



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 06:07 pm BST

PDB ID : 6UXJ  
Title : Structure of serine hydroxymethyltransferase 8 from Glycine max cultivar Essex complexed with PLP-glycine and 5-formyltetrahydrofolate  
Authors : Korasick, D.A.; Tanner, J.J.; Beamer, L.J.  
Deposited on : 2019-11-07  
Resolution : 1.40 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

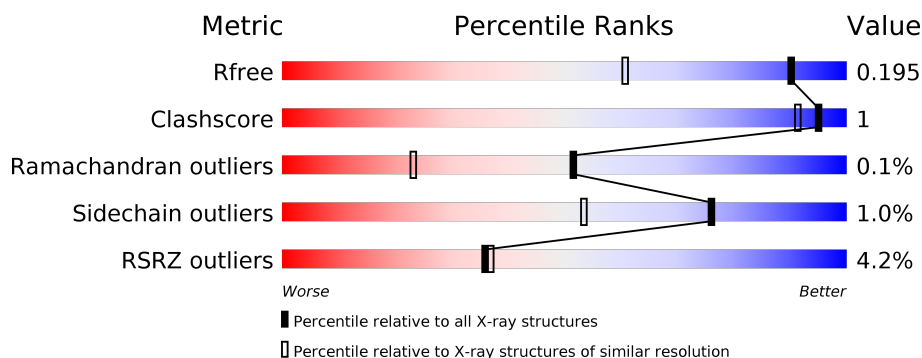
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	473	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
1	B	473	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>
1	C	473	<div> <div>3%</div> <div>96%</div> <div>.</div> </div>
1	D	473	<div> <div>6%</div> <div>97%</div> <div>.</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16819 atoms, of which 0 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.

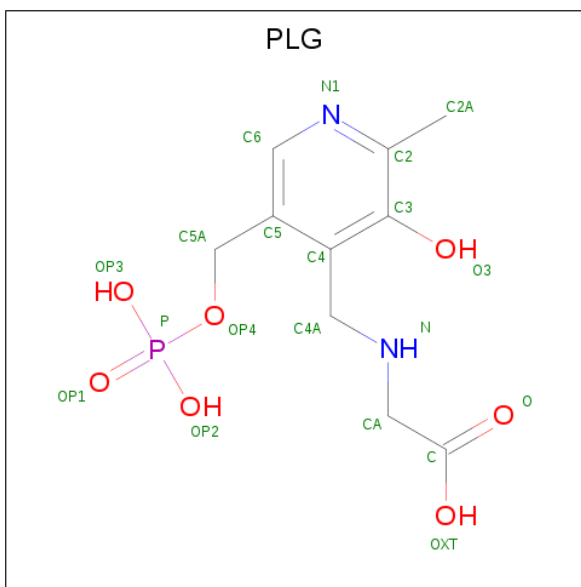
- Molecule 1 is a protein called Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	5	0
			3655	2329	626	683	17			
1	B	472	Total	C	N	O	S	0	9	0
			3684	2350	629	688	17			
1	C	472	Total	C	N	O	S	0	9	0
			3677	2346	628	686	17			
1	D	472	Total	C	N	O	S	0	7	0
			3670	2337	628	688	17			

There are 8 discrepancies between the modelled and reference sequences:

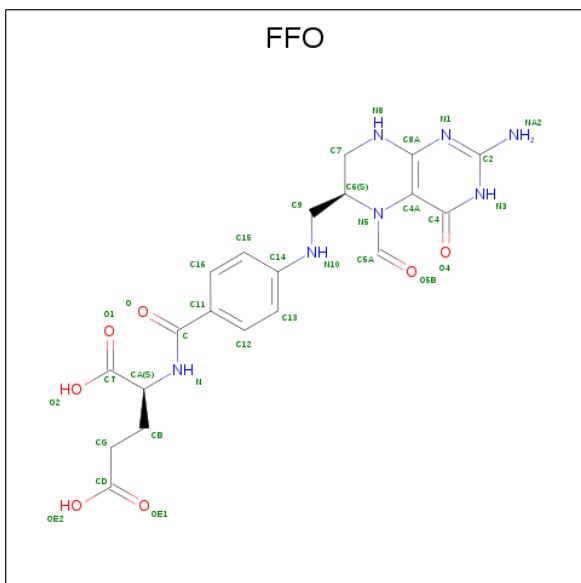
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP K4FZF8
A	0	HIS	-	expression tag	UNP K4FZF8
B	-1	SER	-	expression tag	UNP K4FZF8
B	0	HIS	-	expression tag	UNP K4FZF8
C	-1	SER	-	expression tag	UNP K4FZF8
C	0	HIS	-	expression tag	UNP K4FZF8
D	-1	SER	-	expression tag	UNP K4FZF8
D	0	HIS	-	expression tag	UNP K4FZF8

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>7</sub>P).



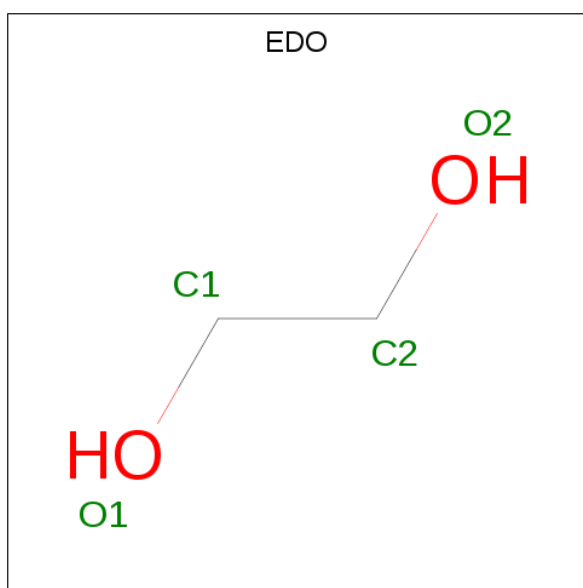
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 20	C 10	N 2	O 7	P 1	0	0
2	B	1	Total 20	C 10	N 2	O 7	P 1	0	0
2	C	1	Total 20	C 10	N 2	O 7	P 1	0	0
2	D	1	Total 20	C 10	N 2	O 7	P 1	0	0

- Molecule 3 is N-[4-({[(6S)-2-amino-5-formyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-glutamic acid (three-letter code: FFO) (formula: C<sub>20</sub>H<sub>23</sub>N<sub>7</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			68	40	14	14		
3	B	1	Total	C	N	O	0	1
			68	40	14	14		
3	C	1	Total	C	N	O	0	1
			68	40	14	14		
3	D	1	Total	C	N	O	0	1
			68	40	14	14		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

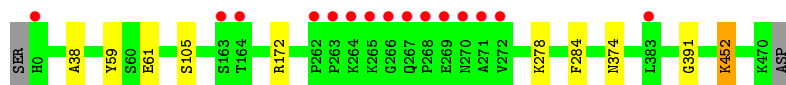
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	406	Total O 406 406	0	0
5	B	415	Total O 416 416	0	1
5	C	449	Total O 449 449	0	0
5	D	442	Total O 442 442	0	0

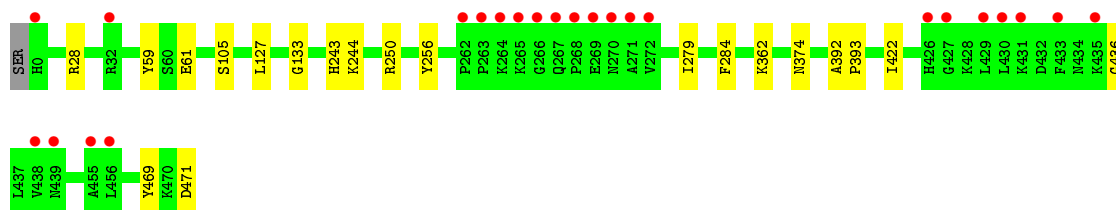
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Serine hydroxymethyltransferase



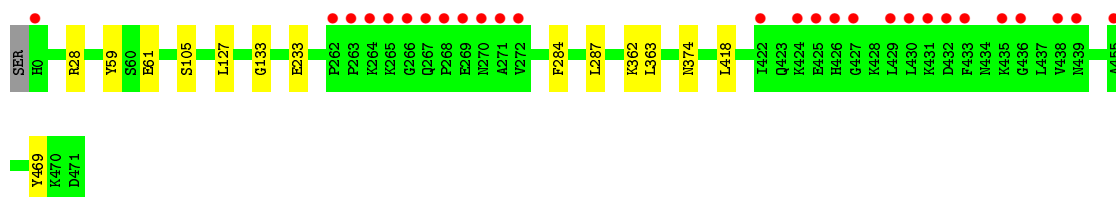
- Molecule 1: Serine hydroxymethyltransferase



- Molecule 1: Serine hydroxymethyltransferase



- Molecule 1: Serine hydroxymethyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.89Å 90.76Å 146.85Å 90.00° 90.81° 90.00°	Depositor
Resolution (Å)	45.38 – 1.40 47.95 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.38-1.40) 98.2 (47.95-1.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, $R_{free}$	0.165 , 0.194 0.165 , 0.195	Depositor DCC
$R_{free}$ test set	21604 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -k,-h,-l 0.000 for k,h,-l 0.013 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FFO, PLG, EDO

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	0.31	0/3755	0.53	0/5083
1	B	0.32	0/3796	0.54	0/5135
1	C	0.32	0/3789	0.55	0/5128
1	D	0.33	0/3776	0.54	0/5109
All	All	0.32	0/15116	0.54	0/20455

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	3655	0	3617	5	0
1	B	3684	0	3663	8	0
1	C	3677	0	3653	10	0
1	D	3670	0	3630	6	0
2	A	20	0	12	2	0
2	B	20	0	12	2	0
2	C	20	0	12	2	0
2	D	20	0	12	2	0
3	A	68	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	68	0	42	0	0
3	C	68	0	42	1	0
3	D	68	0	42	0	0
4	A	16	0	24	0	0
4	B	12	0	18	0	0
4	C	20	0	30	3	0
4	D	20	0	30	0	0
5	A	406	0	0	3	0
5	B	416	0	0	1	0
5	C	449	0	0	3	0
5	D	442	0	0	2	0
All	All	16819	0	14881	37	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 1.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ARG:NH1	1:C:175:GLU:OE1	2.18	0.76
1:C:373[B]:LYS:NZ	5:C:901:HOH:O	2.24	0.70
1:C:142:SER:HA	4:C:805:EDO:H11	1.77	0.65
5:A:625:HOH:O	2:B:501:PLG:H4A1	2.04	0.56
5:C:928:HOH:O	2:D:704:PLG:H4A1	2.07	0.55
2:A:501:PLG:H4A1	5:B:610:HOH:O	2.11	0.51
1:B:422:ILE:HG23	1:B:436:GLY:HA3	1.91	0.51
2:A:501:PLG:O3	2:A:501:PLG:N	2.44	0.51
2:B:501:PLG:O3	2:B:501:PLG:N	2.46	0.49
1:A:172:ARG:NH1	5:A:604:HOH:O	2.45	0.49
1:C:21:ASP:OD2	1:C:25:LYS:NZ	2.43	0.48
2:C:802:PLG:H4A1	5:D:810:HOH:O	2.12	0.48
2:D:704:PLG:N	2:D:704:PLG:O3	2.45	0.48
2:C:802:PLG:O3	2:C:802:PLG:N	2.46	0.48
1:A:278:LYS:HG3	5:A:630:HOH:O	2.14	0.47
1:D:28:ARG:HD2	1:D:469:TYR:HB3	1.98	0.46
1:C:133:GLY:O	3:C:803[B]:FFO:N3	2.45	0.45
1:B:28:ARG:NE	1:B:471:ASP:OXT	2.46	0.44
1:A:38:ALA:HA	1:A:391:GLY:HA3	2.01	0.43
1:D:61:GLU:HB3	1:D:284:PHE:CZ	2.52	0.43
1:A:61:GLU:HB3	1:A:284:PHE:CZ	2.54	0.43
1:C:140:TYR:CE2	4:C:805:EDO:H22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:O	1:B:133:GLY:HA3	2.19	0.42
1:B:61:GLU:HB3	1:B:284:PHE:CZ	2.55	0.42
1:B:28:ARG:HD2	1:B:469:TYR:HB3	2.02	0.42
1:A:452:LYS:HE2	1:A:452:LYS:HB2	1.82	0.41
1:B:243:HIS:ND1	1:B:250:ARG:HA	2.35	0.41
1:D:127:LEU:O	1:D:133:GLY:HA3	2.21	0.41
1:D:363:LEU:HD11	1:D:418:LEU:HG	2.02	0.41
4:C:806:EDO:H22	1:D:287:LEU:HD22	2.02	0.41
1:C:278:LYS:HG3	5:C:971:HOH:O	2.20	0.41
1:C:32:ARG:HD3	1:C:32:ARG:HA	1.86	0.40
1:B:392:ALA:N	1:B:393:PRO:CD	2.84	0.40
1:C:465:SER:O	1:C:470:LYS:NZ	2.52	0.40
1:C:127:LEU:O	1:C:133:GLY:HA3	2.20	0.40
1:D:233[B]:GLU:OE2	5:D:801:HOH:O	2.22	0.40
1:B:256:TYR:HB3	1:B:279[A]:ILE:HD12	2.02	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	474/473 (100%)	461 (97%)	13 (3%)	0	100	100
1	B	479/473 (101%)	469 (98%)	9 (2%)	1 (0%)	47	21
1	C	479/473 (101%)	467 (98%)	12 (2%)	0	100	100
1	D	477/473 (101%)	465 (98%)	12 (2%)	0	100	100
All	All	1909/1892 (101%)	1862 (98%)	46 (2%)	1 (0%)	51	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	LYS

