Full wwPDB EM Validation Report ⓘ

Oct 19, 2023 – 10:58 AM EDT

PDB ID	:	8SS8
EMDB ID	:	EMD-40747
Title	:	Structure of AMPA receptor GluA2 complex with auxiliary subunit TARP gamma-5 bound to competitive antagonist ZK and antiepileptic drug perampanel (closed state)
Authors	:	Gangwar, S.P.; Yen, L.Y.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on	:	2023-05-08
Resolution	:	2.81 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 ⓘ 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:

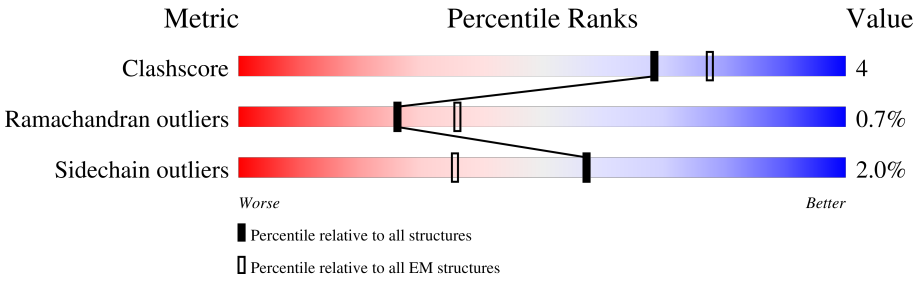
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.81 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	1026	12% 82% 12% 5%
1	B	1026	67% 8% 24%
1	C	1026	12% 83% 11% 5%
1	D	1026	68% 8% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CLR	B	1103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CLR	D	1103	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28487 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	974	Total	C	N	O	S	0	0
			7682	4963	1265	1414	40		
1	B	783	Total	C	N	O	S	0	0
			6177	3969	1022	1156	30		
1	C	974	Total	C	N	O	S	0	0
			7682	4963	1265	1414	40		
1	D	783	Total	C	N	O	S	0	0
			6177	3969	1022	1156	30		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	830	SER	-	linker	UNP P19491
A	831	ALA	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	830	SER	-	linker	UNP P19491
B	831	ALA	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	830	SER	-	linker	UNP P19491
C	831	ALA	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	830	SER	-	linker	UNP P19491

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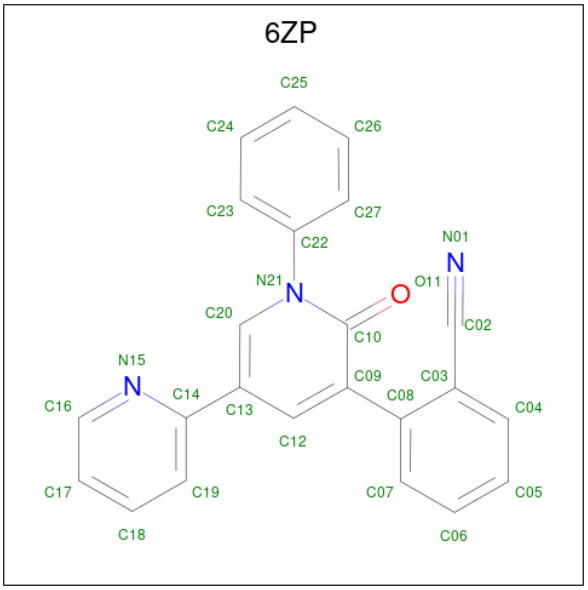
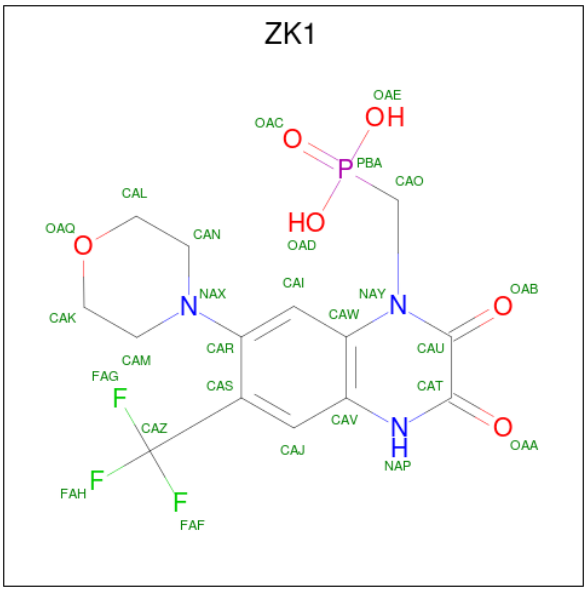
Chain	Residue	Modelled	Actual	Comment	Reference
D	831	ALA	-	linker	UNP P19491

- Molecule 2 is 2-(6'-oxo-1'-phenyl[1',6'-dihydro[2,3'-bipyridine]]-5'-yl)benzonitrile (three-letter code: 6ZP) (formula: $C_{23}H_{15}N_3O$) (labeled as "Ligand of Interest" by depositor).



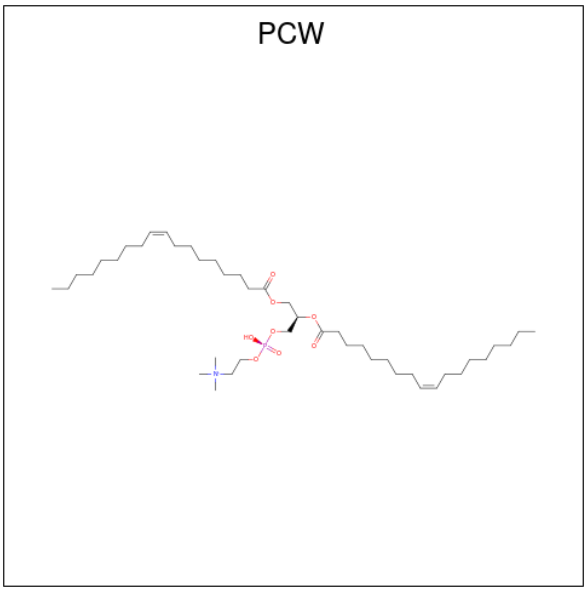
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			27	23	3	1	
2	B	1	Total	C	N	O	0
			27	23	3	1	
2	C	1	Total	C	N	O	0
			27	23	3	1	
2	D	1	Total	C	N	O	0
			27	23	3	1	

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



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

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).

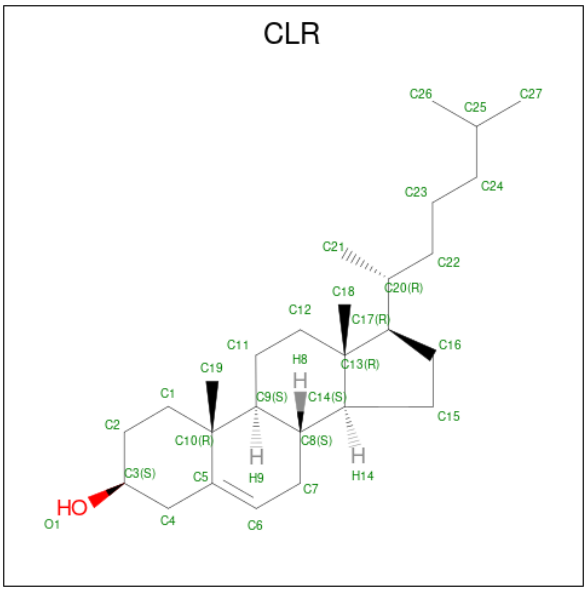


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	B	1	Total	C				0
			11	11				
4	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
4	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	D	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	D	1	Total	C				0
			11	11				

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Na	0
			2	2	

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C O 28 27 1	0
6	D	1	Total C O 28 27 1	0

- Molecule 7 is water.

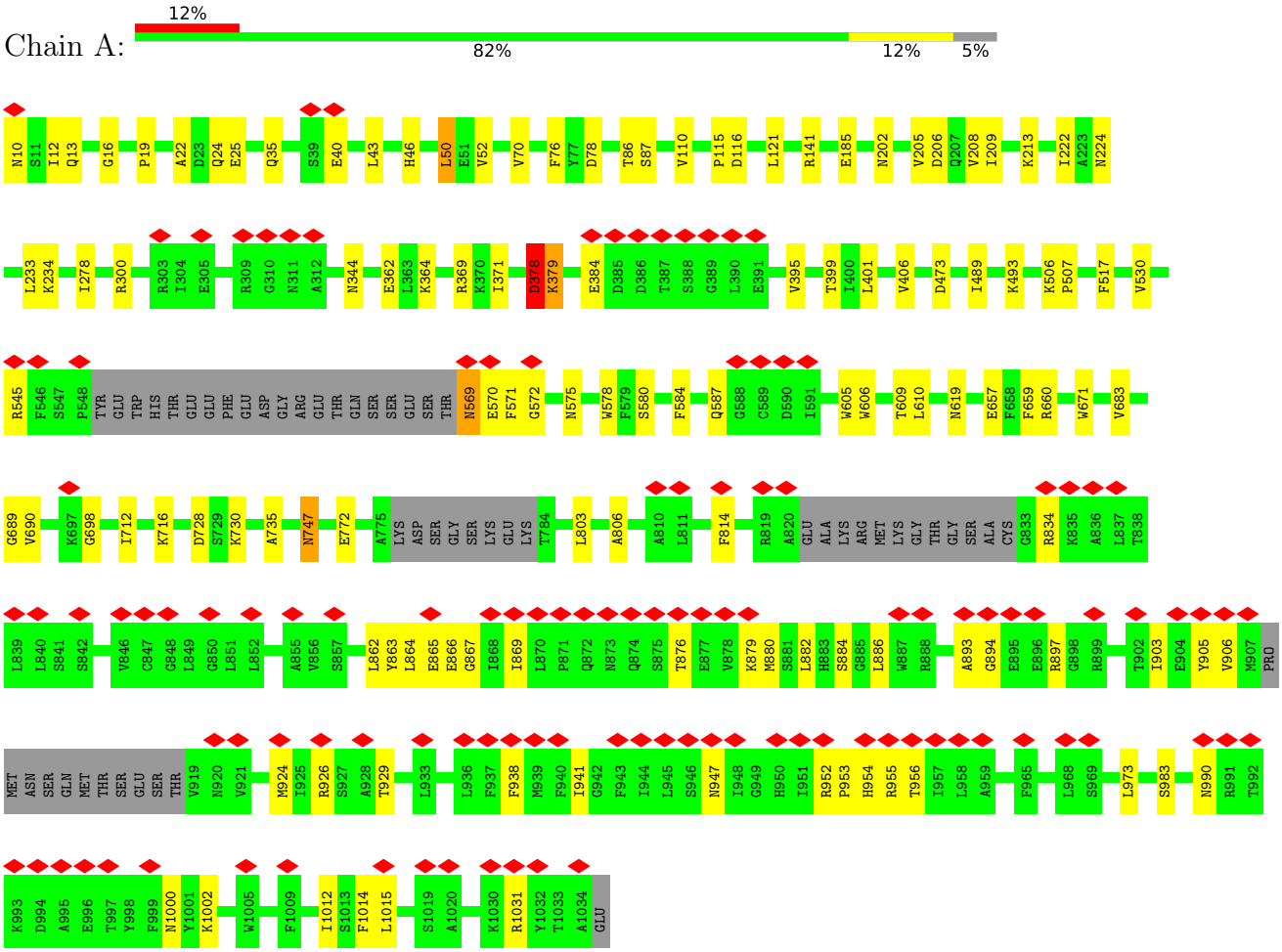
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total O 1 1	0
7	B	3	Total O 3 3	0
7	C	4	Total O 4 4	0
7	D	3	Total O 3 3	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

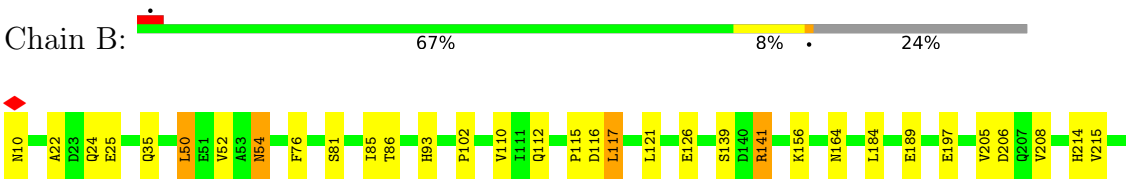
• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

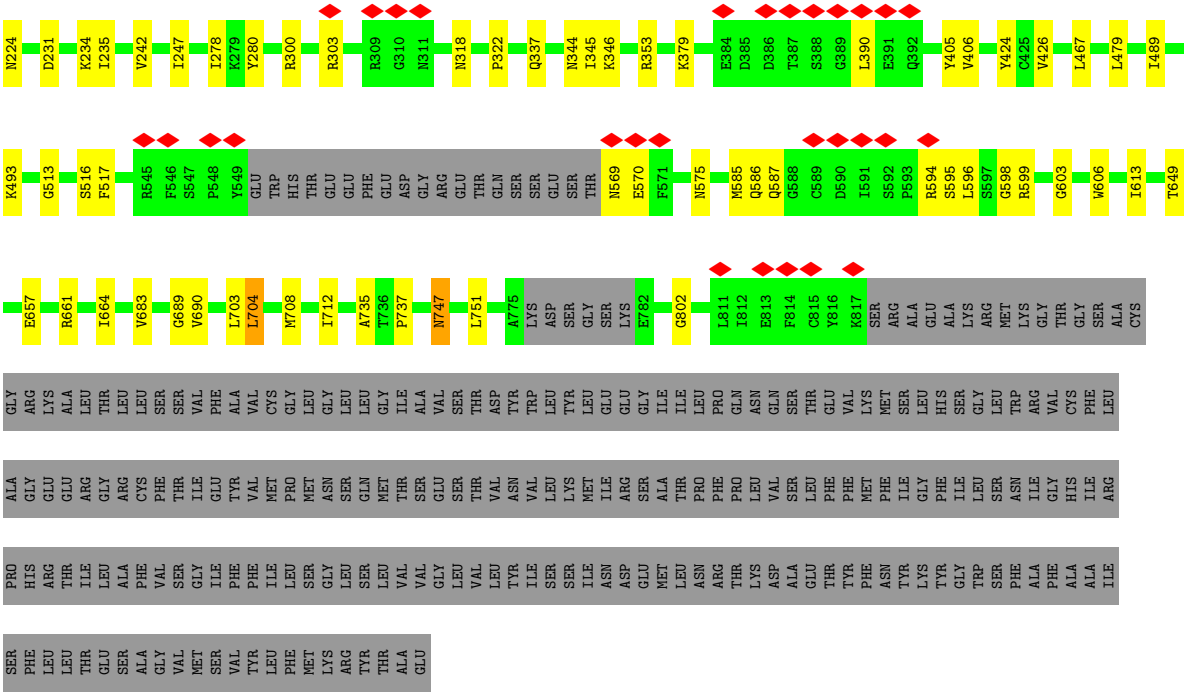
Chain A:



• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

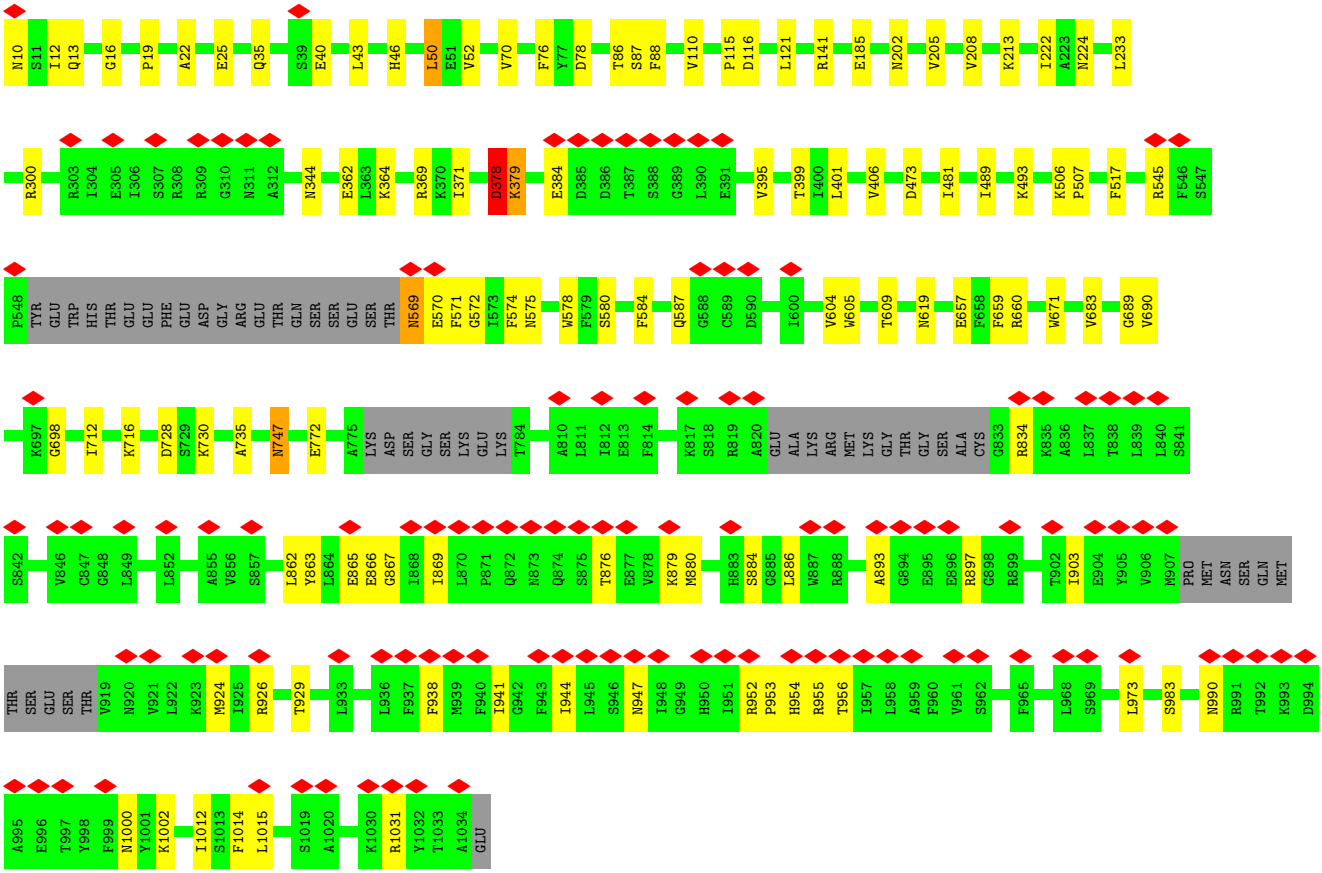
Chain B:





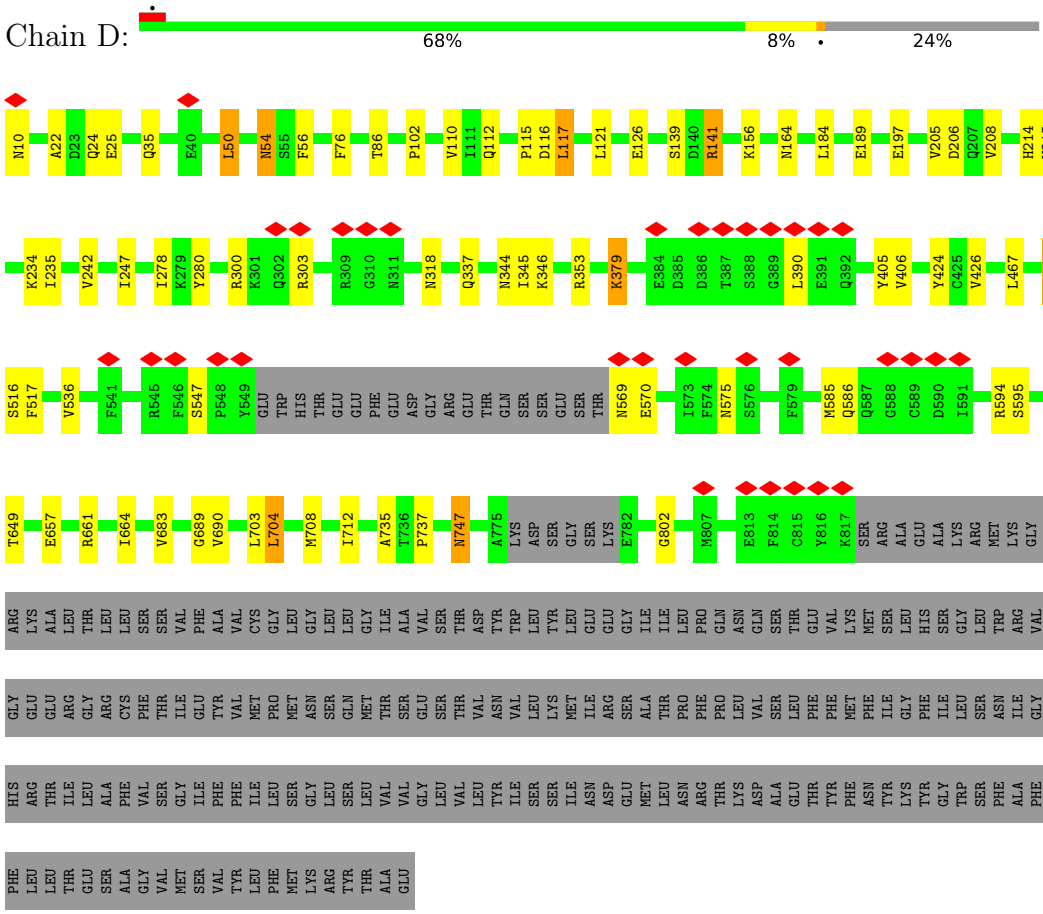
• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

Chain C:



• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	126964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	10.208	Depositor
Minimum map value	-5.570	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.188	Depositor
Recommended contour level	0.95	Depositor
Map size (Å)	384.80002, 384.80002, 384.80002	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9250001, 0.9250001, 0.9250001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZK1, 6ZP, NA, CLR, PCW

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	0.60	0/7848	0.66	5/10606 (0.0%)
1	B	0.60	1/6308 (0.0%)	0.65	7/8523 (0.1%)
1	C	0.60	0/7848	0.66	5/10606 (0.0%)
1	D	0.60	1/6308 (0.0%)	0.65	7/8523 (0.1%)
All	All	0.60	2/28312 (0.0%)	0.66	24/38258 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	C	0	4
1	D	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	ARG	CA-CB	6.40	1.68	1.53
1	D	141	ARG	CA-CB	6.40	1.68	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	117	LEU	CA-CB-CG	9.23	136.53	115.30
1	D	117	LEU	CA-CB-CG	9.22	136.52	115.30
1	B	704	LEU	CA-CB-CG	8.04	133.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	704	LEU	CA-CB-CG	8.04	133.78	115.30
1	C	121	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	121	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	233	LEU	CA-CB-CG	5.44	127.81	115.30
1	C	233	LEU	CA-CB-CG	5.43	127.80	115.30
1	D	121	LEU	CA-CB-CG	5.42	127.76	115.30
1	B	121	LEU	CA-CB-CG	5.42	127.76	115.30
1	B	50	LEU	CA-CB-CG	5.25	127.38	115.30
1	D	50	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	76	PHE	CB-CG-CD1	5.24	124.47	120.80
1	C	76	PHE	CB-CG-CD1	5.24	124.47	120.80
1	B	50	LEU	CB-CG-CD1	5.23	119.88	111.00
1	D	50	LEU	CB-CG-CD1	5.21	119.87	111.00
1	D	76	PHE	CB-CG-CD1	5.15	124.41	120.80
1	B	76	PHE	CB-CG-CD1	5.12	124.38	120.80
1	A	378	ASP	C-N-CA	5.10	134.45	121.70
1	C	378	ASP	C-N-CA	5.08	134.40	121.70
1	A	50	LEU	CB-CG-CD1	5.02	119.54	111.00
1	D	479	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	479	LEU	CA-CB-CG	5.01	126.83	115.30
1	C	50	LEU	CB-CG-CD1	5.00	119.51	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	ASP	Peptide
1	A	506	LYS	Peptide
1	A	955	ARG	Peptide
1	A	956	THR	Peptide
1	B	139	SER	Peptide
1	C	378	ASP	Peptide
1	C	506	LYS	Peptide
1	C	955	ARG	Peptide
1	C	956	THR	Peptide
1	D	139	SER	Peptide

