



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:39 AM UTC

PDB ID : 4J7H / pdb_00004j7h
Title : Crystal structure of EvaA, a 2,3-dehydratase in complex with dTDP-benzene and dTDP-rhamnose
Authors : Holden, H.M.; Kubiak, R.L.; Thoden, J.B.
Deposited on : 2013-02-13
Resolution : 1.69 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) 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

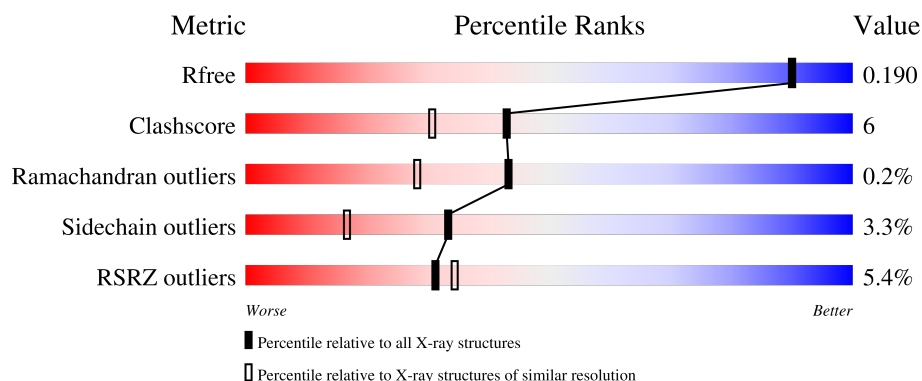
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	471	6% 82% 11% • 5%
1	B	471	5% 84% 9% • 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8138 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.

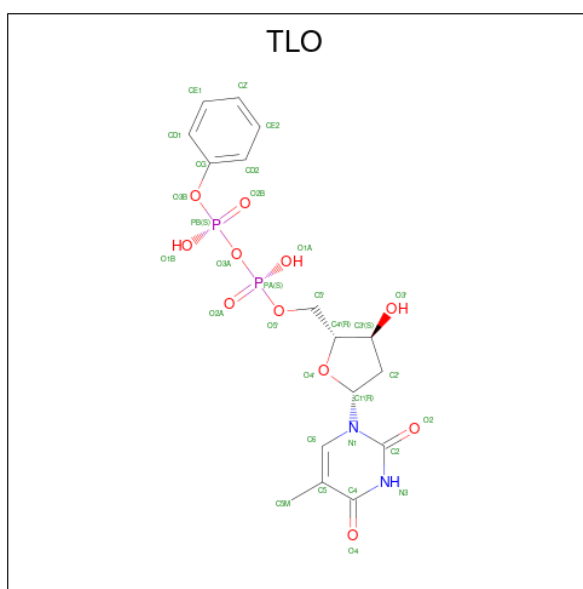
- Molecule 1 is a protein called EvaA 2,3-dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	5	0
			3603	2290	647	654	12			
1	B	444	Total	C	N	O	S	0	7	0
			3581	2274	638	657	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	ALA	ARG	engineered mutation	UNP O52793
B	381	ALA	ARG	engineered mutation	UNP O52793

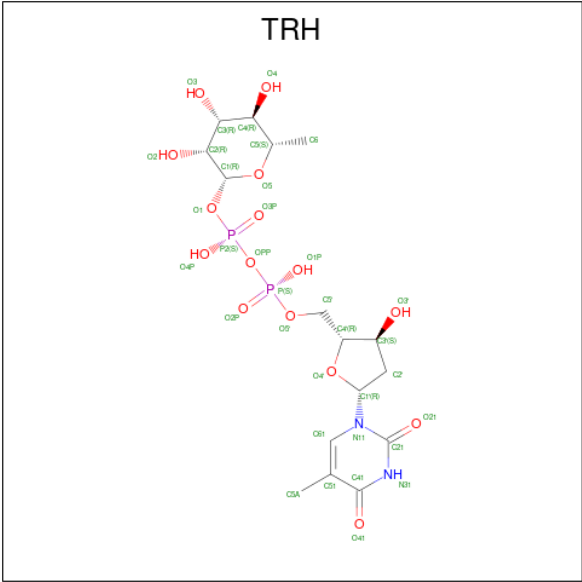
- Molecule 2 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phenoxy)phosphoryl]oxy}phosphoryl]thymidine (CCD ID: TLO) (formula: C₁₆H₂₀N₂O₁₁P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	31	16	2	11	2	0	0

- Molecule 3 is 2'-DEOXY-THYMIDINE-BETA-L-RHAMNOSE (CCD ID: TRH) (formula: C₁₆H₂₆N₂O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	35	16	2	15	2	0	0
3	B	1	35	16	2	15	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

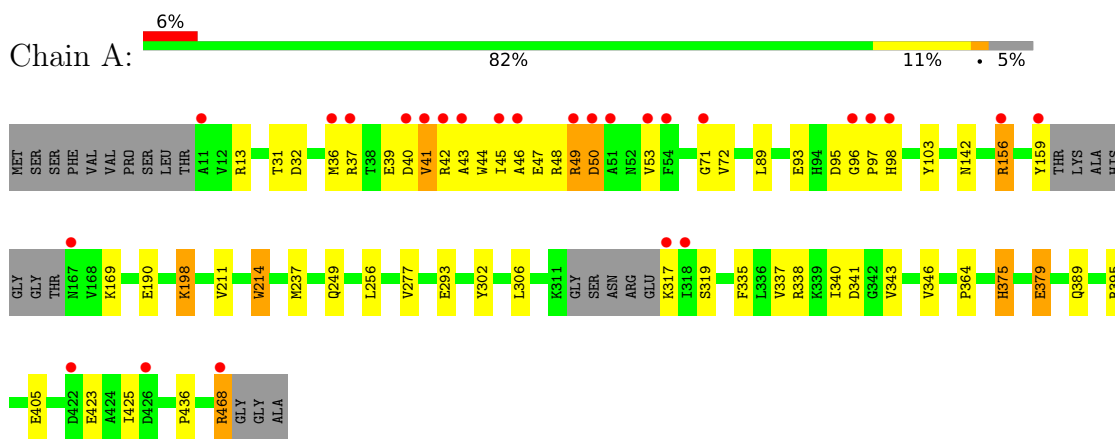
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	418	Total	O	0	0
			418	418		
5	B	380	Total	O	0	0
			380	380		