### 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	385/387 (100%)	381 (99%)	4 (1%)	76	53
1	B	390/387 (101%)	385 (99%)	5 (1%)	69	42
1	C	389/387 (100%)	386 (99%)	3 (1%)	81	62
1	D	387/387 (100%)	383 (99%)	4 (1%)	76	53
All	All	1551/1548 (100%)	1535 (99%)	16 (1%)	76	53

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	105	SER
1	A	374	ASN
1	A	452	LYS
1	B	59	TYR
1	B	105	SER
1	B	362[A]	LYS
1	B	362[B]	LYS
1	B	374	ASN
1	C	59	TYR
1	C	105	SER
1	C	374	ASN
1	D	59	TYR
1	D	105	SER
1	D	362	LYS
1	D	374	ASN

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	D	703	-	3,3,3	0.48	0	2,2,2	0.13	0
3	FFO	D	705[B]	-	28,36,36	4.69	15 (53%)	28,50,50	2.12	7 (25%)
4	EDO	C	804	-	3,3,3	0.42	0	2,2,2	0.31	0
3	FFO	B	502[B]	-	28,36,36	4.91	15 (53%)	28,50,50	1.89	6 (21%)
3	FFO	B	502[A]	-	28,36,36	4.40	14 (50%)	28,50,50	1.99	6 (21%)
4	EDO	D	701	-	3,3,3	0.44	0	2,2,2	0.15	0
4	EDO	C	801	-	3,3,3	0.45	0	2,2,2	0.45	0
4	EDO	D	707	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	C	805	-	3,3,3	0.47	0	2,2,2	0.46	0
4	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.34	0
2	PLG	D	704	-	17,20,20	1.22	3 (17%)	23,28,28	1.61	5 (21%)
4	EDO	C	807	-	3,3,3	0.46	0	2,2,2	0.41	0
2	PLG	B	501	-	17,20,20	1.24	1 (5%)	23,28,28	1.64	6 (26%)
4	EDO	C	806	-	3,3,3	0.48	0	2,2,2	0.24	0
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.31	0
4	EDO	A	506	-	3,3,3	0.48	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	D	706	-	3,3,3	0.46	0	2,2,2	0.30	0
3	FFO	C	803[B]	-	28,36,36	4.54	15 (53%)	28,50,50	2.13	6 (21%)
3	FFO	C	803[A]	-	28,36,36	4.66	14 (50%)	28,50,50	1.95	7 (25%)
3	FFO	A	502[A]	-	28,36,36	4.52	14 (50%)	28,50,50	2.08	7 (25%)
2	PLG	C	802	-	17,20,20	1.20	2 (11%)	23,28,28	1.72	6 (26%)
4	EDO	A	504	-	3,3,3	0.49	0	2,2,2	0.33	0
4	EDO	B	504	-	3,3,3	0.44	0	2,2,2	0.21	0
3	FFO	A	502[B]	-	28,36,36	4.89	15 (53%)	28,50,50	1.90	6 (21%)
2	PLG	A	501	-	17,20,20	1.29	2 (11%)	23,28,28	1.60	6 (26%)
4	EDO	D	702	-	3,3,3	0.49	0	2,2,2	0.33	0
4	EDO	B	505	-	3,3,3	0.48	0	2,2,2	0.25	0
4	EDO	A	503	-	3,3,3	0.47	0	2,2,2	0.41	0
3	FFO	D	705[A]	-	28,36,36	4.69	15 (53%)	28,50,50	1.93	6 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	703	-	-	0/1/1/1	-
3	FFO	D	705[B]	-	-	1/18/37/37	0/2/3/3
4	EDO	C	804	-	-	0/1/1/1	-
3	FFO	B	502[B]	-	-	1/18/37/37	0/2/3/3
3	FFO	B	502[A]	-	-	1/18/37/37	0/2/3/3
4	EDO	D	701	-	-	0/1/1/1	-
4	EDO	C	801	-	-	1/1/1/1	-
4	EDO	D	707	-	-	0/1/1/1	-
4	EDO	C	805	-	-	0/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
2	PLG	D	704	-	-	2/10/12/12	0/1/1/1
4	EDO	C	807	-	-	0/1/1/1	-
2	PLG	B	501	-	-	2/10/12/12	0/1/1/1
4	EDO	C	806	-	-	0/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	D	706	-	-	0/1/1/1	-
3	FFO	C	803[B]	-	-	0/18/37/37	0/2/3/3
3	FFO	C	803[A]	-	-	1/18/37/37	0/2/3/3
3	FFO	A	502[A]	-	-	1/18/37/37	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	C	802	-	-	2/10/12/12	0/1/1/1
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
3	FFO	A	502[B]	-	-	1/18/37/37	0/2/3/3
2	PLG	A	501	-	-	3/10/12/12	0/1/1/1
4	EDO	D	702	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
3	FFO	D	705[A]	-	-	1/18/37/37	0/2/3/3

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[B]	FFO	C7-C6	-11.47	1.38	1.52
3	A	502[B]	FFO	C7-C6	-11.44	1.38	1.52
3	D	705[B]	FFO	C7-C6	-11.14	1.39	1.52
3	C	803[B]	FFO	C7-C6	-11.10	1.39	1.52
3	C	803[A]	FFO	C7-C6	-11.07	1.39	1.52
3	D	705[A]	FFO	C7-C6	-11.05	1.39	1.52
3	B	502[A]	FFO	C7-C6	-10.92	1.39	1.52
3	A	502[A]	FFO	C7-C6	-10.58	1.39	1.52
3	B	502[B]	FFO	C2-N3	9.25	1.51	1.35
3	A	502[B]	FFO	C2-N3	9.19	1.51	1.35
3	D	705[B]	FFO	C2-N3	8.87	1.51	1.35
3	C	803[A]	FFO	C2-N3	8.68	1.50	1.35
3	D	705[A]	FFO	C2-N3	8.65	1.50	1.35
3	C	803[B]	FFO	C2-N3	8.55	1.50	1.35
3	A	502[A]	FFO	C2-N3	8.48	1.50	1.35
3	A	502[B]	FFO	C4-N3	8.29	1.47	1.33
3	B	502[B]	FFO	C4-N3	8.25	1.47	1.33
3	D	705[B]	FFO	C4-N3	8.05	1.47	1.33
3	B	502[A]	FFO	C2-N3	8.03	1.49	1.35
3	D	705[A]	FFO	C4-N3	7.93	1.46	1.33
3	C	803[B]	FFO	C4-N3	7.85	1.46	1.33
3	A	502[B]	FFO	C2-N1	7.84	1.49	1.35
3	B	502[B]	FFO	C2-N1	7.82	1.49	1.35
3	C	803[A]	FFO	C4-N3	7.80	1.46	1.33
3	A	502[A]	FFO	C4-N3	7.77	1.46	1.33
3	B	502[B]	FFO	C7-N8	7.76	1.57	1.44
3	A	502[B]	FFO	C7-N8	7.71	1.57	1.44
3	D	705[A]	FFO	C7-N8	7.58	1.57	1.44
3	D	705[B]	FFO	C7-N8	7.51	1.57	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	705[B]	FFO	C2-N1	7.48	1.48	1.35
3	B	502[B]	FFO	C5A-N5	7.45	1.45	1.35
3	C	803[A]	FFO	C7-N8	7.45	1.57	1.44
3	A	502[A]	FFO	C7-N8	7.43	1.57	1.44
3	D	705[A]	FFO	C2-N1	7.41	1.48	1.35
3	A	502[B]	FFO	C4-C4A	7.36	1.51	1.41
3	C	803[B]	FFO	C7-N8	7.35	1.57	1.44
3	B	502[A]	FFO	C4-N3	7.32	1.45	1.33
3	C	803[A]	FFO	C2-N1	7.30	1.48	1.35
3	A	502[B]	FFO	C5A-N5	7.29	1.45	1.35
3	B	502[B]	FFO	C4-C4A	7.22	1.51	1.41
3	B	502[A]	FFO	C7-N8	7.21	1.56	1.44
3	C	803[A]	FFO	C5A-N5	7.11	1.45	1.35
3	C	803[B]	FFO	C2-N1	7.07	1.48	1.35
3	D	705[A]	FFO	C4-C4A	7.03	1.51	1.41
3	D	705[A]	FFO	C5A-N5	7.03	1.45	1.35
3	A	502[A]	FFO	C2-N1	6.94	1.47	1.35
3	C	803[A]	FFO	C4-C4A	6.93	1.50	1.41
3	D	705[B]	FFO	C5A-N5	6.87	1.44	1.35
3	A	502[B]	FFO	C4A-C8A	6.84	1.54	1.41
3	B	502[B]	FFO	C4A-C8A	6.78	1.54	1.41
3	A	502[A]	FFO	C4-C4A	6.76	1.50	1.41
3	C	803[B]	FFO	C4-C4A	6.59	1.50	1.41
3	B	502[A]	FFO	C2-N1	6.59	1.47	1.35
3	A	502[A]	FFO	C5A-N5	6.56	1.44	1.35
3	D	705[B]	FFO	C4-C4A	6.54	1.50	1.41
3	A	502[A]	FFO	C4A-C8A	6.47	1.54	1.41
3	D	705[A]	FFO	C4A-C8A	6.41	1.54	1.41
3	C	803[A]	FFO	C4A-C8A	6.37	1.53	1.41
3	B	502[A]	FFO	C4-C4A	6.33	1.50	1.41
3	D	705[B]	FFO	C4A-C8A	6.27	1.53	1.41
3	B	502[A]	FFO	C5A-N5	6.18	1.43	1.35
3	C	803[B]	FFO	C5A-N5	6.17	1.43	1.35
3	B	502[A]	FFO	C4A-C8A	5.96	1.53	1.41
3	C	803[B]	FFO	C4A-C8A	5.72	1.52	1.41
3	B	502[B]	FFO	C2-NA2	5.67	1.45	1.33
3	B	502[B]	FFO	C8A-N1	5.66	1.45	1.34
3	A	502[B]	FFO	C8A-N1	5.59	1.45	1.34
3	A	502[B]	FFO	C2-NA2	5.45	1.44	1.33
3	D	705[B]	FFO	C8A-N1	5.42	1.44	1.34
3	D	705[A]	FFO	C8A-N1	5.25	1.44	1.34
3	C	803[B]	FFO	C-N	5.20	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	705[B]	FFO	C2-NA2	5.18	1.44	1.33
3	B	502[B]	FFO	C-N	5.18	1.45	1.34
3	C	803[A]	FFO	C8A-N1	5.14	1.44	1.34
3	A	502[B]	FFO	C-N	5.07	1.45	1.34
3	C	803[A]	FFO	C-N	5.05	1.45	1.34
3	C	803[A]	FFO	C2-NA2	5.01	1.43	1.33
3	D	705[A]	FFO	C2-NA2	5.01	1.43	1.33
3	B	502[A]	FFO	C-N	4.99	1.45	1.34
3	D	705[A]	FFO	C-N	4.99	1.45	1.34
3	D	705[B]	FFO	C-N	4.93	1.44	1.34
3	A	502[A]	FFO	C8A-N1	4.87	1.43	1.34
3	A	502[A]	FFO	C-N	4.81	1.44	1.34
3	C	803[B]	FFO	C2-NA2	4.75	1.43	1.33
3	C	803[B]	FFO	C8A-N1	4.64	1.43	1.34
3	B	502[A]	FFO	C8A-N1	4.62	1.43	1.34
3	A	502[A]	FFO	C2-NA2	4.61	1.43	1.33
3	B	502[A]	FFO	C2-NA2	4.43	1.42	1.33
3	B	502[A]	FFO	C4A-N5	-3.15	1.37	1.41
3	C	803[B]	FFO	C4A-N5	-3.10	1.37	1.41
3	A	502[A]	FFO	C4A-N5	-3.09	1.37	1.41
2	A	501	PLG	C5-C4	-2.98	1.36	1.40
2	B	501	PLG	C5-C4	-2.88	1.36	1.40
3	D	705[A]	FFO	C4A-N5	-2.72	1.37	1.41
3	D	705[B]	FFO	C4A-N5	-2.61	1.38	1.41
2	C	802	PLG	C5-C4	-2.55	1.36	1.40
3	B	502[A]	FFO	O4-C4	-2.53	1.18	1.24
3	C	803[B]	FFO	C14-N10	2.46	1.45	1.38
2	D	704	PLG	C5-C4	-2.45	1.37	1.40
3	D	705[A]	FFO	O4-C4	-2.37	1.18	1.24
3	A	502[B]	FFO	C4A-N5	-2.36	1.38	1.41
3	C	803[A]	FFO	C14-N10	2.34	1.45	1.38
3	C	803[A]	FFO	C4A-N5	-2.34	1.38	1.41
3	B	502[B]	FFO	O4-C4	-2.34	1.18	1.24
3	B	502[B]	FFO	C14-N10	2.32	1.45	1.38
3	A	502[B]	FFO	C14-N10	2.30	1.45	1.38
3	D	705[B]	FFO	C14-N10	2.25	1.45	1.38
3	C	803[B]	FFO	O4-C4	-2.24	1.18	1.24
3	D	705[A]	FFO	C14-N10	2.24	1.45	1.38
3	B	502[A]	FFO	C14-N10	2.24	1.45	1.38
3	D	705[B]	FFO	O-C	-2.23	1.18	1.23
3	A	502[B]	FFO	O4-C4	-2.22	1.19	1.24
3	A	502[A]	FFO	C14-N10	2.21	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	705[B]	FFO	O4-C4	-2.18	1.19	1.24
3	D	705[A]	FFO	O-C	-2.16	1.18	1.23
2	D	704	PLG	C3-C4	-2.15	1.36	1.40
2	C	802	PLG	C3-C4	-2.13	1.36	1.40
3	A	502[B]	FFO	O-C	-2.12	1.19	1.23
3	C	803[A]	FFO	O-C	-2.09	1.19	1.23
2	D	704	PLG	C3-C2	-2.05	1.38	1.40
3	B	502[B]	FFO	O-C	-2.02	1.19	1.23
3	A	502[A]	FFO	O-C	-2.02	1.19	1.23
3	C	803[B]	FFO	O-C	-2.01	1.19	1.23
3	B	502[B]	FFO	C4A-N5	-2.01	1.38	1.41
2	A	501	PLG	C3-C4	-2.00	1.37	1.40

