Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 10:57 PM EDT

PDB ID	:	6DWE
Title	:	Crystal structure of tryptophan synthase from M. tuberculosis - aminoacrylate- and BRD0059-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	:	2018-06-26
Resolution	:	2.69 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 (1)) were used in the production of this report:

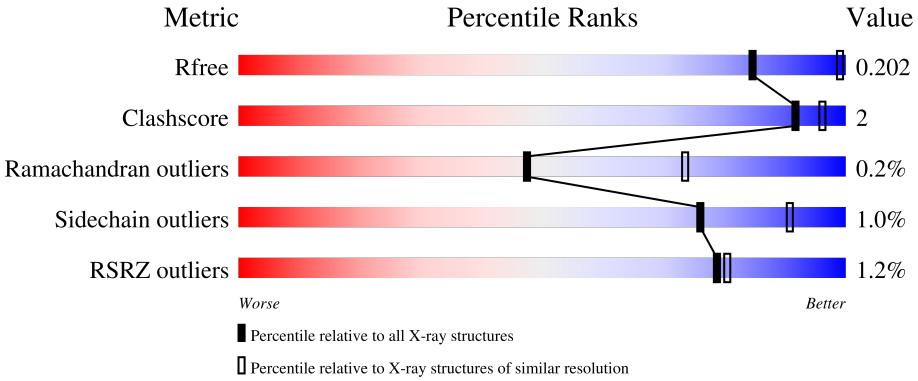
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.69 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.



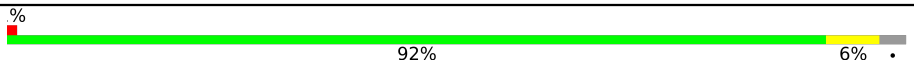
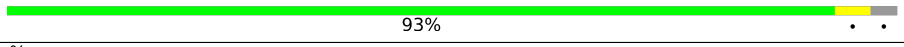
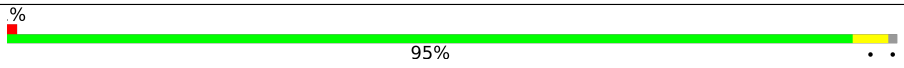
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	A	276	85% 5% 10%
1	C	276	85% 5% 10%
1	E	276	4% 83% 6% 11%
1	G	276	87% 10%
2	B	410	93% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	410	
2	F	410	
2	H	410	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MLA	H	511	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 20363 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	1	0
			1814	1137	327	345	5			
1	G	248	Total	C	N	O	S	0	1	0
			1805	1132	326	342	5			
1	E	246	Total	C	N	O	S	0	1	0
			1781	1118	318	340	5			
1	C	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	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
G	271	HIS	-	expression tag	UNP P9WFY1
G	272	HIS	-	expression tag	UNP P9WFY1
G	273	HIS	-	expression tag	UNP P9WFY1
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	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
C	271	HIS	-	expression tag	UNP P9WFY1
C	272	HIS	-	expression tag	UNP P9WFY1
C	273	HIS	-	expression tag	UNP P9WFY1

Continued on next page...

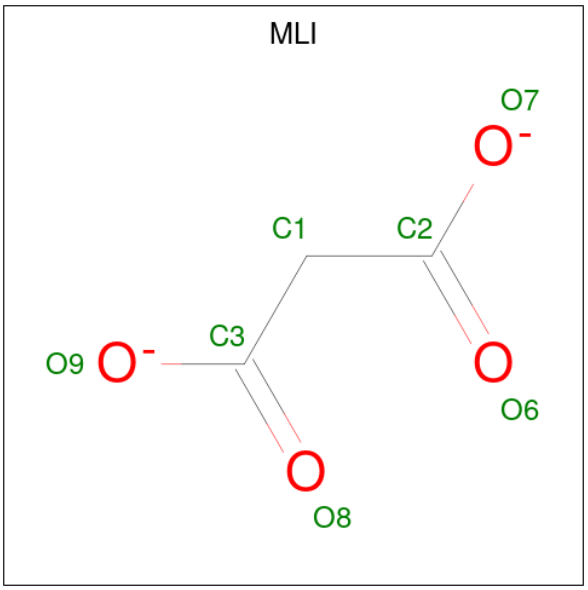
Continued from previous page...

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

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

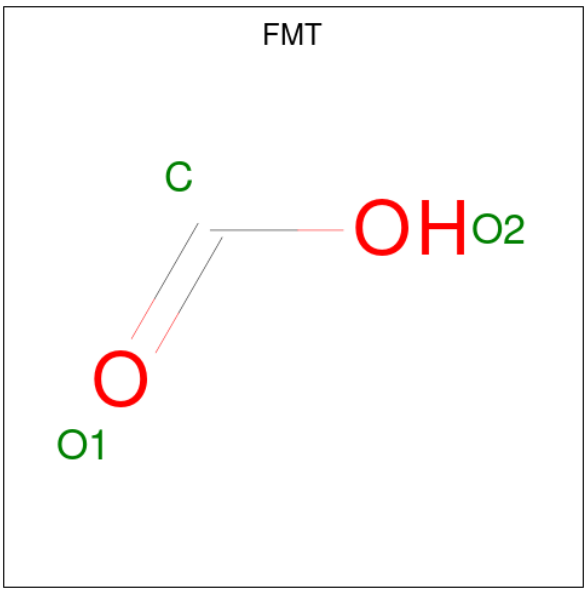
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	5	0
			3044	1898	555	577	14			
2	H	404	Total	C	N	O	S	0	2	0
			3023	1889	546	574	14			
2	F	399	Total	C	N	O	S	0	3	0
			3000	1872	545	570	13			
2	D	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



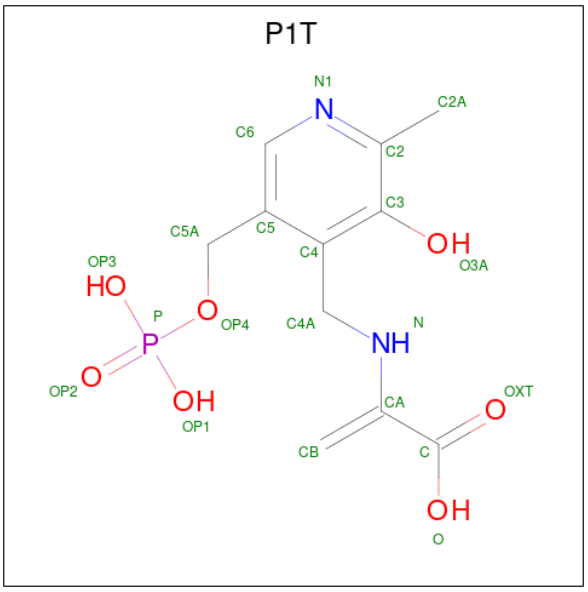
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			3	1	2			
4	A	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3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

Continued on next page...

Continued from previous page...

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

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

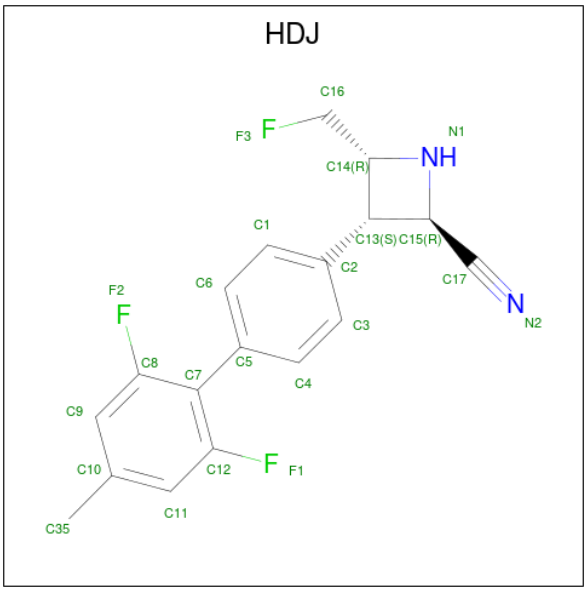


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O P 21 11 2 7 1	0	0
5	H	1	Total C N O P 21 11 2 7 1	0	0
5	F	1	Total C N O P 21 11 2 7 1	0	0
5	D	1	Total C N O P 21 11 2 7 1	0	0

- Molecule 6 is CESIUM ION (three-letter code: CS) (formula: Cs).

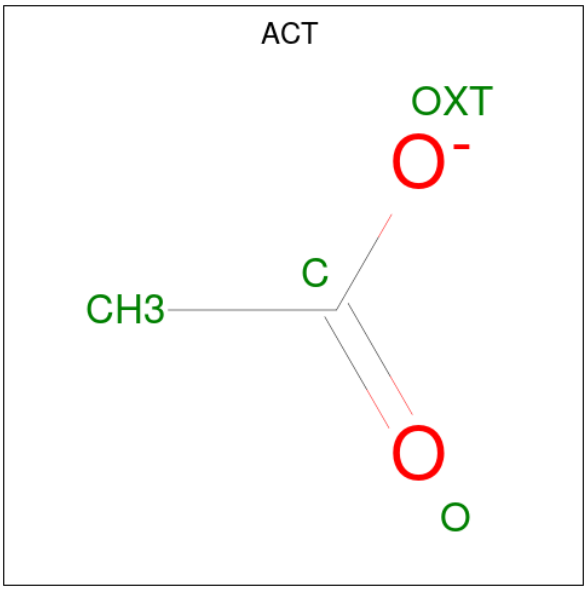
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total Cs 3 3	0	0
6	H	1	Total Cs 1 1	0	0
6	F	3	Total Cs 3 3	0	0
6	D	2	Total Cs 2 2	0	0

- Molecule 7 is (2R,3S,4R)-3-(2',6'-difluoro-4'-methyl[1,1'-biphenyl]-4-yl)-4-(fluoromethyl)azetidine-2-carbonitrile (three-letter code: HDJ) (formula: $C_{18}H_{15}F_3N_2$).



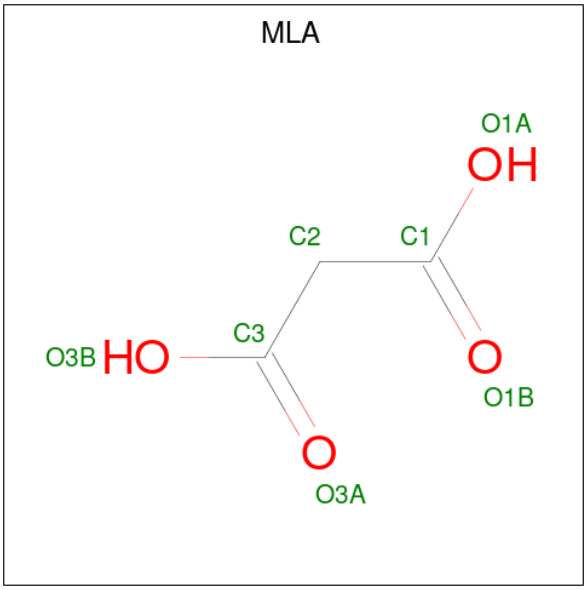
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C F N 23 18 3 2	0	0
7	H	1	Total C F N 23 18 3 2	0	0
7	F	1	Total C F N 23 18 3 2	0	0
7	D	1	Total C F N 23 18 3 2	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



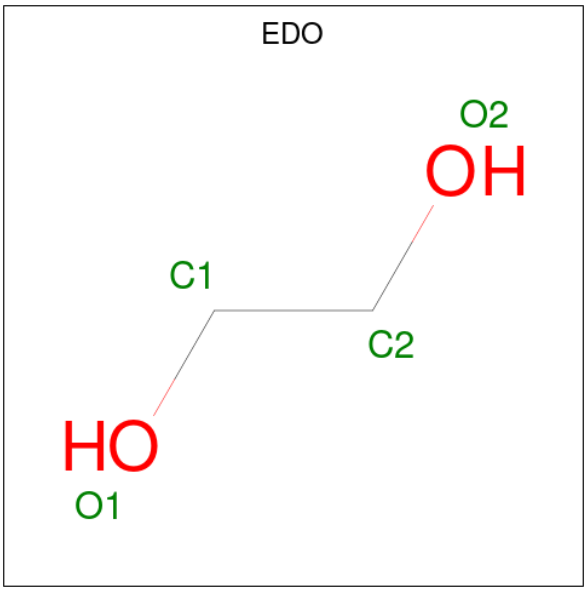
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0
8	H	1	Total C O 4 2 2	0	0
8	H	1	Total C O 4 2 2	0	0

- Molecule 9 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



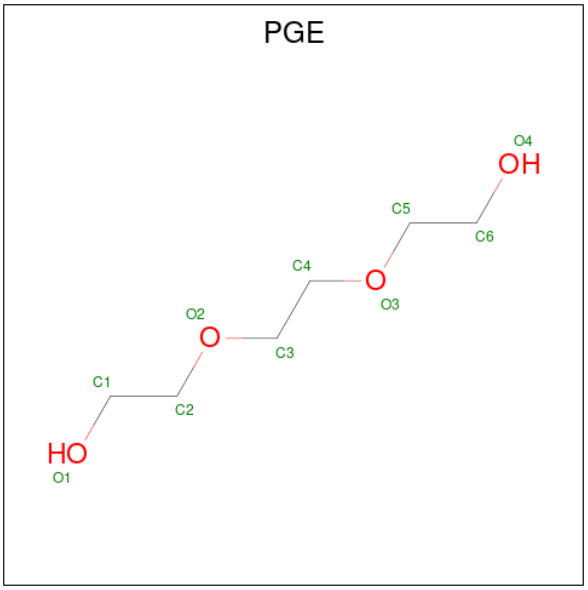
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total C O 7 3 4	0	0
9	F	1	Total C O 7 3 4	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 12 is water.