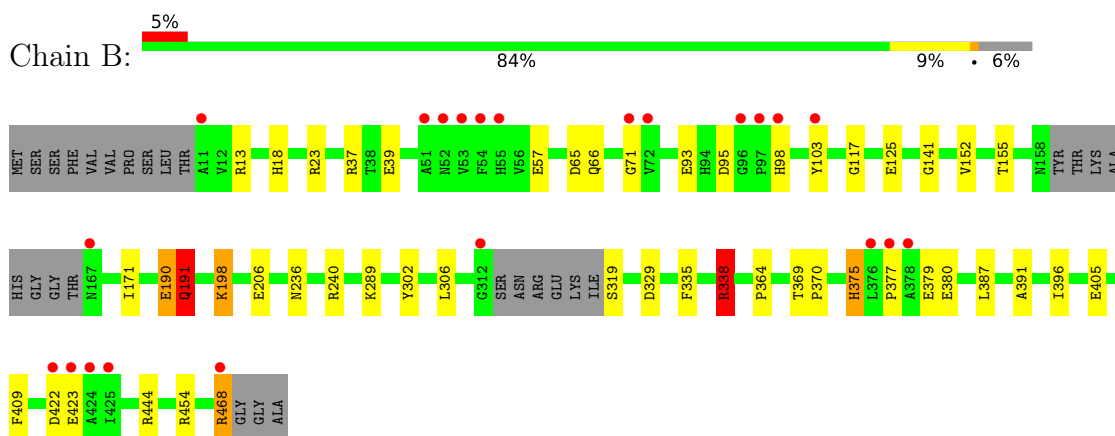
3 Residue-property plots [i](#)

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: EvaA 2,3-dehydratase



- Molecule 1: EvaA 2,3-dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.68Å 108.64Å 110.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.13 – 1.69 110.13 – 1.69	Depositor EDS
% Data completeness (in resolution range)	96.8 (110.13-1.69) 96.8 (110.13-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.191 0.164 , 0.190	Depositor DCC
R_{free} test set	7019 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k 0.013 for -l,-k,-h 0.014 for k,h,-l 0.002 for k,l,h 0.002 for l,h,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8138	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TLO, EDO, TRH

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	0.59	0/3710	1.35	16/5055 (0.3%)
1	B	0.58	0/3694	1.32	7/5038 (0.1%)
All	All	0.58	0/7404	1.34	23/10093 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	GLY	N-CA-C	8.78	122.68	112.50
1	B	444	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	A	71	GLY	N-CA-C	6.62	120.50	112.49
1	A	50	ASP	N-CA-C	6.51	118.37	111.28
1	A	341	ASP	CB-CA-C	-6.45	97.58	110.42
1	A	343	VAL	CB-CA-C	-5.98	103.97	110.85
1	A	142	ASN	CA-C-N	-5.96	113.54	119.56
1	A	142	ASN	C-N-CA	-5.96	113.54	119.56
1	A	211	VAL	CB-CA-C	-5.93	105.18	111.00
1	A	214	TRP	N-CA-C	-5.78	101.64	110.14
1	A	13	ARG	CB-CG-CD	5.76	124.54	111.30
1	A	32	ASP	N-CA-C	5.71	118.03	107.99
1	A	31	THR	CA-C-N	-5.51	114.31	122.41
1	A	31	THR	C-N-CA	-5.51	114.31	122.41
1	A	198	LYS	CA-CB-CG	-5.46	103.19	114.10
1	A	39	GLU	N-CA-C	-5.43	105.36	111.28
1	A	375	HIS	N-CA-C	-5.40	106.47	113.16
1	B	338	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	B	191	GLN	N-CA-CB	5.29	117.79	109.69
1	A	249	GLN	CA-C-O	-5.25	114.71	120.69
1	B	375	HIS	N-CA-C	-5.20	106.62	113.17
1	B	454	ARG	NE-CZ-NH2	5.07	123.76	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	ARG	CB-CG-CD	5.05	122.92	111.30

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	3603	0	3531	49	0
1	B	3581	0	3496	39	0
2	A	31	0	18	1	0
2	B	31	0	18	4	0
3	A	35	0	24	0	0
3	B	35	0	24	0	0
4	A	16	0	24	1	0
4	B	8	0	12	2	0
5	A	418	0	0	5	0
5	B	380	0	0	9	0
All	All	8138	0	7147	90	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 6.

