



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:46 pm BST

PDB ID : 6E9P
Title : Crystal structure of tryptophan synthase from *M. tuberculosis* - open form with BRD0059 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 : 2018-08-01
Resolution : 2.57 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 : 2.11
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) : 2.11

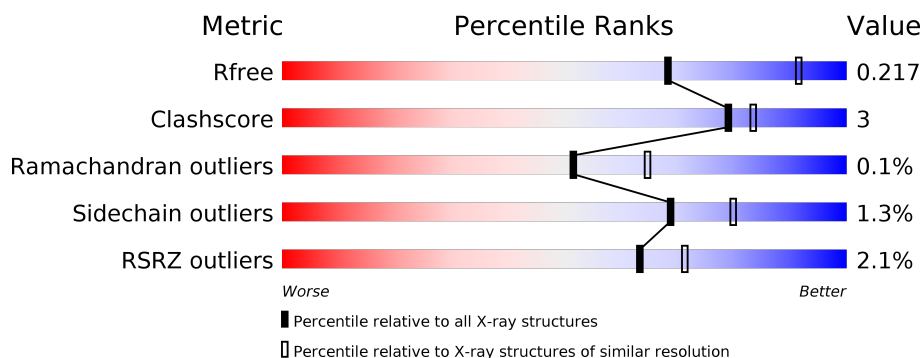
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	<div> <div>2%</div> <div>85% 5% 10%</div> </div>
1	C	276	<div> <div>2%</div> <div>86% 10%</div> </div>
1	E	276	<div> <div>5%</div> <div>78% 12% 11%</div> </div>
1	G	276	<div> <div>3%</div> <div>83% 7% 10%</div> </div>
2	B	410	<div> <div>%</div> <div>90% 9%</div> </div>
2	D	410	<div> <div>%</div> <div>90% 9%</div> </div>

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

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
5	EDO	F	507	-	-	-	X
8	FMT	B	503	-	-	X	-
8	FMT	B	505	-	-	X	-
8	FMT	B	510	-	-	X	-
8	FMT	D	515	-	-	-	X
8	FMT	D	516	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19733 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	249	Total	C	N	O	S	0	0	0
			1799	1129	323	342	5			
1	E	246	Total	C	N	O	S	0	0	0
			1752	1104	306	337	5			
1	G	249	Total	C	N	O	S	0	0	0
			1806	1133	323	345	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	expression tag	UNP P9WIFY1
A	272	HIS	-	expression tag	UNP P9WIFY1
A	273	HIS	-	expression tag	UNP P9WIFY1
A	274	HIS	-	expression tag	UNP P9WIFY1
A	275	HIS	-	expression tag	UNP P9WIFY1
A	276	HIS	-	expression tag	UNP P9WIFY1
C	271	HIS	-	expression tag	UNP P9WIFY1
C	272	HIS	-	expression tag	UNP P9WIFY1
C	273	HIS	-	expression tag	UNP P9WIFY1
C	274	HIS	-	expression tag	UNP P9WIFY1
C	275	HIS	-	expression tag	UNP P9WIFY1
C	276	HIS	-	expression tag	UNP P9WIFY1
E	271	HIS	-	expression tag	UNP P9WIFY1
E	272	HIS	-	expression tag	UNP P9WIFY1
E	273	HIS	-	expression tag	UNP P9WIFY1
E	274	HIS	-	expression tag	UNP P9WIFY1
E	275	HIS	-	expression tag	UNP P9WIFY1
E	276	HIS	-	expression tag	UNP P9WIFY1
G	271	HIS	-	expression tag	UNP P9WIFY1
G	272	HIS	-	expression tag	UNP P9WIFY1
G	273	HIS	-	expression tag	UNP P9WIFY1

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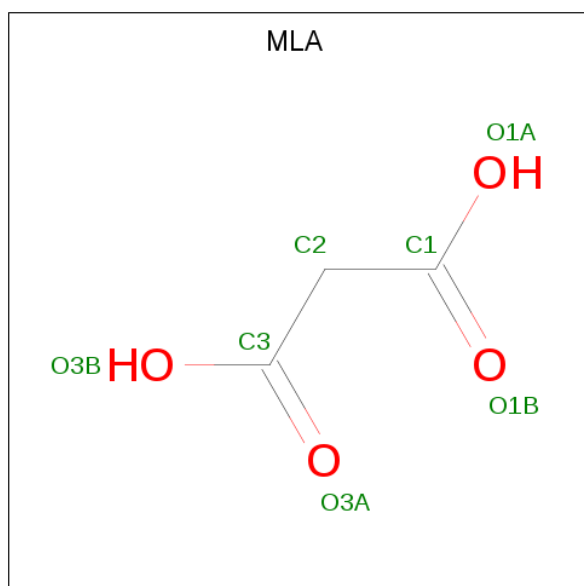
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Chain	Residue	Modelled	Actual	Comment	Reference
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	276	HIS	-	expression tag	UNP P9WFY1

- 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	1	0
			3034	1892	548	580	1	13			
2	D	405	Total	C	N	O	P	S	0	2	0
			3048	1901	552	581	1	13			
2	F	399	Total	C	N	O	P	S	0	0	0
			2984	1864	539	567	1	13			
2	H	400	Total	C	N	O	P	S	0	0	0
			2991	1867	540	570	1	13			

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



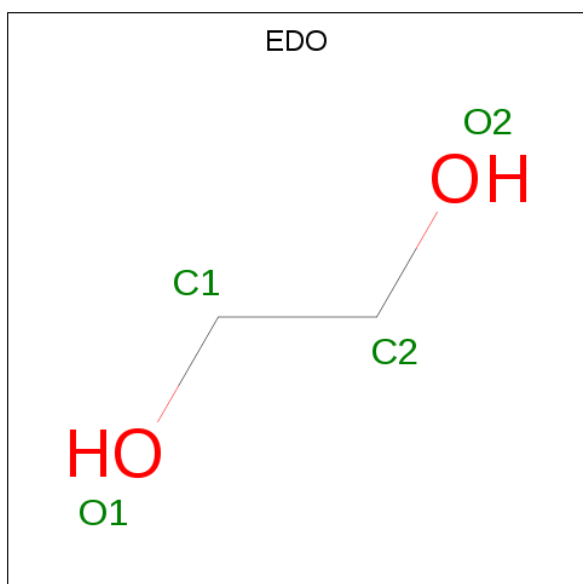
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



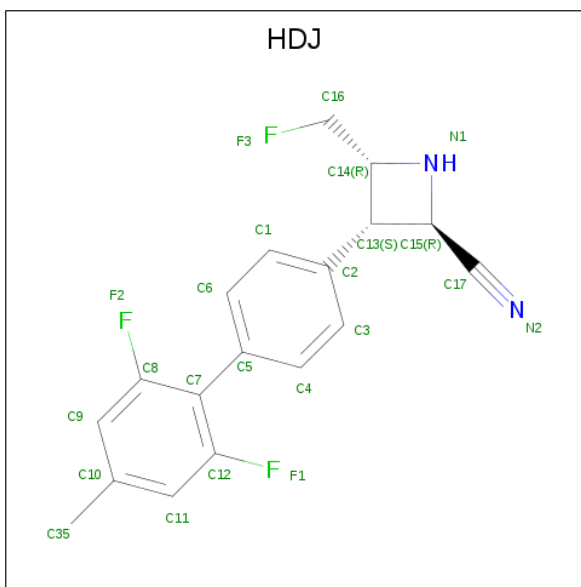
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



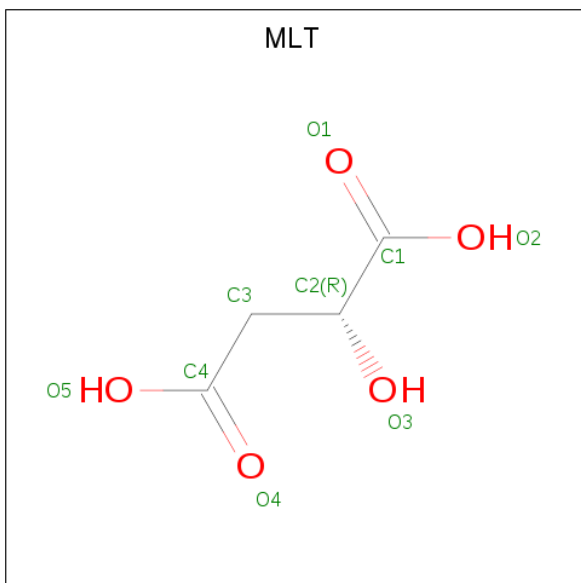
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 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: C₁₈H₁₅F₃N₂).



