Full wwPDB EM Validation Report (i)

Oct 8, 2022 – 04:58 PM EDT

PDB ID	:	7SCB
EMDB ID	:	EMD-25032
Title	:	B-cylinder of Synechocystis PCC 6803 Phycobilisome, complex with OCP - local refinement
Authors	:	Sauer, P.V.; Sutter, M.; Dominguez-Martin, M.A.; Kirst, H.; Kerfeld, C.A.
Deposited on	:	2021-09-27
Resolution	:	2.50 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

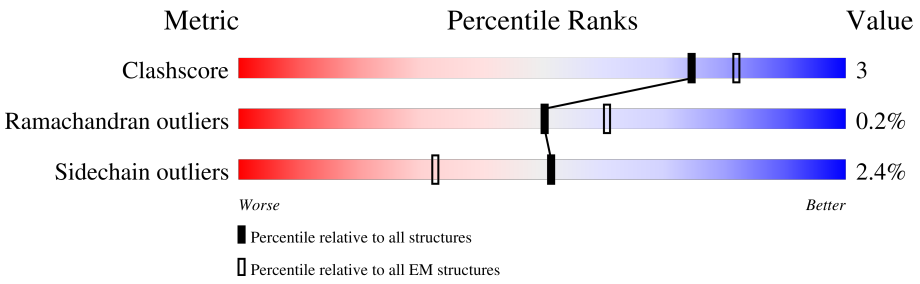
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.50 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	AA	161	54%, 90%, 9%
1	AC	161	47%, 91%, 8%
1	AH	161	89%, 10%
1	AJ	161	93%, 7%
1	AN	161	89%, 10%
1	AP	161	93%, 6%
1	AR	161	88%, 11%
1	AU	161	10%, 91%, 8%

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Mol	Chain	Length	Quality of chain
1	AW	161	86% 12%
1	AY	161	84% 14%
2	AB	161	39% 91% 9%
2	AD	161	47% 87% 12%
2	AF	161	39% 90% 9%
2	AI	161	93% 7%
2	AL	161	91% 9%
2	AO	161	94% 6%
2	AQ	161	96%
2	AS	161	93% 7%
2	AV	161	5% 91% 9%
2	AX	161	91% 9%
2	AZ	161	95% 5%
3	AE	161	44% 84% 15%
4	AK	169	92% 8%
5	BB	67	19% 85% 15%
5	BC	67	13% 88% 12%
6	BE	896	63% 9% 28%
7	BG	249	22% 77%
8	BH	317	6% 46% 7% 47%
9	BI	121	28% 70%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 37229 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 Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	160	1210	754	207	242	7	0	0
1	AC	160	1210	754	207	242	7	0	0
1	AH	160	1210	754	207	242	7	0	0
1	AJ	160	1210	754	207	242	7	0	0
1	AN	160	1210	754	207	242	7	0	0
1	AP	160	1210	754	207	242	7	0	0
1	AR	160	1210	754	207	242	7	0	0
1	AU	160	1210	754	207	242	7	0	0
1	AW	160	1210	754	207	242	7	0	0
1	AY	160	1210	754	207	242	7	0	0

- Molecule 2 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	161	1206	757	202	240	7	0	0
2	AD	161	1206	757	202	240	7	0	0
2	AF	161	1206	757	202	240	7	0	0
2	AI	161	1206	757	202	240	7	0	0
2	AL	161	1206	757	202	240	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AO	161	1206	757	202	240	7	0	0
2	AQ	161	1206	757	202	240	7	0	0
2	AS	161	1206	757	202	240	7	0	0
2	AV	161	1206	757	202	240	7	0	0
2	AX	161	1206	757	202	240	7	0	0
2	AZ	161	1206	757	202	240	7	0	0

- Molecule 3 is a protein called Allophycocyanin subunit alpha-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AE	160	1254	797	212	241	4	0	0

- Molecule 4 is a protein called Allophycocyanin subunit beta-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AK	169	1322	825	229	259	9	0	0

- Molecule 5 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BB	67	546	343	104	94	5	0	0
5	BC	67	546	343	104	94	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	36	TRP	SER	conflict	UNP Q01950
BC	36	TRP	SER	conflict	UNP Q01950

- Molecule 6 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BE	647	5124	3252	904	955	13	0	0

- Molecule 7 is a protein called Phycobilisome rod-core linker polypeptide CpcG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BG	57	451	282	87	80	2	0	0

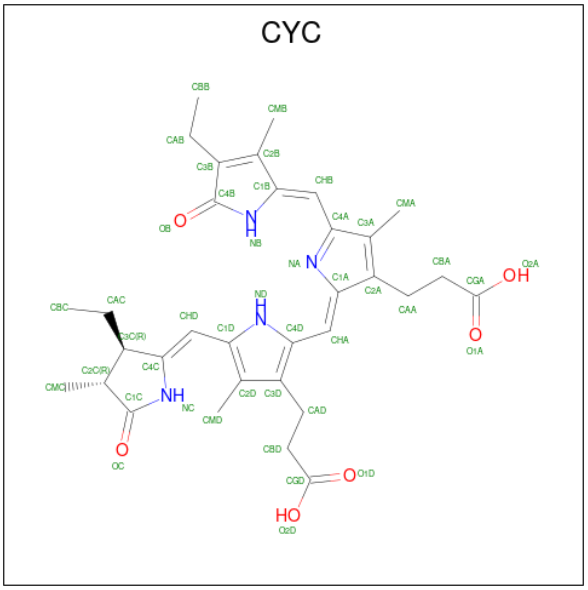
- Molecule 8 is a protein called Orange carotenoid-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BH	169	1269	809	215	237	8	0	0

- Molecule 9 is a protein called Sll1873 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BI	36	277	172	55	49	1	0	0

- Molecule 10 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	AA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	AB	1	43	33	4	6	0
10	AC	1	43	33	4	6	0
10	AD	1	43	33	4	6	0
10	AE	1	43	33	4	6	0
10	AF	1	43	33	4	6	0
10	AH	1	43	33	4	6	0
10	AI	1	43	33	4	6	0
10	AJ	1	43	33	4	6	0
10	AK	1	43	33	4	6	0
10	AL	1	43	33	4	6	0
10	AN	1	43	33	4	6	0
10	AO	1	43	33	4	6	0
10	AP	1	43	33	4	6	0
10	AQ	1	43	33	4	6	0
10	AR	1	43	33	4	6	0
10	AS	1	43	33	4	6	0
10	AU	1	43	33	4	6	0
10	AV	1	43	33	4	6	0
10	AW	1	43	33	4	6	0
10	AX	1	43	33	4	6	0
10	AY	1	43	33	4	6	0

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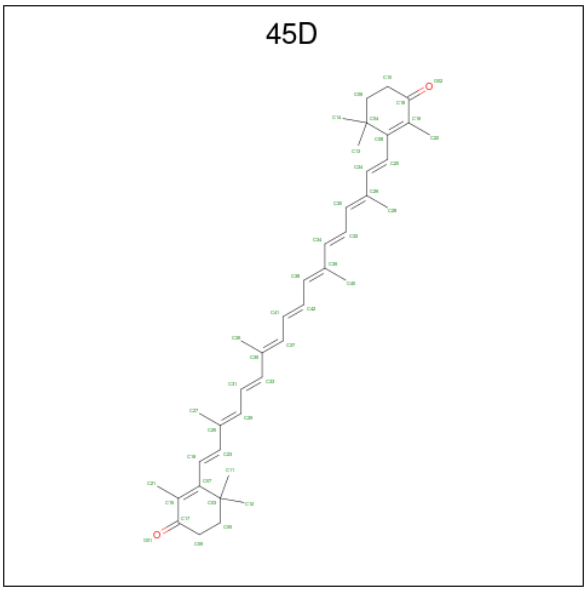
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	AZ	1	43	33	4	6	0
10	BE	1	43	33	4	6	0

- Molecule 11 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



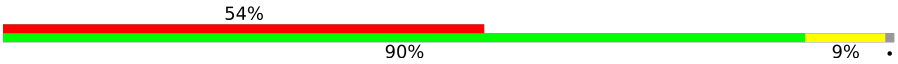
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	BH	1	42	40	2	0

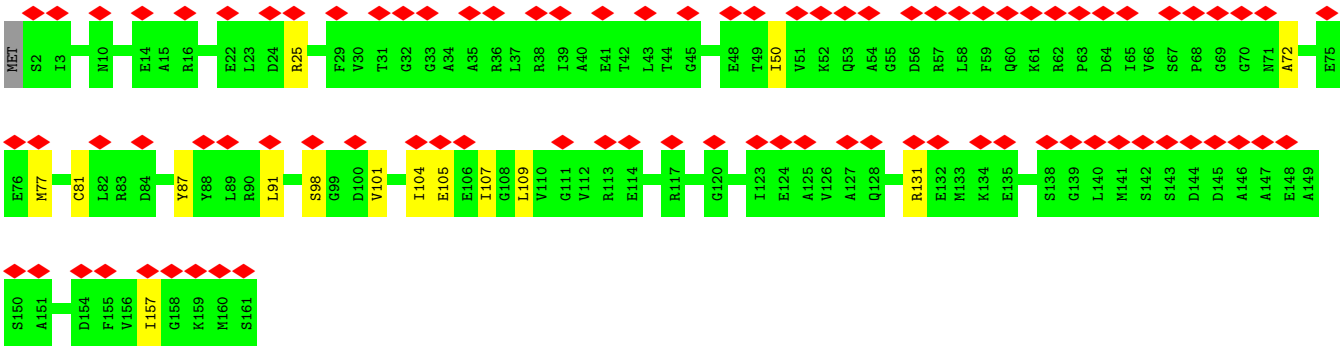
3 Residue-property plots (i)

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: Allophycocyanin alpha chain

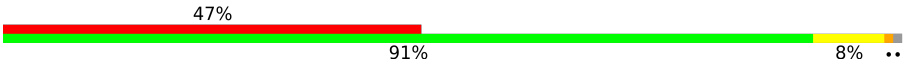
Chain AA:

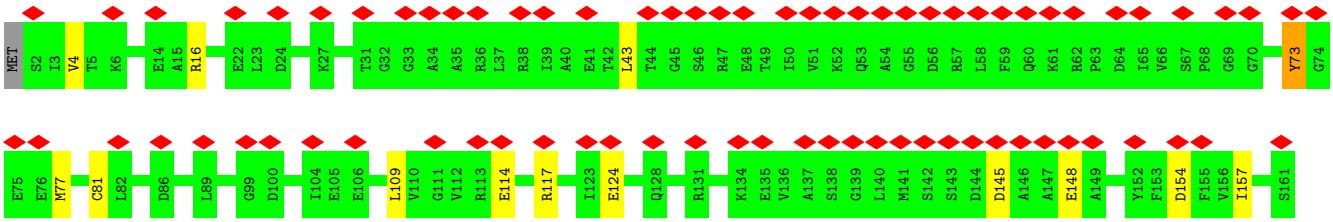




- Molecule 1: Allophycocyanin alpha chain

Chain AC:



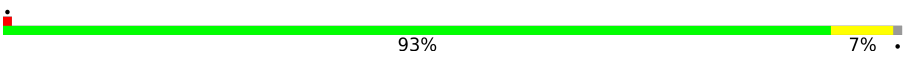


- Molecule 1: Allophycocyanin alpha chain

Chain AH:

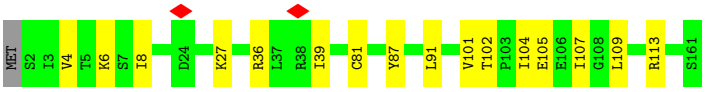
- Molecule 1: Allophycocyanin alpha chain

Chain AJ:



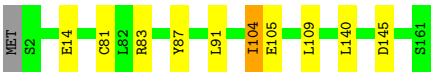
• Molecule 1: Allophycocyanin alpha chain

Chain AN:



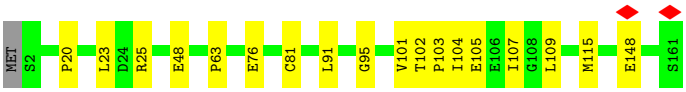
• Molecule 1: Allophycocyanin alpha chain

Chain AP:



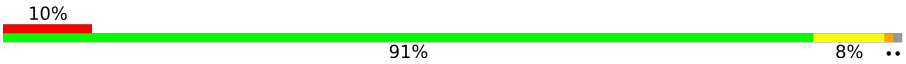
• Molecule 1: Allophycocyanin alpha chain

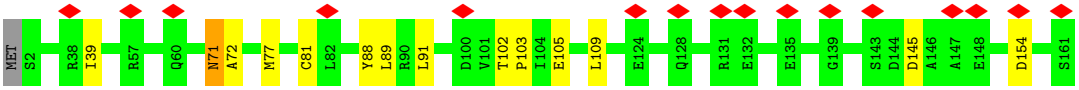
Chain AR:



• Molecule 1: Allophycocyanin alpha chain

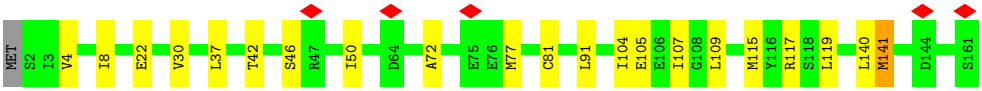
Chain AU:





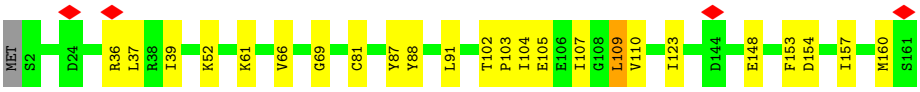
• Molecule 1: Allophycocyanin alpha chain

Chain AW:



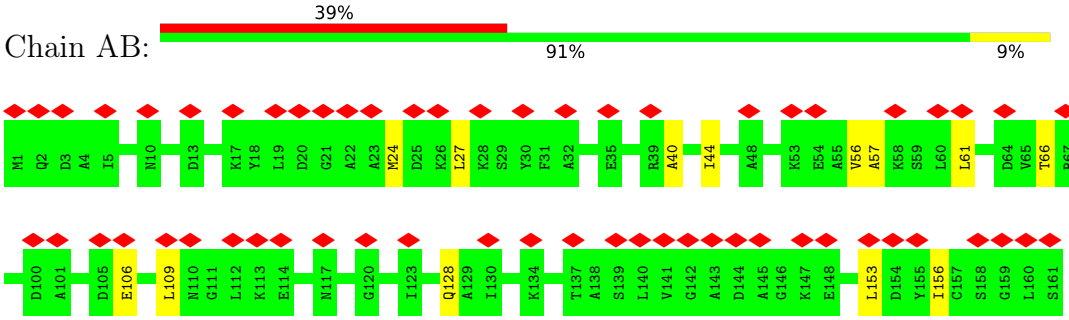
• Molecule 1: Allophycocyanin alpha chain

Chain AY:



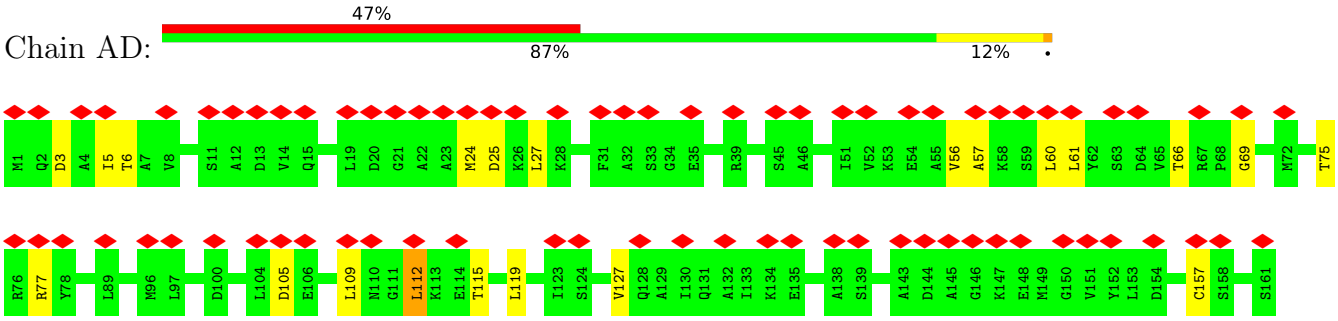
• Molecule 2: Allophycocyanin beta chain

Chain AB:



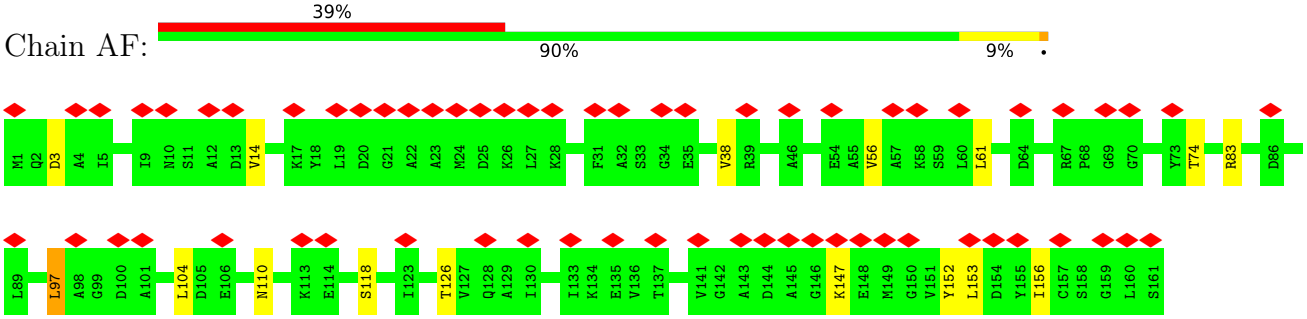
- Molecule 2: Allophycocyanin beta chain

Chain AD:



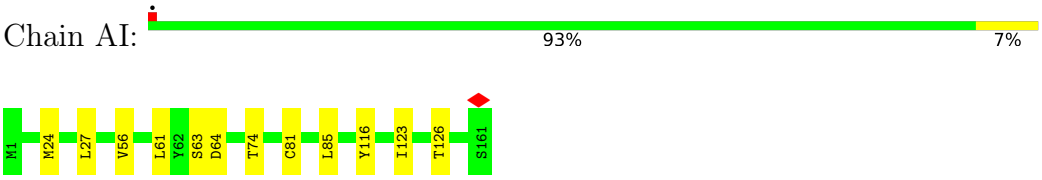
- Molecule 2: Allophycocyanin beta chain

Chain AF:



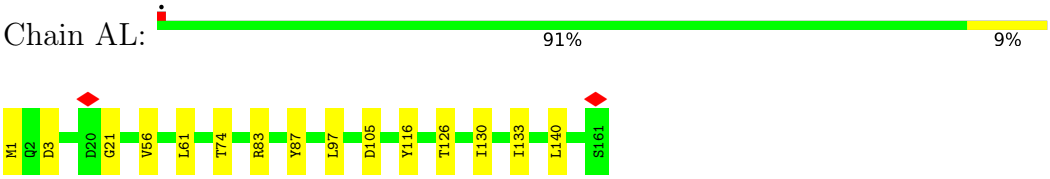
- Molecule 2: Allophycocyanin beta chain

Chain AI:



- Molecule 2: Allophycocyanin beta chain

Chain AL:

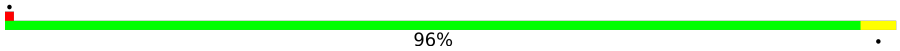


- Molecule 2: Allophycocyanin beta chain

Chain AO:

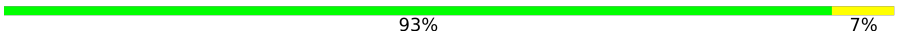
• Molecule 2: Allophycocyanin beta chain

Chain AQ:



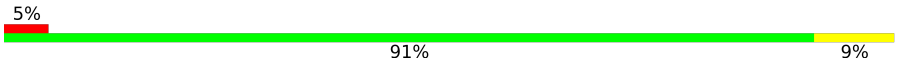
• Molecule 2: Allophycocyanin beta chain

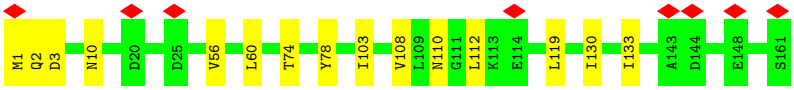
Chain AS:



• Molecule 2: Allophycocyanin beta chain

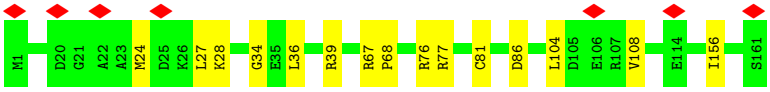
Chain AV:





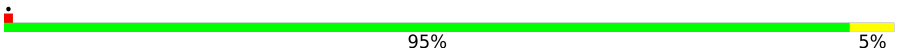
• Molecule 2: Allophycocyanin beta chain

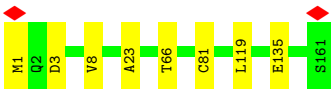
Chain AX:



• Molecule 2: Allophycocyanin beta chain

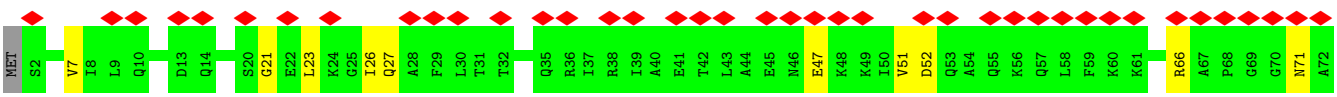
Chain AZ:

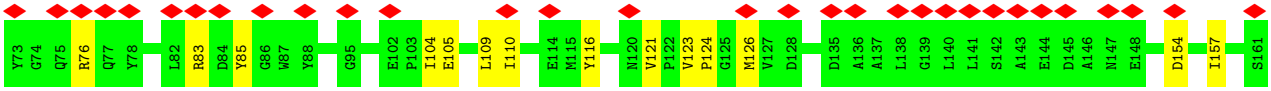




• Molecule 3: Allophycocyanin subunit alpha-B

Chain AE:



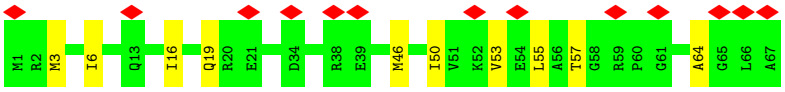


• Molecule 4: Allophycocyanin subunit beta-18

Chain AK:

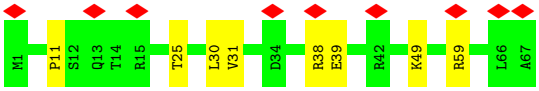
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain BB:



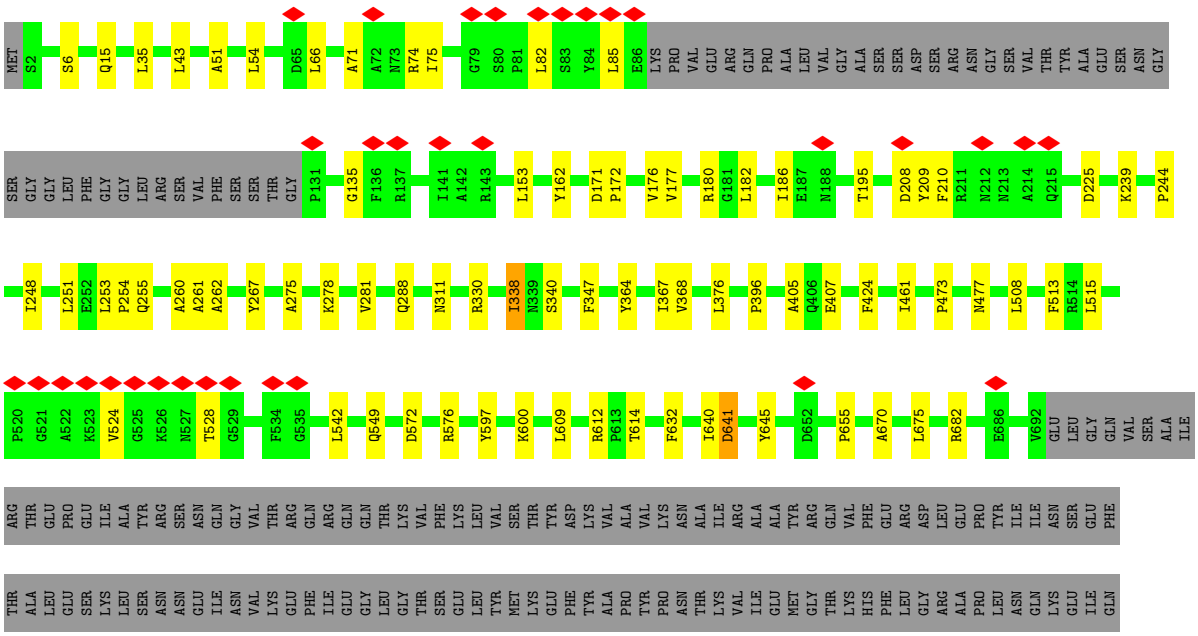
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

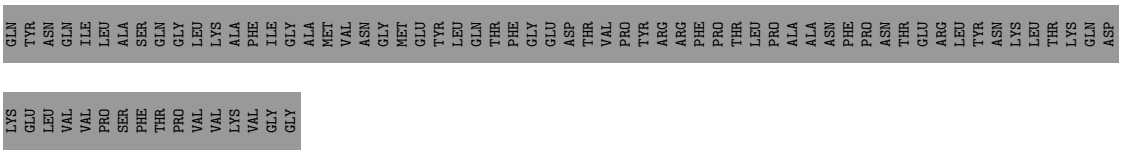
Chain BC:



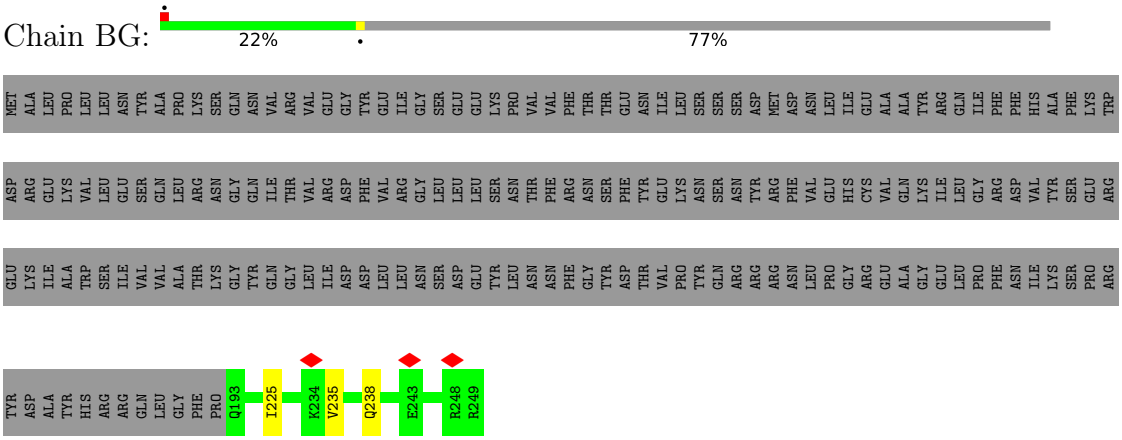
• Molecule 6: Phycobiliprotein ApcE

Chain BE:

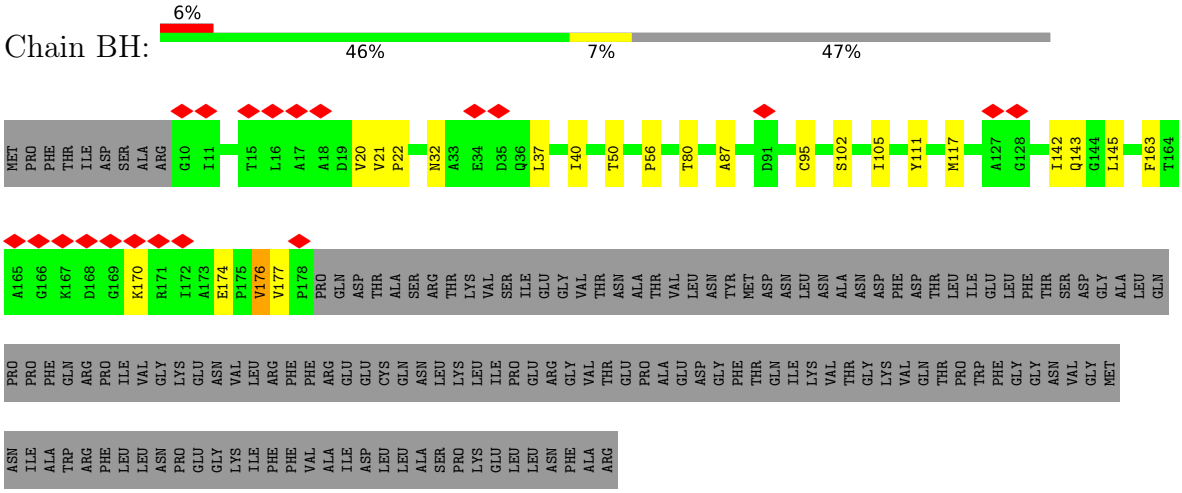




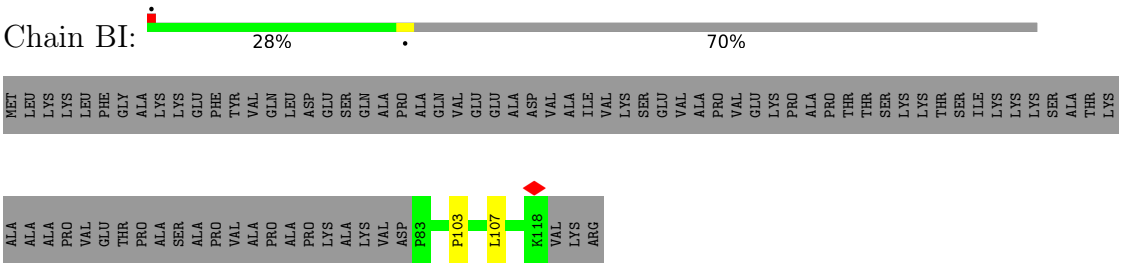
• Molecule 7: Phycobilisome rod-core linker polypeptide CpcG



• Molecule 8: Orange carotenoid-binding protein



• Molecule 9: Sll1873 protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	340838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.860	Depositor
Minimum map value	-0.607	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.457	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, 45D

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	AA	0.28	0/1225	0.57	0/1652
1	AC	0.28	0/1225	0.60	0/1652
1	AH	0.28	0/1225	0.58	0/1652
1	AJ	0.28	0/1225	0.57	0/1652
1	AN	0.28	0/1225	0.58	0/1652
1	AP	0.28	0/1225	0.57	0/1652
1	AR	0.28	0/1225	0.58	0/1652
1	AU	0.29	0/1225	0.58	0/1652
1	AW	0.28	0/1225	0.58	0/1652
1	AY	0.28	0/1225	0.58	0/1652
2	AB	0.27	0/1220	0.59	0/1650
2	AD	0.27	0/1220	0.58	0/1650
2	AF	0.27	0/1220	0.58	0/1650
2	AI	0.27	0/1220	0.56	0/1650
2	AL	0.27	0/1220	0.57	0/1650
2	AO	0.27	0/1220	0.56	0/1650
2	AQ	0.27	0/1220	0.58	0/1650
2	AS	0.27	0/1220	0.57	0/1650
2	AV	0.27	0/1220	0.58	0/1650
2	AX	0.27	0/1220	0.57	0/1650
2	AZ	0.27	0/1220	0.57	0/1650
3	AE	0.27	0/1277	0.57	0/1730
4	AK	0.26	0/1341	0.57	0/1813
5	BB	0.26	0/555	0.60	0/743
5	BC	0.26	0/555	0.59	0/743
6	BE	0.27	0/5236	0.58	0/7076
7	BG	0.27	0/459	0.62	0/620
8	BH	0.27	0/1294	0.59	0/1763
9	BI	0.29	0/283	0.61	0/381
All	All	0.27	0/36670	0.58	0/49539

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1210	0	1210	9	0
1	AC	1210	0	1210	4	0
1	AH	1210	0	1210	8	0
1	AJ	1210	0	1210	6	0
1	AN	1210	0	1210	12	0
1	AP	1210	0	1210	5	0
1	AR	1210	0	1210	12	0
1	AU	1210	0	1210	8	0
1	AW	1210	0	1210	15	0
1	AY	1210	0	1210	16	0
2	AB	1206	0	1218	8	0
2	AD	1206	0	1218	12	0
2	AF	1206	0	1218	11	0
2	AI	1206	0	1218	8	0
2	AL	1206	0	1218	7	0
2	AO	1206	0	1218	5	0
2	AQ	1206	0	1218	6	0
2	AS	1206	0	1218	8	0
2	AV	1206	0	1218	9	0
2	AX	1206	0	1218	8	0
2	AZ	1206	0	1218	3	0
3	AE	1254	0	1250	13	0
4	AK	1322	0	1311	8	0
5	BB	546	0	568	7	0
5	BC	546	0	568	5	0
6	BE	5124	0	5090	41	0
7	BG	451	0	465	2	0
8	BH	1269	0	1275	11	0
9	BI	277	0	283	1	0
10	AA	43	0	37	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AB	43	0	37	3	0
10	AC	43	0	37	1	0
10	AD	43	0	37	1	0
10	AE	43	0	37	2	0
10	AF	43	0	37	3	0
10	AH	43	0	37	3	0
10	AI	43	0	37	3	0
10	AJ	43	0	37	0	0
10	AK	43	0	37	1	0
10	AL	43	0	37	5	0
10	AN	43	0	37	2	0
10	AO	43	0	37	1	0
10	AP	43	0	37	3	0
10	AQ	43	0	37	2	0
10	AR	43	0	37	1	0
10	AS	43	0	37	4	0
10	AU	43	0	37	3	0
10	AV	43	0	37	3	0
10	AW	43	0	37	4	0
10	AX	43	0	37	3	0
10	AY	43	0	37	3	0
10	AZ	43	0	37	2	0
10	BE	43	0	37	2	0
11	BH	42	0	52	3	0
All	All	37229	0	37248	241	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 3.

All (241) 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:AW:105:GLU:HA	1:AW:109:LEU:HB2	1.66	0.76
1:AN:105:GLU:HA	1:AN:109:LEU:HB2	1.68	0.76
10:AL:200:CYC:HAA1	6:BE:424:PHE:HZ	1.51	0.75
6:BE:177:VAL:HG21	6:BE:260:ALA:HB2	1.68	0.74
8:BH:117:MET:HE1	11:BH:400:45D:H311	1.71	0.73
2:AB:106:GLU:HB2	5:BB:57:THR:HG23	1.72	0.72
1:AR:105:GLU:HA	1:AR:109:LEU:HB2	1.70	0.72
1:AJ:105:GLU:HA	1:AJ:109:LEU:HB2	1.75	0.68
1:AP:105:GLU:HA	1:AP:109:LEU:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BE:253:LEU:HB2	6:BE:405:ALA:HB2	1.76	0.67
10:AH:200:CYC:HMD2	10:AH:200:CYC:HC	1.61	0.64
1:AA:87:TYR:HB3	10:AA:200:CYC:HBB3	1.81	0.62
1:AN:91:LEU:HD11	1:AN:107:ILE:HB	1.81	0.62
1:AW:119:LEU:HG	10:AW:200:CYC:HHA	1.82	0.61
1:AY:87:TYR:HB3	10:AY:200:CYC:HBB3	1.83	0.61
10:AQ:200:CYC:HB	10:AQ:200:CYC:HMA1	1.64	0.61
2:AX:36:LEU:HD23	2:AX:39:ARG:HH12	1.66	0.60
4:AK:134:MET:O	4:AK:138:ILE:HG12	2.01	0.60
1:AC:73:TYR:H	1:AC:77:MET:HB2	1.65	0.60
4:AK:123:PRO:HB2	4:AK:126:PRO:HD2	1.83	0.59
1:AN:102:THR:HA	1:AN:105:GLU:HG2	1.84	0.59
2:AO:56:VAL:HG12	2:AO:61:LEU:HG	1.84	0.59
6:BE:195:THR:HG22	10:BE:1000:CYC:H2C	1.85	0.58
3:AE:105:GLU:HA	3:AE:109:LEU:HB2	1.85	0.57
3:AE:71:ASN:HD21	3:AE:121:VAL:HG22	1.70	0.56
8:BH:95:CYS:HB3	8:BH:163:PHE:H	1.70	0.56
10:AL:200:CYC:HAA1	6:BE:424:PHE:CZ	2.38	0.56
4:AK:84:ARG:HD3	6:BE:254:PRO:HD3	1.87	0.55
1:AY:61:LYS:HG3	8:BH:56:PRO:HG2	1.87	0.55
1:AW:91:LEU:HB3	1:AW:104:ILE:HG23	1.89	0.55
6:BE:15:GLN:HB3	6:BE:261:ALA:HA	1.89	0.55
8:BH:50:THR:HG21	8:BH:143:GLN:HE21	1.71	0.55
2:AI:74:THR:HG22	1:AJ:107:ILE:HG23	1.90	0.54
8:BH:102:SER:H	8:BH:105:ILE:HD12	1.72	0.54
1:AA:105:GLU:HA	1:AA:109:LEU:HB3	1.89	0.54
2:AQ:116:TYR:HE2	2:AQ:126:THR:HG21	1.72	0.54
3:AE:123:VAL:N	3:AE:124:PRO:HD2	2.22	0.54
5:BB:6:ILE:HG22	5:BB:53:VAL:HG12	1.90	0.54
1:AH:154:ASP:HA	1:AH:157:ILE:HD12	1.90	0.54
2:AF:56:VAL:HG12	2:AF:61:LEU:HG	1.90	0.54
3:AE:154:ASP:HA	3:AE:157:ILE:HD12	1.90	0.53
8:BH:21:VAL:HB	8:BH:22:PRO:HD3	1.89	0.53
2:AQ:74:THR:HG22	1:AR:107:ILE:HG23	1.90	0.53
2:AS:126:THR:HG22	10:AS:200:CYC:H3C	1.89	0.53
2:AV:74:THR:HG22	1:AW:107:ILE:HG23	1.91	0.52
2:AL:97:LEU:HD13	6:BE:35:LEU:HD12	1.91	0.52
1:AA:72:ALA:HA	1:AA:77:MET:HB3	1.91	0.52
3:AE:23:LEU:HA	3:AE:26:ILE:HD12	1.91	0.52
2:AD:57:ALA:HA	2:AD:61:LEU:HD12	1.90	0.52
10:AE:200:CYC:HMD2	10:AE:200:CYC:HC	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BE:267:TYR:HB3	6:BE:281:VAL:HG22	1.92	0.52
2:AX:67:ARG:HG3	2:AX:68:PRO:HD2	1.92	0.52
1:AW:30:VAL:HG21	2:AX:34:GLY:HA3	1.92	0.52
10:AF:200:CYC:HMA1	10:AF:200:CYC:HB	1.75	0.51
2:AF:83:ARG:HH22	10:AF:200:CYC:HBA2	1.74	0.51
6:BE:275:ALA:HA	6:BE:278:LYS:HB2	1.93	0.51
2:AD:119:LEU:HD13	10:AD:200:CYC:HHA	1.92	0.51
2:AL:56:VAL:HG12	2:AL:61:LEU:HG	1.93	0.51
10:AS:200:CYC:HMA1	10:AS:200:CYC:HB	1.75	0.51
1:AU:81:CYS:HA	10:AU:200:CYC:HHD	1.92	0.51
1:AW:4:VAL:O	1:AW:8:ILE:HG12	2.10	0.51
3:AE:116:TYR:HB3	3:AE:121:VAL:HB	1.92	0.51
2:AL:97:LEU:HD22	6:BE:43:LEU:HD13	1.93	0.50
1:AP:87:TYR:HB3	10:AP:200:CYC:HBB3	1.92	0.50
6:BE:251:LEU:HD11	6:BE:407:GLU:HB3	1.92	0.50
2:AL:116:TYR:HE2	2:AL:126:THR:HG21	1.76	0.50
1:AR:101:VAL:HG23	1:AR:104:ILE:HD12	1.92	0.50
1:AP:91:LEU:HB3	1:AP:104:ILE:HG23	1.93	0.50
1:AR:91:LEU:HB3	1:AR:104:ILE:HG23	1.94	0.50
1:AW:81:CYS:HA	10:AW:200:CYC:HHD	1.94	0.50
2:AI:56:VAL:HG12	2:AI:61:LEU:HG	1.94	0.50
6:BE:612:ARG:HH21	6:BE:614:THR:HA	1.76	0.50
2:AB:40:ALA:O	2:AB:44:ILE:HG12	2.11	0.50
6:BE:244:PRO:HG2	6:BE:248:ILE:HD13	1.94	0.50
6:BE:364:TYR:HA	6:BE:367:ILE:HD12	1.94	0.49
6:BE:670:ALA:HA	6:BE:675:LEU:HD13	1.93	0.49
1:AH:107:ILE:HG23	2:AL:74:THR:HG22	1.95	0.49
1:AA:101:VAL:HG12	1:AA:104:ILE:HD12	1.94	0.49
10:AL:200:CYC:HBC3	10:AL:200:CYC:HHD	1.93	0.49
1:AY:81:CYS:HA	10:AY:200:CYC:HHD	1.94	0.49
2:AD:24:MET:HA	2:AD:27:LEU:HD12	1.93	0.49
3:AE:21:GLY:HA3	1:AJ:3:ILE:HD11	1.93	0.49
1:AN:36:ARG:HA	1:AN:39:ILE:HD12	1.95	0.49
1:AR:81:CYS:HA	10:AR:200:CYC:HAC1	1.84	0.48
2:AX:76:ARG:HB2	1:AY:110:VAL:HG13	1.94	0.48
1:AN:4:VAL:O	1:AN:8:ILE:HG12	2.13	0.48
5:BB:19:GLN:HB2	6:BE:239:LYS:HG2	1.95	0.48
1:AA:81:CYS:HA	10:AA:200:CYC:HAC1	1.86	0.48
1:AR:95:GLY:HA3	1:AR:104:ILE:HD11	1.95	0.48
1:AC:81:CYS:HA	10:AC:200:CYC:HAC1	1.76	0.48
2:AB:153:LEU:HA	2:AB:156:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:105:GLU:HA	1:AU:109:LEU:HB3	1.96	0.48
2:AV:119:LEU:HD13	10:AV:200:CYC:HHA	1.96	0.48
1:AN:91:LEU:HD12	1:AN:104:ILE:HA	1.96	0.48
2:AS:110:ASN:HB3	6:BE:597:TYR:HB2	1.95	0.47
1:AW:81:CYS:HA	10:AW:200:CYC:HAC1	1.90	0.47
10:AB:200:CYC:HC	10:AB:200:CYC:HMD2	1.79	0.47
2:AF:118:SER:HB3	5:BB:55:LEU:HB2	1.96	0.47
1:AY:105:GLU:HA	1:AY:109:LEU:HB3	1.94	0.47
2:AQ:126:THR:HG23	10:AQ:200:CYC:HBC3	1.96	0.47
1:AY:88:TYR:HA	1:AY:91:LEU:HD12	1.95	0.47
2:AI:116:TYR:HE1	10:AI:200:CYC:HHB	1.79	0.47
2:AD:56:VAL:HG13	2:AD:60:LEU:HB2	1.97	0.47
5:BC:31:VAL:HG11	5:BC:39:GLU:HG2	1.97	0.47
1:AA:107:ILE:HG23	2:AF:74:THR:HG22	1.95	0.47
1:AY:81:CYS:HA	10:AY:200:CYC:HAC1	1.84	0.47
1:AY:102:THR:N	1:AY:103:PRO:HD2	2.30	0.47
6:BE:597:TYR:HB3	6:BE:600:LYS:HD2	1.96	0.47
2:AX:24:MET:HA	2:AX:27:LEU:HD12	1.97	0.47
2:AD:112:LEU:HA	2:AD:115:THR:HG22	1.97	0.47
6:BE:368:VAL:HB	6:BE:376:LEU:HD13	1.96	0.47
6:BE:576:ARG:HG3	6:BE:645:TYR:HE1	1.80	0.46
2:AD:5:ILE:HG22	2:AD:27:LEU:HD23	1.97	0.46
1:AY:91:LEU:HD21	1:AY:107:ILE:HB	1.97	0.46
6:BE:82:LEU:HD12	6:BE:85:LEU:HD12	1.97	0.46
8:BH:142:ILE:HA	8:BH:145:LEU:HD12	1.97	0.46
1:AJ:44:THR:HG22	4:AK:18:TYR:HD2	1.79	0.46
4:AK:82:CYS:HA	10:AK:200:CYC:HAC1	1.91	0.46
2:AB:56:VAL:HG12	2:AB:61:LEU:HG	1.98	0.46
3:AE:26:ILE:HD13	2:AF:97:LEU:HD21	1.97	0.46
3:AE:83:ARG:HH22	10:AE:200:CYC:HBA1	1.81	0.46
10:AL:200:CYC:HMD2	10:AL:200:CYC:NC	2.31	0.46
1:AN:87:TYR:HB3	10:AN:200:CYC:HBB3	1.97	0.46
1:AW:42:THR:HG21	1:AW:141:MET:HB3	1.98	0.46
1:AU:39:ILE:HG12	1:AU:145:ASP:HB3	1.98	0.46
8:BH:37:LEU:HD13	8:BH:87:ALA:HB2	1.98	0.46
6:BE:513:PHE:HB3	6:BE:542:LEU:HD12	1.98	0.45
1:AW:119:LEU:HD12	10:AW:200:CYC:HBD1	1.98	0.45
1:AH:83:ARG:HH22	10:AH:200:CYC:HBA2	1.81	0.45
1:AH:102:THR:N	1:AH:103:PRO:HD2	2.31	0.45
1:AR:63:PRO:HD2	1:AY:69:GLY:HA3	1.98	0.45
1:AR:102:THR:N	1:AR:103:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:88:TYR:HA	1:AU:91:LEU:HD12	1.98	0.45
2:AB:24:MET:HA	2:AB:27:LEU:HD12	1.97	0.45
2:AF:153:LEU:HA	2:AF:156:ILE:HD12	1.98	0.45
2:AV:1:MET:HG3	2:AV:103:ILE:HD12	1.98	0.45
2:AX:108:VAL:HA	10:AX:200:CYC:HBB2	1.98	0.45
6:BE:85:LEU:HG	6:BE:153:LEU:HD21	1.98	0.45
1:AA:107:ILE:HD11	5:BB:64:ALA:HB2	1.99	0.45
10:AB:200:CYC:HAA1	6:BE:311:ASN:HB2	1.99	0.45
2:AD:69:GLY:HA2	2:AF:14:VAL:HG13	1.98	0.45
3:AE:7:VAL:HG11	3:AE:26:ILE:HD11	1.98	0.45
2:AV:130:ILE:HA	2:AV:133:ILE:HD12	1.99	0.45
2:AV:56:VAL:HG12	2:AV:60:LEU:HD12	1.97	0.45
1:AA:91:LEU:HD22	1:AA:104:ILE:HA	1.98	0.45
6:BE:576:ARG:HH12	6:BE:641:ASP:HA	1.82	0.45
2:AX:81:CYS:HA	10:AX:200:CYC:HAC1	1.95	0.45
5:BC:30:LEU:HD12	6:BE:572:ASP:HB3	1.98	0.45
2:AI:123:ILE:HA	2:AI:126:THR:HG22	1.99	0.45
2:AS:153:LEU:HA	2:AS:156:ILE:HD12	1.98	0.45
8:BH:111:TYR:HB2	11:BH:400:45D:H341	1.99	0.45
1:AC:114:GLU:HA	1:AC:117:ARG:HB2	1.99	0.44
2:AD:105:ASP:HA	2:AD:109:LEU:HB2	1.99	0.44
2:AI:24:MET:HA	2:AI:27:LEU:HD12	1.99	0.44
2:AV:119:LEU:HD22	10:AV:200:CYC:HBD1	1.99	0.44
1:AY:91:LEU:HB3	1:AY:104:ILE:HG23	1.99	0.44
1:AH:105:GLU:HA	1:AH:109:LEU:HB3	1.99	0.44
1:AN:27:LYS:HG2	2:AO:38:VAL:HG11	1.99	0.44
1:AP:83:ARG:HH22	10:AP:200:CYC:HBA2	1.82	0.44
1:AR:91:LEU:HD22	1:AR:104:ILE:HA	1.98	0.44
1:AH:91:LEU:HB3	1:AH:104:ILE:HG23	2.00	0.44
2:AD:3:ASP:H	2:AD:6:THR:HB	1.83	0.44
1:AJ:91:LEU:HB3	1:AJ:104:ILE:HG23	1.99	0.44
10:AL:200:CYC:HMD2	10:AL:200:CYC:HC	1.82	0.44
2:AQ:56:VAL:HG12	2:AQ:60:LEU:HD12	2.00	0.44
9:BI:103:PRO:HB3	9:BI:107:LEU:HD12	2.00	0.44
2:AO:122:PRO:HB2	2:AO:125:SER:HB2	2.00	0.44
1:AP:81:CYS:HA	10:AP:200:CYC:HHD	1.99	0.44
1:AU:72:ALA:HA	1:AU:77:MET:HB3	1.99	0.44
8:BH:176:VAL:HG22	8:BH:177:VAL:H	1.83	0.44
3:AE:51:VAL:HG23	3:AE:85:TYR:HB3	2.00	0.44
1:AN:81:CYS:HA	10:AN:200:CYC:HAC1	1.91	0.44
2:AQ:115:THR:HG23	6:BE:461:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AY:66:VAL:HG21	7:BG:235:VAL:HG21	1.98	0.44
10:AZ:200:CYC:HAA1	5:BC:25:THR:HG21	1.99	0.44
2:AD:56:VAL:HG12	2:AD:61:LEU:HG	2.00	0.43
2:AD:127:VAL:HG13	2:AD:157:CYS:HB2	1.99	0.43
10:AH:200:CYC:HC	10:AH:200:CYC:CMD	2.28	0.43
2:AI:81:CYS:HA	10:AI:200:CYC:HAC1	1.98	0.43
2:AS:65:VAL:HG11	10:AS:200:CYC:HMC2	1.99	0.43
2:AB:109:LEU:HD11	2:AB:156:ILE:HA	2.01	0.43
2:AI:63:SER:HB3	6:BE:682:ARG:HB2	1.99	0.43
2:AL:83:ARG:HE	2:AL:87:TYR:HE2	1.65	0.43
1:AC:154:ASP:HA	1:AC:157:ILE:HD12	1.99	0.43
2:AQ:78:TYR:CD1	1:AR:115:MET:HG3	2.54	0.43
1:AY:36:ARG:HA	1:AY:39:ILE:HD12	2.00	0.43
6:BE:6:SER:HB3	6:BE:473:PRO:HB2	1.99	0.43
10:AV:200:CYC:NB	10:AV:200:CYC:HMA1	2.34	0.43
2:AX:104:LEU:HD22	2:AX:156:ILE:HD12	2.00	0.43
5:BB:3:MET:H	5:BB:57:THR:HB	1.84	0.43
2:AB:81:CYS:HA	10:AB:200:CYC:HAC1	1.99	0.43
6:BE:609:LEU:HD22	6:BE:640:ILE:HD11	2.01	0.43
1:AW:46:SER:O	1:AW:50:ILE:HG12	2.19	0.43
1:AY:123:ILE:HG13	1:AY:160:MET:HG3	2.00	0.43
6:BE:288:GLN:HG2	6:BE:396:PRO:HB2	2.01	0.43
4:AK:118:ASN:HB3	2:AS:122:PRO:HA	2.00	0.42
2:AS:119:LEU:HB3	2:AS:121:VAL:HG23	2.01	0.42
1:AA:131:ARG:HD3	1:AA:157:ILE:HG21	2.00	0.42
1:AN:101:VAL:HA	1:AN:104:ILE:HD12	2.01	0.42
1:AN:107:ILE:HG23	2:AS:74:THR:HG22	2.01	0.42
1:AU:81:CYS:HA	10:AU:200:CYC:HAC1	1.70	0.42
6:BE:176:VAL:O	6:BE:180:ARG:HB2	2.19	0.42
8:BH:40:ILE:HB	11:BH:400:45D:H421	2.01	0.42
1:AH:13:ALA:HB2	6:BE:330:ARG:HD2	2.01	0.42
2:AV:78:TYR:CD1	1:AW:115:MET:HG3	2.54	0.42
1:AW:72:ALA:HA	1:AW:77:MET:HB3	2.02	0.42
1:AY:153:PHE:O	1:AY:157:ILE:HG12	2.19	0.42
2:AV:2:GLN:HE21	2:AV:10:ASN:HD22	1.68	0.42
1:AJ:153:PHE:O	1:AJ:157:ILE:HG12	2.20	0.42
6:BE:171:ASP:HA	6:BE:172:PRO:HD3	1.92	0.42
1:AH:112:VAL:HG12	1:AH:123:ILE:HD11	2.02	0.42
1:AU:102:THR:N	1:AU:103:PRO:HD2	2.35	0.42
4:AK:167:LEU:HD22	6:BE:477:ASN:HB2	2.02	0.42
2:AD:75:THR:HG23	3:AE:110:ILE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AF:110:ASN:HB3	5:BB:50:ILE:HD12	2.02	0.41
2:AF:126:THR:HG22	10:AF:200:CYC:H3C	2.02	0.41
2:AZ:81:CYS:HA	10:AZ:200:CYC:HAC1	1.89	0.41
6:BE:51:ALA:HA	6:BE:54:LEU:HD12	2.01	0.41
2:AL:130:ILE:HA	2:AL:133:ILE:HD12	2.02	0.41
2:AO:85:LEU:HG	10:AO:200:CYC:HBC1	2.02	0.41
1:AR:25:ARG:HH22	1:AW:22:GLU:HG3	1.86	0.41
10:AS:200:CYC:HMA1	10:AS:200:CYC:NB	2.35	0.41
6:BE:338:ILE:HG23	6:BE:340:SER:H	1.84	0.41
2:AZ:8:VAL:HG13	2:AZ:23:ALA:HB1	2.02	0.41
6:BE:71:ALA:O	6:BE:75:ILE:HG12	2.21	0.41
2:AI:85:LEU:HG	10:AI:200:CYC:HBC1	2.03	0.41
2:AB:57:ALA:HA	2:AB:61:LEU:HD12	2.03	0.41
1:AU:71:ASN:HD21	10:AU:200:CYC:HBD2	1.86	0.41
2:AZ:119:LEU:HD21	5:BC:11:PRO:HB3	2.03	0.41
3:AE:27:GLN:HG3	2:AF:38:VAL:HG11	2.03	0.40
1:AN:113:ARG:HH21	1:AW:117:ARG:HD3	1.86	0.40
2:AS:130:ILE:HA	2:AS:133:ILE:HD12	2.02	0.40
2:AV:110:ASN:HD21	5:BC:49:LYS:HA	1.86	0.40
1:AY:52:LYS:HD2	7:BG:238:GLN:HA	2.01	0.40
6:BE:549:GLN:HG2	6:BE:655:PRO:HB2	2.03	0.40
2:AF:104:LEU:HD11	2:AF:152:TYR:HB3	2.04	0.40
4:AK:90:LEU:HD11	4:AK:138:ILE:HD11	2.04	0.40
2:AO:96:MET:HG3	2:AO:149:MET:HG2	2.02	0.40
1:AR:20:PRO:HA	1:AR:23:LEU:HB2	2.03	0.40
10:AX:200:CYC:HMD2	10:AX:200:CYC:NC	2.37	0.40
6:BE:182:LEU:HD11	10:BE:1000:CYC:CHB	2.51	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	AA	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	AC	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	43
1	AH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	AJ	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
1	AN	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	AP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	AR	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	AU	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	AW	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	AY	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	25	43
2	AB	159/161 (99%)	150 (94%)	9 (6%)	0	100	100
2	AD	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	AF	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	AI	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	AL	159/161 (99%)	154 (97%)	4 (2%)	1 (1%)	25	43
2	AO	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
2	AQ	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	AS	159/161 (99%)	150 (94%)	9 (6%)	0	100	100
2	AV	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	AX	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	AZ	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
3	AE	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
4	AK	167/169 (99%)	161 (96%)	6 (4%)	0	100	100
5	BB	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
5	BC	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
6	BE	643/896 (72%)	598 (93%)	40 (6%)	5 (1%)	19	35
7	BG	55/249 (22%)	54 (98%)	1 (2%)	0	100	100
8	BH	167/317 (53%)	154 (92%)	11 (7%)	2 (1%)	13	24
9	BI	34/121 (28%)	33 (97%)	1 (3%)	0	100	100
All	All	4683/5428 (86%)	4506 (96%)	167 (4%)	10 (0%)	50	68