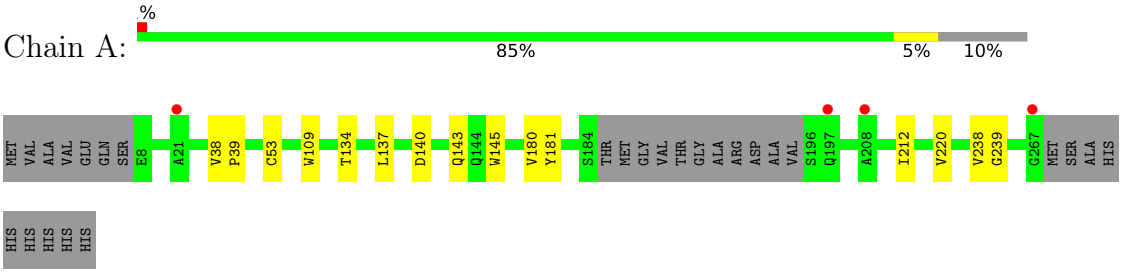
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	51	Total O 51 51	0	0
12	B	153	Total O 153 153	0	0
12	G	74	Total O 74 74	0	2
12	H	148	Total O 149 149	0	1
12	E	24	Total O 24 24	0	0
12	F	129	Total O 129 129	0	4
12	C	43	Total O 43 43	0	0
12	D	139	Total O 139 139	0	0

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.

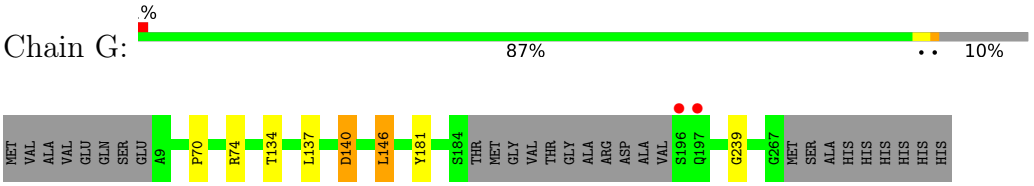
• Molecule 1: Tryptophan synthase alpha chain

Chain A:



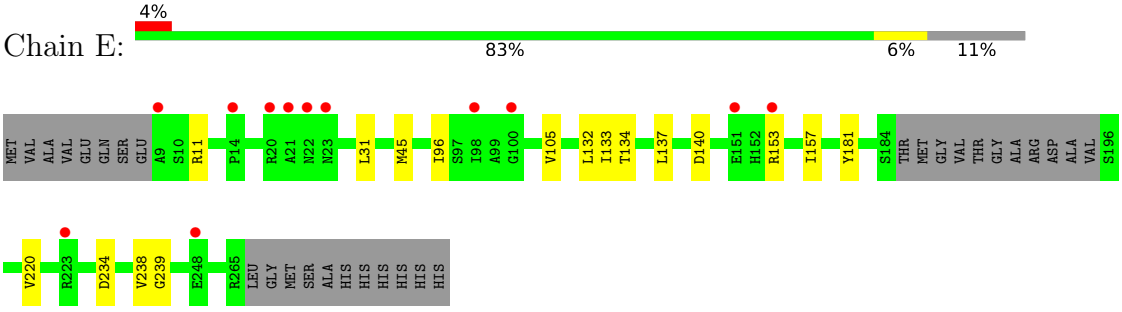
• Molecule 1: Tryptophan synthase alpha chain

Chain G:



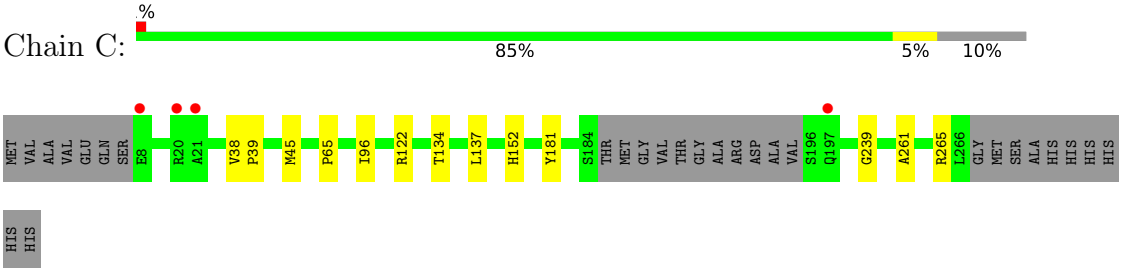
• Molecule 1: Tryptophan synthase alpha chain

Chain E:



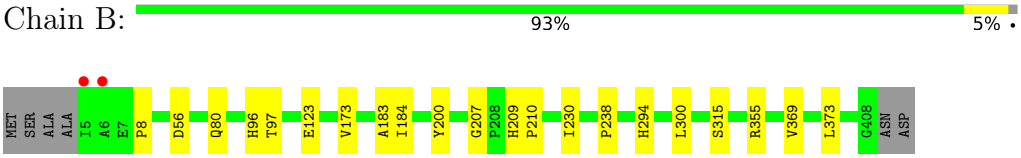
• Molecule 1: Tryptophan synthase alpha chain

Chain C:



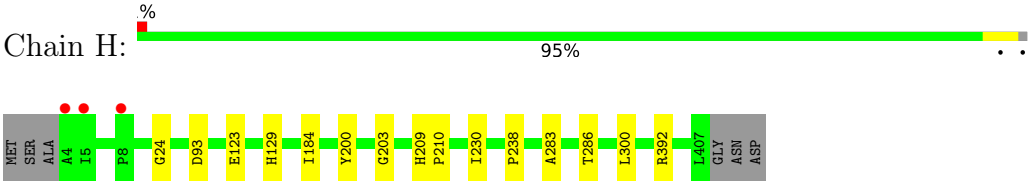
• Molecule 2: Tryptophan synthase beta chain

Chain B:



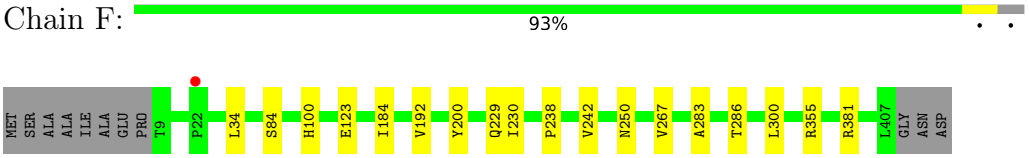
• Molecule 2: Tryptophan synthase beta chain

Chain H:



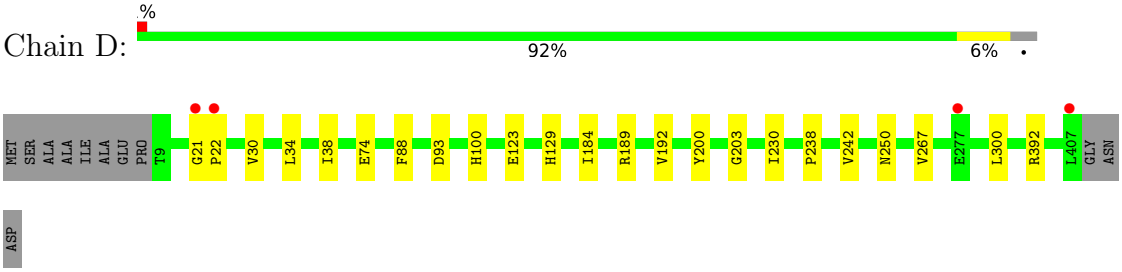
• Molecule 2: Tryptophan synthase beta chain

Chain F:



• Molecule 2: Tryptophan synthase beta chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.09Å 159.40Å 165.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.69 29.90 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.90-2.69) 99.1 (29.90-2.69)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.155 , 0.202 0.155 , 0.202	Depositor DCC
R_{free} test set	1955 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20363	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: HDJ, MLI, FMT, MLA, ACT, CS, P1T, EDO, PGE

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	0.24	0/1843	0.42	0/2514
1	C	0.24	0/1828	0.43	0/2495
1	E	0.24	0/1810	0.42	0/2472
1	G	0.24	0/1834	0.42	0/2502
2	B	0.25	0/3104	0.43	0/4205
2	D	0.25	0/3043	0.43	0/4123
2	F	0.25	0/3060	0.43	0/4146
2	H	0.25	0/3084	0.43	0/4180
All	All	0.25	0/19606	0.43	0/26637

