Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 10:08 AM EDT

PDB ID	:	8EL4
Title	:	Light harvesting phycobiliprotein HaPE555 from the cryptophyte Hemiselmis andersenii CCMP644 in a tight interface filament
Authors	:	Rathbone, H.W.; Michie, K.A.; Laos, A.L.; Curmi, P.M.G.
Deposited on	:	2022-09-23
Resolution	:	1.73 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

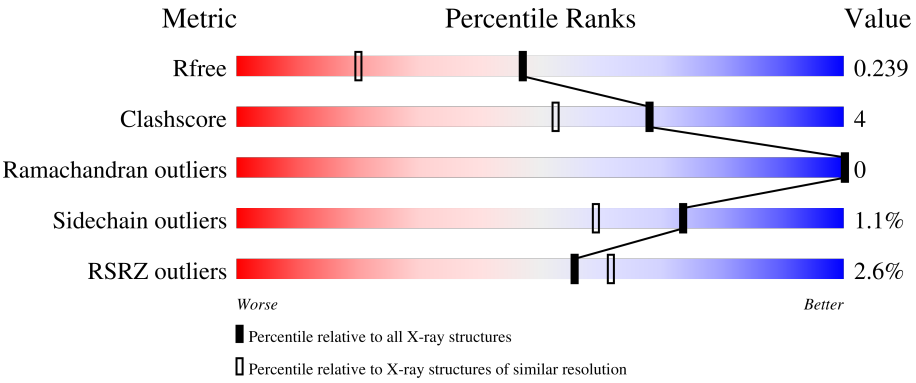
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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.



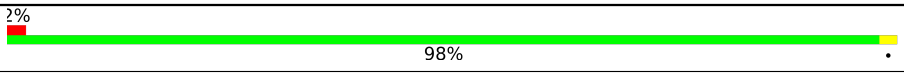
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	67	3% 94%
1	F	67	7% 88% 7%
2	B	177	% 86% 6% 8%
2	D	177	2% 86% 6% 8%
3	C	62	3% 90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	62	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9570 atoms, of which 4655 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Phycoerythrin alpha-1 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	64	Total	C	H	N	O	S	0	64	0
			924	287	459	82	91	5			
1	F	64	Total	C	H	N	O	S	0	64	0
			922	287	457	82	91	5			

- Molecule 2 is a protein called Phycoerythrin550 beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	163	Total	C	H	N	O	S	0	5	0
			2421	745	1213	209	245	9			
2	D	163	Total	C	H	N	O	S	0	8	0
			2484	762	1245	215	253	9			

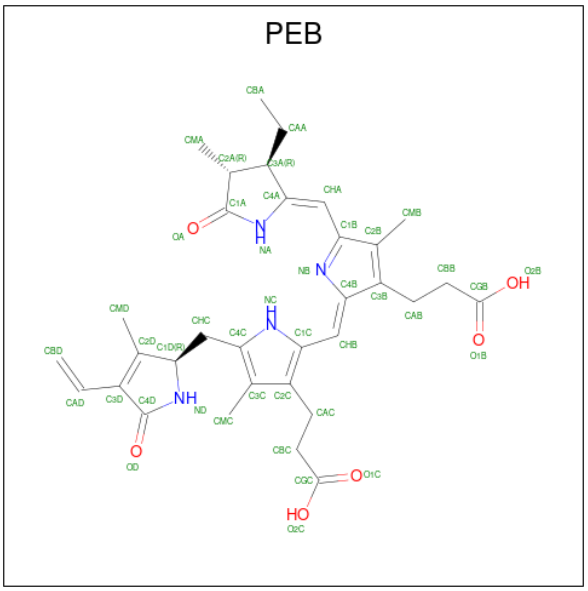
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	VAL	GLU	conflict	UNP U5T8W0
D	172	VAL	GLU	conflict	UNP U5T8W0

- Molecule 3 is a protein called Phycoerythrin alpha-2 subunit.

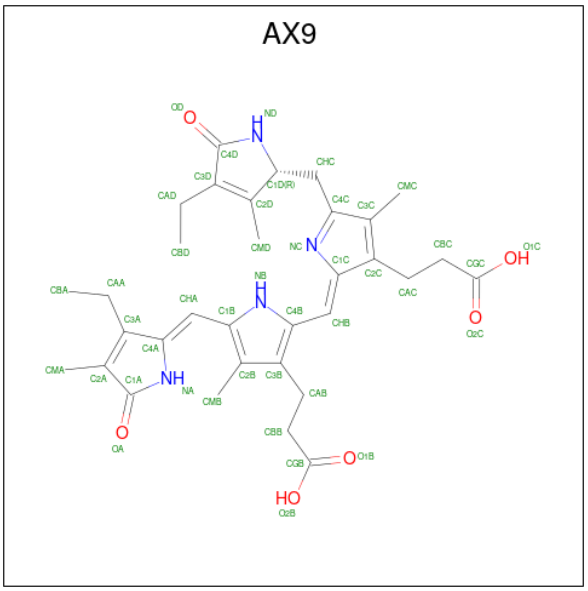
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	62	Total	C	H	N	O	S	0	62	0
			915	280	457	79	93	6			
3	E	62	Total	C	H	N	O	S	0	62	0
			914	280	456	79	93	6			

- Molecule 4 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	1
			80	33	37	4	6		
4	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
4	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
4	C	1	Total	C	H	N	O	0	1
			80	33	37	4	6		
4	D	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
4	D	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
4	E	1	Total	C	H	N	O	0	1
			80	33	37	4	6		
4	F	1	Total	C	H	N	O	0	1
			80	33	37	4	6		

- Molecule 5 is DiCys-(15,16)-Dihydrobiliverdin (three-letter code: AX9) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
5	D	1	Total	C	H	N	O	0	0
			79	33	36	4	6		

- Molecule 6 is water.

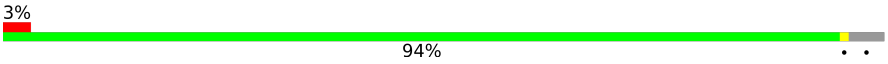
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	2
			36	36		
6	B	65	Total	O	0	3
			65	65		
6	C	27	Total	O	0	1
			27	27		
6	D	57	Total	O	0	2
			57	57		
6	E	4	Total	O	0	2
			4	4		
6	F	3	Total	O	0	1
			3	3		

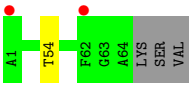
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Phycoerythrin alpha-1 subunit

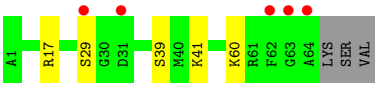
Chain A:





• Molecule 1: Phycoerythrin alpha-1 subunit

Chain F:

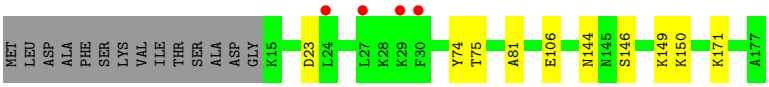


• Molecule 2: Phycoerythrin550 beta subunit

Chain B:

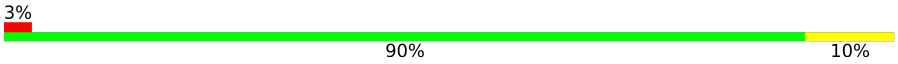
• Molecule 2: Phycoerythrin550 beta subunit

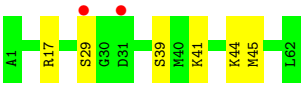
Chain D:



• Molecule 3: Phycoerythrin alpha-2 subunit

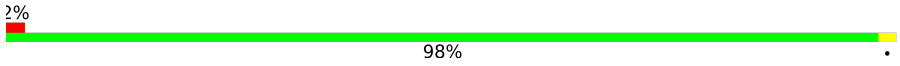
Chain C:





• Molecule 3: Phycoerythrin alpha-2 subunit

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.53Å 71.26Å 48.28Å 90.00° 108.47° 90.00°	Depositor
Resolution (Å)	45.80 – 1.73 45.80 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.80-1.73) 99.3 (45.80-1.73)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.239 0.189 , 0.239	Depositor DCC
R_{free} test set	1972 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9570	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AX9, PEB, LYZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.60	0/459	0.78	0/609
1	F	0.58	0/459	0.71	0/609
2	B	0.58	0/1228	0.74	1/1657 (0.1%)
2	D	0.56	0/1259	0.66	0/1697
3	C	0.58	0/450	0.68	0/597
3	E	0.60	0/450	0.74	0/597
All	All	0.58	0/4305	0.71	1/5766 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	101	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	465	459	451	1	0
1	F	465	457	450	3	0
2	B	1208	1213	1203	9	1
2	D	1239	1245	1232	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	458	457	449	4	0
3	E	458	456	450	1	0
4	A	43	37	37	3	0
4	B	86	74	74	6	0
4	C	43	37	37	0	0
4	D	86	74	74	8	0
4	E	43	37	37	2	0
4	F	43	37	37	0	0
5	B	43	36	0	0	0
5	D	43	36	0	0	0
6	A	36	0	0	0	0
6	B	65	0	0	2	0
6	C	27	0	0	0	0
6	D	57	0	0	1	0
6	E	4	0	0	0	0
6	F	3	0	0	1	0
All	All	4915	4655	4531	35	1

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

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:PEB:HMB2	4:D:202:PEB:HNA	1.48	0.78
1:A:54[A]:THR:HG23	2:B:67:ILE:HD11	1.69	0.73
2:B:67:ILE:HD11	3:E:54[B]:THR:HG23	1.69	0.73
2:D:149:LYS:NZ	6:D:301:HOH:O	2.22	0.72
2:B:149:LYS:NZ	6:B:301:HOH:O	2.26	0.68
4:B:202:PEB:HNA	4:B:202:PEB:HMB2	1.59	0.68
2:B:111:ASN:ND2	6:B:302:HOH:O	2.29	0.65
4:D:203:PEB:HMB2	4:D:203:PEB:HNA	1.66	0.60
2:D:146:SER:O	2:D:150:LYS:NZ	2.31	0.58
4:B:203:PEB:HBA3	4:B:203:PEB:HHA1	1.85	0.58
4:D:203:PEB:HMB2	4:D:203:PEB:NA	2.18	0.58
4:B:203:PEB:HNA	4:B:203:PEB:HMB2	1.71	0.55
4:A:101[A]:PEB:HMB2	4:A:101[A]:PEB:NA	2.23	0.53
4:E:101[B]:PEB:HMB2	4:E:101[B]:PEB:NA	2.23	0.53
4:B:203:PEB:HMB2	4:B:203:PEB:NA	2.25	0.52
4:D:202:PEB:HMB2	4:D:202:PEB:NA	2.22	0.50
1:F:60[B]:LYS:HB2	6:F:201:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39[A]:SER:OG	3:C:41[A]:LYS:HE2	2.13	0.48
1:F:39[B]:SER:OG	1:F:41[B]:LYS:HE2	2.13	0.48
2:B:31:VAL:HG21	2:B:37:ARG:HD2	1.95	0.48
3:C:45[A]:MET:HE2	2:D:81:ALA:HB2	1.96	0.48
2:D:106:GLU:OE1	2:D:171:LYS:NZ	2.47	0.47
4:D:203:PEB:HBA3	4:D:203:PEB:CHA	2.45	0.46
4:A:101[A]:PEB:HMB2	4:A:101[A]:PEB:HNA	1.81	0.46
4:E:101[B]:PEB:HMB2	4:E:101[B]:PEB:HNA	1.81	0.46
4:D:203:PEB:HBA3	4:D:203:PEB:HHA1	1.97	0.46
4:A:101[A]:PEB:O1B	3:C:44[A]:LYS:HG2	2.15	0.45
2:D:74:TYR:CD2	2:D:75:THR:HG23	2.52	0.45
2:D:144[B]:ASN:OD1	2:D:150:LYS:HD2	2.18	0.43
2:B:142:ILE:O	4:B:203:PEB:HAA2	2.19	0.43
2:B:156:GLY:HA3	4:B:203:PEB:CMB	2.49	0.43
3:C:17[A]:ARG:NH1	4:D:203:PEB:HMC2	2.35	0.42
4:D:203:PEB:HMC2	1:F:17[B]:ARG:NH1	2.35	0.42
2:B:58:GLY:O	2:B:62:GLU:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:ASN:OD1	2:D:106:GLU:OE2[1_455]	1.95	0.25

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
1	F	61/67 (91%)	61 (100%)	0	0	100	100
2	B	166/177 (94%)	164 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	170/177 (96%)	166 (98%)	4 (2%)	0	100	100
3	C	59/62 (95%)	59 (100%)	0	0	100	100
3	E	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	576/612 (94%)	568 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	45/48 (94%)	45 (100%)	0	100	100
1	F	45/48 (94%)	44 (98%)	1 (2%)	52	29
2	B	134/140 (96%)	132 (98%)	2 (2%)	65	47
2	D	138/140 (99%)	137 (99%)	1 (1%)	84	75
3	C	48/48 (100%)	47 (98%)	1 (2%)	53	30
3	E	48/48 (100%)	48 (100%)	0	100	100
All	All	458/472 (97%)	453 (99%)	5 (1%)	73	59

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	49	SER
2	B	101	ASP
3	C	29[A]	SER
2	D	23	ASP
1	F	29[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26[A]	GLN
1	A	46[A]	ASN
3	C	56[A]	ASN
1	F	26[B]	GLN
1	F	46[B]	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LYZ	A	4[A]	1	7,9,10	0.63	0	4,10,12	1.03	0
3	LYZ	C	4[A]	3	7,9,10	0.93	0	4,10,12	0.59	0
1	LYZ	F	4[B]	1	7,9,10	0.93	0	4,10,12	0.59	0
3	LYZ	E	4[B]	3	7,9,10	0.63	0	4,10,12	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYZ	A	4[A]	1	-	1/8/9/11	-
3	LYZ	C	4[A]	3	-	1/8/9/11	-
1	LYZ	F	4[B]	1	-	1/8/9/11	-
3	LYZ	E	4[B]	3	-	1/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4[A]	LYZ	O-C-CA-CB
1	F	4[B]	LYZ	O-C-CA-CB
1	A	4[A]	LYZ	OH-CD-CG-CB
3	E	4[B]	LYZ	OH-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
5	AX9	D	201	2	41,46,46	1.71	11 (26%)	41,67,67	1.31	7 (17%)
4	PEB	D	203	2	43,46,46	5.03	34 (79%)	45,67,67	1.76	6 (13%)
4	PEB	A	101[A]	1	43,46,46	4.17	29 (67%)	45,67,67	2.29	12 (26%)
4	PEB	D	202	2	43,46,46	4.47	30 (69%)	45,67,67	2.36	17 (37%)
4	PEB	F	101[B]	1	43,46,46	4.68	31 (72%)	45,67,67	2.19	11 (24%)
5	AX9	B	201	2	41,46,46	1.60	8 (19%)	41,67,67	1.44	6 (14%)
4	PEB	C	101[A]	3	43,46,46	4.68	31 (72%)	45,67,67	2.19	11 (24%)
4	PEB	E	101[B]	3	43,46,46	4.17	29 (67%)	45,67,67	2.29	12 (26%)
4	PEB	B	203	2	43,46,46	4.56	32 (74%)	45,67,67	1.85	12 (26%)
4	PEB	B	202	2	43,46,46	4.31	30 (69%)	45,67,67	2.26	12 (26%)