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	BH	176	VAL
6	BE	135	GLY
6	BE	262	ALA
1	AC	109	LEU
2	AL	21	GLY
6	BE	528	THR
1	AY	109	LEU
6	BE	210	PHE
6	BE	524	VAL
8	BH	20	VAL

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	AA	128/129 (99%)	125 (98%)	3 (2%)	50	76
1	AC	128/129 (99%)	121 (94%)	7 (6%)	21	41
1	AH	128/129 (99%)	125 (98%)	3 (2%)	50	76
1	AJ	128/129 (99%)	126 (98%)	2 (2%)	62	84
1	AN	128/129 (99%)	127 (99%)	1 (1%)	81	93
1	AP	128/129 (99%)	124 (97%)	4 (3%)	40	67
1	AR	128/129 (99%)	125 (98%)	3 (2%)	50	76
1	AU	128/129 (99%)	125 (98%)	3 (2%)	50	76
1	AW	128/129 (99%)	125 (98%)	3 (2%)	50	76
1	AY	128/129 (99%)	125 (98%)	3 (2%)	50	76
2	AB	125/125 (100%)	123 (98%)	2 (2%)	62	84
2	AD	125/125 (100%)	121 (97%)	4 (3%)	39	65
2	AF	125/125 (100%)	122 (98%)	3 (2%)	49	74
2	AI	125/125 (100%)	124 (99%)	1 (1%)	81	93
2	AL	125/125 (100%)	121 (97%)	4 (3%)	39	65
2	AO	125/125 (100%)	124 (99%)	1 (1%)	81	93
2	AQ	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AS	125/125 (100%)	124 (99%)	1 (1%)	81	93
2	AV	125/125 (100%)	122 (98%)	3 (2%)	49	74
2	AX	125/125 (100%)	122 (98%)	3 (2%)	49	74
2	AZ	125/125 (100%)	121 (97%)	4 (3%)	39	65
3	AE	132/133 (99%)	126 (96%)	6 (4%)	27	51
4	AK	140/140 (100%)	137 (98%)	3 (2%)	53	78
5	BB	58/58 (100%)	56 (97%)	2 (3%)	37	63
5	BC	58/58 (100%)	56 (97%)	2 (3%)	37	63
6	BE	541/753 (72%)	527 (97%)	14 (3%)	46	72
7	BG	49/221 (22%)	48 (98%)	1 (2%)	55	79
8	BH	129/257 (50%)	125 (97%)	4 (3%)	40	67
9	BI	30/98 (31%)	30 (100%)	0	100	100
All	All	3792/4383 (86%)	3702 (98%)	90 (2%)	51	74

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	25	ARG
1	AA	50	ILE
1	AA	98	SER
2	AB	66	THR
2	AB	128	GLN
1	AC	4	VAL
1	AC	16	ARG
1	AC	43	LEU
1	AC	73	TYR
1	AC	124	GLU
1	AC	145	ASP
1	AC	148	GLU
2	AD	25	ASP
2	AD	66	THR
2	AD	77	ARG
2	AD	112	LEU
3	AE	47	GLU
3	AE	52	ASP
3	AE	66	ARG
3	AE	76	ARG
3	AE	104	ILE

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Mol	Chain	Res	Type
3	AE	126	MET
2	AF	3	ASP
2	AF	97	LEU
2	AF	147	LYS
1	AH	53	GLN
1	AH	76	GLU
1	AH	84	ASP
2	AI	64	ASP
1	AJ	25	ARG
1	AJ	145	ASP
4	AK	61	GLU
4	AK	105	LEU
4	AK	113	LEU
2	AL	1	MET
2	AL	3	ASP
2	AL	105	ASP
2	AL	140	LEU
1	AN	6	LYS
2	AO	140	LEU
1	AP	14	GLU
1	AP	104	ILE
1	AP	140	LEU
1	AP	145	ASP
1	AR	48	GLU
1	AR	76	GLU
1	AR	148	GLU
2	AS	149	MET
1	AU	71	ASN
1	AU	89	LEU
1	AU	154	ASP
2	AV	3	ASP
2	AV	108	VAL
2	AV	112	LEU
1	AW	37	LEU
1	AW	140	LEU
1	AW	141	MET
2	AX	28	LYS
2	AX	77	ARG
2	AX	86	ASP
1	AY	37	LEU
1	AY	148	GLU
1	AY	154	ASP

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Mol	Chain	Res	Type
2	AZ	1	MET
2	AZ	3	ASP
2	AZ	66	THR
2	AZ	135	GLU
5	BB	16	ILE
5	BB	46	MET
5	BC	38	ARG
5	BC	59	ARG
6	BE	66	LEU
6	BE	74	ARG
6	BE	162	TYR
6	BE	186	ILE
6	BE	208	ASP
6	BE	209	TYR
6	BE	225	ASP
6	BE	255	GLN
6	BE	338	ILE
6	BE	347	PHE
6	BE	508	LEU
6	BE	515	LEU
6	BE	632	PHE
6	BE	641	ASP
7	BG	225	ILE
8	BH	32	ASN
8	BH	80	THR
8	BH	170	LYS
8	BH	174	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	128	GLN
2	AB	110	ASN
3	AE	71	ASN
3	AE	117	ASN
4	AK	72	ASN
2	AO	10	ASN
2	AO	71	ASN
2	AQ	71	ASN
1	AU	71	ASN
2	AV	10	ASN
5	BC	41	GLN

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Mol	Chain	Res	Type
6	BE	30	GLN
6	BE	200	GLN
6	BE	213	ASN
6	BE	215	GLN
6	BE	451	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	CYC	AN	200	1	42,46,46	1.10	1 (2%)	50,67,67	1.08	3 (6%)
10	CYC	AW	200	1	42,46,46	1.08	1 (2%)	50,67,67	0.92	2 (4%)
10	CYC	AJ	200	1	42,46,46	1.09	1 (2%)	50,67,67	0.99	3 (6%)
10	CYC	AH	200	1	42,46,46	1.08	1 (2%)	50,67,67	1.12	5 (10%)
10	CYC	AK	200	4	42,46,46	1.08	1 (2%)	50,67,67	1.11	4 (8%)
10	CYC	AO	200	2	42,46,46	1.06	1 (2%)	50,67,67	1.05	3 (6%)
10	CYC	AZ	200	2	42,46,46	1.10	1 (2%)	50,67,67	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	CYC	AP	200	1	42,46,46	1.08	1 (2%)	50,67,67	1.04	3 (6%)
11	45D	BH	400	-	43,43,43	1.20	7 (16%)	54,60,60	1.53	9 (16%)
10	CYC	AS	200	2	42,46,46	0.99	1 (2%)	50,67,67	1.01	2 (4%)
10	CYC	AU	200	1	42,46,46	1.09	1 (2%)	50,67,67	1.00	3 (6%)
10	CYC	AQ	200	2	42,46,46	1.11	1 (2%)	50,67,67	0.99	2 (4%)
10	CYC	AY	200	1	42,46,46	1.13	1 (2%)	50,67,67	1.09	4 (8%)
10	CYC	AA	200	1	42,46,46	1.11	1 (2%)	50,67,67	1.07	3 (6%)
10	CYC	AI	200	2	42,46,46	1.09	1 (2%)	50,67,67	0.98	2 (4%)
10	CYC	AB	200	2	42,46,46	1.07	1 (2%)	50,67,67	1.04	3 (6%)
10	CYC	AE	200	3	42,46,46	1.16	1 (2%)	50,67,67	1.02	4 (8%)
10	CYC	AL	200	2	42,46,46	1.08	1 (2%)	50,67,67	1.13	4 (8%)
10	CYC	AF	200	2	42,46,46	1.14	1 (2%)	50,67,67	1.07	3 (6%)
10	CYC	AC	200	1	42,46,46	1.11	1 (2%)	50,67,67	0.98	3 (6%)
10	CYC	AD	200	2	42,46,46	1.09	1 (2%)	50,67,67	0.99	3 (6%)
10	CYC	AR	200	1	42,46,46	1.09	1 (2%)	50,67,67	1.00	3 (6%)
10	CYC	BE	1000	6	42,46,46	1.14	1 (2%)	50,67,67	1.01	2 (4%)
10	CYC	AX	200	2	42,46,46	1.12	1 (2%)	50,67,67	0.99	2 (4%)
10	CYC	AV	200	2	42,46,46	1.10	1 (2%)	50,67,67	1.04	3 (6%)

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
10	CYC	AN	200	1	-	13/25/74/74	0/4/4/4
10	CYC	AW	200	1	-	18/25/74/74	0/4/4/4
10	CYC	AJ	200	1	-	12/25/74/74	0/4/4/4
10	CYC	AH	200	1	-	12/25/74/74	0/4/4/4
10	CYC	AK	200	4	-	13/25/74/74	0/4/4/4
10	CYC	AO	200	2	-	11/25/74/74	0/4/4/4
10	CYC	AZ	200	2	-	7/25/74/74	0/4/4/4
10	CYC	AP	200	1	-	14/25/74/74	0/4/4/4
11	45D	BH	400	-	-	15/29/69/69	0/2/2/2
10	CYC	AS	200	2	-	12/25/74/74	0/4/4/4
10	CYC	AU	200	1	-	13/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CYC	AQ	200	2	-	15/25/74/74	0/4/4/4
10	CYC	AY	200	1	-	15/25/74/74	0/4/4/4
10	CYC	AA	200	1	-	17/25/74/74	0/4/4/4
10	CYC	AI	200	2	-	15/25/74/74	0/4/4/4
10	CYC	AB	200	2	-	9/25/74/74	0/4/4/4
10	CYC	AE	200	3	-	13/25/74/74	0/4/4/4
10	CYC	AL	200	2	-	8/25/74/74	0/4/4/4
10	CYC	AF	200	2	-	15/25/74/74	0/4/4/4
10	CYC	AC	200	1	-	9/25/74/74	0/4/4/4
10	CYC	AD	200	2	-	14/25/74/74	0/4/4/4
10	CYC	AR	200	1	-	12/25/74/74	0/4/4/4
10	CYC	BE	1000	6	-	15/25/74/74	0/4/4/4
10	CYC	AX	200	2	-	14/25/74/74	0/4/4/4
10	CYC	AV	200	2	-	16/25/74/74	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AE	200	CYC	CHA-C1A	5.79	1.40	1.35
10	AF	200	CYC	CHA-C1A	5.75	1.39	1.35
10	BE	1000	CYC	CHA-C1A	5.70	1.39	1.35
10	AY	200	CYC	CHA-C1A	5.57	1.39	1.35
10	AX	200	CYC	CHA-C1A	5.55	1.39	1.35
10	AQ	200	CYC	CHA-C1A	5.50	1.39	1.35
10	AV	200	CYC	CHA-C1A	5.47	1.39	1.35
10	AA	200	CYC	CHA-C1A	5.39	1.39	1.35
10	AC	200	CYC	CHA-C1A	5.38	1.39	1.35
10	AU	200	CYC	CHA-C1A	5.35	1.39	1.35
10	AD	200	CYC	CHA-C1A	5.29	1.39	1.35
10	AP	200	CYC	CHA-C1A	5.29	1.39	1.35
10	AN	200	CYC	CHA-C1A	5.28	1.39	1.35
10	AJ	200	CYC	CHA-C1A	5.26	1.39	1.35
10	AR	200	CYC	CHA-C1A	5.25	1.39	1.35
10	AZ	200	CYC	CHA-C1A	5.18	1.39	1.35
10	AI	200	CYC	CHA-C1A	5.15	1.39	1.35
10	AH	200	CYC	CHA-C1A	5.08	1.39	1.35
10	AW	200	CYC	CHA-C1A	5.05	1.39	1.35
10	AB	200	CYC	CHA-C1A	5.00	1.39	1.35
10	AK	200	CYC	CHA-C1A	4.99	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AL	200	CYC	CHA-C1A	4.98	1.39	1.35
10	AO	200	CYC	CHA-C1A	4.95	1.39	1.35
10	AS	200	CYC	CHA-C1A	4.58	1.38	1.35
11	BH	400	45D	C34-C36	3.90	1.54	1.45
11	BH	400	45D	C04-C08	3.07	1.58	1.53
11	BH	400	45D	C09-C17	2.49	1.54	1.50
11	BH	400	45D	C03-C07	2.46	1.57	1.53
11	BH	400	45D	C24-C20	2.17	1.39	1.33
11	BH	400	45D	C27-C25	2.08	1.55	1.50
11	BH	400	45D	C39-C35	2.08	1.55	1.50

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	BH	400	45D	C42-C38-C36	4.66	133.96	127.31
11	BH	400	45D	C06-C04-C08	3.82	116.36	110.48
10	AL	200	CYC	CAC-C3C-C4C	3.66	122.08	112.67
10	AF	200	CYC	CMB-C2B-C1B	3.50	128.53	124.17
10	AY	200	CYC	CMB-C2B-C1B	3.32	128.31	124.17
10	AO	200	CYC	CMB-C2B-C1B	3.25	128.22	124.17
10	AK	200	CYC	CHA-C1A-NA	-3.25	124.32	128.83
10	AN	200	CYC	CMB-C2B-C1B	3.21	128.17	124.17
10	AA	200	CYC	CMB-C2B-C1B	3.19	128.16	124.17
10	AD	200	CYC	CHA-C1A-NA	-3.19	124.40	128.83
10	AZ	200	CYC	CMB-C2B-C1B	3.19	128.15	124.17
10	AB	200	CYC	CMB-C2B-C1B	3.18	128.14	124.17
10	AE	200	CYC	CHA-C1A-NA	-3.17	124.44	128.83
10	AC	200	CYC	CHA-C1A-NA	-3.16	124.44	128.83
10	AL	200	CYC	CMB-C2B-C1B	3.12	128.06	124.17
10	AH	200	CYC	CHA-C1A-NA	-3.09	124.55	128.83
10	AH	200	CYC	CMB-C2B-C1B	3.07	128.00	124.17
10	AI	200	CYC	CMB-C2B-C1B	3.07	128.00	124.17
10	BE	1000	CYC	CHA-C1A-NA	-3.07	124.57	128.83
10	AR	200	CYC	CMB-C2B-C1B	3.05	127.98	124.17
10	AK	200	CYC	CMB-C2B-C1B	3.05	127.98	124.17
10	AV	200	CYC	CHA-C1A-NA	-3.05	124.59	128.83
10	AW	200	CYC	CHA-C1A-NA	-3.05	124.59	128.83
10	AP	200	CYC	CMB-C2B-C1B	3.05	127.97	124.17
10	AU	200	CYC	CHA-C1A-NA	-3.02	124.64	128.83
10	AP	200	CYC	CHA-C1A-NA	-3.01	124.66	128.83
10	AH	200	CYC	CAC-C3C-C4C	2.94	120.23	112.67
10	AU	200	CYC	CMB-C2B-C1B	2.94	127.84	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	AL	200	CYC	CHA-C1A-NA	-2.93	124.77	128.83
10	AS	200	CYC	CMB-C2B-C1B	2.91	127.79	124.17
11	BH	400	45D	C05-C03-C07	2.90	114.95	110.48
10	BE	1000	CYC	CMB-C2B-C1B	2.90	127.79	124.17
10	AJ	200	CYC	CHA-C1A-NA	-2.90	124.81	128.83
10	AJ	200	CYC	CMB-C2B-C1B	2.87	127.75	124.17
10	AI	200	CYC	CHA-C1A-NA	-2.87	124.84	128.83
10	AB	200	CYC	CHA-C1A-NA	-2.87	124.85	128.83
10	AQ	200	CYC	CHA-C1A-NA	-2.87	124.85	128.83
10	AC	200	CYC	CMB-C2B-C1B	2.86	127.74	124.17
10	AN	200	CYC	CHA-C1A-NA	-2.86	124.87	128.83
10	AE	200	CYC	CMB-C2B-C1B	2.83	127.70	124.17
10	AR	200	CYC	CHA-C1A-NA	-2.82	124.92	128.83
10	AZ	200	CYC	CHA-C1A-NA	-2.80	124.94	128.83
10	AS	200	CYC	CHA-C1A-NA	-2.79	124.95	128.83
10	AA	200	CYC	CHA-C1A-NA	-2.79	124.96	128.83
10	AY	200	CYC	CHA-C1A-NA	-2.79	124.96	128.83
10	AQ	200	CYC	CMB-C2B-C1B	2.78	127.64	124.17
10	AV	200	CYC	CMB-C2B-C1B	2.77	127.63	124.17
10	AD	200	CYC	CMB-C2B-C1B	2.77	127.62	124.17
11	BH	400	45D	C10-C18-C16	2.75	121.20	118.65
10	AF	200	CYC	CHA-C1A-NA	-2.74	125.02	128.83
10	AX	200	CYC	CHA-C1A-NA	-2.74	125.03	128.83
10	AP	200	CYC	C1B-NB-C4B	-2.69	107.24	110.67
10	AX	200	CYC	CMB-C2B-C1B	2.63	127.45	124.17
10	AW	200	CYC	CMB-C2B-C1B	2.63	127.45	124.17
10	AK	200	CYC	C1B-NB-C4B	-2.62	107.33	110.67
10	AO	200	CYC	CHA-C1A-NA	-2.61	125.21	128.83
10	AN	200	CYC	C1B-NB-C4B	-2.58	107.38	110.67
10	AY	200	CYC	C1B-NB-C4B	-2.56	107.41	110.67
10	AO	200	CYC	C1B-NB-C4B	-2.50	107.48	110.67
10	AB	200	CYC	C1B-NB-C4B	-2.47	107.53	110.67
10	AA	200	CYC	C1B-NB-C4B	-2.46	107.53	110.67
10	AZ	200	CYC	C1B-NB-C4B	-2.39	107.63	110.67
10	AL	200	CYC	C1B-NB-C4B	-2.30	107.74	110.67
10	AV	200	CYC	C1B-CHB-C4A	2.29	133.69	128.08
11	BH	400	45D	C32-C34-C36	-2.29	119.98	126.42
10	AE	200	CYC	C2C-C3C-C4C	2.26	104.72	101.34
10	AF	200	CYC	C1B-NB-C4B	-2.25	107.80	110.67
11	BH	400	45D	C31-C29-C25	2.25	130.51	127.31
10	AC	200	CYC	C1B-NB-C4B	-2.22	107.84	110.67
10	AY	200	CYC	C1B-CHB-C4A	2.20	133.45	128.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	AK	200	CYC	C2C-C3C-C4C	2.17	104.59	101.34
10	AJ	200	CYC	C1B-NB-C4B	-2.16	107.91	110.67
11	BH	400	45D	C23-C19-C07	-2.15	121.17	127.20
10	AH	200	CYC	C2C-C3C-C4C	2.15	104.55	101.34
10	AU	200	CYC	C1B-NB-C4B	-2.13	107.96	110.67
10	AH	200	CYC	C1B-NB-C4B	-2.12	107.97	110.67
10	AD	200	CYC	C1B-NB-C4B	-2.08	108.02	110.67
11	BH	400	45D	C10-C06-C04	2.08	116.52	113.18
10	AE	200	CYC	C1B-NB-C4B	-2.06	108.05	110.67
11	BH	400	45D	C22-C16-C18	2.02	118.49	115.48
10	AR	200	CYC	C1B-NB-C4B	-2.00	108.12	110.67

There are no chirality outliers.

All (327) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	AA	200	CYC	NA-C1A-CHA-C4D
10	AA	200	CYC	ND-C4D-CHA-C1A
10	AA	200	CYC	C3D-C4D-CHA-C1A
10	AA	200	CYC	NA-C4A-CHB-C1B
10	AA	200	CYC	C3A-C4A-CHB-C1B
10	AA	200	CYC	C2C-C3C-CAC-CBC
10	AA	200	CYC	C4C-C3C-CAC-CBC
10	AA	200	CYC	C2D-C1D-CHD-C4C
10	AB	200	CYC	NA-C4A-CHB-C1B
10	AB	200	CYC	C3A-C4A-CHB-C1B
10	AB	200	CYC	C2C-C3C-CAC-CBC
10	AB	200	CYC	C4C-C3C-CAC-CBC
10	AC	200	CYC	NA-C4A-CHB-C1B
10	AC	200	CYC	C3A-C4A-CHB-C1B
10	AC	200	CYC	C2C-C3C-CAC-CBC
10	AC	200	CYC	C4C-C3C-CAC-CBC
10	AD	200	CYC	NA-C1A-CHA-C4D
10	AD	200	CYC	C2A-C1A-CHA-C4D
10	AD	200	CYC	ND-C4D-CHA-C1A
10	AD	200	CYC	C3D-C4D-CHA-C1A
10	AD	200	CYC	NA-C4A-CHB-C1B
10	AD	200	CYC	C3A-C4A-CHB-C1B
10	AD	200	CYC	C2C-C3C-CAC-CBC
10	AD	200	CYC	C4C-C3C-CAC-CBC
10	AE	200	CYC	NA-C1A-CHA-C4D
10	AE	200	CYC	ND-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
10	AE	200	CYC	C3D-C4D-CHA-C1A
10	AE	200	CYC	NA-C4A-CHB-C1B
10	AE	200	CYC	C3A-C4A-CHB-C1B
10	AE	200	CYC	C4C-C3C-CAC-CBC
10	AE	200	CYC	C3D-CAD-CBD-CGD
10	AF	200	CYC	ND-C4D-CHA-C1A
10	AF	200	CYC	C3D-C4D-CHA-C1A
10	AF	200	CYC	NA-C4A-CHB-C1B
10	AF	200	CYC	C3A-C4A-CHB-C1B
10	AF	200	CYC	NB-C1B-CHB-C4A
10	AF	200	CYC	C2B-C1B-CHB-C4A
10	AF	200	CYC	C2C-C3C-CAC-CBC
10	AF	200	CYC	C4C-C3C-CAC-CBC
10	AH	200	CYC	NA-C4A-CHB-C1B
10	AH	200	CYC	C3A-C4A-CHB-C1B
10	AH	200	CYC	C2C-C3C-CAC-CBC
10	AH	200	CYC	ND-C1D-CHD-C4C
10	AH	200	CYC	C2D-C1D-CHD-C4C
10	AI	200	CYC	NA-C4A-CHB-C1B
10	AI	200	CYC	C3A-C4A-CHB-C1B
10	AI	200	CYC	C2B-C1B-CHB-C4A
10	AI	200	CYC	C2C-C3C-CAC-CBC
10	AI	200	CYC	C4C-C3C-CAC-CBC
10	AI	200	CYC	ND-C1D-CHD-C4C
10	AI	200	CYC	C2D-C1D-CHD-C4C
10	AJ	200	CYC	ND-C4D-CHA-C1A
10	AJ	200	CYC	NA-C4A-CHB-C1B
10	AJ	200	CYC	C3A-C4A-CHB-C1B
10	AJ	200	CYC	C2C-C3C-CAC-CBC
10	AJ	200	CYC	C4C-C3C-CAC-CBC
10	AK	200	CYC	ND-C4D-CHA-C1A
10	AK	200	CYC	C3D-C4D-CHA-C1A
10	AK	200	CYC	NA-C4A-CHB-C1B
10	AK	200	CYC	C3A-C4A-CHB-C1B
10	AK	200	CYC	C4C-C3C-CAC-CBC
10	AL	200	CYC	NA-C4A-CHB-C1B
10	AL	200	CYC	C3A-C4A-CHB-C1B
10	AL	200	CYC	ND-C1D-CHD-C4C
10	AL	200	CYC	C2D-C1D-CHD-C4C
10	AN	200	CYC	ND-C4D-CHA-C1A
10	AN	200	CYC	C3D-C4D-CHA-C1A
10	AN	200	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
10	AN	200	CYC	C3A-C4A-CHB-C1B
10	AN	200	CYC	C2C-C3C-CAC-CBC
10	AN	200	CYC	C4C-C3C-CAC-CBC
10	AO	200	CYC	NA-C4A-CHB-C1B
10	AO	200	CYC	C3A-C4A-CHB-C1B
10	AO	200	CYC	C2C-C3C-CAC-CBC
10	AO	200	CYC	C4C-C3C-CAC-CBC
10	AO	200	CYC	ND-C1D-CHD-C4C
10	AP	200	CYC	ND-C4D-CHA-C1A
10	AP	200	CYC	NA-C4A-CHB-C1B
10	AP	200	CYC	C3A-C4A-CHB-C1B
10	AP	200	CYC	C4C-C3C-CAC-CBC
10	AP	200	CYC	C2D-C1D-CHD-C4C
10	AQ	200	CYC	NA-C1A-CHA-C4D
10	AQ	200	CYC	NA-C4A-CHB-C1B
10	AQ	200	CYC	C3A-C4A-CHB-C1B
10	AQ	200	CYC	NB-C1B-CHB-C4A
10	AQ	200	CYC	C2B-C1B-CHB-C4A
10	AQ	200	CYC	C2C-C3C-CAC-CBC
10	AQ	200	CYC	C4C-C3C-CAC-CBC
10	AQ	200	CYC	ND-C1D-CHD-C4C
10	AQ	200	CYC	C2D-C1D-CHD-C4C
10	AR	200	CYC	ND-C4D-CHA-C1A
10	AR	200	CYC	NA-C4A-CHB-C1B
10	AR	200	CYC	C3A-C4A-CHB-C1B
10	AR	200	CYC	C2C-C3C-CAC-CBC
10	AR	200	CYC	C4C-C3C-CAC-CBC
10	AS	200	CYC	NA-C1A-CHA-C4D
10	AS	200	CYC	ND-C4D-CHA-C1A
10	AS	200	CYC	C3D-C4D-CHA-C1A
10	AS	200	CYC	NA-C4A-CHB-C1B
10	AS	200	CYC	C3A-C4A-CHB-C1B
10	AS	200	CYC	NB-C1B-CHB-C4A
10	AS	200	CYC	C2B-C1B-CHB-C4A
10	AS	200	CYC	C2C-C3C-CAC-CBC
10	AS	200	CYC	C4C-C3C-CAC-CBC
10	AU	200	CYC	NA-C4A-CHB-C1B
10	AU	200	CYC	C3A-C4A-CHB-C1B
10	AU	200	CYC	C4C-C3C-CAC-CBC
10	AU	200	CYC	ND-C1D-CHD-C4C
10	AU	200	CYC	C2D-C1D-CHD-C4C
10	AV	200	CYC	ND-C4D-CHA-C1A

