

wwPDB X-ray Structure Validation Summary Report (i)

Oct 19, 2023 – 04:15 PM EDT

PDB ID	:	7SUT
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		
Resolution	:	1.49 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

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

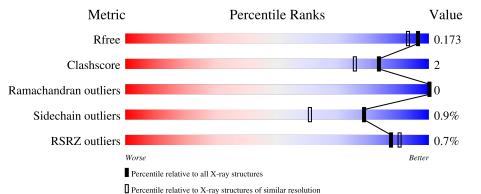
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 <=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	А	80	94%	
1	Е	80	% 94%	
2	В	177	% 93%	6% •
2	D	177		• 9%
2	F	177	95%	5% ·



Continued from previous page...

Mol	Chain	Length	Quality of chain	
2	Н	177	% 	9%
3	С	68	91%	• 7%
3	G	68	3% 	• 7%



2 Entry composition (i)

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			Aton	ns		ZeroOcc	AltConf	Trace	
1	А	78	100001	e	Н 671	N 116	0 136	S 6	0	9	0
1	Е	78	Total 1256	C 399			O 126	${f S}{5}$	0	3	0

• Molecule 2 is a protein called Phycoerythrin550 beta subunit.

Mol	Chain	Residues		Atoms						AltConf	Trace
2	В	174	Total	С	Η	Ν	0	\mathbf{S}	0	18	0
	D	174	2713	831	1362	231	279	10	0	10	0
2	D	161	Total	С	Η	Ν	0	\mathbf{S}	0	4	0
	D	101	2395	737	1204	205	239	10	0		0
2	F	176	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
	Δ Γ	170	2630	808	1324	222	265	11	0	9	
2	Н	161	Total	С	Η	Ν	0	S	0	6	0
	2 H	101	2396	737	1201	206	243	9	0	0	U

There are 4 discrepancies between the modelled and reference sequences:

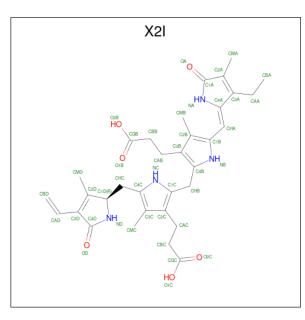
Chain	Residue	Modelled	Actual	Comment	Reference
В	172	VAL	GLU	conflict	UNP U5T8W0
D	172	VAL	GLU	conflict	UNP U5T8W0
F	172	VAL	GLU	conflict	UNP U5T8W0
Н	172	VAL	GLU	conflict	UNP U5T8W0

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

Mol	Chain	Residues		-	Atom	IS		ZeroOcc	AltConf	Trace	
3	3 C 63	Total	С	Η	Ν	0	S	0	2	0	
5		05	1046	325	525	90	100	6	0	2	0
2	С	63	Total	С	Η	Ν	0	S	0	4	0
0	G	05	1075	335	537	92	105	6	0		0



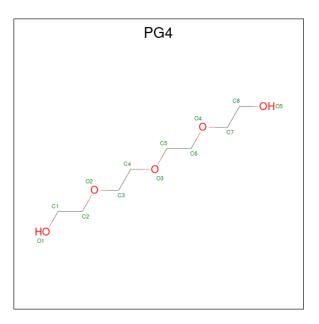
• Molecule 4 is (15,16)-DIHYDROBILIVERDIN (SINGLY LINKED) (three-letter code: X2I) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	
4	Λ	1	1 Total (Η	Ν	Ο	0	0	
4	4 A	1	78	33	35	4	6	0	0	
4	С	1	Total	С	Η	Ν	Ο	0	0	
4	4 0	1	78	33	35	4	6	0	0	
4	E	1	Total	С	Η	Ν	Ο	0	0	
4	Ľ	1	78	33	35	4	6	0	0	
4	С	1	Total	С	Η	Ν	Ο	0	0	
4	4 G	1	78	33	35	4	6	0	U	

• Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).





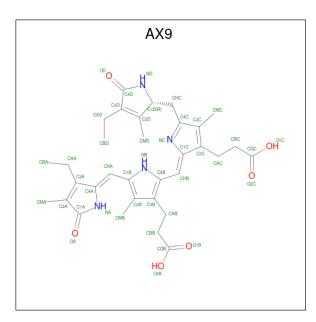
Mol	Chain	Residues	A	Ator	\mathbf{ns}		ZeroOcc	AltConf	
5	Λ	1	Total	С	Η	Ο	0	0	
	D A	1	31	8	18	5	0		
5	Ц	1	Total	С	Η	Ο	0	0	
5	11	1	31	8	18	5	0		

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

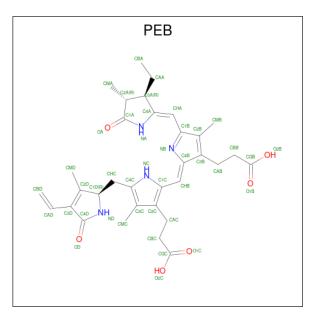
• Molecule 7 is DiCys-(15,16)-Dihydrobiliverdin (three-letter code: AX9) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	В	1	Total	С	Η	Ν	0	0	1
1	D	1	158	66	72	8	12	0	T
7	Л	1	Total	С	Η	Ν	0	0	0
1	D	1	79	33	36	4	6	0	0
7	F	1	Total	С	Η	Ν	0	0	0
1	Г	1	79	33	36	4	6	0	0
7	Н	1	Total	С	Η	Ν	0	0	0
1	11	1	79	33	36	4	6	0	0

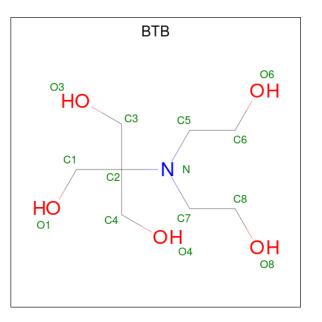
• Molecule 8 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
8	В	1	Total	С	Η	Ν	Ο	0	0
0	D	1	80	33	37	4	6	0	0
8	В	1	Total	С	Η	Ν	Ο	0	0
0	D	I	80	33	37	4	6	0	0
8	Л	1	Total	С	Η	Ν	Ο	0	0
0	D	1	80	33	37	4	6	0	0
8	F	1	Total	\mathbf{C}	Η	Ν	Ο	0	0
0	Г	1	80	33	37	4	6	0	0
8	F	1	Total	\mathbf{C}	Η	Ν	Ο	0	0
0	Г	1	80	33	37	4	6	0	0
8	Н	1	Total	\mathbf{C}	Η	Ν	Ο	0	0
0	11	1	80	33	37	4	6	0	0

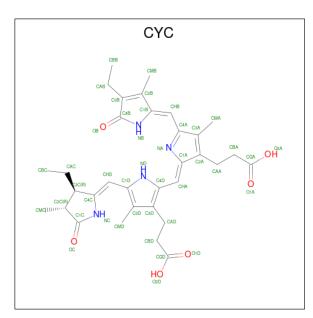
• Molecule 9 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
0	В	1	Total	С	Η	Ν	Ο	0	0
	D	1	33	8	19	1	5		U

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





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
10	Л	1	Total	С	Η	Ν	0	0	0
10	D		80	33	37	4	6	0	
10	Ц	1	Total	С	Η	Ν	Ο	0	0
10	11	1	80	33	37	4	6	0	0

• Molecule 11 is water.

