



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 03:17 PM EDT

PDB ID : 4J7G
Title : Crystal structure of EvaA, a 2,3-dehydratase in complex with dTDP-fucose and dTDP-rhamnose
Authors : Holden, H.M.; Kubiak, R.L.; Thoden, J.B.
Deposited on : 2013-02-13
Resolution : 1.70 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

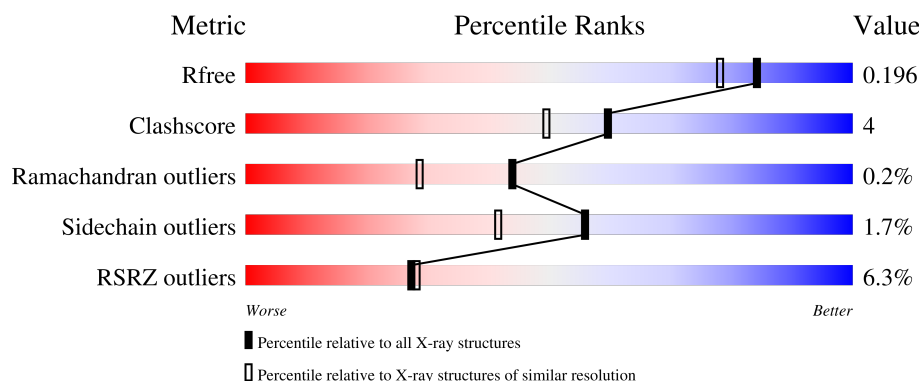
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (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	
1	B	471	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7953 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.

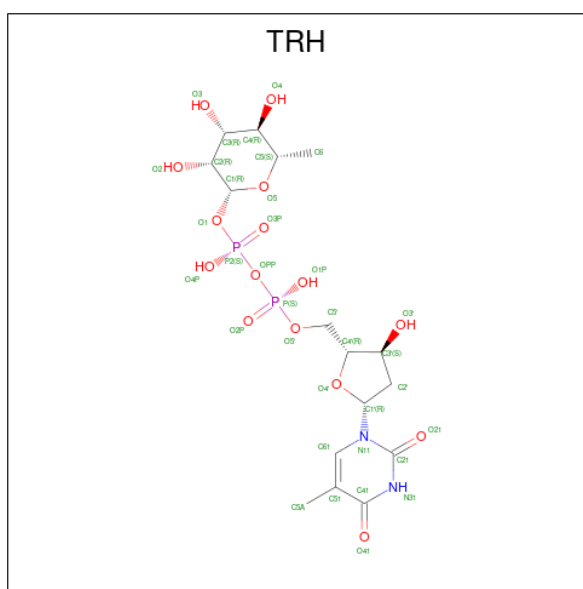
- Molecule 1 is a protein called EvaA 2,3-dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	4	0
			3599	2285	644	658	12			
1	B	446	Total	C	N	O	S	0	4	0
			3580	2276	639	654	11			

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

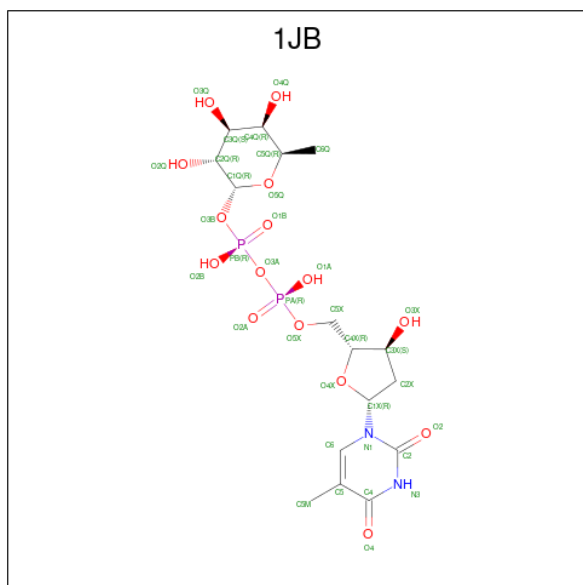
- Molecule 2 is 2'-DEOXY-THYMIDINE-BETA-L-RHAMNOSE (three-letter code: TRH) (formula: C₁₆H₂₆N₂O₁₅P₂).



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

- Molecule 3 is [[(2R,3S,5R)-5-[5-methyl-2,4-bis(oxidanylidene)pyrimidin-1-yl]-3-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2R,3R,4S,5R,6R)-6-methyl-3,4,5-tris(oxidanyl)oxan-2-yl] hydrogen phosphate (three-letter code: 1JB) (formula: C₁₆H₂₆N₂O₁₅P₂).