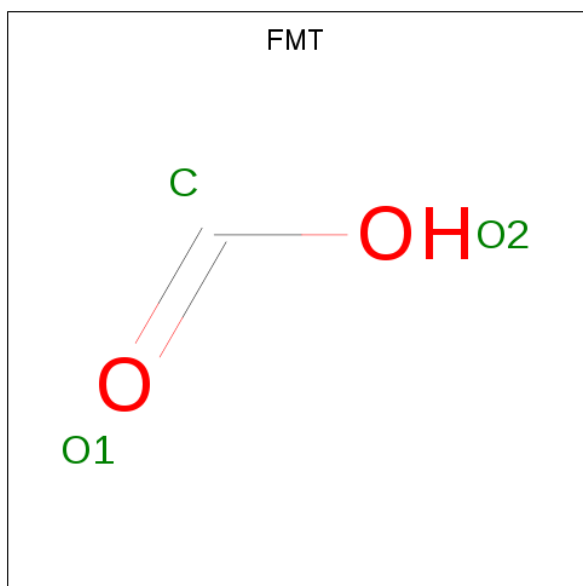
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	F	N	0	0
			23	18	3	2		
6	D	1	Total	C	F	N	0	0
			23	18	3	2		
6	F	1	Total	C	F	N	0	0
			23	18	3	2		
6	H	1	Total	C	F	N	0	0
			23	18	3	2		

- 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	0	1
			18	8	10		

- Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	17	Total O 17 17	0	0

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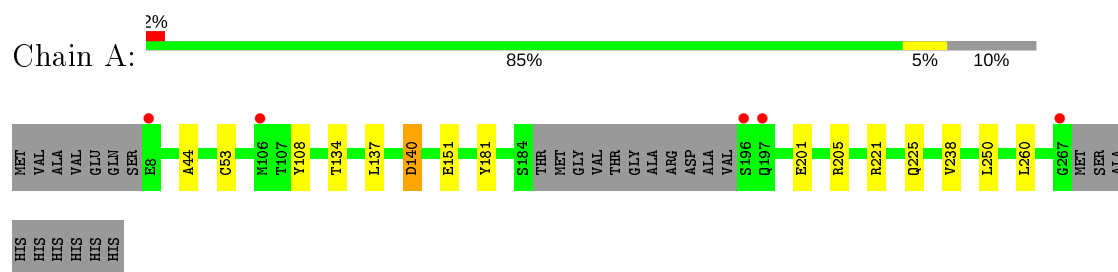
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	38	Total 38	O 38	0	0
9	C	21	Total 21	O 21	0	0
9	D	51	Total 51	O 51	0	0
9	E	2	Total 2	O 2	0	0
9	F	37	Total 37	O 37	0	0
9	G	14	Total 14	O 14	0	0
9	H	42	Total 42	O 42	0	0

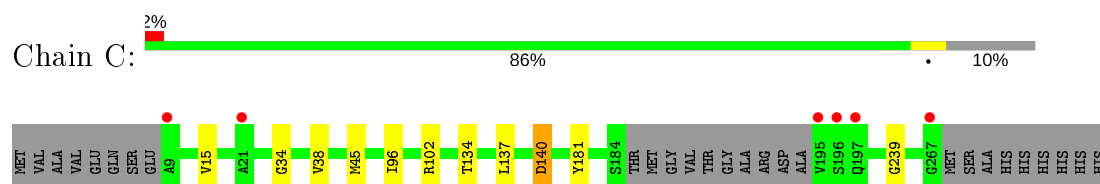
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

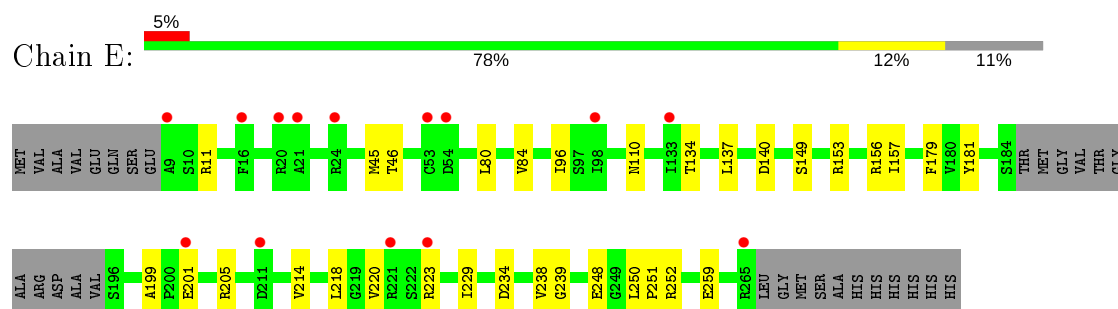
- Molecule 1: Tryptophan synthase alpha chain



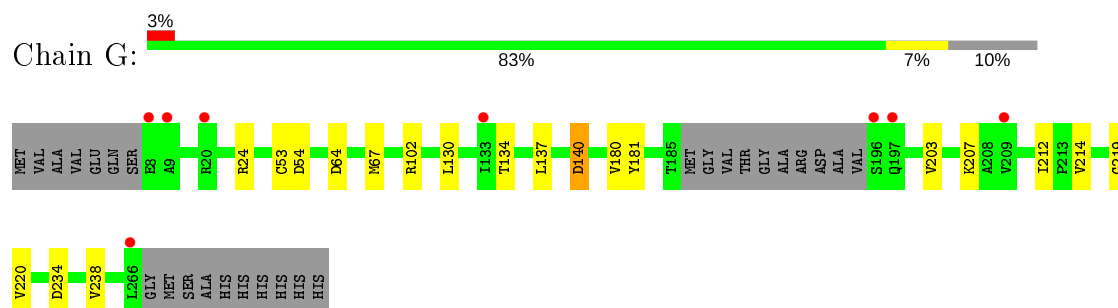
- Molecule 1: Tryptophan synthase alpha chain



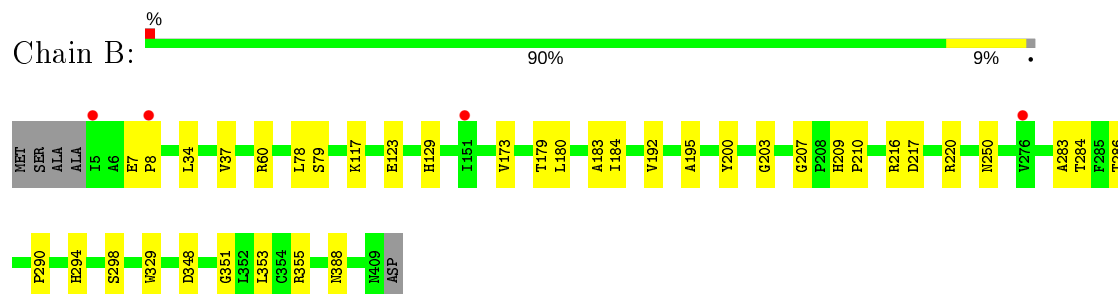
- Molecule 1: Tryptophan synthase alpha chain



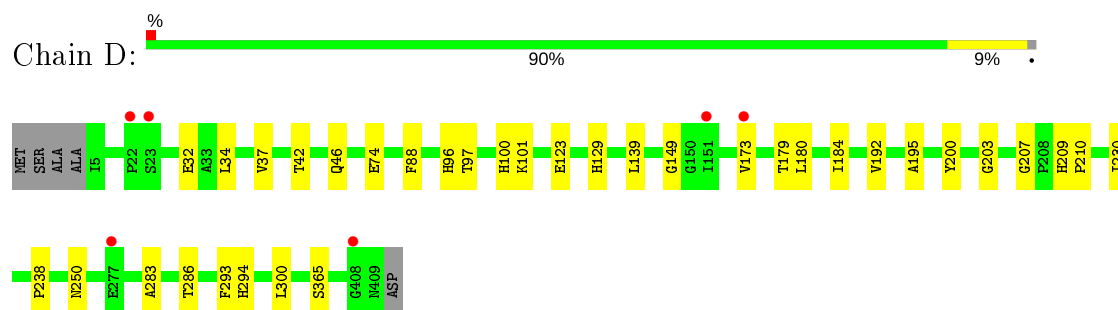
- Molecule 1: Tryptophan synthase alpha chain



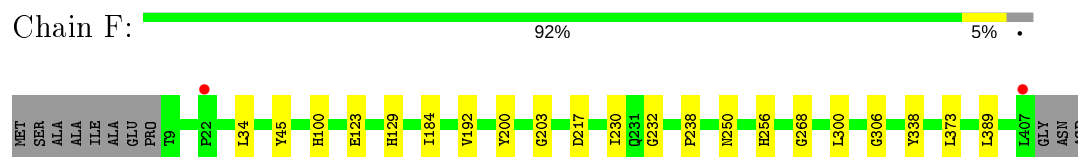
- Molecule 2: Tryptophan synthase beta chain



