Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2023 – 08:11 AM EDT

PDB ID	:	8FSD
Title	:	P130R mutant of soybean SHMT8 in complex with PLP-glycine and formylTHF
Authors	:	Beamer, L.J.; Korasick, D.A.
Deposited on	:	2023-01-09
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:

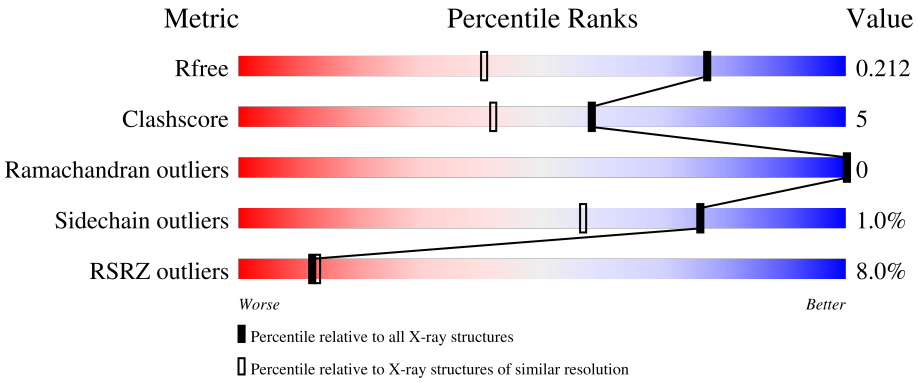
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.49 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}	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	A	491	7% 89% 8% .
1	B	491	9% 81% 14% 5%
1	C	491	3% 90% 6% .
1	D	491	11% 85% 11% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17286 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	472	Total	C	N	O	S	0	15	0
			3706	2362	629	697	18			
1	B	468	Total	C	N	O	S	0	17	0
			3656	2333	615	691	17			
1	C	472	Total	C	N	O	S	0	12	0
			3688	2352	625	691	20			
1	D	469	Total	C	N	O	S	0	31	0
			3763	2402	635	708	18			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0R0IK90
A	-18	GLY	-	expression tag	UNP A0A0R0IK90
A	-17	SER	-	expression tag	UNP A0A0R0IK90
A	-16	SER	-	expression tag	UNP A0A0R0IK90
A	-15	HIS	-	expression tag	UNP A0A0R0IK90
A	-14	HIS	-	expression tag	UNP A0A0R0IK90
A	-13	HIS	-	expression tag	UNP A0A0R0IK90
A	-12	HIS	-	expression tag	UNP A0A0R0IK90
A	-11	HIS	-	expression tag	UNP A0A0R0IK90
A	-10	HIS	-	expression tag	UNP A0A0R0IK90
A	-9	SER	-	expression tag	UNP A0A0R0IK90
A	-8	SER	-	expression tag	UNP A0A0R0IK90
A	-7	GLY	-	expression tag	UNP A0A0R0IK90
A	-6	LEU	-	expression tag	UNP A0A0R0IK90
A	-5	VAL	-	expression tag	UNP A0A0R0IK90
A	-4	PRO	-	expression tag	UNP A0A0R0IK90
A	-3	ARG	-	expression tag	UNP A0A0R0IK90
A	-2	GLY	-	expression tag	UNP A0A0R0IK90
A	-1	SER	-	expression tag	UNP A0A0R0IK90
A	0	HIS	-	expression tag	UNP A0A0R0IK90
A	130	ARG	PRO	engineered mutation	UNP A0A0R0IK90

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP A0A0R0IK90
B	-18	GLY	-	expression tag	UNP A0A0R0IK90
B	-17	SER	-	expression tag	UNP A0A0R0IK90
B	-16	SER	-	expression tag	UNP A0A0R0IK90
B	-15	HIS	-	expression tag	UNP A0A0R0IK90
B	-14	HIS	-	expression tag	UNP A0A0R0IK90
B	-13	HIS	-	expression tag	UNP A0A0R0IK90
B	-12	HIS	-	expression tag	UNP A0A0R0IK90
B	-11	HIS	-	expression tag	UNP A0A0R0IK90
B	-10	HIS	-	expression tag	UNP A0A0R0IK90
B	-9	SER	-	expression tag	UNP A0A0R0IK90
B	-8	SER	-	expression tag	UNP A0A0R0IK90
B	-7	GLY	-	expression tag	UNP A0A0R0IK90
B	-6	LEU	-	expression tag	UNP A0A0R0IK90
B	-5	VAL	-	expression tag	UNP A0A0R0IK90
B	-4	PRO	-	expression tag	UNP A0A0R0IK90
B	-3	ARG	-	expression tag	UNP A0A0R0IK90
B	-2	GLY	-	expression tag	UNP A0A0R0IK90
B	-1	SER	-	expression tag	UNP A0A0R0IK90
B	0	HIS	-	expression tag	UNP A0A0R0IK90
B	130	ARG	PRO	engineered mutation	UNP A0A0R0IK90
C	-19	MET	-	initiating methionine	UNP A0A0R0IK90
C	-18	GLY	-	expression tag	UNP A0A0R0IK90
C	-17	SER	-	expression tag	UNP A0A0R0IK90
C	-16	SER	-	expression tag	UNP A0A0R0IK90
C	-15	HIS	-	expression tag	UNP A0A0R0IK90
C	-14	HIS	-	expression tag	UNP A0A0R0IK90
C	-13	HIS	-	expression tag	UNP A0A0R0IK90
C	-12	HIS	-	expression tag	UNP A0A0R0IK90
C	-11	HIS	-	expression tag	UNP A0A0R0IK90
C	-10	HIS	-	expression tag	UNP A0A0R0IK90
C	-9	SER	-	expression tag	UNP A0A0R0IK90
C	-8	SER	-	expression tag	UNP A0A0R0IK90
C	-7	GLY	-	expression tag	UNP A0A0R0IK90
C	-6	LEU	-	expression tag	UNP A0A0R0IK90
C	-5	VAL	-	expression tag	UNP A0A0R0IK90
C	-4	PRO	-	expression tag	UNP A0A0R0IK90
C	-3	ARG	-	expression tag	UNP A0A0R0IK90
C	-2	GLY	-	expression tag	UNP A0A0R0IK90
C	-1	SER	-	expression tag	UNP A0A0R0IK90
C	0	HIS	-	expression tag	UNP A0A0R0IK90
C	130	ARG	PRO	engineered mutation	UNP A0A0R0IK90

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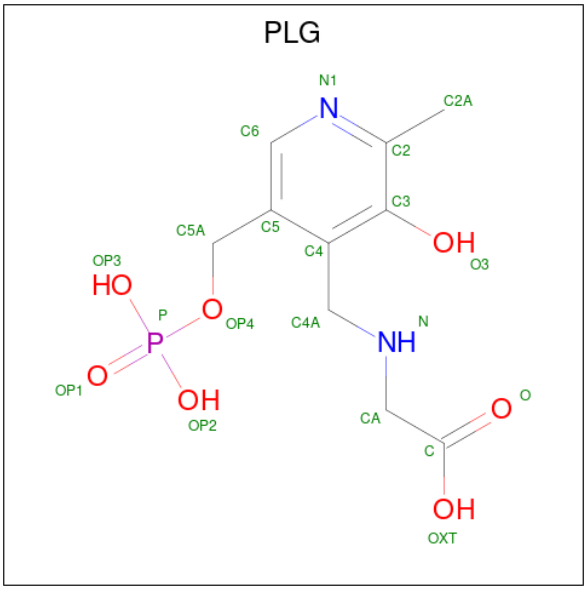
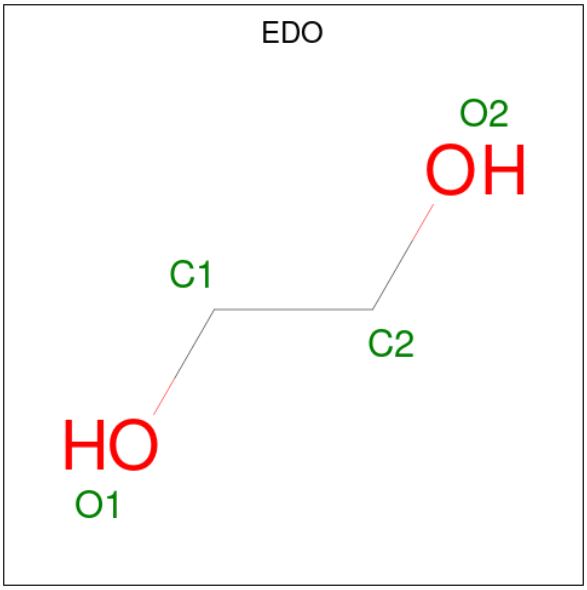
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP A0A0R0IK90
D	-18	GLY	-	expression tag	UNP A0A0R0IK90
D	-17	SER	-	expression tag	UNP A0A0R0IK90
D	-16	SER	-	expression tag	UNP A0A0R0IK90
D	-15	HIS	-	expression tag	UNP A0A0R0IK90
D	-14	HIS	-	expression tag	UNP A0A0R0IK90
D	-13	HIS	-	expression tag	UNP A0A0R0IK90
D	-12	HIS	-	expression tag	UNP A0A0R0IK90
D	-11	HIS	-	expression tag	UNP A0A0R0IK90
D	-10	HIS	-	expression tag	UNP A0A0R0IK90
D	-9	SER	-	expression tag	UNP A0A0R0IK90
D	-8	SER	-	expression tag	UNP A0A0R0IK90
D	-7	GLY	-	expression tag	UNP A0A0R0IK90
D	-6	LEU	-	expression tag	UNP A0A0R0IK90
D	-5	VAL	-	expression tag	UNP A0A0R0IK90
D	-4	PRO	-	expression tag	UNP A0A0R0IK90
D	-3	ARG	-	expression tag	UNP A0A0R0IK90
D	-2	GLY	-	expression tag	UNP A0A0R0IK90
D	-1	SER	-	expression tag	UNP A0A0R0IK90
D	0	HIS	-	expression tag	UNP A0A0R0IK90
D	130	ARG	PRO	engineered mutation	UNP A0A0R0IK90

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: $C_{10}H_{15}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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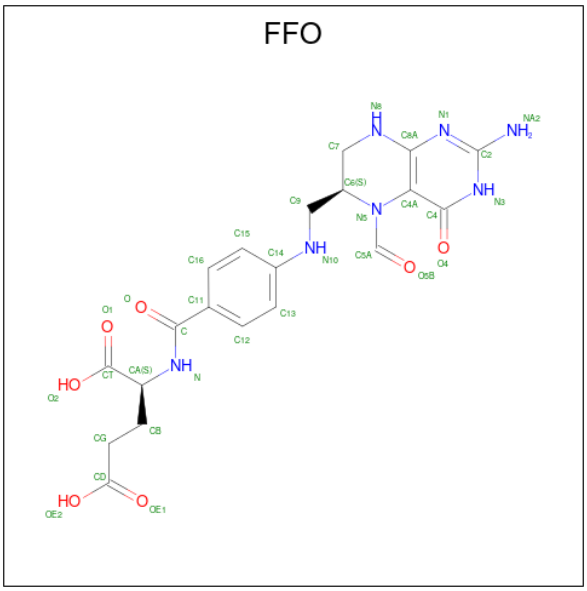
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total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

- Molecule 4 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: $C_{20}H_{23}N_7O_7$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

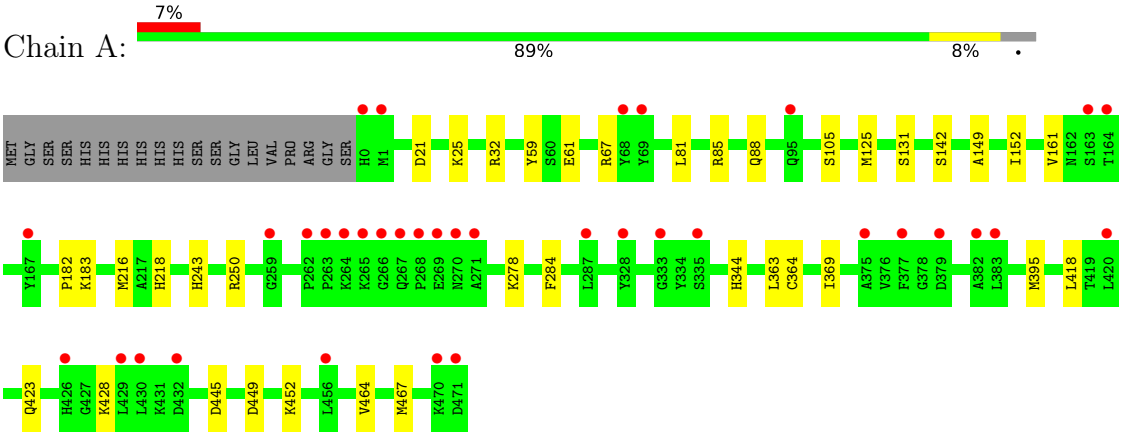
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	478	Total O 478 478	0	0
5	B	444	Total O 444 444	0	0
5	C	569	Total O 569 569	0	0
5	D	526	Total O 526 526	0	0

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.

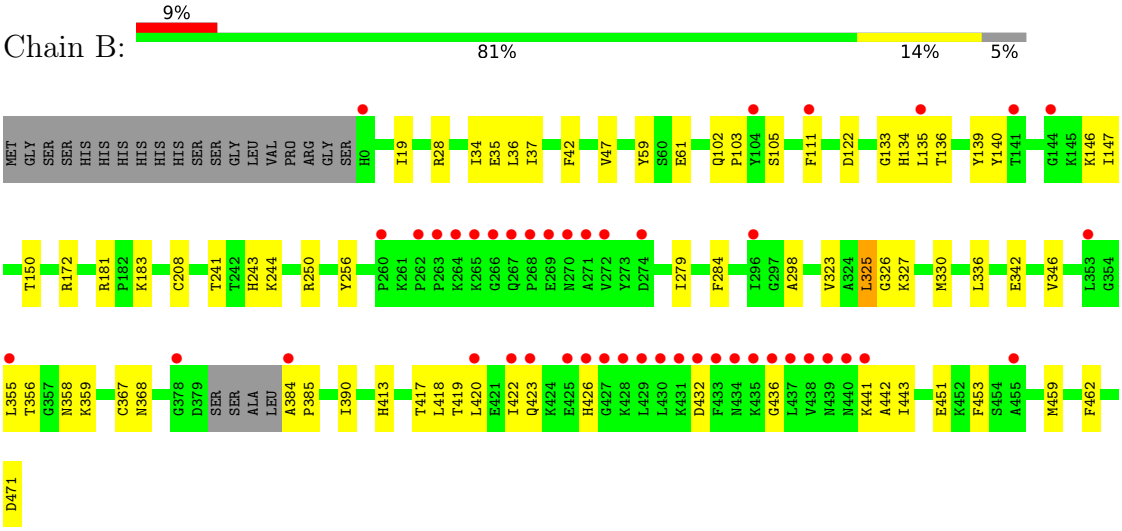
• Molecule 1: Serine hydroxymethyltransferase

Chain A:



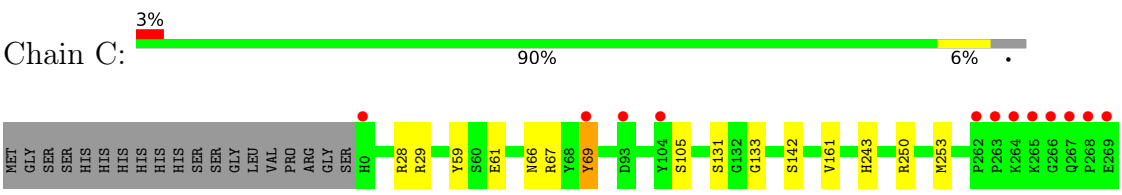
• Molecule 1: Serine hydroxymethyltransferase

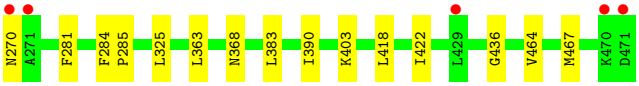
Chain B:



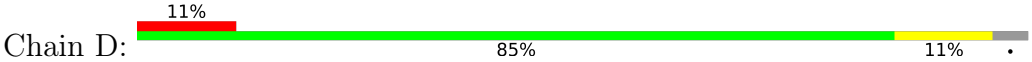
• Molecule 1: Serine hydroxymethyltransferase

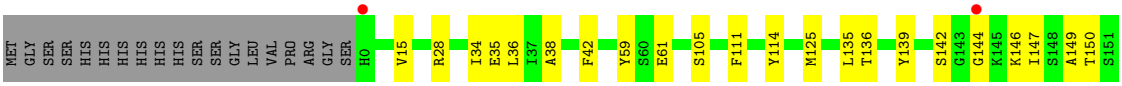
Chain C:

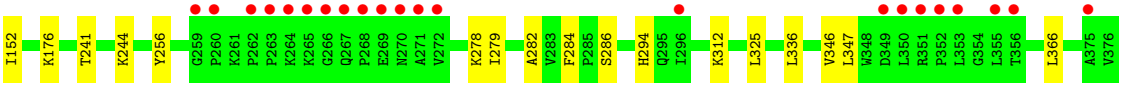


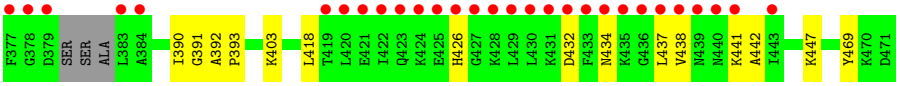


• Molecule 1: Serine hydroxymethyltransferase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.56Å 90.48Å 146.18Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	47.41 – 1.49 47.41 – 1.49	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.41-1.49) 97.4 (47.41-1.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.49Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.184 , 0.213 0.184 , 0.212	Depositor DCC
R_{free} test set	17758 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for -k,-h,-l 0.009 for k,h,-l 0.018 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17286	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLG, EDO, FFO

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	0.34	0/3829	0.61	2/5182 (0.0%)
1	B	0.37	0/3789	0.64	1/5135 (0.0%)
1	C	0.37	0/3807	0.65	1/5152 (0.0%)
1	D	0.38	0/3907	0.63	2/5290 (0.0%)
All	All	0.36	0/15332	0.63	6/20759 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	325	LEU	CB-CG-CD2	-10.68	92.85	111.00
1	D	125	MET	N-CA-CB	6.81	122.85	110.60
1	C	253	MET	N-CA-CB	-5.79	100.18	110.60
1	A	216	MET	CB-CA-C	-5.47	99.46	110.40
1	D	125	MET	CA-CB-CG	5.34	122.38	113.30
1	A	395	MET	CB-CG-SD	-5.14	96.97	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3706	0	3671	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3656	0	3598	57	0
1	C	3688	0	3660	21	0
1	D	3763	0	3715	41	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	28	0	42	1	0
3	B	24	0	36	2	0
3	C	24	0	36	3	0
3	D	28	0	42	8	0
4	A	68	0	42	0	0
4	B	68	0	42	4	0
4	C	68	0	42	3	0
4	D	68	0	42	1	0
5	A	478	0	0	7	0
5	B	444	0	0	6	0
5	C	569	0	0	4	0
5	D	526	0	0	8	0
All	All	17286	0	15016	145	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 5.

All (145) 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:D:346[B]:VAL:HB	1:D:390[B]:ILE:HD11	1.60	0.82
1:B:359[B]:LYS:NZ	1:B:423:GLN:OE1	2.18	0.75
1:B:181[A]:ARG:HB2	3:D:702:EDO:H12	1.71	0.72
1:B:35:GLU:HG3	1:B:42:PHE:HZ	1.58	0.68
1:D:144[B]:GLY:HA2	3:D:702:EDO:H22	1.75	0.68
1:B:181[B]:ARG:HB2	3:D:702:EDO:H12	1.75	0.67
1:B:346:VAL:HG22	1:B:390[B]:ILE:HD11	1.76	0.66
1:B:325:LEU:HD21	1:B:390[B]:ILE:CD1	2.25	0.66
1:D:135:LEU:HD23	1:D:139[A]:TYR:HD2	1.61	0.66
1:A:81[B]:LEU:HD21	1:A:85:ARG:CZ	2.27	0.65
1:D:35:GLU:HG3	1:D:42:PHE:HZ	1.61	0.65
1:B:356:THR:OG1	1:B:358[B]:ASN:OD1	2.11	0.65
1:B:325:LEU:HD21	1:B:390[B]:ILE:HD13	1.79	0.63
1:A:81[B]:LEU:HD22	1:B:19:ILE:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:HIS:O	1:B:417[A]:THR:HG23	1.99	0.63
1:B:355:LEU:HD22	1:B:419:THR:HG22	1.81	0.62
1:A:149:ALA:HA	1:A:152[A]:ILE:HD12	1.80	0.62
5:A:612:HOH:O	2:B:802:PLG:H4A1	2.00	0.61
1:B:134:HIS:CD2	4:B:808[B]:FFO:H5A	2.36	0.60
1:B:418:LEU:HD11	1:B:442:ALA:HB1	1.84	0.59
1:D:426:HIS:O	1:D:432:ASP:HB3	2.02	0.59
1:B:181[B]:ARG:NH1	1:B:208:CYS:HA	2.17	0.58
1:B:136:THR:O	1:B:150[B]:THR:HG21	2.04	0.58
2:C:501:PLG:H4A1	5:D:825:HOH:O	2.04	0.56
1:D:176:LYS:NZ	5:D:811:HOH:O	2.39	0.56
1:A:449:ASP:HA	1:A:452:LYS:HE3	1.87	0.56
1:C:67:ARG:HB3	5:C:618:HOH:O	2.05	0.56
1:D:325:LEU:HD21	1:D:390[B]:ILE:HD13	1.88	0.56
1:D:418:LEU:HD11	1:D:442:ALA:HB1	1.88	0.56
1:B:181[B]:ARG:NH2	1:D:142[B]:SER:O	2.39	0.55
1:A:464:VAL:O	1:A:467:MET:HG2	2.05	0.55
1:A:131:SER:HB3	1:A:161:VAL:HG13	1.88	0.55
1:B:181[B]:ARG:NE	1:D:142[B]:SER:O	2.41	0.54
1:A:142:SER:HA	3:A:503:EDO:H22	1.90	0.53
1:D:256:TYR:HB3	1:D:279[A]:ILE:HD12	1.91	0.53
1:B:181[B]:ARG:CZ	1:D:142[B]:SER:O	2.57	0.52
1:D:150[B]:THR:HG23	5:D:1139:HOH:O	2.09	0.52
1:A:61:GLU:OE1	4:B:808[A]:FFO:H5A	2.10	0.52
5:C:608:HOH:O	2:D:703:PLG:H4A1	2.10	0.52
1:B:133:GLY:O	4:B:808[B]:FFO:N3	2.38	0.52
1:B:150[B]:THR:HG23	5:B:1198:HOH:O	2.09	0.52
1:B:368:ASN:ND2	1:B:451:GLU:OE2	2.43	0.51
1:D:15:VAL:HG22	3:D:707:EDO:H12	1.92	0.51
1:D:136:THR:O	1:D:150[B]:THR:HG21	2.10	0.51
2:C:501:PLG:O3	2:C:501:PLG:N	2.43	0.51
1:D:146[B]:LYS:NZ	5:D:819:HOH:O	2.44	0.51
1:C:29:ARG:HA	3:C:506:EDO:H12	1.93	0.51
1:C:61:GLU:OE1	4:D:708[A]:FFO:H5A	2.11	0.51
1:D:325:LEU:CD2	1:D:390[B]:ILE:HD13	2.40	0.51
1:B:342:GLU:OE2	5:B:901:HOH:O	2.20	0.50
1:A:21:ASP:O	1:A:25:LYS:HG3	2.12	0.50
1:D:312:LYS:HB2	3:D:706:EDO:H22	1.93	0.50
1:C:142:SER:HA	3:C:504:EDO:H22	1.94	0.49
1:D:28[A]:ARG:HD3	5:D:804:HOH:O	2.12	0.49
1:C:383:LEU:HD23	4:C:508[A]:FFO:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:TYR:HB3	1:B:279[A]:ILE:HD12	1.94	0.49
1:A:363:LEU:HD11	1:A:418:LEU:HG	1.94	0.49
2:A:501:PLG:H4A1	5:B:907:HOH:O	2.13	0.49
1:A:67:ARG:HB3	5:A:679:HOH:O	2.12	0.49
1:B:181[B]:ARG:HH12	1:B:208:CYS:HA	1.77	0.48
3:D:707:EDO:H21	5:D:889:HOH:O	2.11	0.48
1:B:346:VAL:HG22	1:B:390[B]:ILE:CD1	2.42	0.48
1:B:323:VAL:O	1:B:327:LYS:HG2	2.14	0.48
1:A:445:ASP:OD1	5:A:601:HOH:O	2.20	0.47
1:B:426:HIS:O	1:B:432:ASP:HB3	2.15	0.47
1:C:69:TYR:HD1	5:C:618:HOH:O	1.98	0.47
1:D:346[B]:VAL:HB	1:D:390[B]:ILE:CD1	2.39	0.47
1:B:241:THR:HG21	1:B:244:LYS:NZ	2.30	0.47
1:C:28:ARG:HA	1:C:467[B]:MET:HE1	1.96	0.47
1:C:66:ASN:HD21	3:C:507:EDO:H21	1.79	0.47
1:A:61:GLU:HB3	1:A:284:PHE:CZ	2.49	0.47
2:B:802:PLG:O3	2:B:802:PLG:N	2.47	0.47
1:B:34:ILE:HG22	1:B:36:LEU:HG	1.97	0.46
1:B:111:PHE:CD2	3:B:801:EDO:H11	2.51	0.46
1:B:326:GLY:O	1:B:330:MET:HB2	2.15	0.46
1:D:336:LEU:HD13	1:D:346[B]:VAL:HG11	1.98	0.46
1:B:422:ILE:HG23	1:B:436:GLY:HA3	1.98	0.46
1:D:135:LEU:HD23	1:D:139[A]:TYR:CD2	2.46	0.46
1:A:88:GLN:NE2	5:A:613:HOH:O	2.42	0.46
1:C:368:ASN:ND2	5:C:623:HOH:O	2.48	0.46
1:D:438:VAL:HA	5:D:1150:HOH:O	2.16	0.45
1:B:139:TYR:HD1	1:B:147:ILE:HB	1.80	0.45
2:A:501:PLG:N	2:A:501:PLG:O3	2.49	0.45
1:B:146:LYS:NZ	5:B:921:HOH:O	2.50	0.45
1:B:61:GLU:HB3	1:B:284:PHE:CZ	2.51	0.45
1:C:363:LEU:HD11	1:C:418:LEU:HG	1.99	0.45
1:C:131:SER:HB3	1:C:161:VAL:HG13	1.99	0.45
1:D:38:ALA:HA	1:D:391:GLY:HA3	1.98	0.45
1:B:35:GLU:HG3	1:B:42:PHE:CZ	2.46	0.44
1:B:181[A]:ARG:HH12	3:B:805:EDO:H21	1.82	0.44
1:A:125:MET:HG3	1:A:182:PRO:HB3	1.99	0.44
1:B:471:ASP:OD1	5:B:902:HOH:O	2.21	0.44
1:D:34:ILE:HG22	1:D:36:LEU:HG	1.99	0.44
1:B:367:CYS:SG	1:B:443:ILE:HG23	2.59	0.43
1:C:383:LEU:HD23	4:C:508[B]:FFO:CD	2.48	0.43
1:D:325:LEU:HD21	1:D:390[A]:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ALA:HA	1:D:286[A]:SER:HB2	2.01	0.43
1:C:284:PHE:CD1	1:C:285:PRO:HA	2.53	0.43
1:C:325:LEU:HD21	1:C:390:ILE:HG21	2.00	0.43
1:D:149:ALA:HA	1:D:152[A]:ILE:HD12	2.01	0.43
1:A:183[B]:LYS:HG2	5:A:721:HOH:O	2.17	0.43
1:D:28[B]:ARG:HD3	1:D:469:TYR:HB3	2.00	0.43
1:D:114:TYR:HE2	1:D:150[B]:THR:HG21	1.84	0.43
1:D:434:ASN:HA	1:D:437:LEU:HD23	2.00	0.43
1:A:423:GLN:CD	1:A:428:LYS:HG2	2.39	0.42
5:A:604:HOH:O	1:B:37:ILE:HD12	2.19	0.42
1:B:181[B]:ARG:NH2	1:B:208:CYS:O	2.51	0.42
1:B:459:MET:HG2	1:B:462:PHE:CZ	2.54	0.42
1:C:281:PHE:HZ	1:D:147[B]:ILE:HD12	1.84	0.42
1:D:278:LYS:HG3	5:D:838:HOH:O	2.19	0.42
1:A:218:HIS:HB3	1:A:344:HIS:CE1	2.54	0.42
1:B:134:HIS:CE1	1:B:136:THR:HG23	2.55	0.42
1:B:102:GLN:N	1:B:103:PRO:CD	2.83	0.42
1:B:453:PHE:HE1	5:B:1181:HOH:O	2.01	0.42
1:C:61:GLU:HB3	1:C:284:PHE:CZ	2.54	0.42
1:A:243:HIS:ND1	1:A:250:ARG:HA	2.35	0.42
1:B:330:MET:HG3	1:B:336:LEU:HG	2.02	0.42
2:D:703:PLG:O3	2:D:703:PLG:N	2.52	0.42
1:D:61:GLU:HB3	1:D:284:PHE:CZ	2.55	0.42
1:D:241:THR:HG21	1:D:244:LYS:NZ	2.35	0.42
1:D:294:HIS:HD1	1:D:294:HIS:H	1.67	0.42
1:B:241:THR:HB	1:B:243:HIS:CE1	2.55	0.41
1:B:243:HIS:ND1	1:B:250:ARG:HA	2.35	0.41
1:D:366:LEU:O	1:D:447:LYS:HD2	2.20	0.41
1:C:61:GLU:HB2	1:C:69:TYR:HE1	1.85	0.41
1:A:364:CYS:HB3	1:A:369:ILE:O	2.20	0.41
1:B:47:VAL:HG13	1:B:298:ALA:HB1	2.01	0.41
1:D:111:PHE:CD2	3:D:709:EDO:H11	2.56	0.41
1:B:122:ASP:CG	1:B:183:LYS:HD3	2.41	0.41
1:B:181[A]:ARG:HA	1:B:181[A]:ARG:HD3	1.91	0.41
1:C:422:ILE:HG23	1:C:436:GLY:HA3	2.03	0.41
1:C:464:VAL:HG13	1:C:467[B]:MET:SD	2.61	0.41
1:A:278:LYS:HG3	5:A:632:HOH:O	2.20	0.41
1:B:384:ALA:HA	1:B:385:PRO:HD2	1.95	0.41
1:C:133:GLY:O	4:C:508[B]:FFO:N3	2.42	0.41
1:D:347:LEU:HD12	1:D:347:LEU:HA	1.92	0.41
1:D:392:ALA:N	1:D:393:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:HA	1:B:172:ARG:NE	2.36	0.40
1:A:32:ARG:HD3	1:A:32:ARG:HA	1.91	0.40
1:B:135:LEU:HD11	4:B:808[A]:FFO:H15	2.03	0.40
1:B:355:LEU:HD11	1:B:420:LEU:HG	2.03	0.40
1:C:243:HIS:ND1	1:C:250:ARG:HA	2.37	0.40
1:D:336:LEU:HD13	1:D:346[B]:VAL:CG1	2.51	0.40
1:B:140:TYR:CG	3:D:701:EDO:H21	2.57	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	485/491 (99%)	472 (97%)	13 (3%)	0	100	100
1	B	481/491 (98%)	468 (97%)	13 (3%)	0	100	100
1	C	482/491 (98%)	470 (98%)	12 (2%)	0	100	100
1	D	496/491 (101%)	480 (97%)	16 (3%)	0	100	100
All	All	1944/1964 (99%)	1890 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	393/402 (98%)	391 (100%)	2 (0%)	88 78
1	B	386/402 (96%)	382 (99%)	4 (1%)	76 57
1	C	391/402 (97%)	386 (99%)	5 (1%)	69 44
1	D	397/402 (99%)	393 (99%)	4 (1%)	76 57
All	All	1567/1608 (98%)	1552 (99%)	15 (1%)	76 57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	105	SER
1	B	28	ARG
1	B	59	TYR
1	B	105	SER
1	B	441	LYS
1	C	59	TYR
1	C	69	TYR
1	C	105	SER
1	C	270	ASN
1	C	403	LYS
1	D	59	TYR
1	D	105	SER
1	D	403	LYS
1	D	441	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	C	66	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

