



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2022 – 04:13 PM EST

PDB ID : 7LKL

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 the product L-tryptophan at the enzyme beta-site at 1.05 Angstrom resolution. One of the beta-Q114 rotamer conformations allows a hydrogen bond to form with the PLP oxygen at the position 3 in the ring

Authors : Hilario, E.; Dunn, M.F.; Mueller, L.J.

Deposited on : 2021-02-02

Resolution : 1.05 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 following versions of software and data (see [references](#) ①) 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

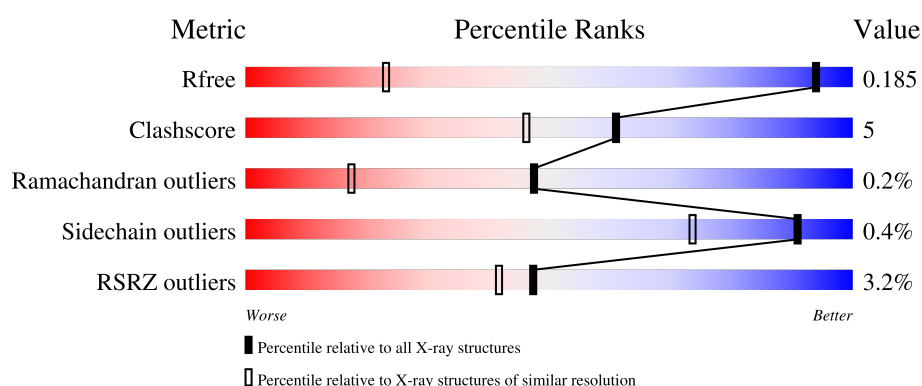
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	<div> <div>5%</div> <div>94%</div> <div>5%</div> </div>
2	B	397	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6290 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.

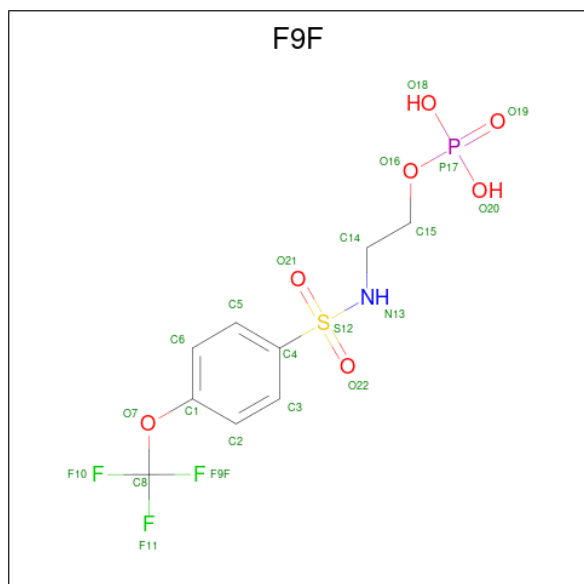
- Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	8	0
			2065	1306	356	395	8			

- 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	25	0
			3168	1988	556	601	23			

- Molecule 3 is 2-([4-(TRIFLUOROMETHOXY)PHENYL]SULFONYL)AMINO)ETHYL DIHYDROGEN PHOSPHATE (three-letter code: F9F) (formula: C₉H₁₁F₃NO₇PS) (labeled as "Ligand of Interest" by depositor).



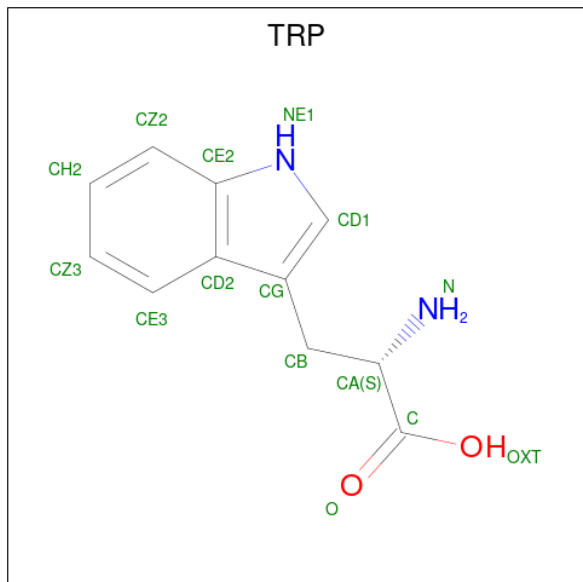
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	S	0	0
			22	9	3	1	7	1	1		

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



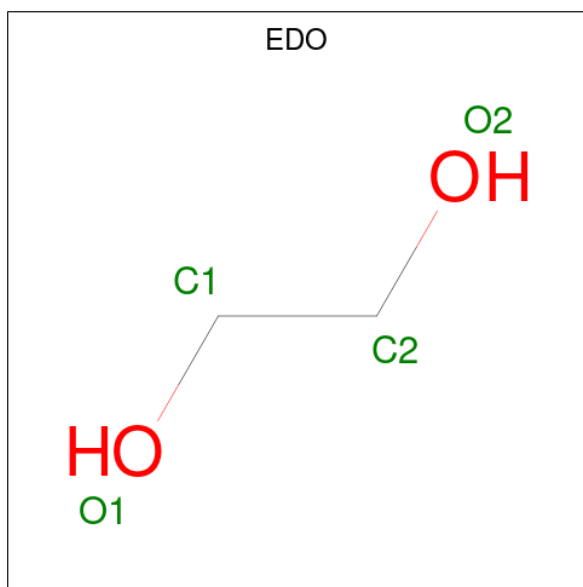
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total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

- Molecule 5 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	11	2	2		
5	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is CESIUM ION (three-letter code: CS) (formula: Cs) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cs 4 4	0	2
7	B	3	Total Cs 4 4	0	1

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

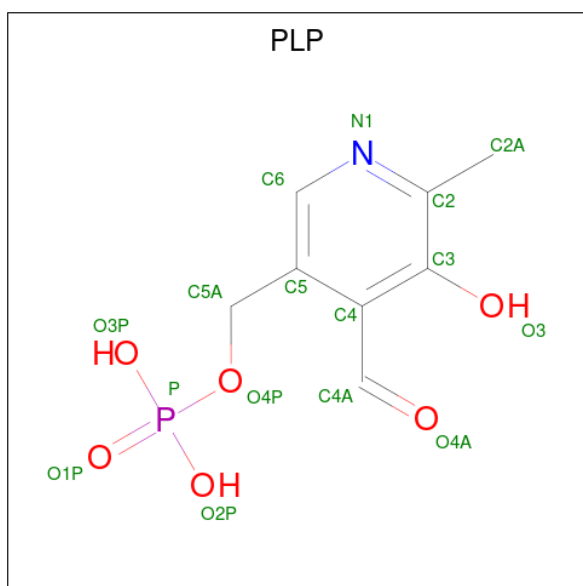
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	B	3	Total Cl 3 3	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 10 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



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

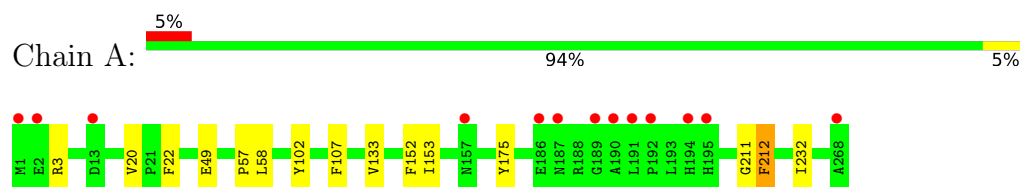
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	365	Total	O	0	11
			376	376		
11	B	475	Total	O	0	18
			493	493		

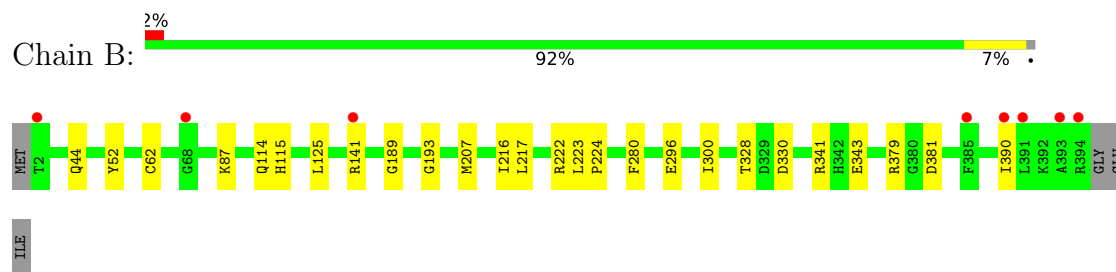
3 Residue-property plots [i](#)

