Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2026 – 10:14 AM EST

PDB ID	:	6UB9 / pdb_00006ub9
Title	:	Crystal structure of tryptophan synthase from M. tuberculosis - AMINOACRYLATE- AND BRD6309-BOUND FORM
Authors	:	Chang, C.; Michalska, K.; Maltseva, N.I.; Jedrzejczak, R.; McCarren, P.; Nag, P.P.; Joachimiak, A.; Satchell, K.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2019-09-11
Resolution	:	2.78 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 (i) 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 (1)) were used in the production of this report:

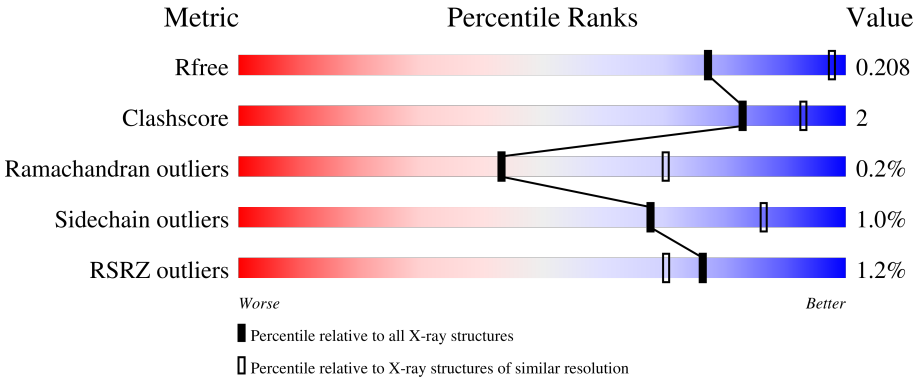
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.78 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	276	86% 5% 10%
1	C	276	85% 5% 10%
1	E	276	2% 81% 8% 11%
1	G	276	84% 6% 10%
2	B	410	90% 9%

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Mol	Chain	Length	Quality of chain
2	D	410	92% 5%
2	F	410	% 91% 6%
2	H	410	% 90% 7%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 19666 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	249	Total	C	N	O	S	0	0	0
			1803	1131	323	344	5			
1	C	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	E	247	Total	C	N	O	S	0	0	0
			1778	1117	318	338	5			
1	G	248	Total	C	N	O	S	0	1	0
			1805	1132	326	342	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	expression tag	UNP P9WFY1
A	272	HIS	-	expression tag	UNP P9WFY1
A	273	HIS	-	expression tag	UNP P9WFY1
A	274	HIS	-	expression tag	UNP P9WFY1
A	275	HIS	-	expression tag	UNP P9WFY1
A	276	HIS	-	expression tag	UNP P9WFY1
C	271	HIS	-	expression tag	UNP P9WFY1
C	272	HIS	-	expression tag	UNP P9WFY1
C	273	HIS	-	expression tag	UNP P9WFY1
C	274	HIS	-	expression tag	UNP P9WFY1
C	275	HIS	-	expression tag	UNP P9WFY1
C	276	HIS	-	expression tag	UNP P9WFY1
E	271	HIS	-	expression tag	UNP P9WFY1
E	272	HIS	-	expression tag	UNP P9WFY1
E	273	HIS	-	expression tag	UNP P9WFY1
E	274	HIS	-	expression tag	UNP P9WFY1
E	275	HIS	-	expression tag	UNP P9WFY1
E	276	HIS	-	expression tag	UNP P9WFY1
G	271	HIS	-	expression tag	UNP P9WFY1
G	272	HIS	-	expression tag	UNP P9WFY1
G	273	HIS	-	expression tag	UNP P9WFY1

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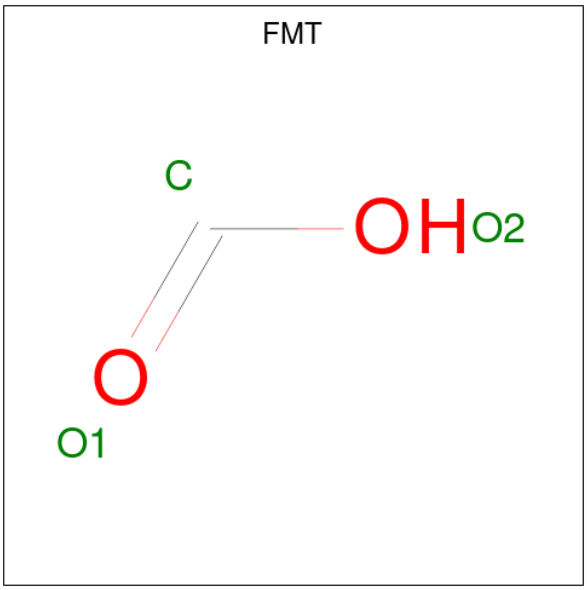
Chain	Residue	Modelled	Actual	Comment	Reference
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	276	HIS	-	expression tag	UNP P9WFY1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	2	0
			3015	1883	546	572	14			
2	D	399	Total	C	N	O	S	0	2	0
			2992	1868	544	567	13			
2	F	400	Total	C	N	O	S	0	2	0
			2996	1870	544	569	13			
2	H	403	Total	C	N	O	S	0	2	0
			3018	1886	545	573	14			

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

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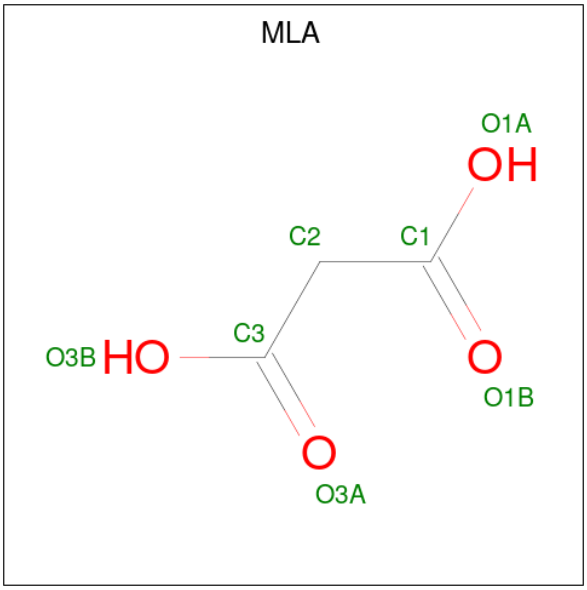
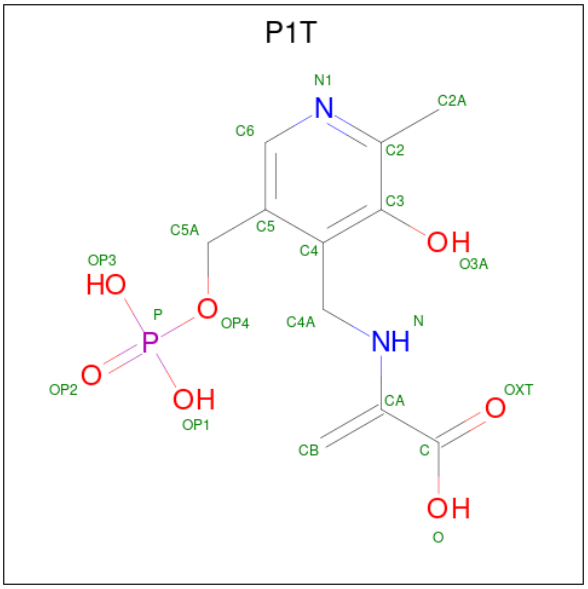
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0

- Molecule 4 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



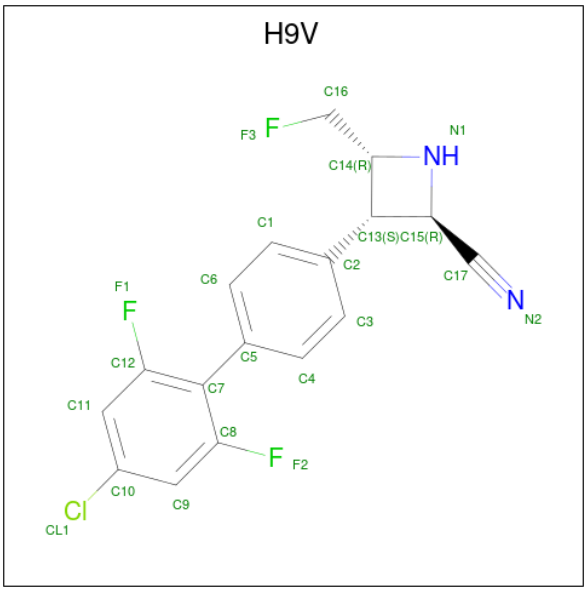
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	E	1	Total C O 7 3 4	0	0
4	F	1	Total C O 7 3 4	0	0
4	G	1	Total C O 7 3 4	0	0

- Molecule 5 is 2-[({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN -4-YL}METHYL)AMINO]ACRYLIC ACID (CCD ID: P1T) (formula: $C_{11}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O P 21 11 2 7 1	0	0
5	D	1	Total C N O P 21 11 2 7 1	0	0
5	F	1	Total C N O P 21 11 2 7 1	0	0
5	H	1	Total C N O P 21 11 2 7 1	0	0

- Molecule 6 is (2R,3S,4R)-3-(4'-chloro-2',6'-difluoro[1,1'-biphenyl]-4-yl)-4-(fluoromethyl)azetidine-2-carbonitrile (CCD ID: H9V) (formula: $C_{17}H_{12}ClF_3N_2$) (labeled as "Ligand of Interest" by depositor).

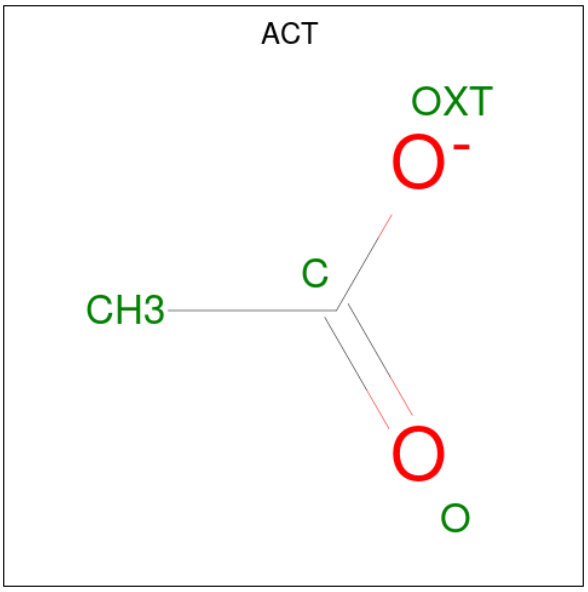


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C Cl F N 23 17 1 3 2	0	0
6	D	1	Total C Cl F N 23 17 1 3 2	0	0
6	F	1	Total C Cl F N 23 17 1 3 2	0	0
6	H	1	Total C Cl F N 23 17 1 3 2	0	0

- Molecule 7 is CESIUM ION (CCD ID: CS) (formula: Cs).

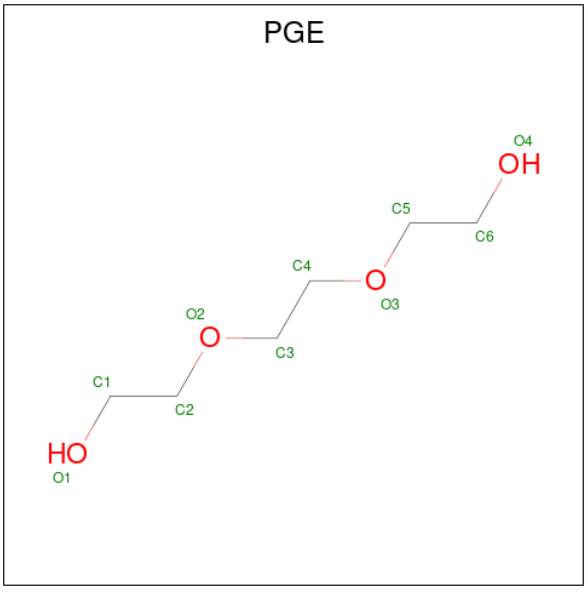
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cs 1 1	0	0
7	D	1	Total Cs 1 1	0	0
7	F	1	Total Cs 1 1	0	0
7	H	1	Total Cs 1 1	0	0

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



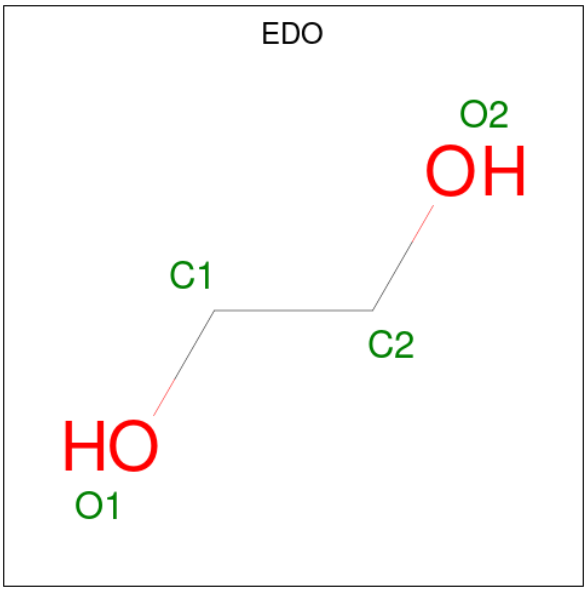
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 10 6 4	0	0
9	F	1	Total C O 10 6 4	0	0

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is water.

