



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 12:39 PM EDT

PDB ID : 8DB0 / pdb_00008db0
Title : Crystal structure of DMATS1 prenyltransferase in complex with L-Trp and DMSPP
Authors : Eaton, S.A.; Ronnebaum, T.A.; Roose, B.W.; Christianson, D.W.
Deposited on : 2022-06-14
Resolution : 2.26 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

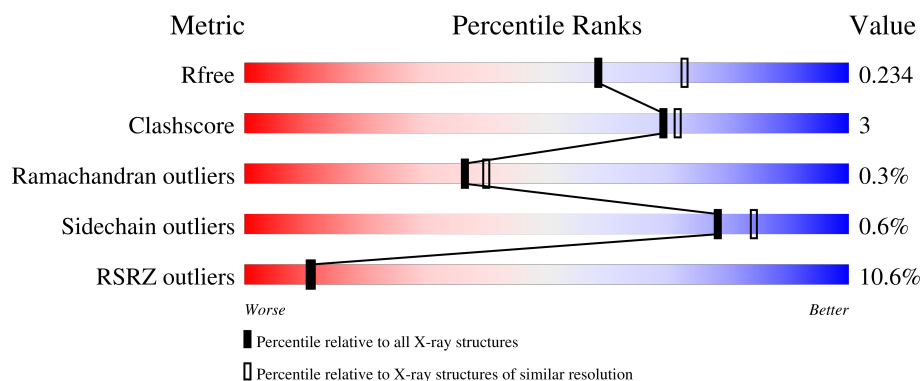
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	419	
1	B	419	
1	C	419	
1	D	419	

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
4	DST	C	501	-	-	X	-

2 Entry composition [i](#)

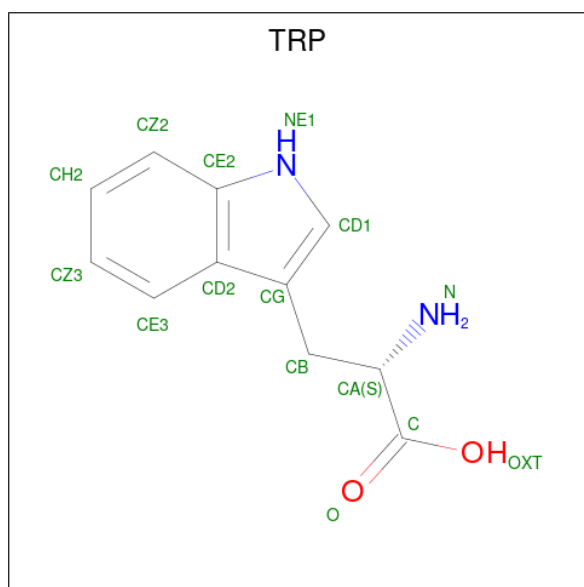
There are 6 unique types of molecules in this entry. The entry contains 12476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dimethylallyltryptophan synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3118	2019	518	573	8			
1	B	389	Total	C	N	O	S	0	0	0
			3036	1964	502	562	8			
1	C	384	Total	C	N	O	S	0	0	0
			2910	1888	482	533	7			
1	D	382	Total	C	N	O	S	0	0	0
			2839	1840	464	528	7			

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



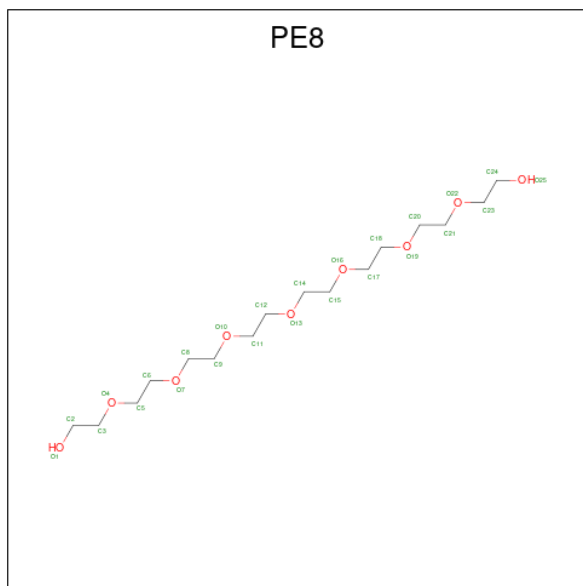
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

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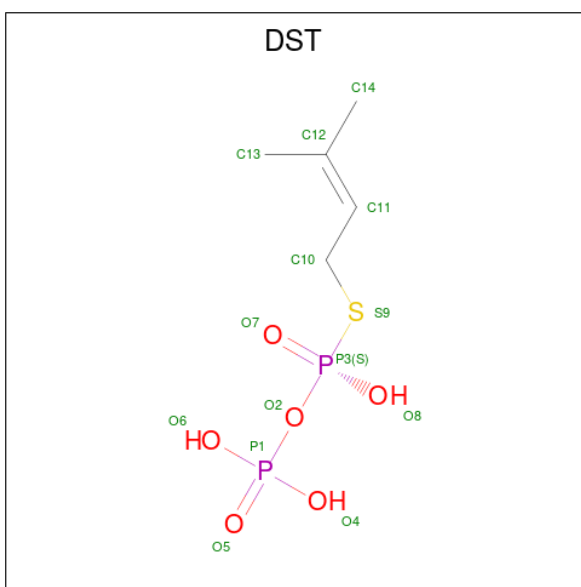
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: $C_{16}H_{34}O_9$).



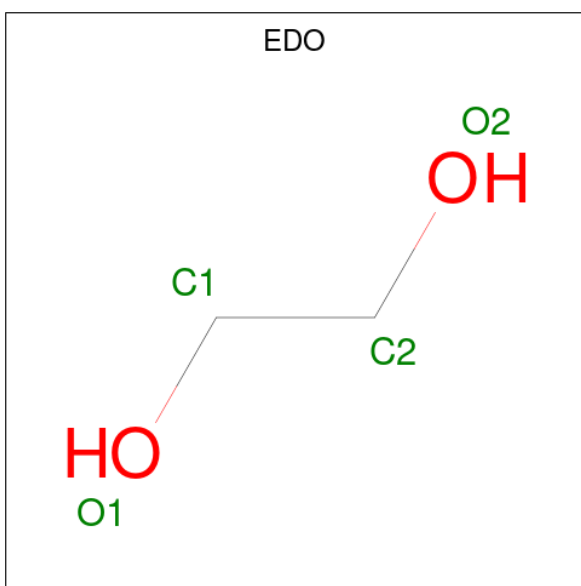
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	16	9		

- Molecule 4 is DIMETHYLALLYL S-THIOLODIPHOSPHATE (CCD ID: DST) (formula: $C_5H_{12}O_6P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	O	P	S	0	0
			14	5	6	2	1		
4	C	1	Total	C	O	P	S	0	0
			14	5	6	2	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is water.

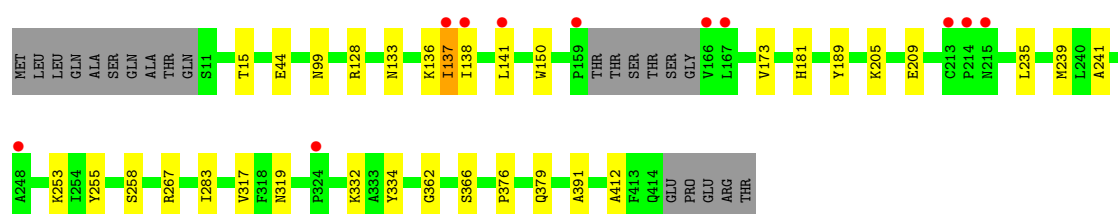
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	200	Total 200	O 200	0	0
6	B	129	Total 129	O 129	0	0
6	C	76	Total 76	O 76	0	0
6	D	51	Total 51	O 51	0	0

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.

