Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 01:53 pm GMT

PDB ID	:	6ZRX
Title	:	Crystal structure of 6-dimethylallyltryptophan synthase from Micromonospora olivasterospora in complex with DMASPP and Trp
Authors	:	Ostertag, E.; Stehle, T.; Zocher, G.
Deposited on	:	2020-07-15
Resolution	:	1.70 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:

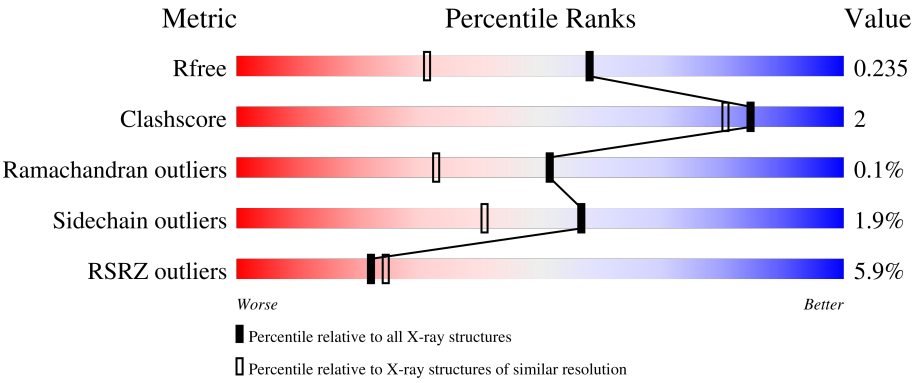
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	AAA	362	6% 89% 9%
1	BBB	362	4% 94%
1	CCC	362	7% 93% 7%
1	DDD	362	6% 94% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12221 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.

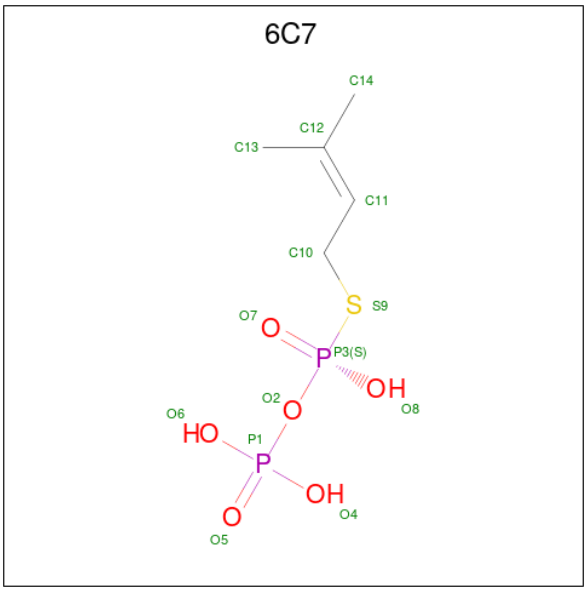
- Molecule 1 is a protein called DMATS type aromatic prenyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	356	Total	C	N	O	S	0	18	0
			2806	1773	501	528	4			
1	BBB	353	Total	C	N	O	S	0	6	0
			2709	1713	482	508	6			
1	CCC	360	Total	C	N	O	S	0	9	0
			2764	1750	496	513	5			
1	DDD	360	Total	C	N	O	S	0	11	0
			2801	1769	509	518	5			

There are 16 discrepancies between the modelled and reference sequences:

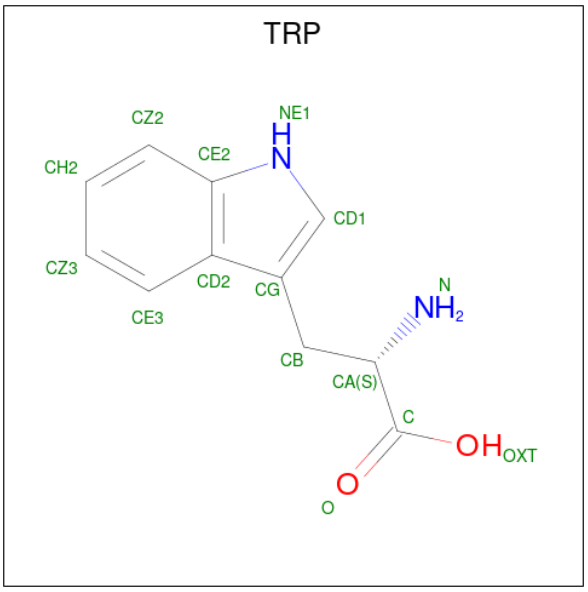
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	359	LEU	-	expression tag	UNP Q2MFY2
AAA	360	VAL	-	expression tag	UNP Q2MFY2
AAA	361	PRO	-	expression tag	UNP Q2MFY2
AAA	362	ARG	-	expression tag	UNP Q2MFY2
BBB	359	LEU	-	expression tag	UNP Q2MFY2
BBB	360	VAL	-	expression tag	UNP Q2MFY2
BBB	361	PRO	-	expression tag	UNP Q2MFY2
BBB	362	ARG	-	expression tag	UNP Q2MFY2
CCC	359	LEU	-	expression tag	UNP Q2MFY2
CCC	360	VAL	-	expression tag	UNP Q2MFY2
CCC	361	PRO	-	expression tag	UNP Q2MFY2
CCC	362	ARG	-	expression tag	UNP Q2MFY2
DDD	359	LEU	-	expression tag	UNP Q2MFY2
DDD	360	VAL	-	expression tag	UNP Q2MFY2
DDD	361	PRO	-	expression tag	UNP Q2MFY2
DDD	362	ARG	-	expression tag	UNP Q2MFY2

- Molecule 2 is S-(3-methylbut-2-en-1-yl) trihydrogen thiodiphosphate (three-letter code: 6C7) (formula: $C_5H_{12}O_6P_2S$) (labeled as "Ligand of Interest" by depositor).



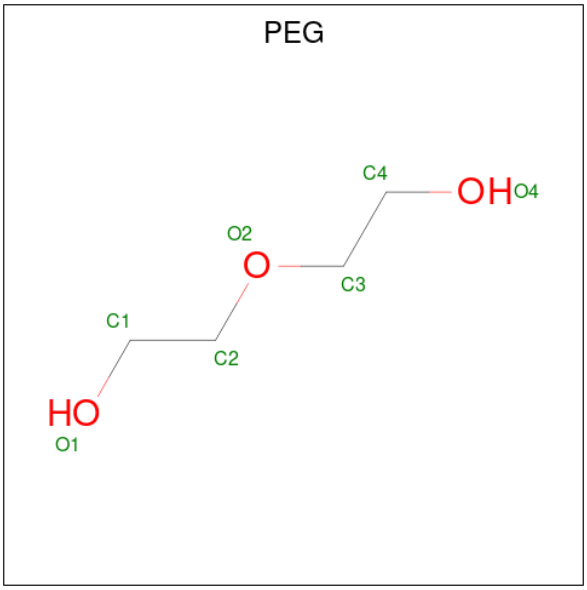
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	O	P	S	0	0
			14	5	6	2	1		
2	BBB	1	Total	C	O	P	S	0	0
			14	5	6	2	1		
2	CCC	1	Total	C	O	P	S	0	0
			14	5	6	2	1		
2	DDD	1	Total	C	O	P	S	0	0
			14	5	6	2	1		

- Molecule 3 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
3	AAA	1	Total C N O 15 11 2 2	0	0
3	BBB	1	Total C N O 15 11 2 2	0	0
3	CCC	1	Total C N O 15 11 2 2	0	0
3	DDD	1	Total C N O 15 11 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 7 4 3	0	0
4	AAA	1	Total C O 7 4 3	0	0
4	BBB	1	Total C O 7 4 3	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 7 4 3	0	0
4	CCC	1	Total C O 7 4 3	0	0
4	CCC	1	Total C O 7 4 3	0	0
4	DDD	1	Total C O 7 4 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	DDD	1	Total Na 1 1	0	0

- Molecule 6 is water.

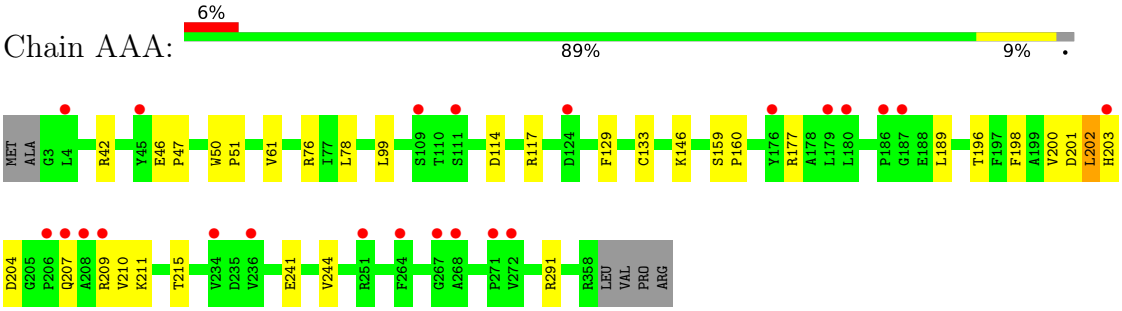
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	251	Total O 251 251	0	0
6	BBB	238	Total O 238 238	0	0
6	CCC	247	Total O 247 247	0	0
6	DDD	235	Total O 235 235	0	0

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.