38 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	$\#\|Z\| > 2$
3	EDO	B	805	-	3,3,3	0.46	0	2,2,2	0.29	0
3	EDO	A	503	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	B	804	-	3,3,3	0.51	0	2,2,2	0.26	0
3	EDO	C	502	-	3,3,3	0.45	0	2,2,2	0.54	0
3	EDO	B	803	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	C	506	-	3,3,3	0.43	0	2,2,2	0.46	0
2	PLG	C	501	-	20,20,20	1.25	2 (10%)	25,28,28	1.51	5 (20%)
2	PLG	A	501	-	20,20,20	1.25	2 (10%)	25,28,28	1.27	4 (16%)
3	EDO	D	702	-	3,3,3	0.36	0	2,2,2	0.70	0
4	FFO	D	708[A]	-	33,36,36	4.17	14 (42%)	36,50,50	1.67	6 (16%)
4	FFO	A	508[B]	-	33,36,36	4.07	14 (42%)	36,50,50	1.63	6 (16%)
3	EDO	D	705	-	3,3,3	0.48	0	2,2,2	0.45	0
3	EDO	B	807	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	D	706	-	3,3,3	0.48	0	2,2,2	0.36	0
3	EDO	A	509	-	3,3,3	0.46	0	2,2,2	0.50	0
2	PLG	B	802	-	20,20,20	1.30	3 (15%)	25,28,28	1.49	4 (16%)
3	EDO	B	801	-	3,3,3	0.59	0	2,2,2	0.06	0
3	EDO	A	505	-	3,3,3	0.45	0	2,2,2	0.41	0
4	FFO	B	808[B]	-	33,36,36	4.20	14 (42%)	36,50,50	1.58	5 (13%)
4	FFO	C	508[B]	-	33,36,36	3.85	13 (39%)	36,50,50	1.71	6 (16%)
3	EDO	C	503	-	3,3,3	0.49	0	2,2,2	0.36	0
3	EDO	C	504	-	3,3,3	0.39	0	2,2,2	0.51	0
4	FFO	A	508[A]	-	33,36,36	4.15	13 (39%)	36,50,50	1.65	6 (16%)
3	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.23	0
3	EDO	D	704	-	3,3,3	0.49	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	D	707	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	A	502	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	A	507	-	3,3,3	0.48	0	2,2,2	0.26	0
4	FFO	B	808[A]	-	33,36,36	4.16	13 (39%)	36,50,50	1.53	4 (11%)
4	FFO	D	708[B]	-	33,36,36	4.16	13 (39%)	36,50,50	1.55	7 (19%)
3	EDO	C	505	-	3,3,3	0.48	0	2,2,2	0.31	0
4	FFO	C	508[A]	-	33,36,36	4.11	14 (42%)	36,50,50	1.64	5 (13%)
3	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.38	0
2	PLG	D	703	-	20,20,20	1.23	2 (10%)	25,28,28	1.51	4 (16%)
3	EDO	B	806	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	D	701	-	3,3,3	0.52	0	2,2,2	0.22	0
3	EDO	C	507	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	D	709	-	3,3,3	0.58	0	2,2,2	0.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	805	-	-	0/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	B	804	-	-	0/1/1/1	-
3	EDO	C	502	-	-	0/1/1/1	-
3	EDO	B	803	-	-	0/1/1/1	-
3	EDO	C	506	-	-	0/1/1/1	-
2	PLG	C	501	-	-	2/12/12/12	0/1/1/1
2	PLG	A	501	-	-	2/12/12/12	0/1/1/1
3	EDO	D	702	-	-	1/1/1/1	-
4	FFO	D	708[A]	-	-	2/24/37/37	0/3/3/3
4	FFO	A	508[B]	-	-	2/24/37/37	0/3/3/3
3	EDO	D	705	-	-	0/1/1/1	-
3	EDO	B	807	-	-	1/1/1/1	-
3	EDO	D	706	-	-	0/1/1/1	-
3	EDO	A	509	-	-	0/1/1/1	-
2	PLG	B	802	-	-	2/12/12/12	0/1/1/1
3	EDO	B	801	-	-	0/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
4	FFO	B	808[B]	-	-	2/24/37/37	0/3/3/3
4	FFO	C	508[B]	-	-	1/24/37/37	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	503	-	-	0/1/1/1	-
3	EDO	C	504	-	-	0/1/1/1	-
4	FFO	A	508[A]	-	-	1/24/37/37	0/3/3/3
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	D	704	-	-	1/1/1/1	-
3	EDO	D	707	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	A	507	-	-	1/1/1/1	-
4	FFO	B	808[A]	-	-	2/24/37/37	0/3/3/3
4	FFO	D	708[B]	-	-	0/24/37/37	0/3/3/3
3	EDO	C	505	-	-	0/1/1/1	-
4	FFO	C	508[A]	-	-	3/24/37/37	0/3/3/3
3	EDO	A	506	-	-	0/1/1/1	-
2	PLG	D	703	-	-	4/12/12/12	0/1/1/1
3	EDO	B	806	-	-	0/1/1/1	-
3	EDO	D	701	-	-	0/1/1/1	-
3	EDO	C	507	-	-	1/1/1/1	-
3	EDO	D	709	-	-	1/1/1/1	-

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	708[A]	FFO	C7-C6	-12.38	1.37	1.52
4	B	808[B]	FFO	C7-C6	-12.24	1.37	1.52
4	C	508[A]	FFO	C7-C6	-12.22	1.37	1.52
4	B	808[A]	FFO	C7-C6	-12.18	1.37	1.52
4	D	708[B]	FFO	C7-C6	-12.02	1.38	1.52
4	B	808[B]	FFO	C7-N8	12.00	1.58	1.46
4	A	508[A]	FFO	C7-C6	-11.98	1.38	1.52
4	A	508[A]	FFO	C7-N8	11.98	1.58	1.46
4	C	508[A]	FFO	C7-N8	11.89	1.58	1.46
4	D	708[B]	FFO	C7-N8	11.89	1.58	1.46
4	A	508[B]	FFO	C7-C6	-11.80	1.38	1.52
4	D	708[A]	FFO	C7-N8	11.74	1.58	1.46
4	A	508[B]	FFO	C7-N8	11.74	1.58	1.46
4	B	808[A]	FFO	C7-N8	11.61	1.58	1.46
4	C	508[B]	FFO	C7-N8	11.06	1.57	1.46
4	C	508[B]	FFO	C7-C6	-10.29	1.40	1.52
4	B	808[B]	FFO	C2-N1	7.15	1.50	1.33
4	D	708[B]	FFO	C2-N1	7.10	1.50	1.33
4	A	508[A]	FFO	C2-N1	7.07	1.50	1.33
4	D	708[A]	FFO	C2-N1	7.00	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	508[A]	FFO	C2-N1	6.96	1.50	1.33
4	B	808[A]	FFO	C2-N1	6.95	1.50	1.33
4	C	508[B]	FFO	C2-N1	6.85	1.49	1.33
4	B	808[B]	FFO	C8A-N1	6.73	1.46	1.36
4	A	508[A]	FFO	C8A-N1	6.72	1.46	1.36
4	A	508[B]	FFO	C2-N1	6.71	1.49	1.33
4	B	808[A]	FFO	C8A-N1	6.67	1.46	1.36
4	D	708[B]	FFO	C8A-N1	6.62	1.45	1.36
4	D	708[A]	FFO	C8A-N1	6.58	1.45	1.36
4	C	508[A]	FFO	C8A-N1	6.54	1.45	1.36
4	B	808[B]	FFO	C-N	6.10	1.47	1.34
4	A	508[B]	FFO	C8A-N1	6.08	1.45	1.36
4	D	708[B]	FFO	C2-N3	6.06	1.52	1.37
4	B	808[A]	FFO	C-N	6.06	1.47	1.34
4	D	708[B]	FFO	C-N	6.05	1.47	1.34
4	D	708[A]	FFO	C-N	5.98	1.47	1.34
4	C	508[B]	FFO	C8A-N1	5.96	1.45	1.36
4	B	808[B]	FFO	C2-N3	5.95	1.52	1.37
4	A	508[B]	FFO	C-N	5.95	1.47	1.34
4	A	508[A]	FFO	C2-N3	5.93	1.52	1.37
4	A	508[A]	FFO	C-N	5.92	1.47	1.34
4	A	508[B]	FFO	C2-N3	5.88	1.52	1.37
4	C	508[B]	FFO	C2-N3	5.86	1.52	1.37
4	C	508[A]	FFO	C-N	5.85	1.46	1.34
4	B	808[A]	FFO	C2-N3	5.82	1.52	1.37
4	C	508[B]	FFO	C-N	5.76	1.46	1.34
4	D	708[A]	FFO	C2-N3	5.74	1.51	1.37
4	C	508[A]	FFO	C2-N3	5.51	1.51	1.37
4	B	808[A]	FFO	C5A-N5	5.18	1.46	1.36
4	D	708[A]	FFO	C5A-N5	5.16	1.46	1.36
4	B	808[B]	FFO	C5A-N5	5.01	1.45	1.36
4	A	508[B]	FFO	C5A-N5	5.01	1.45	1.36
4	C	508[A]	FFO	C5A-N5	5.00	1.45	1.36
4	C	508[B]	FFO	C4-N3	4.99	1.48	1.38
4	B	808[A]	FFO	C4-N3	4.95	1.48	1.38
4	D	708[B]	FFO	C4-N3	4.92	1.48	1.38
4	D	708[B]	FFO	C2-NA2	4.81	1.45	1.34
4	B	808[B]	FFO	C4-N3	4.80	1.47	1.38
4	A	508[A]	FFO	C5A-N5	4.80	1.45	1.36
4	B	808[A]	FFO	C2-NA2	4.79	1.45	1.34
4	D	708[A]	FFO	C4-N3	4.78	1.47	1.38
4	B	808[B]	FFO	C2-NA2	4.77	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	508[B]	FFO	C4-N3	4.77	1.47	1.38
4	D	708[A]	FFO	C2-NA2	4.76	1.45	1.34
4	D	708[B]	FFO	C5A-N5	4.75	1.45	1.36
4	A	508[A]	FFO	C4-N3	4.74	1.47	1.38
4	A	508[A]	FFO	C2-NA2	4.73	1.45	1.34
4	C	508[B]	FFO	C2-NA2	4.63	1.45	1.34
4	C	508[A]	FFO	C4-N3	4.60	1.47	1.38
4	C	508[B]	FFO	C5A-N5	4.56	1.44	1.36
4	A	508[B]	FFO	C2-NA2	4.46	1.44	1.34
4	C	508[A]	FFO	C2-NA2	4.43	1.44	1.34
4	B	808[A]	FFO	C4A-C4	3.33	1.52	1.43
4	A	508[B]	FFO	C14-N10	3.26	1.48	1.38
4	B	808[B]	FFO	C14-N10	3.20	1.48	1.38
4	D	708[B]	FFO	C14-N10	3.20	1.48	1.38
4	D	708[A]	FFO	C4A-C4	3.15	1.51	1.43
4	B	808[A]	FFO	C14-N10	3.14	1.47	1.38
4	C	508[A]	FFO	C4A-C4	3.14	1.51	1.43
4	A	508[B]	FFO	C4A-C4	3.12	1.51	1.43
4	D	708[A]	FFO	C14-N10	3.12	1.47	1.38
4	B	808[B]	FFO	C4A-C4	3.10	1.51	1.43
4	A	508[A]	FFO	C14-N10	3.08	1.47	1.38
2	B	802	PLG	C5-C4	-3.06	1.36	1.40
4	D	708[B]	FFO	C4A-C4	2.99	1.51	1.43
4	C	508[B]	FFO	C14-N10	2.98	1.47	1.38
4	A	508[A]	FFO	C4A-C4	2.94	1.51	1.43
4	C	508[A]	FFO	C14-N10	2.92	1.47	1.38
4	C	508[B]	FFO	C4A-C4	2.90	1.51	1.43
2	A	501	PLG	C5-C4	-2.74	1.36	1.40
2	C	501	PLG	C5-C4	-2.66	1.36	1.40
2	B	802	PLG	C3-C2	-2.49	1.38	1.40
4	D	708[A]	FFO	O4-C4	-2.47	1.18	1.23
4	C	508[B]	FFO	C9-N10	2.47	1.50	1.45
2	D	703	PLG	C5-C4	-2.45	1.37	1.40
4	D	708[B]	FFO	C11-C	2.41	1.55	1.50
4	A	508[A]	FFO	O-C	-2.40	1.18	1.23
4	D	708[A]	FFO	C11-C	2.36	1.55	1.50
4	B	808[B]	FFO	C11-C	2.32	1.55	1.50
4	A	508[B]	FFO	C11-C	2.32	1.55	1.50
4	B	808[A]	FFO	C11-C	2.27	1.54	1.50
4	D	708[A]	FFO	O-C	-2.25	1.18	1.23
4	C	508[A]	FFO	O-C	-2.24	1.18	1.23
4	A	508[B]	FFO	O4-C4	-2.24	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	708[B]	FFO	O-C	-2.23	1.18	1.23
4	B	808[B]	FFO	O-C	-2.22	1.18	1.23
4	B	808[A]	FFO	O-C	-2.22	1.18	1.23
4	A	508[B]	FFO	O-C	-2.21	1.18	1.23
4	C	508[B]	FFO	O-C	-2.19	1.18	1.23
2	B	802	PLG	C3-C4	-2.16	1.36	1.40
4	C	508[A]	FFO	O4-C4	-2.16	1.19	1.23
2	D	703	PLG	C3-C2	-2.14	1.38	1.40
4	A	508[A]	FFO	C11-C	2.14	1.54	1.50
2	A	501	PLG	C3-C2	-2.14	1.38	1.40
4	B	808[B]	FFO	O4-C4	-2.13	1.19	1.23
2	C	501	PLG	C3-C4	-2.10	1.36	1.40
4	C	508[A]	FFO	C11-C	2.08	1.54	1.50

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	708[A]	FFO	C4A-C4-N3	5.42	120.54	110.99
4	A	508[B]	FFO	C4A-C4-N3	5.12	120.01	110.99
4	B	808[B]	FFO	C4A-C4-N3	4.99	119.78	110.99
4	C	508[B]	FFO	C4A-C4-N3	4.95	119.72	110.99
4	C	508[A]	FFO	C4A-C4-N3	4.93	119.67	110.99
4	A	508[A]	FFO	C4A-C4-N3	4.82	119.48	110.99
4	B	808[A]	FFO	C4A-C4-N3	4.72	119.31	110.99
4	D	708[B]	FFO	C4A-C4-N3	4.37	118.70	110.99
4	C	508[B]	FFO	C2-N1-C8A	4.18	120.97	113.43
2	D	703	PLG	OP4-C5A-C5	4.03	117.04	109.35
4	C	508[A]	FFO	C2-N1-C8A	3.92	120.51	113.43
4	A	508[B]	FFO	C2-N1-C8A	3.76	120.21	113.43
4	A	508[A]	FFO	C2-N1-C8A	3.76	120.21	113.43
4	D	708[A]	FFO	C2-N1-C8A	3.70	120.10	113.43
4	B	808[B]	FFO	C2-N1-C8A	3.65	120.03	113.43
4	B	808[A]	FFO	C2-N1-C8A	3.60	119.92	113.43
4	D	708[B]	FFO	C2-N1-C8A	3.54	119.83	113.43
2	B	802	PLG	OP4-C5A-C5	3.39	115.81	109.35
2	C	501	PLG	OP4-C5A-C5	3.20	115.45	109.35
4	A	508[B]	FFO	C2-N3-C4	-3.02	119.60	125.10
2	B	802	PLG	C6-C5-C4	2.95	120.20	118.12
4	B	808[A]	FFO	C6-C9-N10	-2.83	104.85	112.23
2	A	501	PLG	OP4-C5A-C5	2.81	114.71	109.35
4	D	708[A]	FFO	C2-N3-C4	-2.78	120.03	125.10
2	B	802	PLG	C4A-N-CA	-2.77	109.69	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	PLG	C5-C6-N1	-2.73	119.27	123.82
4	C	508[A]	FFO	C6-C9-N10	-2.70	105.18	112.23
2	C	501	PLG	C4A-C4-C5	-2.64	116.78	119.71
4	D	708[A]	FFO	CG-CB-CA	-2.61	108.27	113.16
4	A	508[A]	FFO	O5B-C5A-N5	-2.58	120.24	124.63
4	B	808[B]	FFO	C2-N3-C4	-2.58	120.40	125.10
2	C	501	PLG	C6-C5-C4	2.57	119.94	118.12
4	C	508[B]	FFO	C2-N3-C4	-2.56	120.43	125.10
2	C	501	PLG	C4A-C4-C3	2.53	122.75	120.04
2	C	501	PLG	C5-C6-N1	-2.51	119.64	123.82
4	A	508[A]	FFO	O4-C4-C4A	-2.50	121.41	127.54
4	C	508[B]	FFO	O5B-C5A-N5	-2.49	120.40	124.63
2	D	703	PLG	C4A-C4-C3	2.48	122.70	120.04
4	A	508[A]	FFO	C2-N3-C4	-2.47	120.59	125.10
4	C	508[A]	FFO	C2-N3-C4	-2.43	120.67	125.10
4	D	708[B]	FFO	C6-C9-N10	-2.42	105.91	112.23
4	D	708[B]	FFO	O4-C4-C4A	-2.39	121.67	127.54
4	D	708[B]	FFO	CG-CB-CA	-2.39	108.69	113.16
2	D	703	PLG	C5-C6-N1	-2.37	119.87	123.82
4	A	508[B]	FFO	O4-C4-C4A	-2.36	121.75	127.54
2	D	703	PLG	C6-C5-C4	2.36	119.78	118.12
4	C	508[B]	FFO	O4-C4-C4A	-2.33	121.83	127.54
2	A	501	PLG	C6-C5-C4	2.32	119.76	118.12
4	D	708[B]	FFO	O5B-C5A-N5	-2.32	120.69	124.63
4	B	808[B]	FFO	O4-C4-C4A	-2.31	121.88	127.54
4	D	708[A]	FFO	O4-C4-C4A	-2.30	121.90	127.54
2	A	501	PLG	C5-C6-N1	-2.29	120.00	123.82
4	A	508[B]	FFO	CG-CB-CA	-2.29	108.87	113.16
4	D	708[B]	FFO	C2-N3-C4	-2.25	120.99	125.10
4	D	708[A]	FFO	C6-C9-N10	-2.16	106.61	112.23
4	B	808[B]	FFO	C6-C9-N10	-2.15	106.62	112.23
4	A	508[A]	FFO	CG-CB-CA	-2.11	109.21	113.16
4	C	508[A]	FFO	O4-C4-C4A	-2.08	122.44	127.54
4	C	508[B]	FFO	N3-C2-N1	-2.07	119.46	123.32
4	A	508[B]	FFO	NA2-C2-N3	2.07	121.12	116.71
4	B	808[A]	FFO	N3-C2-N1	-2.06	119.49	123.32
2	A	501	PLG	C4A-C4-C3	2.01	122.19	120.04

