



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 10:46 AM EST

PDB ID : 7LV5  
Title : The internal aldimine form of the wild-type Salmonella typhimurium Tryptophan Synthase in complex with inhibitor N-(4'-trifluoromethoxybenzenesulfonyl)-2-amino-1-ethylphosphate (F9F) at the enzyme alpha-site, cesium ion at the metal coordination site and L-Histidine at the enzyme beta-site at 1.55 Angstrom resolution  
Authors : Hilario, E.; Dunn, M.F.; Mueller, L.J.  
Deposited on : 2021-02-23  
Resolution : 1.60 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	:	2.26
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)	:	2.26

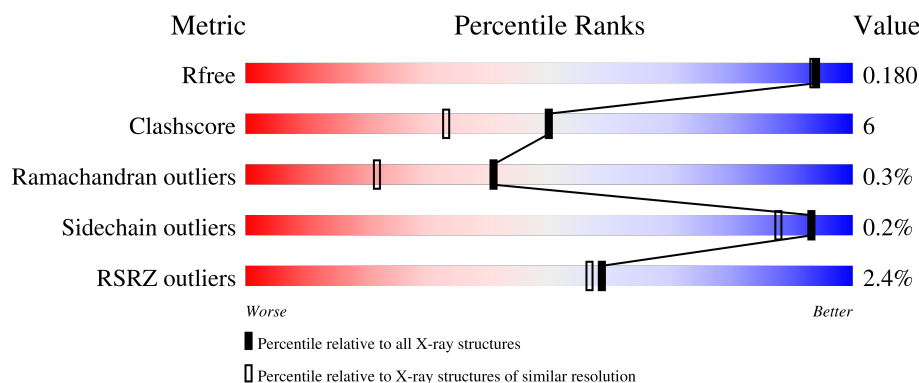
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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	268	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
2	B	397	<div> <div>2%</div> <div>93%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	304	-	-	X	-
7	EDO	B	408	-	-	X	-
7	EDO	B	410	-	-	X	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 5965 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.

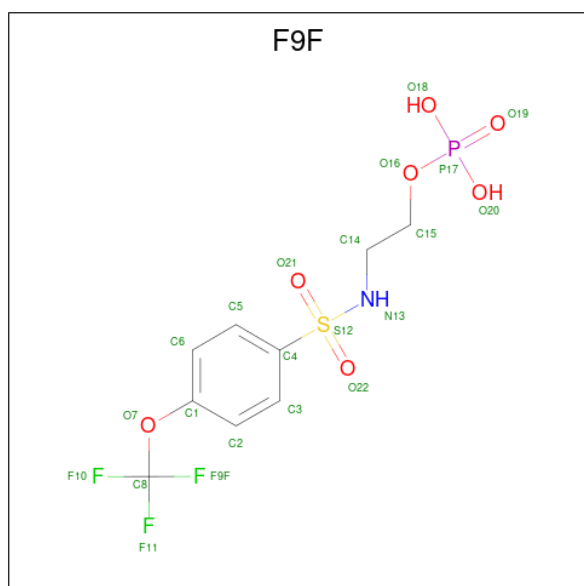
- Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	4	0
			2023	1280	351	383	9			

- Molecule 2 is a protein called Tryptophan synthase beta chain.

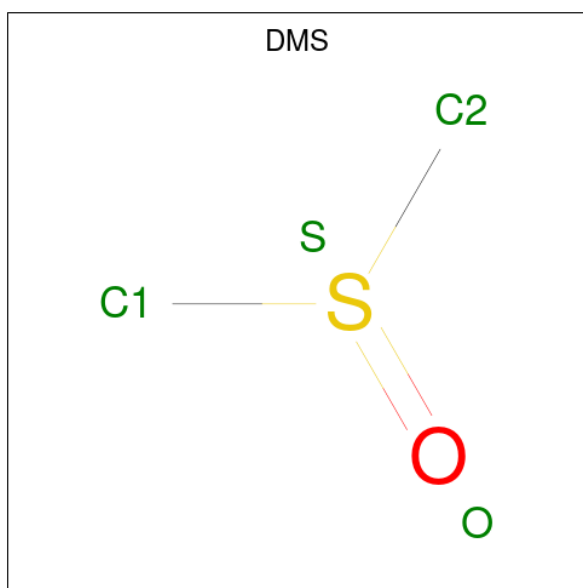
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	393	Total	C	N	O	S	0	12	0
			3077	1928	545	585	19			

- Molecule 3 is 2-([4-(TRIFLUOROMETHOXY)PHENYL]SULFONYL)AMINO)ETHYL DIHYDROGEN PHOSPHATE (three-letter code: F9F) (formula: C<sub>9</sub>H<sub>11</sub>F<sub>3</sub>NO<sub>7</sub>PS) (labeled as "Ligand of Interest" by depositor).



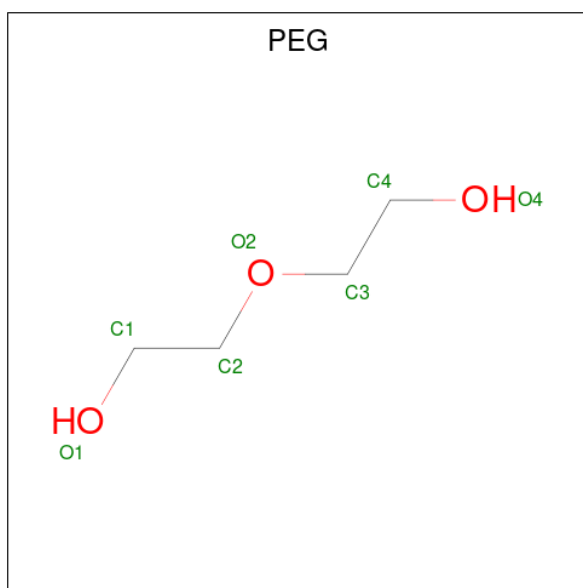
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	S	0	0
			22	9	3	1	7	1	1		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



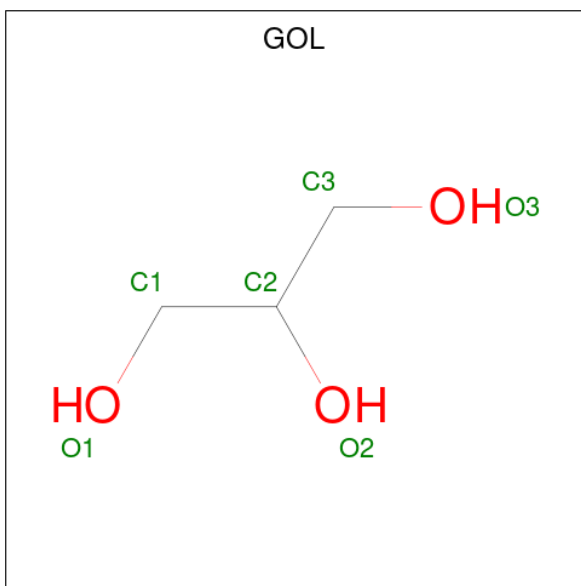
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	S	
			4	2	1	1	
							0
							0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