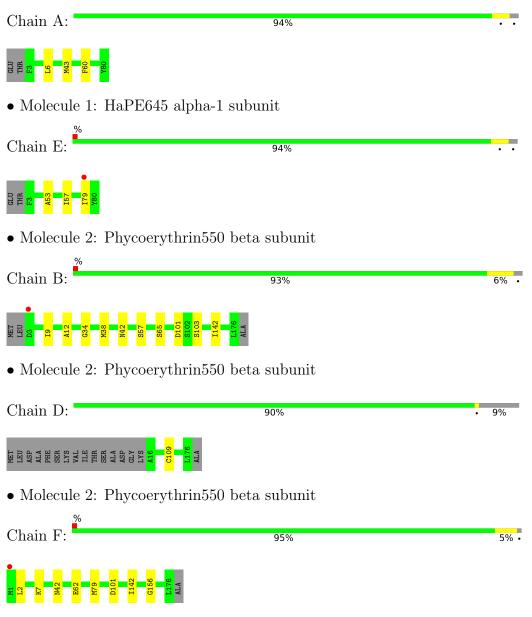
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	65	$\begin{array}{cc} \text{Total} & \text{O} \\ 65 & 65 \end{array}$	0	1
11	В	80	Total O 80 80	0	0
11	С	41	Total O 41 41	0	0
11	D	82	Total O 82 82	0	0
11	Е	45	$\begin{array}{cc} \text{Total} & \text{O} \\ 45 & 45 \end{array}$	0	0
11	F	58	Total O 58 58	0	0
11	G	28	TotalO2828	0	1
11	Н	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0



3 Residue-property plots (i)

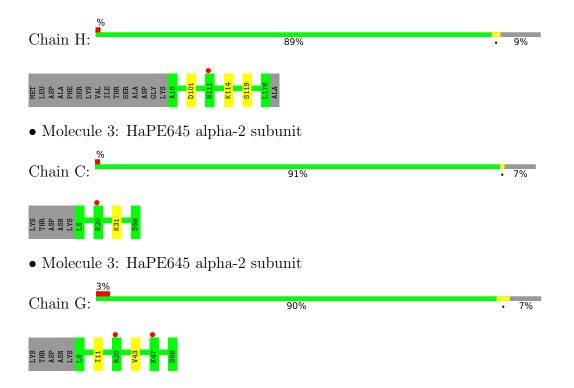
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 2: Phycoerythrin550 beta subunit







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	54.03Å 80.98Å 115.84Å	Deperitor
a, b, c, α , β , γ	90.00° 92.21° 90.00°	Depositor
Resolution (Å)	41.43 - 1.49	Depositor
Resolution (A)	115.75 - 1.49	EDS
% Data completeness	93.3(41.43-1.49)	Depositor
(in resolution range)	$87.8\ (115.75\text{-}1.49)$	EDS
R _{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.78 (at 1.49 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.145 , 0.175	Depositor
II, IIfree	0.142 , 0.173	DCC
R_{free} test set	1871 reflections (1.23%)	wwPDB-VP
Wilson B-factor $(Å^2)$	17.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.46 , 54.7	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	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.

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.



¹Intensities estimated from amplitudes.

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, PG4, CYC, BTB, PEB, AX9, 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		
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.52	0/696	0.69	0/927	
1	Е	0.45	0/647	0.68	0/864	
2	В	0.46	0/1395	0.63	0/1880	
2	D	0.50	0/1211	0.66	0/1634	
2	F	0.42	0/1345	0.62	0/1814	
2	Н	0.40	0/1222	0.60	0/1651	
3	С	0.52	0/528	0.75	0/704	
3	G	0.46	0/545	0.65	0/728	
All	All	0.46	0/7589	0.65	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	А	685	671	662	5	0
1	Е	636	620	616	3	0
2	В	1351	1362	1315	10	0
2	D	1191	1204	1193	0	0
2	F	1306	1324	1297	6	0



7	S	U	Т	

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Н	1195	1201	1180	0	0
3	С	521	525	521	1	0
3	G	538	537	533	3	0
4	А	43	35	0	0	0
4	С	43	35	0	0	0
4	Е	43	35	0	0	0
4	G	43	35	0	0	0
5	А	13	18	18	1	0
5	Н	13	18	18	0	0
6	А	1	0	0	0	0
7	В	86	72	0	0	0
7	D	43	36	0	0	0
7	F	43	36	0	0	0
7	Н	43	36	0	0	0
8	В	86	74	74	6	0
8	D	43	37	37	2	0
8	F	86	74	74	5	0
8	Н	43	37	37	3	0
9	В	14	19	19	0	0
10	D	43	37	37	3	0
10	Н	43	37	37	3	0
11	А	65	0	0	0	0
11	В	80	0	0	0	0
11	С	41	0	0	1	0
11	D	82	0	0	0	0
11	Е	45	0	0	0	0
11	F	58	0	0	0	0
11	G	28	0	0	0	0
11	Н	57	0	0	0	0
All	All	8651	8115	7668	39	0

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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.

The worst 5 of 39 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)
8:F:202:PEB:HNA	8:F:202:PEB:HMB2	1.50	0.76
10:D:202:CYC:HMA1	10:D:202:CYC:HB	1.52	0.74
8:B:202:PEB:HNA	8:B:202:PEB:HMB2	1.54	0.71
8:H:203:PEB:HMB2	8:H:203:PEB:HNA	1.63	0.63



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:202:CYC:HMA1	10:H:202:CYC:HB	1.63	0.62

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	Perce	ntiles
1	А	85/80~(106%)	81 (95%)	4(5%)	0	100	100
1	Ε	79/80~(99%)	75~(95%)	4(5%)	0	100	100
2	В	190/177~(107%)	186~(98%)	4 (2%)	0	100	100
2	D	163/177~(92%)	161 (99%)	2(1%)	0	100	100
2	\mathbf{F}	183/177~(103%)	181 (99%)	2(1%)	0	100	100
2	Н	165/177~(93%)	163~(99%)	2(1%)	0	100	100
3	\mathbf{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 (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	А	77/70~(110%)	77~(100%)	0	100 100
1	Ε	71/70~(101%)	71 (100%)	0	100 100
2	В	155/140 (111%)	154 (99%)	1 (1%)	86 74
2	D	132/140~(94%)	131~(99%)	1 (1%)	81 66
2	\mathbf{F}	147/140~(105%)	145~(99%)	2(1%)	67 42
2	Н	134/140~(96%)	131~(98%)	3(2%)	52 22
3	С	57/60~(95%)	57~(100%)	0	100 100
3	G	59/60~(98%)	59~(100%)	0	100 100
All	All	832/820~(102%)	825~(99%)	7 (1%)	78 66

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	101	ASP
2	Н	101	ASP
2	Н	119	SER
2	Н	114	LYS
2	F	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	Turne	Chain	Res	Link	B	ond leng	gths	B	ond ang	Bond angles		
INIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
5	PG4	Н	204	-	12,12,12	0.16	0	11,11,11	0.62	0		
7	AX9	D	201	2	41,46,46	1.66	8 (19%)	41,67,67	1.15	5 (12%)		
7	AX9	F	201	2	41,46,46	1.58	9 (21%)	41,67,67	1.32	4 (9%)		
8	PEB	В	203	2	43,46,46	3.83	26 (60%)	45,67,67	1.96	16 (35%)		
9	BTB	В	204	-	13,13,13	0.57	0	7,16,16	0.38	0		
7	AX9	В	201[A]	2	$41,\!46,\!46$	1.61	8 (19%)	41,67,67	1.13	4 (9%)		
5	PG4	А	102	-	12,12,12	0.17	0	11,11,11	0.60	0		
7	AX9	В	201[B]	2	41,46,46	1.62	8 (19%)	41,67,67	1.09	3 (7%)		
8	PEB	Н	203	2	43,46,46	4.07	30 (69%)	45,67,67	2.14	15 (33%)		
8	PEB	D	203	2	43,46,46	3.68	26 (60%)	45,67,67	1.77	8 (17%)		
8	PEB	F	203	2	43,46,46	4.28	27 (62%)	45,67,67	1.88	9 (20%)		
8	PEB	F	202	2	43,46,46	4.46	32 (74%)	45,67,67	2.27	16 (35%)		
4	X2I	G	101	3	41,46,46	3.13	8 (19%)	40,67,67	1.45	<mark>6 (15%)</mark>		
8	PEB	В	202	2	43,46,46	3.96	29 (67%)	45,67,67	2.23	12 (26%)		
10	CYC	D	202	2	42,46,46	2.39	12 (28%)	50,67,67	2.48	14 (28%)		
10	CYC	Н	202	2	42,46,46	2.71	14 (33%)	50,67,67	2.31	12 (24%)		
4	X2I	А	101	1	41,46,46	3.27	6 (14%)	40,67,67	1.63	7 (17%)		
7	AX9	Н	201	2	41,46,46	1.60	8 (19%)	41,67,67	1.13	2 (4%)		
4	X2I	Е	101	1	41,46,46	3.03	7 (17%)	40,67,67	1.64	11 (27%)		
4	X2I	С	101	3	41,46,46	2.84	8 (19%)	40,67,67	1.27	4 (10%)		

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	PG4	Н	204	-	-	1/10/10/10	-
7	AX9	D	201	2	-	5/26/74/74	0/4/4/4
7	AX9	F	201	2	-	4/26/74/74	0/4/4/4



