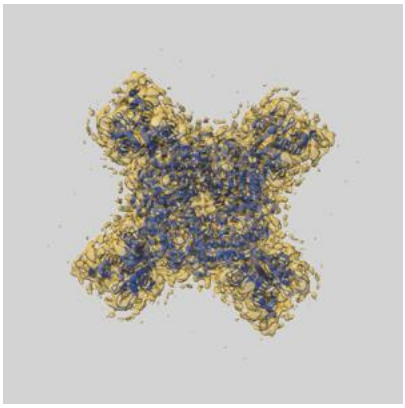
9.1 Map-model overlay



X



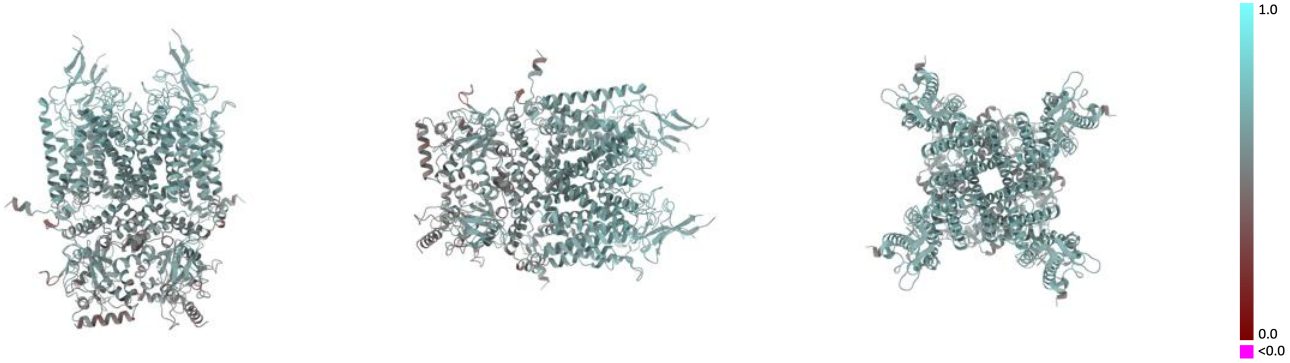
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.574 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.

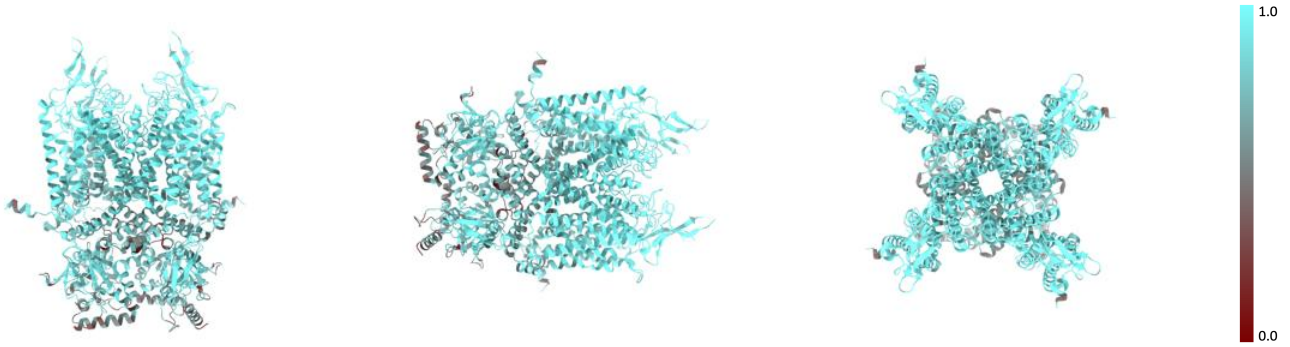
9.2 Q-score mapped to coordinate model (i)



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.