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

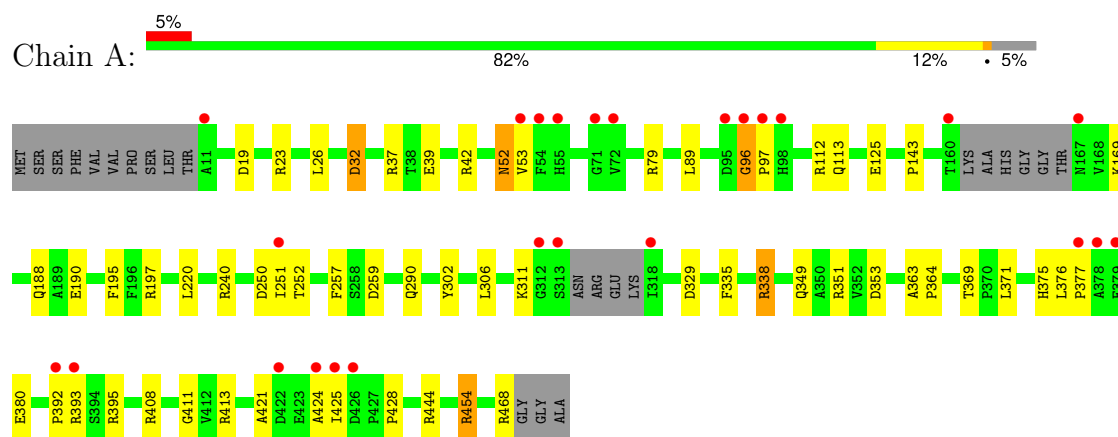
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	352	Total O 352 352	0	0
4	B	282	Total O 282 282	0	0

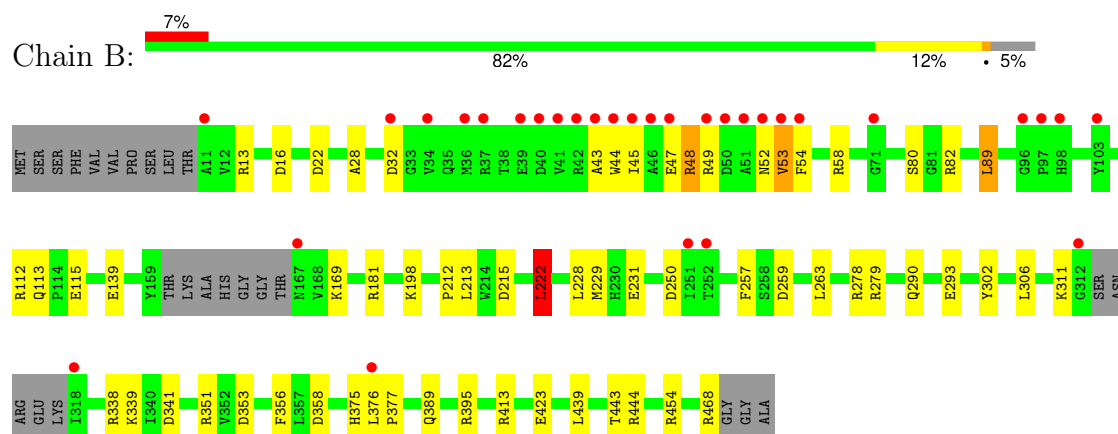
3 Residue-property plots

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	105.83Å 108.22Å 110.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.21 – 1.70 110.21 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (110.21-1.70) 95.5 (110.21-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.172 , 0.197 0.171 , 0.196	Depositor DCC
R_{free} test set	6991 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k 0.012 for -l,-k,-h 0.014 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7953	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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: 1JB, 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	0.58	0/3702	1.34	27/5044 (0.5%)
1	B	0.56	0/3686	1.35	37/5029 (0.7%)
All	All	0.57	0/7388	1.35	64/10073 (0.6%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229[A]	MET	CG-SD-CE	-16.77	73.36	100.20
1	B	229[B]	MET	CG-SD-CE	-16.77	73.36	100.20
1	A	468	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	351	ARG	NE-CZ-NH2	-13.30	113.65	120.30
1	A	444	ARG	NE-CZ-NH1	-10.01	115.29	120.30
1	A	250	ASP	CB-CG-OD2	9.80	127.12	118.30
1	B	395	ARG	NE-CZ-NH2	9.73	125.17	120.30
1	B	454	ARG	NE-CZ-NH1	-9.26	115.67	120.30
1	A	112	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	197	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	395	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	A	468	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	B	278	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	B	395	ARG	NE-CZ-NH1	-7.95	116.32	120.30
1	A	32	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	B	58	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	A	444	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	B	13	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	181	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	B	444	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	A	454	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	190	GLU	CA-CB-CG	-7.17	97.64	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	351	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	16[A]	ASP	CB-CG-OD1	7.10	124.69	118.30
1	B	16[B]	ASP	CB-CG-OD1	7.10	124.69	118.30
1	B	215	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	454	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	353	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	197	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	22	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	439	LEU	CB-CG-CD1	-6.66	99.68	111.00
1	A	395	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	444	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	257	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	B	259	ASP	CB-CG-OD1	6.43	124.09	118.30
1	B	169	LYS	CD-CE-NZ	-6.32	97.17	111.70
1	A	259	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	257	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	A	89	LEU	CB-CG-CD1	-6.07	100.68	111.00
1	B	356	PHE	CB-CG-CD2	-5.96	116.63	120.80
1	B	263	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	A	42	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	A	220	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	A	79	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	413	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	B	89	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	B	222	LEU	CB-CG-CD1	5.54	120.42	111.00
1	A	96	GLY	N-CA-C	-5.51	99.32	113.10
1	A	19	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	250	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	341	ASP	CB-CA-C	-5.44	99.52	110.40
1	B	257	PHE	CB-CG-CD1	5.41	124.59	120.80
1	A	26	LEU	CB-CG-CD1	-5.40	101.81	111.00
1	A	195	PHE	CB-CG-CD2	-5.35	117.05	120.80
1	B	341	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	B	48	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	413	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	13	ARG	CB-CG-CD	5.19	125.10	111.60
1	B	358	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	443	THR	N-CA-CB	5.08	119.96	110.30
1	B	358	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	228	LEU	CB-CG-CD1	-5.03	102.44	111.00
1	B	338	ARG	NE-CZ-NH2	5.03	122.81	120.30