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
5	AX9	D	201	2	-	7/26/74/74	0/4/4/4
4	PEB	D	203	2	-	7/24/74/74	0/4/4/4
4	PEB	A	101[A]	1	-	7/24/74/74	0/4/4/4
4	PEB	D	202	2	-	4/24/74/74	0/4/4/4
4	PEB	F	101[B]	1	-	4/24/74/74	0/4/4/4
5	AX9	B	201	2	-	7/26/74/74	0/4/4/4
4	PEB	C	101[A]	3	-	4/24/74/74	0/4/4/4
4	PEB	E	101[B]	3	-	7/24/74/74	0/4/4/4
4	PEB	B	203	2	-	4/24/74/74	0/4/4/4
4	PEB	B	202	2	-	2/24/74/74	0/4/4/4

All (265) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	203	PEB	CHB-C4B	11.93	1.45	1.35
4	D	203	PEB	C2A-C1A	11.83	1.62	1.52
4	C	101[A]	PEB	C2A-C1A	11.80	1.62	1.52
4	F	101[B]	PEB	C2A-C1A	11.80	1.62	1.52
4	B	203	PEB	C2A-C1A	11.45	1.62	1.52
4	D	202	PEB	CHB-C4B	11.24	1.44	1.35
4	B	202	PEB	CHB-C4B	10.57	1.44	1.35
4	C	101[A]	PEB	CHB-C4B	10.32	1.43	1.35
4	F	101[B]	PEB	CHB-C4B	10.32	1.43	1.35
4	D	203	PEB	CAC-C2C	10.16	1.67	1.52
4	D	203	PEB	C1A-NA	10.04	1.50	1.37
4	D	202	PEB	C2A-C1A	9.80	1.60	1.52
4	B	203	PEB	CAC-C2C	9.77	1.66	1.52
4	A	101[A]	PEB	CHB-C4B	9.60	1.43	1.35
4	E	101[B]	PEB	CHB-C4B	9.60	1.43	1.35
4	B	203	PEB	CHB-C4B	9.31	1.42	1.35
4	B	203	PEB	C1A-NA	9.26	1.49	1.37
4	B	202	PEB	CAC-C2C	9.06	1.65	1.52
4	D	203	PEB	CHA-C1B	8.92	1.61	1.40
4	A	101[A]	PEB	C4D-ND	8.77	1.47	1.35
4	E	101[B]	PEB	C4D-ND	8.77	1.47	1.35
4	D	202	PEB	C1A-NA	8.54	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	203	PEB	C3A-C4A	8.49	1.63	1.50
4	C	101[A]	PEB	CAC-C2C	8.30	1.64	1.52
4	F	101[B]	PEB	CAC-C2C	8.30	1.64	1.52
4	A	101[A]	PEB	C2A-C1A	8.29	1.59	1.52
4	E	101[B]	PEB	C2A-C1A	8.29	1.59	1.52
4	C	101[A]	PEB	C1A-NA	8.23	1.48	1.37
4	F	101[B]	PEB	C1A-NA	8.23	1.48	1.37
4	B	203	PEB	CHA-C1B	8.11	1.59	1.40
4	D	202	PEB	CAC-C2C	8.10	1.63	1.52
4	B	202	PEB	C4D-ND	8.08	1.46	1.35
4	B	202	PEB	C1A-NA	8.08	1.48	1.37
4	C	101[A]	PEB	C4D-ND	8.04	1.46	1.35
4	F	101[B]	PEB	C4D-ND	8.04	1.46	1.35
4	D	202	PEB	CHA-C1B	8.02	1.59	1.40
4	C	101[A]	PEB	CHA-C1B	8.00	1.59	1.40
4	F	101[B]	PEB	CHA-C1B	8.00	1.59	1.40
4	A	101[A]	PEB	CHA-C1B	7.82	1.58	1.40
4	E	101[B]	PEB	CHA-C1B	7.82	1.58	1.40
4	A	101[A]	PEB	C1A-NA	7.54	1.47	1.37
4	E	101[B]	PEB	C1A-NA	7.54	1.47	1.37
4	B	202	PEB	CHA-C1B	7.52	1.58	1.40
4	D	203	PEB	C4D-ND	7.48	1.45	1.35
4	D	202	PEB	C4D-ND	7.27	1.45	1.35
4	A	101[A]	PEB	CAC-C2C	7.13	1.62	1.52
4	E	101[B]	PEB	CAC-C2C	7.13	1.62	1.52
4	B	202	PEB	C3A-C4A	7.01	1.61	1.50
4	C	101[A]	PEB	C3A-C4A	6.84	1.60	1.50
4	F	101[B]	PEB	C3A-C4A	6.84	1.60	1.50
4	C	101[A]	PEB	CMD-C2D	6.76	1.61	1.50
4	F	101[B]	PEB	CMD-C2D	6.76	1.61	1.50
4	B	203	PEB	C3A-C4A	6.73	1.60	1.50
4	B	203	PEB	C4D-ND	6.62	1.44	1.35
4	D	202	PEB	C3A-C4A	6.50	1.60	1.50
4	B	202	PEB	C2A-C1A	6.50	1.57	1.52
4	D	202	PEB	CMD-C2D	6.22	1.60	1.50
4	B	202	PEB	CMD-C2D	6.10	1.60	1.50
4	D	203	PEB	CMB-C2B	5.95	1.63	1.50
4	C	101[A]	PEB	CMB-C2B	5.73	1.62	1.50
4	F	101[B]	PEB	CMB-C2B	5.73	1.62	1.50
4	D	203	PEB	CMD-C2D	5.71	1.59	1.50
4	C	101[A]	PEB	C4A-NA	5.68	1.49	1.37
4	F	101[B]	PEB	C4A-NA	5.68	1.49	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	101[A]	PEB	CMD-C2D	5.66	1.59	1.50
4	E	101[B]	PEB	CMD-C2D	5.66	1.59	1.50
4	D	202	PEB	CMB-C2B	5.50	1.62	1.50
4	B	203	PEB	CBC-CGC	5.39	1.63	1.50
4	B	203	PEB	CMD-C2D	5.35	1.59	1.50
4	D	203	PEB	C1C-CHB	5.31	1.61	1.41
4	C	101[A]	PEB	C1C-CHB	5.30	1.61	1.41
4	F	101[B]	PEB	C1C-CHB	5.30	1.61	1.41
4	A	101[A]	PEB	CBC-CGC	5.25	1.62	1.50
4	E	101[B]	PEB	CBC-CGC	5.25	1.62	1.50
4	D	202	PEB	CBC-CGC	5.20	1.62	1.50
4	D	203	PEB	C4A-NA	5.07	1.48	1.37
4	A	101[A]	PEB	C1C-CHB	5.06	1.60	1.41
4	E	101[B]	PEB	C1C-CHB	5.06	1.60	1.41
4	B	202	PEB	C1C-CHB	5.02	1.60	1.41
4	D	202	PEB	C1C-CHB	4.96	1.60	1.41
4	A	101[A]	PEB	C3A-C4A	4.95	1.58	1.50
4	E	101[B]	PEB	C3A-C4A	4.95	1.58	1.50
4	B	203	PEB	C4A-NA	4.93	1.47	1.37
4	D	202	PEB	C2D-C3D	4.90	1.40	1.34
4	A	101[A]	PEB	CMB-C2B	4.88	1.61	1.50
4	E	101[B]	PEB	CMB-C2B	4.88	1.61	1.50
4	D	203	PEB	CBC-CGC	4.87	1.61	1.50
4	C	101[A]	PEB	C2D-C3D	4.85	1.40	1.34
4	F	101[B]	PEB	C2D-C3D	4.85	1.40	1.34
4	A	101[A]	PEB	C4A-NA	4.84	1.47	1.37
4	E	101[B]	PEB	C4A-NA	4.84	1.47	1.37
4	B	203	PEB	CMB-C2B	4.82	1.61	1.50
4	D	203	PEB	CAB-C3B	4.82	1.63	1.51
5	B	201	AX9	C1C-C2C	-4.81	1.38	1.45
4	B	202	PEB	CBC-CGC	4.80	1.61	1.50
4	B	203	PEB	C1C-CHB	4.76	1.59	1.41
4	C	101[A]	PEB	CBB-CGB	4.71	1.61	1.50
4	F	101[B]	PEB	CBB-CGB	4.71	1.61	1.50
4	D	202	PEB	C4A-NA	4.66	1.47	1.37
4	B	203	PEB	CMA-C2A	4.64	1.63	1.53
4	C	101[A]	PEB	CBC-CGC	4.62	1.61	1.50
4	F	101[B]	PEB	CBC-CGC	4.62	1.61	1.50
4	D	203	PEB	CMA-C2A	4.62	1.63	1.53
4	A	101[A]	PEB	CBB-CGB	4.52	1.61	1.50
4	E	101[B]	PEB	CBB-CGB	4.52	1.61	1.50
5	D	201	AX9	C1C-C2C	-4.50	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	203	PEB	CBB-CGB	4.45	1.60	1.50
4	B	202	PEB	CBB-CGB	4.45	1.60	1.50
4	B	202	PEB	C4A-NA	4.38	1.46	1.37
4	B	202	PEB	CMB-C2B	4.30	1.59	1.50
4	D	202	PEB	CMA-C2A	4.24	1.62	1.53
4	B	202	PEB	C2D-C3D	4.21	1.40	1.34
4	B	203	PEB	CAB-C3B	4.12	1.62	1.51
4	D	203	PEB	C2D-C3D	4.10	1.39	1.34
4	A	101[A]	PEB	CAB-C3B	4.09	1.61	1.51
4	E	101[B]	PEB	CAB-C3B	4.09	1.61	1.51
4	D	202	PEB	CBB-CGB	4.03	1.59	1.50
4	C	101[A]	PEB	O1B-CGB	3.97	1.35	1.22
4	F	101[B]	PEB	O1B-CGB	3.97	1.35	1.22
4	B	202	PEB	CAB-C3B	3.96	1.61	1.51
4	C	101[A]	PEB	C1B-NB	3.95	1.45	1.36
4	F	101[B]	PEB	C1B-NB	3.95	1.45	1.36
4	C	101[A]	PEB	CMA-C2A	3.93	1.61	1.53
4	F	101[B]	PEB	CMA-C2A	3.93	1.61	1.53
4	A	101[A]	PEB	C2D-C3D	3.91	1.39	1.34
4	E	101[B]	PEB	C2D-C3D	3.91	1.39	1.34
4	A	101[A]	PEB	O1B-CGB	3.81	1.34	1.22
4	E	101[B]	PEB	O1B-CGB	3.81	1.34	1.22
4	B	203	PEB	CBB-CGB	3.79	1.59	1.50
4	B	202	PEB	CAD-C3D	3.77	1.57	1.47
4	D	203	PEB	C4B-NB	3.73	1.46	1.38
4	A	101[A]	PEB	CMA-C2A	3.70	1.61	1.53
4	E	101[B]	PEB	CMA-C2A	3.70	1.61	1.53
4	D	203	PEB	O1B-CGB	3.68	1.34	1.22
4	B	202	PEB	O1C-CGC	3.67	1.34	1.22
4	B	203	PEB	C2D-C3D	3.66	1.39	1.34
4	B	203	PEB	O1B-CGB	3.58	1.34	1.22
4	B	203	PEB	O1C-CGC	3.55	1.33	1.22
4	D	202	PEB	CAD-C3D	3.55	1.57	1.47
4	B	203	PEB	C1B-NB	3.51	1.44	1.36
4	B	202	PEB	CMC-C3C	3.49	1.58	1.51
4	B	202	PEB	CHC-C4C	3.47	1.58	1.50
4	D	203	PEB	O1C-CGC	3.42	1.33	1.22
4	C	101[A]	PEB	CAB-C3B	3.41	1.60	1.51
4	F	101[B]	PEB	CAB-C3B	3.41	1.60	1.51
4	C	101[A]	PEB	O1C-CGC	3.38	1.33	1.22
4	F	101[B]	PEB	O1C-CGC	3.38	1.33	1.22
5	B	201	AX9	C4D-ND	3.38	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	101[A]	PEB	CHC-C4C	3.36	1.58	1.50
4	F	101[B]	PEB	CHC-C4C	3.36	1.58	1.50
4	D	202	PEB	CAB-C3B	3.34	1.60	1.51
4	D	202	PEB	O1C-CGC	3.34	1.33	1.22
4	B	203	PEB	C3C-C4C	3.33	1.47	1.42
5	D	201	AX9	C4A-C3A	-3.32	1.38	1.45
4	D	203	PEB	C1B-NB	3.30	1.44	1.36
4	D	203	PEB	CBB-CAB	3.30	1.62	1.52
4	A	101[A]	PEB	O1C-CGC	3.27	1.33	1.22
4	E	101[B]	PEB	O1C-CGC	3.27	1.33	1.22
4	C	101[A]	PEB	CAD-C3D	3.26	1.56	1.47
4	F	101[B]	PEB	CAD-C3D	3.26	1.56	1.47
4	D	203	PEB	C3B-C2B	3.24	1.43	1.36
4	C	101[A]	PEB	CMC-C3C	3.24	1.58	1.51
4	F	101[B]	PEB	CMC-C3C	3.24	1.58	1.51
4	D	202	PEB	O1B-CGB	3.23	1.32	1.22
4	B	203	PEB	CHC-C4C	3.23	1.58	1.50
4	D	203	PEB	C3C-C4C	3.23	1.47	1.42
4	C	101[A]	PEB	C3C-C4C	3.22	1.47	1.42
4	F	101[B]	PEB	C3C-C4C	3.22	1.47	1.42
4	B	202	PEB	C3C-C4C	3.21	1.47	1.42
5	B	201	AX9	C1A-C2A	-3.19	1.39	1.47
4	B	203	PEB	CAA-C3A	3.15	1.60	1.54
4	B	202	PEB	O1B-CGB	3.15	1.32	1.22
4	A	101[A]	PEB	C1B-NB	3.14	1.43	1.36
4	E	101[B]	PEB	C1B-NB	3.14	1.43	1.36
4	D	202	PEB	CHC-C4C	3.14	1.57	1.50
4	C	101[A]	PEB	C4B-NB	3.13	1.45	1.38
4	F	101[B]	PEB	C4B-NB	3.13	1.45	1.38
5	D	201	AX9	CHB-C1C	3.08	1.37	1.35
5	D	201	AX9	C1B-CHA	3.07	1.53	1.41
4	D	203	PEB	CAD-C3D	3.04	1.55	1.47
4	B	202	PEB	C1B-NB	3.00	1.43	1.36
5	D	201	AX9	C4D-ND	2.99	1.39	1.35
4	B	202	PEB	C4B-NB	2.99	1.44	1.38
4	D	202	PEB	CMC-C3C	2.96	1.57	1.51
4	A	101[A]	PEB	C3B-C2B	2.95	1.43	1.36
4	E	101[B]	PEB	C3B-C2B	2.95	1.43	1.36
5	D	201	AX9	C1A-C2A	-2.94	1.39	1.47
5	D	201	AX9	CHC-C1D	-2.92	1.47	1.53
4	D	203	PEB	CMC-C3C	2.91	1.57	1.51
4	B	203	PEB	CHA-C4A	2.89	1.42	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	PEB	CMA-C2A	2.87	1.59	1.53
4	D	202	PEB	C1B-NB	2.87	1.43	1.36
4	D	203	PEB	CHC-C4C	2.86	1.57	1.50
4	A	101[A]	PEB	CAD-C3D	2.85	1.55	1.47
4	E	101[B]	PEB	CAD-C3D	2.85	1.55	1.47
4	D	202	PEB	C3B-C2B	2.85	1.42	1.36
4	B	203	PEB	CAD-C3D	2.81	1.55	1.47
5	B	201	AX9	C4A-C3A	-2.78	1.39	1.45
4	D	202	PEB	C3C-C4C	2.77	1.46	1.42
4	C	101[A]	PEB	CAA-C3A	2.75	1.59	1.54
4	F	101[B]	PEB	CAA-C3A	2.75	1.59	1.54
5	B	201	AX9	C1B-CHA	2.73	1.51	1.41
5	B	201	AX9	CHC-C1D	-2.72	1.47	1.53
5	D	201	AX9	C4B-CHB	2.71	1.51	1.41
4	B	203	PEB	CMC-C3C	2.68	1.57	1.51
4	A	101[A]	PEB	CHC-C4C	2.64	1.56	1.50
4	E	101[B]	PEB	CHC-C4C	2.64	1.56	1.50
4	B	202	PEB	CAA-C3A	2.62	1.59	1.54
4	D	202	PEB	C2C-C3C	2.62	1.45	1.37
4	A	101[A]	PEB	OD-C4D	2.59	1.28	1.23
4	E	101[B]	PEB	OD-C4D	2.59	1.28	1.23
4	D	203	PEB	CAA-C3A	2.57	1.59	1.54
5	B	201	AX9	C4B-CHB	2.56	1.51	1.41
4	B	202	PEB	CBD-CAD	2.55	1.42	1.30
4	D	203	PEB	CHA-C4A	2.54	1.41	1.36
4	C	101[A]	PEB	CBD-CAD	2.53	1.42	1.30
4	F	101[B]	PEB	CBD-CAD	2.53	1.42	1.30
4	D	203	PEB	C1D-C2D	2.51	1.59	1.50
4	B	202	PEB	C2C-C3C	2.51	1.45	1.37
4	D	202	PEB	CBD-CAD	2.50	1.42	1.30
4	A	101[A]	PEB	CAA-C3A	2.47	1.58	1.54
4	E	101[B]	PEB	CAA-C3A	2.47	1.58	1.54
4	D	203	PEB	OD-C4D	2.43	1.28	1.23
4	C	101[A]	PEB	C3B-C2B	2.41	1.41	1.36
4	F	101[B]	PEB	C3B-C2B	2.41	1.41	1.36
4	C	101[A]	PEB	C1D-C2D	2.41	1.58	1.50
4	F	101[B]	PEB	C1D-C2D	2.41	1.58	1.50
4	B	202	PEB	C1D-C2D	2.40	1.58	1.50
4	D	203	PEB	C2C-C3C	2.39	1.44	1.37
5	B	201	AX9	CHC-C4C	2.37	1.53	1.50
4	D	202	PEB	C1D-ND	2.32	1.49	1.45
5	D	201	AX9	C4D-C3D	-2.28	1.43	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	203	PEB	CBD-CAD	2.28	1.41	1.30
4	D	203	PEB	CBD-CAD	2.27	1.41	1.30
4	A	101[A]	PEB	CBD-CAD	2.27	1.41	1.30
4	E	101[B]	PEB	CBD-CAD	2.27	1.41	1.30
4	B	203	PEB	C3B-C2B	2.27	1.41	1.36
4	A	101[A]	PEB	C1D-C2D	2.26	1.58	1.50
4	E	101[B]	PEB	C1D-C2D	2.26	1.58	1.50
4	B	202	PEB	C3B-C2B	2.26	1.41	1.36
5	D	201	AX9	CHC-C4C	2.25	1.52	1.50
4	C	101[A]	PEB	CBB-CAB	2.24	1.59	1.52
4	F	101[B]	PEB	CBB-CAB	2.24	1.59	1.52
4	A	101[A]	PEB	CBB-CAB	2.24	1.59	1.52
4	E	101[B]	PEB	CBB-CAB	2.24	1.59	1.52
4	C	101[A]	PEB	CHA-C4A	2.24	1.41	1.36
4	F	101[B]	PEB	CHA-C4A	2.24	1.41	1.36
4	D	202	PEB	CBB-CAB	2.21	1.59	1.52
4	D	202	PEB	CAA-C3A	2.19	1.58	1.54
4	B	203	PEB	C2A-C3A	2.18	1.60	1.54
5	D	201	AX9	C4C-NC	2.14	1.39	1.35
4	B	202	PEB	CBB-CAB	2.13	1.58	1.52
4	D	203	PEB	C2A-C3A	2.13	1.60	1.54
4	B	203	PEB	C1D-ND	2.12	1.48	1.45
4	B	203	PEB	C2C-C3C	2.12	1.44	1.37
4	C	101[A]	PEB	OD-C4D	2.12	1.27	1.23
4	F	101[B]	PEB	OD-C4D	2.12	1.27	1.23
4	B	203	PEB	C1D-C2D	2.10	1.57	1.50
4	A	101[A]	PEB	C3C-C4C	2.09	1.45	1.42
4	E	101[B]	PEB	C3C-C4C	2.09	1.45	1.42
4	D	202	PEB	C1D-C2D	2.06	1.57	1.50
4	A	101[A]	PEB	C4B-NB	2.05	1.42	1.38
4	E	101[B]	PEB	C4B-NB	2.05	1.42	1.38
4	B	203	PEB	CBB-CAB	2.04	1.58	1.52
4	D	203	PEB	C1B-C2B	2.03	1.50	1.45