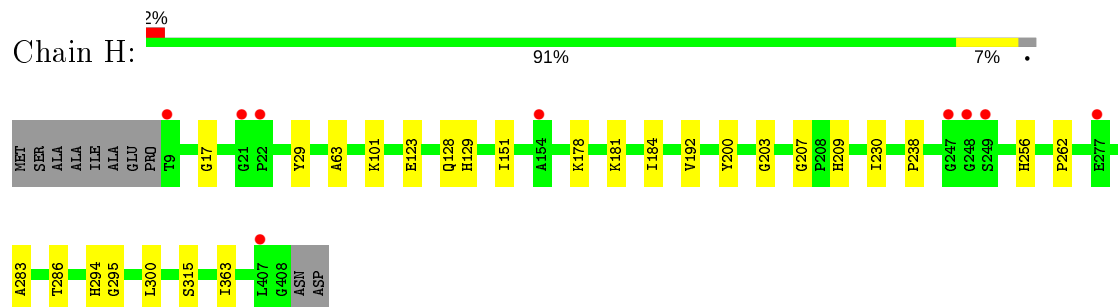
- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.66Å 157.94Å 166.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.34 – 2.57 29.34 – 2.57	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.34-2.57) 97.1 (29.34-2.57)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.57Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.176 , 0.217 0.176 , 0.217	Depositor DCC
R_{free} test set	2168 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19733	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLA, FMT, LLP, EDO, MLT, ACT, HDJ

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	0.28	0/1843	0.45	0/2514
1	C	0.28	0/1828	0.45	0/2495
1	E	0.26	0/1781	0.44	0/2436
1	G	0.27	0/1835	0.45	0/2505
2	B	0.28	0/3070	0.48	0/4161
2	D	0.29	0/3084	0.47	0/4179
2	F	0.29	0/3019	0.47	0/4091
2	H	0.28	0/3026	0.47	0/4100
All	All	0.28	0/19486	0.46	0/26481

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1814	0	1834	8	0
1	C	1799	0	1818	5	0
1	E	1752	0	1750	15	0
1	G	1806	0	1826	12	0
2	B	3034	0	2937	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3048	0	2958	18	0
2	F	2984	0	2893	12	0
2	H	2991	0	2904	14	0
3	A	7	0	2	0	0
3	C	7	0	2	0	0
4	A	4	0	3	0	0
4	B	8	0	6	0	0
4	G	8	0	6	0	0
5	A	4	0	6	2	0
5	B	4	0	6	0	0
5	D	16	0	24	0	0
5	E	4	0	6	0	0
5	F	12	0	18	1	0
5	G	4	0	6	0	0
5	H	8	0	12	1	0
6	B	23	0	0	0	0
6	D	23	0	0	0	0
6	F	23	0	0	0	0
6	H	23	0	0	0	0
7	B	18	0	8	1	0
8	B	18	0	6	9	0
8	C	9	0	3	0	0
8	D	33	0	11	2	0
8	F	12	0	4	1	0
8	H	15	0	5	1	0
9	A	17	0	0	0	0
9	B	38	0	0	0	0
9	C	21	0	0	0	0
9	D	51	0	0	1	0
9	E	2	0	0	0	0
9	F	37	0	0	0	0
9	G	14	0	0	1	0
9	H	42	0	0	0	0
All	All	19733	0	19054	108	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 3.

All (108) 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:79:SER:HB2	8:B:505:FMT:H	1.42	1.02
2:B:329:TRP:CD1	8:B:510:FMT:H	2.28	0.69
2:D:293:PHE:HB3	8:D:512:FMT:H	1.77	0.67
2:D:149:GLY:HA2	2:D:173:VAL:HG22	1.76	0.66
7:B:502[B]:MLT:H2	2:F:232:GLY:HA2	1.77	0.66
2:F:373:LEU:HD12	8:F:505:FMT:H	1.79	0.64
2:D:32:GLU:OE1	9:D:601:HOH:O	2.15	0.62
2:F:123:GLU:HG3	2:F:184:ILE:HG12	1.81	0.60
1:A:108:TYR:HE1	5:A:503:EDO:H12	1.66	0.60
1:E:11:ARG:NH1	1:E:153:ARG:O	2.33	0.60
2:B:329:TRP:NE1	8:B:510:FMT:H	2.18	0.59
1:E:218:LEU:HD12	1:E:229:ILE:HD11	1.83	0.58
2:B:7:GLU:HG2	2:B:220:ARG:HH22	1.69	0.58
2:H:123:GLU:HG3	2:H:184:ILE:HG12	1.87	0.56
2:B:129:HIS:CE1	2:B:203:GLY:HA2	2.41	0.55
1:E:149:SER:OG	1:E:156:ARG:NH1	2.39	0.55
2:D:34:LEU:HD13	2:D:192:VAL:HG22	1.88	0.55
2:B:123:GLU:HG3	2:B:184:ILE:HG12	1.88	0.55
1:G:180:VAL:HG23	1:G:212:ILE:HD13	1.89	0.54
2:B:351:GLY:HA3	8:B:503:FMT:H	1.89	0.54
2:B:283:ALA:HB1	2:B:286:THR:HB	1.89	0.54
2:H:262:PRO:O	5:H:507:EDO:H11	2.08	0.53
1:A:134:THR:HB	1:A:137:LEU:HB3	1.90	0.53
1:A:140:ASP:OD1	1:A:140:ASP:N	2.40	0.52
2:D:123:GLU:HG3	2:D:184:ILE:HG12	1.90	0.52
2:H:315:SER:HB2	2:H:363:ILE:HG22	1.91	0.51
2:B:216:ARG:O	2:B:220:ARG:HG3	2.11	0.51
2:D:207:GLY:HA2	2:D:294:HIS:O	2.09	0.51
2:D:42:THR:O	2:D:46:GLN:HG2	2.11	0.51
1:E:220:VAL:HB	1:E:238:VAL:HG22	1.94	0.50
2:H:230:ILE:HG21	2:H:238:PRO:HD3	1.94	0.50
1:G:220:VAL:HB	1:G:238:VAL:HG22	1.94	0.50
2:B:79:SER:CB	8:B:505:FMT:H	2.29	0.50
1:E:199:ALA:HB2	1:E:218:LEU:HD21	1.93	0.50
2:D:283:ALA:HB1	2:D:286:THR:HB	1.92	0.50
2:B:207:GLY:HA2	2:B:294:HIS:O	2.12	0.50
1:A:108:TYR:CE1	5:A:503:EDO:H12	2.45	0.49
1:G:24:ARG:NH2	1:G:54:ASP:OD2	2.41	0.49
2:F:230:ILE:HG21	2:F:238:PRO:HD3	1.95	0.49
1:C:134:THR:HB	1:C:137:LEU:HB3	1.94	0.49
2:B:284:THR:OG1	8:B:508:FMT:H	2.11	0.49
2:B:329:TRP:HE1	8:B:510:FMT:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:HB	2:B:195:ALA:HB1	1.95	0.49
1:G:219:GLY:N	9:G:602:HOH:O	2.46	0.49
2:B:34:LEU:HD13	2:B:192:VAL:HG22	1.94	0.49
1:E:45:MET:HB3	1:E:96:ILE:HD11	1.95	0.49
1:G:207:LYS:NZ	1:G:234:ASP:OD2	2.37	0.48
2:B:7:GLU:HG3	2:B:8:PRO:HD2	1.95	0.48
1:G:140:ASP:N	1:G:140:ASP:OD1	2.47	0.48
1:E:134:THR:HB	1:E:137:LEU:HB3	1.96	0.48
2:F:129:HIS:CE1	2:F:203:GLY:HA2	2.49	0.48
1:G:134:THR:HB	1:G:137:LEU:HB3	1.95	0.48
1:G:214:VAL:H	1:G:234:ASP:HB2	1.79	0.48
2:D:129:HIS:CE1	2:D:203:GLY:HA2	2.49	0.47
2:H:151:ILE:HG13	2:H:178:LYS:HB2	1.96	0.47
1:C:45:MET:HB3	1:C:96:ILE:HD11	1.96	0.47
2:H:283:ALA:HB1	2:H:286:THR:HB	1.97	0.47
2:B:351:GLY:CA	8:B:503:FMT:H	2.44	0.47
2:B:7:GLU:HG2	2:B:220:ARG:NH2	2.29	0.46
1:A:238:VAL:HG21	1:A:260:LEU:HD13	1.96	0.46
2:D:209:HIS:ND1	2:D:210:PRO:HA	2.31	0.45
2:B:355:ARG:HH11	8:B:503:FMT:C	2.29	0.45
2:B:60:ARG:HE	8:D:505:FMT:C	2.29	0.45
2:B:78:LEU:HD11	2:B:353:LEU:HD13	1.98	0.45
2:D:101:LLP:NZ	2:D:101:LLP:O3	2.47	0.45
2:F:34:LEU:HD13	2:F:192:VAL:HG22	1.99	0.45
2:D:139:LEU:O	5:F:507:EDO:H12	2.17	0.45
2:D:230:ILE:HG21	2:D:238:PRO:HD3	2.00	0.44
1:A:221:ARG:NH2	1:A:225:GLN:HE22	2.15	0.44
1:C:34:GLY:HA2	1:C:38:VAL:HA	2.00	0.44
2:H:17:GLY:HA3	2:H:209:HIS:HB2	2.00	0.44
1:C:15:VAL:HG22	1:C:102:ARG:HE	1.81	0.44
2:D:37:VAL:HB	2:D:195:ALA:HB1	2.00	0.43
2:H:29:TYR:O	2:H:295:GLY:HA2	2.18	0.43
1:G:67:MET:HE3	2:H:192:VAL:HG21	1.99	0.43
1:A:44:ALA:HA	1:A:250:LEU:HD11	1.99	0.43
1:G:102:ARG:HG2	1:G:130:LEU:HD11	1.99	0.43
2:B:290:PRO:HA	2:B:298:SER:O	2.18	0.43
2:B:173:VAL:HG21	2:B:183:ALA:HA	2.00	0.43
2:D:96:HIS:O	2:D:97:THR:OG1	2.28	0.43
1:E:250:LEU:N	1:E:251:PRO:HD2	2.33	0.43
2:B:179:THR:OG1	2:B:180:LEU:N	2.51	0.42
1:E:201:GLU:O	1:E:205:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ASP:OD1	1:C:140:ASP:N	2.51	0.42
2:D:74:GLU:HB2	2:D:88:PHE:CE2	2.55	0.42
1:E:110:ASN:ND2	2:F:306:GLY:O	2.52	0.42
2:H:129:HIS:CE1	2:H:203:GLY:HA2	2.55	0.42
1:G:64:ASP:OD2	2:H:181:LYS:NZ	2.32	0.42
2:B:209:HIS:ND1	2:B:210:PRO:HA	2.35	0.42
2:H:101:LLP:HO3	2:H:128:GLN:HG2	1.84	0.42
2:H:63:ALA:O	8:H:505:FMT:O2	2.37	0.42
2:F:100:HIS:CE1	2:F:250:ASN:HB3	2.54	0.41
2:F:268:GLY:O	2:F:338:TYR:HA	2.20	0.41
2:B:217:ASP:HA	2:B:220:ARG:HG3	2.01	0.41
1:E:223:ARG:HB2	1:E:259:GLU:HB3	2.03	0.41
2:F:45:TYR:OH	2:F:217:ASP:OD2	2.35	0.41
2:B:117:LYS:NZ	2:B:195:ALA:O	2.49	0.41
2:H:207:GLY:HA2	2:H:294:HIS:O	2.21	0.41
1:E:248:GLU:CD	1:E:252:ARG:HG2	2.42	0.41
2:D:100:HIS:NE2	2:D:250:ASN:HB3	2.35	0.41
1:E:214:VAL:H	1:E:234:ASP:HB2	1.86	0.41
2:F:389:LEU:HA	2:F:389:LEU:HD12	1.93	0.41
1:E:80:LEU:HA	1:E:84:VAL:HG12	2.04	0.40
1:E:157:ILE:HG12	1:E:179:PHE:CE1	2.57	0.40
2:F:123:GLU:HG3	2:F:184:ILE:CG1	2.51	0.40
1:G:203:VAL:HG22	1:G:214:VAL:HG11	2.03	0.40
1:A:201:GLU:O	1:A:205:ARG:HG3	2.21	0.40
2:D:179:THR:OG1	2:D:180:LEU:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	241 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	245/276 (89%)	241 (98%)	3 (1%)	1 (0%)	34	45
1	E	242/276 (88%)	235 (97%)	6 (2%)	1 (0%)	34	45
1	G	245/276 (89%)	240 (98%)	5 (2%)	0	100	100
2	B	403/410 (98%)	393 (98%)	10 (2%)	0	100	100
2	D	404/410 (98%)	391 (97%)	13 (3%)	0	100	100
2	F	396/410 (97%)	385 (97%)	11 (3%)	0	100	100
2	H	397/410 (97%)	389 (98%)	8 (2%)	0	100	100
All	All	2578/2744 (94%)	2515 (98%)	61 (2%)	2 (0%)	51	65