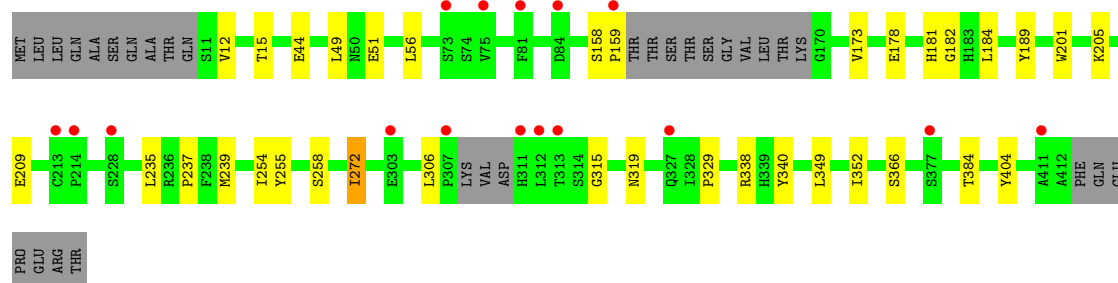
• Molecule 1: Dimethylallyltryptophan synthase 1

Chain A: 



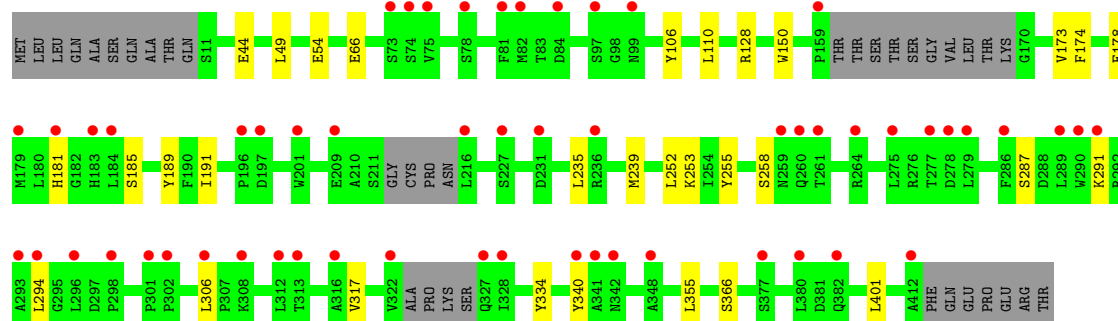
• Molecule 1: Dimethylallyltryptophan synthase 1

Chain B: 

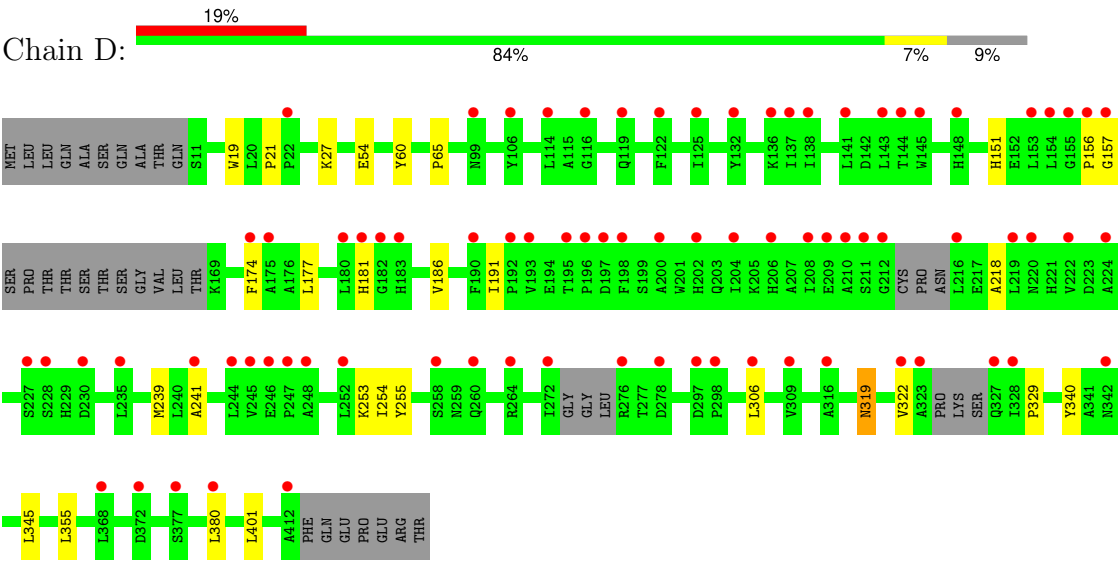


• Molecule 1: Dimethylallyltryptophan synthase 1

Chain C: 



● Molecule 1: Dimethylallyltryptophan synthase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.50Å 108.40Å 182.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.14 – 2.26 93.14 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (93.14-2.26) 95.2 (93.14-2.26)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.206 , 0.232 0.207 , 0.234	Depositor DCC
R_{free} test set	1999 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12476	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: EDO, DST, PE8

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	0.27	0/3215	0.49	0/4396
1	B	0.24	0/3131	0.47	0/4285
1	C	0.35	0/2998	0.55	0/4110
1	D	0.25	0/2924	0.45	0/4017
All	All	0.28	0/12268	0.49	0/16808

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	3118	0	2967	20	0
1	B	3036	0	2872	20	0
1	C	2910	0	2679	19	0
1	D	2839	0	2530	17	0
2	A	15	0	9	0	0
2	B	15	0	9	2	0
2	C	15	0	9	5	0
2	D	15	0	9	0	0
3	A	25	0	34	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	10	3	0
4	C	14	0	10	6	0
5	C	4	0	6	3	0
6	A	200	0	0	1	0
6	B	129	0	0	0	0
6	C	76	0	0	0	0
6	D	51	0	0	1	0
All	All	12476	0	11144	80	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 (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLY:HA3	3:A:502:PE8:H201	1.62	0.81
1:A:376:PRO:HB3	1:A:412:ALA:HB1	1.67	0.77
1:B:51:GLU:OE2	1:B:182:GLY:N	2.22	0.73
4:C:501:DST:H111	2:C:503:TRP:CE2	2.25	0.72
1:C:317:VAL:HG13	1:C:334:TYR:HB2	1.71	0.71
1:C:235:LEU:HD23	1:C:258:SER:HB2	1.70	0.71
1:B:235:LEU:HD23	1:B:258:SER:HB2	1.72	0.71
1:A:99:ASN:HB3	3:A:502:PE8:H202	1.74	0.68
1:D:345:LEU:HB2	1:D:380:LEU:HG	1.77	0.66
1:C:287:SER:OG	1:C:291:LYS:NZ	2.31	0.64
1:A:15:THR:HG23	1:D:54:GLU:HG2	1.82	0.62
1:D:253:LYS:NZ	6:D:603:HOH:O	2.35	0.60
1:B:15:THR:HG23	1:C:54:GLU:HG2	1.85	0.59
4:C:501:DST:H102	2:C:503:TRP:CZ2	2.38	0.58
1:B:201:TRP:HZ3	1:B:254:ILE:HD13	1.69	0.58
1:A:133:ASN:HA	1:A:136:LYS:HE2	1.85	0.57
1:B:404:TYR:CE2	4:B:501:DST:H102	2.40	0.57
1:A:235:LEU:HD23	1:A:258:SER:HB2	1.88	0.55
1:D:218:ALA:HB3	1:D:322:VAL:HG13	1.88	0.55
1:B:205:LYS:NZ	1:B:209:GLU:OE2	2.32	0.55
1:A:317:VAL:HG13	1:A:334:TYR:HB2	1.89	0.54
1:A:137:ILE:HG22	1:A:138:ILE:HG13	1.90	0.54
1:C:44:GLU:HB3	1:C:366:SER:HB3	1.88	0.54
1:B:44:GLU:HB3	1:B:366:SER:HB3	1.90	0.54
1:B:272:ILE:HD13	1:B:329:PRO:HG2	1.89	0.53
1:D:218:ALA:HB1	1:D:329:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:HIS:CE1	1:D:156:PRO:HB2	2.45	0.51
4:B:501:DST:H142	2:B:502:TRP:CD1	2.47	0.50
1:A:205:LYS:HE2	1:A:209:GLU:OE2	2.12	0.50
4:C:501:DST:H111	2:C:503:TRP:CZ2	2.46	0.50
1:D:27:LYS:HD3	1:D:65:PRO:HA	1.94	0.50
4:C:501:DST:C13	5:C:502:EDO:H11	2.42	0.49
1:D:21:PRO:O	1:D:60:TYR:OH	2.26	0.49
1:A:99:ASN:CB	3:A:502:PE8:H202	2.43	0.49
1:B:239:MET:HB3	1:B:255:TYR:HB2	1.96	0.48
3:A:502:PE8:H231	6:A:767:HOH:O	2.12	0.48
1:C:128:ARG:HB2	1:C:150:TRP:CH2	2.49	0.48
1:D:355:LEU:HD21	1:D:401:LEU:HD12	1.96	0.48
1:D:239:MET:HB3	1:D:255:TYR:HB2	1.94	0.47
1:D:241:ALA:HB3	1:D:253:LYS:HB2	1.95	0.47
1:B:306:LEU:HD23	1:B:340:TYR:CG	2.49	0.47
1:A:137:ILE:CG2	1:A:138:ILE:HG13	2.44	0.47
1:D:306:LEU:HD13	1:D:340:TYR:CG	2.50	0.47
1:A:267:ARG:HG3	1:A:283:ILE:HG21	1.96	0.46
1:B:178:GLU:O	1:B:184:LEU:HD12	2.16	0.46
4:C:501:DST:C13	5:C:502:EDO:O2	2.63	0.46
4:C:501:DST:H142	2:C:503:TRP:CD1	2.50	0.46
1:C:239:MET:HB3	1:C:255:TYR:HB2	1.98	0.45
1:D:254:ILE:O	1:D:319:ASN:HA	2.16	0.45
1:C:173:VAL:HA	1:C:189:TYR:O	2.17	0.45
1:C:294:LEU:HD22	1:C:340:TYR:HB2	1.99	0.45
1:B:49:LEU:HD23	1:C:49:LEU:HD23	1.99	0.44
1:A:44:GLU:HB3	1:A:366:SER:HB3	2.00	0.43
1:A:128:ARG:HH21	1:A:150:TRP:CD1	2.35	0.43
1:D:177:LEU:HD23	1:D:186:VAL:HG22	2.00	0.43
1:C:178:GLU:HB2	1:C:185:SER:HB2	2.01	0.43
1:B:12:VAL:HG12	1:B:56:LEU:HD12	2.01	0.43
1:C:174:PHE:CE2	1:C:191:ILE:HD11	2.54	0.42
1:A:173:VAL:HA	1:A:189:TYR:O	2.19	0.42
1:A:332:LYS:HD3	1:A:391:ALA:HB1	2.01	0.42
1:D:156:PRO:O	1:D:157:GLY:C	2.63	0.42
1:B:49:LEU:HB3	1:C:49:LEU:HD23	2.02	0.42
1:C:306:LEU:HD23	1:C:340:TYR:CG	2.55	0.42
1:A:241:ALA:HB3	1:A:253:LYS:HB2	2.01	0.42
1:A:376:PRO:HG2	1:A:379:GLN:HB2	2.02	0.42
1:B:173:VAL:HA	1:B:189:TYR:O	2.19	0.42
1:B:338:ARG:HA	1:B:384:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:SER:O	1:B:315:GLY:HA3	2.20	0.41
1:D:174:PHE:CE2	1:D:191:ILE:HD11	2.55	0.41
1:B:158:SER:HA	1:B:159:PRO:HD3	1.95	0.41
1:B:201:TRP:HB2	1:B:237:PRO:HG2	2.02	0.41
1:B:349:LEU:HD23	1:B:352:ILE:HD11	2.01	0.41
4:B:501:DST:H111	2:B:502:TRP:CZ2	2.56	0.41
1:C:106:TYR:HA	5:C:502:EDO:H21	2.02	0.41
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.88	0.41
1:C:334:TYR:CD2	2:C:503:TRP:HH2	2.40	0.40
1:C:355:LEU:HD21	1:C:401:LEU:HD12	2.02	0.40
1:C:66:GLU:HB2	1:C:110:LEU:HD22	2.03	0.40
1:A:137:ILE:HG21	1:D:19:TRP:CH2	2.56	0.40
1:A:239:MET:HB3	1:A:255:TYR:HB2	2.03	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	394/419 (94%)	383 (97%)	10 (2%)	1 (0%)	36	40
1	B	383/419 (91%)	375 (98%)	7 (2%)	1 (0%)	36	40
1	C	376/419 (90%)	367 (98%)	8 (2%)	1 (0%)	36	40
1	D	372/419 (89%)	363 (98%)	8 (2%)	1 (0%)	36	40
All	All	1525/1676 (91%)	1488 (98%)	33 (2%)	4 (0%)	36	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	HIS
1	B	181	HIS