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101[A]	PEB	C1C-CHB-C4B	-9.08	117.96	128.81
4	F	101[B]	PEB	C1C-CHB-C4B	-9.08	117.96	128.81
4	A	101[A]	PEB	C1C-CHB-C4B	-8.81	118.28	128.81
4	E	101[B]	PEB	C1C-CHB-C4B	-8.81	118.28	128.81
4	B	202	PEB	C1C-CHB-C4B	-7.77	119.53	128.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	202	PEB	C1C-CHB-C4B	-7.06	120.37	128.81
4	A	101[A]	PEB	CAB-CBB-CGB	-6.07	100.55	113.60
4	E	101[B]	PEB	CAB-CBB-CGB	-6.07	100.55	113.60
4	B	202	PEB	OA-C1A-C2A	-5.15	122.08	126.17
4	D	203	PEB	CHC-C1D-ND	-5.06	108.07	113.95
4	D	202	PEB	CBB-CAB-C3B	-5.05	98.60	112.63
4	D	202	PEB	CHA-C4A-NA	4.79	130.90	125.20
4	A	101[A]	PEB	CHC-C1D-ND	-4.67	108.53	113.95
4	E	101[B]	PEB	CHC-C1D-ND	-4.67	108.53	113.95
4	B	202	PEB	CHC-C1D-ND	-4.65	108.54	113.95
4	B	203	PEB	C1C-CHB-C4B	-4.55	123.37	128.81
4	D	203	PEB	CHC-C4C-C3C	-4.53	122.61	130.34
4	D	203	PEB	C1C-CHB-C4B	-4.49	123.45	128.81
4	D	202	PEB	CBC-CAC-C2C	-4.35	105.20	112.62
4	B	203	PEB	CHC-C1D-ND	-4.11	109.18	113.95
4	C	101[A]	PEB	CAC-CBC-CGC	-4.05	102.41	113.76
4	F	101[B]	PEB	CAC-CBC-CGC	-4.05	102.41	113.76
5	B	201	AX9	CHC-C1D-ND	-3.96	108.72	113.72
4	B	203	PEB	CHC-C4C-C3C	-3.67	124.07	130.34
4	B	202	PEB	CMB-C2B-C1B	3.60	130.60	125.06
4	C	101[A]	PEB	CAB-CBB-CGB	-3.58	105.89	113.60
4	F	101[B]	PEB	CAB-CBB-CGB	-3.58	105.89	113.60
4	B	202	PEB	CBB-CAB-C3B	-3.55	102.75	112.63
4	C	101[A]	PEB	CBC-CAC-C2C	-3.55	106.57	112.62
4	F	101[B]	PEB	CBC-CAC-C2C	-3.55	106.57	112.62
4	B	202	PEB	CHA-C4A-NA	3.51	129.37	125.20
4	B	202	PEB	C2A-C1A-NA	3.50	111.29	108.27
4	B	203	PEB	OA-C1A-C2A	3.49	128.94	126.17
4	B	203	PEB	CAC-CBC-CGC	3.43	123.38	113.76
4	D	202	PEB	CBA-CAA-C3A	-3.30	106.12	113.47
4	A	101[A]	PEB	CBC-CAC-C2C	-3.24	107.08	112.62
4	E	101[B]	PEB	CBC-CAC-C2C	-3.24	107.08	112.62
4	B	203	PEB	OA-C1A-NA	-3.18	121.09	124.94
4	D	202	PEB	CAB-C3B-C4B	-3.18	119.39	125.01
4	C	101[A]	PEB	CMB-C2B-C1B	3.17	129.94	125.06
4	F	101[B]	PEB	CMB-C2B-C1B	3.17	129.94	125.06
4	B	202	PEB	CHB-C4B-C3B	-3.17	118.01	125.32
4	D	202	PEB	CHA-C1B-NB	-3.14	118.37	124.93
4	D	202	PEB	CHC-C1D-ND	-3.11	110.34	113.95
5	D	201	AX9	CHC-C1D-ND	-3.05	109.87	113.72
4	D	202	PEB	CMB-C2B-C1B	3.04	129.74	125.06
4	D	202	PEB	C4B-C3B-C2B	3.02	110.13	106.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	101[A]	PEB	CAC-CBC-CGC	-3.00	105.35	113.76
4	E	101[B]	PEB	CAC-CBC-CGC	-3.00	105.35	113.76
5	B	201	AX9	CAA-C3A-C4A	2.98	128.40	124.38
4	C	101[A]	PEB	C2A-C1A-NA	2.97	110.84	108.27
4	F	101[B]	PEB	C2A-C1A-NA	2.97	110.84	108.27
4	D	202	PEB	C1B-C2B-C3B	-2.92	103.16	106.51
4	A	101[A]	PEB	CHC-C4C-C3C	-2.89	125.40	130.34
4	E	101[B]	PEB	CHC-C4C-C3C	-2.89	125.40	130.34
4	C	101[A]	PEB	CMD-C2D-C3D	-2.89	125.99	130.06
4	F	101[B]	PEB	CMD-C2D-C3D	-2.89	125.99	130.06
5	D	201	AX9	CAD-C3D-C4D	2.85	125.88	121.38
5	B	201	AX9	CAD-C3D-C4D	2.83	125.85	121.38
4	C	101[A]	PEB	CHC-C1D-ND	-2.82	110.67	113.95
4	F	101[B]	PEB	CHC-C1D-ND	-2.82	110.67	113.95
4	B	202	PEB	CBA-CAA-C3A	-2.80	107.23	113.47
4	D	203	PEB	C2A-C1A-NA	2.77	110.66	108.27
4	A	101[A]	PEB	C2A-C1A-NA	2.71	110.61	108.27
4	E	101[B]	PEB	C2A-C1A-NA	2.71	110.61	108.27
4	C	101[A]	PEB	CMA-C2A-C1A	-2.71	106.57	112.40
4	F	101[B]	PEB	CMA-C2A-C1A	-2.71	106.57	112.40
4	D	202	PEB	CHC-C4C-C3C	-2.63	125.86	130.34
4	B	202	PEB	CHA-C1B-NB	-2.61	119.48	124.93
4	D	203	PEB	CHA-C1B-NB	-2.54	119.62	124.93
4	B	203	PEB	CHA-C1B-NB	-2.50	119.69	124.93
4	B	202	PEB	CAC-CBC-CGC	-2.50	106.76	113.76
4	A	101[A]	PEB	CMD-C2D-C3D	-2.43	126.64	130.06
4	E	101[B]	PEB	CMD-C2D-C3D	-2.43	126.64	130.06
4	D	203	PEB	O2C-CGC-CBC	2.41	121.78	114.03
5	B	201	AX9	O1C-CGC-CBC	2.39	121.72	114.03
4	A	101[A]	PEB	CMA-C2A-C1A	-2.39	107.26	112.40
4	E	101[B]	PEB	CMA-C2A-C1A	-2.39	107.26	112.40
4	A	101[A]	PEB	CBA-CAA-C3A	-2.38	108.18	113.47
4	E	101[B]	PEB	CBA-CAA-C3A	-2.38	108.18	113.47
4	C	101[A]	PEB	CBA-CAA-C3A	-2.35	108.23	113.47
4	F	101[B]	PEB	CBA-CAA-C3A	-2.35	108.23	113.47
4	D	202	PEB	OD-C4D-ND	-2.34	122.47	125.93
4	A	101[A]	PEB	C4B-C3B-C2B	2.32	109.36	106.78
4	E	101[B]	PEB	C4B-C3B-C2B	2.32	109.36	106.78
4	D	202	PEB	C2A-C1A-NA	2.32	110.27	108.27
4	A	101[A]	PEB	O2C-CGC-CBC	2.32	121.48	114.03
4	E	101[B]	PEB	O2C-CGC-CBC	2.32	121.48	114.03
5	D	201	AX9	CAC-CBC-CGC	-2.24	108.79	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	202	PEB	OA-C1A-C2A	-2.18	124.44	126.17
4	B	203	PEB	O2B-CGB-CBB	2.18	121.04	114.03
5	B	201	AX9	C1D-CHC-C4C	-2.13	108.73	113.37
5	D	201	AX9	CMD-C2D-C3D	-2.13	124.56	127.77
4	C	101[A]	PEB	C4B-NB-C1B	-2.13	102.50	106.51
4	F	101[B]	PEB	C4B-NB-C1B	-2.13	102.50	106.51
4	D	202	PEB	C2A-C3A-C4A	2.09	104.47	101.34
4	B	203	PEB	CBC-CAC-C2C	-2.08	109.08	112.62
5	D	201	AX9	CAA-C3A-C4A	2.08	127.18	124.38
4	D	202	PEB	CAB-CBB-CGB	-2.07	109.14	113.60
4	B	203	PEB	CBB-CAB-C3B	-2.07	106.87	112.63
5	D	201	AX9	C4A-NA-C1A	-2.07	108.04	110.67
4	B	203	PEB	CHA-C1B-C2B	2.06	130.19	124.90
5	B	201	AX9	CHB-C1C-C2C	-2.04	120.61	125.32
4	B	202	PEB	CMA-C2A-C1A	-2.02	108.05	112.40
4	B	203	PEB	CMB-C2B-C1B	2.01	128.16	125.06
5	D	201	AX9	CMA-C2A-C1A	2.00	126.10	121.39