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	176 (98%)	4 (2%)	52	66
1	C	178/200 (89%)	176 (99%)	2 (1%)	73	83
1	E	171/200 (86%)	168 (98%)	3 (2%)	59	73
1	G	180/200 (90%)	177 (98%)	3 (2%)	60	74
2	B	298/301 (99%)	294 (99%)	4 (1%)	69	80
2	D	300/301 (100%)	297 (99%)	3 (1%)	76	84
2	F	292/301 (97%)	289 (99%)	3 (1%)	76	84
2	H	294/301 (98%)	291 (99%)	3 (1%)	76	84
All	All	1893/2004 (94%)	1868 (99%)	25 (1%)	69	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	140	ASP
1	A	151	GLU
1	A	181	TYR
2	B	200	TYR
2	B	250	ASN
2	B	348	ASP
2	B	388	ASN
1	C	140	ASP
1	C	181	TYR
2	D	200	TYR
2	D	300	LEU
2	D	365	SER
1	E	46	THR
1	E	140	ASP
1	E	181	TYR
2	F	200	TYR
2	F	256	HIS
2	F	300	LEU
1	G	53	CYS
1	G	140	ASP
1	G	181	TYR
2	H	200	TYR
2	H	256	HIS
2	H	300	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	250	ASN
2	B	388	ASN

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	2.55	6 (26%)	25,32,34	1.32	4 (16%)
2	LLP	F	101	2	23,24,25	2.53	6 (26%)	25,32,34	1.32	4 (16%)
2	LLP	H	101	2	23,24,25	2.65	6 (26%)	25,32,34	1.20	2 (8%)
2	LLP	B	101	2	23,24,25	2.61	7 (30%)	25,32,34	1.29	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	-	3/16/17/19	0/1/1/1
2	LLP	B	101	2	-	5/16/17/19	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	101	LLP	C4-C4'	8.41	1.62	1.46
2	B	101	LLP	C4-C4'	8.04	1.61	1.46
2	D	101	LLP	C4-C4'	7.91	1.61	1.46
2	F	101	LLP	C4-C4'	7.82	1.61	1.46
2	H	101	LLP	C4'-NZ	5.13	1.44	1.27
2	D	101	LLP	C4'-NZ	5.05	1.44	1.27
2	F	101	LLP	C4'-NZ	4.97	1.44	1.27
2	B	101	LLP	C4'-NZ	4.90	1.43	1.27
2	B	101	LLP	C4-C5	-4.03	1.36	1.42
2	F	101	LLP	C4-C5	-3.86	1.37	1.42
2	D	101	LLP	C4-C5	-3.64	1.37	1.42
2	B	101	LLP	C2'-C2	3.41	1.56	1.50
2	H	101	LLP	C4-C5	-3.39	1.37	1.42
2	D	101	LLP	C2'-C2	3.28	1.55	1.50
2	H	101	LLP	C2'-C2	3.28	1.55	1.50
2	F	101	LLP	C2'-C2	3.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	101	LLP	C6-N1	3.08	1.40	1.34
2	B	101	LLP	C6-N1	3.03	1.40	1.34
2	F	101	LLP	C6-N1	3.01	1.40	1.34
2	D	101	LLP	C6-N1	3.00	1.40	1.34
2	H	101	LLP	C5'-C5	2.40	1.57	1.50
2	D	101	LLP	C5'-C5	2.13	1.56	1.50
2	B	101	LLP	C5'-C5	2.13	1.56	1.50
2	F	101	LLP	C5'-C5	2.08	1.56	1.50
2	B	101	LLP	C3-C2	2.02	1.42	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	101	LLP	C4-C4'-NZ	-3.68	107.41	124.31
2	D	101	LLP	C4-C4'-NZ	-3.44	108.50	124.31
2	B	101	LLP	C4-C4'-NZ	-3.12	110.00	124.31
2	H	101	LLP	C4-C4'-NZ	-3.12	110.00	124.31
2	D	101	LLP	CE-NZ-C4'	-2.60	110.92	118.90
2	B	101	LLP	CE-NZ-C4'	-2.59	110.94	118.90
2	H	101	LLP	CE-NZ-C4'	-2.43	111.43	118.90
2	B	101	LLP	C5-C6-N1	-2.38	119.85	123.82
2	B	101	LLP	C3-C4-C5	2.30	120.03	118.26
2	F	101	LLP	CE-NZ-C4'	-2.27	111.93	118.90
2	F	101	LLP	C5-C6-N1	-2.22	120.11	123.82
2	F	101	LLP	C3-C4-C5	2.14	119.91	118.26
2	D	101	LLP	C3-C4-C5	2.14	119.91	118.26
2	D	101	LLP	C5-C6-N1	-2.02	120.46	123.82

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	101	LLP	C5'-OP4-P-OP3
2	F	101	LLP	CD-CE-NZ-C4'
2	H	101	LLP	CD-CE-NZ-C4'
2	D	101	LLP	CD-CE-NZ-C4'
2	B	101	LLP	CD-CE-NZ-C4'
2	F	101	LLP	C5'-OP4-P-OP3
2	D	101	LLP	C3-C4-C4'-NZ
2	F	101	LLP	C3-C4-C4'-NZ
2	B	101	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	101	LLP	1	0
2	H	101	LLP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