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	7682	0	7701	64	0
1	B	6177	0	6164	47	0
1	C	7682	0	7701	57	0
1	D	6177	0	6164	44	0
2	A	27	0	0	1	0
2	B	27	0	0	1	0
2	C	27	0	0	1	0
2	D	27	0	0	1	0
3	A	27	0	13	0	0
3	B	27	0	13	1	0
3	C	27	0	13	0	0
3	D	27	0	13	1	0
4	A	147	0	207	5	0
4	B	95	0	125	4	0
4	C	147	0	207	6	0
4	D	95	0	125	5	0
5	A	2	0	0	0	0
6	B	28	0	37	3	0
6	D	28	0	37	4	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	C	4	0	0	0	0
7	D	3	0	0	0	0
All	All	28487	0	28520	214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (214) 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)
6:B:1103:CLR:C15	6:B:1103:CLR:C16	1.78	1.61
6:D:1103:CLR:C15	6:D:1103:CLR:C16	1.78	1.57
1:B:493:LYS:HG2	1:B:747:ASN:HD21	1.58	0.69
1:D:493:LYS:HG2	1:D:747:ASN:HD21	1.58	0.69
1:D:337:GLN:HE22	1:D:346:LYS:HD3	1.59	0.67
1:B:337:GLN:HE22	1:B:346:LYS:HD3	1.59	0.67
1:C:863:TYR:HB2	1:C:1002:LYS:HB3	1.79	0.64
1:A:863:TYR:HB2	1:A:1002:LYS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ILE:HD11	1:C:43:LEU:HG	1.79	0.64
1:A:12:ILE:HD11	1:A:43:LEU:HG	1.79	0.64
4:A:1104:PCW:H342	4:A:1106:PCW:H161	1.81	0.63
1:D:594:ARG:HA	1:D:599:ARG:HH21	1.64	0.63
1:A:1012:ILE:HG12	4:A:1104:PCW:H442	1.81	0.63
1:C:867:GLY:HA2	1:C:879:LYS:HG2	1.81	0.63
1:A:867:GLY:HA2	1:A:879:LYS:HG2	1.81	0.63
1:B:594:ARG:HA	1:B:599:ARG:HH21	1.64	0.62
1:A:610:LEU:HD11	1:B:613:ILE:HG12	1.81	0.62
1:C:52:VAL:HG12	1:C:78:ASP:HB2	1.83	0.61
1:C:493:LYS:HG2	1:C:747:ASN:HD21	1.66	0.60
1:A:866:GLU:HB3	1:A:880:MET:HB3	1.84	0.59
1:C:1012:ILE:HG12	4:C:1104:PCW:H442	1.84	0.59
1:C:866:GLU:HB3	1:C:880:MET:HB3	1.84	0.59
1:A:52:VAL:HG12	1:A:78:ASP:HB2	1.83	0.59
1:B:102:PRO:HA	1:B:112:GLN:HG2	1.85	0.59
1:C:862:LEU:HB3	1:C:884:SER:HB2	1.85	0.59
1:A:493:LYS:HG2	1:A:747:ASN:HD21	1.66	0.59
1:D:102:PRO:HA	1:D:112:GLN:HG2	1.85	0.59
1:A:862:LEU:HB3	1:A:884:SER:HB2	1.85	0.58
1:C:517:PHE:HA	2:C:1101:6ZP:C07	2.34	0.58
1:C:584:PHE:HA	1:C:609:THR:HG21	1.85	0.58
1:A:606:TRP:CG	1:B:587:GLN:HG3	2.39	0.58
1:A:584:PHE:HA	1:A:609:THR:HG21	1.85	0.57
1:A:952:ARG:HB2	1:A:954:HIS:HD2	1.70	0.57
1:C:952:ARG:HB2	1:C:954:HIS:HD2	1.69	0.57
1:B:606:TRP:CG	1:C:587:GLN:HG3	2.40	0.56
1:D:708:MET:HG3	3:D:1102:ZK1:HAK	1.86	0.56
1:A:869:ILE:HG22	1:A:876:THR:HG22	1.88	0.56
1:D:197:GLU:HA	1:D:224:ASN:HD21	1.71	0.55
1:A:86:THR:HG22	1:A:110:VAL:HG21	1.87	0.55
1:B:126:GLU:OE2	1:B:156:LYS:NZ	2.39	0.55
1:B:197:GLU:HA	1:B:224:ASN:HD21	1.71	0.55
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.87	0.55
1:A:545:ARG:NH1	1:A:571:PHE:O	2.40	0.55
4:C:1104:PCW:H342	4:C:1106:PCW:H161	1.88	0.55
1:C:869:ILE:HG22	1:C:876:THR:HG22	1.88	0.55
1:C:86:THR:HG22	1:C:110:VAL:HG21	1.87	0.55
1:B:708:MET:HG3	3:B:1102:ZK1:HAK	1.88	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.87	0.54
1:A:903:ILE:O	1:A:926:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:903:ILE:O	1:C:926:ARG:NH1	2.40	0.54
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.89	0.54
1:A:657:GLU:OE2	1:A:660:ARG:NH1	2.41	0.54
1:C:657:GLU:OE2	1:C:660:ARG:NH1	2.41	0.54
1:C:545:ARG:NH1	1:C:571:PHE:O	2.40	0.54
1:A:728:ASP:OD2	1:A:730:LYS:NZ	2.42	0.53
1:B:517:PHE:HA	2:B:1101:6ZP:C07	2.39	0.53
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.89	0.53
1:D:126:GLU:OE2	1:D:156:LYS:NZ	2.39	0.53
1:C:728:ASP:OD2	1:C:730:LYS:NZ	2.42	0.52
1:A:40:GLU:OE1	1:A:300:ARG:NH1	2.40	0.52
1:D:205:VAL:HA	1:D:208:VAL:HG22	1.91	0.52
1:A:13:GLN:HG3	1:A:70:VAL:HG12	1.92	0.52
1:B:205:VAL:HA	1:B:208:VAL:HG22	1.91	0.52
1:A:362:GLU:HG3	1:A:371:ILE:HG12	1.90	0.52
1:A:587:GLN:HE22	1:D:586:GLN:HG2	1.75	0.52
1:C:362:GLU:HG3	1:C:371:ILE:HG12	1.90	0.52
1:D:184:LEU:HB3	1:D:189:GLU:HB2	1.91	0.52
1:D:570:GLU:O	1:D:575:ASN:ND2	2.43	0.52
1:C:13:GLN:HG3	1:C:70:VAL:HG12	1.92	0.52
1:C:40:GLU:HB3	1:C:300:ARG:HH22	1.75	0.52
1:C:973:LEU:HD12	1:C:1014:PHE:HB2	1.92	0.52
1:C:40:GLU:OE1	1:C:300:ARG:NH1	2.40	0.51
1:B:184:LEU:HB3	1:B:189:GLU:HB2	1.91	0.51
1:B:570:GLU:O	1:B:575:ASN:ND2	2.43	0.51
1:A:973:LEU:HD12	1:A:1014:PHE:HB2	1.92	0.51
1:A:87:SER:OG	1:B:54:ASN:ND2	2.44	0.51
1:D:599:ARG:O	1:D:603:GLY:N	2.44	0.51
1:C:87:SER:OG	1:D:54:ASN:ND2	2.43	0.50
1:A:185:GLU:OE2	1:A:213:LYS:NZ	2.40	0.50
1:D:467:LEU:HD22	1:D:737:PRO:HD3	1.94	0.50
6:D:1103:CLR:H273	4:D:1106:PCW:H222	1.93	0.50
1:A:40:GLU:HB3	1:A:300:ARG:HH22	1.75	0.49
1:C:1014:PHE:HD2	1:C:1015:LEU:HD12	1.77	0.49
1:A:690:VAL:HG21	1:A:712:ILE:HD13	1.95	0.49
1:C:690:VAL:HG21	1:C:712:ILE:HD13	1.95	0.49
1:D:517:PHE:HA	2:D:1101:6ZP:C07	2.42	0.49
1:B:595:SER:HB3	1:B:598:GLY:H	1.77	0.49
1:B:599:ARG:O	1:B:603:GLY:N	2.44	0.49
1:B:467:LEU:HD22	1:B:737:PRO:HD3	1.94	0.49
1:D:595:SER:HB3	1:D:598:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ASP:OD1	1:D:234:LYS:NZ	2.35	0.48
1:A:517:PHE:HA	2:A:1101:6ZP:C07	2.43	0.48
1:B:596:LEU:HD13	1:C:574:PHE:HE1	1.78	0.48
1:B:214:HIS:HB2	1:B:235:ILE:HG13	1.96	0.48
1:A:202:ASN:HA	1:A:205:VAL:HG12	1.96	0.48
1:C:19:PRO:HG3	1:C:52:VAL:HG21	1.96	0.48
1:A:803:LEU:HD21	1:D:536:VAL:HG12	1.96	0.47
1:C:865:GLU:HB2	1:C:1000:ASN:HB2	1.95	0.47
1:A:865:GLU:HB2	1:A:1000:ASN:HB2	1.96	0.47
1:C:489:ILE:HD12	1:C:735:ALA:HB1	1.95	0.47
1:A:1014:PHE:HD2	1:A:1015:LEU:HD12	1.77	0.47
4:A:1106:PCW:H331	4:A:1106:PCW:H221	1.96	0.47
4:B:1104:PCW:H141	4:B:1104:PCW:H19	1.97	0.47
1:C:202:ASN:HA	1:C:205:VAL:HG12	1.96	0.47
1:C:924:MET:HB3	1:C:983:SER:HB3	1.96	0.47
1:D:214:HIS:HB2	1:D:235:ILE:HG13	1.96	0.47
6:D:1103:CLR:H20	6:D:1103:CLR:H182	1.68	0.47
1:A:379:LYS:HD2	1:A:379:LYS:HA	1.79	0.47
1:B:215:VAL:HG11	1:D:215:VAL:HG11	1.97	0.47
1:C:604:VAL:HG11	1:D:802:GLY:HA3	1.96	0.47
4:D:1104:PCW:H141	4:D:1104:PCW:H19	1.96	0.47
1:A:19:PRO:HG3	1:A:52:VAL:HG21	1.97	0.47
4:C:1104:PCW:H39	4:C:1104:PCW:H361	1.79	0.47
1:A:489:ILE:HD12	1:A:735:ALA:HB1	1.95	0.46
1:A:924:MET:HB3	1:A:983:SER:HB3	1.96	0.46
1:A:716:LYS:HG3	1:A:772:GLU:HB3	1.97	0.46
1:B:86:THR:HG22	1:B:110:VAL:HG21	1.97	0.46
1:D:24:GLN:HE21	1:D:278:ILE:HG13	1.81	0.46
1:C:716:LYS:HG3	1:C:772:GLU:HB3	1.97	0.46
1:B:802:GLY:HA2	4:B:1105:PCW:H19	1.98	0.46
4:C:1104:PCW:H32	4:C:1104:PCW:H121	1.77	0.46
1:B:405:TYR:HA	1:B:424:TYR:HB3	1.99	0.45
1:D:86:THR:HG22	1:D:110:VAL:HG21	1.97	0.45
1:D:683:VAL:HG11	1:D:689:GLY:HA2	1.98	0.45
1:D:405:TYR:HA	1:D:424:TYR:HB3	1.98	0.45
1:A:683:VAL:HG11	1:A:689:GLY:HA2	1.99	0.45
4:B:1105:PCW:H73	4:B:1105:PCW:H41	1.79	0.45
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.99	0.45
4:D:1105:PCW:H73	4:D:1105:PCW:H41	1.80	0.45
1:C:938:PHE:HA	1:C:941:ILE:HG22	1.99	0.45
1:C:185:GLU:OE2	1:C:213:LYS:NZ	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:VAL:HG11	1:C:689:GLY:HA2	1.99	0.45
1:A:587:GLN:NE2	1:D:586:GLN:HG2	2.31	0.45
1:A:938:PHE:HA	1:A:941:ILE:HG22	1.99	0.45
1:B:683:VAL:HG11	1:B:689:GLY:HA2	1.98	0.44
1:C:886:LEU:HD11	1:C:929:THR:HA	1.99	0.44
4:D:1105:PCW:H181	4:D:1105:PCW:H151	1.75	0.44
1:B:690:VAL:HG21	1:B:712:ILE:HD13	1.99	0.44
1:B:586:GLN:HG2	1:C:587:GLN:HE22	1.82	0.44
4:B:1104:PCW:H342	4:B:1104:PCW:H372	1.88	0.44
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.99	0.44
1:B:24:GLN:HE21	1:B:278:ILE:HG13	1.81	0.44
1:A:572:GLY:H	1:A:575:ASN:HB2	1.83	0.44
1:C:572:GLY:H	1:C:575:ASN:HB2	1.83	0.44
4:C:1103:PCW:H83	4:C:1103:PCW:H42	1.83	0.44
1:B:184:LEU:HD22	1:B:189:GLU:HG3	2.00	0.43
1:D:690:VAL:HG21	1:D:712:ILE:HD13	1.99	0.43
1:C:379:LYS:HA	1:C:379:LYS:HD2	1.79	0.43
6:B:1103:CLR:H182	6:B:1103:CLR:H20	1.69	0.43
1:D:657:GLU:O	1:D:661:ARG:HG2	2.19	0.43
1:A:401:LEU:HD23	1:A:406:VAL:HG12	2.01	0.43
1:A:806:ALA:HB2	1:D:600:ILE:HB	2.01	0.43
4:A:1104:PCW:H32	4:A:1104:PCW:H121	1.74	0.43
1:C:364:LYS:HE3	1:C:369:ARG:HH11	1.84	0.43
1:C:401:LEU:HD23	1:C:406:VAL:HG12	2.01	0.43
1:C:952:ARG:HB2	1:C:954:HIS:CD2	2.53	0.43
1:A:886:LEU:HD11	1:A:929:THR:HA	1.99	0.43
1:A:206:ASP:OD1	1:A:234:LYS:NZ	2.39	0.43
4:C:1104:PCW:H42	4:C:1104:PCW:H72	1.80	0.43
1:D:184:LEU:HD22	1:D:189:GLU:HG3	2.00	0.43
1:A:578:TRP:CD2	1:D:599:ARG:HD2	2.52	0.43
1:B:493:LYS:HD2	1:C:481:ILE:HG21	2.00	0.43
1:B:22:ALA:HB1	1:B:25:GLU:HB2	2.01	0.42
1:B:206:ASP:OD1	1:B:234:LYS:NZ	2.35	0.42
1:A:364:LYS:HE3	1:A:369:ARG:HH11	1.84	0.42
1:D:247:ILE:HD11	1:D:280:TYR:HB2	2.01	0.42
1:D:22:ALA:HB1	1:D:25:GLU:HB2	2.01	0.42
1:B:52:VAL:O	1:B:81:SER:OG	2.33	0.42
1:C:222:ILE:HG22	1:C:224:ASN:HB3	2.01	0.42
1:A:16:GLY:N	1:A:46:HIS:O	2.52	0.42
1:A:580:SER:O	1:A:605:TRP:NE1	2.51	0.42
1:C:16:GLY:N	1:C:46:HIS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:PHE:HE1	1:D:56:PHE:HA	1.85	0.42
1:B:657:GLU:O	1:B:661:ARG:HG2	2.19	0.42
1:D:231:ASP:HB2	1:D:234:LYS:HE2	2.01	0.42
1:B:513:GLY:N	1:B:516:SER:OG	2.52	0.42
1:C:580:SER:O	1:C:605:TRP:NE1	2.51	0.42
1:D:513:GLY:N	1:D:516:SER:OG	2.52	0.42
1:A:953:PRO:HB3	1:A:1031:ARG:HH21	1.85	0.41
1:B:406:VAL:HG22	1:B:426:VAL:HG23	2.02	0.41
1:C:569:ASN:HD22	1:C:570:GLU:H	1.68	0.41
1:A:395:VAL:HG13	1:A:473:ASP:HB2	2.03	0.41
1:A:569:ASN:HD22	1:A:570:GLU:H	1.68	0.41
1:A:222:ILE:HG22	1:A:224:ASN:HB3	2.01	0.41
1:A:530:VAL:HG21	4:A:1106:PCW:H242	2.02	0.41
1:B:247:ILE:HD11	1:B:280:TYR:HB2	2.01	0.41
1:B:596:LEU:HD13	1:C:574:PHE:CE1	2.54	0.41
6:B:1103:CLR:H231	6:B:1103:CLR:H272	1.77	0.41
1:D:300:ARG:O	1:D:303:ARG:NH2	2.54	0.41
1:A:814:PHE:CG	1:D:547:SER:HB3	2.55	0.41
1:B:85:ILE:HD13	1:B:85:ILE:HA	1.93	0.41
1:B:300:ARG:O	1:B:303:ARG:NH2	2.54	0.41
1:C:395:VAL:HG13	1:C:473:ASP:HB2	2.03	0.41
1:D:379:LYS:HD3	1:D:379:LYS:HA	1.90	0.41
1:A:880:MET:HA	1:A:894:GLY:HA3	2.02	0.41
1:A:905:TYR:HD2	1:A:906:VAL:HG12	1.86	0.41
1:C:953:PRO:HB3	1:C:1031:ARG:HH21	1.86	0.41
6:D:1103:CLR:H231	6:D:1103:CLR:H272	1.76	0.41
1:A:209:ILE:HD12	1:A:234:LYS:HE2	2.03	0.41
1:A:587:GLN:HG3	1:D:606:TRP:CG	2.56	0.41
1:D:345:ILE:HG12	1:D:353:ARG:HH12	1.85	0.41
1:A:22:ALA:HB1	1:A:25:GLU:HB2	2.03	0.40
1:A:864:LEU:HB3	1:A:882:LEU:HB3	2.03	0.40
1:A:952:ARG:HB2	1:A:954:HIS:CD2	2.53	0.40
1:B:345:ILE:HG12	1:B:353:ARG:HH12	1.85	0.40
1:B:493:LYS:HG3	1:B:751:LEU:HD21	2.03	0.40
1:D:406:VAL:HG22	1:D:426:VAL:HG23	2.02	0.40
4:D:1104:PCW:H372	4:D:1104:PCW:H342	1.87	0.40
1:B:231:ASP:HB2	1:B:234:LYS:HE2	2.02	0.40
1:C:22:ALA:HB1	1:C:25:GLU:HB2	2.03	0.40
1:A:24:GLN:HE21	1:A:278:ILE:HD12	1.86	0.40
1:C:941:ILE:HA	1:C:944:ILE:HG12	2.03	0.40
1:B:93:HIS:CD2	1:B:322:PRO:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ARG:HD2	1:C:578:TRP:CD2	2.56	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	964/1026 (94%)	889 (92%)	67 (7%)	8 (1%)	19	47
1	B	777/1026 (76%)	716 (92%)	57 (7%)	4 (0%)	29	59
1	C	964/1026 (94%)	889 (92%)	67 (7%)	8 (1%)	19	47
1	D	777/1026 (76%)	716 (92%)	57 (7%)	4 (0%)	29	59
All	All	3482/4104 (85%)	3210 (92%)	248 (7%)	24 (1%)	26	51

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	LYS
1	C	379	LYS
1	A	115	PRO
1	B	115	PRO
1	B	379	LYS
1	C	115	PRO
1	D	115	PRO
1	D	379	LYS
1	A	378	ASP
1	A	893	ALA
1	C	378	ASP
1	C	893	ALA
1	B	116	ASP
1	D	116	ASP

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Mol	Chain	Res	Type
1	A	384	GLU
1	A	507	PRO
1	B	664	ILE
1	C	384	GLU
1	C	507	PRO
1	D	664	ILE
1	A	116	ASP
1	C	116	ASP
1	A	698	GLY
1	C	698	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	831/877 (95%)	817 (98%)	14 (2%)	60	86
1	B	668/877 (76%)	653 (98%)	15 (2%)	52	81
1	C	831/877 (95%)	817 (98%)	14 (2%)	60	86
1	D	668/877 (76%)	652 (98%)	16 (2%)	49	80
All	All	2998/3508 (86%)	2939 (98%)	59 (2%)	57	83

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	35	GLN
1	A	50	LEU
1	A	141	ARG
1	A	208	VAL
1	A	344	ASN
1	A	399	THR
1	A	569	ASN
1	A	619	ASN
1	A	747	ASN
1	A	834	ARG

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Mol	Chain	Res	Type
1	A	897	ARG
1	A	947	ASN
1	A	990	ASN
1	B	10	ASN
1	B	35	GLN
1	B	50	LEU
1	B	54	ASN
1	B	117	LEU
1	B	141	ARG
1	B	164	ASN
1	B	242	VAL
1	B	318	ASN
1	B	344	ASN
1	B	390	LEU
1	B	569	ASN
1	B	585	MET
1	B	704	LEU
1	B	747	ASN
1	C	10	ASN
1	C	35	GLN
1	C	50	LEU
1	C	141	ARG
1	C	208	VAL
1	C	344	ASN
1	C	399	THR
1	C	569	ASN
1	C	619	ASN
1	C	747	ASN
1	C	834	ARG
1	C	897	ARG
1	C	947	ASN
1	C	990	ASN
1	D	10	ASN
1	D	35	GLN
1	D	50	LEU
1	D	54	ASN
1	D	117	LEU
1	D	141	ARG
1	D	164	ASN
1	D	242	VAL
1	D	318	ASN
1	D	344	ASN

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Mol	Chain	Res	Type
1	D	390	LEU
1	D	479	LEU
1	D	569	ASN
1	D	585	MET
1	D	704	LEU
1	D	747	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	214	HIS
1	A	344	ASN
1	A	569	ASN
1	A	619	ASN
1	A	726	ASN
1	A	747	ASN
1	A	883	HIS
1	A	947	ASN
1	A	954	HIS
1	A	990	ASN
1	B	10	ASN
1	B	54	ASN
1	B	164	ASN
1	B	167	ASN
1	B	214	HIS
1	B	224	ASN
1	B	318	ASN
1	B	337	GLN
1	B	344	ASN
1	B	435	HIS
1	B	747	ASN
1	C	10	ASN
1	C	214	HIS
1	C	344	ASN
1	C	569	ASN
1	C	619	ASN
1	C	726	ASN
1	C	747	ASN
1	C	883	HIS
1	C	947	ASN
1	C	954	HIS

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Mol	Chain	Res	Type
1	C	990	ASN
1	D	10	ASN
1	D	54	ASN
1	D	164	ASN
1	D	167	ASN
1	D	214	HIS
1	D	224	ASN
1	D	318	ASN
1	D	337	GLN
1	D	344	ASN
1	D	435	HIS
1	D	747	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 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
4	PCW	D	1104	-	42,42,53	1.21	3 (7%)	48,50,61	1.18	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CLR	D	1103	-	31,31,31	9.07	22 (70%)	48,48,48	5.07	19 (39%)
4	PCW	A	1104	-	42,42,53	1.23	4 (9%)	48,50,61	1.13	3 (6%)
2	6ZP	A	1101	-	30,30,30	1.03	1 (3%)	35,41,41	0.93	1 (2%)
4	PCW	D	1106	-	10,10,53	0.77	0	9,9,61	0.35	0
3	ZK1	A	1102	-	28,29,29	2.83	9 (32%)	42,45,45	1.99	11 (26%)
4	PCW	B	1105	-	40,40,53	1.25	4 (10%)	45,48,61	1.03	3 (6%)
3	ZK1	D	1102	-	28,29,29	2.76	7 (25%)	42,45,45	1.75	9 (21%)
2	6ZP	C	1101	-	30,30,30	1.03	1 (3%)	35,41,41	0.93	1 (2%)
3	ZK1	B	1102	-	28,29,29	2.77	7 (25%)	42,45,45	1.72	9 (21%)
4	PCW	B	1104	-	42,42,53	1.21	3 (7%)	48,50,61	1.15	4 (8%)
2	6ZP	B	1101	-	30,30,30	1.02	1 (3%)	35,41,41	0.89	1 (2%)
4	PCW	A	1106	-	50,50,53	1.14	3 (6%)	56,58,61	1.00	3 (5%)
4	PCW	C	1104	-	42,42,53	1.23	4 (9%)	48,50,61	1.13	4 (8%)
4	PCW	A	1103	-	41,41,53	1.23	4 (9%)	47,49,61	1.05	3 (6%)
4	PCW	A	1105	-	10,10,53	0.78	0	9,9,61	0.31	0
4	PCW	B	1106	-	10,10,53	0.77	0	9,9,61	0.35	0
4	PCW	C	1106	-	50,50,53	1.14	3 (6%)	56,58,61	1.00	3 (5%)
2	6ZP	D	1101	-	30,30,30	1.02	1 (3%)	35,41,41	0.90	1 (2%)
4	PCW	C	1105	-	10,10,53	0.79	0	9,9,61	0.29	0
4	PCW	C	1103	-	41,41,53	1.24	4 (9%)	47,49,61	1.05	3 (6%)
6	CLR	B	1103	-	31,31,31	9.07	23 (74%)	48,48,48	5.05	20 (41%)
4	PCW	D	1105	-	40,40,53	1.25	4 (10%)	45,48,61	1.05	3 (6%)
3	ZK1	C	1102	-	28,29,29	2.88	9 (32%)	42,45,45	1.93	13 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	D	1104	-	-	26/46/46/57	-
6	CLR	D	1103	-	3/3/10/11	7/10/68/68	0/4/4/4
4	PCW	A	1104	-	-	25/46/46/57	-
2	6ZP	A	1101	-	-	0/13/14/14	0/4/4/4
4	PCW	D	1106	-	-	4/8/8/57	-
3	ZK1	A	1102	-	-	5/13/23/23	0/3/3/3
4	PCW	B	1105	-	-	22/44/44/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZK1	D	1102	-	-	5/13/23/23	0/3/3/3
2	6ZP	C	1101	-	-	0/13/14/14	0/4/4/4
3	ZK1	B	1102	-	-	5/13/23/23	0/3/3/3
4	PCW	B	1104	-	-	26/46/46/57	-
2	6ZP	B	1101	-	-	0/13/14/14	0/4/4/4
4	PCW	A	1106	-	-	27/54/54/57	-
4	PCW	C	1104	-	-	30/46/46/57	-
4	PCW	A	1103	-	-	24/45/45/57	-
4	PCW	A	1105	-	-	3/8/8/57	-
4	PCW	B	1106	-	-	4/8/8/57	-
4	PCW	C	1106	-	-	28/54/54/57	-
2	6ZP	D	1101	-	-	0/13/14/14	0/4/4/4
4	PCW	C	1103	-	-	24/45/45/57	-
6	CLR	B	1103	-	3/3/10/11	7/10/68/68	0/4/4/4
4	PCW	C	1105	-	-	5/8/8/57	-
4	PCW	D	1105	-	-	21/44/44/57	-
3	ZK1	C	1102	-	-	5/13/23/23	0/3/3/3