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Mol	Chain	Res	Type	Atoms
10	AV	200	CYC	C3D-C4D-CHA-C1A
10	AV	200	CYC	NA-C4A-CHB-C1B
10	AV	200	CYC	C3A-C4A-CHB-C1B
10	AV	200	CYC	NB-C1B-CHB-C4A
10	AV	200	CYC	C2B-C1B-CHB-C4A
10	AV	200	CYC	C2C-C3C-CAC-CBC
10	AV	200	CYC	C4C-C3C-CAC-CBC
10	AW	200	CYC	NA-C1A-CHA-C4D
10	AW	200	CYC	C2A-C1A-CHA-C4D
10	AW	200	CYC	ND-C4D-CHA-C1A
10	AW	200	CYC	C3D-C4D-CHA-C1A
10	AW	200	CYC	NA-C4A-CHB-C1B
10	AW	200	CYC	C3A-C4A-CHB-C1B
10	AW	200	CYC	C2C-C3C-CAC-CBC
10	AW	200	CYC	C4C-C3C-CAC-CBC
10	AW	200	CYC	NC-C4C-CHD-C1D
10	AW	200	CYC	ND-C1D-CHD-C4C
10	AW	200	CYC	C2D-C1D-CHD-C4C
10	AX	200	CYC	NA-C4A-CHB-C1B
10	AX	200	CYC	C3A-C4A-CHB-C1B
10	AX	200	CYC	NB-C1B-CHB-C4A
10	AX	200	CYC	C2B-C1B-CHB-C4A
10	AX	200	CYC	C2C-C3C-CAC-CBC
10	AX	200	CYC	C4C-C3C-CAC-CBC
10	AX	200	CYC	ND-C1D-CHD-C4C
10	AX	200	CYC	C2D-C1D-CHD-C4C
10	AY	200	CYC	ND-C4D-CHA-C1A
10	AY	200	CYC	C3D-C4D-CHA-C1A
10	AY	200	CYC	NA-C4A-CHB-C1B
10	AY	200	CYC	C3A-C4A-CHB-C1B
10	AY	200	CYC	C4C-C3C-CAC-CBC
10	AY	200	CYC	C2D-C1D-CHD-C4C
10	AZ	200	CYC	NA-C4A-CHB-C1B
10	AZ	200	CYC	C3A-C4A-CHB-C1B
10	AZ	200	CYC	C2C-C3C-CAC-CBC
10	AZ	200	CYC	C4C-C3C-CAC-CBC
10	BE	1000	CYC	NA-C1A-CHA-C4D
10	BE	1000	CYC	C2A-C1A-CHA-C4D
10	BE	1000	CYC	ND-C4D-CHA-C1A
10	BE	1000	CYC	C3D-C4D-CHA-C1A
10	BE	1000	CYC	NA-C4A-CHB-C1B
10	BE	1000	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
10	BE	1000	CYC	C2B-C1B-CHB-C4A
10	BE	1000	CYC	ND-C1D-CHD-C4C
10	BE	1000	CYC	C2D-C1D-CHD-C4C
11	BH	400	45D	C31-C33-C35-C39
11	BH	400	45D	C32-C34-C36-C38
11	BH	400	45D	C32-C34-C36-C40
10	AI	200	CYC	NB-C1B-CHB-C4A
10	BE	1000	CYC	NB-C1B-CHB-C4A
10	AH	200	CYC	C2A-CAA-CBA-CGA
10	AK	200	CYC	C2A-CAA-CBA-CGA
10	AP	200	CYC	C2A-CAA-CBA-CGA
10	AX	200	CYC	C2A-CAA-CBA-CGA
11	BH	400	45D	C19-C23-C25-C27
11	BH	400	45D	C20-C24-C26-C28
11	BH	400	45D	C19-C23-C25-C29
11	BH	400	45D	C31-C33-C35-C37
10	AF	200	CYC	NA-C1A-CHA-C4D
10	AI	200	CYC	NA-C1A-CHA-C4D
10	AJ	200	CYC	NA-C1A-CHA-C4D
10	AP	200	CYC	NA-C1A-CHA-C4D
10	AV	200	CYC	NA-C1A-CHA-C4D
10	AA	200	CYC	NB-C1B-CHB-C4A
10	AD	200	CYC	NB-C1B-CHB-C4A
10	AW	200	CYC	NB-C1B-CHB-C4A
10	AY	200	CYC	NB-C1B-CHB-C4A
10	AA	200	CYC	C2B-C1B-CHB-C4A
10	AE	200	CYC	C2A-CAA-CBA-CGA
10	AF	200	CYC	C2A-CAA-CBA-CGA
10	AE	200	CYC	C2A-C1A-CHA-C4D
11	BH	400	45D	C36-C38-C42-C41
10	AA	200	CYC	C2A-CAA-CBA-CGA
10	AC	200	CYC	C2A-CAA-CBA-CGA
10	AI	200	CYC	C2A-CAA-CBA-CGA
11	BH	400	45D	C20-C24-C26-C30
10	AD	200	CYC	C2B-C1B-CHB-C4A
10	AW	200	CYC	C2B-C1B-CHB-C4A
11	BH	400	45D	C03-C07-C19-C23
11	BH	400	45D	C15-C07-C19-C23
11	BH	400	45D	C16-C08-C20-C24
10	AQ	200	CYC	C2A-CAA-CBA-CGA
10	AA	200	CYC	C2A-C1A-CHA-C4D
10	AI	200	CYC	C2A-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
10	AQ	200	CYC	C2A-C1A-CHA-C4D
10	AS	200	CYC	C2A-C1A-CHA-C4D
10	AJ	200	CYC	C2A-CAA-CBA-CGA
10	AU	200	CYC	NC-C4C-CHD-C1D
10	AK	200	CYC	C2C-C3C-CAC-CBC
10	AP	200	CYC	C2C-C3C-CAC-CBC
10	AU	200	CYC	C2C-C3C-CAC-CBC
10	AV	200	CYC	C3D-CAD-CBD-CGD
10	AY	200	CYC	C2C-C3C-CAC-CBC
10	AY	200	CYC	C2B-C1B-CHB-C4A
10	AR	200	CYC	NA-C1A-CHA-C4D
10	AU	200	CYC	C2A-CAA-CBA-CGA
10	AF	200	CYC	C2A-C1A-CHA-C4D
10	AP	200	CYC	C2A-C1A-CHA-C4D
10	AO	200	CYC	NB-C1B-CHB-C4A
11	BH	400	45D	C26-C30-C32-C34
10	AN	200	CYC	C2A-CAA-CBA-CGA
10	AR	200	CYC	C2A-CAA-CBA-CGA
11	BH	400	45D	C04-C08-C20-C24
10	AH	200	CYC	C4C-C3C-CAC-CBC
10	AW	200	CYC	C2A-CAA-CBA-CGA
10	AK	200	CYC	NB-C1B-CHB-C4A
10	BE	1000	CYC	C3D-CAD-CBD-CGD
10	AH	200	CYC	NA-C1A-CHA-C4D
10	AK	200	CYC	NA-C1A-CHA-C4D
10	AY	200	CYC	C2B-C3B-CAB-CBB
10	AN	200	CYC	C3D-CAD-CBD-CGD
10	AR	200	CYC	C3D-CAD-CBD-CGD
10	AN	200	CYC	NB-C1B-CHB-C4A
10	AX	200	CYC	C2B-C3B-CAB-CBB
10	AV	200	CYC	C2A-C1A-CHA-C4D
11	BH	400	45D	C25-C29-C31-C33
10	AA	200	CYC	C2B-C3B-CAB-CBB
10	AC	200	CYC	CAD-CBD-CGD-O2D
10	AJ	200	CYC	CAD-CBD-CGD-O2D
10	AN	200	CYC	CAD-CBD-CGD-O1D
10	AU	200	CYC	CAD-CBD-CGD-O2D
10	AZ	200	CYC	CAD-CBD-CGD-O2D
10	AE	200	CYC	CAD-CBD-CGD-O2D
10	AV	200	CYC	CAD-CBD-CGD-O1D
10	AC	200	CYC	CAA-CBA-CGA-O2A
10	AW	200	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
10	BE	1000	CYC	CAD-CBD-CGD-O2D
10	AA	200	CYC	CAD-CBD-CGD-O2D
10	AL	200	CYC	CAA-CBA-CGA-O2A
10	AY	200	CYC	CAA-CBA-CGA-O2A
10	AB	200	CYC	CAA-CBA-CGA-O1A
10	AH	200	CYC	CAD-CBD-CGD-O1D
10	AK	200	CYC	CAD-CBD-CGD-O1D
10	AO	200	CYC	CAD-CBD-CGD-O1D
10	AX	200	CYC	CAA-CBA-CGA-O1A
10	AX	200	CYC	CAD-CBD-CGD-O1D
10	AB	200	CYC	CAA-CBA-CGA-O2A
10	AP	200	CYC	CAD-CBD-CGD-O2D
10	AA	200	CYC	CAA-CBA-CGA-O1A
10	AJ	200	CYC	CAA-CBA-CGA-O1A
10	AW	200	CYC	CAD-CBD-CGD-O2D
10	AB	200	CYC	C2A-CAA-CBA-CGA
10	AI	200	CYC	CAA-CBA-CGA-O2A
10	AL	200	CYC	CAD-CBD-CGD-O2D
10	AR	200	CYC	CAD-CBD-CGD-O1D
10	AZ	200	CYC	CAD-CBD-CGD-O1D
10	AD	200	CYC	CAD-CBD-CGD-O1D
10	AI	200	CYC	CAA-CBA-CGA-O1A
10	AP	200	CYC	CAA-CBA-CGA-O1A
10	AY	200	CYC	CAD-CBD-CGD-O1D
10	AK	200	CYC	CAD-CBD-CGD-O2D
10	AW	200	CYC	CAD-CBD-CGD-O1D
10	AL	200	CYC	CAD-CBD-CGD-O1D
10	AO	200	CYC	CAA-CBA-CGA-O1A
10	AH	200	CYC	CAD-CBD-CGD-O2D
10	AJ	200	CYC	CAA-CBA-CGA-O2A
10	AQ	200	CYC	CAA-CBA-CGA-O1A
10	AQ	200	CYC	CAD-CBD-CGD-O1D
10	AS	200	CYC	CAA-CBA-CGA-O1A
10	AU	200	CYC	CAA-CBA-CGA-O2A
10	AX	200	CYC	CAD-CBD-CGD-O2D
10	AY	200	CYC	CAD-CBD-CGD-O2D
10	AR	200	CYC	CAA-CBA-CGA-O1A
10	AR	200	CYC	CAA-CBA-CGA-O2A
10	AV	200	CYC	CAA-CBA-CGA-O1A
10	AX	200	CYC	CAA-CBA-CGA-O2A
10	AY	200	CYC	CAA-CBA-CGA-O1A
10	BE	1000	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
10	AA	200	CYC	CAA-CBA-CGA-O2A
10	AL	200	CYC	CAA-CBA-CGA-O1A
10	AP	200	CYC	CAD-CBD-CGD-O1D
10	AS	200	CYC	CAA-CBA-CGA-O2A
10	AU	200	CYC	CAD-CBD-CGD-O1D
10	AO	200	CYC	C2B-C1B-CHB-C4A
10	AB	200	CYC	CAD-CBD-CGD-O1D
10	AC	200	CYC	CAD-CBD-CGD-O1D
10	AO	200	CYC	CAD-CBD-CGD-O2D
10	AR	200	CYC	CAD-CBD-CGD-O2D
10	AO	200	CYC	CAA-CBA-CGA-O2A
10	AU	200	CYC	CAA-CBA-CGA-O1A
10	AV	200	CYC	CAD-CBD-CGD-O2D
10	AC	200	CYC	CAA-CBA-CGA-O1A
10	AJ	200	CYC	CAD-CBD-CGD-O1D
10	AN	200	CYC	CAD-CBD-CGD-O2D
10	AQ	200	CYC	CAD-CBD-CGD-O2D
10	AV	200	CYC	CAA-CBA-CGA-O2A
10	AW	200	CYC	CAA-CBA-CGA-O1A
10	AZ	200	CYC	NC-C4C-CHD-C1D
10	AF	200	CYC	CAD-CBD-CGD-O1D
10	AA	200	CYC	CAD-CBD-CGD-O1D
10	AJ	200	CYC	C2A-C1A-CHA-C4D
10	AB	200	CYC	CAD-CBD-CGD-O2D
10	AD	200	CYC	CAD-CBD-CGD-O2D
10	AE	200	CYC	CAD-CBD-CGD-O1D
10	AP	200	CYC	CAA-CBA-CGA-O2A
10	AY	200	CYC	NA-C1A-CHA-C4D
10	AQ	200	CYC	CAA-CBA-CGA-O2A
10	BE	1000	CYC	CAA-CBA-CGA-O2A
10	AD	200	CYC	CAA-CBA-CGA-O2A
10	AK	200	CYC	CAA-CBA-CGA-O1A
10	AK	200	CYC	CAA-CBA-CGA-O2A
10	AI	200	CYC	CAD-CBD-CGD-O1D
10	BE	1000	CYC	CAA-CBA-CGA-O1A
10	AH	200	CYC	CAA-CBA-CGA-O2A
10	AD	200	CYC	CAA-CBA-CGA-O1A
10	AF	200	CYC	CAD-CBD-CGD-O2D
10	AH	200	CYC	CAA-CBA-CGA-O1A
10	AN	200	CYC	C2B-C1B-CHB-C4A
10	AF	200	CYC	CAA-CBA-CGA-O2A
10	AI	200	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
10	AV	200	CYC	C2A-CAA-CBA-CGA
10	AU	200	CYC	NB-C1B-CHB-C4A
10	AF	200	CYC	CAA-CBA-CGA-O1A
10	AE	200	CYC	C2C-C3C-CAC-CBC
10	AP	200	CYC	C2B-C3B-CAB-CBB
10	AE	200	CYC	NB-C1B-CHB-C4A
10	AN	200	CYC	CAA-CBA-CGA-O2A

There are no ring outliers.

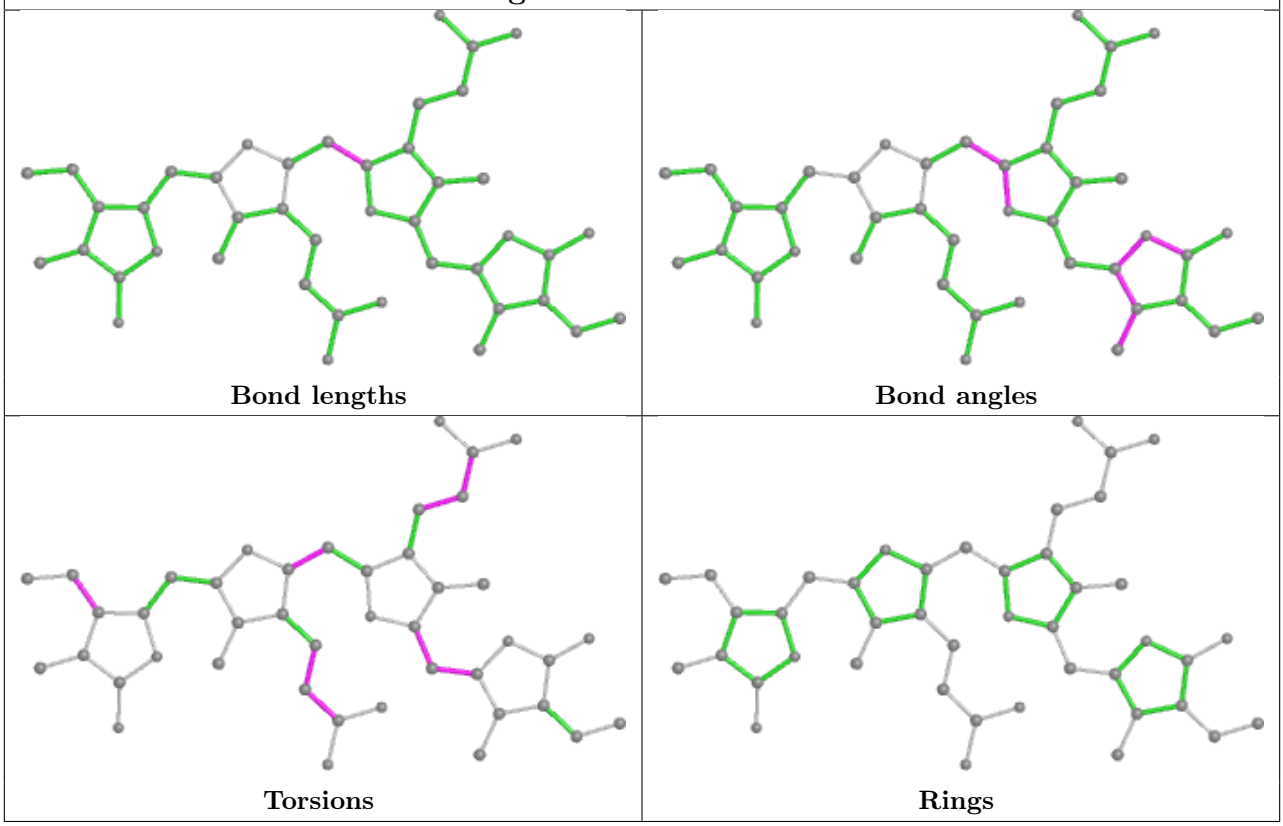
24 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	AN	200	CYC	2	0
10	AW	200	CYC	4	0
10	AH	200	CYC	3	0
10	AK	200	CYC	1	0
10	AO	200	CYC	1	0
10	AZ	200	CYC	2	0
10	AP	200	CYC	3	0
11	BH	400	45D	3	0
10	AS	200	CYC	4	0
10	AU	200	CYC	3	0
10	AQ	200	CYC	2	0
10	AY	200	CYC	3	0
10	AA	200	CYC	2	0
10	AI	200	CYC	3	0
10	AB	200	CYC	3	0
10	AE	200	CYC	2	0
10	AL	200	CYC	5	0
10	AF	200	CYC	3	0
10	AC	200	CYC	1	0
10	AD	200	CYC	1	0
10	AR	200	CYC	1	0
10	BE	1000	CYC	2	0
10	AX	200	CYC	3	0
10	AV	200	CYC	3	0

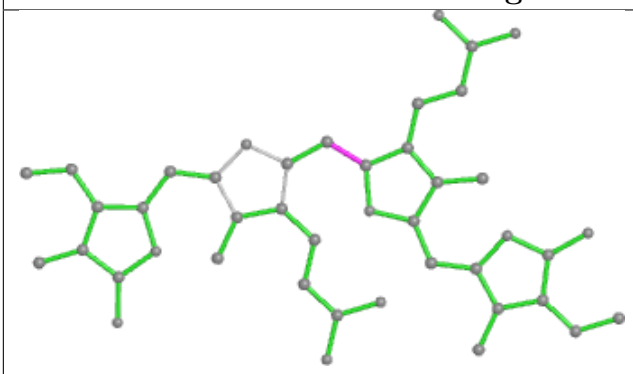
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

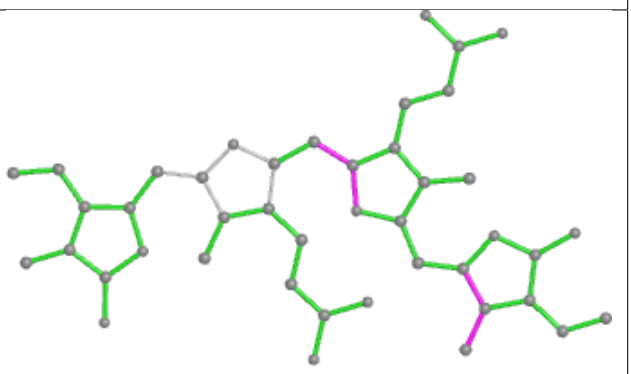
Ligand CYC AN 200



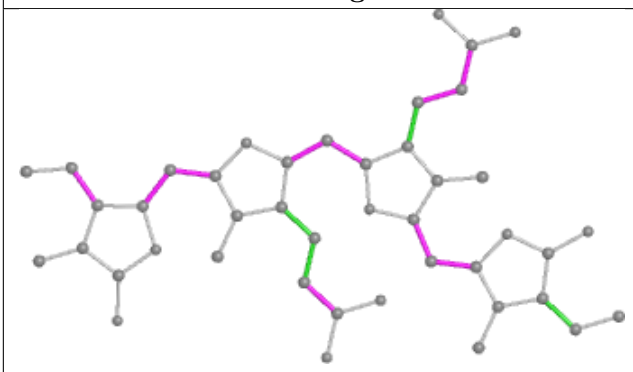
Ligand CYC AW 200



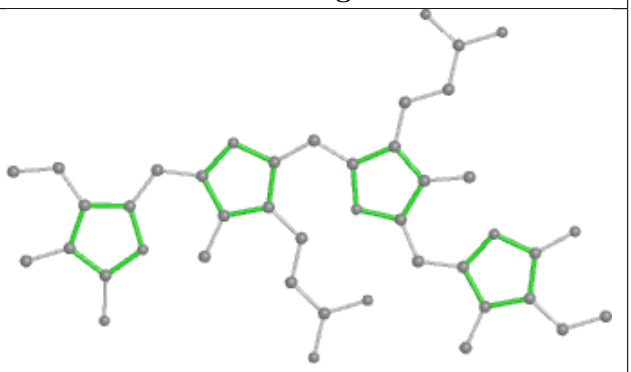
Bond lengths



Bond angles

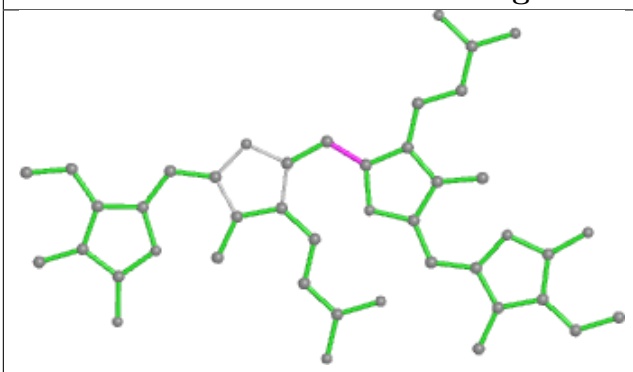


Torsions

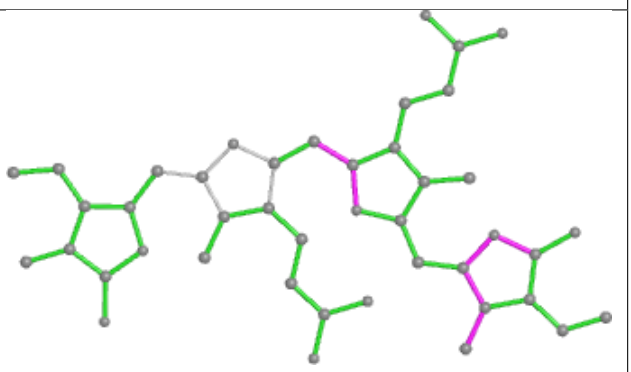


Rings

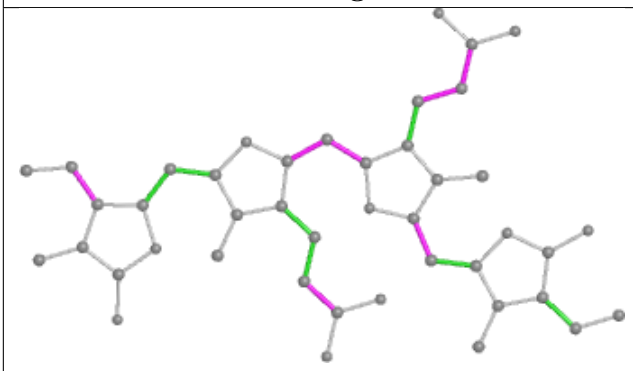
Ligand CYC AJ 200



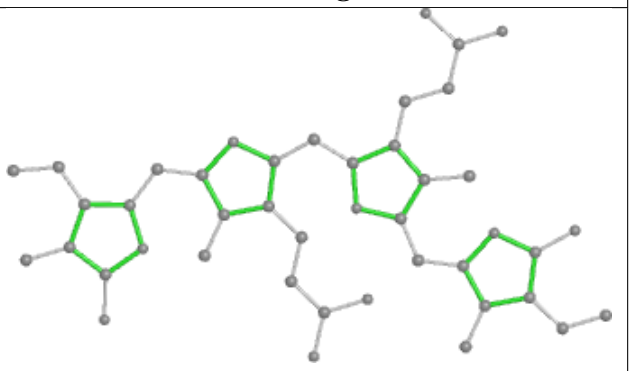
Bond lengths



Bond angles

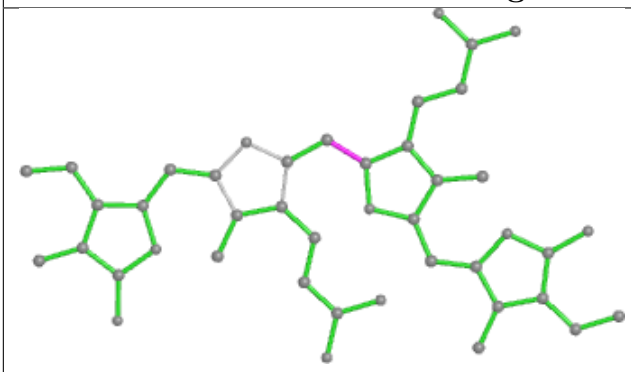


Torsions

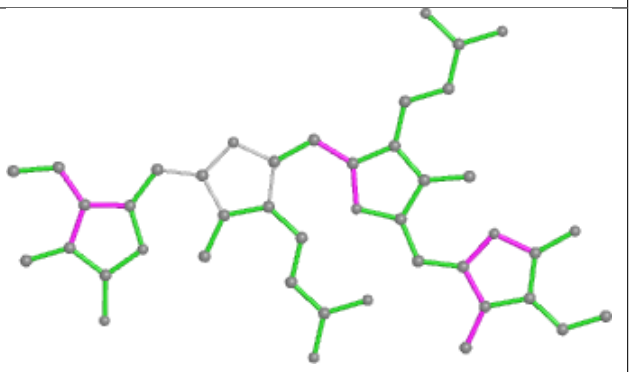


Rings

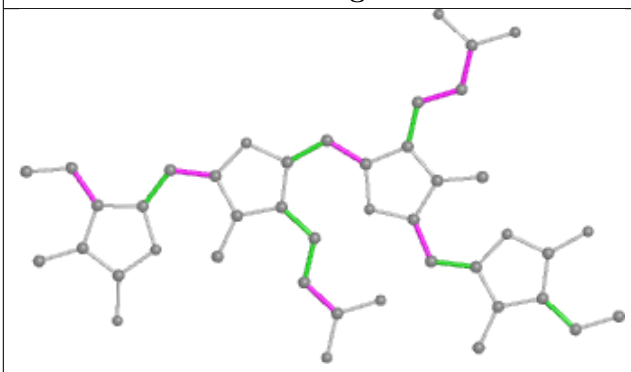
Ligand CYC AH 200



Bond lengths



Bond angles



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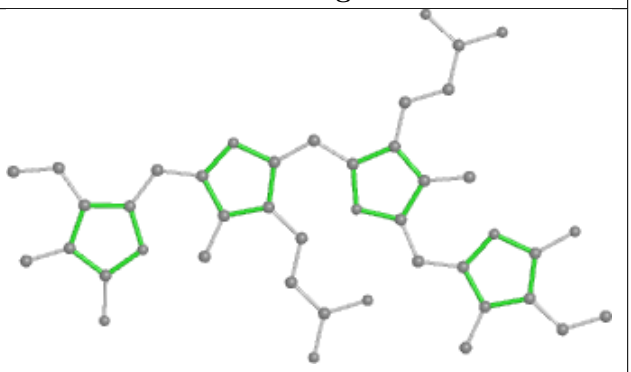