55 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	$\# Z > 2$
5	EDO	F	507	-	3,3,3	0.50	0	2,2,2	0.16	0
5	EDO	B	511	-	3,3,3	0.48	0	2,2,2	0.23	0
6	HDJ	B	501	-	23,25,25	1.22	1 (4%)	23,36,36	1.73	5 (21%)
8	FMT	H	503	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	D	503	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	F	504	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	G	503	-	1,3,3	1.34	0	0,3,3	0.00	-
3	MLA	C	501	-	0,6,6	0.00	-	0,7,7	0.00	-
8	FMT	H	502	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	C	504	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	F	502	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	D	515	-	0,2,2	0.00	-	0,1,1	0.00	-
7	MLT	B	502[A]	-	2,8,8	0.41	0	3,10,10	0.80	0
8	FMT	H	505	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	F	506	-	3,3,3	0.47	0	2,2,2	0.33	0
7	MLT	B	502[B]	-	2,8,8	0.42	0	3,10,10	0.52	0
8	FMT	D	516	-	0,2,2	0.00	-	0,1,1	0.00	-
6	HDJ	D	501	-	23,25,25	1.25	1 (4%)	23,36,36	1.64	5 (21%)
8	FMT	B	503	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ACT	B	506	-	1,3,3	1.72	0	0,3,3	0.00	-
8	FMT	D	513	-	0,2,2	0.00	-	0,1,1	0.00	-
6	HDJ	F	501	-	23,25,25	1.14	2 (8%)	23,36,36	1.46	2 (8%)
8	FMT	B	509	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	D	507	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	F	503	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	B	508	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	A	503	-	3,3,3	0.48	0	2,2,2	0.21	0
8	FMT	D	512	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	H	508	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ACT	B	504	-	1,3,3	1.13	0	0,3,3	0.00	-
8	FMT	B	505	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	C	502	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	F	505	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ACT	G	501	-	1,3,3	1.41	0	0,3,3	0.00	-
8	FMT	H	504	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	D	514	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	C	503	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	B	507	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ACT	A	502	-	1,3,3	1.71	0	0,3,3	0.00	-
8	FMT	D	502	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	D	506	-	0,2,2	0.00	-	0,1,1	0.00	-
6	HDJ	H	501	-	23,25,25	1.46	2 (8%)	23,36,36	1.65	6 (26%)
5	EDO	H	507	-	3,3,3	0.46	0	2,2,2	0.26	0
5	EDO	D	508	-	3,3,3	0.46	0	2,2,2	0.36	0
8	FMT	D	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	E	501	-	3,3,3	0.49	0	2,2,2	0.29	0
3	MLA	A	501	-	0,6,6	0.00	-	0,7,7	0.00	-
5	EDO	D	510	-	3,3,3	0.49	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FMT	D	505	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	B	510	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	F	508	-	3,3,3	0.48	0	2,2,2	0.34	0
5	EDO	G	502	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	H	506	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	D	511	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EDO	D	509	-	3,3,3	0.52	0	2,2,2	0.20	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
5	EDO	F	506	-	-	0/1/1/1	-
5	EDO	F	507	-	-	0/1/1/1	-
5	EDO	B	511	-	-	0/1/1/1	-
5	EDO	H	507	-	-	0/1/1/1	-
6	HDJ	D	501	-	-	2/8/24/24	0/3/3/3
6	HDJ	B	501	-	-	2/8/24/24	0/3/3/3
5	EDO	E	501	-	-	0/1/1/1	-
6	HDJ	F	501	-	-	1/8/24/24	0/3/3/3
5	EDO	D	509	-	-	0/1/1/1	-
3	MLA	A	501	-	-	0/0/4/4	-
7	MLT	B	502[B]	-	-	0/2/8/8	-
3	MLA	C	501	-	-	0/0/4/4	-
5	EDO	H	506	-	-	1/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	D	510	-	-	0/1/1/1	-
5	EDO	F	508	-	-	0/1/1/1	-
6	HDJ	H	501	-	-	1/8/24/24	0/3/3/3
5	EDO	D	508	-	-	0/1/1/1	-
7	MLT	B	502[A]	-	-	2/2/8/8	-
5	EDO	D	511	-	-	0/1/1/1	-
5	EDO	G	502	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	501	HDJ	C13-C15	-6.07	1.50	1.56
6	D	501	HDJ	C13-C15	-5.00	1.51	1.56
6	B	501	HDJ	C13-C15	-4.77	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	501	HDJ	C13-C15	-4.27	1.52	1.56
6	F	501	HDJ	C15-C17	-2.24	1.46	1.48
6	H	501	HDJ	C15-C17	-2.23	1.46	1.48

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	HDJ	C8-C7-C12	4.94	119.41	114.56
6	D	501	HDJ	C8-C7-C12	4.62	119.10	114.56
6	H	501	HDJ	C8-C7-C12	4.49	118.97	114.56
6	F	501	HDJ	C8-C7-C12	4.16	118.64	114.56
6	B	501	HDJ	C9-C8-C7	-3.21	119.78	123.45
6	H	501	HDJ	C9-C8-C7	-3.10	119.91	123.45
6	D	501	HDJ	C9-C8-C7	-3.03	119.99	123.45
6	F	501	HDJ	C9-C8-C7	-3.00	120.02	123.45
6	B	501	HDJ	C5-C7-C12	-2.99	116.33	120.92
6	H	501	HDJ	C5-C7-C12	-2.61	116.90	120.92
6	D	501	HDJ	C6-C5-C7	-2.59	116.50	120.79
6	D	501	HDJ	C5-C7-C12	-2.48	117.11	120.92
6	H	501	HDJ	C6-C5-C7	-2.46	116.71	120.79
6	B	501	HDJ	C6-C5-C7	-2.25	117.07	120.79
6	B	501	HDJ	C5-C7-C8	2.11	124.16	120.92
6	H	501	HDJ	C4-C5-C7	2.05	124.20	120.79
6	H	501	HDJ	C11-C12-C7	-2.05	121.11	123.45
6	D	501	HDJ	C11-C12-C7	-2.02	121.14	123.45

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	506	EDO	O1-C1-C2-O2
7	B	502[A]	MLT	O3-C2-C3-C4
7	B	502[A]	MLT	C1-C2-C3-C4
5	G	502	EDO	O1-C1-C2-O2
6	D	501	HDJ	C15-C13-C2-C3
6	B	501	HDJ	C15-C13-C2-C1
6	B	501	HDJ	C15-C13-C2-C3
6	D	501	HDJ	C15-C13-C2-C1
6	F	501	HDJ	C15-C13-C2-C1
6	H	501	HDJ	C15-C13-C2-C1

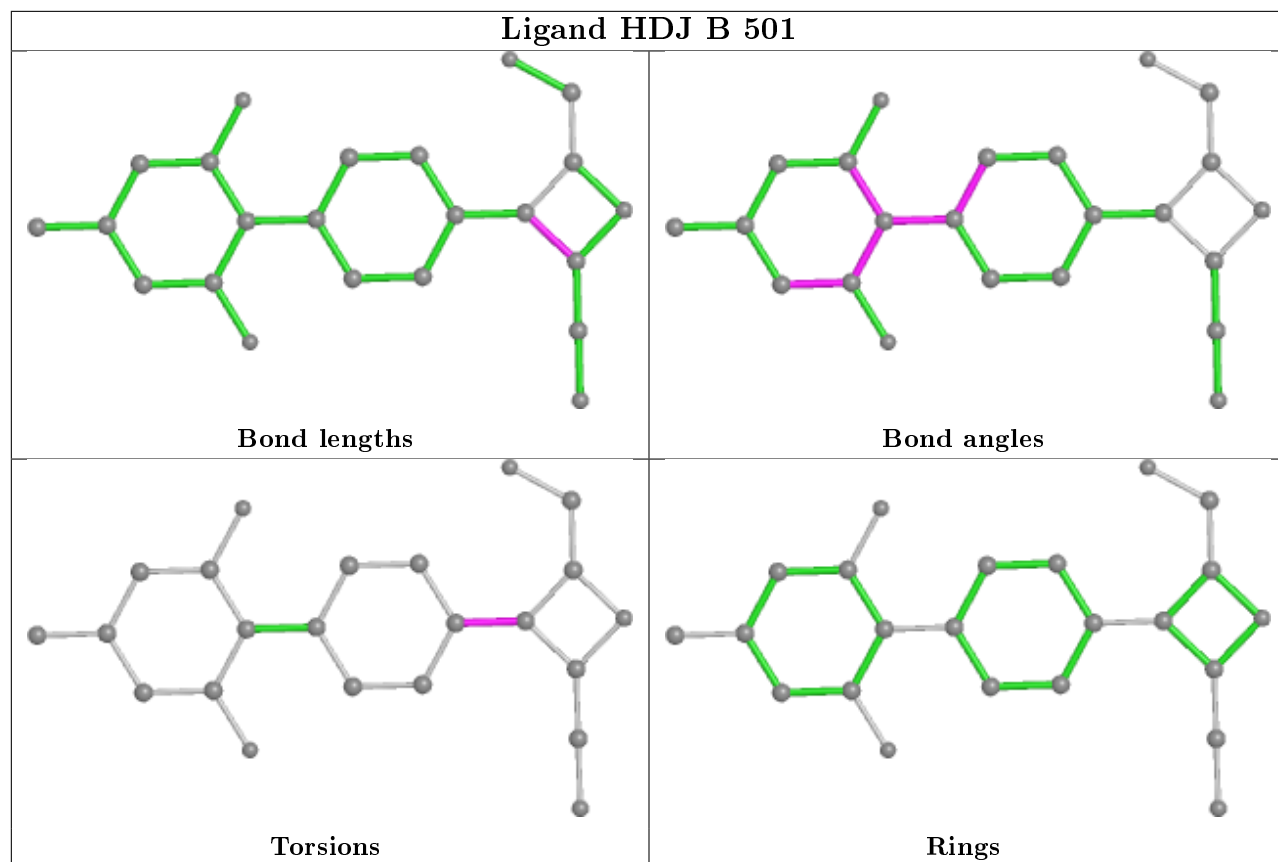
There are no ring outliers.