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1103	CLR	C8-C14	-28.66	0.98	1.53
6	B	1103	CLR	C8-C14	-28.60	0.99	1.53
6	D	1103	CLR	C12-C11	-20.25	1.10	1.53
6	B	1103	CLR	C12-C11	-20.20	1.10	1.53
6	B	1103	CLR	C7-C8	-18.77	1.21	1.53
6	D	1103	CLR	C7-C8	-18.75	1.21	1.53
6	B	1103	CLR	C12-C13	-13.06	1.30	1.54
6	D	1103	CLR	C12-C13	-13.04	1.30	1.54
6	B	1103	CLR	C13-C17	10.10	1.74	1.55
6	D	1103	CLR	C13-C17	9.97	1.74	1.55
6	B	1103	CLR	C15-C14	9.21	1.73	1.54
6	D	1103	CLR	C15-C14	9.17	1.73	1.54
6	B	1103	CLR	C7-C6	8.94	1.69	1.50
6	D	1103	CLR	C7-C6	8.92	1.69	1.50
6	B	1103	CLR	C16-C15	8.85	1.78	1.54
6	D	1103	CLR	C16-C15	8.81	1.78	1.54
6	D	1103	CLR	C10-C5	-8.71	1.35	1.52
6	B	1103	CLR	C10-C5	-8.60	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1103	CLR	C20-C17	-8.40	1.39	1.54
6	B	1103	CLR	C20-C17	-8.34	1.39	1.54
3	B	1102	ZK1	OAA-CAT	8.25	1.39	1.23
3	D	1102	ZK1	OAA-CAT	8.21	1.39	1.23
6	B	1103	CLR	C4-C5	8.15	1.69	1.51
6	D	1103	CLR	C4-C5	8.15	1.69	1.51
3	C	1102	ZK1	OAA-CAT	7.89	1.38	1.23
3	A	1102	ZK1	OAA-CAT	7.80	1.38	1.23
3	D	1102	ZK1	OAB-CAU	7.80	1.39	1.23
6	D	1103	CLR	C13-C14	7.80	1.69	1.55
3	B	1102	ZK1	OAB-CAU	7.78	1.39	1.23
6	B	1103	CLR	C13-C14	7.75	1.69	1.55
3	C	1102	ZK1	OAB-CAU	7.54	1.39	1.23
3	A	1102	ZK1	OAB-CAU	7.50	1.38	1.23
6	D	1103	CLR	C16-C17	6.56	1.68	1.54
6	B	1103	CLR	C16-C17	6.52	1.67	1.54
6	B	1103	CLR	C1-C10	5.66	1.65	1.54
6	D	1103	CLR	C1-C10	5.59	1.64	1.54
2	D	1101	6ZP	C09-C10	-4.85	1.38	1.46
2	B	1101	6ZP	C09-C10	-4.85	1.38	1.46
2	C	1101	6ZP	C09-C10	-4.73	1.38	1.46
2	A	1101	6ZP	C09-C10	-4.72	1.38	1.46
6	D	1103	CLR	C11-C9	4.66	1.61	1.53
6	B	1103	CLR	C11-C9	4.60	1.61	1.53
3	C	1102	ZK1	CAV-CAW	-4.54	1.35	1.40
3	A	1102	ZK1	CAV-CAW	-4.28	1.35	1.40
3	C	1102	ZK1	CAV-NAP	-4.25	1.32	1.39
6	B	1103	CLR	C22-C20	4.10	1.64	1.54
3	C	1102	ZK1	CAW-NAY	-4.10	1.33	1.41
6	D	1103	CLR	C22-C20	4.10	1.64	1.54
3	A	1102	ZK1	CAW-NAY	-4.08	1.34	1.41
3	A	1102	ZK1	CAV-NAP	-4.08	1.32	1.39
6	D	1103	CLR	C1-C2	4.05	1.62	1.53
6	B	1103	CLR	C1-C2	4.04	1.62	1.53
3	C	1102	ZK1	CAT-NAP	-4.00	1.30	1.35
3	A	1102	ZK1	CAU-NAY	-3.91	1.30	1.38
3	C	1102	ZK1	CAU-NAY	-3.83	1.31	1.38
3	D	1102	ZK1	CAW-NAY	-3.82	1.34	1.41
3	B	1102	ZK1	CAV-NAP	-3.81	1.33	1.39
3	B	1102	ZK1	CAW-NAY	-3.79	1.34	1.41
3	D	1102	ZK1	CAV-NAP	-3.72	1.33	1.39
3	A	1102	ZK1	CAT-NAP	-3.71	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1103	CLR	C2-C3	-3.62	1.43	1.51
3	B	1102	ZK1	CAT-NAP	-3.58	1.30	1.35
6	D	1103	CLR	C2-C3	-3.54	1.43	1.51
3	D	1102	ZK1	CAT-NAP	-3.54	1.31	1.35
3	D	1102	ZK1	CAU-NAY	-3.45	1.31	1.38
3	B	1102	ZK1	CAV-CAW	-3.43	1.36	1.40
3	B	1102	ZK1	CAU-NAY	-3.38	1.31	1.38
3	D	1102	ZK1	CAV-CAW	-3.30	1.36	1.40
4	A	1104	PCW	O3-C11	3.29	1.43	1.33
4	A	1106	PCW	O3-C11	3.27	1.42	1.33
4	C	1104	PCW	O3-C11	3.26	1.42	1.33
4	C	1106	PCW	O3-C11	3.25	1.42	1.33
4	D	1104	PCW	O2-C31	3.17	1.43	1.34
4	B	1104	PCW	O2-C31	3.14	1.43	1.34
4	C	1103	PCW	O3-C11	3.13	1.42	1.33
4	A	1103	PCW	O3-C11	3.10	1.42	1.33
4	D	1105	PCW	O3-C11	3.08	1.42	1.33
6	B	1103	CLR	C10-C9	3.08	1.61	1.56
6	D	1103	CLR	C6-C5	3.06	1.39	1.33
4	B	1105	PCW	O3-C11	3.06	1.42	1.33
6	B	1103	CLR	C6-C5	3.01	1.39	1.33
4	D	1105	PCW	O2-C31	2.95	1.42	1.34
6	D	1103	CLR	C10-C9	2.93	1.60	1.56
4	B	1105	PCW	O2-C31	2.92	1.42	1.34
4	A	1104	PCW	O2-C31	2.91	1.42	1.34
4	C	1103	PCW	O2-C31	2.89	1.42	1.34
4	A	1103	PCW	O2-C31	2.89	1.42	1.34
6	B	1103	CLR	C18-C13	2.88	1.59	1.54
4	C	1104	PCW	O2-C31	2.83	1.42	1.34
4	C	1106	PCW	O2-C31	2.73	1.42	1.34
4	B	1104	PCW	O3-C11	2.71	1.41	1.33
6	D	1103	CLR	C18-C13	2.67	1.59	1.54
4	A	1106	PCW	O2-C2	-2.66	1.39	1.46
4	A	1106	PCW	O2-C31	2.66	1.41	1.34
4	D	1104	PCW	O3-C11	2.63	1.41	1.33
4	B	1105	PCW	O2-C2	-2.62	1.40	1.46
4	D	1105	PCW	O2-C2	-2.61	1.40	1.46
4	C	1106	PCW	O2-C2	-2.60	1.40	1.46
4	A	1103	PCW	O2-C2	-2.57	1.40	1.46
4	C	1103	PCW	O2-C2	-2.55	1.40	1.46
4	A	1104	PCW	O2-C2	-2.41	1.40	1.46
4	C	1104	PCW	O2-C2	-2.36	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1104	PCW	O2-C2	-2.35	1.40	1.46
4	B	1104	PCW	O2-C2	-2.34	1.40	1.46
6	B	1103	CLR	C4-C3	2.23	1.56	1.52
6	D	1103	CLR	C4-C3	2.22	1.56	1.52
3	A	1102	ZK1	PBA-OAD	-2.19	1.49	1.54
3	C	1102	ZK1	PBA-OAD	-2.16	1.50	1.54
4	C	1103	PCW	P-O4P	2.12	1.67	1.59
4	A	1103	PCW	P-O4P	2.12	1.67	1.59
3	C	1102	ZK1	PBA-OAE	-2.12	1.50	1.54
3	A	1102	ZK1	PBA-OAE	-2.12	1.50	1.54
6	B	1103	CLR	C21-C20	2.09	1.58	1.53
4	D	1105	PCW	P-O4P	2.04	1.67	1.59
4	B	1105	PCW	P-O4P	2.02	1.67	1.59
4	C	1104	PCW	P-O4P	2.01	1.67	1.59
4	A	1104	PCW	P-O4P	2.00	1.67	1.59

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1103	CLR	C18-C13-C12	-15.12	86.71	110.59
6	D	1103	CLR	C18-C13-C12	-14.63	87.49	110.59
6	D	1103	CLR	C18-C13-C14	-12.87	87.70	111.71
6	B	1103	CLR	C18-C13-C14	-12.31	88.76	111.71
6	D	1103	CLR	C17-C13-C14	11.73	113.97	100.07
6	B	1103	CLR	C17-C13-C14	11.39	113.56	100.07
6	D	1103	CLR	C18-C13-C17	-11.03	91.14	111.71
6	B	1103	CLR	C12-C13-C17	10.95	132.95	116.57
6	D	1103	CLR	C12-C13-C17	10.84	132.79	116.57
6	B	1103	CLR	C18-C13-C17	-10.61	91.92	111.71
6	B	1103	CLR	C7-C6-C5	-9.10	108.27	125.06
6	D	1103	CLR	C4-C5-C6	-8.68	108.10	120.61
6	D	1103	CLR	C7-C6-C5	-8.57	109.25	125.06
6	B	1103	CLR	C4-C5-C6	-8.52	108.32	120.61
6	B	1103	CLR	C14-C8-C9	7.58	119.23	109.09
6	D	1103	CLR	C14-C8-C9	7.52	119.16	109.09
6	D	1103	CLR	C10-C5-C6	-7.42	111.55	122.90
6	B	1103	CLR	C10-C5-C6	-7.39	111.60	122.90
6	D	1103	CLR	C7-C8-C9	7.30	118.56	109.71
6	B	1103	CLR	C7-C8-C9	7.28	118.53	109.71
6	D	1103	CLR	C19-C10-C9	-5.42	105.22	111.68
6	B	1103	CLR	C19-C10-C9	-5.37	105.28	111.68
3	A	1102	ZK1	CAI-CAR-NAX	-5.24	114.77	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1102	ZK1	CAI-CAR-NAX	-5.12	114.94	122.52
3	A	1102	ZK1	CAN-NAX-CAM	5.08	122.73	111.52
6	D	1103	CLR	C8-C7-C6	5.02	119.94	112.73
3	D	1102	ZK1	CAN-NAX-CAM	4.96	122.46	111.52
6	B	1103	CLR	C8-C7-C6	4.82	119.65	112.73
3	B	1102	ZK1	CAN-NAX-CAM	4.77	122.04	111.52
3	C	1102	ZK1	CAN-NAX-CAM	4.67	121.83	111.52
3	A	1102	ZK1	CAS-CAR-NAX	4.56	125.15	119.92
6	B	1103	CLR	C12-C11-C9	4.49	120.89	113.11
3	C	1102	ZK1	CAS-CAR-NAX	4.47	125.04	119.92
6	D	1103	CLR	C12-C11-C9	4.46	120.85	113.11
6	B	1103	CLR	C13-C14-C8	4.32	120.78	114.38
4	D	1104	PCW	O2-C31-C32	4.24	120.64	111.50
6	D	1103	CLR	C13-C14-C8	4.24	120.66	114.38
4	B	1104	PCW	O2-C31-C32	4.23	120.62	111.50
4	A	1104	PCW	O2-C31-C32	4.11	120.35	111.50
4	C	1104	PCW	O2-C31-C32	4.06	120.26	111.50
3	A	1102	ZK1	CAV-NAP-CAT	-4.05	119.65	124.80
3	D	1102	ZK1	CAV-NAP-CAT	-3.97	119.75	124.80
6	B	1103	CLR	C12-C13-C14	3.96	113.42	107.27
4	D	1104	PCW	C8-N-C6	3.90	119.01	108.97
4	A	1106	PCW	C8-N-C6	3.88	118.96	108.97
4	C	1106	PCW	C8-N-C6	3.87	118.93	108.97
4	A	1106	PCW	O2-C31-C32	3.85	119.80	111.50
4	C	1106	PCW	O2-C31-C32	3.85	119.79	111.50
4	A	1103	PCW	O2-C31-C32	3.84	119.78	111.50
4	C	1103	PCW	O2-C31-C32	3.83	119.76	111.50
3	B	1102	ZK1	CAV-NAP-CAT	-3.82	119.94	124.80
3	D	1102	ZK1	CAI-CAR-NAX	-3.81	116.89	122.52
3	B	1102	ZK1	CAI-CAR-NAX	-3.78	116.93	122.52
6	D	1103	CLR	C12-C13-C14	3.76	113.11	107.27
4	A	1104	PCW	C8-N-C6	3.76	118.64	108.97
4	C	1104	PCW	C8-N-C6	3.74	118.60	108.97
4	A	1103	PCW	C8-N-C6	3.57	118.15	108.97
4	C	1103	PCW	C8-N-C6	3.57	118.15	108.97
4	B	1105	PCW	O2-C31-C32	3.45	118.94	111.50
4	D	1105	PCW	O2-C31-C32	3.45	118.94	111.50
3	C	1102	ZK1	CAV-NAP-CAT	-3.45	120.42	124.80
4	B	1104	PCW	C8-N-C6	3.41	117.73	108.97
4	D	1105	PCW	C8-N-C6	3.27	117.38	108.97
4	B	1105	PCW	C8-N-C6	3.26	117.34	108.97
6	D	1103	CLR	C11-C12-C13	3.08	118.07	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1103	CLR	C11-C12-C13	3.06	118.03	112.78
3	D	1102	ZK1	CAS-CAR-NAX	2.95	123.30	119.92
2	A	1101	6ZP	C20-C13-C12	2.92	120.00	117.38
2	D	1101	6ZP	C20-C13-C12	2.92	119.99	117.38
2	C	1101	6ZP	C20-C13-C12	2.90	119.98	117.38
6	B	1103	CLR	C9-C10-C5	2.90	114.20	109.65
3	B	1102	ZK1	CAS-CAR-NAX	2.89	123.23	119.92
4	C	1104	PCW	O3-C11-C12	2.86	120.88	111.91
2	B	1101	6ZP	C20-C13-C12	2.86	119.94	117.38
3	C	1102	ZK1	CAL-OAQ-CAK	2.82	119.31	109.89
4	D	1105	PCW	O3-C11-C12	2.82	120.76	111.91
4	A	1104	PCW	O3-C11-C12	2.82	120.75	111.91
3	B	1102	ZK1	CAT-CAU-NAY	2.80	120.53	117.32
3	D	1102	ZK1	CAT-CAU-NAY	2.79	120.52	117.32
6	D	1103	CLR	C9-C10-C5	2.79	114.02	109.65
3	A	1102	ZK1	CAU-CAT-NAP	2.78	120.35	117.49
3	D	1102	ZK1	CAW-NAY-CAU	-2.68	119.48	122.79
4	B	1105	PCW	O3-C11-C12	2.67	120.30	111.91
3	B	1102	ZK1	CAW-NAY-CAU	-2.65	119.51	122.79
3	D	1102	ZK1	CAU-CAT-NAP	2.64	120.21	117.49
3	A	1102	ZK1	CAT-CAU-NAY	2.64	120.34	117.32
3	D	1102	ZK1	FAG-CAZ-CAS	-2.63	108.12	112.70
3	A	1102	ZK1	CAO-NAY-CAU	2.62	119.06	116.51
3	A	1102	ZK1	FAG-CAZ-CAS	-2.62	108.14	112.70
3	A	1102	ZK1	CAW-NAY-CAU	-2.61	119.56	122.79
3	C	1102	ZK1	CAO-NAY-CAU	2.60	119.05	116.51
6	B	1103	CLR	C21-C20-C17	2.56	116.84	112.92
3	B	1102	ZK1	FAG-CAZ-CAS	-2.53	108.30	112.70
6	D	1103	CLR	C10-C9-C8	2.52	116.51	112.73
3	C	1102	ZK1	CAT-CAU-NAY	2.50	120.19	117.32
4	D	1104	PCW	C3-C2-C1	-2.48	105.92	111.79
3	B	1102	ZK1	CAU-CAT-NAP	2.43	119.99	117.49
3	A	1102	ZK1	CAL-CAN-NAX	2.42	114.48	110.02
3	C	1102	ZK1	OAQ-CAL-CAN	2.41	117.11	111.80
4	B	1104	PCW	C3-C2-C1	-2.41	106.09	111.79
6	B	1103	CLR	C10-C9-C8	2.40	116.33	112.73
3	C	1102	ZK1	CAW-NAY-CAU	-2.39	119.83	122.79
3	C	1102	ZK1	FAG-CAZ-CAS	-2.38	108.56	112.70
3	C	1102	ZK1	CAU-CAT-NAP	2.36	119.92	117.49
4	C	1103	PCW	O3-C11-C12	2.36	119.31	111.91
4	C	1106	PCW	O3-C11-C12	2.33	119.23	111.91
4	A	1103	PCW	O3-C11-C12	2.32	119.19	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1102	ZK1	CAK-CAM-NAX	2.32	114.30	110.02
4	A	1106	PCW	O3-C11-C12	2.32	119.18	111.91
4	D	1104	PCW	O3-C11-C12	2.21	118.86	111.91
4	B	1104	PCW	O3-C11-C12	2.21	118.85	111.91
6	D	1103	CLR	C21-C20-C17	2.21	116.30	112.92
3	C	1102	ZK1	OAD-PBA-CAO	2.20	111.37	106.66
3	B	1102	ZK1	CAK-CAM-NAX	2.13	113.96	110.02
3	A	1102	ZK1	CAK-CAM-NAX	2.10	113.89	110.02
4	C	1104	PCW	C2-O2-C31	-2.03	112.80	117.79
3	C	1102	ZK1	CAK-CAM-NAX	2.02	113.75	110.02
6	B	1103	CLR	C1-C10-C9	2.01	111.54	108.73

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1103	CLR	C17
6	B	1103	CLR	C9
6	B	1103	CLR	C13
6	D	1103	CLR	C17
6	D	1103	CLR	C9
6	D	1103	CLR	C13