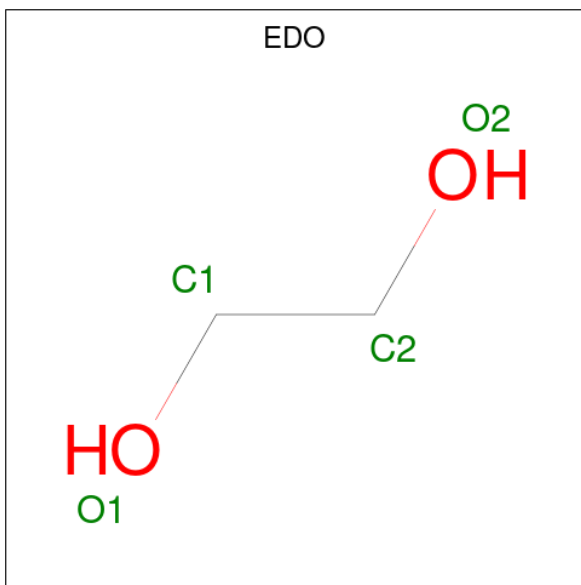
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O		
			7	4	3		
						0	0
5	B	1	Total	C	O		
			7	4	3		
						0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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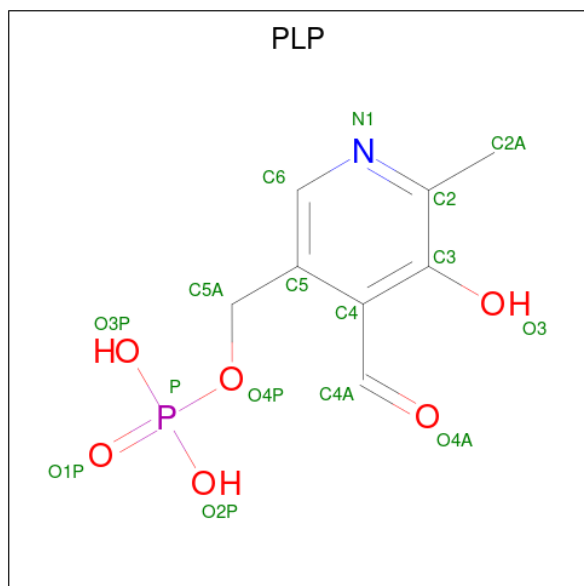
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is CESIUM ION (three-letter code: CS) (formula: Cs) (labeled as "Ligand of Interest" by depositor).

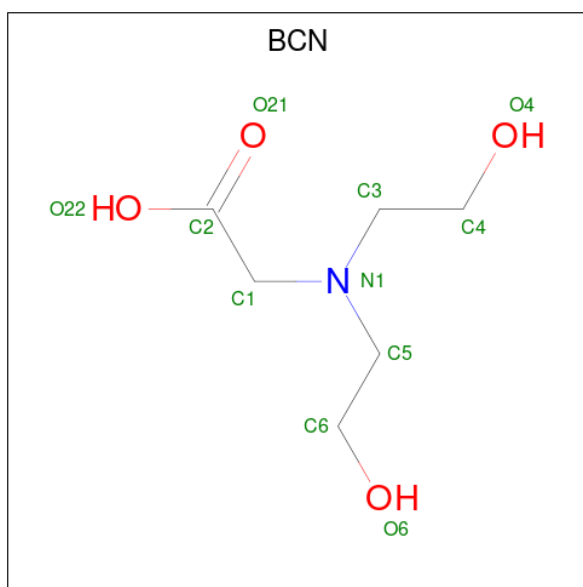
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cs	0	0
			1	1		
8	B	3	Total	Cs	0	1
			4	4		

- Molecule 9 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



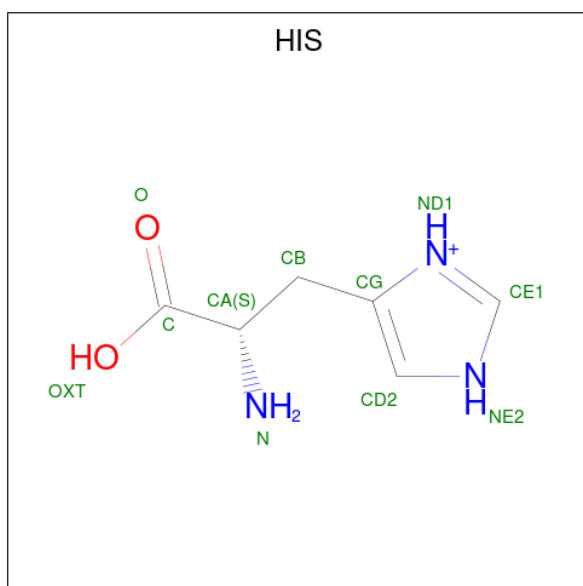
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 10 is BICINE (three-letter code: BCN) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 11 is HISTIDINE (three-letter code: HIS) (formula:  $C_6H_{10}N_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total 1	Cl 1	0	0

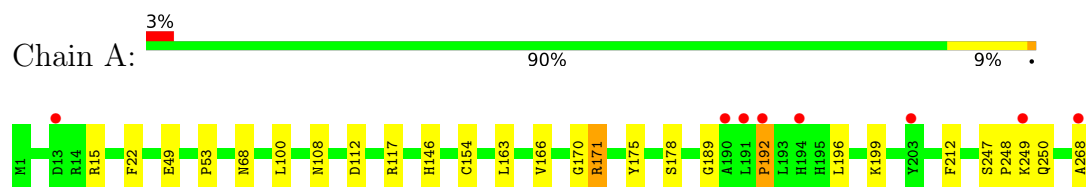
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	284	Total 285	O 285	0	1
13	B	461	Total 471	O 471	0	10

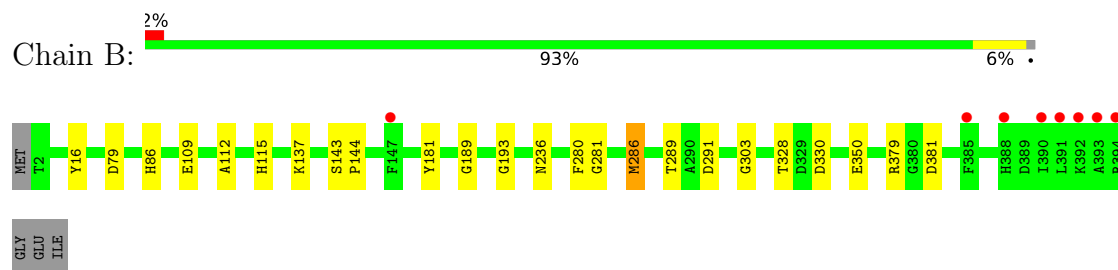
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Tryptophan synthase alpha chain



- Molecule 2: Tryptophan synthase beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.15Å 59.18Å 67.35Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	39.14 – 1.60 39.15 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.8 (39.14-1.60) 89.8 (39.15-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.129 , 0.179 0.129 , 0.180	Depositor DCC
$R_{free}$ test set	4139 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5965	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 6.21% 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: PEG, EDO, BCN, F9F, CS, DMS, CL, PLP, GOL

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	0.36	0/2062	0.65	1/2802 (0.0%)
2	B	0.41	0/3137	0.66	0/4236
All	All	0.39	0/5199	0.66	1/7038 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ARG	CG-CD-NE	-5.10	101.09	111.80

