Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:49 PM BST

PDB ID	:	6UAP
Title	:	Crystal structure of tryptophan synthase from M. tuberculosis - open form with BRD6309 bound
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	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

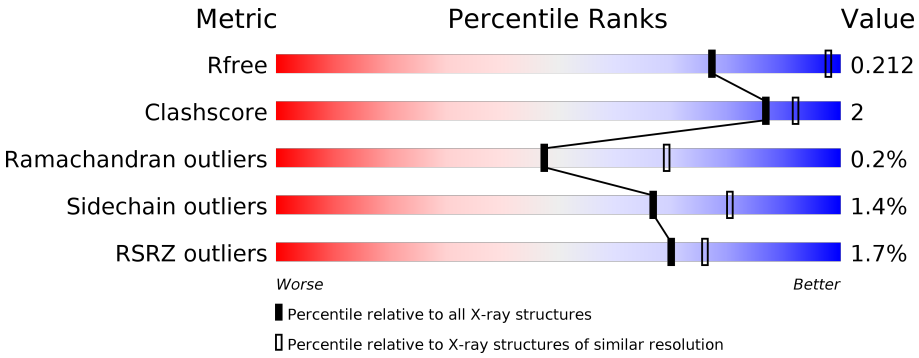
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.75 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 on 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	2% 85% 5% 10%
1	C	276	3% 86% • • 9%
1	E	276	3% 82% 7% • 11%
1	G	276	3% 80% 8% • 11%
2	B	410	91% 8% •
2	D	410	% 93% 6% •

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Mol	Chain	Length	Quality of chain
2	F	410	92% 5%
2	H	410	% 92% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MLA	B	504	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19739 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	C	250	Total	C	N	O	S	0	1	0
			1810	1135	325	345	5			
1	E	247	Total	C	N	O	S	0	0	0
			1761	1109	311	336	5			
1	G	247	Total	C	N	O	S	0	0	0
			1750	1103	313	329	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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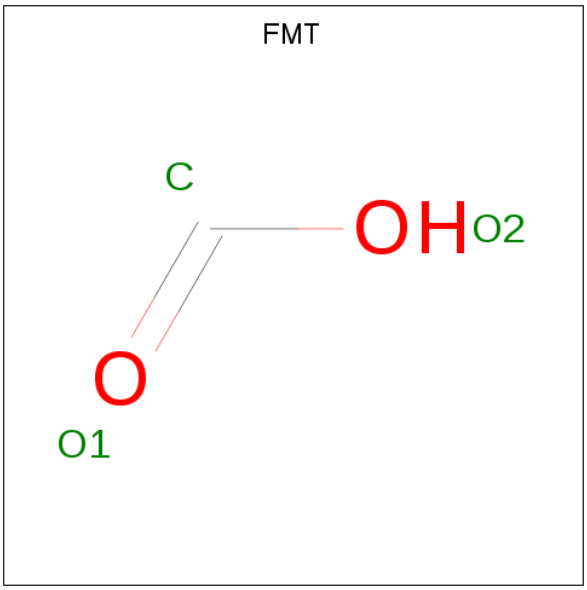
Chain	Residue	Modelled	Actual	Comment	Reference
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	276	HIS	-	expression tag	UNP P9WFY1

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	P	S	0	0	0
			3020	1886	546	574	1	13			
2	D	406	Total	C	N	O	P	S	0	0	0
			3029	1891	547	577	1	13			
2	F	400	Total	C	N	O	P	S	0	0	0
			2992	1869	540	569	1	13			
2	H	400	Total	C	N	O	P	S	11	1	0
			3002	1873	544	571	1	13			

- Molecule 3 is FORMIC ACID (three-letter code: 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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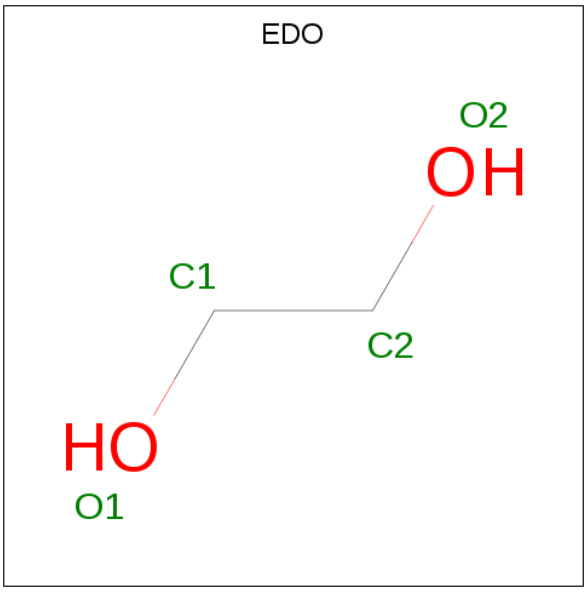
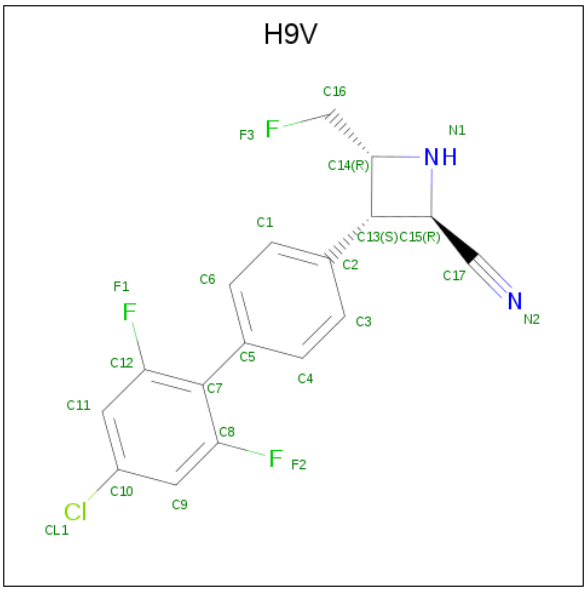
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	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	F	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	G	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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is (2R,3S,4R)-3-(4'-chloro-2',6'-difluoro[1,1'-biphenyl]-4-yl)-4-(fluoromethyl)azetidine-2-carbonitrile (three-letter code: H9V) (formula: $C_{17}H_{12}ClF_3N_2$) (labeled as "Ligand of Interest" by author).



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

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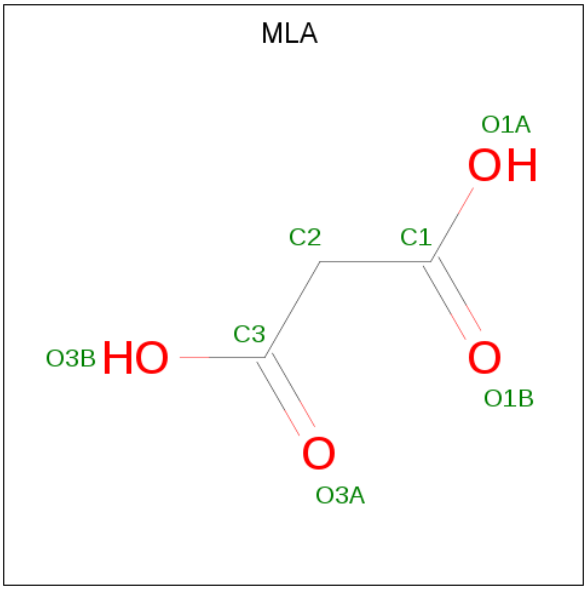
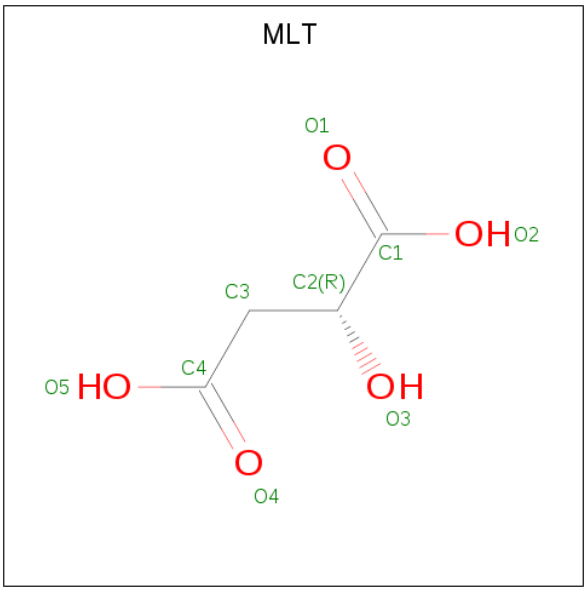
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	Cl	F	N	0	0
			23	17	1	3	2		
5	F	1	Total	C	Cl	F	N	0	0
			23	17	1	3	2		
5	H	1	Total	C	Cl	F	N	0	0
			23	17	1	3	2		