All (303) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1103	PCW	O4P-C4-C5-N
4	A	1103	PCW	O31-C31-O2-C2
4	A	1103	PCW	C1-O3P-P-O4P
4	A	1104	PCW	C12-C11-O3-C3
4	A	1104	PCW	O11-C11-O3-C3
4	A	1104	PCW	C1-O3P-P-O1P
4	A	1106	PCW	O4P-C4-C5-N
4	A	1106	PCW	O31-C31-O2-C2
4	A	1106	PCW	C1-O3P-P-O2P
4	A	1106	PCW	C4-O4P-P-O1P
4	A	1106	PCW	C4-O4P-P-O3P
4	B	1104	PCW	C32-C31-O2-C2
4	B	1104	PCW	C1-O3P-P-O2P
4	B	1105	PCW	C19-C20-C21-C22
4	C	1103	PCW	O4P-C4-C5-N
4	C	1103	PCW	O31-C31-O2-C2
4	C	1103	PCW	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
4	C	1104	PCW	C12-C11-O3-C3
4	C	1104	PCW	O11-C11-O3-C3
4	C	1104	PCW	C4-O4P-P-O2P
4	C	1106	PCW	O4P-C4-C5-N
4	C	1106	PCW	O31-C31-O2-C2
4	C	1106	PCW	C1-O3P-P-O2P
4	C	1106	PCW	C4-O4P-P-O1P
4	D	1104	PCW	C32-C31-O2-C2
4	D	1104	PCW	C1-O3P-P-O2P
4	D	1105	PCW	C19-C20-C21-C22
6	B	1103	CLR	C16-C17-C20-C21
6	B	1103	CLR	C16-C17-C20-C22
6	D	1103	CLR	C16-C17-C20-C21
6	D	1103	CLR	C16-C17-C20-C22
4	B	1104	PCW	O11-C11-O3-C3
4	D	1104	PCW	O11-C11-O3-C3
4	B	1104	PCW	O31-C31-O2-C2
4	D	1104	PCW	O31-C31-O2-C2
4	B	1104	PCW	C12-C11-O3-C3
4	D	1104	PCW	C12-C11-O3-C3
4	A	1103	PCW	C32-C31-O2-C2
4	A	1106	PCW	C32-C31-O2-C2
4	C	1103	PCW	C32-C31-O2-C2
4	C	1106	PCW	C32-C31-O2-C2
6	B	1103	CLR	C13-C17-C20-C21
6	D	1103	CLR	C13-C17-C20-C21
6	B	1103	CLR	C13-C17-C20-C22
6	D	1103	CLR	C13-C17-C20-C22
4	B	1105	PCW	C15-C16-C17-C18
4	A	1104	PCW	C2-C1-O3P-P
4	C	1104	PCW	C2-C1-O3P-P
4	C	1104	PCW	C32-C31-O2-C2
4	A	1104	PCW	C11-C12-C13-C14
6	B	1103	CLR	C20-C22-C23-C24
6	D	1103	CLR	C20-C22-C23-C24
6	D	1103	CLR	C22-C23-C24-C25
4	D	1104	PCW	C4-C5-N-C6
4	B	1104	PCW	C11-C12-C13-C14
4	C	1104	PCW	C11-C12-C13-C14
4	D	1104	PCW	C11-C12-C13-C14
4	A	1104	PCW	C17-C18-C19-C20
4	C	1104	PCW	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
6	B	1103	CLR	C22-C23-C24-C25
4	A	1106	PCW	C31-C32-C33-C34
4	A	1103	PCW	C4-O4P-P-O3P
4	B	1105	PCW	C4-O4P-P-O3P
4	C	1103	PCW	C4-O4P-P-O3P
4	C	1106	PCW	C4-O4P-P-O3P
4	D	1104	PCW	C1-O3P-P-O4P
4	D	1105	PCW	C4-O4P-P-O3P
4	C	1103	PCW	C31-C32-C33-C34
4	A	1103	PCW	C31-C32-C33-C34
4	C	1104	PCW	O31-C31-O2-C2
4	A	1104	PCW	C32-C31-O2-C2
4	D	1105	PCW	C14-C15-C16-C17
4	A	1106	PCW	C14-C15-C16-C17
4	D	1104	PCW	C13-C14-C15-C16
4	A	1104	PCW	O31-C31-O2-C2
4	A	1106	PCW	C35-C36-C37-C38
4	C	1106	PCW	C35-C36-C37-C38
4	B	1104	PCW	C13-C14-C15-C16
4	C	1104	PCW	C17-C18-C19-C20
4	C	1103	PCW	C21-C22-C23-C24
4	B	1105	PCW	C14-C15-C16-C17
4	C	1106	PCW	C14-C15-C16-C17
4	A	1104	PCW	C31-C32-C33-C34
4	A	1103	PCW	C13-C14-C15-C16
4	C	1103	PCW	C24-C25-C26-C27
4	A	1103	PCW	C22-C23-C24-C25
4	B	1104	PCW	C15-C16-C17-C18
4	C	1103	PCW	C13-C14-C15-C16
4	B	1104	PCW	C40-C41-C42-C43
4	C	1104	PCW	C36-C37-C38-C39
4	C	1106	PCW	C20-C21-C22-C23
4	A	1106	PCW	C12-C13-C14-C15
4	C	1104	PCW	C14-C15-C16-C17
4	D	1104	PCW	C15-C16-C17-C18
4	D	1106	PCW	C14-C15-C16-C17
4	D	1104	PCW	C4-C5-N-C8
4	B	1105	PCW	C34-C35-C36-C37
4	B	1106	PCW	C14-C15-C16-C17
4	C	1106	PCW	C15-C16-C17-C18
4	B	1106	PCW	C15-C16-C17-C18
4	C	1105	PCW	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
4	D	1106	PCW	C15-C16-C17-C18
4	A	1106	PCW	C12-C11-O3-C3
4	A	1103	PCW	C12-C13-C14-C15
4	A	1104	PCW	C14-C15-C16-C17
4	D	1104	PCW	C32-C33-C34-C35
4	C	1104	PCW	C34-C35-C36-C37
4	A	1104	PCW	C12-C13-C14-C15
4	A	1106	PCW	C16-C17-C18-C19
4	C	1106	PCW	C40-C41-C42-C43
4	D	1104	PCW	C35-C36-C37-C38
4	D	1105	PCW	C34-C35-C36-C37
4	A	1104	PCW	C34-C35-C36-C37
4	D	1104	PCW	C4-C5-N-C7
4	B	1104	PCW	C32-C33-C34-C35
4	C	1104	PCW	C13-C14-C15-C16
4	A	1106	PCW	O11-C11-O3-C3
4	C	1103	PCW	C22-C23-C24-C25
4	A	1106	PCW	C40-C41-C42-C43
4	C	1106	PCW	C16-C17-C18-C19
4	D	1104	PCW	C36-C37-C38-C39
4	B	1105	PCW	O31-C31-O2-C2
4	D	1105	PCW	O31-C31-O2-C2
4	C	1106	PCW	C12-C11-O3-C3
4	A	1106	PCW	C42-C43-C44-C45
4	C	1106	PCW	C12-C13-C14-C15
4	C	1106	PCW	C21-C22-C23-C24
4	C	1104	PCW	C35-C36-C37-C38
4	B	1105	PCW	C31-C32-C33-C34
4	B	1105	PCW	C32-C31-O2-C2
4	D	1105	PCW	C32-C31-O2-C2
4	D	1105	PCW	C15-C16-C17-C18
4	B	1105	PCW	C35-C36-C37-C38
4	B	1105	PCW	C12-C13-C14-C15
4	B	1104	PCW	C36-C37-C38-C39
4	B	1105	PCW	C36-C37-C38-C39
4	A	1103	PCW	C21-C22-C23-C24
4	C	1103	PCW	C11-C12-C13-C14
4	A	1104	PCW	C1-O3P-P-O4P
4	B	1104	PCW	C1-O3P-P-O4P
4	C	1104	PCW	C4-O4P-P-O3P
4	C	1106	PCW	C22-C23-C24-C25
4	C	1106	PCW	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
4	C	1106	PCW	C42-C43-C44-C45
4	D	1105	PCW	C35-C36-C37-C38
4	A	1104	PCW	O3P-C1-C2-C3
4	C	1104	PCW	O3P-C1-C2-C3
4	A	1104	PCW	C16-C17-C18-C19
4	A	1104	PCW	C36-C37-C38-C39
4	B	1104	PCW	C16-C17-C18-C19
4	D	1104	PCW	C40-C41-C42-C43
4	D	1105	PCW	C36-C37-C38-C39
4	D	1105	PCW	C31-C32-C33-C34
4	A	1103	PCW	C14-C15-C16-C17
4	C	1103	PCW	C32-C33-C34-C35
4	C	1106	PCW	O11-C11-O3-C3
4	C	1104	PCW	C12-C13-C14-C15
4	C	1103	PCW	C12-C11-O3-C3
4	A	1106	PCW	C21-C22-C23-C24
4	A	1103	PCW	C32-C33-C34-C35
4	A	1104	PCW	C13-C14-C15-C16
4	B	1104	PCW	C35-C36-C37-C38
4	A	1106	PCW	C20-C21-C22-C23
4	C	1104	PCW	C16-C17-C18-C19
4	C	1103	PCW	C12-C13-C14-C15
4	D	1104	PCW	C42-C43-C44-C45
4	A	1106	PCW	C15-C16-C17-C18
4	C	1106	PCW	C33-C34-C35-C36
4	C	1103	PCW	C14-C15-C16-C17
4	C	1104	PCW	C42-C43-C44-C45
4	A	1105	PCW	C13-C14-C15-C16
4	D	1105	PCW	O3P-C1-C2-C3
4	A	1106	PCW	C22-C23-C24-C25
4	C	1103	PCW	O11-C11-O3-C3
4	A	1104	PCW	C42-C43-C44-C45
4	D	1104	PCW	C16-C17-C18-C19
4	C	1104	PCW	C33-C34-C35-C36
4	A	1103	PCW	C12-C11-O3-C3
4	C	1106	PCW	C13-C14-C15-C16
4	A	1103	PCW	C1-C2-C3-O3
4	B	1104	PCW	C1-C2-C3-O3
4	C	1103	PCW	C1-C2-C3-O3
4	D	1104	PCW	C1-C2-C3-O3
4	B	1105	PCW	C11-C12-C13-C14
4	A	1104	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	1105	PCW	O3P-C1-C2-O2
4	D	1105	PCW	O3P-C1-C2-O2
4	B	1106	PCW	C16-C17-C18-C19
4	D	1106	PCW	C16-C17-C18-C19
4	C	1105	PCW	C13-C14-C15-C16
4	C	1105	PCW	C15-C16-C17-C18
4	A	1103	PCW	O2-C2-C3-O3
4	B	1104	PCW	O2-C2-C3-O3
4	C	1103	PCW	O2-C2-C3-O3
4	A	1103	PCW	C20-C21-C22-C23
4	B	1105	PCW	O3P-C1-C2-C3
4	A	1106	PCW	C36-C37-C38-C39
4	D	1105	PCW	C32-C33-C34-C35
4	D	1105	PCW	C12-C13-C14-C15
4	B	1105	PCW	C1-C2-C3-O3
4	D	1105	PCW	C1-C2-C3-O3
4	C	1104	PCW	O3P-C1-C2-O2
4	A	1103	PCW	C33-C34-C35-C36
4	B	1105	PCW	O2-C2-C3-O3
4	D	1104	PCW	O2-C2-C3-O3
4	D	1105	PCW	O2-C2-C3-O3
4	A	1104	PCW	C35-C36-C37-C38
4	C	1103	PCW	C33-C34-C35-C36
3	A	1102	ZK1	NAY-CAO-PBA-OAD
3	A	1102	ZK1	NAY-CAO-PBA-OAE
3	B	1102	ZK1	NAY-CAO-PBA-OAD
3	B	1102	ZK1	NAY-CAO-PBA-OAE
3	C	1102	ZK1	NAY-CAO-PBA-OAD
3	C	1102	ZK1	NAY-CAO-PBA-OAE
3	D	1102	ZK1	NAY-CAO-PBA-OAD
3	D	1102	ZK1	NAY-CAO-PBA-OAE
4	A	1103	PCW	O11-C11-O3-C3
3	A	1102	ZK1	NAY-CAO-PBA-OAC
3	B	1102	ZK1	NAY-CAO-PBA-OAC
3	C	1102	ZK1	NAY-CAO-PBA-OAC
3	D	1102	ZK1	NAY-CAO-PBA-OAC
4	C	1104	PCW	C1-O3P-P-O4P
4	B	1105	PCW	C32-C33-C34-C35
4	A	1103	PCW	C4-O4P-P-O1P
4	A	1104	PCW	C1-O3P-P-O2P
4	A	1104	PCW	C4-O4P-P-O1P
4	A	1106	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
4	B	1105	PCW	C4-O4P-P-O2P
4	C	1103	PCW	C4-O4P-P-O1P
4	C	1104	PCW	C1-O3P-P-O2P
4	C	1104	PCW	C4-O4P-P-O1P
4	C	1106	PCW	C4-O4P-P-O2P
4	D	1105	PCW	C4-O4P-P-O2P
4	A	1103	PCW	C5-C4-O4P-P
4	C	1103	PCW	C5-C4-O4P-P
4	C	1106	PCW	C41-C42-C43-C44
4	A	1106	PCW	C41-C42-C43-C44
4	B	1104	PCW	C4-C5-N-C6
6	D	1103	CLR	C23-C24-C25-C27
4	B	1104	PCW	O4P-C4-C5-N
4	C	1106	PCW	C1-C2-C3-O3
4	D	1104	PCW	O4P-C4-C5-N
4	A	1106	PCW	O2-C2-C3-O3
4	C	1106	PCW	O2-C2-C3-O3
3	C	1102	ZK1	CAI-CAR-NAX-CAN
4	D	1105	PCW	C33-C34-C35-C36
4	A	1103	PCW	C24-C25-C26-C27
3	B	1102	ZK1	CAI-CAR-NAX-CAN
4	D	1104	PCW	C2-C1-O3P-P
4	D	1105	PCW	C4-C5-N-C6
6	B	1103	CLR	C23-C24-C25-C27
3	D	1102	ZK1	CAI-CAR-NAX-CAN
4	A	1105	PCW	C16-C17-C18-C19
4	C	1106	PCW	C1-O3P-P-O4P
4	A	1106	PCW	C1-C2-C3-O3
4	B	1106	PCW	C13-C14-C15-C16
4	A	1106	PCW	C32-C33-C34-C35
4	D	1104	PCW	C34-C35-C36-C37
4	D	1106	PCW	C13-C14-C15-C16
3	A	1102	ZK1	CAI-CAR-NAX-CAM
3	A	1102	ZK1	CAI-CAR-NAX-CAN
4	C	1103	PCW	C17-C18-C19-C20
4	A	1106	PCW	C33-C34-C35-C36
4	A	1105	PCW	C19-C20-C21-C22
4	B	1104	PCW	C2-C1-O3P-P
4	A	1103	PCW	C25-C26-C27-C28
4	C	1103	PCW	C20-C21-C22-C23
4	C	1104	PCW	C41-C42-C43-C44
4	D	1105	PCW	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
4	A	1106	PCW	C37-C38-C39-C40
4	D	1105	PCW	C4-C5-N-C7
4	A	1103	PCW	C15-C16-C17-C18
3	D	1102	ZK1	CAI-CAR-NAX-CAM
4	B	1104	PCW	C39-C40-C41-C42
4	D	1104	PCW	C39-C40-C41-C42
3	B	1102	ZK1	CAI-CAR-NAX-CAM
4	C	1103	PCW	C25-C26-C27-C28
4	C	1104	PCW	O3-C11-C12-C13
4	C	1104	PCW	C37-C38-C39-C40
4	C	1105	PCW	C19-C20-C21-C22
4	A	1104	PCW	C37-C38-C39-C40
4	C	1106	PCW	C37-C38-C39-C40
4	B	1104	PCW	C4-C5-N-C7
4	B	1105	PCW	C33-C34-C35-C36
3	C	1102	ZK1	CAI-CAR-NAX-CAM
4	D	1104	PCW	O2-C31-C32-C33
4	B	1104	PCW	C34-C35-C36-C37
4	B	1105	PCW	C4-C5-N-C6
4	B	1105	PCW	C4-C5-N-C7
4	A	1103	PCW	C11-C12-C13-C14
4	B	1104	PCW	O2-C31-C32-C33
4	A	1104	PCW	O3-C11-C12-C13
4	C	1106	PCW	C17-C18-C19-C20
4	C	1105	PCW	C16-C17-C18-C19
4	B	1104	PCW	O31-C31-C32-C33
4	C	1104	PCW	O11-C11-C12-C13
4	B	1104	PCW	C4-O4P-P-O2P
4	C	1104	PCW	C1-O3P-P-O1P
4	B	1104	PCW	C42-C43-C44-C45
4	A	1104	PCW	O11-C11-C12-C13
4	D	1104	PCW	O31-C31-C32-C33
4	C	1104	PCW	C4-C5-N-C6
4	B	1105	PCW	C13-C14-C15-C16

There are no ring outliers.

18 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1104	PCW	2	0
6	D	1103	CLR	4	0
4	A	1104	PCW	3	0

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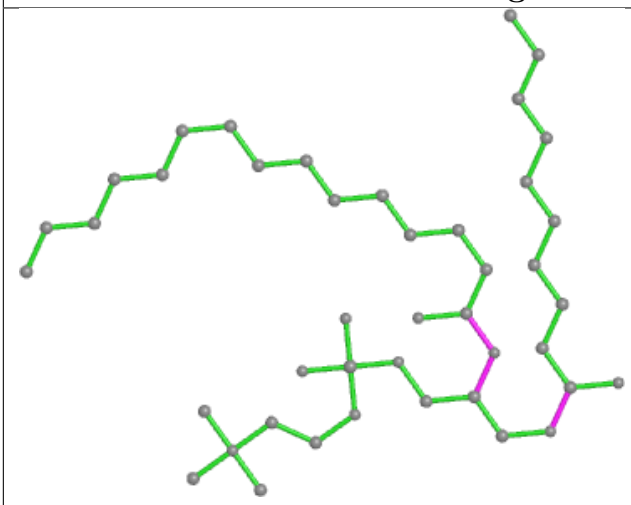
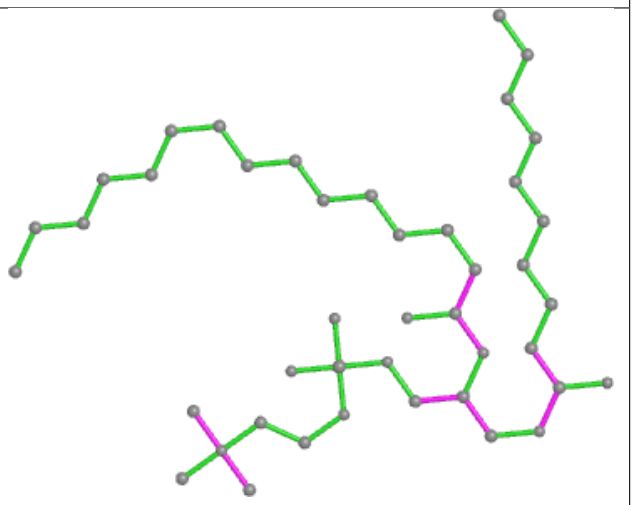
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	6ZP	1	0
4	D	1106	PCW	1	0
4	B	1105	PCW	2	0
3	D	1102	ZK1	1	0
2	C	1101	6ZP	1	0
3	B	1102	ZK1	1	0
4	B	1104	PCW	2	0
2	B	1101	6ZP	1	0
4	A	1106	PCW	3	0
4	C	1104	PCW	5	0
4	C	1106	PCW	1	0
2	D	1101	6ZP	1	0
4	C	1103	PCW	1	0
6	B	1103	CLR	3	0
4	D	1105	PCW	2	0

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.