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEB	В	203	2	-	5/24/74/74	0/4/4/4
9	BTB	В	204	-	-	0/21/21/21	-
7	AX9	В	201[A]	2	-	6/26/74/74	0/4/4/4
5	PG4	А	102	-	-	4/10/10/10	-
7	AX9	В	201[B]	2	-	5/26/74/74	0/4/4/4
8	PEB	Н	203	2	-	7/24/74/74	0/4/4/4
8	PEB	D	203	2	-	6/24/74/74	0/4/4/4
8	PEB	F	203	2	-	5/24/74/74	0/4/4/4
8	PEB	F	202	2	-	6/24/74/74	0/4/4/4
4	X2I	G	101	3	-	9/22/58/58	0/4/4/4
8	PEB	В	202	2	-	4/24/74/74	0/4/4/4
10	CYC	D	202	2	-	9/25/74/74	0/4/4/4
10	CYC	Н	202	2	-	5/25/74/74	0/4/4/4
4	X2I	А	101	1	-	8/22/58/58	0/4/4/4
7	AX9	Н	201	2	-	4/26/74/74	0/4/4/4
4	X2I	Е	101	1	-	9/22/58/58	0/4/4/4
4	X2I	С	101	3	-	10/22/58/58	0/4/4/4

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The worst 5 of 266 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
4	А	101	X2I	CHB-C1C	-19.20	1.37	1.51
4	G	101	X2I	CHB-C1C	-17.84	1.38	1.51
4	Е	101	X2I	CHB-C1C	-17.33	1.38	1.51
4	С	101	X2I	CHB-C1C	-15.77	1.39	1.51
8	F	202	PEB	CHB-C4B	11.19	1.44	1.35

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
10	D	202	CYC	OC-C1C-C2C	-9.88	118.32	126.17
8	F	202	PEB	C1C-CHB-C4B	-8.11	119.12	128.81
10	Н	202	CYC	OC-C1C-C2C	-7.87	119.91	126.17
10	D	202	CYC	C2C-C1C-NC	7.84	115.03	108.27
10	Н	202	CYC	C2C-C1C-NC	7.75	114.95	108.27

There are no chirality outliers.

5 of 112 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	А	101	X2I	NB-C1B-CHA-C4A
4	А	101	X2I	C2B-C1B-CHA-C4A
4	А	101	X2I	C2C-C1C-CHB-C4B
4	С	101	X2I	NB-C1B-CHA-C4A
4	С	101	X2I	C2B-C1B-CHA-C4A

There are no ring outliers.

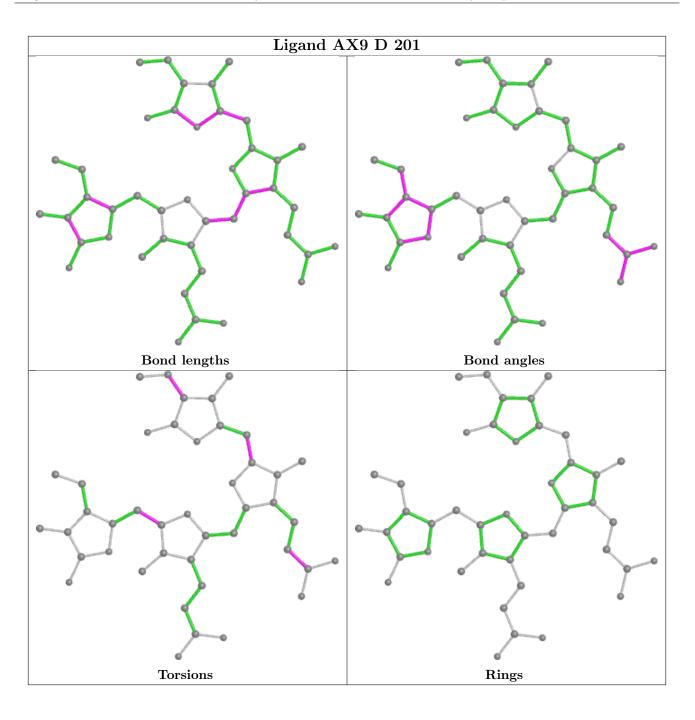
9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	В	203	PEB	4	0
5	А	102	PG4	1	0
8	Н	203	PEB	3	0
8	D	203	PEB	2	0
8	F	203	PEB	4	0
8	F	202	PEB	1	0
8	В	202	PEB	2	0
10	D	202	CYC	3	0
10	Н	202	CYC	3	0