- Molecule 6 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



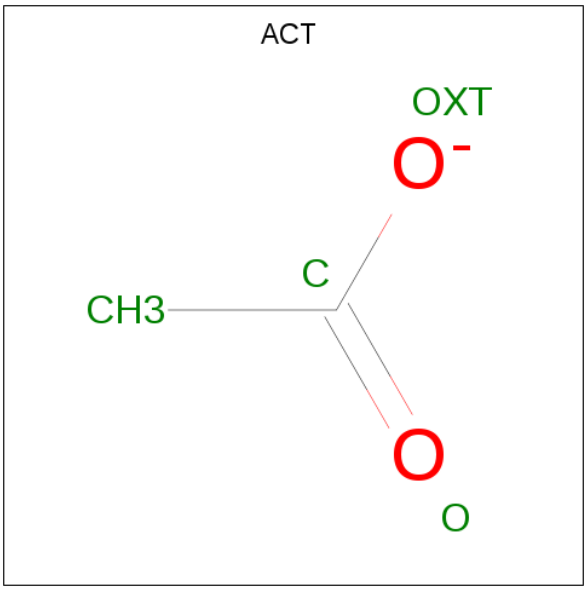
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	3	4		
6	C	1	Total	C	O	0	0
			7	3	4		
6	F	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 9 4 5	0	0
7	D	1	Total C O 9 4 5	0	0
7	D	1	Total C O 9 4 5	0	0
7	F	1	Total C O 9 4 5	0	0
7	H	1	Total C O 9 4 5	0	0

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



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

- Molecule 9 is water.

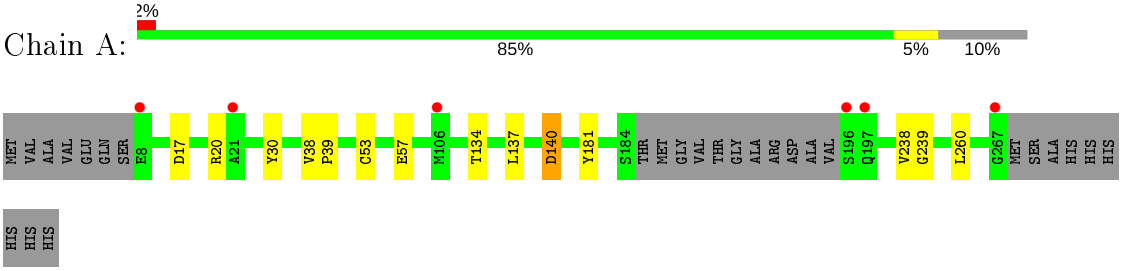
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	26	Total O 26 26	0	0
9	B	52	Total O 52 52	0	0
9	C	26	Total O 26 26	0	0
9	D	52	Total O 52 52	0	0
9	E	13	Total O 13 13	0	0
9	F	52	Total O 52 52	0	0
9	G	19	Total O 19 19	0	0
9	H	62	Total O 62 62	0	0

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.

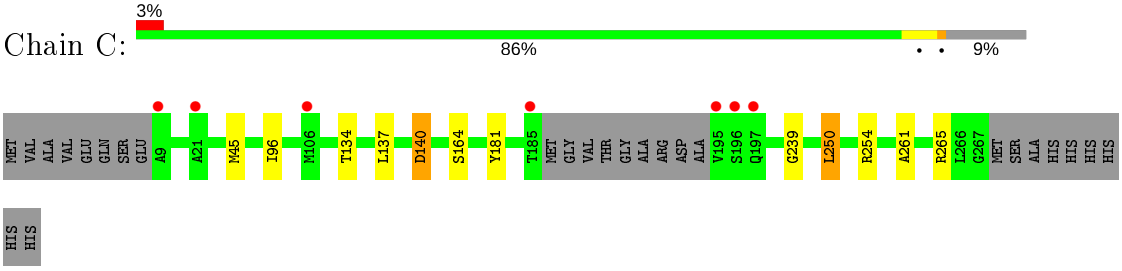
- Molecule 1: Tryptophan synthase alpha chain

Chain A:



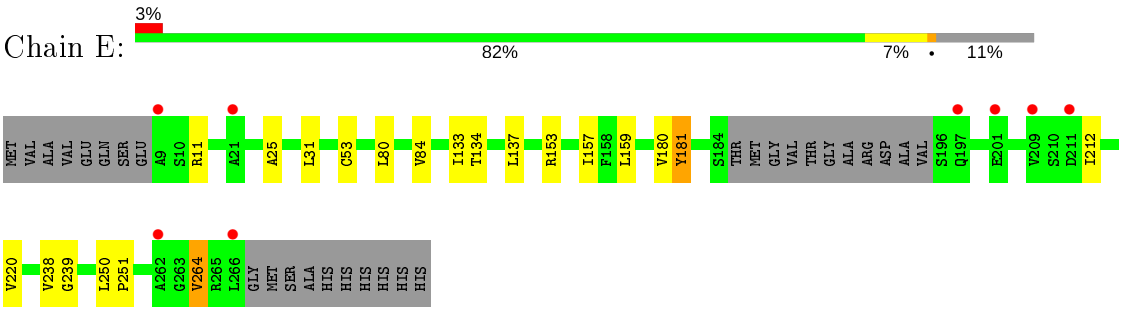
- Molecule 1: Tryptophan synthase alpha chain

Chain C:



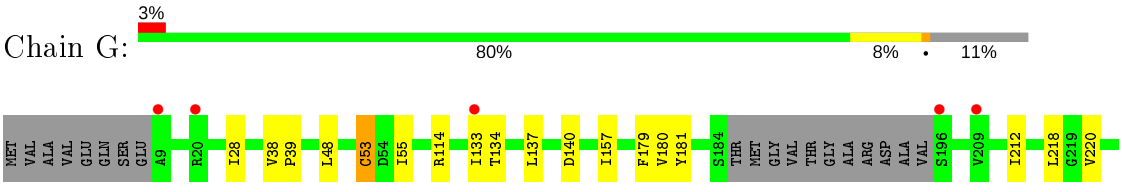
- Molecule 1: Tryptophan synthase alpha chain

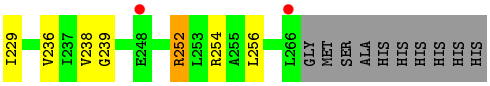
Chain E:



- Molecule 1: Tryptophan synthase alpha chain

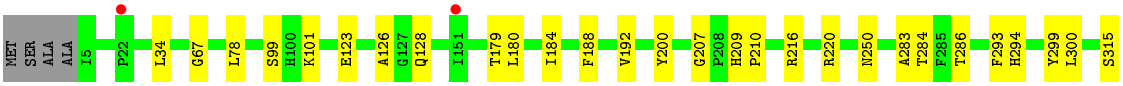
Chain G:





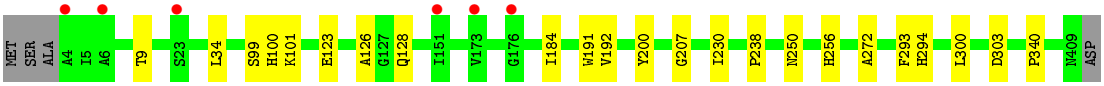
• Molecule 2: Tryptophan synthase beta chain

Chain B:



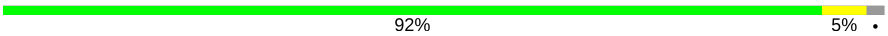
• Molecule 2: Tryptophan synthase beta chain

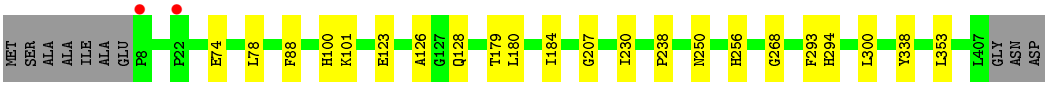
Chain D:



• Molecule 2: Tryptophan synthase beta chain

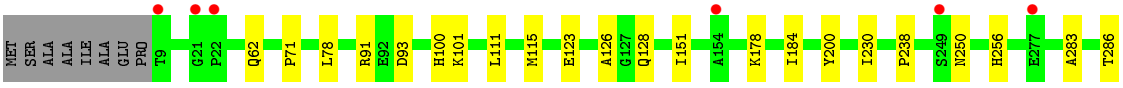
Chain F:





• 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	134.78Å 157.88Å 166.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.65 – 2.75 29.65 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.65-2.75) 99.2 (29.65-2.74)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.171 , 0.211 0.171 , 0.212	Depositor DCC
R_{free} test set	1854 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19739	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: MLA, H9V, FMT, LLP, EDO, MLT, ACT

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	0.25	0/1843	0.42	0/2514
1	C	0.24	0/1839	0.42	0/2510
1	E	0.24	0/1790	0.41	0/2448
1	G	0.24	0/1779	0.41	0/2434
2	B	0.25	0/3056	0.43	0/4143
2	D	0.25	0/3065	0.43	0/4155
2	F	0.25	0/3028	0.43	0/4103
2	H	0.25	0/3037	0.44	0/4114
All	All	0.25	0/19437	0.43	0/26421