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	2023	0	2008	30	0
2	B	3077	0	3021	28	0
3	A	22	0	9	2	0
4	A	4	0	6	2	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
6	A	6	0	8	15	0
7	A	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	16	0	24	12	0
8	A	1	0	0	0	0
8	B	4	0	0	0	0
9	B	15	0	6	0	0
10	B	11	0	12	0	0
11	B	11	0	6	2	0
12	B	1	0	0	0	0
13	A	285	0	0	4	0
13	B	471	0	0	5	0
All	All	5965	0	5126	60	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 6.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:THR:CB	7:B:410:EDO:H21	1.94	0.98
2:B:330:ASP:HB2	7:B:410:EDO:H22	1.46	0.95
2:B:328:THR:HB	7:B:410:EDO:H21	1.49	0.91
2:B:291:ASP:HB2	7:B:408:EDO:H12	1.52	0.90
1:A:108:ASN:HA	13:A:518:HOH:O	1.76	0.84
2:B:289:THR:OG1	7:B:408:EDO:H11	1.78	0.83
2:B:379[B]:ARG:NH2	13:B:755[B]:HOH:O	1.94	0.78
1:A:249:LYS:HB2	6:A:304:GOL:H11	1.67	0.77
1:A:15:ARG:O	1:A:268:ALA:HB2	1.85	0.76
2:B:109:GLU:OE2	11:B:409:HIS:HE1	1.71	0.74
2:B:328:THR:OG1	7:B:410:EDO:H21	1.88	0.73
1:A:247:SER:HB3	6:A:304:GOL:O1	1.91	0.71
1:A:249:LYS:HB2	6:A:304:GOL:C1	2.22	0.70
2:B:181[B]:TYR:CE2	13:B:546:HOH:O	2.45	0.68
2:B:291:ASP:CB	7:B:408:EDO:H12	2.26	0.66
2:B:289:THR:CB	7:B:408:EDO:H11	2.25	0.65
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.80	0.64
2:B:112:ALA:HB3	13:B:513:HOH:O	1.97	0.62
2:B:181[B]:TYR:CZ	13:B:546:HOH:O	2.55	0.57
1:A:117:ARG:HG2	4:A:302:DMS:C2	2.35	0.56
1:A:249:LYS:CB	6:A:304:GOL:H11	2.38	0.54
1:A:249:LYS:N	6:A:304:GOL:H11	2.23	0.54
1:A:248:PRO:HD2	6:A:304:GOL:H2	1.90	0.53
1:A:248:PRO:HD2	6:A:304:GOL:H31	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:THR:OG1	7:B:410:EDO:C2	2.55	0.52
1:A:154[B]:CYS:SG	1:A:166:VAL:HG11	2.49	0.52
2:B:303:GLY:HA3	2:B:350:GLU:OE2	2.11	0.51
2:B:289:THR:HB	7:B:408:EDO:H11	1.93	0.50
2:B:137:LYS:HE3	13:B:665:HOH:O	2.10	0.50
2:B:79:ASP:HB2	2:B:379[A]:ARG:HB3	1.95	0.48
1:A:170:GLY:O	1:A:171:ARG:NH2	2.40	0.48
2:B:379[B]:ARG:HD2	2:B:381:ASP:OD1	2.14	0.48
1:A:247:SER:HA	6:A:304:GOL:H2	1.97	0.47
1:A:163:LEU:HD21	1:A:196:LEU:HD22	1.96	0.47
2:B:291:ASP:HB2	7:B:408:EDO:C1	2.35	0.46
1:A:249:LYS:H	6:A:304:GOL:H31	1.81	0.46
1:A:178[B]:SER:HB3	1:A:189:GLY:HA3	1.97	0.46
1:A:248:PRO:HD2	6:A:304:GOL:C3	2.45	0.46
1:A:249:LYS:H	6:A:304:GOL:C3	2.29	0.46
1:A:249:LYS:H	6:A:304:GOL:H11	1.80	0.46
2:B:109:GLU:OE2	11:B:409:HIS:CE1	2.60	0.46
1:A:250:GLN:H	6:A:304:GOL:H11	1.82	0.45
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.51	0.45
2:B:193:GLY:HA2	2:B:280:PHE:O	2.16	0.45
1:A:192:PRO:HB3	13:A:573:HOH:O	2.18	0.44
2:B:143[A]:SER:OG	2:B:144:PRO:HD3	2.17	0.44
1:A:175:TYR:CE2	3:A:301:F9F:H5	2.53	0.43
1:A:249:LYS:HB2	6:A:304:GOL:H32	2.00	0.43
1:A:249:LYS:CA	6:A:304:GOL:H11	2.48	0.43
1:A:100:LEU:C	1:A:100:LEU:HD13	2.38	0.43
7:A:305:EDO:H21	13:A:499:HOH:O	2.20	0.42
2:B:330:ASP:CB	7:B:410:EDO:H22	2.33	0.42
1:A:117:ARG:HG2	4:A:302:DMS:H23	2.01	0.42
1:A:199:LYS:HA	1:A:199:LYS:HD2	1.90	0.41
1:A:53:PRO:HA	1:A:68:ASN:OD1	2.21	0.41
3:A:301:F9F:H3	13:A:516:HOH:O	2.21	0.41
2:B:86:HIS:CE1	2:B:236:ASN:HB3	2.56	0.41
2:B:16:TYR:O	2:B:281:GLY:HA2	2.21	0.40
2:B:286:MET:HB3	2:B:286:MET:HE3	1.58	0.40
1:A:22:PHE:HA	1:A:49:GLU:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	270/268 (101%)	266 (98%)	2 (1%)	2 (1%)	22	7
2	B	404/397 (102%)	396 (98%)	8 (2%)	0	100	100
All	All	674/665 (101%)	662 (98%)	10 (2%)	2 (0%)	41	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	PRO
1	A	212	PHE

### 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	207/208 (100%)	207 (100%)	0	100	100
2	B	316/311 (102%)	315 (100%)	1 (0%)	92	87
All	All	523/519 (101%)	522 (100%)	1 (0%)	93	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	286	MET

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

Mol	Chain	Res	Type
1	A	146	HIS
1	A	210	GLN
2	B	36	GLN
2	B	42	GLN
2	B	63	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	EDO	B	406	-	3,3,3	0.11	0	2,2,2	0.18	0
7	EDO	B	408	-	3,3,3	0.31	0	2,2,2	0.91	0
11	HIS	B	409	-	4,11,11	0.98	0	3,14,14	1.30	0
7	EDO	B	410	-	3,3,3	0.31	0	2,2,2	1.12	0
3	F9F	A	301	-	22,22,22	0.48	0	32,33,33	0.71	0
10	BCN	B	404	-	7,10,10	0.24	0	8,11,11	0.79	0
7	EDO	B	405	-	3,3,3	0.08	0	2,2,2	0.26	0
5	PEG	B	407	-	6,6,6	0.25	0	5,5,5	0.20	0
7	EDO	A	305	-	3,3,3	0.20	0	2,2,2	0.40	0
6	GOL	A	304	-	5,5,5	0.14	0	5,5,5	0.60	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	A	303	-	6,6,6	0.11	0	5,5,5	0.09	0
4	DMS	A	302	-	3,3,3	0.21	0	3,3,3	0.07	0
9	PLP	B	401	2	15,15,16	0.79	1 (6%)	20,22,23	1.25	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	406	-	-	0/1/1/1	-
7	EDO	B	408	-	-	1/1/1/1	-
11	HIS	B	409	-	-	0/4/8/8	0/1/1/1
7	EDO	B	410	-	-	1/1/1/1	-
3	F9F	A	301	-	-	6/20/20/20	0/1/1/1
10	BCN	B	404	-	-	2/8/10/10	-
7	EDO	B	405	-	-	1/1/1/1	-
5	PEG	B	407	-	-	0/4/4/4	-
7	EDO	A	305	-	-	1/1/1/1	-
6	GOL	A	304	-	-	3/4/4/4	-
5	PEG	A	303	-	-	1/4/4/4	-
9	PLP	B	401	2	-	0/6/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	401	PLP	C4A-C4	-2.08	1.47	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	401	PLP	O4P-C5A-C5	3.21	115.47	109.35
9	B	401	PLP	C4A-C4-C5	2.89	123.91	120.94