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	803[B]	FFO	C4-C4A-C8A	6.92	119.85	114.44
3	A	502[A]	FFO	C4-C4A-C8A	6.88	119.82	114.44
3	D	705[B]	FFO	C4-C4A-C8A	6.74	119.71	114.44
3	B	502[A]	FFO	C4-C4A-C8A	6.50	119.52	114.44
3	D	705[A]	FFO	C4-C4A-C8A	6.48	119.51	114.44
3	A	502[B]	FFO	C4-C4A-C8A	5.72	118.91	114.44
3	C	803[A]	FFO	C4-C4A-C8A	5.67	118.88	114.44
3	B	502[B]	FFO	C4-C4A-C8A	5.23	118.53	114.44
3	C	803[B]	FFO	O5B-C5A-N5	-5.11	117.96	125.36
2	C	802	PLG	OP4-C5A-C5	4.50	117.92	109.35
2	D	704	PLG	OP4-C5A-C5	4.47	117.86	109.35
3	B	502[B]	FFO	C4A-N5-C6	-4.08	112.08	119.31
2	A	501	PLG	OP4-C5A-C5	4.06	117.08	109.35
3	A	502[B]	FFO	C4A-N5-C6	-3.99	112.23	119.31
3	C	803[A]	FFO	C4A-N5-C6	-3.95	112.30	119.31
3	D	705[B]	FFO	C4A-N5-C6	-3.82	112.53	119.31
3	D	705[A]	FFO	C4A-N5-C6	-3.74	112.67	119.31
3	B	502[A]	FFO	O5B-C5A-N5	-3.69	120.01	125.36
2	B	501	PLG	OP4-C5A-C5	3.69	116.38	109.35
3	A	502[A]	FFO	C4A-N5-C6	-3.69	112.77	119.31
3	D	705[B]	FFO	O5B-C5A-N5	-3.67	120.04	125.36
3	B	502[B]	FFO	N3-C2-N1	-3.58	119.81	125.42
3	B	502[A]	FFO	C4A-N5-C6	-3.57	112.97	119.31
3	D	705[B]	FFO	N3-C2-N1	-3.44	120.02	125.42
3	A	502[A]	FFO	O5B-C5A-N5	-3.41	120.42	125.36
3	C	803[B]	FFO	C4A-N5-C6	-3.39	113.30	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	803[A]	FFO	N3-C2-N1	-3.36	120.15	125.42
3	A	502[A]	FFO	C4-N3-C2	3.24	121.07	115.93
3	A	502[B]	FFO	N3-C2-N1	-3.20	120.40	125.42
2	B	501	PLG	C-CA-N	-3.19	104.92	111.43
3	C	803[A]	FFO	C4-N3-C2	3.12	120.89	115.93
3	D	705[A]	FFO	O5B-C5A-N5	-3.12	120.85	125.36
2	C	802	PLG	C-CA-N	-3.05	105.20	111.43
3	C	803[B]	FFO	N3-C2-N1	-2.99	120.73	125.42
3	D	705[B]	FFO	C4-N3-C2	2.97	120.65	115.93
3	B	502[B]	FFO	C4-N3-C2	2.92	120.58	115.93
2	A	501	PLG	C-CA-N	-2.90	105.51	111.43
3	C	803[B]	FFO	C2-N1-C8A	2.89	121.01	114.54
2	D	704	PLG	C-CA-N	-2.84	105.64	111.43
3	A	502[B]	FFO	C4-N3-C2	2.79	120.36	115.93
3	C	803[A]	FFO	O5B-C5A-N5	-2.78	121.33	125.36
2	C	802	PLG	C4A-C4-C3	2.76	123.00	120.04
3	A	502[A]	FFO	N3-C2-N1	-2.76	121.09	125.42
3	D	705[B]	FFO	C2-N1-C8A	2.71	120.61	114.54
3	B	502[B]	FFO	C2-N1-C8A	2.70	120.60	114.54
2	B	501	PLG	C5-C6-N1	-2.67	119.37	123.82
3	B	502[A]	FFO	N3-C2-N1	-2.62	121.31	125.42
3	B	502[A]	FFO	C4-N3-C2	2.56	120.00	115.93
3	D	705[A]	FFO	N3-C2-N1	-2.55	121.41	125.42
3	A	502[B]	FFO	C2-N1-C8A	2.55	120.25	114.54
2	B	501	PLG	C4A-C4-C5	-2.54	116.88	119.71
3	C	803[A]	FFO	C2-N1-C8A	2.53	120.20	114.54
3	A	502[A]	FFO	C4A-C4-N3	-2.53	117.95	123.14
2	B	501	PLG	C4A-C4-C3	2.52	122.74	120.04
2	C	802	PLG	C6-C5-C4	2.47	119.87	118.12
2	D	704	PLG	C5-C6-N1	-2.47	119.71	123.82
2	A	501	PLG	C4A-C4-C3	2.46	122.67	120.04
2	C	802	PLG	C4A-C4-C5	-2.44	117.00	119.71
3	B	502[A]	FFO	C2-N1-C8A	2.43	119.98	114.54
3	D	705[A]	FFO	C2-N1-C8A	2.39	119.90	114.54
2	C	802	PLG	C5-C6-N1	-2.37	119.87	123.82
2	B	501	PLG	C6-C5-C4	2.36	119.79	118.12
3	D	705[A]	FFO	C4-N3-C2	2.34	119.65	115.93
2	D	704	PLG	C4A-C4-C3	2.33	122.54	120.04
3	B	502[B]	FFO	O5B-C5A-N5	-2.32	122.00	125.36
3	C	803[A]	FFO	NA2-C2-N1	2.27	120.79	117.25
2	A	501	PLG	C5-C6-N1	-2.27	120.04	123.82
3	A	502[B]	FFO	O5B-C5A-N5	-2.25	122.10	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	704	PLG	C6-C5-C4	2.21	119.68	118.12
3	A	502[A]	FFO	C2-N1-C8A	2.18	119.42	114.54
3	C	803[B]	FFO	C4-N3-C2	2.17	119.37	115.93
2	A	501	PLG	C4A-C4-C5	-2.15	117.32	119.71
2	A	501	PLG	C6-C5-C4	2.12	119.62	118.12
3	D	705[B]	FFO	NA2-C2-N1	2.01	120.38	117.25

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	704	PLG	C5-C4-C4A-N
2	B	501	PLG	C5-C4-C4A-N
2	C	802	PLG	C3-C4-C4A-N
2	C	802	PLG	C5-C4-C4A-N
2	A	501	PLG	C3-C4-C4A-N
2	A	501	PLG	C5-C4-C4A-N
2	D	704	PLG	C3-C4-C4A-N
2	A	501	PLG	C5A-OP4-P-OP1
3	A	502[A]	FFO	CT-CA-N-C
3	A	502[B]	FFO	CT-CA-N-C
4	C	801	EDO	O1-C1-C2-O2
2	B	501	PLG	C3-C4-C4A-N
4	A	503	EDO	O1-C1-C2-O2
4	A	504	EDO	O1-C1-C2-O2
4	D	702	EDO	O1-C1-C2-O2
3	D	705[B]	FFO	CT-CA-N-C
3	B	502[A]	FFO	CT-CA-N-C
3	B	502[B]	FFO	CT-CA-N-C
3	C	803[A]	FFO	CT-CA-N-C
3	D	705[A]	FFO	CT-CA-N-C

There are no ring outliers.

7 monomers are involved in 12 short contacts:

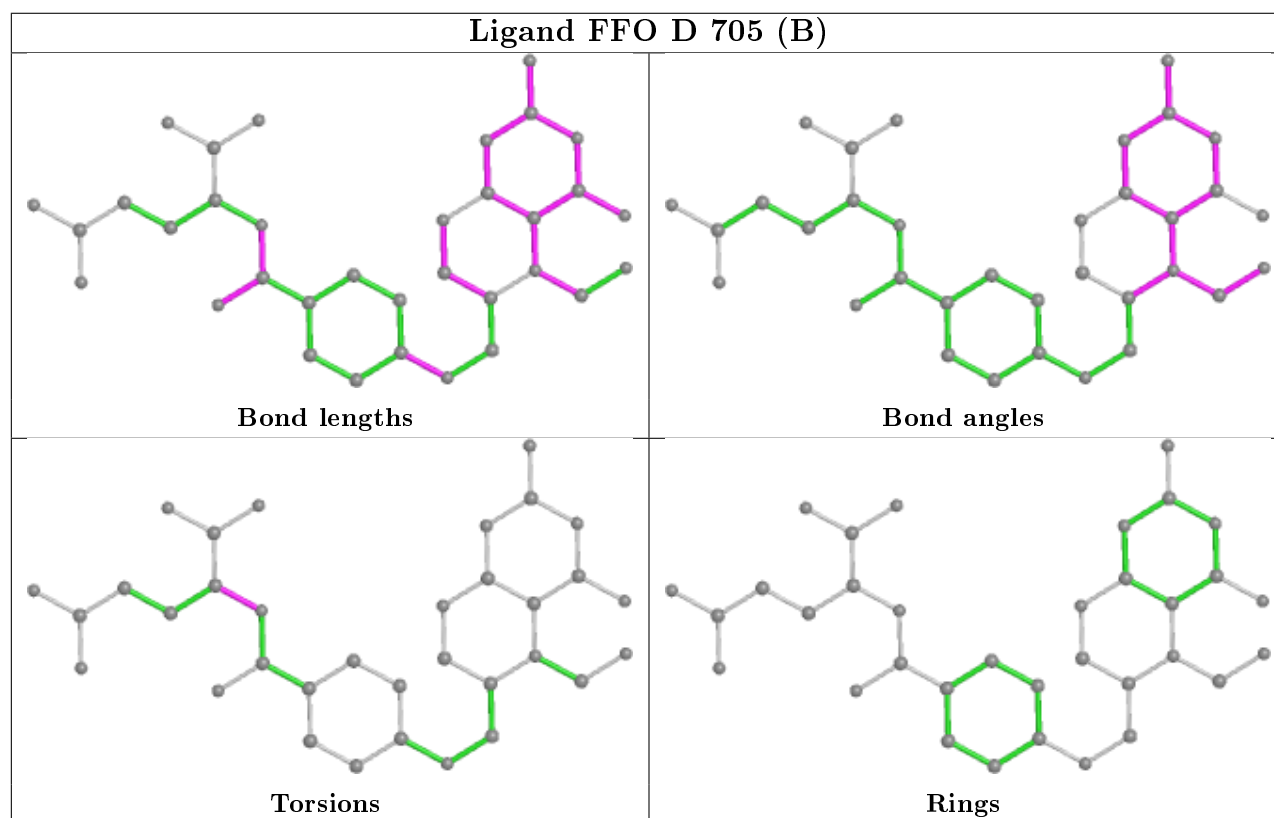
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	805	EDO	2	0
2	D	704	PLG	2	0
2	B	501	PLG	2	0
4	C	806	EDO	1	0
3	C	803[B]	FFO	1	0

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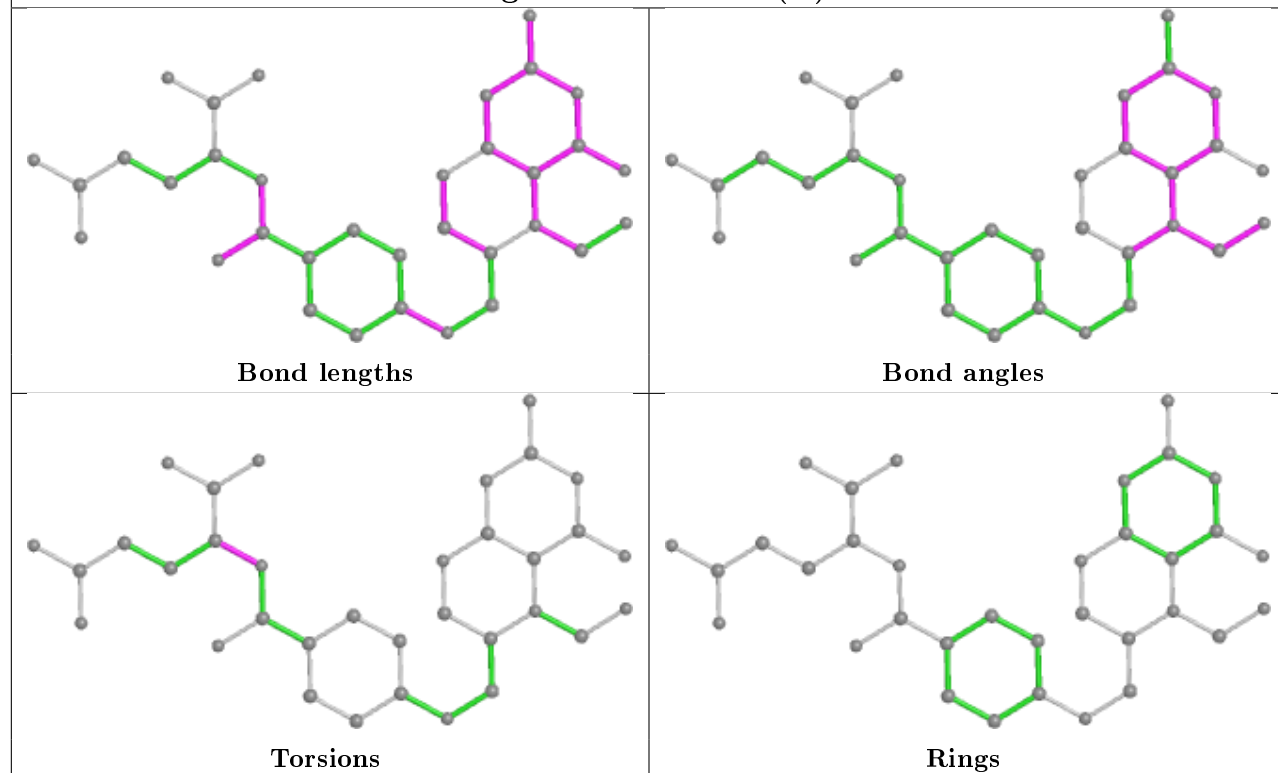
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	PLG	2	0
2	A	501	PLG	2	0