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Mol	Chain	Res	Type
1	A	181	HIS
1	D	181	HIS

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	323/363 (89%)	320 (99%)	3 (1%)	70	79
1	B	315/363 (87%)	313 (99%)	2 (1%)	78	84
1	C	283/363 (78%)	282 (100%)	1 (0%)	84	89
1	D	265/363 (73%)	264 (100%)	1 (0%)	84	89
All	All	1186/1452 (82%)	1179 (99%)	7 (1%)	78	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ILE
1	A	141	LEU
1	A	319	ASN
1	B	272	ILE
1	B	319	ASN
1	C	253	LYS
1	D	319	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	119	GLN
1	A	221	HIS
1	A	260	GLN
1	A	387	GLN
1	B	202	HIS
1	B	220	ASN

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Mol	Chain	Res	Type
1	B	221	HIS
1	B	342	ASN
1	B	387	GLN
1	B	408	GLN
1	C	39	ASN
1	C	129	ASN
1	C	387	GLN
1	D	151	HIS
1	D	360	HIS
1	D	365	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
2	TRP	C	503	-	15,16,16	1.39	1 (6%)	18,22,22	1.47	3 (16%)
4	DST	B	501	-	10,13,13	1.61	2 (20%)	12,19,19	1.37	2 (16%)
2	TRP	D	501	-	15,16,16	1.45	2 (13%)	18,22,22	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	502	-	3,3,3	0.68	0	2,2,2	0.36	0
2	TRP	B	502	-	15,16,16	1.43	1 (6%)	18,22,22	1.29	4 (22%)
4	DST	C	501	-	10,13,13	1.86	2 (20%)	12,19,19	0.91	1 (8%)
2	TRP	A	501	-	15,16,16	1.43	2 (13%)	18,22,22	1.11	1 (5%)
3	PE8	A	502	-	24,24,24	0.54	0	23,23,23	0.38	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
2	TRP	C	503	-	-	1/8/8/8	0/2/2/2
4	DST	B	501	-	-	0/7/13/13	-
2	TRP	D	501	-	-	0/8/8/8	0/2/2/2
5	EDO	C	502	-	-	1/1/1/1	-
2	TRP	B	502	-	-	0/8/8/8	0/2/2/2
4	DST	C	501	-	-	0/7/13/13	-
2	TRP	A	501	-	-	0/8/8/8	0/2/2/2
3	PE8	A	502	-	-	12/22/22/22	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	DST	C10-S9	-4.78	1.78	1.84
4	B	501	DST	C10-S9	-3.54	1.79	1.84
2	D	501	TRP	CD2-CE2	-3.25	1.37	1.41
2	A	501	TRP	CD2-CE2	-3.15	1.37	1.41
2	C	503	TRP	CD2-CE2	-3.14	1.37	1.41
2	B	502	TRP	CD2-CE2	-2.74	1.38	1.41
4	B	501	DST	P3-O8	-2.69	1.50	1.56
4	C	501	DST	P3-O8	-2.34	1.50	1.56
2	D	501	TRP	CD1-NE1	-2.26	1.33	1.37
2	A	501	TRP	CD1-NE1	-2.05	1.33	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	DST	C14-C12-C13	3.16	121.86	114.59
2	C	503	TRP	CA-CB-CG	-2.90	107.99	113.49
2	C	503	TRP	CG-CD1-NE1	-2.67	107.38	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TRP	CG-CD1-NE1	-2.61	107.44	110.31
2	C	503	TRP	CZ2-CE2-CD2	-2.58	119.69	122.19
4	B	501	DST	C14-C12-C11	-2.47	115.24	122.66
2	D	501	TRP	CG-CD1-NE1	-2.43	107.64	110.31
2	B	502	TRP	CG-CD1-NE1	-2.36	107.72	110.31
2	D	501	TRP	CZ2-CE2-CD2	-2.32	119.94	122.19
2	B	502	TRP	CZ2-CE2-CD2	-2.21	120.05	122.19
2	B	502	TRP	OXT-C-O	-2.17	119.15	124.08
2	B	502	TRP	CE3-CD2-CE2	2.08	121.00	118.84
4	C	501	DST	O6-P1-O2	2.04	111.49	104.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

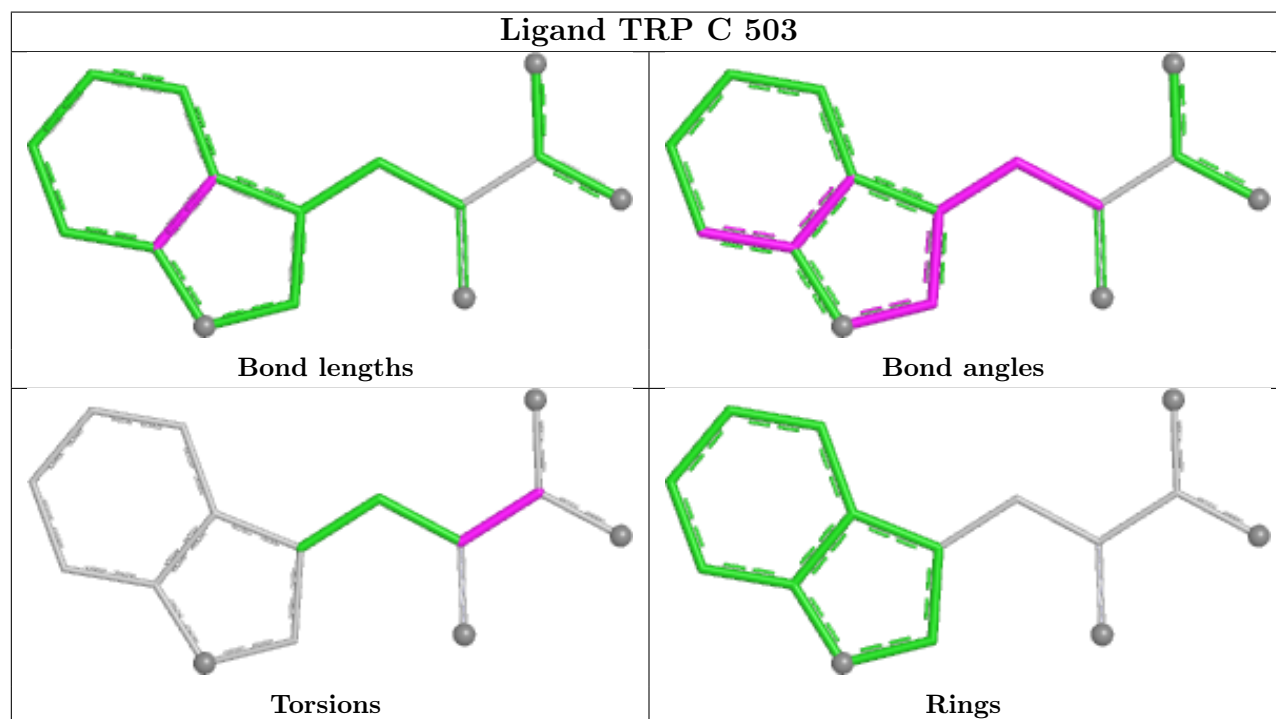
Mol	Chain	Res	Type	Atoms
3	A	502	PE8	O10-C11-C12-O13
3	A	502	PE8	O16-C17-C18-O19
3	A	502	PE8	O4-C5-C6-O7
3	A	502	PE8	O7-C8-C9-O10
3	A	502	PE8	O19-C20-C21-O22
3	A	502	PE8	O22-C23-C24-O25
5	C	502	EDO	O1-C1-C2-O2
3	A	502	PE8	C14-C15-O16-C17
3	A	502	PE8	O13-C14-C15-O16
3	A	502	PE8	C24-C23-O22-C21
3	A	502	PE8	C11-C12-O13-C14
2	C	503	TRP	O-C-CA-N
3	A	502	PE8	C17-C18-O19-C20
3	A	502	PE8	C12-C11-O10-C9

There are no ring outliers.