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLG	C3-C4-C4A-N
2	A	501	PLG	C5-C4-C4A-N
2	B	802	PLG	C3-C4-C4A-N
2	B	802	PLG	C5-C4-C4A-N
2	C	501	PLG	C3-C4-C4A-N
2	C	501	PLG	C5-C4-C4A-N
2	D	703	PLG	C3-C4-C4A-N
2	D	703	PLG	C5-C4-C4A-N
4	C	508[A]	FFO	C13-C14-N10-C9
4	C	508[A]	FFO	C15-C14-N10-C9
3	A	504	EDO	O1-C1-C2-O2
3	A	505	EDO	O1-C1-C2-O2
4	A	508[B]	FFO	C13-C14-N10-C9
2	D	703	PLG	C5A-OP4-P-OP1
4	C	508[A]	FFO	CT-CA-CB-CG
4	C	508[B]	FFO	CT-CA-CB-CG
4	A	508[B]	FFO	C15-C14-N10-C9
3	D	709	EDO	O1-C1-C2-O2
4	D	708[A]	FFO	C13-C14-N10-C9
4	B	808[B]	FFO	CA-CB-CG-CD
3	A	507	EDO	O1-C1-C2-O2
4	A	508[A]	FFO	C13-C14-N10-C9
4	B	808[A]	FFO	CA-CB-CG-CD
4	D	708[A]	FFO	C15-C14-N10-C9
3	D	704	EDO	O1-C1-C2-O2
4	B	808[A]	FFO	C15-C14-N10-C9
2	D	703	PLG	C5A-OP4-P-OP2
3	C	507	EDO	O1-C1-C2-O2
3	D	702	EDO	O1-C1-C2-O2
3	B	807	EDO	O1-C1-C2-O2
4	B	808[B]	FFO	OE2-CD-CG-CB

There are no ring outliers.

20 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	805	EDO	1	0
3	A	503	EDO	1	0
3	C	506	EDO	1	0
2	C	501	PLG	2	0
2	A	501	PLG	2	0
3	D	702	EDO	3	0
4	D	708[A]	FFO	1	0

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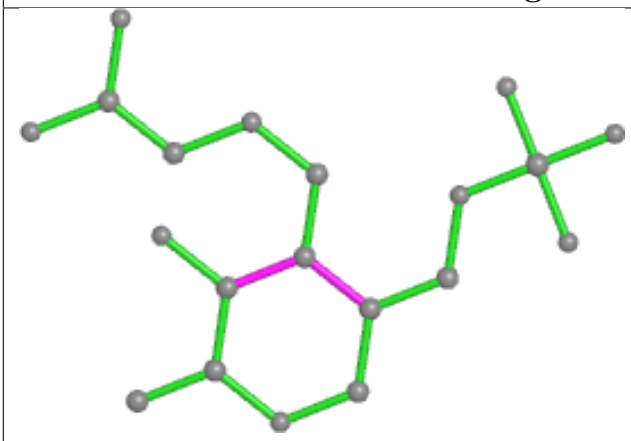
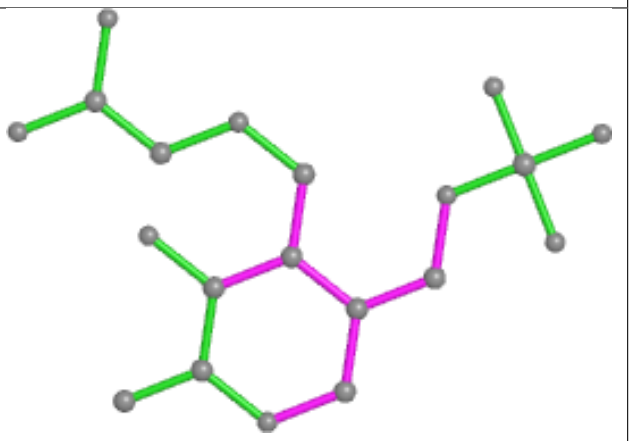
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	706	EDO	1	0
2	B	802	PLG	2	0
3	B	801	EDO	1	0
4	B	808[B]	FFO	2	0
4	C	508[B]	FFO	2	0
3	C	504	EDO	1	0
3	D	707	EDO	2	0
4	B	808[A]	FFO	2	0
4	C	508[A]	FFO	1	0
2	D	703	PLG	2	0
3	D	701	EDO	1	0
3	C	507	EDO	1	0
3	D	709	EDO	1	0

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

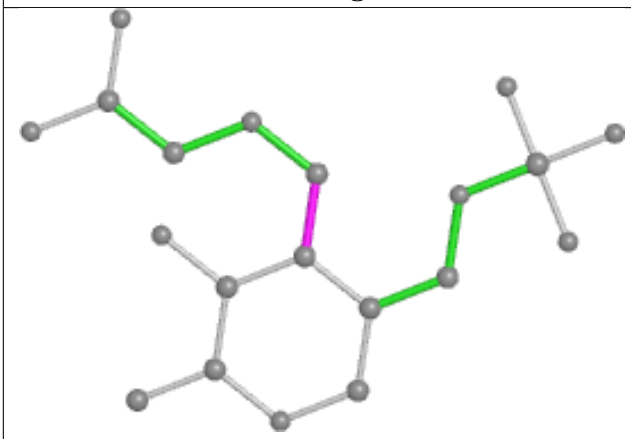
Ligand PLG C 501



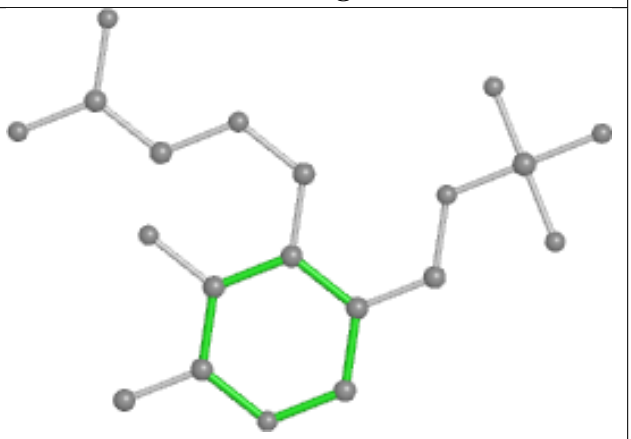
Bond lengths



Bond angles

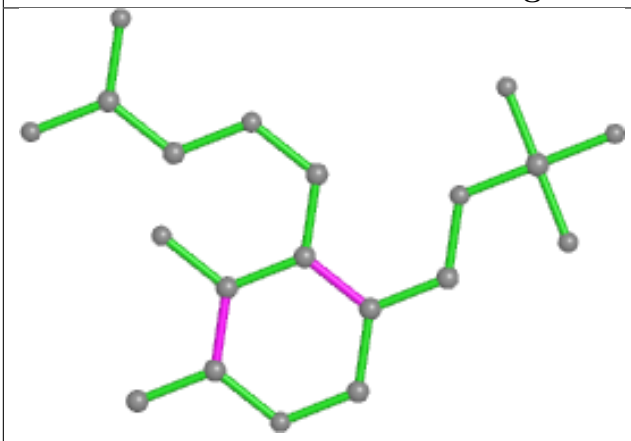


Torsions



Rings

Ligand PLG A 501



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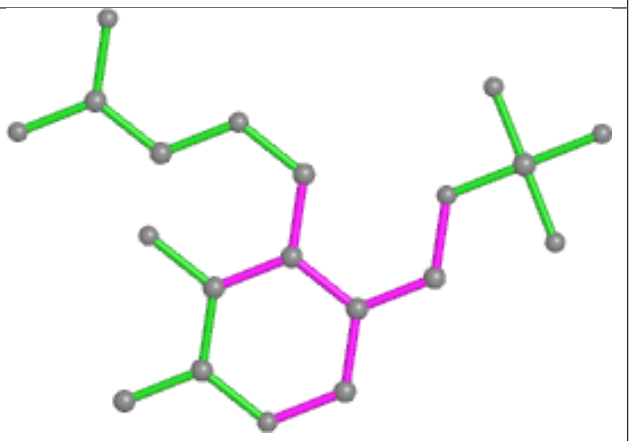
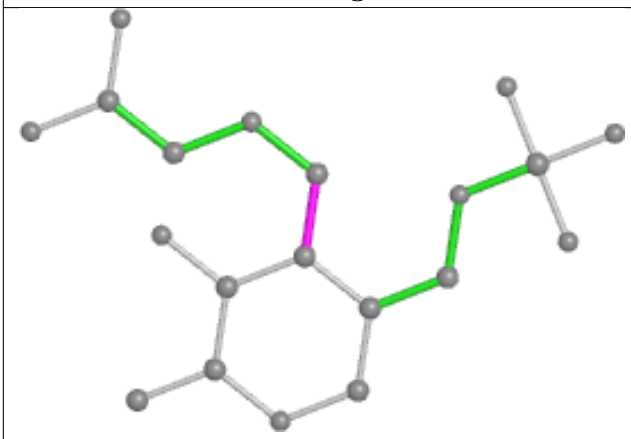
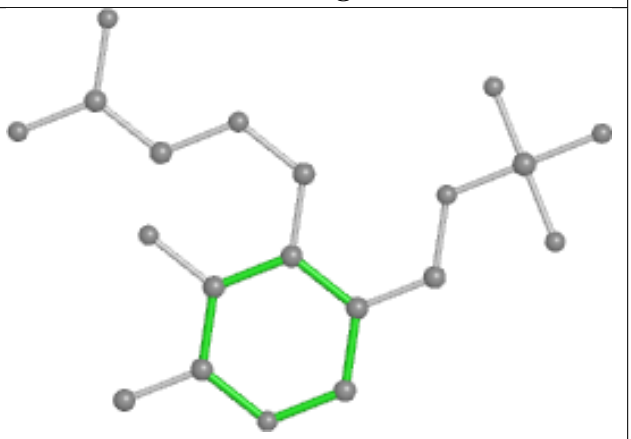


Bond angles

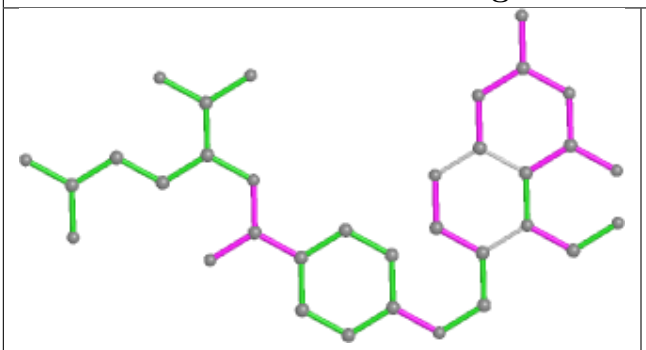


Torsions



Rings

Ligand FFO D 708 (A)



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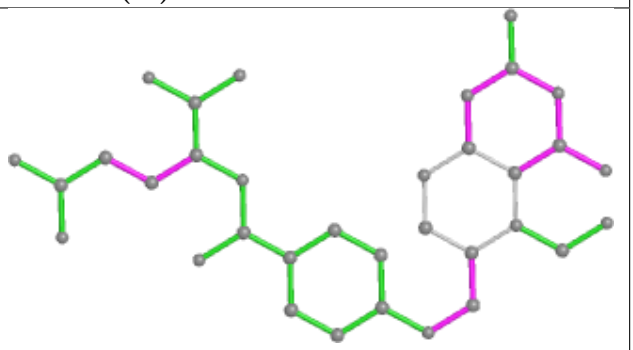
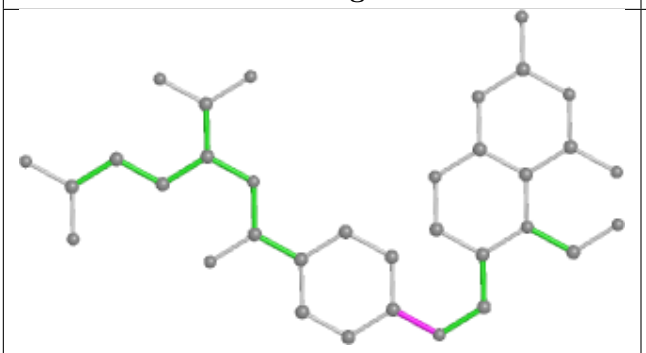
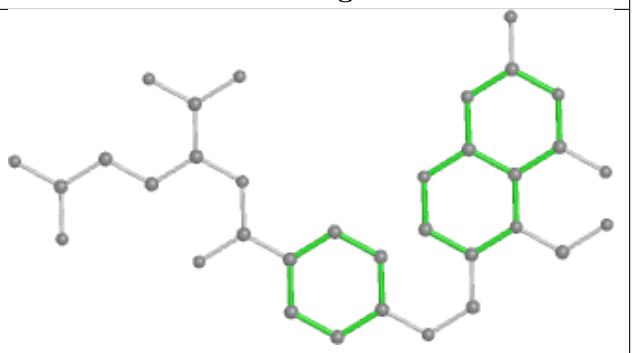


Bond angles

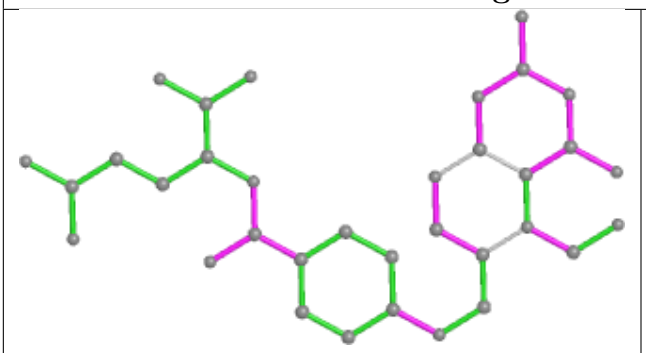


Torsions



Rings

Ligand FFO A 508 (B)



