



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:02 AM UTC

PDB ID : 7SUT / pdb_00007sut
Title : Light harvesting phycobiliprotein HaPE645 from the cryptophyte *Hemiselmis andersenii* CCMP644
Authors : Rathbone, H.W.; Michie, K.A.; Laos, A.L.; Curmi, P.M.G.
Deposited on : 2021-11-18
Resolution : 1.49 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

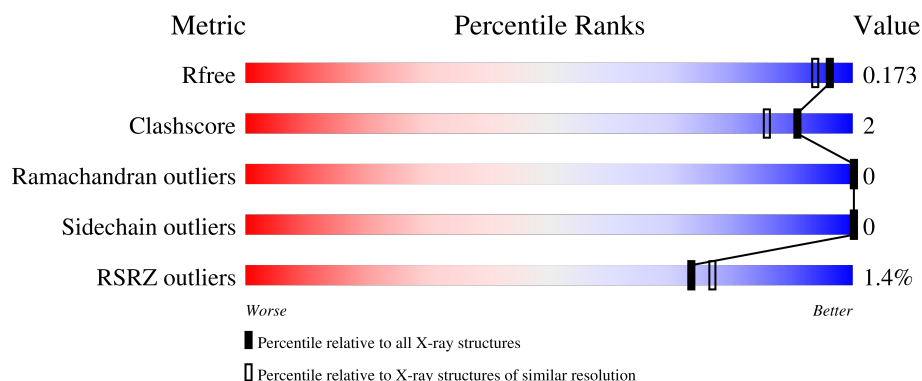
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

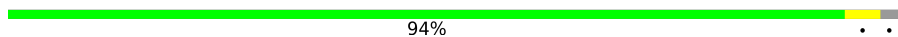
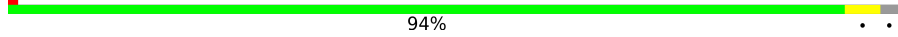
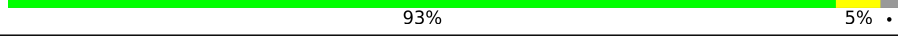
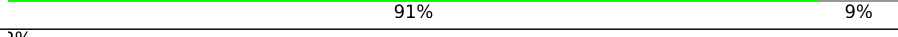
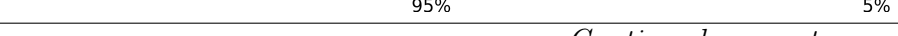
The reported resolution of this entry is 1.49 Å.

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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 $\leq 5\%$. 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	80	 94%
1	E	80	 94%
2	B	177	 93% 5%
2	D	177	 91% 9%
2	F	177	 95% 5%

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Mol	Chain	Length	Quality of chain
2	H	177	% 91% 9%
3	C	68	3% 91% 7%
3	G	68	4% 90% 7%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16766 atoms, of which 8115 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 HaPE645 alpha-1 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	78	Total	C	H	N	O	S	0	9	0
			1356	427	671	116	136	6			
1	E	78	Total	C	H	N	O	S	0	3	0
			1256	399	620	106	126	5			

- Molecule 2 is a protein called Phycoerythrin550 beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	174	Total	C	H	N	O	S	0	18	0
			2713	831	1362	231	279	10			
2	D	161	Total	C	H	N	O	S	0	4	0
			2395	737	1204	205	239	10			
2	F	176	Total	C	H	N	O	S	0	9	0
			2630	808	1324	222	265	11			
2	H	161	Total	C	H	N	O	S	0	6	0
			2396	737	1201	206	243	9			

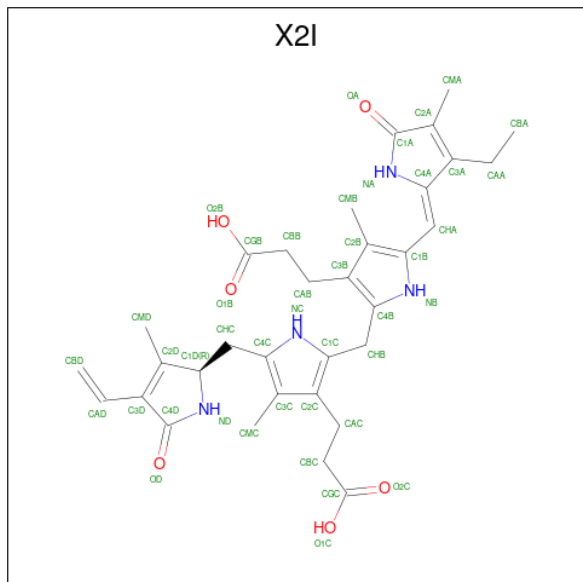
There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called HaPE645 alpha-2 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	63	Total	C	H	N	O	S	0	2	0
			1046	325	525	90	100	6			
3	G	63	Total	C	H	N	O	S	0	4	0
			1075	335	537	92	105	6			

- Molecule 4 is (15,16)-DIHYDROBILIVERDIN (SINGLY LINKED) (CCD ID: X2I) (formula: $\text{C}_{33}\text{H}_{40}\text{N}_4\text{O}_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 78	C 33	H 35	N 4	O 6	0	0
4	C	1	Total 78	C 33	H 35	N 4	O 6	0	0
4	E	1	Total 78	C 33	H 35	N 4	O 6	0	0
4	G	1	Total 78	C 33	H 35	N 4	O 6	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

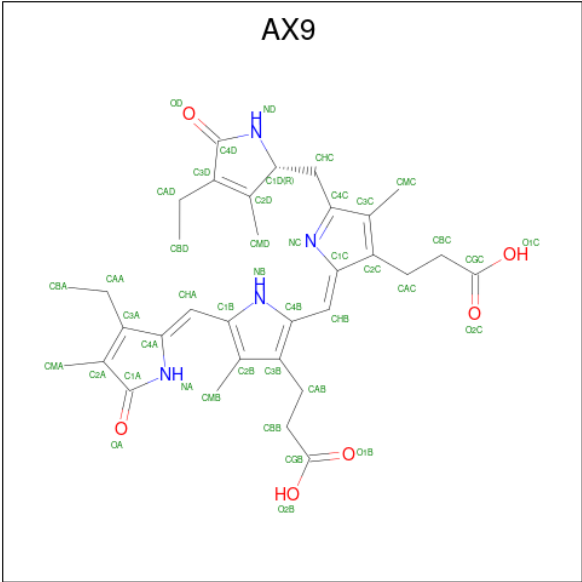


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			31	8	18	5		
5	H	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

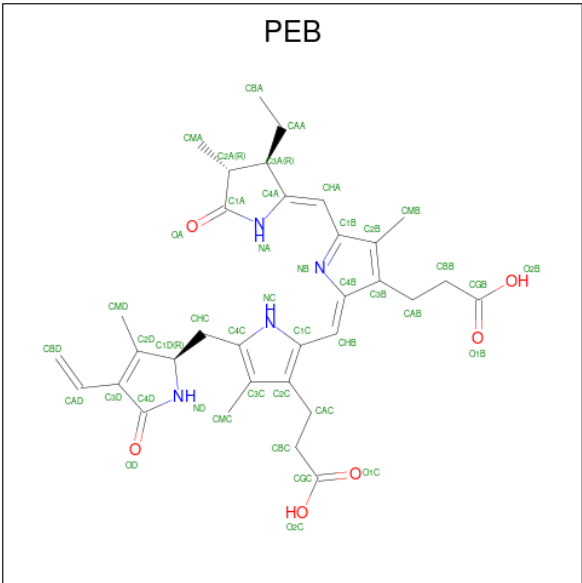
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DiCys-(15,16)-Dihydrobiliverdin (CCD ID: AX9) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



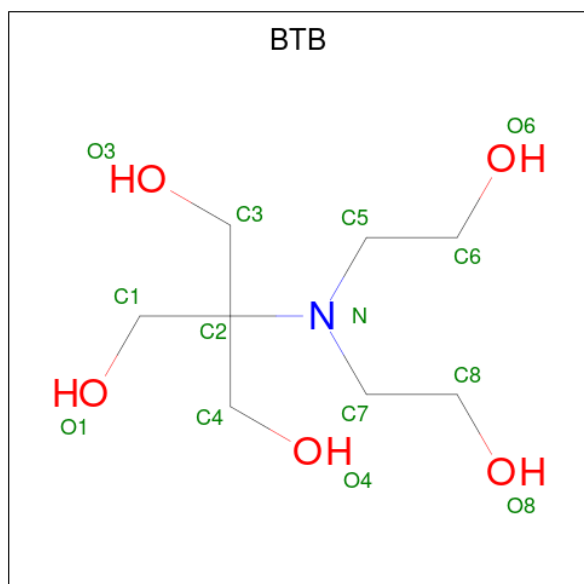
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	0	1
			158	66	72	8	12		
7	D	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
7	F	1	Total	C	H	N	O	0	0
			79	33	36	4	6		
7	H	1	Total	C	H	N	O	0	0
			79	33	36	4	6		

- Molecule 8 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



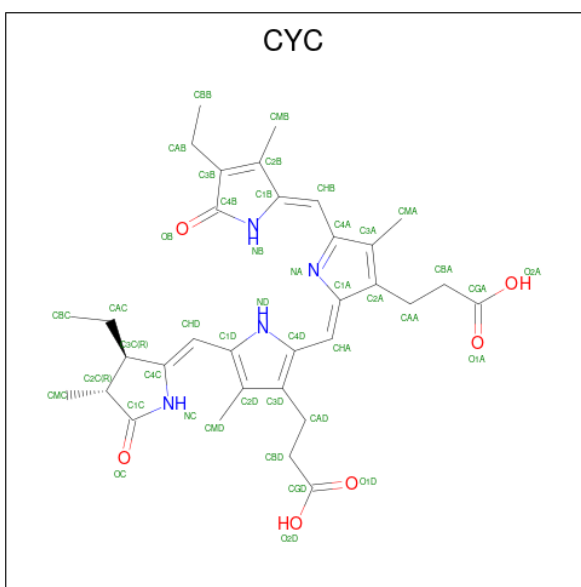
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
8	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
8	D	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
8	F	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
8	F	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
8	H	1	Total	C	H	N	O	0	0
			80	33	37	4	6		

- Molecule 9 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			33	8	19	1	5		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
10	D	1	Total 80	C 33	H 37	N 4	O 6	0	0
10	H	1	Total 80	C 33	H 37	N 4	O 6	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	65	Total O 65 65	0	1
11	B	80	Total O 80 80	0	0
11	C	41	Total O 41 41	0	0
11	D	82	Total O 82 82	0	0
11	E	45	Total O 45 45	0	0
11	F	58	Total O 58 58	0	0
11	G	28	Total O 28 28	0	1
11	H	57	Total O 57 57	0	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 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: HaPE645 alpha-1 subunit

Chain A:  94% . .



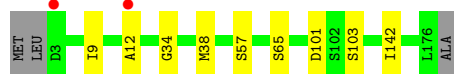
- Molecule 1: HaPE645 alpha-1 subunit

Chain E:  94% . .



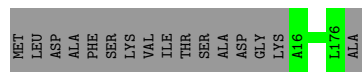
- Molecule 2: Phycoerythrin550 beta subunit

Chain B:  93% 5% .



- Molecule 2: Phycoerythrin550 beta subunit

Chain D:  91% 9%

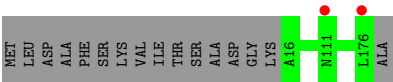
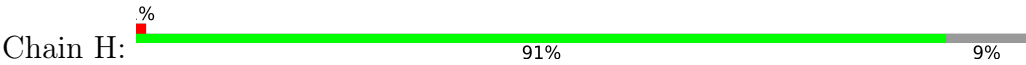


- Molecule 2: Phycoerythrin550 beta subunit

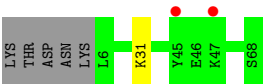
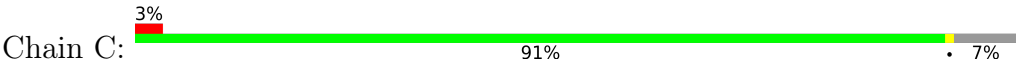
Chain F:  95% 5% .



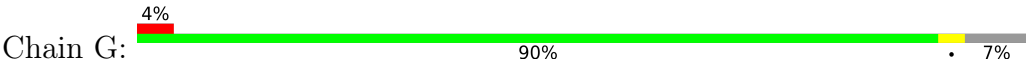
- Molecule 2: Phycoerythrin550 beta subunit



• Molecule 3: HaPE645 alpha-2 subunit



• Molecule 3: HaPE645 alpha-2 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.03Å 80.98Å 115.84Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	41.43 – 1.49 41.43 – 1.49	Depositor EDS
% Data completeness (in resolution range)	93.3 (41.43-1.49) 87.8 (41.43-1.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 1.49Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.145 , 0.175 0.144 , 0.173	Depositor DCC
R_{free} test set	1871 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	16766	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CL, BTB, PEB, CYC, AX9, PG4, X2I

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	0.42	0/696	0.57	0/927
1	E	0.40	0/647	0.58	0/864
2	B	0.40	0/1395	0.56	0/1880
2	D	0.46	0/1211	0.62	0/1634
2	F	0.36	0/1345	0.55	0/1814
2	H	0.33	0/1222	0.51	0/1651
3	C	0.45	0/528	0.65	0/704
3	G	0.36	0/545	0.52	0/728
All	All	0.40	0/7589	0.57	0/10202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	685	671	662	6	0
1	E	636	620	616	3	0
2	B	1351	1362	1315	11	0
2	D	1191	1204	1193	0	0
2	F	1306	1324	1297	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1195	1201	1180	0	0
3	C	521	525	521	1	0
3	G	538	537	533	3	0
4	A	43	35	0	0	0
4	C	43	35	0	0	0
4	E	43	35	0	0	0
4	G	43	35	0	0	0
5	A	13	18	18	1	0
5	H	13	18	18	0	0
6	A	1	0	0	0	0
7	B	86	72	0	0	0
7	D	43	36	0	0	0
7	F	43	36	0	0	0
7	H	43	36	0	0	0
8	B	86	74	74	3	0
8	D	43	37	37	0	0
8	F	86	74	74	3	0
8	H	43	37	37	1	0
9	B	14	19	19	0	0
10	D	43	37	37	1	0
10	H	43	37	37	0	0
11	A	65	0	0	0	0
11	B	80	0	0	0	0
11	C	41	0	0	1	0
11	D	82	0	0	0	0
11	E	45	0	0	0	0
11	F	58	0	0	0	0
11	G	28	0	0	0	0
11	H	57	0	0	0	0
All	All	8651	8115	7668	27	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 2.

All (27) 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)
2:F:142:ILE:O	8:F:203:PEB:HAA2	2.04	0.58
8:H:203:PEB:HBA3	8:H:203:PEB:HHA1	1.86	0.57
1:A:6:LEU:CD1	2:B:12:ALA:HB1	2.35	0.56
1:A:43[B]:MET:HG3	2:B:9:ILE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:11[B]:ILE:HD13	3:G:43:VAL:HG13	1.93	0.51
1:E:53:ALA:HB1	2:F:79:MET:HB3	1.92	0.51
2:F:2:LEU:O	2:F:7:LYS:HE2	2.13	0.49
3:G:11[B]:ILE:HD12	3:G:43:VAL:HG22	1.95	0.49
3:G:11[B]:ILE:CD1	3:G:43:VAL:HG13	2.43	0.48
5:A:102:PG4:C7	2:B:65:SER:HB2	2.44	0.47
1:A:43[B]:MET:CG	2:B:9:ILE:HA	2.44	0.47
10:D:202:CYC:HMA1	10:D:202:CYC:HB	1.80	0.47
1:A:43[A]:MET:HE3	2:B:9:ILE:HA	1.97	0.46
8:B:203:PEB:HBA3	8:B:203:PEB:HHA1	1.97	0.46
8:F:202:PEB:CMB	8:F:202:PEB:HNA	2.28	0.46
8:B:202:PEB:CMB	8:B:202:PEB:HNA	2.29	0.45
1:A:60:PHE:CE1	2:B:57:SER:HB2	2.52	0.45
2:B:101:ASP:OD2	2:B:103[B]:SER:HB2	2.17	0.44
2:B:101:ASP:OD2	2:B:103[A]:SER:OG	2.25	0.43
1:E:57:ILE:HG13	2:F:79:MET:HG2	1.99	0.43
3:C:31[A]:LYS:HE3	11:C:209:HOH:O	2.18	0.43
2:B:34:GLY:O	2:B:38:MET:HG2	2.18	0.43
1:E:79:ILE:HD11	2:F:62:GLU:HG2	2.00	0.42
1:A:43[A]:MET:HE3	2:B:9:ILE:HG12	2.02	0.42
2:B:142:ILE:O	8:B:203:PEB:HAA2	2.19	0.42
2:F:36:LYS:NZ	2:F:157:ASP:O	2.40	0.41
2:F:156:GLY:HA3	8:F:203:PEB:CMB	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 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	85/80 (106%)	81 (95%)	4 (5%)	0	100	100
1	E	79/80 (99%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	190/177 (107%)	186 (98%)	4 (2%)	0	100	100
2	D	163/177 (92%)	161 (99%)	2 (1%)	0	100	100
2	F	183/177 (103%)	181 (99%)	2 (1%)	0	100	100
2	H	165/177 (93%)	163 (99%)	2 (1%)	0	100	100
3	C	63/68 (93%)	63 (100%)	0	0	100	100
3	G	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
All	All	993/1004 (99%)	974 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	77/70 (110%)	77 (100%)	0	100	100
1	E	71/70 (101%)	71 (100%)	0	100	100
2	B	155/140 (111%)	155 (100%)	0	100	100
2	D	132/140 (94%)	132 (100%)	0	100	100
2	F	147/140 (105%)	147 (100%)	0	100	100
2	H	134/140 (96%)	134 (100%)	0	100	100
3	C	57/60 (95%)	57 (100%)	0	100	100
3	G	59/60 (98%)	59 (100%)	0	100	100
All	All	832/820 (102%)	832 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	145	ASN

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Mol	Chain	Res	Type
2	F	25	GLN
2	F	145	ASN
2	H	111	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	CYC	H	202	2	46,46,46	2.81	12 (26%)	63,67,67	2.16	14 (22%)
7	AX9	B	201[B]	2	45,46,46	1.81	7 (15%)	54,67,67	1.20	5 (9%)
8	PEB	F	203	2	46,46,46	4.11	33 (71%)	56,67,67	2.01	17 (30%)
4	X2I	E	101	1	46,46,46	1.59	7 (15%)	59,67,67	1.64	16 (27%)
8	PEB	H	203	2	46,46,46	3.93	32 (69%)	56,67,67	2.29	22 (39%)
5	PG4	A	102	-	12,12,12	0.17	0	11,11,11	0.59	0
8	PEB	B	202	2	46,46,46	3.78	33 (71%)	56,67,67	2.11	18 (32%)
7	AX9	B	201[A]	2	45,46,46	1.79	7 (15%)	54,67,67	1.22	6 (11%)
7	AX9	D	201	2	45,46,46	1.67	8 (17%)	54,67,67	1.15	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	X2I	C	101	3	46,46,46	1.59	7 (15%)	59,67,67	1.50	11 (18%)
8	PEB	D	203	2	46,46,46	3.48	30 (65%)	56,67,67	1.87	18 (32%)
4	X2I	A	101	1	46,46,46	1.45	5 (10%)	59,67,67	1.63	15 (25%)
10	CYC	D	202	2	46,46,46	2.48	11 (23%)	63,67,67	2.41	16 (25%)
8	PEB	B	203	2	46,46,46	3.60	31 (67%)	56,67,67	1.97	21 (37%)
5	PG4	H	204	-	12,12,12	0.16	0	11,11,11	0.61	0
4	X2I	G	101	3	46,46,46	1.64	7 (15%)	59,67,67	1.73	15 (25%)
8	PEB	F	202	2	46,46,46	4.33	34 (73%)	56,67,67	2.20	24 (42%)
9	BTB	B	204	-	13,13,13	0.63	0	7,16,16	0.41	0
7	AX9	H	201	2	45,46,46	1.82	9 (20%)	54,67,67	1.09	3 (5%)
7	AX9	F	201	2	45,46,46	1.79	8 (17%)	54,67,67	1.29	5 (9%)

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	H	202	2	-	6/26/74/74	0/4/4/4
7	AX9	B	201[B]	2	-	4/26/74/74	0/4/4/4
8	PEB	F	203	2	-	5/26/74/74	0/4/4/4
4	X2I	E	101	1	-	7/26/58/58	0/4/4/4
8	PEB	H	203	2	-	7/26/74/74	0/4/4/4
5	PG4	A	102	-	-	4/10/10/10	-
8	PEB	B	202	2	-	4/26/74/74	0/4/4/4
7	AX9	B	201[A]	2	-	7/26/74/74	0/4/4/4
7	AX9	D	201	2	-	5/26/74/74	0/4/4/4
4	X2I	C	101	3	-	7/26/58/58	0/4/4/4
8	PEB	D	203	2	-	6/26/74/74	0/4/4/4
4	X2I	A	101	1	-	7/26/58/58	0/4/4/4
10	CYC	D	202	2	-	8/26/74/74	0/4/4/4
8	PEB	B	203	2	-	4/26/74/74	0/4/4/4
5	PG4	H	204	-	-	1/10/10/10	-
4	X2I	G	101	3	-	6/26/58/58	0/4/4/4
8	PEB	F	202	2	-	6/26/74/74	0/4/4/4
9	BTB	B	204	-	-	0/21/21/21	-
7	AX9	H	201	2	-	4/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AX9	F	201	2	-	4/26/74/74	0/4/4/4