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	303	PEG	O2-C3-C4-O4
7	B	405	EDO	O1-C1-C2-O2

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
7	B	408	EDO	O1-C1-C2-O2
7	B	410	EDO	O1-C1-C2-O2
6	A	304	GOL	O2-C2-C3-O3
3	A	301	F9F	C3-C4-S12-O21
7	A	305	EDO	O1-C1-C2-O2
3	A	301	F9F	C5-C4-S12-O21
6	A	304	GOL	C1-C2-C3-O3
3	A	301	F9F	N13-C14-C15-O16
10	B	404	BCN	C2-C1-N1-C5
10	B	404	BCN	C2-C1-N1-C3
3	A	301	F9F	C2-C1-O7-C8
3	A	301	F9F	C6-C1-O7-C8
3	A	301	F9F	C3-C4-S12-N13
6	A	304	GOL	O1-C1-C2-C3

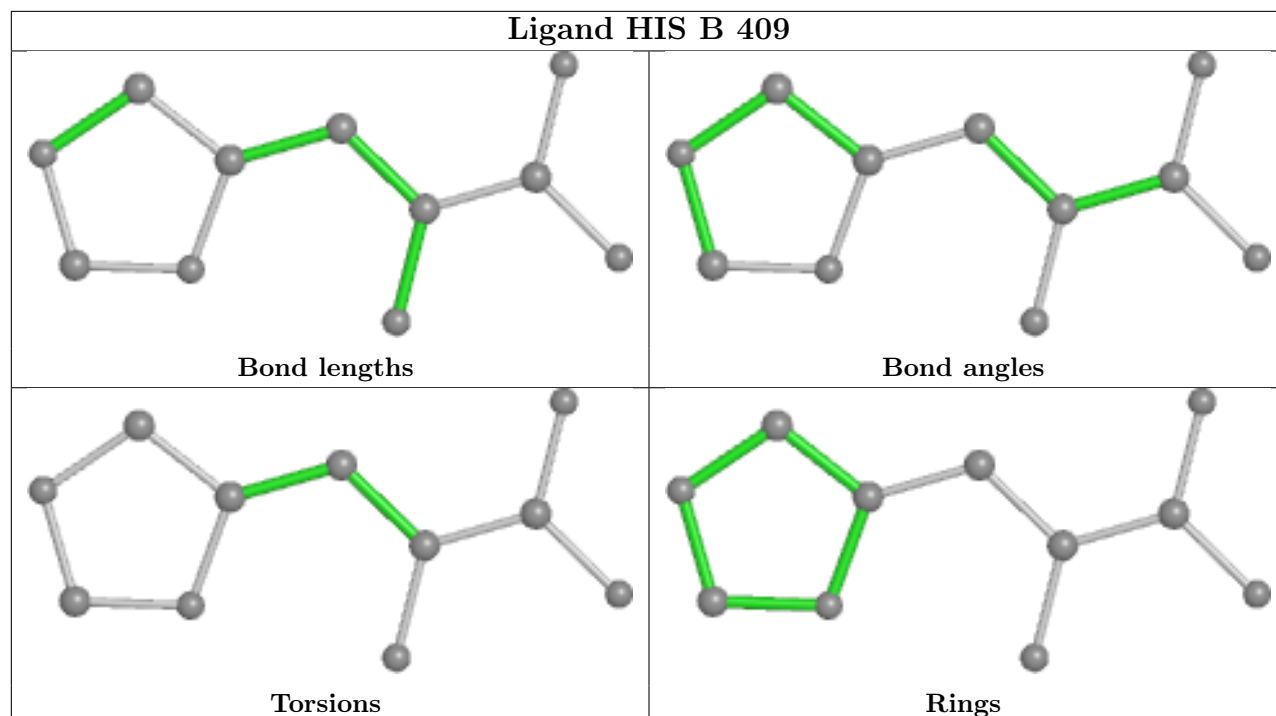
There are no ring outliers.

7 monomers are involved in 34 short contacts:

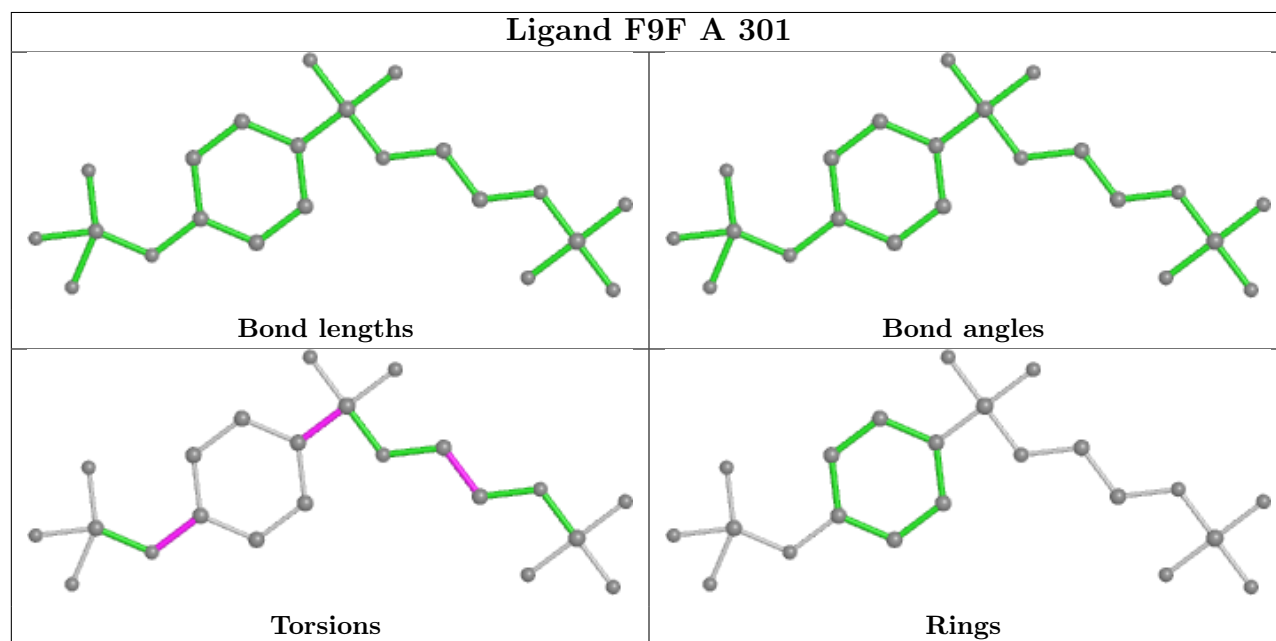
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	408	EDO	6	0
11	B	409	HIS	2	0
7	B	410	EDO	6	0
3	A	301	F9F	2	0
7	A	305	EDO	1	0
6	A	304	GOL	15	0
4	A	302	DMS	2	0