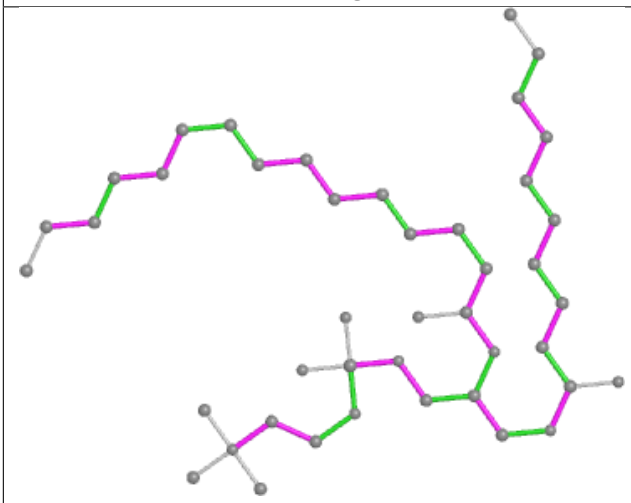
Ligand PCW D 1104



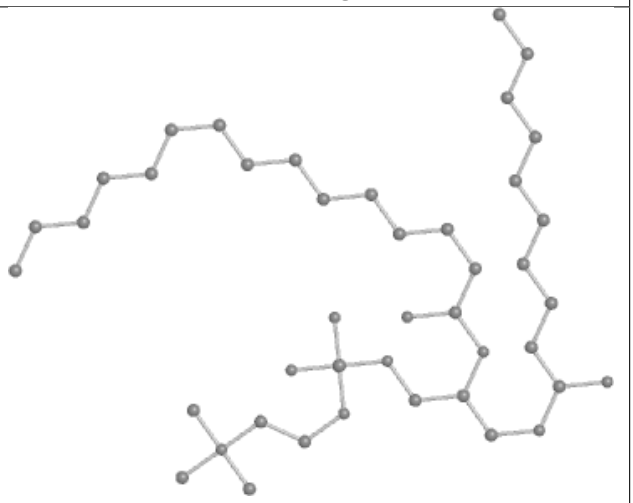
Bond lengths



Bond angles

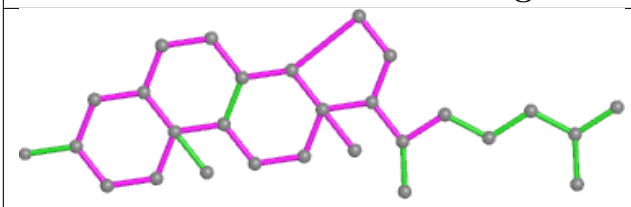


Torsions

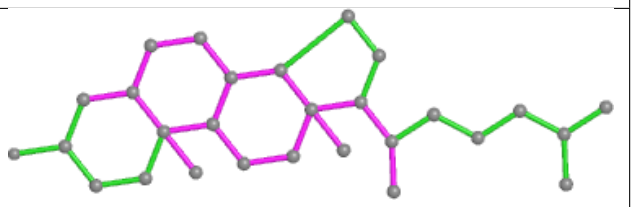


Rings

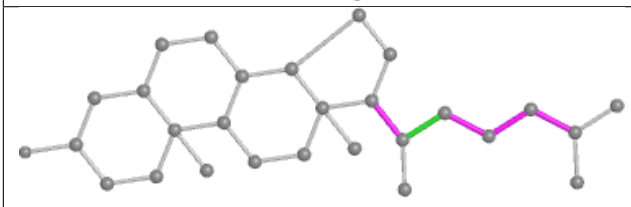
Ligand CLR D 1103



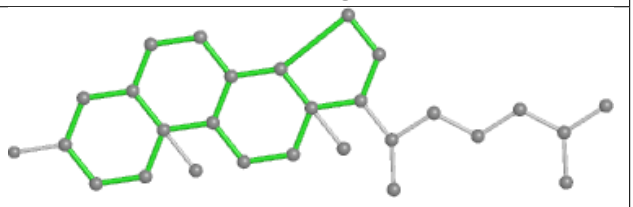
Bond lengths



Bond angles

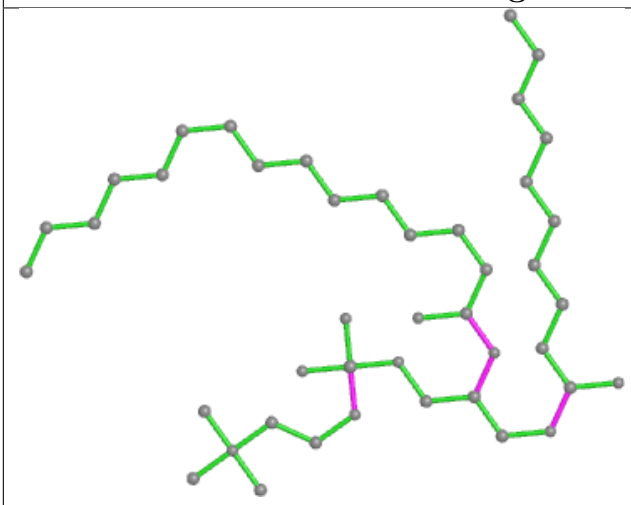


Torsions

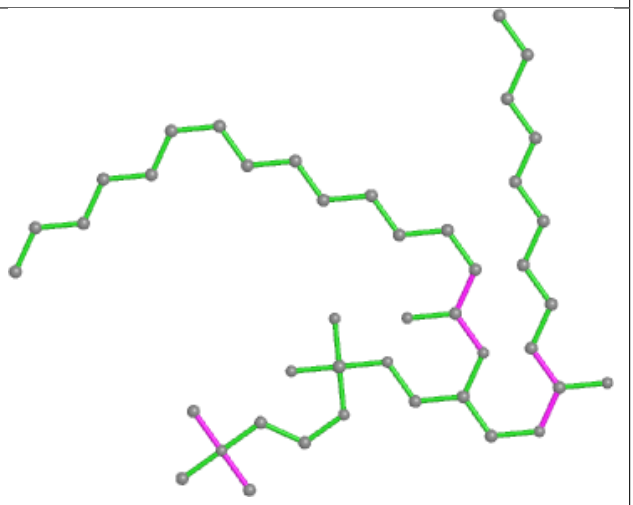


Rings

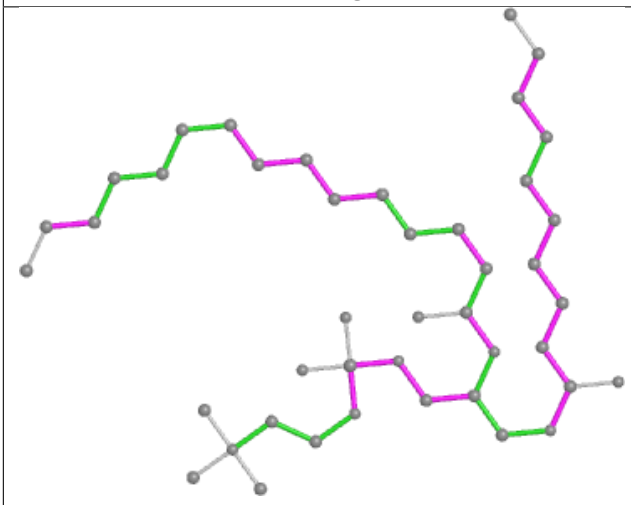
Ligand PCW A 1104



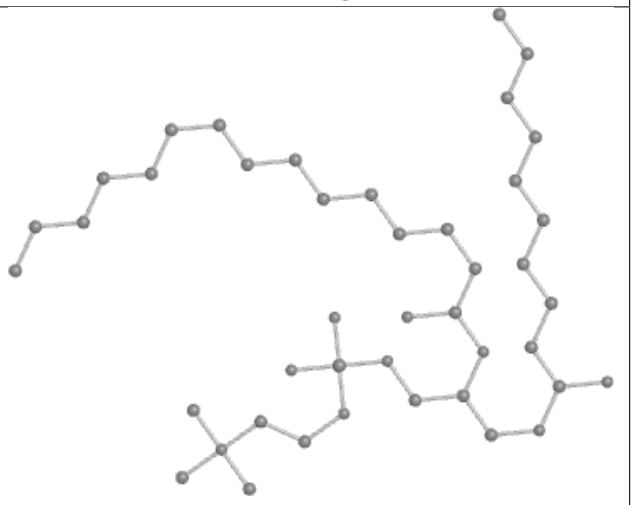
Bond lengths



Bond angles

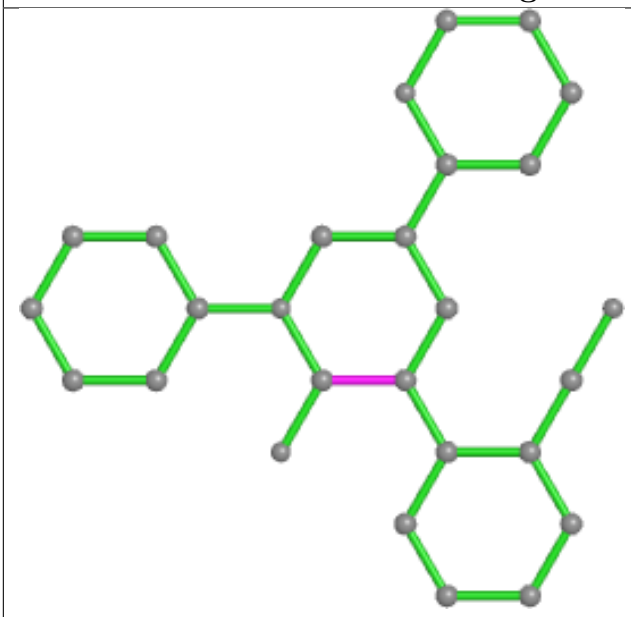


Torsions

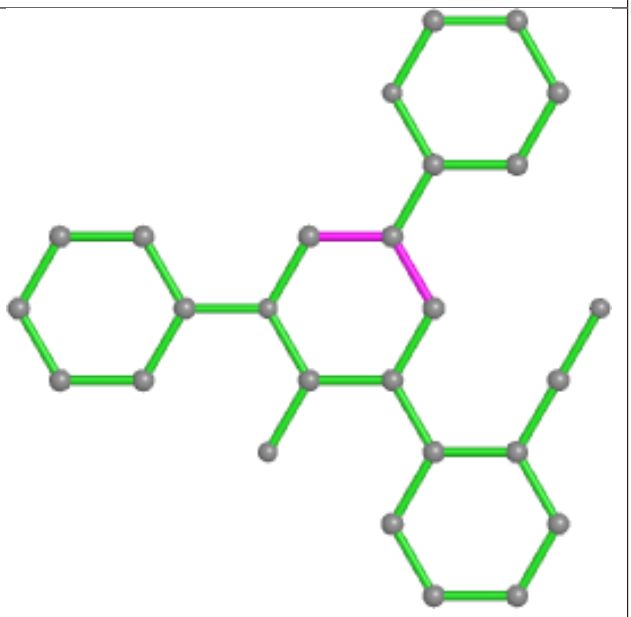


Rings

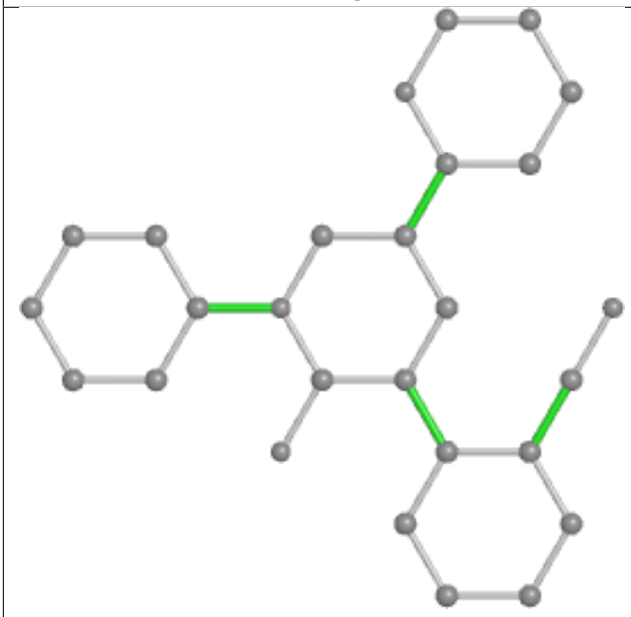
Ligand 6ZP A 1101



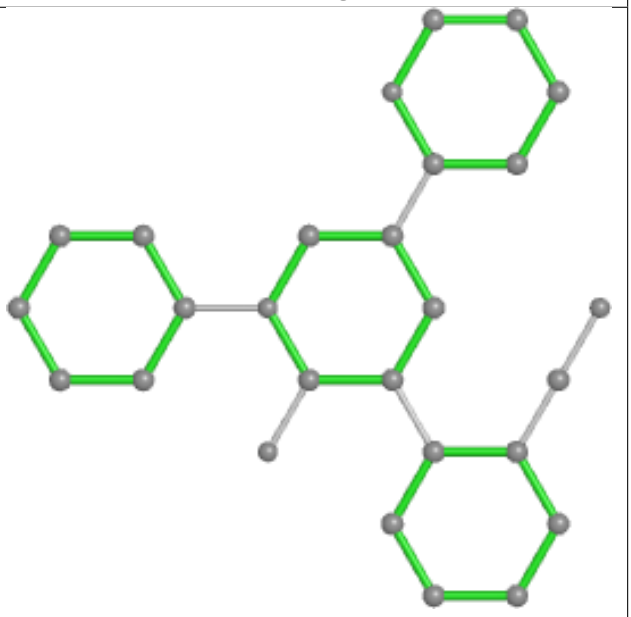
Bond lengths



Bond angles

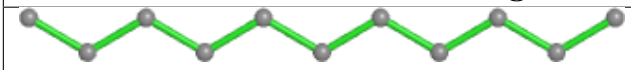


Torsions

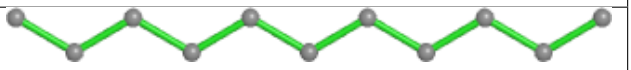


Rings

Ligand PCW D 1106



Bond lengths

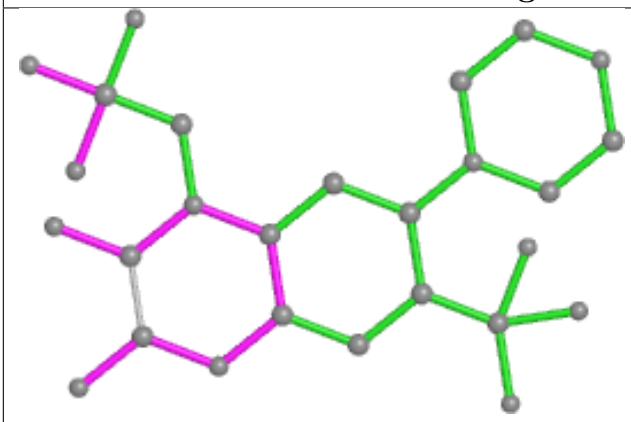


Bond angles

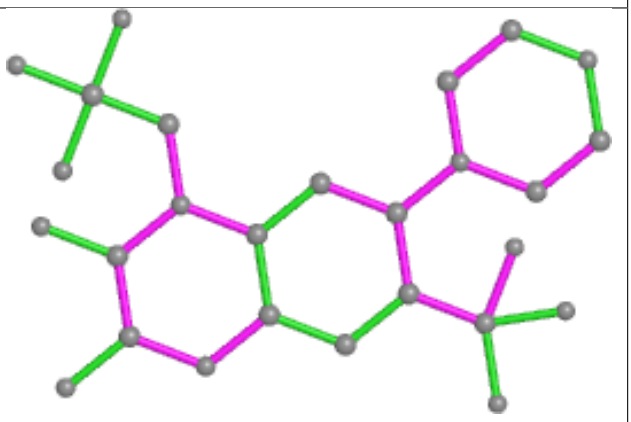
Torsions

Rings

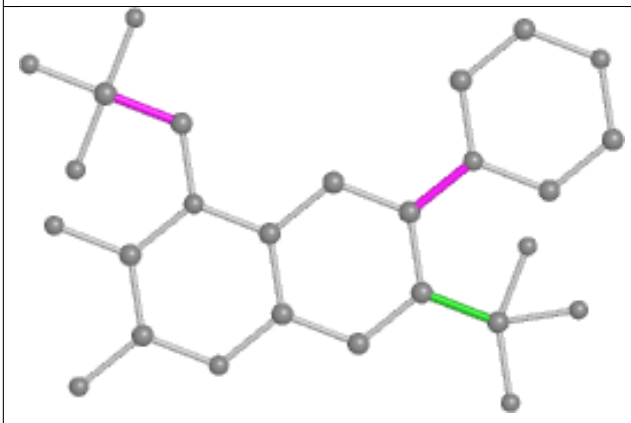
Ligand ZK1 A 1102



Bond lengths



Bond angles



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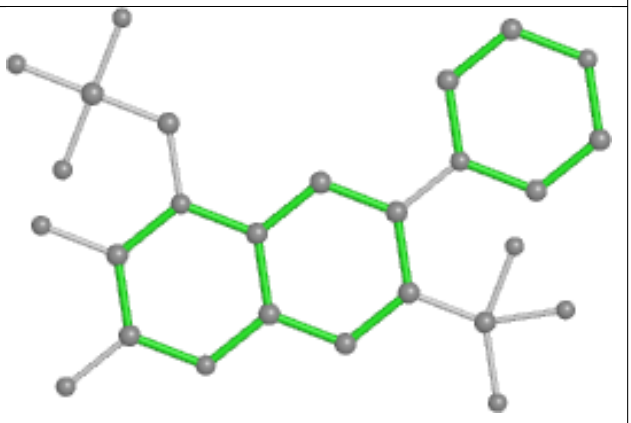
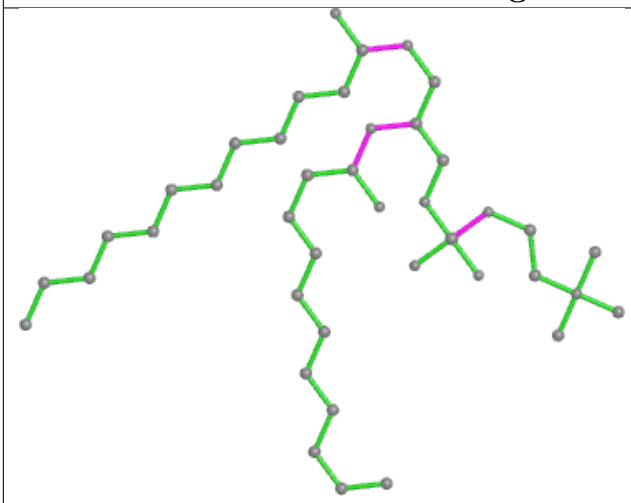
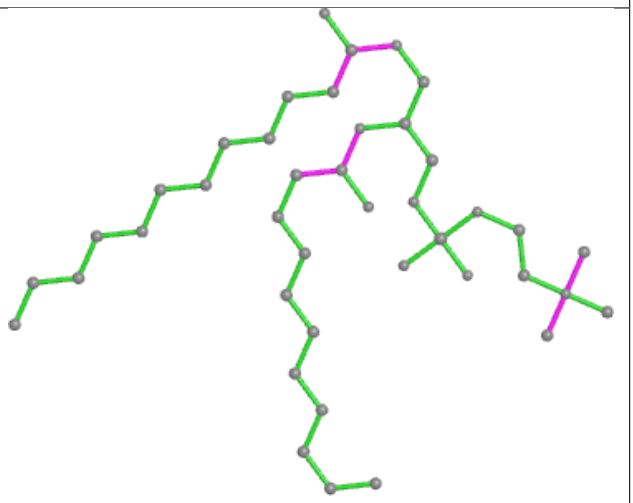


Rings

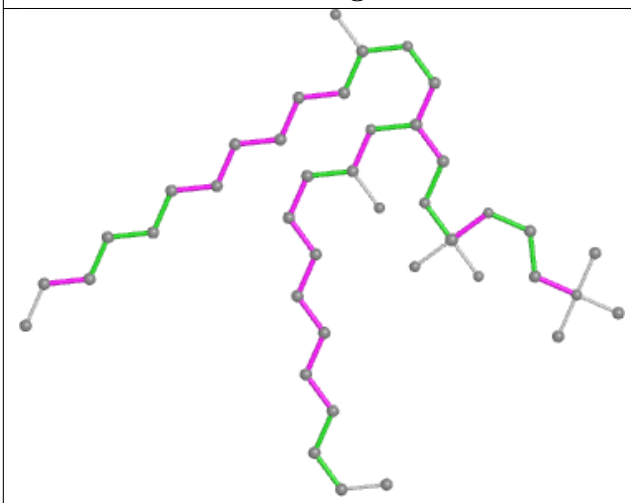
Ligand PCW B 1105



Bond lengths



Bond angles



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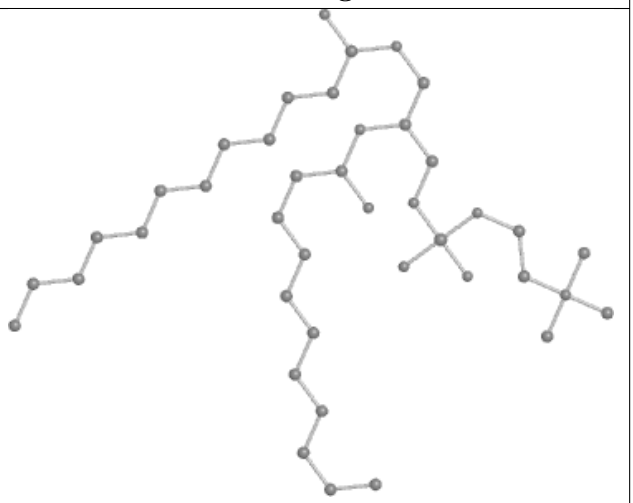
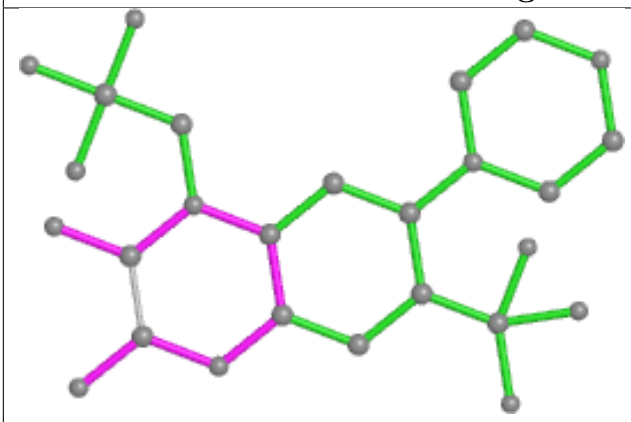
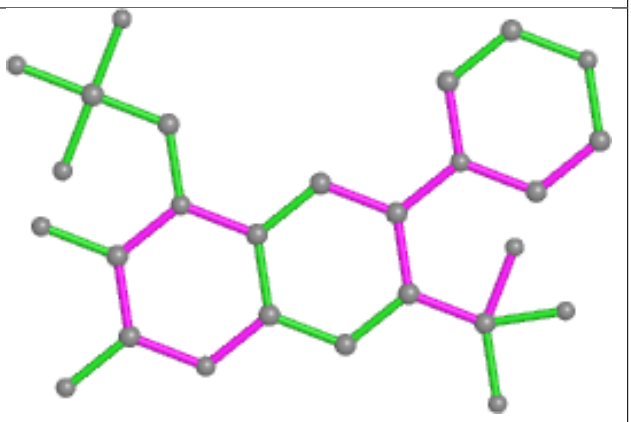


Rings

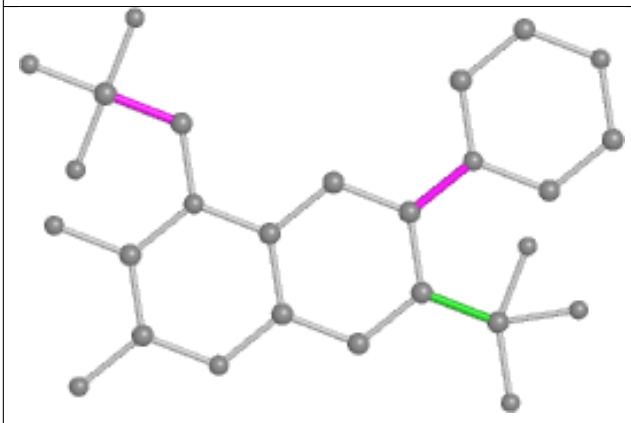
Ligand ZK1 D 1102



Bond lengths



Bond angles



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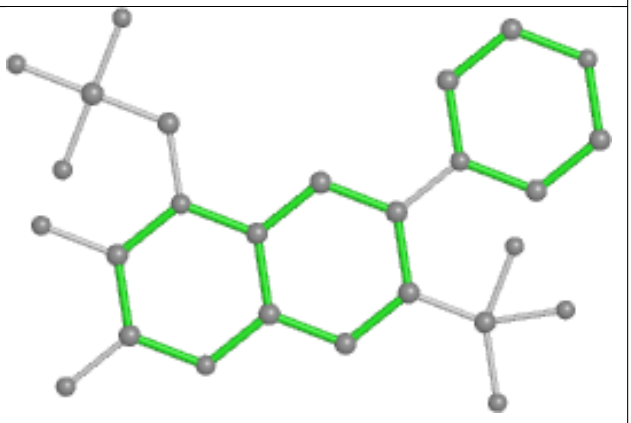
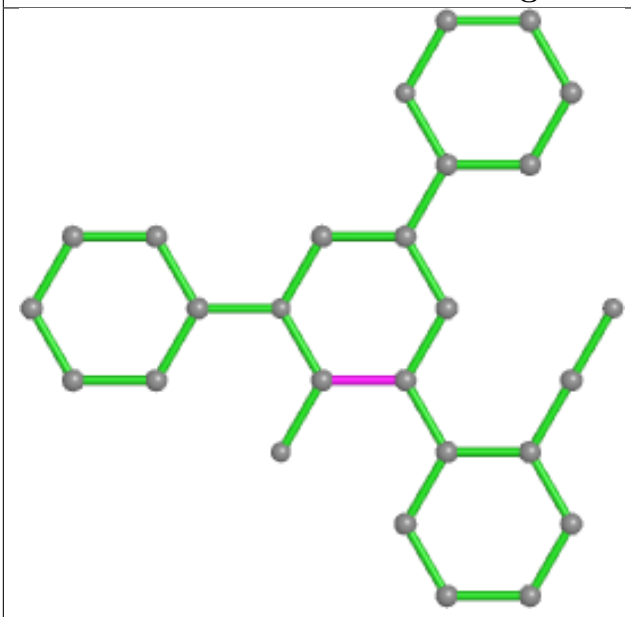
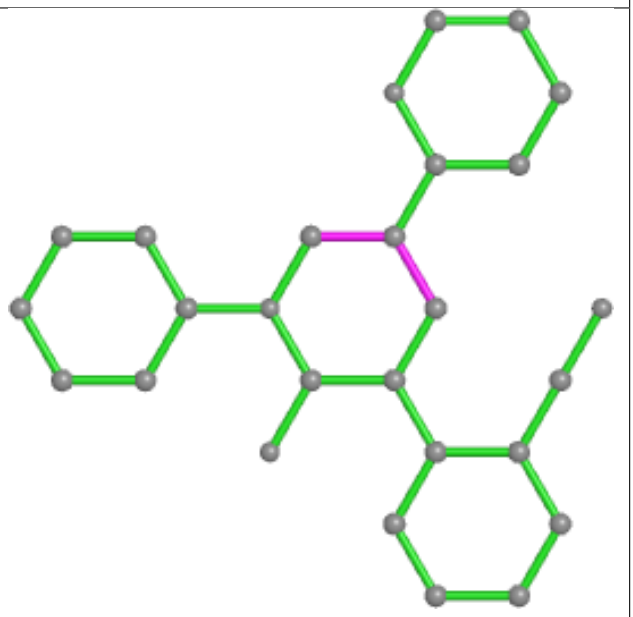


Rings

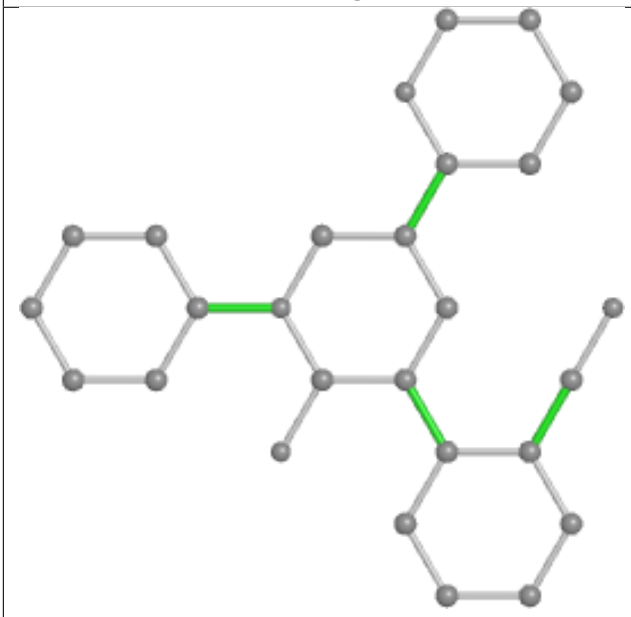
Ligand 6ZP C 1101



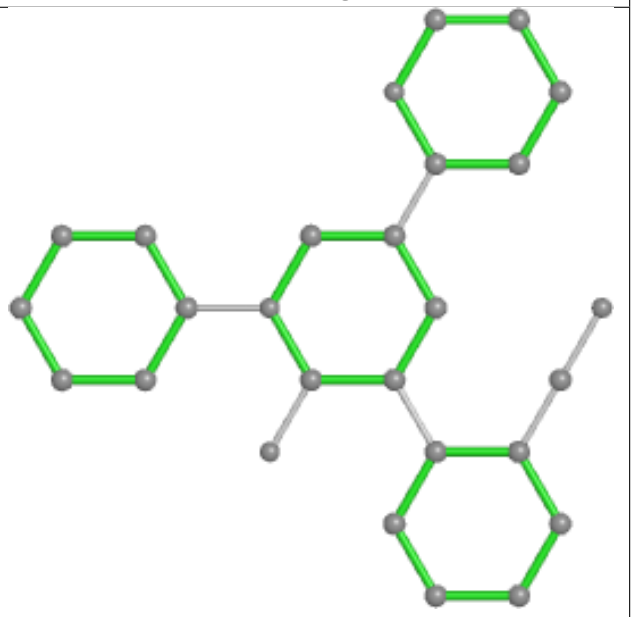
Bond lengths



Bond angles

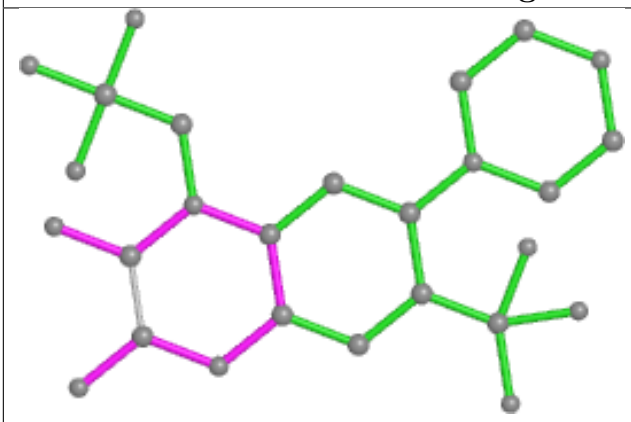


Torsions

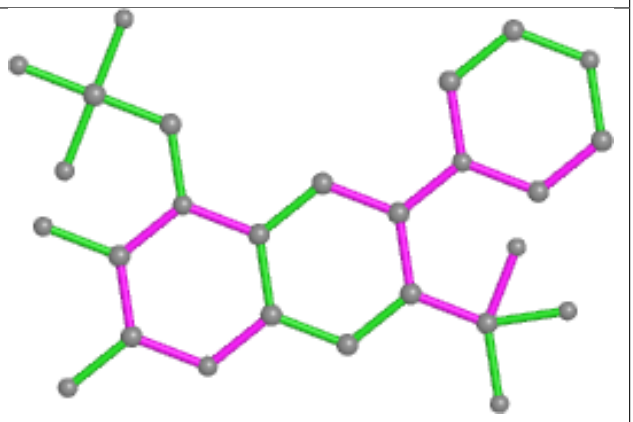


Rings

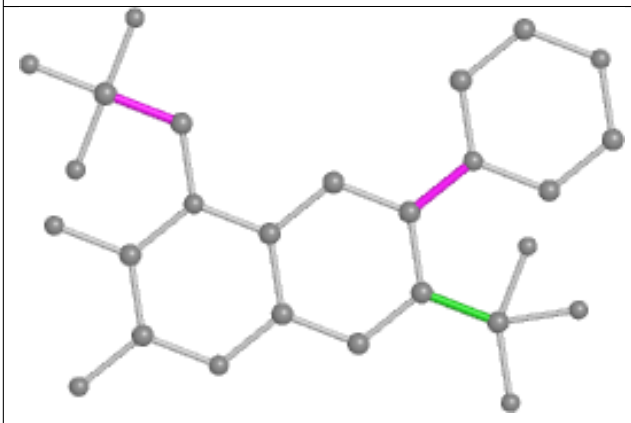
Ligand ZK1 B 1102



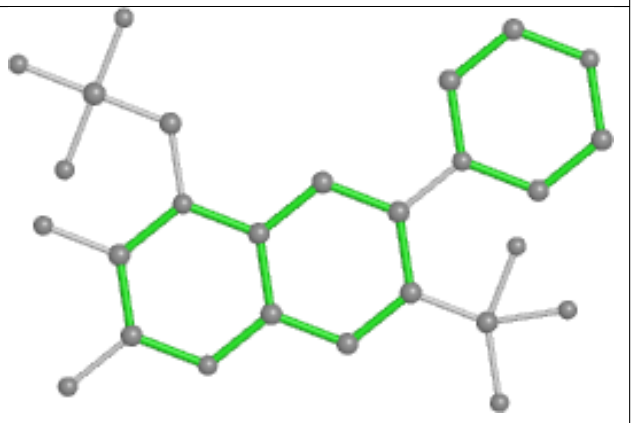
Bond lengths



Bond angles

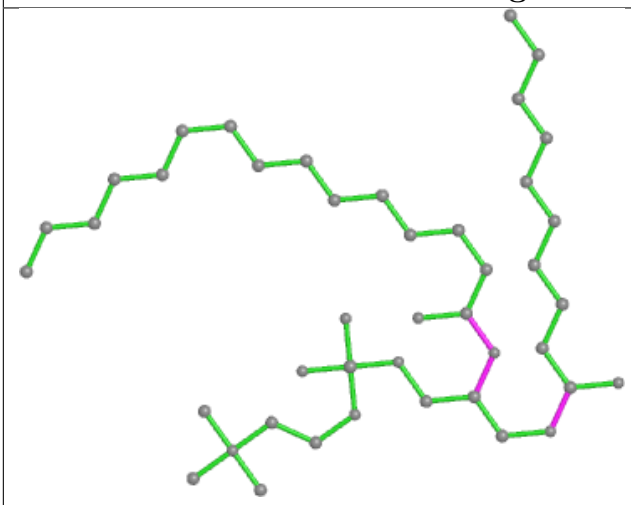


Torsions

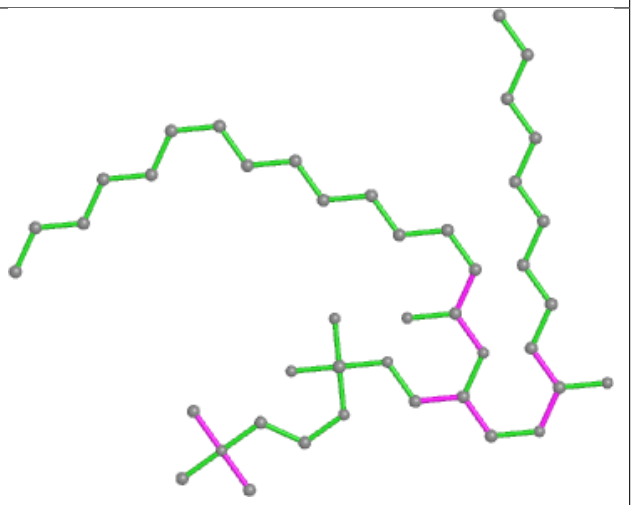


Rings

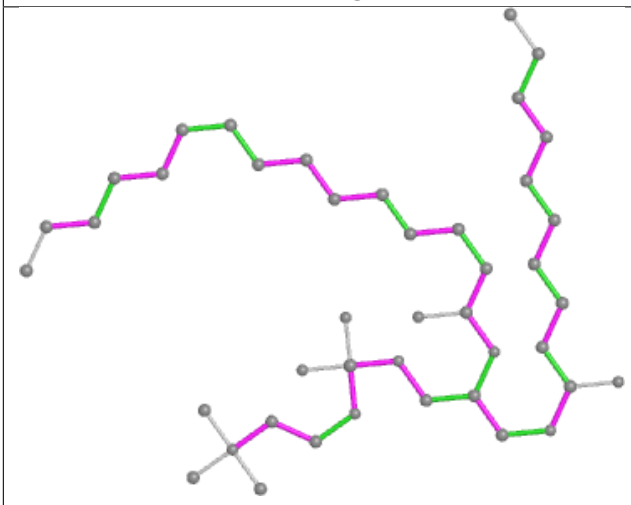
Ligand PCW B 1104



Bond lengths



Bond angles



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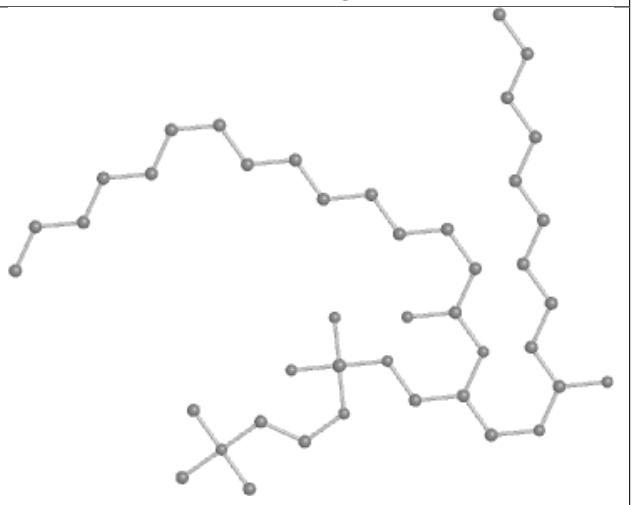
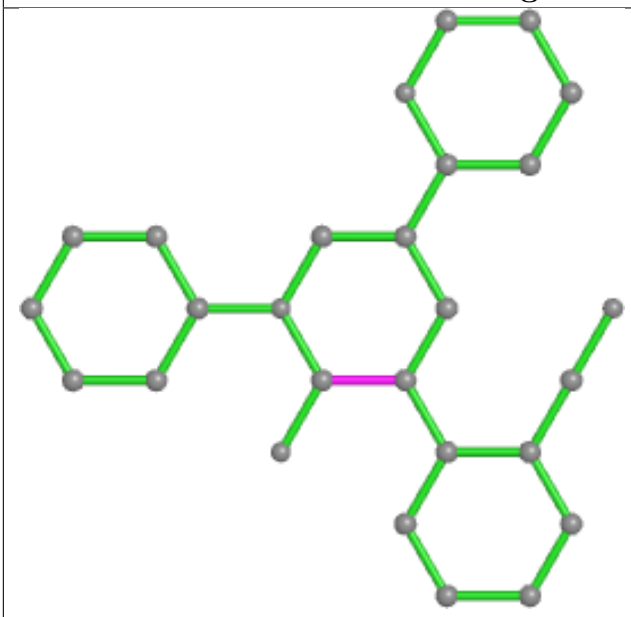
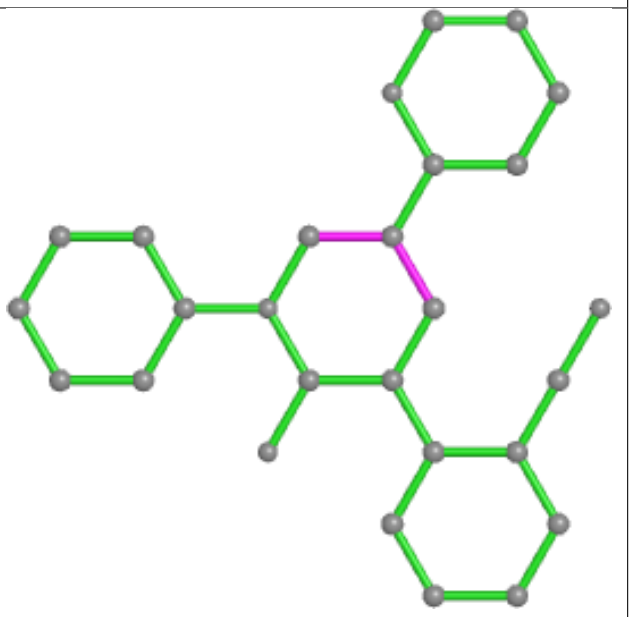