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: 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, α , β , γ	181.74Å 59.81Å 67.30Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	28.92 – 1.05 28.90 – 1.05	Depositor EDS
% Data completeness (in resolution range)	93.6 (28.92-1.05) 93.6 (28.90-1.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.154 , 0.176 0.163 , 0.185	Depositor DCC
R_{free} test set	15525 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	8.8	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6290	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CS, F9F, CL, DMS, PLP, PEG

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	0.60	0/2105	0.69	0/2863
2	B	0.58	0/3227	0.72	0/4357
All	All	0.59	0/5332	0.71	0/7220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2065	0	2037	15	0
2	B	3168	0	3116	24	0
3	A	22	0	9	2	0
4	A	24	0	36	5	0
4	B	28	0	42	3	0
5	A	15	0	9	0	0
5	B	15	0	9	0	0
6	A	4	0	5	3	0
6	B	32	0	48	0	0
7	A	4	0	0	1	0
7	B	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
8	B	3	0	0	0	0
9	B	21	0	30	7	0
10	B	15	0	6	1	0
11	A	376	0	0	5	0
11	B	493	0	0	16	0
All	All	6290	0	5347	49	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 (49) 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)
4:A:309:DMS:H11	11:A:539[A]:HOH:O	1.62	1.00
9:B:505:PEG:H32	11:B:901:HOH:O	1.70	0.89
4:A:309:DMS:H22	11:A:539[A]:HOH:O	1.73	0.89
2:B:125:LEU:HD11	9:B:513:PEG:H31	1.59	0.84
4:B:515:DMS:S	11:B:778:HOH:O	2.37	0.82
2:B:223:LEU:HD23	11:B:878:HOH:O	1.81	0.80
7:A:311[B]:CS:CS	11:A:547:HOH:O	2.29	0.78
2:B:217[A]:LEU:HG	11:B:878:HOH:O	1.87	0.74
1:A:107:PHE:CE2	6:A:308:EDO:H22	2.29	0.68
1:A:133[A]:VAL:HG12	1:A:152:PHE:CD2	2.30	0.67
1:A:58:LEU:CD2	11:B:751:HOH:O	2.43	0.67
4:B:515:DMS:H21	11:B:761:HOH:O	1.97	0.63
1:A:107:PHE:CD2	6:A:308:EDO:H21	2.35	0.61
2:B:330:ASP:HB2	9:B:511:PEG:H12	1.82	0.60
2:B:44[A]:GLN:HG3	11:B:750:HOH:O	2.03	0.58
1:A:107:PHE:CE2	6:A:308:EDO:C2	2.86	0.57
4:B:504:DMS:H23	11:B:1060:HOH:O	2.05	0.56
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.38	0.55
2:B:114[A]:GLN:NE2	11:B:603:HOH:O	2.41	0.54
1:A:133[A]:VAL:HG12	1:A:152:PHE:HD2	1.69	0.54
2:B:52:TYR:HB2	9:B:513:PEG:H12	1.89	0.54
2:B:141:ARG:CZ	11:B:749:HOH:O	2.57	0.52
2:B:328:THR:OG1	9:B:511:PEG:H22	2.10	0.52
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.45	0.51
1:A:22:PHE:HA	1:A:49[A]:GLU:O	2.10	0.50
2:B:216[B]:ILE:HG22	2:B:222[B]:ARG:O	2.11	0.50
1:A:175:TYR:CE2	3:A:301:F9F:H5	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379[A]:ARG:HD2	2:B:381:ASP:OD1	2.12	0.49
1:A:58:LEU:HD23	11:B:751:HOH:O	2.09	0.49
2:B:193:GLY:HA2	2:B:280:PHE:O	2.14	0.47
2:B:125:LEU:CD1	9:B:513:PEG:H31	2.39	0.47
2:B:216[A]:ILE:HG23	11:B:878:HOH:O	2.15	0.47
2:B:216[A]:ILE:HG21	2:B:224:PRO:HD3	1.98	0.46
2:B:341:ARG:NH1	11:B:604:HOH:O	2.43	0.46
1:A:153:ILE:HD13	1:A:175:TYR:HB3	1.98	0.46
1:A:20:VAL:O	1:A:232:ILE:HA	2.17	0.44
2:B:87:LYS:HE3	11:B:696:HOH:O	2.18	0.43
2:B:87:LYS:NZ	10:B:520:PLP:O3	2.52	0.42
2:B:216[A]:ILE:CG2	11:B:878:HOH:O	2.66	0.42
4:A:309:DMS:C2	11:A:539[A]:HOH:O	2.48	0.42
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.55	0.42
2:B:62[B]:CYS:HB2	2:B:343:GLU:OE2	2.19	0.41
9:B:505:PEG:H42	9:B:505:PEG:H21	1.79	0.41
1:A:3:ARG:NH1	4:A:307:DMS:H23	2.36	0.41
1:A:211:GLY:O	1:A:212:PHE:HB2	2.21	0.40
2:B:62[B]:CYS:HB2	2:B:343:GLU:CD	2.41	0.40
3:A:301:F9F:H3	11:A:507:HOH:O	2.21	0.40
2:B:114[B]:GLN:HG3	11:B:620:HOH:O	2.20	0.40
1:A:3:ARG:HH12	4:A:307:DMS:C2	2.34	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	275/268 (103%)	271 (98%)	3 (1%)	1 (0%)	34	11
2	B	416/397 (105%)	410 (99%)	6 (1%)	0	100	100
All	All	691/665 (104%)	681 (99%)	9 (1%)	1 (0%)	47	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE

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	213/208 (102%)	213 (100%)	0	100	100
2	B	329/311 (106%)	327 (99%)	2 (1%)	86	62
All	All	542/519 (104%)	540 (100%)	2 (0%)	91	73