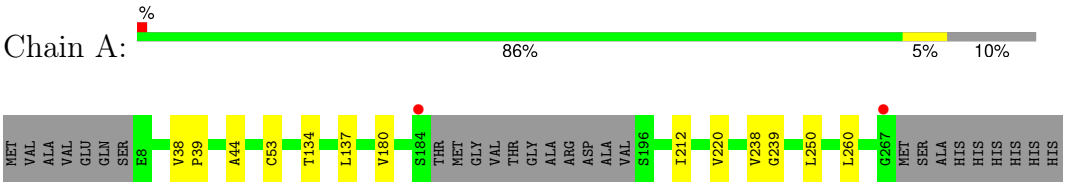
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	8	Total O 8 8	0	0
11	B	40	Total O 40 40	0	0
11	C	6	Total O 6 6	0	0
11	D	40	Total O 40 40	0	0
11	E	2	Total O 2 2	0	0
11	F	25	Total O 25 25	0	0
11	G	11	Total O 11 11	0	0
11	H	40	Total O 40 40	0	0

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.

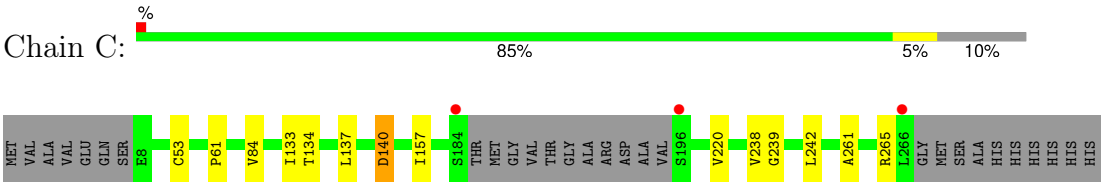
• Molecule 1: Tryptophan synthase alpha chain

Chain A:



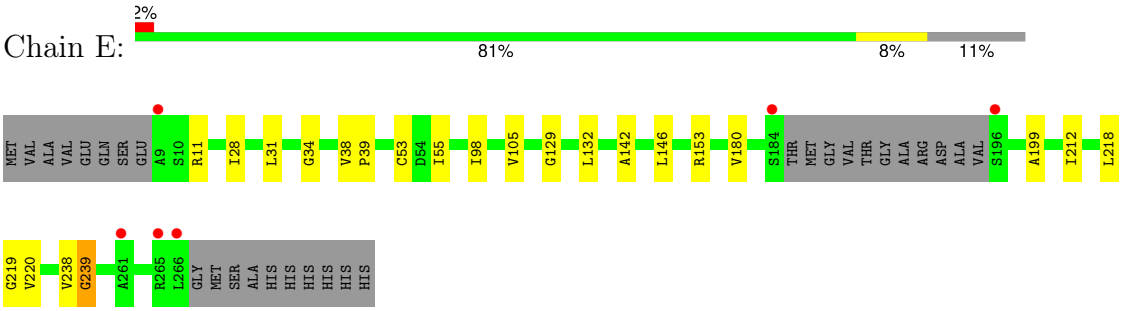
• Molecule 1: Tryptophan synthase alpha chain

Chain C:



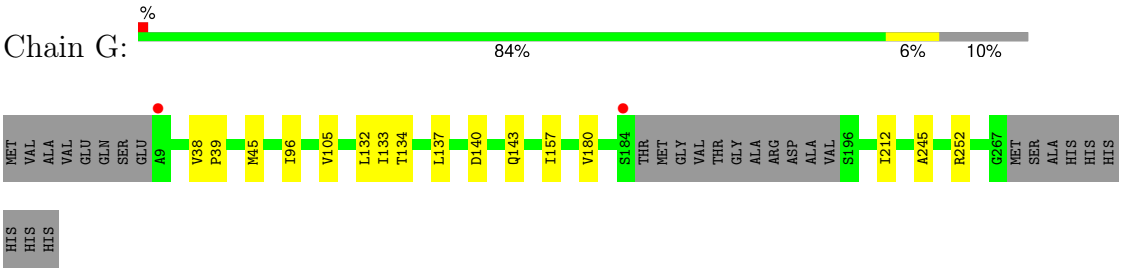
• Molecule 1: Tryptophan synthase alpha chain

Chain E:



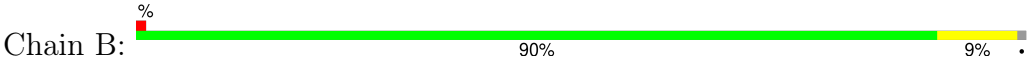
• Molecule 1: Tryptophan synthase alpha chain

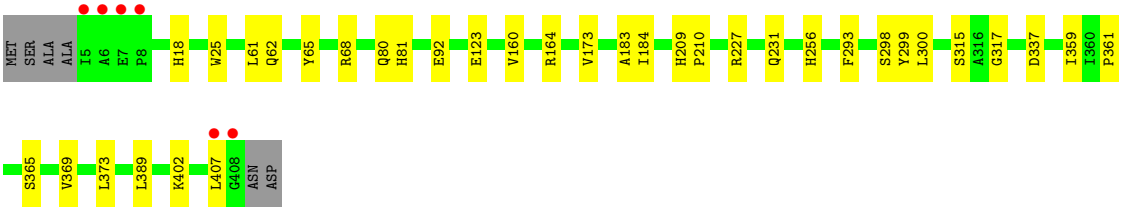
Chain G:



• Molecule 2: Tryptophan synthase beta chain

Chain B:





• Molecule 2: Tryptophan synthase beta chain

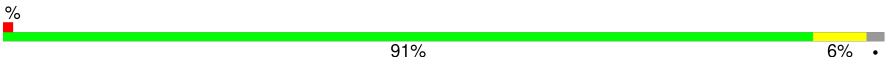
Chain D:

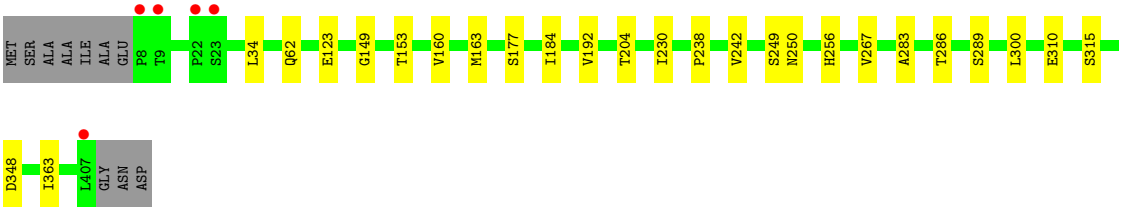




• Molecule 2: Tryptophan synthase beta chain

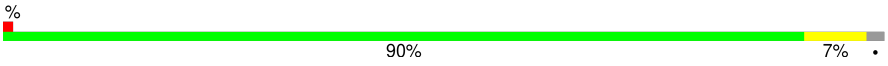
Chain F:

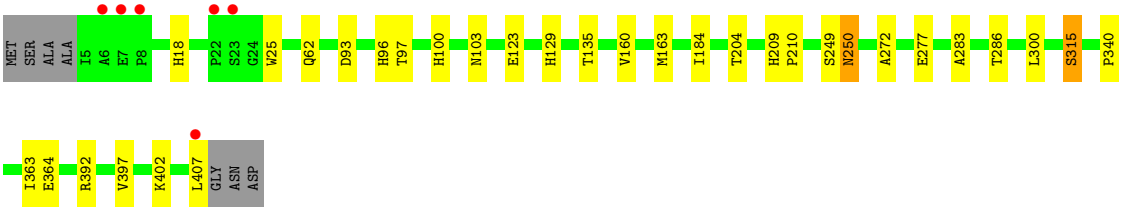




• Molecule 2: Tryptophan synthase beta chain

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.37Å 159.62Å 164.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.78 29.89 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.6 (29.89-2.78) 93.5 (29.89-2.78)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.169 , 0.210 0.173 , 0.208	Depositor DCC
R_{free} test set	1677 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 25.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19666	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, FMT, MLA, EDO, CS, ACT, P1T, H9V

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	0.13	0/1832	0.31	0/2500
1	C	0.12	0/1828	0.31	0/2495
1	E	0.11	0/1807	0.30	0/2468
1	G	0.13	0/1834	0.33	0/2502
2	B	0.14	0/3076	0.34	0/4169
2	D	0.14	0/3052	0.33	0/4135
2	F	0.14	0/3056	0.34	0/4141
2	H	0.14	0/3079	0.33	0/4173
All	All	0.13	0/19564	0.33	0/26583