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

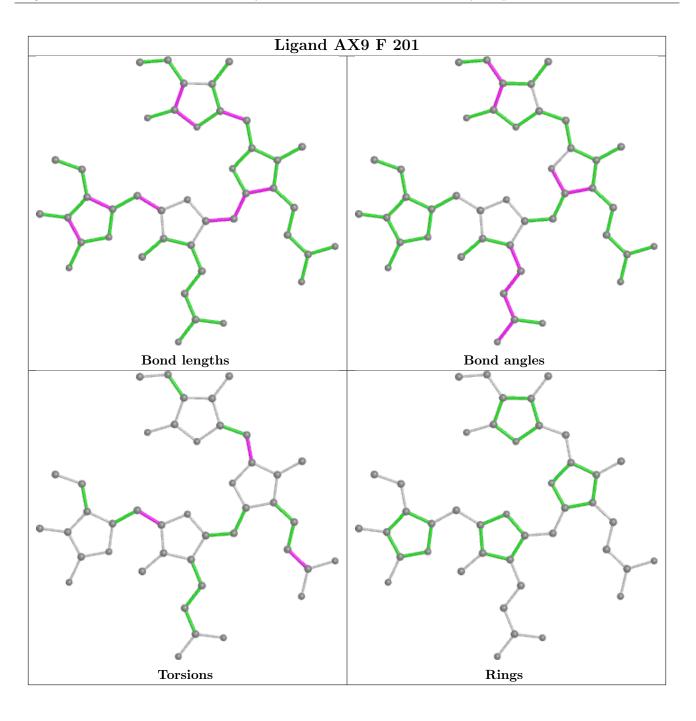




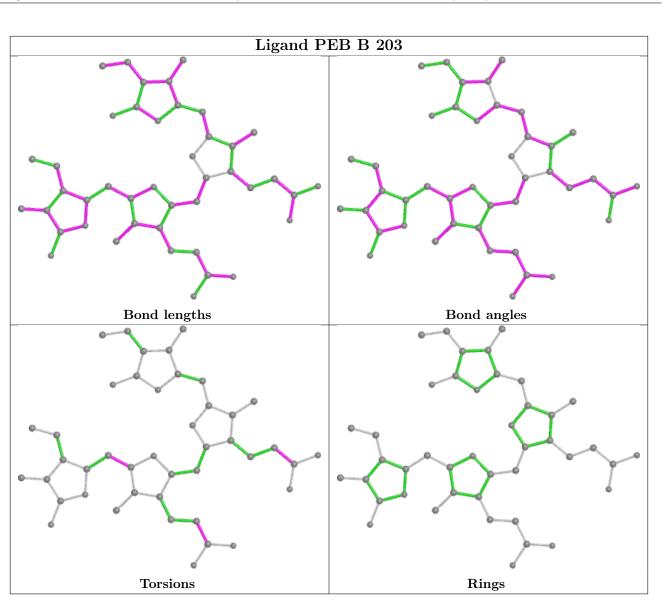






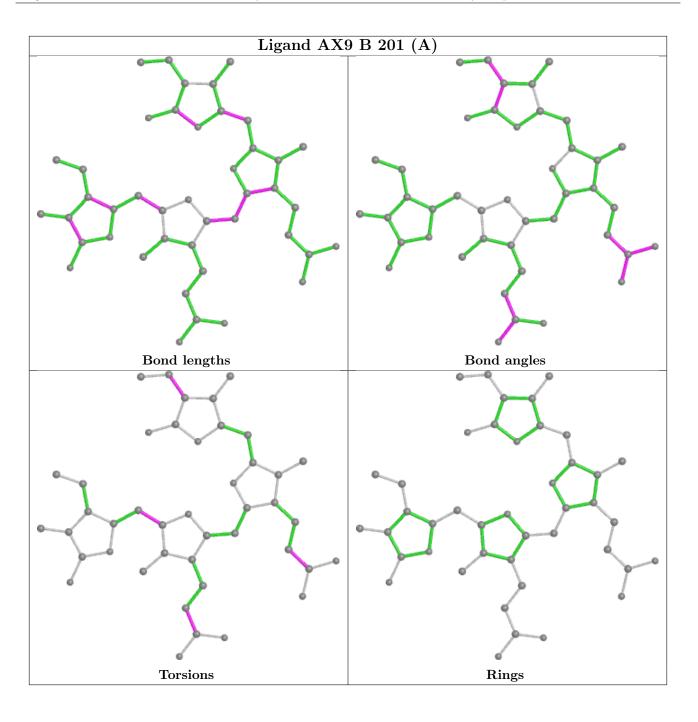






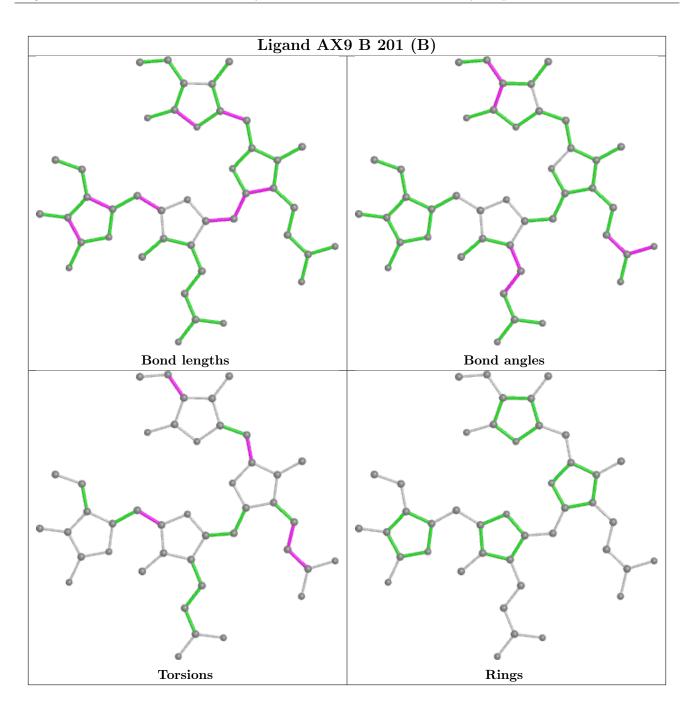




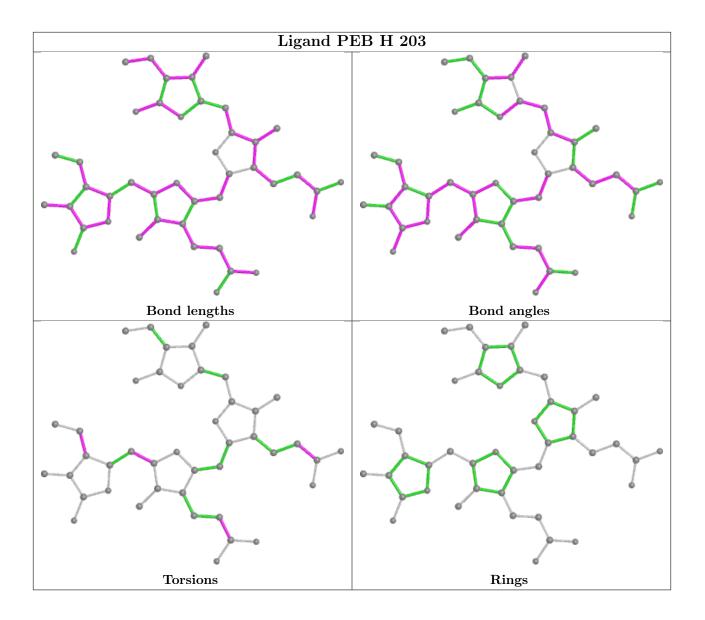






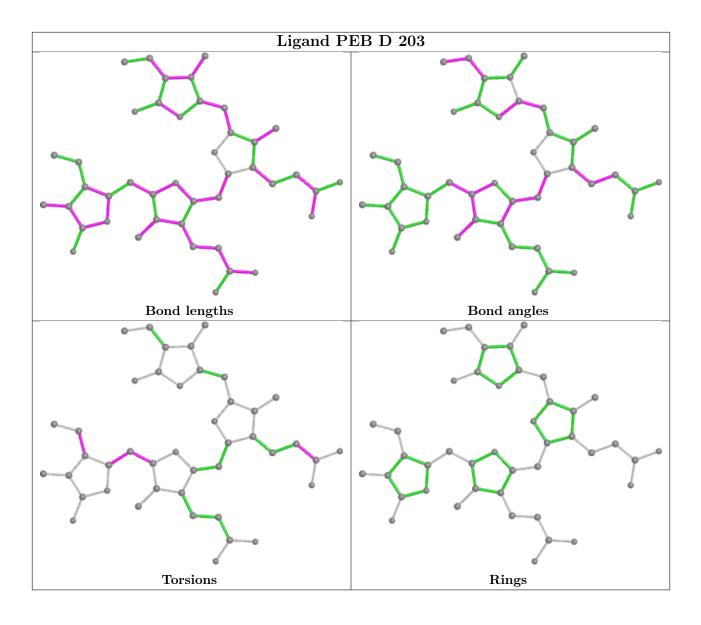






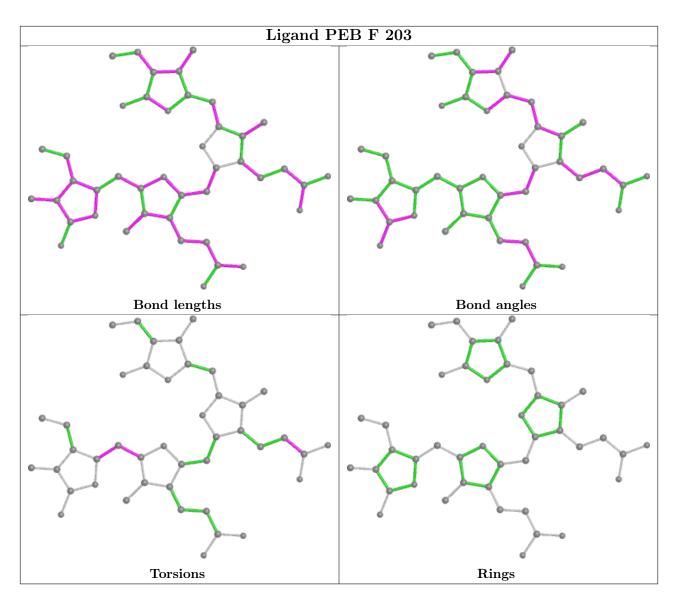




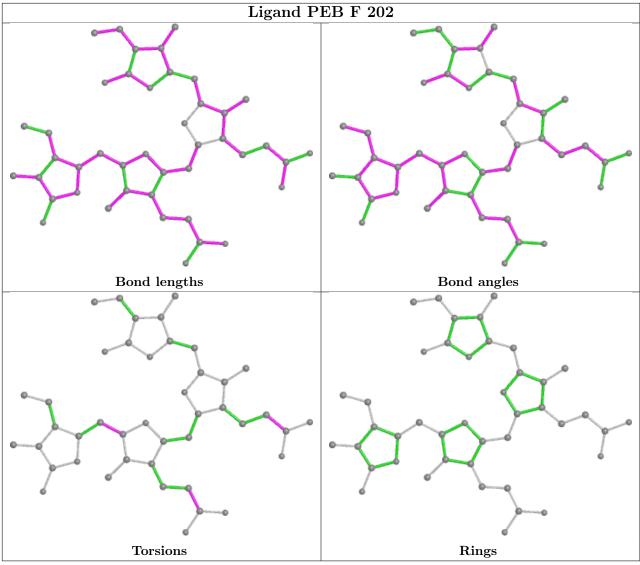




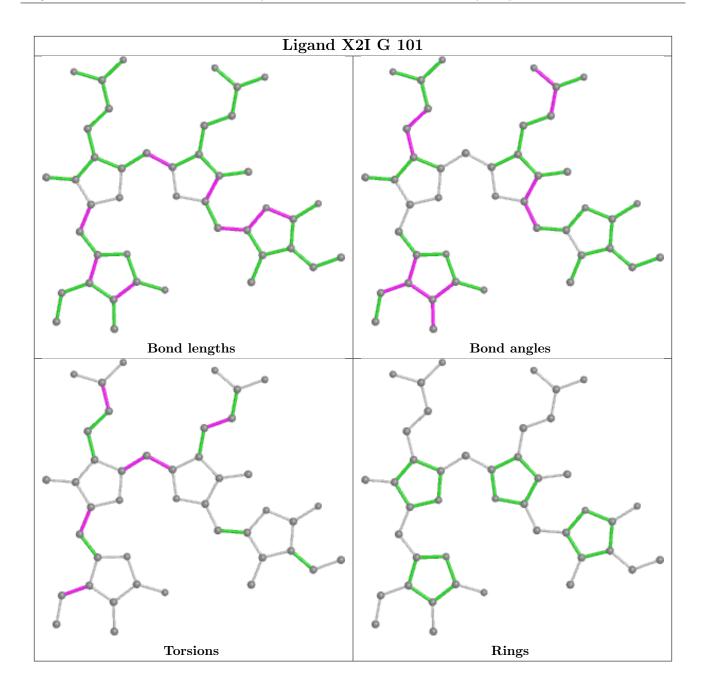






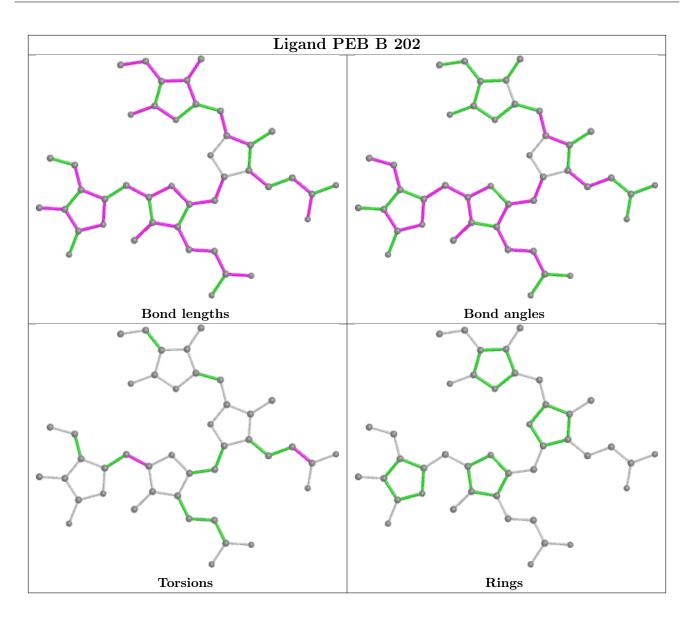




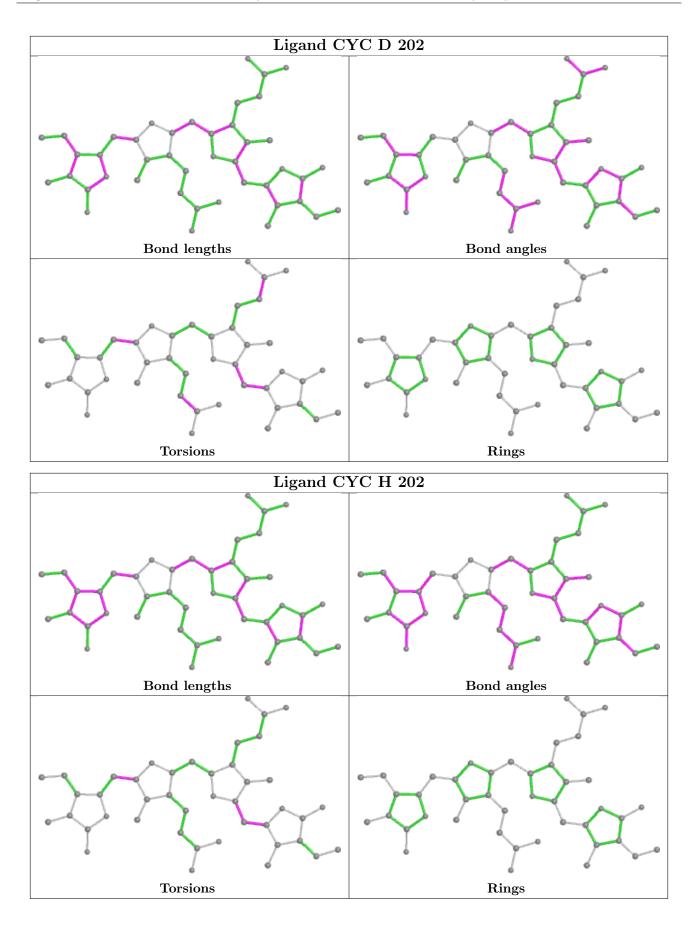




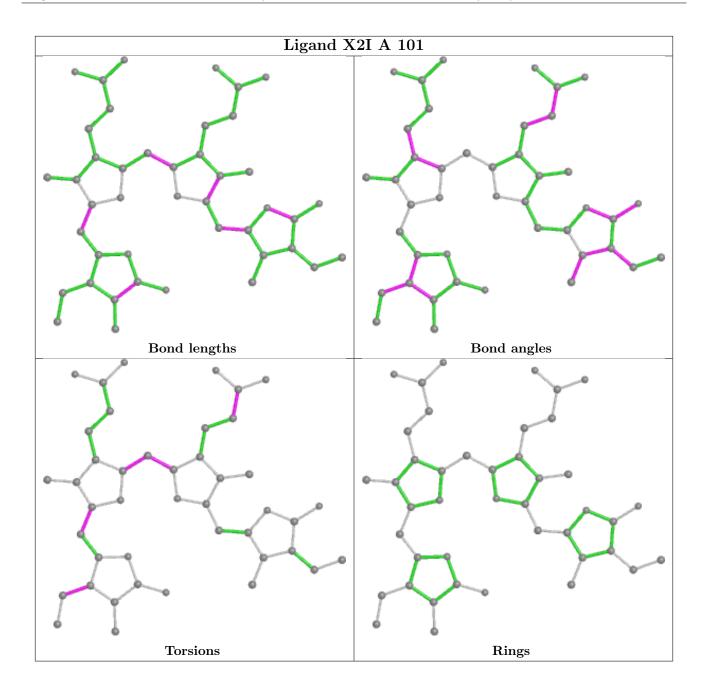






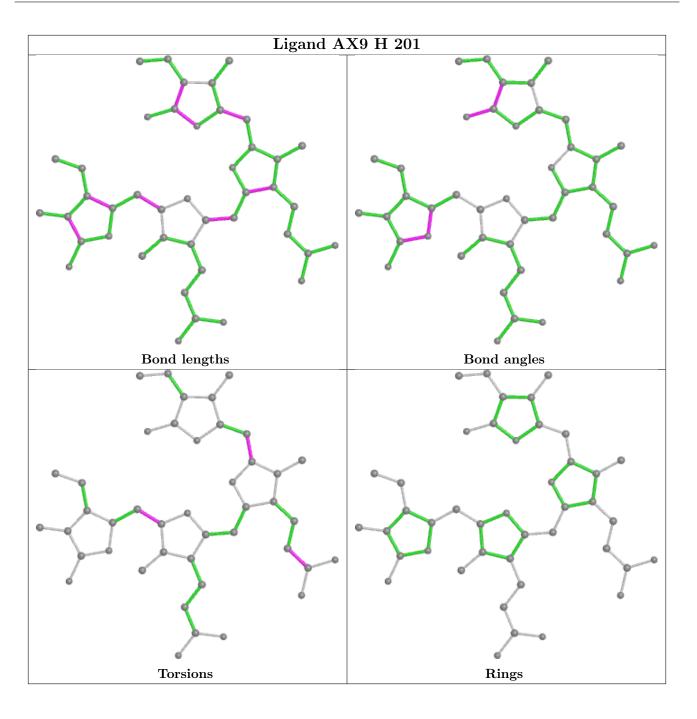




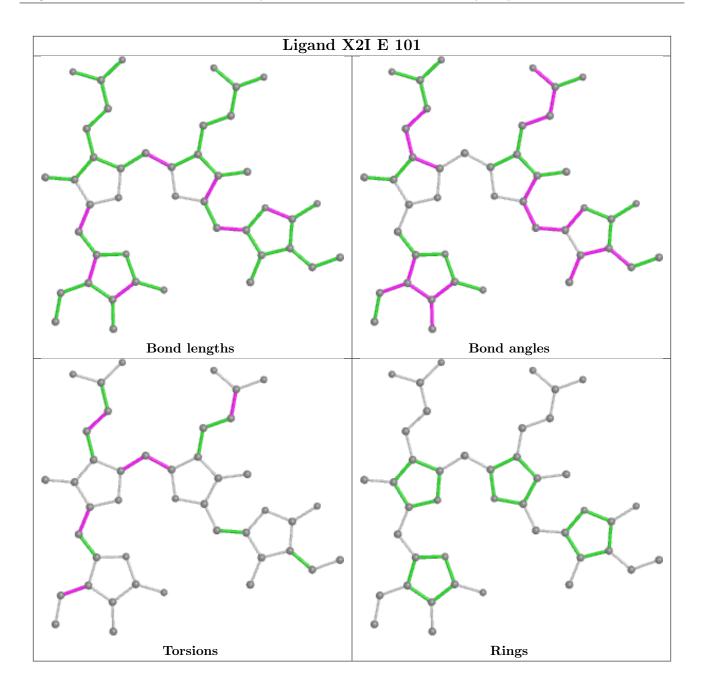




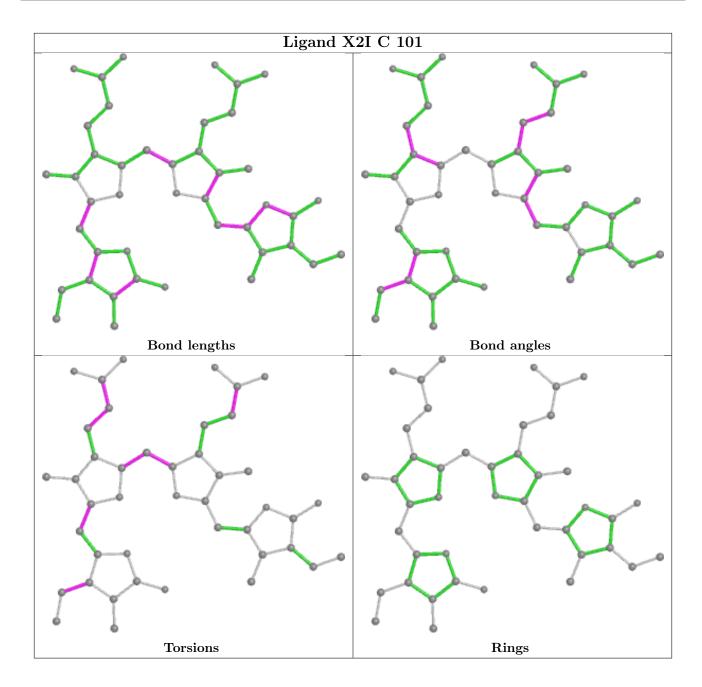












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	78/80~(97%)	-0.47	0 100 100	15, 20, 34, 59	0
1	Ε	78/80~(97%)	-0.33	1 (1%) 77 81	20, 26, 48, 55	0