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	207	MET
2	B	296	GLU

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 41 ligands modelled in this entry, 12 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	PLP	B	520	2	15,15,16	0.98	1 (6%)	20,22,23	1.27	2 (10%)
3	F9F	A	301	-	22,22,22	0.50	0	32,33,33	0.79	0
4	DMS	B	510	-	3,3,3	0.26	0	3,3,3	0.16	0
4	DMS	B	515	-	3,3,3	0.30	0	3,3,3	0.35	0
5	TRP	A	303	-	12,16,16	0.65	0	12,22,22	0.82	0
4	DMS	B	514	-	3,3,3	0.21	0	3,3,3	0.12	0
4	DMS	A	305	-	3,3,3	0.16	0	3,3,3	0.10	0
6	EDO	B	512	-	3,3,3	0.06	0	2,2,2	0.43	0
4	DMS	B	504	-	3,3,3	0.25	0	3,3,3	0.41	0
9	PEG	B	505	-	6,6,6	0.27	0	5,5,5	0.26	0
6	EDO	B	517	-	3,3,3	0.19	0	2,2,2	0.48	0
6	EDO	B	509	-	3,3,3	0.07	0	2,2,2	0.31	0
4	DMS	A	307	-	3,3,3	0.11	0	3,3,3	0.73	0
4	DMS	A	306	-	3,3,3	0.37	0	3,3,3	0.16	0
6	EDO	B	507	-	3,3,3	0.30	0	2,2,2	0.10	0
4	DMS	A	309	-	3,3,3	0.16	0	3,3,3	0.27	0
6	EDO	B	516	-	3,3,3	0.09	0	2,2,2	0.28	0
9	PEG	B	511	-	6,6,6	0.11	0	5,5,5	0.13	0
6	EDO	B	518	-	3,3,3	0.04	0	2,2,2	0.09	0
4	DMS	A	304	-	3,3,3	0.23	0	3,3,3	0.20	0
4	DMS	B	503	-	3,3,3	0.16	0	3,3,3	0.18	0
6	EDO	B	519	-	3,3,3	0.15	0	2,2,2	0.04	0
6	EDO	B	506	-	3,3,3	0.13	0	2,2,2	0.13	0
9	PEG	B	513	-	6,6,6	0.16	0	5,5,5	0.51	0
6	EDO	A	308	-	3,3,3	1.95	1 (33%)	2,2,2	0.55	0
5	TRP	B	501	-	12,16,16	0.68	0	12,22,22	0.92	1 (8%)
4	DMS	B	502	-	3,3,3	0.93	0	3,3,3	0.48	0
4	DMS	A	302	-	3,3,3	0.21	0	3,3,3	0.28	0
4	DMS	B	508	-	3,3,3	0.21	0	3,3,3	0.07	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
6	EDO	B	506	-	-	1/1/1/1	-
9	PEG	B	505	-	-	2/4/4/4	-
10	PLP	B	520	2	-	0/6/6/8	0/1/1/1
6	EDO	B	517	-	-	1/1/1/1	-
3	F9F	A	301	-	-	6/20/20/20	0/1/1/1
5	TRP	A	303	-	-	0/3/8/8	0/2/2/2
6	EDO	B	509	-	-	1/1/1/1	-
9	PEG	B	513	-	-	2/4/4/4	-
6	EDO	B	507	-	-	0/1/1/1	-
6	EDO	A	308	-	-	0/1/1/1	-
6	EDO	B	516	-	-	1/1/1/1	-
5	TRP	B	501	-	-	0/3/8/8	0/2/2/2
6	EDO	B	518	-	-	1/1/1/1	-
9	PEG	B	511	-	-	0/4/4/4	-
6	EDO	B	512	-	-	1/1/1/1	-
6	EDO	B	519	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	308	EDO	O2-C2	-3.12	1.25	1.42
10	B	520	PLP	C4A-C4	-2.54	1.46	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	520	PLP	C4A-C4-C5	2.95	123.98	120.94
10	B	520	PLP	O4P-C5A-C5	2.41	113.94	109.35
5	B	501	TRP	CH2-CZ2-CE2	-2.09	117.08	120.08

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	505	PEG	C4-C3-O2-C2
9	B	513	PEG	O1-C1-C2-O2
9	B	505	PEG	O2-C3-C4-O4
6	B	509	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	512	EDO	O1-C1-C2-O2
6	B	517	EDO	O1-C1-C2-O2
9	B	513	PEG	O2-C3-C4-O4
3	A	301	F9F	C3-C4-S12-O21
6	B	516	EDO	O1-C1-C2-O2
3	A	301	F9F	C5-C4-S12-O21
3	A	301	F9F	N13-C14-C15-O16
6	B	506	EDO	O1-C1-C2-O2
6	B	518	EDO	O1-C1-C2-O2
3	A	301	F9F	C6-C1-O7-C8
3	A	301	F9F	C3-C4-S12-N13
3	A	301	F9F	C2-C1-O7-C8

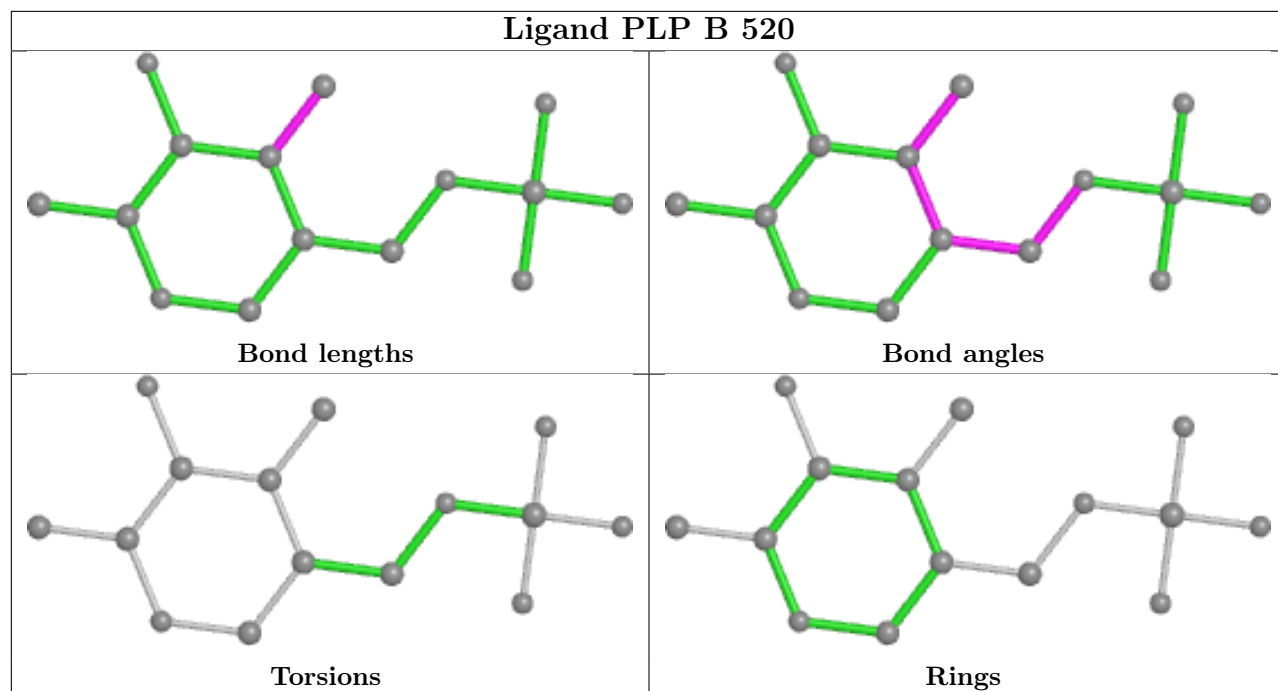
There are no ring outliers.

10 monomers are involved in 21 short contacts:

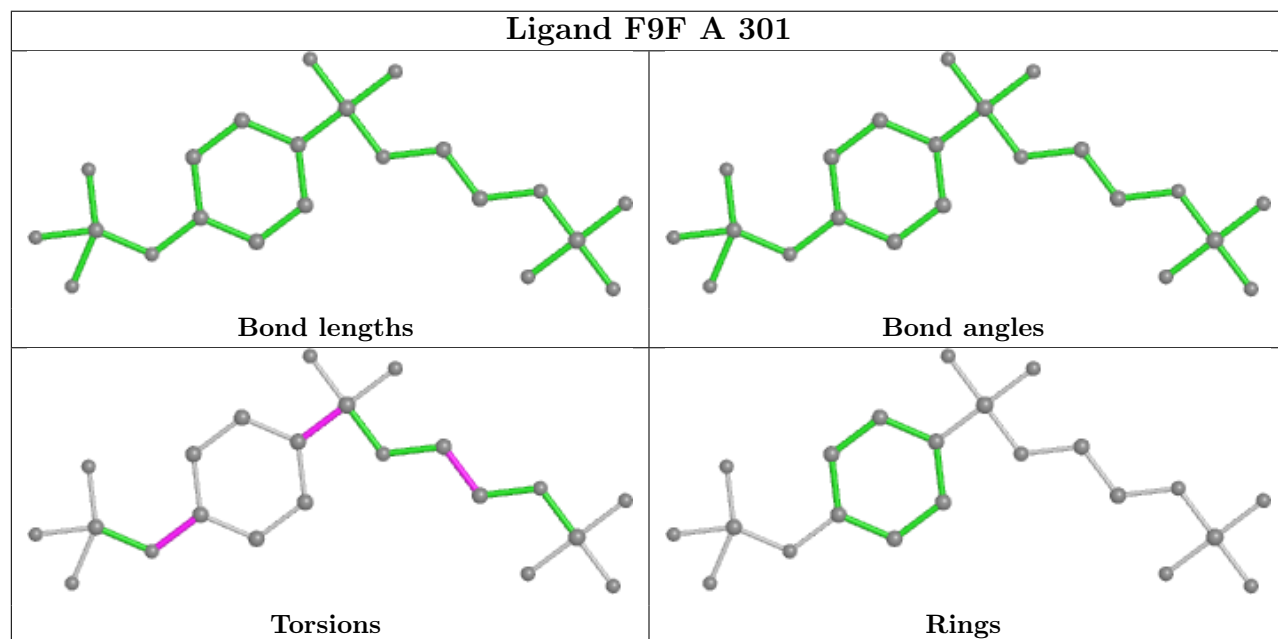
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	520	PLP	1	0
3	A	301	F9F	2	0
4	B	515	DMS	2	0
4	B	504	DMS	1	0
9	B	505	PEG	2	0
4	A	307	DMS	2	0
4	A	309	DMS	3	0
9	B	511	PEG	2	0
9	B	513	PEG	3	0
6	A	308	EDO	3	0