Rings

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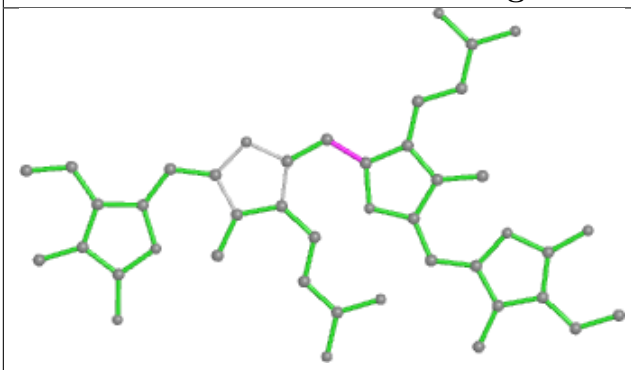
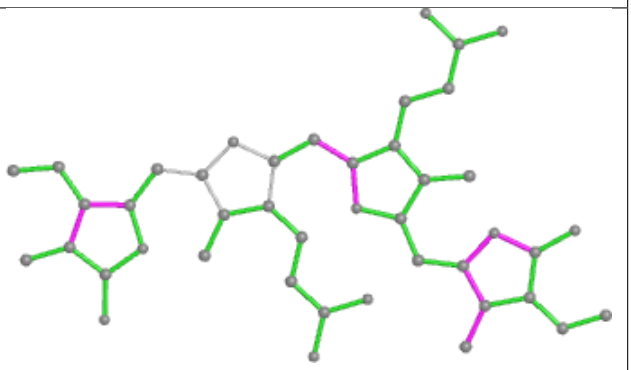
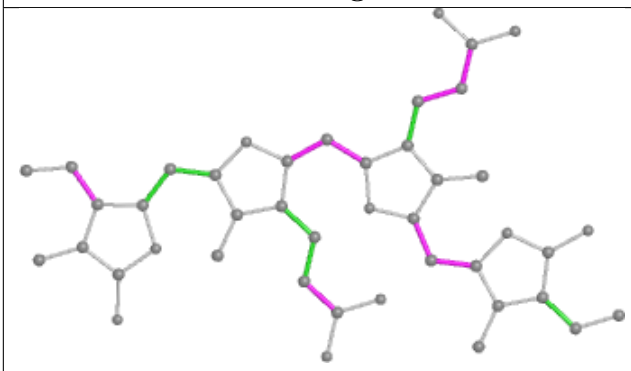


Bond lengths



Bond angles



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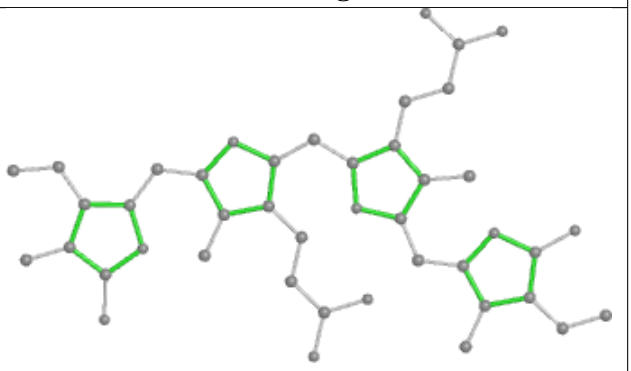
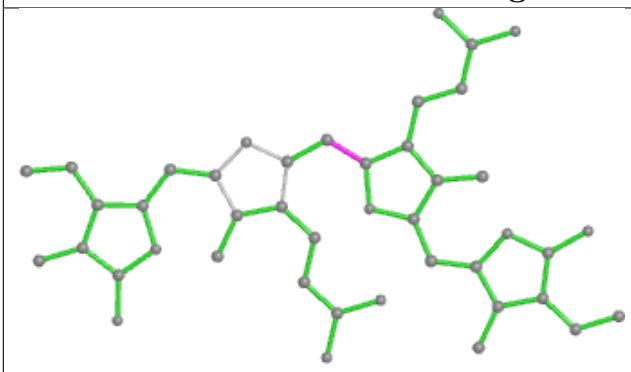
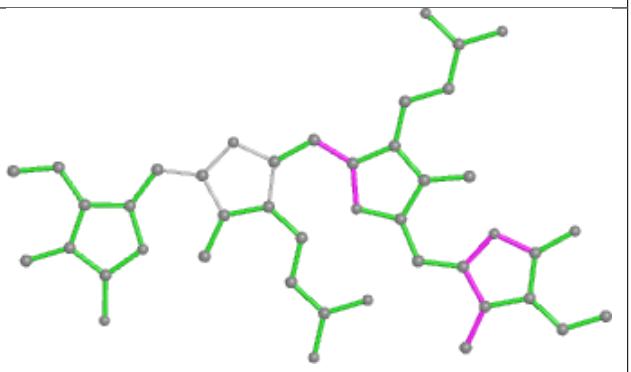


Rings

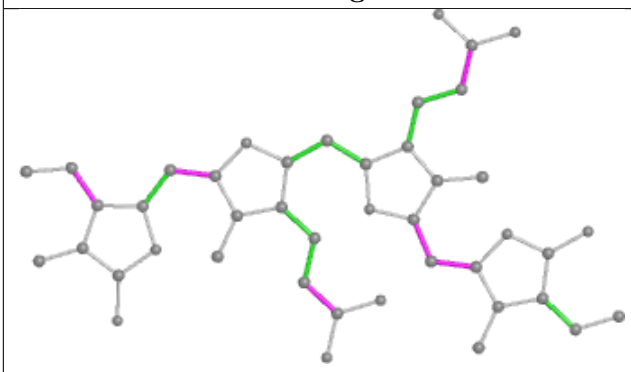
Ligand CYC AO 200



Bond lengths



Bond angles



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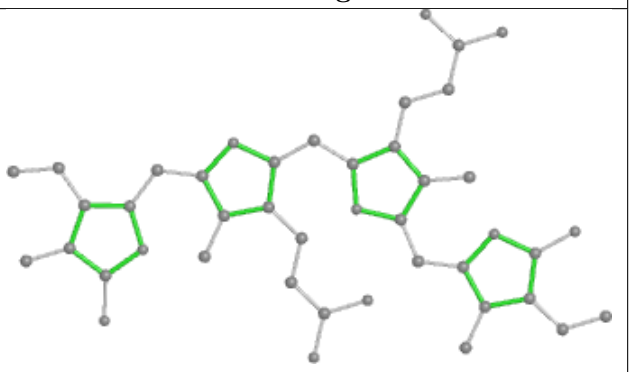
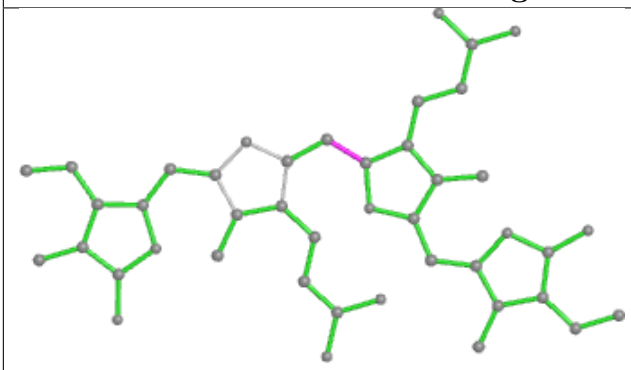
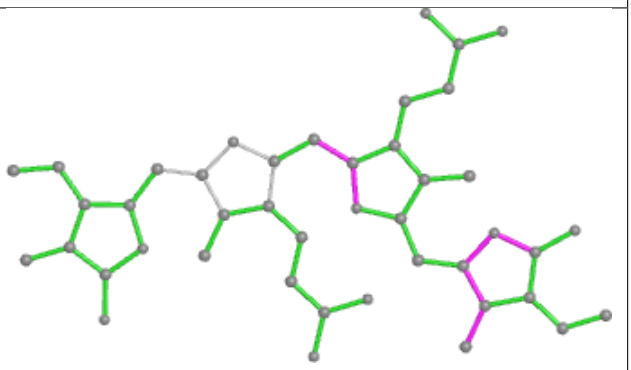


Rings

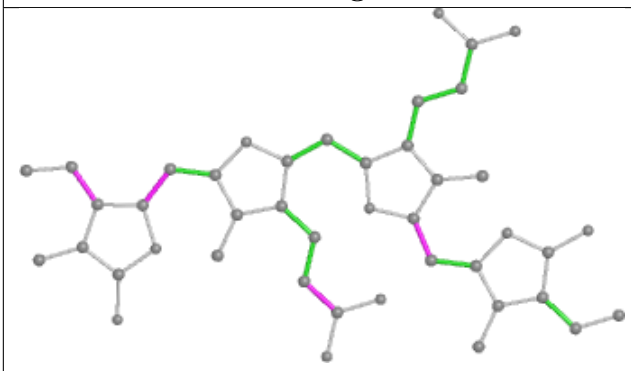
Ligand CYC AZ 200



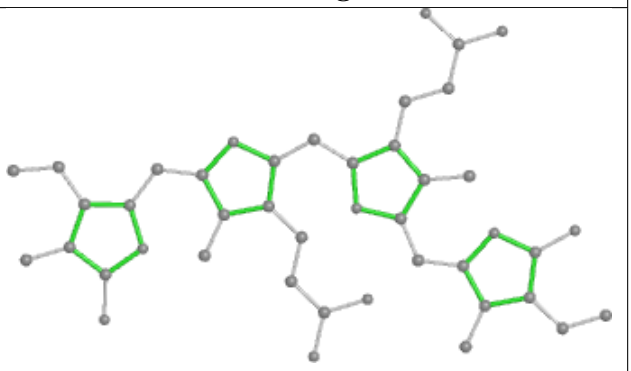
Bond lengths



Bond angles

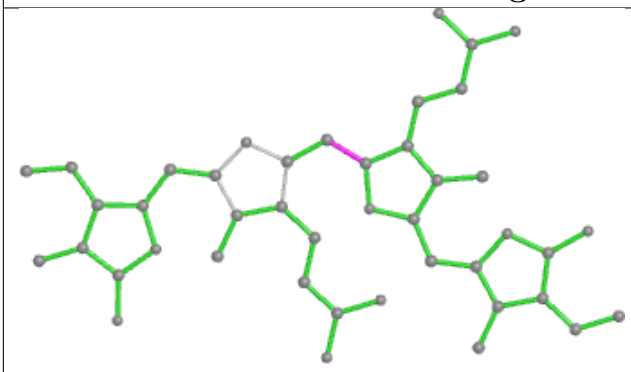


Torsions



Rings

Ligand CYC AP 200



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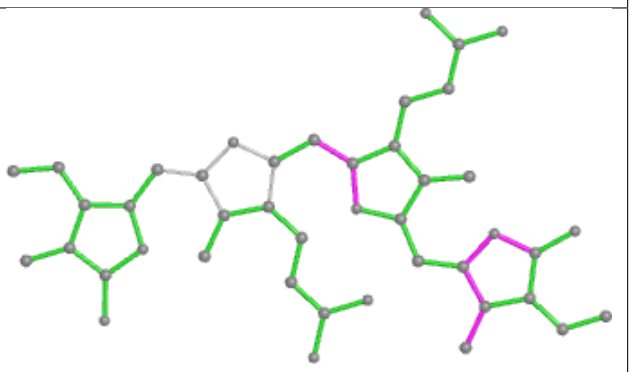
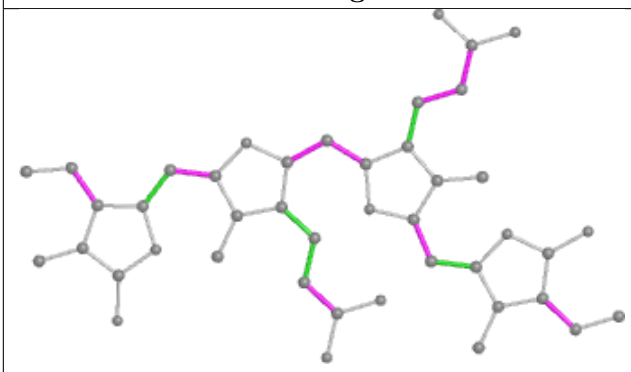


Bond angles



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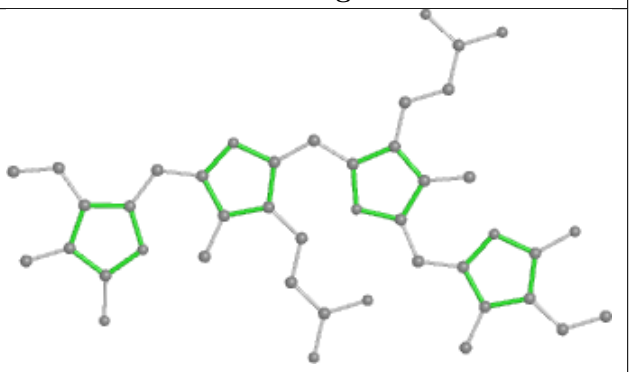

Rings

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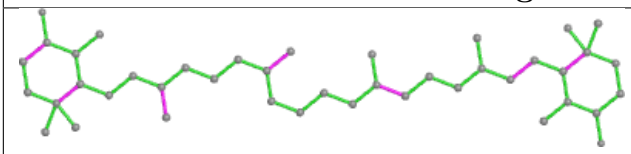

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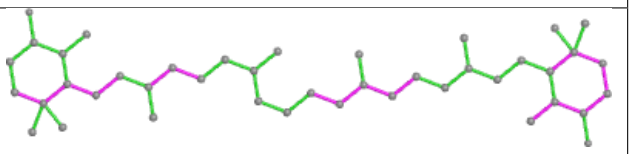

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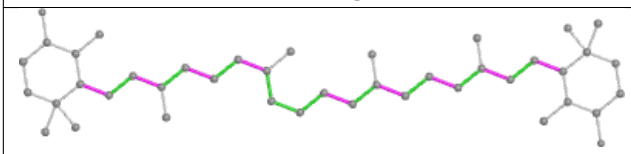

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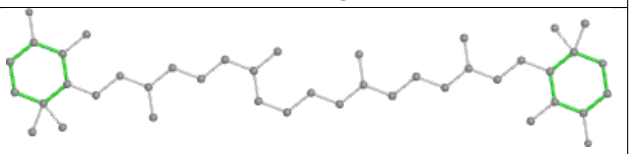
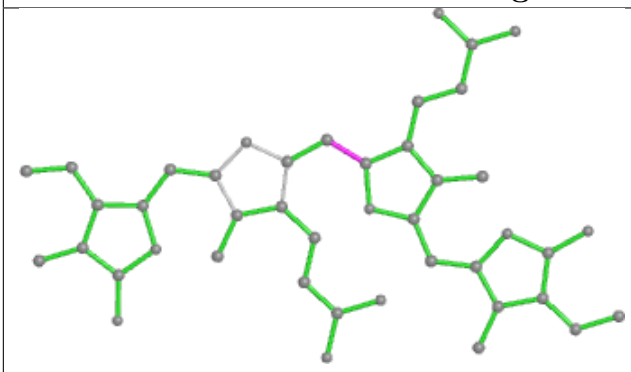


Rings

Ligand CYC AS 200



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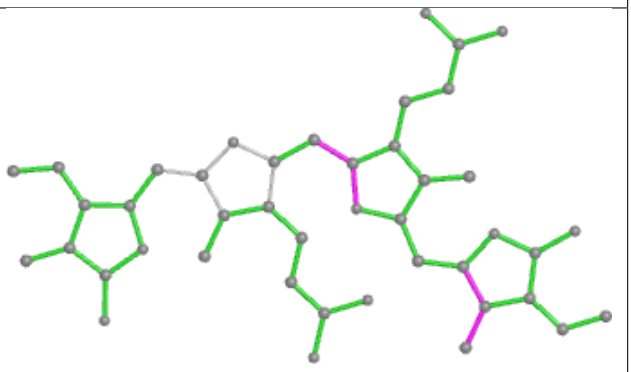

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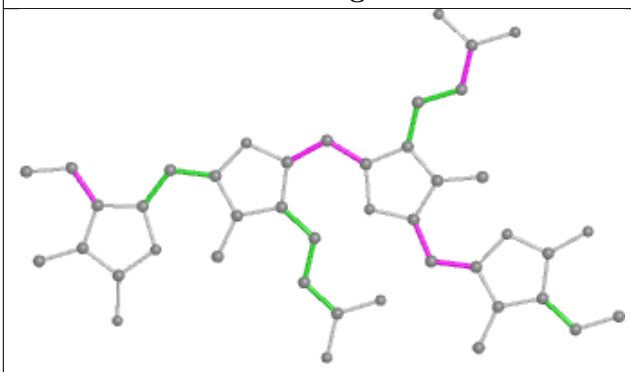

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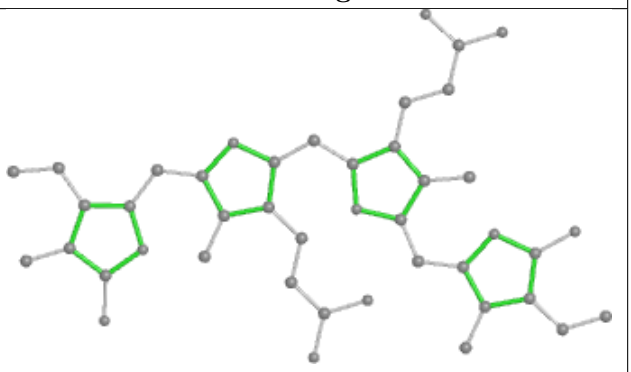

Rings

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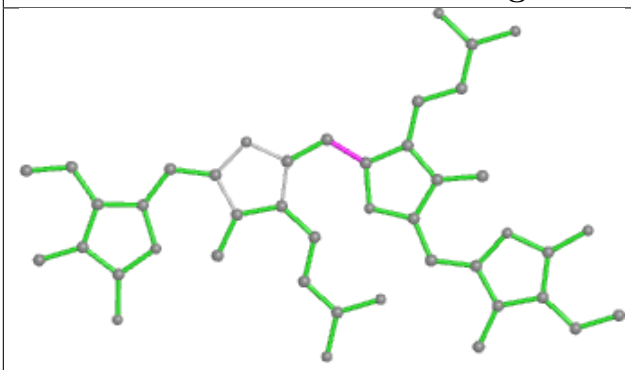

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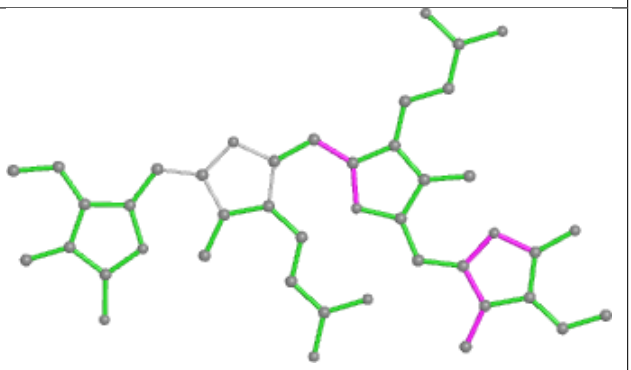

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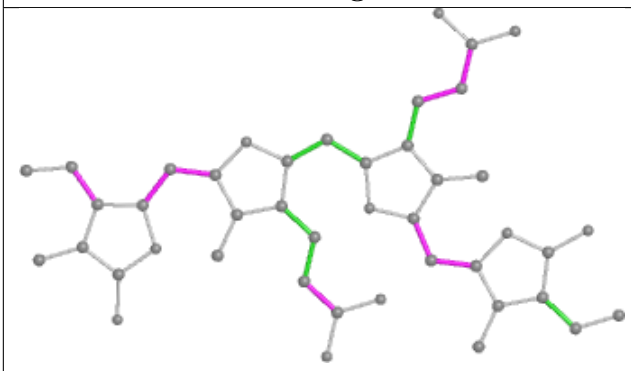

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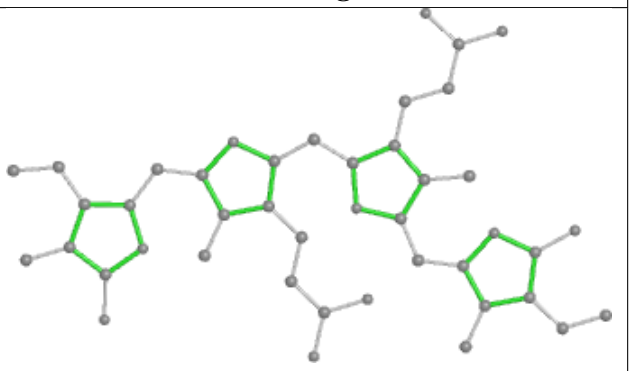
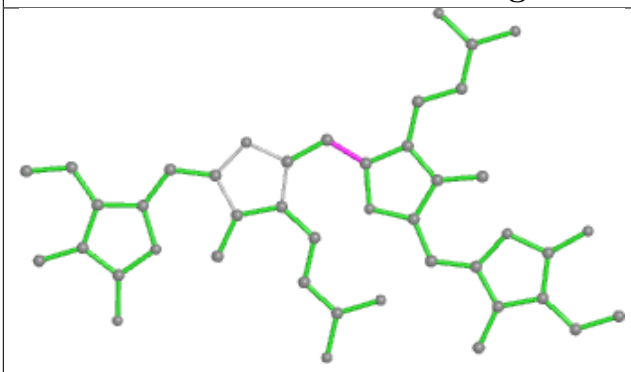


Rings

Ligand CYC AQ 200



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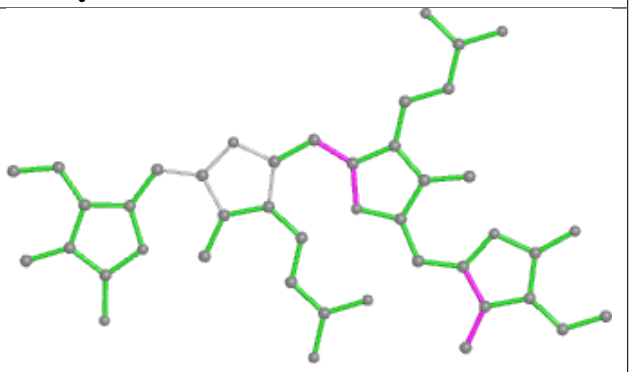

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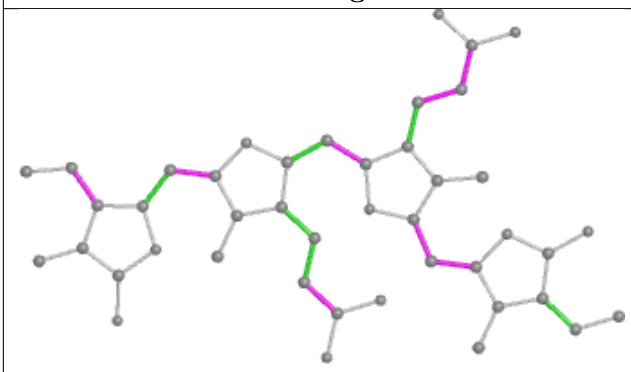

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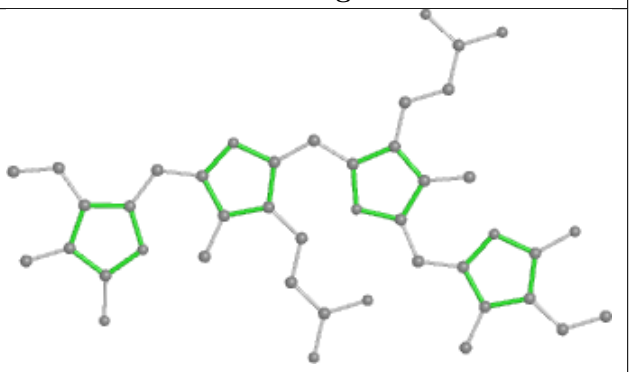