All (281) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	202	CYC	C1C-NC	-9.77	1.24	1.37
10	D	202	CYC	C1C-NC	-9.12	1.25	1.37
8	F	202	PEB	C4D-ND	8.94	1.46	1.35
8	F	202	PEB	CHB-C1C	8.88	1.60	1.40
8	F	202	PEB	C1A-NA	8.87	1.49	1.37
8	H	203	PEB	CHB-C1C	8.73	1.60	1.40
8	F	203	PEB	CHB-C1C	8.57	1.59	1.40
8	B	202	PEB	CHB-C1C	8.40	1.59	1.40
8	B	203	PEB	C2A-C1A	8.28	1.59	1.52
8	F	203	PEB	CHA-C1B	8.25	1.59	1.40
8	H	203	PEB	C1A-NA	8.23	1.48	1.37
8	F	203	PEB	C1A-NA	8.14	1.48	1.37
8	F	202	PEB	CHA-C1B	8.09	1.59	1.40
8	H	203	PEB	CHA-C1B	8.08	1.59	1.40
8	D	203	PEB	C1A-NA	7.98	1.48	1.37
8	B	203	PEB	CHB-C1C	7.67	1.57	1.40
8	F	202	PEB	CHC-C4C	7.62	1.59	1.50
8	F	203	PEB	C2A-C1A	7.57	1.58	1.52
8	D	203	PEB	CHB-C1C	7.55	1.57	1.40
8	B	202	PEB	CHA-C1B	7.44	1.57	1.40
8	B	202	PEB	C1A-NA	7.37	1.47	1.37
8	F	202	PEB	C2A-C1A	7.33	1.58	1.52
8	F	203	PEB	C4D-ND	7.32	1.44	1.35
8	B	203	PEB	C1A-NA	7.25	1.47	1.37
8	B	203	PEB	CHA-C1B	7.08	1.57	1.40
8	B	202	PEB	C4D-ND	7.04	1.43	1.35
8	D	203	PEB	CHA-C1B	6.98	1.56	1.40
10	H	202	CYC	CHD-C1D	6.59	1.55	1.40
8	B	203	PEB	C4D-ND	6.56	1.43	1.35
8	B	202	PEB	CHC-C4C	6.55	1.57	1.50
8	H	203	PEB	C2A-C1A	6.54	1.57	1.52
8	D	203	PEB	C4D-ND	6.52	1.43	1.35
8	H	203	PEB	C4D-ND	6.46	1.43	1.35
8	F	203	PEB	CHC-C4C	6.44	1.57	1.50
8	F	202	PEB	C4C-C3C	6.31	1.46	1.38
10	H	202	CYC	CHA-C4D	6.30	1.54	1.40
8	H	203	PEB	CMD-C2D	6.24	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	202	PEB	CMD-C2D	6.19	1.60	1.50
10	H	202	CYC	CHB-C4A	6.12	1.54	1.40
8	B	202	PEB	C2A-C1A	6.07	1.57	1.52
8	F	203	PEB	CMD-C2D	5.88	1.59	1.50
8	D	203	PEB	C2A-C1A	5.82	1.57	1.52
8	F	203	PEB	C4A-NA	5.75	1.48	1.37
8	F	202	PEB	CMB-C2B	5.72	1.62	1.50
10	D	202	CYC	CHA-C4D	5.71	1.53	1.40
8	F	203	PEB	CAC-C2C	5.69	1.66	1.51
10	H	202	CYC	C4C-NC	-5.65	1.26	1.37
8	B	202	PEB	CMD-C2D	5.62	1.59	1.50
8	H	203	PEB	CHC-C4C	5.58	1.56	1.50
8	F	202	PEB	C4A-NA	5.52	1.48	1.37
8	F	203	PEB	CMB-C2B	5.45	1.61	1.50
8	H	203	PEB	CAC-C2C	5.43	1.65	1.51
8	B	202	PEB	C4C-C3C	5.37	1.45	1.38
8	F	202	PEB	CAC-C2C	5.35	1.65	1.51
10	D	202	CYC	CHB-C4A	5.31	1.52	1.40
8	B	202	PEB	CMB-C2B	5.31	1.61	1.50
8	H	203	PEB	C4C-C3C	5.31	1.45	1.38
8	B	203	PEB	CHC-C4C	5.25	1.56	1.50
7	F	201	AX9	CHB-C4B	5.20	1.52	1.40
4	G	101	X2I	CHA-C1B	5.16	1.52	1.40
8	H	203	PEB	C4A-NA	5.14	1.47	1.37
7	B	201[A]	AX9	CHB-C4B	5.10	1.51	1.40
8	B	202	PEB	CAC-C2C	5.06	1.64	1.51
8	B	202	PEB	C4A-NA	5.01	1.47	1.37
4	C	101	X2I	CHA-C1B	5.00	1.51	1.40
8	F	203	PEB	C4C-C3C	5.00	1.45	1.38
7	F	201	AX9	CHA-C1B	4.98	1.51	1.40
10	H	202	CYC	C4B-C3B	-4.98	1.39	1.48
7	B	201[B]	AX9	C1C-C2C	-4.93	1.38	1.45
8	B	202	PEB	CBC-CGC	4.89	1.61	1.50
8	F	202	PEB	CBC-CGC	4.89	1.61	1.50
8	H	203	PEB	CMB-C2B	4.86	1.60	1.50
8	B	203	PEB	CMB-C2B	4.82	1.60	1.50
7	B	201[A]	AX9	CHA-C1B	4.82	1.51	1.40
10	D	202	CYC	CHD-C1D	4.79	1.51	1.40
7	D	201	AX9	CHB-C4B	4.78	1.51	1.40
8	F	203	PEB	CBC-CGC	4.77	1.61	1.50
4	A	101	X2I	CHA-C1B	4.71	1.51	1.40
8	H	203	PEB	CBC-CGC	4.71	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	203	PEB	CMD-C2D	4.70	1.58	1.50
7	D	201	AX9	C4D-ND	4.70	1.40	1.35
4	E	101	X2I	CHA-C1B	4.69	1.50	1.40
7	F	201	AX9	C1C-C2C	-4.68	1.38	1.45
7	H	201	AX9	C1C-C2C	-4.67	1.38	1.45
10	D	202	CYC	C4C-NC	-4.66	1.28	1.37
7	B	201[B]	AX9	CHB-C4B	4.65	1.50	1.40
8	D	203	PEB	CHC-C4C	4.65	1.55	1.50
8	D	203	PEB	CMD-C2D	4.63	1.57	1.50
7	B	201[B]	AX9	CHA-C1B	4.62	1.50	1.40
10	D	202	CYC	C4B-C3B	-4.62	1.39	1.48
8	F	203	PEB	CBB-CGB	4.61	1.61	1.50
7	H	201	AX9	CHB-C4B	4.61	1.50	1.40
8	D	203	PEB	CMB-C2B	4.60	1.60	1.50
8	B	203	PEB	C4A-NA	4.59	1.46	1.37
8	B	203	PEB	CAC-C2C	4.58	1.63	1.51
4	E	101	X2I	C1A-C2A	-4.56	1.37	1.48
8	B	203	PEB	CBC-CGC	4.50	1.61	1.50
8	D	203	PEB	CAC-C2C	4.49	1.62	1.51
4	G	101	X2I	C1A-C2A	-4.47	1.37	1.48
8	D	203	PEB	CBB-CGB	4.44	1.60	1.50
7	B	201[A]	AX9	C1C-C2C	-4.41	1.38	1.45
8	D	203	PEB	CBC-CGC	4.40	1.60	1.50
7	H	201	AX9	CHA-C1B	4.32	1.50	1.40
8	F	203	PEB	C1C-NC	4.31	1.45	1.37
8	H	203	PEB	CBB-CGB	4.25	1.60	1.50
8	F	202	PEB	C2D-C3D	4.25	1.40	1.34
8	F	202	PEB	C3A-C4A	4.21	1.59	1.50
8	F	202	PEB	CMA-C2A	4.15	1.62	1.53
8	H	203	PEB	C2D-C3D	4.15	1.39	1.34
8	F	202	PEB	C4C-NC	4.10	1.46	1.37
10	H	202	CYC	CAC-C3C	-4.08	1.46	1.54
4	C	101	X2I	C4A-C3A	-4.00	1.37	1.44
8	B	203	PEB	C4C-C3C	3.99	1.43	1.38
8	F	203	PEB	CMA-C2A	3.99	1.61	1.53
8	F	202	PEB	CBB-CGB	3.99	1.59	1.50
8	F	202	PEB	C1C-NC	3.97	1.44	1.37
8	H	203	PEB	CAB-C3B	3.97	1.61	1.51
8	F	203	PEB	CAB-C3B	3.96	1.61	1.51
8	B	202	PEB	C3A-C4A	3.95	1.59	1.50
8	D	203	PEB	C4C-C3C	3.94	1.43	1.38
4	A	101	X2I	C1A-C2A	-3.92	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	101	X2I	C4D-ND	3.91	1.39	1.35
8	F	203	PEB	O1B-CGB	3.90	1.34	1.22
7	D	201	AX9	C1C-C2C	-3.89	1.39	1.45
4	C	101	X2I	C1A-C2A	-3.87	1.38	1.48
8	D	203	PEB	CAB-C3B	3.85	1.61	1.51
7	H	201	AX9	C1A-C2A	-3.84	1.38	1.48
8	B	203	PEB	C3A-C4A	3.84	1.58	1.50
8	F	203	PEB	C3A-C4A	3.84	1.58	1.50
8	B	202	PEB	CBB-CGB	3.84	1.59	1.50
8	H	203	PEB	CMA-C2A	3.79	1.61	1.53
8	D	203	PEB	C4A-NA	3.74	1.44	1.37
8	F	202	PEB	O1C-CGC	3.73	1.34	1.22
8	H	203	PEB	C1C-NC	3.69	1.44	1.37
4	E	101	X2I	C4D-ND	3.66	1.39	1.35
8	F	202	PEB	CAD-C3D	3.66	1.57	1.47
8	F	202	PEB	O1B-CGB	3.65	1.34	1.22
8	H	203	PEB	O1B-CGB	3.64	1.34	1.22
4	A	101	X2I	C4D-ND	3.63	1.39	1.35
4	C	101	X2I	C4D-ND	3.57	1.39	1.35
4	G	101	X2I	C4A-C3A	-3.57	1.38	1.44
8	D	203	PEB	CMA-C2A	3.56	1.60	1.53
7	H	201	AX9	C4D-ND	3.53	1.39	1.35
7	B	201[A]	AX9	C1A-C2A	-3.53	1.39	1.48
8	D	203	PEB	C2D-C3D	3.51	1.39	1.34
7	B	201[B]	AX9	C1A-C2A	-3.49	1.39	1.48
8	B	203	PEB	CBB-CGB	3.46	1.58	1.50
10	D	202	CYC	CAC-C3C	-3.46	1.47	1.54
4	E	101	X2I	C4A-C3A	-3.45	1.38	1.44
7	B	201[B]	AX9	C4D-ND	3.42	1.39	1.35
10	H	202	CYC	C1A-C2A	-3.41	1.40	1.45
8	F	203	PEB	C4C-NC	3.40	1.44	1.37
7	H	201	AX9	C4A-C3A	-3.38	1.38	1.44
8	B	203	PEB	CAB-C3B	3.38	1.60	1.51
10	H	202	CYC	C2C-C3C	3.38	1.63	1.54
8	D	203	PEB	O1B-CGB	3.37	1.33	1.22
7	B	201[A]	AX9	C4D-ND	3.36	1.39	1.35
8	H	203	PEB	CAD-C3D	3.36	1.56	1.47
8	F	202	PEB	C1B-NB	3.35	1.44	1.36
8	B	202	PEB	C1C-NC	3.33	1.43	1.37
8	F	203	PEB	O1C-CGC	3.31	1.32	1.22
8	F	203	PEB	C2D-C3D	3.30	1.38	1.34
10	D	202	CYC	C2C-C3C	3.30	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	203	PEB	CMA-C2A	3.29	1.60	1.53
8	B	202	PEB	C2D-C3D	3.26	1.38	1.34
8	F	202	PEB	CAB-C3B	3.26	1.59	1.51
8	B	203	PEB	O1C-CGC	3.23	1.32	1.22
8	B	202	PEB	C3B-C2B	3.22	1.43	1.36
4	A	101	X2I	CHB-C1C	-3.22	1.37	1.49
8	H	203	PEB	O1C-CGC	3.20	1.32	1.22
8	H	203	PEB	C1B-NB	3.19	1.43	1.36
7	D	201	AX9	CHA-C1B	3.18	1.47	1.40
7	B	201[B]	AX9	CHC-C1D	-3.16	1.47	1.53
8	D	203	PEB	C3B-C2B	3.15	1.43	1.36
4	G	101	X2I	CHC-C1D	-3.15	1.47	1.53
7	F	201	AX9	C1A-C2A	-3.15	1.40	1.48
10	H	202	CYC	C2C-C1C	-3.14	1.49	1.52
8	H	203	PEB	C4C-NC	3.12	1.44	1.37
10	H	202	CYC	C1B-C2B	-3.11	1.39	1.45
8	F	202	PEB	CAA-C3A	3.10	1.59	1.54
4	E	101	X2I	CHC-C1D	-3.09	1.47	1.53
7	B	201[A]	AX9	CHC-C1D	-3.08	1.47	1.53
8	F	203	PEB	C3B-C2B	3.08	1.43	1.36
8	H	203	PEB	C3B-C2B	3.08	1.43	1.36
8	B	203	PEB	C3B-C2B	3.06	1.43	1.36
8	B	202	PEB	CAB-C3B	3.06	1.59	1.51
8	F	202	PEB	CHB-C4B	3.06	1.44	1.38
8	B	202	PEB	O1C-CGC	3.06	1.32	1.22
8	B	202	PEB	C1B-NB	3.05	1.43	1.36
8	H	203	PEB	CMC-C3C	3.05	1.57	1.50
8	H	203	PEB	C3A-C4A	3.04	1.57	1.50
8	B	203	PEB	C1C-NC	3.04	1.43	1.37
8	D	203	PEB	C3A-C4A	3.04	1.57	1.50
8	B	203	PEB	O1B-CGB	3.03	1.32	1.22
8	B	202	PEB	O1B-CGB	3.02	1.32	1.22
10	D	202	CYC	C1A-C2A	-3.01	1.41	1.45
7	B	201[B]	AX9	C4A-C3A	-3.01	1.39	1.44
4	C	101	X2I	CHC-C1D	-3.00	1.47	1.53
8	F	202	PEB	CMC-C3C	3.00	1.56	1.50
8	D	203	PEB	CHC-C1D	-2.98	1.47	1.53
7	F	201	AX9	C4D-C3D	-2.98	1.42	1.48
8	F	202	PEB	C1D-C2D	2.96	1.60	1.50
8	B	202	PEB	CAD-C3D	2.96	1.55	1.47
8	F	203	PEB	C1B-NB	2.95	1.43	1.36
8	B	203	PEB	C2D-C3D	2.95	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	101	X2I	CHB-C1C	-2.94	1.38	1.49
8	F	203	PEB	CAD-C3D	2.92	1.55	1.47
8	F	202	PEB	CHA-C4A	2.92	1.41	1.36
8	D	203	PEB	O1C-CGC	2.87	1.31	1.22
8	F	203	PEB	CMC-C3C	2.87	1.56	1.50
8	B	202	PEB	CMA-C2A	2.87	1.59	1.53
8	D	203	PEB	C4C-NC	2.86	1.43	1.37
8	F	202	PEB	C3B-C2B	2.86	1.42	1.36
4	E	101	X2I	CHB-C1C	-2.84	1.38	1.49
8	B	202	PEB	C1D-C2D	2.83	1.59	1.50
7	F	201	AX9	C4D-ND	2.83	1.38	1.35
8	B	202	PEB	C4C-NC	2.82	1.43	1.37
10	D	202	CYC	C1B-C2B	-2.81	1.40	1.45
7	D	201	AX9	C1D-ND	-2.81	1.41	1.45
8	F	203	PEB	CAA-C3A	2.81	1.59	1.54
7	B	201[A]	AX9	C4A-C3A	-2.77	1.39	1.44
7	F	201	AX9	CHC-C1D	-2.76	1.47	1.53
8	F	203	PEB	CBC-CAC	2.75	1.61	1.51
7	D	201	AX9	C1A-C2A	-2.74	1.41	1.48
8	B	203	PEB	CMC-C3C	2.74	1.56	1.50
4	A	101	X2I	CHC-C1D	-2.69	1.48	1.53
8	B	202	PEB	CHB-C4B	2.68	1.43	1.38
8	B	202	PEB	CAA-C3A	2.67	1.59	1.54
8	F	203	PEB	CHB-C4B	2.67	1.43	1.38
4	G	101	X2I	C1D-ND	-2.65	1.42	1.45
4	C	101	X2I	C1D-ND	-2.62	1.42	1.45
8	B	203	PEB	CAA-C3A	2.61	1.59	1.54
8	B	203	PEB	CHB-C4B	2.57	1.43	1.38
7	H	201	AX9	CHC-C1D	-2.55	1.48	1.53
4	C	101	X2I	CHB-C1C	-2.53	1.39	1.49
8	D	203	PEB	C1B-NB	2.49	1.42	1.36
8	F	203	PEB	CHA-C4A	2.49	1.40	1.36
8	D	203	PEB	CMC-C3C	2.47	1.55	1.50
8	F	203	PEB	C2A-C3A	2.46	1.61	1.54
8	F	202	PEB	CBD-CAD	2.43	1.42	1.30
8	B	203	PEB	CAD-C3D	2.43	1.53	1.47
7	D	201	AX9	CHC-C1D	-2.41	1.48	1.53
8	B	202	PEB	CBB-CAB	2.41	1.60	1.51
7	H	201	AX9	C4D-C3D	-2.41	1.43	1.48
8	F	202	PEB	CBB-CAB	2.40	1.60	1.51
8	H	203	PEB	CBB-CAB	2.39	1.60	1.51
8	B	203	PEB	C1B-NB	2.37	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	203	PEB	CHA-C4A	2.34	1.40	1.36
8	F	202	PEB	CBC-CAC	2.34	1.60	1.51
8	H	203	PEB	OD-C4D	2.33	1.28	1.23
8	F	203	PEB	CBB-CAB	2.33	1.60	1.51
8	B	202	PEB	CMC-C3C	2.32	1.55	1.50
8	F	202	PEB	C4B-NB	2.29	1.43	1.38
8	B	203	PEB	C1D-C2D	2.28	1.58	1.50
8	D	203	PEB	CHB-C4B	2.28	1.43	1.38
8	H	203	PEB	CHB-C4B	2.28	1.43	1.38
8	D	203	PEB	C1C-NC	2.25	1.41	1.37
8	H	203	PEB	CBC-CAC	2.25	1.59	1.51
8	D	203	PEB	CAD-C3D	2.20	1.53	1.47
7	F	201	AX9	C4A-C3A	-2.20	1.40	1.44
8	B	203	PEB	CBC-CAC	2.19	1.59	1.51
8	D	203	PEB	C4B-NB	2.18	1.43	1.38
8	F	203	PEB	C4B-NB	2.17	1.43	1.38
8	H	203	PEB	C4B-NB	2.16	1.43	1.38
8	B	202	PEB	C4B-NB	2.16	1.43	1.38
8	B	202	PEB	CBD-CAD	2.16	1.40	1.30
8	B	203	PEB	C4C-NC	2.15	1.41	1.37
7	D	201	AX9	C4A-C3A	-2.13	1.41	1.44
4	E	101	X2I	CHC-C4C	2.13	1.52	1.50
8	B	202	PEB	CBC-CAC	2.11	1.59	1.51
8	B	203	PEB	CBD-CAD	2.10	1.40	1.30
8	D	203	PEB	CBC-CAC	2.08	1.59	1.51
8	H	203	PEB	CBD-CAD	2.07	1.40	1.30
8	H	203	PEB	CAA-C3A	2.05	1.57	1.54
10	D	202	CYC	C4A-C3A	-2.04	1.41	1.45
10	H	202	CYC	C4A-C3A	-2.03	1.41	1.45
8	D	203	PEB	CBB-CAB	2.03	1.59	1.51
8	F	202	PEB	OD-C4D	2.03	1.27	1.23
8	B	202	PEB	OD-C4D	2.02	1.27	1.23
8	F	203	PEB	CBD-CAD	2.01	1.40	1.30
7	H	201	AX9	C1D-ND	-2.00	1.42	1.45