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101[A]	PEB	NB-C1B-CHA-C4A
4	A	101[A]	PEB	C2B-C1B-CHA-C4A
4	B	202	PEB	NB-C1B-CHA-C4A
4	B	202	PEB	C2B-C1B-CHA-C4A
4	B	203	PEB	NB-C1B-CHA-C4A
4	B	203	PEB	C2B-C1B-CHA-C4A
4	C	101[A]	PEB	NB-C1B-CHA-C4A
4	C	101[A]	PEB	C2B-C1B-CHA-C4A
4	D	202	PEB	NB-C1B-CHA-C4A
4	D	203	PEB	C1C-C2C-CAC-CBC
4	D	203	PEB	C3C-C2C-CAC-CBC
4	D	203	PEB	NB-C1B-CHA-C4A
4	E	101[B]	PEB	NB-C1B-CHA-C4A
4	E	101[B]	PEB	C2B-C1B-CHA-C4A
4	F	101[B]	PEB	NB-C1B-CHA-C4A
4	F	101[B]	PEB	C2B-C1B-CHA-C4A
5	B	201	AX9	NB-C1B-CHA-C4A
5	B	201	AX9	NC-C4C-CHC-C1D
5	D	201	AX9	NB-C1B-CHA-C4A
5	D	201	AX9	NC-C4C-CHC-C1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	203	PEB	C2B-C1B-CHA-C4A
4	D	202	PEB	C2B-C1B-CHA-C4A
4	D	203	PEB	NA-C4A-CHA-C1B
4	A	101[A]	PEB	C3B-CAB-CBB-CGB
4	E	101[B]	PEB	C3B-CAB-CBB-CGB
5	D	201	AX9	C2D-C3D-CAD-CBD
4	D	202	PEB	C1C-C2C-CAC-CBC
4	D	202	PEB	C3C-C2C-CAC-CBC
4	A	101[A]	PEB	C4B-C3B-CAB-CBB
4	E	101[B]	PEB	C4B-C3B-CAB-CBB
5	B	201	AX9	C2C-CAC-CBC-CGC
4	A	101[A]	PEB	CAB-CBB-CGB-O1B
4	E	101[B]	PEB	CAB-CBB-CGB-O1B
4	A	101[A]	PEB	C2B-C3B-CAB-CBB
4	E	101[B]	PEB	C2B-C3B-CAB-CBB
5	D	201	AX9	CAB-CBB-CGB-O1B
5	B	201	AX9	CAB-CBB-CGB-O1B
5	D	201	AX9	CAB-CBB-CGB-O2B
4	C	101[A]	PEB	CAC-CBC-CGC-O2C
4	F	101[B]	PEB	CAC-CBC-CGC-O2C
5	B	201	AX9	CAB-CBB-CGB-O2B
4	B	203	PEB	CAC-CBC-CGC-O2C
4	A	101[A]	PEB	CAB-CBB-CGB-O2B
4	B	203	PEB	CAC-CBC-CGC-O1C
4	E	101[B]	PEB	CAB-CBB-CGB-O2B
4	C	101[A]	PEB	CAC-CBC-CGC-O1C
4	F	101[B]	PEB	CAC-CBC-CGC-O1C
5	D	201	AX9	CAC-CBC-CGC-O1C
4	D	203	PEB	CAC-CBC-CGC-O2C
5	B	201	AX9	CAC-CBC-CGC-O1C
5	D	201	AX9	CAC-CBC-CGC-O2C
4	D	203	PEB	CAC-CBC-CGC-O1C
5	B	201	AX9	CAC-CBC-CGC-O2C

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	203	PEB	6	0
4	A	101[A]	PEB	3	0
4	D	202	PEB	2	0
4	E	101[B]	PEB	2	0

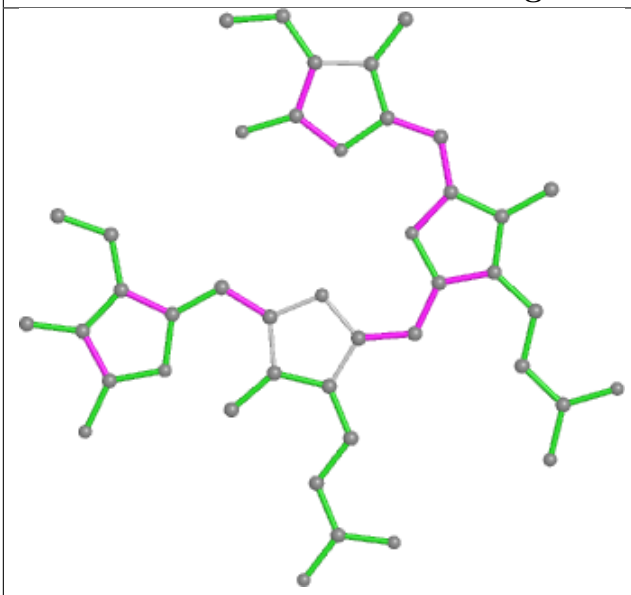
Continued on next page...

Continued from previous page...

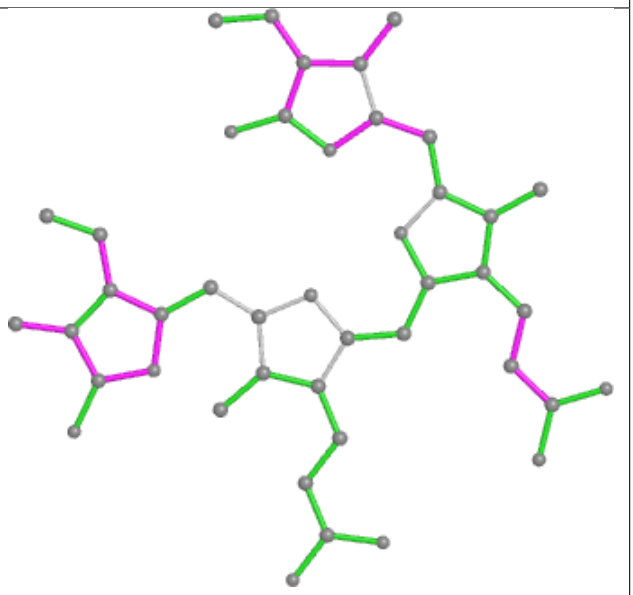
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	203	PEB	5	0
4	B	202	PEB	1	0

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

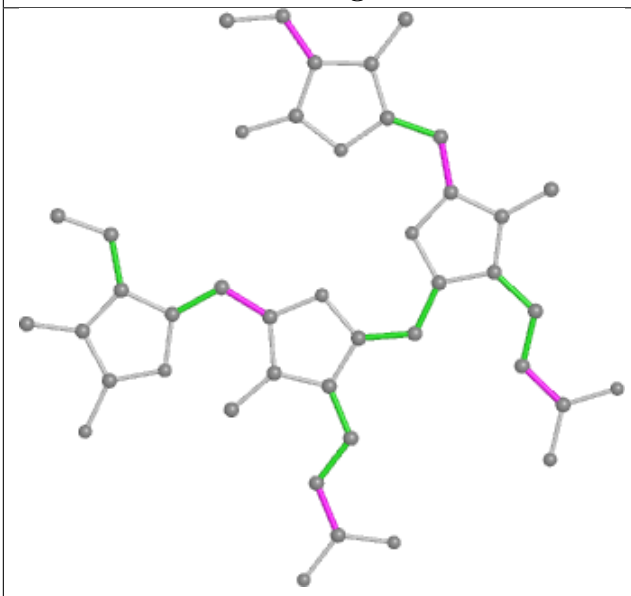
Ligand AX9 D 201



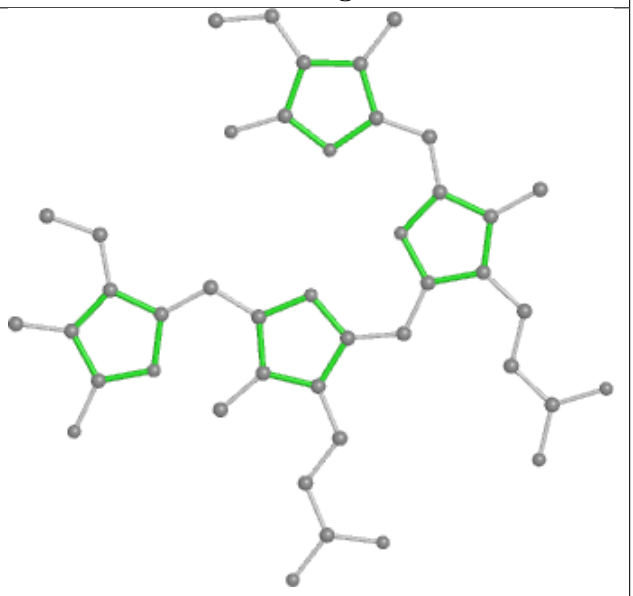
Bond lengths



Bond angles

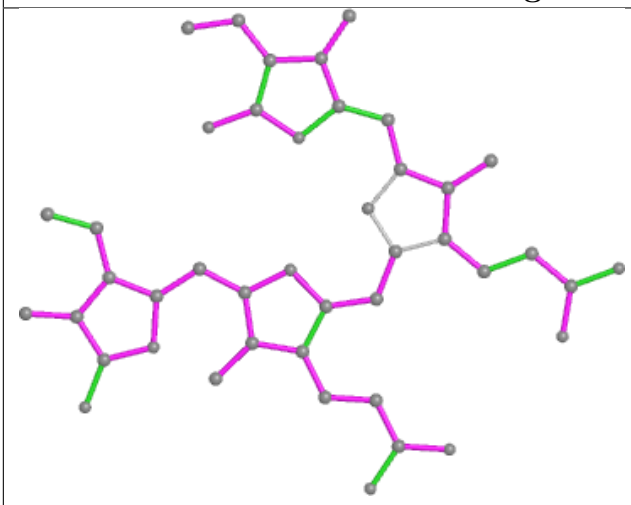


Torsions

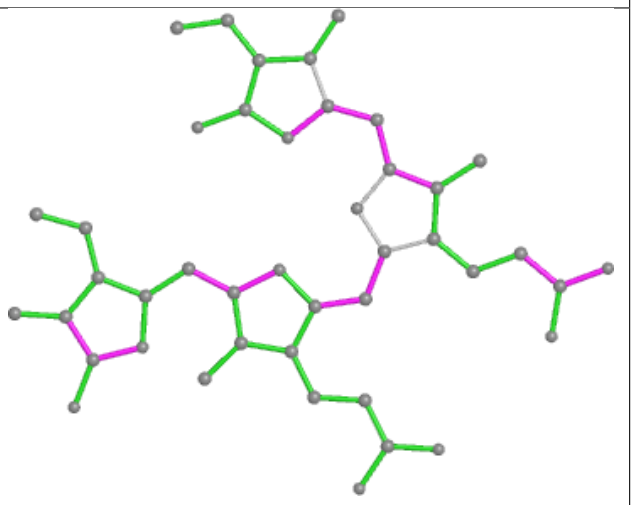


Rings

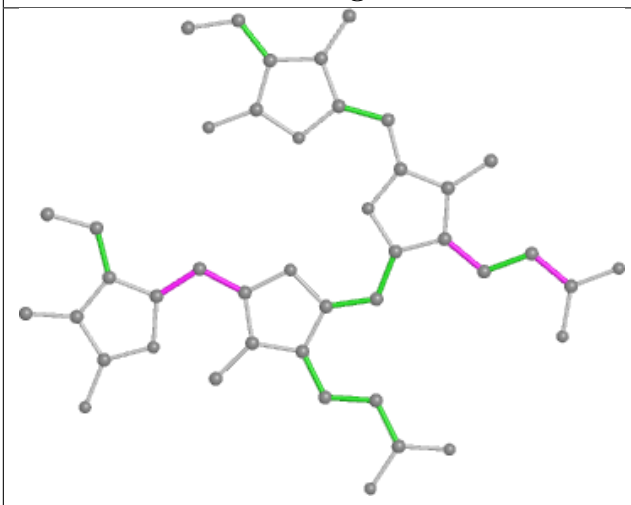
Ligand PEB D 203



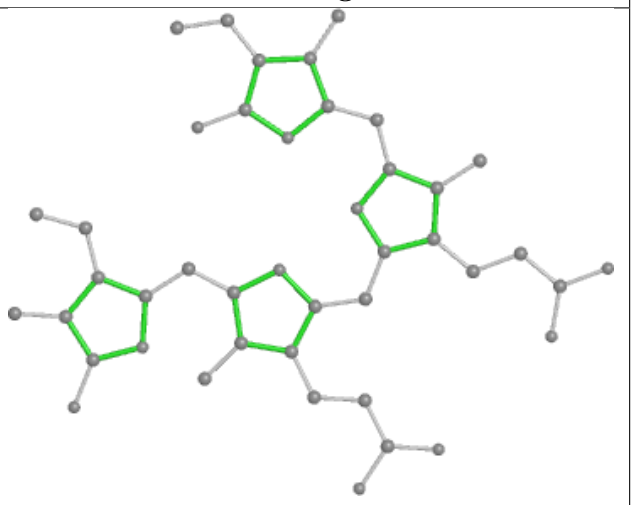
Bond lengths



Bond angles

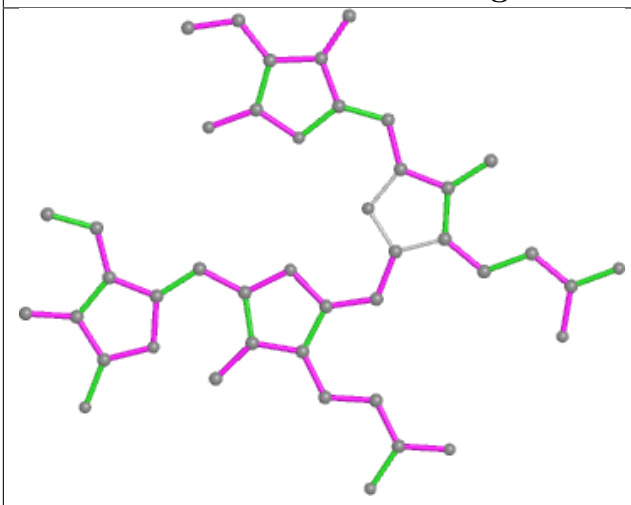


Torsions

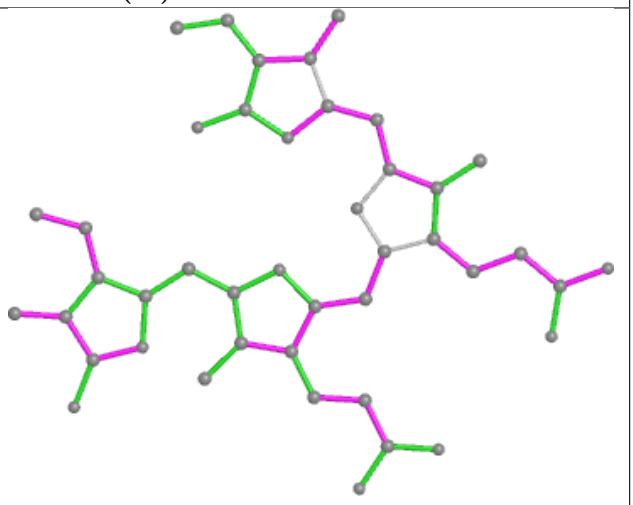


Rings

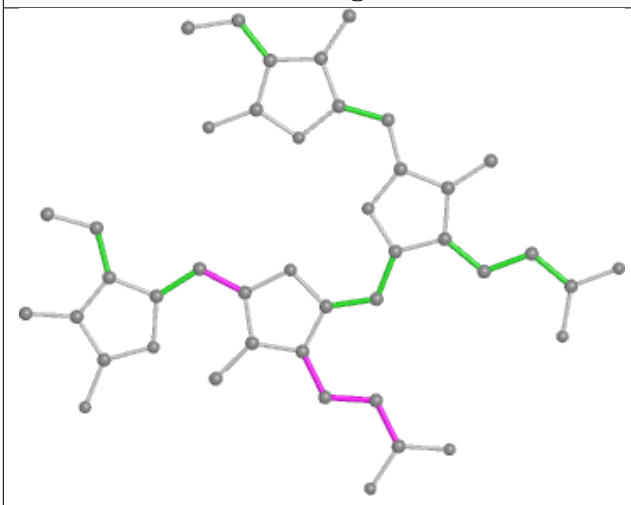
Ligand PEB A 101 (A)