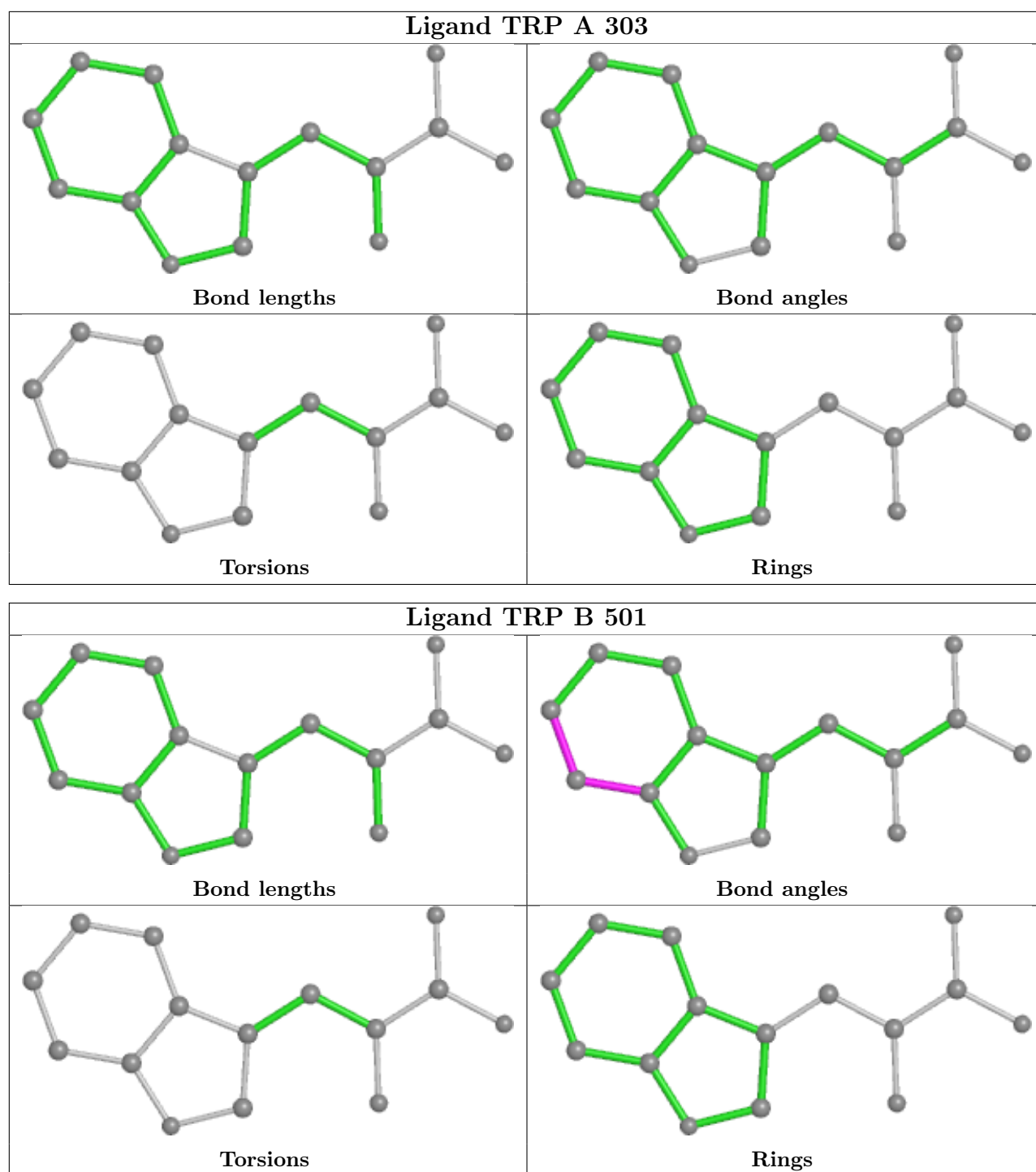
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 PLP B 520



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	268/268 (100%)	0.10	13 (4%) 29 26	7, 12, 26, 48	0
2	B	393/397 (98%)	0.00	8 (2%) 65 58	5, 10, 19, 45	0
All	All	661/665 (99%)	0.04	21 (3%) 47 42	5, 11, 23, 48	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	12.8
2	B	393	ALA	5.1
2	B	385	PHE	4.8
2	B	391	LEU	4.4
1	A	1	MET	3.3
1	A	192	PRO	3.3
2	B	394	ARG	3.2
1	A	191	LEU	3.0
1	A	268	ALA	3.0
1	A	13[A]	ASP	2.9
2	B	2	THR	2.9
1	A	187	ASN	2.8
1	A	186	GLU	2.7
2	B	390	ILE	2.5
1	A	189	GLY	2.4
2	B	141	ARG	2.3
1	A	195	HIS	2.2
1	A	194	HIS	2.2
1	A	157	ASN	2.1
1	A	2	GLU	2.1
2	B	68	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	B	512	4/4	0.63	0.21	24,29,29,35	0
6	EDO	B	518	4/4	0.65	0.16	32,34,35,41	0
9	PEG	B	511	7/7	0.77	0.23	25,29,34,39	0
6	EDO	B	506	4/4	0.82	0.23	26,27,33,37	0
4	DMS	B	514	4/4	0.82	0.26	22,35,35,36	0
4	DMS	A	307	4/4	0.83	0.21	15,25,26,26	0
4	DMS	B	515	4/4	0.85	0.14	11,17,27,33	0
9	PEG	B	513	7/7	0.85	0.20	13,18,27,29	7
6	EDO	B	517	4/4	0.86	0.17	19,24,28,30	0
9	PEG	B	505	7/7	0.87	0.20	20,26,35,36	0
6	EDO	B	516	4/4	0.88	0.15	35,37,38,39	0
6	EDO	A	308	4/4	0.88	0.21	8,10,17,22	0
6	EDO	B	509	4/4	0.91	0.19	33,35,37,44	0
8	CL	B	526	1/1	0.92	0.05	55,55,55,55	0
8	CL	B	525	1/1	0.93	0.04	54,54,54,54	0
4	DMS	A	305	4/4	0.93	0.14	22,30,37,38	0
4	DMS	A	304	4/4	0.93	0.16	35,36,38,41	0
4	DMS	B	504	4/4	0.93	0.17	21,25,26,31	0
6	EDO	B	519	4/4	0.93	0.16	23,23,29,32	0
6	EDO	B	507	4/4	0.94	0.13	15,24,25,30	0
5	TRP	A	303	15/15	0.94	0.20	18,20,23,24	0
8	CL	A	312	1/1	0.95	0.14	31,31,31,31	0
4	DMS	A	306	4/4	0.95	0.17	18,18,18,20	0
5	TRP	B	501	15/15	0.96	0.09	13,14,15,15	0
4	DMS	A	309	4/4	0.96	0.19	18,18,19,19	0
4	DMS	B	508	4/4	0.96	0.18	28,29,29,29	0
4	DMS	B	510	4/4	0.96	0.20	36,37,40,42	0

Continued on next page...