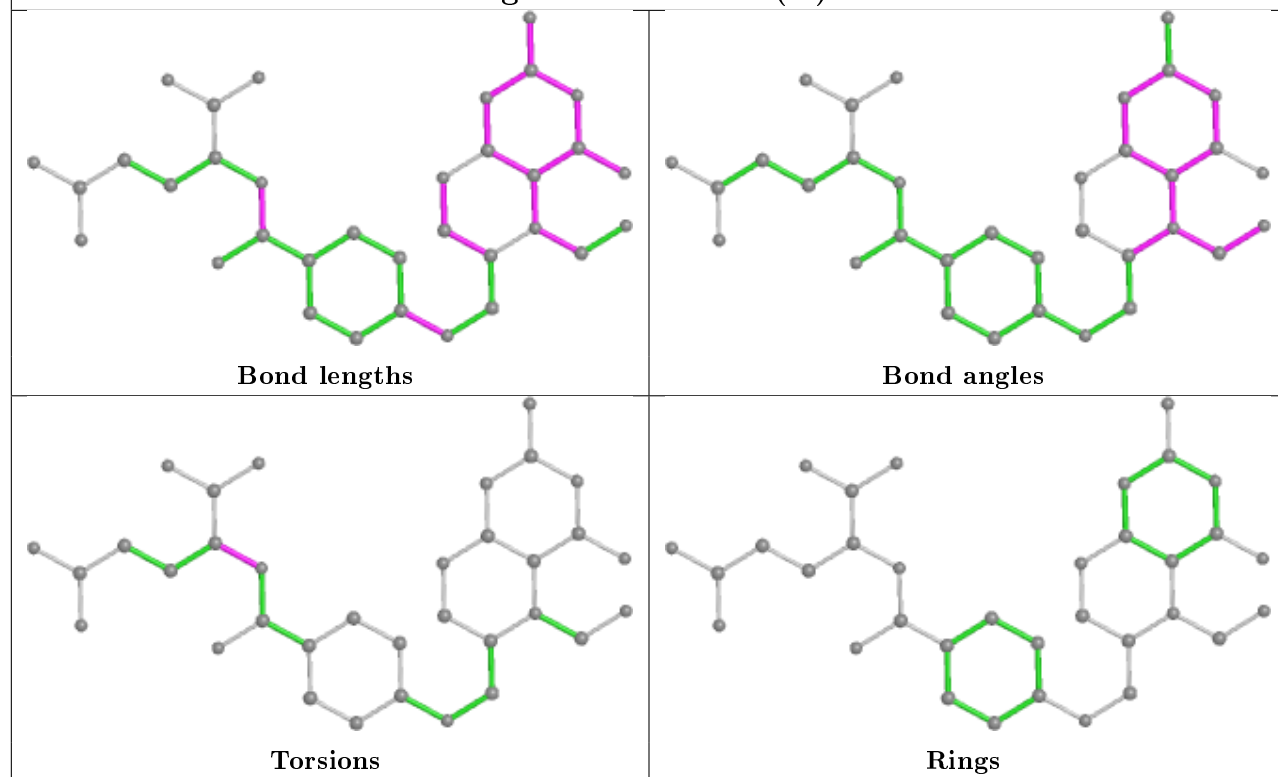
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

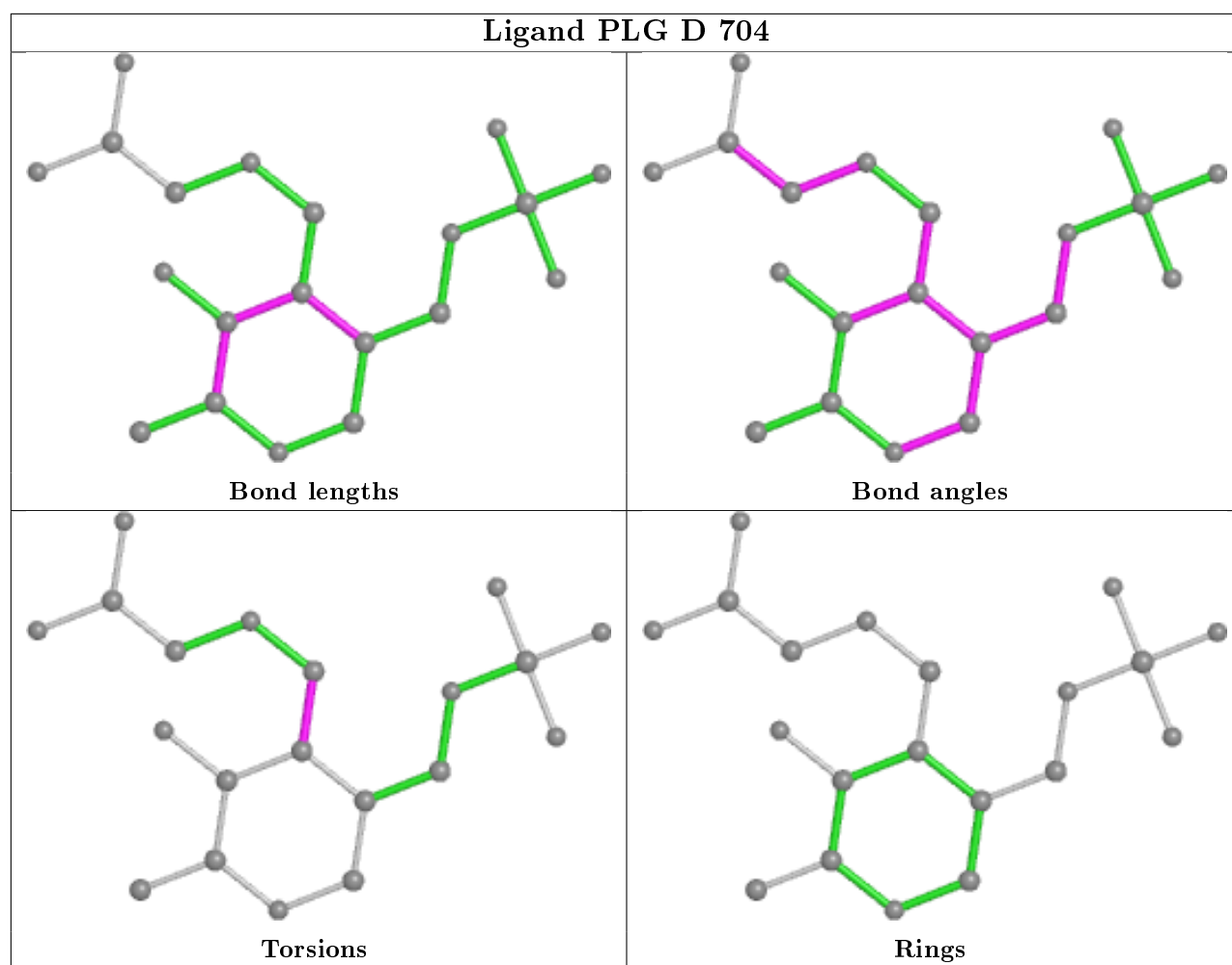


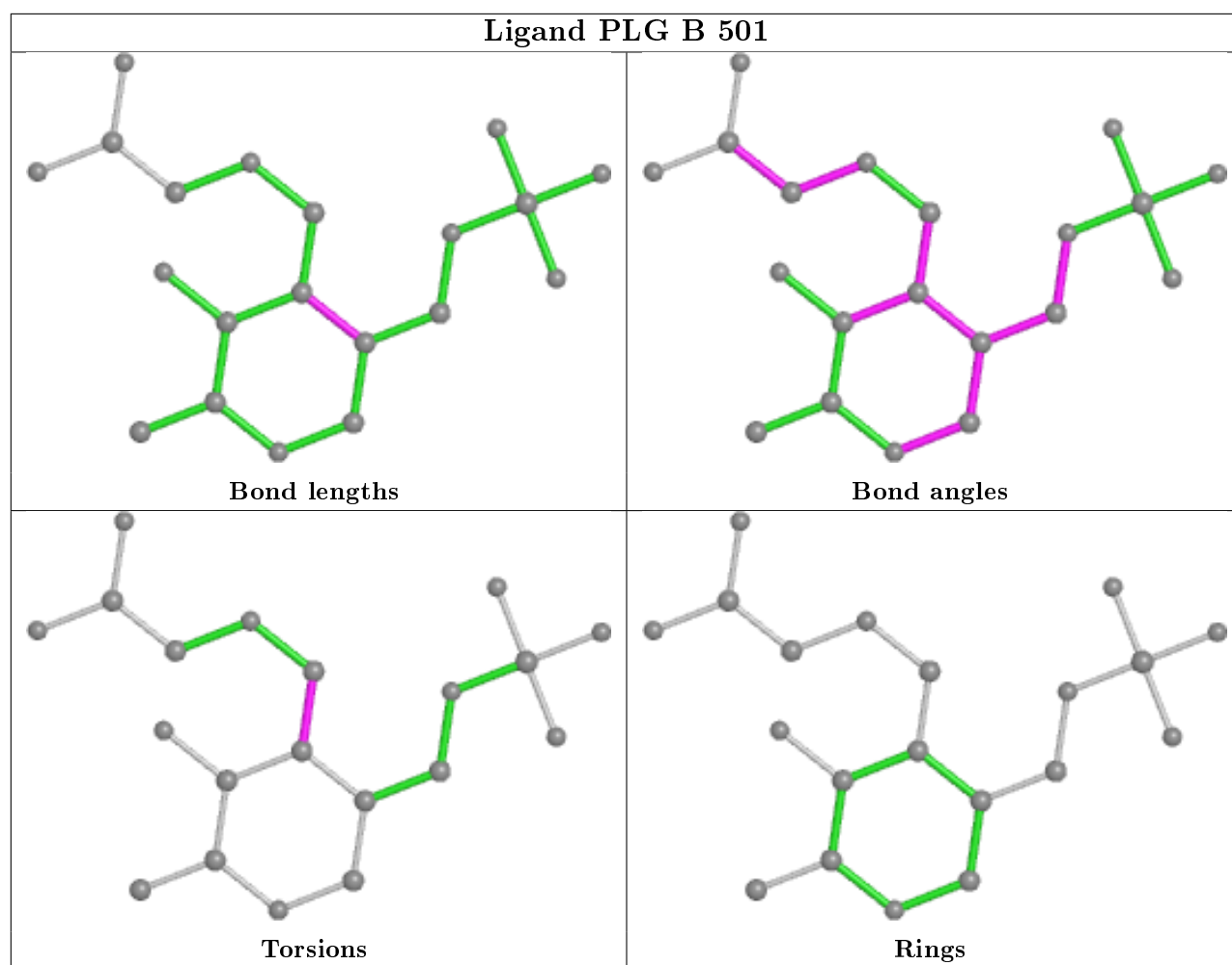
## Ligand FFO B 502 (B)



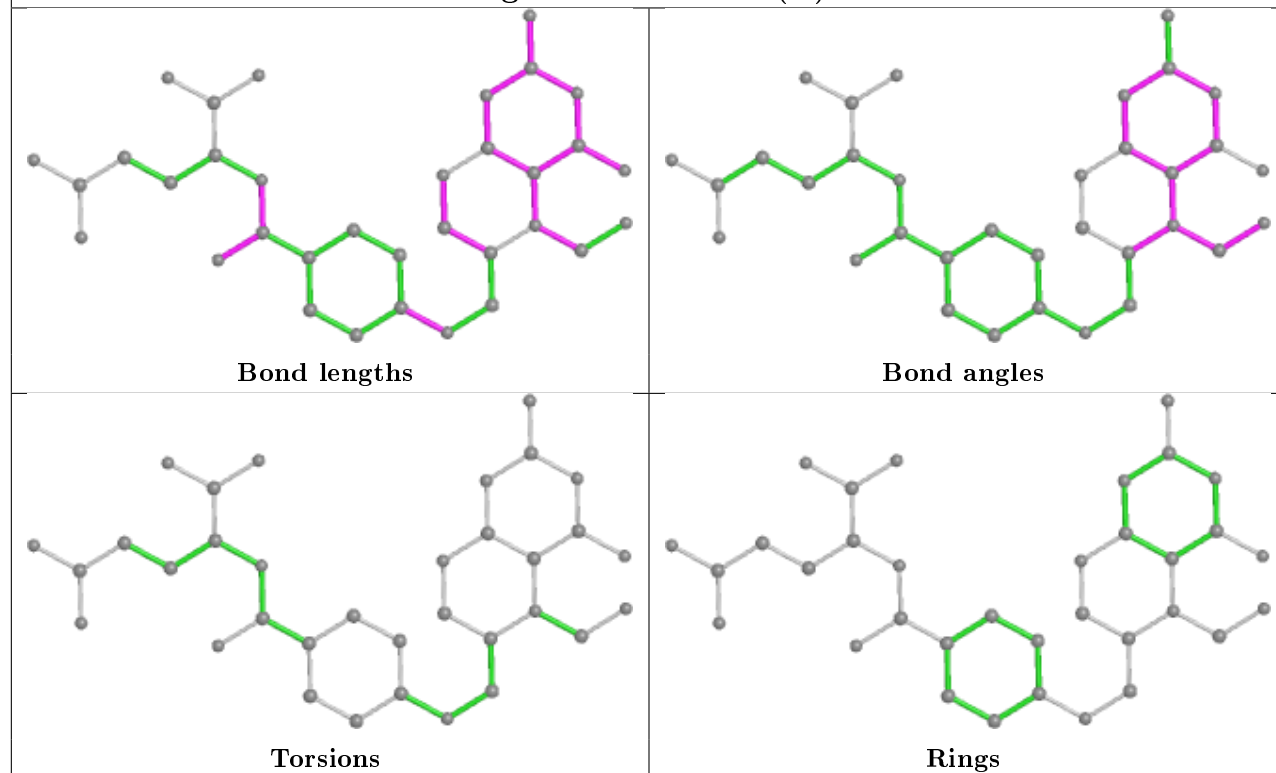
## Ligand FFO B 502 (A)