12 monomers are involved in 18 short contacts:

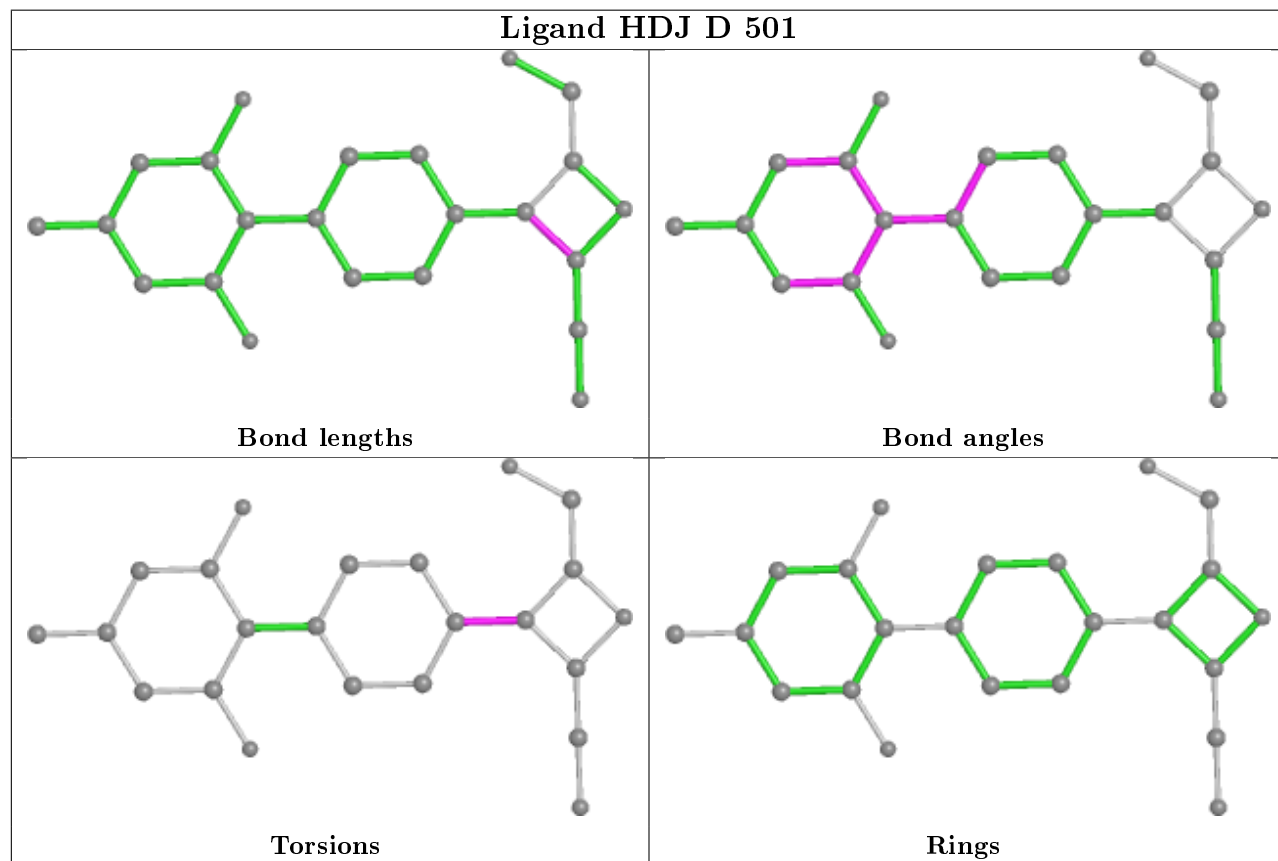
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	507	EDO	1	0
8	H	505	FMT	1	0
7	B	502[B]	MLT	1	0
8	B	503	FMT	3	0
8	B	508	FMT	1	0
5	A	503	EDO	2	0
8	D	512	FMT	1	0
8	B	505	FMT	2	0
8	F	505	FMT	1	0
5	H	507	EDO	1	0
8	D	505	FMT	1	0
8	B	510	FMT	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