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	A	1803	0	1822	6	0
1	C	1799	0	1819	7	0
1	E	1778	0	1791	12	0
1	G	1805	0	1828	8	0
2	B	3015	0	2929	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2992	0	2914	11	0
2	F	2996	0	2912	11	0
2	H	3018	0	2939	16	0
3	A	6	0	2	0	0
3	B	15	0	4	0	0
3	C	3	0	1	0	0
3	E	3	0	1	0	0
3	F	6	0	2	0	0
3	H	12	0	4	0	0
4	A	7	0	2	0	0
4	C	7	0	2	0	0
4	E	7	0	2	2	0
4	F	7	0	2	0	0
4	G	7	0	2	0	0
5	B	21	0	11	1	0
5	D	21	0	11	0	0
5	F	21	0	11	1	0
5	H	21	0	11	0	0
6	B	23	0	0	0	0
6	D	23	0	0	0	0
6	F	23	0	0	0	0
6	H	23	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
8	B	4	0	3	0	0
9	D	10	0	14	0	0
9	F	10	0	14	0	0
10	H	4	0	6	0	0
11	A	8	0	0	0	0
11	B	40	0	0	1	0
11	C	6	0	0	0	0
11	D	40	0	0	1	0
11	E	2	0	0	0	0
11	F	25	0	0	1	0
11	G	11	0	0	0	0
11	H	40	0	0	0	0
All	All	19666	0	19059	92	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 (92) 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:123:GLU:HG3	2:B:184:ILE:HG12	1.62	0.81
2:H:62[B]:GLN:HE22	2:H:103:ASN:HA	1.51	0.74
2:B:62[B]:GLN:HE21	2:B:68:ARG:HG3	1.59	0.66
2:B:402:LYS:HG2	2:B:407:LEU:HD12	1.80	0.64
2:D:62[B]:GLN:HE22	2:D:103:ASN:HA	1.61	0.64
1:E:219:GLY:H	4:E:502:MLA:HC21	1.62	0.64
2:F:62:GLN:NE2	11:F:602:HOH:O	2.32	0.62
1:A:134:THR:HB	1:A:137:LEU:HB3	1.82	0.61
2:B:62[A]:GLN:NE2	11:B:601:HOH:O	2.34	0.59
2:H:402:LYS:HG3	2:H:407:LEU:HD11	1.85	0.57
2:H:123:GLU:HG3	2:H:184:ILE:HG12	1.86	0.56
2:F:242:VAL:HG12	2:F:267:VAL:HB	1.89	0.55
2:D:230:ILE:HG21	2:D:238:PRO:HD3	1.89	0.53
2:D:311:SER:O	11:D:601:HOH:O	2.18	0.53
2:D:160:VAL:HA	2:D:163:MET:HE3	1.91	0.53
1:E:11:ARG:NH1	1:E:153:ARG:O	2.42	0.53
1:C:220:VAL:HB	1:C:238:VAL:HG22	1.91	0.53
2:D:242:VAL:HG12	2:D:267:VAL:HB	1.89	0.52
2:F:283:ALA:HB1	2:F:286:THR:HB	1.91	0.52
1:E:220:VAL:HB	1:E:238:VAL:HG22	1.92	0.52
2:F:123:GLU:HG3	2:F:184:ILE:HG12	1.92	0.52
2:H:283:ALA:HB1	2:H:286:THR:HB	1.92	0.51
2:D:123:GLU:HG3	2:D:184:ILE:HG12	1.93	0.51
1:E:180:VAL:HG23	1:E:212:ILE:HD13	1.93	0.51
1:G:140:ASP:O	1:G:143:GLN:NE2	2.44	0.51
2:B:62[B]:GLN:NE2	2:B:68:ARG:HG3	2.26	0.50
2:F:160:VAL:HA	2:F:163:MET:HE3	1.94	0.49
2:B:68:ARG:NH1	2:B:92:GLU:OE1	2.35	0.49
2:H:160:VAL:HA	2:H:163:MET:HE3	1.93	0.49
1:C:261:ALA:O	1:C:265:ARG:NH1	2.46	0.48
2:H:123:GLU:O	2:H:129:HIS:HD2	1.97	0.48
2:B:209:HIS:ND1	2:B:210:PRO:HA	2.28	0.48
2:D:74:GLU:HB2	2:D:88:PHE:CE2	2.49	0.48
1:A:180:VAL:HG23	1:A:212:ILE:HD13	1.95	0.47
1:C:140:ASP:OD1	1:C:140:ASP:N	2.48	0.47
2:D:129:HIS:CE1	2:D:203:GLY:HA2	2.50	0.47
1:G:133:ILE:HG12	1:G:157:ILE:HB	1.96	0.47
1:E:28:ILE:HG12	1:E:55:ILE:HB	1.97	0.47
2:B:80:GLN:HG3	2:B:81:HIS:ND1	2.30	0.46
2:D:209:HIS:ND1	2:D:210:PRO:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:THR:HB	1:G:137:LEU:HB3	1.98	0.46
1:C:61:PRO:HG2	1:C:84:VAL:HG11	1.97	0.45
1:A:238:VAL:HG21	1:A:260:LEU:HD13	1.99	0.45
2:H:204:THR:HA	2:H:249:SER:HB3	1.98	0.45
1:E:142:ALA:O	1:E:146:LEU:HG	2.16	0.45
1:E:105:VAL:HB	1:E:132:LEU:HD12	1.99	0.44
1:A:38:VAL:HB	1:A:39:PRO:HD3	2.00	0.44
1:C:134:THR:HB	1:C:137:LEU:HB3	2.00	0.44
2:F:230:ILE:HG21	2:F:238:PRO:HD3	1.99	0.44
2:H:272:ALA:HB2	2:H:340:PRO:HB2	2.00	0.44
1:A:44:ALA:HA	1:A:250:LEU:HD21	1.99	0.44
2:F:177:SER:HB3	2:F:310:GLU:CD	2.42	0.44
2:H:315:SER:HB2	2:H:363:ILE:HG22	1.98	0.44
1:E:239:GLY:N	4:E:502:MLA:O1B	2.50	0.44
1:G:245:ALA:HB1	1:G:252:ARG:HG3	2.01	0.43
2:B:18:HIS:HA	2:B:25:TRP:O	2.19	0.43
2:H:209:HIS:ND1	2:H:210:PRO:HA	2.32	0.43
1:G:180:VAL:HG23	1:G:212:ILE:HD13	2.00	0.43
2:H:93:ASP:HB2	2:H:392:ARG:HB3	1.99	0.43
2:F:204:THR:HA	2:F:249:SER:HB3	2.01	0.43
2:F:315:SER:HB2	2:F:363:ILE:HG22	1.99	0.43
2:B:298:SER:OG	2:B:299:TYR:N	2.51	0.42
1:E:38:VAL:HB	1:E:39:PRO:HD3	2.00	0.42
2:B:173:VAL:HG21	2:B:183:ALA:HA	2.00	0.42
2:B:61:LEU:O	2:B:65:TYR:HB3	2.19	0.42
2:B:293:PHE:HB2	2:B:300:LEU:HD13	2.00	0.42
1:G:38:VAL:HB	1:G:39:PRO:HD3	2.00	0.42
2:D:113:ARG:HD3	2:D:113:ARG:HA	1.82	0.42
1:G:105:VAL:HB	1:G:132:LEU:HD12	2.01	0.42
2:B:369:VAL:O	2:B:373:LEU:HG	2.20	0.42
1:G:45:MET:HB3	1:G:96:ILE:HD11	2.01	0.42
2:H:277:GLU:H	2:H:277:GLU:CD	2.28	0.42
2:B:365:SER:HB3	2:B:389:LEU:HD12	2.02	0.42
2:D:207:GLY:HA2	2:D:294:HIS:O	2.20	0.42
1:E:31:LEU:HD23	1:E:31:LEU:HA	1.94	0.41
1:A:220:VAL:HB	1:A:238:VAL:HG22	2.02	0.41
2:H:315:SER:OG	2:H:364:GLU:HG3	2.20	0.41
2:B:160:VAL:O	2:B:164:ARG:HG3	2.19	0.41
1:C:238:VAL:HG12	1:C:242:LEU:HG	2.02	0.41
1:E:199:ALA:HB2	1:E:218:LEU:HD21	2.03	0.41
2:H:96:HIS:O	2:H:97:THR:OG1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:GLY:CA	5:B:501:P1T:H4A1	2.51	0.40
1:E:34:GLY:HA2	1:E:38:VAL:HA	2.01	0.40
2:H:100:HIS:NE2	2:H:250:ASN:HB3	2.36	0.40
2:B:227:ARG:O	2:B:231:GLN:HG3	2.21	0.40
2:B:361:PRO:HB3	2:B:389:LEU:HD11	2.03	0.40
1:C:133:ILE:HG12	1:C:157:ILE:HB	2.03	0.40
5:F:501:P1T:O3A	5:F:501:P1T:N	2.54	0.40
2:F:34:LEU:HG	2:F:192:VAL:HG22	2.04	0.40
2:B:359:ILE:HG21	2:B:389:LEU:HD21	2.01	0.40
2:F:149:GLY:O	2:F:153:THR:HG23	2.22	0.40
2:H:18:HIS:HA	2:H:25:TRP:O	2.21	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	245/276 (89%)	242 (99%)	2 (1%)	1 (0%)	30	57
1	C	244/276 (88%)	238 (98%)	5 (2%)	1 (0%)	30	57
1	E	243/276 (88%)	234 (96%)	7 (3%)	2 (1%)	16	40
1	G	245/276 (89%)	240 (98%)	5 (2%)	0	100	100
2	B	404/410 (98%)	395 (98%)	9 (2%)	0	100	100
2	D	399/410 (97%)	388 (97%)	11 (3%)	0	100	100
2	F	400/410 (98%)	386 (96%)	14 (4%)	0	100	100
2	H	403/410 (98%)	391 (97%)	12 (3%)	0	100	100
All	All	2583/2744 (94%)	2514 (97%)	65 (2%)	4 (0%)	43	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	129	GLY
1	C	239	GLY
1	E	239	GLY
1	A	239	GLY

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	179/200 (90%)	178 (99%)	1 (1%)	78	91
1	C	179/200 (90%)	177 (99%)	2 (1%)	65	85
1	E	175/200 (88%)	173 (99%)	2 (1%)	65	85
1	G	179/200 (90%)	179 (100%)	0	100	100
2	B	298/302 (99%)	295 (99%)	3 (1%)	68	86
2	D	297/302 (98%)	296 (100%)	1 (0%)	86	94
2	F	297/302 (98%)	292 (98%)	5 (2%)	53	80
2	H	300/302 (99%)	295 (98%)	5 (2%)	53	80
All	All	1904/2008 (95%)	1885 (99%)	19 (1%)	68	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
2	B	256	HIS
2	B	315	SER
2	B	337	ASP
1	C	53	CYS
1	C	140	ASP
2	D	300	LEU
1	E	53	CYS
1	E	98	ILE
2	F	250	ASN
2	F	256	HIS
2	F	289	SER

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Mol	Chain	Res	Type
2	F	300	LEU
2	F	348	ASP
2	H	135	THR
2	H	250	ASN
2	H	300	LEU
2	H	315	SER
2	H	397	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	46	GLN
2	B	100	HIS
2	B	129	HIS
1	C	152	HIS
2	D	129	HIS
2	D	312	HIS
2	F	81	HIS
2	F	129	HIS
2	F	250	ASN
2	F	312	HIS
2	F	388	ASN
2	H	100	HIS
2	H	250	ASN
2	H	388	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	FMT	C	502	-	2,2,2	0.68	0	1,1,1	0.62	0
9	PGE	D	504	-	9,9,9	0.32	0	8,8,8	0.36	0
3	FMT	B	504	-	2,2,2	0.68	0	1,1,1	0.62	0
6	H9V	D	502	-	24,25,25	1.84	5 (20%)	26,36,36	1.83	6 (23%)
3	FMT	B	506	-	2,2,2	0.70	0	1,1,1	0.59	0
5	P1T	H	502	-	20,21,21	2.67	4 (20%)	29,30,30	1.86	7 (24%)
9	PGE	F	507	-	9,9,9	0.31	0	8,8,8	0.28	0
10	EDO	H	506	-	3,3,3	0.46	0	2,2,2	0.30	0
4	MLA	A	502	-	6,6,6	1.10	0	7,7,7	1.04	0
4	MLA	G	501	-	6,6,6	1.09	0	7,7,7	1.07	0
3	FMT	E	501	-	2,2,2	0.68	0	1,1,1	0.59	0
3	FMT	B	505	-	2,2,2	0.65	0	1,1,1	0.62	0
6	H9V	B	502	-	24,25,25	1.94	4 (16%)	26,36,36	1.79	8 (30%)
3	FMT	B	509	-	2,2,2	0.60	0	1,1,1	0.65	0
8	ACT	B	507	-	3,3,3	0.79	0	3,3,3	0.81	0
3	FMT	F	504	-	2,2,2	0.69	0	1,1,1	0.57	0
3	FMT	A	501	-	2,2,2	0.71	0	1,1,1	0.55	0
3	FMT	H	508	-	2,2,2	0.71	0	1,1,1	0.56	0
3	FMT	H	507	-	2,2,2	0.69	0	1,1,1	0.58	0
3	FMT	A	503	-	2,2,2	0.66	0	1,1,1	0.66	0
3	FMT	F	505	-	2,2,2	0.69	0	1,1,1	0.57	0
6	H9V	F	502	-	24,25,25	1.76	4 (16%)	26,36,36	1.83	5 (19%)
6	H9V	H	503	-	24,25,25	1.79	3 (12%)	26,36,36	1.94	8 (30%)
4	MLA	F	506	-	6,6,6	1.13	0	7,7,7	1.03	0
5	P1T	F	501	-	20,21,21	2.61	4 (20%)	29,30,30	2.11	10 (34%)
3	FMT	H	501	-	2,2,2	0.65	0	1,1,1	0.63	0
4	MLA	E	502	-	6,6,6	1.09	0	7,7,7	1.08	0
3	FMT	B	508	-	2,2,2	0.75	0	1,1,1	0.80	0
5	P1T	B	501	-	20,21,21	2.70	4 (20%)	29,30,30	1.91	8 (27%)
3	FMT	H	505	-	2,2,2	0.67	0	1,1,1	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	P1T	D	501	-	20,21,21	2.74	4 (20%)	29,30,30	1.88	6 (20%)
4	MLA	C	501	-	6,6,6	1.17	0	7,7,7	1.00	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	H9V	F	502	-	-	1/8/24/24	0/3/3/3
5	P1T	B	501	-	-	5/14/15/15	0/1/1/1
6	H9V	B	502	-	-	1/8/24/24	0/3/3/3
6	H9V	H	503	-	-	1/8/24/24	0/3/3/3
9	PGE	D	504	-	-	2/7/7/7	-
6	H9V	D	502	-	-	3/8/24/24	0/3/3/3
4	MLA	F	506	-	-	2/4/4/4	-
5	P1T	D	501	-	-	5/14/15/15	0/1/1/1
5	P1T	F	501	-	-	8/14/15/15	0/1/1/1
5	P1T	H	502	-	-	3/14/15/15	0/1/1/1
9	PGE	F	507	-	-	3/7/7/7	-
4	MLA	C	501	-	-	0/4/4/4	-
4	MLA	A	502	-	-	0/4/4/4	-
4	MLA	G	501	-	-	0/4/4/4	-
10	EDO	H	506	-	-	0/1/1/1	-
4	MLA	E	502	-	-	0/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	P1T	C3-C2	7.61	1.48	1.41
5	D	501	P1T	C3-C2	7.55	1.48	1.41
5	H	502	P1T	C3-C2	7.36	1.48	1.41
5	F	501	P1T	C3-C2	7.25	1.48	1.41
5	D	501	P1T	C3-C4	6.03	1.48	1.40
5	D	501	P1T	C5-C4	5.92	1.48	1.40
5	H	502	P1T	C3-C4	5.86	1.48	1.40
5	B	501	P1T	C5-C4	5.83	1.48	1.40
5	B	501	P1T	C3-C4	5.75	1.48	1.40
5	F	501	P1T	C5-C4	5.62	1.48	1.40
5	F	501	P1T	C3-C4	5.58	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	502	P1T	C5-C4	5.53	1.48	1.40
6	B	502	H9V	C2-C13	-5.26	1.39	1.51
6	B	502	H9V	C7-C5	-5.26	1.40	1.50
6	D	502	H9V	C2-C13	-5.07	1.39	1.51
6	H	503	H9V	C2-C13	-4.95	1.40	1.51
6	H	503	H9V	C7-C5	-4.94	1.41	1.50
6	F	502	H9V	C7-C5	-4.88	1.41	1.50
6	D	502	H9V	C7-C5	-4.68	1.41	1.50
6	F	502	H9V	C2-C13	-4.57	1.40	1.51
5	H	502	P1T	CA-C	-3.62	1.44	1.49
6	B	502	H9V	C15-C17	3.56	1.53	1.48
5	D	501	P1T	CA-C	-3.38	1.44	1.49
6	D	502	H9V	C15-C17	3.28	1.53	1.48
5	B	501	P1T	CA-C	-3.27	1.45	1.49
6	H	503	H9V	C14-N1	3.17	1.52	1.48
5	F	501	P1T	CA-C	-3.16	1.45	1.49
6	F	502	H9V	C14-N1	3.14	1.51	1.48
6	D	502	H9V	F1-C12	-2.99	1.27	1.35
6	B	502	H9V	C14-N1	2.73	1.51	1.48
6	D	502	H9V	C14-N1	2.48	1.51	1.48
6	F	502	H9V	C17-N2	-2.31	1.09	1.14