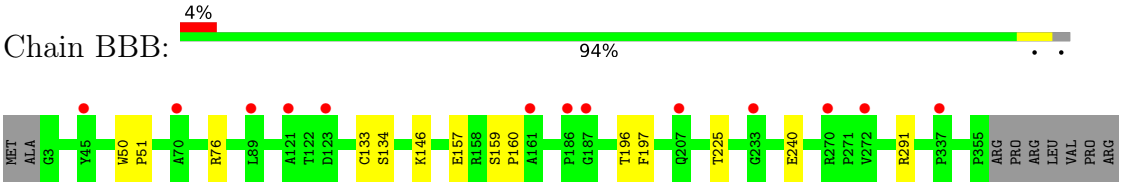
• Molecule 1: DMATS type aromatic prenyltransferase

Chain AAA:



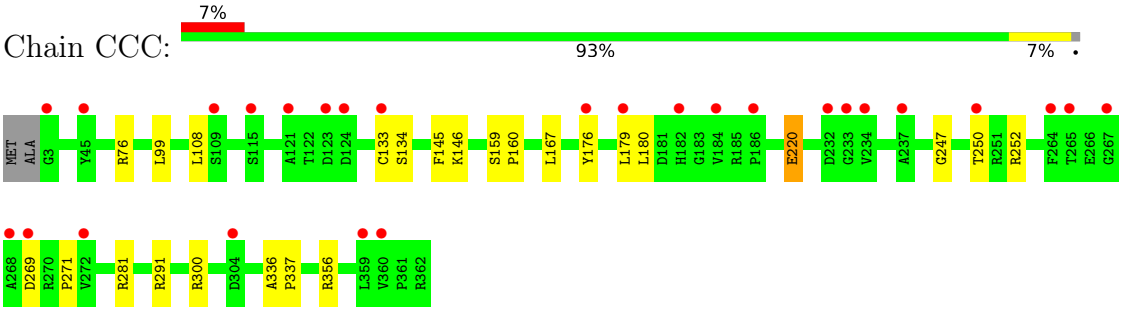
• Molecule 1: DMATS type aromatic prenyltransferase

Chain BBB:



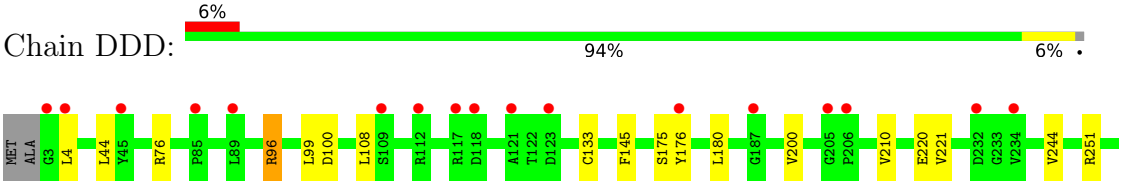
• Molecule 1: DMATS type aromatic prenyltransferase

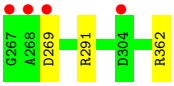
Chain CCC:



• Molecule 1: DMATS type aromatic prenyltransferase

Chain DDD:




G267
A268
D269
R291
D304
R362

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.02Å 98.47Å 89.19Å 90.00° 107.49° 90.00°	Depositor
Resolution (Å)	39.67 – 1.70 39.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.67-1.70) 98.7 (39.64-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.202 , 0.230 0.211 , 0.235	Depositor DCC
R_{free} test set	1671 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12221	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2293e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NA, 6C7, 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	AAA	0.66	0/2887	0.71	0/3944
1	BBB	0.66	0/2778	0.70	0/3791
1	CCC	0.68	0/2835	0.73	0/3874
1	DDD	0.66	0/2881	0.71	0/3934
All	All	0.66	0/11381	0.71	0/15543

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

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	AAA	2806	0	2741	20	0
1	BBB	2709	0	2652	5	0
1	CCC	2764	0	2703	15	0
1	DDD	2801	0	2767	13	0
2	AAA	14	0	0	1	0
2	BBB	14	0	0	0	0
2	CCC	14	0	0	0	0
2	DDD	14	0	0	0	0
3	AAA	15	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	15	0	9	0	0
3	CCC	15	0	9	0	0
3	DDD	15	0	9	0	0
4	AAA	14	0	20	0	0
4	BBB	11	0	15	1	0
4	CCC	21	0	30	0	0
4	DDD	7	0	10	0	0
5	DDD	1	0	0	0	0
6	AAA	251	0	0	1	0
6	BBB	238	0	0	1	0
6	CCC	247	0	0	0	0
6	DDD	235	0	0	1	0
All	All	12221	0	10974	52	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 2.

All (52) 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:AAA:201[B]:ASP:O	1:AAA:203[B]:HIS:N	2.26	0.68
1:AAA:201[A]:ASP:CG	1:AAA:209[A]:ARG:H	1.98	0.67
1:CCC:99:LEU:HD11	1:CCC:133[B]:CYS:SG	2.36	0.66
1:CCC:179:LEU:HD21	1:CCC:271:PRO:HG2	1.78	0.63
1:DDD:176:TYR:CE2	1:DDD:180:LEU:HD11	2.37	0.60
1:AAA:42[B]:ARG:NH2	1:AAA:47:PRO:O	2.33	0.59
1:CCC:269:ASP:HB3	1:DDD:4:LEU:HA	1.85	0.59
1:DDD:96[A]:ARG:NH1	1:DDD:100:ASP:OD2	2.32	0.56
1:BBB:225:THR:HG21	1:BBB:240:GLU:HG2	1.86	0.56
1:AAA:42[B]:ARG:NE	1:AAA:46:GLU:OE2	2.41	0.54
1:CCC:179:LEU:HD21	1:CCC:271:PRO:CG	2.37	0.54
1:CCC:269:ASP:HA	1:DDD:4:LEU:HB3	1.91	0.53
1:CCC:167:LEU:HD13	1:CCC:176:TYR:HB2	1.92	0.52
1:DDD:175[A]:SER:OG	1:DDD:269:ASP:O	2.26	0.52
1:DDD:200[B]:VAL:HG12	1:DDD:210:VAL:HG22	1.92	0.52
1:AAA:42[B]:ARG:CZ	1:AAA:46:GLU:OE2	2.59	0.51
1:AAA:200[A]:VAL:HG12	1:AAA:210[A]:VAL:HG22	1.92	0.50
1:BBB:196:THR:HG22	1:BBB:197:PHE:CE2	2.46	0.50
1:CCC:281:ARG:O	1:CCC:356:ARG:NH2	2.46	0.48
1:AAA:196:THR:HG21	1:AAA:215:THR:OG1	2.14	0.47
1:BBB:50:TRP:CD2	1:BBB:51:PRO:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:134:SER:HB3	1:CCC:146:LYS:HB3	1.97	0.47
1:AAA:42[B]:ARG:NH1	1:AAA:46:GLU:OE2	2.48	0.47
1:CCC:247:GLY:O	1:CCC:250:THR:HG23	2.15	0.47
1:AAA:42[B]:ARG:NH2	6:AAA:508:HOH:O	2.48	0.46
1:DDD:176:TYR:CZ	1:DDD:180:LEU:HD11	2.50	0.46
1:DDD:99:LEU:HD11	1:DDD:133[A]:CYS:SG	2.55	0.46
1:CCC:336:ALA:HB1	1:CCC:337:PRO:HA	1.97	0.45
1:AAA:114:ASP:OD1	1:AAA:117:ARG:NH1	2.49	0.45
1:AAA:198:PHE:CE2	1:AAA:210[B]:VAL:HG11	2.51	0.45
1:DDD:362:ARG:CB	6:DDD:795:HOH:O	2.65	0.45
1:CCC:99:LEU:CD1	1:CCC:133[B]:CYS:SG	3.05	0.45
1:CCC:108:LEU:HD11	1:CCC:145:PHE:CD1	2.52	0.45
1:CCC:159:SER:OG	1:CCC:160:PRO:HD3	2.17	0.45
1:AAA:201[A]:ASP:OD2	1:AAA:209[A]:ARG:N	2.49	0.44
1:AAA:50:TRP:CD2	1:AAA:51:PRO:HD2	2.53	0.44
1:DDD:4:LEU:CD1	1:DDD:44:LEU:HD12	2.48	0.44
1:AAA:159:SER:OG	1:AAA:160:PRO:HD3	2.18	0.44
1:AAA:211[A]:LYS:HE2	1:AAA:211[A]:LYS:HB3	1.79	0.43
1:DDD:96[A]:ARG:HD3	1:DDD:100:ASP:OD2	2.19	0.43
1:AAA:146:LYS:NZ	2:AAA:401:6C7:O5	2.51	0.43
4:BBB:503:PEG:H41	6:BBB:666:HOH:O	2.18	0.43
1:AAA:99:LEU:HD11	1:AAA:133:CYS:HB3	2.01	0.43
1:BBB:134:SER:HB3	1:BBB:146:LYS:HB2	2.01	0.42
1:DDD:108:LEU:HD11	1:DDD:145:PHE:CD1	2.55	0.42
1:DDD:221[B]:VAL:HG23	1:DDD:251:ARG:O	2.19	0.42
1:AAA:241:GLU:HA	1:AAA:244:VAL:HG12	2.01	0.41
1:AAA:160:PRO:HB3	1:AAA:189:LEU:HD21	2.02	0.41
1:BBB:159:SER:OG	1:BBB:160:PRO:HD3	2.19	0.41
1:CCC:167:LEU:HD12	1:CCC:176:TYR:CD1	2.56	0.41
1:CCC:220:GLU:HG2	1:CCC:252:ARG:HG2	2.03	0.41
1:AAA:61:VAL:HA	1:AAA:78:LEU:O	2.20	0.41

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	AAA	372/362 (103%)	363 (98%)	7 (2%)	2 (0%)	29	13
1	BBB	357/362 (99%)	352 (99%)	5 (1%)	0	100	100
1	CCC	367/362 (101%)	362 (99%)	5 (1%)	0	100	100
1	DDD	369/362 (102%)	363 (98%)	6 (2%)	0	100	100
All	All	1465/1448 (101%)	1440 (98%)	23 (2%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	202[A]	LEU
1	AAA	202[B]	LEU

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	AAA	292/290 (101%)	282 (97%)	10 (3%)	37	18
1	BBB	280/290 (97%)	275 (98%)	5 (2%)	59	43
1	CCC	285/290 (98%)	280 (98%)	5 (2%)	59	43
1	DDD	294/290 (101%)	288 (98%)	6 (2%)	55	38
All	All	1151/1160 (99%)	1125 (98%)	26 (2%)	57	33

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	76	ARG
1	AAA	129	PHE
1	AAA	177	ARG
1	AAA	202[A]	LEU
1	AAA	202[B]	LEU
1	AAA	204[A]	ASP