Rings

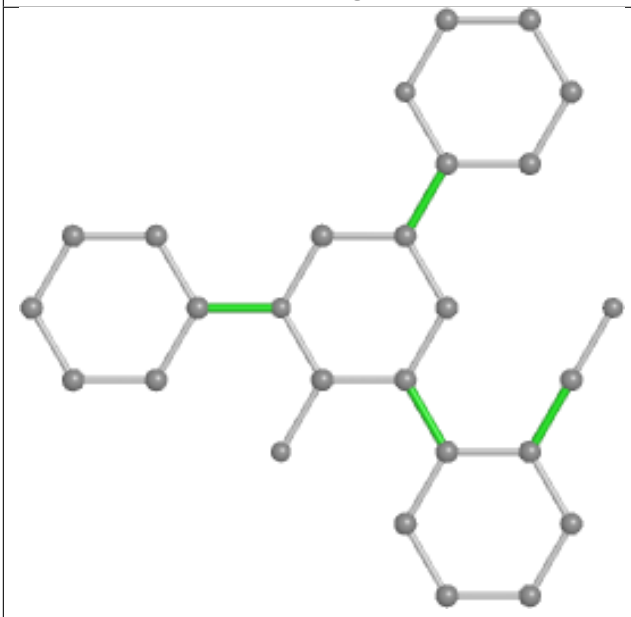
Ligand 6ZP B 1101



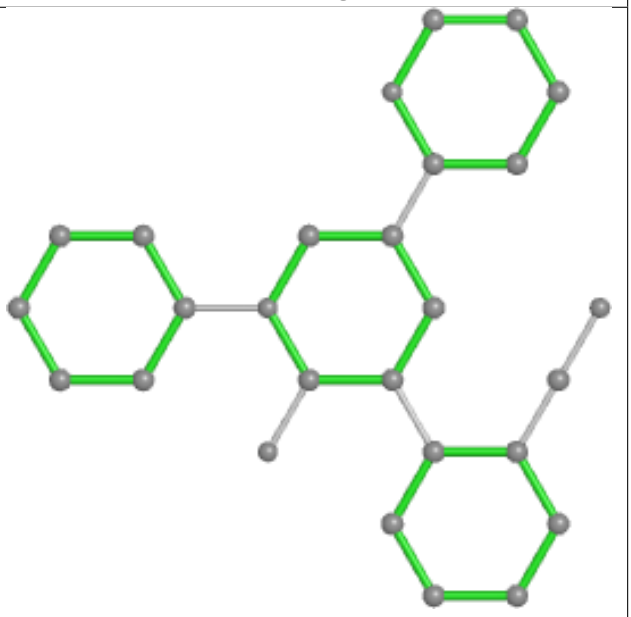
Bond lengths



Bond angles

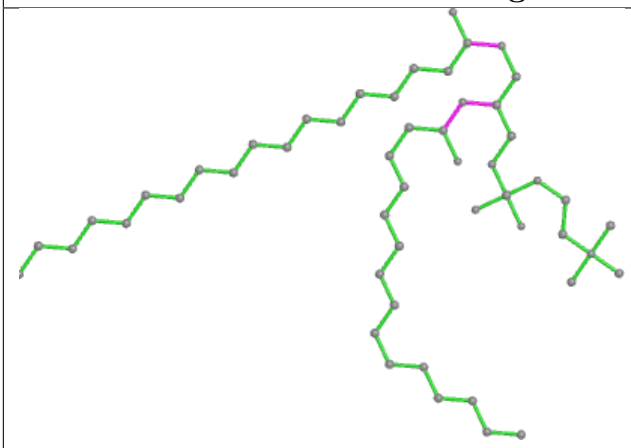


Torsions

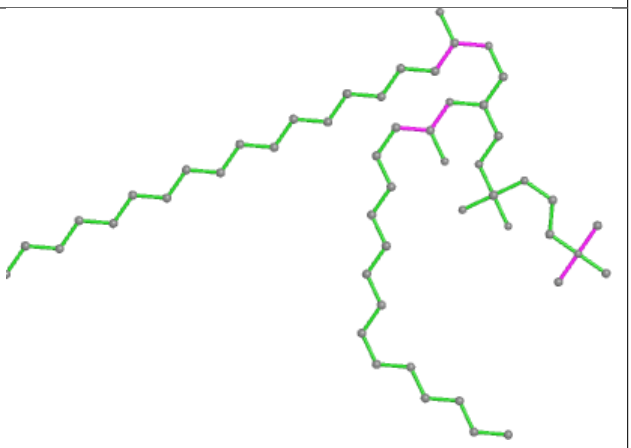


Rings

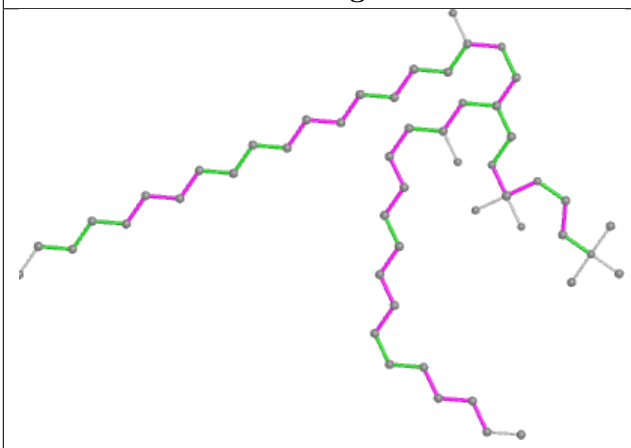
Ligand PCW A 1106



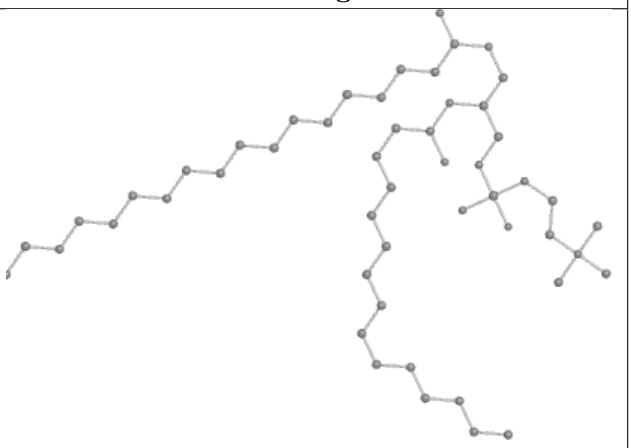
Bond lengths



Bond angles

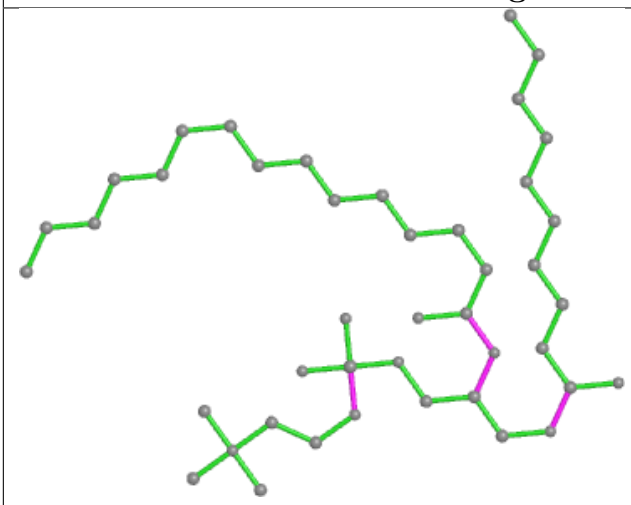


Torsions

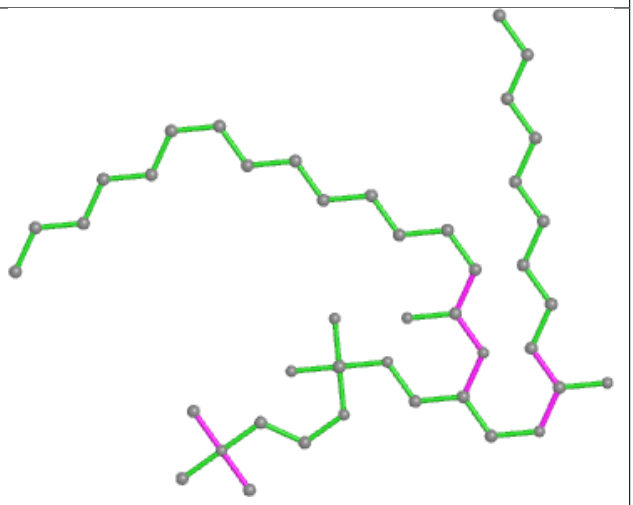


Rings

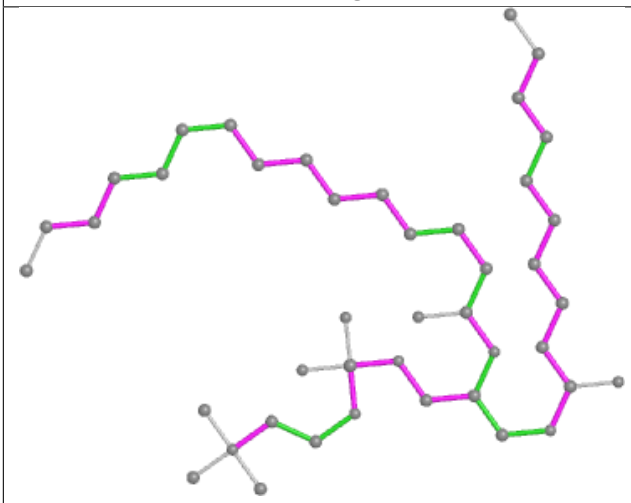
Ligand PCW C 1104



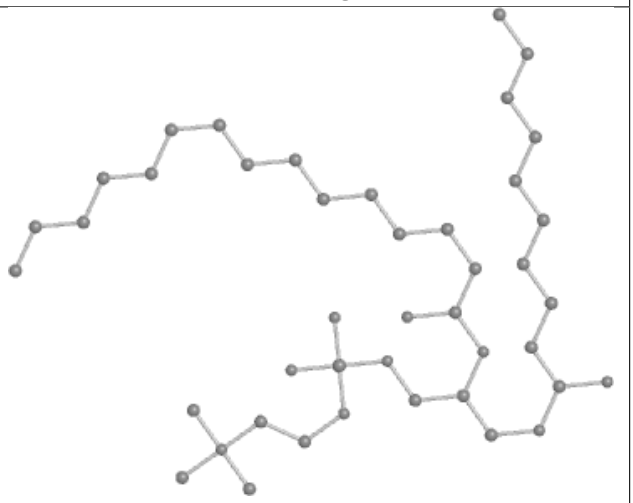
Bond lengths



Bond angles

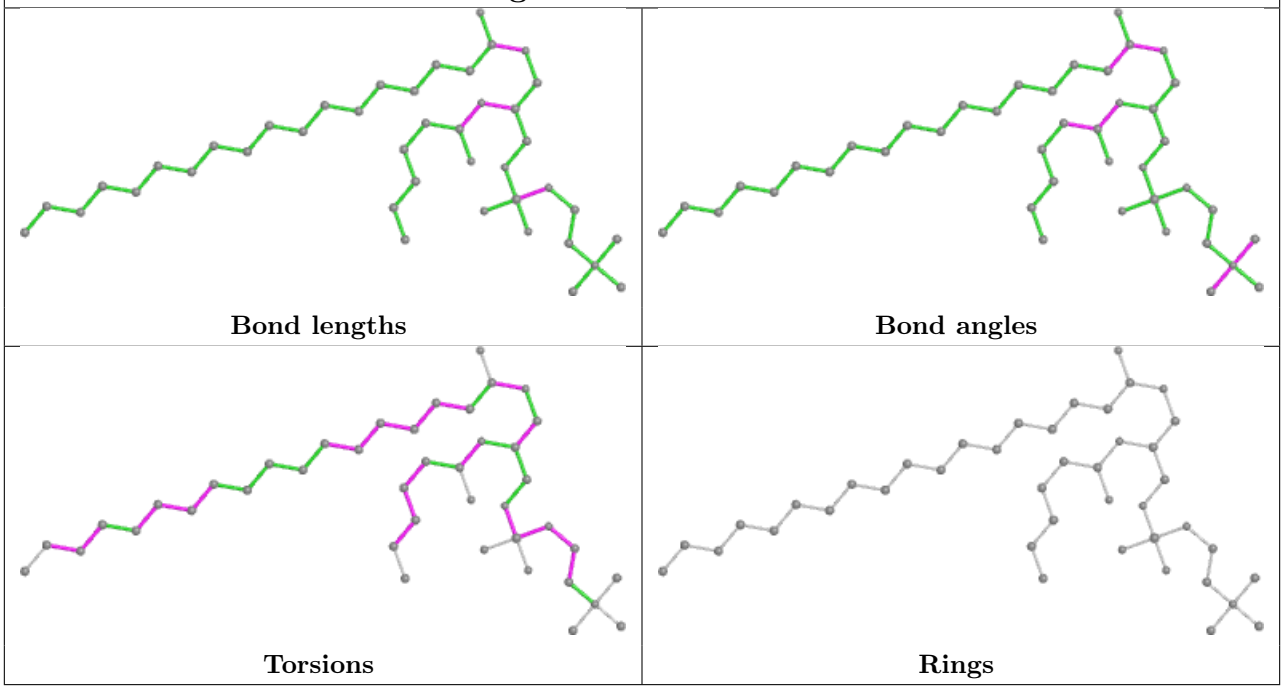


Torsions

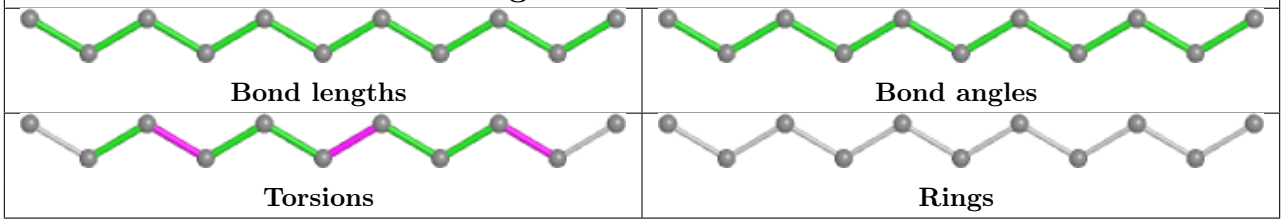


Rings

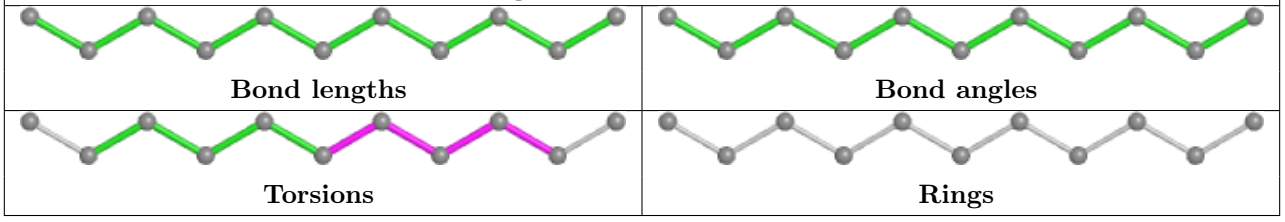
Ligand PCW A 1103



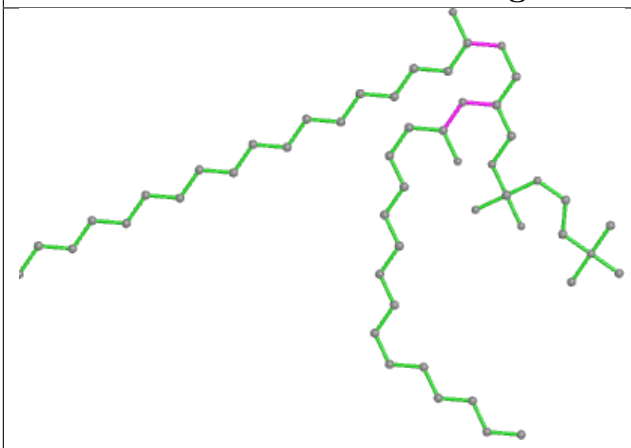
Ligand PCW A 1105



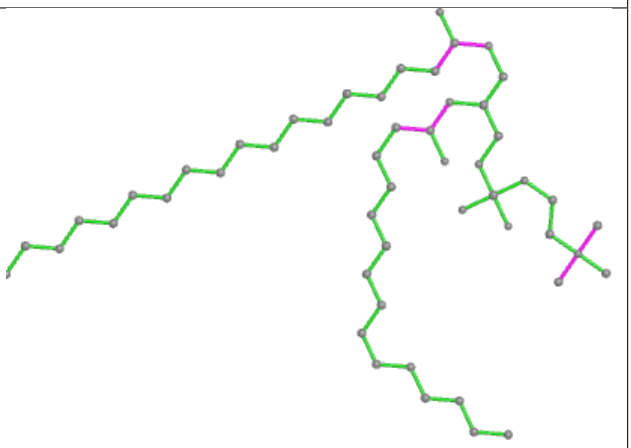
Ligand PCW B 1106



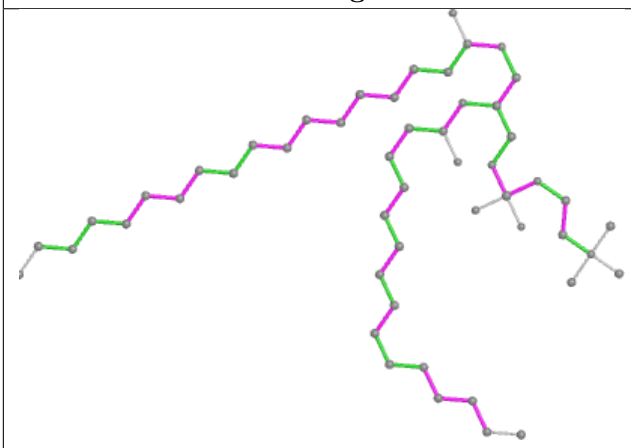
Ligand PCW C 1106



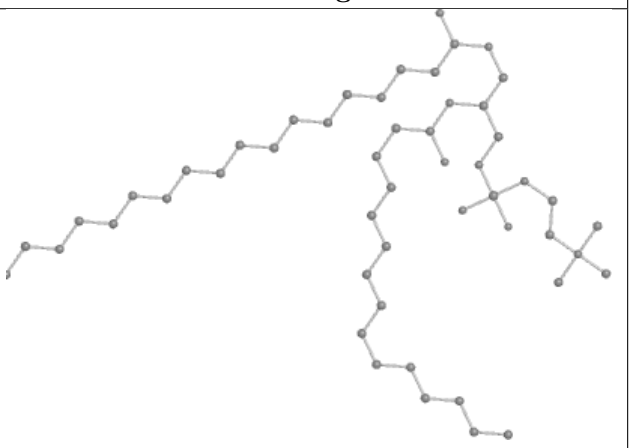
Bond lengths



Bond angles

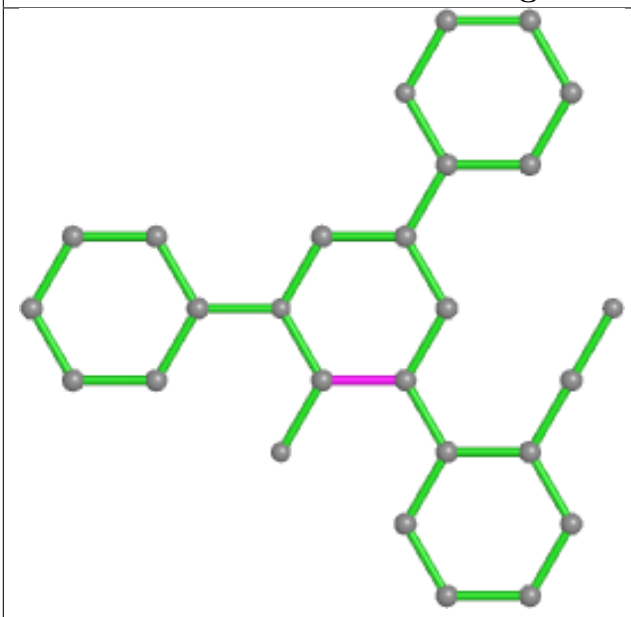


Torsions

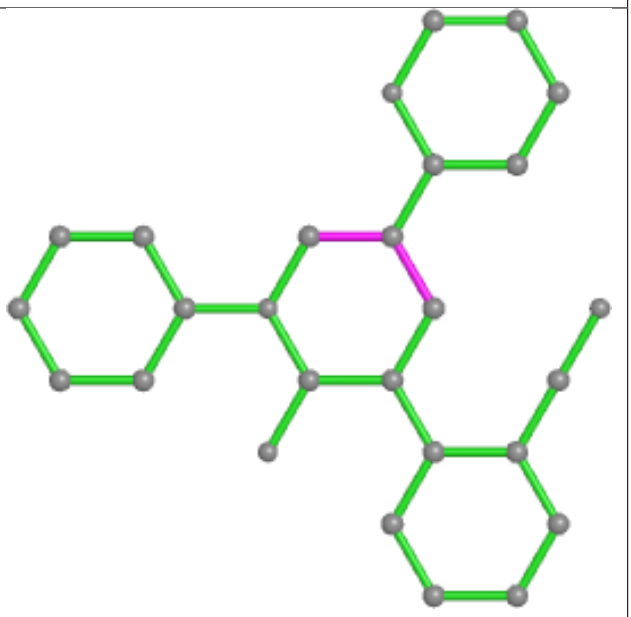


Rings

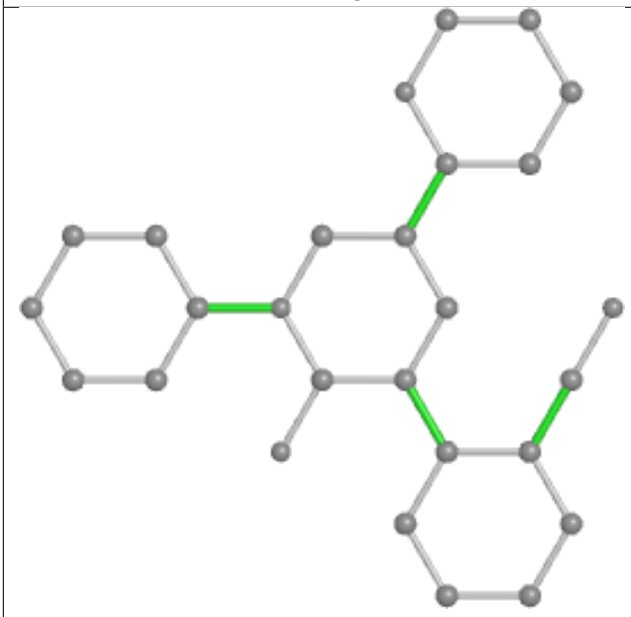
Ligand 6ZP D 1101



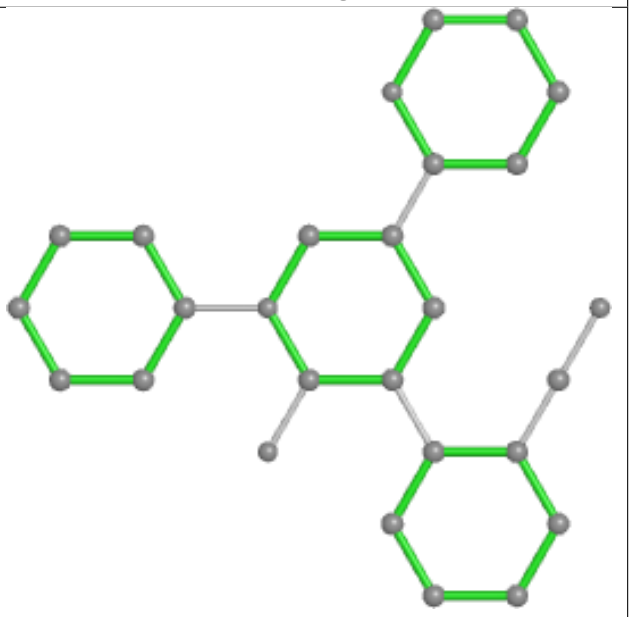
Bond lengths



Bond angles

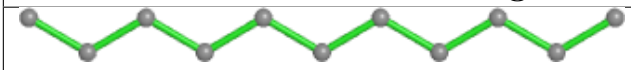


Torsions

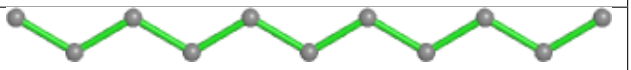


Rings

Ligand PCW C 1105



Bond lengths

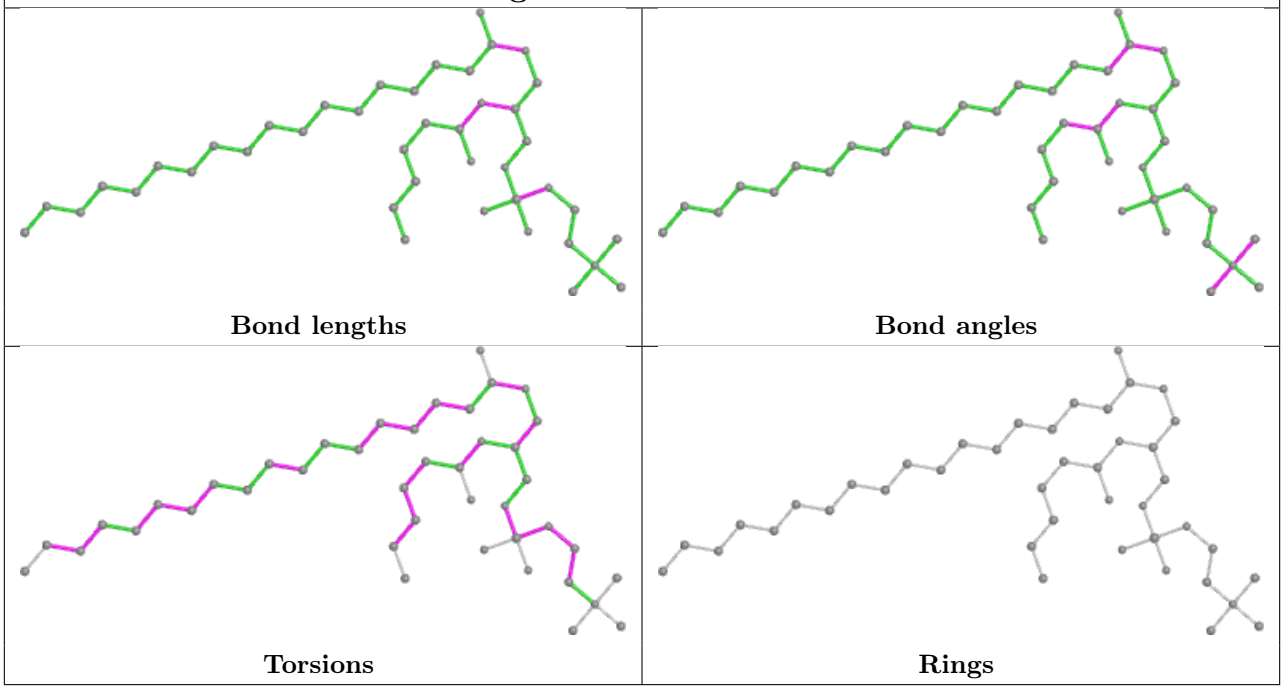


Bond angles

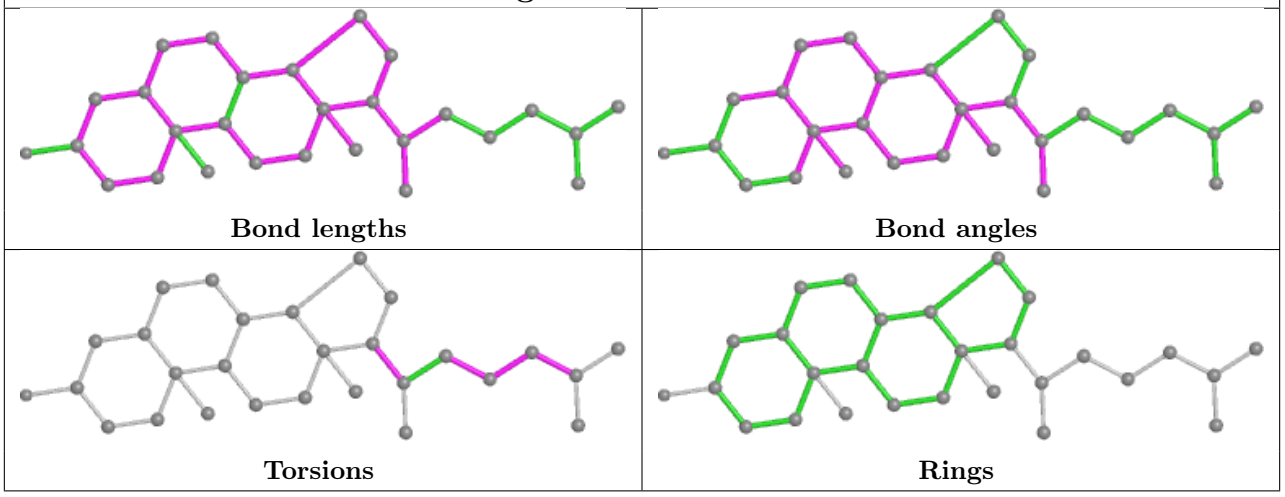
Torsions

Rings

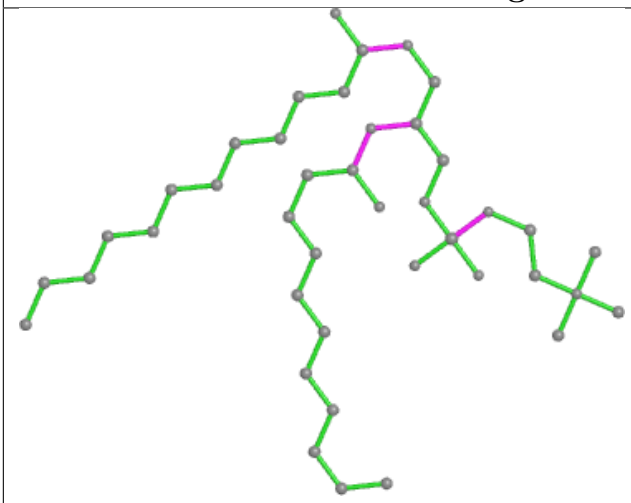
Ligand PCW C 1103



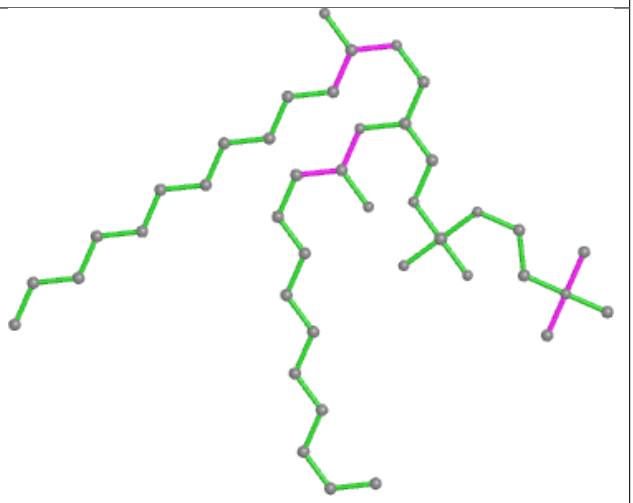
Ligand CLR B 1103



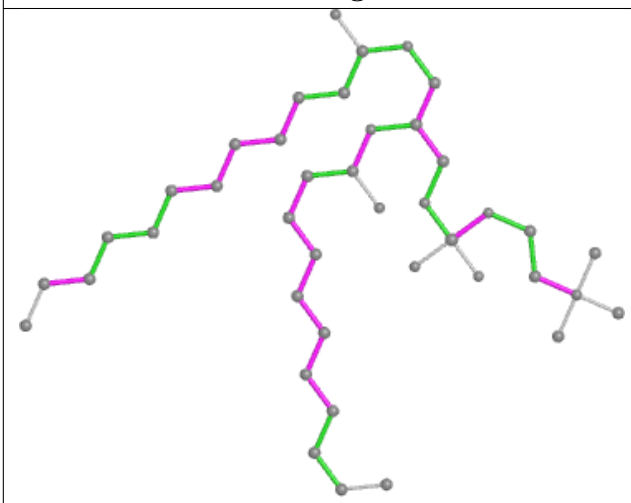
Ligand PCW D 1105



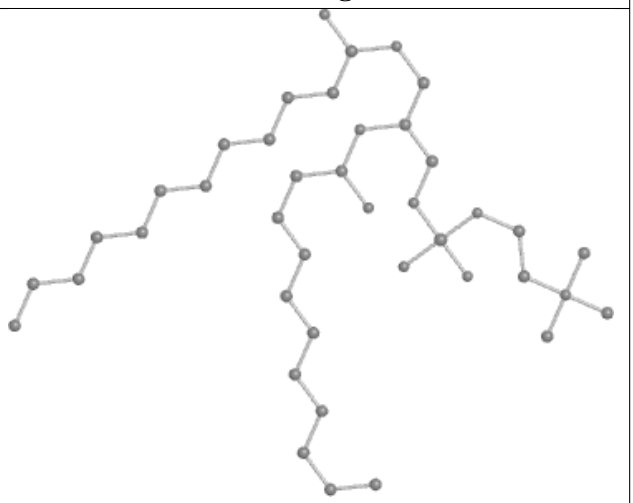
Bond lengths



Bond angles

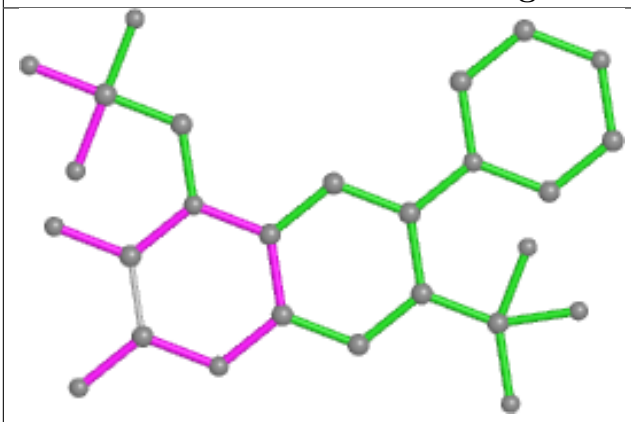