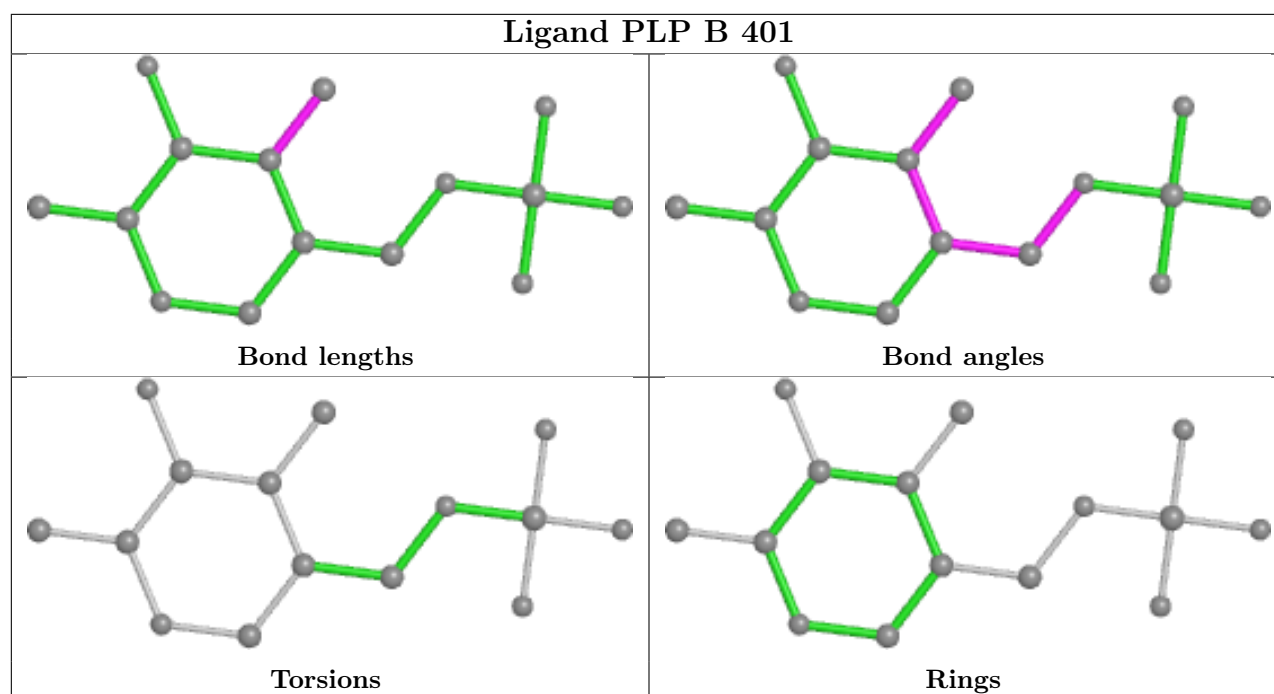
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 HIS B 409



## Ligand F9F A 301





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	268/268 (100%)	-0.43	8 (2%)	50	48	10, 17, 39, 64	0
2	B	393/397 (98%)	-0.47	8 (2%)	65	64	8, 13, 27, 74	0
All	All	661/665 (99%)	-0.46	16 (2%)	59	56	8, 15, 33, 74	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	393	ALA	5.6
1	A	192	PRO	3.8
2	B	391	LEU	3.8
1	A	194	HIS	3.7
2	B	392	LYS	3.5
1	A	268	ALA	3.5
2	B	390	ILE	3.1
2	B	388	HIS	2.9
1	A	190	ALA	2.7
2	B	394	ARG	2.6
2	B	147	PHE	2.5
2	B	385	PHE	2.5
1	A	191	LEU	2.3
1	A	249	LYS	2.1
1	A	13	ASP	2.1
1	A	203	TYR	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

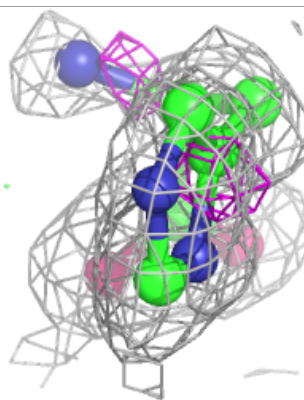
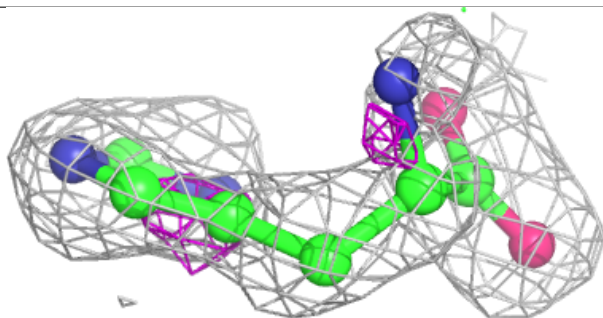
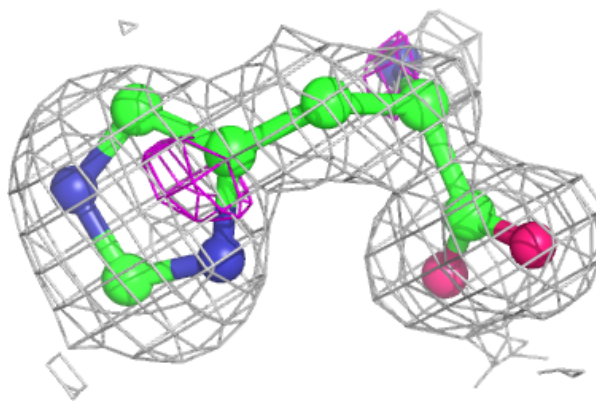
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	EDO	A	305	4/4	0.84	0.16	24,27,28,29	0
6	GOL	A	304	6/6	0.85	0.28	32,36,41,47	0
4	DMS	A	302	4/4	0.85	0.27	58,59,76,77	0
12	CL	B	412	1/1	0.85	0.08	75,75,75,75	0
7	EDO	B	406	4/4	0.86	0.18	51,53,56,64	0
7	EDO	B	405	4/4	0.87	0.08	41,42,47,50	0
5	PEG	B	407	7/7	0.88	0.15	40,41,44,54	0
7	EDO	B	410	4/4	0.92	0.13	20,23,25,32	0
5	PEG	A	303	7/7	0.93	0.07	48,52,54,55	0
11	HIS	B	409	11/11	0.94	0.09	24,33,39,40	0
10	BCN	B	404	11/11	0.95	0.10	14,24,28,30	0
7	EDO	B	408	4/4	0.96	0.17	26,33,37,41	0
3	F9F	A	301	22/22	0.98	0.05	14,15,20,21	0
8	CS	B	403[A]	1/1	0.99	0.03	24,24,24,24	1
8	CS	B	403[B]	1/1	0.99	0.03	32,32,32,32	1
9	PLP	B	401	15/16	0.99	0.09	9,11,18,19	0
8	CS	B	402	1/1	1.00	0.02	19,19,19,19	1
8	CS	B	411	1/1	1.00	0.02	35,35,35,35	1
8	CS	A	306	1/1	1.00	0.02	15,15,15,15	1