All (90) 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:41:VAL:CG1	1:A:45:ILE:CD1	2.39	1.00
1:A:41:VAL:HG13	1:A:45:ILE:CD1	1.95	0.96
1:A:338[B]:ARG:NH2	5:A:996:HOH:O	2.03	0.92
1:A:41:VAL:HG12	1:A:45:ILE:HD13	1.55	0.87
1:A:237:MET:CE	1:A:405:GLU:HG3	2.06	0.86
1:A:338[B]:ARG:NH1	1:A:425:ILE:H	1.76	0.82
1:A:41:VAL:HG12	1:A:45:ILE:CD1	2.12	0.77
1:A:338[B]:ARG:HH11	1:A:425:ILE:H	1.32	0.77
1:A:41:VAL:HG13	1:A:45:ILE:HD12	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLU:HB3	5:A:998:HOH:O	1.85	0.76
1:A:42:ARG:O	1:A:46:ALA:N	2.22	0.72
1:A:45:ILE:O	1:A:49:ARG:HB2	1.91	0.70
1:B:338:ARG:HD3	5:B:964:HOH:O	1.91	0.70
1:A:237:MET:HE2	1:A:405:GLU:HG3	1.77	0.66
1:B:191:GLN:HE21	1:B:191:GLN:H	1.45	0.64
1:B:37:ARG:HB3	1:B:39:GLU:OE1	1.97	0.64
1:A:45:ILE:O	1:A:49:ARG:N	2.23	0.62
1:A:45:ILE:HG21	1:A:49:ARG:CZ	2.30	0.61
1:A:41:VAL:CG1	1:A:45:ILE:HD11	2.30	0.61
1:A:41:VAL:CG1	1:A:45:ILE:HD13	2.18	0.61
1:B:18:HIS:ND1	5:B:778:HOH:O	2.23	0.61
1:A:43:ALA:O	1:A:47:GLU:N	2.25	0.59
1:A:237:MET:HE1	1:A:405:GLU:HG3	1.82	0.58
1:B:329:ASP:HB3	1:B:369:THR:CG2	2.33	0.58
1:A:190:GLU:OE2	1:A:198:LYS:HD3	2.02	0.58
1:A:41:VAL:O	1:A:45:ILE:HD12	2.04	0.57
1:A:98:HIS:HD2	5:A:994:HOH:O	1.86	0.57
1:A:41:VAL:HG13	1:A:45:ILE:HD11	1.83	0.57
1:B:39:GLU:H	1:B:39:GLU:CD	2.13	0.57
1:B:155:THR:HG23	2:B:501:TLO:CD2	2.36	0.56
1:A:338[B]:ARG:NH1	1:A:425:ILE:O	2.39	0.56
1:B:405:GLU:HB2	5:B:914:HOH:O	2.07	0.54
1:A:375:HIS:CD2	1:A:375:HIS:H	2.26	0.54
1:B:206:GLU:OE2	5:B:887:HOH:O	2.19	0.54
2:B:501:TLO:O2B	2:B:501:TLO:H5'	2.07	0.53
1:B:468:ARG:HD3	5:B:935:HOH:O	2.09	0.53
1:A:169:LYS:HD3	1:A:214:TRP:CE3	2.45	0.52
1:A:338[B]:ARG:NH1	1:A:425:ILE:N	2.52	0.52
1:B:93:GLU:O	1:B:103:TYR:HA	2.09	0.52
1:A:379:GLU:O	1:A:379:GLU:HG2	2.07	0.52
1:A:389:GLN:NE2	5:A:1010:HOH:O	2.29	0.52
1:B:155:THR:HG23	2:B:501:TLO:CG	2.41	0.51
1:B:335:PHE:CE1	1:B:364:PRO:HA	2.46	0.51
1:A:395:ARG:HD2	4:A:505:EDO:H11	1.92	0.50
1:B:375:HIS:H	1:B:375:HIS:CD2	2.29	0.50
1:A:41:VAL:CG1	1:A:45:ILE:HD12	2.30	0.50
1:A:45:ILE:CG2	1:A:49:ARG:CZ	2.89	0.50
1:B:65:ASP:O	1:B:66:GLN:HB2	2.11	0.49
1:B:98:HIS:HD2	5:B:827:HOH:O	1.94	0.49
1:A:93:GLU:O	1:A:103:TYR:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ALA:O	5:B:868:HOH:O	2.20	0.49
1:A:95:ASP:OD2	1:A:95:ASP:O	2.30	0.48
1:B:23[A]:ARG:HD2	1:B:125:GLU:OE2	2.14	0.47
1:A:337:VAL:HG22	1:A:346:VAL:HG12	1.97	0.46
1:A:389:GLN:HE21	1:A:389:GLN:HA	1.81	0.46
1:B:396:ILE:HD11	5:B:868:HOH:O	2.16	0.46
1:B:377:PRO:HG2	1:B:380:GLU:OE2	2.16	0.46
1:B:95:ASP:OD2	1:B:95:ASP:C	2.57	0.46
1:A:338[B]:ARG:HD2	1:A:340:ILE:HG12	1.97	0.45
1:B:377:PRO:CD	1:B:380:GLU:OE2	2.65	0.45
1:A:335:PHE:CE1	1:A:364:PRO:HA	2.52	0.44
1:B:387:LEU:HD13	4:B:504:EDO:H11	1.99	0.44
1:A:89:LEU:HD11	1:A:277:VAL:CG1	2.47	0.44
1:B:152:VAL:HG11	1:B:171:ILE:HD13	1.99	0.44
1:A:40:ASP:O	1:A:43:ALA:HB3	2.18	0.44
1:A:256:LEU:HD23	5:A:754:HOH:O	2.18	0.44
2:A:501:TLO:O2B	2:A:501:TLO:H5'	2.18	0.44
1:A:46:ALA:O	1:A:50:ASP:N	2.30	0.43
1:B:377:PRO:CG	1:B:380:GLU:OE2	2.66	0.43
1:A:96:GLY:HA3	1:A:97:PRO:HD2	1.85	0.43
1:A:44:TRP:O	1:A:48:ARG:HG2	2.18	0.43
1:B:37:ARG:NH2	1:B:39:GLU:HG3	2.33	0.43
1:B:422:ASP:HB2	4:B:504:EDO:O1	2.18	0.43
1:B:338:ARG:CD	5:B:964:HOH:O	2.58	0.43
1:B:289:LYS:HB2	1:B:289:LYS:HE2	1.82	0.43
1:B:117:GLY:CA	1:B:155:THR:HG22	2.49	0.43
1:A:36:MET:HE3	1:A:36:MET:HB2	1.75	0.42
1:A:190:GLU:OE1	1:A:405:GLU:OE2	2.36	0.42
1:A:43:ALA:HA	1:A:46:ALA:HB3	2.02	0.42
1:A:156:ARG:HA	1:A:159:TYR:CE2	2.55	0.42
1:B:155:THR:CG2	2:B:501:TLO:CD2	2.98	0.42
1:B:377:PRO:HD2	1:B:380:GLU:OE2	2.19	0.42
1:B:191:GLN:H	1:B:191:GLN:NE2	2.12	0.42
1:B:190:GLU:HG3	1:B:198:LYS:HG2	2.02	0.41
1:B:236:ASN:O	1:B:240:ARG:HG3	2.20	0.41
1:B:329:ASP:HB3	1:B:369:THR:HG23	2.03	0.41
1:A:468[A]:ARG:HH11	1:A:468[A]:ARG:HD3	1.74	0.41
1:B:141:GLY:HA3	1:B:409:PHE:O	2.21	0.41
1:B:37:ARG:NH2	1:B:39:GLU:CG	2.84	0.40
1:B:468:ARG:HD3	1:B:468:ARG:HH21	1.58	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	444/471 (94%)	435 (98%)	8 (2%)	1 (0%)	43	28
1	B	445/471 (94%)	434 (98%)	10 (2%)	1 (0%)	43	28
All	All	889/942 (94%)	869 (98%)	18 (2%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	TYR
1	B	302	TYR

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	385/398 (97%)	370 (96%)	15 (4%)	28	12
1	B	384/398 (96%)	373 (97%)	11 (3%)	37	20
All	All	769/796 (97%)	743 (97%)	26 (3%)	33	16

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	41	VAL
1	A	49	ARG
1	A	53	VAL