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Mol	Chain	Res	Type
1	AAA	204[B]	ASP
1	AAA	207[A]	GLN
1	AAA	207[B]	GLN
1	AAA	291	ARG
1	BBB	76	ARG
1	BBB	133[A]	CYS
1	BBB	133[B]	CYS
1	BBB	157	GLU
1	BBB	291	ARG
1	CCC	76	ARG
1	CCC	180	LEU
1	CCC	220	GLU
1	CCC	291	ARG
1	CCC	300	ARG
1	DDD	76	ARG
1	DDD	96[A]	ARG
1	DDD	96[B]	ARG
1	DDD	220	GLU
1	DDD	244	VAL
1	DDD	291	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	TRP	DDD	502	-	14,16,16	0.77	0	16,22,22	1.11	1 (6%)
4	PEG	BBB	504	-	3,3,6	0.15	0	2,2,5	0.22	0
3	TRP	BBB	502	-	14,16,16	0.67	0	16,22,22	1.07	1 (6%)
2	6C7	DDD	501	-	9,13,13	1.11	1 (11%)	11,19,19	0.80	1 (9%)
2	6C7	CCC	501	-	9,13,13	1.03	1 (11%)	11,19,19	0.96	1 (9%)
4	PEG	CCC	503	-	6,6,6	0.21	0	5,5,5	0.09	0
4	PEG	AAA	404	-	6,6,6	0.21	0	5,5,5	0.13	0
3	TRP	CCC	502	-	14,16,16	0.76	0	16,22,22	0.99	1 (6%)
4	PEG	CCC	504	-	6,6,6	0.13	0	5,5,5	0.08	0
2	6C7	AAA	401	-	9,13,13	1.12	1 (11%)	11,19,19	1.05	1 (9%)
4	PEG	CCC	505	-	6,6,6	0.16	0	5,5,5	0.09	0
3	TRP	AAA	402	-	14,16,16	0.71	0	16,22,22	1.01	1 (6%)
4	PEG	AAA	403	-	6,6,6	0.19	0	5,5,5	0.08	0
4	PEG	BBB	503	-	6,6,6	0.24	0	5,5,5	0.10	0
2	6C7	BBB	501	-	9,13,13	1.17	1 (11%)	11,19,19	1.03	1 (9%)
4	PEG	DDD	504	-	6,6,6	0.18	0	5,5,5	0.10	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	TRP	DDD	502	-	-	0/7/8/8	0/2/2/2
4	PEG	BBB	504	-	-	0/1/1/4	-
3	TRP	BBB	502	-	-	0/7/8/8	0/2/2/2
2	6C7	DDD	501	-	-	3/7/13/13	-
2	6C7	CCC	501	-	-	2/7/13/13	-
4	PEG	CCC	503	-	-	0/4/4/4	-
4	PEG	AAA	404	-	-	2/4/4/4	-
3	TRP	CCC	502	-	-	0/7/8/8	0/2/2/2
4	PEG	CCC	504	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6C7	AAA	401	-	-	1/7/13/13	-
4	PEG	CCC	505	-	-	0/4/4/4	-
3	TRP	AAA	402	-	-	0/7/8/8	0/2/2/2
4	PEG	AAA	403	-	-	1/4/4/4	-
4	PEG	BBB	503	-	-	0/4/4/4	-
2	6C7	BBB	501	-	-	2/7/13/13	-
4	PEG	DDD	504	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	501	6C7	P3-O8	-2.75	1.49	1.56
2	DDD	501	6C7	P3-O8	-2.72	1.49	1.56
2	AAA	401	6C7	P3-O8	-2.62	1.50	1.56
2	BBB	501	6C7	P3-O8	-2.60	1.50	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	401	6C7	O8-P3-O7	2.89	116.82	109.82
2	BBB	501	6C7	O8-P3-O7	2.72	116.42	109.82
3	DDD	502	TRP	OXT-C-CA	2.39	121.53	113.38
3	BBB	502	TRP	OXT-C-CA	2.38	121.48	113.38
2	CCC	501	6C7	O8-P3-O7	2.33	115.46	109.82
3	AAA	402	TRP	OXT-C-CA	2.09	120.52	113.38
3	CCC	502	TRP	CH2-CZ2-CE2	-2.09	117.08	120.08
2	DDD	501	6C7	O8-P3-O7	2.07	114.82	109.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	501	6C7	P3-O2-P1-O4
2	BBB	501	6C7	P3-O2-P1-O6
2	CCC	501	6C7	P3-O2-P1-O4
4	CCC	504	PEG	O2-C3-C4-O4
2	DDD	501	6C7	P3-O2-P1-O5
4	AAA	404	PEG	C1-C2-O2-C3
4	AAA	404	PEG	C4-C3-O2-C2
4	CCC	504	PEG	O1-C1-C2-O2
4	CCC	504	PEG	C4-C3-O2-C2

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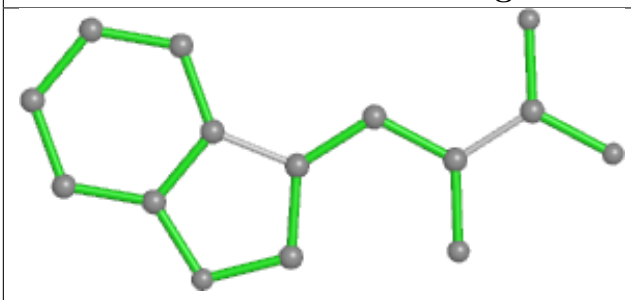
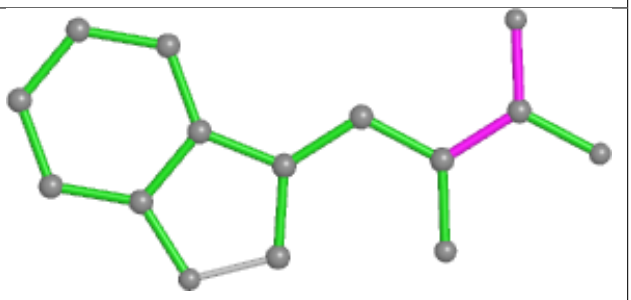
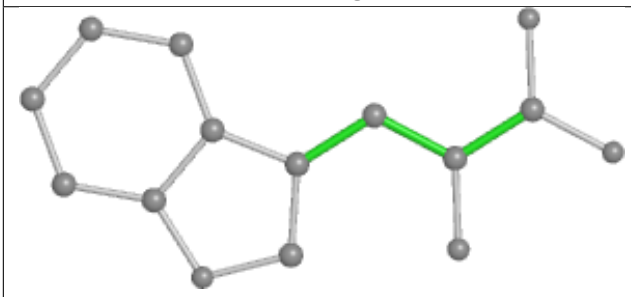
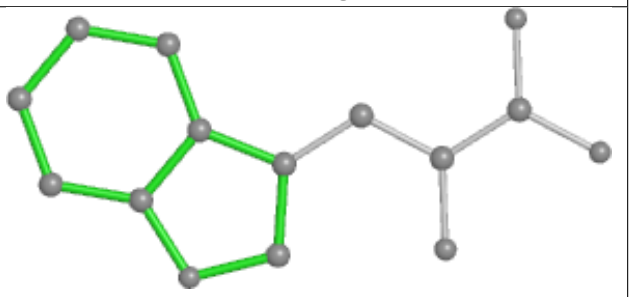
Mol	Chain	Res	Type	Atoms
4	AAA	403	PEG	O1-C1-C2-O2
4	DDD	504	PEG	O1-C1-C2-O2
2	AAA	401	6C7	P3-O2-P1-O6
2	CCC	501	6C7	P3-O2-P1-O6
2	DDD	501	6C7	P3-O2-P1-O4
2	DDD	501	6C7	P3-O2-P1-O6

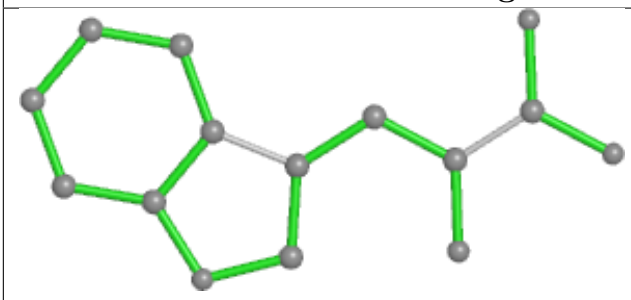
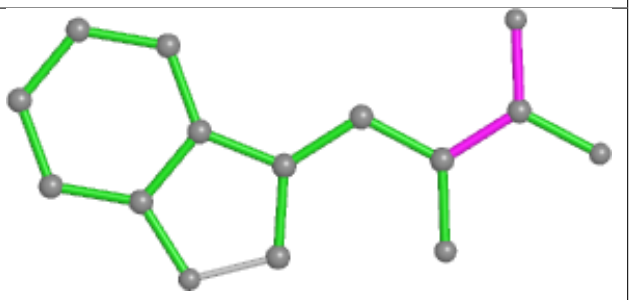
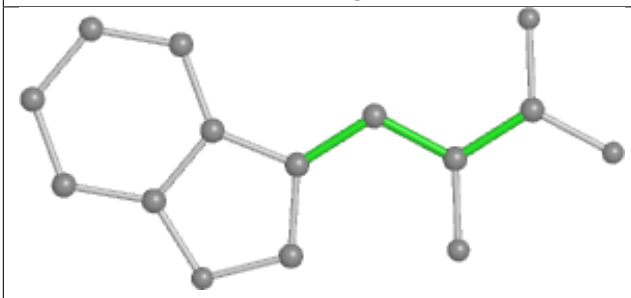
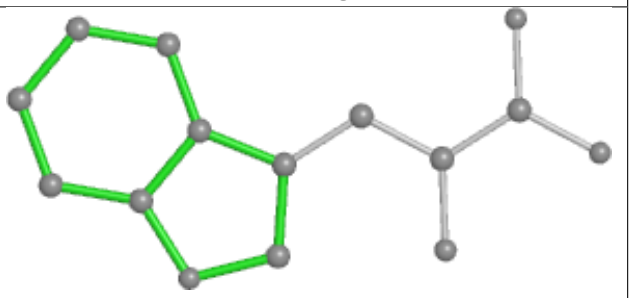
There are no ring outliers.

2 monomers are involved in 2 short contacts:

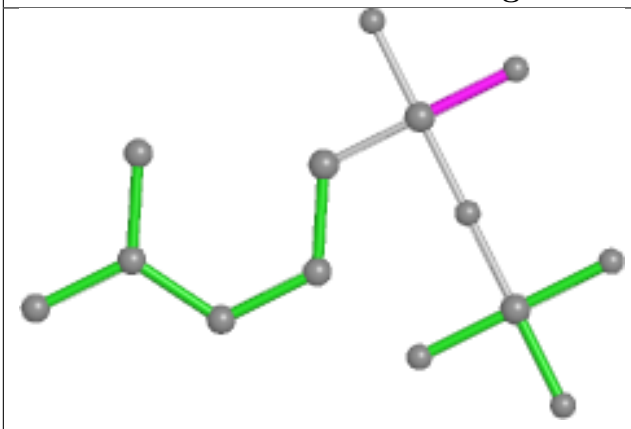
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401	6C7	1	0
4	BBB	503	PEG	1	0

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.