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	1810	0	1824	5	0
1	E	1761	0	1760	10	0
1	G	1750	0	1747	11	0
2	B	3020	0	2930	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3029	0	2939	11	0
2	F	2992	0	2904	11	0
2	H	3002	0	2916	13	0
3	A	6	0	2	0	0
3	B	15	0	5	0	0
3	C	6	0	2	0	0
3	D	18	0	6	0	0
3	F	15	0	5	0	0
3	G	3	0	1	0	0
3	H	6	0	2	0	0
4	A	4	0	6	0	0
4	D	4	0	6	0	0
5	B	23	0	0	0	0
5	D	23	0	0	0	0
5	F	23	0	0	0	0
5	H	23	0	0	0	0
6	B	7	0	2	0	0
6	C	7	0	2	0	0
6	F	7	0	2	0	0
7	B	9	0	4	1	0
7	D	18	0	7	2	0
7	F	9	0	4	2	0
7	H	9	0	4	1	0
8	D	16	0	12	1	0
8	G	4	0	3	0	0
8	H	4	0	3	0	0
9	A	26	0	0	0	0
9	B	52	0	0	0	0
9	C	26	0	0	0	0
9	D	52	0	0	0	0
9	E	13	0	0	0	0
9	F	52	0	0	0	0
9	G	19	0	0	0	0
9	H	62	0	0	1	0
All	All	19739	0	18932	82	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 (82) 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:H:71:PRO:HD2	2:H:91:ARG:HB2	1.76	0.67
2:F:128:GLN:H	7:F:507:MLT:H32	1.61	0.66
1:C:140:ASP:OD1	1:C:140:ASP:N	2.31	0.64
2:F:123:GLU:HG3	2:F:184:ILE:HG12	1.80	0.63
2:D:303:ASP:HB2	8:D:514:ACT:H1	1.80	0.63
2:F:126:ALA:H	7:F:507:MLT:H31	1.63	0.63
2:H:126:ALA:H	7:H:503:MLT:H31	1.63	0.63
2:D:123:GLU:HG3	2:D:184:ILE:HG12	1.83	0.61
1:E:134:THR:HB	1:E:137:LEU:HB3	1.86	0.57
1:A:140:ASP:OD1	1:A:140:ASP:N	2.38	0.57
1:G:28:ILE:HG12	1:G:55:ILE:HB	1.87	0.57
2:B:123:GLU:HG3	2:B:184:ILE:HG12	1.86	0.56
1:G:252:ARG:HH11	1:G:256:LEU:HB2	1.71	0.56
2:B:216:ARG:O	2:B:220:ARG:HG3	2.08	0.54
1:E:11:ARG:NH1	1:E:153:ARG:O	2.40	0.54
1:C:250:LEU:HD21	1:C:254:ARG:HH21	1.73	0.53
2:D:293:PHE:HB2	2:D:300:LEU:HD22	1.90	0.52
1:G:134:THR:HB	1:G:137:LEU:HB3	1.90	0.52
2:B:34:LEU:HD13	2:B:192:VAL:HG22	1.89	0.52
1:G:180:VAL:HG23	1:G:212:ILE:HD13	1.91	0.52
2:F:230:ILE:HG21	2:F:238:PRO:HD3	1.92	0.51
2:H:62:GLN:NE2	9:H:602:HOH:O	2.41	0.50
1:A:238:VAL:HG21	1:A:260:LEU:HD13	1.93	0.49
1:A:17:ASP:OD1	1:A:20:ARG:NH2	2.45	0.49
1:C:134:THR:HB	1:C:137:LEU:HB3	1.94	0.49
2:D:99:SER:HB2	2:D:128:GLN:HE21	1.78	0.49
1:E:220:VAL:HB	1:E:238:VAL:HG22	1.94	0.49
2:H:78:LEU:HD11	2:H:353:LEU:HD13	1.95	0.48
2:D:128:GLN:H	7:D:510:MLT:H2	1.79	0.48
2:H:100:HIS:CE1	2:H:250:ASN:HB3	2.49	0.47
2:H:93:ASP:HB2	2:H:392:ARG:HB3	1.96	0.47
2:B:179:THR:OG1	2:B:180:LEU:N	2.47	0.47
1:E:159:LEU:HG	1:E:181:TYR:HB3	1.95	0.47
1:E:25:ALA:HB3	1:E:264:VAL:HG12	1.96	0.47
1:C:45:MET:HB3	1:C:96:ILE:HD11	1.96	0.47
2:B:126:ALA:H	7:B:505:MLT:C2	2.27	0.47
2:D:272:ALA:HB2	2:D:340:PRO:HB2	1.97	0.46
1:G:157:ILE:HG12	1:G:179:PHE:CE1	2.51	0.46
2:B:293:PHE:HB2	2:B:300:LEU:HD13	1.96	0.46
2:B:78:LEU:HD11	2:B:353:LEU:HD13	1.96	0.46
2:F:179:THR:OG1	2:F:180:LEU:N	2.46	0.46
1:A:134:THR:HB	1:A:137:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:GLY:HA2	2:B:294:HIS:O	2.16	0.46
2:B:67:GLY:HA2	2:H:71:PRO:HG3	1.98	0.46
1:G:133:ILE:HG12	1:G:157:ILE:HB	1.98	0.46
1:G:38:VAL:HB	1:G:39:PRO:HD3	1.98	0.46
2:B:283:ALA:HB1	2:B:286:THR:HB	1.98	0.45
2:B:99:SER:HB3	2:B:128:GLN:HE21	1.82	0.45
2:D:34:LEU:HD13	2:D:192:VAL:HG22	1.97	0.45
1:E:180:VAL:HG23	1:E:212:ILE:HD13	1.98	0.45
2:F:100:HIS:CE1	2:F:250:ASN:HB3	2.52	0.44
2:H:230:ILE:HG21	2:H:238:PRO:HD3	2.00	0.44
2:H:123:GLU:HG3	2:H:184:ILE:HG12	1.98	0.44
1:A:30:TYR:HA	1:A:57:GLU:HB2	2.00	0.44
2:F:78:LEU:HD11	2:F:353:LEU:HD13	2.00	0.44
2:H:151:ILE:HG13	2:H:178:LYS:HB2	2.00	0.44
1:A:38:VAL:HB	1:A:39:PRO:HD3	1.98	0.44
2:F:207:GLY:HA2	2:F:294:HIS:O	2.18	0.44
1:G:218:LEU:HD11	1:G:229:ILE:HD11	1.99	0.44
1:E:133:ILE:HG12	1:E:157:ILE:HB	1.99	0.43
1:G:229:ILE:HG22	1:G:236:VAL:HG22	2.01	0.43
2:F:293:PHE:HB2	2:F:300:LEU:HD13	1.99	0.43
2:D:100:HIS:NE2	2:D:250:ASN:HB3	2.33	0.43
2:B:315:SER:HB3	2:B:363:ILE:HG22	2.01	0.43
2:F:74:GLU:HB2	2:F:88:PHE:CE2	2.54	0.42
2:B:284:THR:HG22	2:B:299:TYR:HB3	2.01	0.42
1:C:261:ALA:O	1:C:265:ARG:NH2	2.46	0.42
1:G:220:VAL:HB	1:G:238:VAL:HG22	2.01	0.42
2:B:216:ARG:HD3	2:B:220:ARG:HD2	2.02	0.42
1:E:250:LEU:N	1:E:251:PRO:HD2	2.34	0.42
2:F:268:GLY:O	2:F:338:TYR:HA	2.20	0.42
2:D:207:GLY:HA2	2:D:294:HIS:O	2.20	0.41
2:H:111:LEU:O	2:H:115:MET:HG3	2.20	0.41
1:E:80:LEU:HA	1:E:84:VAL:HG12	2.02	0.41
2:B:209:HIS:ND1	2:B:210:PRO:HA	2.36	0.41
1:G:48:LEU:O	1:G:53:CYS:HB2	2.21	0.41
2:D:126:ALA:HB3	7:D:510:MLT:O1	2.21	0.40
2:D:230:ILE:HG21	2:D:238:PRO:HD3	2.04	0.40
1:E:31:LEU:HA	1:E:31:LEU:HD23	1.95	0.40
2:H:100:HIS:NE2	2:H:250:ASN:HB3	2.36	0.40
2:H:283:ALA:HB1	2:H:286:THR:HB	2.03	0.40
2:B:188:PHE:O	2:B:192:VAL:HG23	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	246/276 (89%)	238 (97%)	7 (3%)	1 (0%)	34	55
1	C	247/276 (90%)	242 (98%)	4 (2%)	1 (0%)	34	55
1	E	243/276 (88%)	237 (98%)	5 (2%)	1 (0%)	34	55
1	G	243/276 (88%)	237 (98%)	5 (2%)	1 (0%)	34	55
2	B	402/410 (98%)	389 (97%)	13 (3%)	0	100	100
2	D	403/410 (98%)	393 (98%)	10 (2%)	0	100	100
2	F	397/410 (97%)	385 (97%)	12 (3%)	0	100	100
2	H	398/410 (97%)	392 (98%)	6 (2%)	0	100	100
All	All	2579/2744 (94%)	2513 (97%)	62 (2%)	4 (0%)	47	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	239	GLY
1	A	239	GLY
1	C	239	GLY
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%)	177 (98%)	3 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	179/200 (90%)	175 (98%)	4 (2%)	52 71
1	E	171/200 (86%)	168 (98%)	3 (2%)	59 75
1	G	167/200 (84%)	161 (96%)	6 (4%)	35 55
2	B	296/301 (98%)	293 (99%)	3 (1%)	76 85
2	D	297/301 (99%)	293 (99%)	4 (1%)	69 82
2	F	294/301 (98%)	293 (100%)	1 (0%)	92 95
2	H	295/301 (98%)	292 (99%)	3 (1%)	76 85
All	All	1879/2004 (94%)	1852 (99%)	27 (1%)	67 80