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	501	P1T	CB-CA-N	-6.08	110.87	125.84
5	D	501	P1T	CB-CA-N	-5.72	111.75	125.84
5	H	502	P1T	CB-CA-N	-5.39	112.56	125.84
5	B	501	P1T	CB-CA-N	-5.30	112.78	125.84
6	D	502	H9V	C10-C11-C12	4.27	121.14	117.54
6	F	502	H9V	C10-C9-C8	4.00	120.91	117.54
5	D	501	P1T	CB-CA-C	-3.91	110.43	120.72
6	F	502	H9V	C10-C11-C12	3.86	120.80	117.54
5	B	501	P1T	CB-CA-C	-3.76	110.84	120.72
6	D	502	H9V	C10-C9-C8	3.72	120.68	117.54
6	H	503	H9V	C10-C11-C12	3.58	120.56	117.54
5	F	501	P1T	CB-CA-C	-3.55	111.39	120.72
5	F	501	P1T	C-CA-N	3.52	124.04	113.09
6	H	503	H9V	C15-C17-N2	-3.50	173.89	177.70
5	H	502	P1T	CB-CA-C	-3.49	111.53	120.72
5	D	501	P1T	C-CA-N	3.46	123.86	113.09
6	F	502	H9V	C2-C13-C14	3.33	125.93	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	502	H9V	C10-C9-C8	3.29	120.32	117.54
6	H	503	H9V	C10-C9-C8	3.26	120.29	117.54
6	H	503	H9V	C2-C13-C14	3.11	125.42	118.21
5	B	501	P1T	C-CA-N	3.08	122.66	113.09
6	B	502	H9V	C10-C11-C12	2.84	119.94	117.54
5	H	502	P1T	C-CA-N	2.81	121.83	113.09
6	B	502	H9V	C4-C5-C7	2.67	125.37	120.80
5	F	501	P1T	C6-C5-C4	2.61	120.04	118.06
6	B	502	H9V	C12-C7-C8	2.57	117.00	114.55
5	F	501	P1T	OP4-C5A-C5	-2.55	104.58	109.36
6	D	502	H9V	F1-C12-C7	2.53	123.29	119.54
5	H	502	P1T	O-C-CA	2.49	119.59	114.25
5	F	501	P1T	C4A-N-CA	-2.47	120.51	125.68
6	F	502	H9V	C11-C10-C9	-2.47	118.64	121.64
6	D	502	H9V	C11-C10-C9	-2.46	118.65	121.64
6	D	502	H9V	C9-C10-CL1	2.46	122.25	119.17
6	F	502	H9V	F2-C8-C7	2.45	123.17	119.54
6	H	503	H9V	C6-C1-C2	-2.45	118.73	121.18
6	D	502	H9V	F2-C8-C7	2.42	123.13	119.54
6	B	502	H9V	C6-C5-C7	-2.42	116.65	120.80
5	B	501	P1T	O-C-CA	2.27	119.12	114.25
5	F	501	P1T	C4A-C4-C3	2.26	122.98	119.98
6	B	502	H9V	C4-C3-C2	-2.25	118.94	121.18
5	B	501	P1T	C4A-C4-C3	2.23	122.95	119.98
6	B	502	H9V	F2-C8-C7	2.23	122.84	119.54
5	B	501	P1T	C6-N1-C2	2.22	123.22	119.20
5	D	501	P1T	C6-N1-C2	2.21	123.20	119.20
6	H	503	H9V	C4-C5-C7	2.19	124.55	120.80
5	F	501	P1T	C6-N1-C2	2.16	123.12	119.20
5	H	502	P1T	C4A-N-CA	-2.15	121.17	125.68
5	B	501	P1T	OP4-C5A-C5	-2.15	105.33	109.36
5	H	502	P1T	C4A-C4-C3	2.14	122.83	119.98
5	D	501	P1T	O-C-CA	2.12	118.80	114.25
5	B	501	P1T	C4A-N-CA	-2.08	121.32	125.68
5	F	501	P1T	C3-C4-C5	-2.07	116.85	118.73
6	B	502	H9V	C11-C12-C7	-2.07	121.03	123.42
6	H	503	H9V	F1-C12-C7	2.06	122.59	119.54
5	H	502	P1T	C6-N1-C2	2.05	122.91	119.20
5	D	501	P1T	C3-C4-C5	-2.05	116.88	118.73
5	F	501	P1T	O-C-CA	2.04	118.62	114.25
6	H	503	H9V	F2-C8-C7	2.01	122.52	119.54

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	P1T	C5-C4-C4A-N
5	B	501	P1T	C-CA-N-C4A
5	B	501	P1T	O-C-CA-CB
5	B	501	P1T	OXT-C-CA-CB
5	D	501	P1T	C5-C4-C4A-N
5	D	501	P1T	C3-C4-C4A-N
5	F	501	P1T	C5A-OP4-P-OP1
5	F	501	P1T	C5-C4-C4A-N
5	H	502	P1T	C5-C4-C4A-N
9	F	507	PGE	O2-C3-C4-O3
9	D	504	PGE	O3-C5-C6-O4
5	B	501	P1T	C3-C4-C4A-N
5	D	501	P1T	C-CA-N-C4A
5	F	501	P1T	C-CA-N-C4A
5	H	502	P1T	C-CA-N-C4A
5	D	501	P1T	O-C-CA-CB
5	D	501	P1T	OXT-C-CA-CB
5	F	501	P1T	O-C-CA-CB
5	F	501	P1T	OXT-C-CA-CB
6	D	502	H9V	C4-C5-C7-C12
5	F	501	P1T	C5A-OP4-P-OP3
9	D	504	PGE	C3-C4-O3-C5
6	B	502	H9V	C4-C5-C7-C12
6	F	502	H9V	C4-C5-C7-C12
6	H	503	H9V	C4-C5-C7-C12
5	F	501	P1T	C3-C4-C4A-N
5	H	502	P1T	C3-C4-C4A-N
6	D	502	H9V	C4-C5-C7-C8
5	F	501	P1T	C5A-OP4-P-OP2
6	D	502	H9V	C6-C5-C7-C12
4	F	506	MLA	O1B-C1-C2-C3
4	F	506	MLA	O1A-C1-C2-C3
9	F	507	PGE	C3-C4-O3-C5
9	F	507	PGE	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	501	P1T	1	0
4	E	502	MLA	2	0

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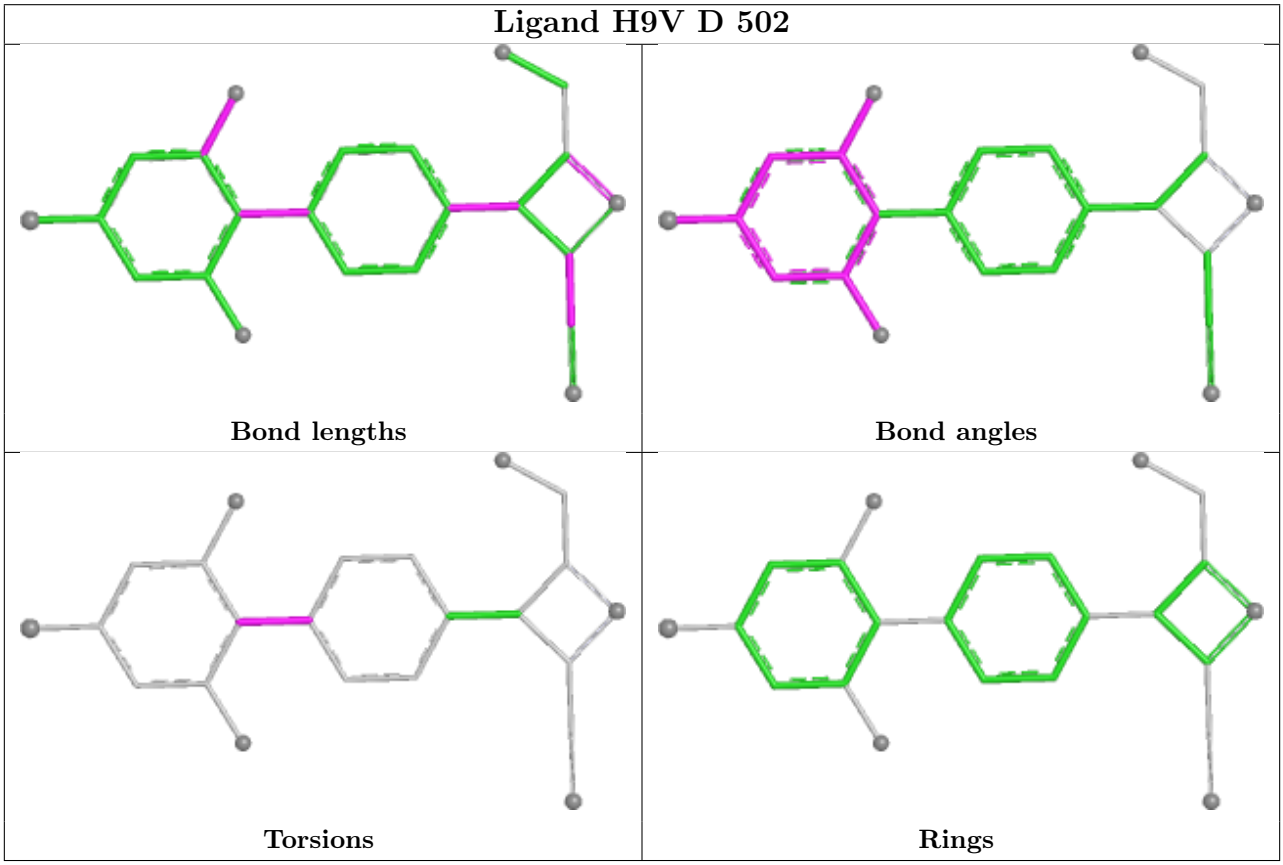
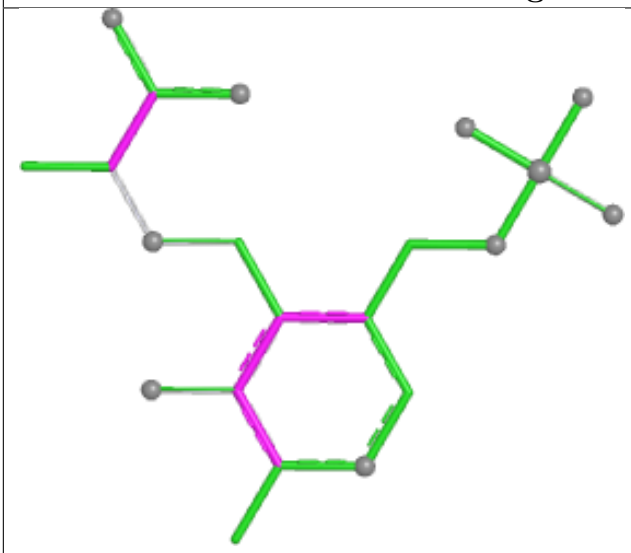
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	P1T	1	0