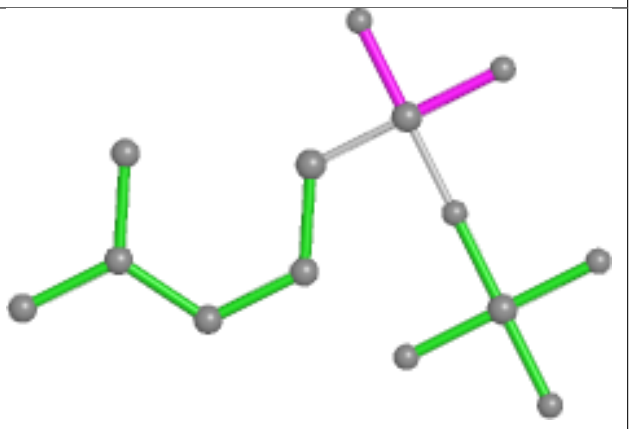
Ligand TRP DDD 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand TRP BBB 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

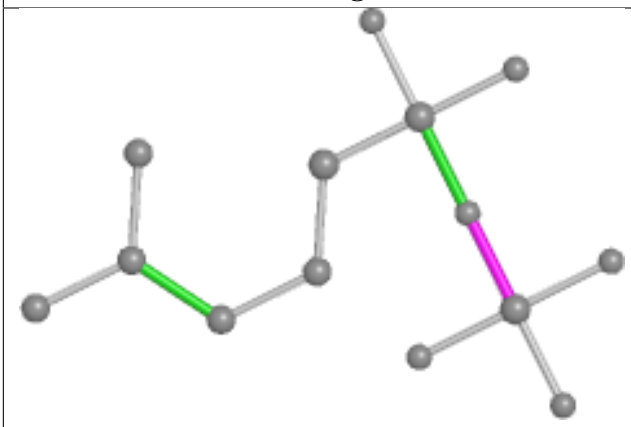
Ligand 6C7 DDD 501



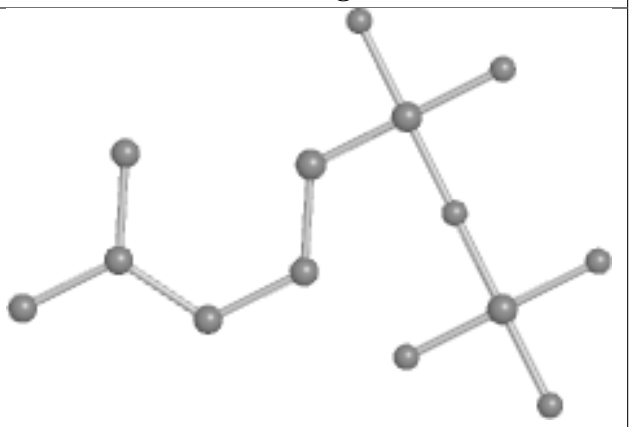
Bond lengths



Bond angles

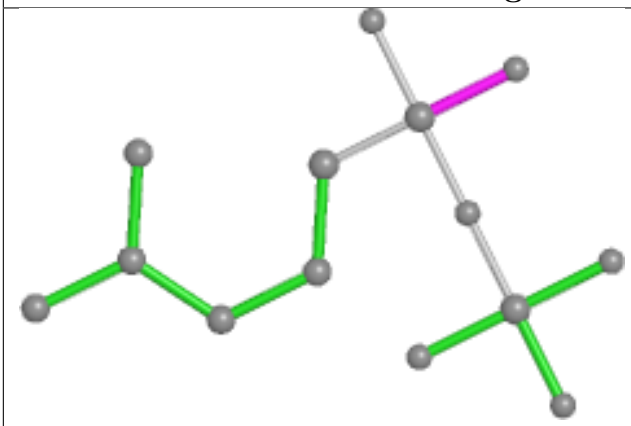


Torsions

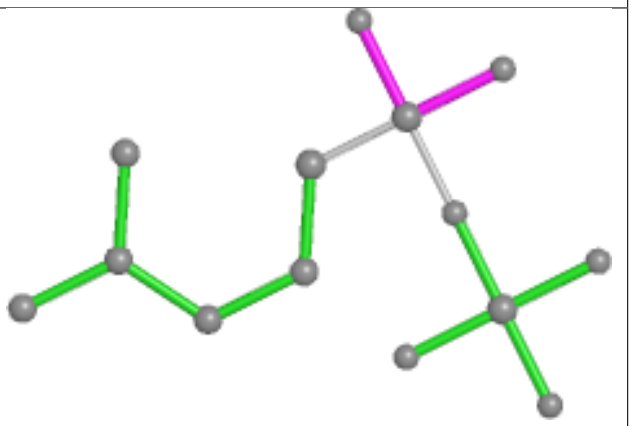


Rings

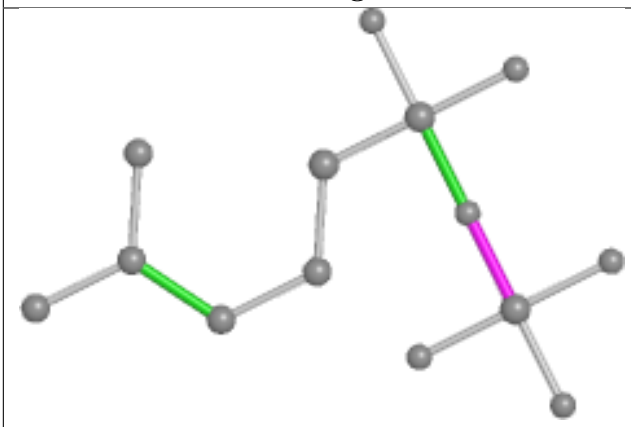
Ligand 6C7 CCC 501



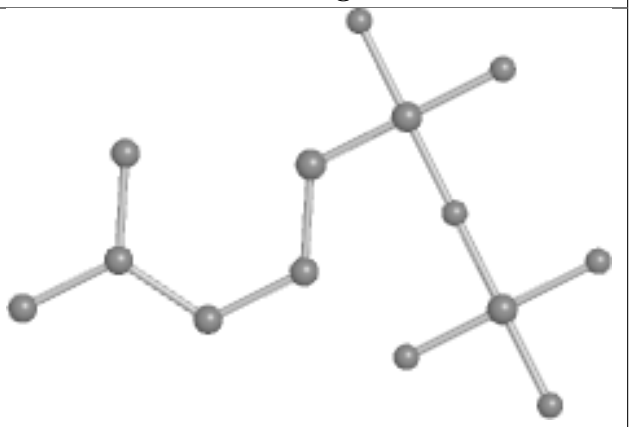
Bond lengths



Bond angles

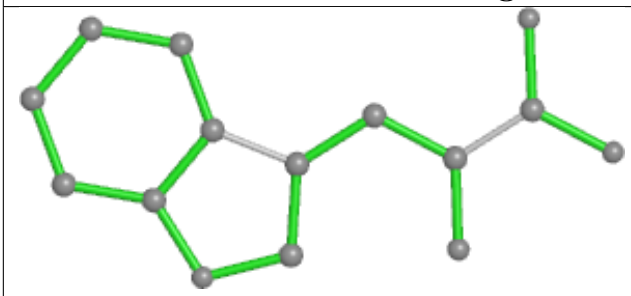


Torsions

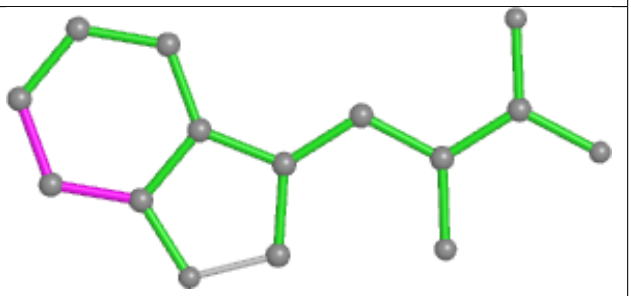


Rings

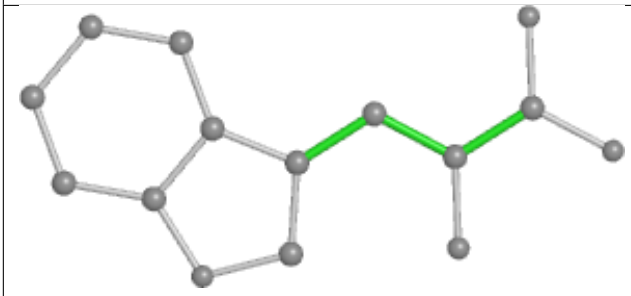
Ligand TRP CCC 502



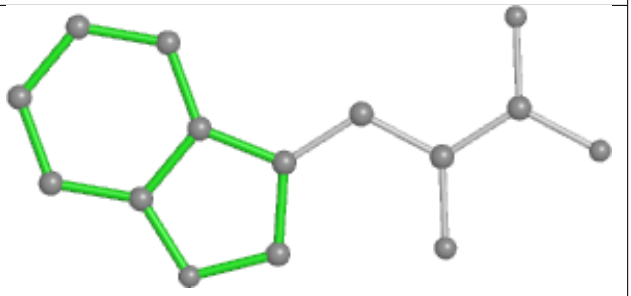
Bond lengths



Bond angles

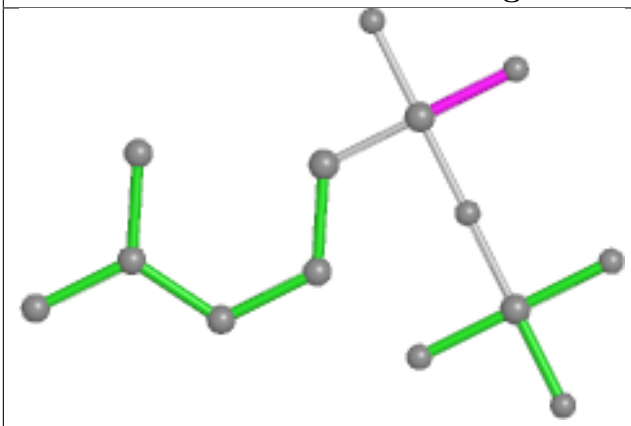


Torsions



Rings

Ligand 6C7 AAA 401



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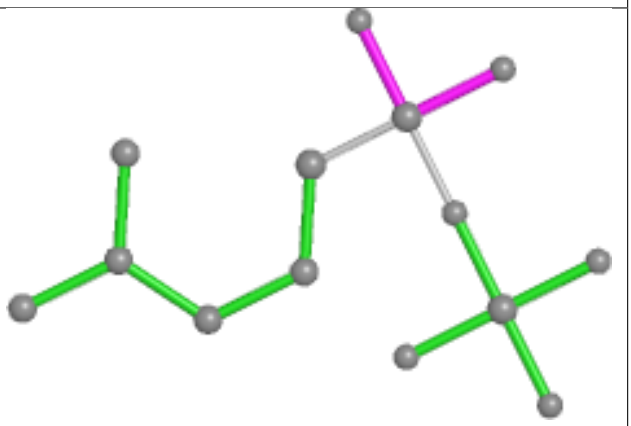