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	140	ASP
1	A	181	TYR
2	B	200	TYR
2	B	250	ASN
2	B	388	ASN
1	C	140	ASP
1	C	164	SER
1	C	181	TYR
1	C	250	LEU
2	D	9	THR
2	D	191	TRP
2	D	200	TYR
2	D	256	HIS
1	E	53	CYS
1	E	181	TYR
1	E	264	VAL
2	F	256	HIS
1	G	53	CYS
1	G	114	ARG
1	G	140	ASP
1	G	181	TYR
1	G	252	ARG
1	G	254	ARG
2	H	128	GLN
2	H	200	TYR
2	H	256	HIS

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	LLP	D	101	2	23,24,25	2.60	6 (26%)	25,32,34	1.29	4 (16%)
2	LLP	F	101	2	23,24,25	2.60	6 (26%)	25,32,34	1.26	4 (16%)
2	LLP	H	101	2	23,24,25	2.61	6 (26%)	25,32,34	1.25	3 (12%)
2	LLP	B	101	2	23,24,25	2.61	6 (26%)	25,32,34	1.30	4 (16%)

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
2	LLP	D	101	2	-	6/16/17/19	0/1/1/1
2	LLP	F	101	2	-	5/16/17/19	0/1/1/1
2	LLP	H	101	2	-	7/16/17/19	0/1/1/1
2	LLP	B	101	2	-	4/16/17/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	101	LLP	C4-C4'	8.15	1.62	1.46
2	B	101	LLP	C4-C4'	8.10	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	101	LLP	C4-C4'	8.06	1.62	1.46
2	D	101	LLP	C4-C4'	8.06	1.62	1.46
2	D	101	LLP	C4'-NZ	4.95	1.43	1.27
2	H	101	LLP	C4'-NZ	4.94	1.43	1.27
2	B	101	LLP	C4'-NZ	4.93	1.43	1.27
2	F	101	LLP	C4'-NZ	4.92	1.43	1.27
2	D	101	LLP	C4-C5	-4.05	1.36	1.42
2	B	101	LLP	C4-C5	-4.00	1.36	1.42
2	F	101	LLP	C4-C5	-3.99	1.36	1.42
2	H	101	LLP	C4-C5	-3.99	1.36	1.42
2	F	101	LLP	C2'-C2	3.39	1.56	1.50
2	B	101	LLP	C2'-C2	3.37	1.56	1.50
2	D	101	LLP	C2'-C2	3.37	1.56	1.50
2	H	101	LLP	C2'-C2	3.35	1.56	1.50
2	D	101	LLP	C6-N1	3.03	1.40	1.34
2	F	101	LLP	C6-N1	3.02	1.40	1.34
2	B	101	LLP	C6-N1	3.01	1.40	1.34
2	H	101	LLP	C6-N1	2.95	1.40	1.34
2	B	101	LLP	C5'-C5	2.13	1.56	1.50
2	D	101	LLP	C5'-C5	2.13	1.56	1.50
2	F	101	LLP	C5'-C5	2.12	1.56	1.50
2	H	101	LLP	C5'-C5	2.08	1.56	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	101	LLP	C4-C4'-NZ	-3.32	109.07	124.31
2	F	101	LLP	C4-C4'-NZ	-3.27	109.30	124.31
2	B	101	LLP	C4-C4'-NZ	-3.22	109.55	124.31
2	H	101	LLP	C4-C4'-NZ	-3.12	110.00	124.31
2	B	101	LLP	CE-NZ-C4'	-2.96	109.82	118.90
2	F	101	LLP	CE-NZ-C4'	-2.89	110.02	118.90
2	H	101	LLP	CE-NZ-C4'	-2.84	110.18	118.90
2	D	101	LLP	CE-NZ-C4'	-2.78	110.37	118.90
2	B	101	LLP	C5-C6-N1	-2.26	120.06	123.82
2	H	101	LLP	C5-C6-N1	-2.24	120.08	123.82
2	D	101	LLP	C3-C4-C5	2.18	119.93	118.26
2	D	101	LLP	C5-C6-N1	-2.17	120.20	123.82
2	B	101	LLP	C3-C4-C5	2.13	119.90	118.26
2	F	101	LLP	C5-C6-N1	-2.12	120.28	123.82
2	F	101	LLP	C3-C4-C5	2.04	119.83	118.26

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	101	LLP	C4-C4'-NZ-CE
2	D	101	LLP	C5'-OP4-P-OP1
2	D	101	LLP	C5'-OP4-P-OP3
2	F	101	LLP	C4-C4'-NZ-CE
2	F	101	LLP	C5'-OP4-P-OP2
2	F	101	LLP	C5'-OP4-P-OP3
2	F	101	LLP	CG-CD-CE-NZ
2	H	101	LLP	C4-C4'-NZ-CE
2	H	101	LLP	C5'-OP4-P-OP2
2	H	101	LLP	C5'-OP4-P-OP3
2	H	101	LLP	C-CA-CB-CG
2	B	101	LLP	C4-C4'-NZ-CE
2	B	101	LLP	C-CA-CB-CG
2	D	101	LLP	CG-CD-CE-NZ
2	B	101	LLP	C5'-OP4-P-OP3
2	H	101	LLP	CD-CE-NZ-C4'
2	B	101	LLP	CD-CE-NZ-C4'
2	D	101	LLP	CD-CE-NZ-C4'
2	F	101	LLP	CD-CE-NZ-C4'
2	H	101	LLP	CE-CD-CG-CB
2	D	101	LLP	C5'-OP4-P-OP2
2	H	101	LLP	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

43 ligands are modelled in this entry.

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	B	503	-	0,2,2	0.00	-	0,1,1	0.00	-
5	H9V	D	501	-	23,25,25	2.13	5 (21%)	25,36,36	2.73	10 (40%)
3	FMT	D	509	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	505	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	504	-	0,2,2	0.00	-	0,1,1	0.00	-
7	MLT	H	503	-	2,8,8	0.54	0	3,10,10	1.37	1 (33%)
8	ACT	G	502	-	1,3,3	1.33	0	0,3,3	0.00	-
6	MLA	F	506	-	0,6,6	0.00	-	0,7,7	0.00	-
4	EDO	A	503	-	3,3,3	0.45	0	2,2,2	0.36	0
3	FMT	D	505	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	502	-	0,2,2	0.00	-	0,1,1	0.00	-
8	ACT	D	502	-	1,3,3	1.39	0	0,3,3	0.00	-
3	FMT	G	501	-	0,2,2	0.00	-	0,1,1	0.00	-
6	MLA	C	502	-	0,6,6	0.00	-	0,7,7	0.00	-
8	ACT	D	503	-	1,3,3	1.08	0	0,3,3	0.00	-
3	FMT	F	502	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	505	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	501	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	501	-	0,2,2	0.00	-	0,1,1	0.00	-
8	ACT	D	513	-	1,3,3	1.20	0	0,3,3	0.00	-
5	H9V	F	501	-	23,25,25	1.97	4 (17%)	25,36,36	1.98	8 (32%)
3	FMT	C	503	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	503	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	506	-	0,2,2	0.00	-	0,1,1	0.00	-
6	MLA	B	504	-	0,6,6	0.00	-	0,7,7	0.00	-
7	MLT	D	510	-	2,8,8	0.33	0	3,10,10	0.86	0
8	ACT	D	514	-	1,3,3	1.37	0	0,3,3	0.00	-
3	FMT	F	508	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	H9V	H	501	-	23,25,25	1.83	3 (13%)	25,36,36	2.06	9 (36%)
3	FMT	A	502	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	507	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	D	512	-	3,3,3	0.46	0	2,2,2	0.37	0
3	FMT	B	507	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	508	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	506	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	508	-	0,2,2	0.00	-	0,1,1	0.00	-
7	MLT	B	505	-	2,8,8	0.55	0	3,10,10	0.92	0
7	MLT	D	511	-	2,8,8	0.44	0	3,10,10	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	ACT	H	504	-	1,3,3	1.28	0	0,3,3	0.00	-
7	MLT	F	507	-	2,8,8	0.47	0	3,10,10	1.02	0
3	FMT	H	502	-	0,2,2	0.00	-	0,1,1	0.00	-
5	H9V	B	501	-	23,25,25	2.02	4 (17%)	25,36,36	2.07	8 (32%)