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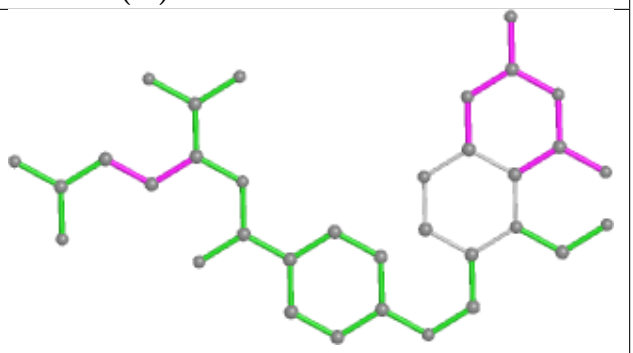
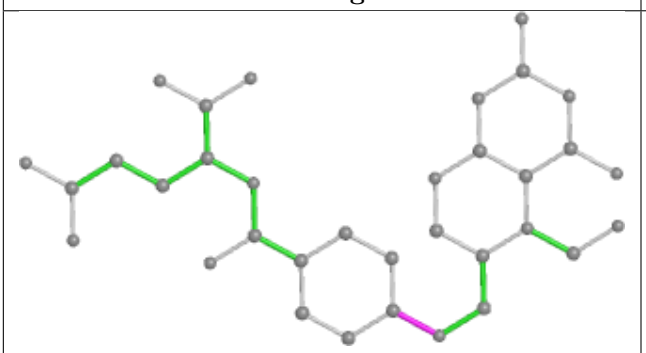
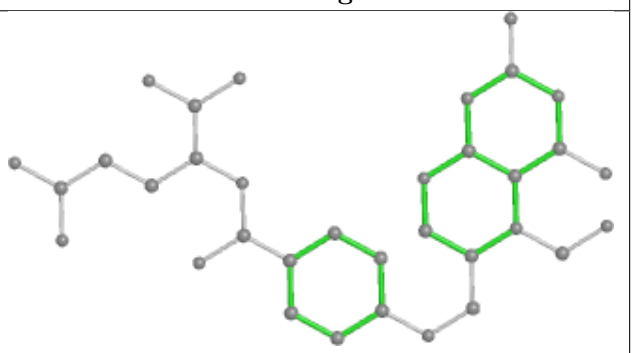


Bond angles

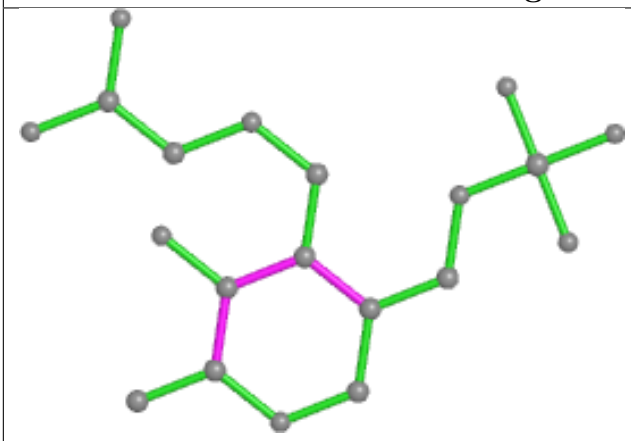


Torsions

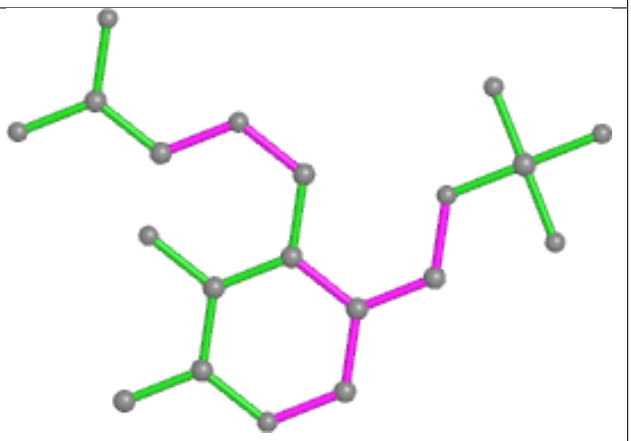


Rings

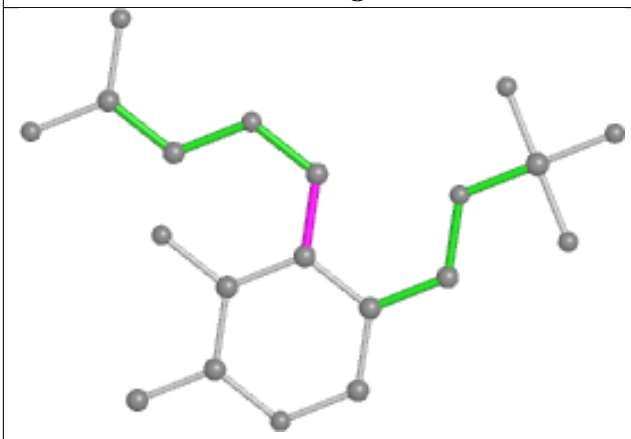
Ligand PLG B 802



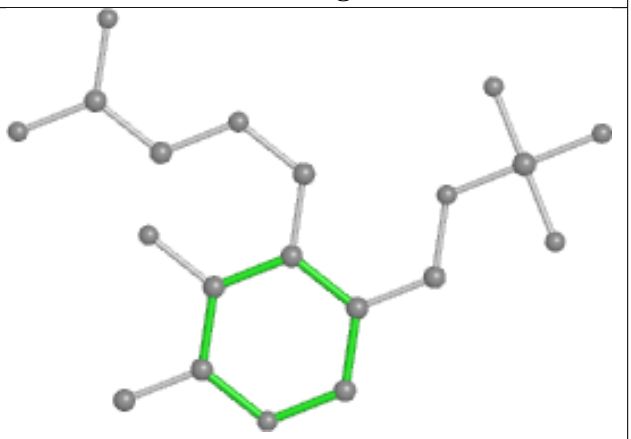
Bond lengths



Bond angles

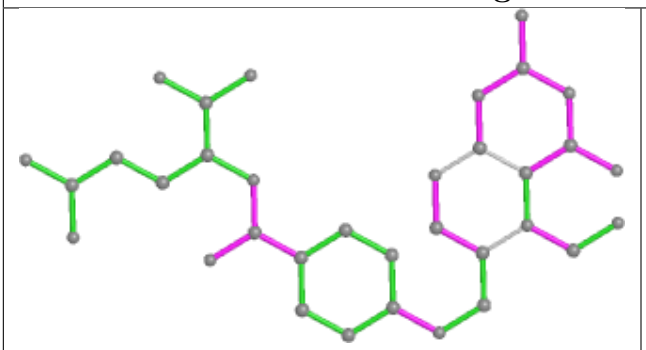


Torsions

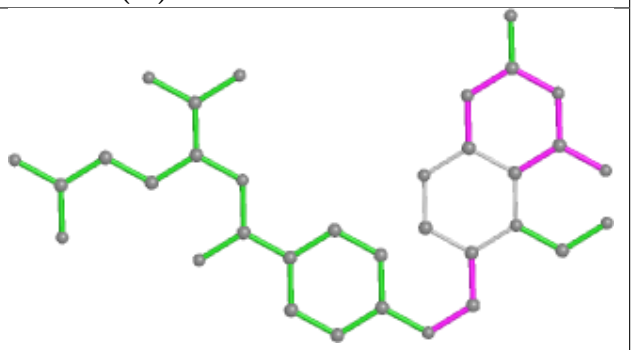


Rings

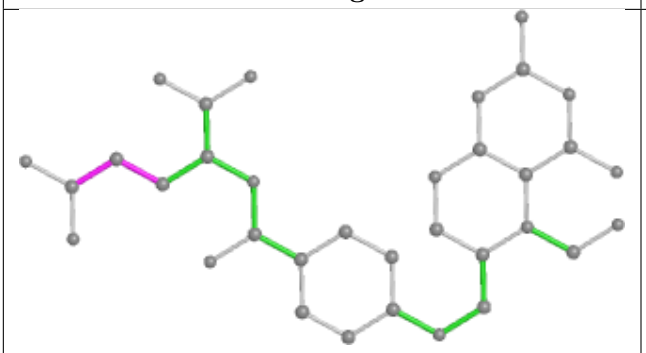
Ligand FFO B 808 (B)



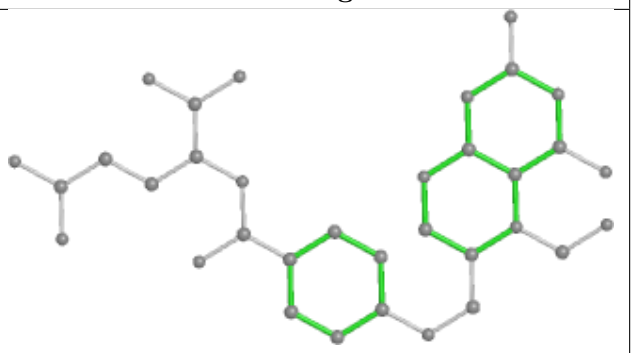
Bond lengths



Bond angles

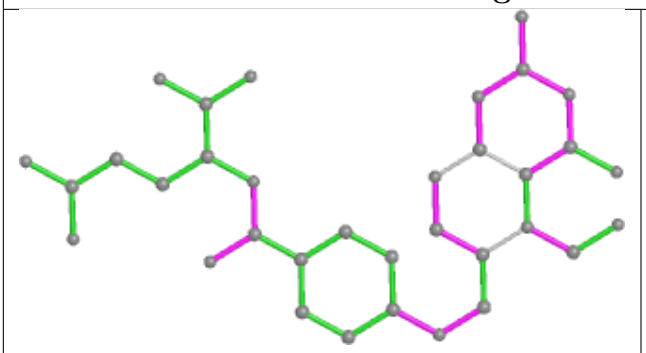


Torsions

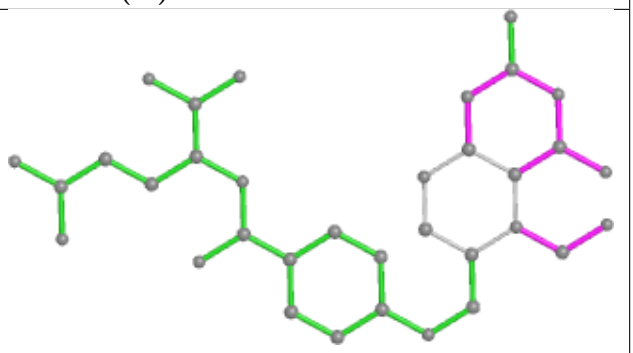


Rings

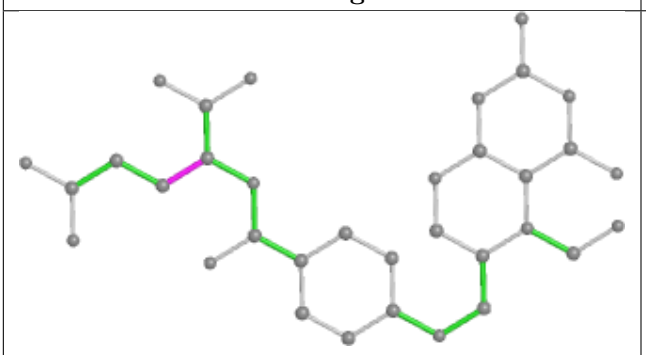
Ligand FFO C 508 (B)



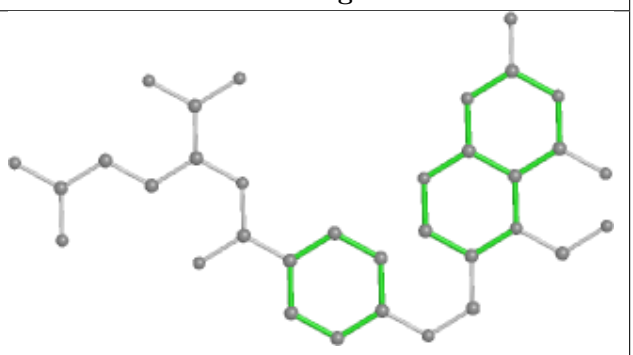
Bond lengths



Bond angles

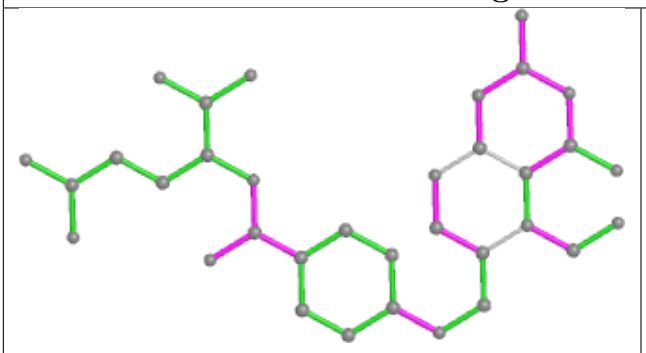


Torsions



Rings

Ligand FFO A 508 (A)



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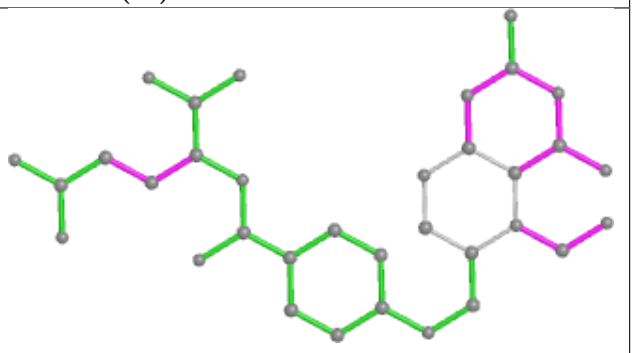
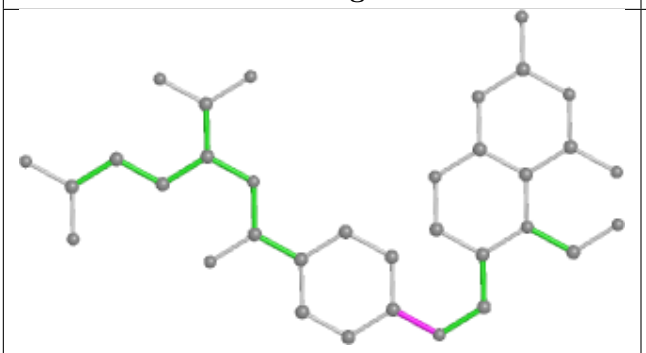
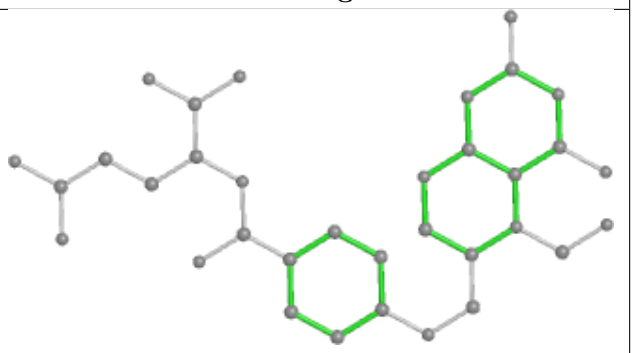


Bond angles

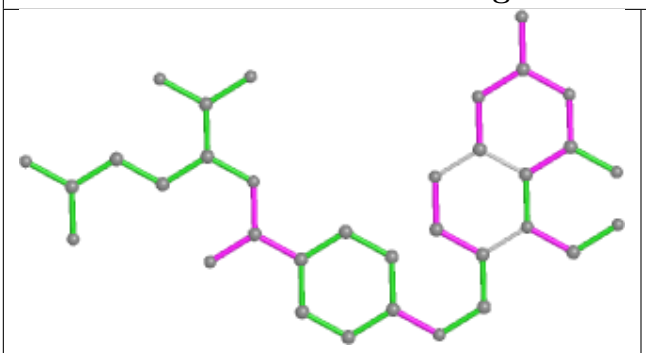


Torsions



Rings

Ligand FFO B 808 (A)



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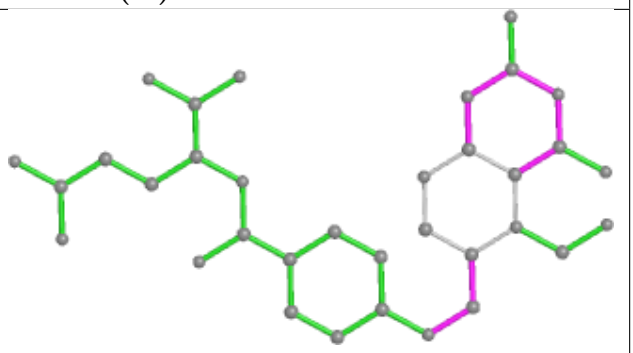
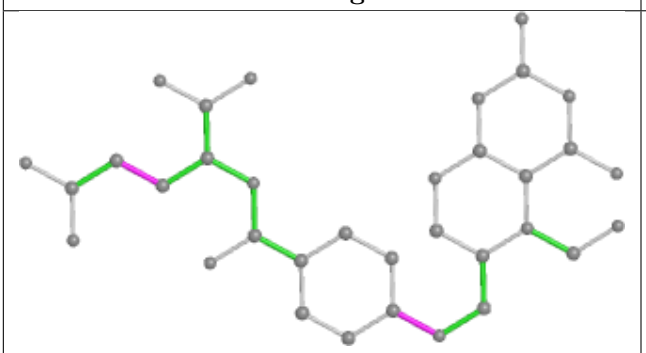
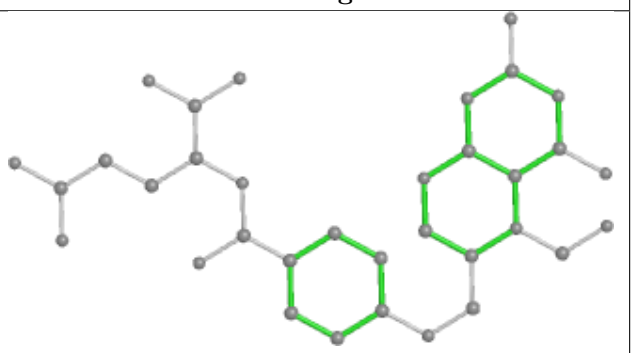