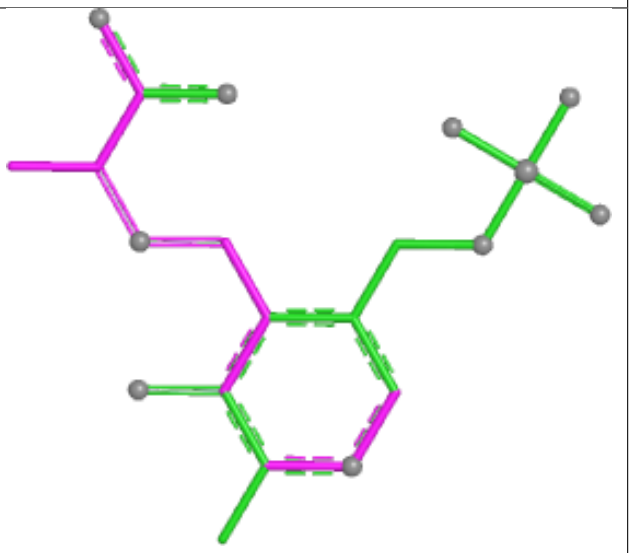
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



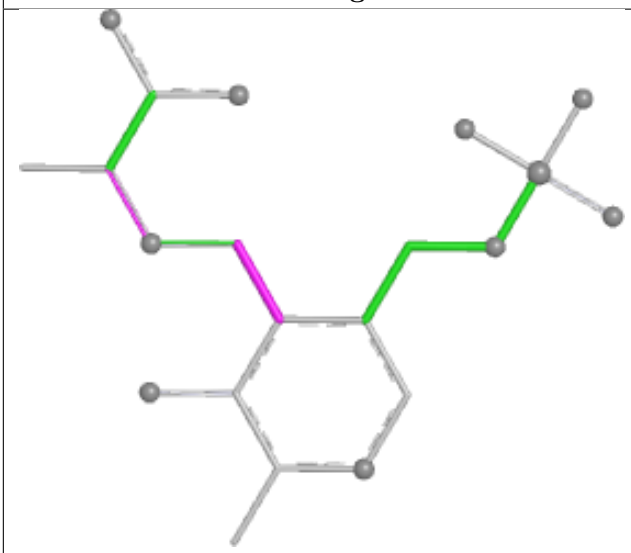
Ligand P1T H 502



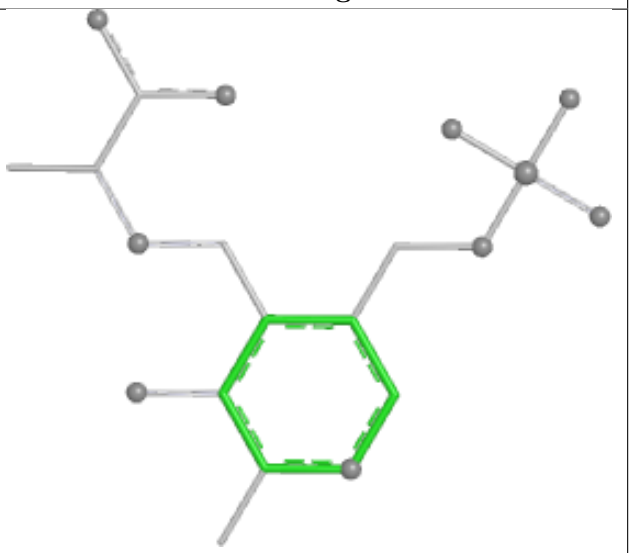
Bond lengths



Bond angles

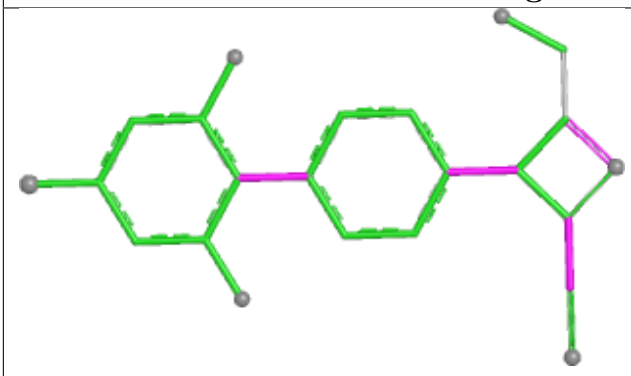


Torsions

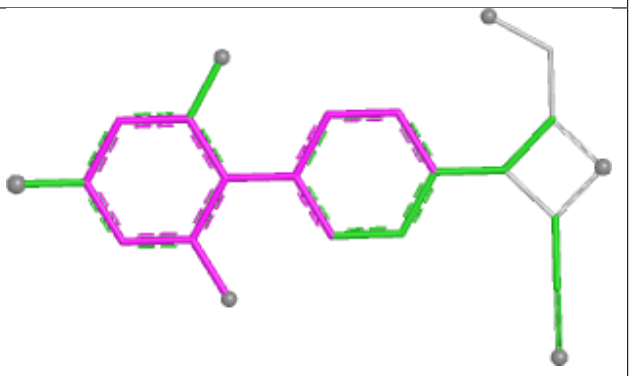


Rings

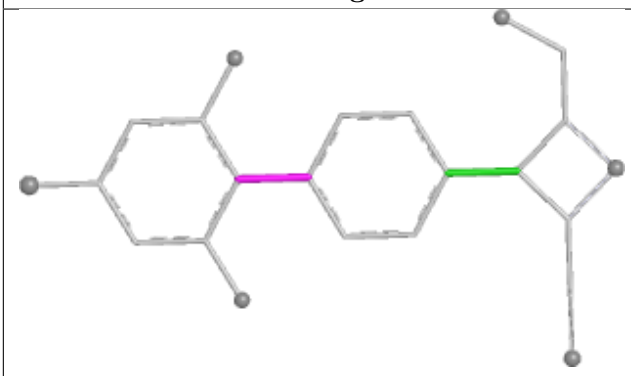
Ligand H9V B 502



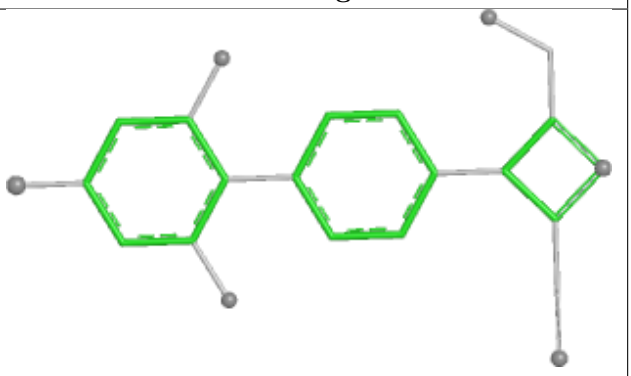
Bond lengths



Bond angles

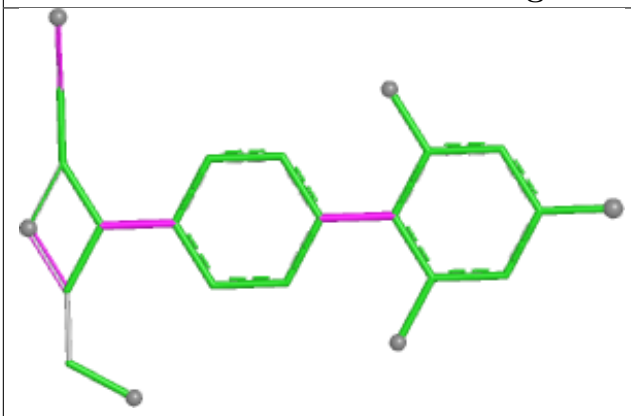


Torsions

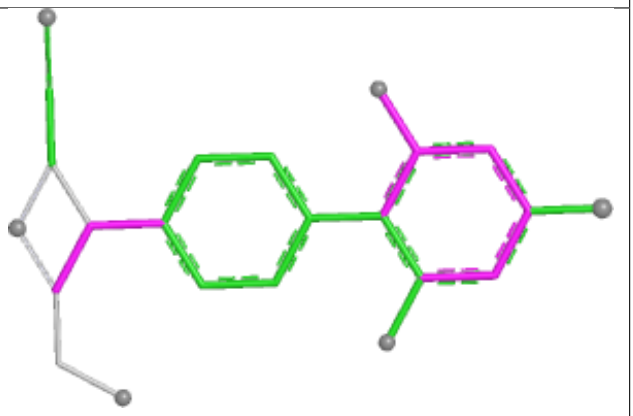


Rings

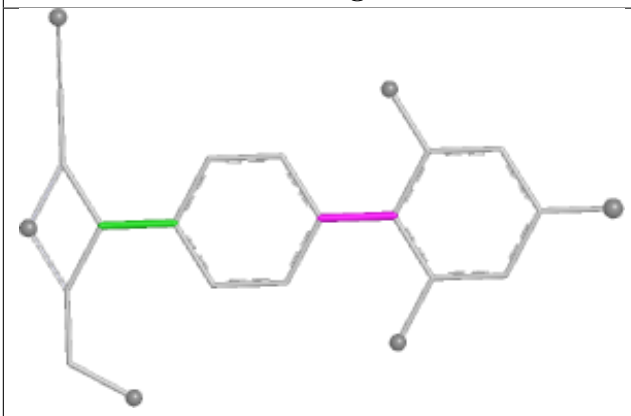
Ligand H9V F 502



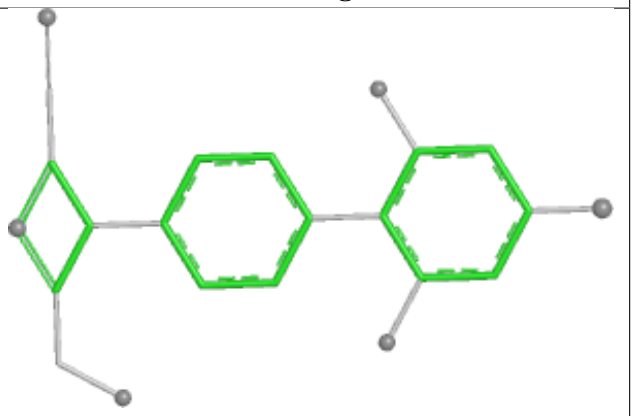
Bond lengths



Bond angles

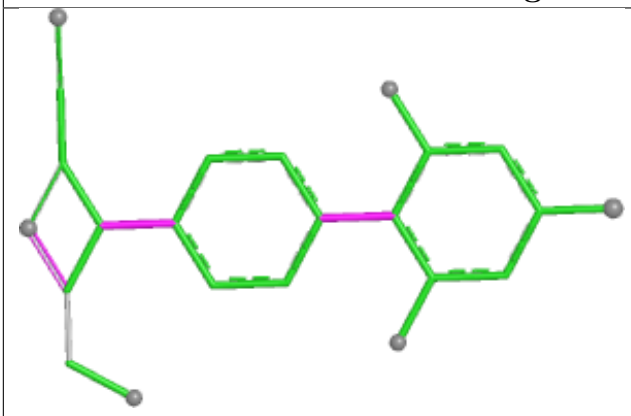


Torsions

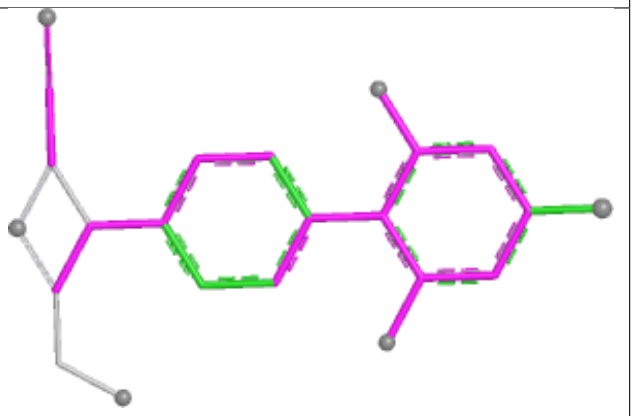


Rings

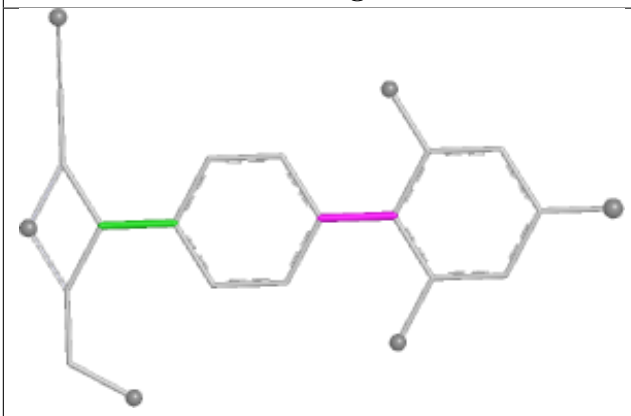
Ligand H9V H 503



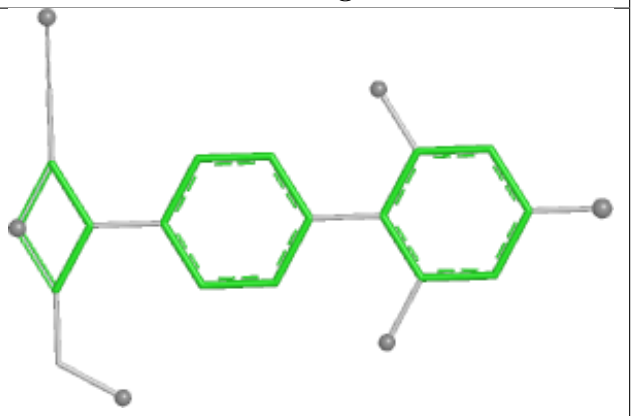
Bond lengths



Bond angles

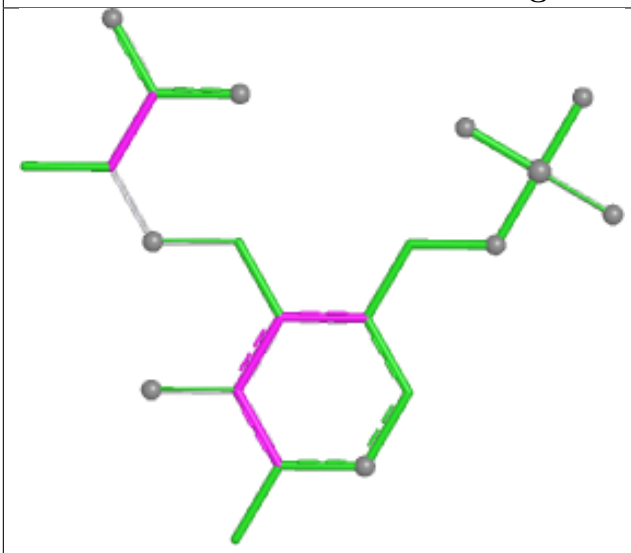


Torsions

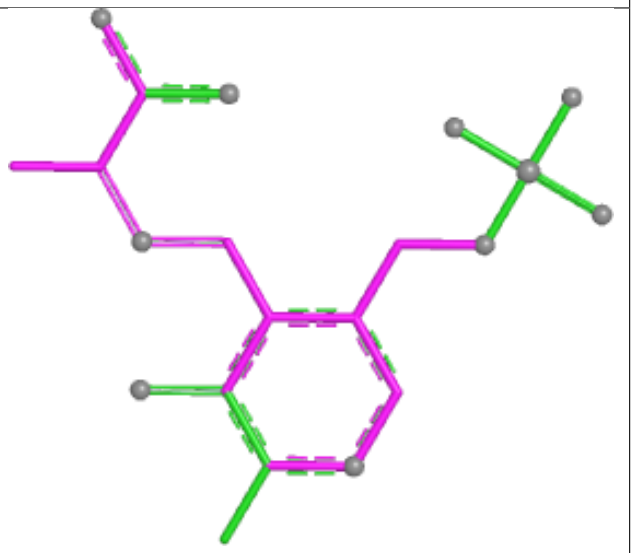


Rings

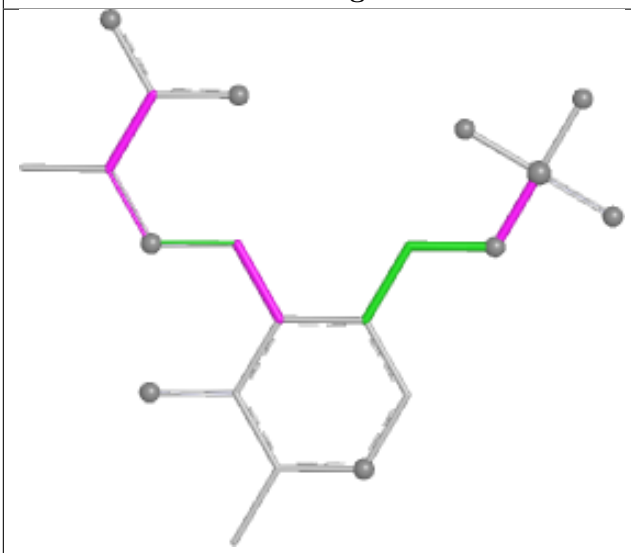
Ligand P1T F 501



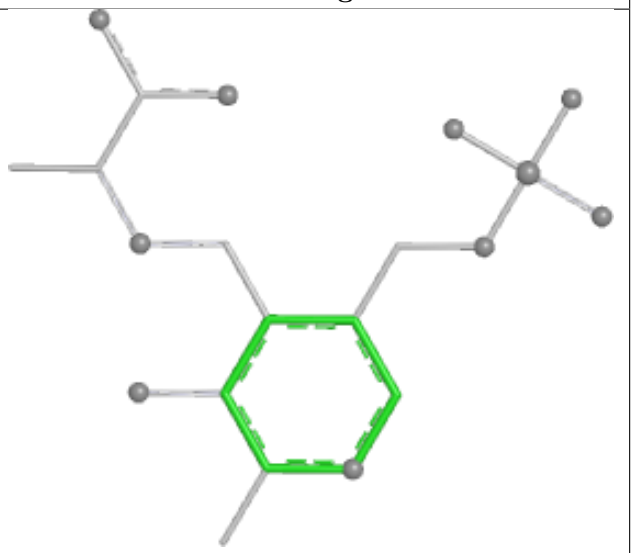
Bond lengths



Bond angles

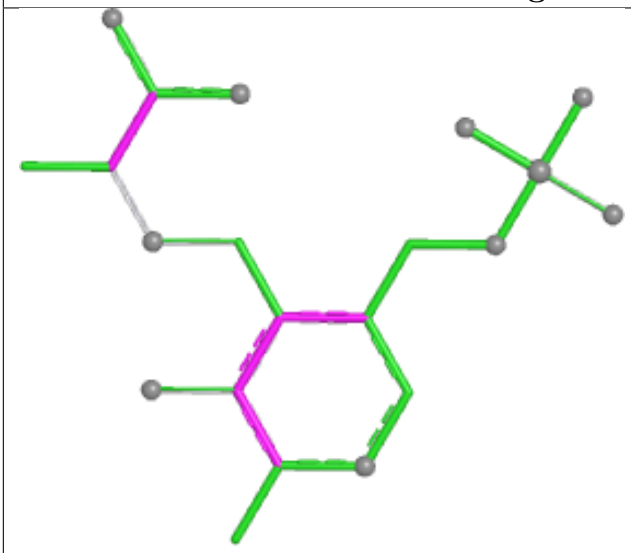


Torsions

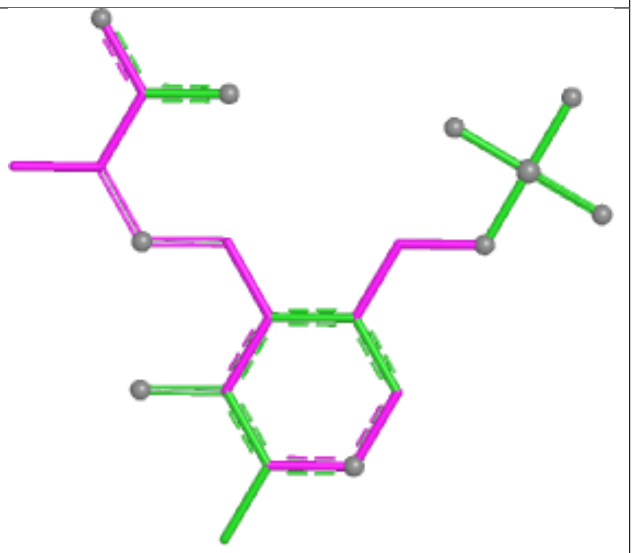


Rings

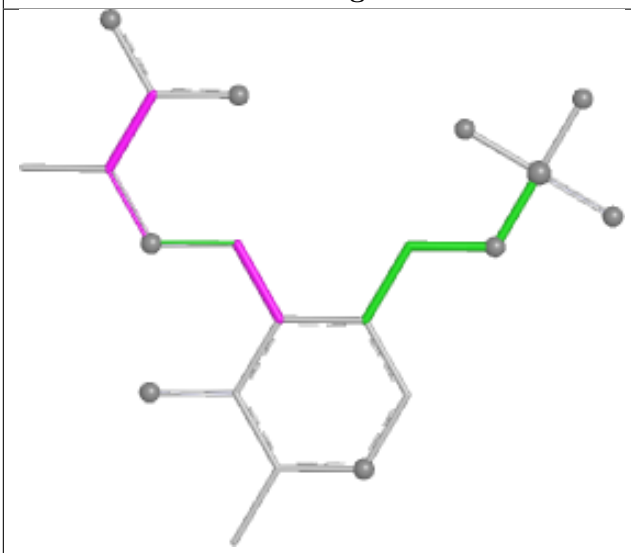
Ligand P1T B 501



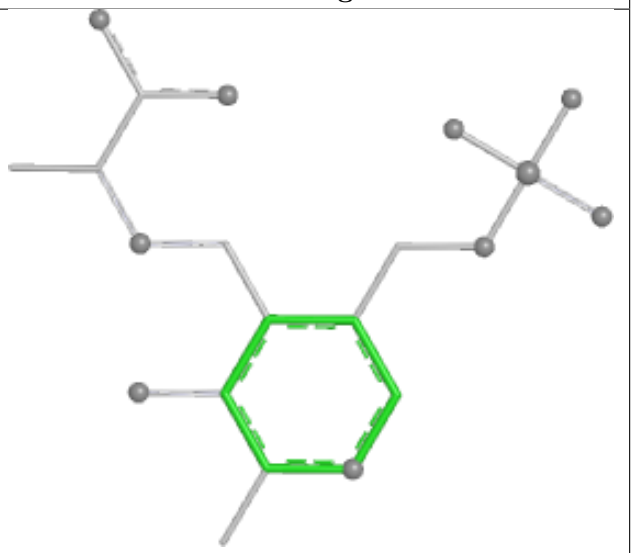
Bond lengths



Bond angles

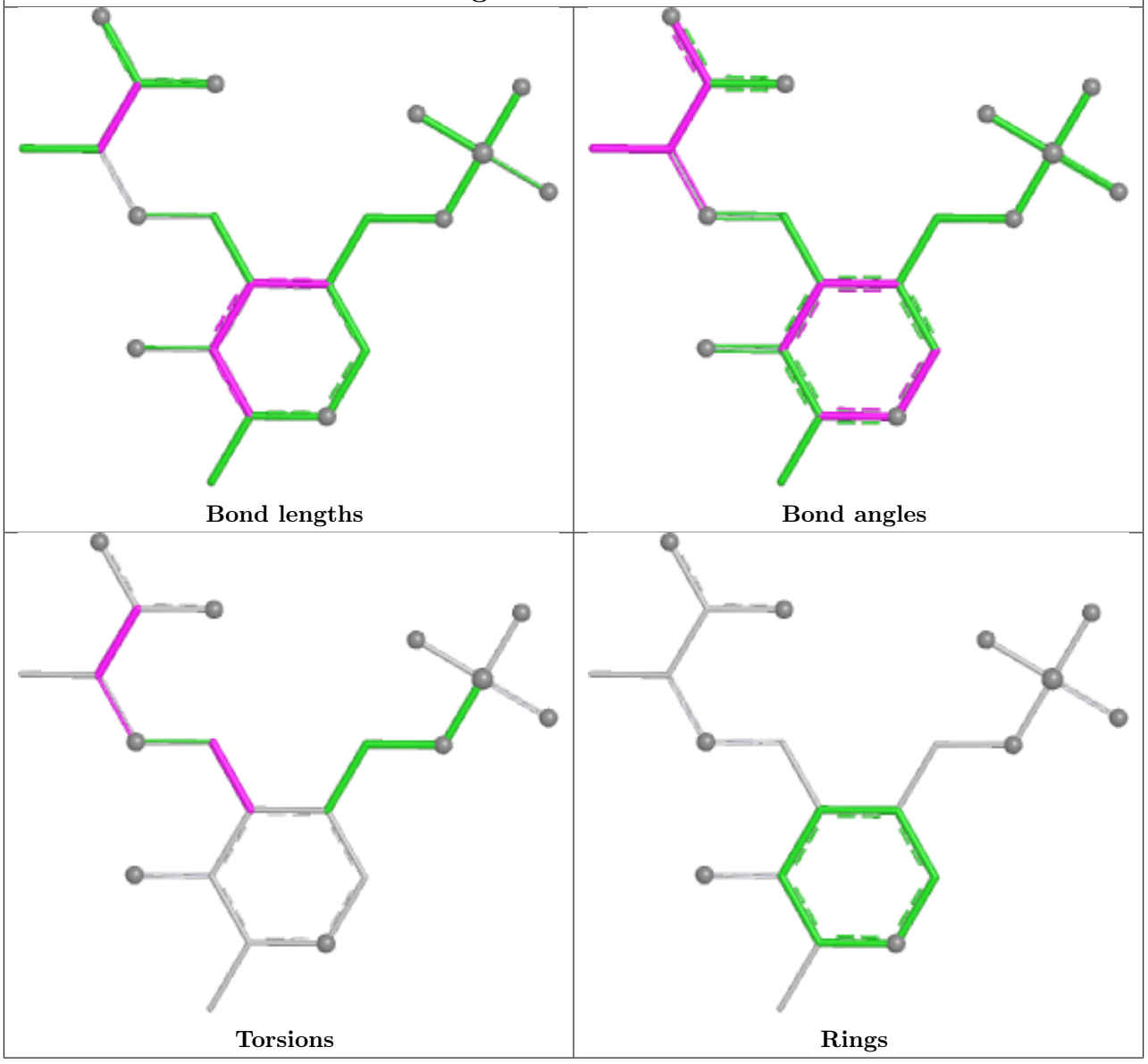


Torsions



Rings

Ligand P1T D 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, 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	249/276 (90%)	-0.41	2 (0%)	82	77	30, 47, 74, 115	0
1	C	248/276 (89%)	-0.26	3 (1%)	76	70	28, 51, 86, 121	0
1	E	247/276 (89%)	0.14	6 (2%)	59	52	39, 71, 105, 124	0