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
5	H9V	D	501	-	-	3/8/24/24	0/3/3/3
6	MLA	F	506	-	-	0/0/4/4	-
5	H9V	H	501	-	-	3/8/24/24	0/3/3/3
7	MLT	H	503	-	-	2/2/8/8	-
4	EDO	D	512	-	-	0/1/1/1	-
5	H9V	F	501	-	-	3/8/24/24	0/3/3/3
4	EDO	A	503	-	-	0/1/1/1	-
6	MLA	B	504	-	-	0/0/4/4	-
7	MLT	D	510	-	-	2/2/8/8	-
6	MLA	C	502	-	-	0/0/4/4	-
7	MLT	B	505	-	-	2/2/8/8	-
7	MLT	D	511	-	-	0/2/8/8	-
7	MLT	F	507	-	-	2/2/8/8	-
5	H9V	B	501	-	-	3/8/24/24	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	H9V	C14-N1	5.41	1.53	1.48
5	B	501	H9V	C2-C13	-5.15	1.40	1.51
5	D	501	H9V	C2-C13	-5.10	1.40	1.51
5	F	501	H9V	C2-C13	-5.03	1.40	1.51
5	B	501	H9V	C7-C5	-5.00	1.41	1.50
5	F	501	H9V	C7-C5	-4.86	1.41	1.50
5	D	501	H9V	C7-C5	-4.78	1.41	1.50
5	H	501	H9V	C2-C13	-4.73	1.41	1.51
5	H	501	H9V	C7-C5	-4.65	1.41	1.50
5	B	501	H9V	C14-N1	4.33	1.52	1.48
5	H	501	H9V	C14-N1	4.26	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	501	H9V	C14-N1	4.07	1.51	1.48
5	F	501	H9V	C15-C17	3.28	1.53	1.48
5	B	501	H9V	C15-C17	3.07	1.52	1.48
5	D	501	H9V	C15-C17	-2.69	1.45	1.48
5	D	501	H9V	C17-N2	-2.13	1.10	1.14

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	501	H9V	C15-C17-N2	-7.65	169.37	177.70
5	D	501	H9V	C10-C11-C12	5.01	121.17	117.48
5	D	501	H9V	C10-C9-C8	4.82	121.03	117.48
5	H	501	H9V	C10-C11-C12	4.67	120.92	117.48
5	H	501	H9V	C10-C9-C8	4.65	120.91	117.48
5	B	501	H9V	C10-C11-C12	4.61	120.88	117.48
5	F	501	H9V	C10-C11-C12	4.59	120.86	117.48
5	B	501	H9V	C10-C9-C8	4.48	120.78	117.48
5	F	501	H9V	C10-C9-C8	4.40	120.72	117.48
5	D	501	H9V	C6-C1-C2	-3.69	117.48	121.20
5	B	501	H9V	F2-C8-C7	3.22	124.11	119.52
5	D	501	H9V	F2-C8-C7	3.19	124.06	119.52
5	D	501	H9V	F1-C12-C7	3.05	123.87	119.52
5	H	501	H9V	F2-C8-C7	3.02	123.82	119.52
5	F	501	H9V	F2-C8-C7	2.95	123.72	119.52
5	B	501	H9V	F1-C12-C7	2.83	123.55	119.52
5	H	501	H9V	F1-C12-C7	2.72	123.39	119.52
5	B	501	H9V	C6-C1-C2	-2.63	118.55	121.20
5	F	501	H9V	F1-C12-C7	2.60	123.22	119.52
5	B	501	H9V	C12-C7-C8	2.59	117.10	114.56
5	H	501	H9V	C6-C1-C2	-2.52	118.66	121.20
5	B	501	H9V	C11-C12-C7	-2.45	120.66	123.45
5	D	501	H9V	C11-C10-C9	-2.38	118.70	121.66
5	F	501	H9V	C12-C7-C8	2.28	116.80	114.56
5	H	501	H9V	C15-C17-N2	-2.27	175.23	177.70
5	F	501	H9V	C6-C1-C2	-2.26	118.92	121.20
5	F	501	H9V	C11-C12-C7	-2.23	120.91	123.45
5	D	501	H9V	C11-C12-C7	-2.22	120.91	123.45
7	H	503	MLT	C3-C2-C1	-2.18	108.32	111.10
5	H	501	H9V	C11-C10-C9	-2.16	118.98	121.66
5	D	501	H9V	C4-C5-C7	2.15	124.36	120.79
5	B	501	H9V	C9-C8-C7	-2.14	121.01	123.45
5	D	501	H9V	C12-C7-C8	2.10	116.62	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	501	H9V	C11-C10-C9	-2.08	119.08	121.66
5	H	501	H9V	C9-C8-C7	-2.02	121.15	123.45
5	H	501	H9V	C11-C12-C7	-2.00	121.16	123.45

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	H	503	MLT	C1-C2-C3-C4
7	H	503	MLT	O3-C2-C3-C4
7	D	510	MLT	C1-C2-C3-C4
7	D	510	MLT	O3-C2-C3-C4
7	F	507	MLT	C1-C2-C3-C4
7	F	507	MLT	O3-C2-C3-C4
7	B	505	MLT	O3-C2-C3-C4
5	D	501	H9V	C4-C5-C7-C12
5	F	501	H9V	C4-C5-C7-C12
5	H	501	H9V	C4-C5-C7-C12
5	B	501	H9V	C4-C5-C7-C12
5	D	501	H9V	C4-C5-C7-C8
7	B	505	MLT	C1-C2-C3-C4
5	D	501	H9V	C6-C5-C7-C12
5	H	501	H9V	C4-C5-C7-C8
5	H	501	H9V	C6-C5-C7-C12
5	B	501	H9V	C4-C5-C7-C8
5	B	501	H9V	C6-C5-C7-C12
5	F	501	H9V	C4-C5-C7-C8
5	F	501	H9V	C6-C5-C7-C12

There are no ring outliers.

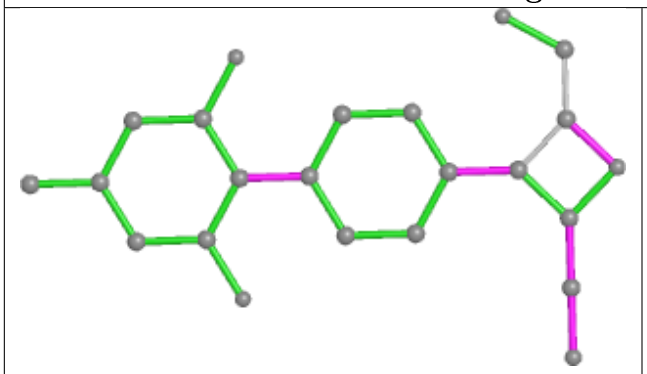
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	503	MLT	1	0
7	D	510	MLT	2	0
8	D	514	ACT	1	0
7	B	505	MLT	1	0
7	F	507	MLT	2	0

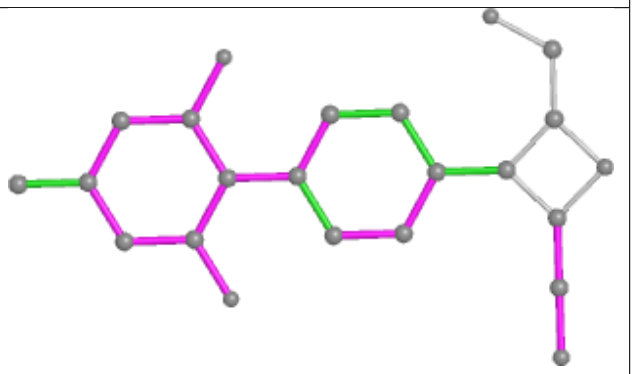
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