Bond angles

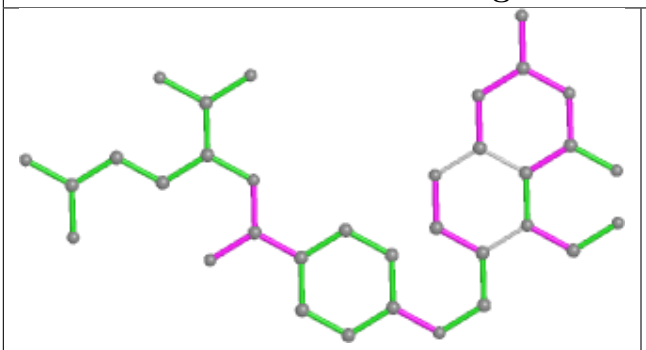


Torsions

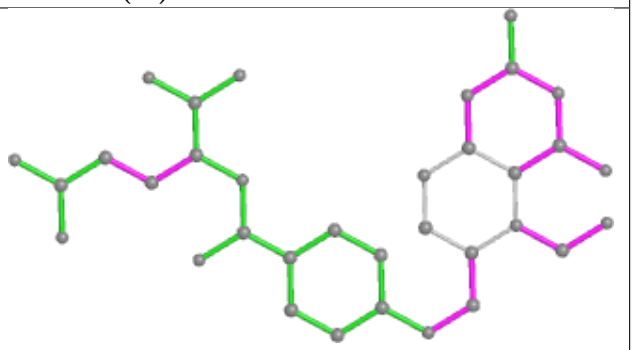


Rings

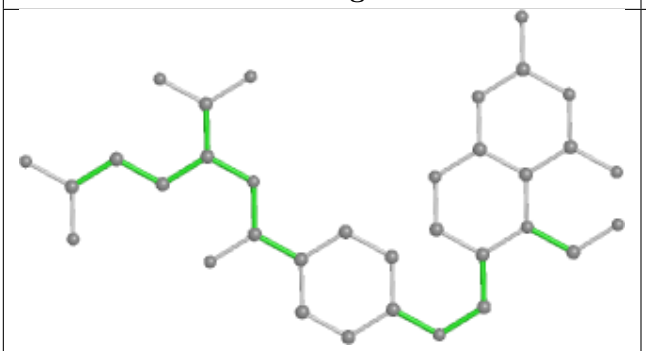
Ligand FFO D 708 (B)



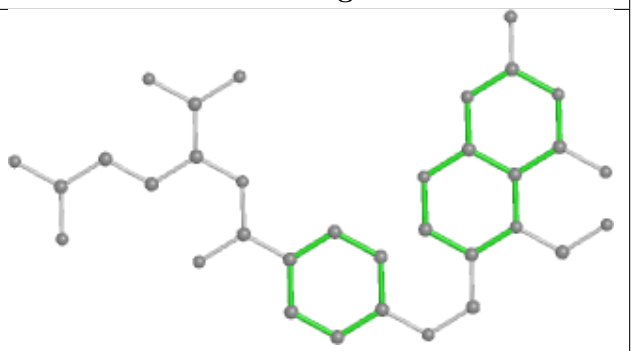
Bond lengths



Bond angles

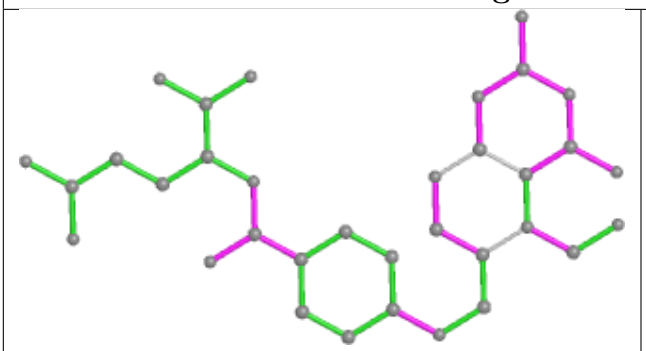


Torsions



Rings

Ligand FFO C 508 (A)



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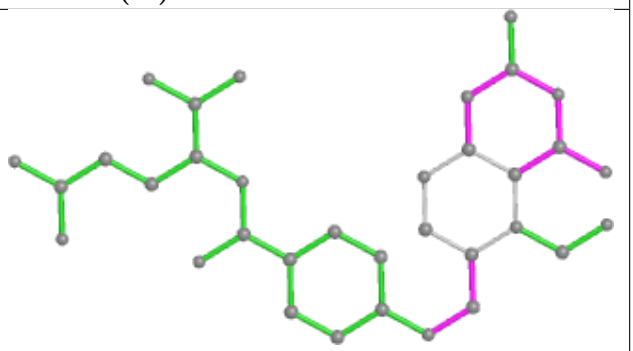
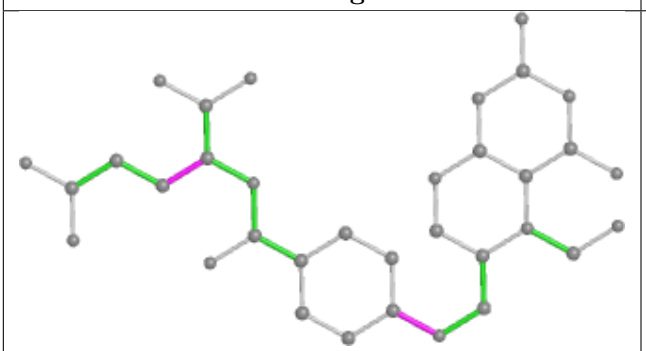
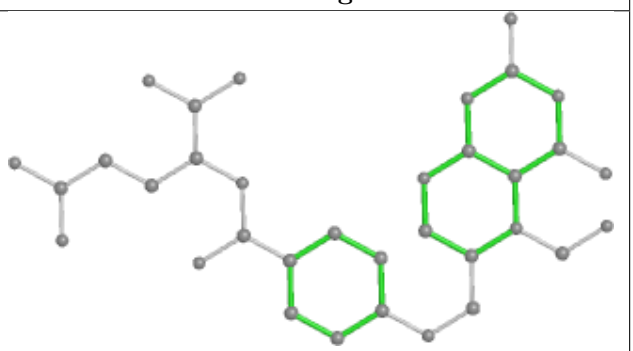


Bond angles

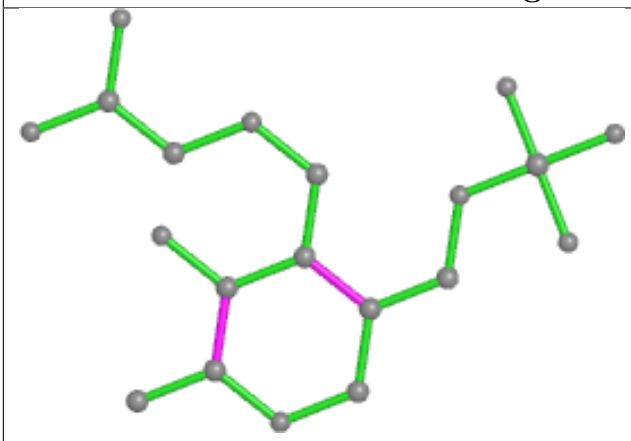


Torsions

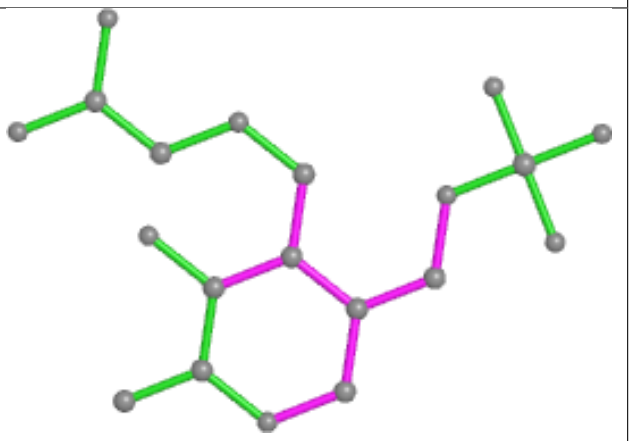


Rings

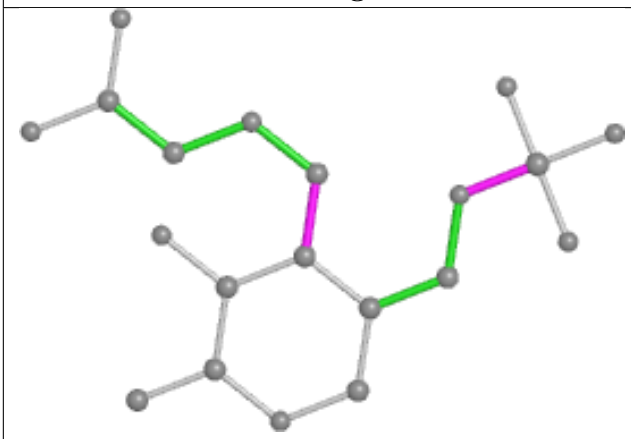
Ligand PLG D 703



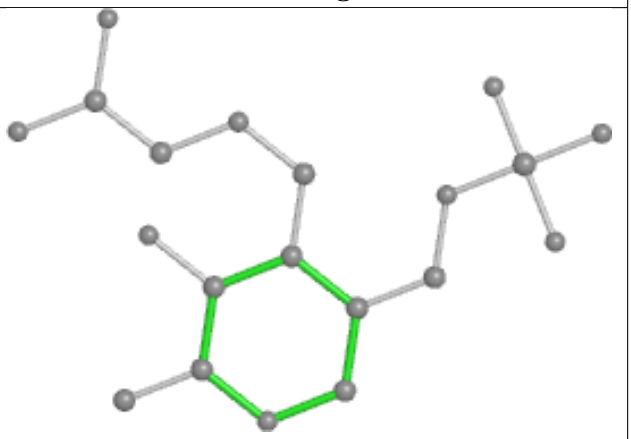
Bond lengths



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	472/491 (96%)	0.47	36 (7%) 13 14	18, 28, 57, 91	0
1	B	468/491 (95%)	0.56	45 (9%) 8 8	16, 25, 62, 86	0
1	C	472/491 (96%)	0.24	17 (3%) 42 47	16, 22, 41, 92	0
1	D	469/491 (95%)	0.67	53 (11%) 5 5	15, 23, 65, 79	0
All	All	1881/1964 (95%)	0.48	151 (8%) 12 13	15, 25, 59, 92	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	GLY	10.8
1	B	266	GLY	9.9
1	D	266	GLY	9.4
1	D	268	PRO	8.8
1	C	266	GLY	8.6
1	D	427	GLY	8.3
1	B	268	PRO	8.3
1	B	438	VAL	7.6
1	D	429	LEU	7.5
1	B	426	HIS	7.3
1	D	433	PHE	7.1
1	A	268	PRO	7.0
1	D	262	PRO	6.8
1	D	270	ASN	6.7
1	D	426	HIS	6.7
1	B	263	PRO	6.6
1	D	263	PRO	6.6
1	D	267	GLN	6.5
1	D	264	LYS	6.4
1	B	269	GLU	6.4
1	B	429	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	378	GLY	6.2
1	D	438	VAL	6.2
1	D	420	LEU	6.0
1	B	265	LYS	6.0
1	B	270	ASN	5.6
1	D	430	LEU	5.6
1	A	267	GLN	5.6
1	D	265	LYS	5.6
1	A	269	GLU	5.5
1	B	431	LYS	5.4
1	D	269	GLU	5.4
1	B	262	PRO	5.4
1	D	271	ALA	5.3
1	D	422	ILE	5.3
1	A	264	LYS	5.3
1	B	267	GLN	5.1
1	A	263	PRO	5.1
1	A	262	PRO	5.0
1	B	422	ILE	5.0
1	D	432	ASP	4.9
1	B	433	PHE	4.9
1	A	265	LYS	4.9
1	C	269	GLU	4.8
1	B	264	LYS	4.8
1	C	268	PRO	4.7
1	D	424	LYS	4.7
1	B	271	ALA	4.6
1	D	351	ARG	4.4
1	D	355	LEU	4.4
1	A	270	ASN	4.4
1	B	427	GLY	4.3
1	C	270	ASN	4.3
1	A	164	THR	4.3
1	A	69[A]	TYR	4.2
1	B	430	LEU	4.1
1	A	163	SER	4.1
1	C	267	GLN	4.0
1	D	0	HIS	4.0
1	A	271	ALA	4.0
1	B	432	ASP	3.9
1	D	439	ASN	3.9
1	D	423	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	353	LEU	3.8
1	C	264	LYS	3.8
1	D	384	ALA	3.7
1	A	430	LEU	3.7
1	B	435	LYS	3.7
1	D	431	LYS	3.7
1	D	434	ASN	3.6
1	D	428	LYS	3.6
1	D	383	LEU	3.5
1	C	262	PRO	3.5
1	D	272	VAL	3.4
1	B	420	LEU	3.4
1	A	377	PHE	3.4
1	B	428	LYS	3.3
1	D	425	GLU	3.3
1	A	471	ASP	3.2
1	C	471	ASP	3.2
1	B	353	LEU	3.2
1	A	0	HIS	3.2
1	D	436	GLY	3.2
1	A	333	GLY	3.1
1	B	423	GLN	3.1
1	A	383	LEU	3.1
1	C	263	PRO	3.1
1	C	0	HIS	3.0
1	B	439	ASN	3.0
1	B	434	ASN	3.0
1	D	437	LEU	3.0
1	D	378	GLY	2.9
1	B	272	VAL	2.9
1	C	69	TYR	2.9
1	D	435	LYS	2.9
1	D	350	LEU	2.8
1	B	141	THR	2.8
1	B	384	ALA	2.8
1	B	437	LEU	2.7
1	C	429	LEU	2.7
1	A	287	LEU	2.7
1	A	429	LEU	2.7
1	A	1[A]	MET	2.7
1	B	425	GLU	2.6
1	C	470	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	441	LYS	2.5
1	C	265	LYS	2.5
1	C	93	ASP	2.5
1	A	167	TYR	2.5
1	B	144	GLY	2.5
1	A	68	TYR	2.5
1	D	260	PRO	2.5
1	D	441	LYS	2.5
1	A	382	ALA	2.4
1	B	455	ALA	2.4
1	A	95[A]	GLN	2.4
1	D	419	THR	2.4
1	B	440	ASN	2.4
1	A	420	LEU	2.4
1	D	349	ASP	2.3
1	D	375	ALA	2.3
1	C	271	ALA	2.3
1	D	443	ILE	2.3
1	A	335	SER	2.3
1	C	104	TYR	2.3
1	D	421	GLU	2.3
1	D	296	ILE	2.3
1	B	135	LEU	2.3
1	B	104	TYR	2.3
1	B	0	HIS	2.2
1	D	356	THR	2.2
1	D	259	GLY	2.2
1	B	436	GLY	2.2
1	B	260	PRO	2.2
1	B	296	ILE	2.2
1	D	377	PHE	2.1
1	B	355	LEU	2.1
1	A	328	TYR	2.1
1	A	259	GLY	2.1
1	A	375	ALA	2.1
1	B	111	PHE	2.1
1	A	432	ASP	2.1
1	B	274[A]	ASP	2.1
1	A	379	ASP	2.1
1	D	352	PRO	2.1
1	A	426	HIS	2.1
1	D	144[A]	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	379	ASP	2.0
1	A	470	LYS	2.0
1	D	440	ASN	2.0
1	A	456	LEU	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
3	EDO	B	804	4/4	0.69	0.17	52,52,52,52	0
3	EDO	B	806	4/4	0.69	0.31	56,63,72,81	0
3	EDO	C	506	4/4	0.69	0.17	38,43,50,57	4
3	EDO	A	504	4/4	0.70	0.16	29,41,45,50	4
3	EDO	A	507	4/4	0.72	0.26	49,50,51,56	4
3	EDO	B	801	4/4	0.76	0.23	42,42,42,42	0
3	EDO	A	505	4/4	0.76	0.18	48,51,57,65	0
3	EDO	B	805	4/4	0.77	0.15	42,45,59,70	0
3	EDO	A	503	4/4	0.79	0.14	54,54,55,55	0
3	EDO	D	709	4/4	0.80	0.21	31,34,36,40	0
3	EDO	A	506	4/4	0.82	0.13	51,53,61,67	0
3	EDO	D	707	4/4	0.84	0.13	28,32,40,42	4
3	EDO	B	807	4/4	0.85	0.13	53,58,59,100	0
4	FFO	B	808[A]	34/34	0.85	0.18	16,42,69,75	34
4	FFO	B	808[B]	34/34	0.85	0.18	18,41,78,84	34
4	FFO	D	708[A]	34/34	0.85	0.18	12,37,72,85	34
4	FFO	D	708[B]	34/34	0.85	0.18	14,34,74,87	34
3	EDO	C	505	4/4	0.86	0.23	44,46,60,99	0
3	EDO	B	803	4/4	0.86	0.20	57,57,57,57	0