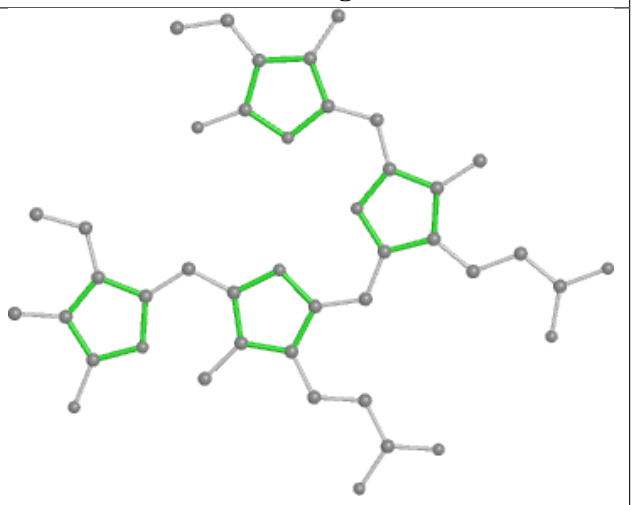
Bond lengths



Bond angles

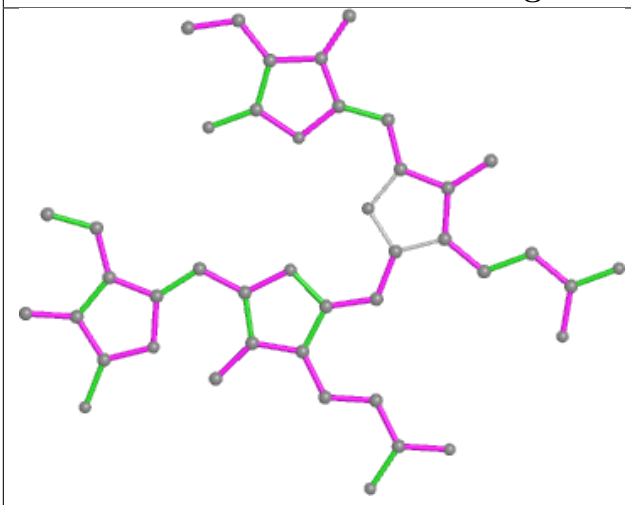


Torsions

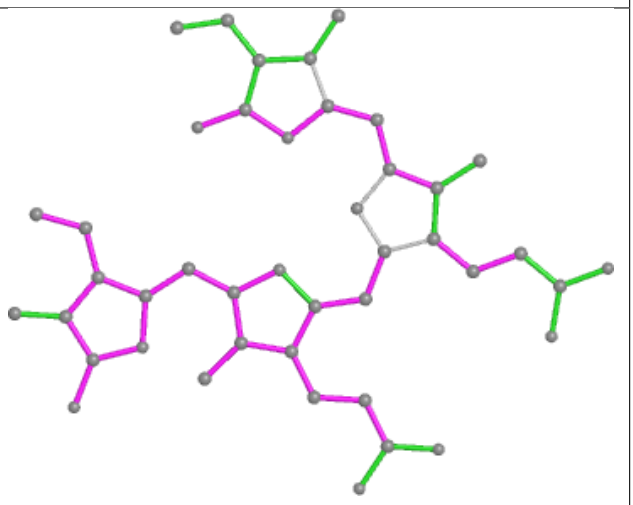


Rings

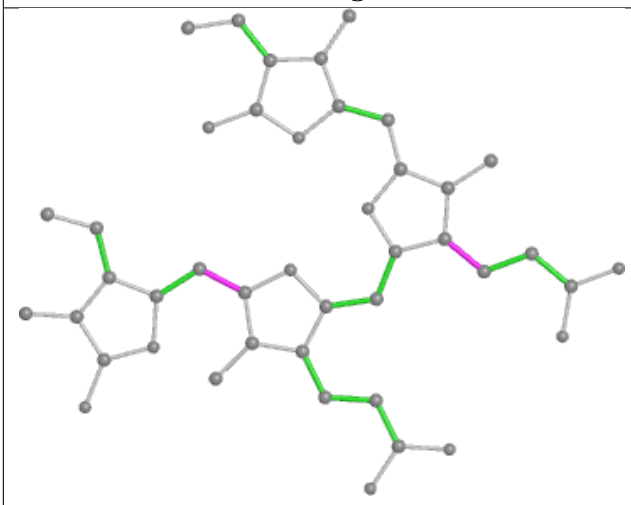
Ligand PEB D 202



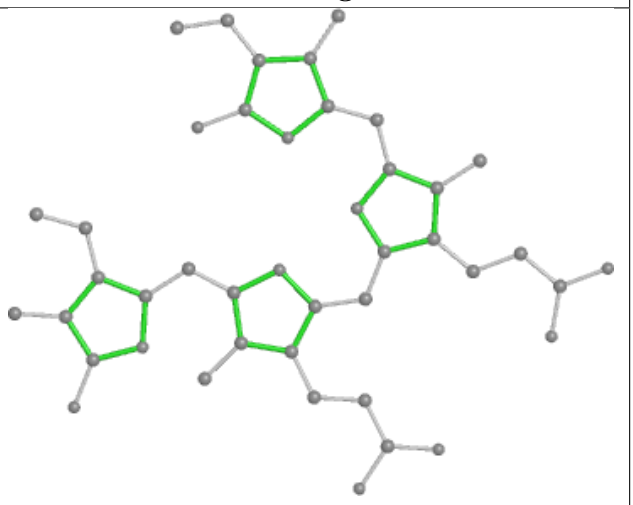
Bond lengths



Bond angles

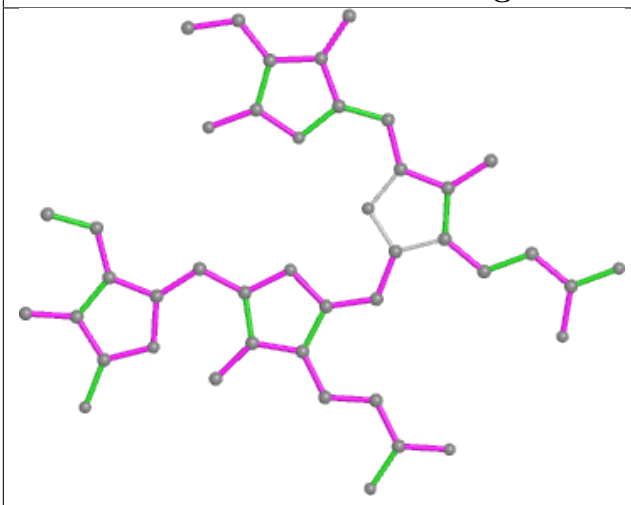


Torsions

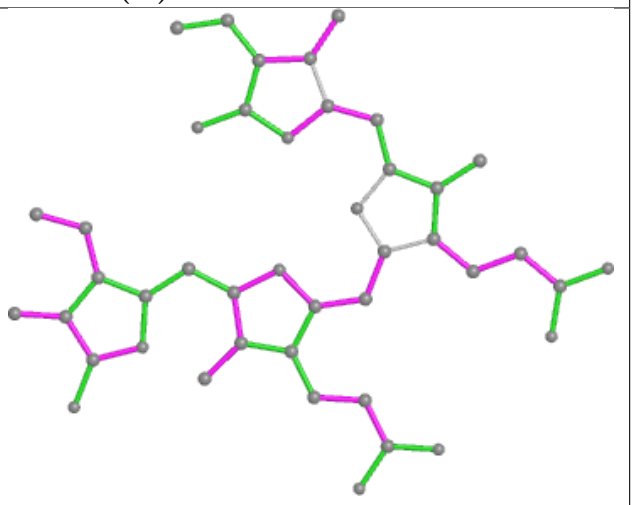


Rings

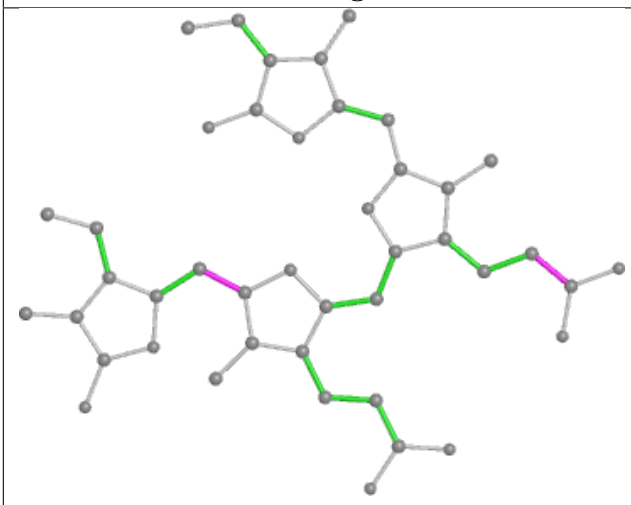
Ligand PEB F 101 (B)



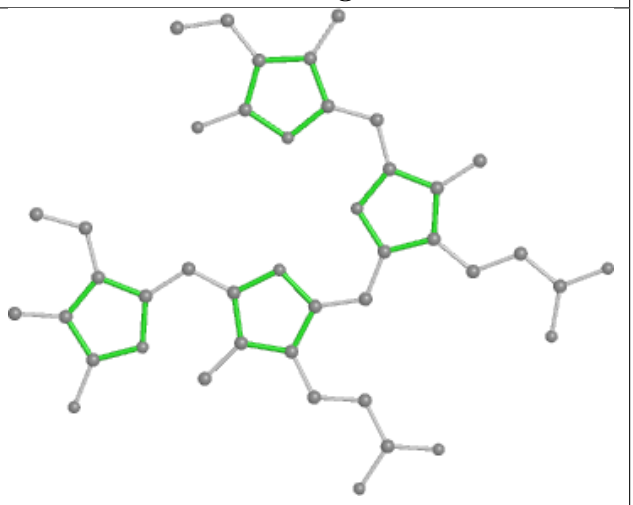
Bond lengths



Bond angles

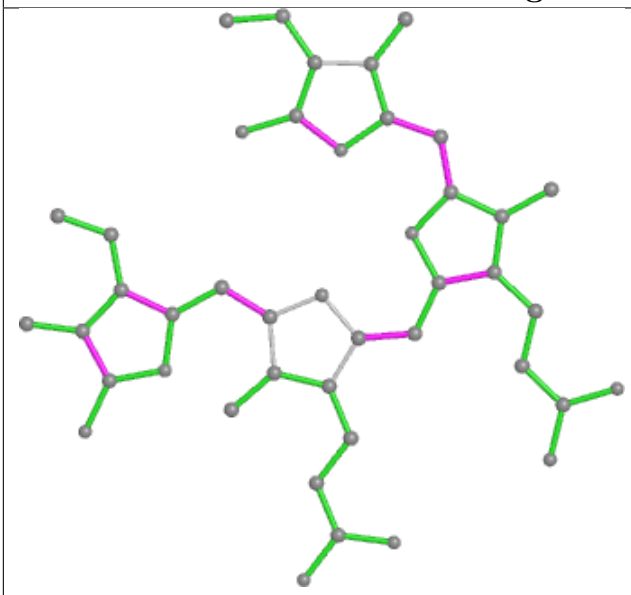


Torsions

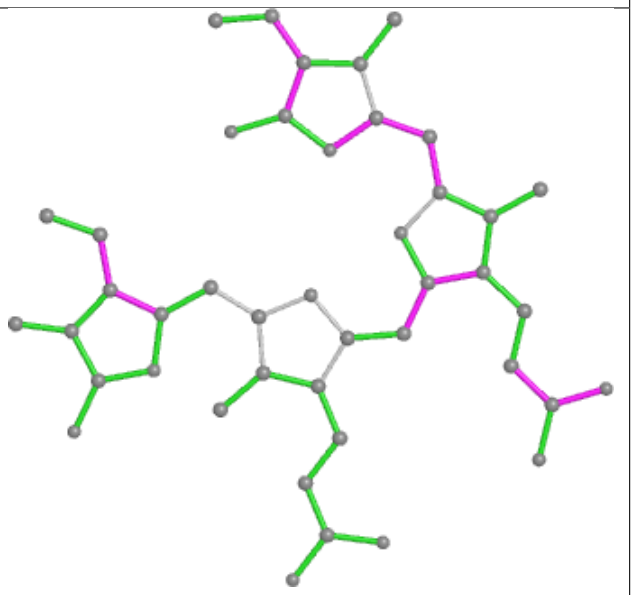


Rings

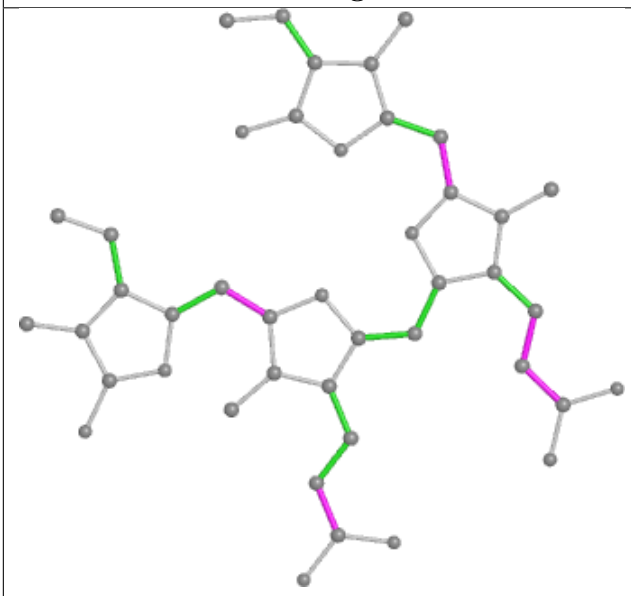
Ligand AX9 B 201



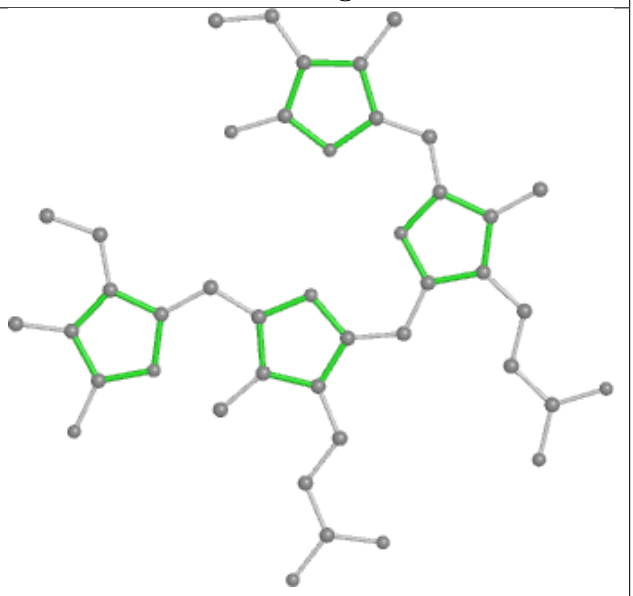
Bond lengths



Bond angles

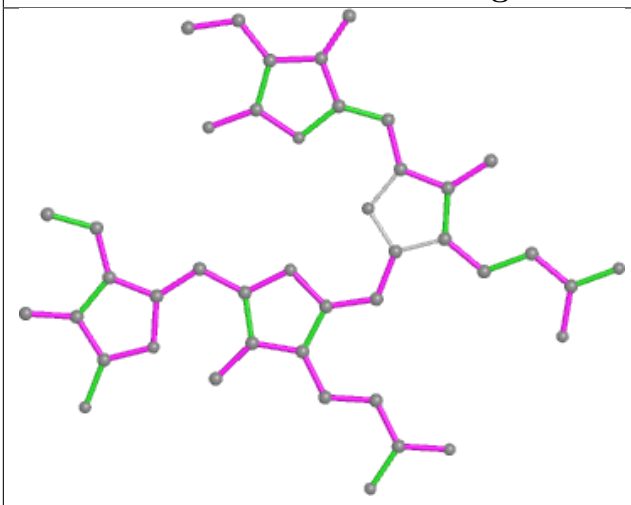


Torsions

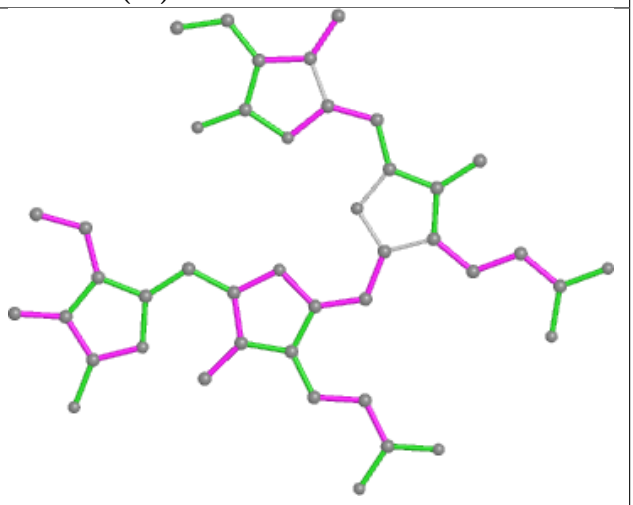


Rings

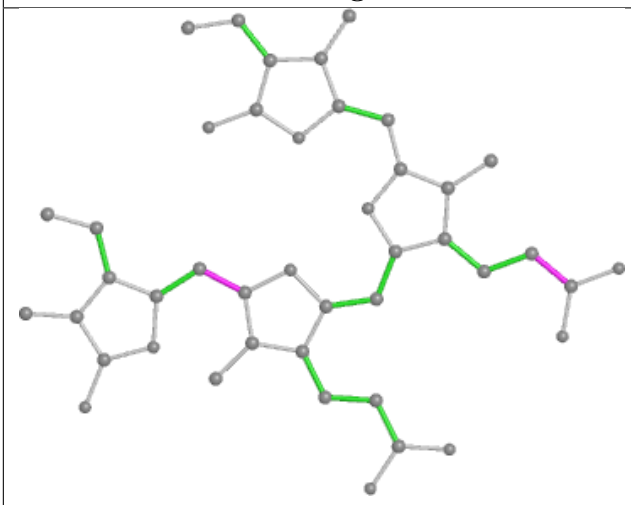
Ligand PEB C 101 (A)