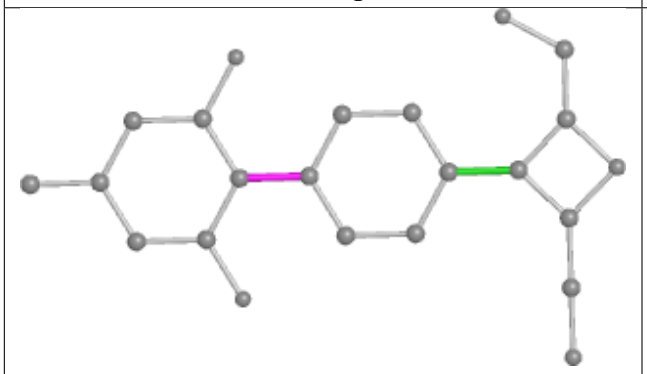
Ligand H9V D 501



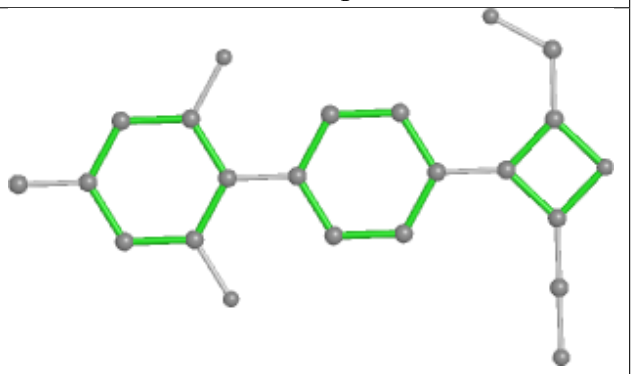
Bond lengths



Bond angles

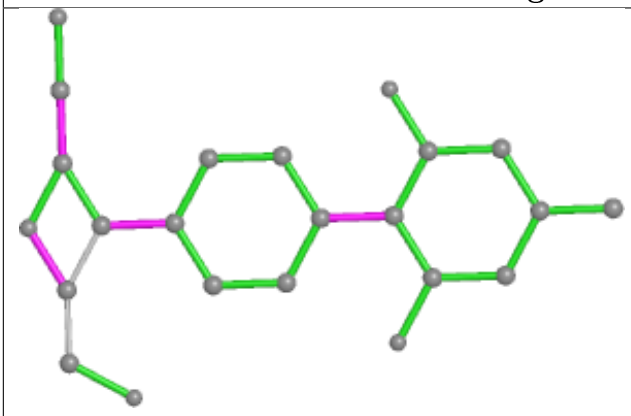


Torsions

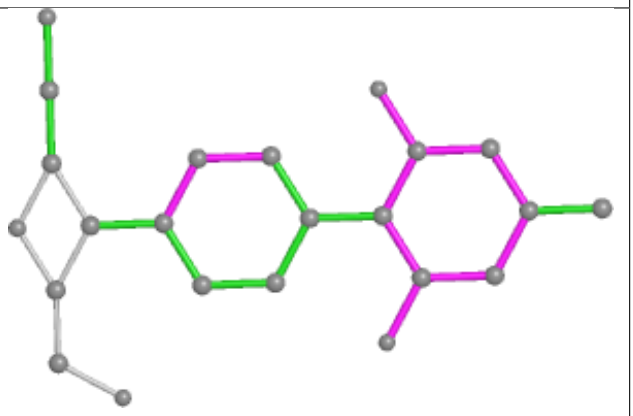


Rings

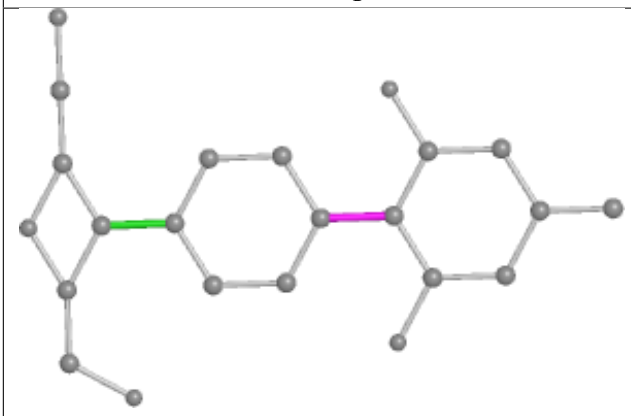
Ligand H9V F 501



Bond lengths



Bond angles



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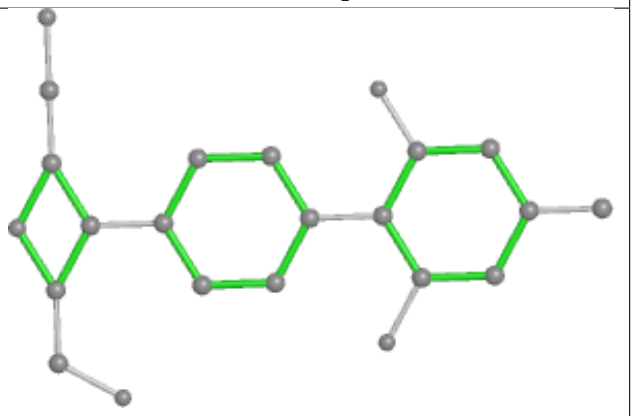
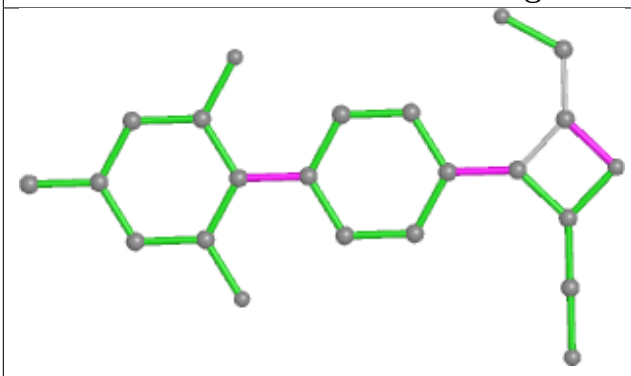
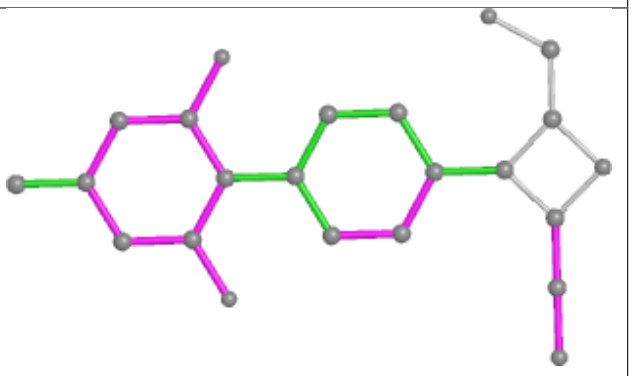