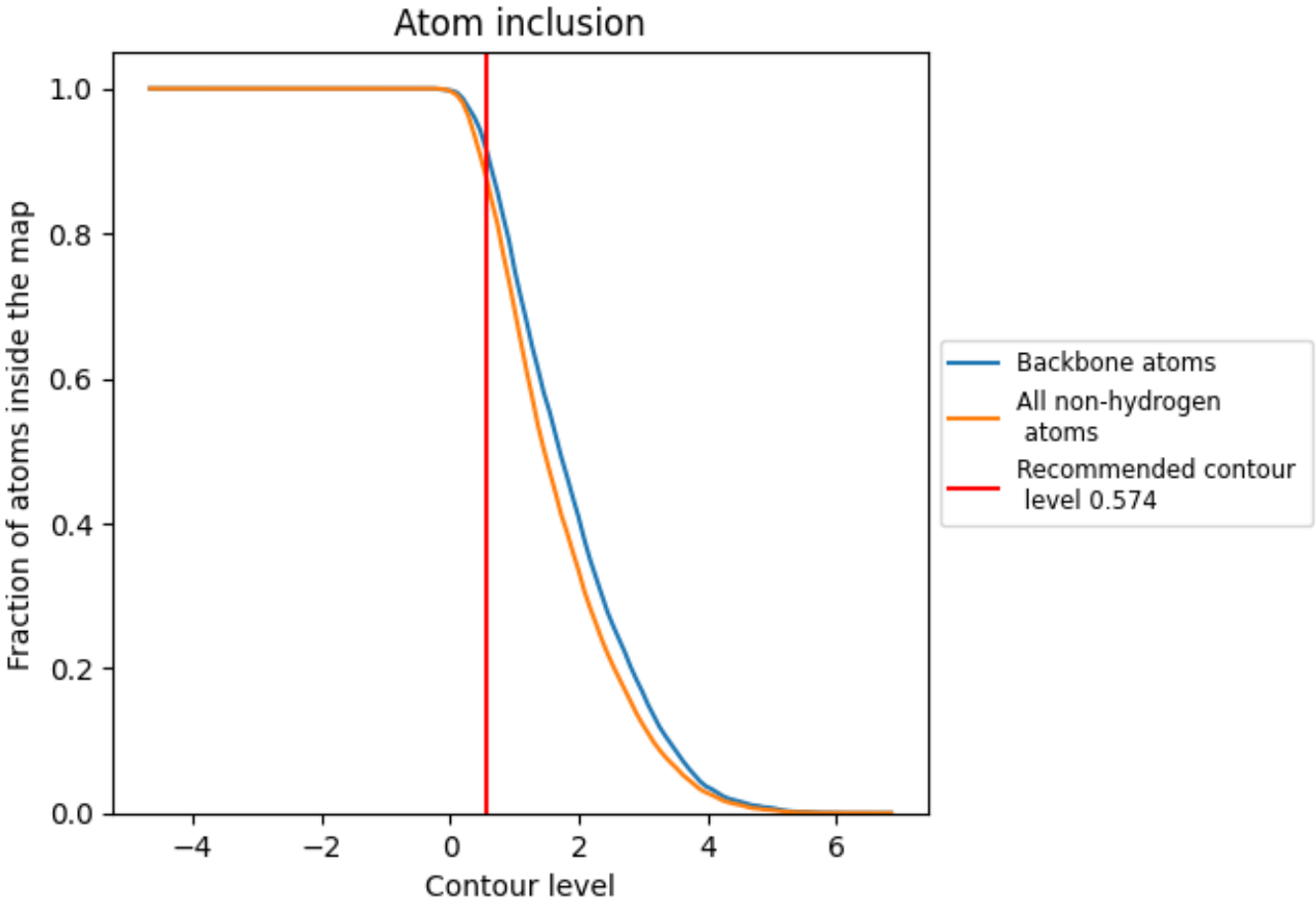
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.574).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.574) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8724	0.5820
A	0.8733	0.5830
B	0.8686	0.5810
C	0.8735	0.5830
D	0.8740	0.5820