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	1814	0	1834	6	0
1	C	1799	0	1819	6	0
1	E	1781	0	1792	7	0
1	G	1805	0	1828	4	0
2	B	3044	0	2953	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2983	0	2907	11	0
2	F	3000	0	2917	9	0
2	H	3023	0	2944	8	0
3	A	7	0	2	0	0
3	C	7	0	2	0	0
3	E	7	0	2	0	0
3	G	7	0	2	0	0
4	A	6	0	2	0	0
4	B	18	0	6	1	0
4	C	3	0	1	0	0
4	D	21	0	7	0	0
4	F	24	0	8	1	0
4	G	12	0	4	0	0
4	H	15	0	5	0	0
5	B	21	0	11	0	0
5	D	21	0	11	1	0
5	F	21	0	11	0	0
5	H	21	0	11	0	0
6	B	3	0	0	0	0
6	D	2	0	0	0	0
6	F	3	0	0	0	0
6	H	1	0	0	0	0
7	B	23	0	0	0	0
7	D	23	0	0	0	0
7	F	23	0	0	0	0
7	H	23	0	0	0	0
8	B	4	0	0	0	0
8	H	8	0	6	1	0
9	F	7	0	2	0	0
9	H	7	0	2	0	0
10	F	4	0	6	3	0
11	D	10	0	14	0	0
12	A	51	0	0	0	0
12	B	153	0	0	0	0
12	C	43	0	0	0	0
12	D	139	0	0	0	0
12	E	24	0	0	0	0
12	F	129	0	0	0	0
12	G	74	0	0	0	0
12	H	149	0	0	0	0
All	All	20363	0	19109	61	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 (61) 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	1.77	0.67
2:H:123:GLU:HG3	2:H:184:ILE:HG12	1.80	0.64
2:F:242:VAL:HG12	2:F:267:VAL:HB	1.81	0.63
1:C:261:ALA:O	1:C:265:ARG:NH1	2.36	0.59
1:G:140:ASP:N	1:G:140:ASP:OD1	2.33	0.58
1:C:65:PRO:O	2:D:189[A]:ARG:NH2	2.38	0.56
1:E:134:THR:HB	1:E:137:LEU:HB3	1.88	0.55
2:F:229:GLN:HG2	10:F:514:EDO:H12	1.89	0.55
1:A:134:THR:HB	1:A:137:LEU:HB3	1.88	0.54
2:F:123:GLU:HG3	2:F:184:ILE:HG12	1.89	0.54
2:D:230:ILE:HG21	2:D:238:PRO:HD3	1.90	0.53
1:E:45:MET:HB3	1:E:96:ILE:HD11	1.93	0.51
1:C:134:THR:HB	1:C:137:LEU:HB3	1.92	0.51
2:B:96:HIS:O	2:B:97:THR:OG1	2.28	0.50
1:G:134:THR:HB	1:G:137:LEU:HB3	1.92	0.50
2:D:123:GLU:HG3	2:D:184:ILE:HG12	1.94	0.49
1:E:220:VAL:HB	1:E:238:VAL:HG22	1.95	0.49
2:B:173:VAL:HG21	2:B:183:ALA:HA	1.94	0.47
1:A:220:VAL:HB	1:A:238:VAL:HG22	1.97	0.47
2:F:230:ILE:HG21	2:F:238:PRO:HD3	1.97	0.47
2:H:283:ALA:HB1	2:H:286:THR:HB	1.95	0.47
1:E:11:ARG:NH1	1:E:153:ARG:O	2.48	0.46
2:B:56:ASP:HB2	10:F:514:EDO:H21	1.98	0.46
2:B:355:ARG:HD3	4:B:506:FMT:H	1.97	0.46
2:H:24:GLY:HA2	8:H:510:ACT:H1	1.97	0.46
2:H:230:ILE:HG21	2:H:238:PRO:HD3	1.97	0.46
2:D:30:VAL:HG21	2:D:38:ILE:HD12	1.98	0.46
2:F:283:ALA:HB1	2:F:286:THR:HB	1.98	0.45
2:B:369:VAL:O	2:B:373:LEU:HG	2.17	0.44
1:A:109:TRP:CH2	1:A:145:TRP:HB2	2.52	0.44
2:F:355:ARG:HD3	4:F:510:FMT:H	2.00	0.44
2:D:93:ASP:HB2	2:D:392:ARG:HB3	1.99	0.44
2:H:129:HIS:CE1	2:H:203:GLY:HA2	2.53	0.44
2:B:209:HIS:ND1	2:B:210:PRO:HA	2.33	0.43
2:H:209:HIS:ND1	2:H:210:PRO:HA	2.32	0.43
2:F:34:LEU:HG	2:F:192:VAL:HG22	1.99	0.43
1:E:31:LEU:HD23	1:E:31:LEU:HA	1.92	0.43
1:E:105:VAL:HB	1:E:132:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:GLU:HB2	2:D:88:PHE:CE2	2.54	0.43
2:F:84:SER:HB3	2:F:381:ARG:HG3	2.00	0.43
1:C:122:ARG:HB2	1:C:152:HIS:CE1	2.53	0.42
1:A:180:VAL:HG23	1:A:212:ILE:HD13	2.01	0.42
2:H:93:ASP:HB2	2:H:392:ARG:HB3	2.00	0.42
1:E:133:ILE:HG12	1:E:157:ILE:HB	2.01	0.42
1:A:140:ASP:O	1:A:143:GLN:NE2	2.52	0.42
2:D:21:GLY:HA3	2:D:22:PRO:HD3	1.89	0.42
2:B:207:GLY:HA2	2:B:294:HIS:O	2.20	0.42
1:C:45:MET:HB3	1:C:96:ILE:HD11	2.00	0.42
1:A:38:VAL:HB	1:A:39:PRO:HD3	2.01	0.42
5:D:501:P1T:O3A	5:D:501:P1T:N	2.50	0.41
1:G:70:PRO:O	1:G:74:ARG:HG2	2.21	0.41
1:C:38:VAL:HB	1:C:39:PRO:HD3	2.02	0.41
1:G:146:LEU:HD12	1:G:146:LEU:HA	1.90	0.41
2:D:100:HIS:CE1	2:D:250:ASN:HB3	2.56	0.41
2:B:230:ILE:HG21	2:B:238:PRO:HD3	2.02	0.41
2:F:100:HIS:NE2	2:F:250:ASN:HB3	2.35	0.41
2:D:34:LEU:HG	2:D:192:VAL:HG22	2.02	0.41
2:D:242:VAL:HG12	2:D:267:VAL:HB	2.02	0.41
2:B:56:ASP:CB	10:F:514:EDO:H21	2.51	0.40
2:H:123:GLU:O	2:H:129:HIS:HD2	2.04	0.40
2:D:129:HIS:CE1	2:D:203:GLY:HA2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/276 (89%)	240 (98%)	5 (2%)	1 (0%)	34	60
1	C	244/276 (88%)	237 (97%)	6 (2%)	1 (0%)	34	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	243/276 (88%)	235 (97%)	7 (3%)	1 (0%)	34 60
1	G	245/276 (89%)	240 (98%)	4 (2%)	1 (0%)	34 60
2	B	407/410 (99%)	394 (97%)	12 (3%)	1 (0%)	47 73
2	D	398/410 (97%)	387 (97%)	11 (3%)	0	100 100
2	F	400/410 (98%)	388 (97%)	12 (3%)	0	100 100
2	H	404/410 (98%)	394 (98%)	10 (2%)	0	100 100
All	All	2587/2744 (94%)	2515 (97%)	67 (3%)	5 (0%)	47 73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	239	GLY
1	A	239	GLY
1	E	239	GLY
2	B	8	PRO
1	G	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	180/200 (90%)	178 (99%)	2 (1%)	73 90
1	C	179/200 (90%)	178 (99%)	1 (1%)	86 95
1	E	176/200 (88%)	173 (98%)	3 (2%)	60 84
1	G	179/200 (90%)	176 (98%)	3 (2%)	60 84
2	B	300/302 (99%)	296 (99%)	4 (1%)	69 87
2	D	296/302 (98%)	294 (99%)	2 (1%)	84 94
2	F	298/302 (99%)	296 (99%)	2 (1%)	84 94
2	H	300/302 (99%)	298 (99%)	2 (1%)	84 94
All	All	1908/2008 (95%)	1889 (99%)	19 (1%)	76 91

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

Mol	Chain	Res	Type
1	A	53	CYS
1	A	181	TYR
2	B	80	GLN
2	B	200	TYR
2	B	300	LEU
2	B	315	SER
1	G	140	ASP
1	G	146	LEU
1	G	181	TYR
2	H	200	TYR
2	H	300	LEU
1	E	140	ASP
1	E	181	TYR
1	E	234	ASP
2	F	200	TYR
2	F	300	LEU
1	C	181	TYR
2	D	200	TYR
2	D	300	LEU

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 61 ligands modelled in this entry, 9 are monoatomic - leaving 52 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	$\#\|Z\| > 2$
4	FMT	D	506	-	2,2,2	0.70	0	1,1,1	0.59	0
4	FMT	H	503	-	2,2,2	0.69	0	1,1,1	0.60	0
4	FMT	H	504	-	2,2,2	0.68	0	1,1,1	0.62	0
4	FMT	A	302	-	2,2,2	0.71	0	1,1,1	0.57	0
4	FMT	F	508	-	2,2,2	0.68	0	1,1,1	0.64	0
4	FMT	G	304	-	2,2,2	0.71	0	1,1,1	0.58	0
4	FMT	D	505	-	2,2,2	0.70	0	1,1,1	0.60	0
4	FMT	D	504	-	2,2,2	0.69	0	1,1,1	0.60	0
9	MLA	F	515	-	6,6,6	1.08	0	7,7,7	1.00	0
4	FMT	F	510	-	2,2,2	0.67	0	1,1,1	0.60	0
3	MLI	C	301	-	6,6,6	1.09	0	7,7,7	0.94	0
4	FMT	F	511	-	2,2,2	0.70	0	1,1,1	0.60	0
8	ACT	H	510	-	3,3,3	0.78	0	3,3,3	0.75	0
7	HDJ	D	511	-	23,25,25	1.15	1 (4%)	23,36,36	1.44	3 (13%)
4	FMT	B	507	-	2,2,2	0.70	0	1,1,1	0.60	0
4	FMT	B	506	-	2,2,2	0.70	0	1,1,1	0.59	0
4	FMT	D	510	-	2,2,2	0.70	0	1,1,1	0.61	0
5	P1T	F	501	-	20,21,21	2.61	4 (20%)	28,30,30	1.62	8 (28%)
4	FMT	F	509	-	2,2,2	0.70	0	1,1,1	0.59	0
3	MLI	E	301	-	6,6,6	1.09	0	7,7,7	1.03	0
4	FMT	B	510	-	2,2,2	0.69	0	1,1,1	0.61	0
9	MLA	H	511	-	6,6,6	1.16	0	7,7,7	1.51	2 (28%)
4	FMT	D	509	-	2,2,2	0.70	0	1,1,1	0.60	0
4	FMT	G	305	-	2,2,2	0.69	0	1,1,1	0.61	0
7	HDJ	H	508	-	23,25,25	1.14	1 (4%)	23,36,36	1.74	5 (21%)
7	HDJ	F	513	-	23,25,25	1.31	1 (4%)	23,36,36	1.56	4 (17%)
3	MLI	A	301	-	6,6,6	1.08	0	7,7,7	0.96	0
5	P1T	B	501	-	20,21,21	2.68	4 (20%)	28,30,30	1.52	6 (21%)
4	FMT	F	512	-	2,2,2	0.70	0	1,1,1	0.59	0
8	ACT	B	512	2	3,3,3	0.80	0	3,3,3	0.74	0
4	FMT	B	509	-	2,2,2	0.70	0	1,1,1	0.58	0
8	ACT	H	509	-	3,3,3	0.77	0	3,3,3	0.70	0
4	FMT	F	505	-	2,2,2	0.67	0	1,1,1	0.63	0
4	FMT	B	508	-	2,2,2	0.70	0	1,1,1	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	F	506	-	2,2,2	0.70	0	1,1,1	0.60	0
4	FMT	D	507	-	2,2,2	0.68	0	1,1,1	0.60	0
5	P1T	H	501	-	20,21,21	2.65	4 (20%)	28,30,30	1.57	7 (25%)
4	FMT	G	303	-	2,2,2	0.71	0	1,1,1	0.58	0
3	MLI	G	301	-	6,6,6	1.09	0	7,7,7	0.95	0
4	FMT	G	302	-	2,2,2	0.71	0	1,1,1	0.58	0
5	P1T	D	501	-	20,21,21	2.76	4 (20%)	28,30,30	2.08	7 (25%)
10	EDO	F	514	-	3,3,3	0.47	0	2,2,2	0.19	0
4	FMT	B	505	-	2,2,2	0.70	0	1,1,1	0.60	0
4	FMT	C	302	-	2,2,2	0.68	0	1,1,1	0.62	0
4	FMT	F	507	-	2,2,2	0.69	0	1,1,1	0.59	0
4	FMT	D	508	-	2,2,2	0.70	0	1,1,1	0.57	0
4	FMT	H	505	-	2,2,2	0.70	0	1,1,1	0.59	0
4	FMT	H	507	-	2,2,2	0.71	0	1,1,1	0.58	0
11	PGE	D	512	-	9,9,9	0.30	0	8,8,8	0.34	0
4	FMT	H	506	-	2,2,2	0.68	0	1,1,1	0.59	0
7	HDJ	B	511	-	23,25,25	1.18	1 (4%)	23,36,36	1.63	5 (21%)
4	FMT	A	303	-	2,2,2	0.69	0	1,1,1	0.59	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	MLI	E	301	-	-	4/4/4/4	-
3	MLI	G	301	-	-	0/4/4/4	-
9	MLA	F	515	-	-	2/4/4/4	-
9	MLA	H	511	-	-	0/4/4/4	-
7	HDJ	H	508	-	-	1/8/24/24	0/3/3/3
7	HDJ	F	513	-	-	1/8/24/24	0/3/3/3
3	MLI	A	301	-	-	2/4/4/4	-
5	P1T	B	501	-	-	10/14/15/15	0/1/1/1
3	MLI	C	301	-	-	0/4/4/4	-
11	PGE	D	512	-	-	3/7/7/7	-
5	P1T	D	501	-	-	3/14/15/15	0/1/1/1
7	HDJ	B	511	-	-	1/8/24/24	0/3/3/3
7	HDJ	D	511	-	-	0/8/24/24	0/3/3/3
5	P1T	H	501	-	-	6/14/15/15	0/1/1/1
10	EDO	F	514	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	P1T	F	501	-	-	9/14/15/15	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	P1T	C3-C2	8.09	1.49	1.40
5	B	501	P1T	C3-C2	8.02	1.48	1.40
5	F	501	P1T	C3-C2	7.96	1.48	1.40
5	H	501	P1T	C3-C2	7.92	1.48	1.40
5	D	501	P1T	C5-C4	5.85	1.48	1.40
5	B	501	P1T	C5-C4	5.70	1.48	1.40
5	D	501	P1T	C3-C4	5.61	1.48	1.40
5	H	501	P1T	C3-C4	5.60	1.48	1.40
7	F	513	HDJ	C13-C15	-5.57	1.50	1.56
5	F	501	P1T	C5-C4	5.52	1.48	1.40
5	H	501	P1T	C5-C4	5.50	1.48	1.40
5	B	501	P1T	C3-C4	5.48	1.48	1.40
5	F	501	P1T	C3-C4	5.30	1.48	1.40
7	B	511	HDJ	C13-C15	-4.84	1.51	1.56
7	D	511	HDJ	C13-C15	-4.63	1.51	1.56
7	H	508	HDJ	C13-C15	-4.52	1.52	1.56
5	D	501	P1T	CA-C	-3.43	1.44	1.49
5	B	501	P1T	CA-C	-2.67	1.45	1.49
5	H	501	P1T	CA-C	-2.65	1.46	1.49
5	F	501	P1T	CA-C	-2.39	1.46	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	501	P1T	CB-CA-N	-6.01	111.33	125.91
7	F	513	HDJ	C8-C7-C12	4.96	119.43	114.56
7	H	508	HDJ	C8-C7-C12	4.96	119.43	114.56
5	D	501	P1T	C-CA-N	4.89	124.51	112.45
7	B	511	HDJ	C8-C7-C12	4.82	119.29	114.56
7	D	511	HDJ	C8-C7-C12	4.66	119.14	114.56
5	D	501	P1T	CB-CA-C	-3.98	110.25	120.72
7	H	508	HDJ	C15-C17-N2	-3.31	174.10	177.70
5	H	501	P1T	C4A-C4-C3	3.13	123.39	120.04
7	F	513	HDJ	C11-C12-C7	-3.08	119.94	123.45
7	H	508	HDJ	C11-C12-C7	-3.04	119.98	123.45
7	B	511	HDJ	C11-C12-C7	-2.97	120.06	123.45
5	F	501	P1T	C-CA-N	2.87	119.52	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	511	HDJ	C11-C12-C7	-2.84	120.21	123.45
5	B	501	P1T	C-CA-N	2.74	119.21	112.45
5	F	501	P1T	C6-C5-C4	2.61	119.96	118.12
5	F	501	P1T	OP4-C5A-C5	-2.59	104.42	109.35
5	B	501	P1T	C4A-C4-C3	2.52	122.75	120.04
5	F	501	P1T	C4A-C4-C3	2.48	122.70	120.04
5	H	501	P1T	C-CA-N	2.40	118.38	112.45
5	B	501	P1T	C4A-N-CA	-2.38	120.48	125.82
5	H	501	P1T	OP4-C5A-C5	-2.37	104.83	109.35
7	H	508	HDJ	C9-C8-C7	-2.37	120.75	123.45
5	F	501	P1T	CB-CA-N	-2.35	120.21	125.91
5	D	501	P1T	C4A-N-CA	-2.33	120.57	125.82
7	F	513	HDJ	C9-C8-C7	-2.33	120.79	123.45
7	B	511	HDJ	C9-C8-C7	-2.32	120.80	123.45
7	D	511	HDJ	C9-C8-C7	-2.30	120.82	123.45
5	H	501	P1T	O-C-CA	2.29	119.10	114.14
7	B	511	HDJ	C6-C5-C7	-2.28	117.02	120.79
5	B	501	P1T	CB-CA-N	-2.26	120.42	125.91
7	H	508	HDJ	C5-C7-C8	-2.24	117.47	120.92
5	H	501	P1T	C6-N1-C2	2.23	123.30	119.17
5	H	501	P1T	C6-C5-C4	2.22	119.69	118.12
5	B	501	P1T	C6-N1-C2	2.20	123.24	119.17
5	F	501	P1T	C6-N1-C2	2.19	123.23	119.17
5	D	501	P1T	C6-N1-C2	2.19	123.22	119.17
5	D	501	P1T	C4A-C4-C3	2.18	122.38	120.04
5	F	501	P1T	C4A-N-CA	-2.17	120.94	125.82
5	D	501	P1T	O-C-CA	2.15	118.79	114.14
5	F	501	P1T	O-C-CA	2.13	118.75	114.14
7	F	513	HDJ	C5-C7-C8	-2.09	117.72	120.92
7	B	511	HDJ	C5-C7-C8	-2.07	117.73	120.92
9	H	511	MLA	O1A-C1-C2	2.05	121.10	114.54
5	B	501	P1T	O-C-CA	2.05	118.58	114.14
9	H	511	MLA	O3B-C3-C2	2.04	121.07	114.54
5	H	501	P1T	OP3-P-OP1	2.03	115.38	107.64