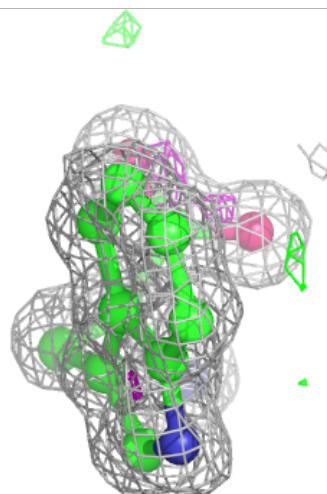
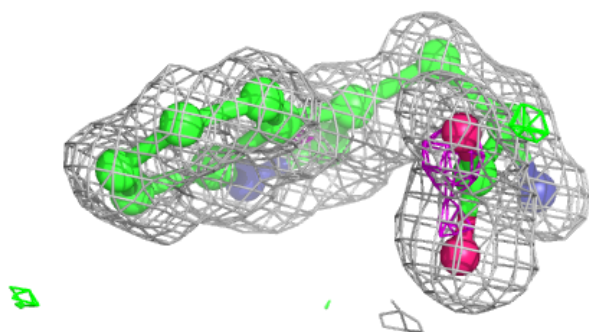
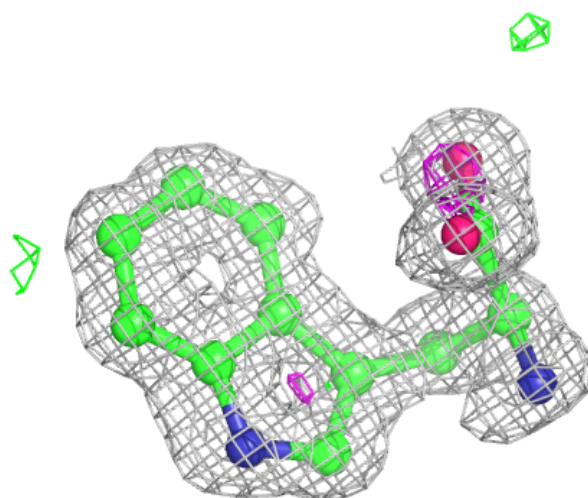
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DMS	B	502	4/4	0.98	0.10	7,12,12,16	0
4	DMS	B	503	4/4	0.98	0.15	16,23,23,23	0
4	DMS	A	302	4/4	0.98	0.10	11,15,15,17	0
7	CS	A	311[B]	1/1	0.99	0.09	11,11,11,11	1
3	F9F	A	301	22/22	0.99	0.05	9,10,13,13	0
8	CL	B	524	1/1	0.99	0.05	31,31,31,31	0
7	CS	A	311[A]	1/1	0.99	0.09	16,16,16,16	0
10	PLP	B	520	15/16	0.99	0.07	6,8,12,12	0
7	CS	B	521	1/1	1.00	0.02	18,18,18,18	1
7	CS	B	522[A]	1/1	1.00	0.04	11,11,11,11	1
7	CS	B	522[C]	1/1	1.00	0.04	18,18,18,18	1
7	CS	B	523	1/1	1.00	0.02	12,12,12,12	0
7	CS	A	310[A]	1/1	1.00	0.06	19,19,19,19	1
7	CS	A	310[B]	1/1	1.00	0.06	31,31,31,31	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.

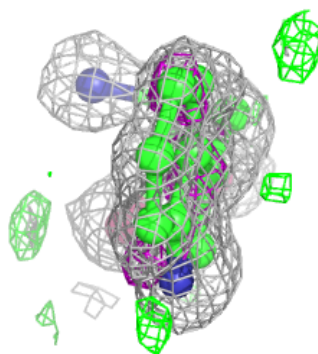
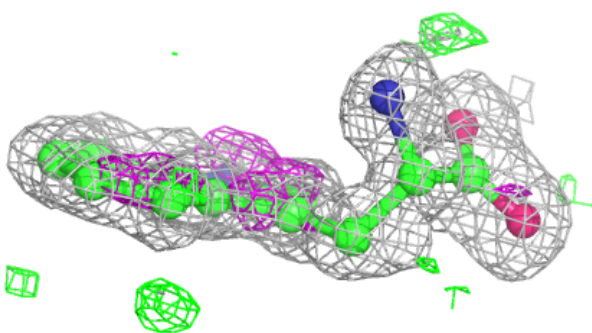
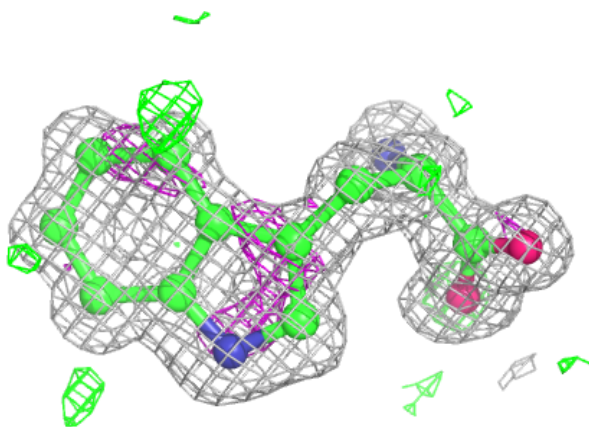
Electron density around TRP A 303:

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



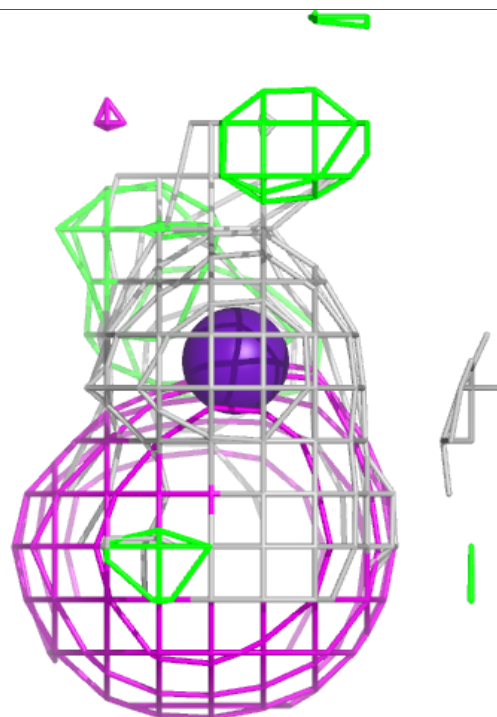
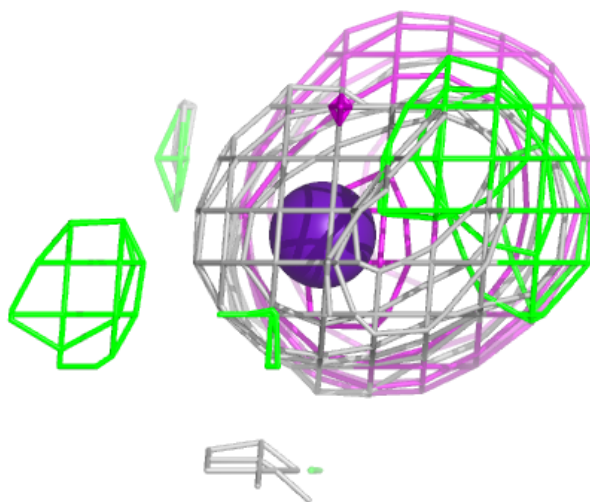
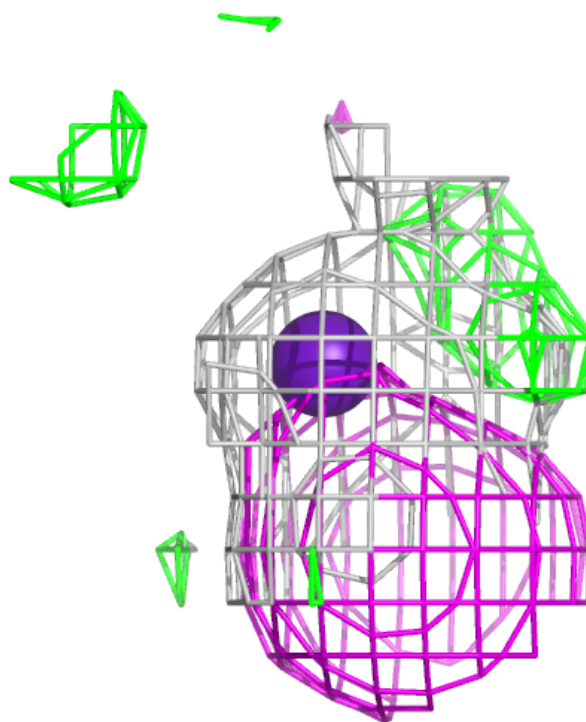
Electron density around TRP B 501:

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



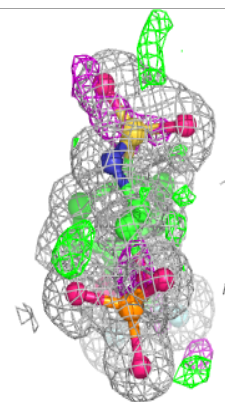
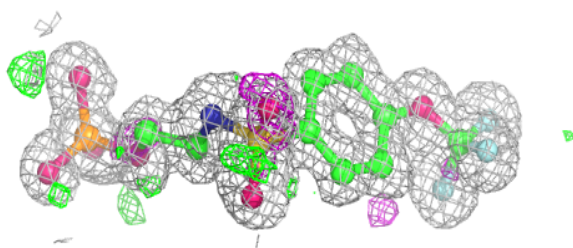
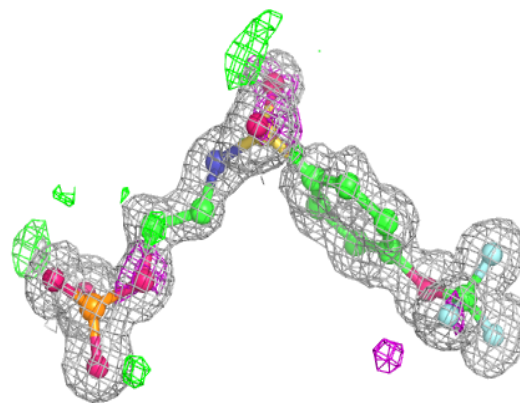
Electron density around CS A 311 (B):

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



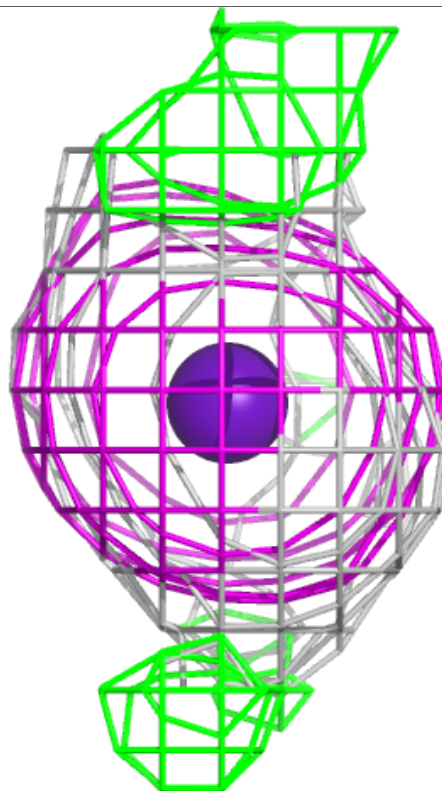
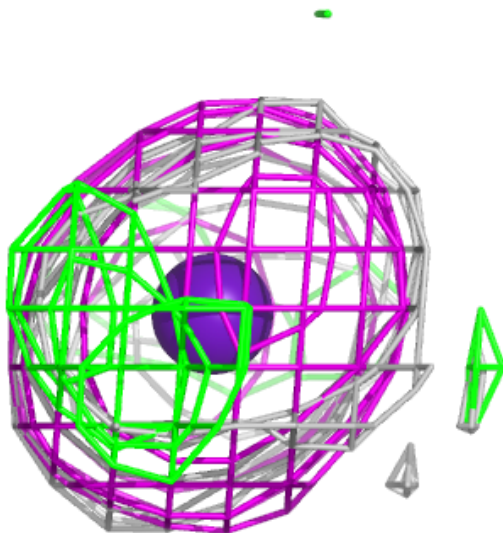
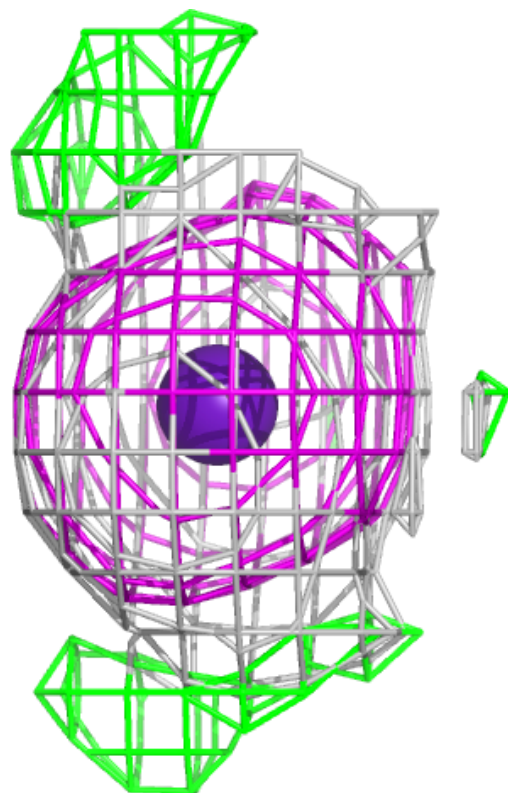
Electron density around F9F A 301:

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



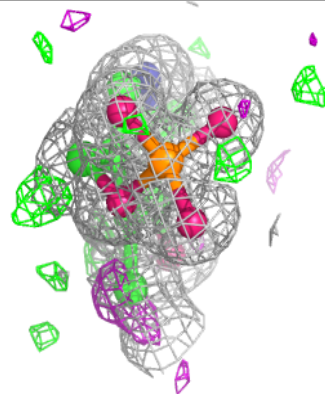
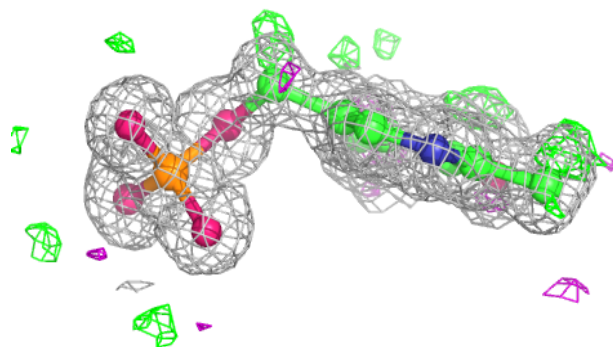
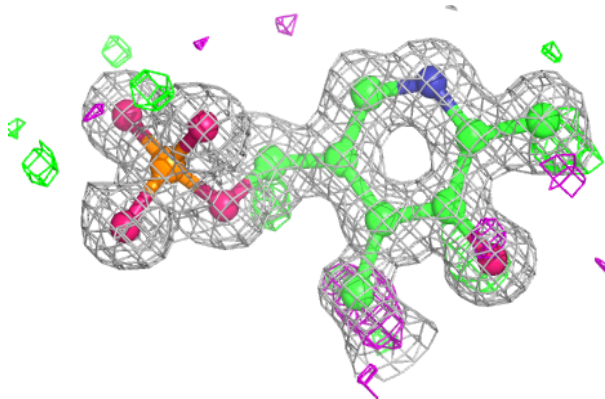
Electron density around CS A 311 (A):