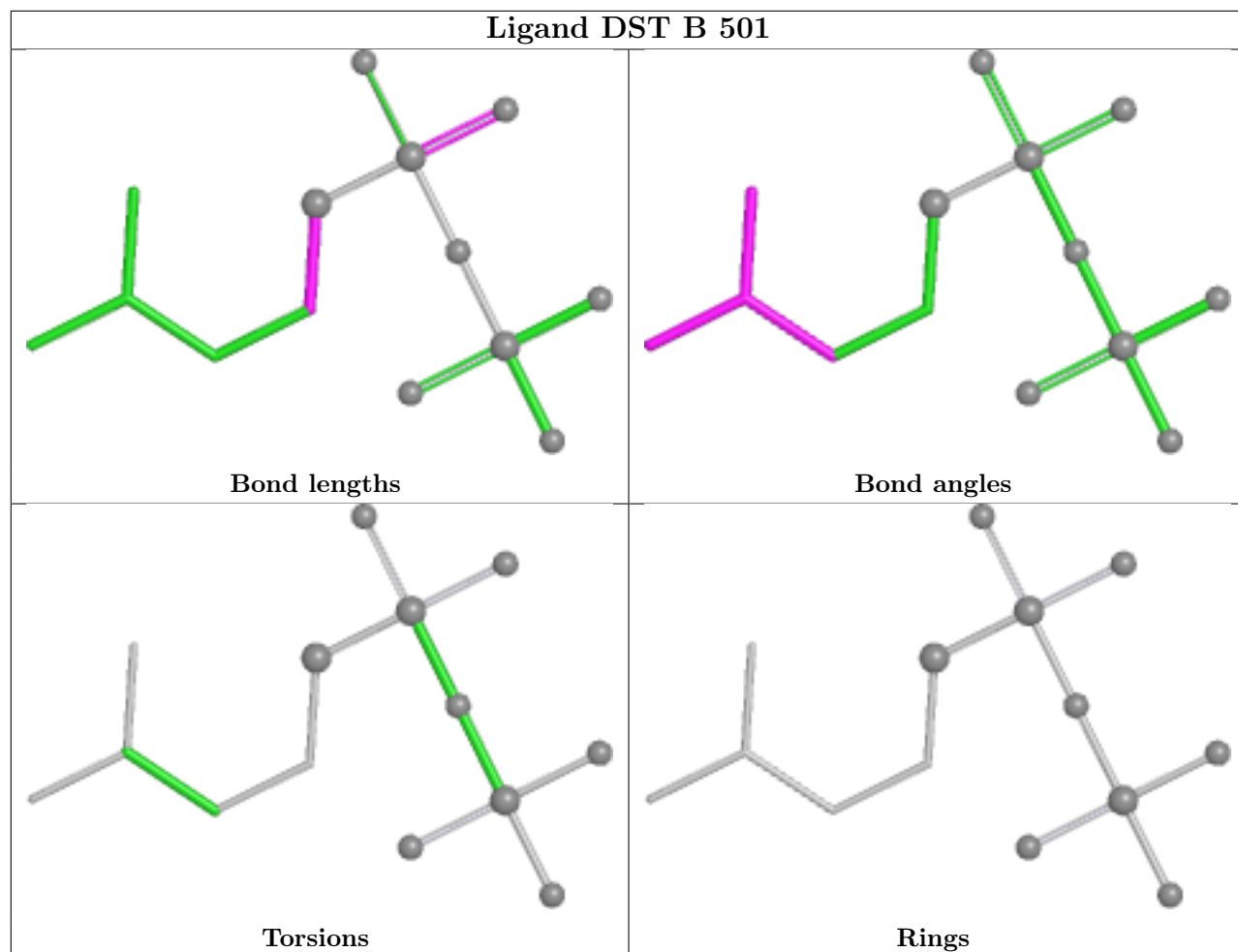
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	503	TRP	5	0
4	B	501	DST	3	0
5	C	502	EDO	3	0
2	B	502	TRP	2	0
4	C	501	DST	6	0
3	A	502	PE8	4	0

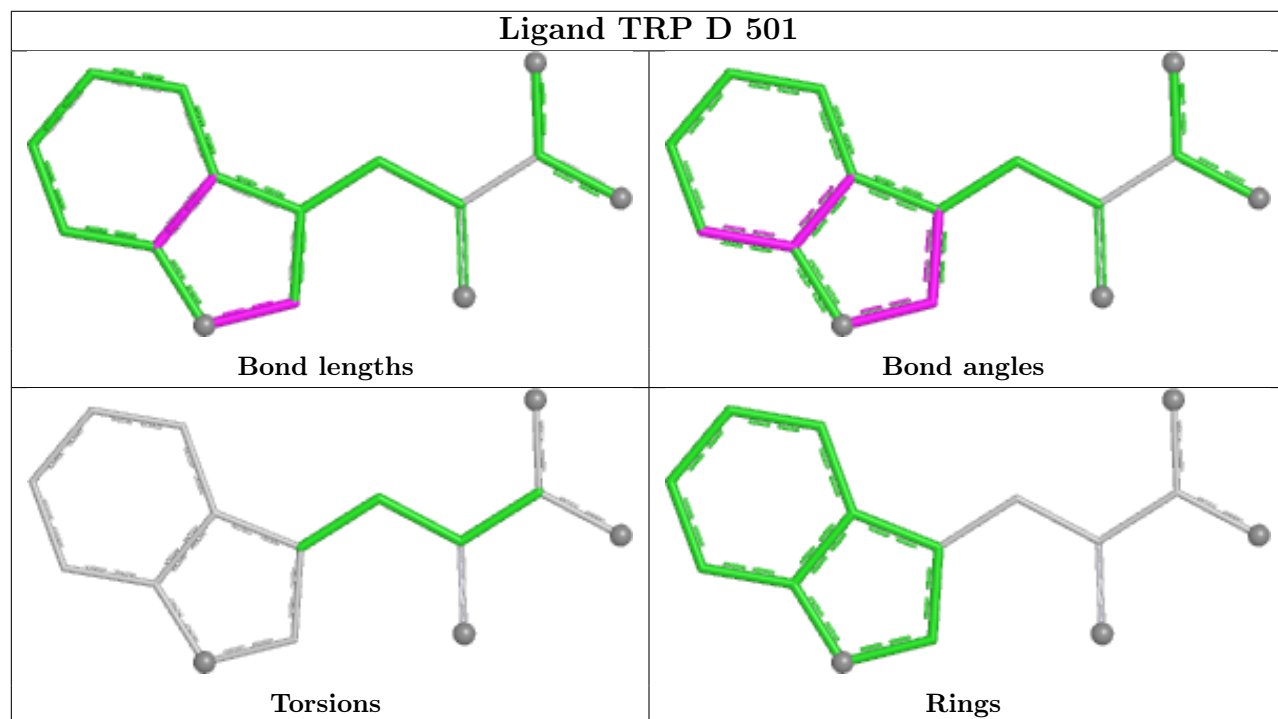
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