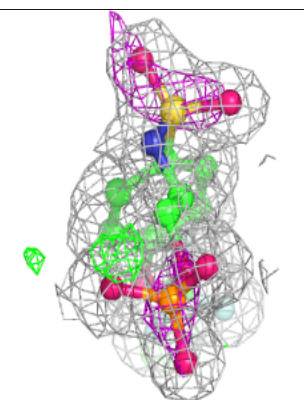
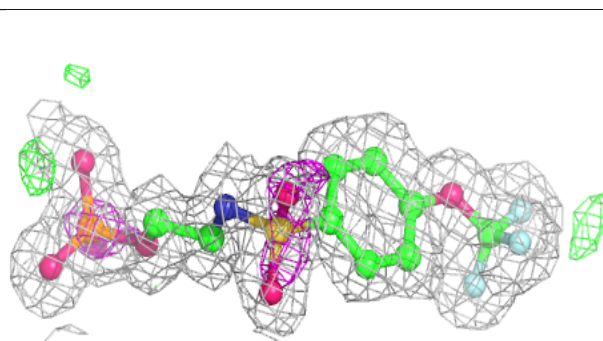
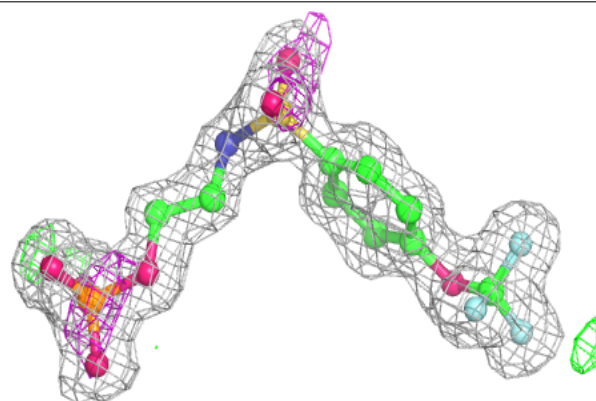
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HIS B 409:**

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

**Electron density around F9F A 301:**

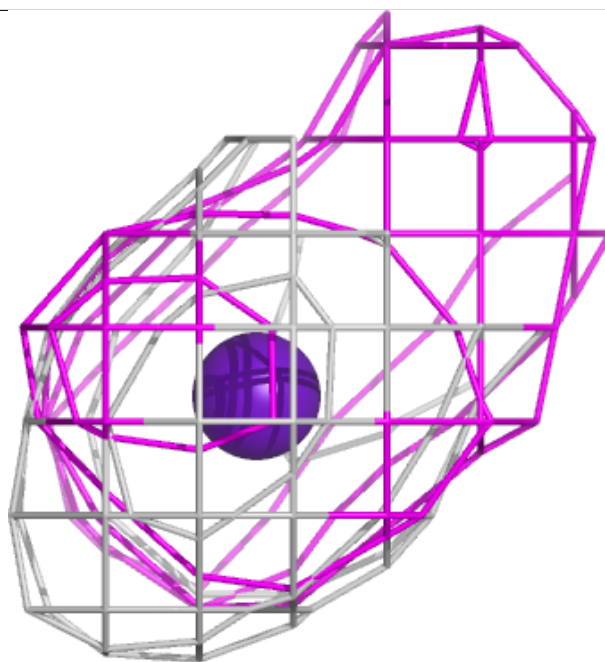
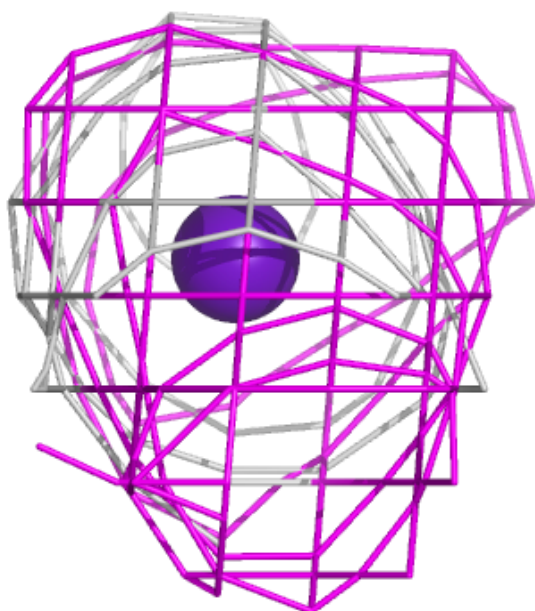
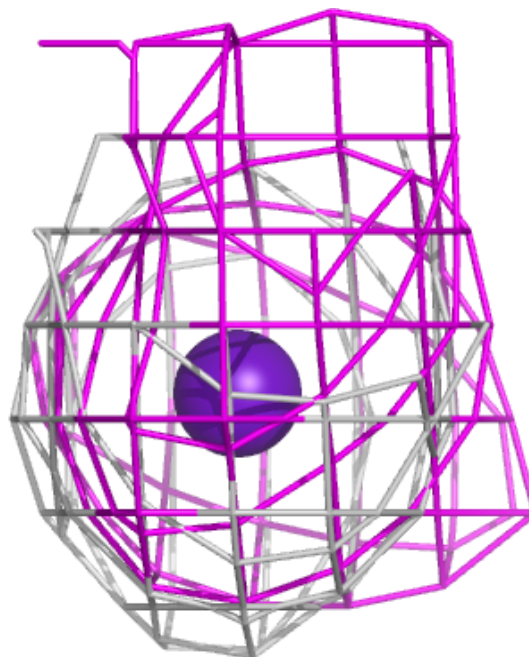
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CS B 403 (A):**