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



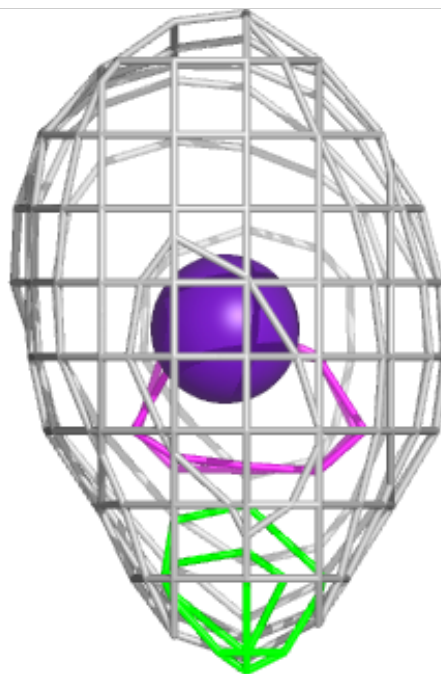
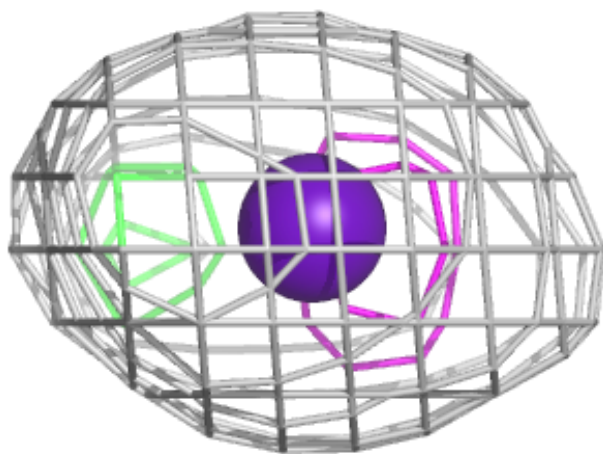
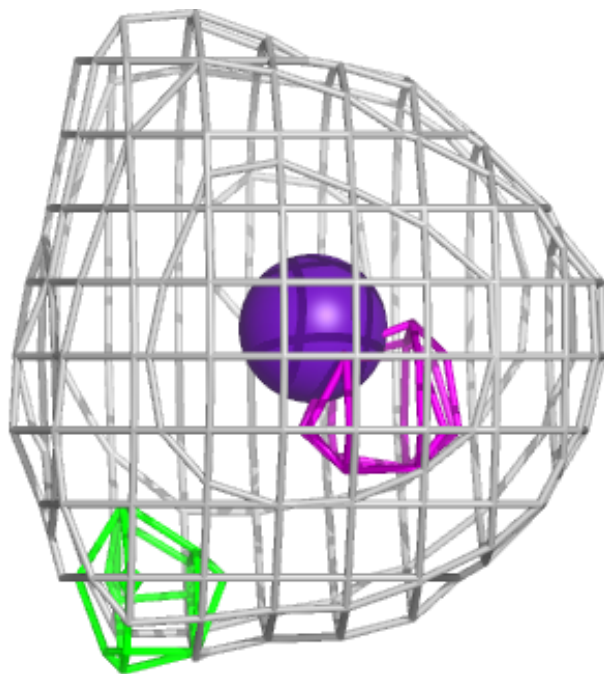
Electron density around PLP B 520:

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



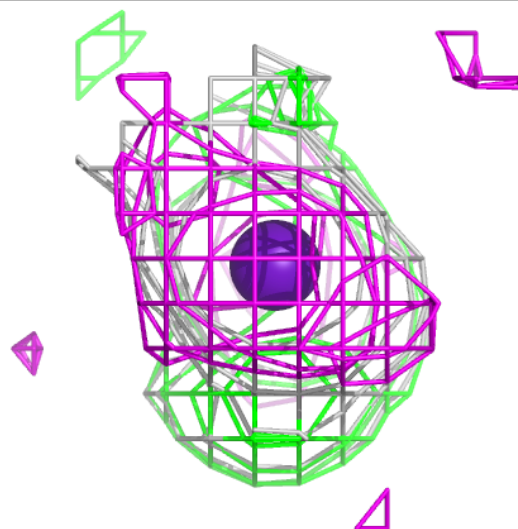
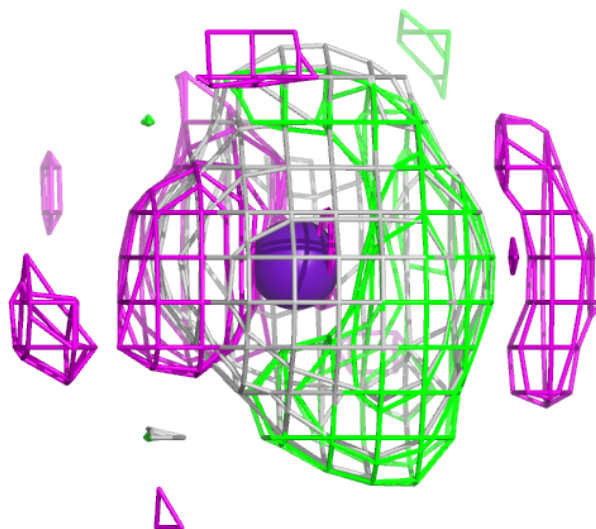
Electron density around CS B 521:

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



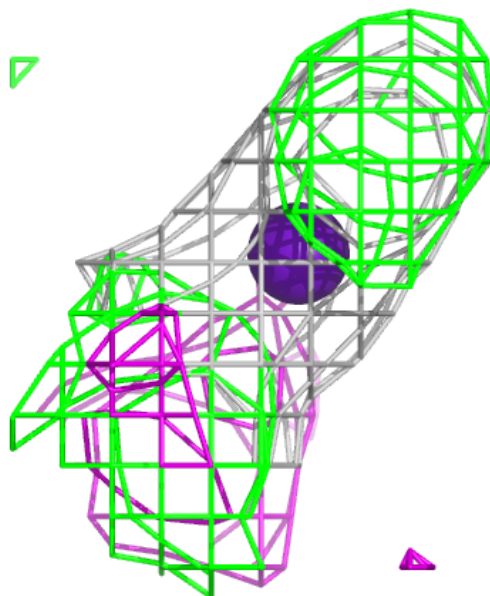
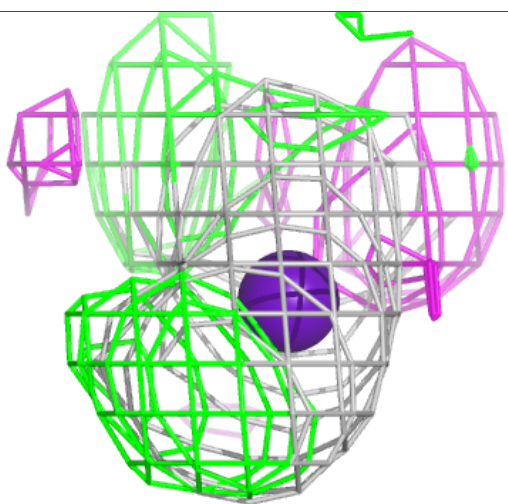
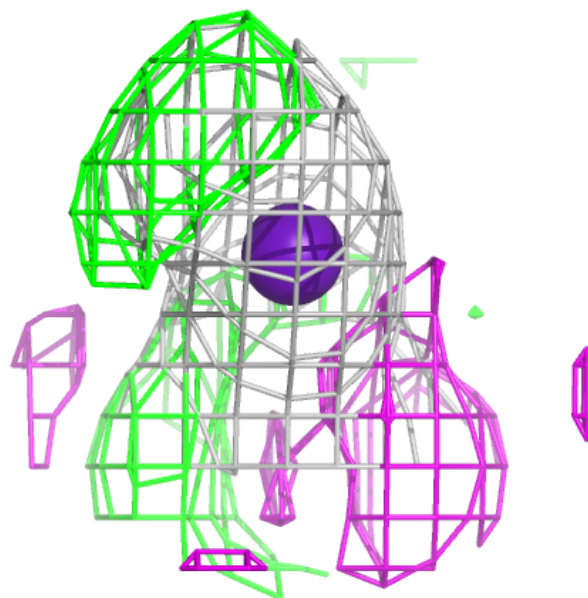
Electron density around CS B 522 (A):