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	P1T	C5A-OP4-P-OP1
5	B	501	P1T	C5A-OP4-P-OP2
5	B	501	P1T	C5-C4-C4A-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	501	P1T	O-C-CA-N
5	B	501	P1T	OXT-C-CA-N
5	H	501	P1T	C5A-OP4-P-OP1
5	H	501	P1T	C5A-OP4-P-OP2
5	H	501	P1T	C5-C4-C4A-N
5	F	501	P1T	C5A-OP4-P-OP1
5	F	501	P1T	C5A-OP4-P-OP3
5	F	501	P1T	C5-C4-C4A-N
5	F	501	P1T	C3-C4-C4A-N
5	D	501	P1T	C5-C4-C4A-N
11	D	512	PGE	O3-C5-C6-O4
5	B	501	P1T	C3-C4-C4A-N
5	H	501	P1T	C3-C4-C4A-N
3	A	301	MLI	C2-C1-C3-O9
5	B	501	P1T	C-CA-N-C4A
5	H	501	P1T	C-CA-N-C4A
5	F	501	P1T	C-CA-N-C4A
5	D	501	P1T	C-CA-N-C4A
5	F	501	P1T	C5A-OP4-P-OP2
3	E	301	MLI	C2-C1-C3-O9
9	F	515	MLA	O1A-C1-C2-C3
3	A	301	MLI	C2-C1-C3-O8
5	F	501	P1T	OXT-C-CA-N
5	B	501	P1T	C5A-OP4-P-OP3
5	H	501	P1T	C5A-OP4-P-OP3
11	D	512	PGE	C3-C4-O3-C5
3	E	301	MLI	C2-C1-C3-O8
9	F	515	MLA	O1B-C1-C2-C3
5	B	501	P1T	O-C-CA-CB
5	B	501	P1T	OXT-C-CA-CB
3	E	301	MLI	C3-C1-C2-O7
5	D	501	P1T	C3-C4-C4A-N
7	B	511	HDJ	C15-C13-C2-C1
7	H	508	HDJ	C15-C13-C2-C1
7	F	513	HDJ	C15-C13-C2-C1
11	D	512	PGE	O1-C1-C2-O2
3	E	301	MLI	C3-C1-C2-O6
5	F	501	P1T	O-C-CA-CB
5	F	501	P1T	OXT-C-CA-CB
10	F	514	EDO	O1-C1-C2-O2

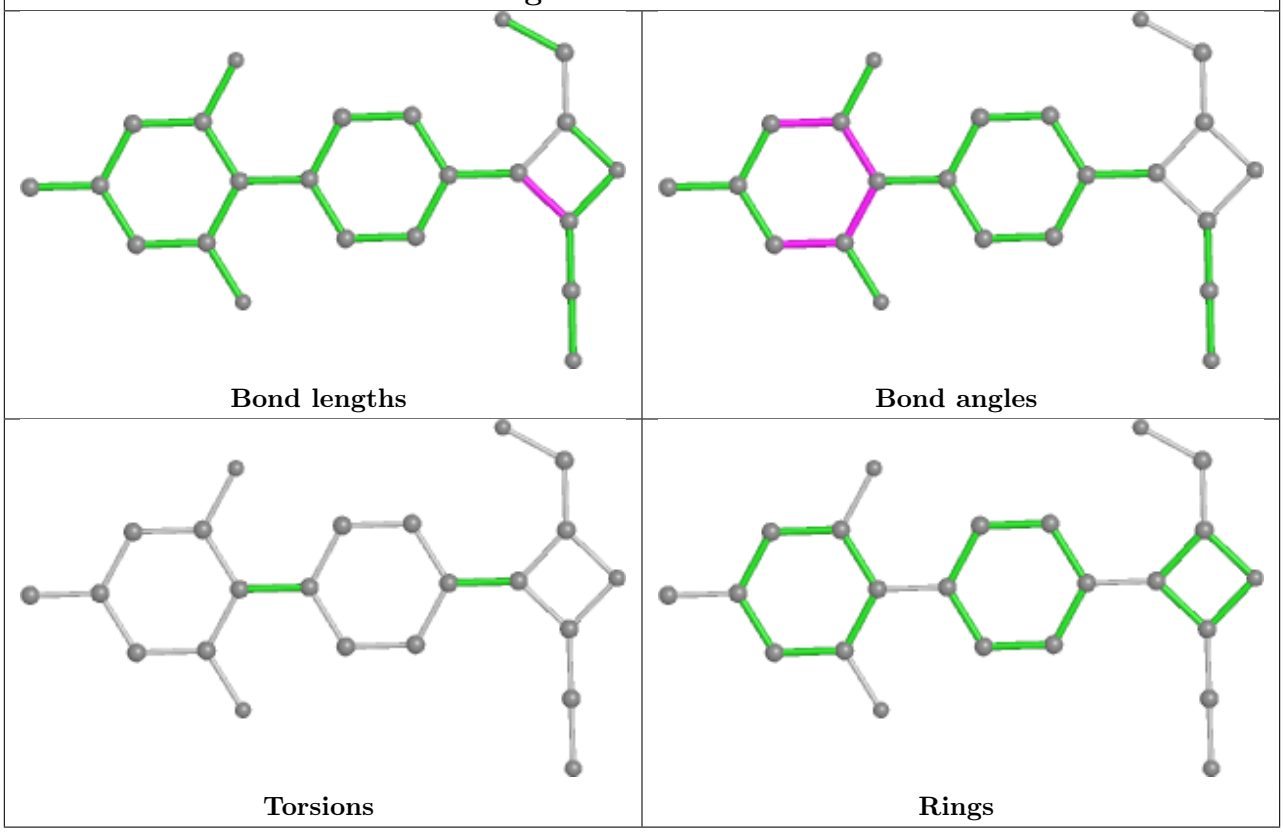
There are no ring outliers.

5 monomers are involved in 7 short contacts:

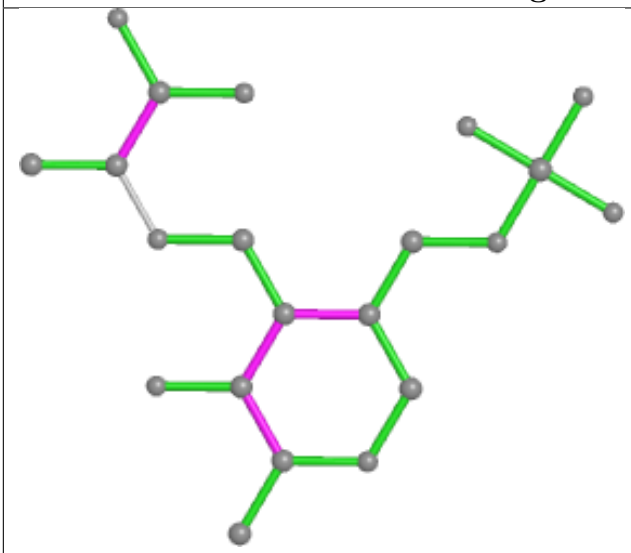
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	510	FMT	1	0
8	H	510	ACT	1	0
4	B	506	FMT	1	0
5	D	501	P1T	1	0
10	F	514	EDO	3	0

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 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.