Torsions

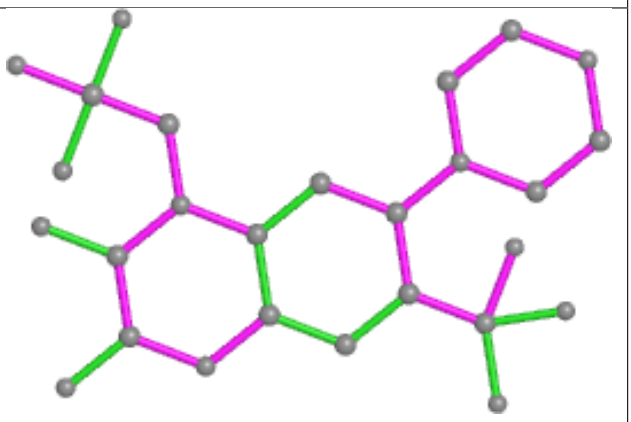


Rings

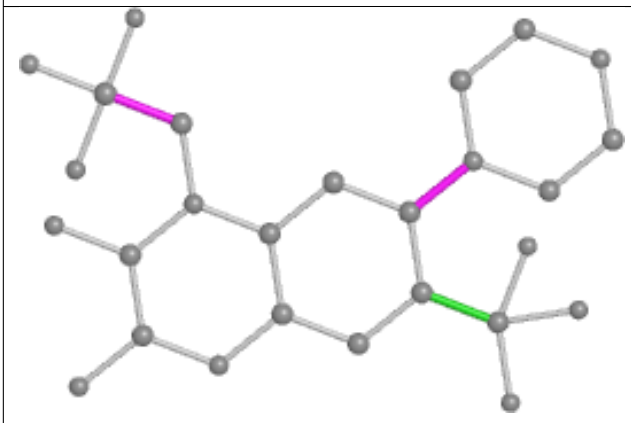
Ligand ZK1 C 1102



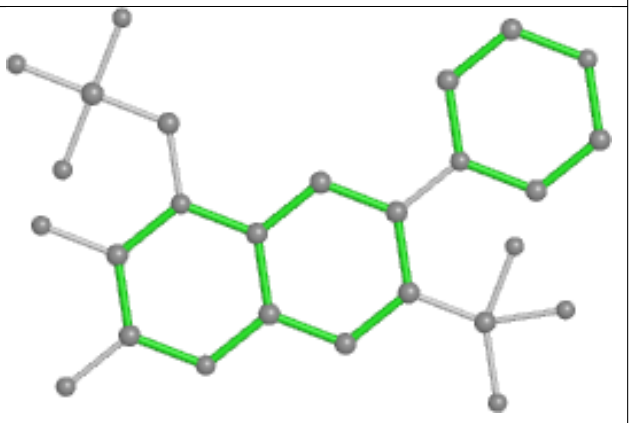
Bond lengths



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.

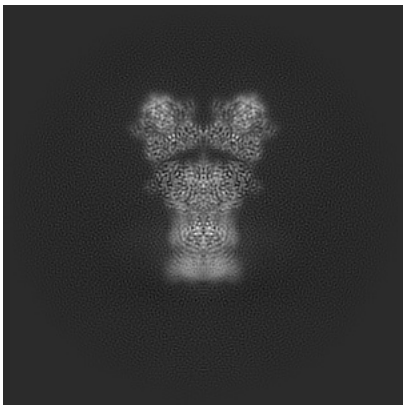
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40747. These allow visual inspection of the internal detail of the map and identification of artifacts.

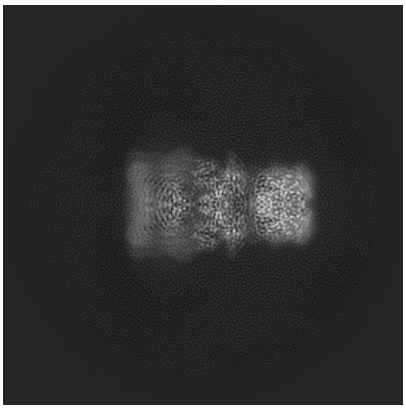
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

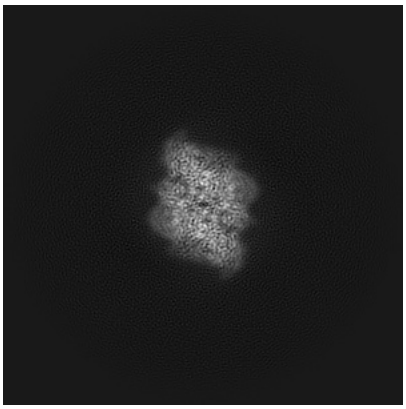
6.1.1 Primary map



X

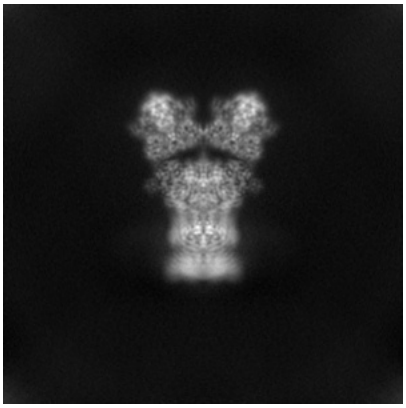


Y

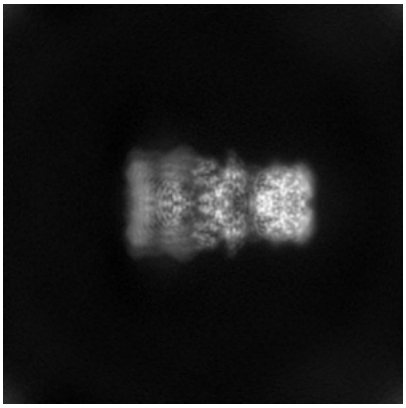


Z

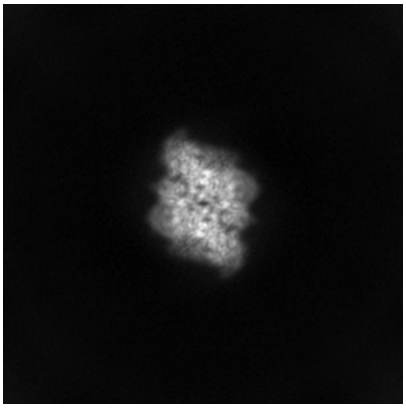
6.1.2 Raw map



X



Y

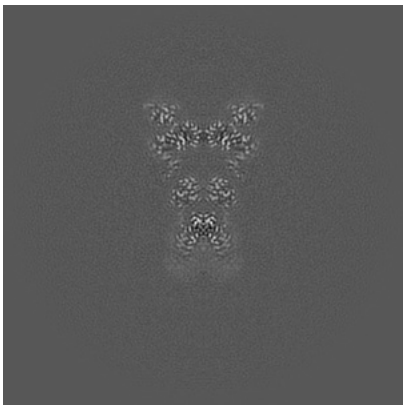


Z

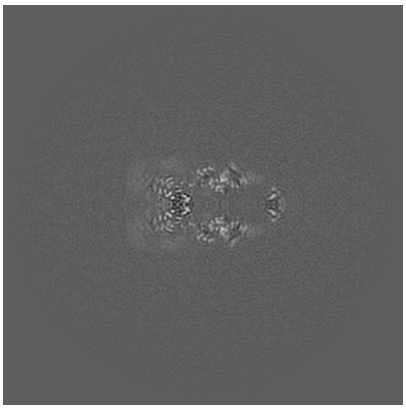
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

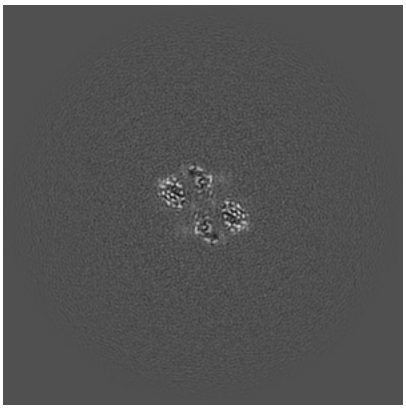
6.2.1 Primary map



X Index: 208

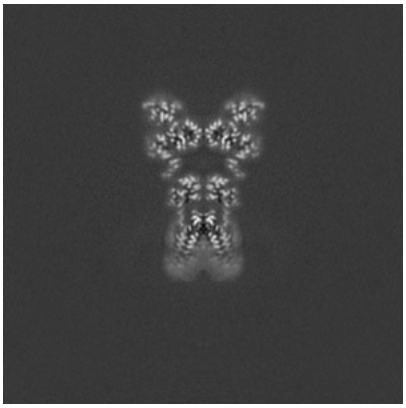


Y Index: 208

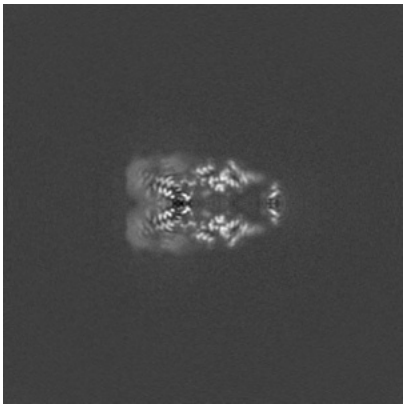


Z Index: 208

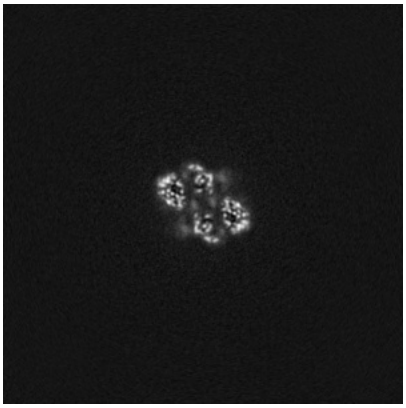
6.2.2 Raw map



X Index: 208



Y Index: 208

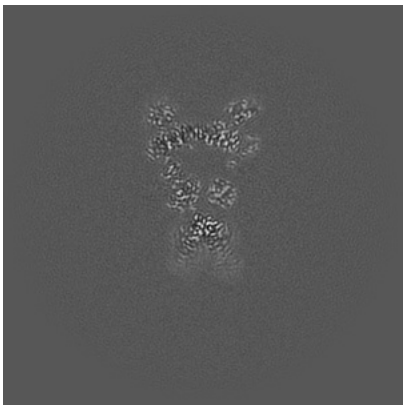


Z Index: 208

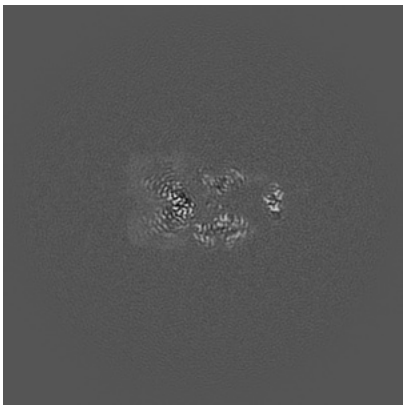
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

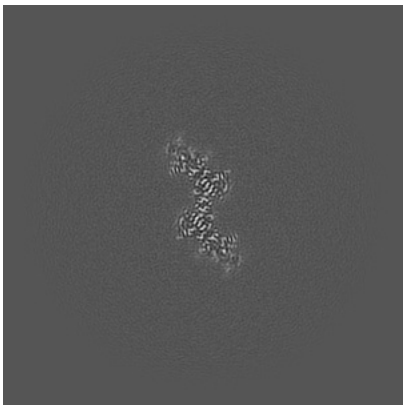
6.3.1 Primary map



X Index: 212

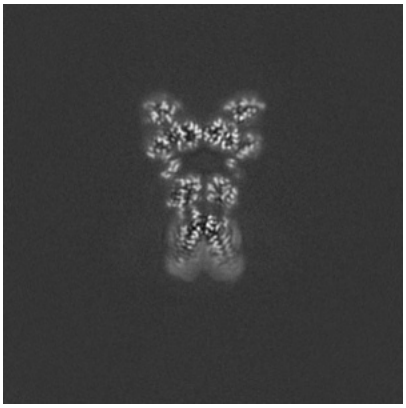


Y Index: 211

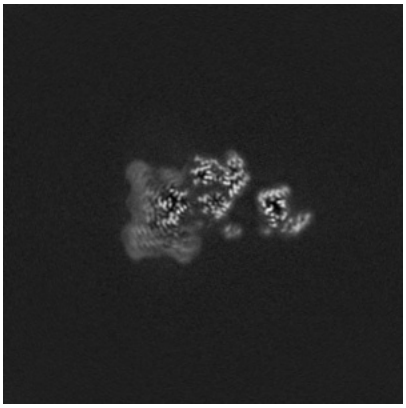


Z Index: 278

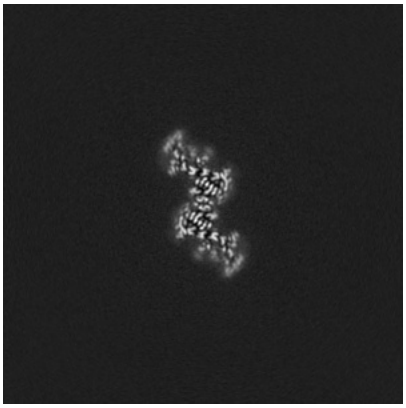
6.3.2 Raw map



X Index: 210



Y Index: 195

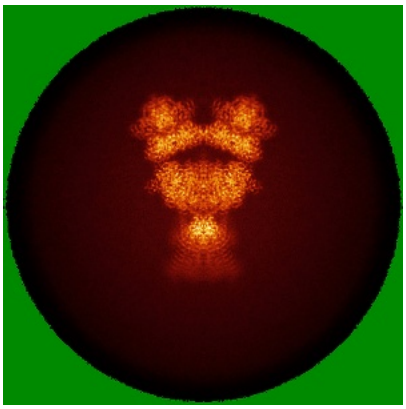


Z Index: 279

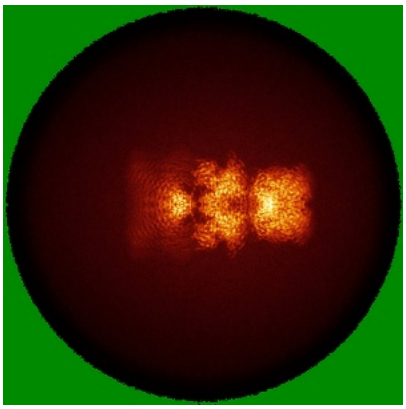
The images above show the largest variance slices of the map in three orthogonal directions.