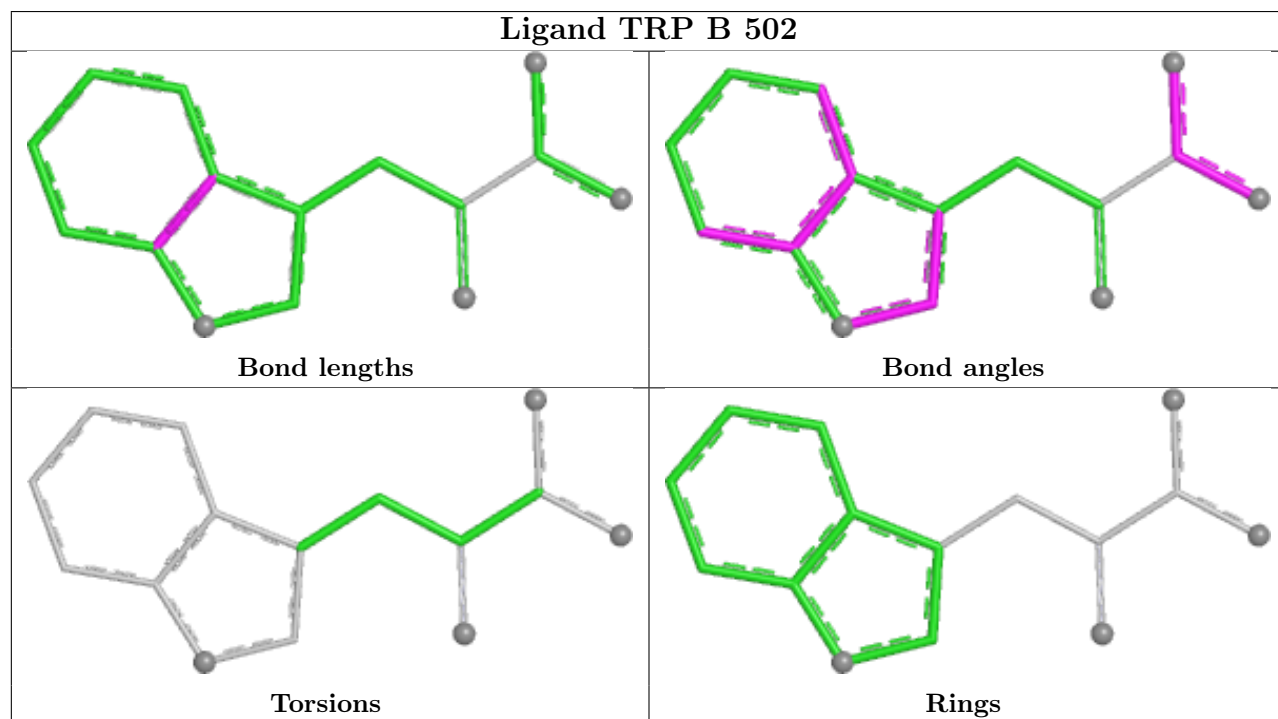
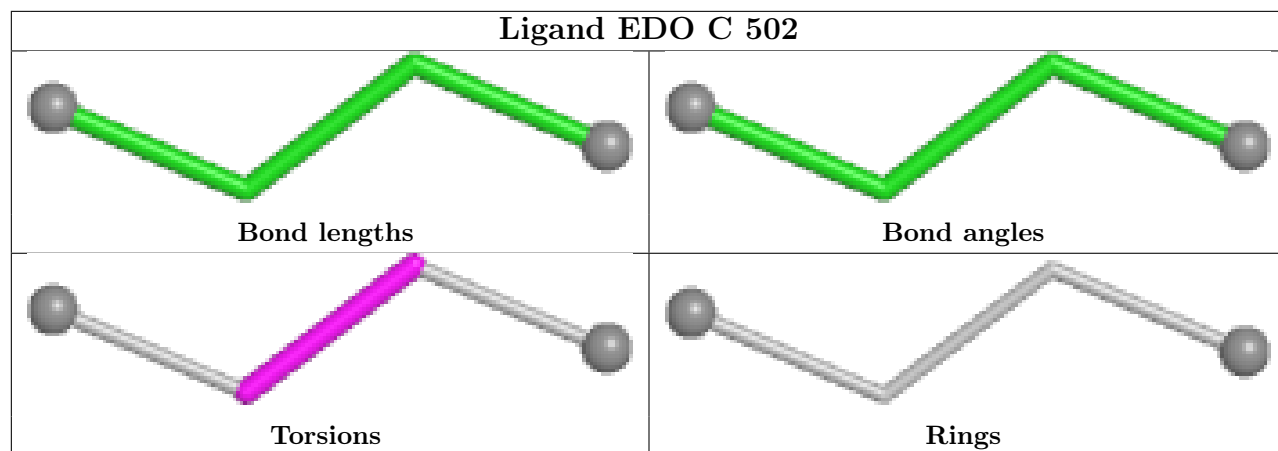