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	3599	0	3508	35	0
1	B	3580	0	3484	28	0
2	A	35	0	24	0	0
2	B	35	0	24	0	0
3	A	35	0	25	0	0
3	B	35	0	25	0	0
4	A	352	0	0	3	0
4	B	282	0	0	5	0
All	All	7953	0	7090	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLY:C	1:A:97:PRO:CA	2.39	0.91
1:A:338[A]:ARG:HH11	1:A:425:ILE:H	1.22	0.85
1:A:113:GLN:NE2	4:A:673:HOH:O	2.06	0.83
1:A:96:GLY:C	1:A:97:PRO:CD	2.54	0.76
1:B:49:ARG:O	1:B:52:ASN:HB3	1.89	0.72
1:A:52:ASN:HD22	1:A:53:VAL:N	1.87	0.72
1:A:371:LEU:O	1:A:371:LEU:HD23	1.91	0.70
1:B:80:SER:OG	1:B:82:ARG:HG2	1.95	0.66
1:B:389:GLN:NE2	4:B:758:HOH:O	2.19	0.66
1:A:113:GLN:HE22	1:A:408:ARG:HH11	1.45	0.65
1:A:376:LEU:HB3	1:A:377:PRO:HD2	1.84	0.59
1:A:23[B]:ARG:NH1	1:A:125:GLU:OE2	2.32	0.58
1:B:375:HIS:H	1:B:375:HIS:CD2	2.22	0.57
1:B:53:VAL:HG12	1:B:54:PHE:N	2.19	0.57
1:B:139:GLU:OE2	4:B:826:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLN:OE1	4:B:674:HOH:O	2.17	0.55
1:B:49:ARG:HA	1:B:52:ASN:HB3	1.89	0.54
1:A:338[A]:ARG:NH1	1:A:425:ILE:H	2.01	0.54
1:A:143:PRO:HG3	1:A:411:GLY:HA2	1.91	0.53
1:A:169:LYS:HE3	4:A:951:HOH:O	2.07	0.53
1:B:45:ILE:O	1:B:49:ARG:N	2.33	0.52
1:B:112:ARG:HD2	1:B:279:ARG:HD3	1.91	0.52
1:B:49:ARG:O	1:B:52:ASN:CA	2.58	0.52
1:A:338[B]:ARG:HG2	1:A:421:ALA:HB3	1.93	0.51
1:B:49:ARG:C	1:B:52:ASN:H	2.14	0.51
1:A:349:GLN:HG2	1:A:363:ALA:HB3	1.92	0.51
1:B:231:GLU:OE2	1:B:468:ARG:NH2	2.44	0.51
1:B:49:ARG:O	1:B:52:ASN:N	2.44	0.49
1:A:338[B]:ARG:HD2	1:A:424:ALA:HA	1.94	0.49
1:B:49:ARG:O	1:B:52:ASN:CB	2.58	0.49
1:A:52:ASN:HD22	1:A:53:VAL:H	1.60	0.49
1:B:389:GLN:HE21	1:B:389:GLN:HA	1.78	0.49
1:B:28:ALA:HA	1:B:222:LEU:HB3	1.95	0.48
1:A:52:ASN:HD22	1:A:52:ASN:C	2.14	0.47
1:A:335:PHE:CE1	1:A:364:PRO:HA	2.50	0.47
1:A:251:ILE:HG13	1:A:252:THR:HG23	1.97	0.47
1:A:52:ASN:C	1:A:52:ASN:ND2	2.69	0.46
1:B:112:ARG:HH11	1:B:112:ARG:HD3	1.63	0.45
1:B:115:GLU:O	1:B:198:LYS:NZ	2.49	0.45
1:A:329:ASP:HB3	1:A:369:THR:CG2	2.46	0.45
1:A:37:ARG:NE	1:A:39:GLU:OE1	2.49	0.45
1:B:353:ASP:OD2	4:B:875:HOH:O	2.21	0.45
1:A:96:GLY:CA	1:A:97:PRO:CD	2.95	0.44
1:A:52:ASN:ND2	1:A:53:VAL:N	2.61	0.43
1:A:37:ARG:HH21	1:A:39:GLU:CD	2.22	0.43
1:A:393:ARG:HD3	1:B:213:LEU:HD23	2.01	0.42
1:B:43:ALA:O	1:B:47:GLU:CB	2.67	0.42
1:A:375:HIS:CD2	1:A:375:HIS:H	2.37	0.42
1:A:188:GLN:HB3	1:A:454:ARG:CZ	2.50	0.42
1:A:290:GLN:NE2	4:A:827:HOH:O	2.34	0.42
1:A:392:PRO:HA	1:B:212:PRO:HA	2.02	0.41
1:A:371:LEU:HD23	1:A:371:LEU:C	2.41	0.41
1:B:376:LEU:HB3	1:B:377:PRO:HD2	2.03	0.41
1:A:338[A]:ARG:HH11	1:A:425:ILE:N	2.04	0.41
1:B:44:TRP:O	1:B:48:ARG:HG2	2.21	0.41
1:B:290:GLN:NE2	4:B:796:HOH:O	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PRO:HG2	1:A:380:GLU:OE1	2.21	0.40
1:B:89:LEU:HD12	1:B:89:LEU:HA	1.89	0.40
1:A:311:LYS:HB2	1:A:311:LYS:HE3	1.92	0.40
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.87	0.40
1:B:43:ALA:O	1:B:47:GLU:HB2	2.22	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	444/471 (94%)	433 (98%)	10 (2%)	1 (0%)	44	29
1	B	444/471 (94%)	424 (96%)	19 (4%)	1 (0%)	44	29
All	All	888/942 (94%)	857 (96%)	29 (3%)	2 (0%)	44	29