2	В	174/177~(98%)	-0.41	1 (0%) 89 91	15, 21, 43, 62	0
2	D	161/177~(90%)	-0.52	0 100 100	14, 19, 33, 48	0
2	F	176/177~(99%)	-0.39	1 (0%) 89 91	19, 28, 43, 66	0
2	Η	161/177~(90%)	-0.38	1 (0%) 89 91	19, 29, 47, 58	0
3	С	63/68~(92%)	-0.42	1 (1%) 72 77	16, 20, 39, 58	0
3	G	63/68~(92%)	-0.22	2 (3%) 47 52	21, 28, 50, 59	0
All	All	954/1004~(95%)	-0.41	7 (0%) 87 90	14, 24, 44, 66	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	47	LYS	2.6
2	F	1	MET	2.2
2	В	3	ASP	2.1
3	G	20	ARG	2.0
2	Н	111	ASN	2.0

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 monosaccharides in this entry.



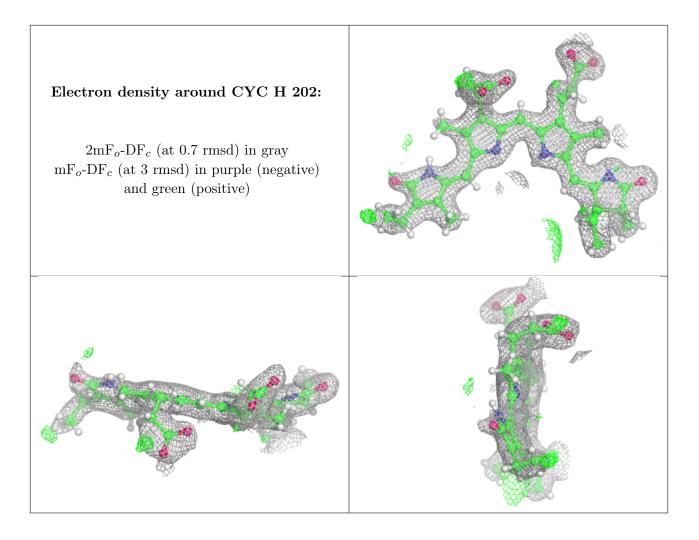
6.4 Ligands (i)

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.

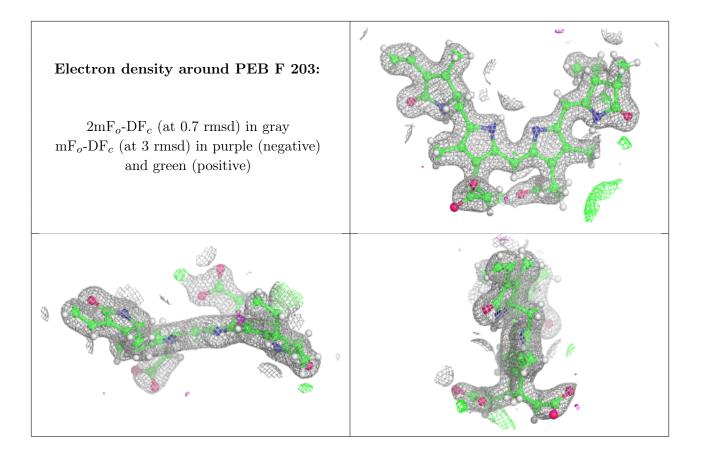
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
5	PG4	А	102	13/13	0.87	0.12	33,51,70,72	0