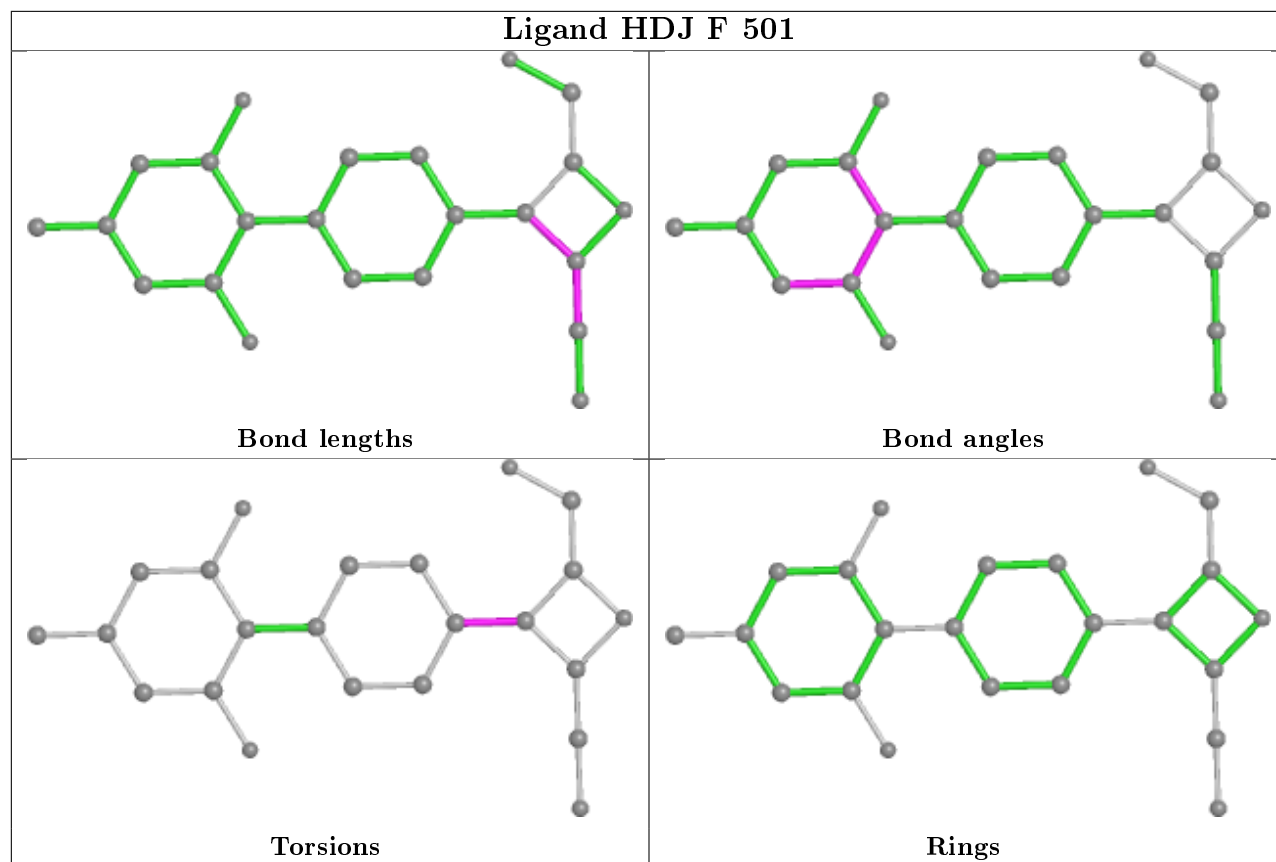
Ligand HDJ B 501



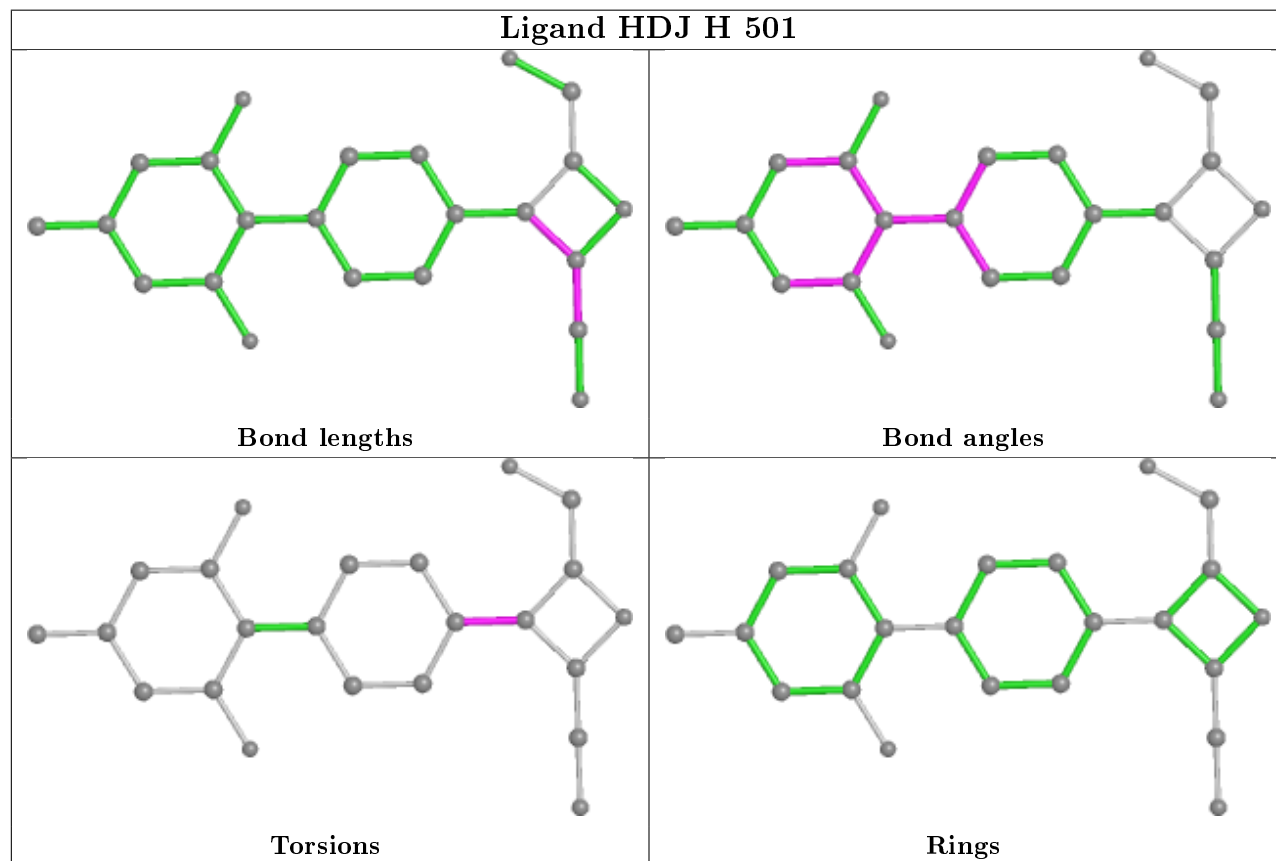
Ligand HDJ D 501



Ligand HDJ F 501



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	249/276 (90%)	-0.30	5 (2%) 65 73	29, 40, 61, 91	0
1	C	249/276 (90%)	-0.28	6 (2%) 59 67	26, 41, 60, 104	0
1	E	246/276 (89%)	0.32	14 (5%) 23 30	37, 70, 101, 117	0
1	G	249/276 (90%)	-0.08	8 (3%) 47 57	29, 49, 83, 115	0
2	B	404/410 (98%)	-0.44	4 (0%) 82 87	22, 34, 57, 103	0
2	D	404/410 (98%)	-0.38	6 (1%) 73 80	21, 32, 60, 97	0
2	F	398/410 (97%)	-0.45	2 (0%) 91 94	23, 35, 53, 76	0
2	H	399/410 (97%)	-0.28	9 (2%) 60 68	22, 33, 54, 94	0
All	All	2598/2744 (94%)	-0.27	54 (2%) 63 71	21, 38, 77, 117	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	8	GLU	6.4
2	H	22	PRO	4.7
1	C	195	VAL	4.4
2	F	22	PRO	3.9
1	C	196	SER	3.7
1	G	9	ALA	3.7
2	H	154	ALA	3.6
1	A	196	SER	3.5
2	H	9	THR	3.5
1	E	9	ALA	3.1
1	G	266	LEU	3.1
2	B	8	PRO	3.1
1	C	21	ALA	3.0
1	G	209	VAL	3.0
1	E	21	ALA	2.9
1	C	267	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	98	ILE	2.8
2	D	23	SER	2.8
2	D	151	ILE	2.8
2	F	407	LEU	2.8
2	B	5	ILE	2.7
1	G	197	GLN	2.7
1	A	8	GLU	2.6
2	B	151	ILE	2.5
1	E	24	ARG	2.5
2	H	21	GLY	2.5
2	H	247	GLY	2.5
2	D	22	PRO	2.5
2	D	173	VAL	2.5
1	E	133	ILE	2.4
1	E	265	ARG	2.4
1	C	197	GLN	2.3
1	A	267	GLY	2.3
1	E	211	ASP	2.3
2	H	407	LEU	2.3
2	H	249	SER	2.3
1	G	196	SER	2.2
1	E	201	GLU	2.2
1	G	133	ILE	2.2
2	B	276	VAL	2.2
1	G	20	ARG	2.2
2	D	277	GLU	2.2
1	E	53	CYS	2.2
1	E	54	ASP	2.1
1	E	221	ARG	2.1
1	C	9	ALA	2.1
2	H	248	GLY	2.1
1	A	197	GLN	2.1
2	H	277	GLU	2.1
1	E	223	ARG	2.1
1	A	106	MET	2.0
2	D	408	GLY	2.0
1	E	20	ARG	2.0
1	E	16	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LLP	D	101	24/25	0.98	0.21	21,30,37,38	0
2	LLP	F	101	24/25	0.98	0.19	22,30,34,36	0
2	LLP	H	101	24/25	0.98	0.18	25,29,34,37	0
2	LLP	B	101	24/25	0.98	0.20	27,36,40,43	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FMT	D	515	3/3	0.50	0.64	72,72,73,74	0
5	EDO	F	507	4/4	0.60	0.54	63,63,65,66	0
5	EDO	A	503	4/4	0.73	0.39	58,58,60,61	0
8	FMT	D	516	3/3	0.75	0.46	61,61,62,64	0
8	FMT	D	514	3/3	0.77	0.19	66,66,67,67	0
8	FMT	B	510	3/3	0.80	0.46	66,66,67,68	0
8	FMT	C	502	3/3	0.81	0.48	59,59,64,66	0
4	ACT	B	506	4/4	0.83	0.41	64,69,71,71	0
8	FMT	D	506	3/3	0.83	0.17	58,58,60,61	0
5	EDO	D	509	4/4	0.83	0.47	46,52,53,55	0
7	MLT	B	502[A]	9/9	0.85	0.28	63,64,64,64	9
7	MLT	B	502[B]	9/9	0.85	0.28	61,64,64,64	9
5	EDO	F	508	4/4	0.86	0.29	54,55,57,57	0
8	FMT	B	505	3/3	0.86	0.31	52,52,53,55	0
8	FMT	F	503	3/3	0.87	0.27	57,57,58,58	0
8	FMT	F	505	3/3	0.87	0.34	46,46,52,52	0
8	FMT	B	503	3/3	0.88	0.21	43,43,51,52	0
8	FMT	D	512	3/3	0.88	0.27	60,60,62,64	0