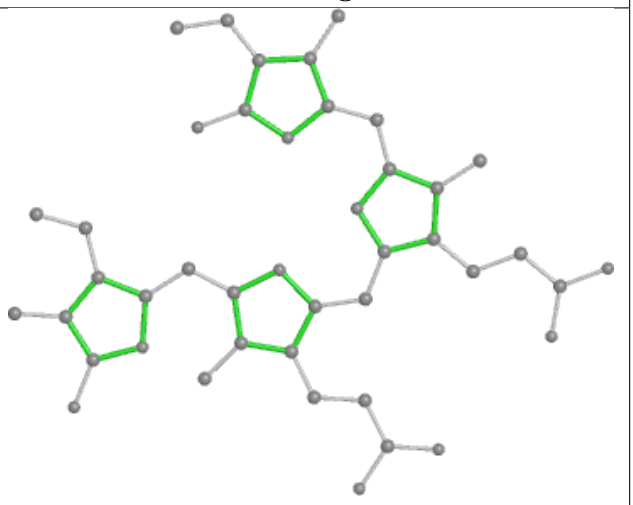
Bond lengths



Bond angles

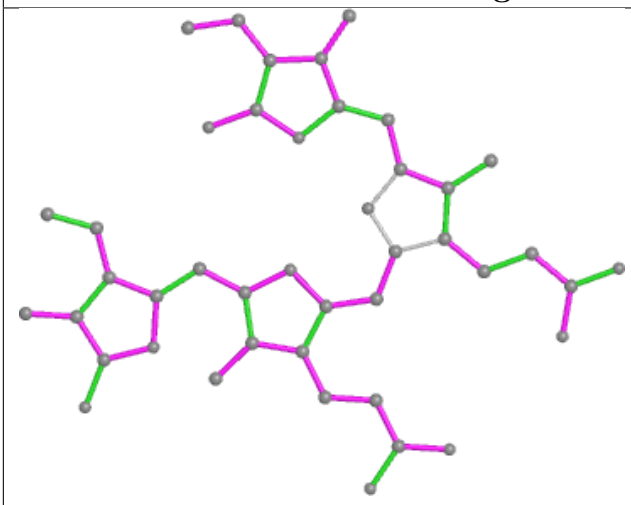


Torsions

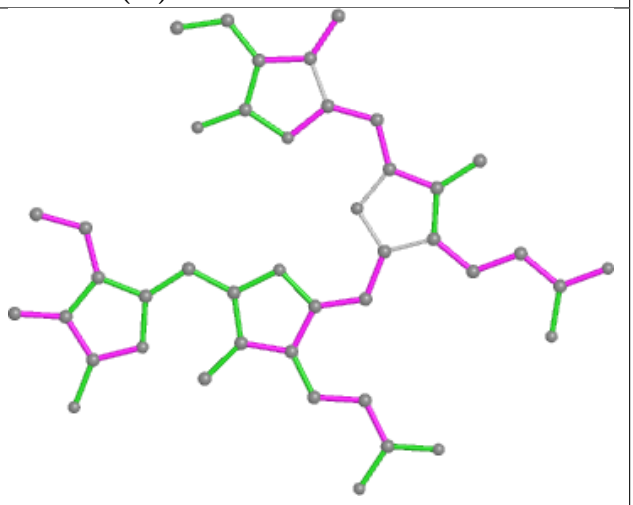


Rings

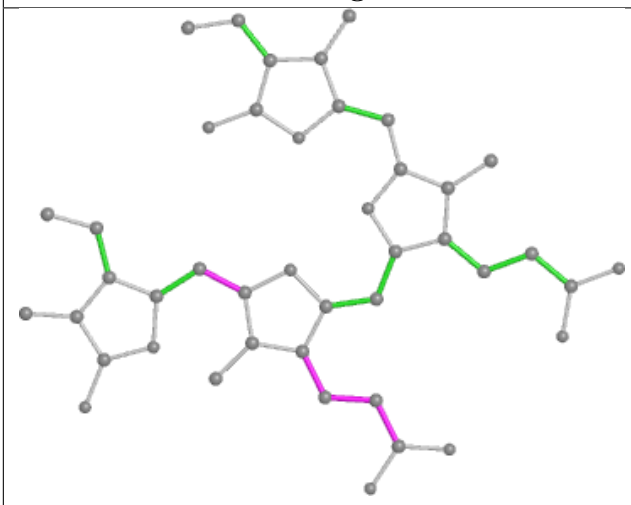
Ligand PEB E 101 (B)



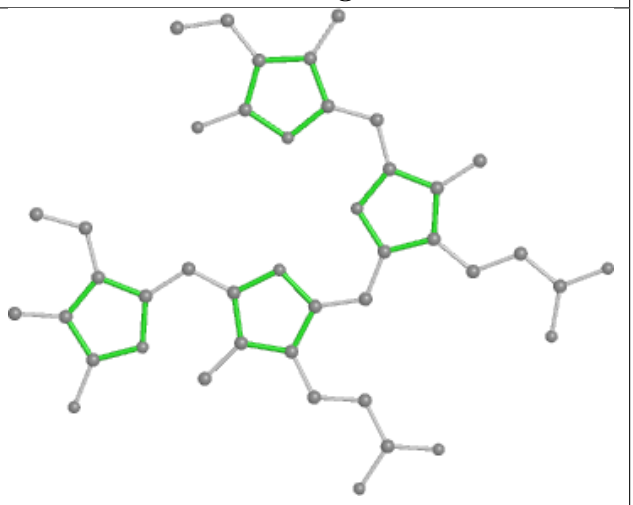
Bond lengths



Bond angles

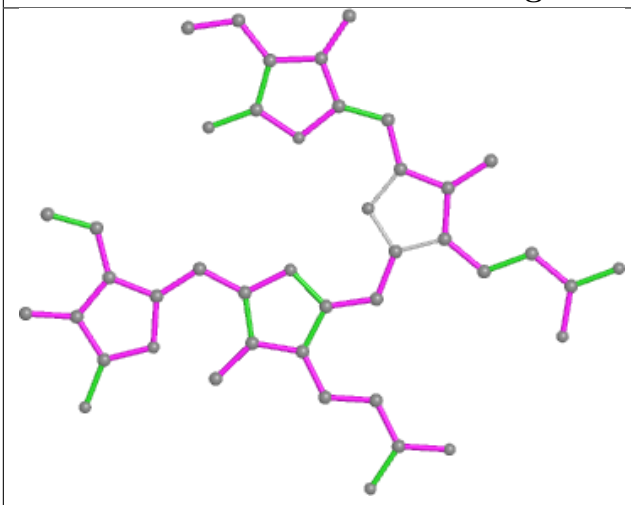


Torsions

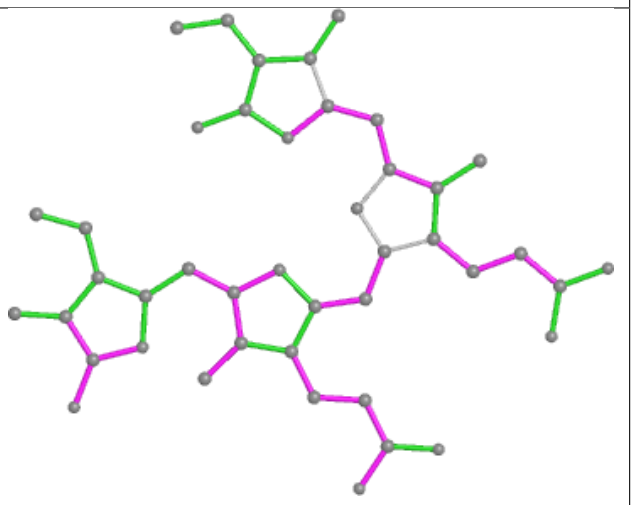


Rings

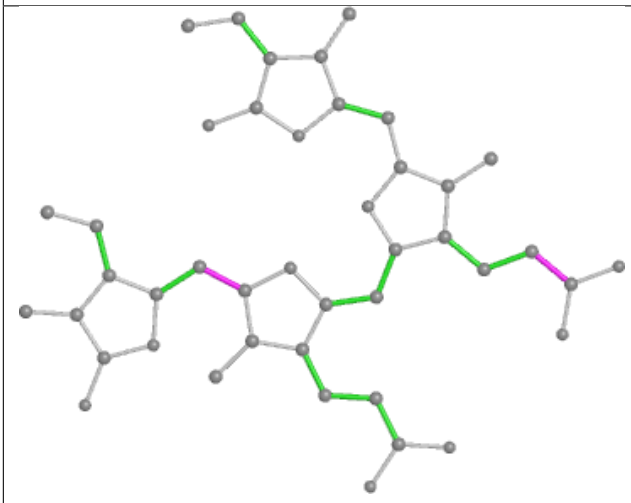
Ligand PEB B 203



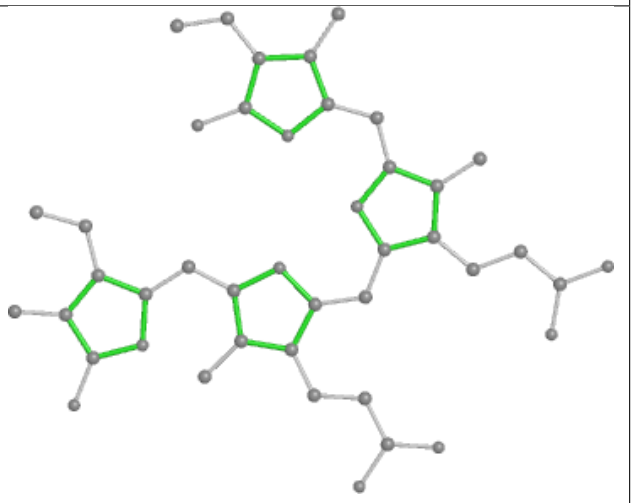
Bond lengths



Bond angles

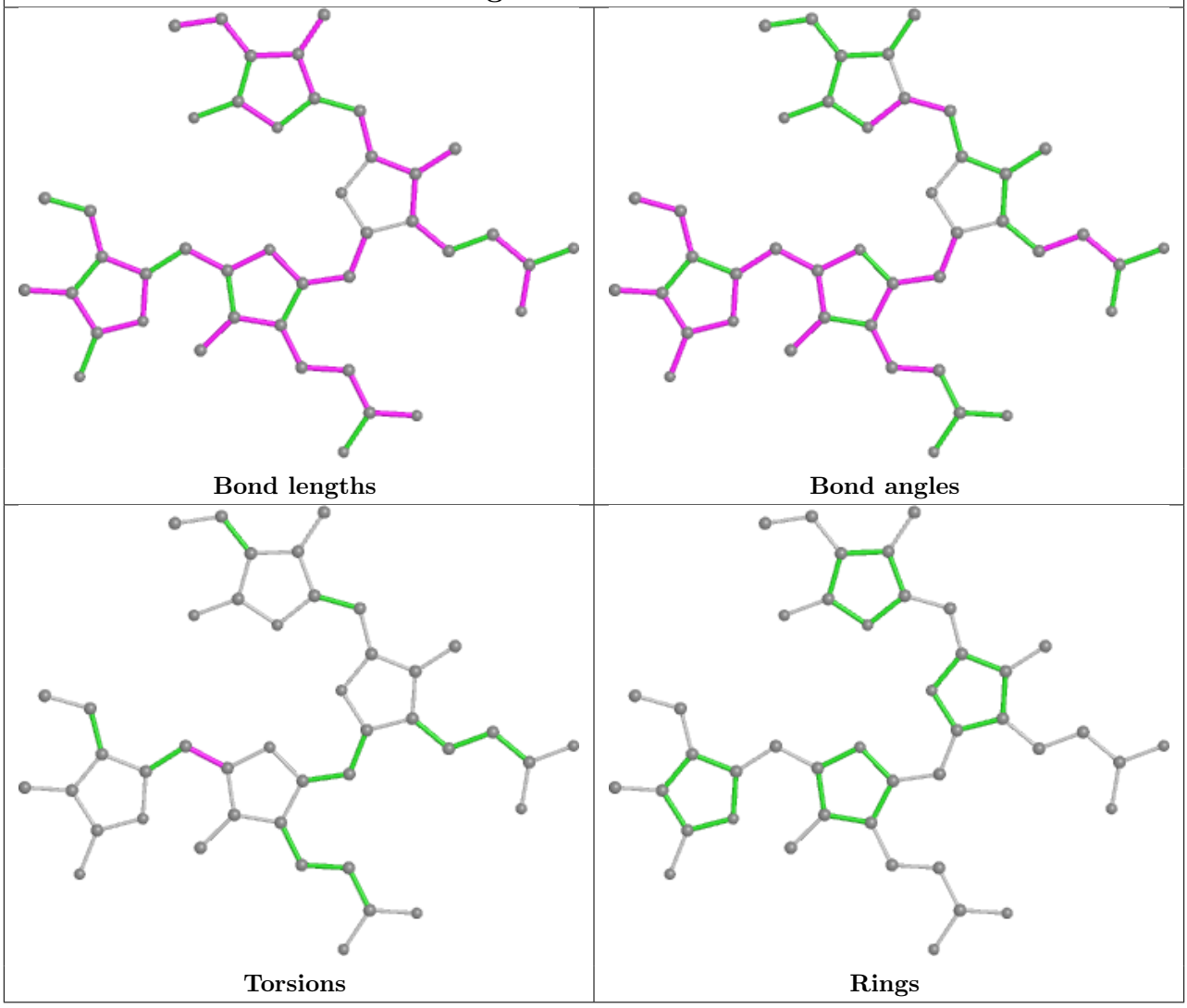


Torsions



Rings

Ligand PEB B 202



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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	63/67 (94%)	-0.14	2 (3%)	47	53	22, 31, 47, 63	63 (100%)
1	F	63/67 (94%)	0.15	5 (7%)	12	16	22, 34, 63, 94	63 (100%)
2	B	163/177 (92%)	-0.25	1 (0%)	89	92	21, 32, 50, 61	0
2	D	163/177 (92%)	-0.11	4 (2%)	57	63	22, 35, 59, 88	0
3	C	61/62 (98%)	0.05	2 (3%)	46	52	22, 35, 63, 94	61 (100%)
3	E	61/62 (98%)	-0.22	1 (1%)	72	78	22, 31, 47, 63	61 (100%)
All	All	574/612 (93%)	-0.12	15 (2%)	56	61	21, 33, 58, 94	248 (43%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	31[B]	ASP	8.0
3	C	31[A]	ASP	8.0
2	D	30	PHE	6.8
1	F	29[B]	SER	4.1
3	C	29[A]	SER	4.1
2	D	27	LEU	3.3
1	A	62[A]	PHE	3.0
1	F	63[B]	GLY	3.0
1	F	64[B]	ALA	2.9
2	D	29	LYS	2.6
1	F	62[B]	PHE	2.5
2	D	24	LEU	2.2
1	A	1[A]	ALA	2.2
3	E	1[B]	ALA	2.2
2	B	27	LEU	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LYZ	A	4[A]	10/11	0.95	0.11	37,55,82,93	21
3	LYZ	E	4[B]	10/11	0.95	0.11	37,55,82,93	21
3	LYZ	C	4[A]	10/11	0.96	0.05	32,44,62,66	21
1	LYZ	F	4[B]	10/11	0.96	0.05	32,44,62,66	21