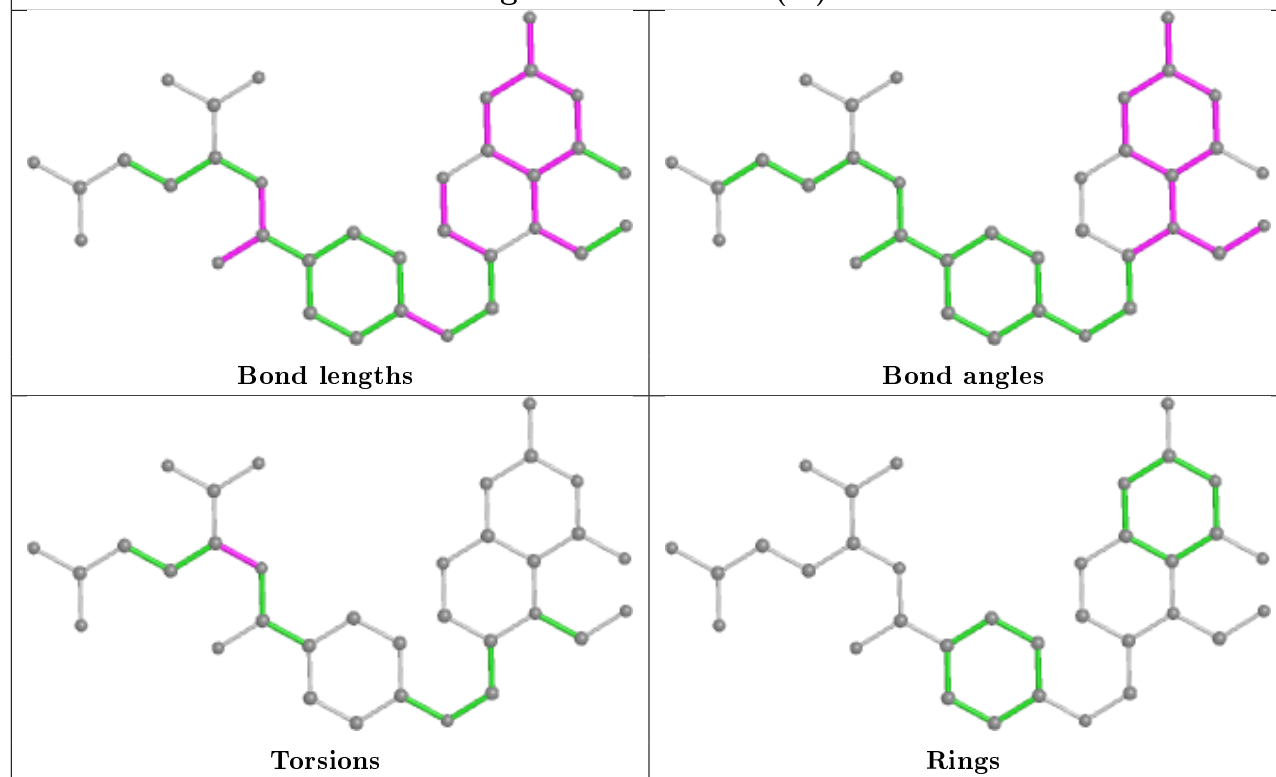


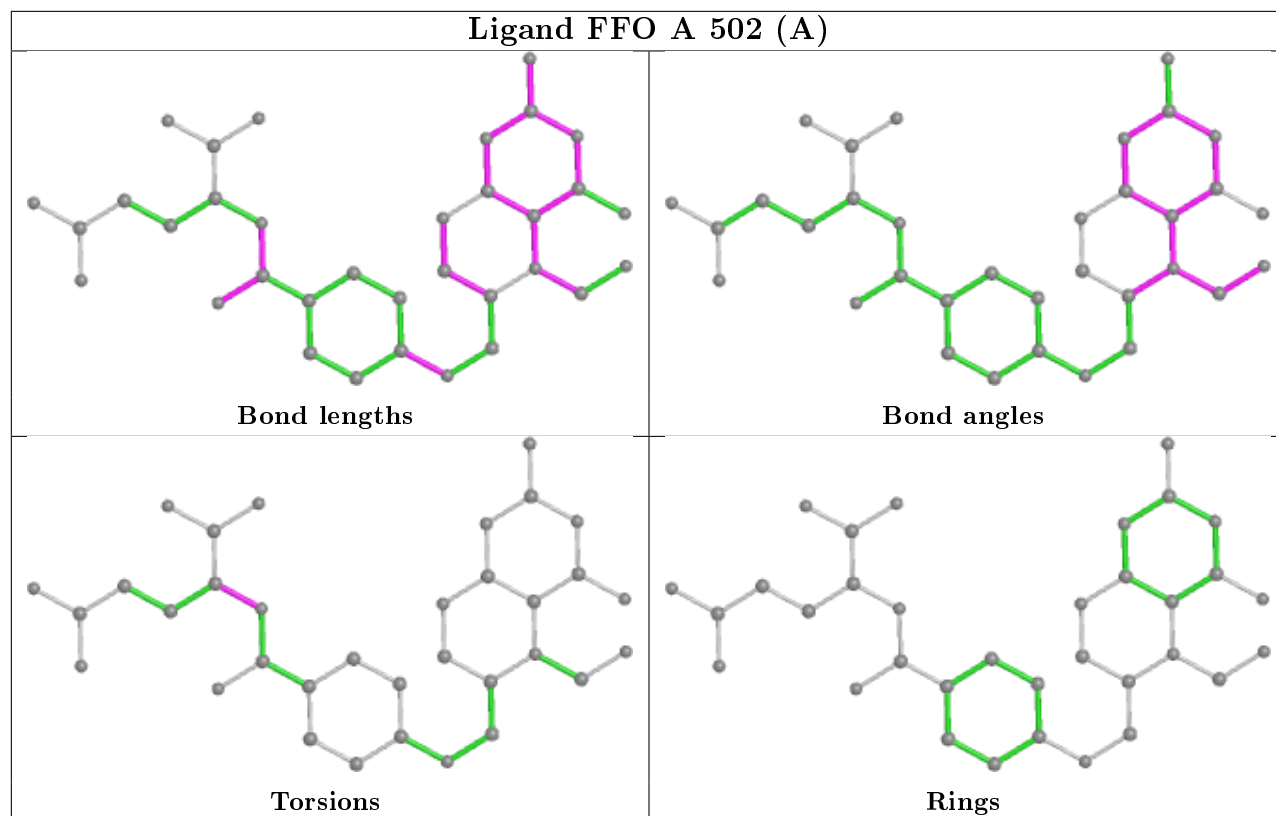


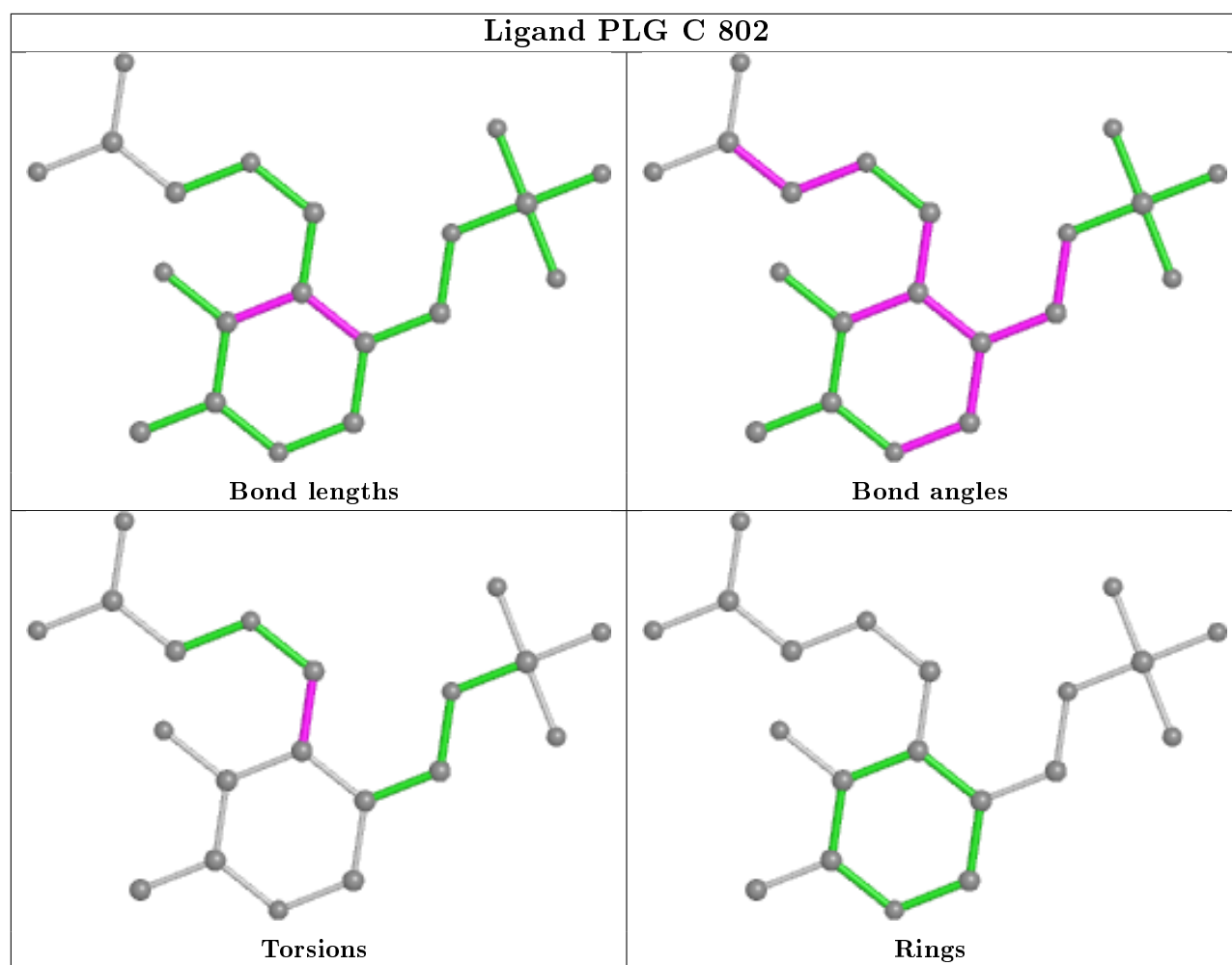
## Ligand FFO C 803 (B)