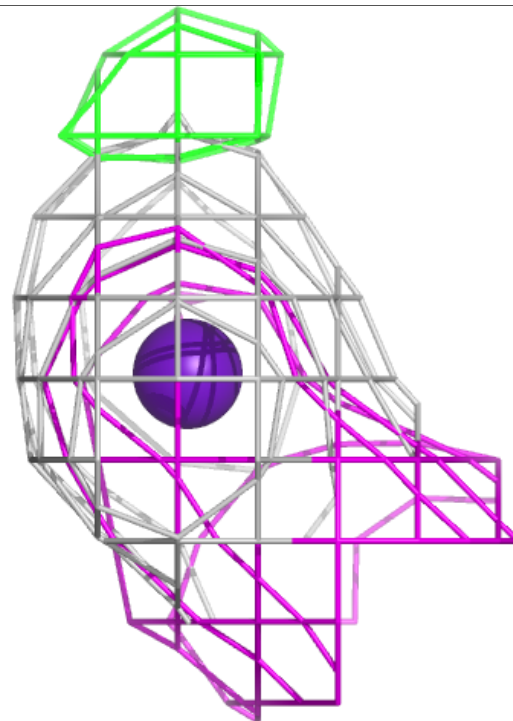
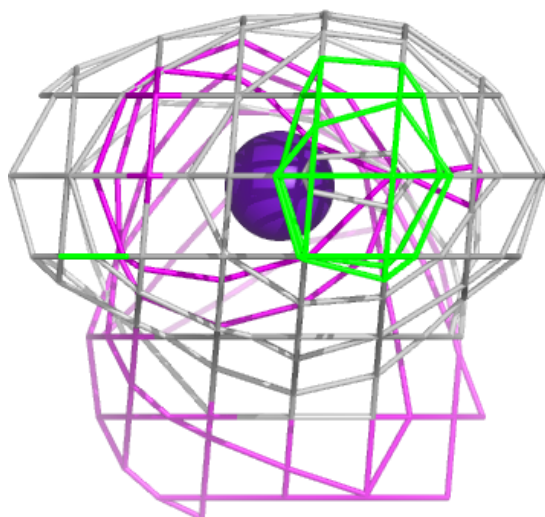
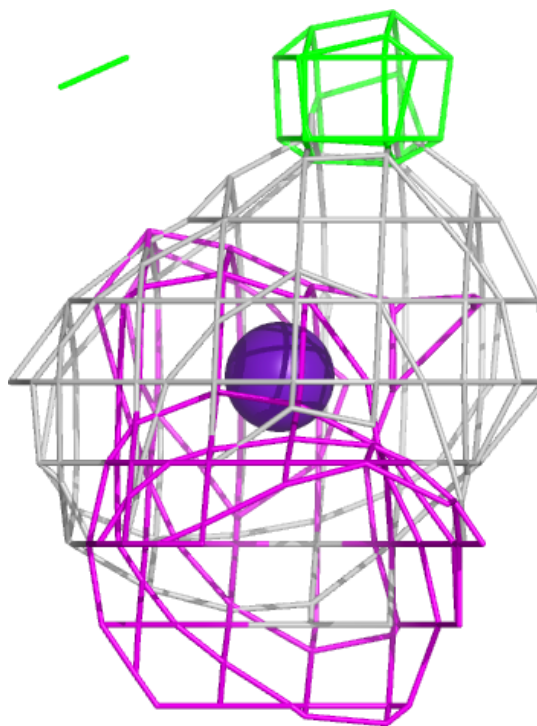
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





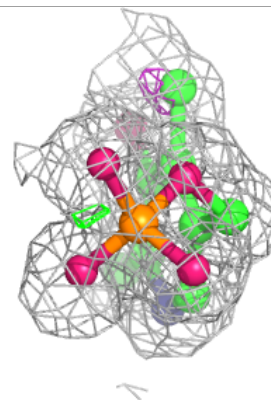
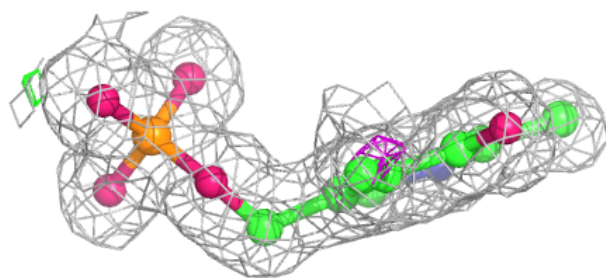
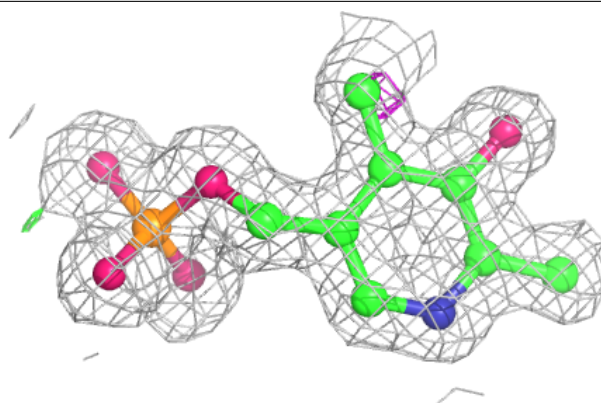
**Electron density around CS B 403 (B):**

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



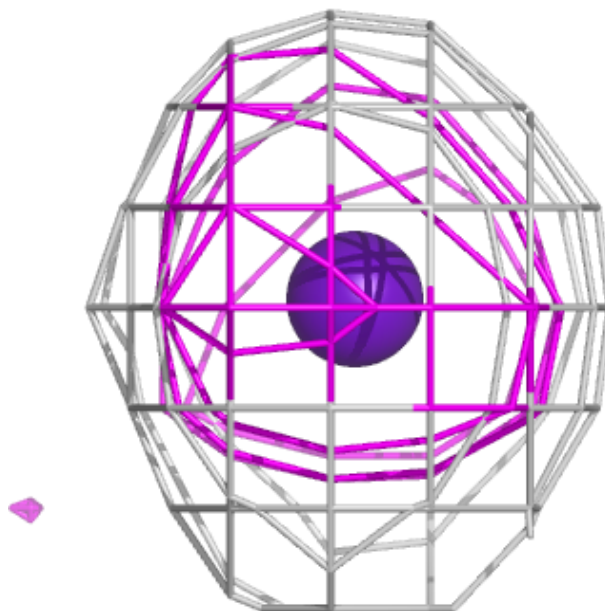
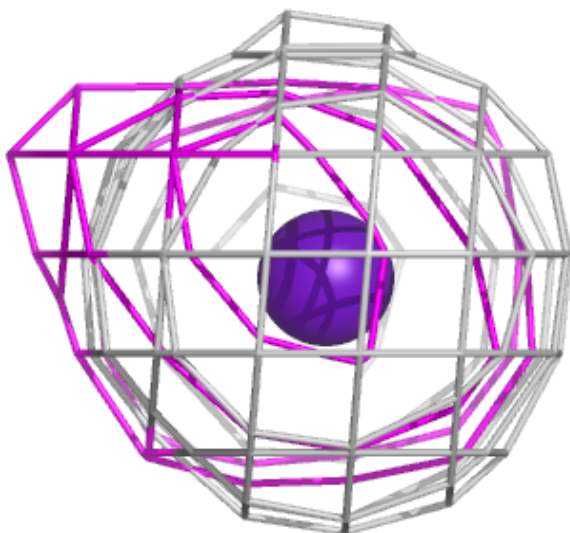
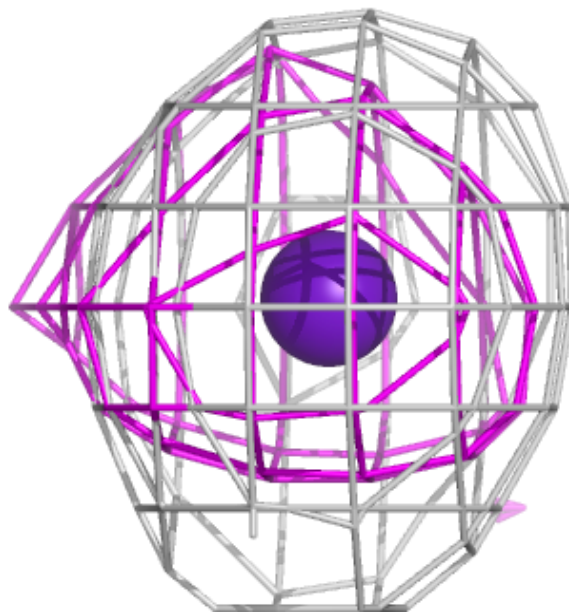
**Electron density around PLP B 401:**