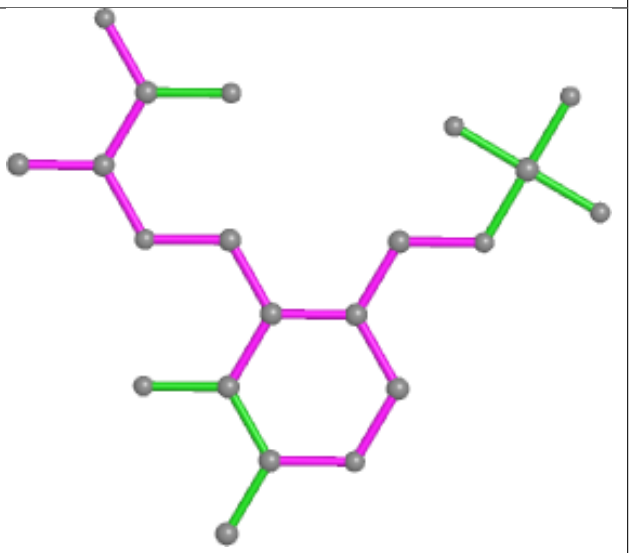
Ligand HDJ D 511



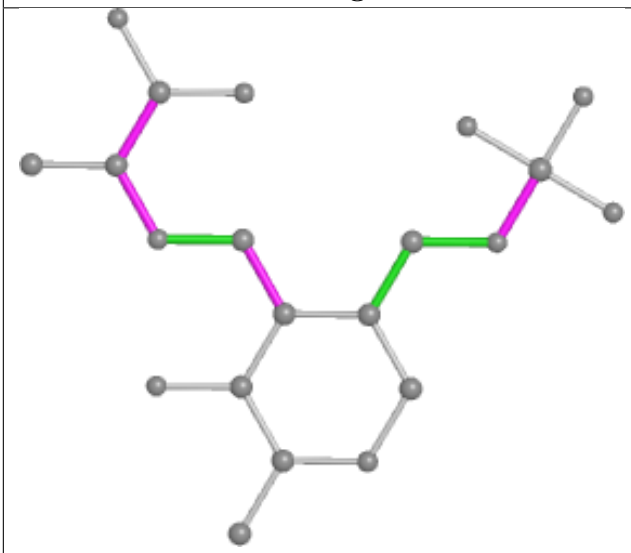
Ligand P1T F 501



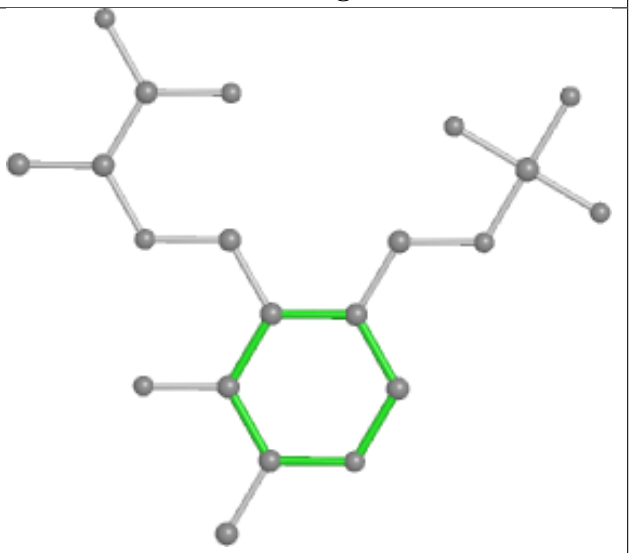
Bond lengths



Bond angles

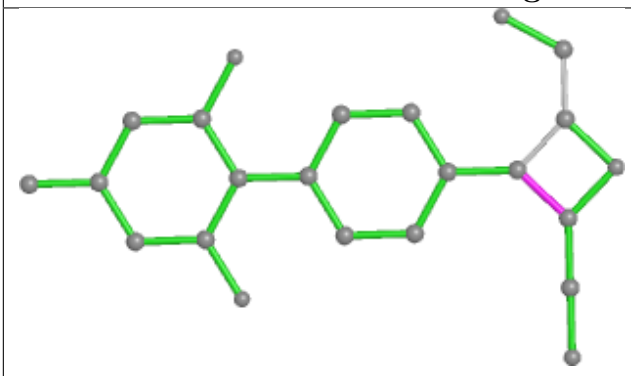


Torsions

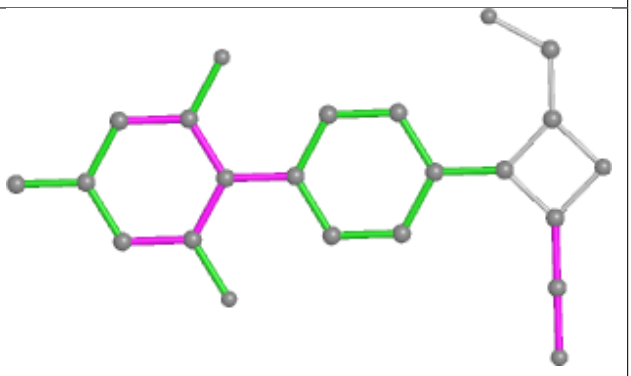


Rings

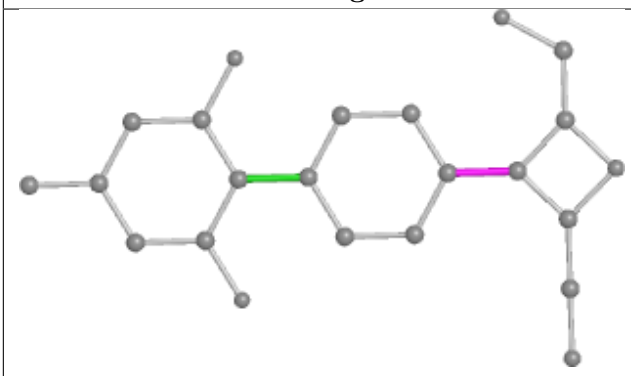
Ligand HDJ H 508



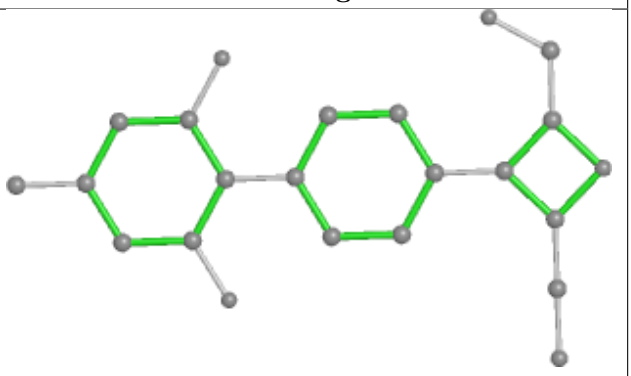
Bond lengths



Bond angles

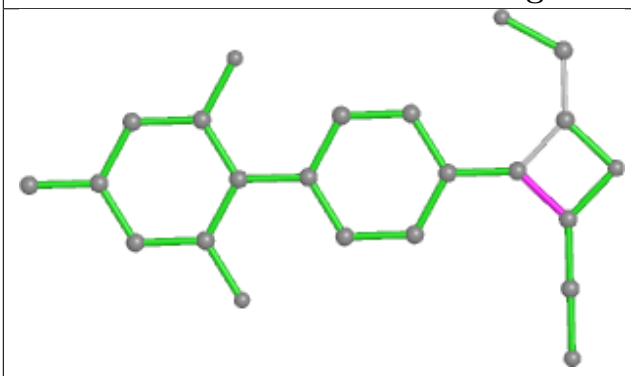


Torsions

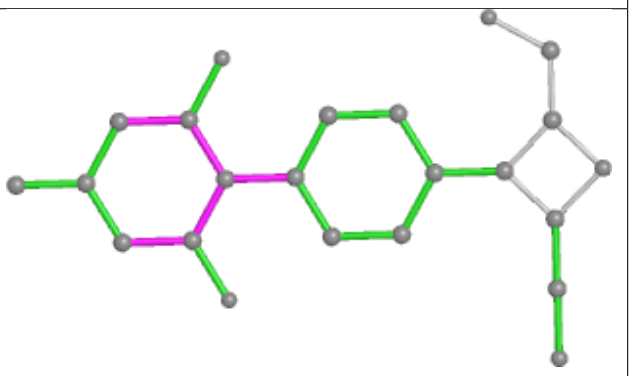


Rings

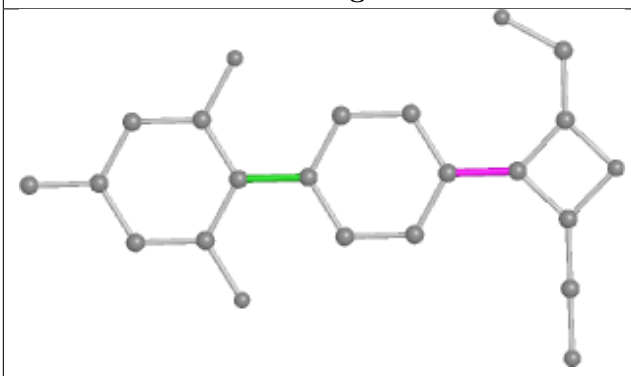
Ligand HDJ F 513



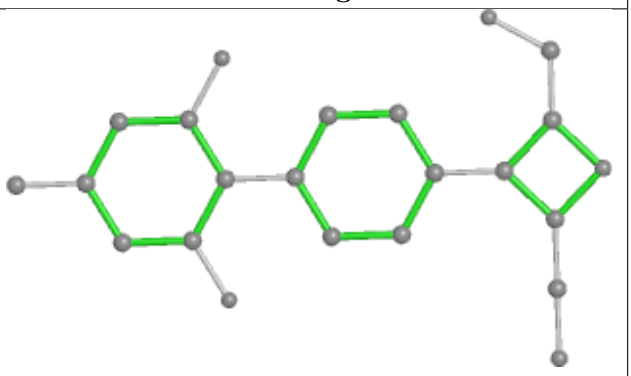
Bond lengths



Bond angles

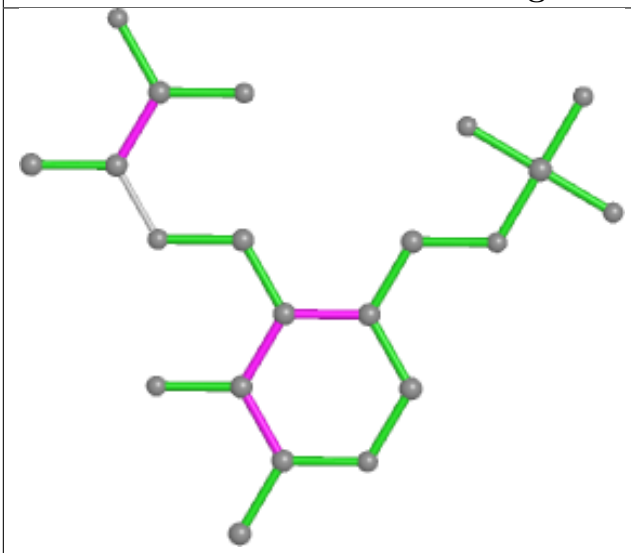


Torsions

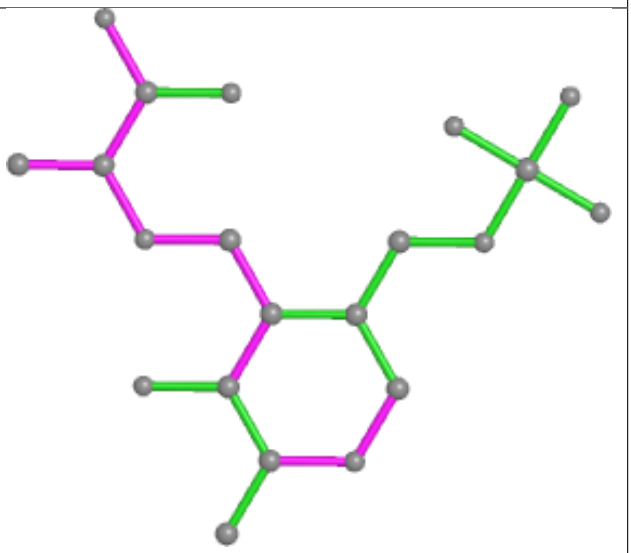


Rings

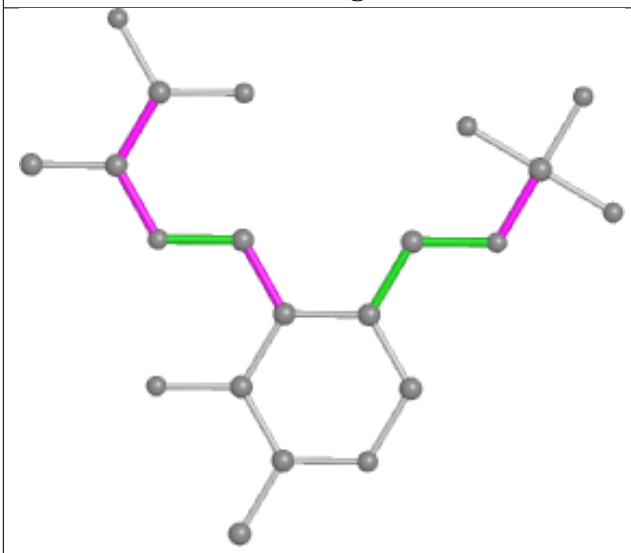
Ligand P1T B 501



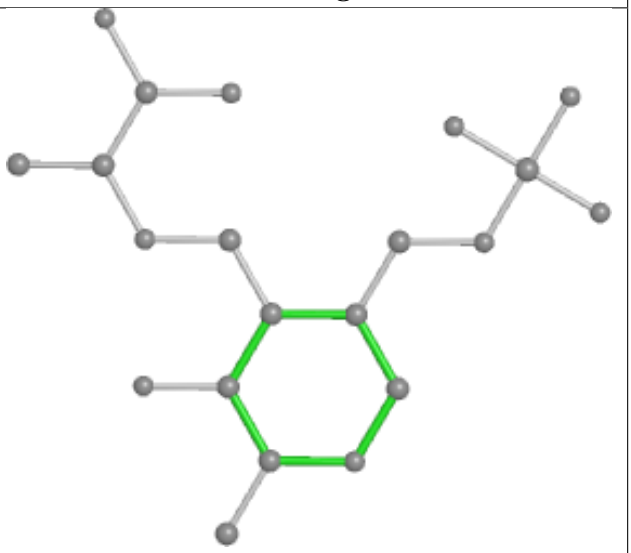
Bond lengths



Bond angles

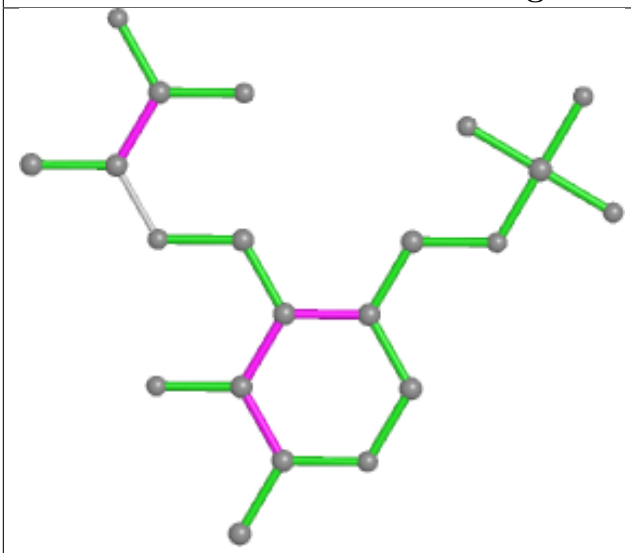


Torsions

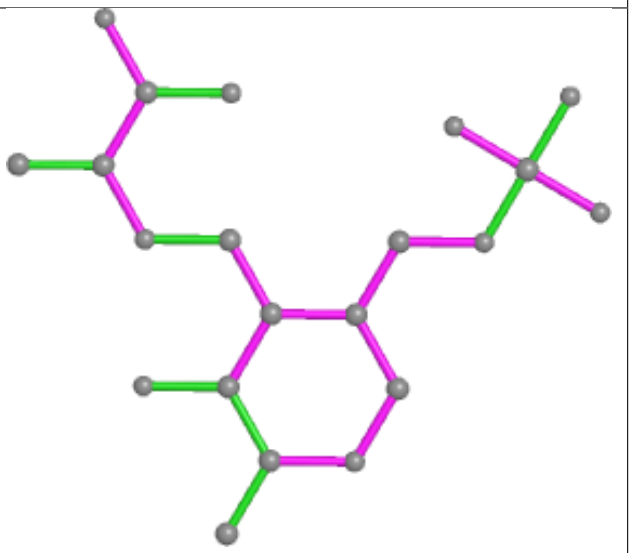


Rings

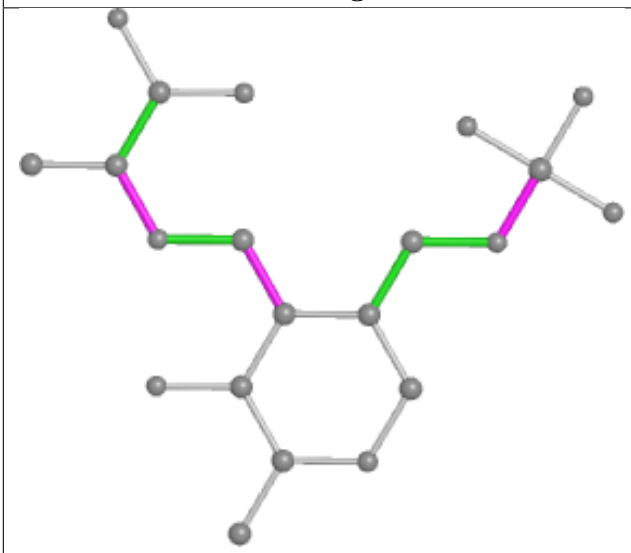
Ligand P1T H 501



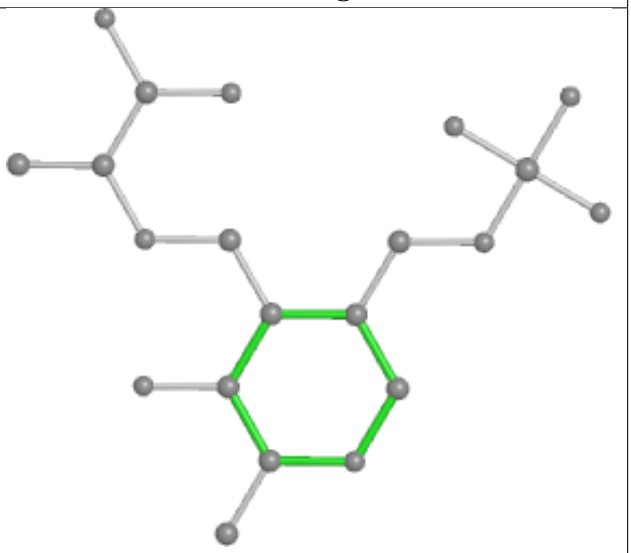
Bond lengths



Bond angles

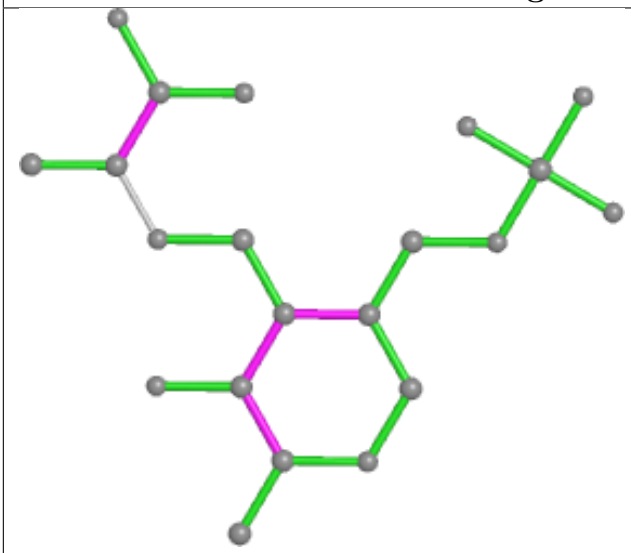


Torsions

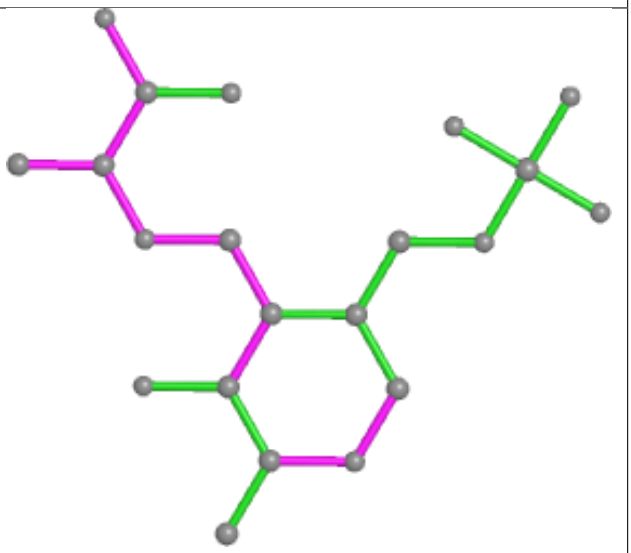


Rings

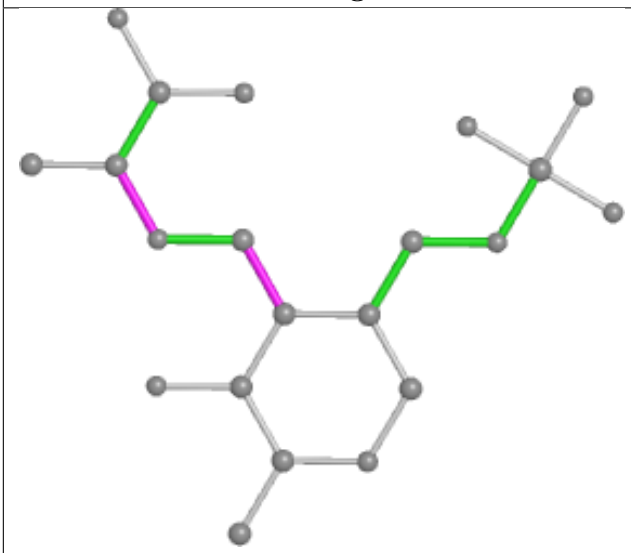
Ligand P1T D 501



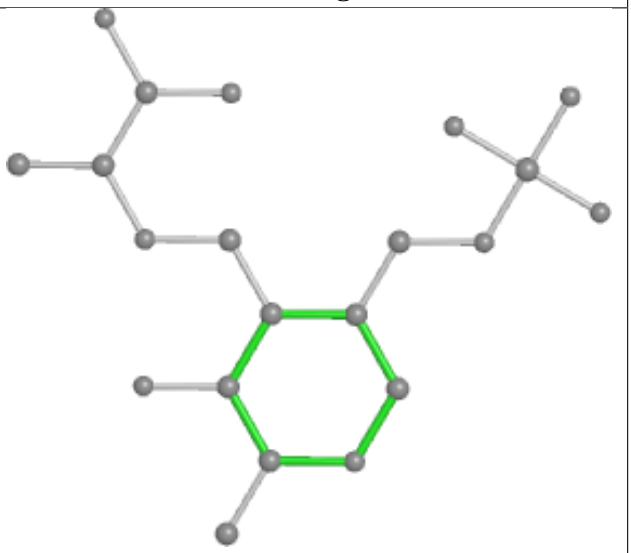
Bond lengths



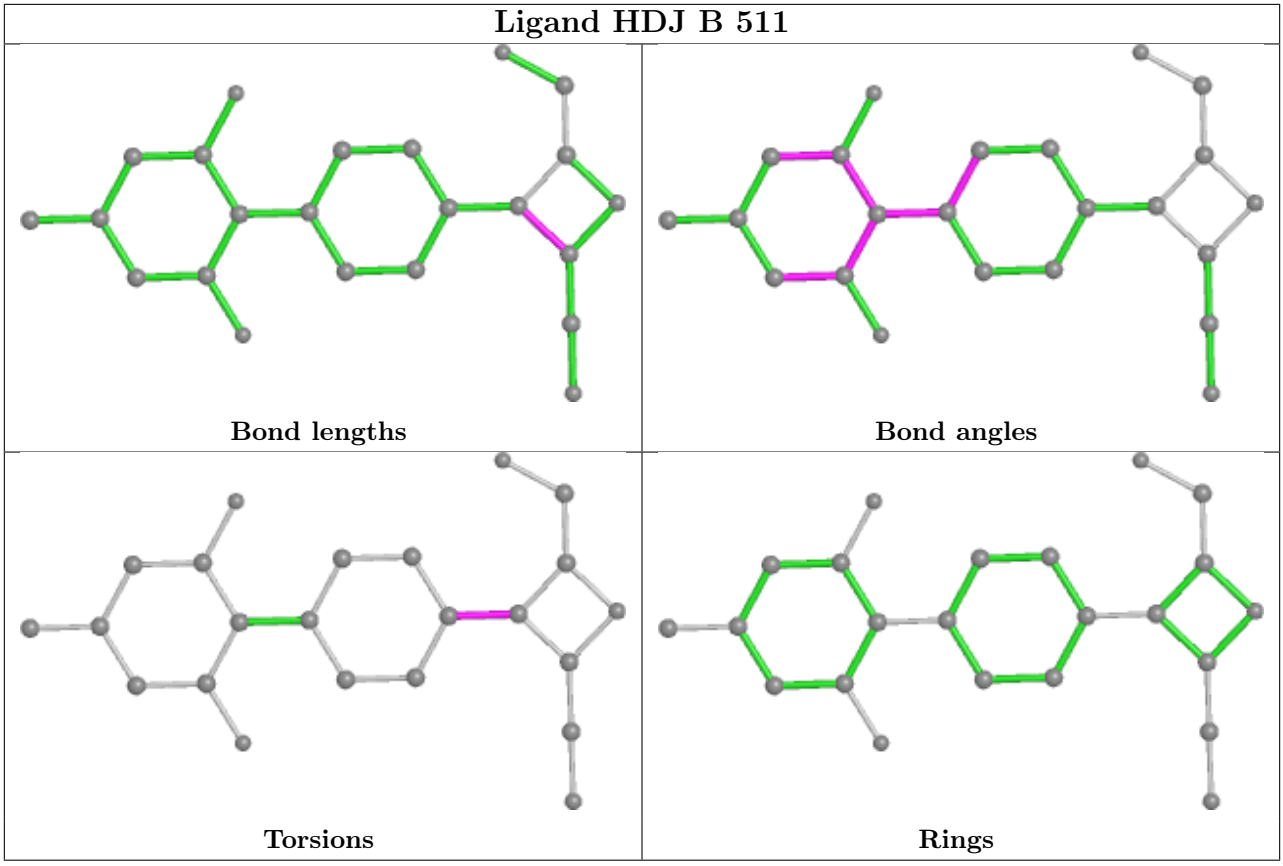
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	249/276 (90%)	-0.44	4 (1%)	72	74	26, 44, 70, 107	0
1	C	248/276 (89%)	-0.31	4 (1%)	72	74	28, 50, 87, 124	0
1	E	246/276 (89%)	-0.02	12 (4%)	29	28	39, 69, 108, 134	0
1	G	248/276 (89%)	-0.55	2 (0%)	86	87	27, 42, 65, 106	0
2	B	404/410 (98%)	-0.68	2 (0%)	91	92	20, 31, 56, 127	0
2	D	399/410 (97%)	-0.63	4 (1%)	82	83	20, 31, 52, 88	0
2	F	399/410 (97%)	-0.70	1 (0%)	94	95	18, 32, 57, 118	0
2	H	404/410 (98%)	-0.68	3 (0%)	87	89	17, 29, 53, 146	0
All	All	2597/2744 (94%)	-0.54	32 (1%)	79	80	17, 36, 80, 146	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	GLU	4.8
1	A	267	GLY	3.1
2	D	22	PRO	3.0
1	E	22	ASN	2.9
1	C	21	ALA	2.8
1	E	9	ALA	2.7
1	C	197	GLN	2.6
1	E	21	ALA	2.6
1	E	23	ASN	2.6
2	B	6	ALA	2.5
2	H	8	PRO	2.5
2	F	22	PRO	2.4
1	G	197	GLN	2.4
1	E	98	ILE	2.4
1	E	20	ARG	2.4
2	D	21	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	5	ILE	2.3
1	E	100	GLY	2.3