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	202	CYC	OC-C1C-C2C	-9.88	118.32	126.17
10	D	202	CYC	C2C-C1C-NC	8.10	115.03	108.29
10	H	202	CYC	C2C-C1C-NC	8.01	114.95	108.29
10	H	202	CYC	OC-C1C-C2C	-7.87	119.91	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	202	CYC	C3C-C4C-NC	5.97	115.63	107.94
8	H	203	PEB	C1A-NA-C4A	-5.78	106.16	113.41
10	H	202	CYC	C3C-C4C-NC	5.60	115.15	107.94
8	B	202	PEB	CBB-CAB-C3B	-5.15	98.29	112.53
8	B	202	PEB	CMB-C2B-C1B	5.13	133.07	125.10
8	F	202	PEB	C1A-NA-C4A	-5.00	107.13	113.41
8	F	202	PEB	C1D-CHC-C4C	-4.93	105.02	113.32
4	A	101	X2I	OD-C4D-ND	-4.80	119.42	126.02
8	F	203	PEB	CAC-CBC-CGC	-4.64	101.36	113.67
4	G	101	X2I	CAA-C3A-C4A	4.59	130.36	124.39
10	D	202	CYC	CHB-C4A-C3A	4.59	136.67	124.87
8	F	203	PEB	C1D-CHC-C4C	-4.44	105.85	113.32
8	B	202	PEB	C1A-NA-C4A	-4.40	107.88	113.41
8	H	203	PEB	CHC-C1D-ND	-4.35	108.39	113.73
8	B	202	PEB	CHA-C1B-NB	-4.34	115.57	124.95
8	D	203	PEB	C1A-NA-C4A	-4.33	107.97	113.41
8	H	203	PEB	C2A-C1A-NA	4.32	111.88	108.29
8	F	202	PEB	CBB-CAB-C3B	-4.31	100.62	112.53
8	F	203	PEB	C1A-NA-C4A	-4.18	108.17	113.41
8	F	202	PEB	C1C-CHB-C4B	-4.17	119.12	128.22
8	D	203	PEB	CHA-C1B-NB	-4.17	115.96	124.95
8	F	202	PEB	CBA-CAA-C3A	-4.16	104.58	113.41
4	E	101	X2I	CAA-C3A-C4A	4.14	129.77	124.39
10	D	202	CYC	CHB-C4A-NA	-4.13	116.02	124.95
8	H	203	PEB	CHB-C1C-C2C	-4.13	118.35	127.22
8	D	203	PEB	C3A-C4A-NA	4.07	113.19	107.94
4	G	101	X2I	CHC-C4C-NC	3.97	126.41	121.10
8	B	203	PEB	C1A-NA-C4A	-3.91	108.50	113.41
4	E	101	X2I	CMD-C2D-C3D	-3.89	124.43	129.95
8	B	203	PEB	C3C-C4C-NC	3.85	111.43	108.31
8	H	203	PEB	CAC-CBC-CGC	-3.85	103.46	113.67
8	B	203	PEB	CAC-CBC-CGC	-3.79	103.61	113.67
8	H	203	PEB	C1D-CHC-C4C	-3.75	107.01	113.32
8	B	202	PEB	C1C-CHB-C4B	-3.72	120.10	128.22
4	E	101	X2I	CHC-C4C-NC	3.69	126.03	121.10
8	H	203	PEB	C3A-C4A-NA	3.68	112.69	107.94
8	H	203	PEB	C1B-CHA-C4A	-3.66	119.82	127.25
10	D	202	CYC	CAB-C3B-C4B	3.62	126.96	121.37
8	B	203	PEB	CHB-C1C-C2C	-3.59	119.51	127.22
8	F	202	PEB	CMB-C2B-C1B	3.58	130.66	125.10
8	F	203	PEB	C1B-CHA-C4A	-3.57	119.99	127.25
8	D	203	PEB	CHB-C1C-C2C	-3.55	119.58	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	202	CYC	CHB-C4A-C3A	3.55	134.00	124.87
8	B	202	PEB	C1D-CHC-C4C	-3.55	107.35	113.32
4	A	101	X2I	CAA-C3A-C4A	3.53	128.98	124.39
8	F	203	PEB	CHB-C1C-C2C	-3.51	119.68	127.22
8	B	203	PEB	C3A-C4A-NA	3.47	112.42	107.94
8	F	202	PEB	CHB-C1C-C2C	-3.47	119.77	127.22
8	H	203	PEB	CMB-C2B-C1B	3.43	130.42	125.10
4	G	101	X2I	CHB-C4B-NB	3.34	128.83	122.04
4	A	101	X2I	CMD-C2D-C3D	-3.32	125.24	129.95
8	B	203	PEB	CHA-C1B-NB	-3.31	117.80	124.95
8	B	202	PEB	CBA-CAA-C3A	-3.30	106.41	113.41
7	F	201	AX9	CAD-C3D-C4D	3.27	126.43	121.37
4	C	101	X2I	CHC-C4C-NC	3.26	125.46	121.10
4	C	101	X2I	C1C-CHB-C4B	3.26	128.32	115.77
8	F	202	PEB	CHA-C1B-NB	-3.24	117.96	124.95
4	C	101	X2I	CHB-C1C-C2C	-3.23	123.90	130.07
8	D	203	PEB	C1B-CHA-C4A	-3.19	120.78	127.25
4	C	101	X2I	CHA-C1B-NB	-3.16	118.14	125.29
4	G	101	X2I	CHB-C1C-C2C	-3.14	124.06	130.07
4	G	101	X2I	CHB-C1C-NC	3.13	128.40	122.04
4	C	101	X2I	CHB-C1C-NC	3.12	128.38	122.04
8	F	203	PEB	OA-C1A-C2A	3.11	128.65	126.17
8	F	203	PEB	C1C-CHB-C4B	-3.09	121.48	128.22
4	A	101	X2I	CAD-C3D-C2D	-3.07	118.47	128.43
8	B	203	PEB	C1C-CHB-C4B	-3.06	121.54	128.22
4	A	101	X2I	C1C-CHB-C4B	3.06	127.54	115.77
8	D	203	PEB	CMB-C2B-C1B	3.03	129.81	125.10
4	G	101	X2I	C1D-ND-C4D	-3.03	108.75	113.42
8	D	203	PEB	CHB-C4B-C3B	-3.01	118.46	125.40
8	F	202	PEB	C1D-ND-C4D	-3.00	108.81	113.42
10	H	202	CYC	CAB-C3B-C4B	2.99	126.00	121.37
8	B	203	PEB	CMB-C2B-C1B	2.99	129.75	125.10
8	F	202	PEB	CMD-C2D-C3D	-2.99	125.71	129.95
4	G	101	X2I	CHB-C4B-C3B	-2.98	124.37	130.07
4	E	101	X2I	CHB-C1C-C2C	-2.97	124.38	130.07
8	B	202	PEB	CHB-C1C-C2C	-2.97	120.83	127.22
4	G	101	X2I	CMA-C2A-C1A	2.96	127.39	121.21
4	A	101	X2I	CHB-C1C-NC	2.95	128.03	122.04
8	H	203	PEB	CHA-C1B-NB	-2.95	118.59	124.95
8	F	203	PEB	C1C-NC-C4C	-2.94	104.36	109.60
7	B	201[B]	AX9	CHB-C1C-NC	2.93	130.76	124.60
8	H	203	PEB	C1C-CHB-C4B	-2.90	121.88	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	202	CYC	CMA-C3A-C4A	2.89	129.58	125.10
8	B	202	PEB	CHA-C1B-C2B	2.88	132.28	124.87
4	E	101	X2I	CHB-C1C-NC	2.88	127.89	122.04
8	H	203	PEB	OA-C1A-C2A	-2.83	123.92	126.17
8	B	203	PEB	CHC-C1D-ND	-2.82	110.27	113.73
8	F	202	PEB	CAC-CBC-CGC	-2.81	106.22	113.67
8	B	203	PEB	O2B-CGB-CBB	2.81	122.87	114.00
10	D	202	CYC	C1B-NB-C4B	-2.80	107.23	110.66
8	F	202	PEB	C2A-C1A-NA	2.79	110.61	108.29
8	F	203	PEB	C3C-C4C-NC	2.77	110.56	108.31
10	H	202	CYC	CBD-CAD-C3D	-2.77	104.87	112.53
4	G	101	X2I	C1C-CHB-C4B	2.74	126.34	115.77
8	D	203	PEB	CHA-C1B-C2B	2.74	131.92	124.87
8	F	203	PEB	CHC-C1D-ND	-2.74	110.37	113.73
8	B	202	PEB	CHC-C4C-NC	2.73	124.75	121.10
4	E	101	X2I	CMA-C2A-C1A	2.72	126.89	121.21
7	F	201	AX9	CHB-C1C-NC	2.71	130.28	124.60
8	B	203	PEB	C1D-CHC-C4C	-2.70	108.77	113.32
4	E	101	X2I	CAA-C3A-C2A	-2.70	122.59	127.56
10	D	202	CYC	CAD-CBD-CGD	-2.69	106.52	113.67
7	F	201	AX9	C2C-C1C-NC	-2.69	106.23	110.04
10	D	202	CYC	O2D-CGD-CBD	2.68	122.45	114.00
10	H	202	CYC	CHB-C4A-NA	-2.67	119.18	124.95
8	H	203	PEB	C1D-ND-C4D	-2.67	109.31	113.42
8	H	203	PEB	C3C-C4C-NC	2.66	110.47	108.31
8	H	203	PEB	CHB-C1C-NC	2.63	131.22	125.29
8	F	203	PEB	OA-C1A-NA	-2.62	121.84	124.93
4	G	101	X2I	CAA-C3A-C2A	-2.62	122.75	127.56
10	D	202	CYC	CMA-C3A-C4A	2.61	129.15	125.10
4	A	101	X2I	CHB-C1C-C2C	-2.57	125.15	130.07
7	B	201[A]	AX9	O1C-CGC-CBC	2.56	122.10	114.00
8	B	202	PEB	CHB-C4B-C3B	-2.55	119.50	125.40
8	F	203	PEB	CHC-C4C-NC	2.54	124.49	121.10
8	F	203	PEB	CAC-C2C-C1C	-2.54	121.75	125.77
8	H	203	PEB	C1C-NC-C4C	-2.53	105.09	109.60
8	F	202	PEB	C3A-C4A-NA	2.52	111.19	107.94
8	B	203	PEB	C1B-CHA-C4A	-2.52	122.13	127.25
8	D	203	PEB	C1C-CHB-C4B	-2.52	122.72	128.22
4	G	101	X2I	CMB-C2B-C1B	2.51	129.27	125.62
8	B	203	PEB	C1C-NC-C4C	-2.51	105.13	109.60
4	G	101	X2I	O1C-CGC-CBC	2.51	121.93	114.00
8	B	202	PEB	C1B-CHA-C4A	-2.51	122.16	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	203	PEB	C3A-C4A-NA	2.49	111.15	107.94
4	C	101	X2I	CHA-C1B-C2B	2.49	133.62	127.53
8	F	202	PEB	CHA-C4A-NA	2.48	128.73	125.63
10	D	202	CYC	CAC-C3C-C4C	2.48	119.03	112.67
8	B	202	PEB	C3A-C4A-NA	2.47	111.13	107.94
8	B	202	PEB	CAB-CBB-CGB	-2.46	107.14	113.67
4	A	101	X2I	CHA-C1B-NB	-2.46	119.74	125.29
4	C	101	X2I	CHB-C4B-NB	2.45	127.02	122.04
4	E	101	X2I	CHB-C4B-NB	2.44	127.00	122.04
7	D	201	AX9	CAA-C3A-C4A	2.43	127.55	124.39
4	C	101	X2I	C4C-NC-C1C	-2.41	108.39	110.53
7	F	201	AX9	O2B-CGB-CBB	2.41	121.61	114.00
8	F	202	PEB	CAA-C3A-C4A	-2.41	106.50	112.67
8	F	202	PEB	CHC-C4C-NC	2.40	124.32	121.10
8	F	203	PEB	C2C-C1C-NC	2.40	110.58	107.57
8	D	203	PEB	C1D-ND-C4D	-2.40	109.73	113.42
8	F	202	PEB	C2C-C1C-NC	2.38	110.56	107.57
8	B	203	PEB	CBB-CAB-C3B	-2.38	105.95	112.53
8	B	203	PEB	CHA-C1B-C2B	2.37	130.97	124.87
10	D	202	CYC	C3B-C4B-NB	2.37	108.66	106.77
8	F	203	PEB	C1D-ND-C4D	-2.37	109.78	113.42
8	B	203	PEB	O1B-CGB-CBB	-2.36	115.59	123.09
7	B	201[A]	AX9	CAD-C3D-C4D	2.36	125.02	121.37
8	H	203	PEB	CAC-C2C-C1C	-2.36	122.03	125.77
8	F	202	PEB	OD-C4D-ND	-2.35	122.78	126.02
4	A	101	X2I	CAC-CBC-CGC	-2.35	107.43	113.67
8	D	203	PEB	CHC-C1D-ND	-2.35	110.85	113.73
4	E	101	X2I	C4C-NC-C1C	-2.34	108.45	110.53
4	A	101	X2I	CHB-C4B-NB	2.34	126.80	122.04
8	B	203	PEB	CHB-C1C-NC	2.34	130.58	125.29
8	D	203	PEB	CBC-CAC-C2C	-2.33	106.08	112.53
8	B	202	PEB	CHB-C4B-NB	2.33	129.49	124.60
7	H	201	AX9	OD-C4D-C3D	-2.33	125.58	128.03
8	B	202	PEB	C1D-ND-C4D	-2.33	109.84	113.42
4	C	101	X2I	CAA-C3A-C4A	2.30	127.38	124.39
7	B	201[A]	AX9	O2B-CGB-CBB	2.30	121.25	114.00
4	E	101	X2I	CAC-CBC-CGC	-2.28	107.61	113.67
4	A	101	X2I	CHB-C4B-C3B	-2.28	125.71	130.07
4	E	101	X2I	C1C-CHB-C4B	2.28	124.54	115.77
8	H	203	PEB	C2C-C1C-NC	2.27	110.42	107.57
7	D	201	AX9	O1C-CGC-CBC	2.27	121.17	114.00
10	H	202	CYC	CAC-C3C-C4C	2.27	118.50	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	203	PEB	CHB-C4B-NB	2.26	129.35	124.60
10	D	202	CYC	CHD-C1D-ND	-2.26	120.19	125.29
8	F	202	PEB	CBC-CAC-C2C	-2.26	106.29	112.53
4	A	101	X2I	CHC-C4C-NC	2.26	124.12	121.10
8	F	202	PEB	CHA-C1B-C2B	2.26	130.67	124.87
7	B	201[B]	AX9	O1C-CGC-CBC	2.24	121.09	114.00
8	D	203	PEB	CBD-CAD-C3D	-2.24	116.35	127.53
10	D	202	CYC	O2D-CGD-O1D	-2.23	117.59	123.33
8	F	202	PEB	C1C-NC-C4C	-2.23	105.63	109.60
4	E	101	X2I	CHB-C4B-C3B	-2.23	125.81	130.07
4	A	101	X2I	CMB-C2B-C1B	2.23	128.86	125.62
8	H	203	PEB	CHC-C4C-NC	2.22	124.07	121.10
8	B	202	PEB	CBC-CAC-C2C	-2.22	106.39	112.53
8	F	202	PEB	CAB-CBB-CGB	-2.21	107.79	113.67
7	D	201	AX9	C1D-ND-C4D	-2.21	110.02	113.42
7	D	201	AX9	C4A-NA-C1A	-2.21	107.95	110.66
10	H	202	CYC	O2D-CGD-CBD	2.19	120.93	114.00
8	D	203	PEB	C1C-NC-C4C	-2.19	105.70	109.60
7	B	201[A]	AX9	CHB-C1C-NC	2.18	129.17	124.60
8	B	203	PEB	OD-C4D-ND	-2.17	123.03	126.02
7	F	201	AX9	CBB-CAB-C3B	-2.16	106.57	112.53
8	D	203	PEB	C2C-C1C-NC	2.15	110.27	107.57
4	C	101	X2I	CMA-C2A-C1A	2.15	125.71	121.21
8	B	203	PEB	C2A-C1A-NA	2.15	110.07	108.29
4	A	101	X2I	CHA-C1B-C2B	2.15	132.79	127.53
7	H	201	AX9	C4A-NA-C1A	-2.14	108.03	110.66
8	D	203	PEB	CHB-C1C-NC	2.14	130.12	125.29
7	H	201	AX9	CHB-C1C-NC	2.14	129.09	124.60
7	B	201[B]	AX9	CMB-C2B-C1B	2.14	128.72	125.62
10	H	202	CYC	CHD-C1D-ND	-2.13	120.48	125.29
4	C	101	X2I	CHB-C4B-C3B	-2.13	126.00	130.07
10	H	202	CYC	C1B-NB-C4B	-2.12	108.06	110.66
8	F	202	PEB	C1B-CHA-C4A	-2.12	122.96	127.25
4	E	101	X2I	CAD-C3D-C2D	-2.11	121.56	128.43
8	B	203	PEB	CMD-C2D-C3D	-2.11	126.96	129.95
4	G	101	X2I	CHA-C1B-NB	-2.10	120.55	125.29
4	G	101	X2I	CHA-C1B-C2B	2.09	132.65	127.53
8	F	202	PEB	C2A-C3A-C4A	2.09	104.47	101.34
7	B	201[B]	AX9	CAD-C3D-C4D	2.09	124.60	121.37
8	B	203	PEB	O2C-CGC-CBC	2.08	120.58	114.00
8	H	203	PEB	CHA-C1B-C2B	2.08	130.22	124.87
8	B	202	PEB	C2A-C1A-NA	2.08	110.02	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	203	PEB	O2B-CGB-CBB	2.08	120.57	114.00
7	B	201[A]	AX9	C1D-ND-C4D	-2.08	110.23	113.42
7	D	201	AX9	CHA-C1B-NB	-2.07	120.60	125.29
7	D	201	AX9	O1C-CGC-O2C	-2.07	118.01	123.33
7	B	201[A]	AX9	O1C-CGC-O2C	-2.07	118.02	123.33
7	D	201	AX9	C4A-C3A-C2A	-2.07	105.88	107.84
4	E	101	X2I	O1C-CGC-CBC	2.07	120.53	114.00
4	A	101	X2I	CMC-C3C-C4C	-2.06	124.76	126.97
4	E	101	X2I	CHC-C1D-ND	-2.05	111.21	113.73
8	H	203	PEB	CAB-CBB-CGB	-2.05	108.23	113.67
4	G	101	X2I	C4A-NA-C1A	-2.04	108.16	110.66
10	H	202	CYC	C3B-C4B-NB	2.03	108.39	106.77
10	D	202	CYC	C1C-NC-C4C	-2.03	110.86	113.41
8	F	203	PEB	CMD-C2D-C3D	-2.02	127.08	129.95
8	D	203	PEB	CAC-CBC-CGC	-2.02	108.30	113.67
10	H	202	CYC	CBC-CAC-C3C	-2.02	109.12	113.41
7	B	201[B]	AX9	C1D-ND-C4D	-2.02	110.31	113.42
10	D	202	CYC	O2A-CGA-O1A	-2.02	118.14	123.33
4	E	101	X2I	C1D-ND-C4D	-2.01	110.32	113.42

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	202	PEB	NB-C1B-CHA-C4A
8	B	202	PEB	C2B-C1B-CHA-C4A
8	B	203	PEB	NB-C1B-CHA-C4A
8	B	203	PEB	C2B-C1B-CHA-C4A
8	D	203	PEB	NA-C4A-CHA-C1B
8	D	203	PEB	NB-C1B-CHA-C4A
8	D	203	PEB	C2B-C1B-CHA-C4A
8	F	202	PEB	NB-C1B-CHA-C4A
8	F	203	PEB	NA-C4A-CHA-C1B
8	F	203	PEB	NB-C1B-CHA-C4A
8	H	203	PEB	NB-C1B-CHA-C4A
10	D	202	CYC	C3A-C4A-CHB-C1B
10	H	202	CYC	C3A-C4A-CHB-C1B
7	B	201[A]	AX9	NB-C1B-CHA-C4A
7	B	201[B]	AX9	NB-C1B-CHA-C4A
7	D	201	AX9	NB-C1B-CHA-C4A
7	F	201	AX9	NB-C1B-CHA-C4A
7	H	201	AX9	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
10	D	202	CYC	ND-C1D-CHD-C4C
10	H	202	CYC	ND-C1D-CHD-C4C
7	B	201[A]	AX9	C2B-C1B-CHA-C4A
7	B	201[B]	AX9	C2B-C1B-CHA-C4A
7	D	201	AX9	C2B-C1B-CHA-C4A
7	F	201	AX9	C2B-C1B-CHA-C4A
7	H	201	AX9	C2B-C1B-CHA-C4A
10	H	202	CYC	C2D-C1D-CHD-C4C
8	F	203	PEB	C2B-C1B-CHA-C4A
8	H	203	PEB	C2B-C1B-CHA-C4A
4	A	101	X2I	NB-C1B-CHA-C4A
4	E	101	X2I	NB-C1B-CHA-C4A
4	G	101	X2I	NB-C1B-CHA-C4A
4	A	101	X2I	C2B-C1B-CHA-C4A
4	C	101	X2I	C2B-C1B-CHA-C4A
4	E	101	X2I	C2B-C1B-CHA-C4A
4	G	101	X2I	C2B-C1B-CHA-C4A
10	D	202	CYC	C2D-C1D-CHD-C4C
4	C	101	X2I	NB-C1B-CHA-C4A
4	A	101	X2I	C2A-C3A-CAA-CBA
4	G	101	X2I	C2A-C3A-CAA-CBA
4	E	101	X2I	C2A-C3A-CAA-CBA
5	A	102	PG4	O4-C7-C8-O5
10	D	202	CYC	NA-C4A-CHB-C1B
10	H	202	CYC	NA-C4A-CHB-C1B
10	H	202	CYC	NB-C1B-CHB-C4A
8	F	202	PEB	C2B-C1B-CHA-C4A
5	A	102	PG4	O3-C5-C6-O4
4	G	101	X2I	C4A-C3A-CAA-CBA
7	B	201[B]	AX9	C2D-C3D-CAD-CBD
4	A	101	X2I	C4A-C3A-CAA-CBA
4	E	101	X2I	C3B-CAB-CBB-CGB
7	B	201[B]	AX9	C2C-CAC-CBC-CGC
7	B	201[A]	AX9	C2D-C3D-CAD-CBD
8	D	203	PEB	C4A-C3A-CAA-CBA
5	A	102	PG4	C5-C6-O4-C7
10	H	202	CYC	C2B-C1B-CHB-C4A
5	H	204	PG4	O1-C1-C2-O2
4	E	101	X2I	C4A-C3A-CAA-CBA
8	H	203	PEB	CAC-CBC-CGC-O2C
8	F	203	PEB	CAC-CBC-CGC-O1C
10	D	202	CYC	CAD-CBD-CGD-O1D