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

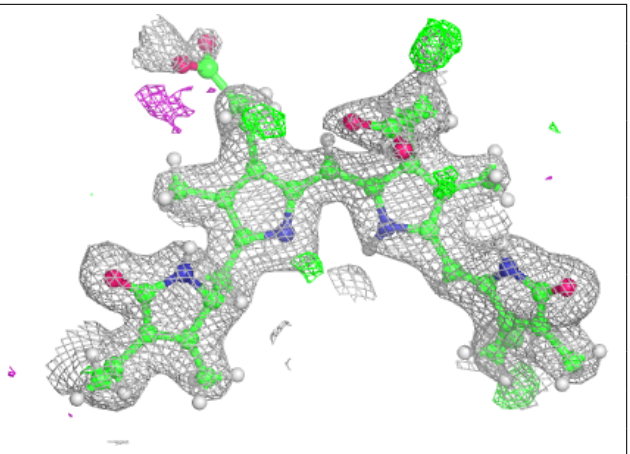
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

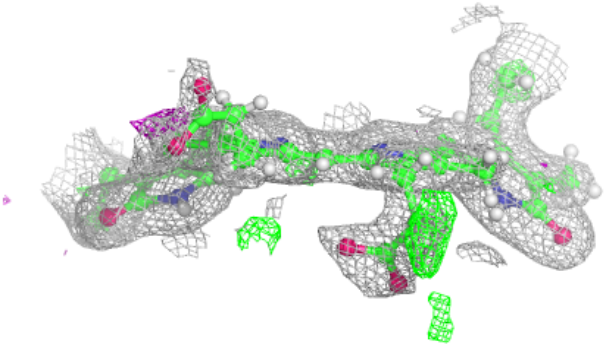
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	AX9	B	201	43/43	0.90	0.11	20,36,53,72	2
4	PEB	D	203	43/43	0.91	0.10	24,36,47,69	0
4	PEB	D	202	43/43	0.92	0.09	22,32,42,52	0
5	AX9	D	201	43/43	0.92	0.09	20,34,49,59	2
4	PEB	E	101[B]	43/43	0.93	0.11	19,27,56,67	80
4	PEB	A	101[A]	43/43	0.93	0.11	19,27,56,67	80
4	PEB	B	203	43/43	0.93	0.09	22,29,41,49	0
4	PEB	F	101[B]	43/43	0.94	0.10	22,36,55,73	80
4	PEB	C	101[A]	43/43	0.94	0.10	22,36,55,73	80
4	PEB	B	202	43/43	0.94	0.08	21,29,37,41	0

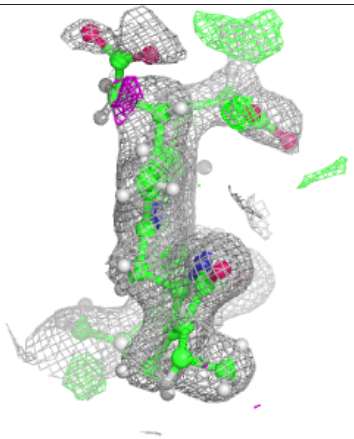
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AX9 B 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

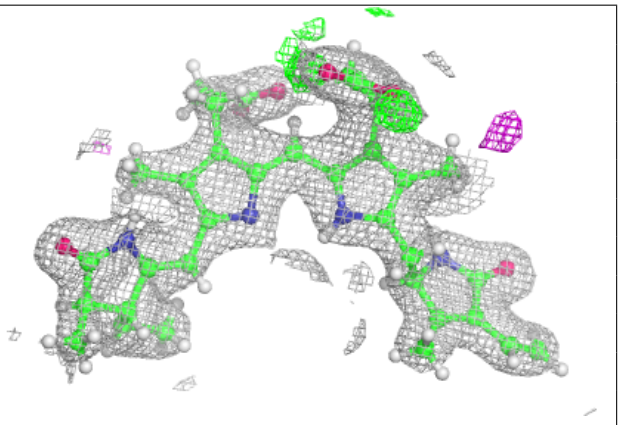


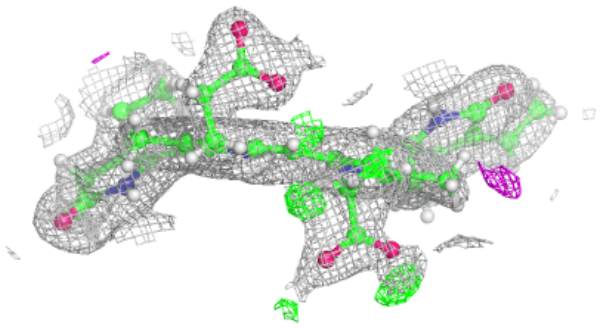


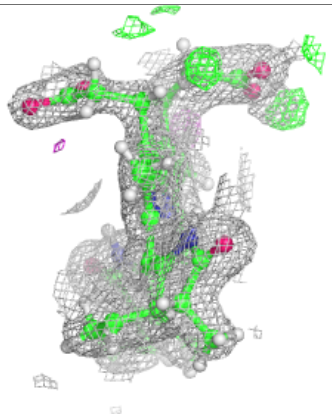


Electron density around PEB D 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

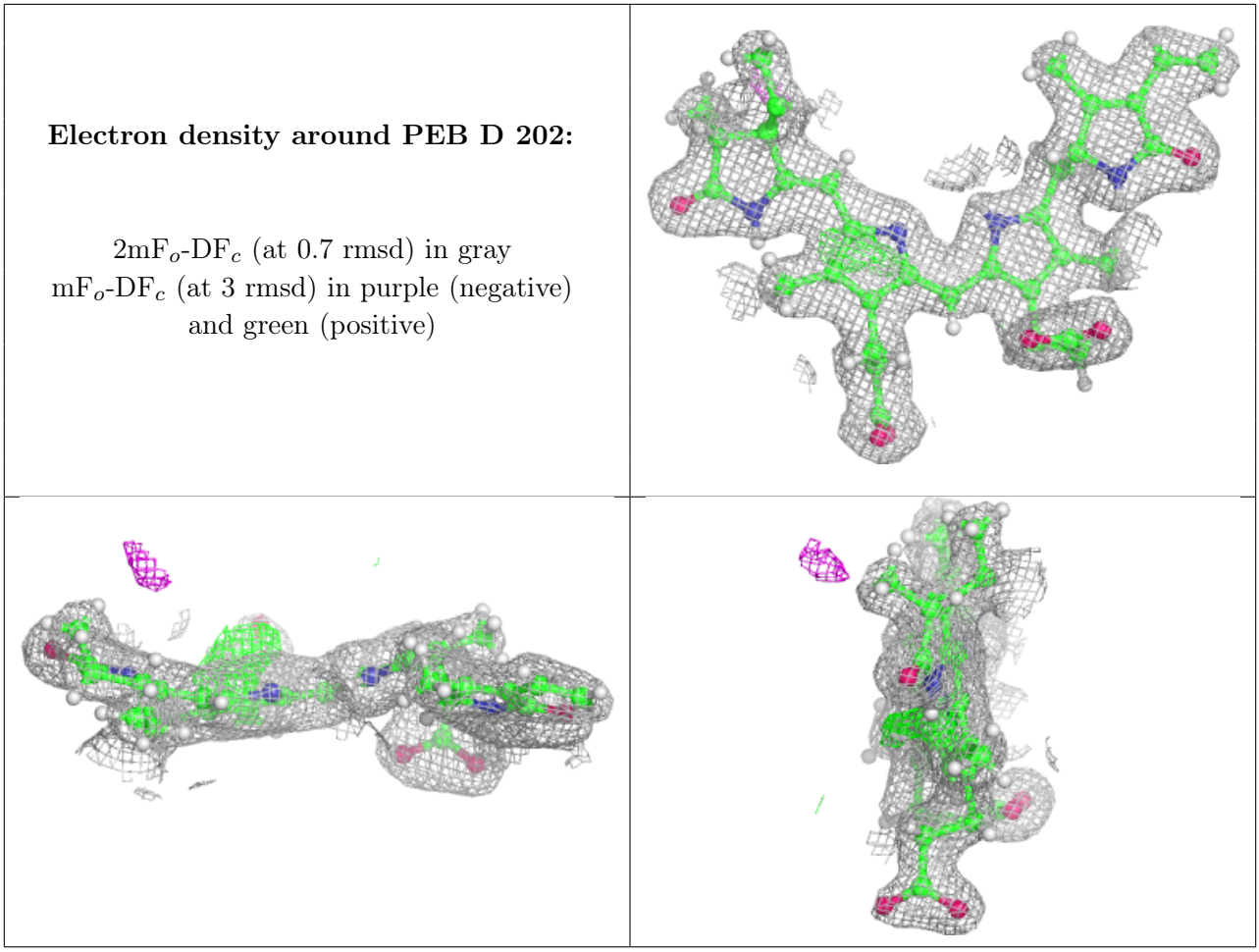






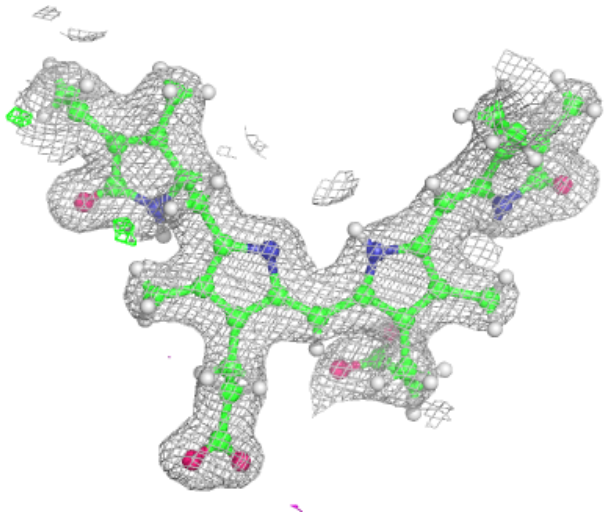
Electron density around PEB D 202:

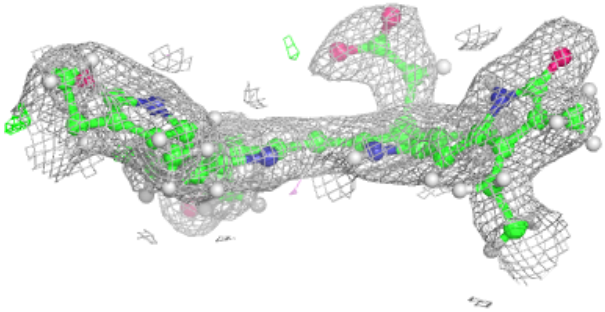
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

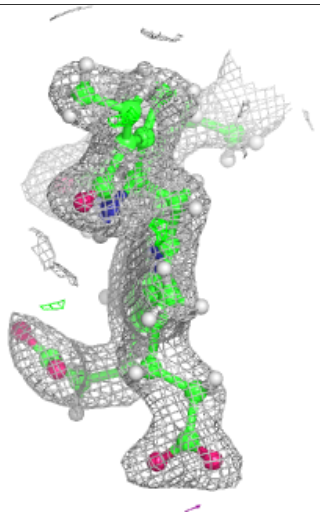


Electron density around AX9 D 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

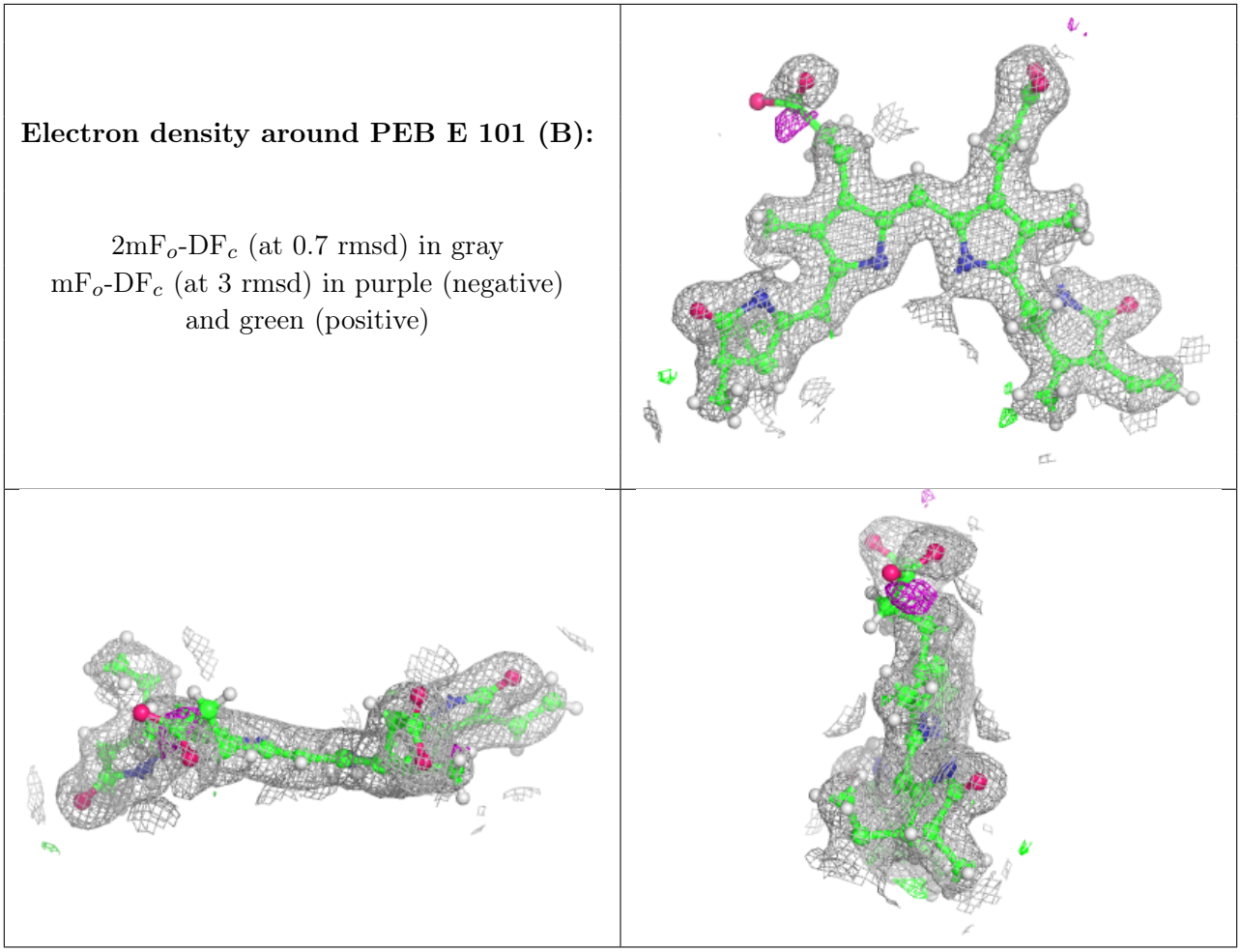






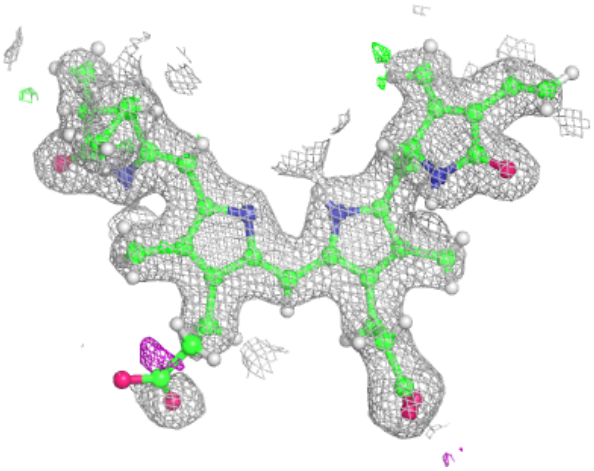
Electron density around PEB E 101 (B):