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/398 (96%)	377 (98%)	6 (2%)	58	44
1	B	381/398 (96%)	373 (98%)	8 (2%)	48	32
All	All	764/796 (96%)	750 (98%)	14 (2%)	56	39

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	52	ASN
1	A	306	LEU
1	A	338[A]	ARG
1	A	338[B]	ARG
1	A	428	PRO
1	B	32	ASP
1	B	53	VAL
1	B	222	LEU
1	B	293	GLU
1	B	306	LEU
1	B	311	LYS
1	B	339	LYS
1	B	423	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	113	GLN
1	A	135	GLN
1	A	375	HIS
1	B	98	HIS
1	B	135	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 ⓘ

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 ⓘ

4 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	1JB	B	502	-	36,37,37	1.29	4 (11%)	54,57,57	2.57	25 (46%)
2	TRH	A	501	-	36,37,37	1.28	4 (11%)	54,57,57	2.24	13 (24%)
3	1JB	A	502	-	36,37,37	1.14	4 (11%)	54,57,57	2.18	17 (31%)
2	TRH	B	501	-	36,37,37	1.23	3 (8%)	54,57,57	2.07	15 (27%)

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	1JB	B	502	-	-	7/21/53/53	0/3/3/3
2	TRH	A	501	-	-	2/21/53/53	0/3/3/3
3	1JB	A	502	-	-	8/21/53/53	0/3/3/3
2	TRH	B	501	-	-	1/21/53/53	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	TRH	P2-OPP	3.34	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TRH	C61-C51	3.32	1.40	1.34
3	B	502	1JB	C4-C5	-3.21	1.39	1.44
3	B	502	1JB	PB-O3A	3.19	1.62	1.59
2	A	501	TRH	C41-C51	-3.18	1.39	1.44
2	B	501	TRH	C61-C51	3.18	1.39	1.34
3	B	502	1JB	C6-C5	2.72	1.39	1.34
2	B	501	TRH	C41-C51	-2.67	1.40	1.44
3	A	502	1JB	C4-C5	-2.66	1.40	1.44
2	A	501	TRH	P2-OPP	2.65	1.62	1.59
3	A	502	1JB	PB-O3A	2.47	1.62	1.59
3	A	502	1JB	C6-C5	2.46	1.38	1.34
3	B	502	1JB	C2-N1	-2.46	1.34	1.38
2	A	501	TRH	P-OPP	2.42	1.62	1.59
3	A	502	1JB	C2-N1	-2.13	1.35	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TRH	O5-C1-O1	-8.60	100.12	111.36
2	B	501	TRH	O5-C1-O1	-7.74	101.24	111.36
2	A	501	TRH	O41-C41-C51	-7.13	116.77	124.92
3	B	502	1JB	O5Q-C1Q-O3B	-6.88	102.37	111.36
3	B	502	1JB	O4Q-C4Q-C5Q	-5.78	96.99	109.74
3	A	502	1JB	C5-C4-N3	5.64	120.23	115.32
3	A	502	1JB	C4-N3-C2	-5.60	120.00	127.34
3	B	502	1JB	C5-C4-N3	5.25	119.89	115.32
3	B	502	1JB	O5Q-C5Q-C4Q	5.06	118.66	109.55
3	A	502	1JB	N3-C2-N1	4.85	121.21	114.89
3	B	502	1JB	O4-C4-C5	-4.79	119.44	124.92
3	A	502	1JB	O5Q-C5Q-C4Q	4.58	117.79	109.55
2	B	501	TRH	O41-C41-C51	-4.56	119.70	124.92
2	A	501	TRH	C61-N11-C21	-4.33	116.99	121.30
3	B	502	1JB	O2B-PB-O3A	-4.31	95.62	107.27
3	B	502	1JB	C1Q-O5Q-C5Q	4.21	120.81	113.63
2	B	501	TRH	C61-N11-C21	-4.07	117.25	121.30