5	PG4	Н	204	13/13	0.90	0.11	34,47,63,75	0
10	CYC	Н	202	43/43	0.93	0.10	22,38,83,100	4
8	PEB	F	203	43/43	0.94	0.10	19,30,54,67	4
8	PEB	В	202	43/43	0.95	0.09	16,24,34,40	4
8	PEB	F	202	43/43	0.95	0.09	22,32,45,50	4
4	X2I	Е	101	43/43	0.95	0.08	21,32,51,73	4
10	CYC	D	202	43/43	0.95	0.07	15,27,42,67	4
4	X2I	G	101	43/43	0.95	0.08	22,30,41,80	4
8	PEB	Н	203	43/43	0.96	0.08	21,29,40,44	4
9	BTB	В	204	14/14	0.96	0.08	14,18,21,22	33
7	AX9	F	201	43/43	0.96	0.07	13,24,47,59	8
8	PEB	В	203	43/43	0.96	0.07	16,22,33,36	4
4	X2I	А	101	43/43	0.97	0.07	14,21,28,58	4
8	PEB	D	203	43/43	0.97	0.08	13,19,33,49	4
7	AX9	Н	201	43/43	0.97	0.06	13,24,31,38	8
4	X2I	С	101	43/43	0.97	0.07	15,21,31,37	4
7	AX9	D	201	43/43	0.98	0.07	13,17,24,28	8
7	AX9	В	201[A]	43/43	0.98	0.07	9,19,31,35	79
7	AX9	В	201[B]	43/43	0.98	0.07	8,17,23,27	79
6	CL	А	103	1/1	0.99	0.04	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.