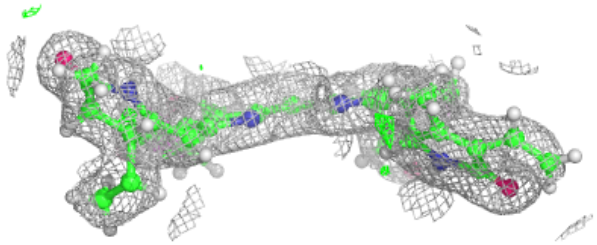
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

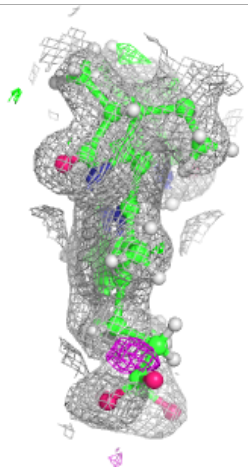


Electron density around PEB A 101 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

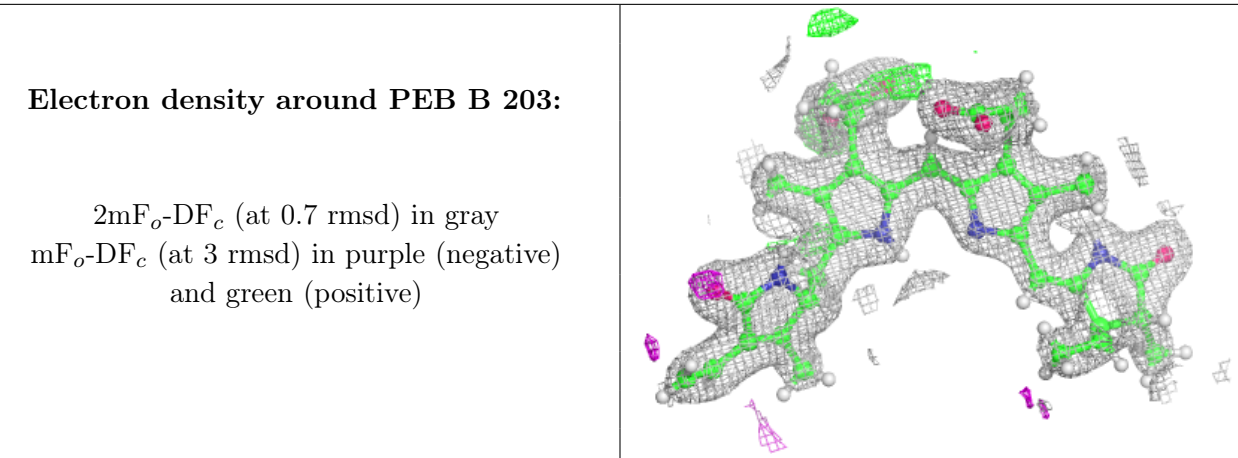


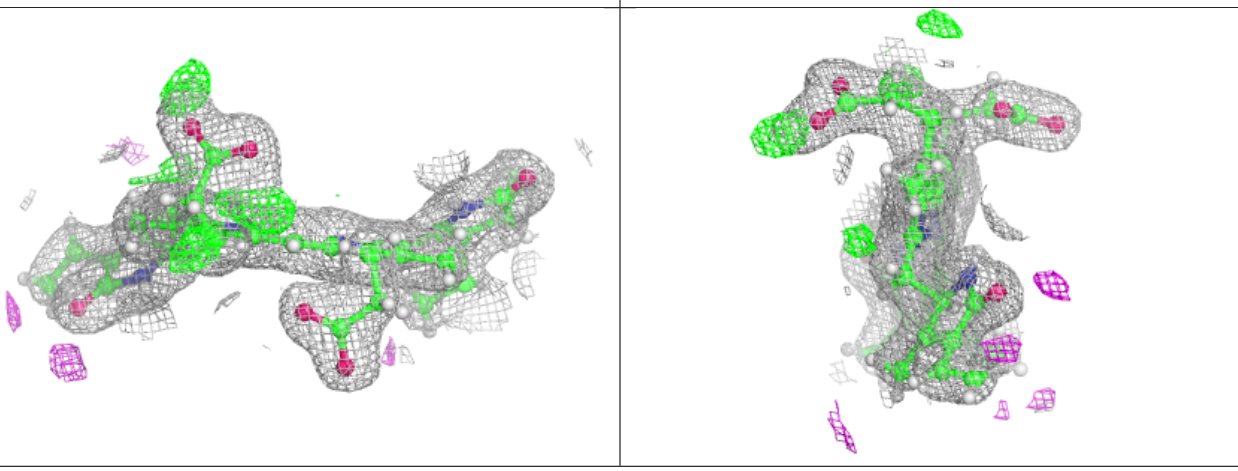




Electron density around PEB B 203:

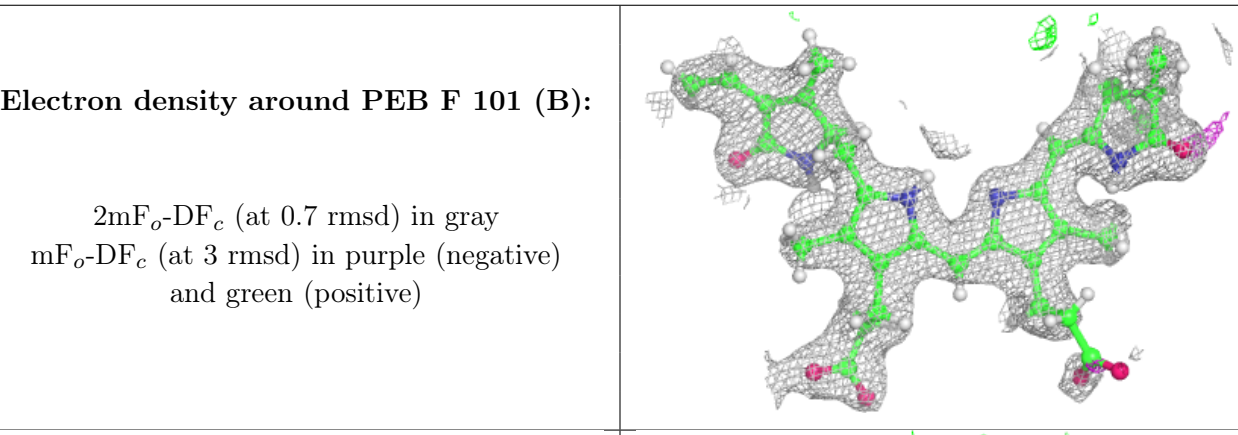
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

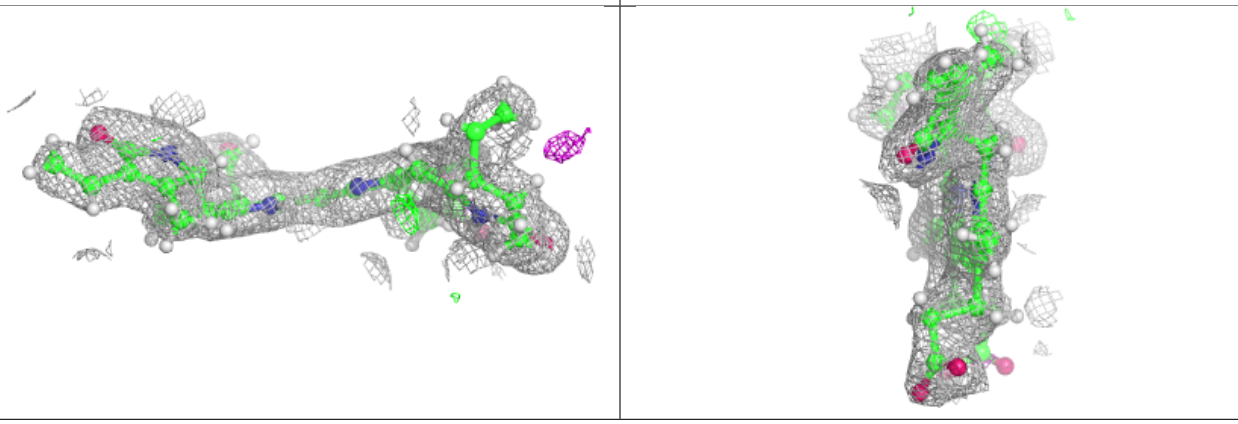




Electron density around PEB F 101 (B):

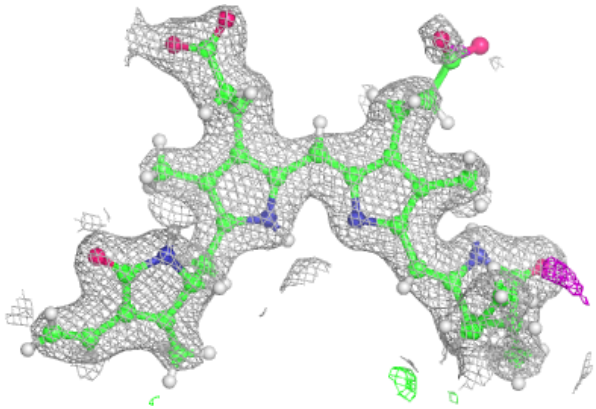
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

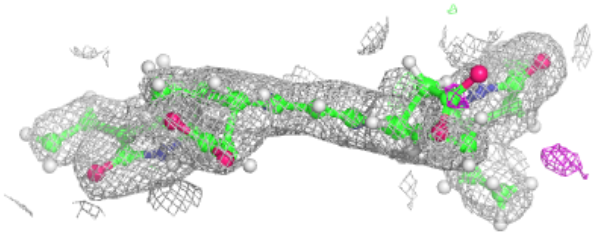


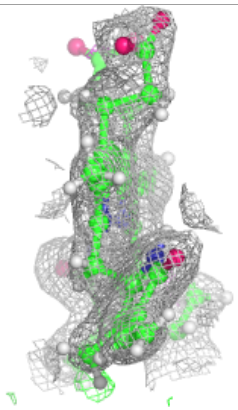


Electron density around PEB C 101 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

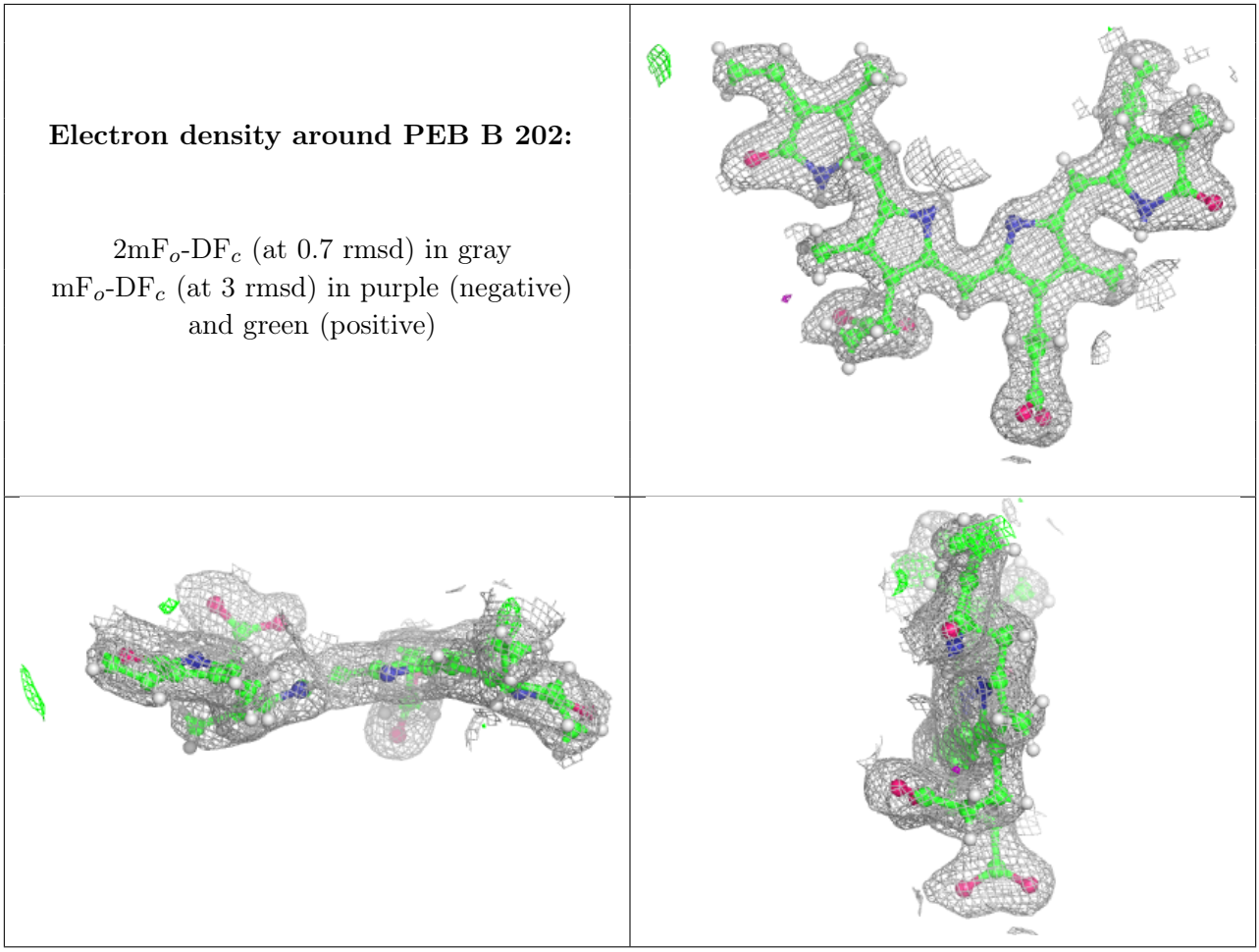






Electron density around PEB B 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.