1	G	248/276 (89%)	-0.47	2 (0%)	82	77	26, 44, 64, 96	1 (0%)
2	B	404/410 (98%)	-0.56	6 (1%)	72	65	15, 32, 54, 128	2 (0%)
2	D	399/410 (97%)	-0.67	1 (0%)	90	88	16, 32, 52, 100	2 (0%)
2	F	400/410 (97%)	-0.63	5 (1%)	75	69	14, 34, 56, 100	2 (0%)
2	H	403/410 (98%)	-0.59	6 (1%)	72	65	15, 31, 53, 133	2 (0%)
All	All	2598/2744 (94%)	-0.47	31 (1%)	76	70	14, 38, 80, 133	9 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	8	PRO	4.6
2	B	6	ALA	4.1
2	F	8	PRO	3.9
1	C	266	LEU	3.8
1	E	266	LEU	3.7
2	B	408	GLY	3.3
2	B	7	GLU	3.1
2	H	8	PRO	3.0
1	E	184	SER	2.7
1	E	196	SER	2.7
2	H	407	LEU	2.6
1	A	184	SER	2.5
2	D	407	LEU	2.5
2	H	7	GLU	2.4
1	G	184	SER	2.4
2	F	407	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	196	SER	2.3
2	F	23	SER	2.3
1	E	9	ALA	2.2
2	H	22	PRO	2.2
1	G	9	ALA	2.2
1	A	267	GLY	2.2
2	H	6	ALA	2.1
1	E	265	ARG	2.1
2	B	5	ILE	2.1
2	H	23	SER	2.1
1	C	184	SER	2.1
2	F	9	THR	2.0
1	E	261	ALA	2.0
2	F	22	PRO	2.0
2	B	407	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides 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
3	FMT	B	508	3/3	0.40	0.24	53,53,53,55	0
4	MLA	C	501	7/7	0.67	0.15	69,69,71,71	0
8	ACT	B	507	4/4	0.71	0.25	72,73,73,74	0
9	PGE	D	504	10/10	0.80	0.17	64,68,72,72	0
4	MLA	G	501	7/7	0.81	0.14	66,67,73,73	0
6	H9V	D	502	23/23	0.81	0.28	58,60,60,61	23
4	MLA	A	502	7/7	0.81	0.10	65,66,68,69	0
4	MLA	F	506	7/7	0.81	0.19	82,84,90,90	0

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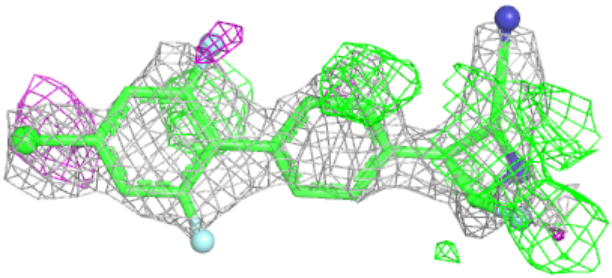
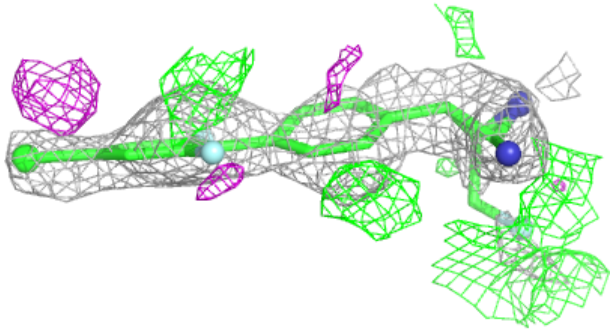
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	EDO	H	506	4/4	0.82	0.14	55,56,56,57	0
4	MLA	E	502	7/7	0.83	0.12	83,83,84,84	0
9	PGE	F	507	10/10	0.84	0.13	67,71,75,75	0
3	FMT	A	501	3/3	0.86	0.19	61,61,62,62	0