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

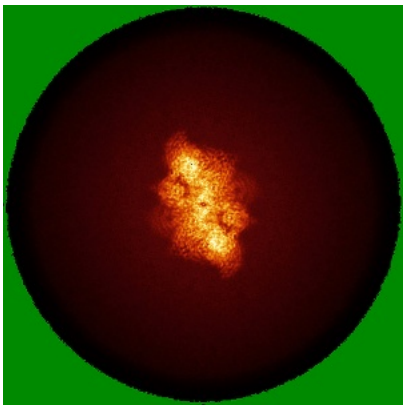
6.4.1 Primary map



X

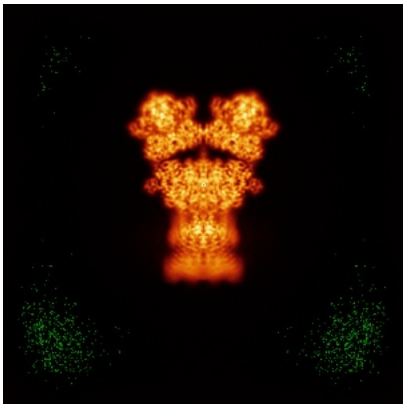


Y

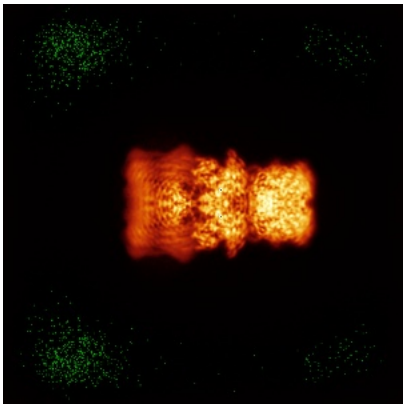


Z

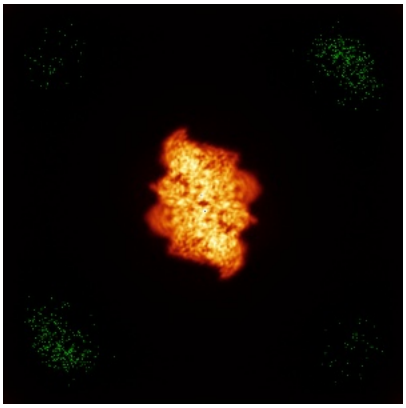
6.4.2 Raw map



X



Y



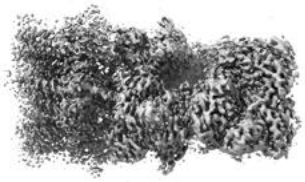
Z

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

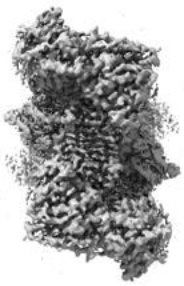
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



Y

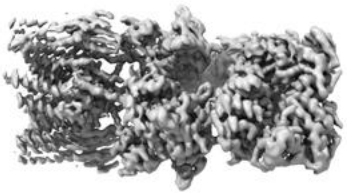


Z

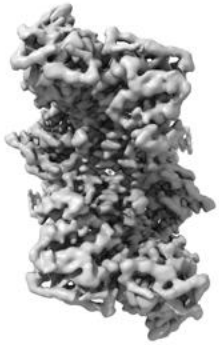
The images above show the 3D surface view of the map at the recommended contour level 0.95. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X



Y



Z

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

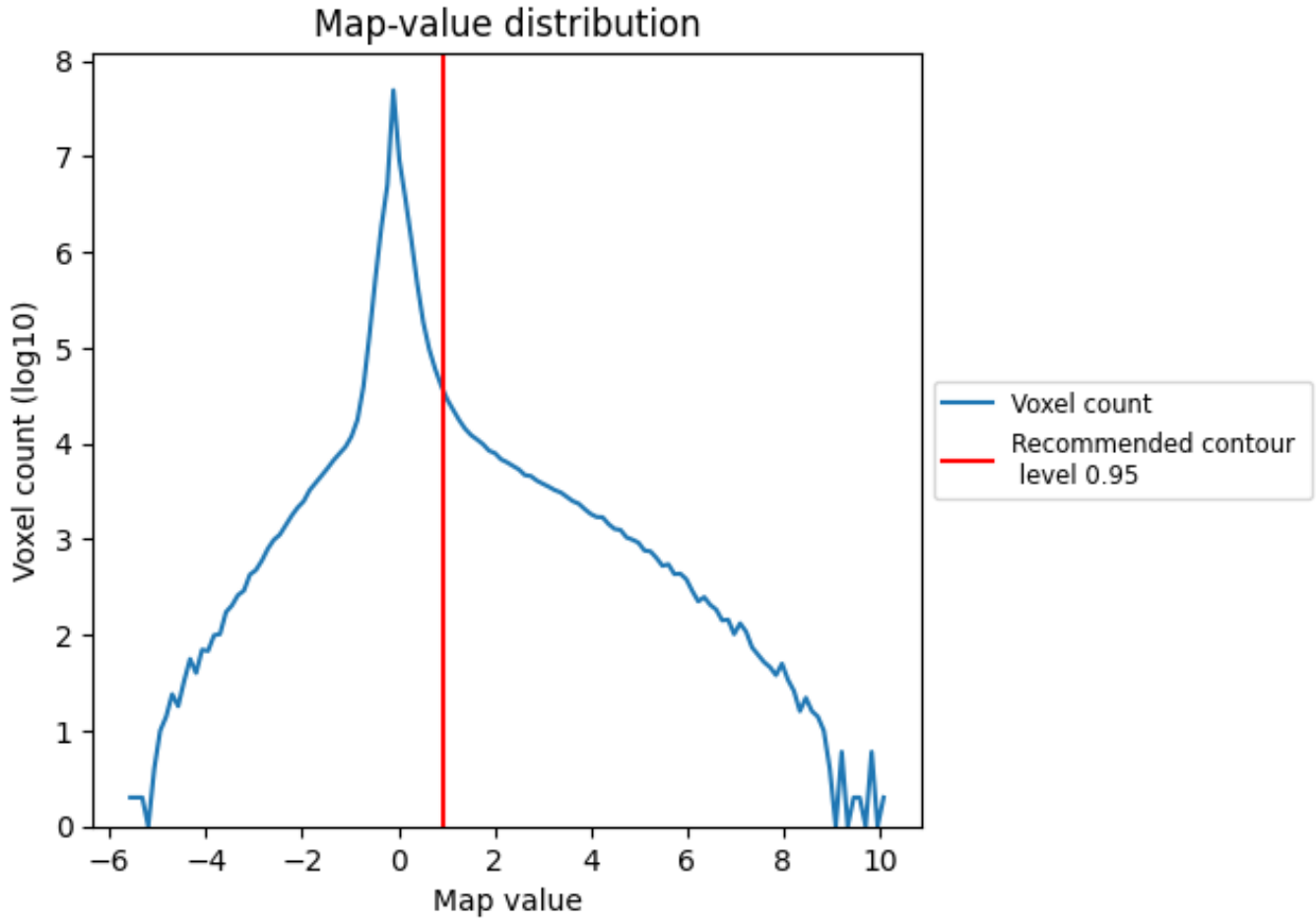
6.6 Mask visualisation (i)

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

7 Map analysis

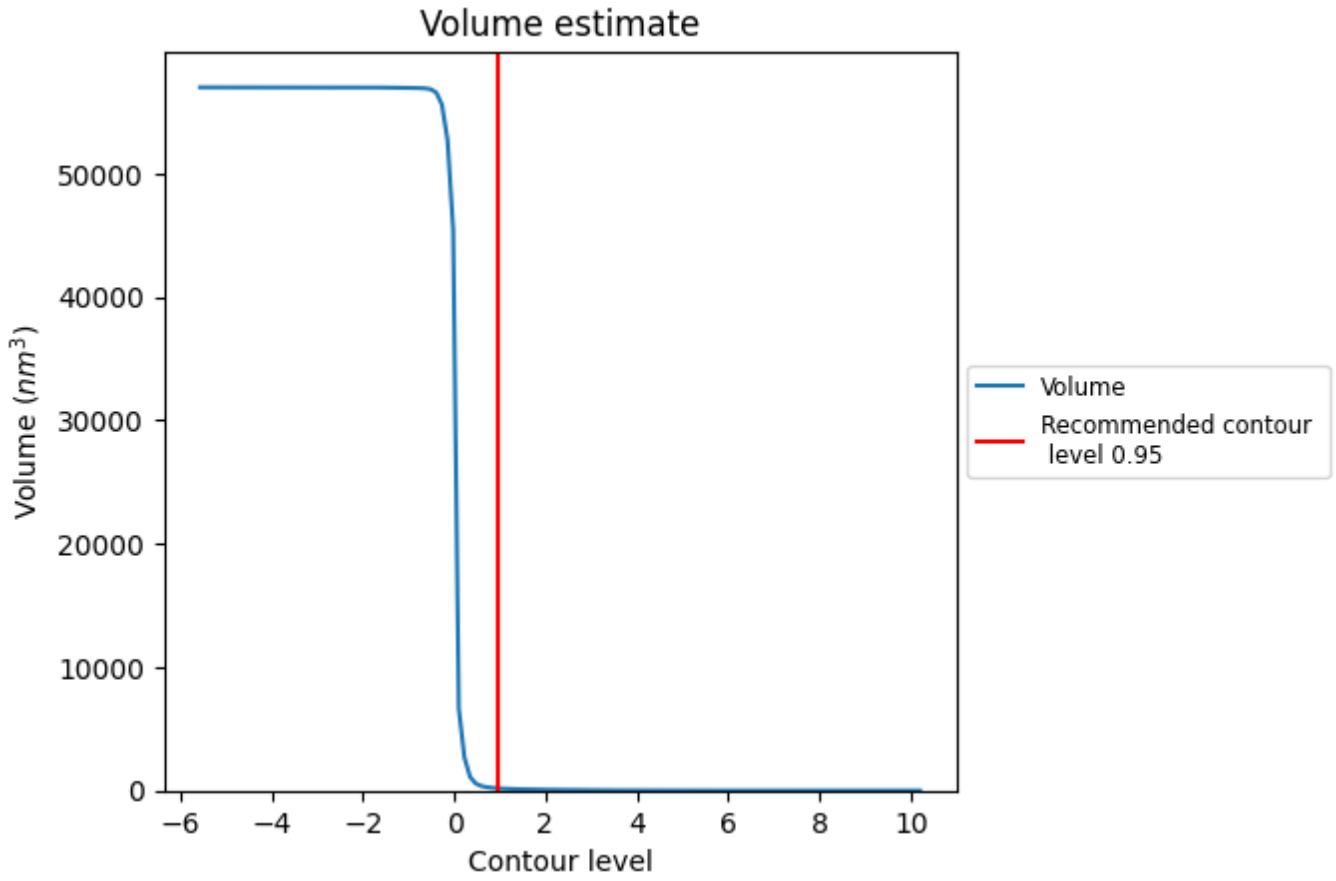
This section contains the results of statistical analysis of the map.

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.

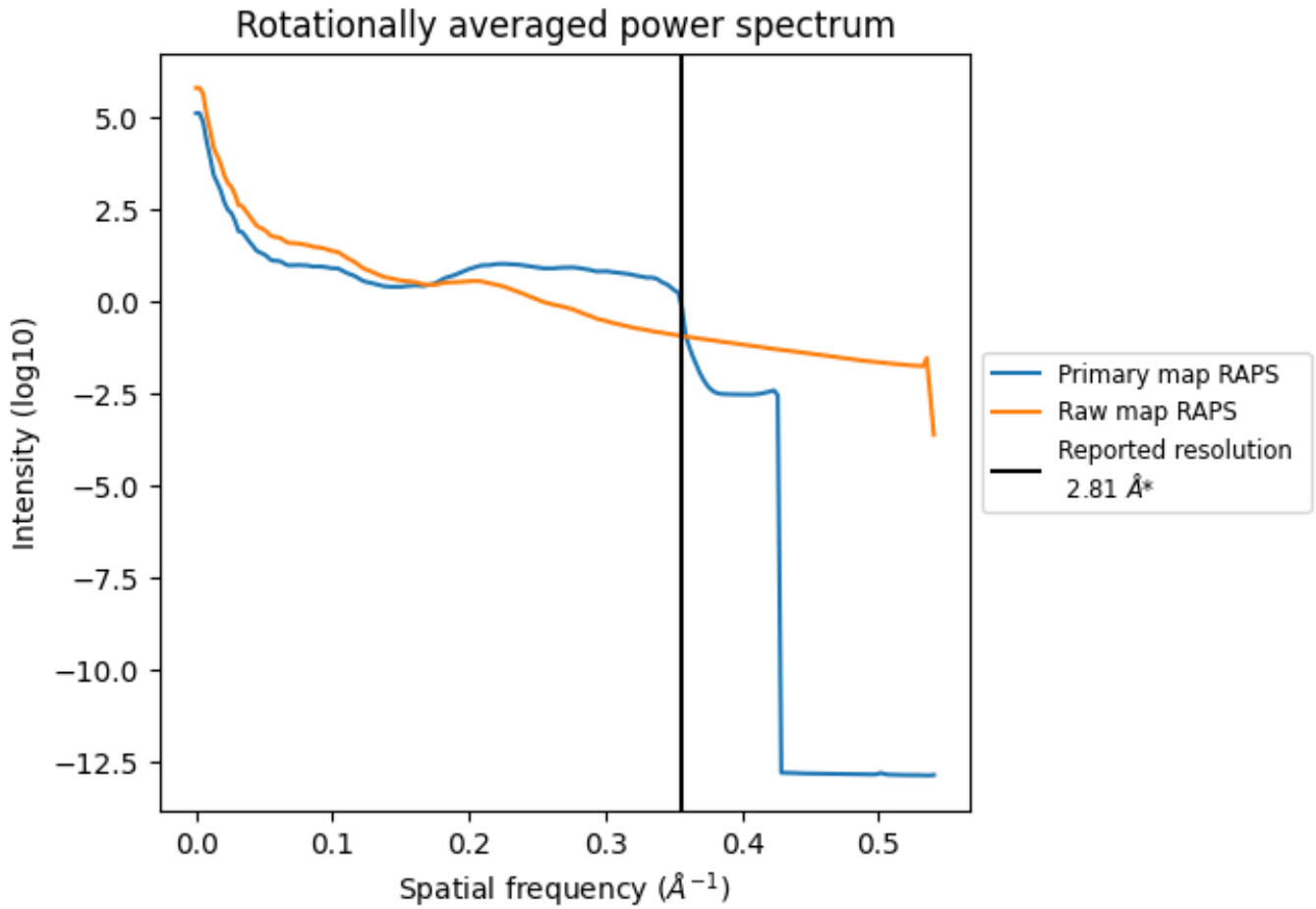
7.2 Volume estimate



The volume at the recommended contour level is 184 nm^3; this corresponds to an approximate mass of 166 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)

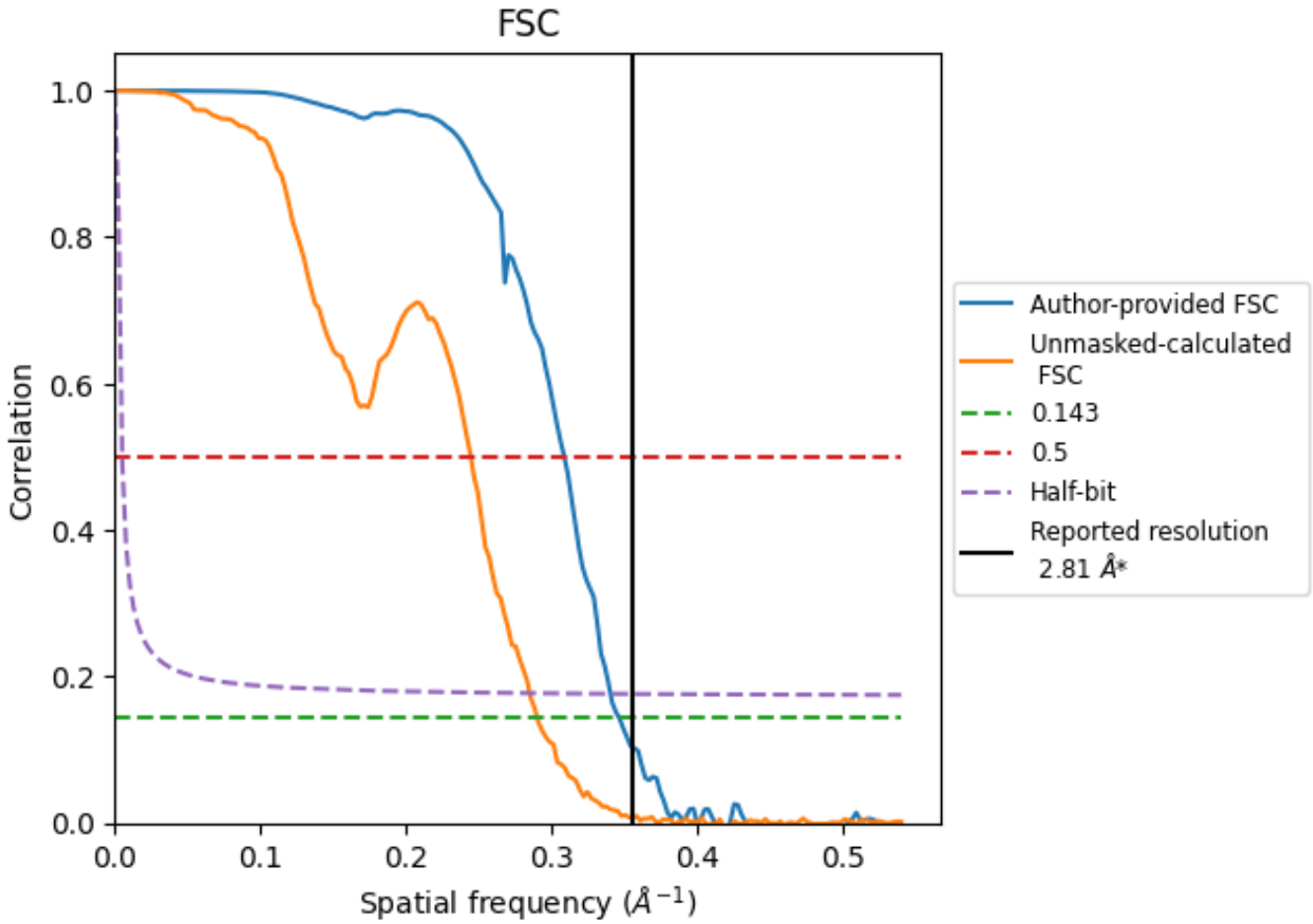


*Reported resolution corresponds to spatial frequency of 0.356 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8.2 Resolution estimates (i)

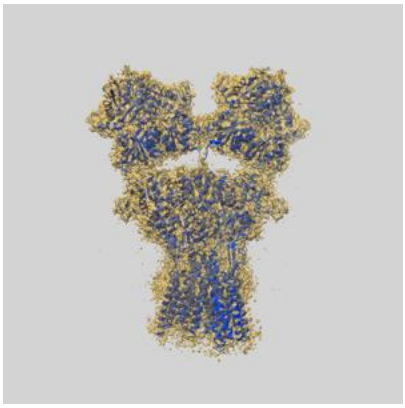
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.89	3.24	2.94
Unmasked-calculated*	3.44	4.09	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.81 by more than 10 %

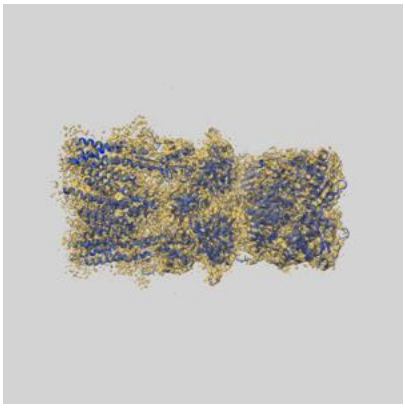
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40747 and PDB model 8SS8. Per-residue inclusion information can be found in section 3 on page 10.

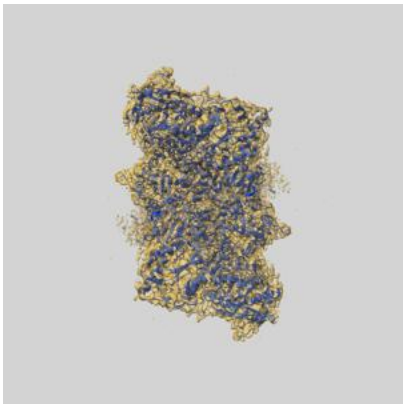
9.1 Map-model overlay



X



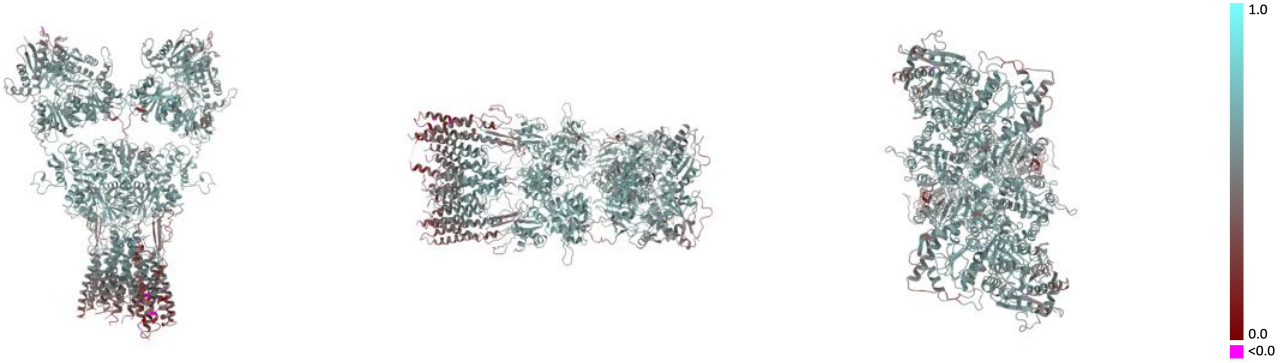
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.95 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.

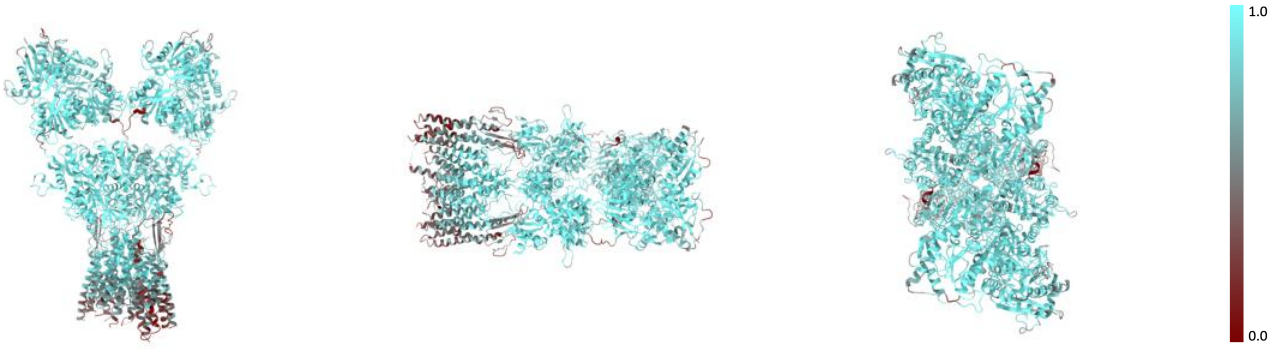
9.2 Q-score mapped to coordinate model (i)



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.

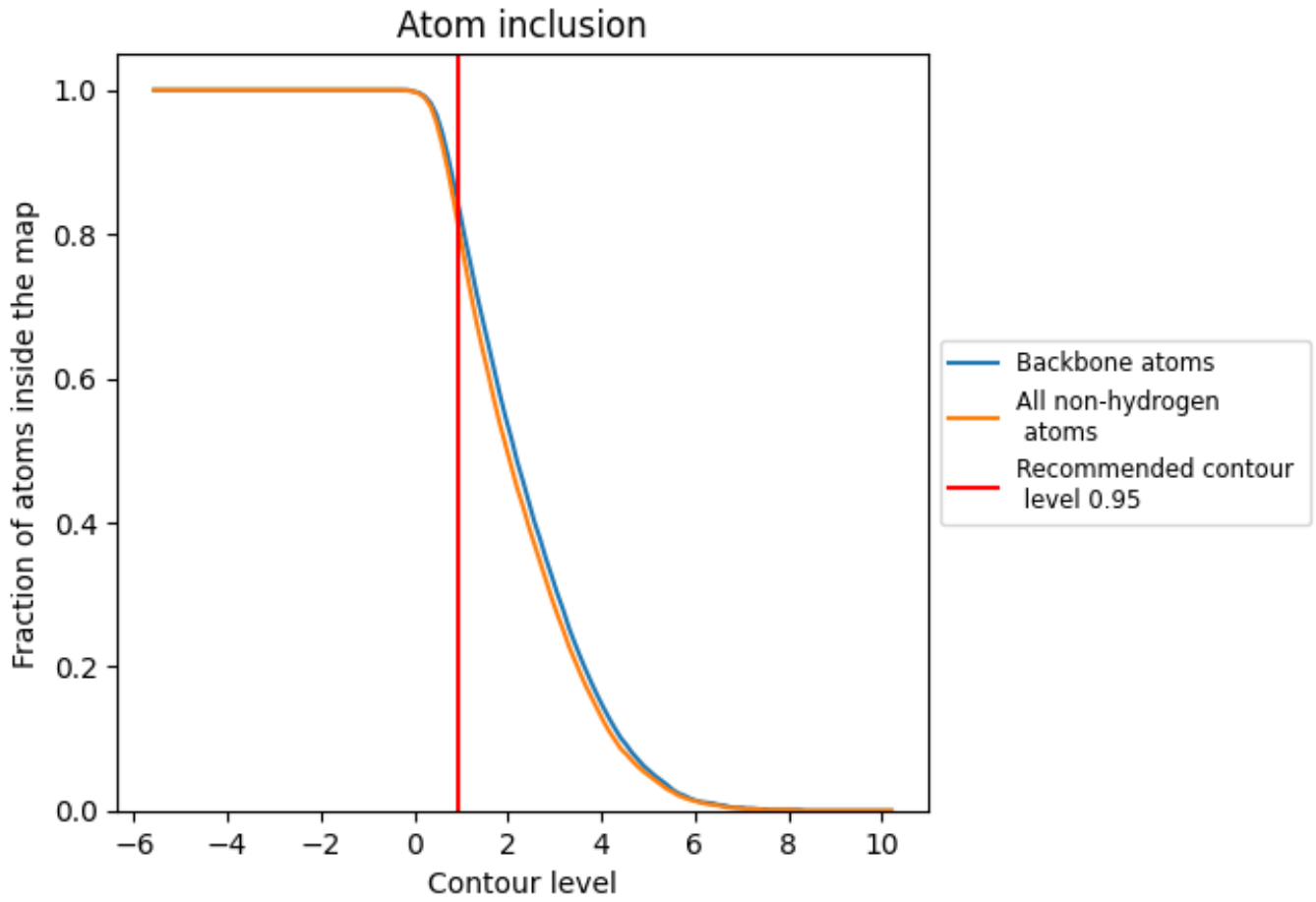
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.95).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.5300
A	0.7760	0.5140
B	0.8570	0.5510
C	0.7720	0.5120
D	0.8520	0.5490