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Mol	Chain	Res	Type
1	A	72	VAL
1	A	156	ARG
1	A	293	GLU
1	A	306	LEU
1	A	317	LYS
1	A	319	SER
1	A	379	GLU
1	A	423	GLU
1	A	436	PRO
1	A	468[A]	ARG
1	A	468[B]	ARG
1	B	57	GLU
1	B	190	GLU
1	B	191	GLN
1	B	198	LYS
1	B	306	LEU
1	B	319	SER
1	B	338	ARG
1	B	370	PRO
1	B	379	GLU
1	B	423	GLU
1	B	468	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	147	GLN
1	A	290	GLN
1	A	375	HIS
1	A	389	GLN
1	B	66	GLN
1	B	98	HIS
1	B	147	GLN
1	B	191	GLN
1	B	290	GLN
1	B	375	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	TRH	A	502	-	36,37,37	1.36	6 (16%)	54,57,57	1.89	15 (27%)
4	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.79	0
2	TLO	B	501	-	33,33,33	1.08	3 (9%)	46,49,49	2.49	18 (39%)
3	TRH	B	502	-	36,37,37	1.37	7 (19%)	54,57,57	1.95	14 (25%)
2	TLO	A	501	-	33,33,33	1.13	3 (9%)	46,49,49	1.93	16 (34%)
4	EDO	B	503	-	3,3,3	0.42	0	2,2,2	0.73	0
4	EDO	A	505	-	3,3,3	0.46	0	2,2,2	0.49	0
4	EDO	A	506	-	3,3,3	0.45	0	2,2,2	1.45	0
4	EDO	A	504	-	3,3,3	0.42	0	2,2,2	0.19	0
4	EDO	A	503	-	3,3,3	0.39	0	2,2,2	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRH	A	502	-	-	3/21/53/53	0/3/3/3
4	EDO	B	504	-	-	1/1/1/1	-
2	TLO	B	501	-	-	2/21/33/33	0/3/3/3
3	TRH	B	502	-	-	1/21/53/53	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLO	A	501	-	-	2/21/33/33	0/3/3/3
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	TRH	C41-C51	-3.84	1.38	1.44
3	A	502	TRH	C61-C51	3.65	1.40	1.34
3	A	502	TRH	C41-C51	-3.07	1.39	1.44
3	B	502	TRH	C21-N11	-3.07	1.33	1.38
2	A	501	TLO	C2-N1	-3.06	1.33	1.38
3	A	502	TRH	P-OPP	2.93	1.62	1.59
3	B	502	TRH	P-OPP	2.91	1.62	1.59
3	A	502	TRH	C21-N11	-2.65	1.34	1.38
3	A	502	TRH	P2-OPP	2.63	1.62	1.59
2	A	501	TLO	C4-C5	2.52	1.48	1.44
2	B	501	TLO	C6-C5	2.50	1.38	1.34
3	B	502	TRH	C61-C51	2.48	1.38	1.34
2	A	501	TLO	C6-C5	2.42	1.38	1.34
2	B	501	TLO	C2-N1	-2.39	1.34	1.38
3	B	502	TRH	C41-N31	-2.39	1.34	1.38
2	B	501	TLO	C4-C5	2.27	1.48	1.44
3	A	502	TRH	C61-N11	-2.12	1.34	1.38
3	B	502	TRH	P2-OPP	2.04	1.61	1.59
3	B	502	TRH	C61-N11	-2.00	1.34	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	TLO	C4-N3-C2	-6.30	119.08	127.34
2	B	501	TLO	N3-C2-N1	5.80	122.44	114.89
3	B	502	TRH	O4P-P2-OPP	5.57	122.32	107.27
2	B	501	TLO	O1B-PB-O3A	-5.29	92.97	107.27
3	A	502	TRH	C6-C5-C4	-5.11	103.74	113.08
3	B	502	TRH	C51-C41-N31	5.10	119.76	115.32
2	B	501	TLO	C5-C4-N3	4.86	119.55	115.32
2	A	501	TLO	O3A-PA-O2A	-4.49	97.19	110.70
3	A	502	TRH	O4P-P2-OPP	4.37	119.09	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	TRH	O5-C1-O1	-4.04	106.08	111.36
2	B	501	TLO	O3A-PA-O2A	-4.02	98.60	110.70
2	B	501	TLO	C5M-C5-C4	3.98	123.04	118.78
3	A	502	TRH	O41-C41-C51	-3.82	120.55	124.92
3	A	502	TRH	C41-N31-C21	-3.80	122.36	127.34
3	A	502	TRH	N31-C21-N11	3.77	119.80	114.89
2	B	501	TLO	O4-C4-C5	-3.62	120.78	124.92
2	A	501	TLO	O2-C2-N1	-3.59	118.12	122.80
2	A	501	TLO	O1B-PB-O3A	-3.56	97.64	107.27
3	A	502	TRH	C51-C41-N31	3.55	118.41	115.32
3	B	502	TRH	C41-N31-C21	-3.54	122.70	127.34
2	B	501	TLO	C5-C6-N1	-3.47	119.54	123.31
2	B	501	TLO	CE2-CD2-CG	3.43	124.17	118.98
2	B	501	TLO	O1B-PB-O3B	3.37	115.85	104.94
3	B	502	TRH	O4-C4-C3	-3.36	102.46	110.38
2	A	501	TLO	C5M-C5-C4	3.25	122.25	118.78
3	B	502	TRH	O41-C41-C51	-3.21	121.25	124.92
2	A	501	TLO	O4'-C4'-C3'	3.15	112.84	105.65
3	B	502	TRH	O5-C5-C6	3.15	113.72	106.74
2	A	501	TLO	N3-C2-N1	3.12	118.95	114.89
2	A	501	TLO	C6-C5-C4	-3.00	115.55	118.02
3	A	502	TRH	C3-C4-C5	-2.98	105.28	109.81
2	B	501	TLO	O1A-PA-O2A	2.98	126.30	112.44
2	A	501	TLO	O1B-PB-O3B	2.91	114.36	104.94
3	B	502	TRH	N31-C21-N11	2.80	118.54	114.89
2	B	501	TLO	C1'-N1-C6	-2.73	116.15	120.74
3	A	502	TRH	C51-C61-N11	-2.65	120.44	123.31
2	B	501	TLO	CD2-CG-CD1	-2.62	116.33	120.16
2	A	501	TLO	C4-N3-C2	-2.61	123.91	127.34
2	A	501	TLO	O1A-PA-O2A	2.60	124.56	112.44
2	A	501	TLO	CE1-CD1-CG	2.54	122.83	118.98
2	B	501	TLO	O2-C2-N1	-2.52	119.51	122.80
3	B	502	TRH	C3-C4-C5	-2.51	106.00	109.81
3	A	502	TRH	O3'-C3'-C4'	-2.50	100.58	110.07
3	B	502	TRH	O4'-C4'-C3'	2.47	111.29	105.65
3	A	502	TRH	O1-C1-C2	2.47	112.91	108.38
2	B	501	TLO	C5M-C5-C6	-2.40	119.61	122.85
3	B	502	TRH	O3'-C3'-C4'	-2.38	101.05	110.07
3	B	502	TRH	C4-C3-C2	2.38	115.01	110.83
3	A	502	TRH	O1-P2-O3P	2.38	117.41	109.81
2	A	501	TLO	CZ-CE1-CD1	-2.38	117.31	120.24
3	A	502	TRH	O5-C5-C6	2.35	111.95	106.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	TRH	C3'-C2'-C1'	2.34	108.33	102.60
2	A	501	TLO	C3'-C2'-C1'	2.30	108.23	102.60
2	B	501	TLO	O3'-C3'-C4'	-2.30	101.34	110.07
2	A	501	TLO	O3'-C3'-C4'	-2.30	101.37	110.07
2	A	501	TLO	C5-C4-N3	2.28	117.30	115.32
3	A	502	TRH	C4-C3-C2	2.26	114.80	110.83
2	A	501	TLO	O4-C4-C5	-2.20	122.41	124.92
2	B	501	TLO	C1'-N1-C2	2.13	121.82	117.66
3	A	502	TRH	O4'-C1'-C2'	-2.09	102.35	106.25
2	B	501	TLO	CZ-CE2-CD2	-2.08	117.68	120.24
3	B	502	TRH	C61-C51-C41	-2.05	116.33	118.02
3	B	502	TRH	O21-C21-N31	-2.01	117.78	121.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	TLO	PA-O3A-PB-O3B
2	A	501	TLO	PA-O3A-PB-O3B
4	B	504	EDO	O1-C1-C2-O2
3	A	502	TRH	O5-C1-O1-P2
3	B	502	TRH	O5-C1-O1-P2
3	A	502	TRH	P-OPP-P2-O3P
3	A	502	TRH	P-OPP-P2-O4P
2	A	501	TLO	CG-O3B-PB-O2B
2	B	501	TLO	CG-O3B-PB-O2B