2	A	501	TRH	C51-C41-N31	3.90	118.72	115.32
2	A	501	TRH	N31-C21-N11	3.85	119.90	114.89
2	B	501	TRH	N31-C21-N11	3.67	119.67	114.89
3	B	502	1JB	C2Q-C3Q-C4Q	3.65	117.24	110.83
2	B	501	TRH	C1-O5-C5	-3.65	107.41	113.63
3	A	502	1JB	O5Q-C1Q-O3B	-3.58	106.69	111.36
3	B	502	1JB	C6Q-C5Q-C4Q	3.57	119.62	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TRH	C5A-C51-C41	3.53	122.55	118.78
3	A	502	1JB	C2X-C1X-N1	-3.51	105.05	113.81
3	A	502	1JB	C2X-C3X-C4X	3.44	109.77	102.80
3	B	502	1JB	C4-N3-C2	-3.39	122.89	127.34
2	A	501	TRH	C61-C51-C41	-3.30	115.30	118.02
3	A	502	1JB	O1A-PA-O3A	3.30	116.18	107.27
3	A	502	1JB	C5M-C5-C4	3.24	122.24	118.78
3	A	502	1JB	O3X-C3X-C2X	-3.11	100.06	110.88
2	B	501	TRH	C2'-C1'-N11	-3.07	106.14	113.81
2	A	501	TRH	O5-C5-C4	-3.06	104.04	109.55
3	B	502	1JB	C5M-C5-C4	3.05	122.04	118.78
3	B	502	1JB	C3Q-C4Q-C5Q	-2.99	105.27	109.81
3	A	502	1JB	O2-C2-N1	-2.91	119.01	122.80
2	B	501	TRH	OPP-P2-O3P	-2.91	101.96	110.70
3	B	502	1JB	O2-C2-N1	-2.84	119.10	122.80
2	B	501	TRH	C1'-N11-C61	2.72	125.31	120.74
2	B	501	TRH	O21-C21-N31	-2.68	116.55	121.49
3	B	502	1JB	C2X-C3X-C4X	2.65	108.18	102.80
2	B	501	TRH	C5A-C51-C41	2.63	121.59	118.78
3	B	502	1JB	O3Q-C3Q-C2Q	2.60	116.51	110.38
2	A	501	TRH	C41-N31-C21	-2.58	123.95	127.34
2	A	501	TRH	OPP-P2-O3P	-2.55	103.04	110.70
2	A	501	TRH	C1-C2-C3	-2.52	104.70	110.01
2	B	501	TRH	O3-C3-C4	-2.52	104.43	110.38
3	A	502	1JB	C5-C6-N1	-2.50	120.60	123.31
3	B	502	1JB	O1A-PA-O3A	2.45	113.89	107.27
3	B	502	1JB	O5Q-C5Q-C6Q	2.41	112.09	106.74
3	B	502	1JB	O4X-C1X-C2X	2.39	110.72	106.25
3	A	502	1JB	O4X-C1X-N1	2.33	112.00	107.86
2	A	501	TRH	O41-C41-N31	2.33	124.49	120.11
2	B	501	TRH	C51-C41-N31	2.32	117.34	115.32
2	B	501	TRH	O4P-P2-OPP	2.30	113.48	107.27
3	A	502	1JB	O5Q-C5Q-C6Q	2.27	111.78	106.74
2	B	501	TRH	C61-C51-C41	-2.20	116.21	118.02
3	B	502	1JB	C2X-C1X-N1	-2.18	108.37	113.81
3	B	502	1JB	O3Q-C3Q-C4Q	-2.17	105.26	110.38
3	A	502	1JB	C5M-C5-C6	-2.15	119.94	122.85
3	A	502	1JB	O4Q-C4Q-C5Q	-2.13	105.03	109.74
2	A	501	TRH	O4P-P2-OPP	2.12	112.99	107.27
3	B	502	1JB	C5-C6-N1	-2.09	121.04	123.31
3	B	502	1JB	N3-C2-N1	2.08	117.60	114.89
3	A	502	1JB	O3A-PA-O2A	-2.07	104.49	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	1JB	C6-C5-C4	-2.05	116.33	118.02
3	B	502	1JB	O3X-C3X-C2X	-2.04	103.81	110.88
2	B	501	TRH	O4-C4-C5	-2.03	105.27	109.74
3	B	502	1JB	O2Q-C2Q-C3Q	-2.01	105.64	110.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