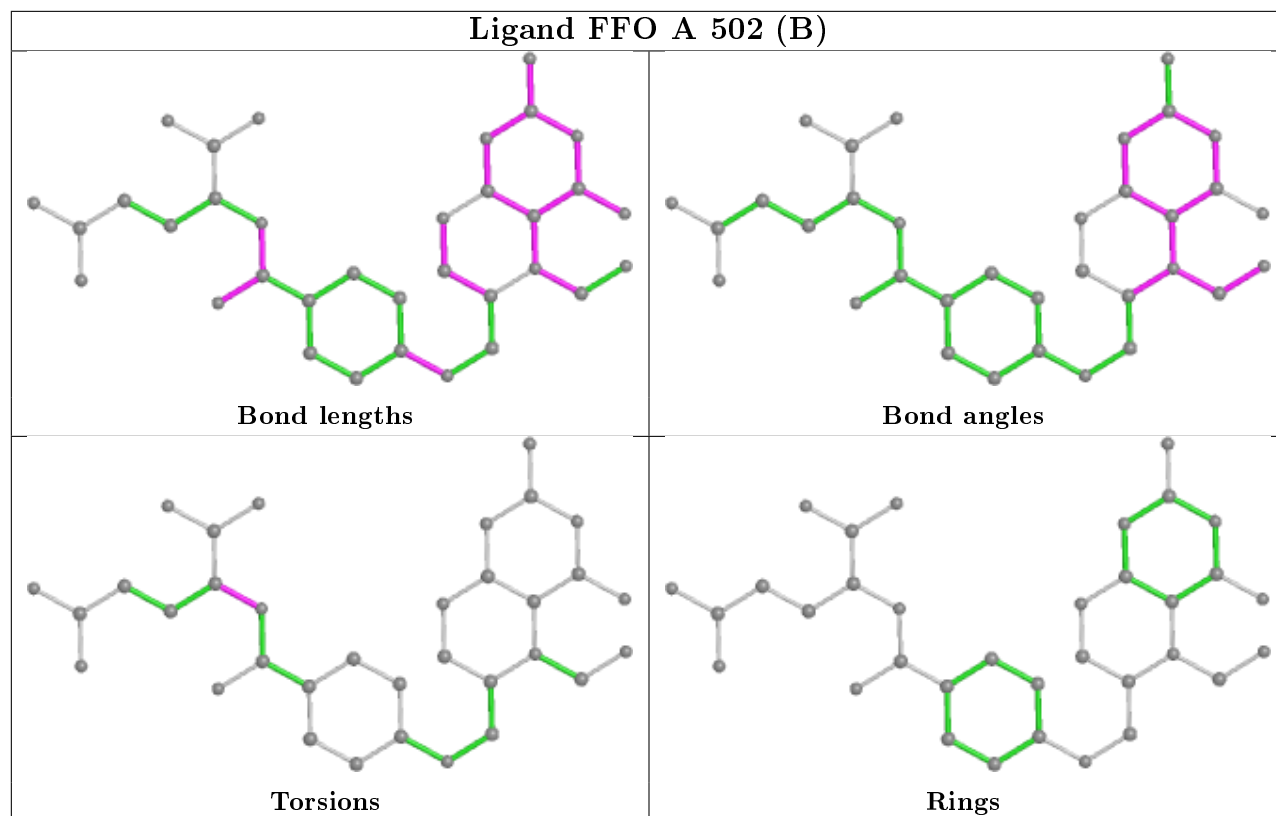


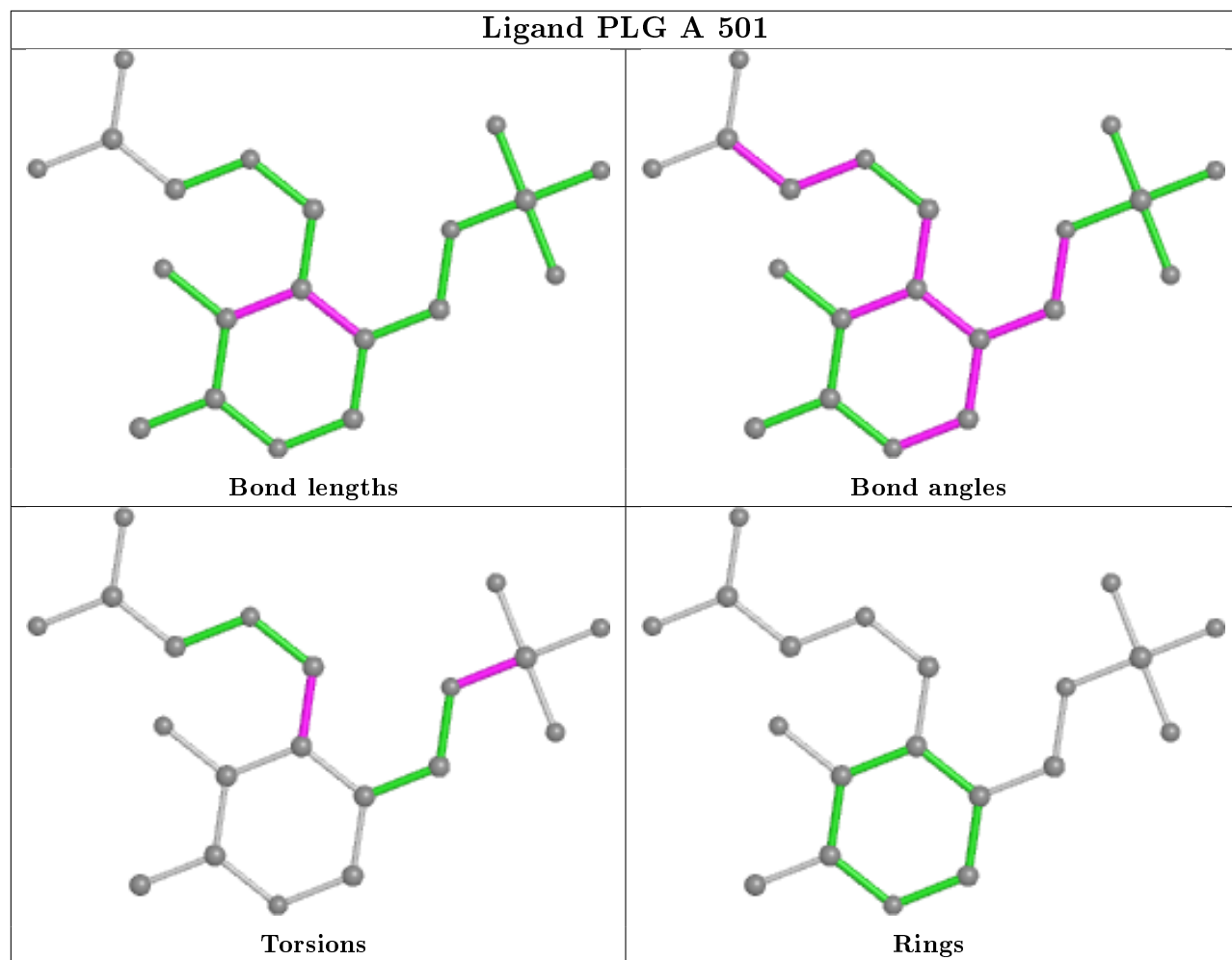
## Ligand FFO C 803 (A)

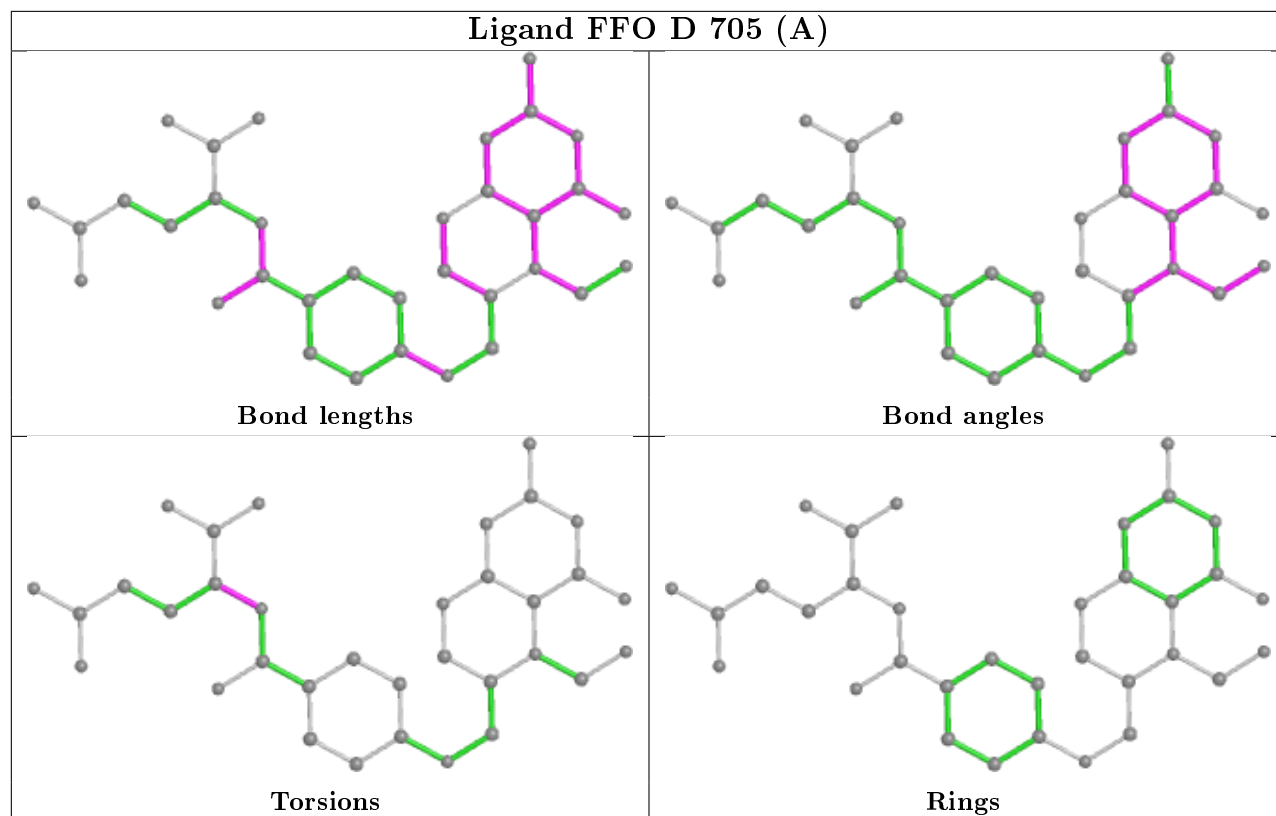












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	471/473 (99%)	-0.18	15 (3%)	47 46	11, 17, 33, 66	0
1	B	472/473 (99%)	-0.16	24 (5%)	28 27	10, 16, 42, 72	0
1	C	472/473 (99%)	-0.28	13 (2%)	53 52	10, 14, 29, 59	0
1	D	472/473 (99%)	-0.06	27 (5%)	23 22	10, 15, 43, 75	0
All	All	1887/1892 (99%)	-0.17	79 (4%)	36 37	10, 16, 38, 75	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	266	GLY	10.6
1	A	266	GLY	9.0
1	B	266	GLY	8.0
1	D	265	LYS	6.9
1	C	266	GLY	6.4
1	D	438	VAL	6.2
1	A	268	PRO	6.2
1	B	265	LYS	6.1
1	A	263	PRO	5.9
1	D	0	HIS	5.6
1	D	264	LYS	5.6
1	B	268	PRO	5.5
1	B	263	PRO	5.3
1	D	429	LEU	5.3
1	D	267	GLN	5.2
1	A	0	HIS	5.2
1	C	-1	SER	4.9
1	C	0	HIS	4.9
1	D	262	PRO	4.9
1	B	456	LEU	4.9
1	D	263	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	4.8
1	A	265	LYS	4.8
1	D	268	PRO	4.7
1	D	439	ASN	4.6
1	B	429	LEU	4.6
1	B	270	ASN	4.6
1	D	270	ASN	4.4
1	B	267	GLN	4.3
1	B	438	VAL	4.1
1	B	262	PRO	4.1
1	A	264	LYS	4.1
1	D	426	HIS	4.1
1	A	270	ASN	4.0
1	B	271	ALA	4.0
1	D	271	ALA	4.0
1	A	267	GLN	3.9
1	B	269	GLU	3.8
1	A	269	GLU	3.7
1	B	264	LYS	3.7
1	C	268	PRO	3.6
1	B	455	ALA	3.6
1	C	269	GLU	3.5
1	B	426	HIS	3.4
1	D	269	GLU	3.4
1	D	430	LEU	3.3
1	D	435	LYS	3.3
1	D	433	PHE	3.2
1	B	430	LEU	3.1
1	C	270	ASN	3.1
1	B	435	LYS	3.0
1	A	164	THR	3.0
1	D	424	LYS	2.9
1	B	439	ASN	2.9
1	C	265	LYS	2.8
1	B	272	VAL	2.8
1	B	433	PHE	2.7
1	B	427	GLY	2.7
1	B	431	LYS	2.7
1	C	263	PRO	2.6
1	D	455	ALA	2.6
1	D	425	GLU	2.6
1	D	272	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	383	LEU	2.5
1	D	432	ASP	2.5
1	C	267	GLN	2.5
1	D	431	LYS	2.4
1	A	271	ALA	2.4
1	C	429	LEU	2.4
1	A	262	PRO	2.4
1	A	163	SER	2.4
1	D	436	GLY	2.4
1	B	32	ARG	2.3
1	D	422	ILE	2.3
1	A	383	LEU	2.3
1	A	272	VAL	2.3
1	C	262	PRO	2.2
1	D	427	GLY	2.2
1	C	272	VAL	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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	C	807	4/4	0.79	0.14	37,37,39,40	0
4	EDO	C	801	4/4	0.84	0.12	41,42,44,45	0
4	EDO	A	503	4/4	0.84	0.12	35,35,36,38	0
4	EDO	D	706	4/4	0.85	0.12	35,35,36,38	0
4	EDO	B	503	4/4	0.87	0.10	31,32,32,33	0
4	EDO	A	504	4/4	0.88	0.11	37,37,38,38	0
4	EDO	D	707	4/4	0.90	0.11	28,28,29,31	0