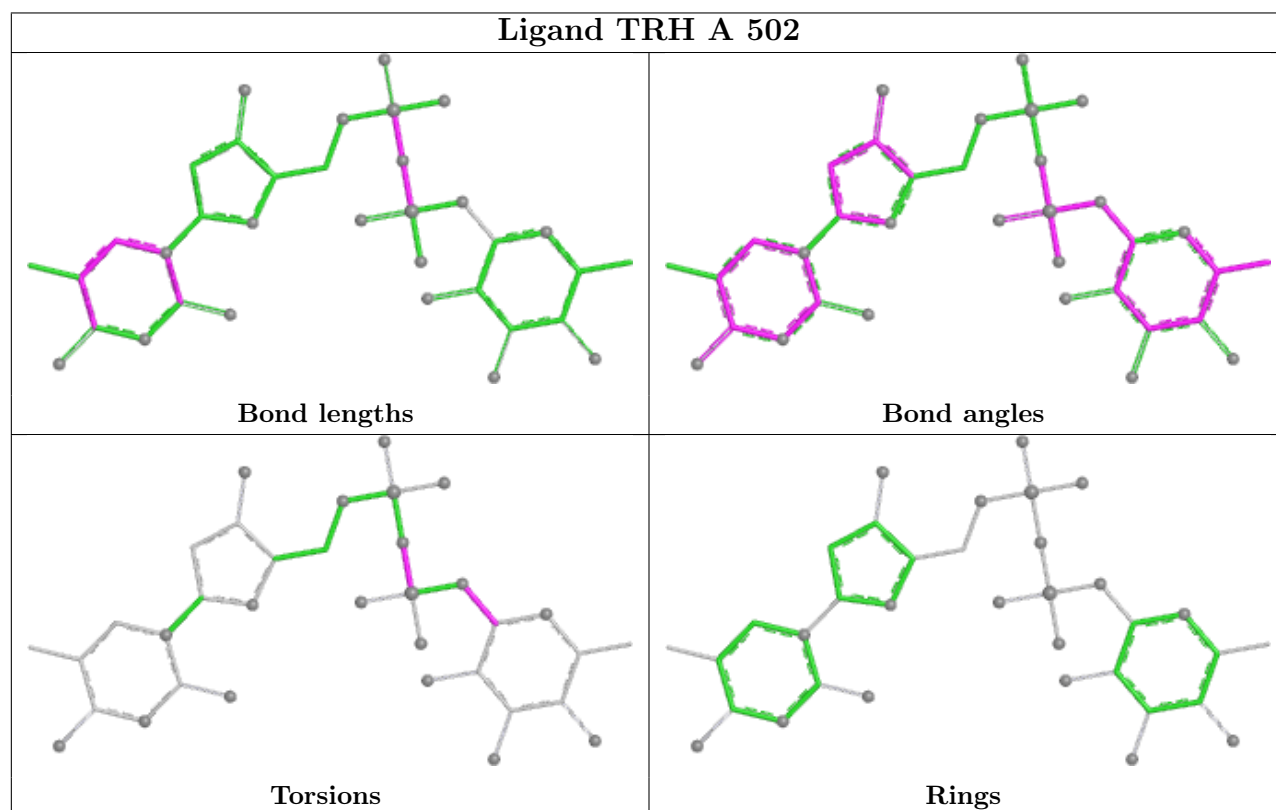
There are no ring outliers.

4 monomers are involved in 8 short contacts:

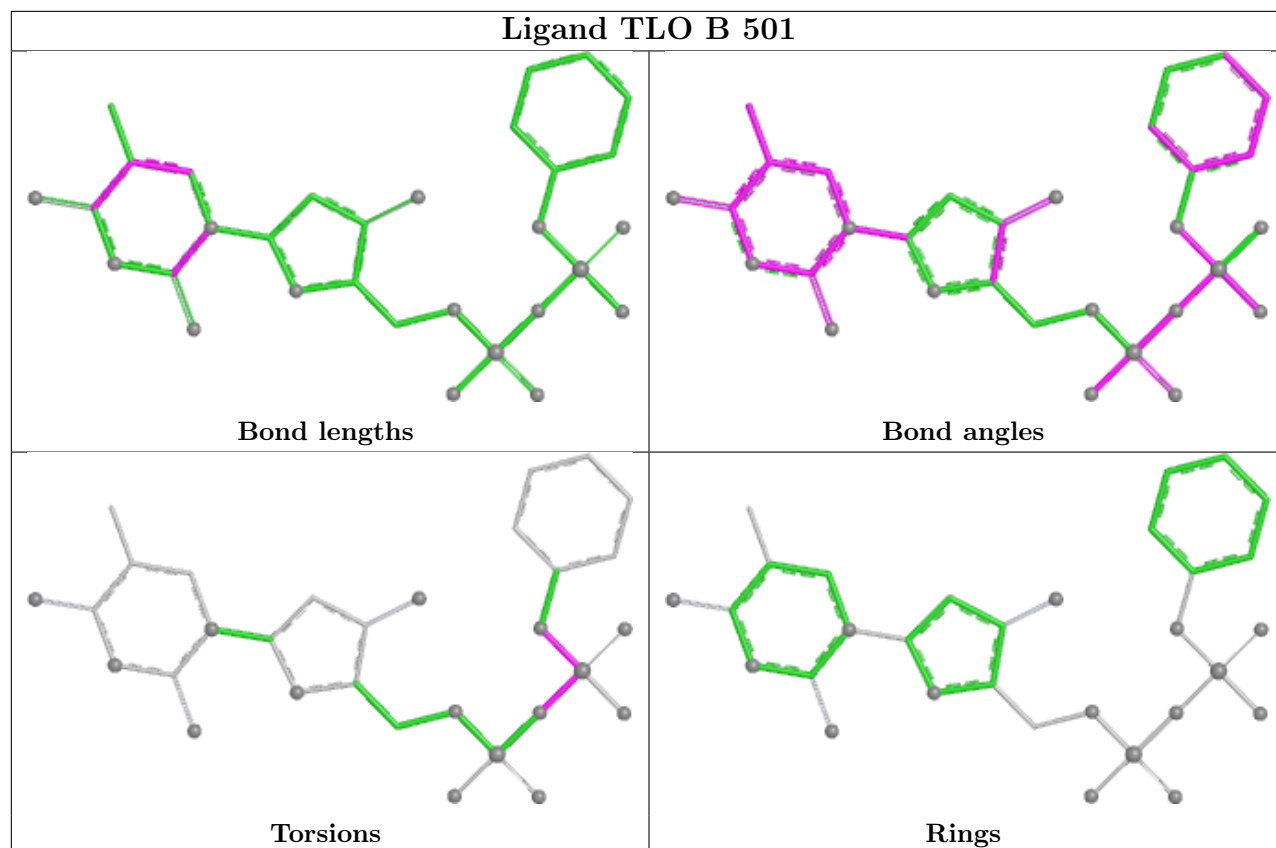
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	EDO	2	0
2	B	501	TLO	4	0
2	A	501	TLO	1	0
4	A	505	EDO	1	0