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



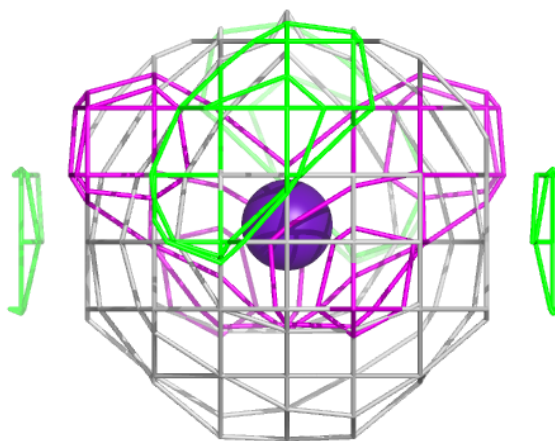
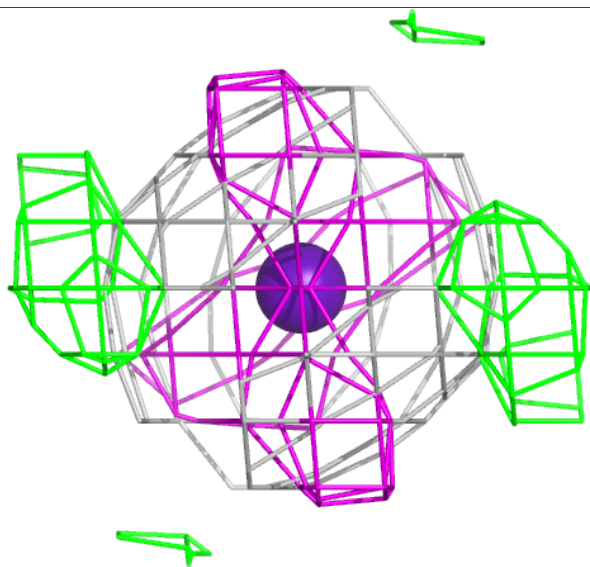
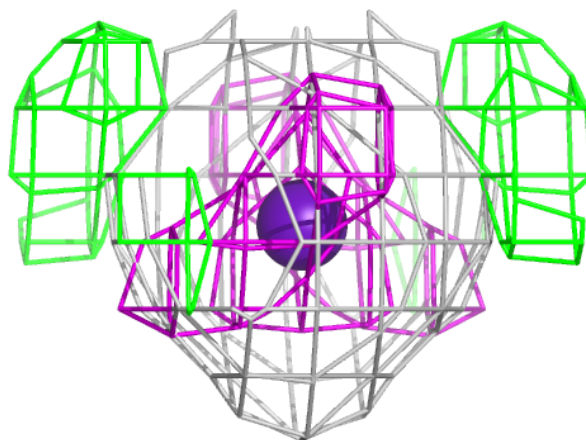
**Electron density around CS B 402:**

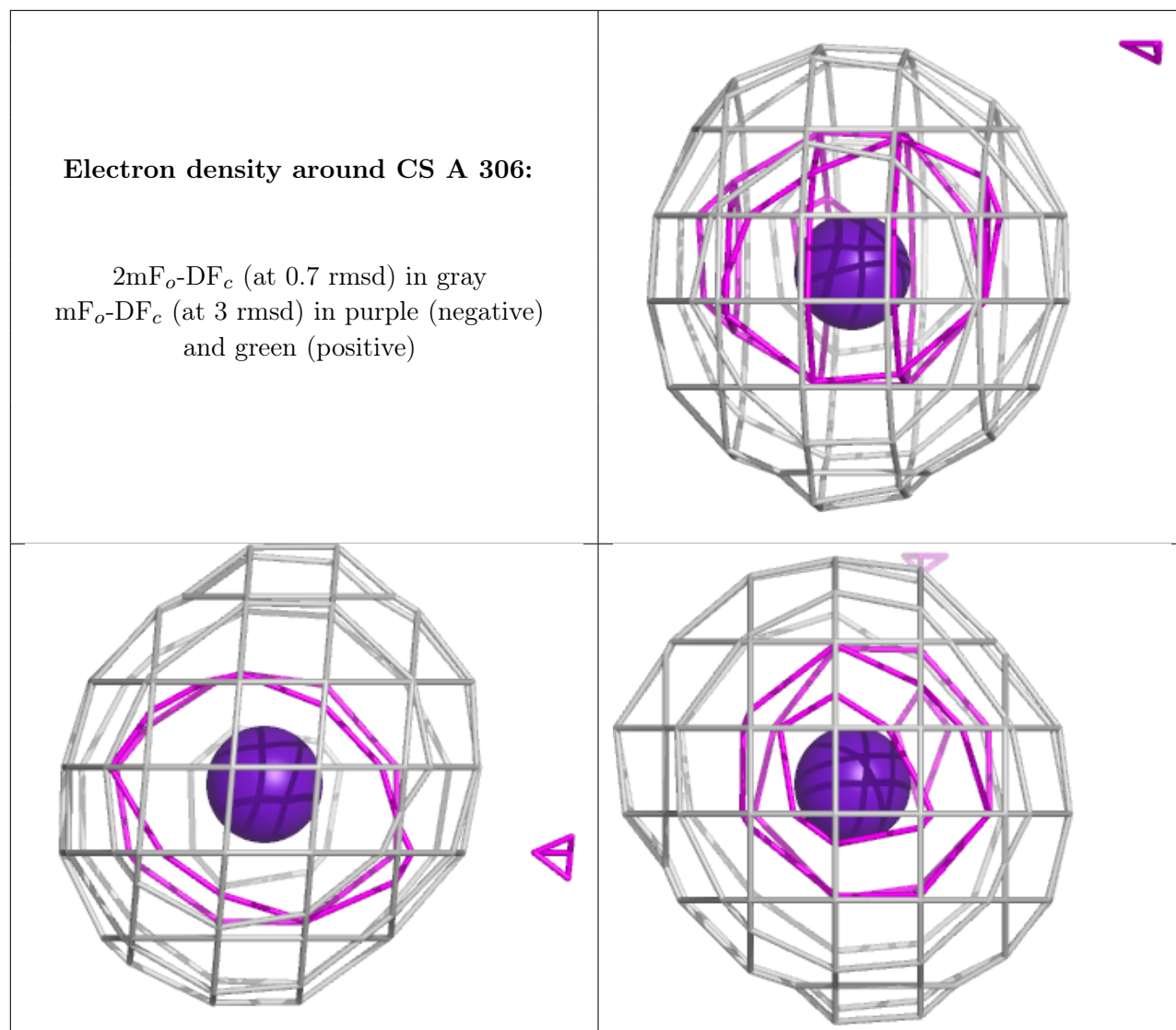
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CS B 411:**

$2mF_o-DF_c$  (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.