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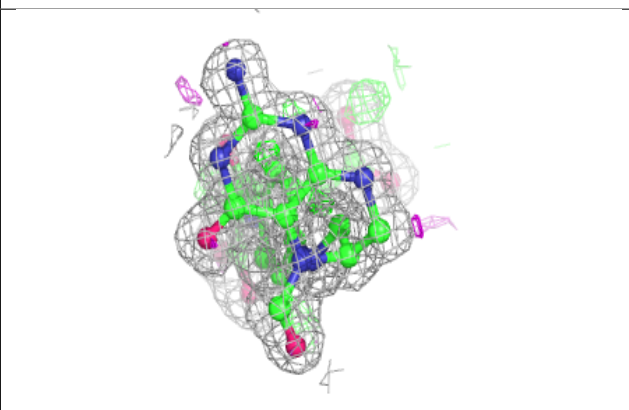
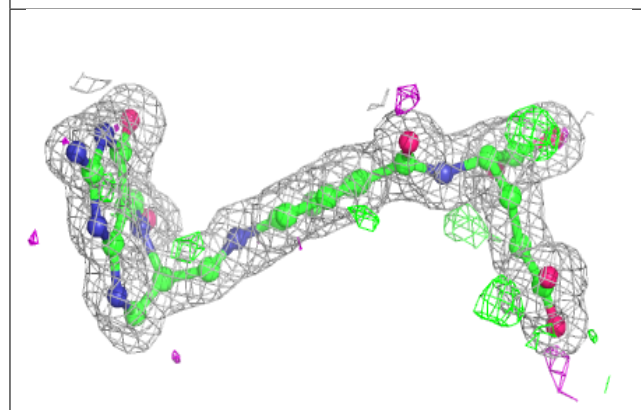
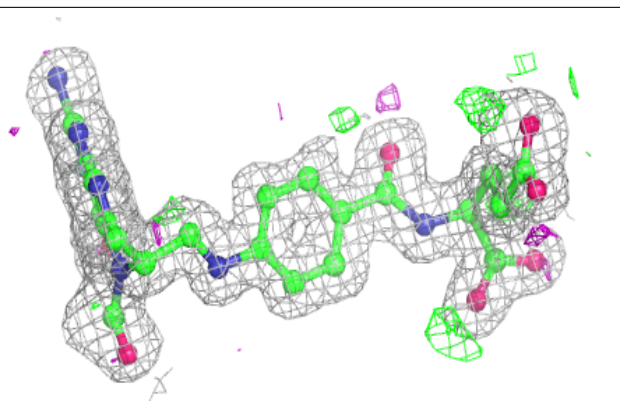
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	506	4/4	0.91	0.08	21,21,22,22	0
4	EDO	D	702	4/4	0.92	0.13	34,34,35,37	0
4	EDO	C	805	4/4	0.92	0.10	33,35,38,41	0
3	FFO	A	502[A]	34/34	0.95	0.09	11,12,23,25	34
3	FFO	B	502[B]	34/34	0.95	0.09	14,19,24,25	34
3	FFO	A	502[B]	34/34	0.95	0.09	12,19,25,25	34
3	FFO	B	502[A]	34/34	0.95	0.09	9,12,23,26	34
3	FFO	D	705[B]	34/34	0.95	0.09	9,13,25,26	34
3	FFO	D	705[A]	34/34	0.95	0.09	11,15,24,25	34
4	EDO	B	504	4/4	0.96	0.07	16,17,18,18	0
3	FFO	C	803[B]	34/34	0.96	0.08	7,12,23,26	34
3	FFO	C	803[A]	34/34	0.96	0.08	10,13,23,26	34
4	EDO	B	505	4/4	0.96	0.11	26,26,27,27	0
4	EDO	D	701	4/4	0.96	0.08	16,17,17,19	0
4	EDO	A	505	4/4	0.96	0.10	19,20,20,22	0
4	EDO	C	806	4/4	0.97	0.13	25,25,26,26	0
4	EDO	C	804	4/4	0.97	0.06	16,16,17,18	0
4	EDO	D	703	4/4	0.98	0.08	17,18,18,18	0
2	PLG	D	704	20/20	0.98	0.09	10,12,14,14	0
2	PLG	C	802	20/20	0.98	0.08	10,11,12,14	0
2	PLG	A	501	20/20	0.98	0.08	11,13,15,16	0
2	PLG	B	501	20/20	0.99	0.08	11,12,14,14	0

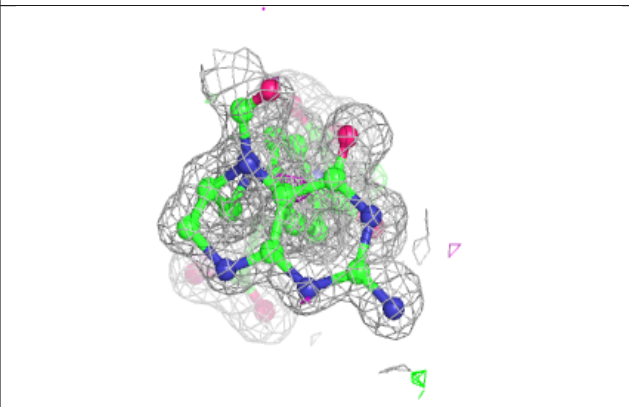
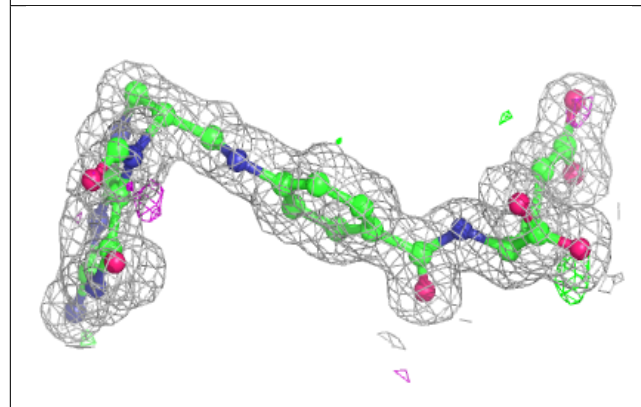
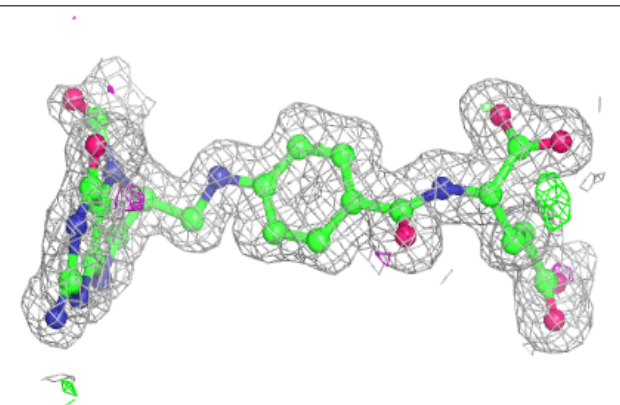
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FFO A 502 (A):**

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

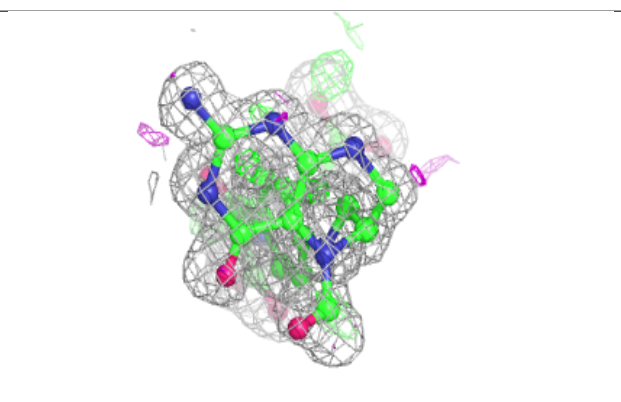
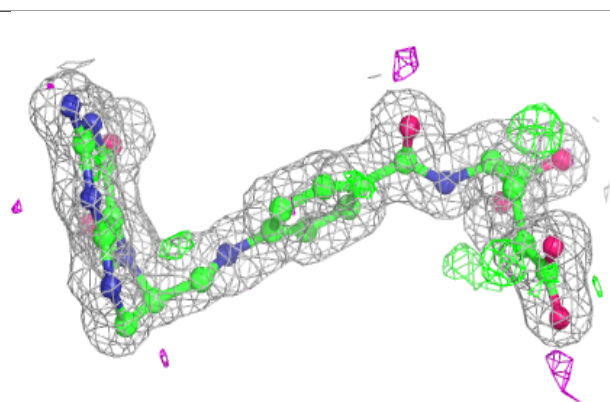
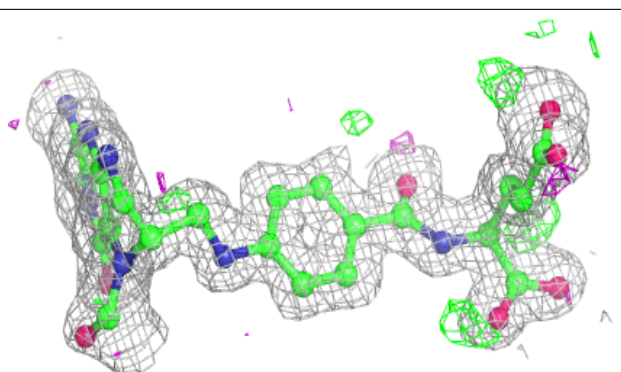
**Electron density around FFO B 502 (B):**

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

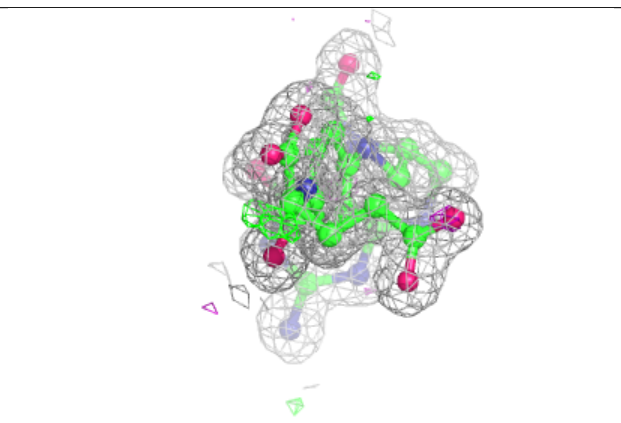
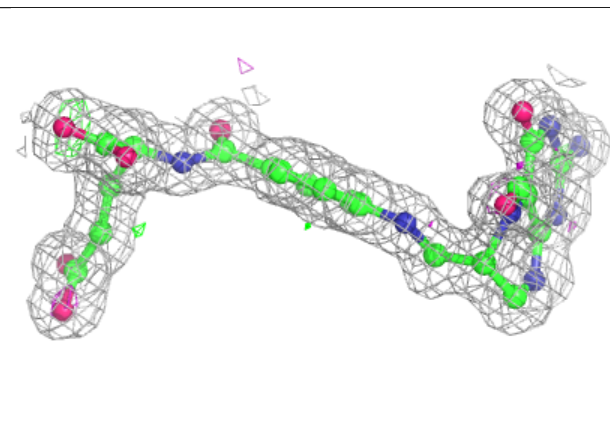
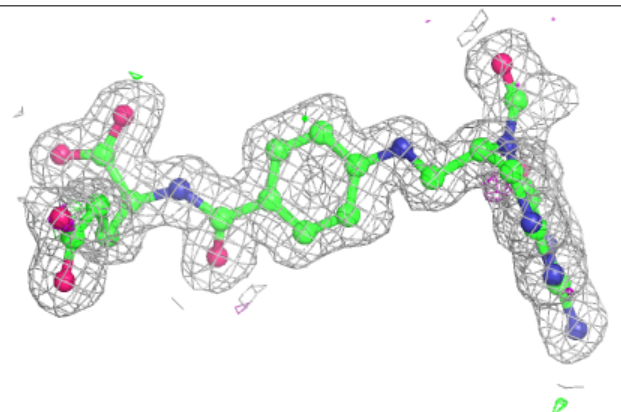


**Electron density around FFO A 502 (B):**

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

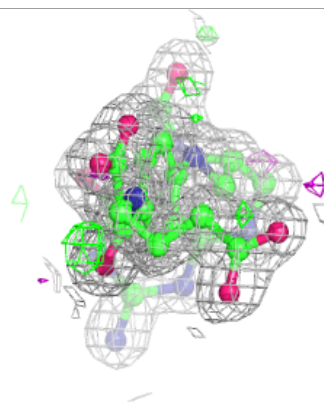
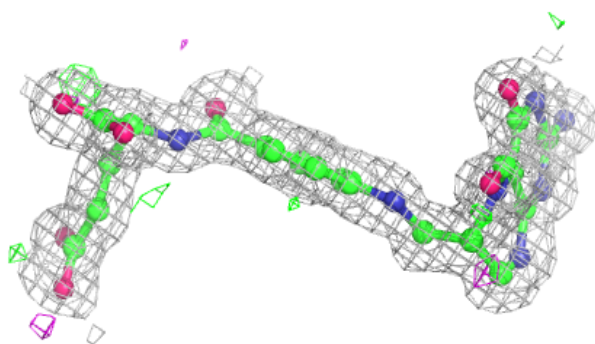
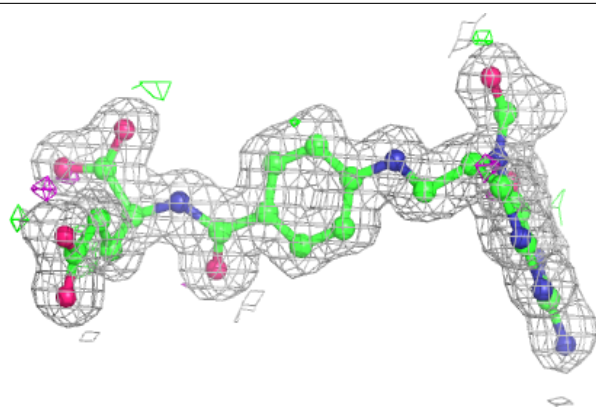
**Electron density around FFO B 502 (A):**