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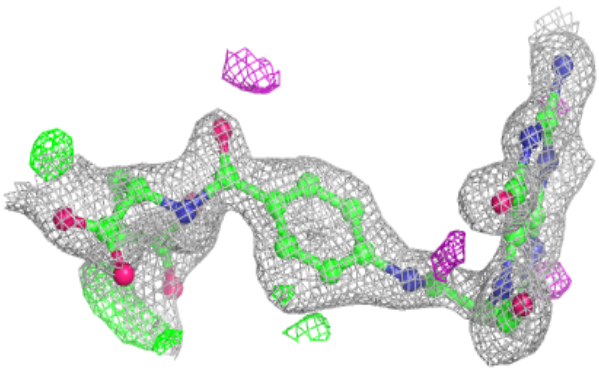
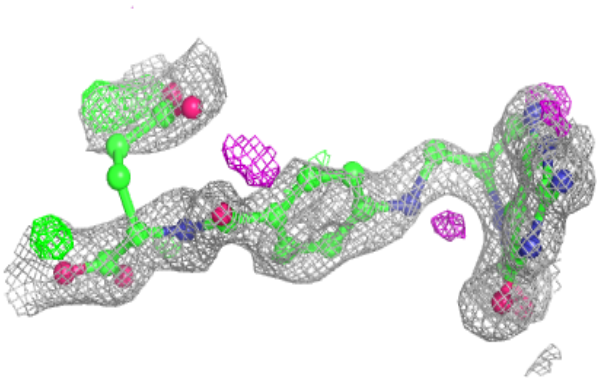
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	D	705	4/4	0.86	0.21	53,53,53,53	0
3	EDO	D	706	4/4	0.87	0.12	29,39,43,46	4
3	EDO	D	702	4/4	0.88	0.12	49,49,50,50	0
3	EDO	C	502	4/4	0.88	0.16	23,23,24,24	0
3	EDO	C	507	4/4	0.88	0.10	36,49,59,60	0
3	EDO	C	504	4/4	0.90	0.12	47,47,47,47	0
3	EDO	A	502	4/4	0.91	0.10	19,20,20,21	4
3	EDO	D	704	4/4	0.91	0.16	34,34,35,35	0
3	EDO	C	503	4/4	0.92	0.12	29,29,30,30	0
4	FFO	A	508[A]	34/34	0.93	0.11	13,27,56,74	34
4	FFO	A	508[B]	34/34	0.93	0.11	12,30,58,68	34
3	EDO	D	701	4/4	0.93	0.11	49,49,50,50	0
4	FFO	C	508[B]	34/34	0.94	0.12	5,17,49,65	34
3	EDO	A	509	4/4	0.94	0.10	19,26,28,31	0
4	FFO	C	508[A]	34/34	0.94	0.12	6,23,44,61	34
2	PLG	C	501	20/20	0.97	0.11	16,17,18,19	0
2	PLG	D	703	20/20	0.97	0.13	16,17,20,21	0
2	PLG	A	501	20/20	0.97	0.10	19,21,22,22	0
2	PLG	B	802	20/20	0.98	0.12	18,19,21,21	0

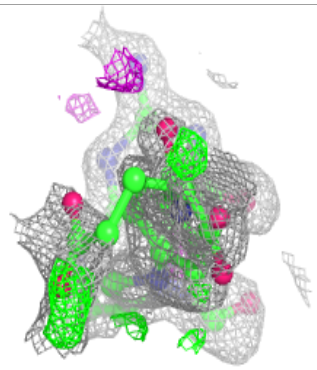
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FFO B 808 (A):

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

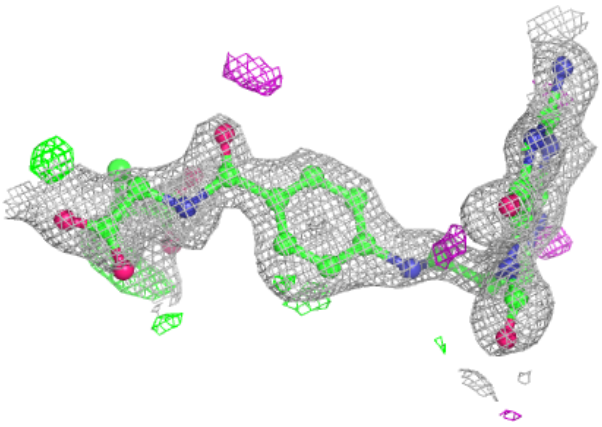


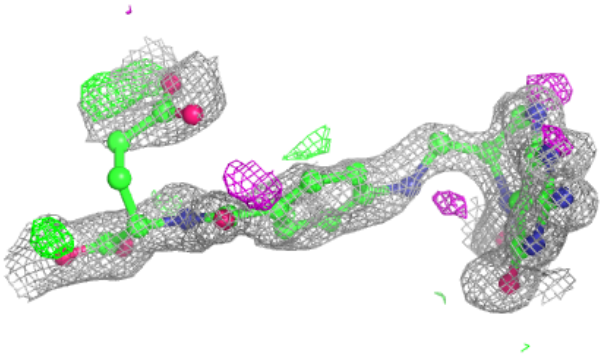


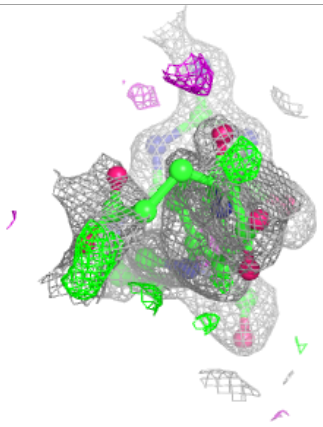


Electron density around FFO B 808 (B):

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

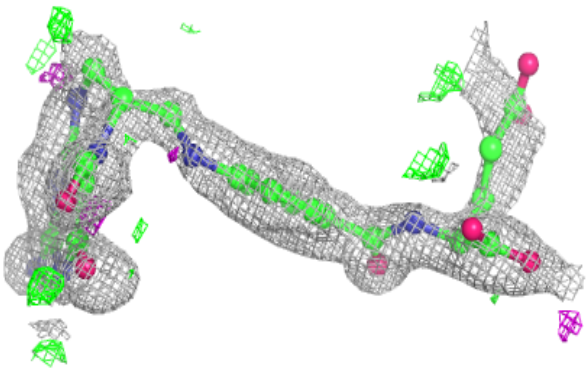


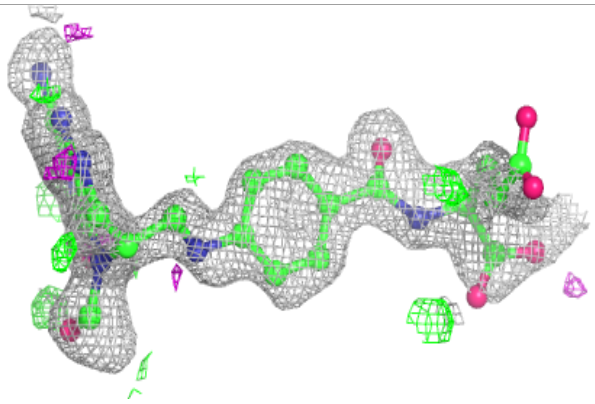


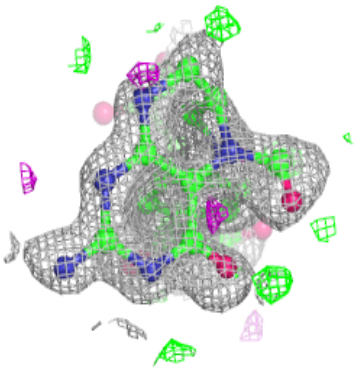


Electron density around FFO D 708 (A):

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

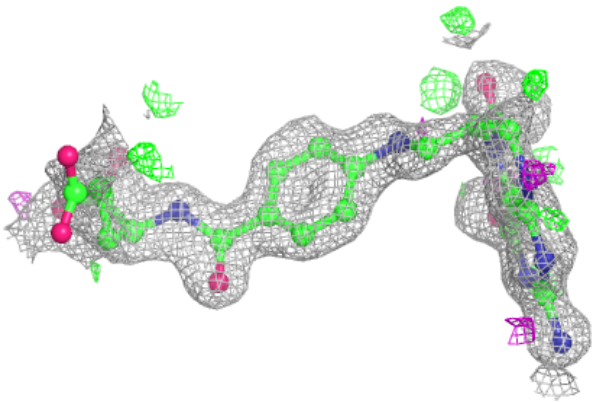


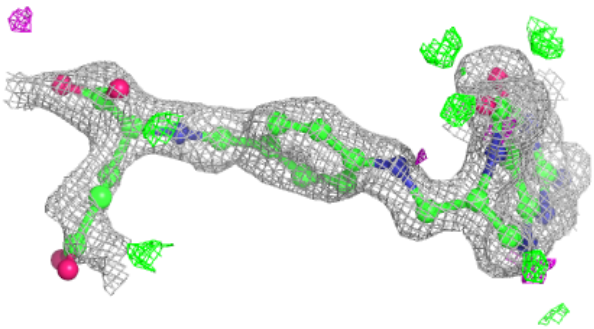


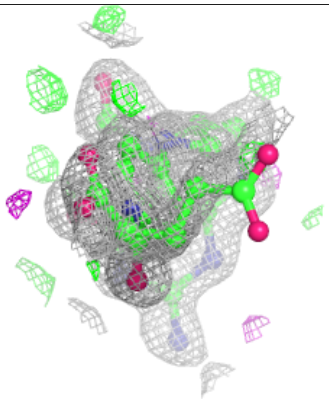


Electron density around FFO D 708 (B):

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

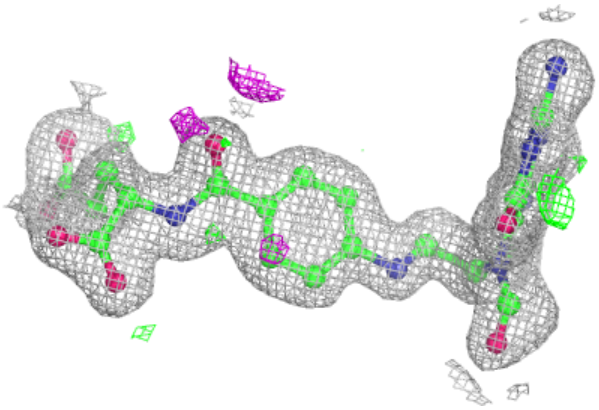


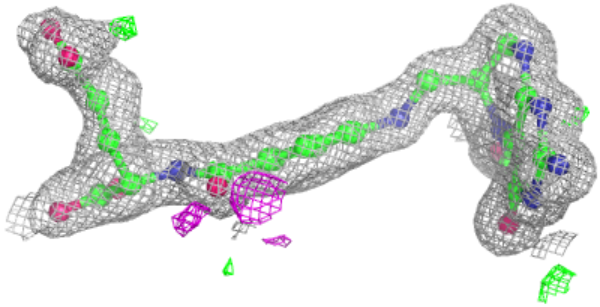


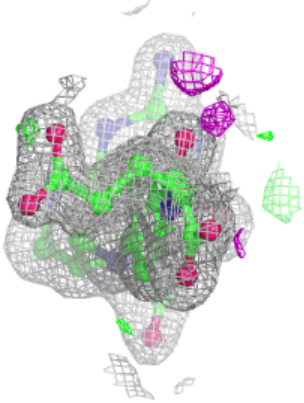


Electron density around FFO A 508 (A):

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

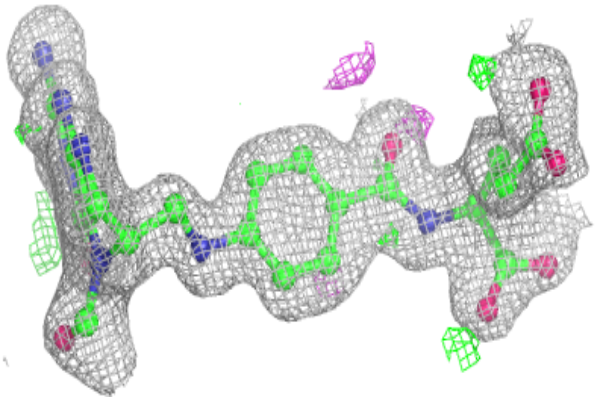


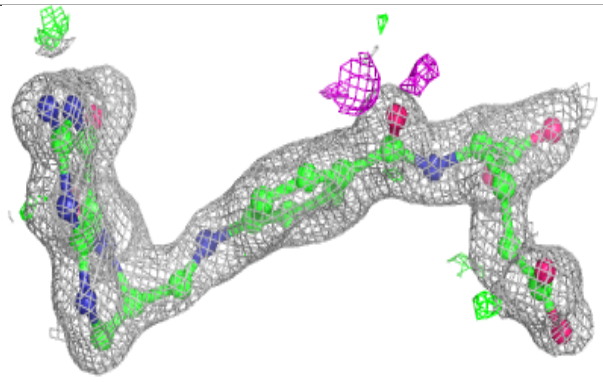


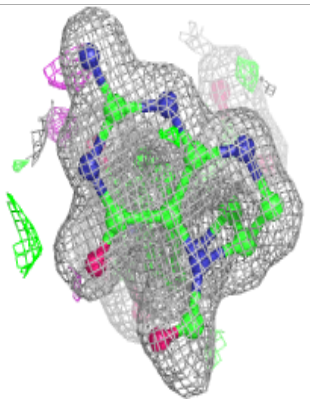


Electron density around FFO A 508 (B):

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

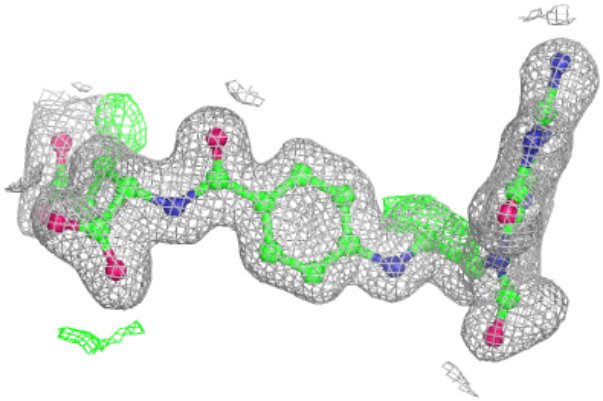


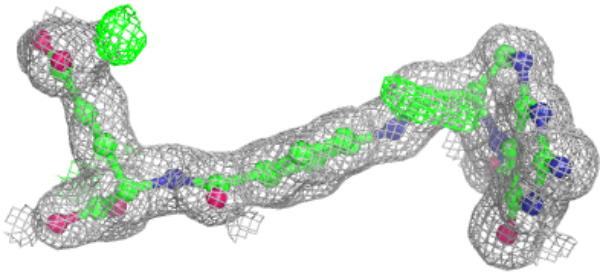


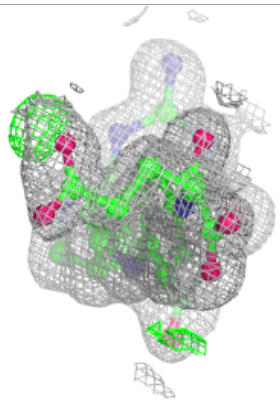


Electron density around FFO C 508 (B):