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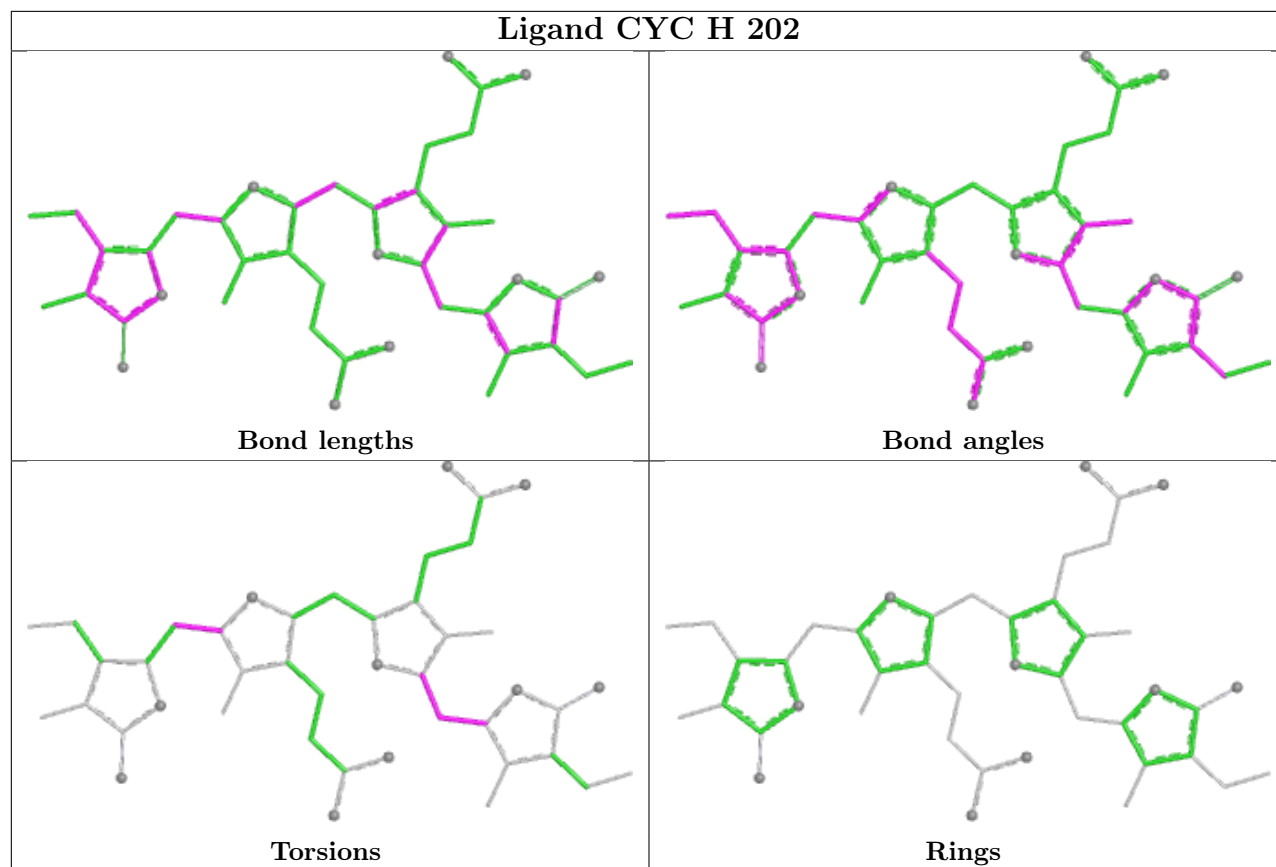
Mol	Chain	Res	Type	Atoms
4	G	101	X2I	CAB-CBB-CGB-O1B
8	F	203	PEB	CAC-CBC-CGC-O2C
8	H	203	PEB	CAC-CBC-CGC-O1C
7	B	201[A]	AX9	CAC-CBC-CGC-O2C
8	B	203	PEB	CAC-CBC-CGC-O1C
4	A	101	X2I	CAC-CBC-CGC-O2C
8	D	203	PEB	CAC-CBC-CGC-O2C
4	C	101	X2I	CAB-CBB-CGB-O2B
8	D	203	PEB	CAC-CBC-CGC-O1C
7	D	201	AX9	C2D-C3D-CAD-CBD
4	G	101	X2I	CAB-CBB-CGB-O2B
7	B	201[A]	AX9	CAB-CBB-CGB-O2B
10	D	202	CYC	CAD-CBD-CGD-O2D
8	B	203	PEB	CAC-CBC-CGC-O2C
4	A	101	X2I	CAC-CBC-CGC-O1C
4	C	101	X2I	CAB-CBB-CGB-O1B
7	B	201[A]	AX9	CAB-CBB-CGB-O1B
7	B	201[A]	AX9	CAC-CBC-CGC-O1C
7	F	201	AX9	CAC-CBC-CGC-O1C
8	F	202	PEB	CAC-CBC-CGC-O2C
8	H	203	PEB	C4A-C3A-CAA-CBA
7	D	201	AX9	CAC-CBC-CGC-O1C
7	H	201	AX9	CAC-CBC-CGC-O1C
8	B	202	PEB	CAC-CBC-CGC-O2C
10	D	202	CYC	CAA-CBA-CGA-O2A
8	F	202	PEB	CAB-CBB-CGB-O1B
4	C	101	X2I	CAC-CBC-CGC-O1C
4	C	101	X2I	CAC-CBC-CGC-O2C
7	D	201	AX9	CAC-CBC-CGC-O2C
8	F	202	PEB	CAC-CBC-CGC-O1C
8	B	202	PEB	CAC-CBC-CGC-O1C
7	H	201	AX9	CAC-CBC-CGC-O2C
7	F	201	AX9	CAC-CBC-CGC-O2C
4	E	101	X2I	CAC-CBC-CGC-O1C
10	D	202	CYC	CAA-CBA-CGA-O1A
4	E	101	X2I	CAC-CBC-CGC-O2C
4	A	101	X2I	C3B-CAB-CBB-CGB
4	C	101	X2I	C2A-C3A-CAA-CBA
5	A	102	PG4	C4-C3-O2-C2
8	H	203	PEB	CAB-CBB-CGB-O1B
8	F	202	PEB	CAB-CBB-CGB-O2B
8	H	203	PEB	CAB-CBB-CGB-O2B

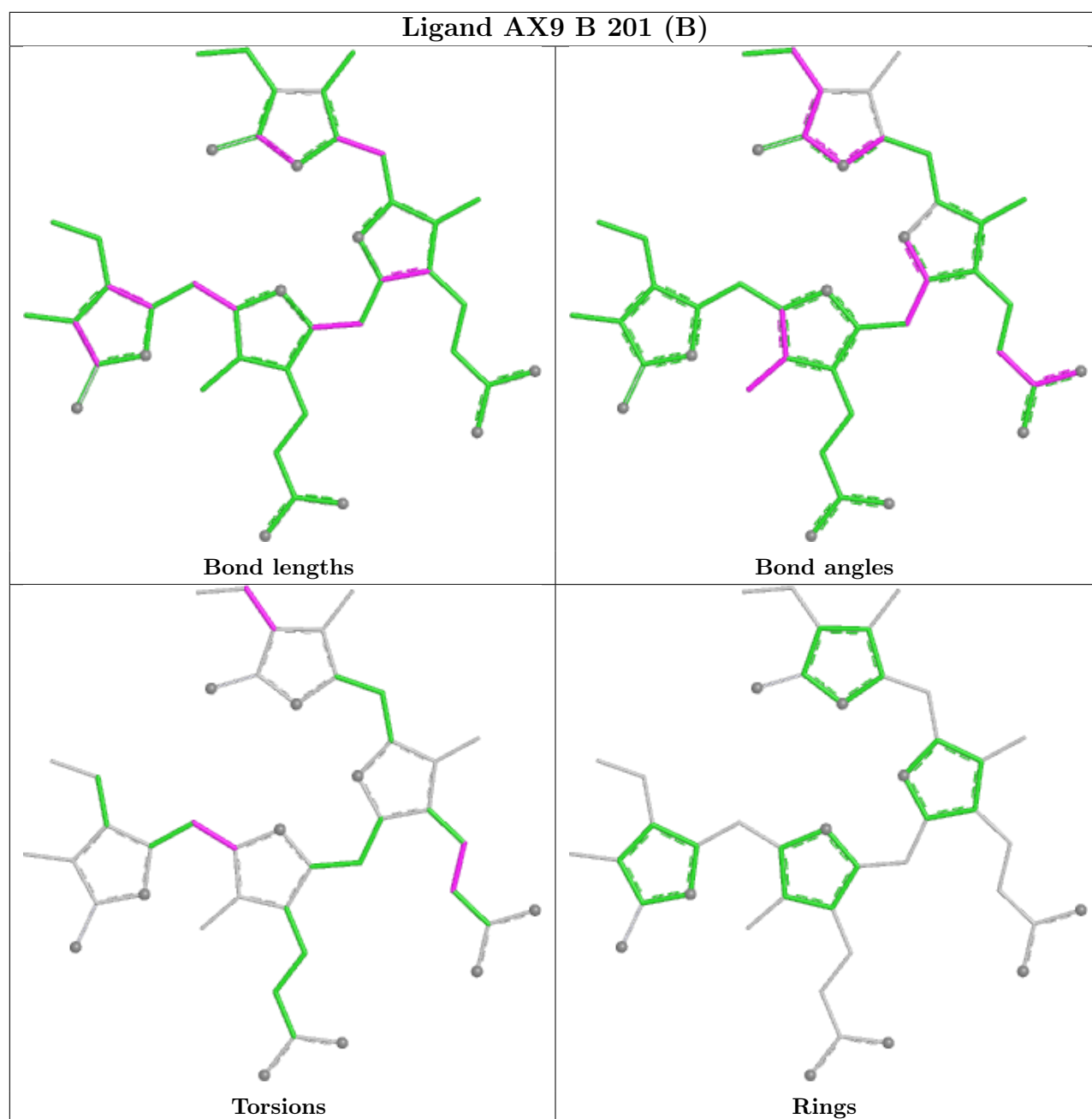
There are no ring outliers.

7 monomers are involved in 9 short contacts:

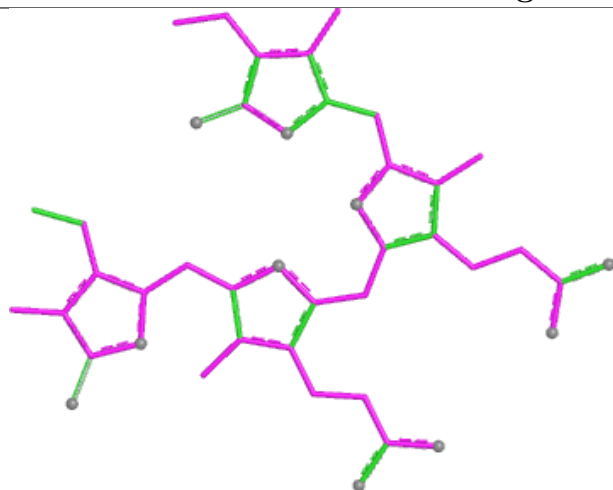
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	203	PEB	2	0
8	H	203	PEB	1	0
5	A	102	PG4	1	0
8	B	202	PEB	1	0
10	D	202	CYC	1	0
8	B	203	PEB	2	0
8	F	202	PEB	1	0

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 than 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.