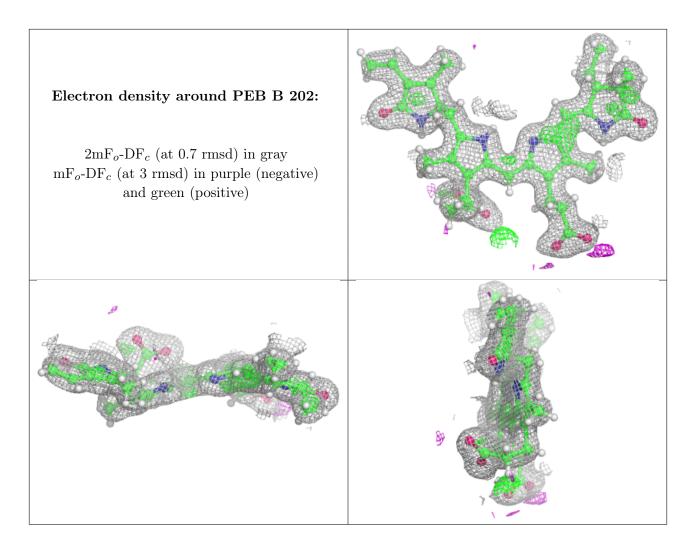




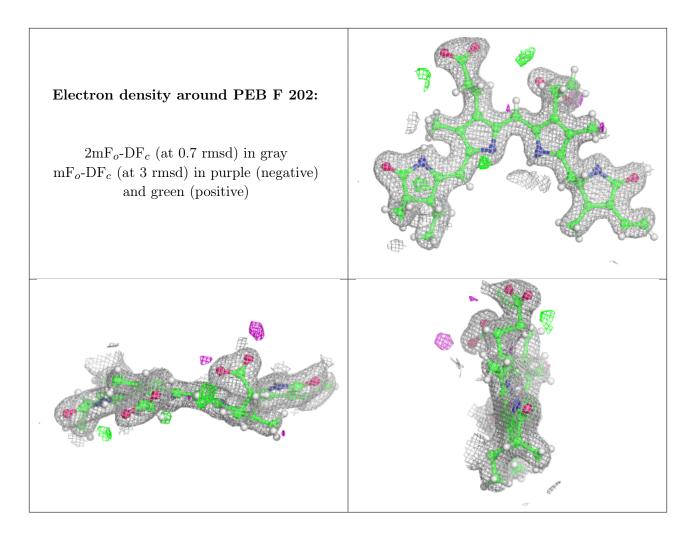




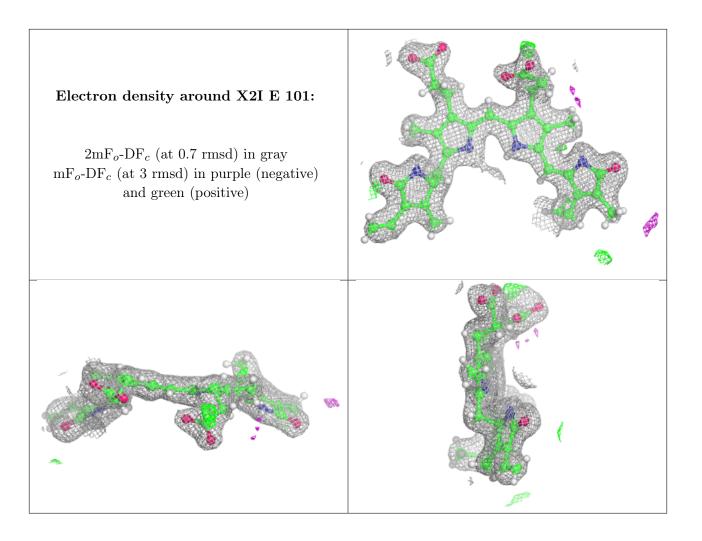




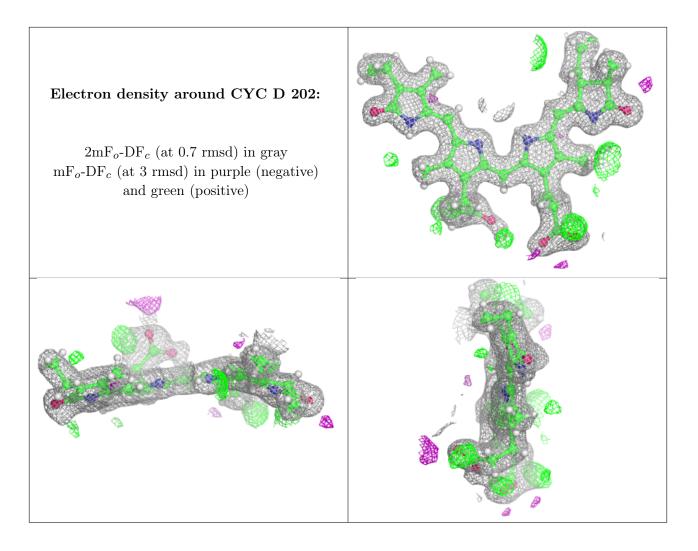




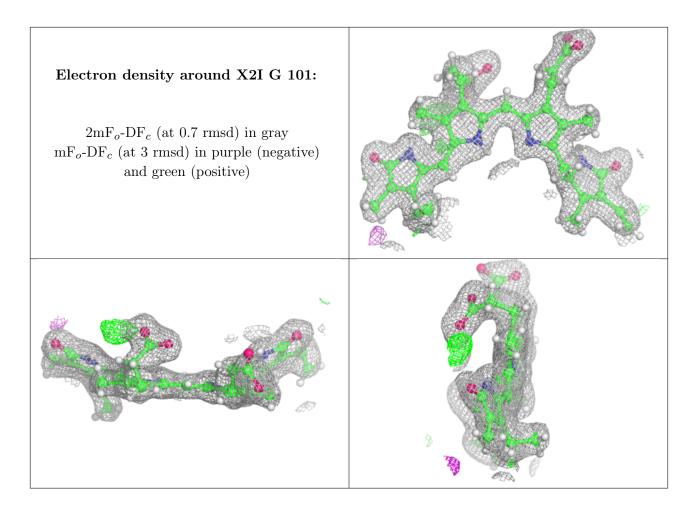




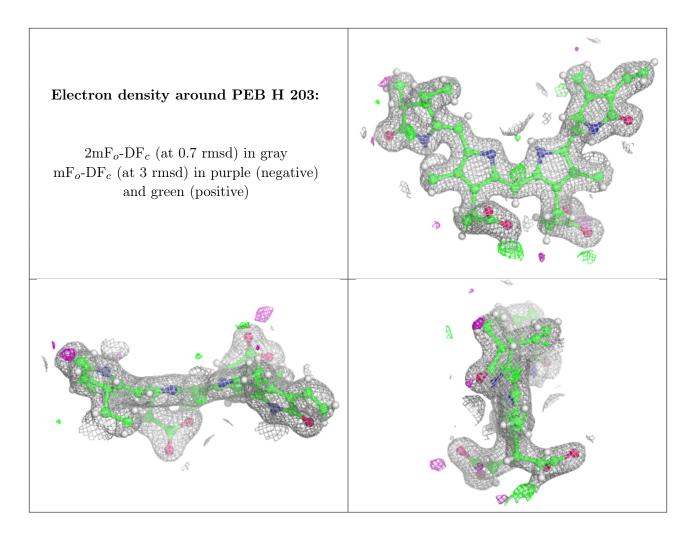




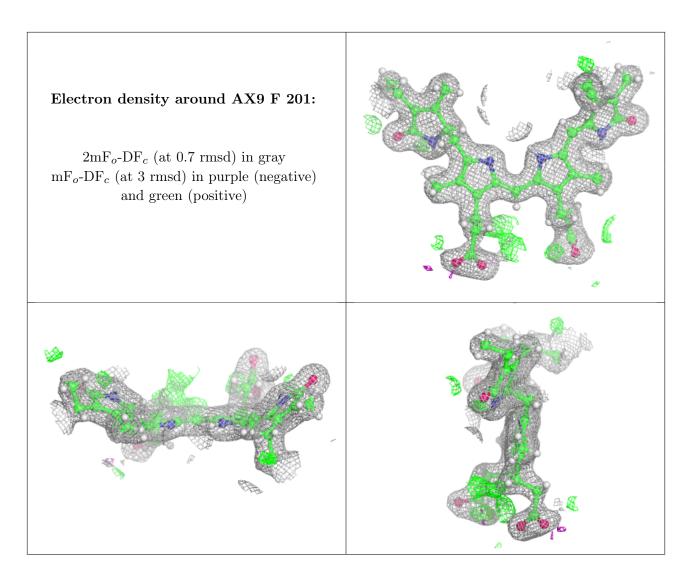




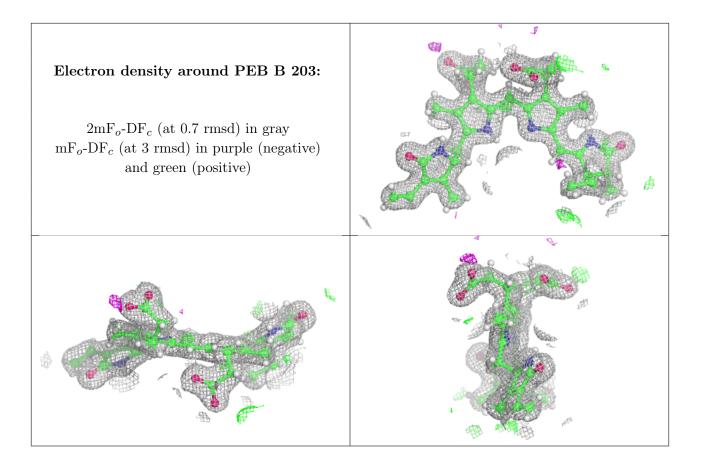