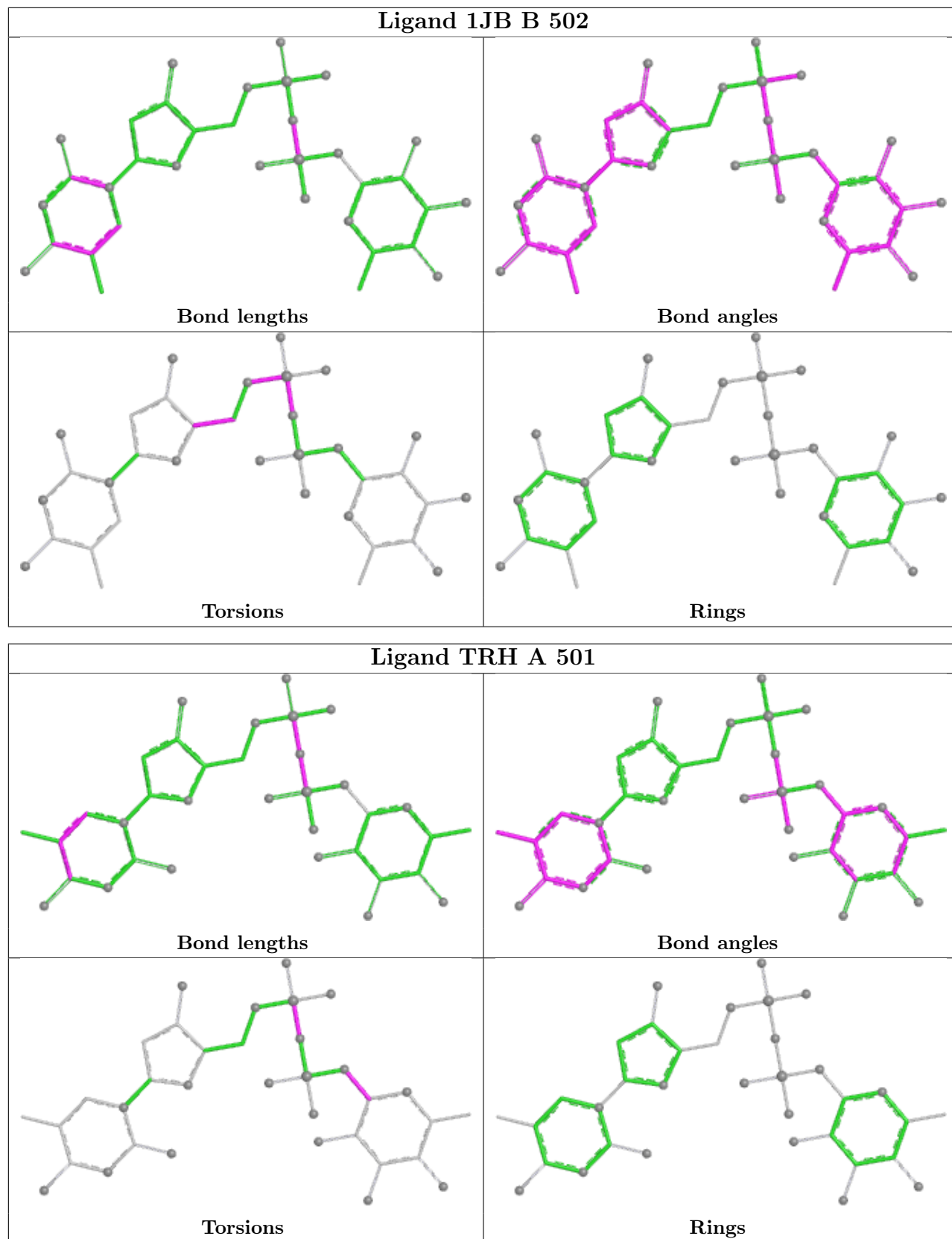
Mol	Chain	Res	Type	Atoms
2	A	501	TRH	O5-C1-O1-P2
3	A	502	1JB	C5X-O5X-PA-O2A
3	B	502	1JB	C3X-C4X-C5X-O5X
3	A	502	1JB	C3X-C4X-C5X-O5X
3	A	502	1JB	PA-O3A-PB-O3B
3	A	502	1JB	PB-O3A-PA-O2A
3	A	502	1JB	O4X-C4X-C5X-O5X
3	A	502	1JB	C5X-O5X-PA-O3A
3	A	502	1JB	C5X-O5X-PA-O1A
3	B	502	1JB	C5X-O5X-PA-O3A
3	B	502	1JB	C5X-O5X-PA-O1A
3	B	502	1JB	C5X-O5X-PA-O2A
3	B	502	1JB	O4X-C4X-C5X-O5X
3	B	502	1JB	PB-O3A-PA-O2A
2	B	501	TRH	O5-C1-O1-P2
2	A	501	TRH	P2-OPP-P-O1P
3	A	502	1JB	PB-O3A-PA-O1A
3	B	502	1JB	PB-O3A-PA-O1A

There are no ring outliers.