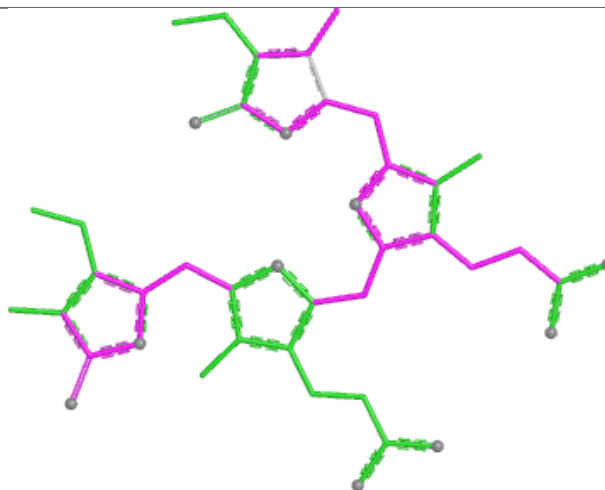




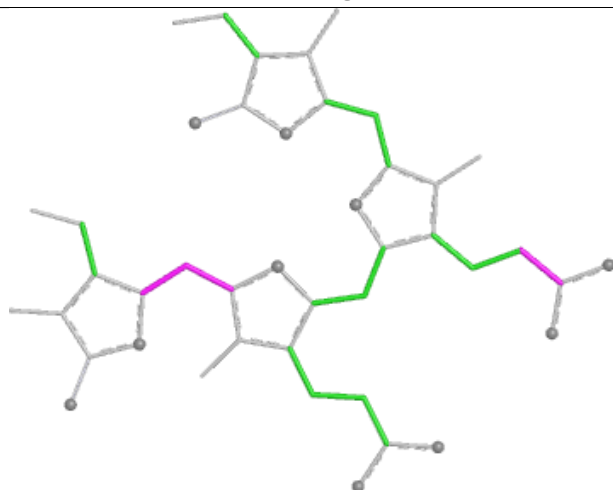
Ligand PEB F 203



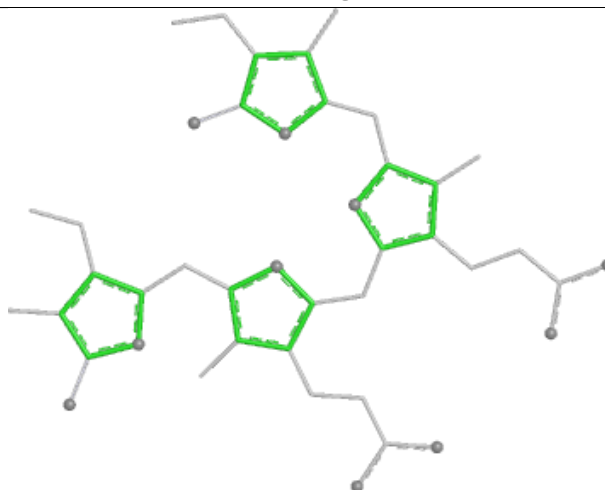
Bond lengths



Bond angles

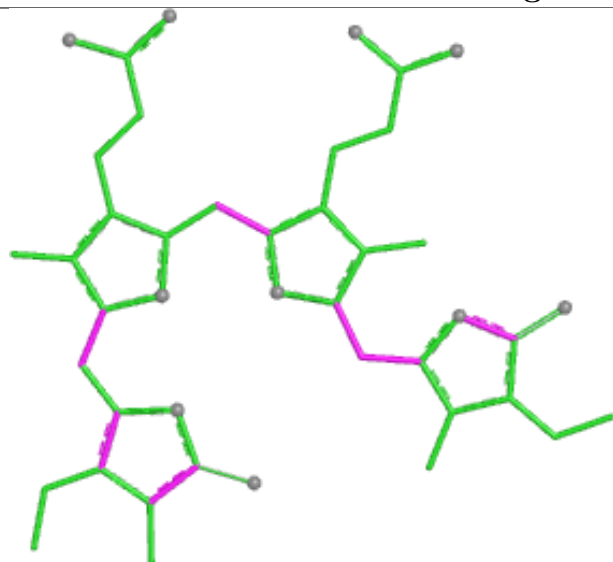


Torsions

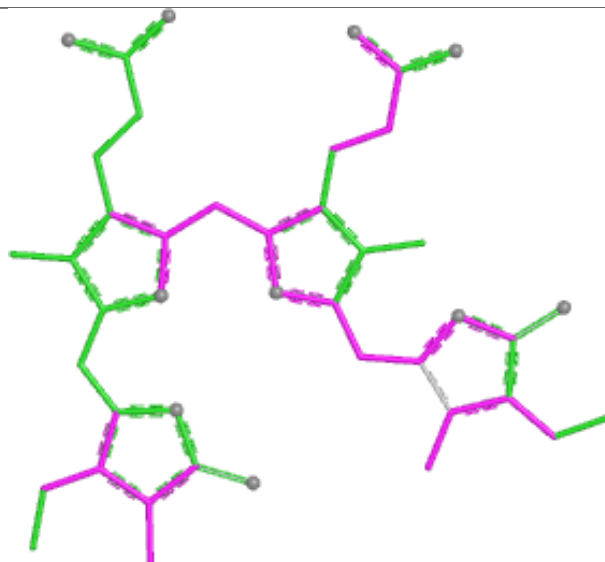


Rings

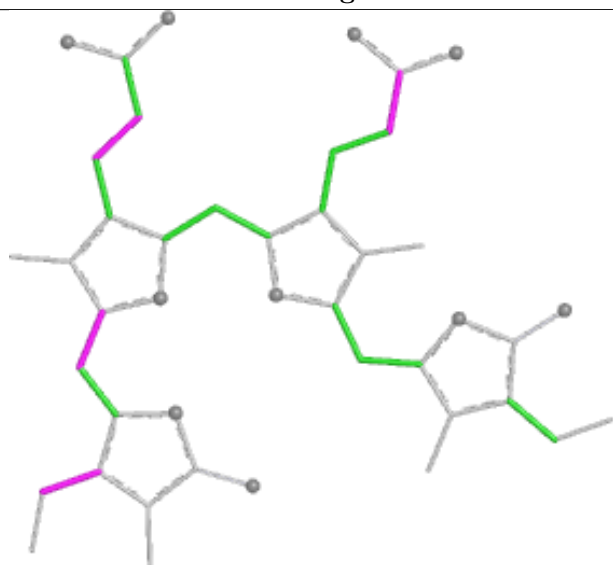
Ligand X2I E 101



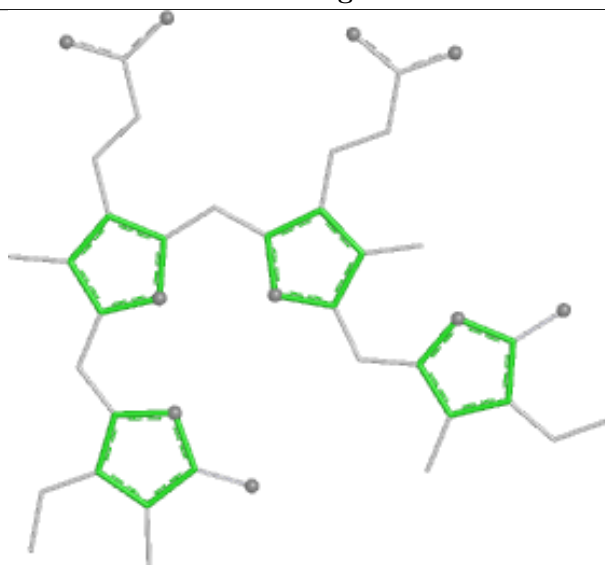
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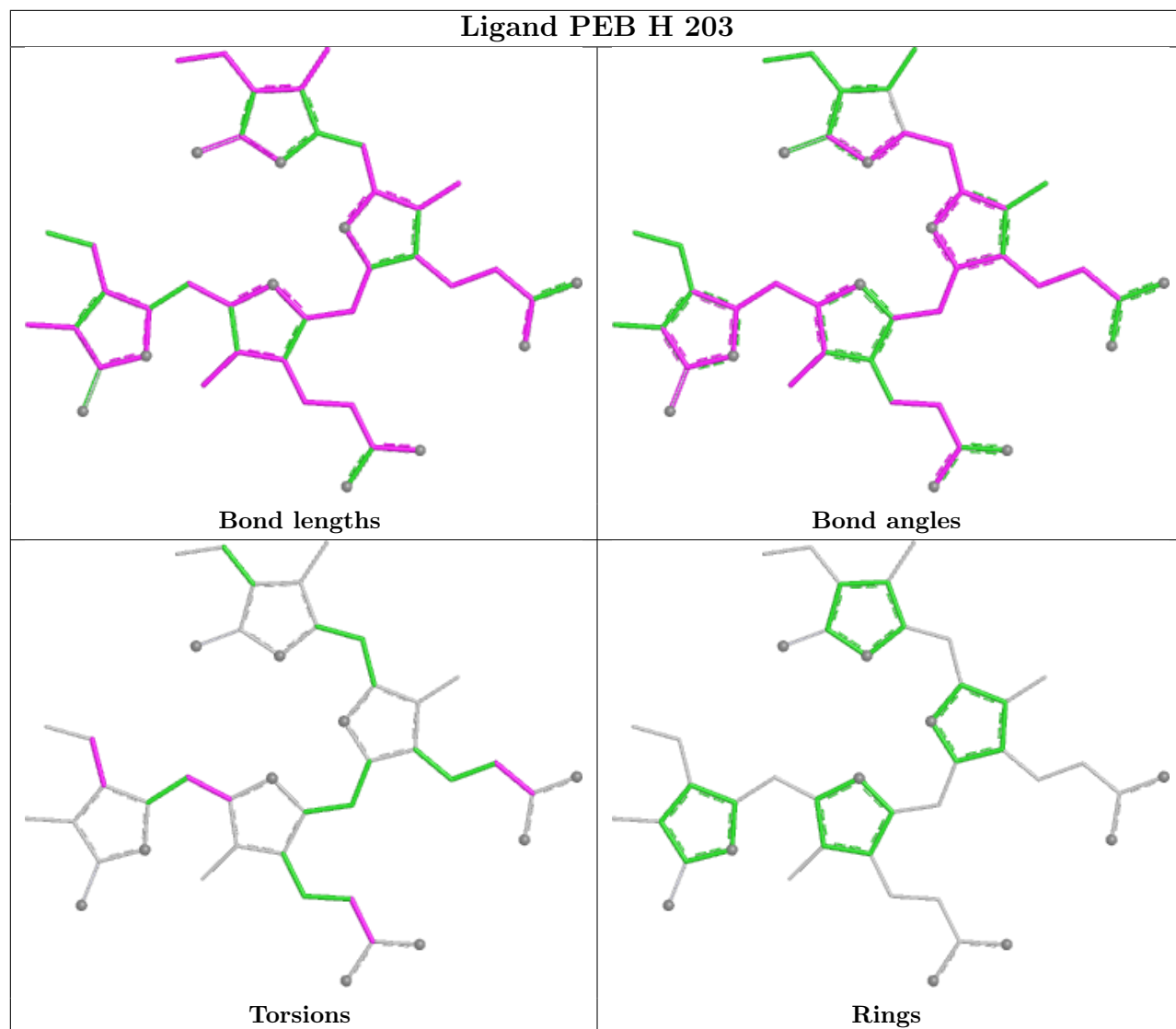
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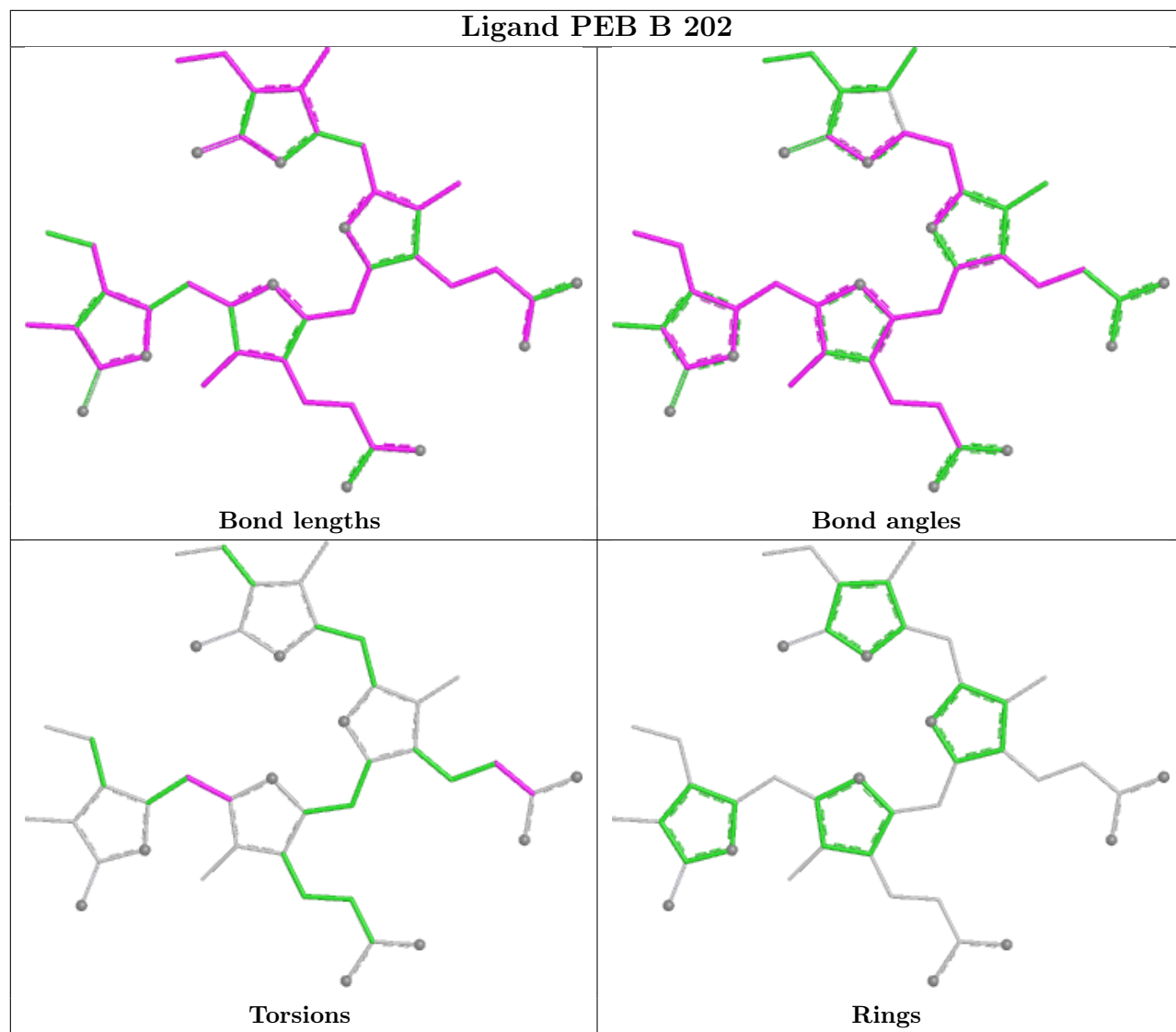