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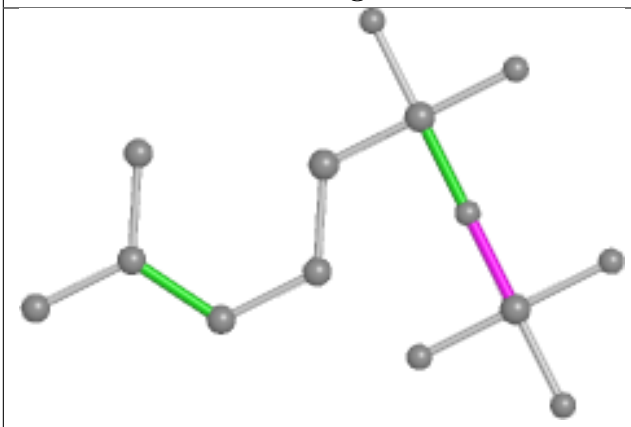
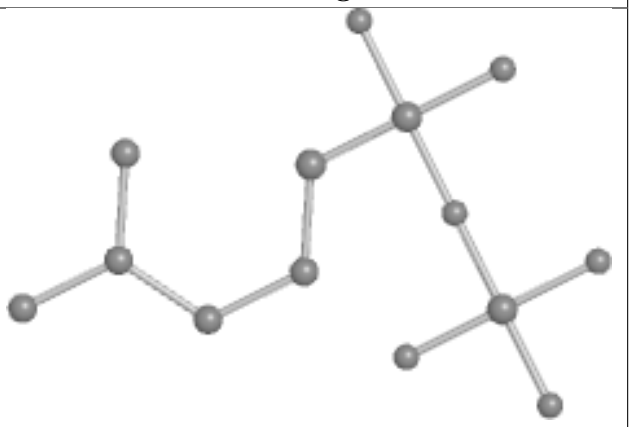
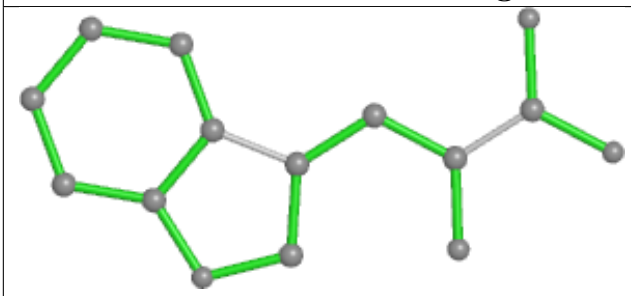


Torsions

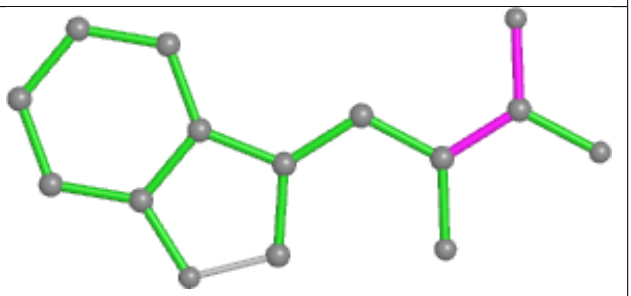


Rings

Ligand TRP AAA 402



Bond lengths



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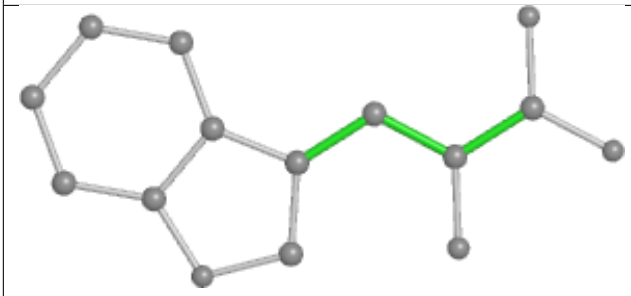

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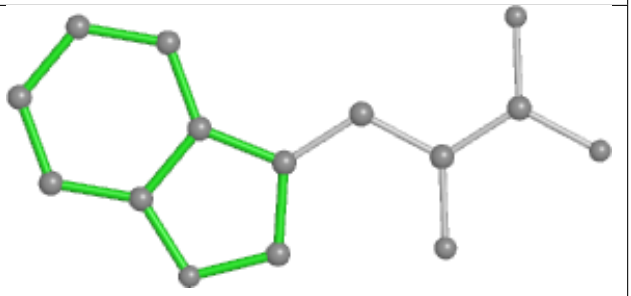
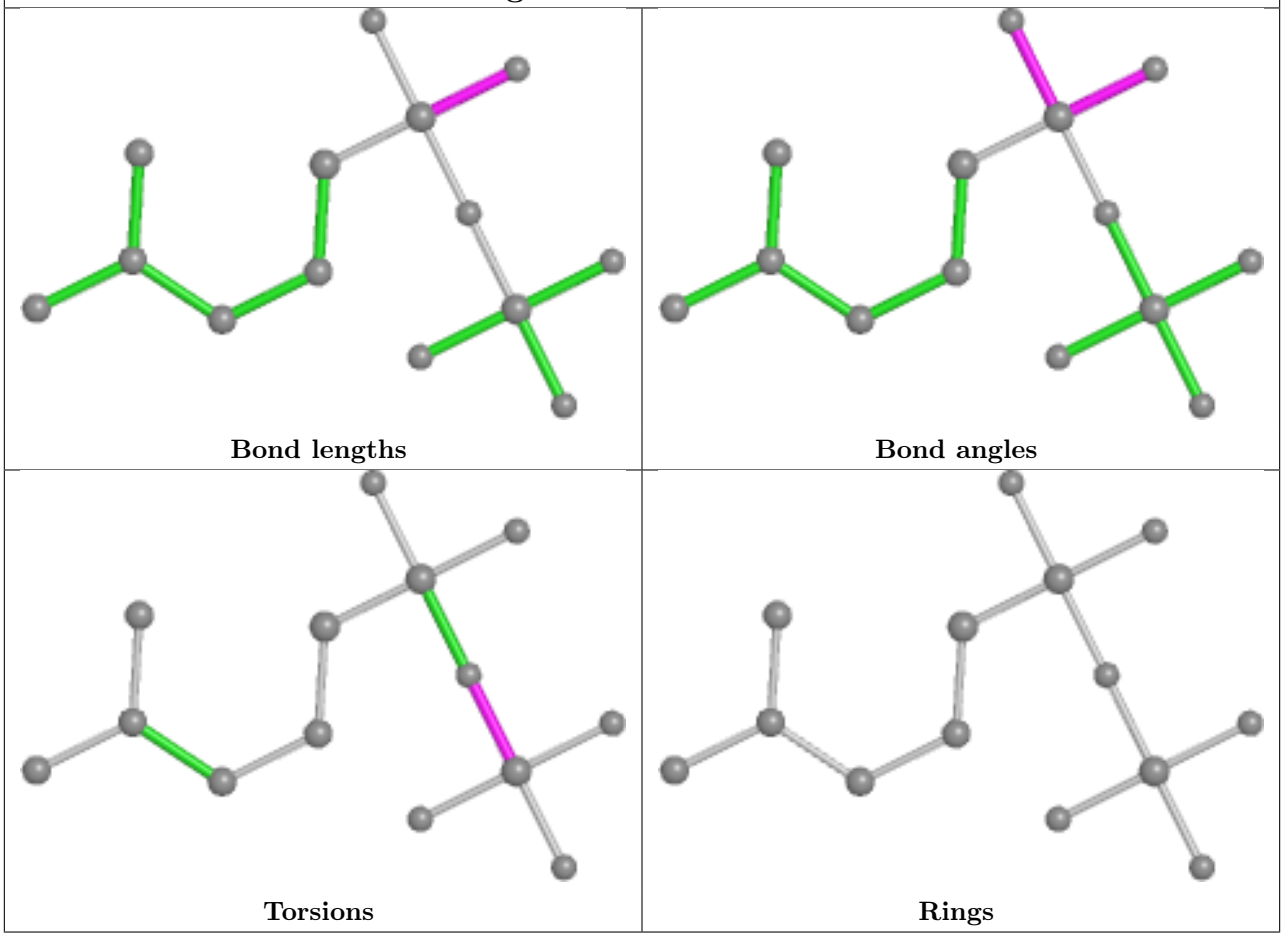