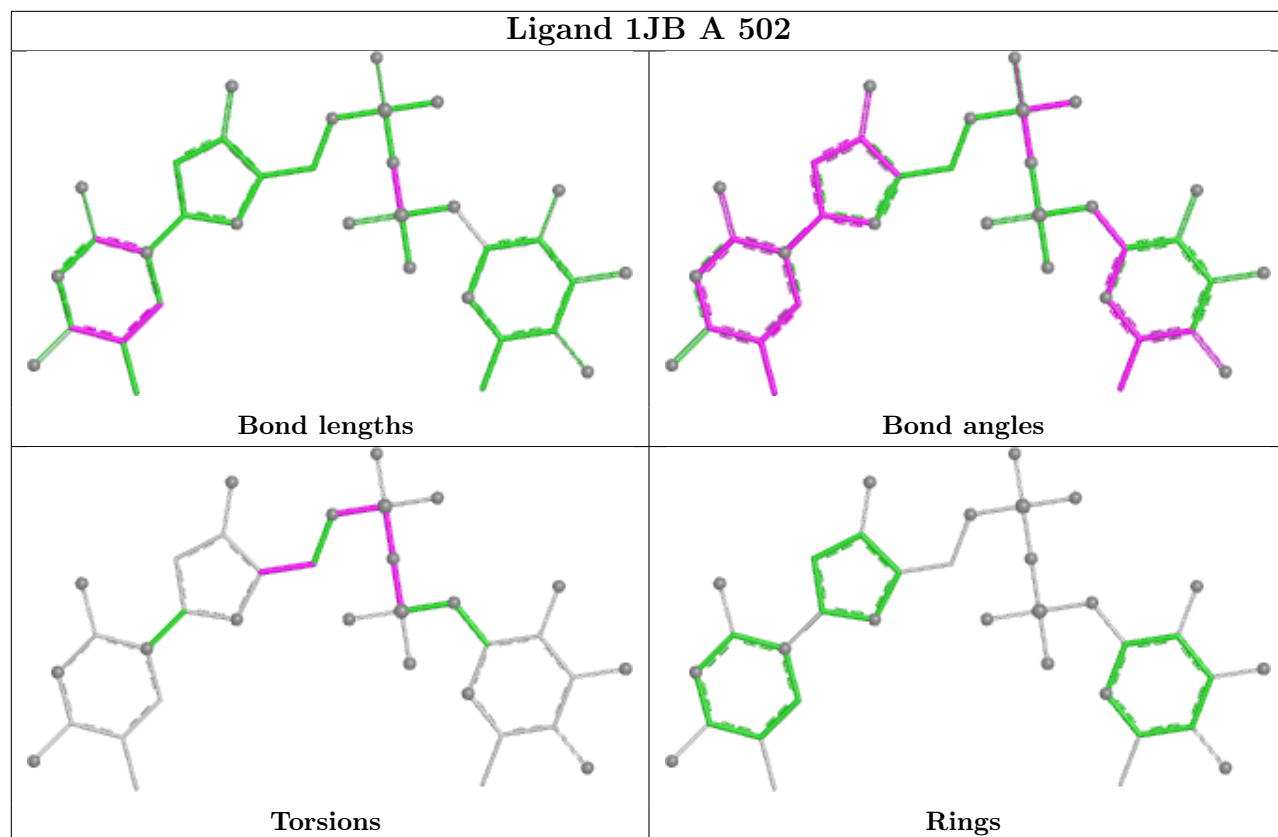
No monomer is involved in short contacts.