1	G	196	SER	2.2
1	C	20	ARG	2.2
2	H	4	ALA	2.2
2	B	5	ILE	2.2
1	A	208	ALA	2.1
1	E	14	PRO	2.1
1	A	21	ALA	2.1
1	E	248	GLU	2.1
2	D	407	LEU	2.1
2	D	277	GLU	2.1
1	E	223	ARG	2.1
1	E	151	GLU	2.0
1	A	197	GLN	2.0
1	E	153	ARG	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
6	CS	D	503	1/1	0.65	0.20	185,185,185,185	1
9	MLA	H	511	7/7	0.66	0.44	100,100,110,115	0
6	CS	B	503	1/1	0.71	0.16	112,112,112,112	1
4	FMT	B	508	3/3	0.75	0.32	64,64,80,85	0
4	FMT	B	509	3/3	0.79	0.33	78,78,84,86	0
8	ACT	B	512	4/4	0.80	0.31	58,63,70,73	0
4	FMT	D	508	3/3	0.80	0.24	54,54,68,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	H	507	3/3	0.81	0.23	52,52,56,63	0
3	MLI	C	301	7/7	0.81	0.19	63,72,76,79	0
8	ACT	H	510	4/4	0.81	0.22	67,81,81,83	0
4	FMT	G	302	3/3	0.81	0.41	63,63,65,72	0
4	FMT	G	304	3/3	0.83	0.55	72,72,78,79	0
4	FMT	F	509	3/3	0.84	0.26	59,59,65,67	0
6	CS	B	504	1/1	0.85	0.08	111,111,111,111	1
11	PGE	D	512	10/10	0.85	0.47	63,80,88,90	0
6	CS	F	504	1/1	0.86	0.08	106,106,106,106	1
4	FMT	F	511	3/3	0.87	0.28	88,88,93,94	0
8	ACT	H	509	4/4	0.88	0.22	46,58,69,70	0
4	FMT	D	509	3/3	0.88	0.33	60,60,64,64	0
4	FMT	F	512	3/3	0.88	0.25	57,57,60,64	0
10	EDO	F	514	4/4	0.88	0.44	64,65,66,68	0
4	FMT	A	302	3/3	0.88	0.39	50,50,57,61	0
9	MLA	F	515	7/7	0.89	0.28	87,88,92,92	0
4	FMT	B	510	3/3	0.89	0.36	84,84,84,84	0
4	FMT	H	505	3/3	0.89	0.41	75,75,81,83	0
4	FMT	D	510	3/3	0.90	0.42	75,75,79,79	0
4	FMT	D	505	3/3	0.90	0.12	66,66,71,72	0
4	FMT	G	303	3/3	0.90	0.35	50,50,64,66	0
4	FMT	H	506	3/3	0.90	0.21	68,68,72,72	0
4	FMT	D	506	3/3	0.91	0.20	77,77,78,82	0
4	FMT	G	305	3/3	0.92	0.26	64,64,69,73	0
4	FMT	F	510	3/3	0.93	0.12	60,60,61,62	0
7	HDJ	D	511	23/23	0.93	0.20	47,60,74,77	0
4	FMT	D	507	3/3	0.93	0.14	59,59,63,63	0
4	FMT	A	303	3/3	0.94	0.46	68,68,71,72	0
4	FMT	B	507	3/3	0.94	0.18	67,67,79,86	0
3	MLI	A	301	7/7	0.94	0.12	45,54,59,62	0
3	MLI	E	301	7/7	0.94	0.15	68,71,77,81	0
6	CS	F	503	1/1	0.94	0.16	118,118,118,118	1
4	FMT	F	506	3/3	0.95	0.20	38,38,47,48	0
4	FMT	H	503	3/3	0.95	0.16	60,60,74,84	0
4	FMT	F	507	3/3	0.96	0.09	44,44,48,51	0
7	HDJ	B	511	23/23	0.96	0.18	24,36,45,50	0
7	HDJ	H	508	23/23	0.96	0.19	32,38,54,56	0
7	HDJ	F	513	23/23	0.96	0.15	25,38,57,63	0
4	FMT	D	504	3/3	0.96	0.21	40,40,41,43	0
4	FMT	B	506	3/3	0.96	0.16	33,33,34,44	0
4	FMT	B	505	3/3	0.97	0.11	48,48,53,54	0
4	FMT	C	302	3/3	0.97	0.09	40,40,44,55	0