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

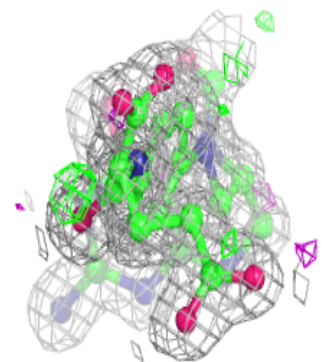
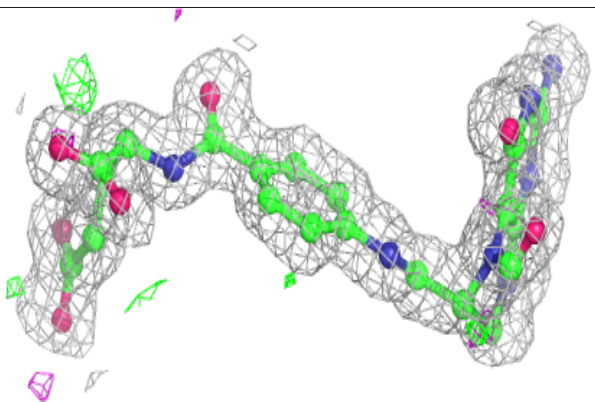
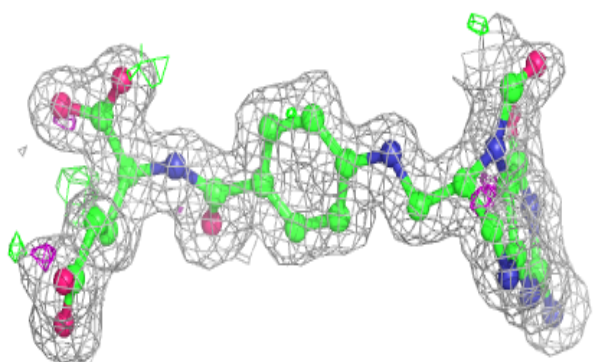


**Electron density around FFO D 705 (B):**

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

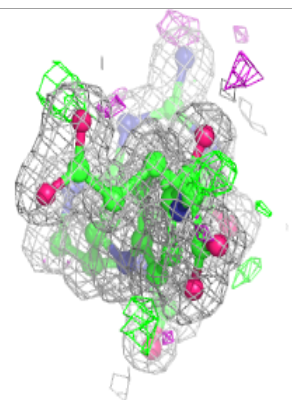
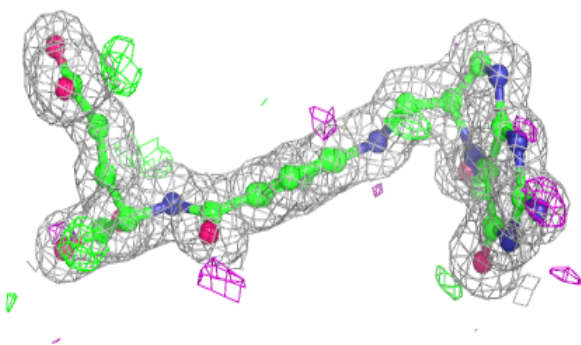
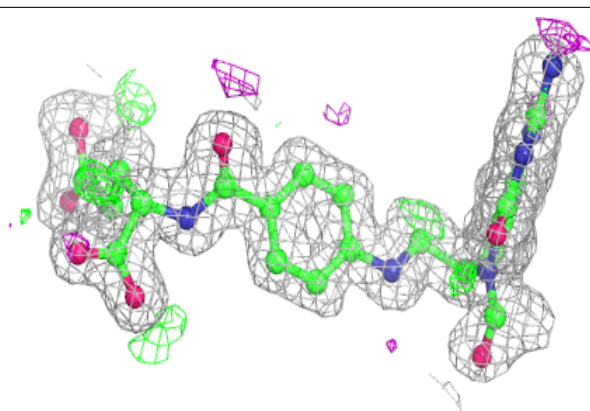
**Electron density around FFO D 705 (A):**

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and green (positive)

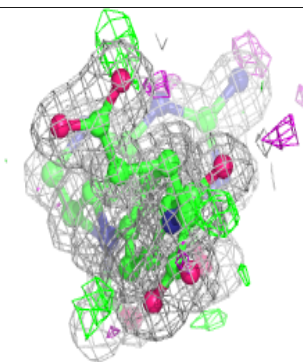
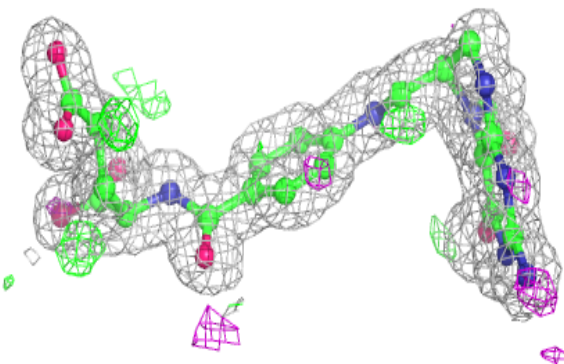
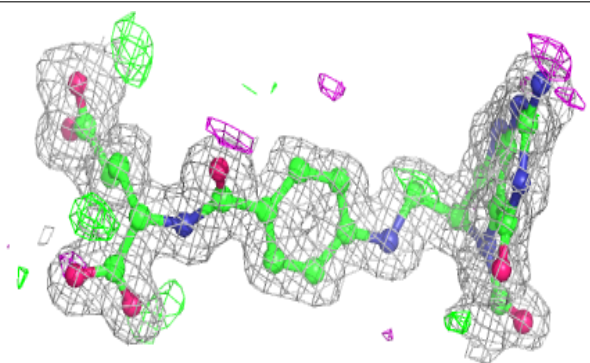


**Electron density around FFO C 803 (B):**

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

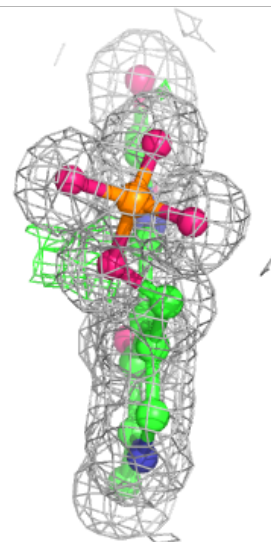
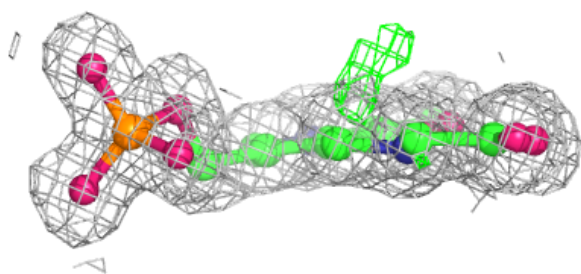
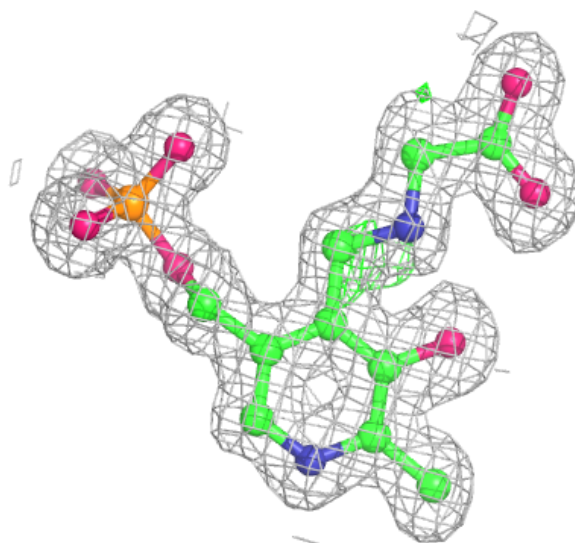
**Electron density around FFO C 803 (A):**

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



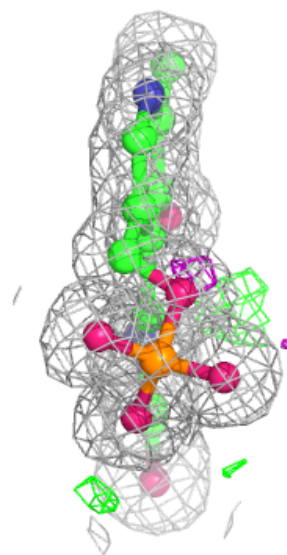
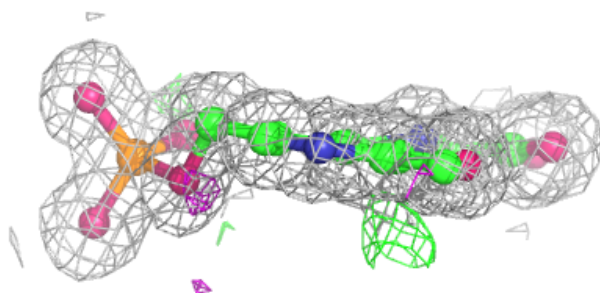
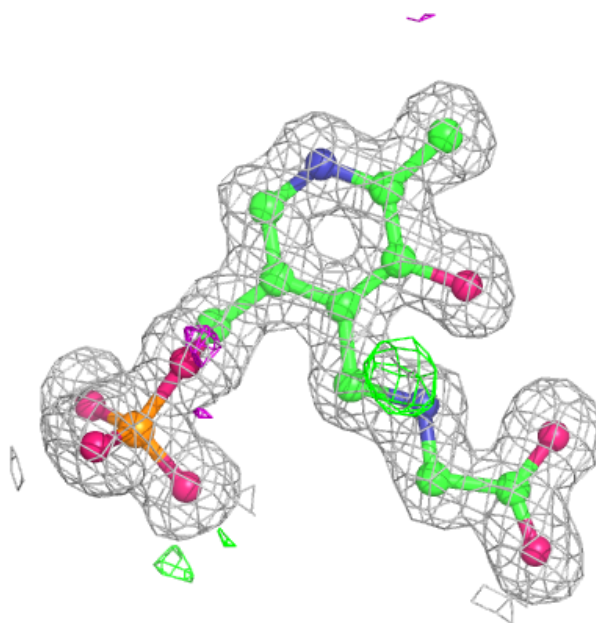
**Electron density around PLG D 704:**

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



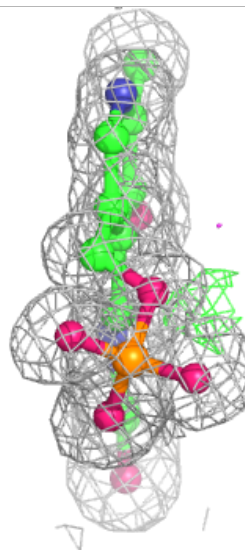
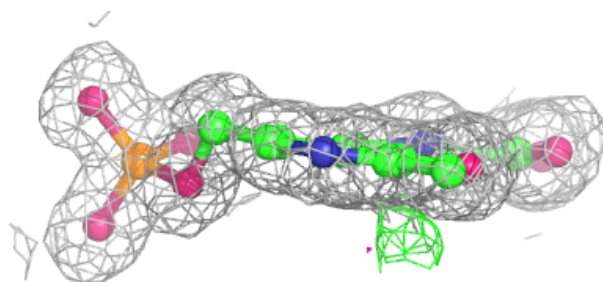
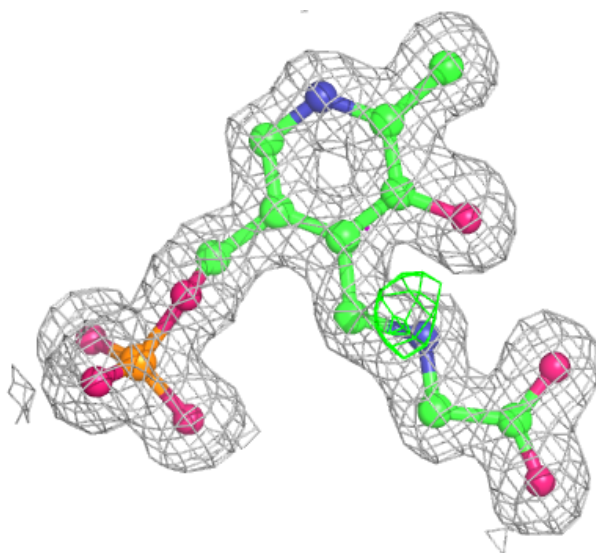
**Electron density around PLG C 802:**

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



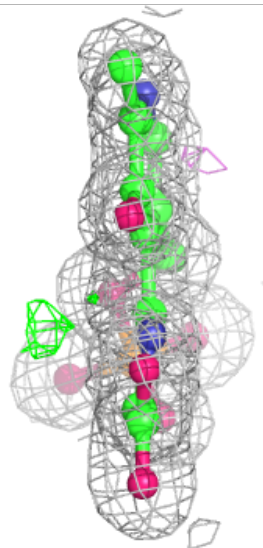
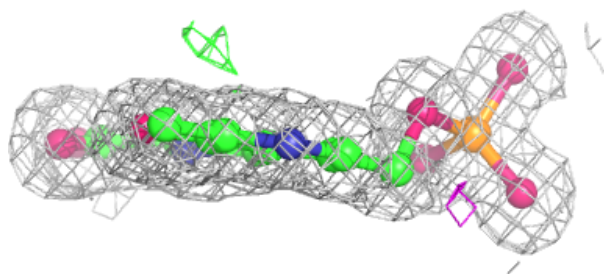
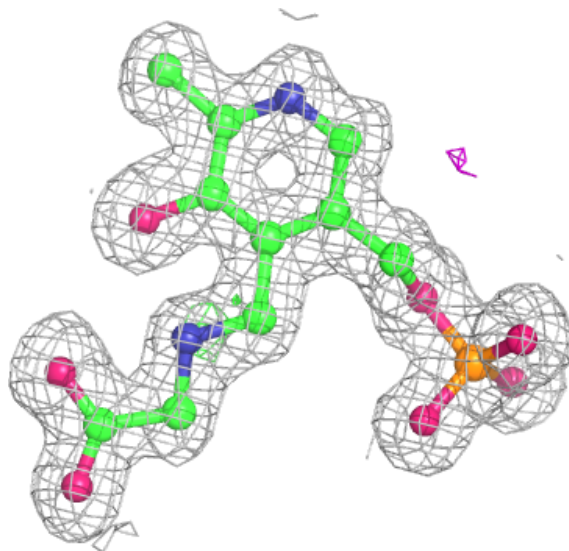
**Electron density around PLG A 501:**

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



**Electron density around PLG B 501:**

$2mF_o-DF_c$  (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.