Rings

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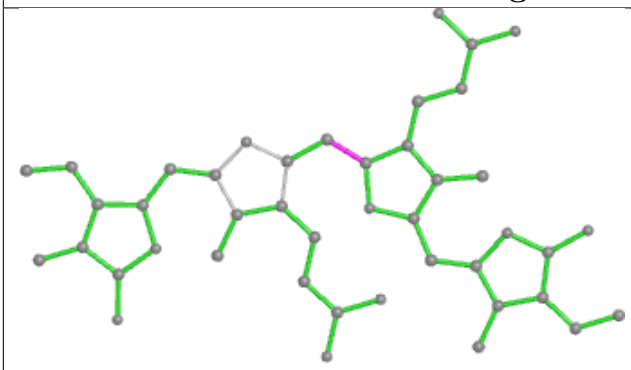

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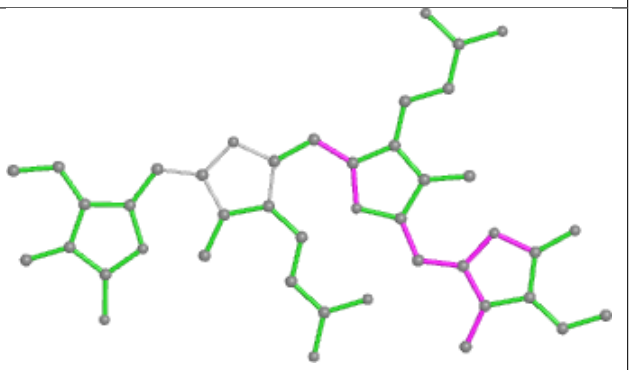

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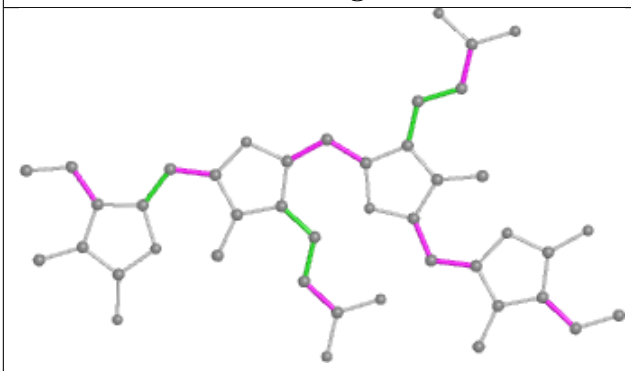

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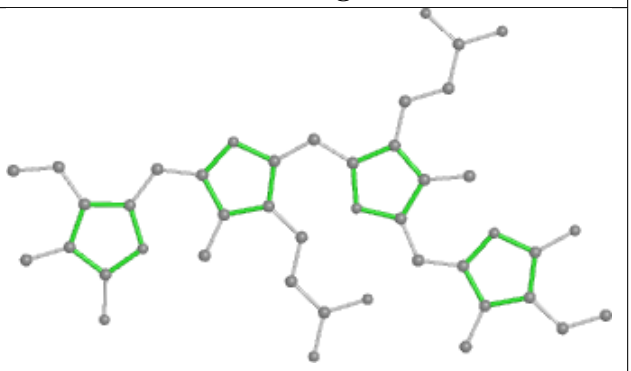

Rings

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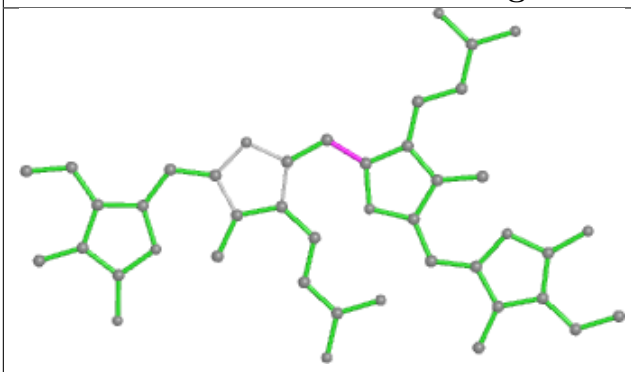

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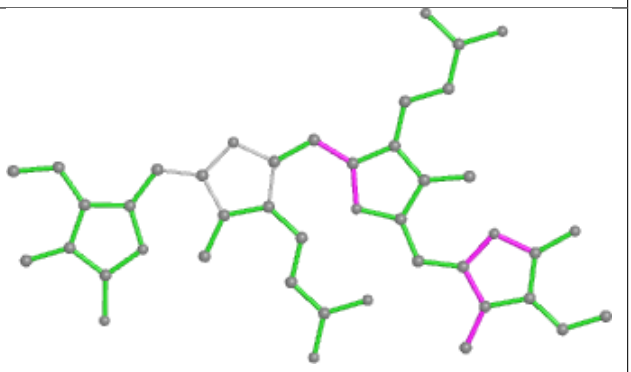

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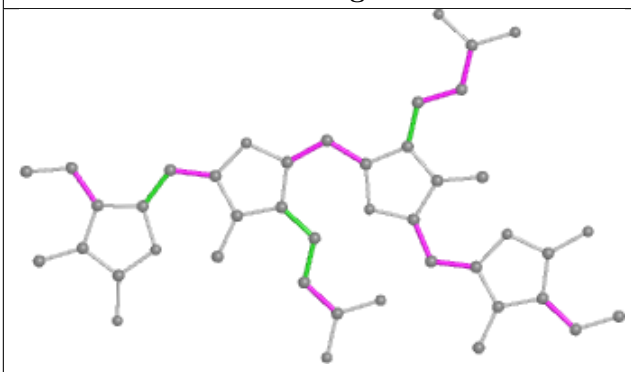

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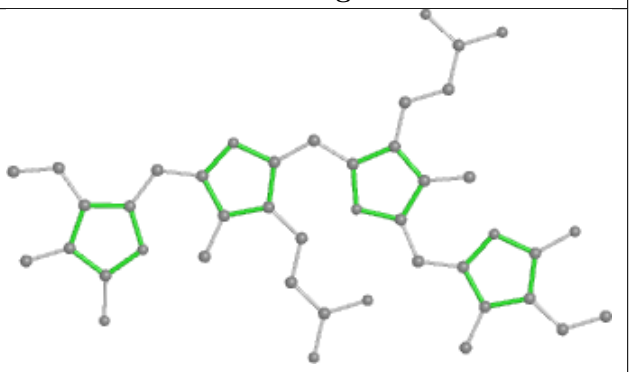

Rings

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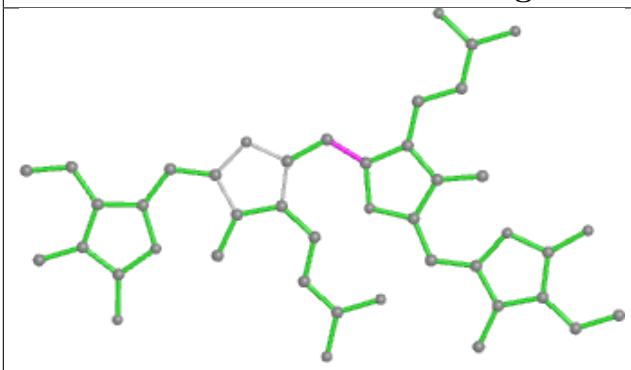

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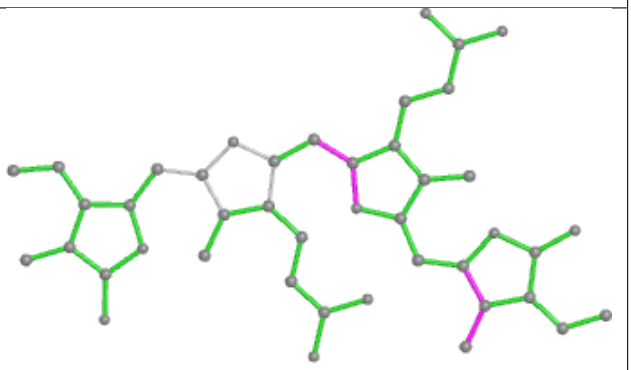

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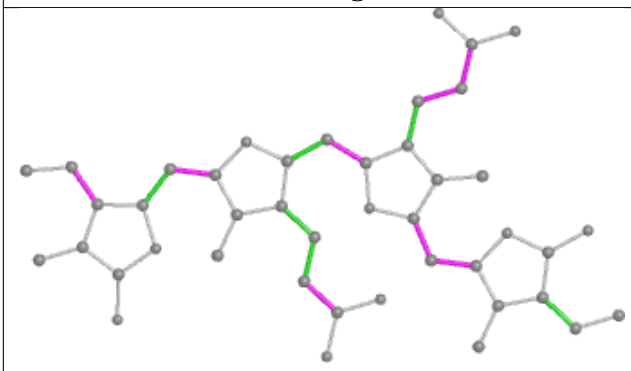

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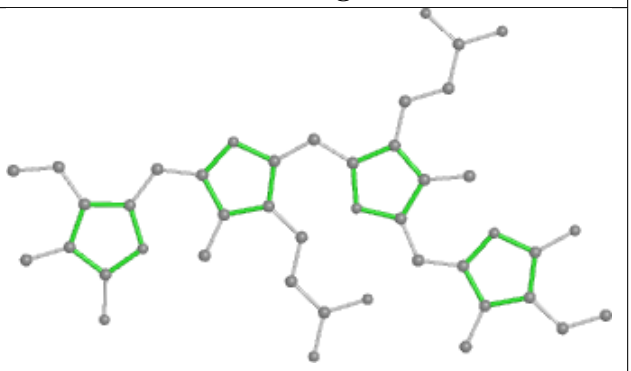

Rings

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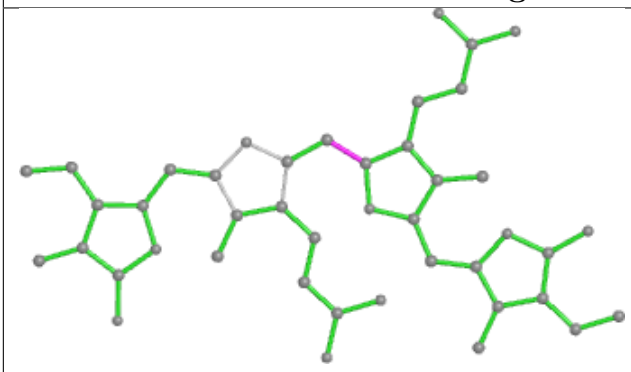

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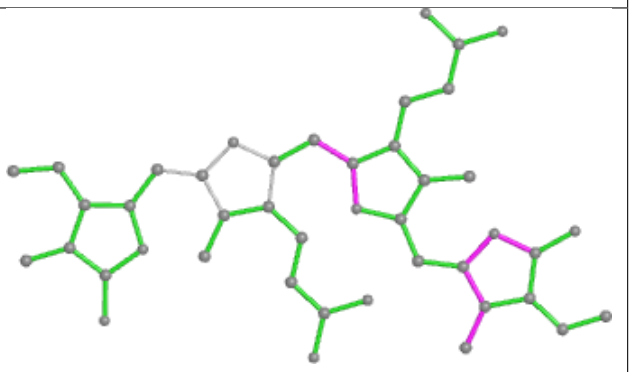

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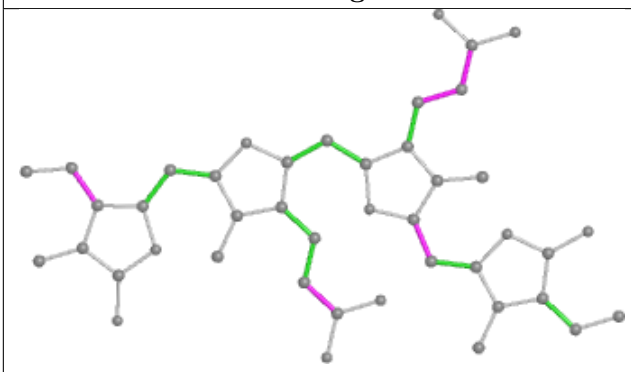

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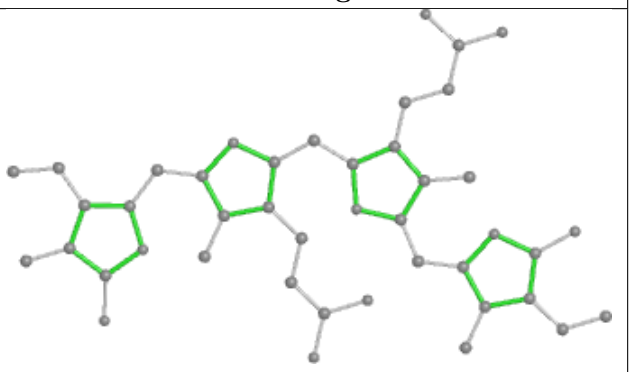

Rings

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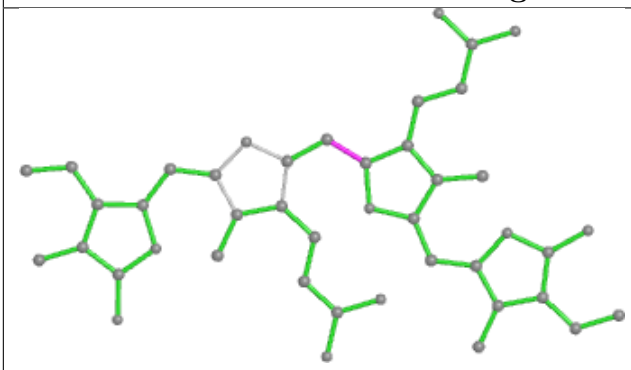

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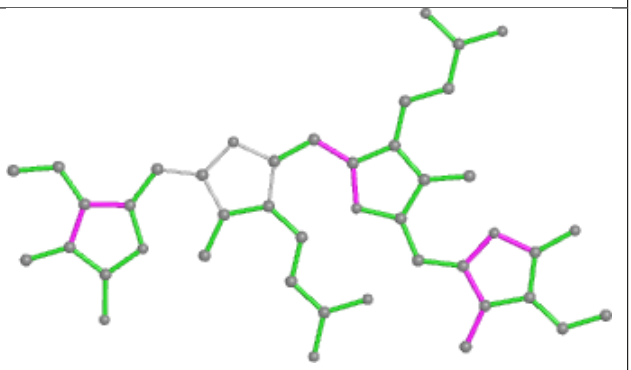

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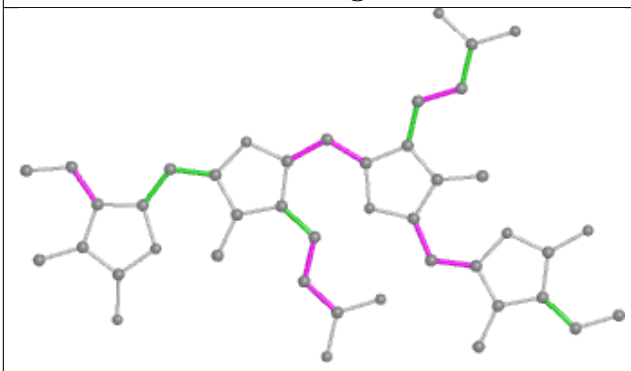

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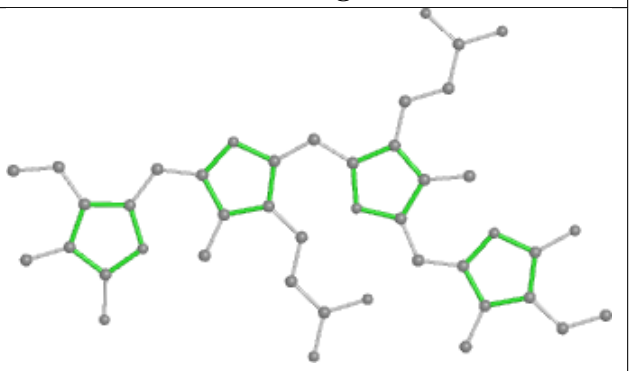

Rings

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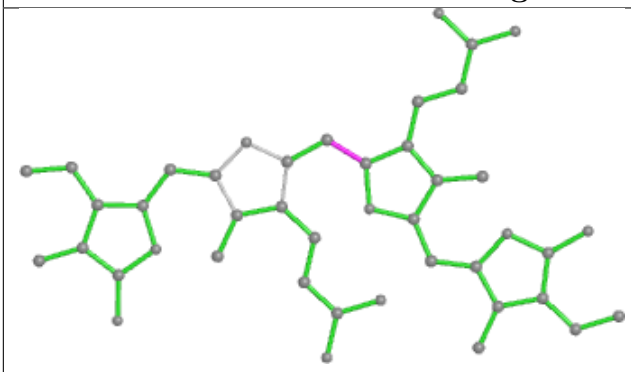

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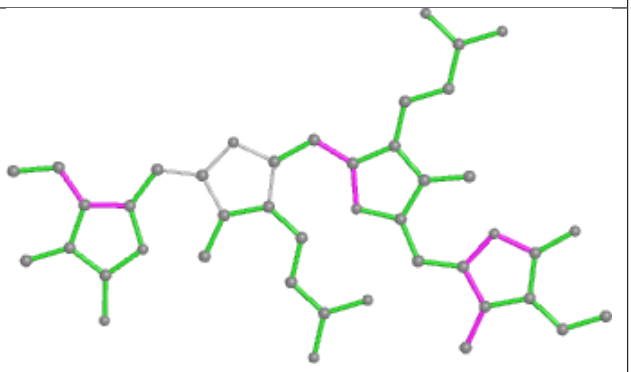

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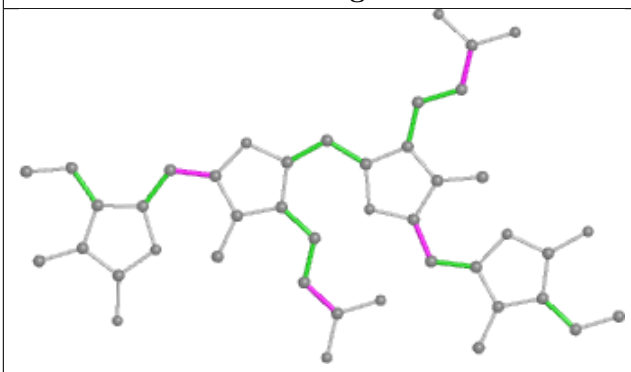

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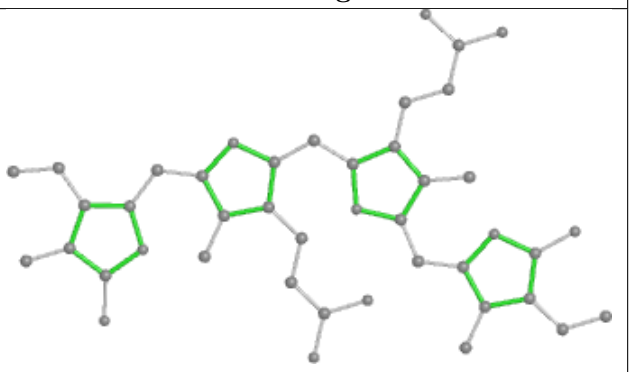

Rings

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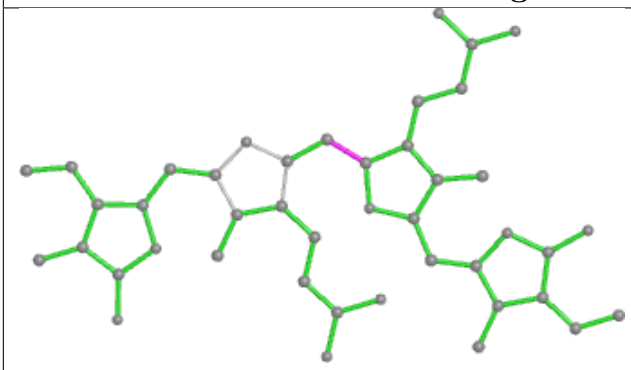

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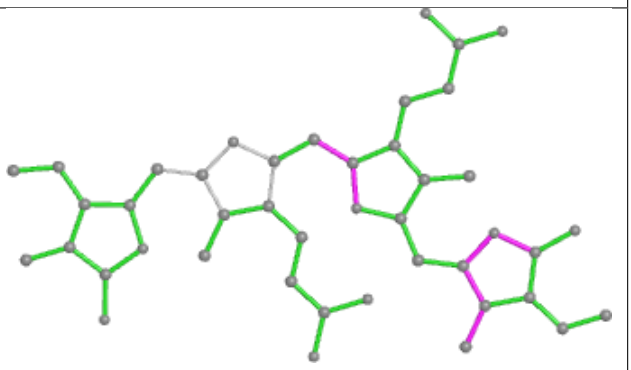
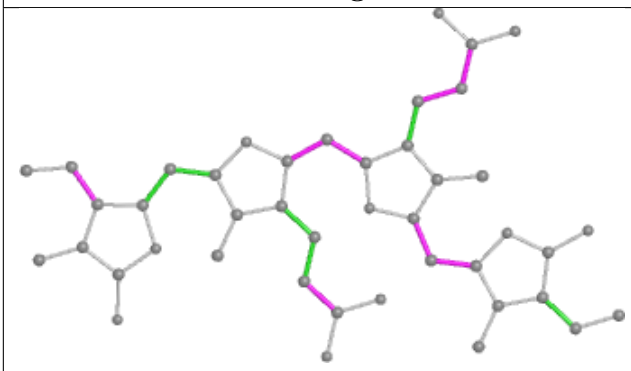


Bond angles



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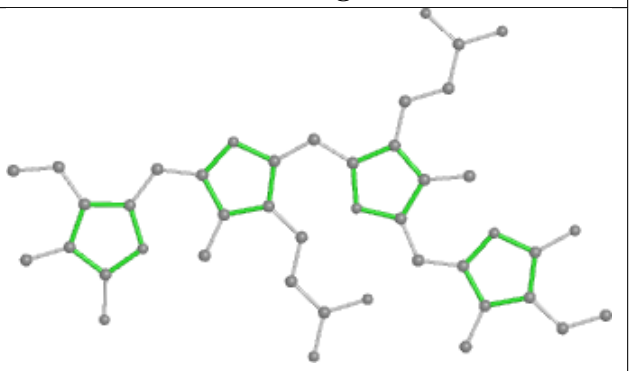

Rings

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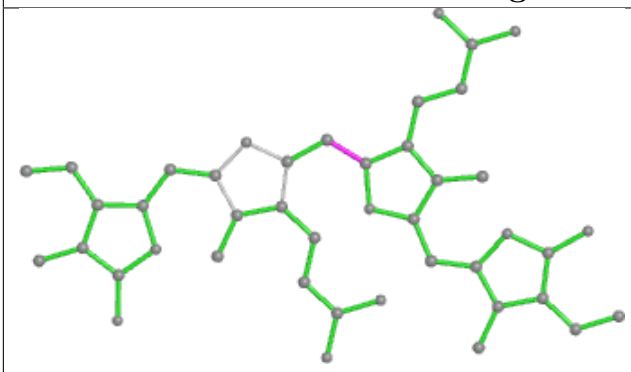

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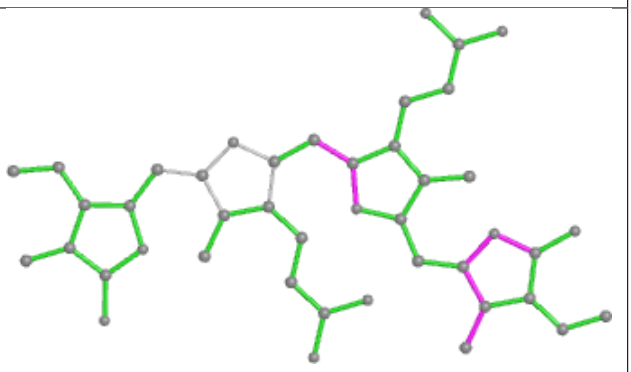
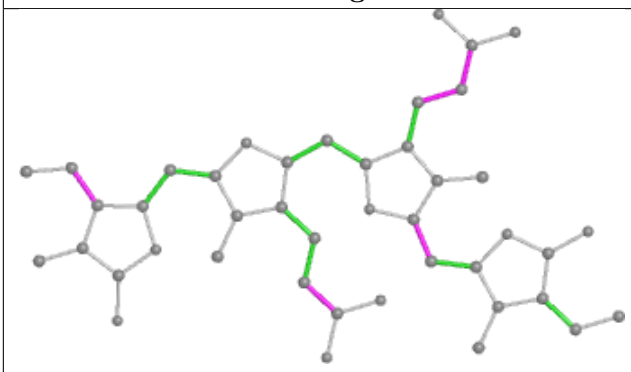


Bond angles



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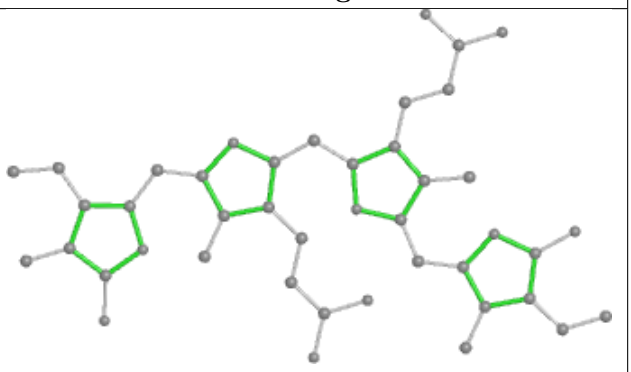
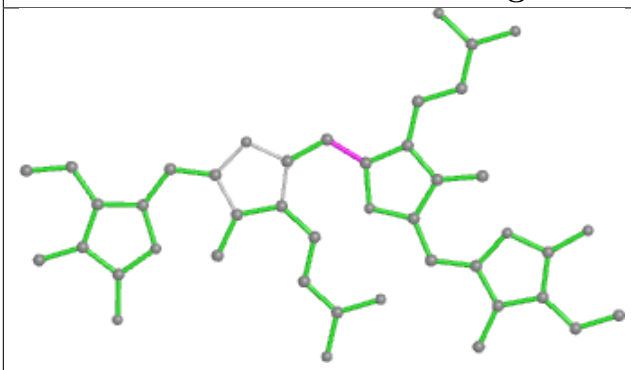
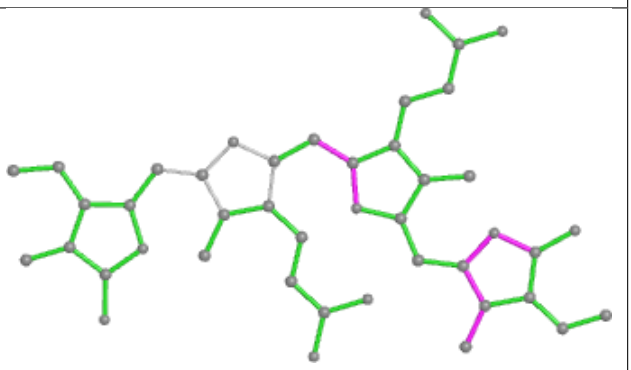