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

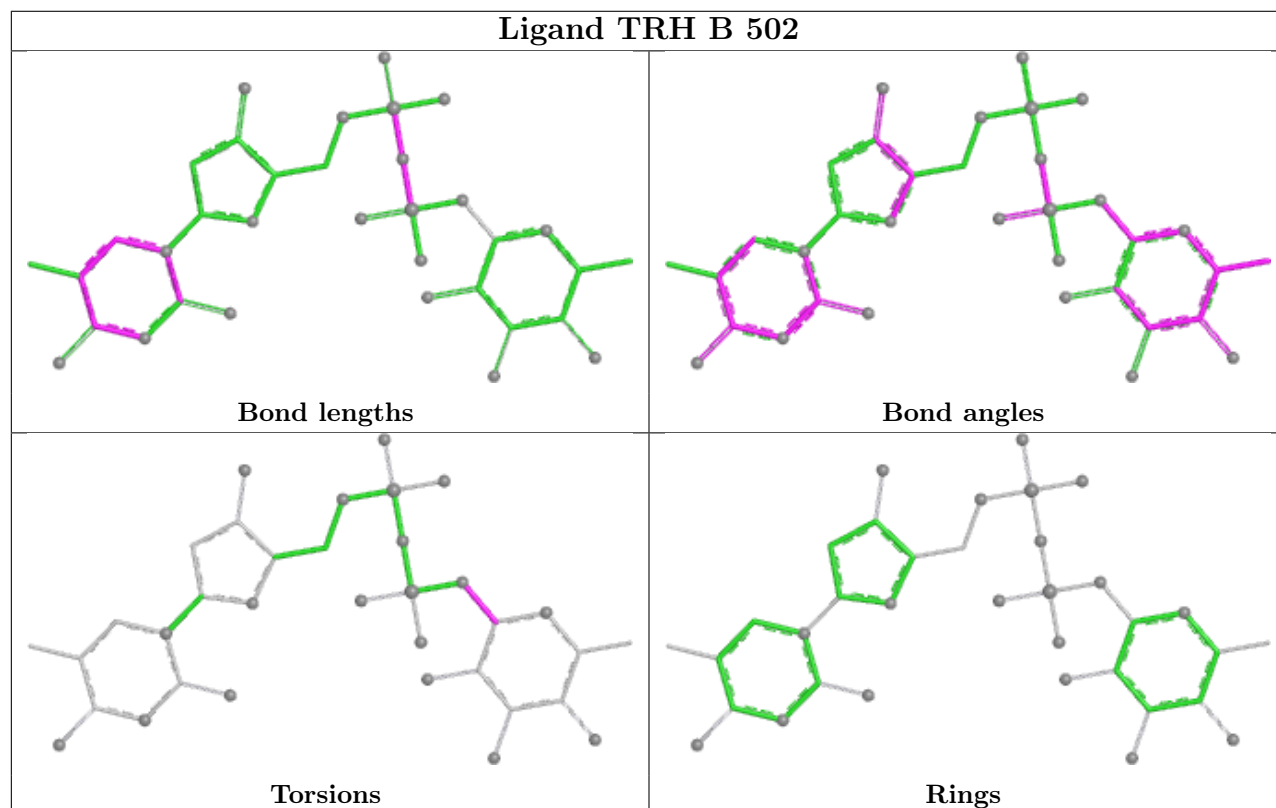
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