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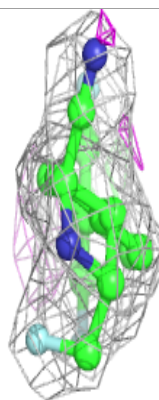
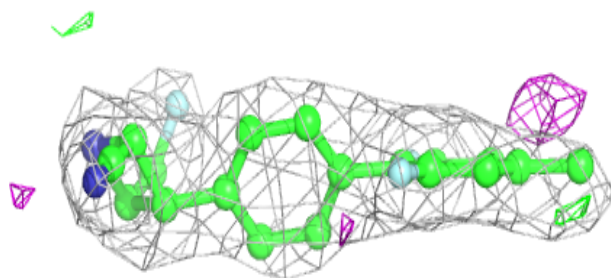
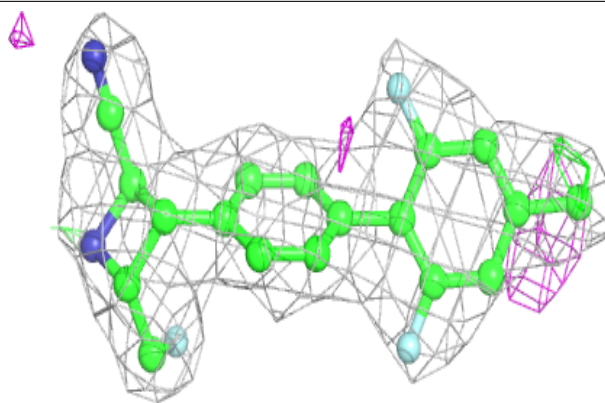
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FMT	H	505	3/3	0.88	0.32	61,61,64,65	0
5	EDO	H	506	4/4	0.89	0.27	51,53,55,56	0
8	FMT	D	505	3/3	0.89	0.38	51,51,52,52	0
8	FMT	H	503	3/3	0.89	0.17	52,52,54,56	0
8	FMT	C	503	3/3	0.89	0.47	59,59,60,60	0
8	FMT	D	502	3/3	0.89	0.25	48,48,50,51	0
5	EDO	D	511	4/4	0.89	0.39	45,47,50,51	0
8	FMT	D	503	3/3	0.90	0.19	54,54,59,61	0
5	EDO	H	507	4/4	0.90	0.19	53,55,55,55	0
5	EDO	E	501	4/4	0.90	0.19	48,51,55,56	0
8	FMT	B	508	3/3	0.90	0.23	65,65,66,66	0
4	ACT	G	501	4/4	0.91	0.23	57,61,61,64	0
5	EDO	B	511	4/4	0.91	0.21	49,49,53,54	0
8	FMT	B	509	3/3	0.91	0.20	64,64,66,66	0
8	FMT	F	504	3/3	0.91	0.24	51,51,53,55	0
5	EDO	G	502	4/4	0.91	0.22	51,52,53,54	0
5	EDO	D	508	4/4	0.92	0.20	48,53,56,57	0
4	ACT	A	502	4/4	0.92	0.28	66,67,68,68	0
5	EDO	F	506	4/4	0.92	0.26	53,53,54,56	0
5	EDO	D	510	4/4	0.92	0.22	47,47,48,49	0
4	ACT	B	504	4/4	0.93	0.27	66,67,67,67	0
3	MLA	A	501	7/7	0.94	0.11	45,47,49,49	0
6	HDJ	D	501	23/23	0.94	0.17	36,44,49,51	0
3	MLA	C	501	7/7	0.94	0.13	57,59,59,60	0
8	FMT	H	502	3/3	0.94	0.20	59,59,59,60	0
8	FMT	D	513	3/3	0.94	0.17	51,51,54,55	0
8	FMT	H	504	3/3	0.94	0.34	57,57,58,61	0
8	FMT	F	502	3/3	0.94	0.10	45,45,48,50	0
8	FMT	B	507	3/3	0.94	0.12	46,46,48,49	0
6	HDJ	F	501	23/23	0.95	0.14	34,39,43,45	0
6	HDJ	B	501	23/23	0.95	0.15	39,45,47,47	0
8	FMT	D	504	3/3	0.96	0.14	60,60,61,63	0
6	HDJ	H	501	23/23	0.96	0.16	32,37,42,46	0
4	ACT	G	503	4/4	0.97	0.12	46,50,51,51	0
8	FMT	H	508	3/3	0.97	0.33	62,62,63,63	0
8	FMT	C	504	3/3	0.97	0.15	49,49,50,51	0
8	FMT	D	507	3/3	0.98	0.15	47,47,48,51	0

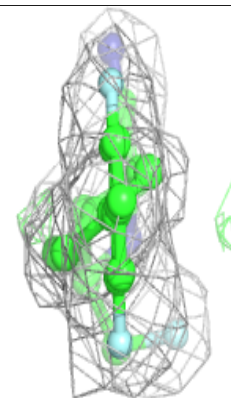
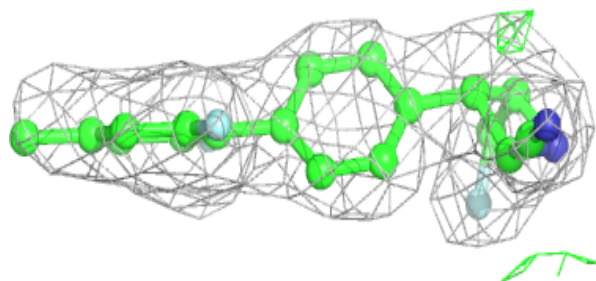
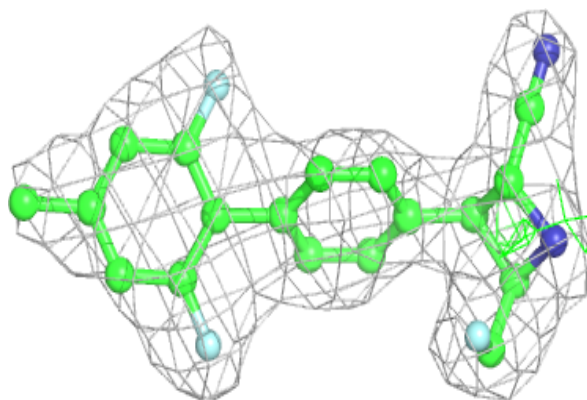
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDJ D 501:

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

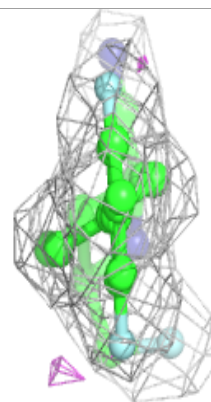
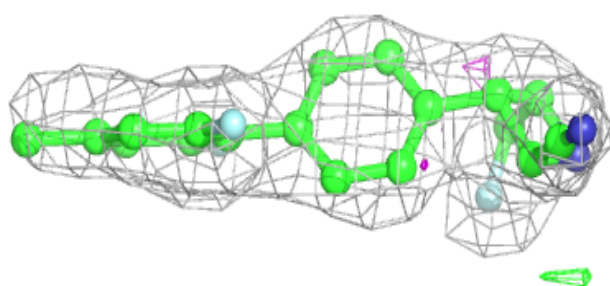
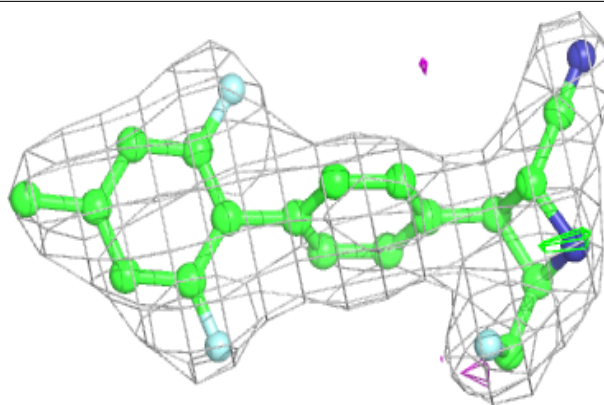
**Electron density around HDJ F 501:**

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and green (positive)

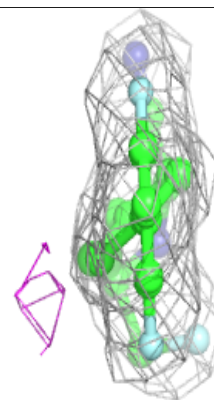
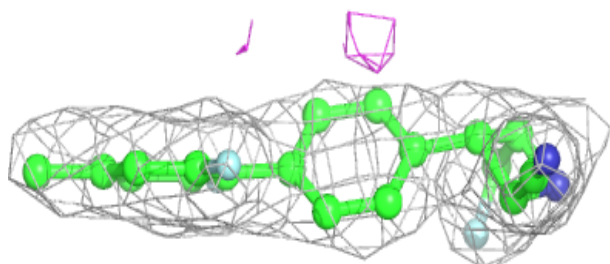
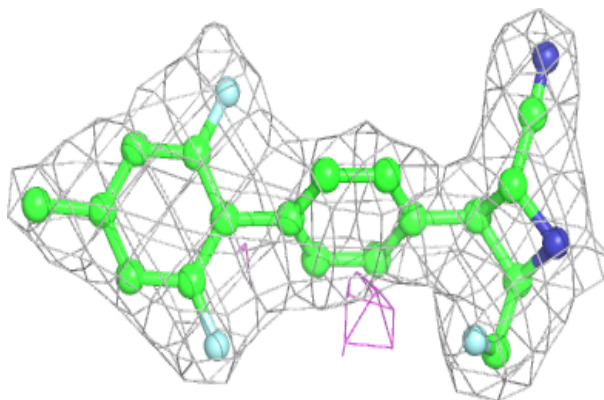


Electron density around HDJ B 501:

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

**Electron density around HDJ 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.