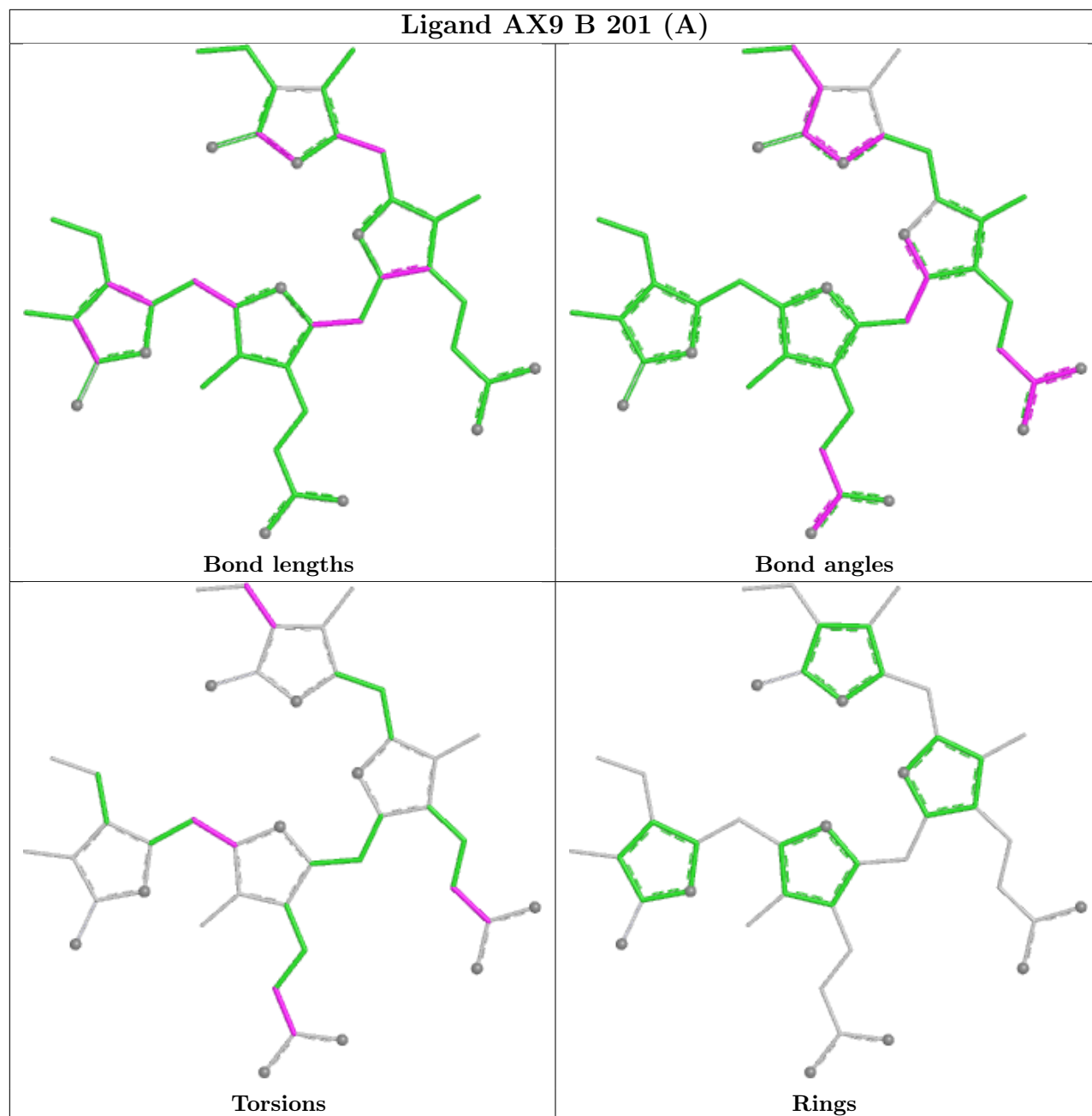
Torsions

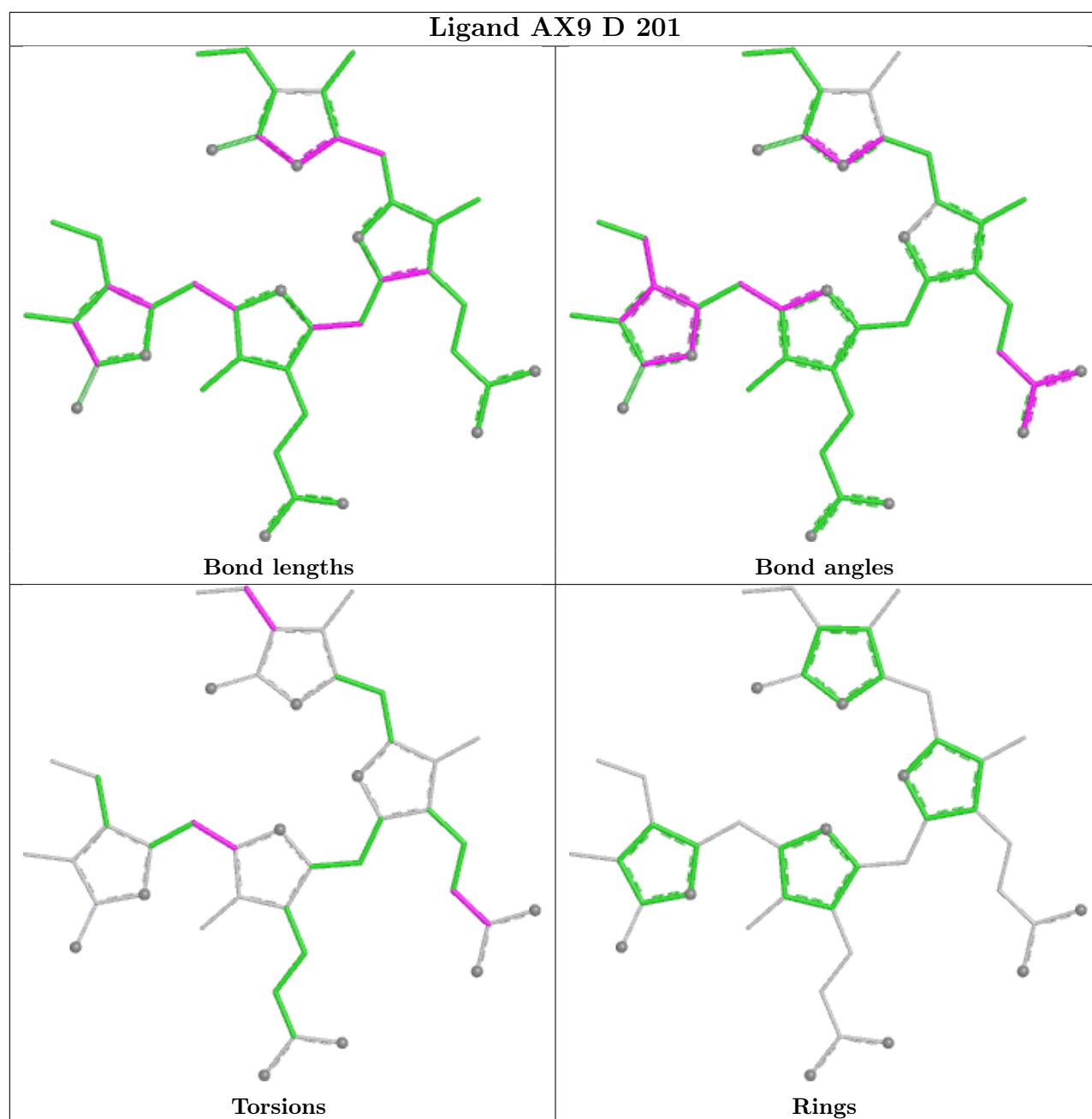


Rings

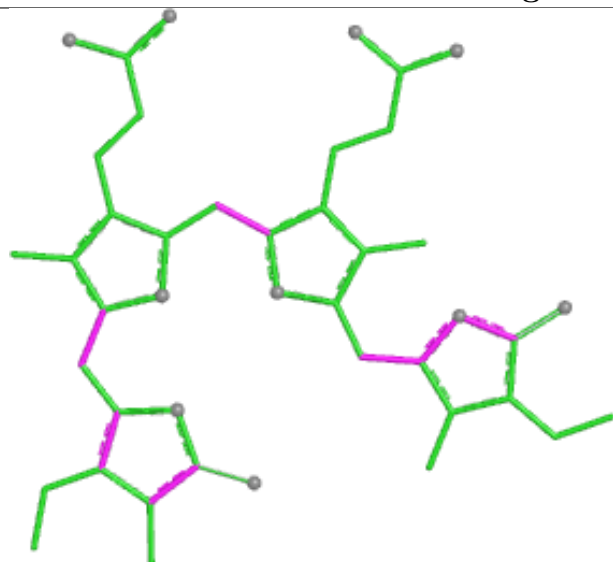




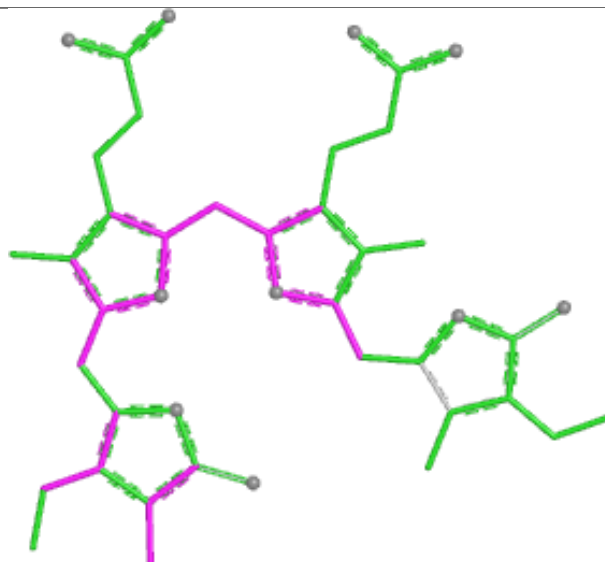




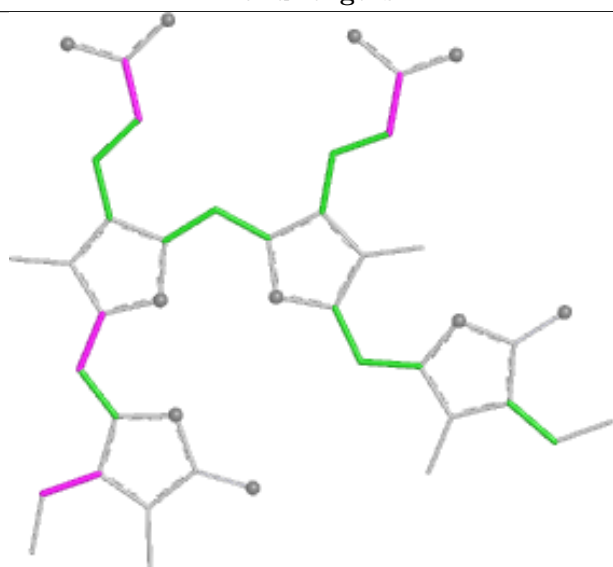
Ligand X2I C 101



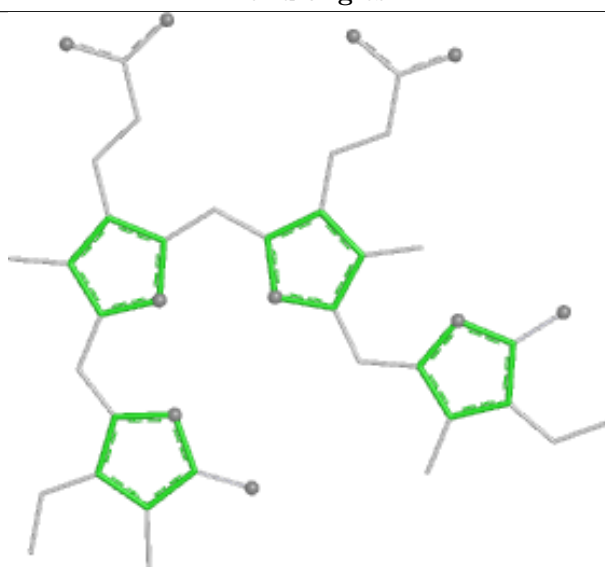
Bond lengths



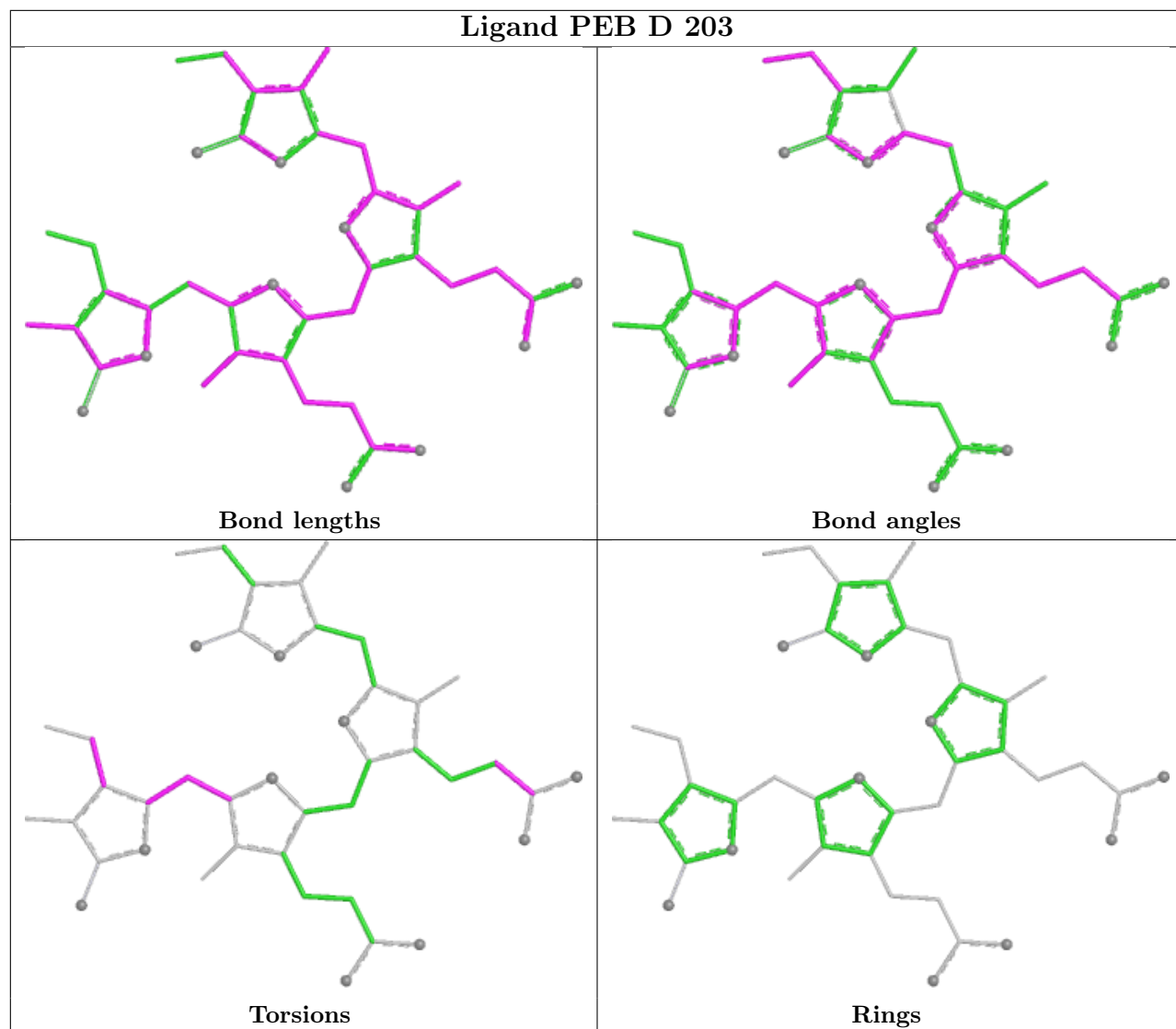
Bond angles



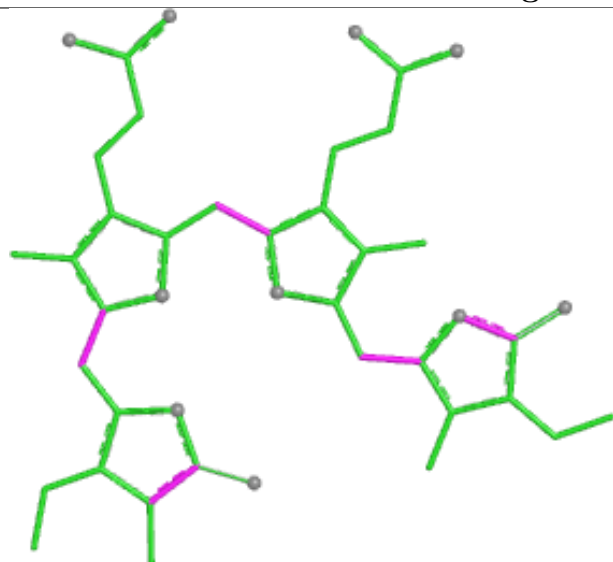
Torsions



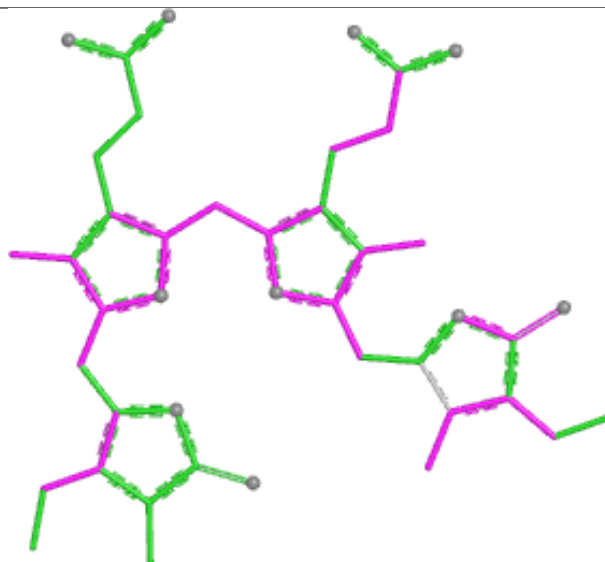
Rings



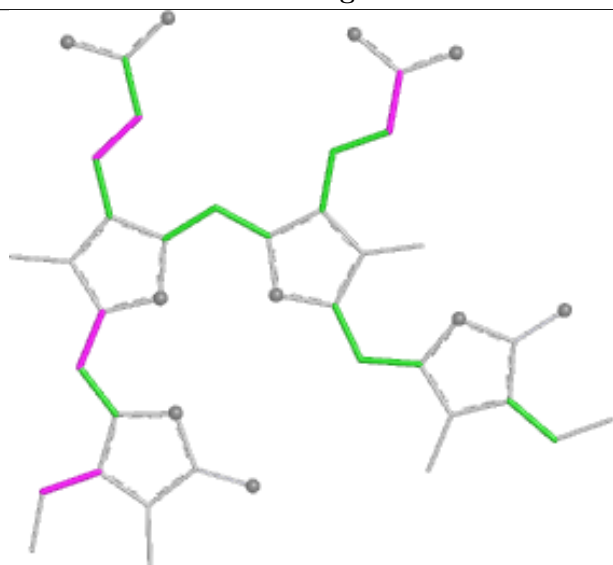
Ligand X2I A 101



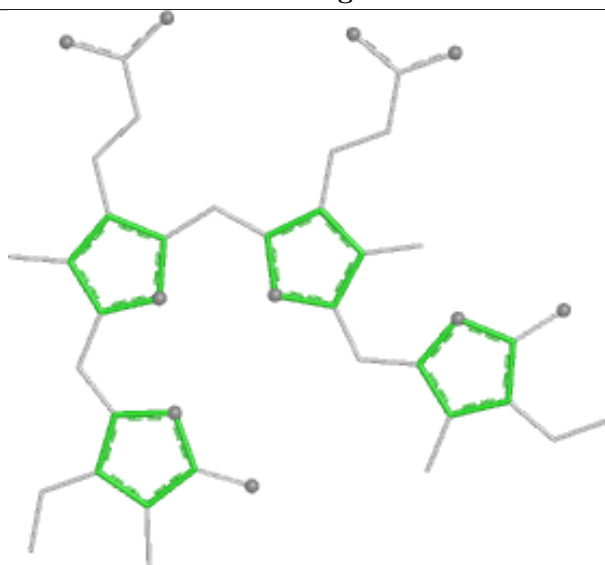
Bond lengths



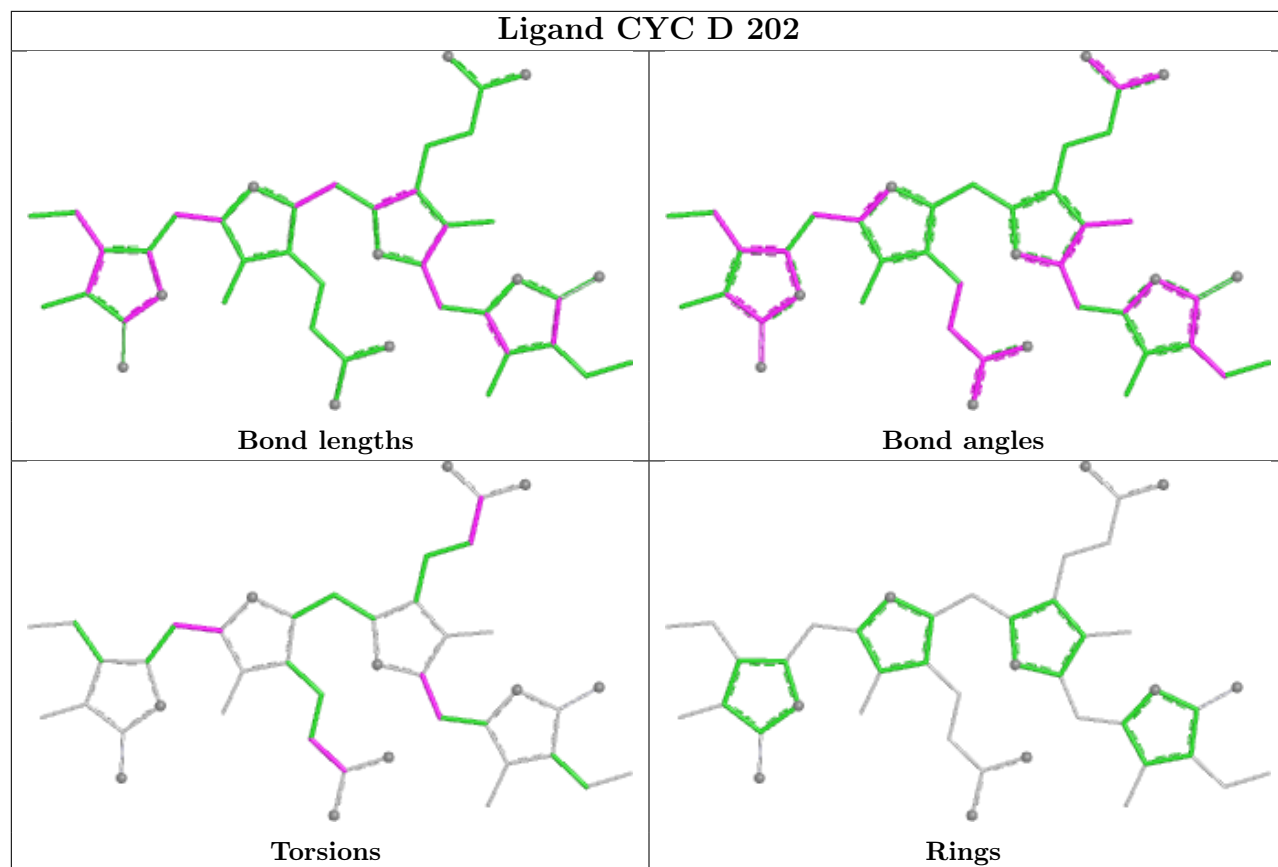
Bond angles

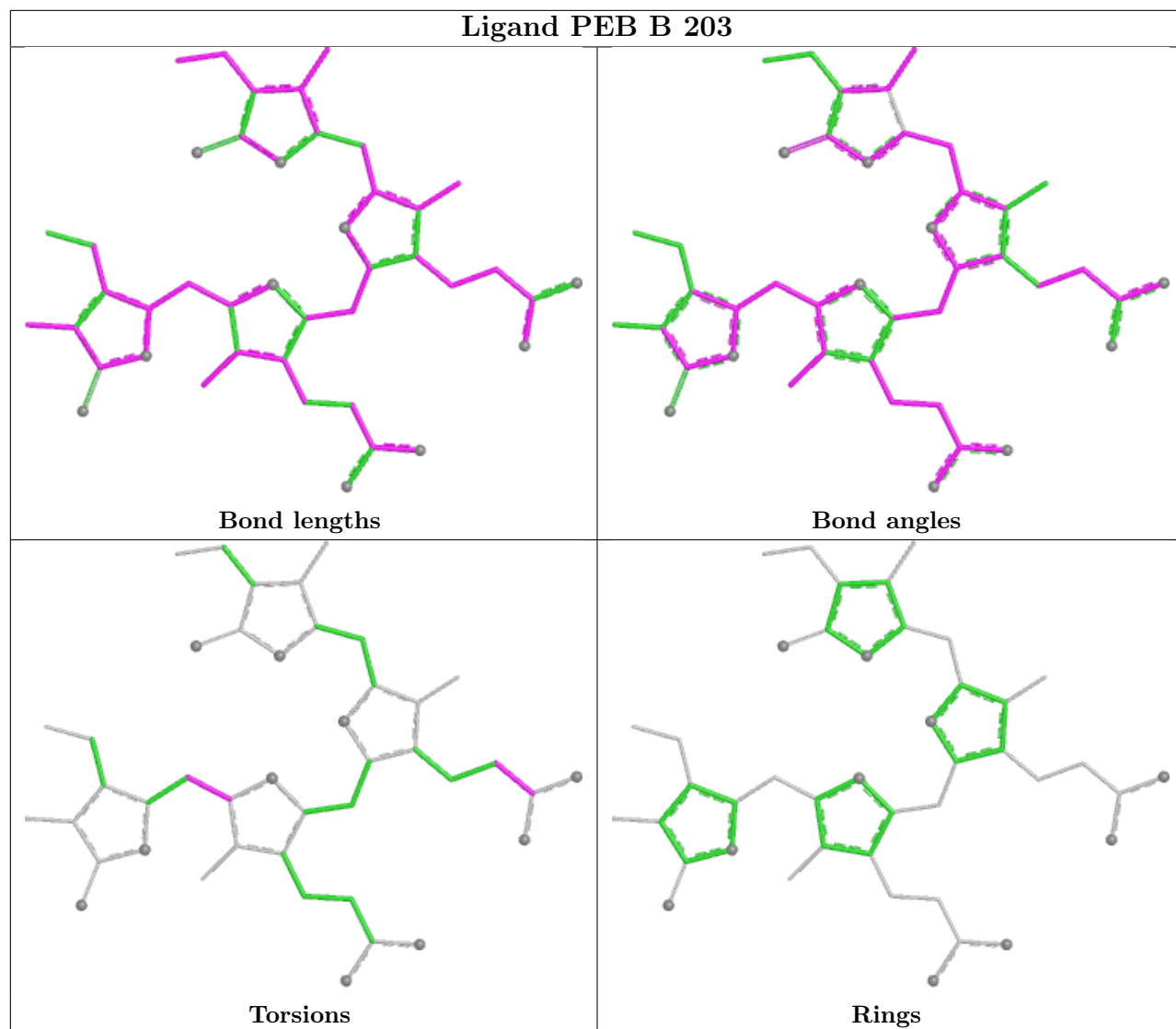


Torsions

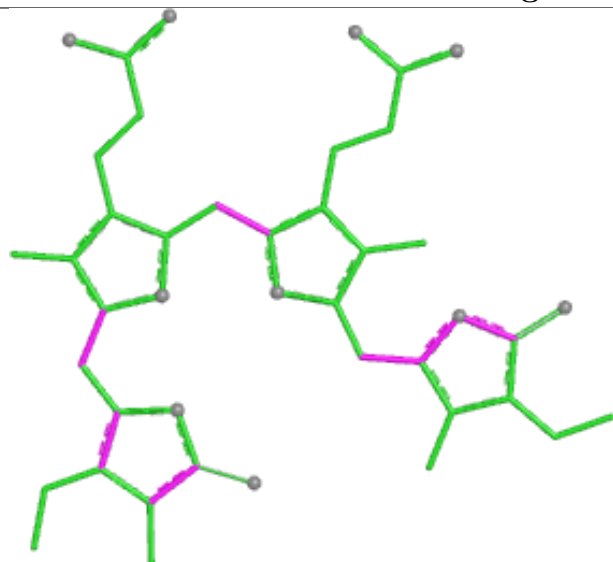


Rings

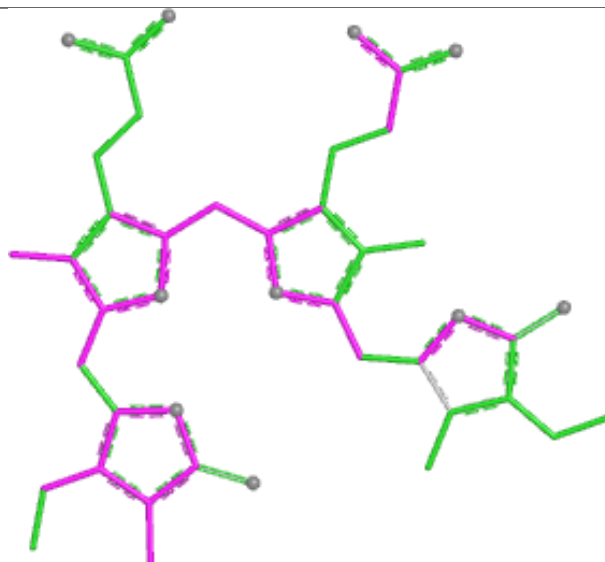




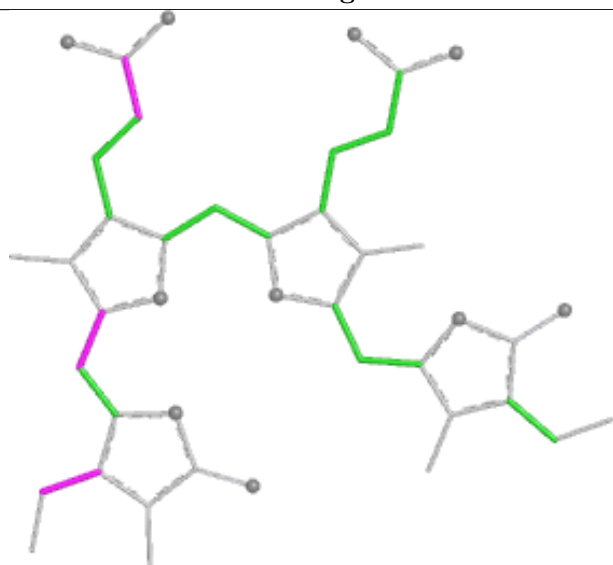
Ligand X2I G 101



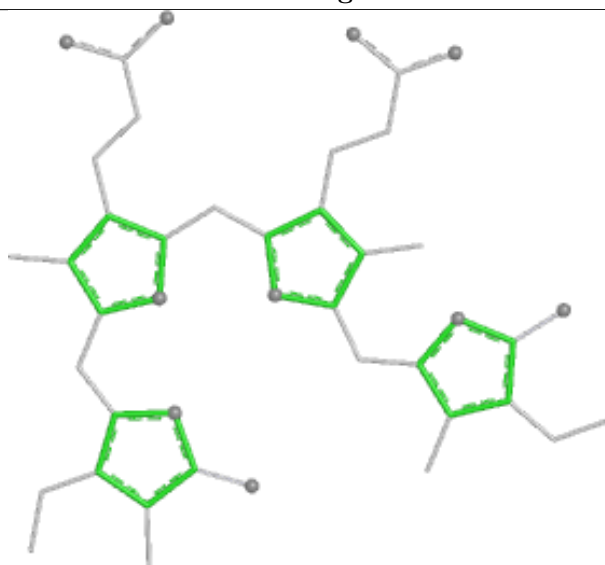
Bond lengths



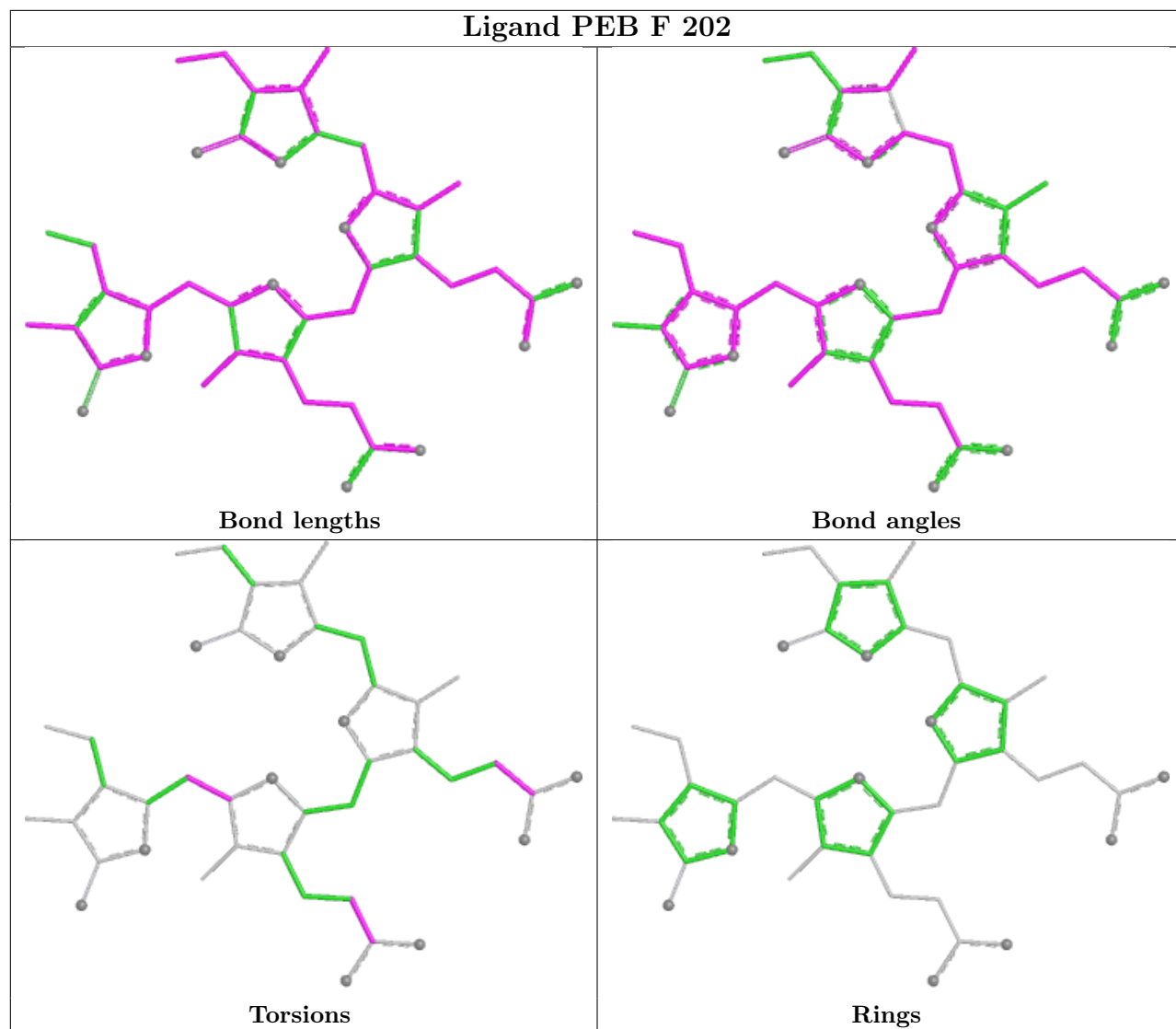
Bond angles

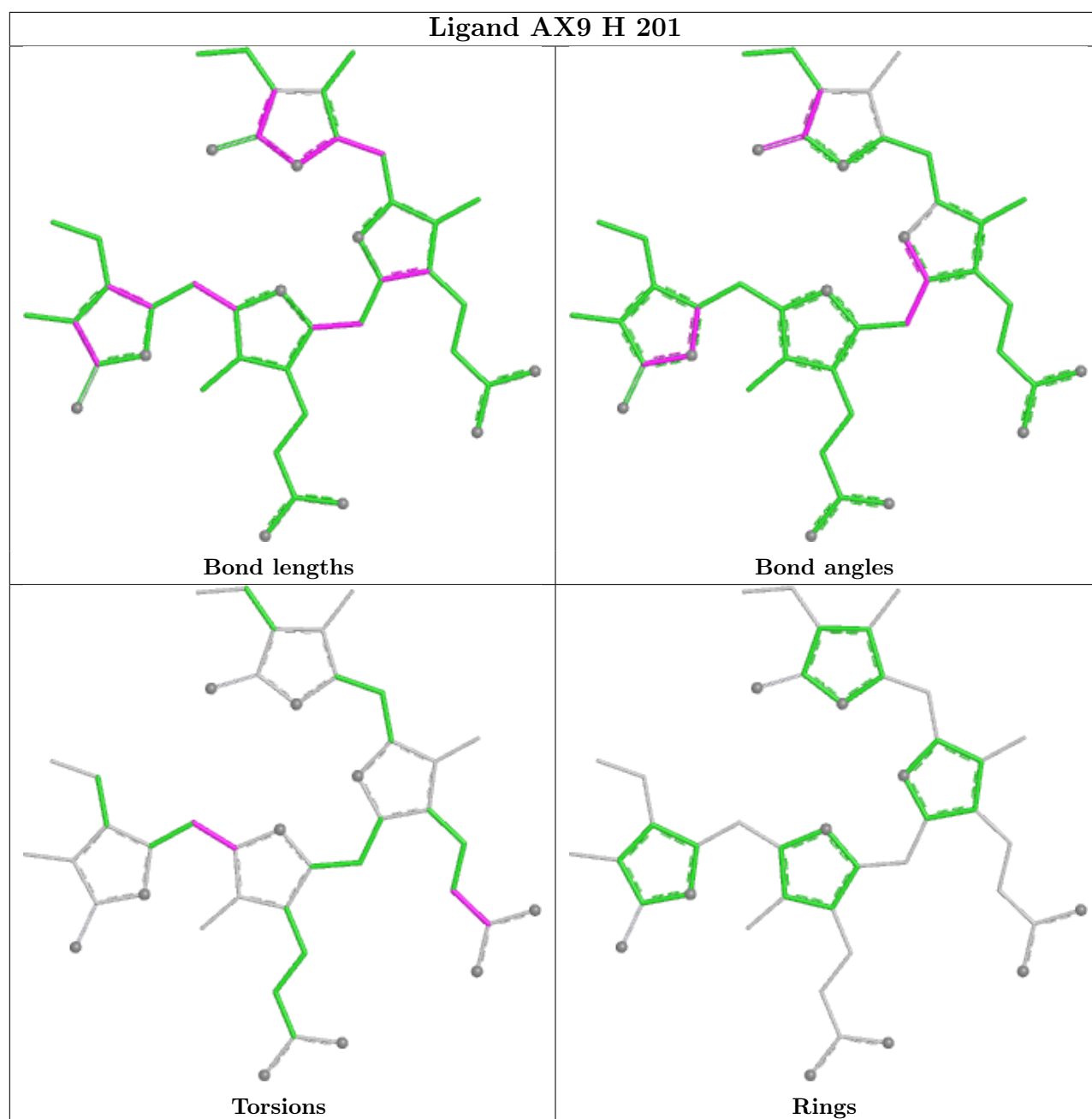


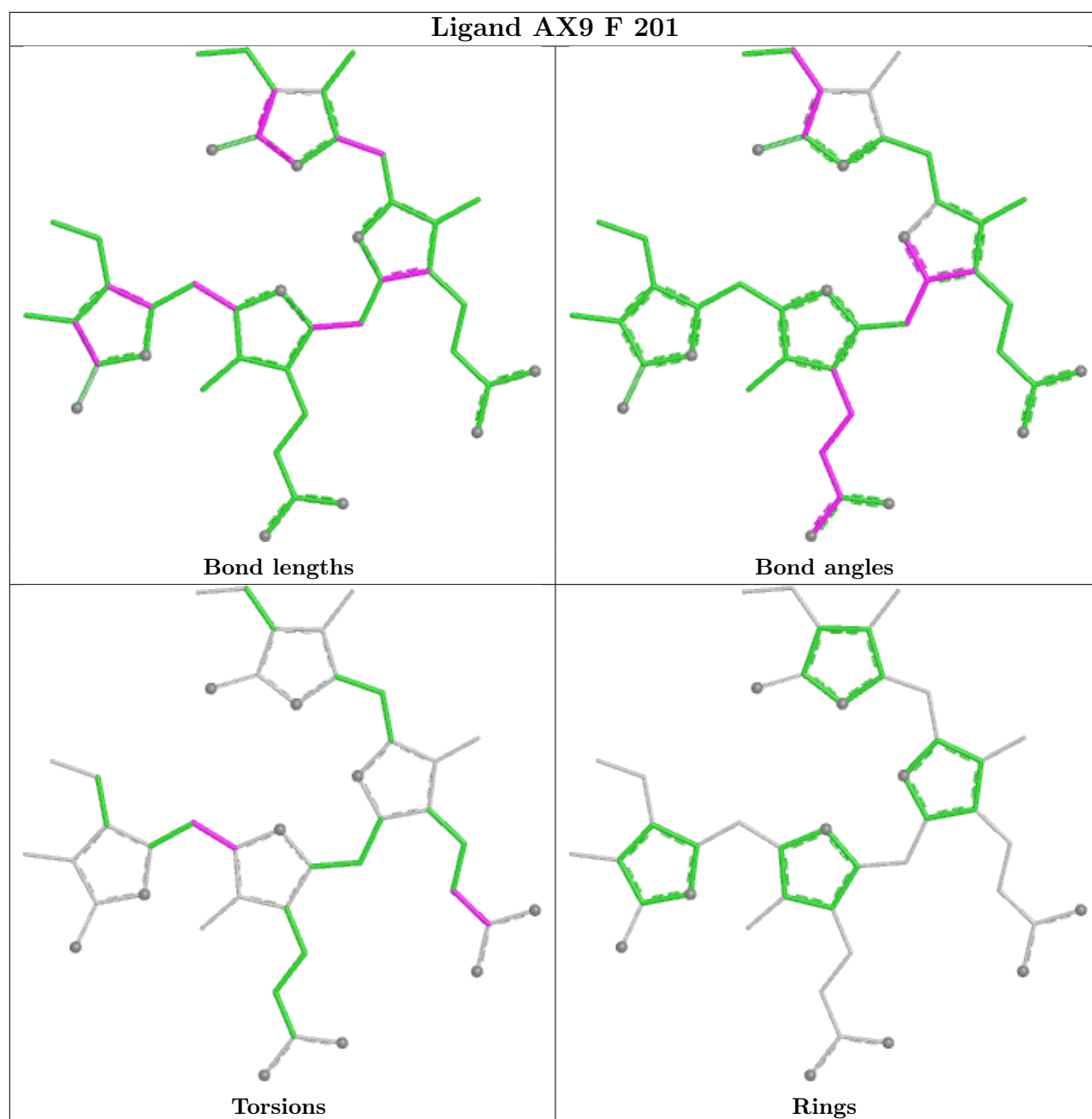
Torsions



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 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, 95th 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	78/80 (97%)	-0.52	0 100 100	9, 21, 37, 78	9 (11%)
1	E	78/80 (97%)	-0.21	1 (1%) 75 78	12, 29, 55, 65	3 (3%)
2	B	174/177 (98%)	-0.37	2 (1%) 78 81	9, 23, 47, 79	14 (8%)
2	D	161/177 (90%)	-0.62	0 100 100	10, 21, 38, 55	3 (1%)
2	F	176/177 (99%)	-0.15	3 (1%) 69 72	11, 31, 48, 78	5 (2%)
2	H	161/177 (90%)	-0.17	2 (1%) 76 80	12, 31, 53, 65	4 (2%)
3	C	63/68 (92%)	-0.51	2 (3%) 50 54	16, 22, 43, 75	2 (3%)
3	G	63/68 (92%)	0.00	3 (4%) 35 39	13, 30, 57, 74	4 (6%)
All	All	954/1004 (95%)	-0.32	13 (1%) 73 77	9, 27, 49, 79	44 (4%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	45[A]	TYR	5.3
3	C	45[A]	TYR	3.9
2	F	176	LEU	3.1
2	F	1	MET	3.0
2	B	3	ASP	2.6
1	E	79	ILE	2.3
3	G	6	LEU	2.3
3	C	47	LYS	2.3
2	H	111	ASN	2.2
2	F	101	ASP	2.2
3	G	47	LYS	2.2
2	H	176	LEU	2.1
2	B	12	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

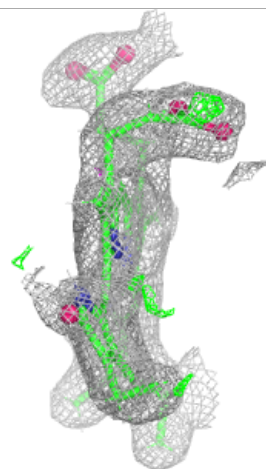
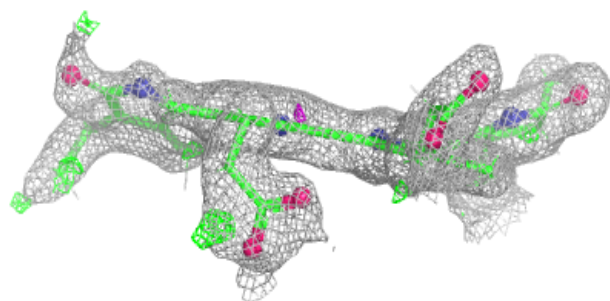