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

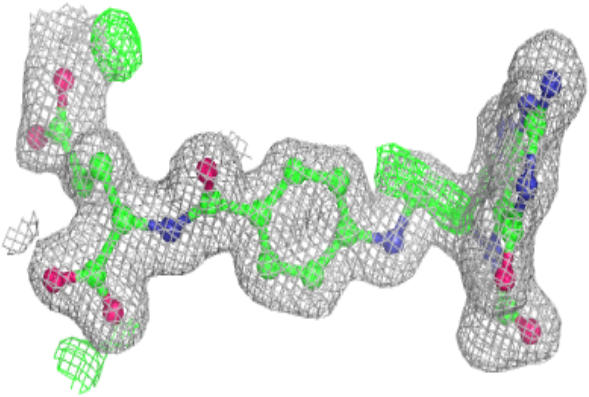


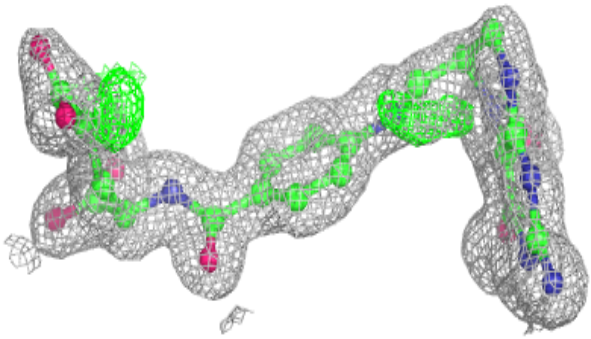


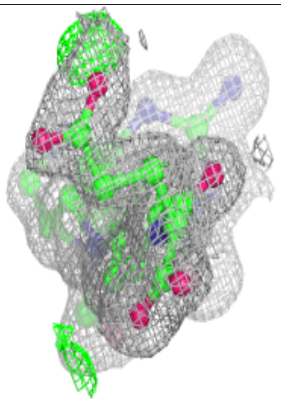


Electron density around FFO C 508 (A):

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

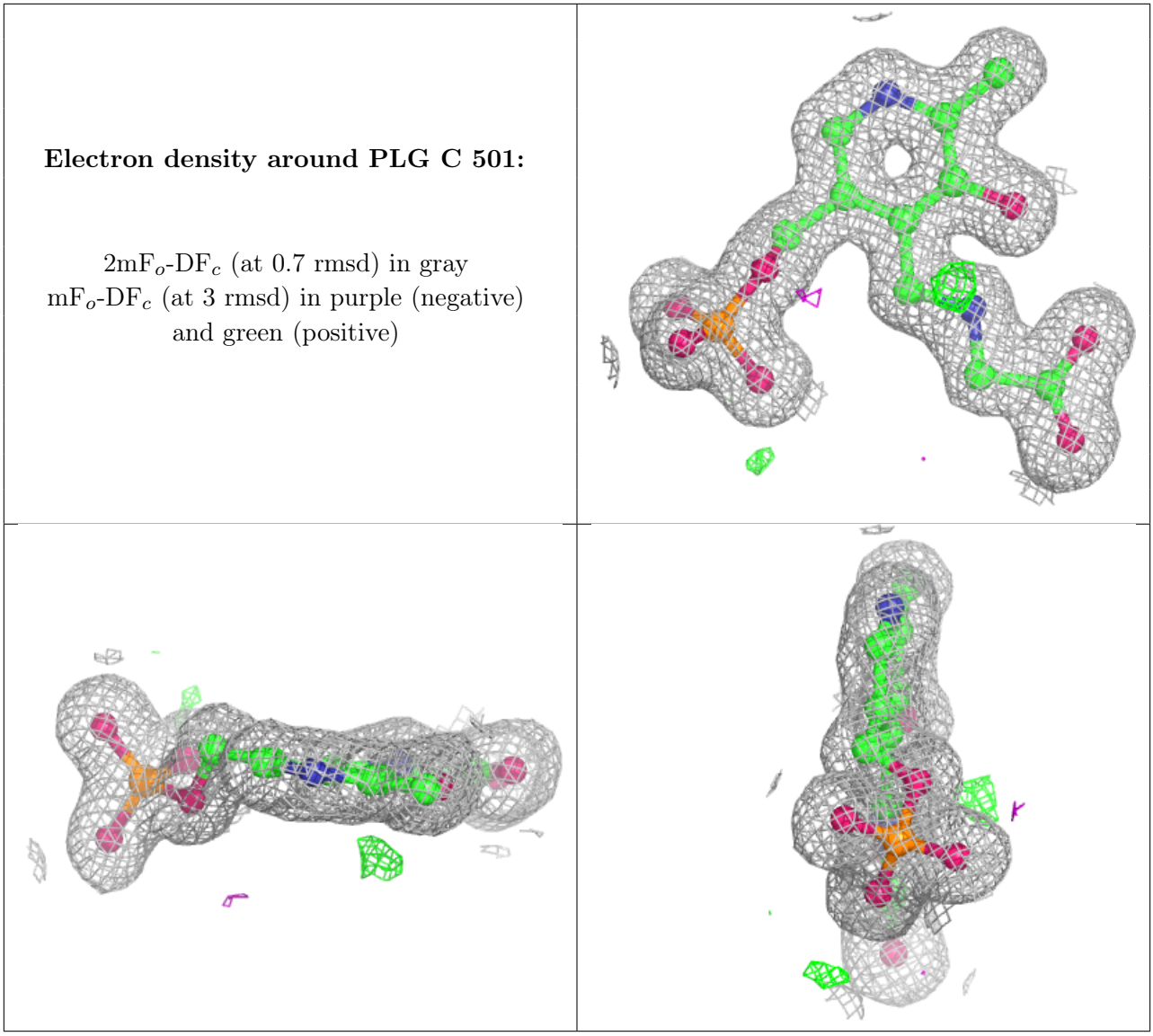






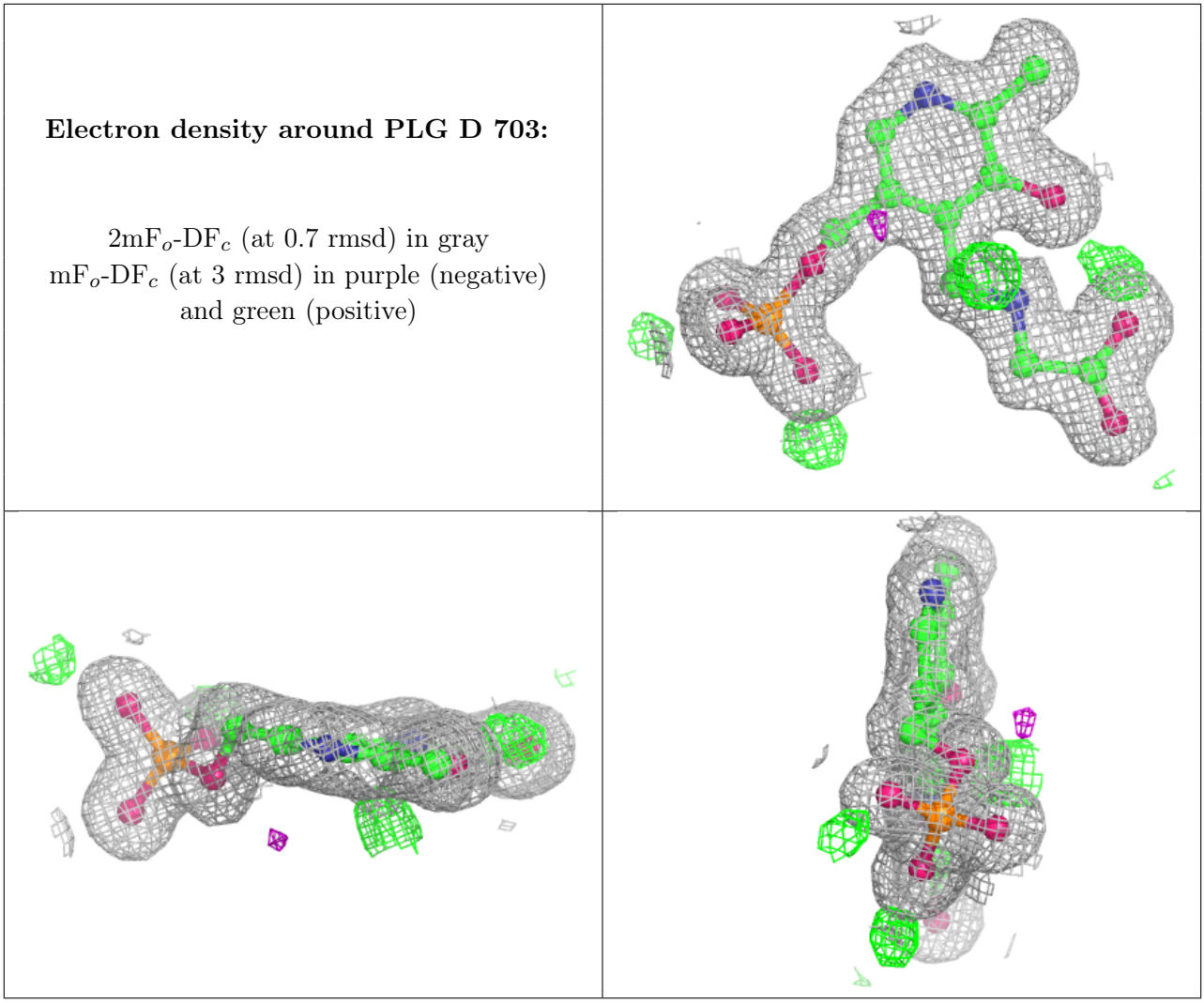
Electron density around PLG C 501:

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



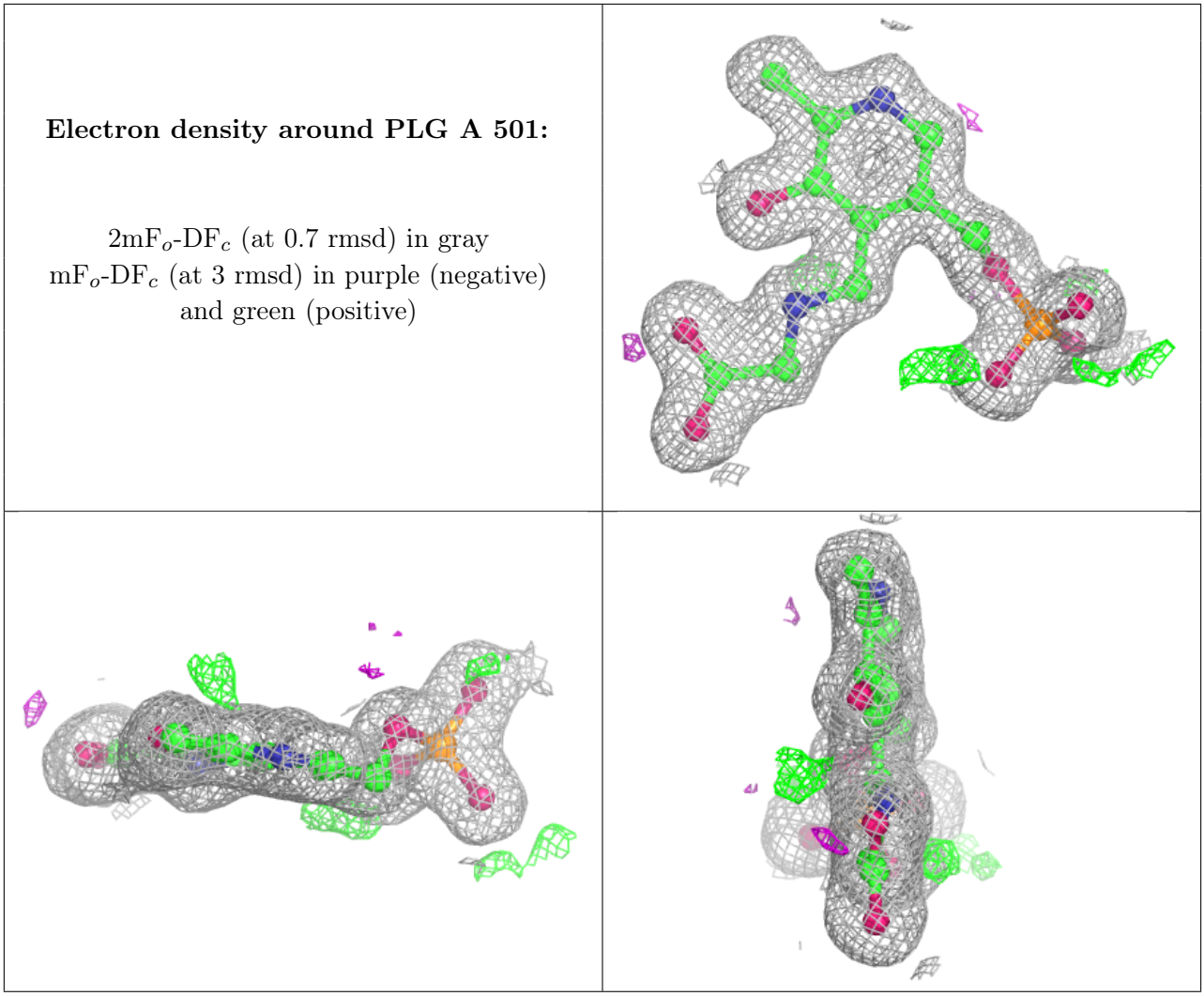
Electron density around PLG D 703:

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



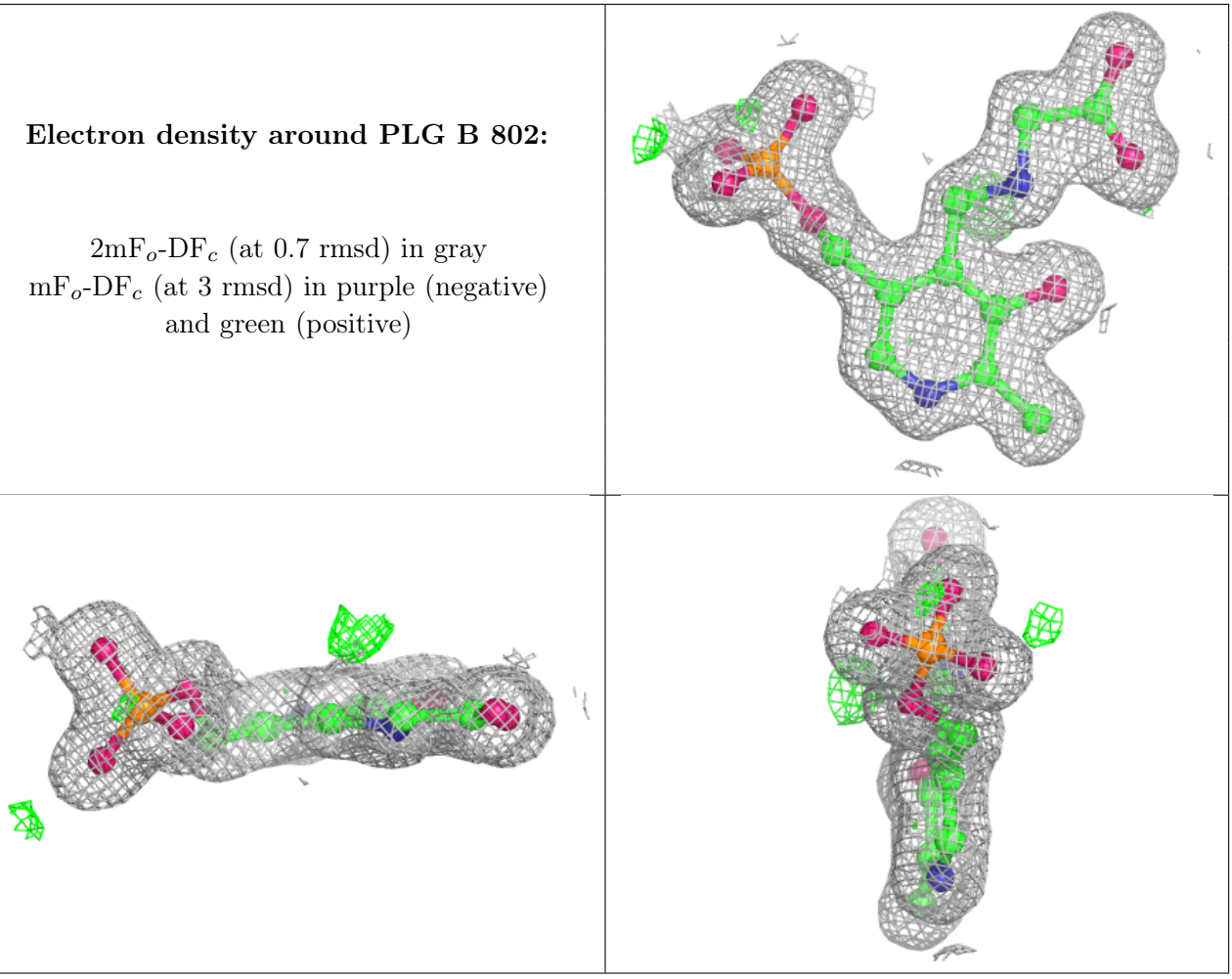
Electron density around PLG A 501:

$2mF_o$-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 802:

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



6.5 Other polymers

There are no such residues in this entry.