3	FMT	E	501	3/3	0.87	0.16	60,60,60,61	0
3	FMT	A	503	3/3	0.88	0.11	46,46,46,46	0
3	FMT	B	506	3/3	0.88	0.11	52,52,53,53	0
3	FMT	F	505	3/3	0.90	0.11	44,44,45,45	0
6	H9V	B	502	23/23	0.91	0.12	37,44,59,70	0
6	H9V	H	503	23/23	0.91	0.12	40,42,56,62	0
6	H9V	F	502	23/23	0.93	0.12	43,49,59,68	0
3	FMT	H	508	3/3	0.93	0.08	59,59,59,60	0
3	FMT	F	504	3/3	0.94	0.09	57,57,57,58	0
3	FMT	B	509	3/3	0.94	0.07	23,23,25,26	0
3	FMT	H	507	3/3	0.95	0.11	59,59,59,60	0
3	FMT	B	504	3/3	0.95	0.07	54,54,54,55	0
3	FMT	H	505	3/3	0.95	0.12	43,43,44,44	0
3	FMT	B	505	3/3	0.96	0.08	38,38,39,39	0
3	FMT	H	501	3/3	0.96	0.09	46,46,46,46	0
5	P1T	B	501	21/21	0.97	0.06	24,25,38,40	0
7	CS	F	503	1/1	0.97	0.11	138,138,138,138	0
3	FMT	C	502	3/3	0.97	0.10	41,41,42,42	0
7	CS	H	504	1/1	0.98	0.04	72,72,72,72	1
5	P1T	H	502	21/21	0.98	0.06	20,23,38,39	0
5	P1T	D	501	21/21	0.98	0.06	23,27,33,34	0
7	CS	B	503	1/1	0.98	0.14	120,120,120,120	0
5	P1T	F	501	21/21	0.98	0.06	26,30,38,38	0
7	CS	D	503	1/1	0.99	0.04	47,47,47,47	1

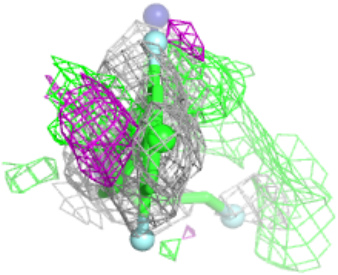
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H9V D 502:

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

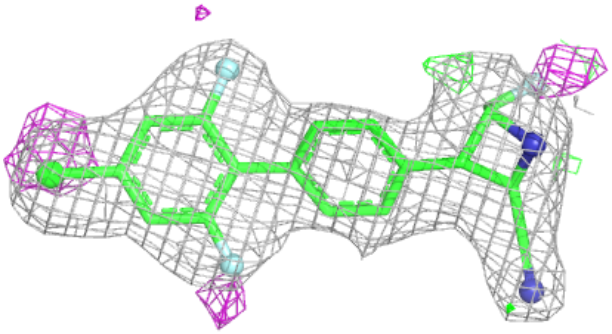


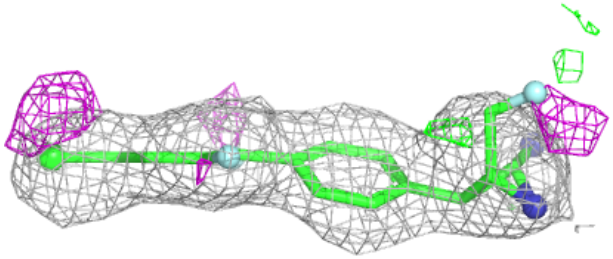


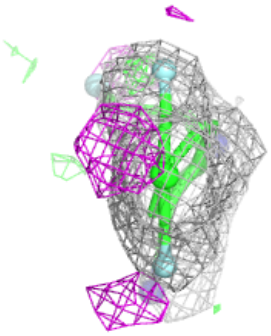


Electron density around H9V B 502:

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

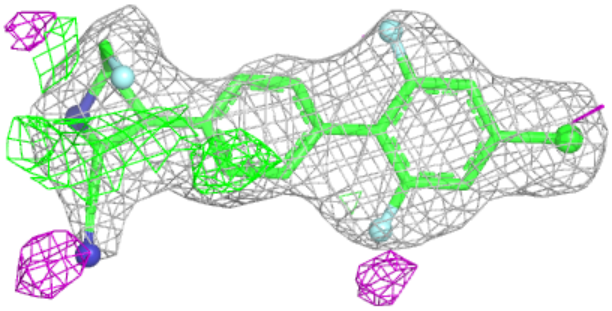


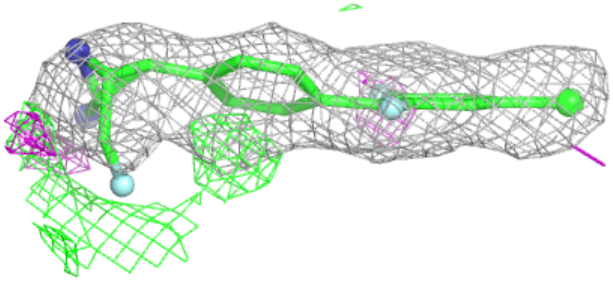


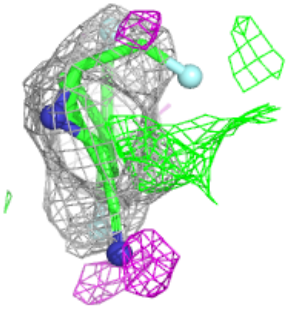


Electron density around H9V H 503:

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

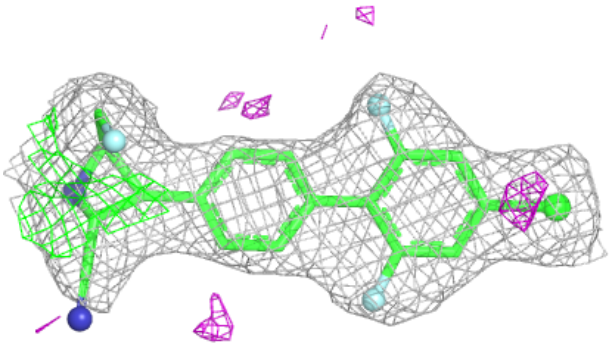


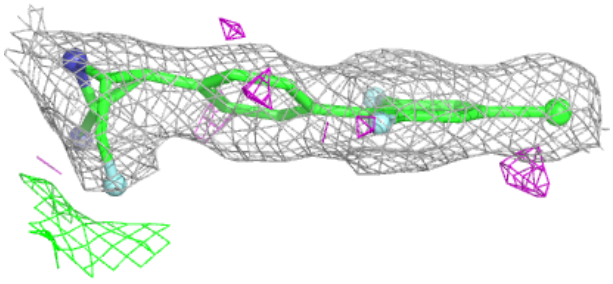


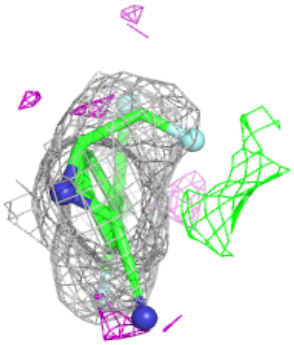


Electron density around H9V F 502:

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

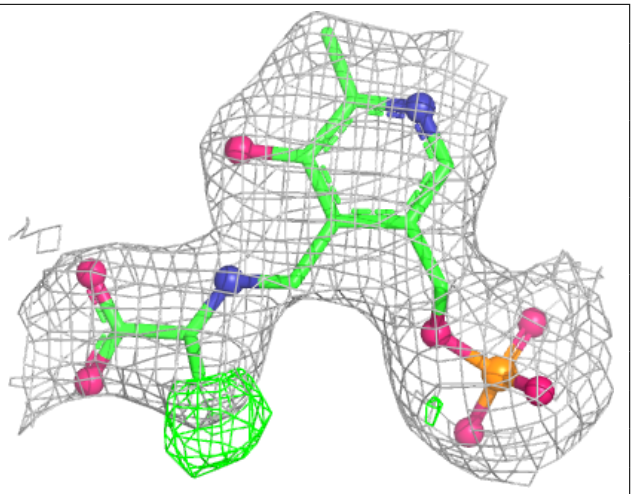


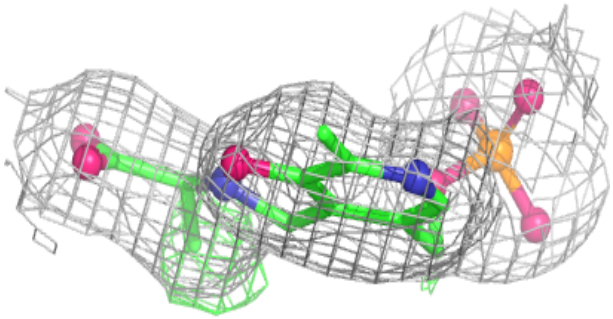


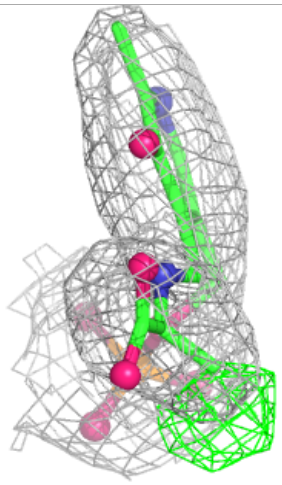


Electron density around P1T B 501:

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

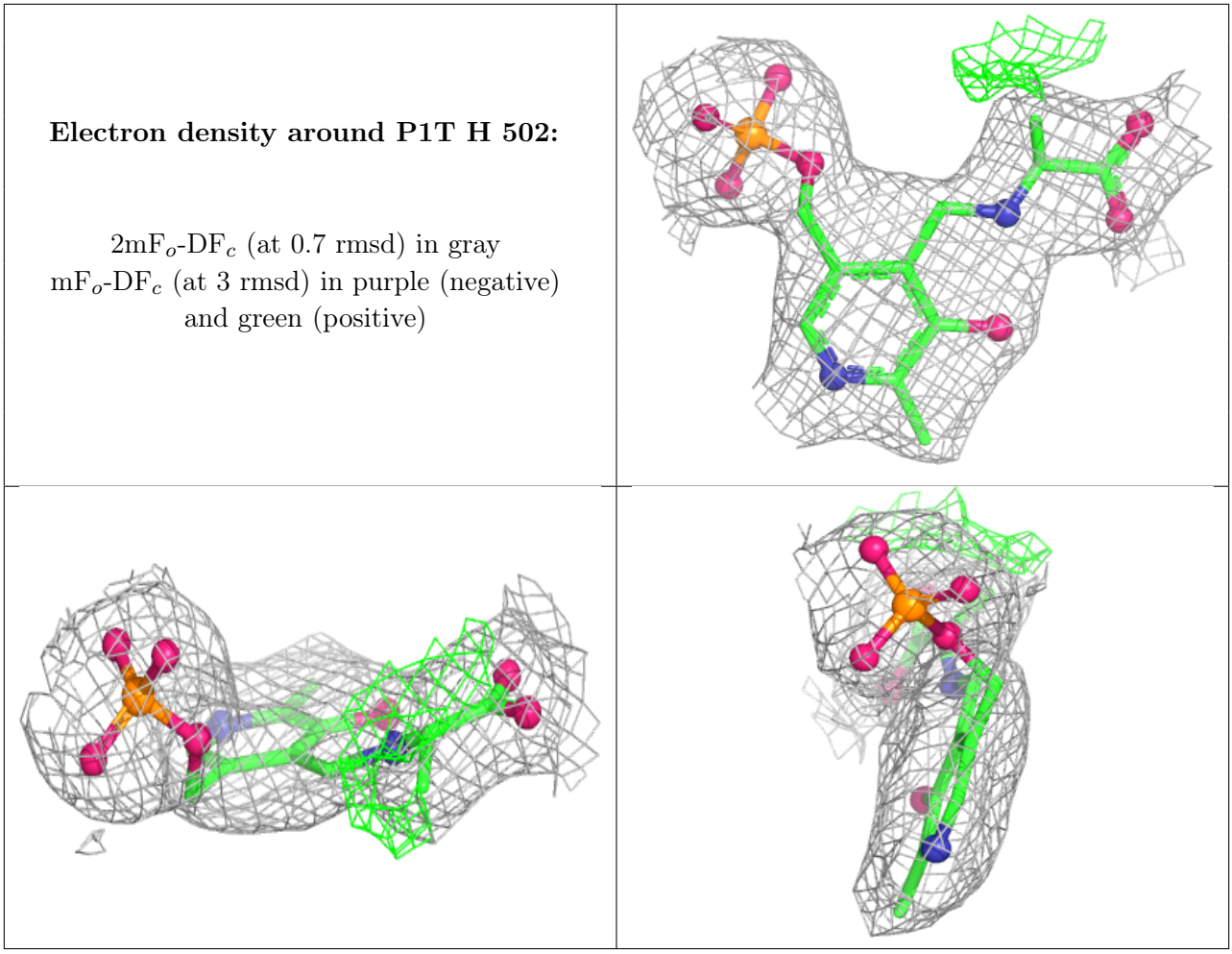






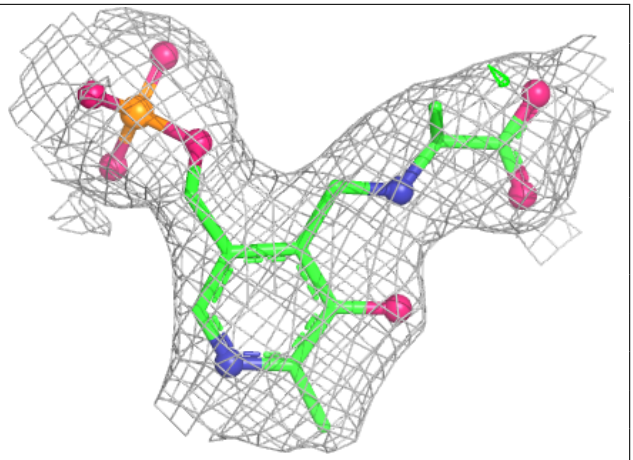
Electron density around P1T H 502:

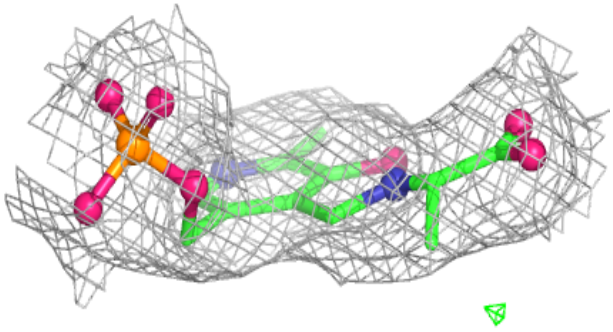
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

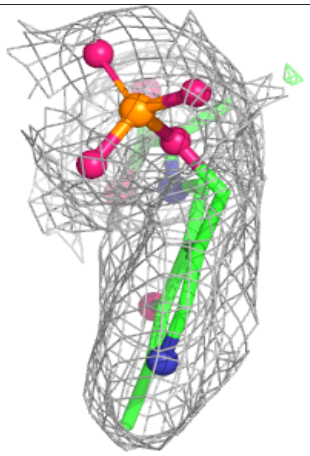


Electron density around P1T D 501:

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

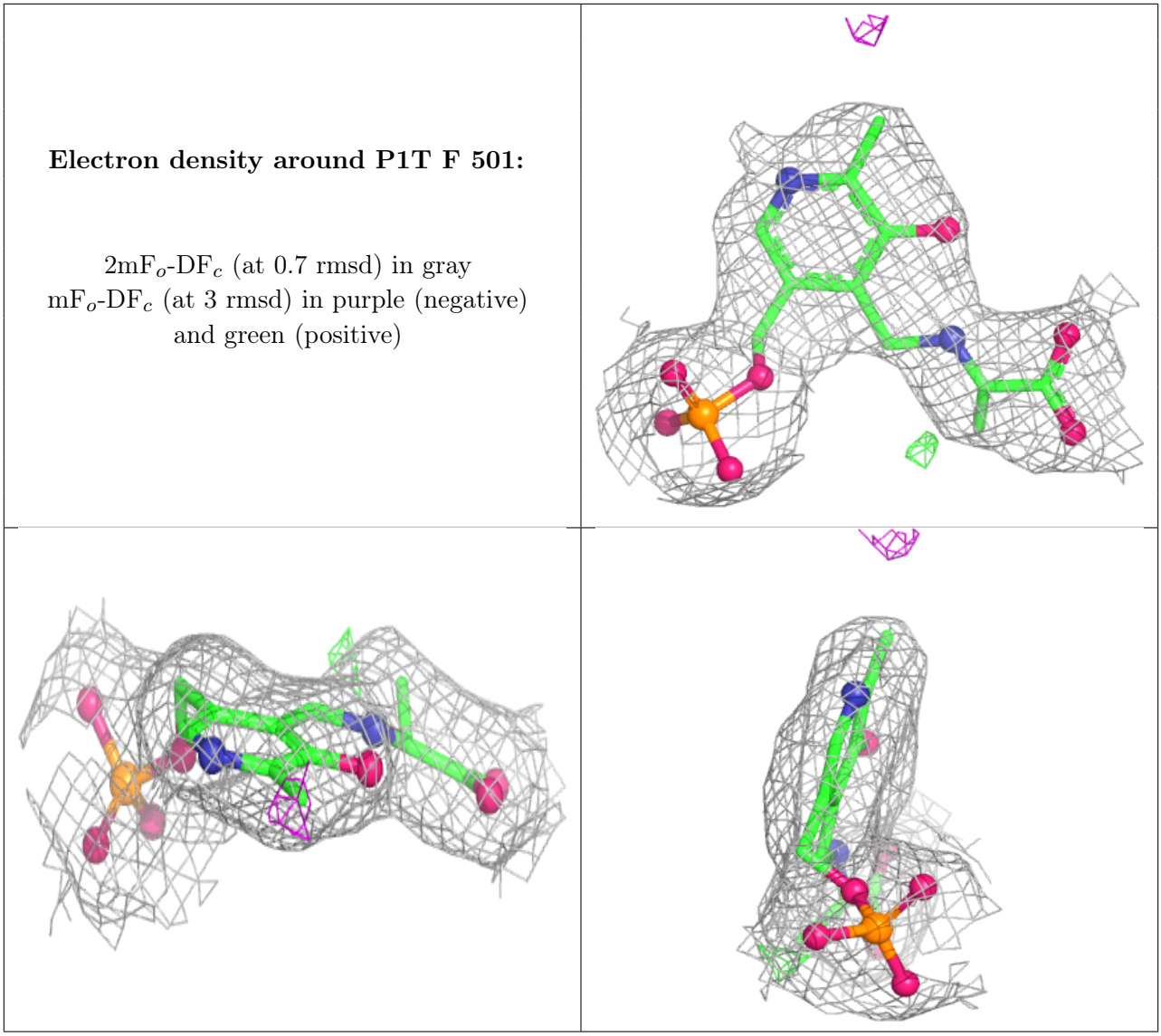






Electron density around P1T F 501:

$2mF_o$-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

There are no such residues in this entry.