Rings

Ligand 6C7 BBB 501



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	AAA	356/362 (98%)	0.28	23 (6%)	18	21	12, 24, 41, 53	1 (0%)
1	BBB	353/362 (97%)	0.15	13 (3%)	41	46	14, 24, 43, 54	0
1	CCC	360/362 (99%)	0.26	27 (7%)	14	16	12, 24, 44, 55	0
1	DDD	360/362 (99%)	0.18	21 (5%)	23	25	12, 22, 42, 56	0
All	All	1429/1448 (98%)	0.22	84 (5%)	22	24	12, 23, 43, 56	1 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	267	GLY	6.2
1	DDD	45	TYR	6.0
1	AAA	267	GLY	5.6
1	CCC	360	VAL	5.5
1	BBB	187	GLY	5.2
1	BBB	186	PRO	4.2
1	CCC	265	THR	4.1
1	CCC	45	TYR	4.0
1	CCC	176	TYR	3.8
1	AAA	268	ALA	3.8
1	AAA	180	LEU	3.7
1	DDD	123	ASP	3.6
1	DDD	109	SER	3.5
1	BBB	207	GLN	3.4
1	AAA	208[A]	ALA	3.3
1	CCC	304	ASP	3.3
1	BBB	70	ALA	3.3
1	AAA	203[A]	HIS	3.2
1	CCC	269	ASP	3.2
1	AAA	209[A]	ARG	3.2
1	BBB	337	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	DDD	176	TYR	3.2
1	AAA	207[A]	GLN	3.2
1	AAA	186	PRO	3.2
1	CCC	186	PRO	3.2
1	CCC	233	GLY	3.2
1	AAA	176	TYR	3.2
1	CCC	3	GLY	3.1
1	CCC	182	HIS	3.1
1	CCC	268	ALA	3.1
1	DDD	85	PRO	3.0
1	DDD	121	ALA	3.0
1	AAA	272	VAL	3.0
1	BBB	161	ALA	2.9
1	DDD	3	GLY	2.9
1	BBB	45	TYR	2.8
1	BBB	89	LEU	2.8
1	DDD	206	PRO	2.7
1	CCC	121	ALA	2.7
1	CCC	234	VAL	2.7
1	CCC	123	ASP	2.6
1	CCC	250	THR	2.6
1	CCC	264	PHE	2.6
1	AAA	206[A]	PRO	2.6
1	AAA	264	PHE	2.6
1	DDD	269	ASP	2.6
1	AAA	4	LEU	2.6
1	CCC	133[A]	CYS	2.6
1	CCC	109	SER	2.5
1	AAA	187	GLY	2.5
1	CCC	237	ALA	2.5
1	BBB	233	GLY	2.5
1	DDD	205	GLY	2.5
1	AAA	236	VAL	2.5
1	CCC	267	GLY	2.5
1	DDD	234	VAL	2.5
1	AAA	179	LEU	2.4
1	DDD	4	LEU	2.4
1	CCC	184	VAL	2.4
1	DDD	112	ARG	2.4
1	AAA	271	PRO	2.3
1	BBB	123	ASP	2.3
1	AAA	234	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	CCC	272	VAL	2.3
1	AAA	251	ARG	2.3
1	DDD	304	ASP	2.3
1	CCC	359	LEU	2.2
1	CCC	115	SER	2.2
1	CCC	124	ASP	2.2
1	BBB	272	VAL	2.2
1	CCC	179	LEU	2.2
1	AAA	45	TYR	2.1
1	DDD	117	ARG	2.1
1	DDD	268	ALA	2.1
1	DDD	89	LEU	2.1
1	DDD	232	ASP	2.1
1	DDD	187	GLY	2.1
1	DDD	118	ASP	2.1
1	CCC	232	ASP	2.1
1	BBB	121	ALA	2.0
1	AAA	124	ASP	2.0
1	AAA	109	SER	2.0
1	BBB	270	ARG	2.0
1	AAA	111	SER	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
4	PEG	AAA	403	7/7	0.78	0.11	39,40,43,45	0
4	PEG	BBB	503	7/7	0.82	0.12	46,46,47,48	0

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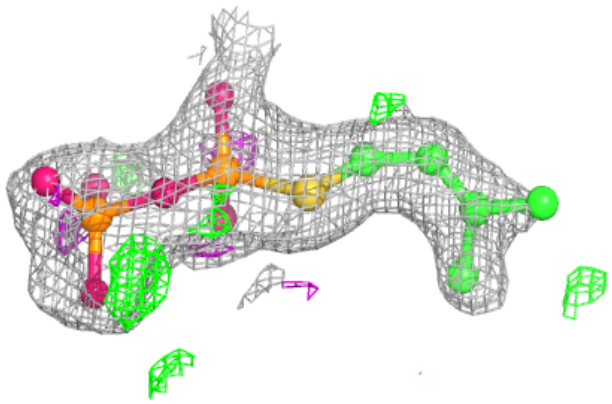
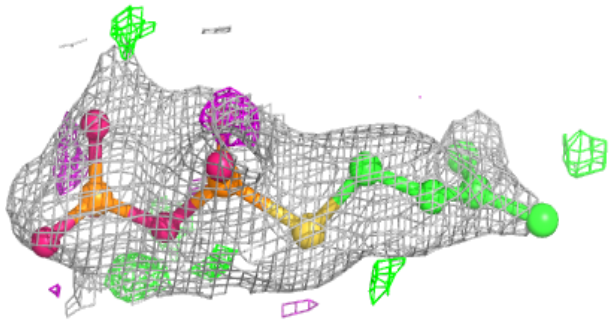
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	BBB	504	4/7	0.82	0.25	41,42,43,44	0
4	PEG	CCC	505	7/7	0.82	0.13	42,43,44,44	0
4	PEG	DDD	504	7/7	0.83	0.14	47,47,49,49	0
4	PEG	CCC	503	7/7	0.84	0.12	28,34,36,37	0
4	PEG	CCC	504	7/7	0.84	0.11	49,49,50,53	0
2	6C7	BBB	501	14/14	0.89	0.14	40,44,49,51	0
4	PEG	AAA	404	7/7	0.92	0.07	26,31,35,36	0
2	6C7	AAA	401	14/14	0.93	0.11	32,37,40,41	0
3	TRP	BBB	502	15/15	0.95	0.08	16,16,17,17	0
5	NA	DDD	503	1/1	0.95	0.09	26,26,26,26	0
3	TRP	AAA	402	15/15	0.96	0.07	15,15,16,16	0
3	TRP	CCC	502	15/15	0.96	0.08	14,14,15,16	0
3	TRP	DDD	502	15/15	0.96	0.09	13,13,14,14	0
2	6C7	DDD	501	14/14	0.97	0.07	22,24,27,28	0
2	6C7	CCC	501	14/14	0.97	0.08	24,25,31,32	0

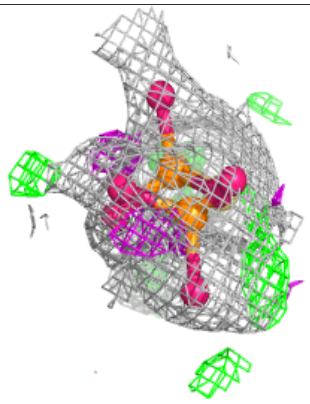
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6C7 BBB 501:

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

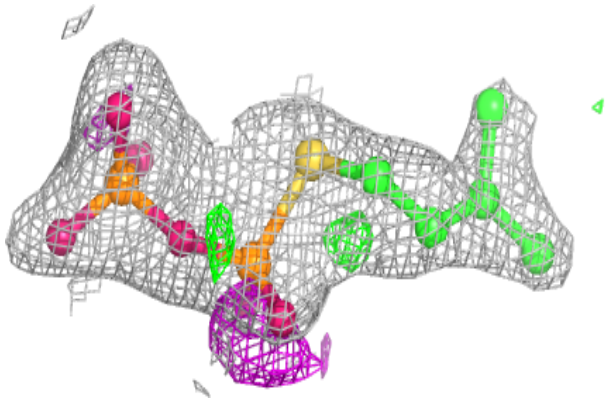


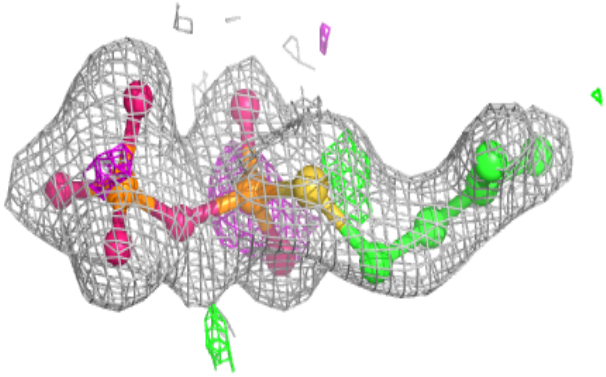


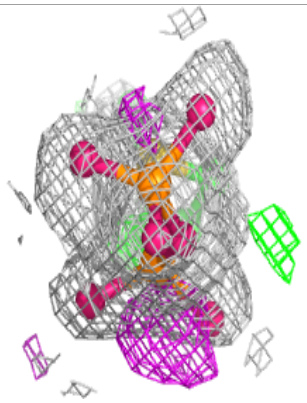


Electron density around 6C7 AAA 401:

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

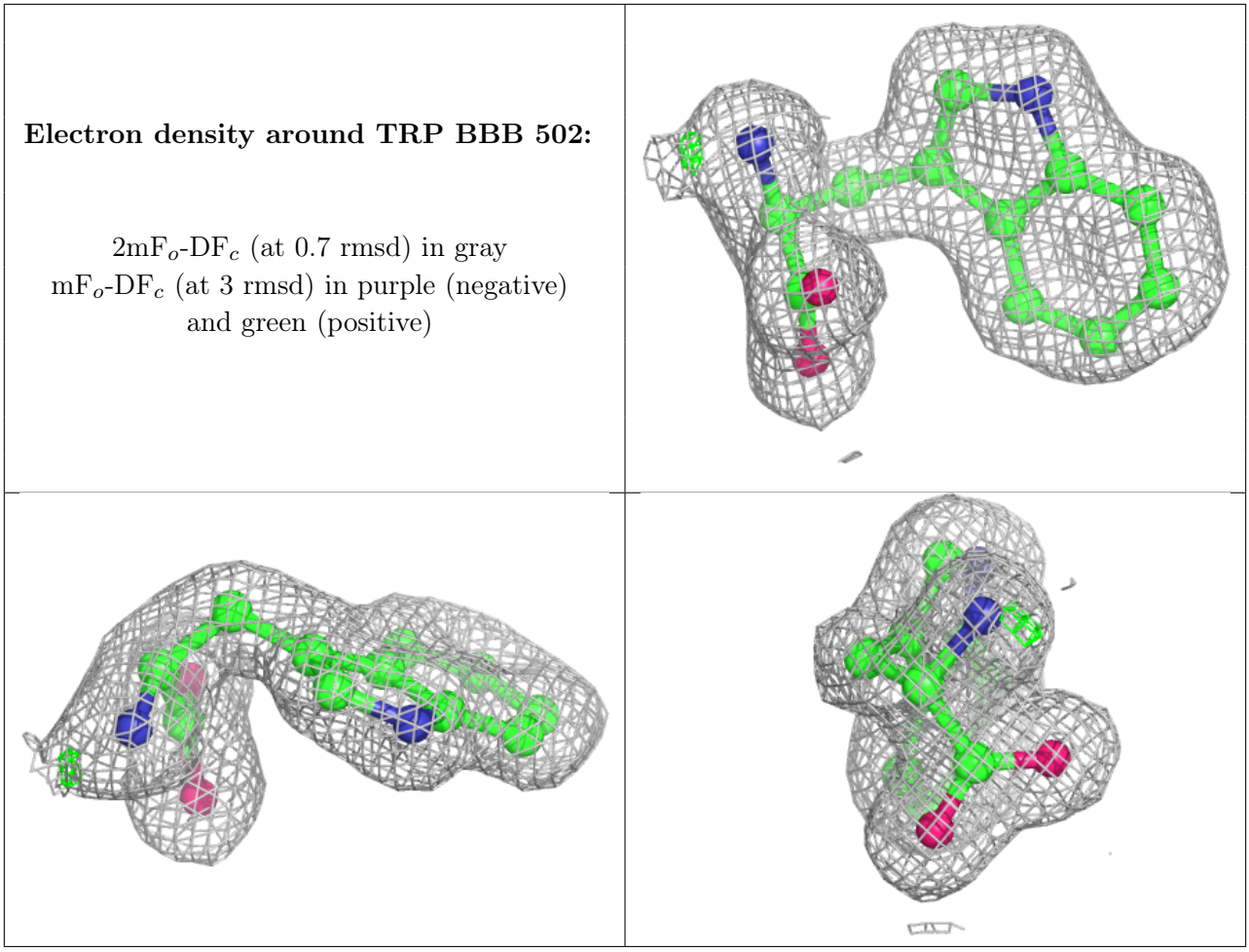






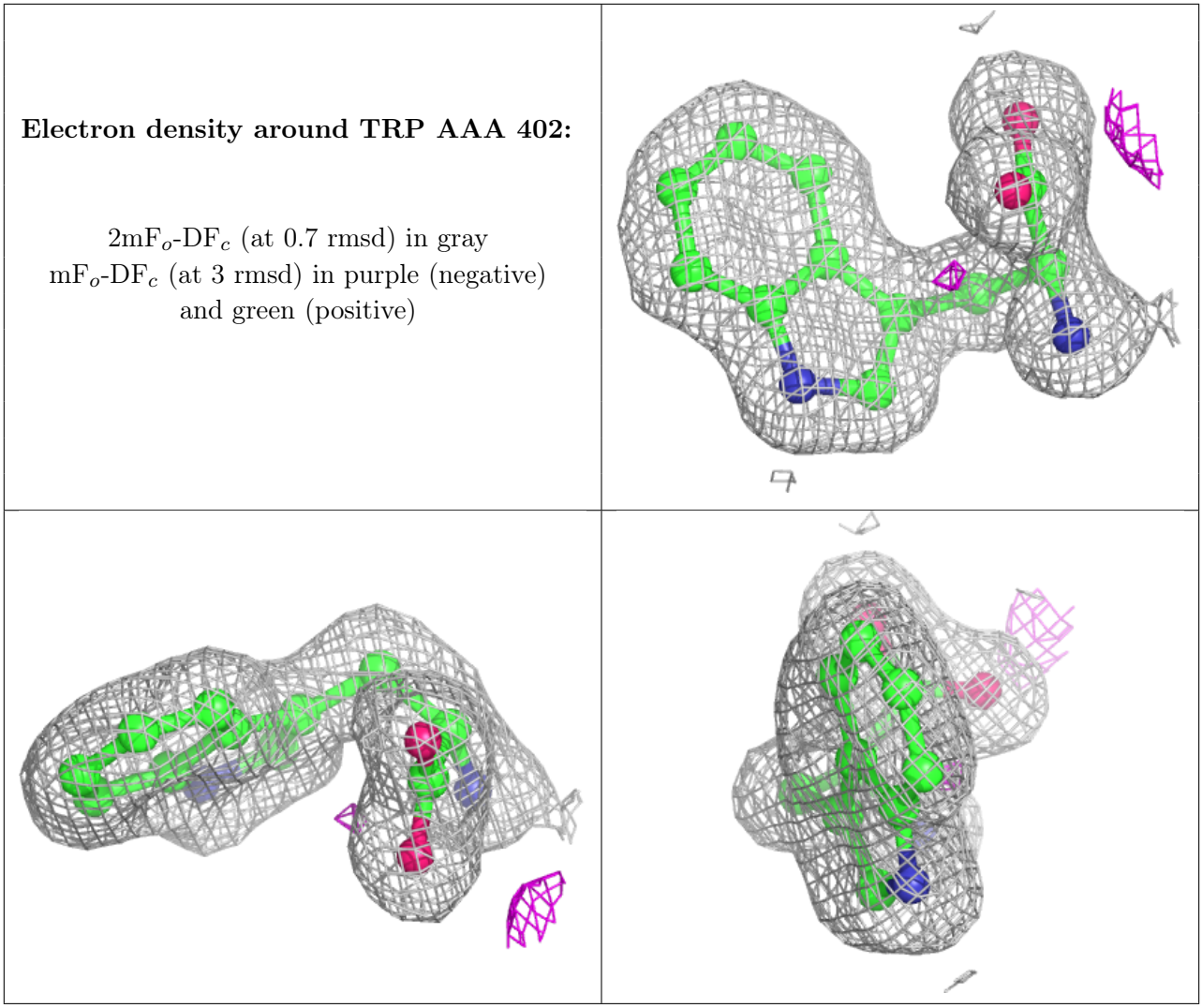
Electron density around TRP BBB 502:

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



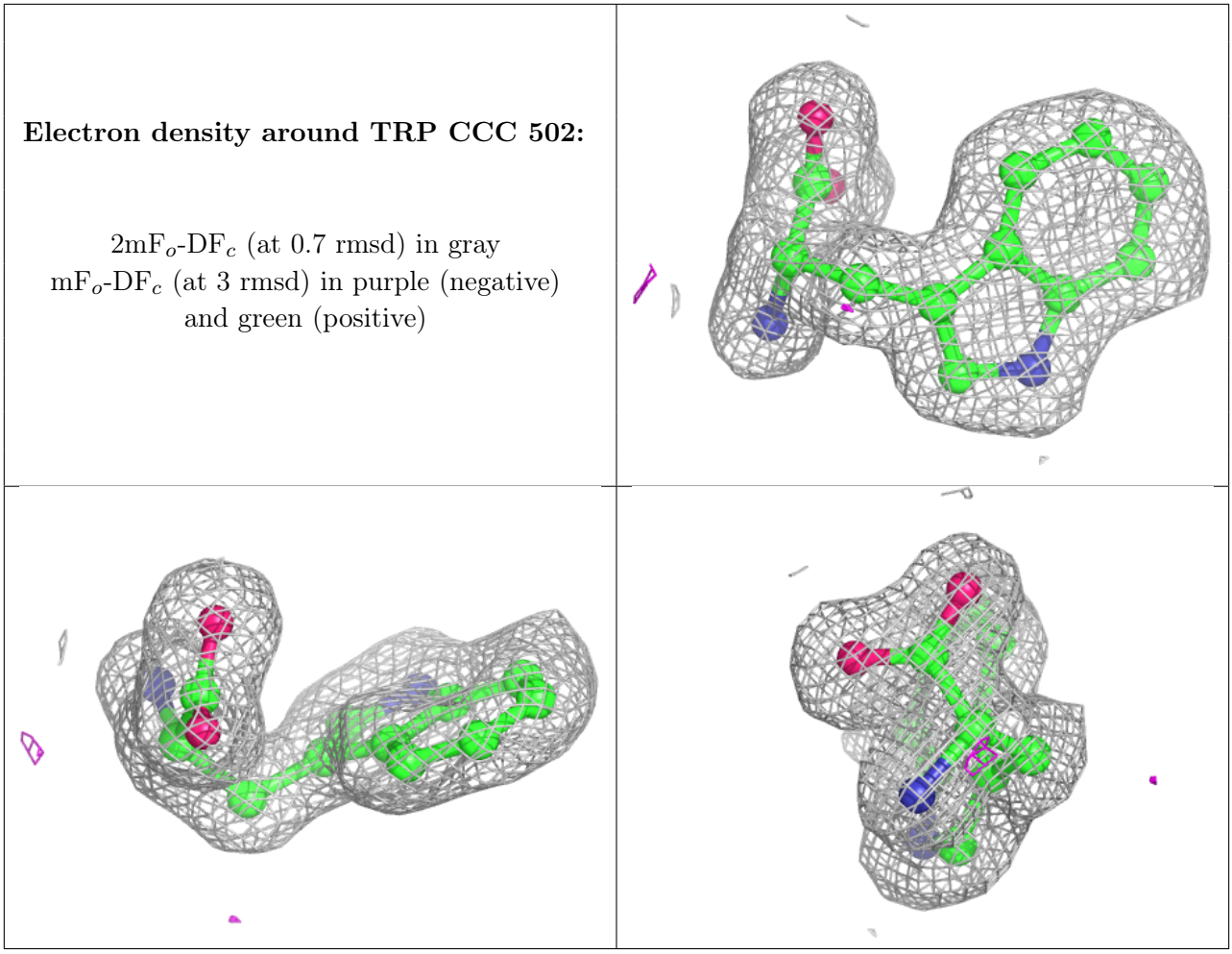
Electron density around TRP AAA 402:

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



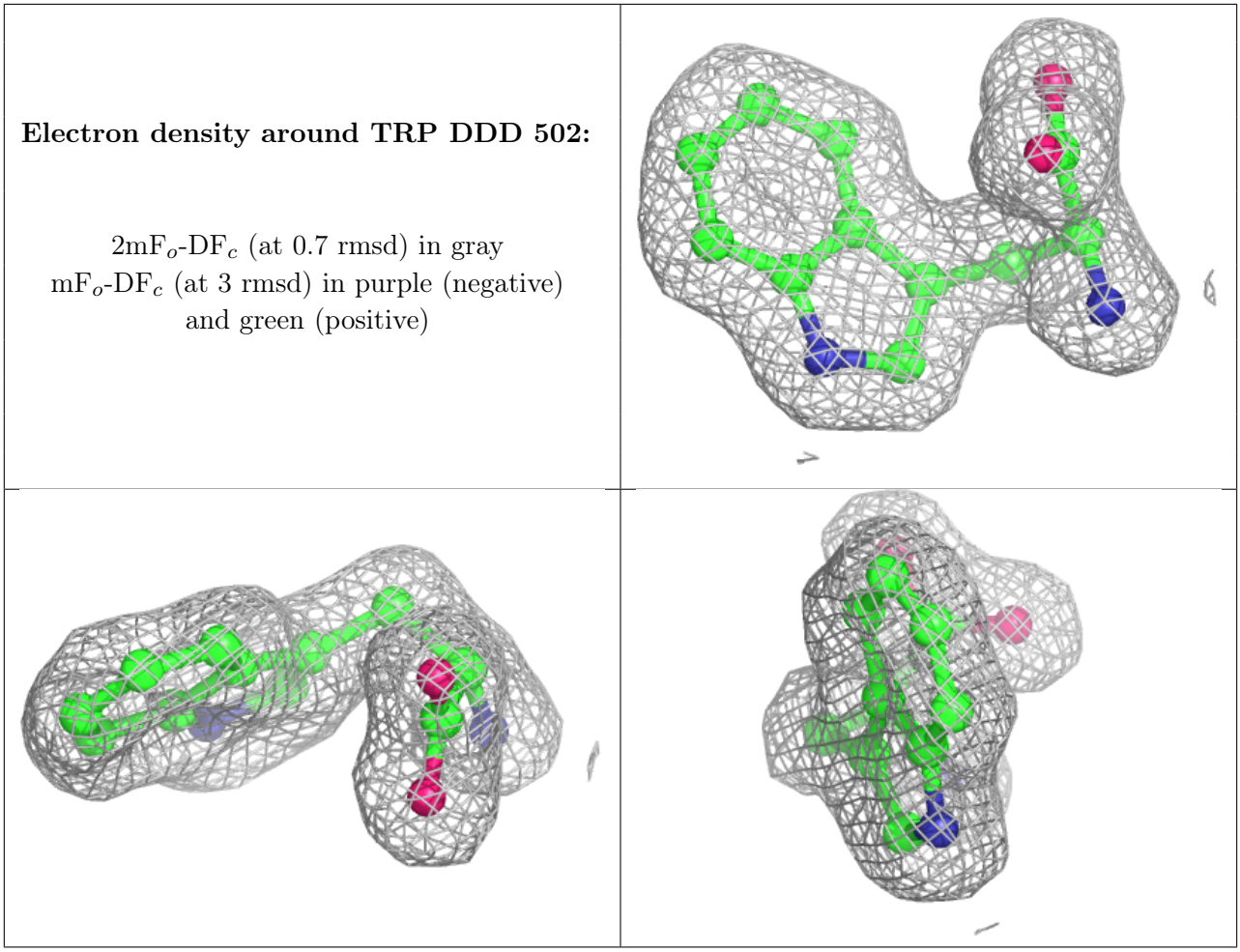
Electron density around TRP CCC 502:

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



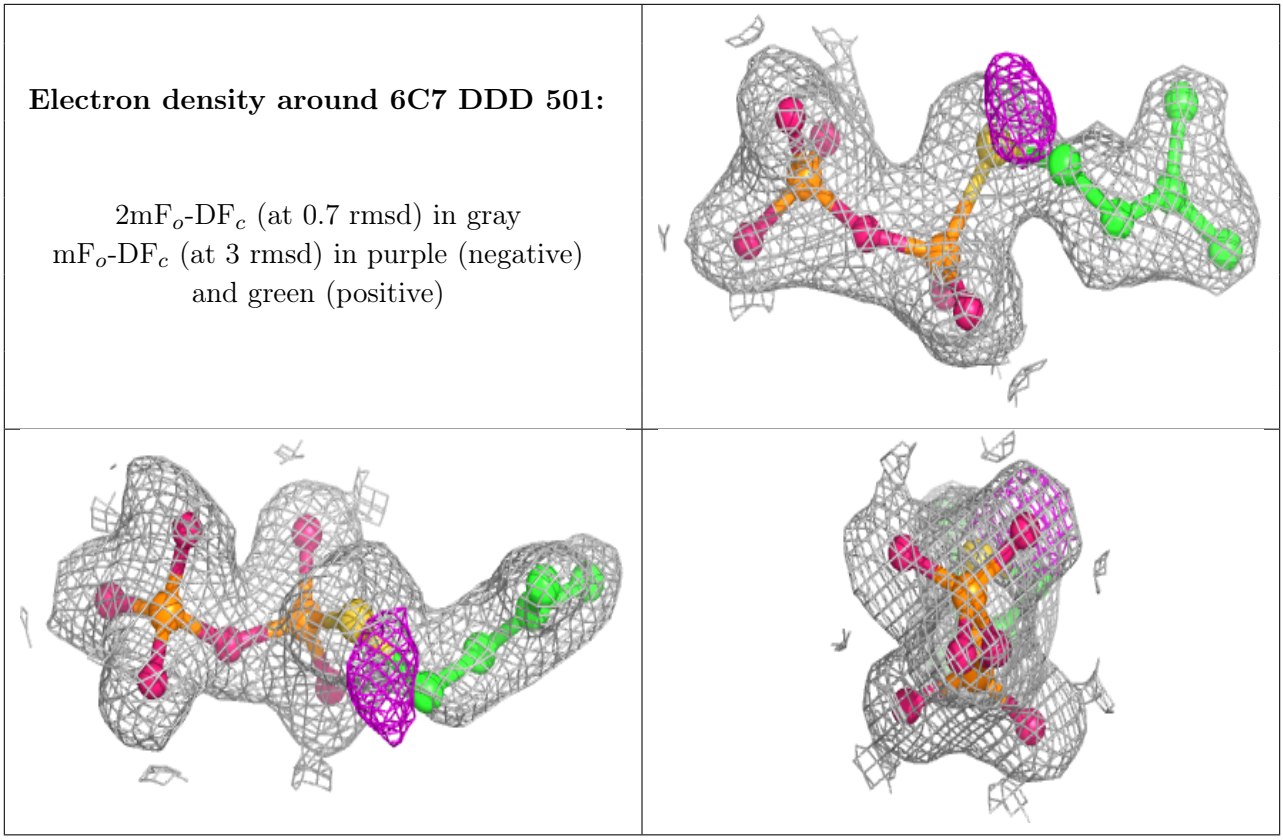
Electron density around TRP DDD 502:

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



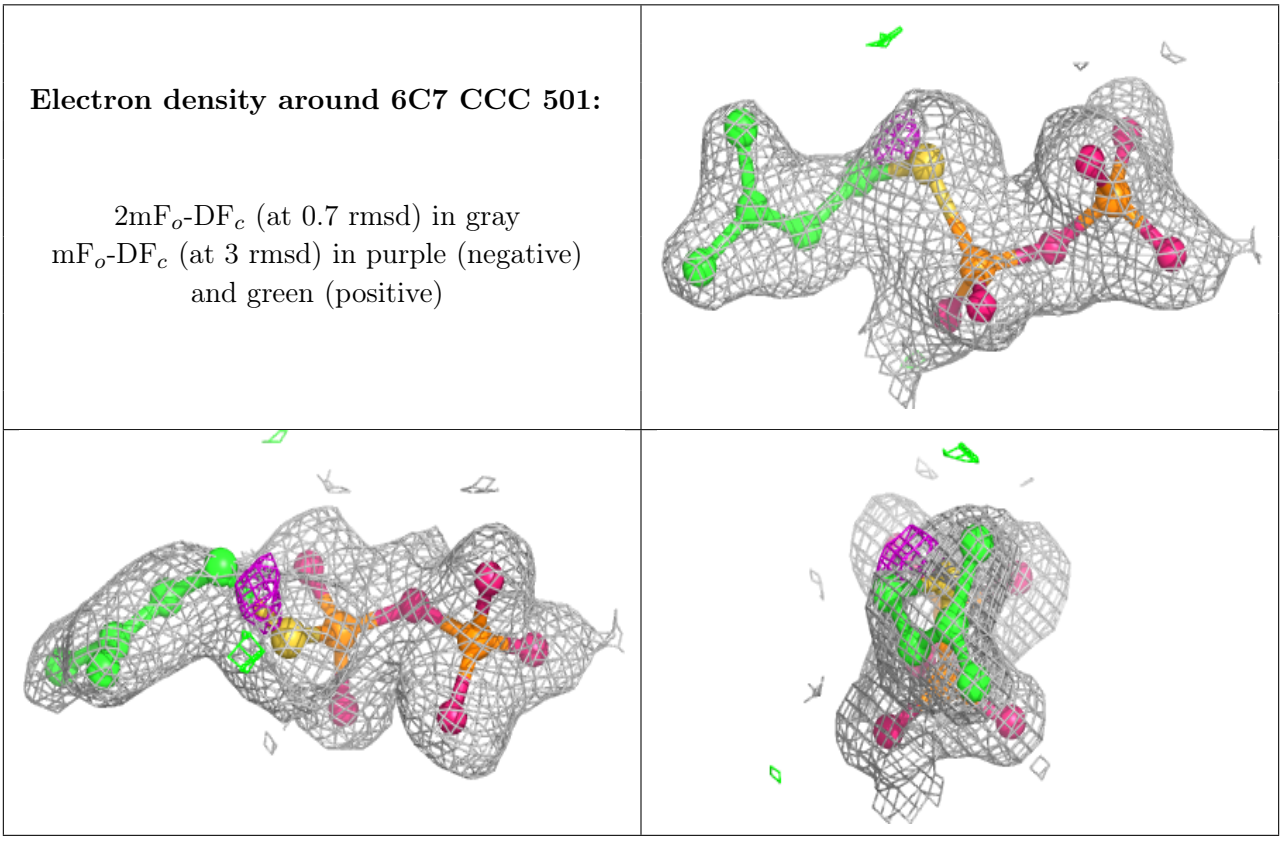
Electron density around 6C7 DDD 501:

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



Electron density around 6C7 CCC 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.