Continued on next page...

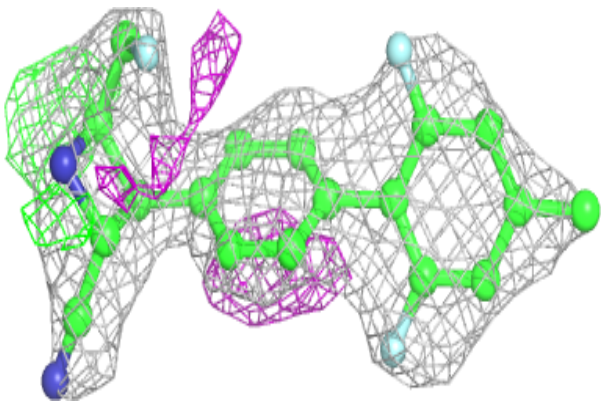
Continued from previous page...

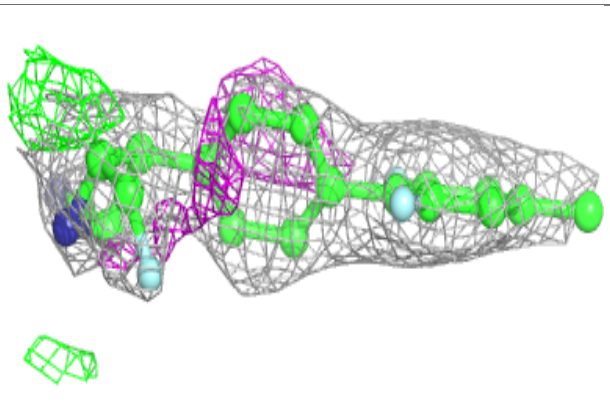
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	H	504	3/3	0.97	0.21	53,53,55,56	0
4	FMT	F	505	3/3	0.97	0.22	62,62,66,72	0
3	MLI	G	301	7/7	0.97	0.10	50,58,61,62	0
4	FMT	F	508	3/3	0.98	0.15	40,40,42,42	0
5	P1T	D	501	21/21	0.98	0.20	20,28,39,40	0
6	CS	D	502	1/1	0.98	0.12	71,71,71,71	1
6	CS	H	502	1/1	0.98	0.12	68,68,68,68	1
6	CS	F	502	1/1	0.98	0.10	76,76,76,76	1
6	CS	B	502	1/1	0.99	0.13	67,67,67,67	1
5	P1T	H	501	21/21	0.99	0.24	17,24,34,35	0
5	P1T	F	501	21/21	0.99	0.22	20,28,46,47	0
5	P1T	B	501	21/21	0.99	0.23	15,23,38,42	0

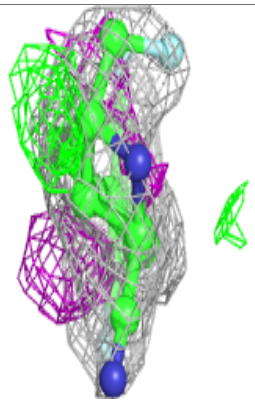
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDJ D 511:

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

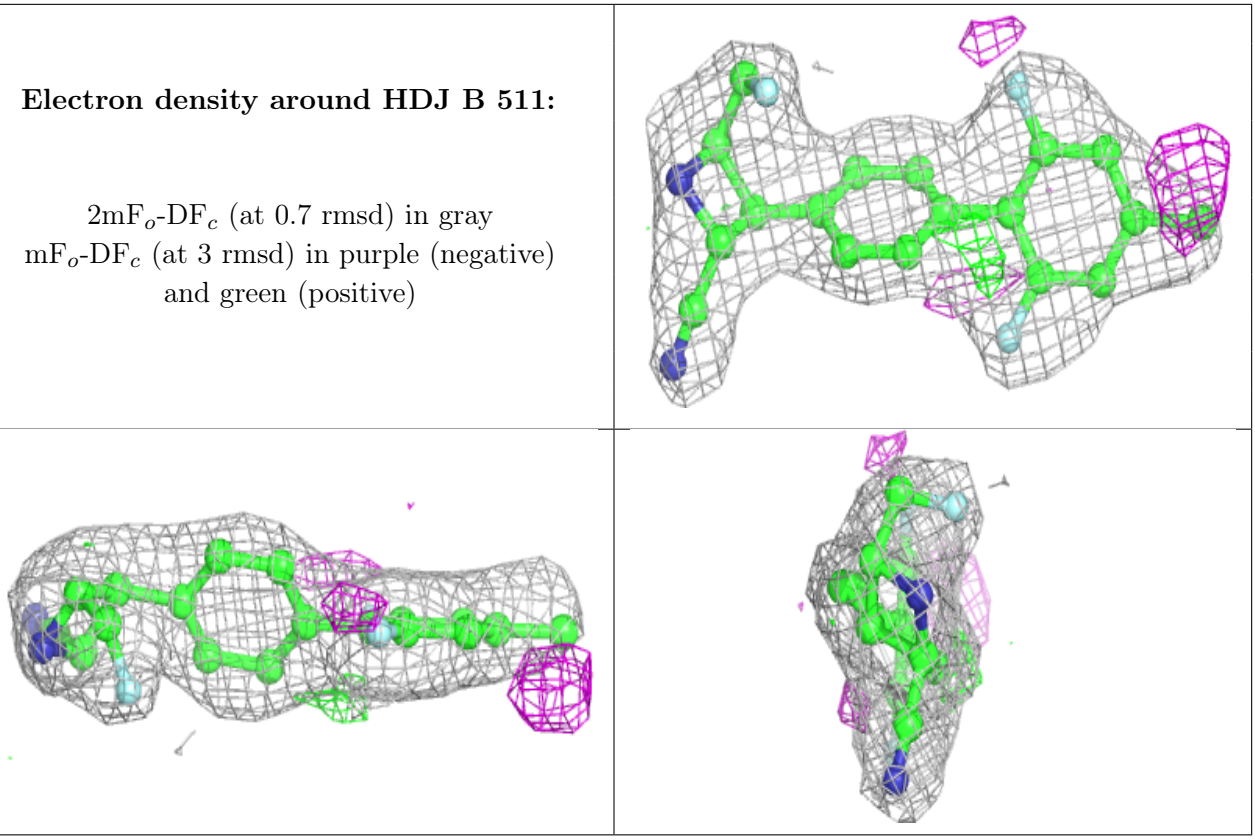






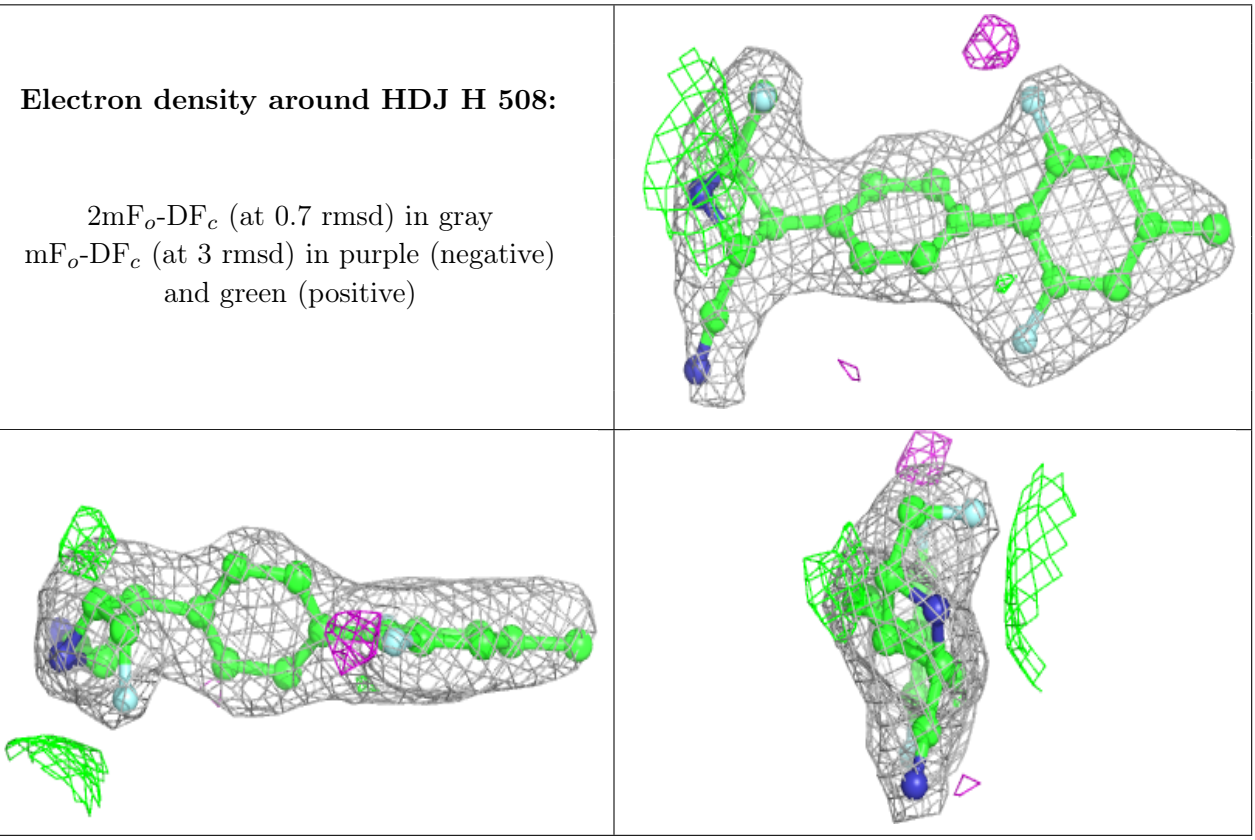
Electron density around HDJ B 511:

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



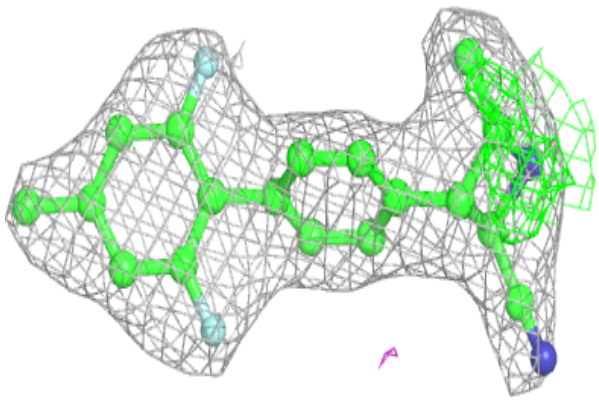
Electron density around HDJ H 508:

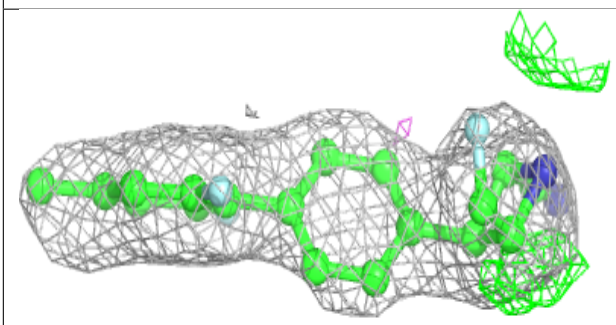
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

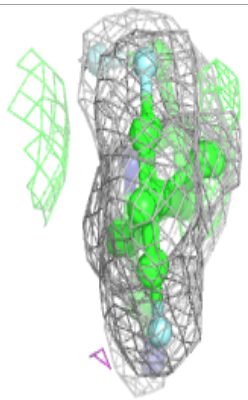


Electron density around HDJ F 513:

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

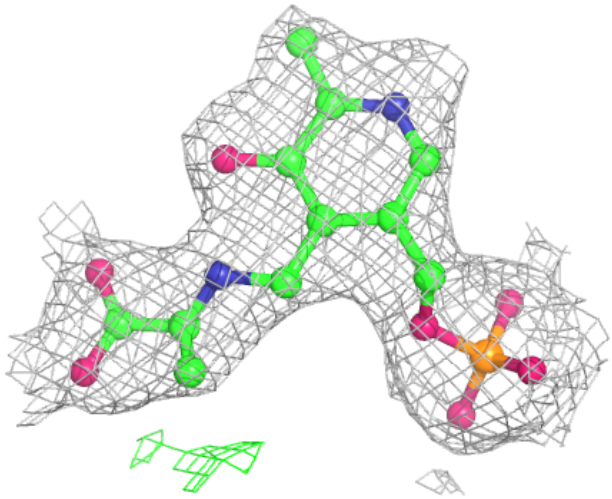


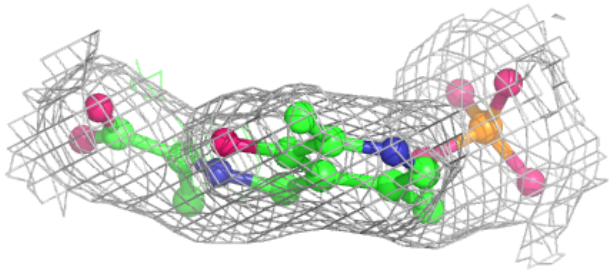


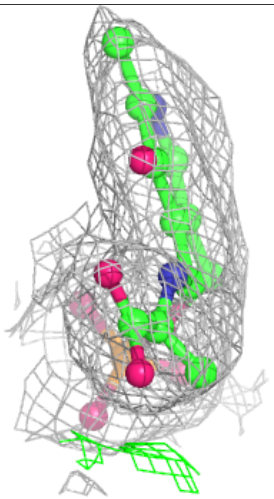


Electron density around P1T D 501:

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

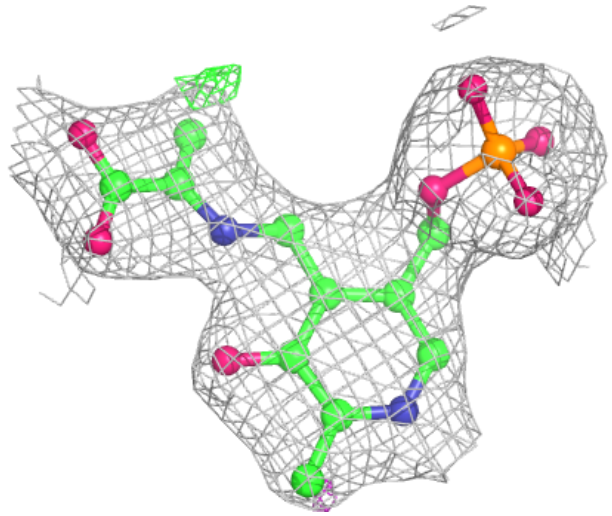


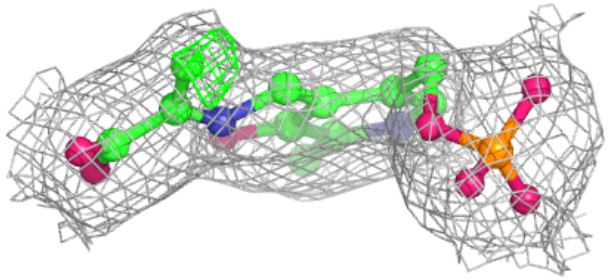


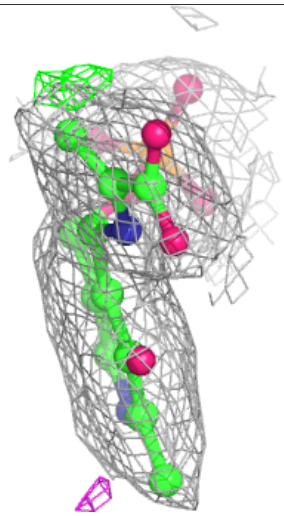


Electron density around P1T H 501:

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

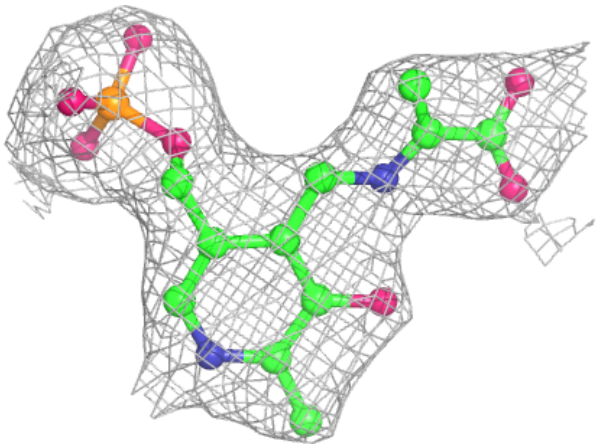


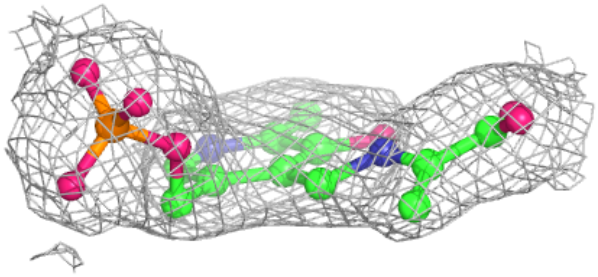


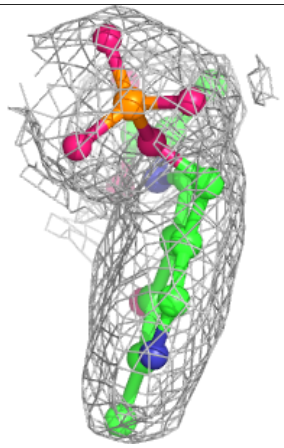


Electron density around P1T F 501:

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

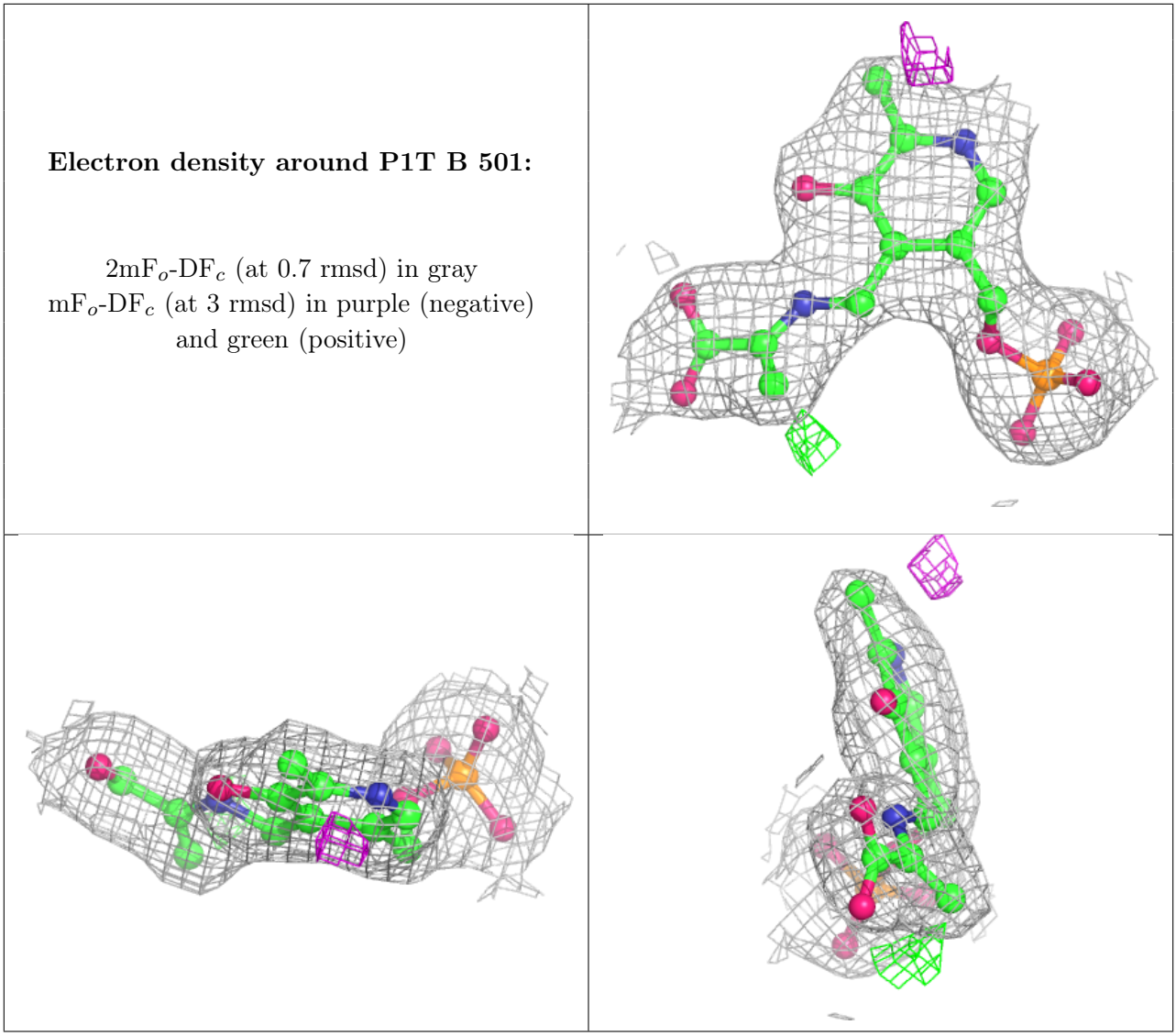






Electron density around P1T B 501:

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



6.5 Other polymers

There are no such residues in this entry.