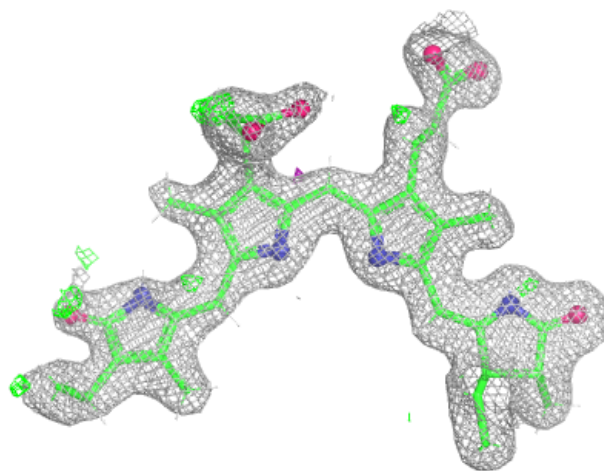
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PG4	A	102	13/13	0.87	0.14	33,51,70,72	0
5	PG4	H	204	13/13	0.91	0.11	34,47,63,75	0
10	CYC	H	202	43/43	0.93	0.11	22,38,83,100	4
8	PEB	B	202	43/43	0.94	0.09	16,24,34,40	4
8	PEB	F	202	43/43	0.94	0.09	22,32,45,50	4
8	PEB	F	203	43/43	0.94	0.10	19,30,54,67	4
4	X2I	G	101	43/43	0.94	0.09	22,30,41,80	4
7	AX9	B	201[A]	43/43	0.95	0.07	9,19,31,35	79
7	AX9	B	201[B]	43/43	0.95	0.07	8,17,23,27	79
8	PEB	H	203	43/43	0.95	0.08	21,29,40,44	4
10	CYC	D	202	43/43	0.95	0.09	15,27,42,67	4
4	X2I	E	101	43/43	0.95	0.08	21,32,51,73	4
9	BTB	B	204	14/14	0.96	0.07	14,18,21,22	33
8	PEB	B	203	43/43	0.96	0.07	16,22,33,36	4
7	AX9	F	201	43/43	0.96	0.07	13,24,47,59	8
4	X2I	A	101	43/43	0.97	0.06	14,21,28,58	4
8	PEB	D	203	43/43	0.97	0.06	13,19,33,49	4
7	AX9	H	201	43/43	0.97	0.06	13,24,31,38	8
4	X2I	C	101	43/43	0.97	0.06	15,21,31,37	4
7	AX9	D	201	43/43	0.98	0.05	13,17,24,28	8
6	CL	A	103	1/1	0.99	0.07	32,32,32,32	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.

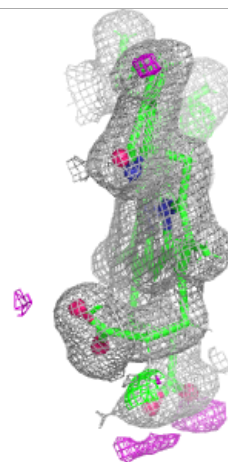
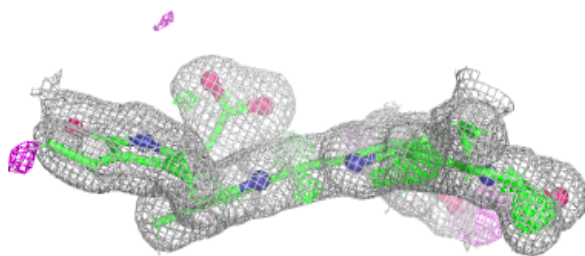
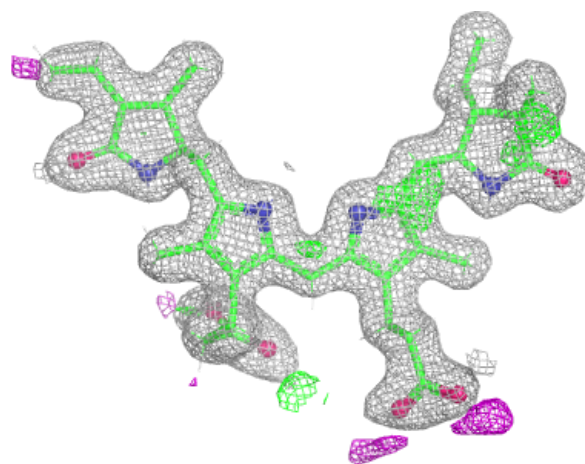
Electron density around CYC H 202:

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



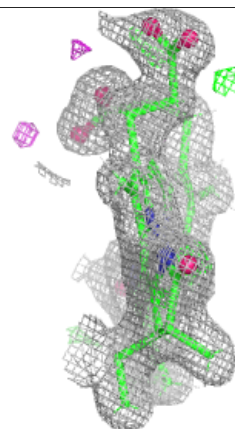
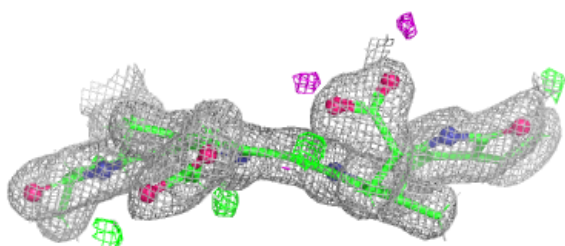
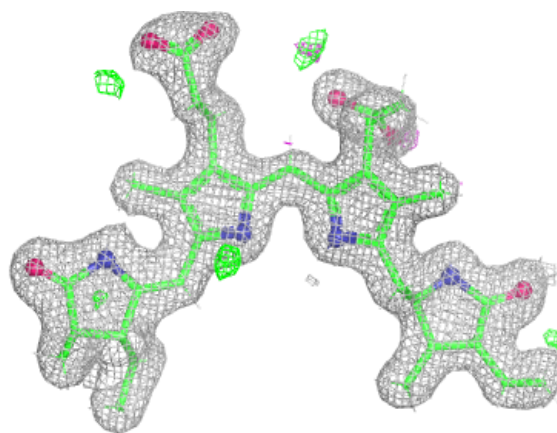
Electron density around PEB B 202:

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and green (positive)

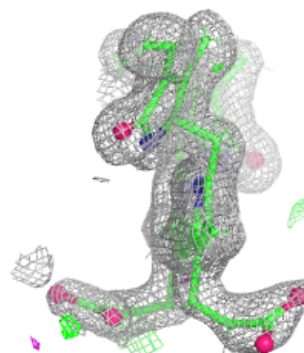
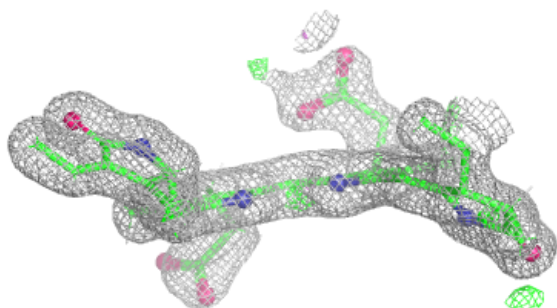
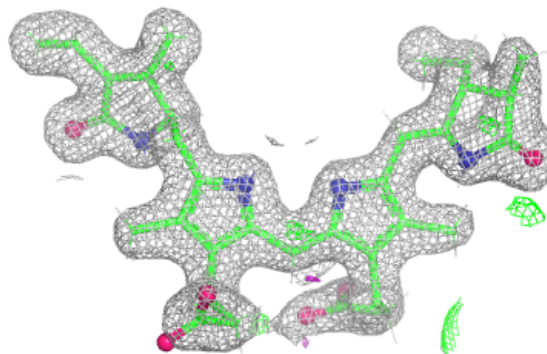


Electron density around PEB F 202:

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and green (positive)

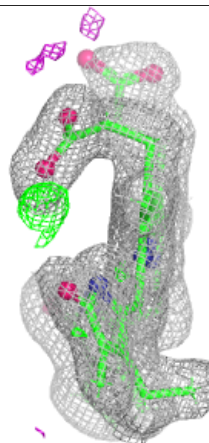
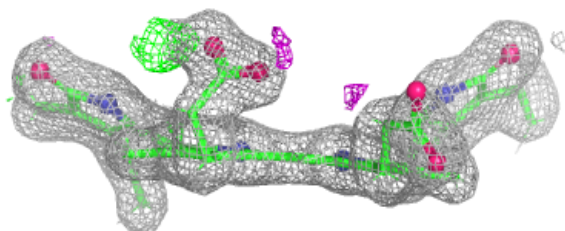
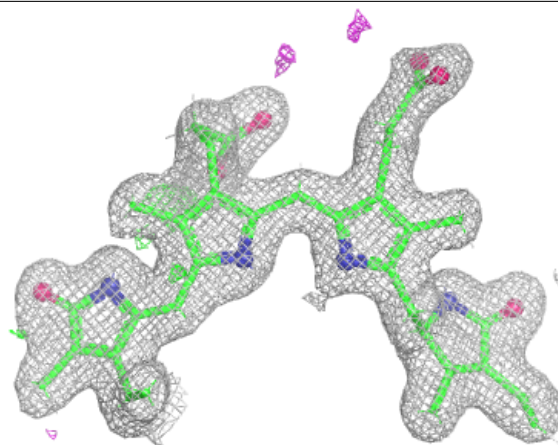
**Electron density around PEB F 203:**

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and green (positive)



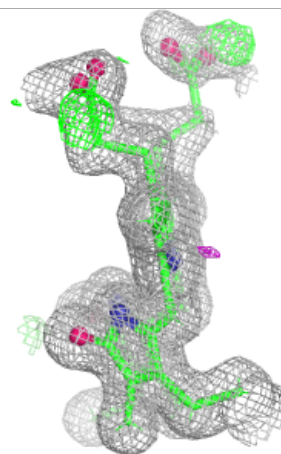
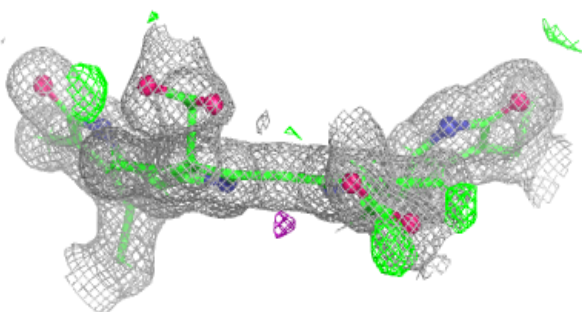
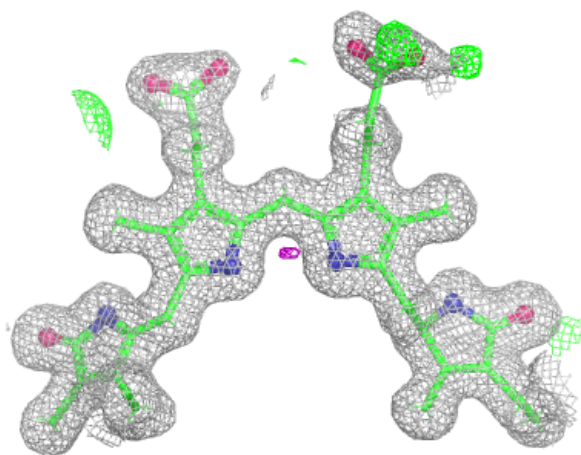
Electron density around X2I G 101:

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and green (positive)



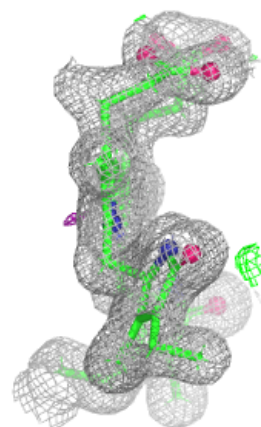
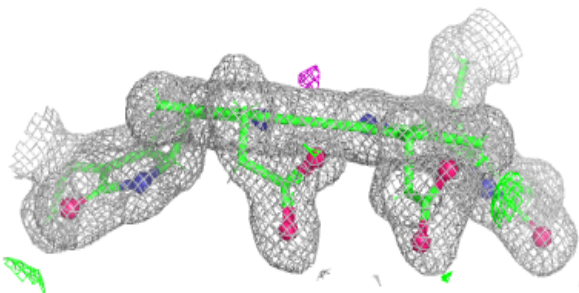
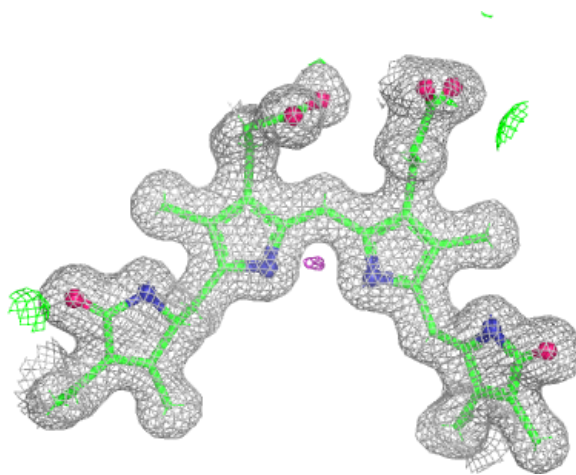
Electron density around AX9 B 201 (A):

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and green (positive)



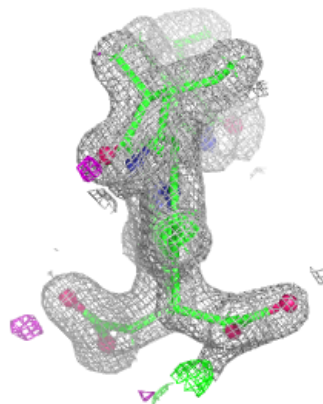
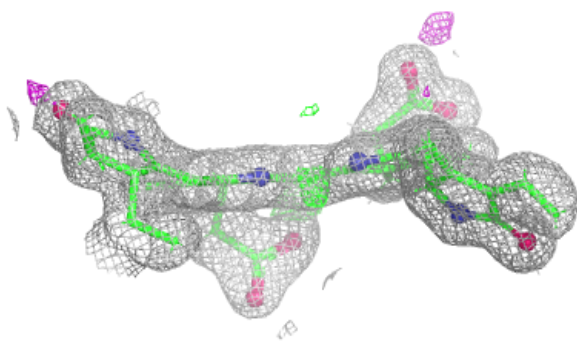
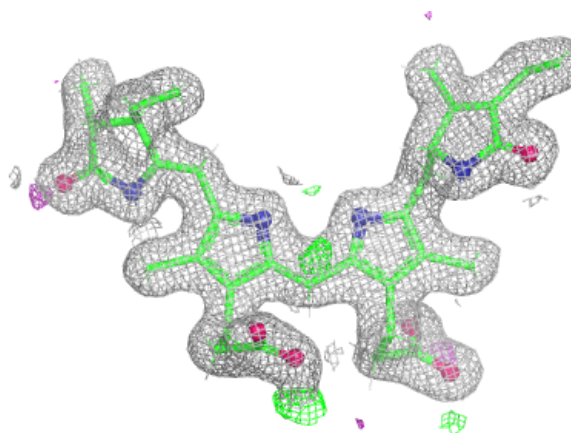
Electron density around AX9 B 201 (B):

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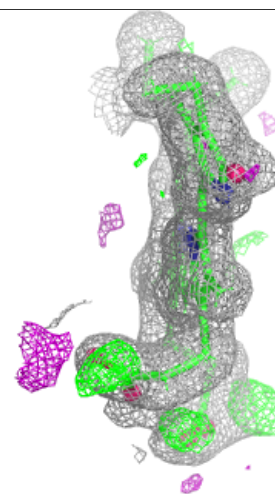
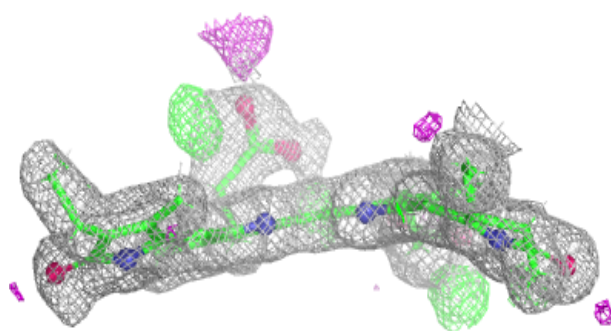
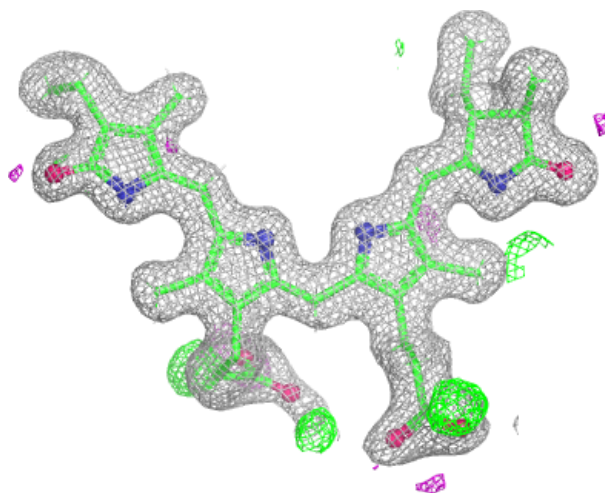
Electron density around PEB H 203:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



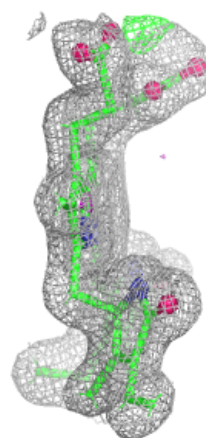
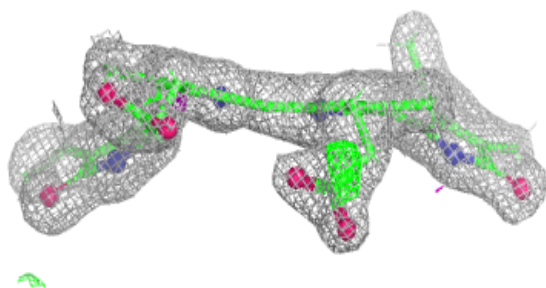
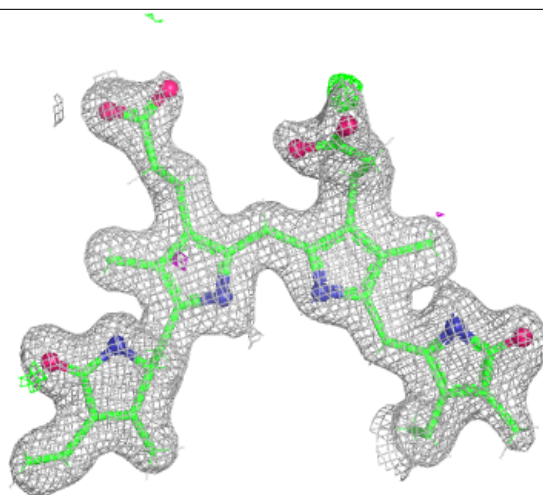
Electron density around CYC D 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



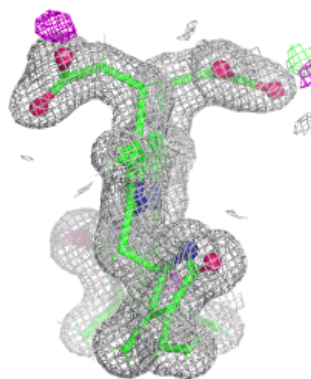
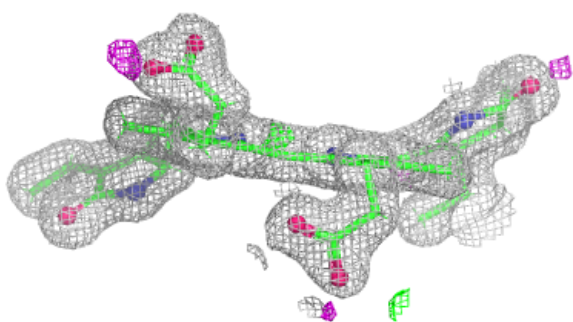
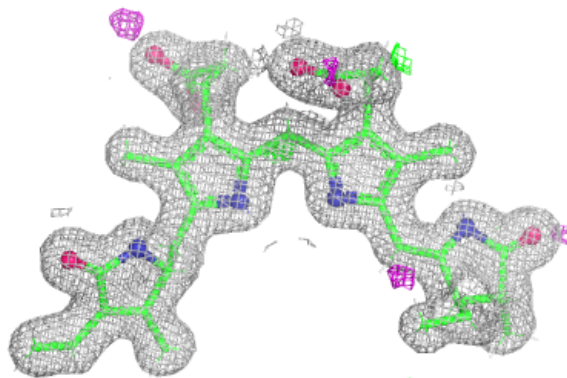
Electron density around X2I E 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



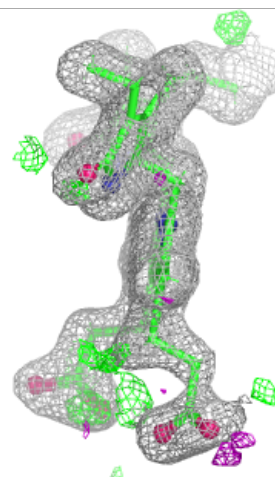
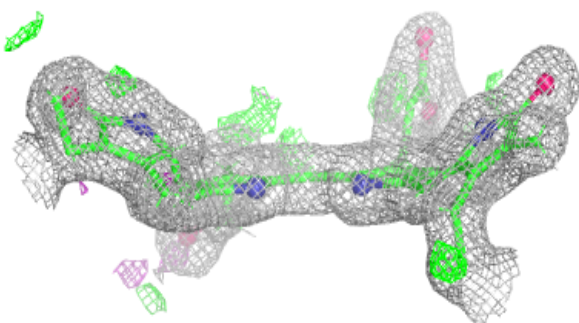
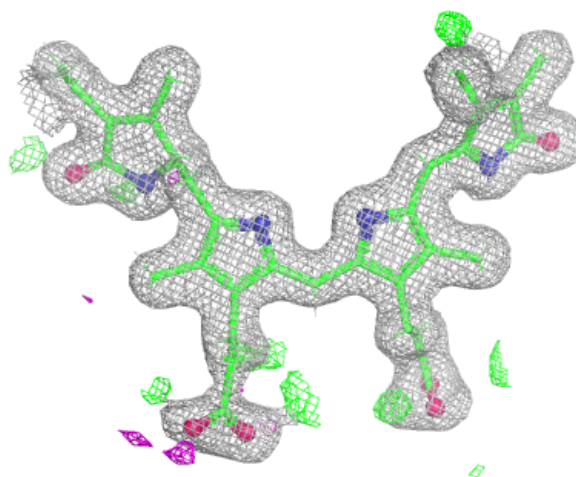
Electron density around PEB B 203:

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and green (positive)



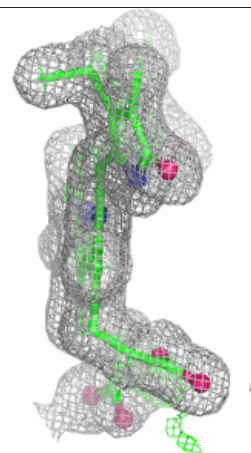
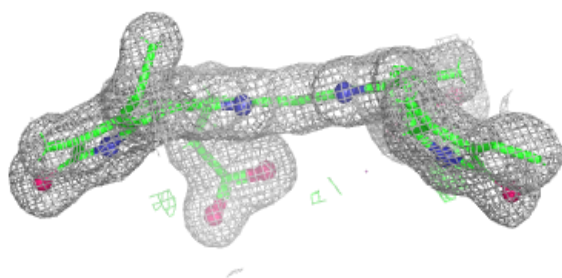
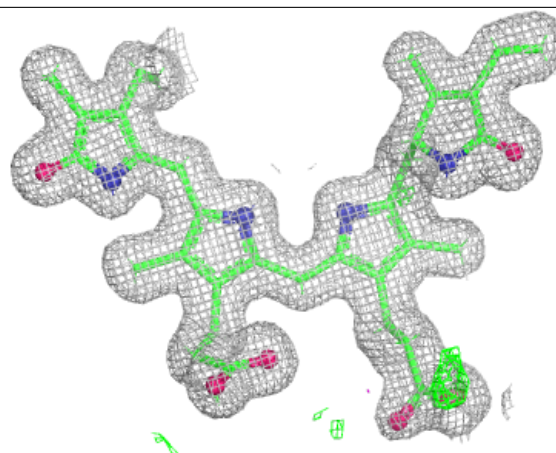
Electron density around AX9 F 201:

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and green (positive)



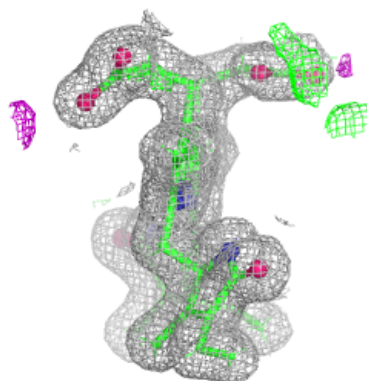
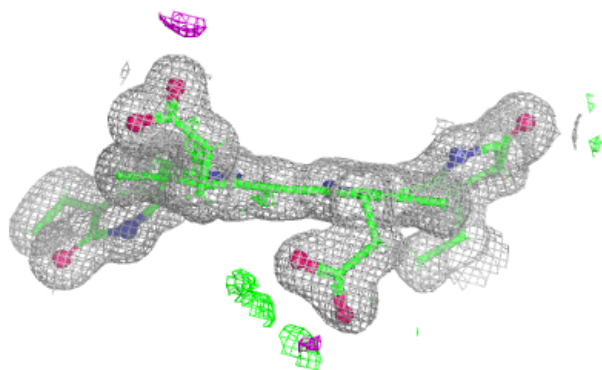
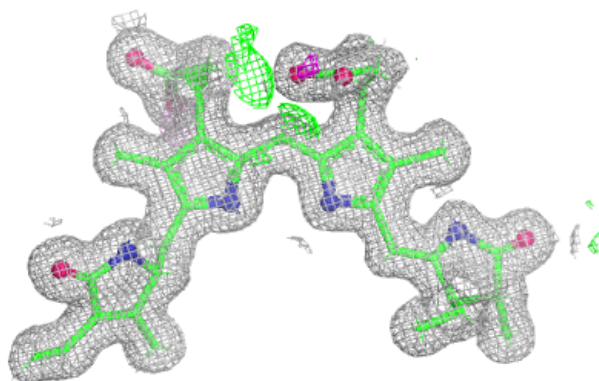
Electron density around X2I A 101:

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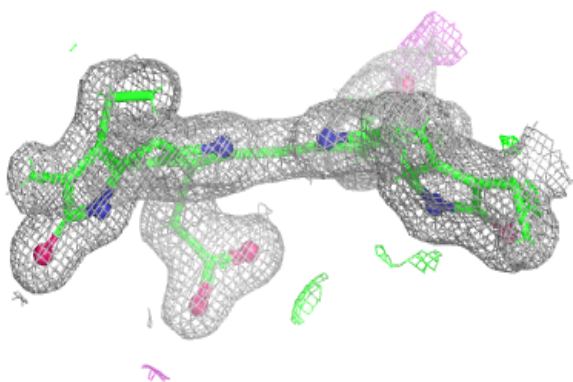
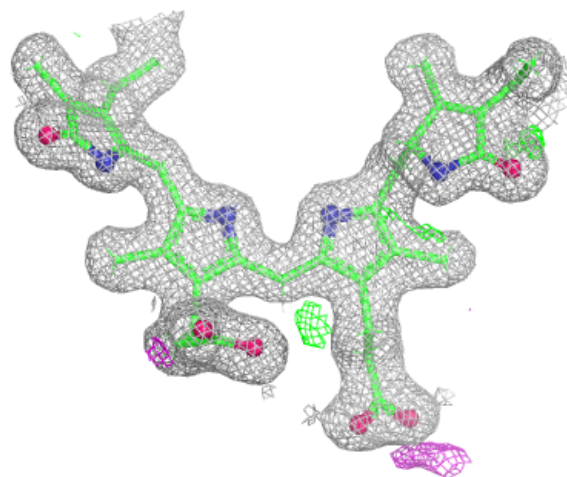
Electron density around PEB D 203:

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and green (positive)



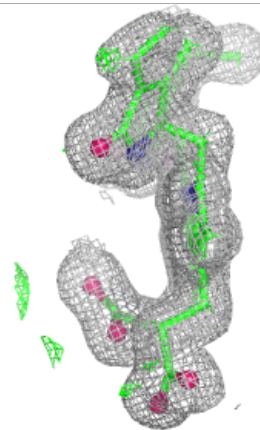
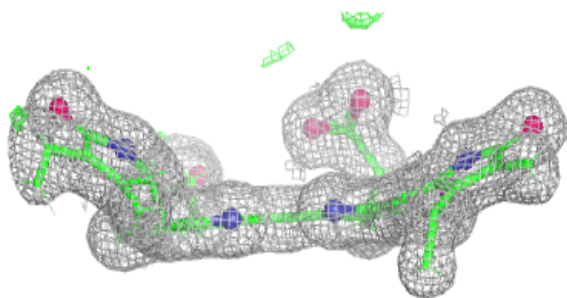
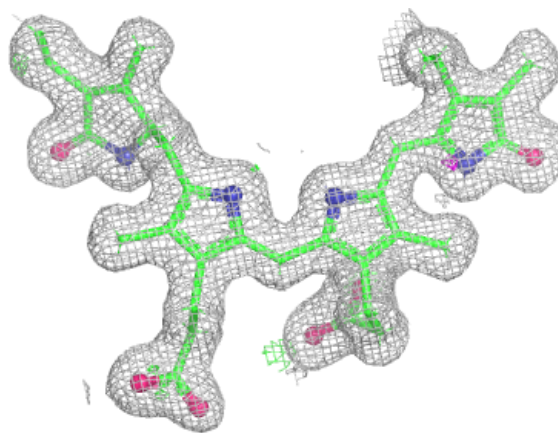
Electron density around AX9 H 201:

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and green (positive)



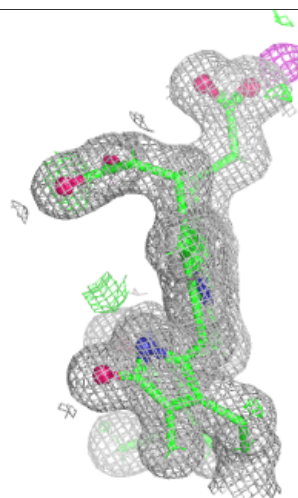
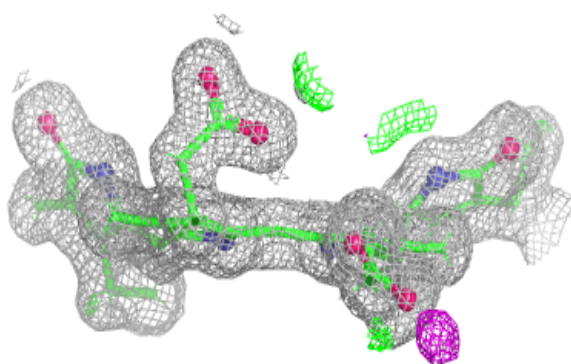
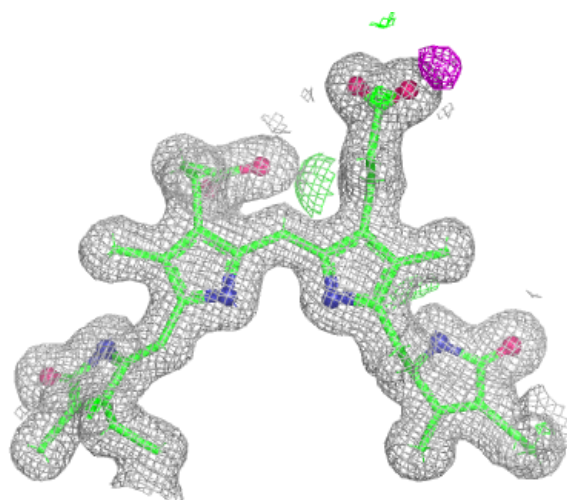
Electron density around X2I C 101:

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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)



6.5 Other polymers [i](#)

There are no such residues in this entry.