Rings

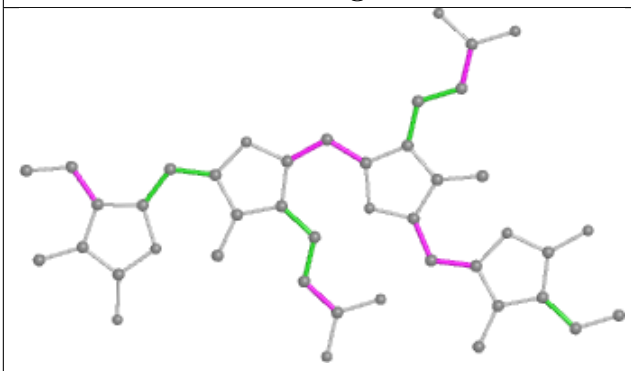
Ligand CYC AD 200



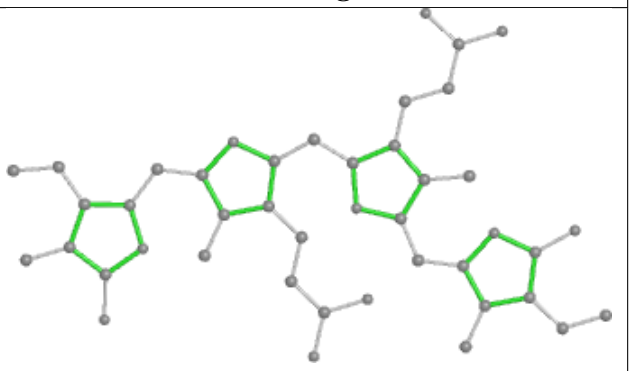
Bond lengths



Bond angles

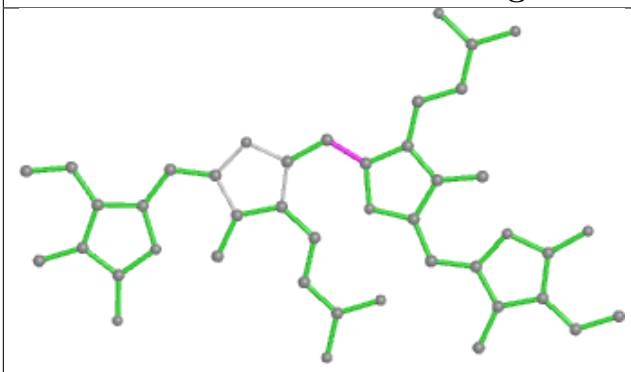


Torsions

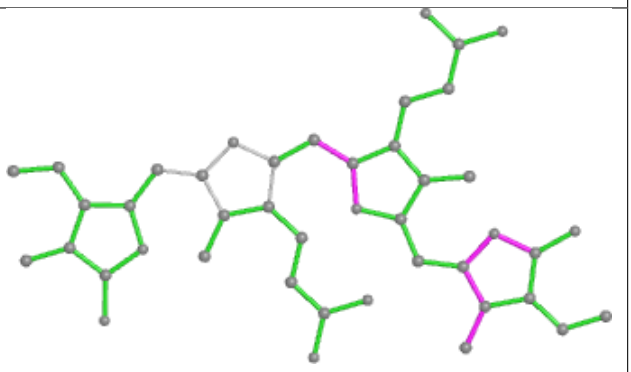


Rings

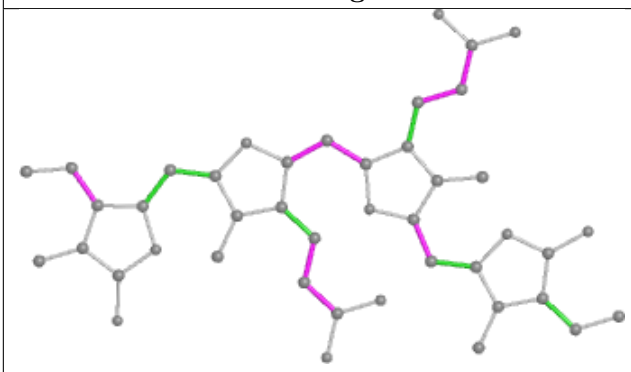
Ligand CYC AR 200



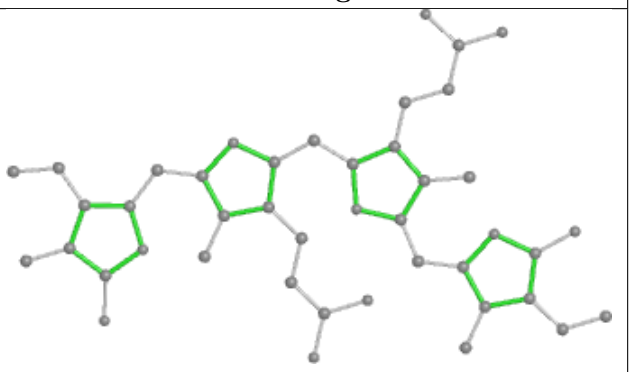
Bond lengths



Bond angles

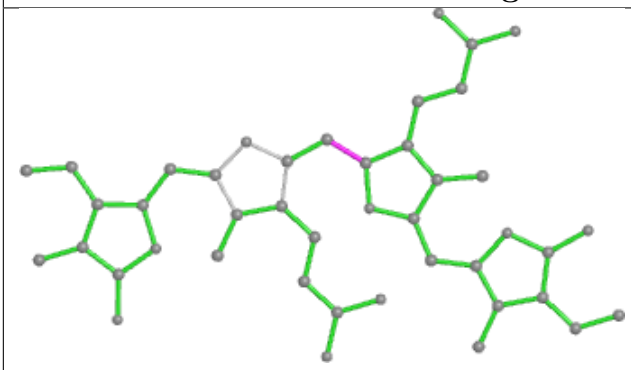


Torsions

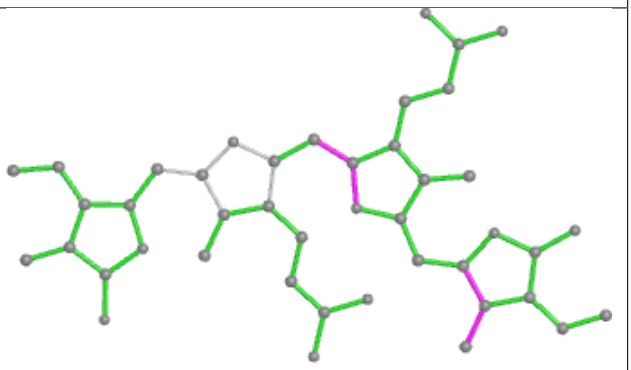


Rings

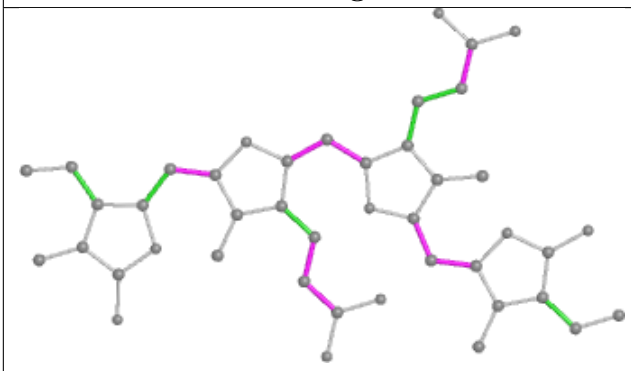
Ligand CYC BE 1000



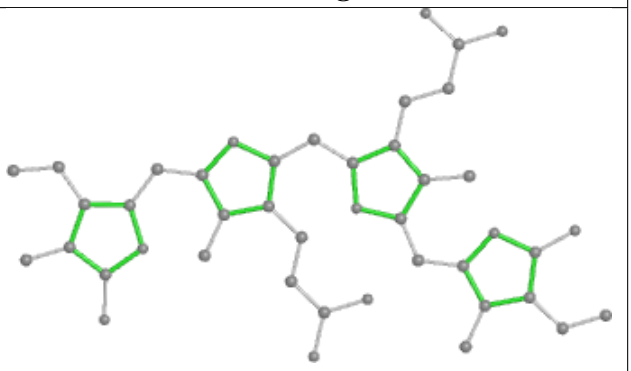
Bond lengths



Bond angles

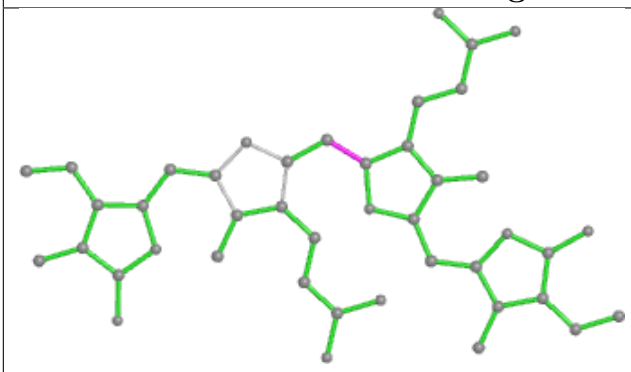


Torsions

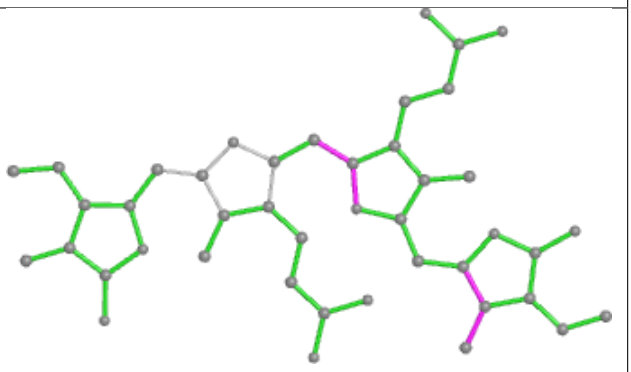


Rings

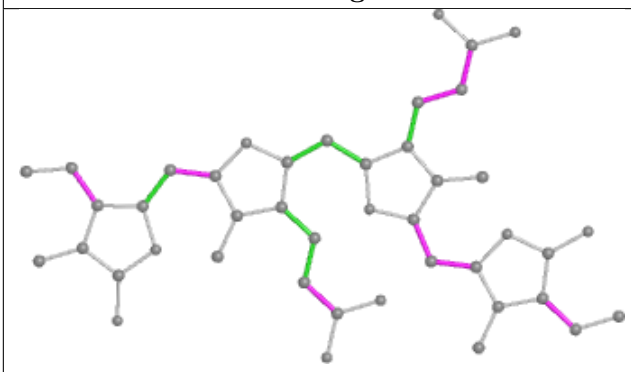
Ligand CYC AX 200



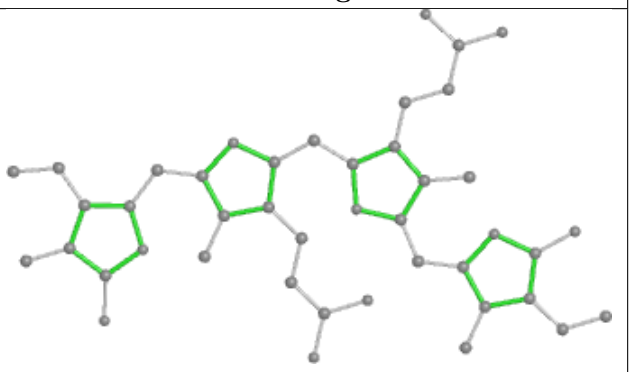
Bond lengths



Bond angles

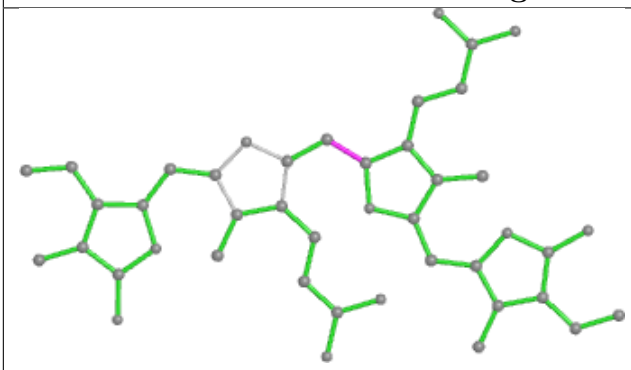


Torsions

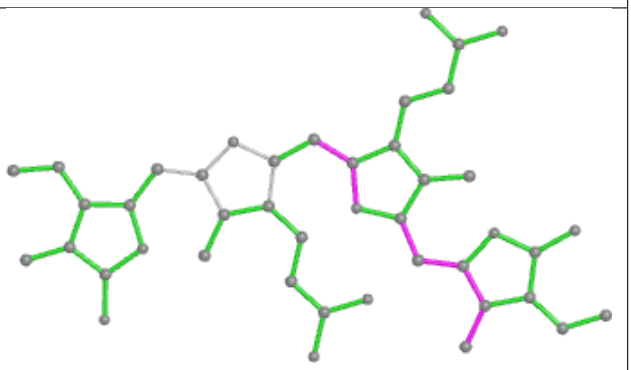


Rings

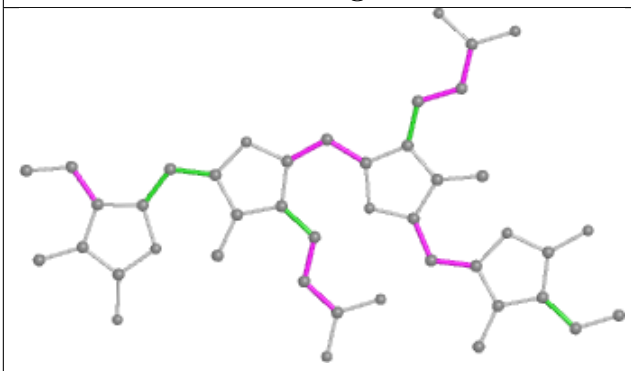
Ligand CYC AV 200



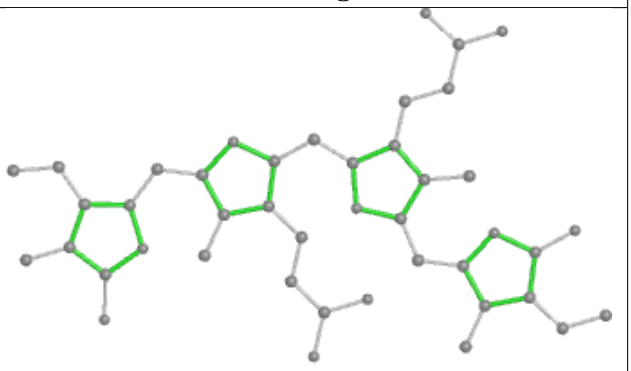
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

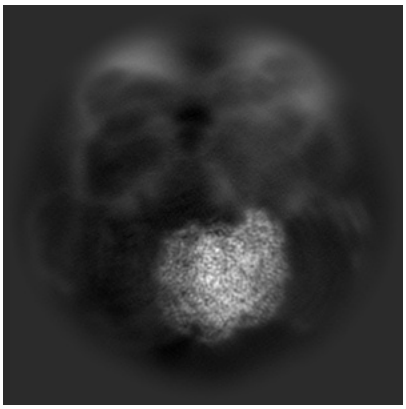
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25032. These allow visual inspection of the internal detail of the map and identification of artifacts.

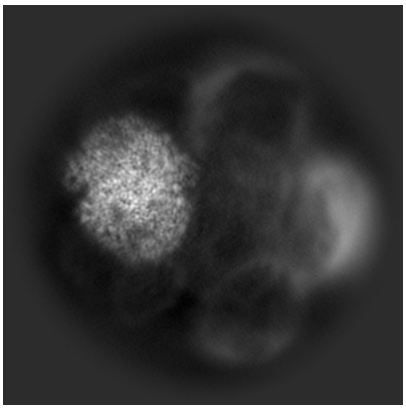
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

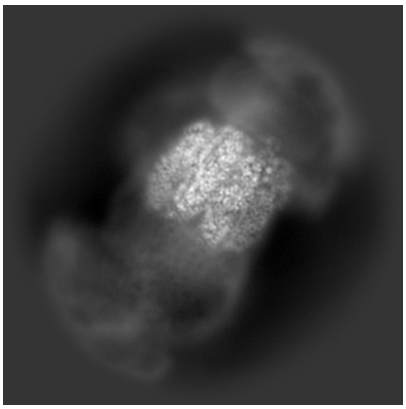
6.1.1 Primary map



X

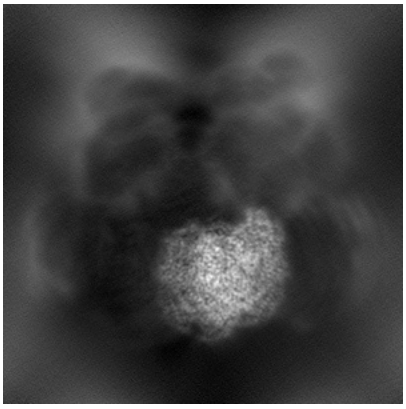


Y

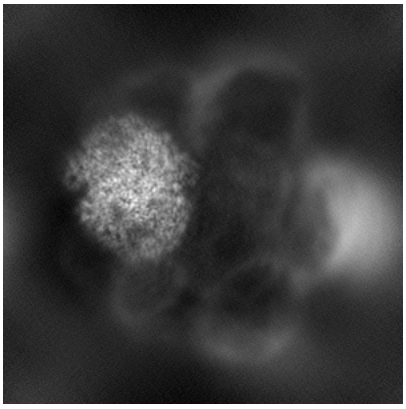


Z

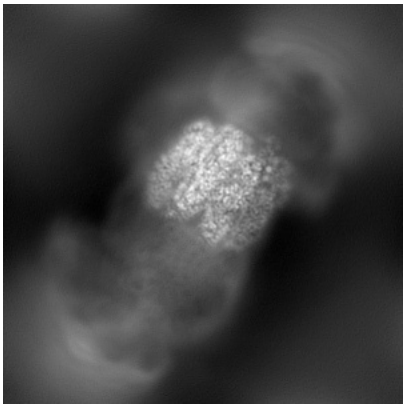
6.1.2 Raw map



X



Y

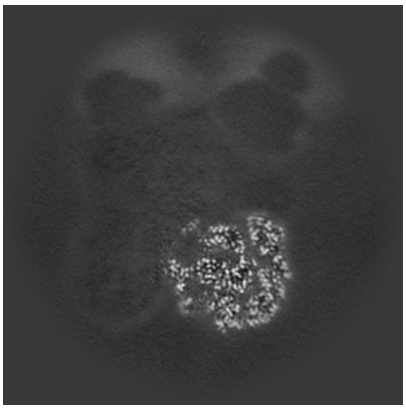


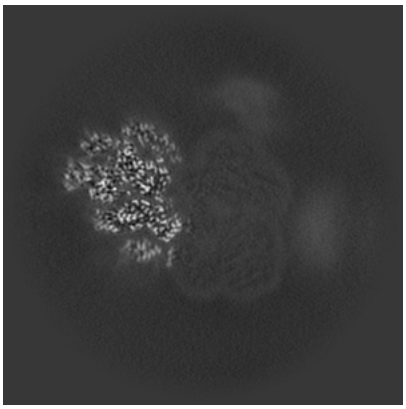
Z

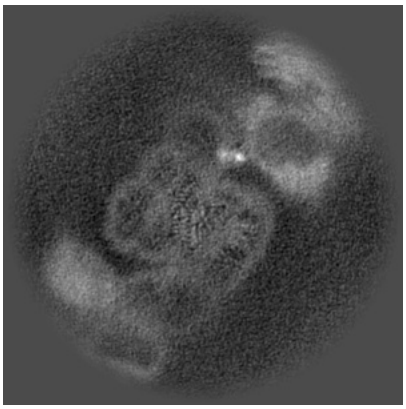
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

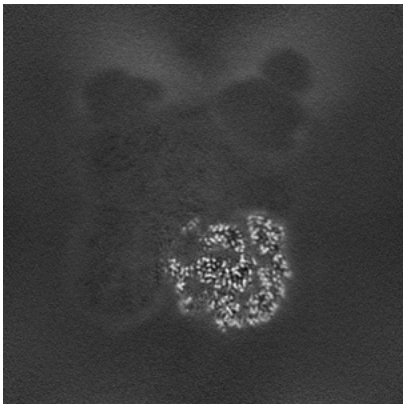
6.2.1 Primary map

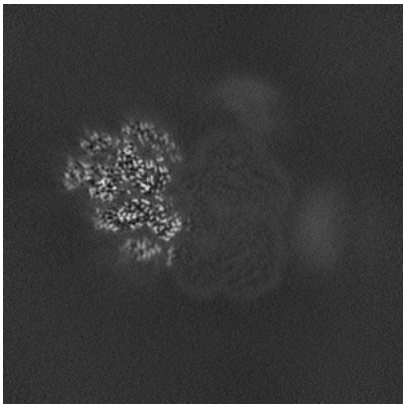

X Index: 180

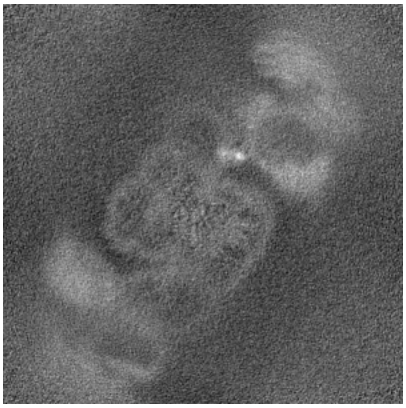

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

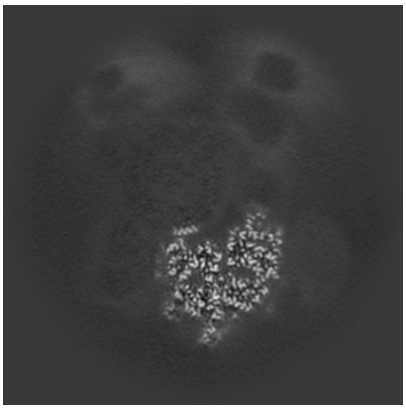

Y Index: 180

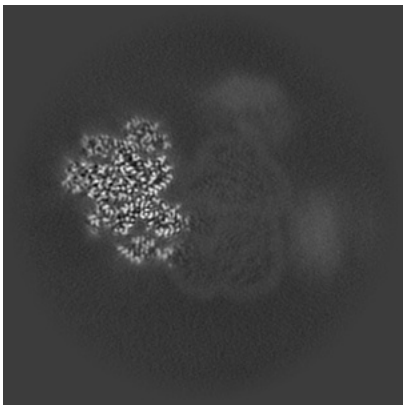

Z Index: 180

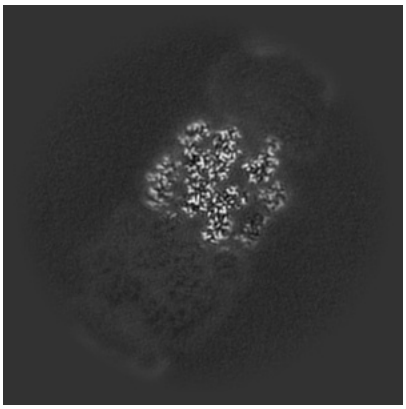
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

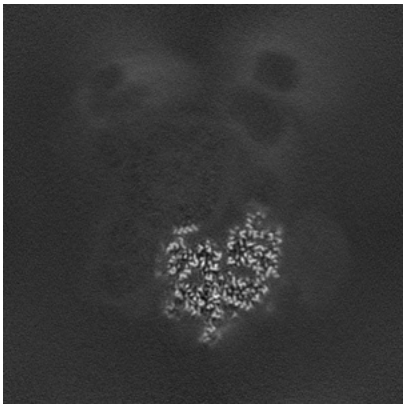
6.3.1 Primary map

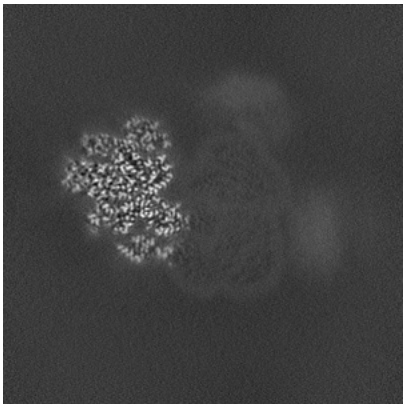

X Index: 196

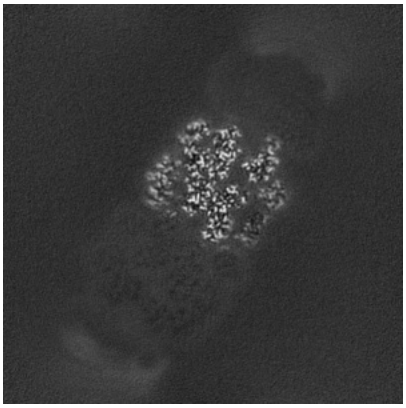

Y Index: 185


Z Index: 128

6.3.2 Raw map


X Index: 196

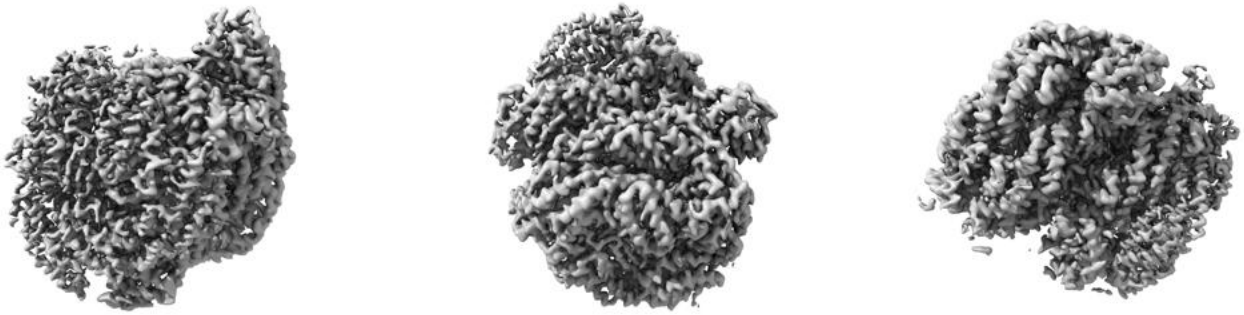

Y Index: 185


Z Index: 128

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

6.4 Orthogonal surface views (i)

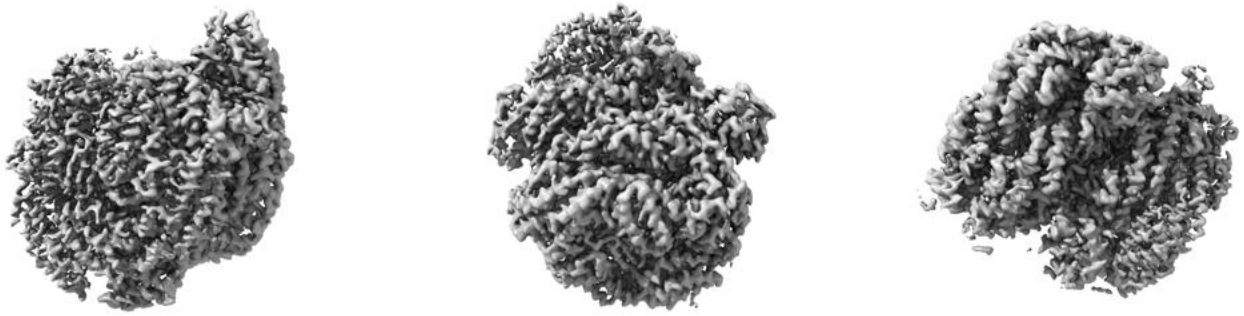
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.457. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