Ligand DST B 501

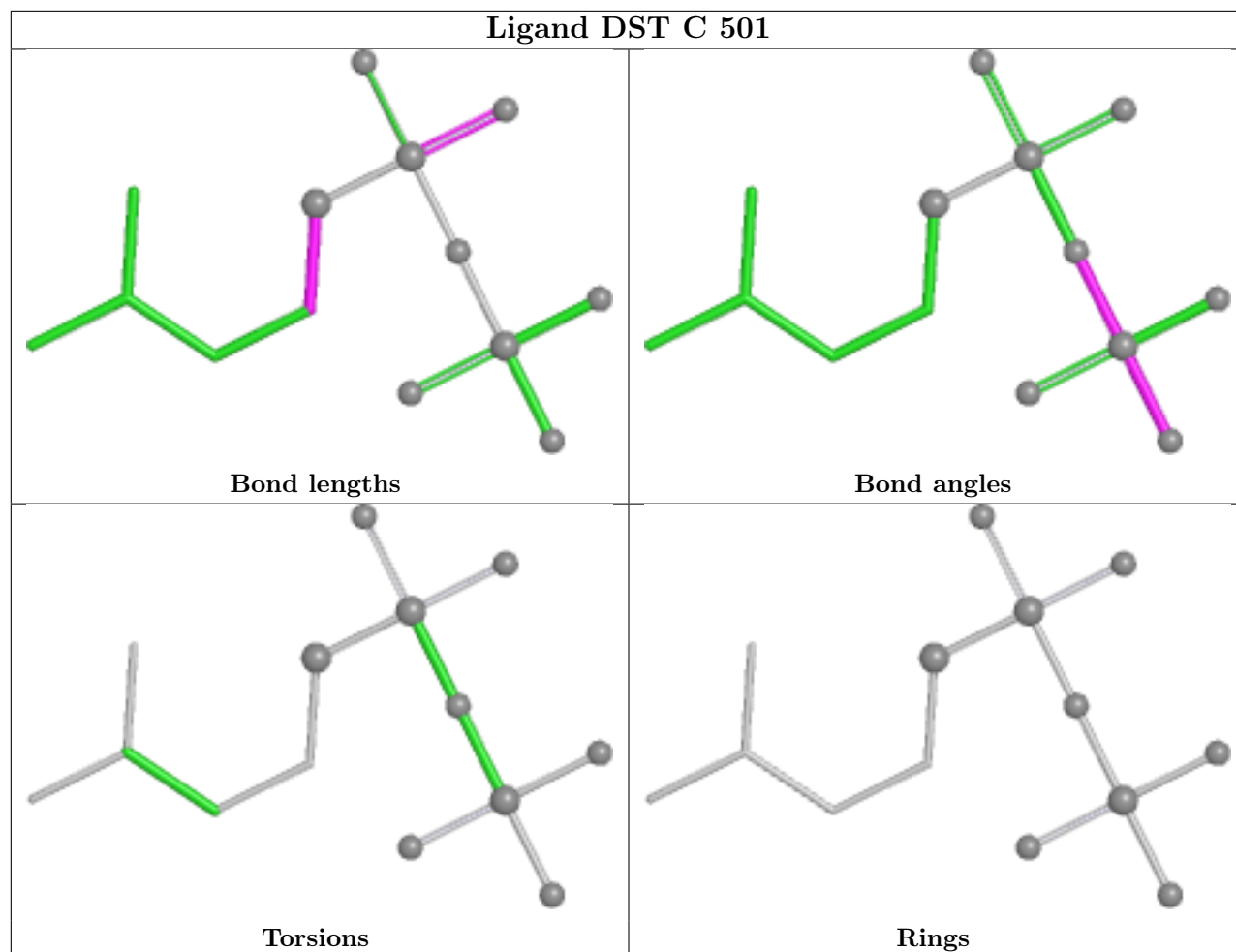


Ligand TRP D 501

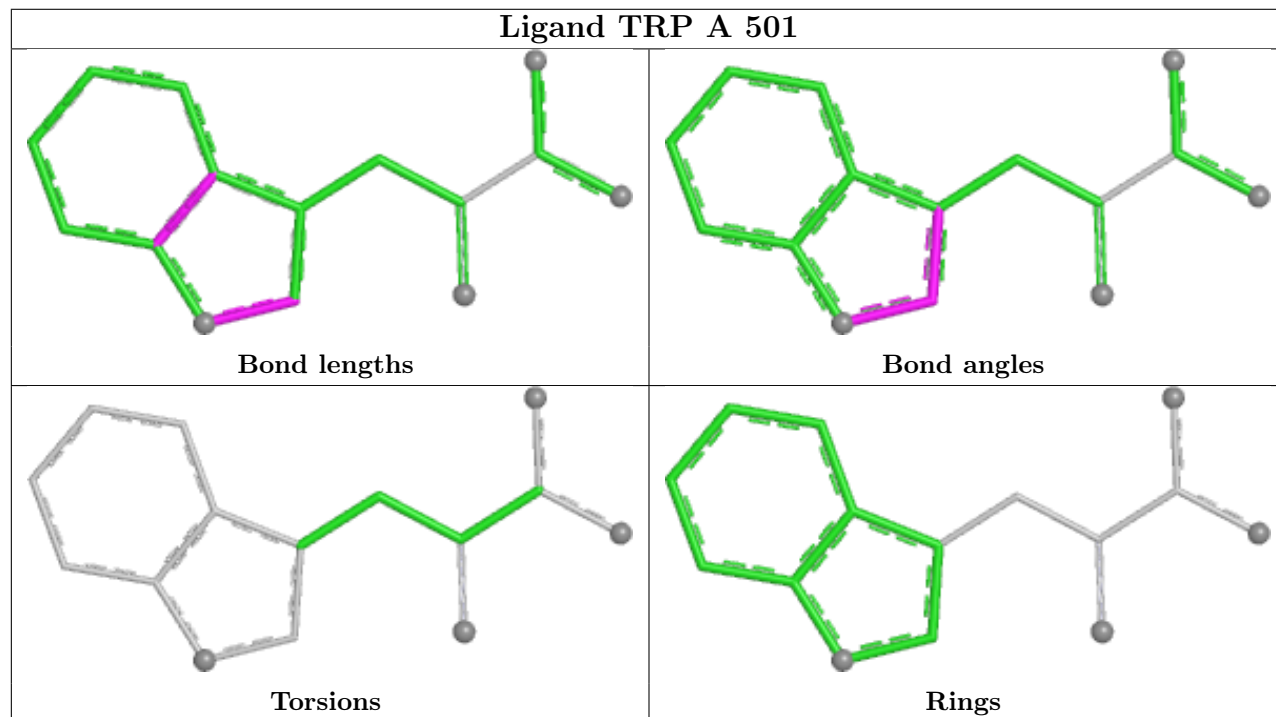


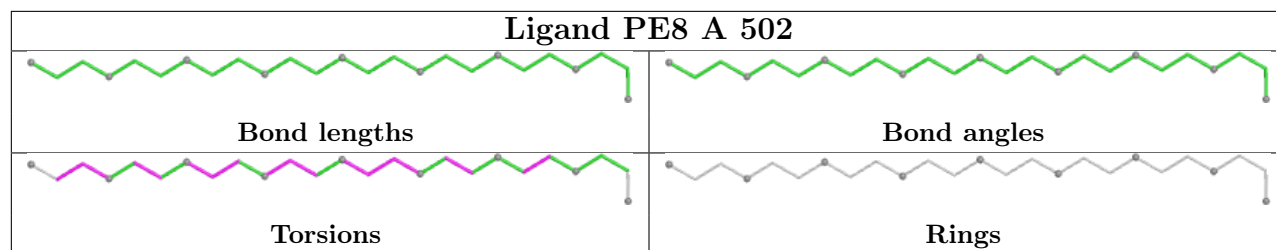


Ligand DST C 501



Ligand TRP A 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	398/419 (94%)	0.09	11 (2%) 55 55	26, 45, 84, 121	0
1	B	389/419 (92%)	0.26	16 (4%) 41 41	25, 48, 83, 97	0
1	C	384/419 (91%)	0.98	56 (14%) 6 5	38, 73, 105, 116	0
1	D	382/419 (91%)	1.36	81 (21%) 2 2	51, 85, 122, 144	0
All	All	1553/1676 (92%)	0.67	164 (10%) 11 11	25, 63, 109, 144	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	323	ALA	6.2
1	D	204	ILE	5.9
1	D	157	GLY	5.2
1	C	293	ALA	5.2
1	D	198	PHE	4.7
1	D	212	GLY	4.6
1	C	290	TRP	4.3
1	D	228	SER	4.1
1	C	159	PRO	4.1
1	C	74	SER	4.0
1	D	145	TRP	3.6
1	C	341	ALA	3.6
1	C	216	LEU	3.5
1	D	230	ASP	3.5
1	D	322	VAL	3.5
1	A	324	PRO	3.4
1	D	412	ALA	3.4
1	D	197	ASP	3.4
1	D	227	SER	3.3
1	C	289	LEU	3.3
1	D	180	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	277	THR	3.3
1	C	302	PRO	3.2
1	D	219	LEU	3.2
1	D	182	GLY	3.2
1	B	159	PRO	3.2
1	D	156	PRO	3.1
1	A	137	ILE	3.1
1	D	144	THR	3.1
1	D	122	PHE	3.1
1	C	99	ASN	3.1
1	C	279	LEU	3.1
1	C	275	LEU	3.1
1	D	327	GLN	3.0
1	C	316	ALA	3.0
1	D	200	ALA	3.0
1	C	322	VAL	3.0
1	D	272	ILE	3.0
1	D	211	SER	3.0
1	C	73	SER	2.9
1	D	206	HIS	2.9
1	A	214	PRO	2.9
1	C	306	LEU	2.9
1	C	308	LYS	2.9
1	D	181	HIS	2.9
1	D	306	LEU	2.9
1	A	213	CYS	2.9
1	D	246	GLU	2.9
1	D	216	LEU	2.8
1	D	137	ILE	2.8
1	C	259	ASN	2.8
1	C	298	PRO	2.8
1	D	192	PRO	2.8
1	D	244	LEU	2.8
1	D	224	ALA	2.8
1	B	311	HIS	2.8
1	D	195	THR	2.8
1	C	231	ASP	2.8
1	B	213	CYS	2.8
1	B	377	SER	2.8
1	D	153	LEU	2.8
1	D	210	ALA	2.8
1	D	148	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	84	ASP	2.7
1	D	190	PHE	2.7
1	D	202	HIS	2.7
1	D	220	ASN	2.7
1	A	166	VAL	2.7
1	D	209	GLU	2.7
1	D	183	HIS	2.7
1	A	159	PRO	2.7
1	C	183	HIS	2.6
1	D	248	ALA	2.6
1	D	316	ALA	2.6
1	D	125	ILE	2.6
1	D	247	PRO	2.6
1	C	294	LEU	2.6
1	D	141	LEU	2.6
1	C	348	ALA	2.6
1	C	97	SER	2.6
1	C	377	SER	2.6
1	D	328	ILE	2.6
1	C	342	ASN	2.6
1	D	222	VAL	2.6
1	C	181	HIS	2.6
1	C	340	TYR	2.6
1	D	136	LYS	2.6
1	D	119	GLN	2.5
1	A	248	ALA	2.5
1	B	214	PRO	2.5
1	C	313	THR	2.5
1	A	138	ILE	2.5
1	B	313	THR	2.5
1	D	196	PRO	2.5
1	C	227	SER	2.5
1	D	245	VAL	2.5
1	C	196	PRO	2.5
1	C	201	TRP	2.4
1	D	380	LEU	2.4
1	B	228	SER	2.4
1	A	167	LEU	2.4
1	C	312	LEU	2.4
1	C	264	ARG	2.4
1	B	312	LEU	2.4
1	D	106	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	412	ALA	2.4
1	B	73	SER	2.4
1	C	75	VAL	2.4
1	D	208	ILE	2.4
1	A	141	LEU	2.4
1	C	296	LEU	2.4
1	C	260	GLN	2.4
1	D	99	ASN	2.3
1	D	342	ASN	2.3
1	D	175	ALA	2.3
1	D	235	LEU	2.3
1	B	84	ASP	2.3
1	B	81	PHE	2.3
1	C	286	PHE	2.3
1	D	143	LEU	2.3
1	B	303	GLU	2.3
1	C	327	GLN	2.3
1	C	382	GLN	2.3
1	C	328	ILE	2.3
1	D	309	VAL	2.3
1	D	297	ASP	2.3
1	C	301	PRO	2.3
1	D	241	ALA	2.3
1	D	276	ARG	2.3
1	B	327	GLN	2.3
1	D	174	PHE	2.2
1	D	252	LEU	2.2
1	D	116	GLY	2.2
1	D	377	SER	2.2
1	C	380	LEU	2.2
1	D	154	LEU	2.2
1	C	278	ASP	2.2
1	D	193	VAL	2.2
1	A	215	ASN	2.2
1	C	82	MET	2.2
1	D	372	ASP	2.2
1	D	138	ILE	2.1
1	D	368	LEU	2.1
1	C	179	MET	2.1
1	C	81	PHE	2.1
1	C	291	LYS	2.1
1	B	411	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	261	THR	2.1
1	B	307	PRO	2.1
1	D	260	GLN	2.1
1	D	132	TYR	2.1
1	D	278	ASP	2.1
1	D	155	GLY	2.1
1	C	236	ARG	2.1
1	C	78	SER	2.1
1	D	258	SER	2.1
1	D	264	ARG	2.1
1	C	184	LEU	2.0
1	D	114	LEU	2.0
1	D	298	PRO	2.0
1	B	75	VAL	2.0
1	C	209	GLU	2.0
1	C	197	ASP	2.0
1	D	22	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