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



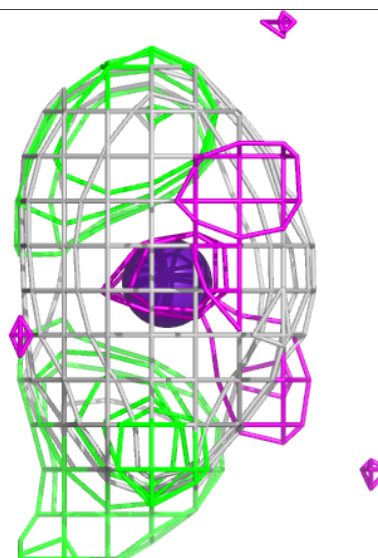
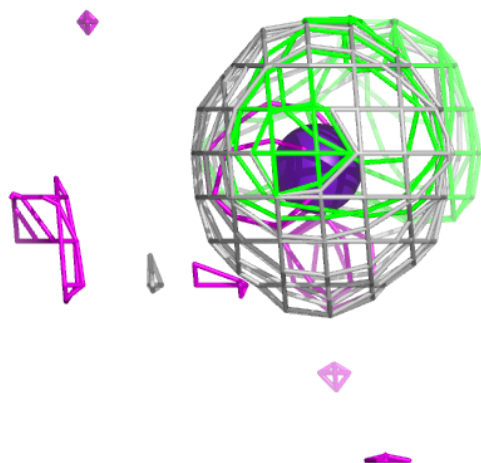
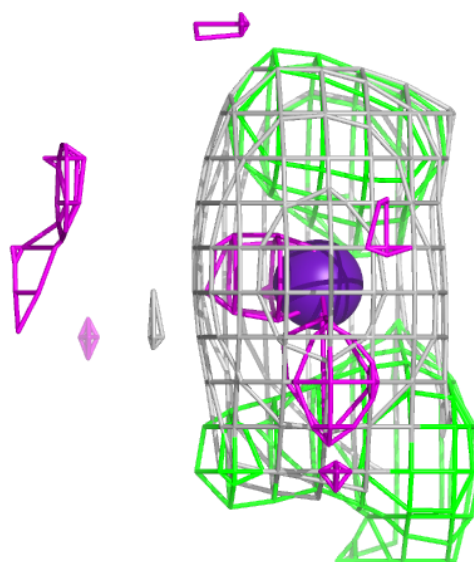
Electron density around CS B 522 (C):

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



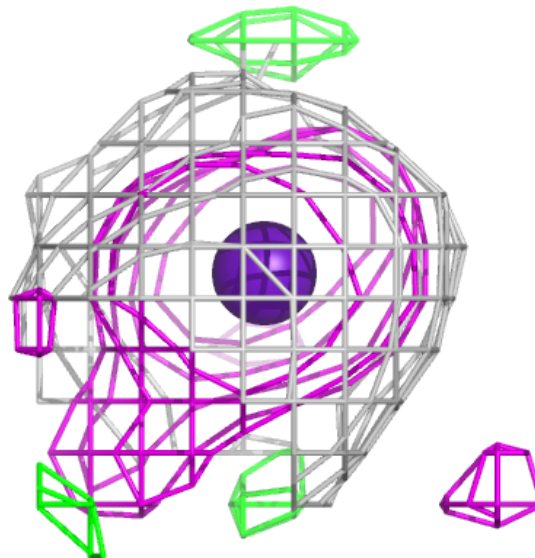
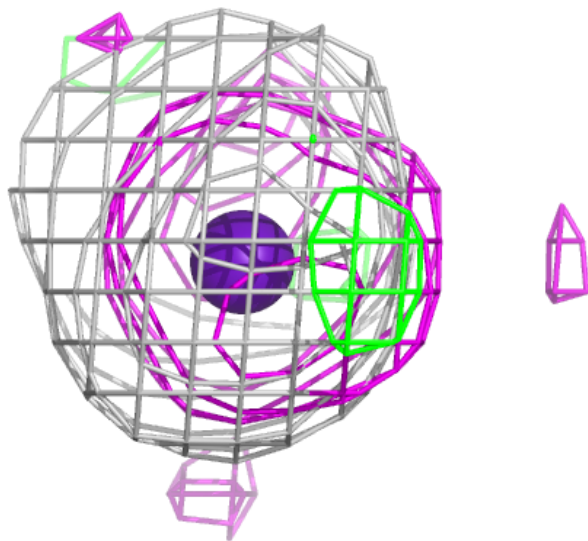
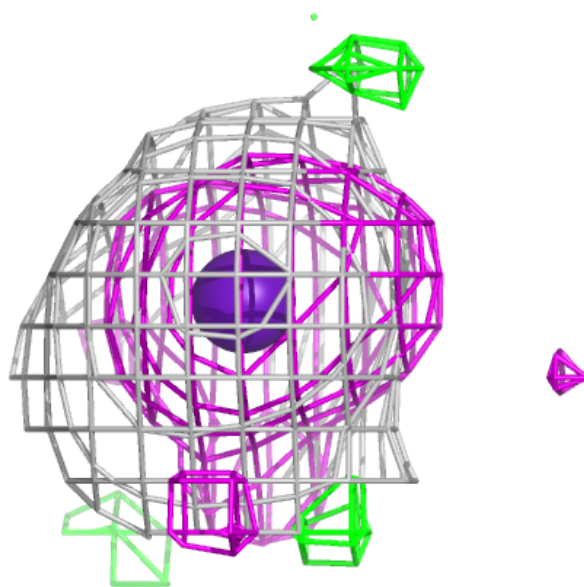
Electron density around CS B 523:

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



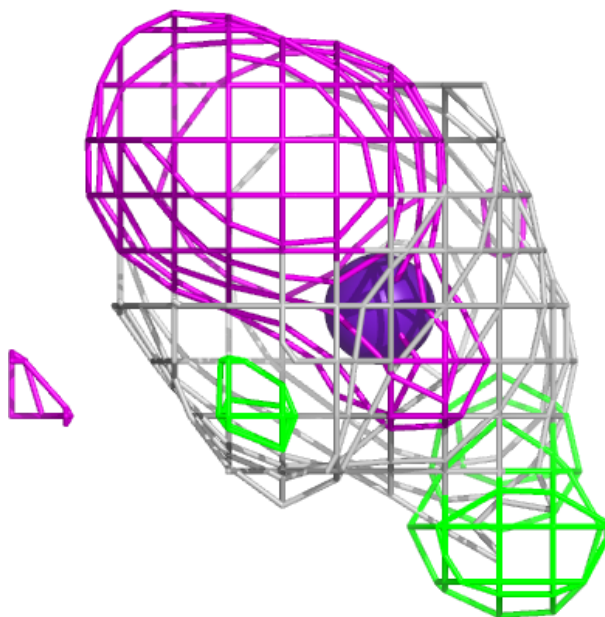
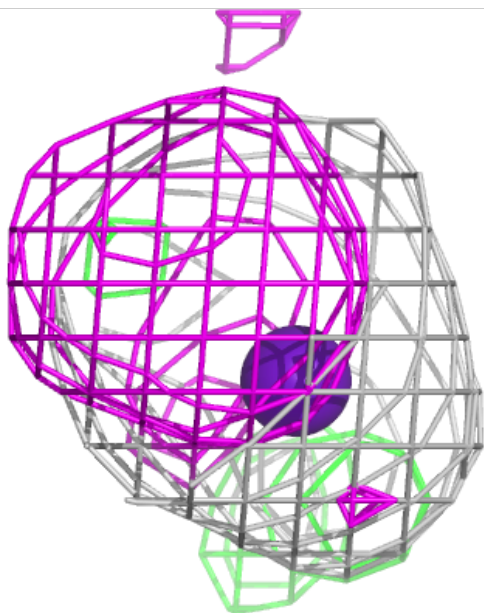
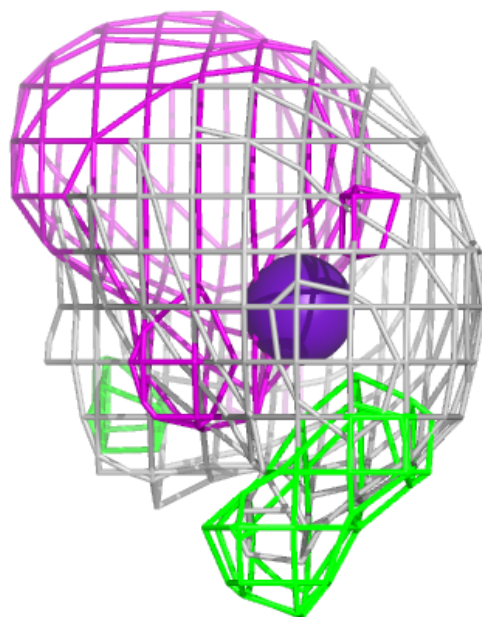
Electron density around CS A 310 (A):

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



Electron density around CS A 310 (B):

$2mF_o - DF_c$ (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.