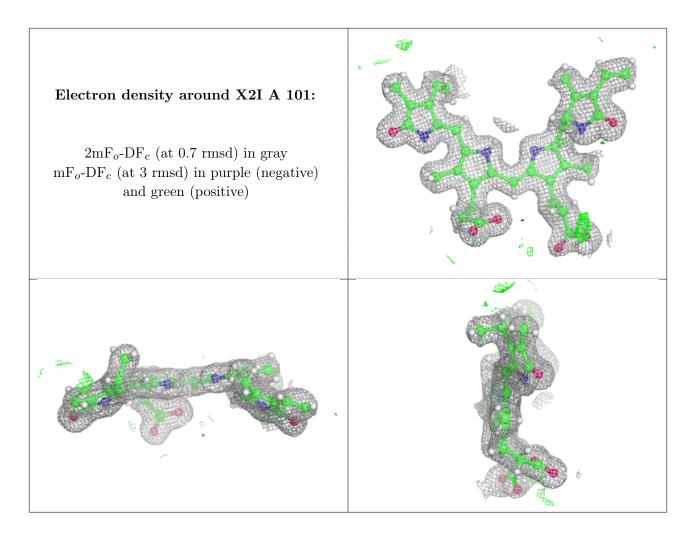




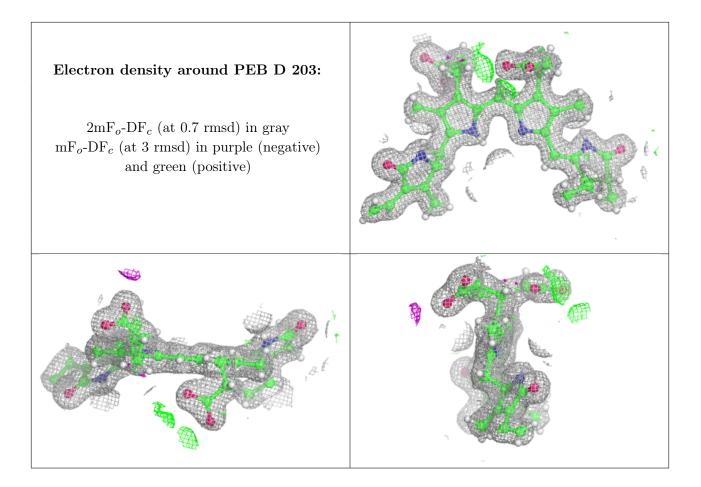




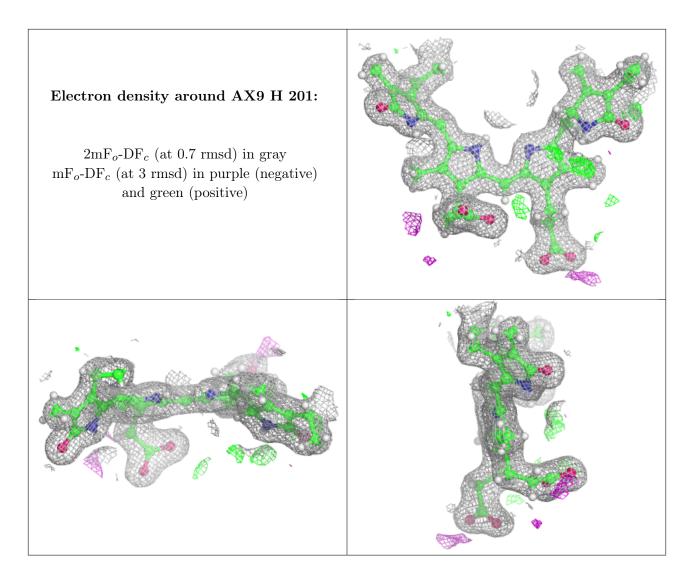




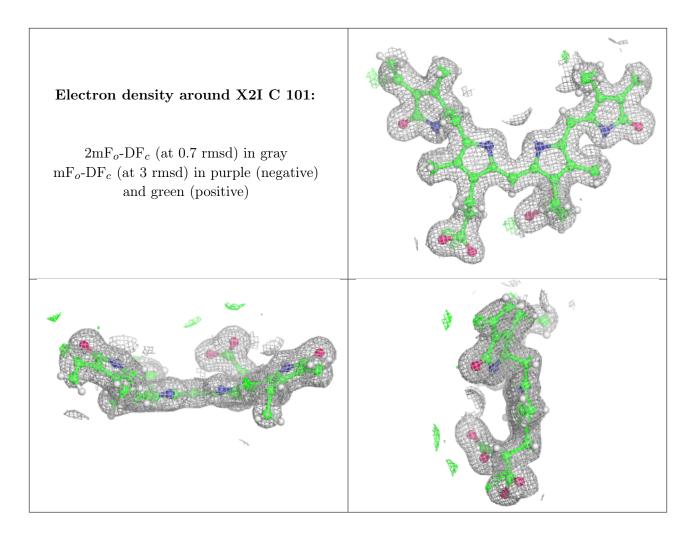




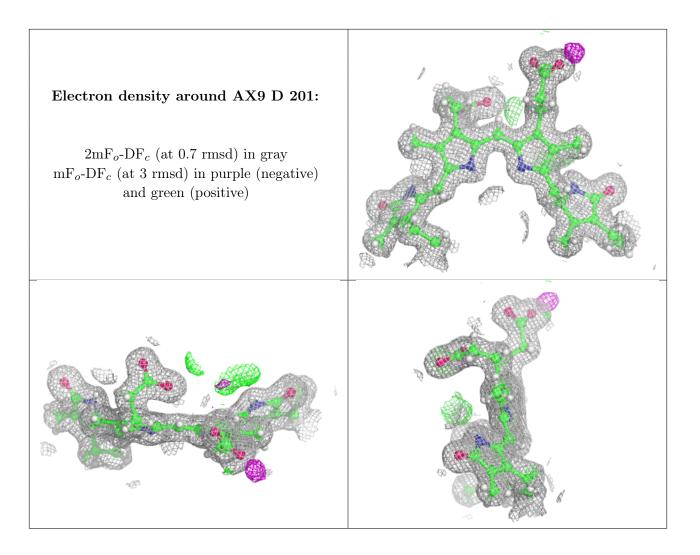




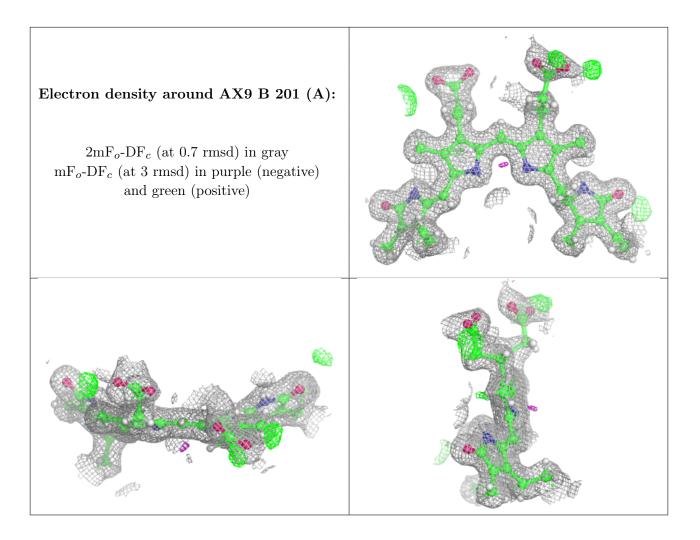




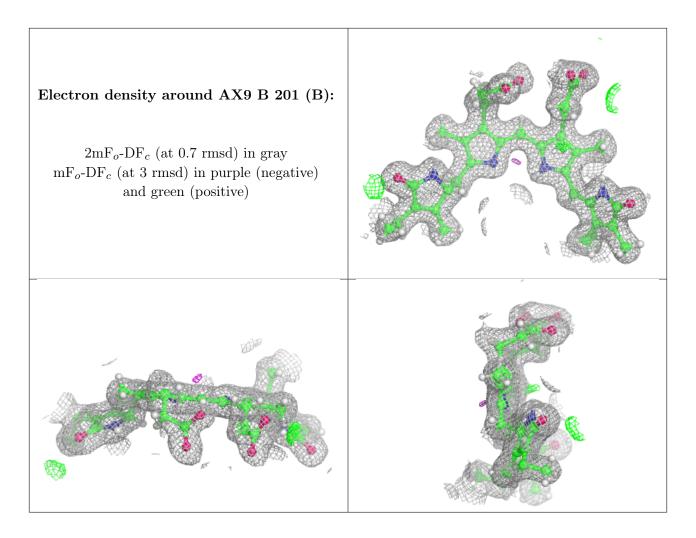












6.5 Other polymers (i)

There are no such residues in this entry.