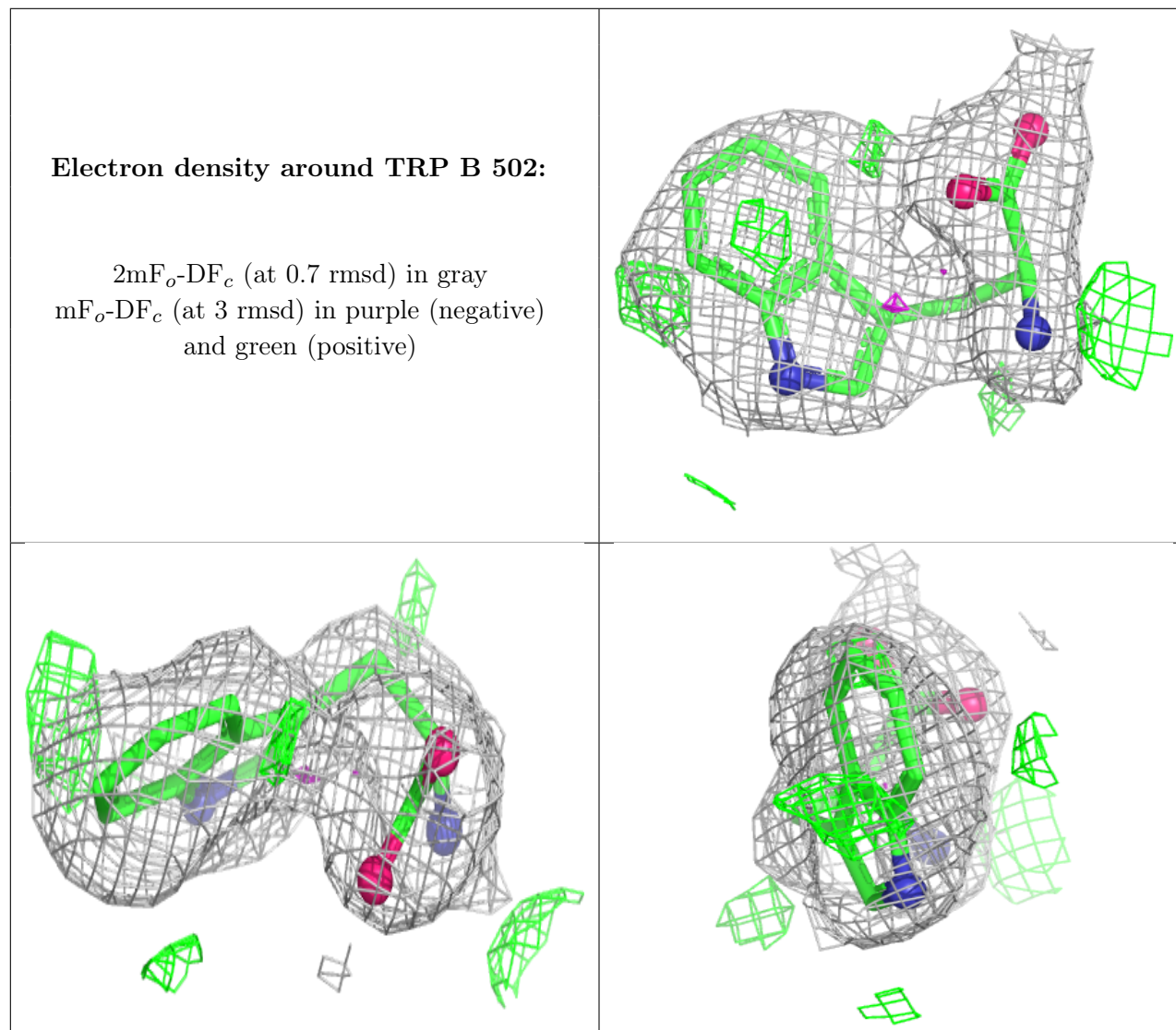
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRP	B	502	15/15	0.83	0.17	51,55,59,60	15
4	DST	B	501	14/14	0.83	0.19	53,58,67,67	14
4	DST	C	501	14/14	0.86	0.15	58,69,76,78	14
3	PE8	A	502	25/25	0.87	0.15	40,52,56,57	25
5	EDO	C	502	4/4	0.87	0.17	51,52,55,63	4
2	TRP	D	501	15/15	0.88	0.15	54,78,81,82	15

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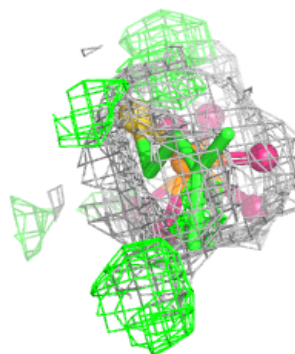
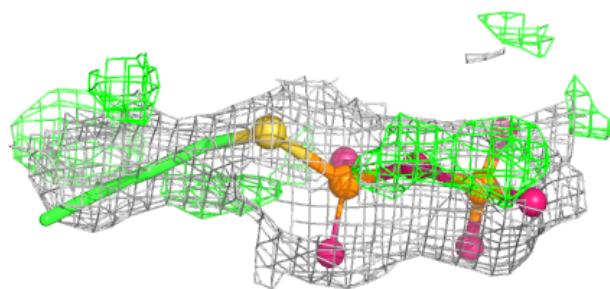
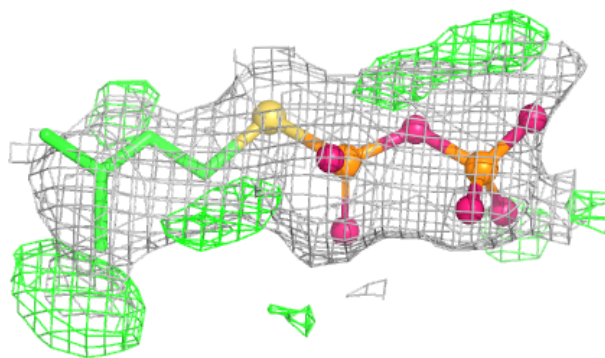
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRP	C	503	15/15	0.90	0.13	54,68,71,71	0
2	TRP	A	501	15/15	0.95	0.07	30,33,35,35	0

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.

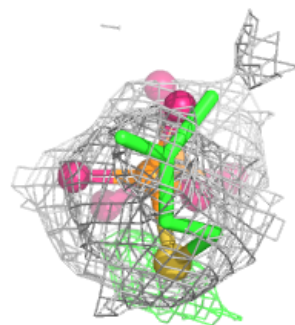
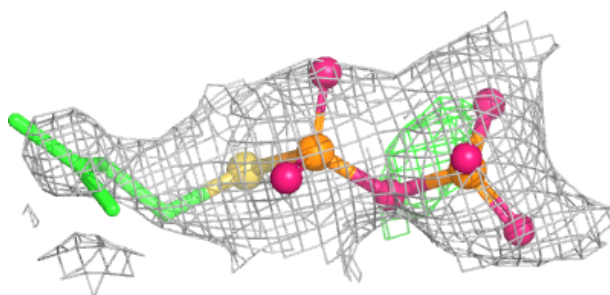
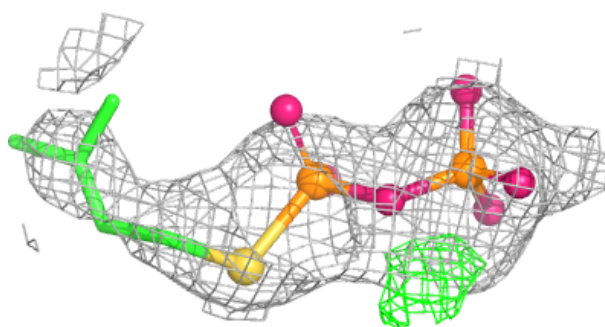


Electron density around DST B 501:

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

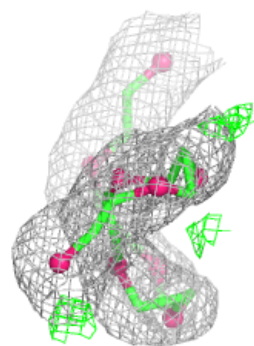
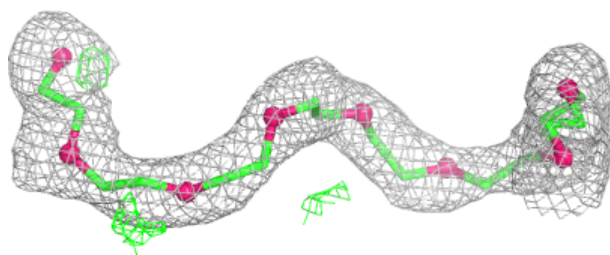
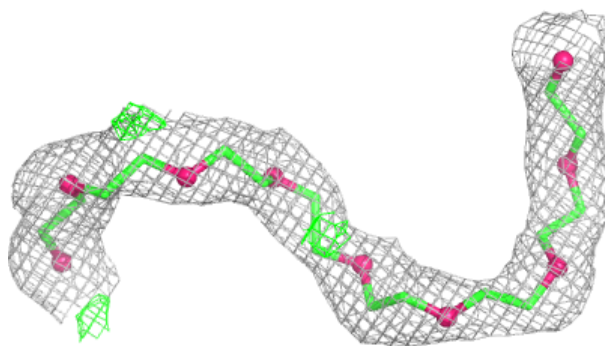
**Electron density around DST C 501:**