Rings

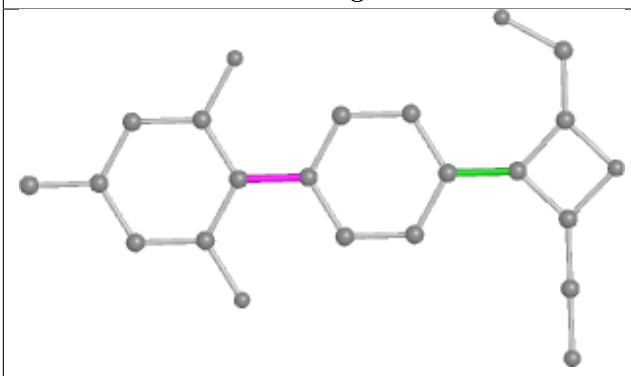
Ligand H9V H 501



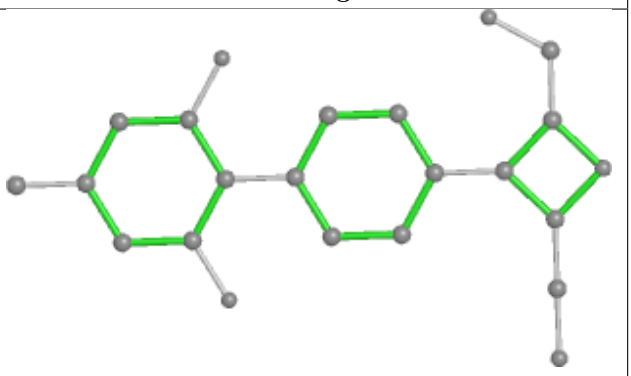
Bond lengths



Bond angles

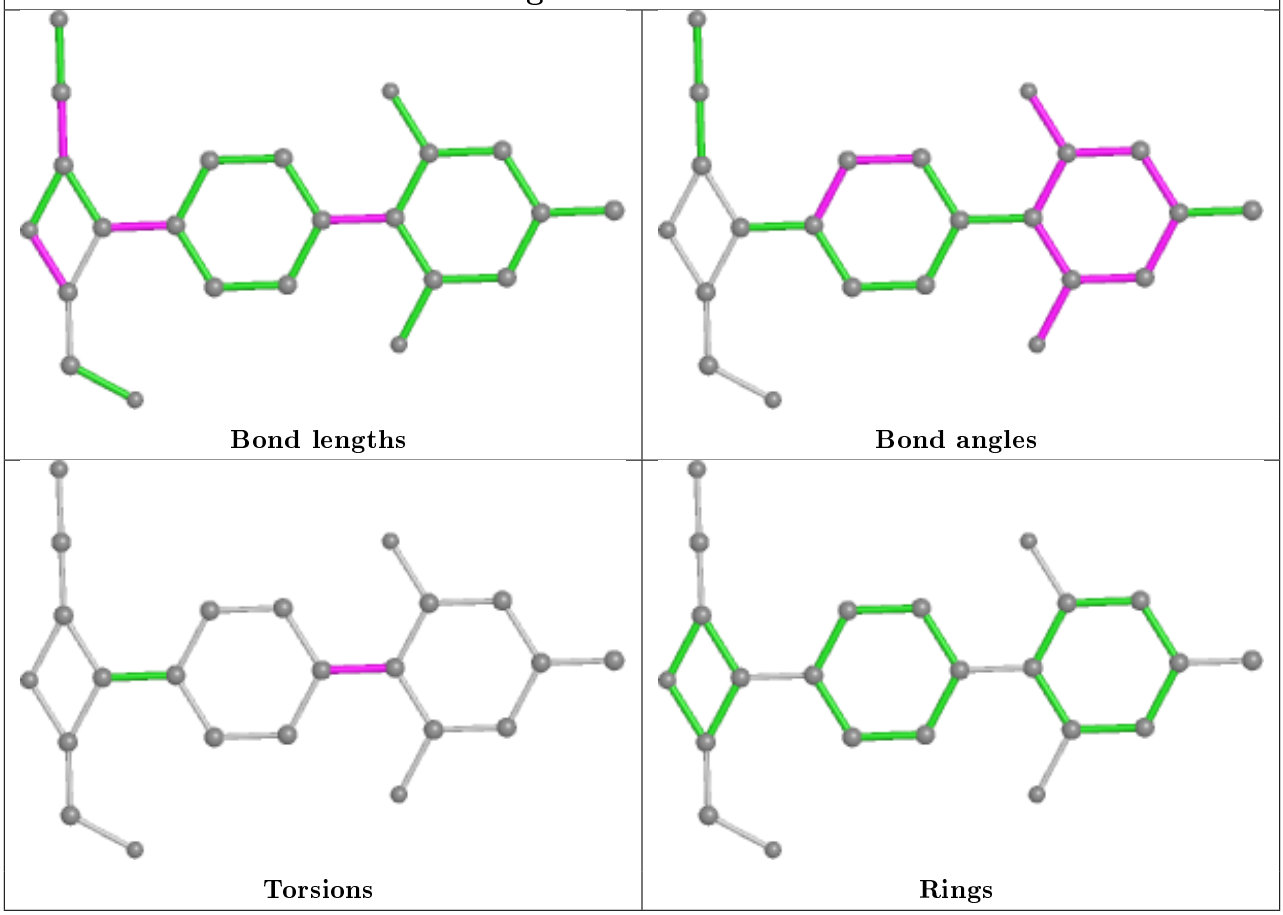


Torsions



Rings

Ligand H9V B 501



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%)	-0.25	6 (2%)	59	66	31, 45, 70, 117	0
1	C	250/276 (90%)	-0.25	7 (2%)	53	60	30, 47, 70, 124	0
1	E	247/276 (89%)	0.04	8 (3%)	47	54	40, 67, 100, 117	0
1	G	247/276 (89%)	-0.12	7 (2%)	53	60	33, 56, 89, 117	0
2	B	404/410 (98%)	-0.47	2 (0%)	91	93	26, 38, 66, 133	0
2	D	405/410 (98%)	-0.38	6 (1%)	73	79	25, 37, 73, 132	0
2	F	399/410 (97%)	-0.48	2 (0%)	91	93	26, 39, 63, 133	0
2	H	399/410 (97%)	-0.30	6 (1%)	73	79	27, 39, 65, 116	0
All	All	2600/2744 (94%)	-0.31	44 (1%)	70	76	25, 43, 81, 133	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	VAL	5.7
2	F	8	PRO	5.7
1	E	9	ALA	4.3
1	A	267	GLY	4.2
2	H	22	PRO	4.0
2	D	4	ALA	3.4
1	E	266	LEU	3.3
1	C	21	ALA	3.3
1	C	196	SER	3.3
1	A	8	GLU	3.3
1	G	266	LEU	3.3
2	F	22	PRO	3.3
2	D	151	ILE	3.2
1	E	197	GLN	3.1
1	E	21	ALA	3.0
1	C	9	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	6	ALA	2.7
1	G	209	VAL	2.7
1	A	197	GLN	2.6
2	H	277	GLU	2.6
2	D	176	GLY	2.5
2	B	22	PRO	2.5
1	E	262	ALA	2.5
1	C	185	THR	2.5
1	A	196	SER	2.5
1	A	21	ALA	2.5
1	G	9	ALA	2.4
2	H	154	ALA	2.4
1	G	196	SER	2.4
1	E	211	ASP	2.4
2	H	9	THR	2.2
2	D	23	SER	2.2
2	D	173	VAL	2.2
2	B	151	ILE	2.2
1	A	106	MET	2.1
1	G	133	ILE	2.1
1	C	197	GLN	2.1
1	E	209	VAL	2.1
1	C	106	MET	2.1
1	G	20	ARG	2.1
1	G	248	GLU	2.1
2	H	249	SER	2.1
2	H	21	GLY	2.0
1	E	201	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	LLP	D	101	24/25	0.98	0.19	27,33,41,43	0
2	LLP	F	101	24/25	0.98	0.19	27,35,40,44	0
2	LLP	H	101	24/25	0.98	0.22	28,34,44,49	0
2	LLP	B	101	24/25	0.99	0.20	24,36,41,43	0

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
7	MLT	D	511	9/9	0.70	0.28	81,87,90,91	0
7	MLT	D	510	9/9	0.74	0.32	64,67,69,71	9
6	MLA	B	504	7/7	0.76	0.54	99,100,102,103	0
7	MLT	B	505	9/9	0.77	0.34	46,55,62,62	9
6	MLA	F	506	7/7	0.81	0.38	90,90,92,93	0
7	MLT	H	503	9/9	0.82	0.30	83,84,88,88	0
8	ACT	D	503	4/4	0.82	0.36	87,87,87,88	0
3	FMT	F	508	3/3	0.84	0.33	59,59,62,63	0
3	FMT	F	505	3/3	0.86	0.20	55,55,56,57	0
3	FMT	B	506	3/3	0.86	0.35	68,68,71,72	0
3	FMT	D	509	3/3	0.86	0.20	51,51,53,53	0
3	FMT	C	503	3/3	0.88	0.39	61,61,62,62	0
4	EDO	A	503	4/4	0.88	0.26	51,53,54,55	0
3	FMT	D	508	3/3	0.89	0.21	68,68,70,70	0
3	FMT	G	501	3/3	0.89	0.38	62,62,66,68	0
8	ACT	D	514	4/4	0.89	0.37	65,69,70,70	0
7	MLT	F	507	9/9	0.89	0.22	65,70,77,78	0
6	MLA	C	502	7/7	0.90	0.19	70,71,78,79	0
5	H9V	D	501	23/23	0.90	0.25	60,62,68,85	0
8	ACT	D	513	4/4	0.90	0.27	68,71,72,73	0
3	FMT	H	502	3/3	0.90	0.22	63,63,65,66	0
5	H9V	B	501	23/23	0.90	0.24	50,58,64,74	0
3	FMT	A	502	3/3	0.91	0.44	56,56,58,58	0
4	EDO	D	512	4/4	0.92	0.15	58,60,61,62	0
3	FMT	B	507	3/3	0.92	0.14	57,57,60,61	0
3	FMT	H	505	3/3	0.92	0.20	55,55,56,59	0
5	H9V	F	501	23/23	0.92	0.20	41,49,61,79	0
5	H9V	H	501	23/23	0.93	0.22	41,56,62,75	0
3	FMT	D	506	3/3	0.93	0.20	54,54,57,60	0
3	FMT	B	508	3/3	0.94	0.21	58,58,59,60	0
3	FMT	A	501	3/3	0.95	0.36	64,64,65,67	0
8	ACT	H	504	4/4	0.95	0.31	62,62,62,63	0