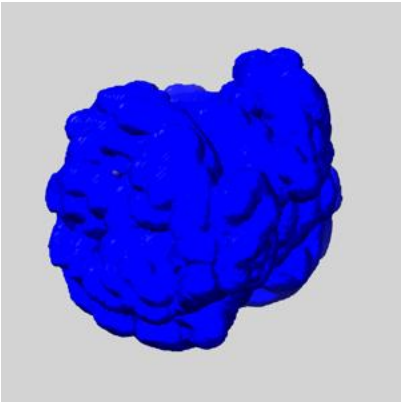
6.5 Mask visualisation (i)

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

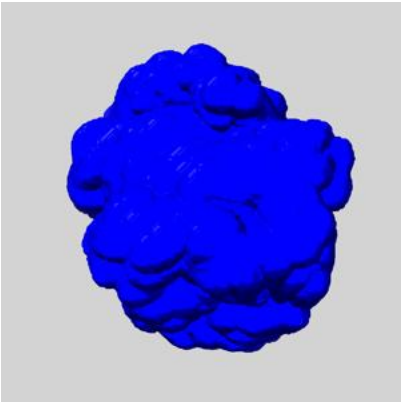
A mask typically either:

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

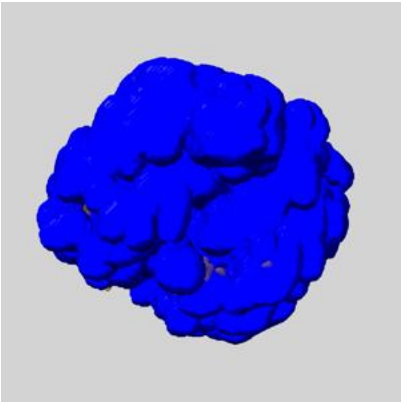
6.5.1 emd_25032_msk_1.map (i)



X



Y

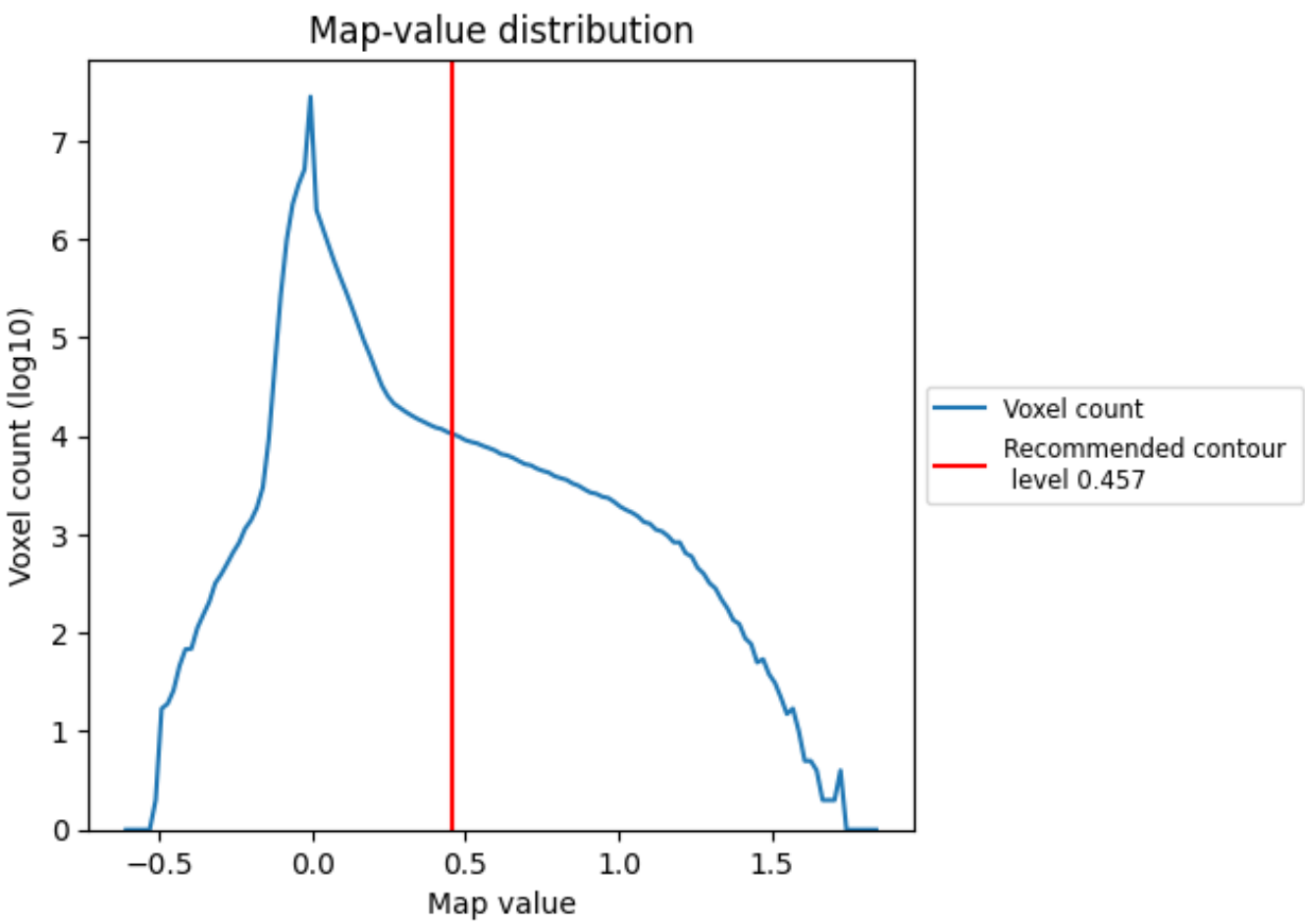


Z

7 Map analysis (i)

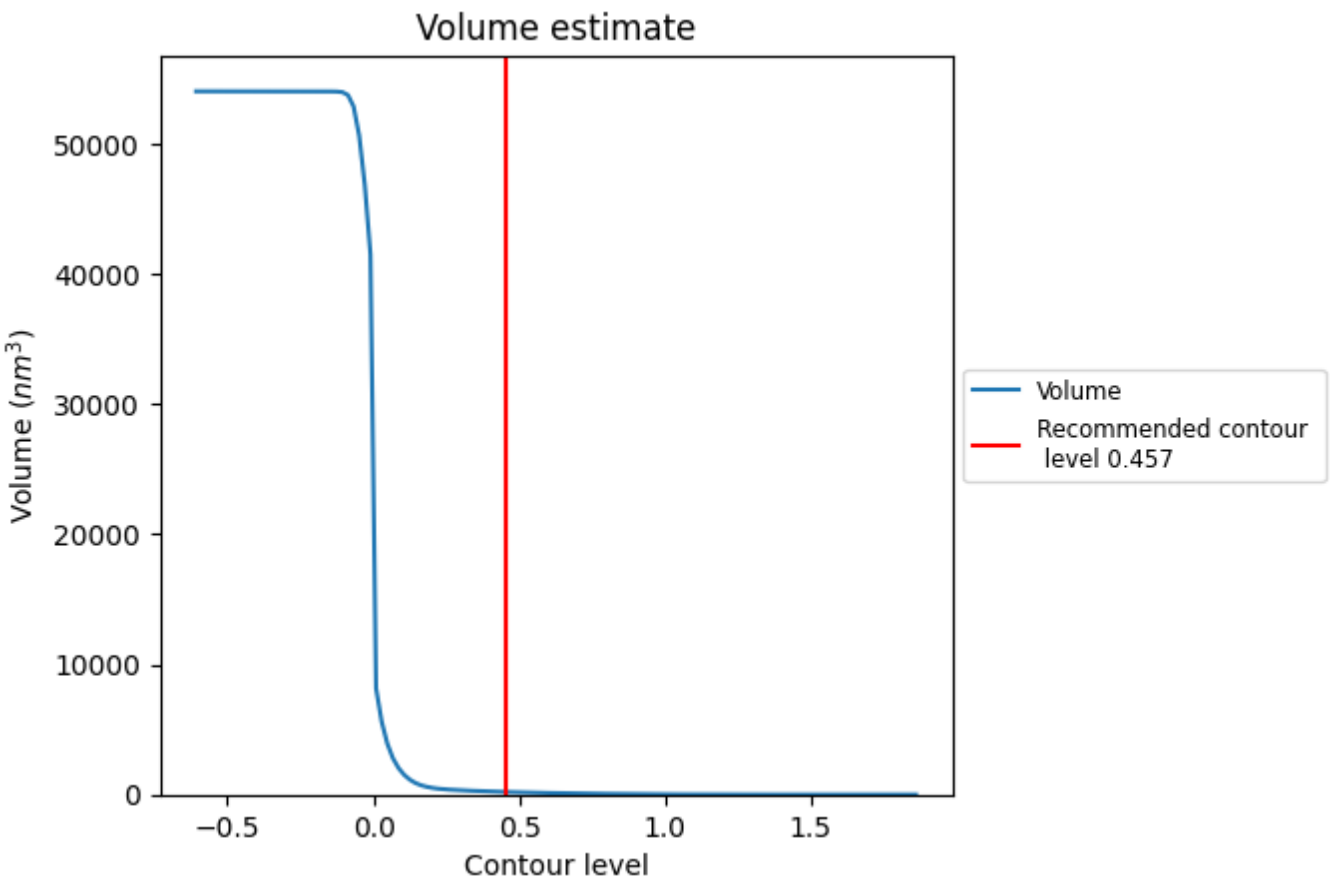
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

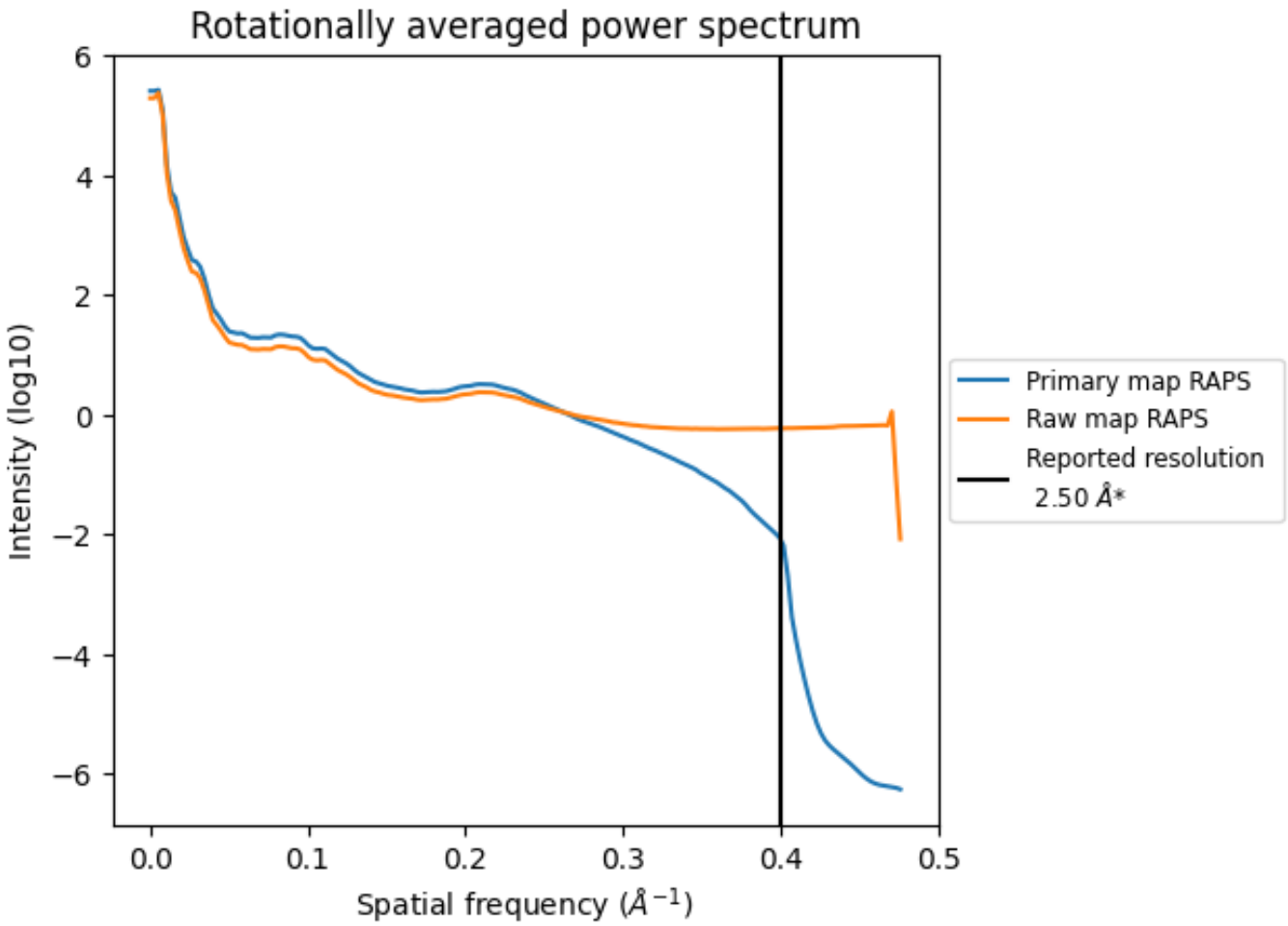
7.2 Volume estimate (i)



The volume at the recommended contour level is 197 nm^3; this corresponds to an approximate mass of 178 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)

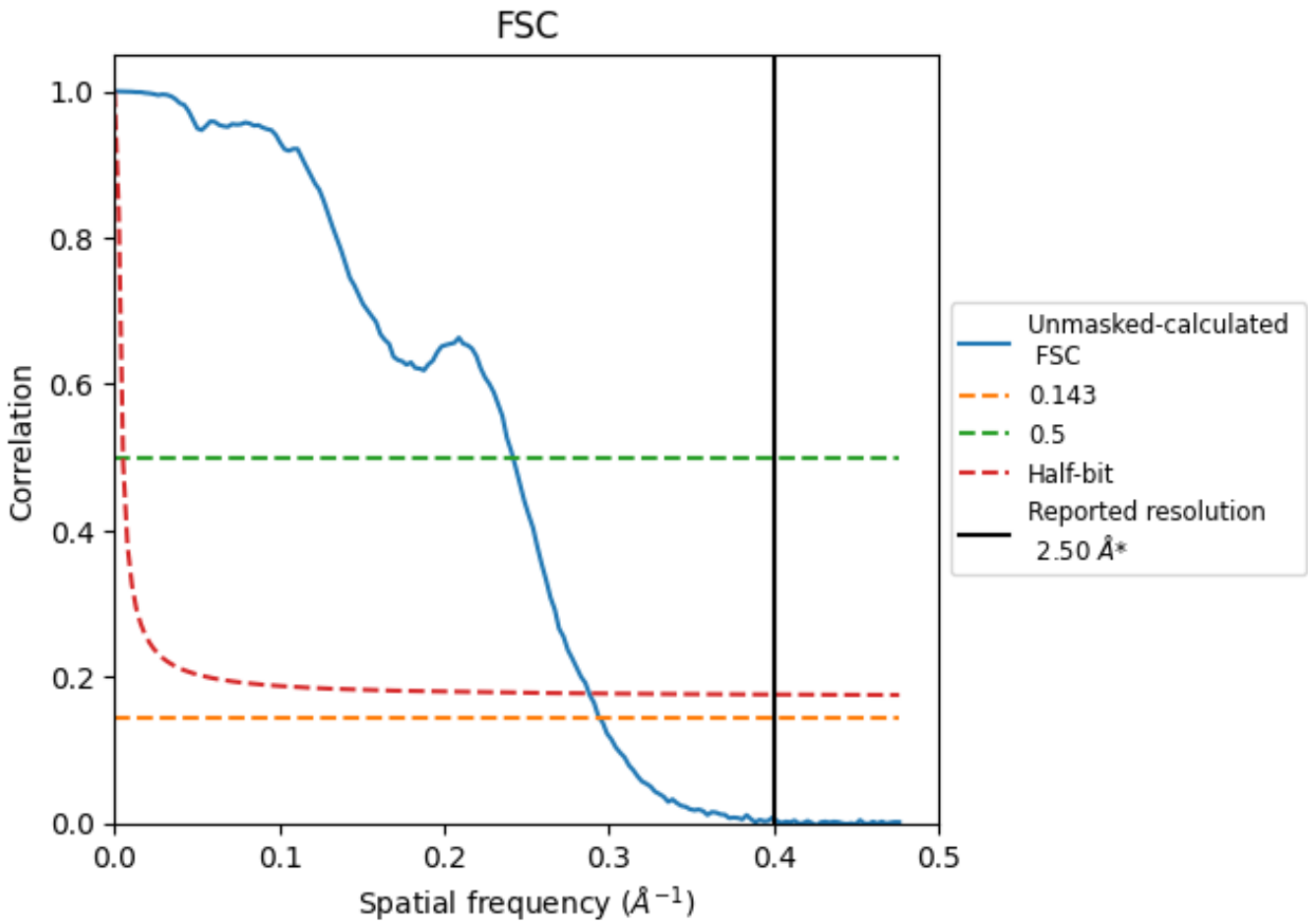


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

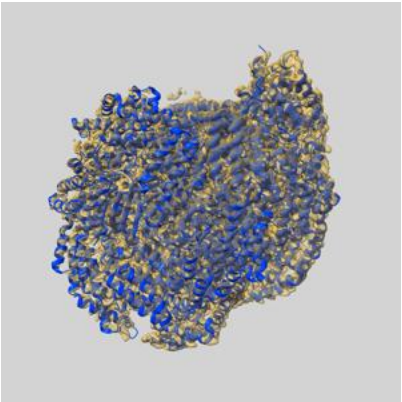
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	4.14	3.47

*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 3.40 differs from the reported value 2.5 by more than 10 %

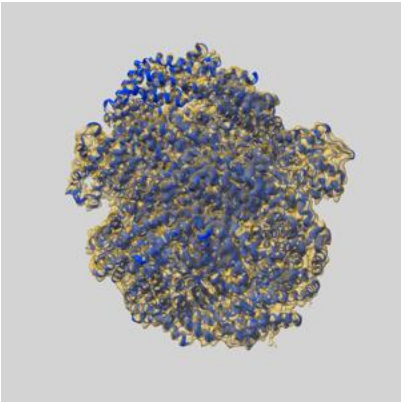
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25032 and PDB model 7SCB. Per-residue inclusion information can be found in section 3 on page 9.

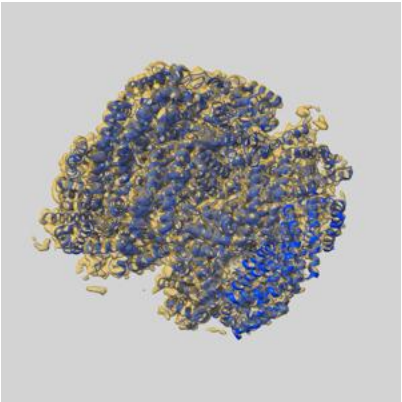
9.1 Map-model overlay (i)



X



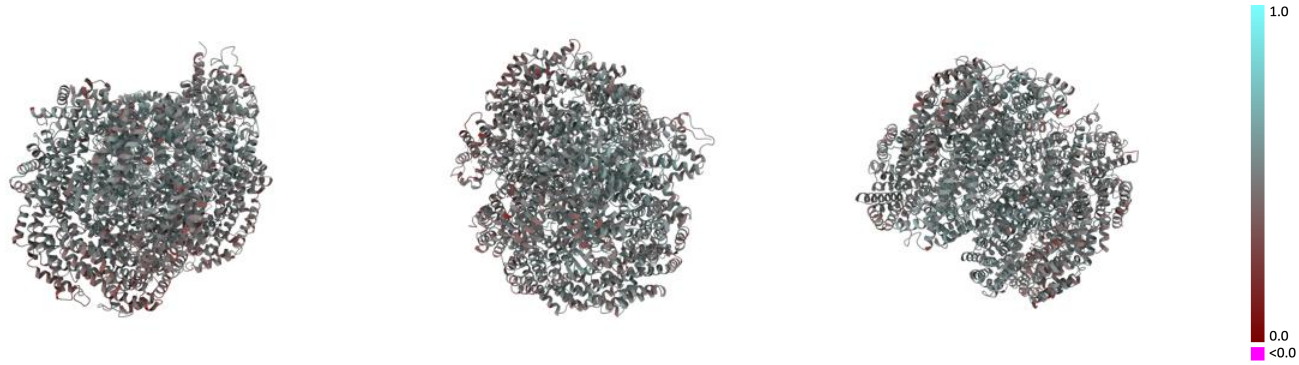
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.457 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.

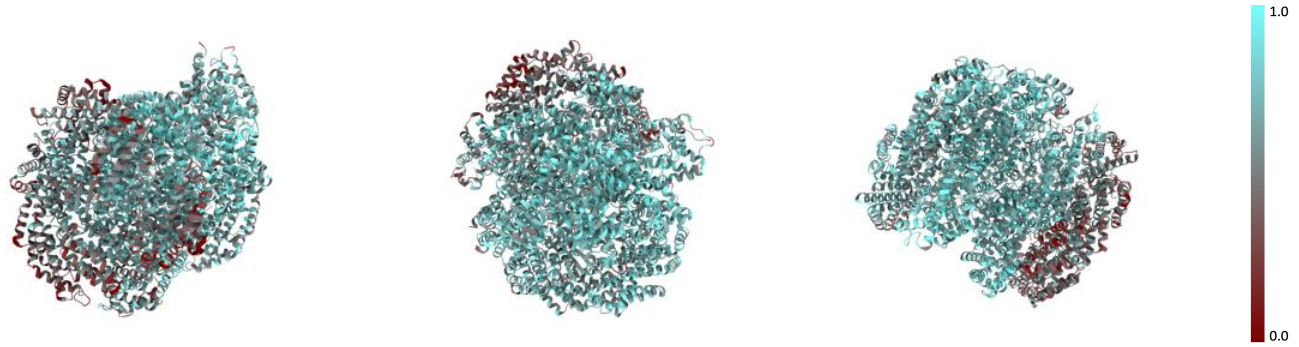
9.2 Q-score mapped to coordinate model (i)



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.

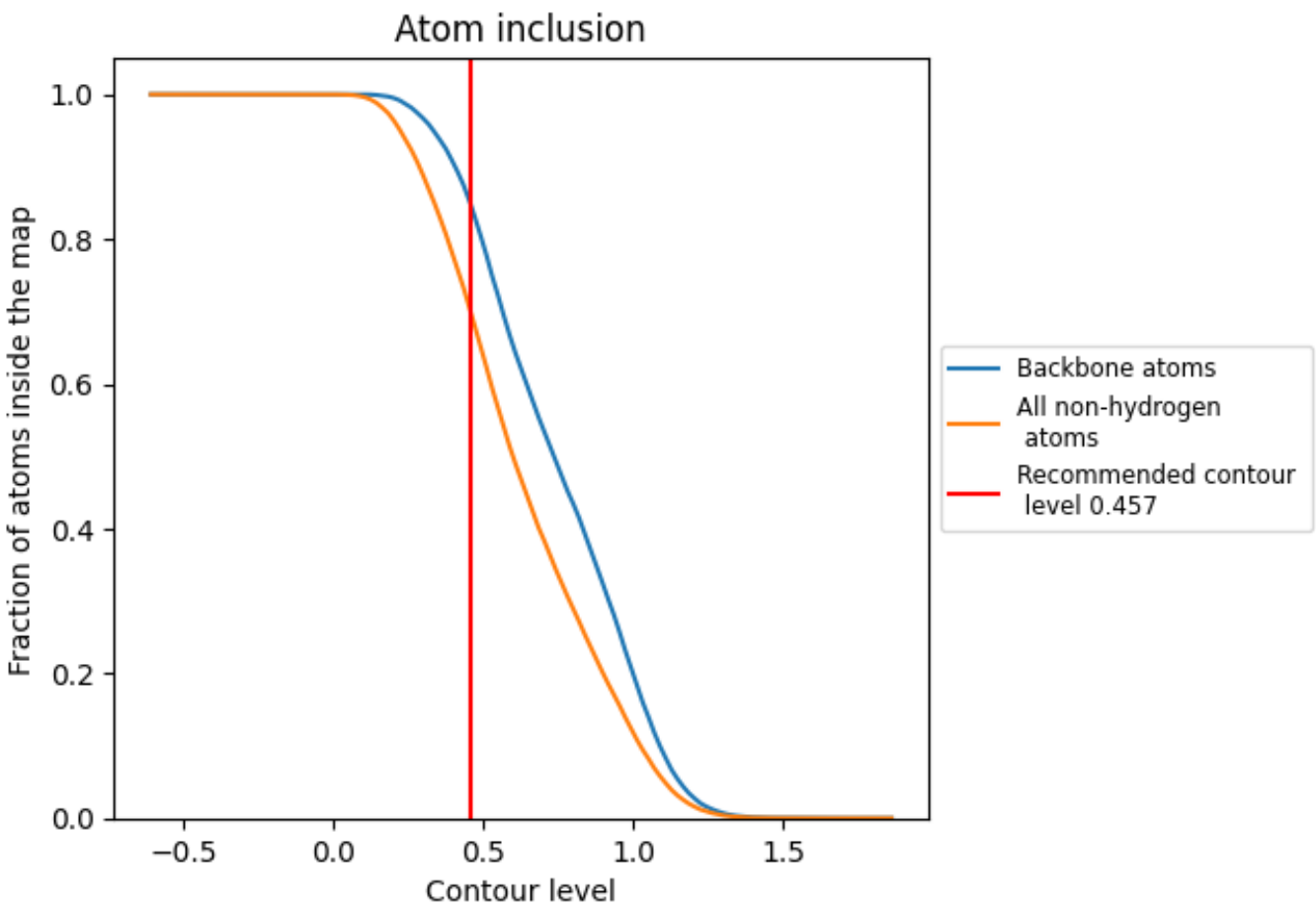
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.457).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.457) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7006	0.4970
AA	0.3970	0.4710
AB	0.4811	0.4880
AC	0.4208	0.4510
AD	0.4310	0.4420
AE	0.4500	0.4460
AF	0.4606	0.4820
AH	0.7998	0.5130
AI	0.8366	0.5450
AJ	0.8056	0.5180
AK	0.7894	0.5080
AL	0.8144	0.5110
AN	0.7711	0.4800
AO	0.8210	0.5360
AP	0.8146	0.5290
AQ	0.8284	0.5460
AR	0.8269	0.5240
AS	0.8202	0.5190
AU	0.6604	0.4740
AV	0.7126	0.4780
AW	0.7383	0.4670
AX	0.7406	0.4690
AY	0.7769	0.4910
AZ	0.7479	0.4930
BB	0.5541	0.5160
BC	0.6034	0.5250
BE	0.7738	0.5070
BG	0.7523	0.4860
BH	0.6672	0.4860
BI	0.6654	0.4520