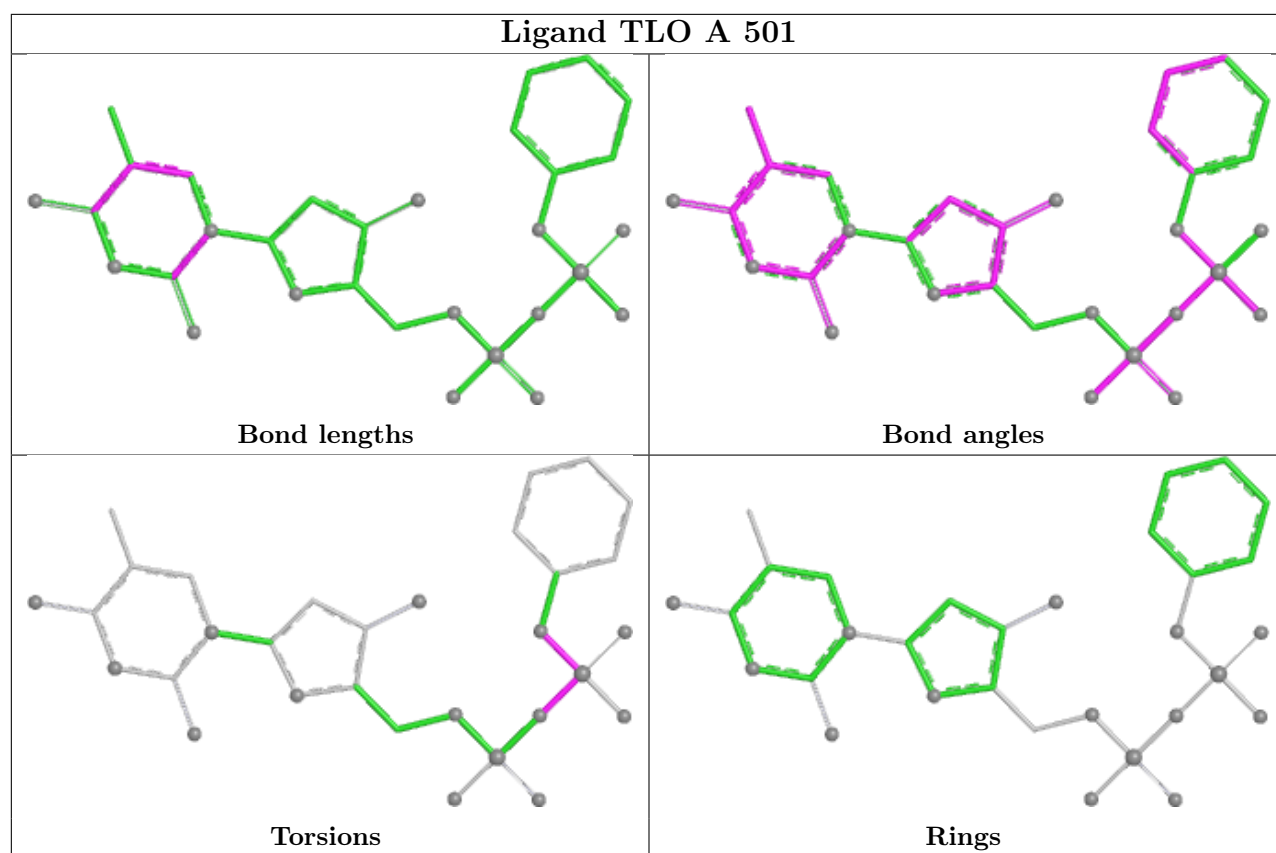


Ligand TLO B 501



Ligand TRH B 502





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	446/471 (94%)	-0.08	26 (5%)	29 32	9, 18, 42, 65	5 (1%)
1	B	444/471 (94%)	-0.13	22 (4%)	34 38	7, 18, 42, 56	7 (1%)
All	All	890/942 (94%)	-0.11	48 (5%)	31 34	7, 18, 42, 65	12 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	VAL	6.8
1	A	159	TYR	6.6
1	A	97	PRO	5.0
1	B	424	ALA	4.7
1	A	53	VAL	4.5
1	B	97	PRO	4.3
1	B	53	VAL	4.0
1	B	425	ILE	3.9
1	A	43	ALA	3.8
1	B	71	GLY	3.5
1	A	71	GLY	3.4
1	A	45	ILE	3.4
1	A	318	ILE	3.3
1	A	46	ALA	3.2
1	B	11	ALA	3.2
1	A	36	MET	3.1
1	B	55	HIS	3.0
1	B	51	ALA	3.0
1	B	167	ASN	3.0
1	B	376	LEU	2.9
1	A	42	ARG	2.9
1	A	51	ALA	2.9
1	A	11	ALA	2.9
1	B	312	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	98	HIS	2.8
1	B	98	HIS	2.8
1	A	49	ARG	2.7
1	B	423	GLU	2.7
1	A	40	ASP	2.6
1	B	377	PRO	2.6
1	A	37	ARG	2.6
1	B	72	VAL	2.5
1	A	317	LYS	2.5
1	B	54	PHE	2.4
1	B	468	ARG	2.4
1	A	50	ASP	2.4
1	A	468[A]	ARG	2.4
1	B	422	ASP	2.2
1	A	96	GLY	2.2
1	A	156	ARG	2.2
1	B	103	TYR	2.2
1	A	54	PHE	2.2
1	A	167	ASN	2.2
1	A	426	ASP	2.1
1	B	96	GLY	2.1
1	B	52	ASN	2.1
1	B	378	ALA	2.1
1	A	422	ASP	2.1

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](#)

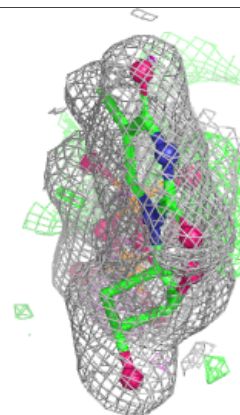
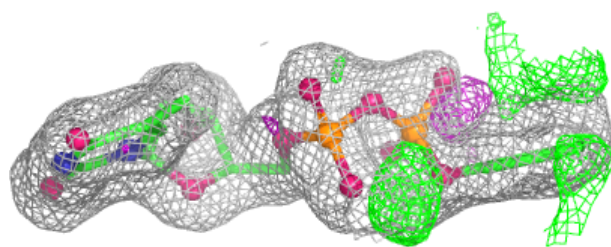
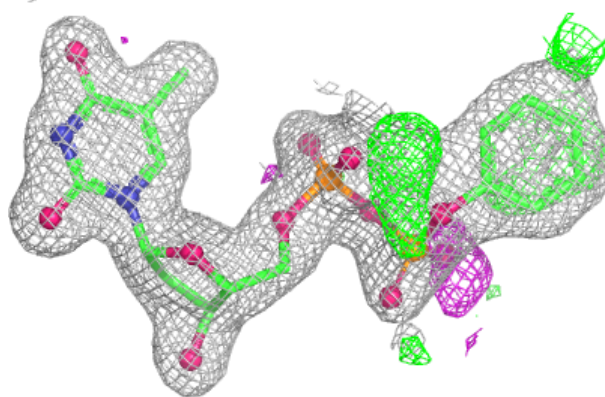
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	EDO	A	506	4/4	0.69	0.24	47,51,53,55	0
4	EDO	A	503	4/4	0.77	0.19	38,43,44,48	0
4	EDO	B	503	4/4	0.81	0.21	46,50,51,55	0
4	EDO	A	505	4/4	0.86	0.14	40,40,44,47	0
4	EDO	B	504	4/4	0.86	0.16	31,31,34,35	0
4	EDO	A	504	4/4	0.92	0.12	24,28,29,33	0
2	TLO	B	501	31/31	0.94	0.09	18,30,46,52	0
3	TRH	B	502	35/35	0.94	0.09	17,24,28,31	0
3	TRH	A	502	35/35	0.95	0.08	17,21,29,30	0
2	TLO	A	501	31/31	0.96	0.07	18,28,39,46	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.