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

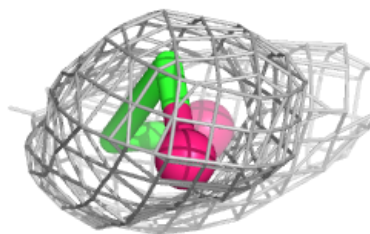
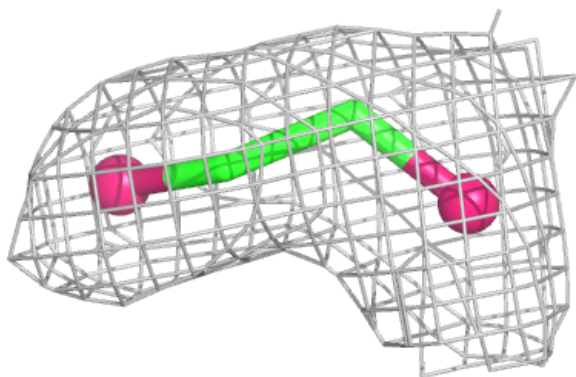
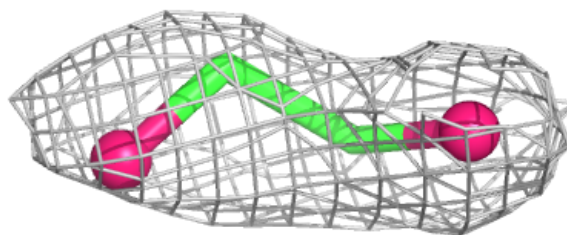


Electron density around PE8 A 502:

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

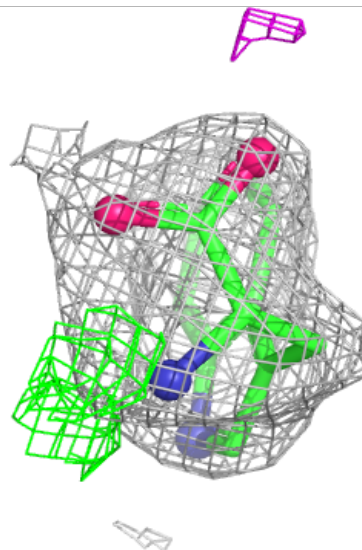
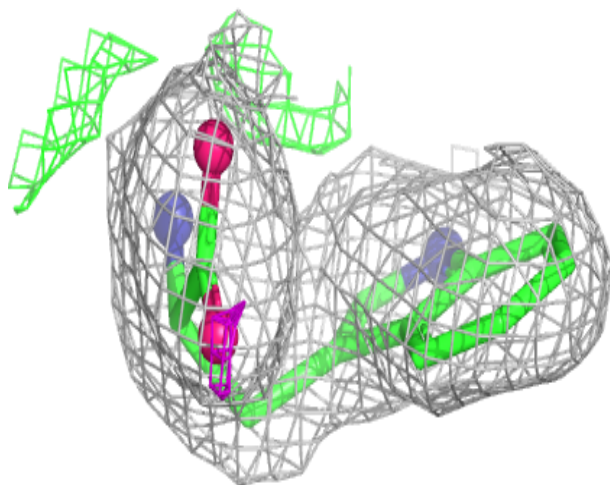
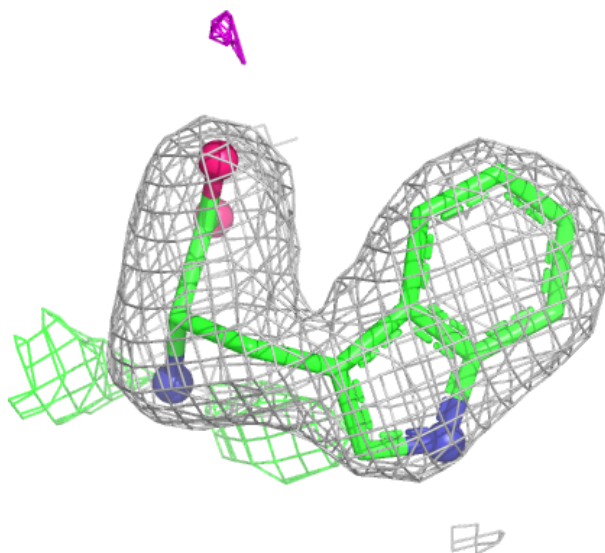
**Electron density around EDO C 502:**

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



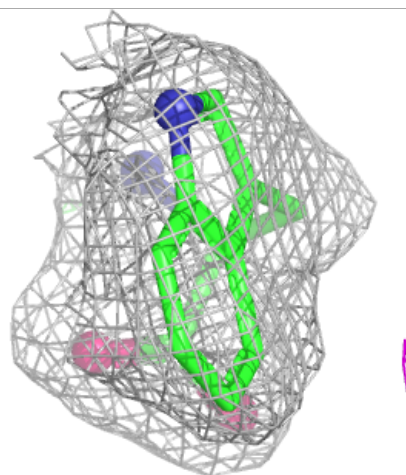
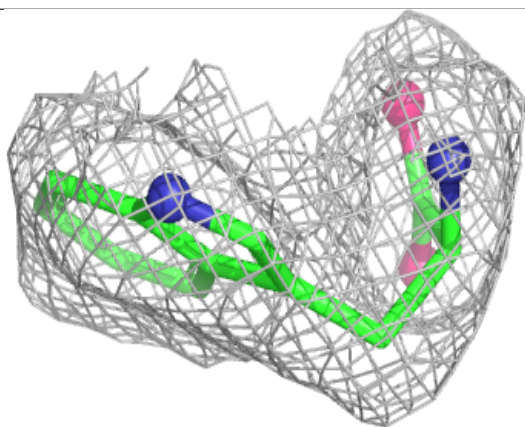
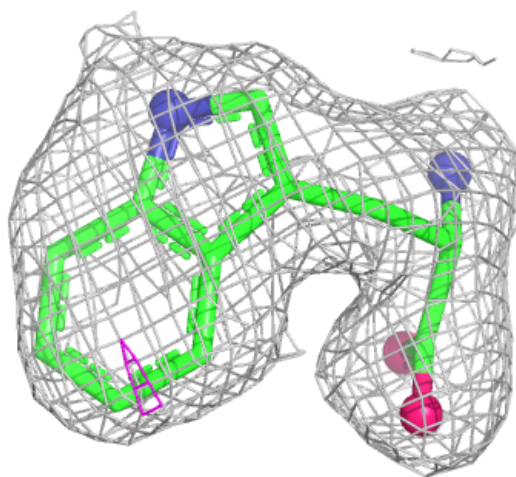
Electron density around TRP D 501:

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



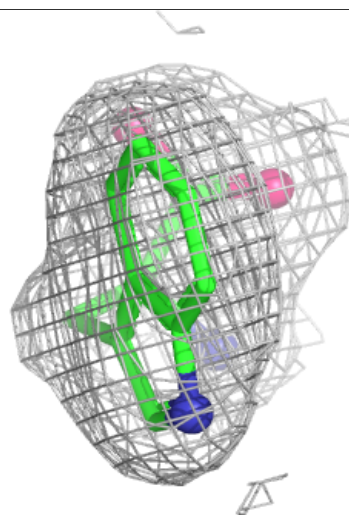
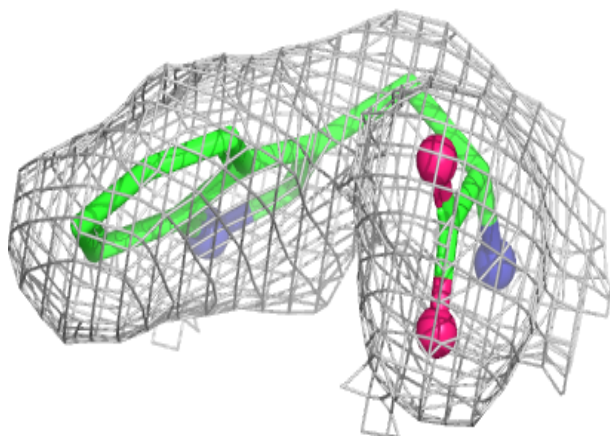
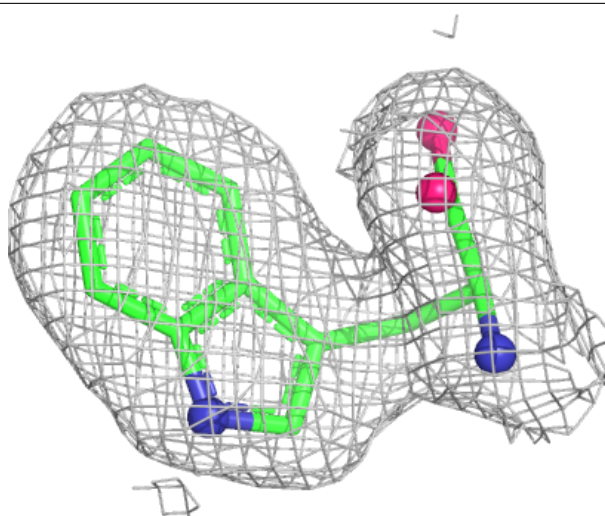
Electron density around TRP C 503:

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



Electron density around TRP A 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.