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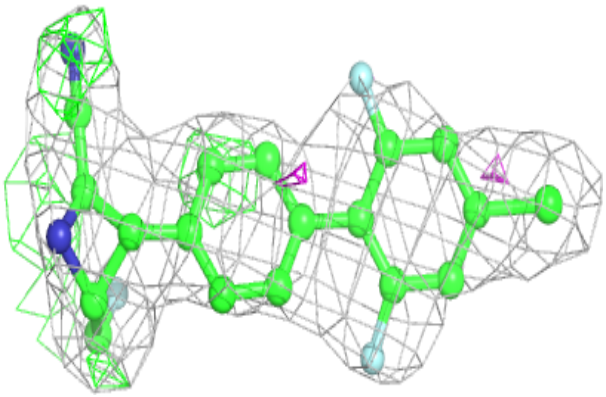
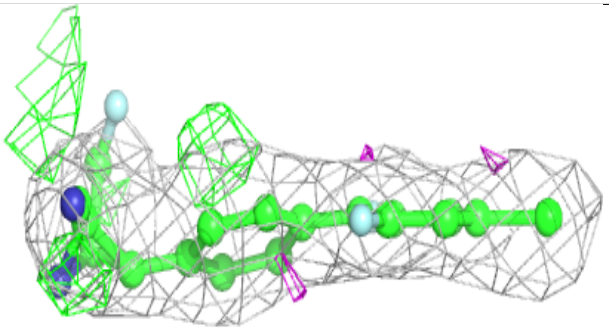
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMT	C	501	3/3	0.95	0.36	60,60,61,61	0
8	ACT	G	502	4/4	0.95	0.15	54,54,54,55	0
3	FMT	B	502	3/3	0.95	0.16	57,57,58,60	0
3	FMT	F	504	3/3	0.96	0.17	49,49,49,50	0
3	FMT	D	504	3/3	0.96	0.09	48,48,48,49	0
8	ACT	D	502	4/4	0.96	0.26	47,52,53,55	0
3	FMT	D	507	3/3	0.96	0.18	43,43,47,50	0
3	FMT	B	503	3/3	0.96	0.23	47,47,50,52	0
3	FMT	D	505	3/3	0.97	0.12	54,54,55,57	0
3	FMT	F	503	3/3	0.97	0.26	58,58,59,60	0
3	FMT	F	502	3/3	0.98	0.08	48,48,48,49	0

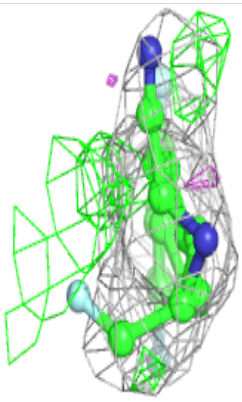
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H9V 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)

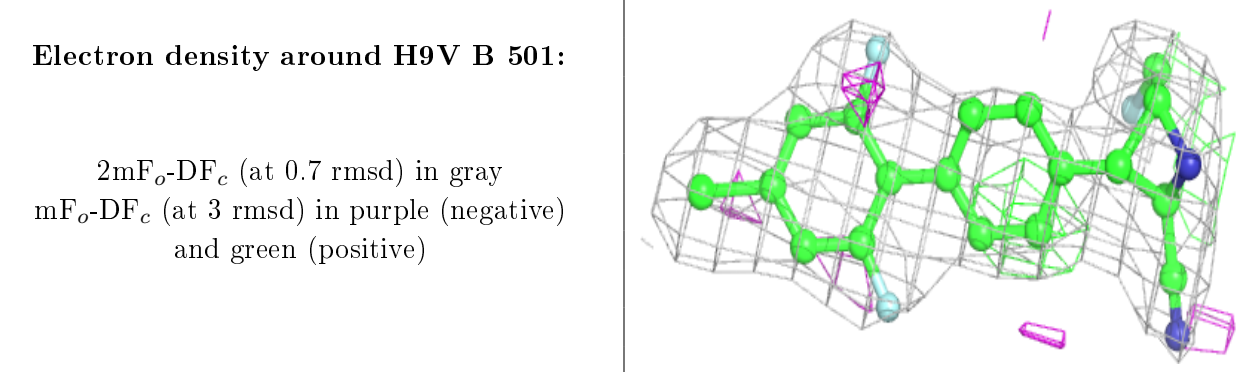






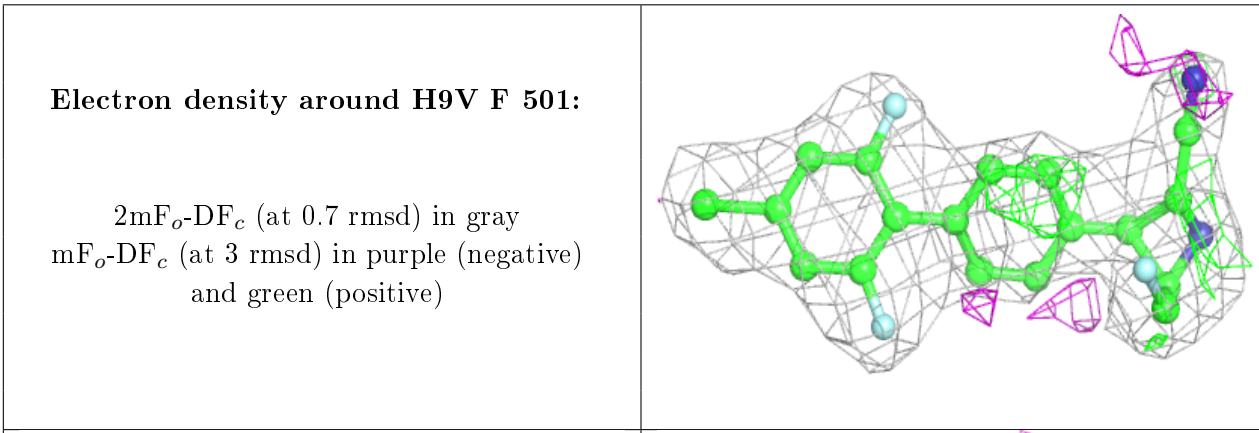
Electron density around H9V B 501:

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



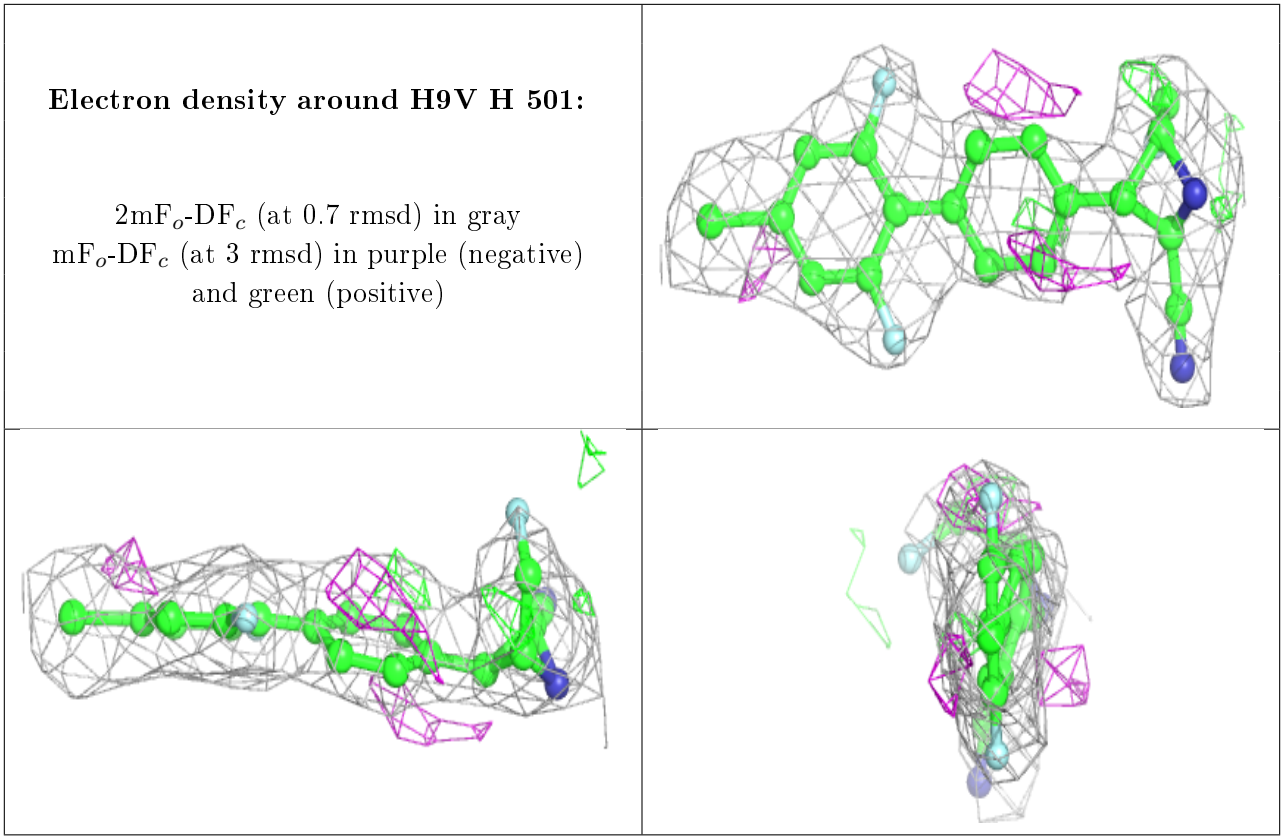
Electron density around H9V F 501:

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



Electron density around H9V 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)



6.5 Other polymers

There are no such residues in this entry.