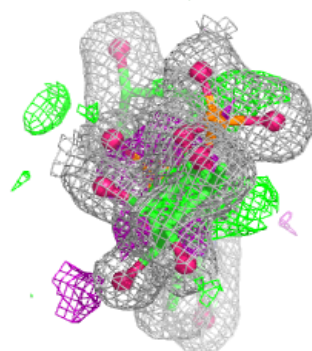
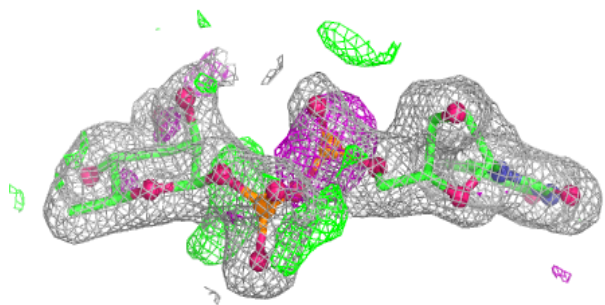
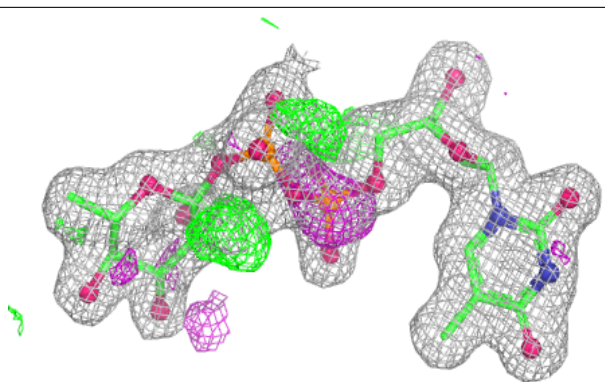
Electron density around TLO B 501:

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

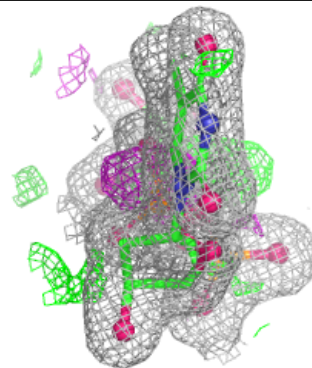
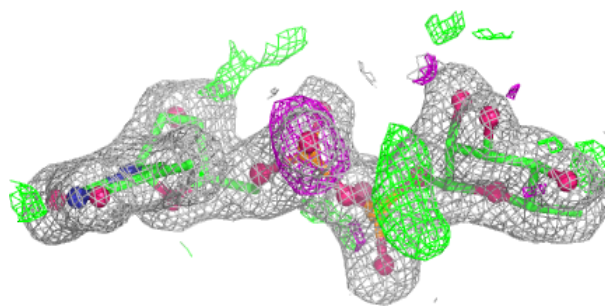
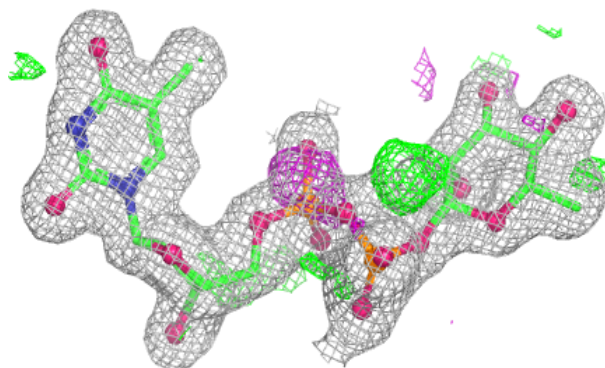


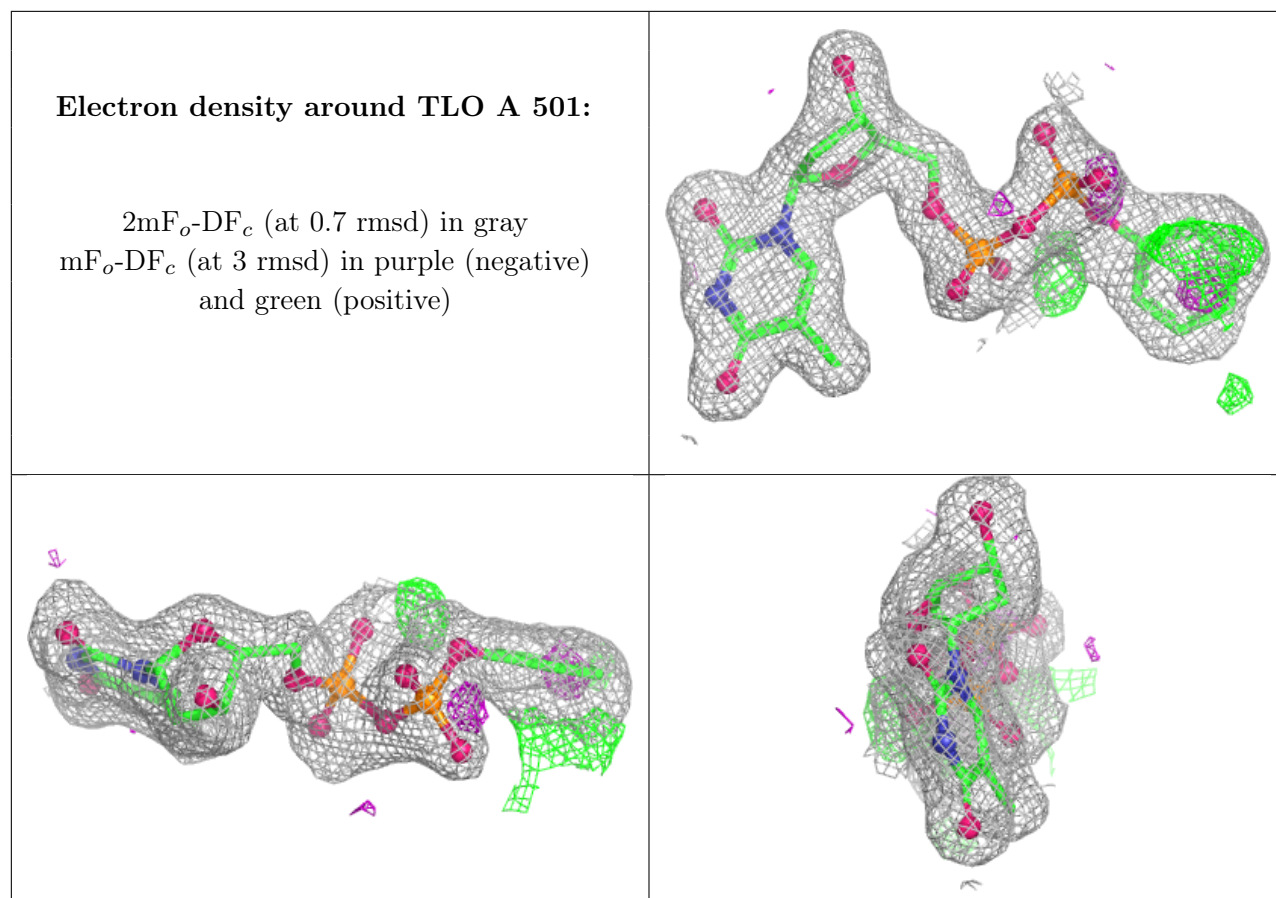
Electron density around TRH B 502:

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

**Electron density around TRH 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.