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

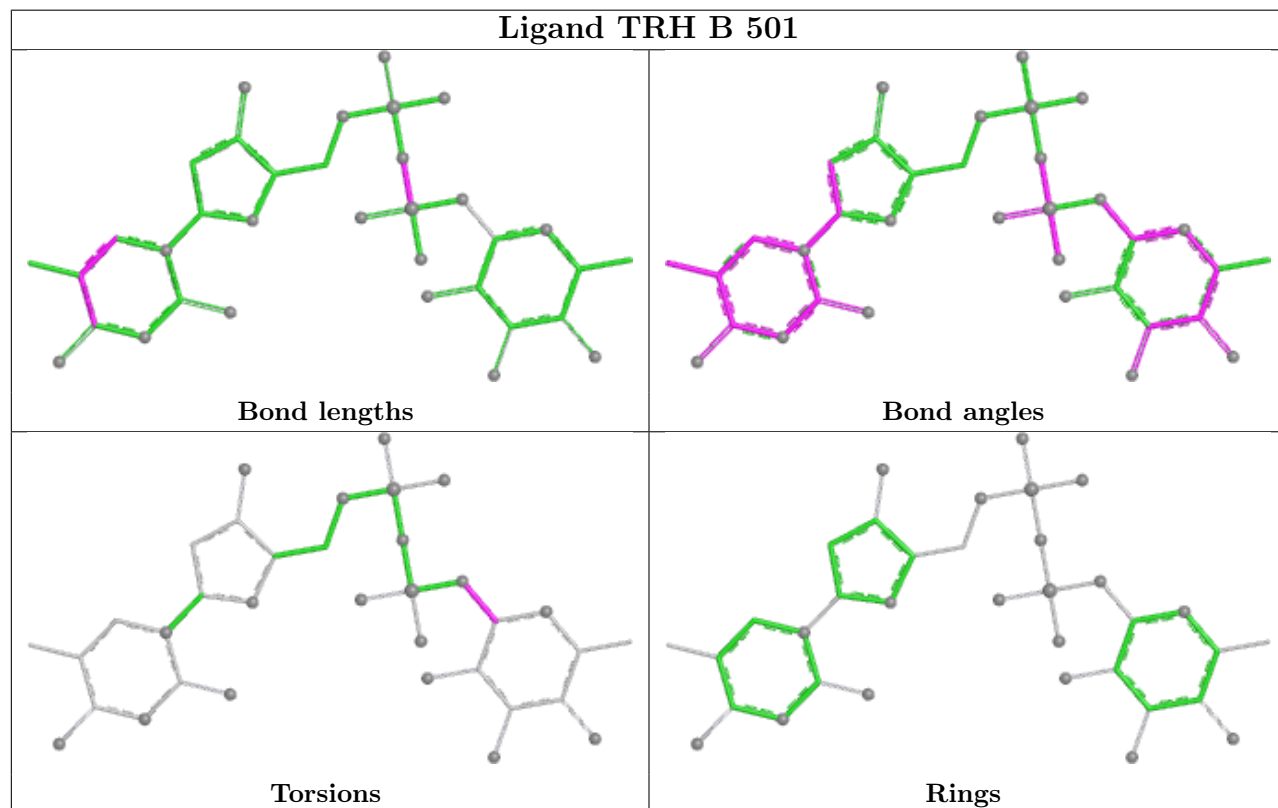
equivalents in the CSD to analyse the geometry.



Ligand 1JB A 502



Ligand TRH B 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	448/471 (95%)	-0.06	25 (5%) 31 33	12, 23, 47, 64	4 (0%)
1	B	446/471 (94%)	0.03	31 (6%) 24 24	12, 24, 48, 72	4 (0%)
All	All	894/942 (94%)	-0.02	56 (6%) 27 28	12, 24, 48, 72	8 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	VAL	7.2
1	A	318	ILE	5.7
1	B	312	GLY	4.8
1	A	160	THR	4.6
1	B	43	ALA	4.4
1	B	71	GLY	4.4
1	B	46	ALA	3.9
1	B	54	PHE	3.8
1	A	98	HIS	3.7
1	B	98	HIS	3.7
1	A	97	PRO	3.6
1	A	392	PRO	3.5
1	A	95	ASP	3.5
1	A	422	ASP	3.4
1	B	97	PRO	3.4
1	A	53	VAL	3.3
1	B	45	ILE	3.3
1	B	318	ILE	3.3
1	B	11	ALA	3.3
1	A	393	ARG	3.2
1	A	378	ALA	3.1
1	A	96	GLY	3.1
1	B	42	ARG	3.0
1	B	49	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	251	ILE	3.0
1	B	167	ASN	2.9
1	A	251	ILE	2.8
1	A	425	ILE	2.8
1	A	424	ALA	2.8
1	B	44	TRP	2.8
1	B	32	ASP	2.7
1	A	11	ALA	2.7
1	A	377	PRO	2.7
1	B	96	GLY	2.5
1	B	52	ASN	2.4
1	B	53	VAL	2.4
1	A	71	GLY	2.4
1	B	252	THR	2.4
1	A	313	SER	2.4
1	B	39	GLU	2.3
1	A	379	GLU	2.3
1	B	40	ASP	2.3
1	B	34	VAL	2.2
1	A	55	HIS	2.2
1	B	376	LEU	2.2
1	B	51	ALA	2.2
1	B	36	MET	2.2
1	A	426	ASP	2.2
1	A	312	GLY	2.2
1	A	54	PHE	2.1
1	B	47	GLU	2.1
1	A	167	ASN	2.1
1	B	103	TYR	2.1
1	B	37	ARG	2.0
1	B	50	ASP	2.0
1	A	72	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

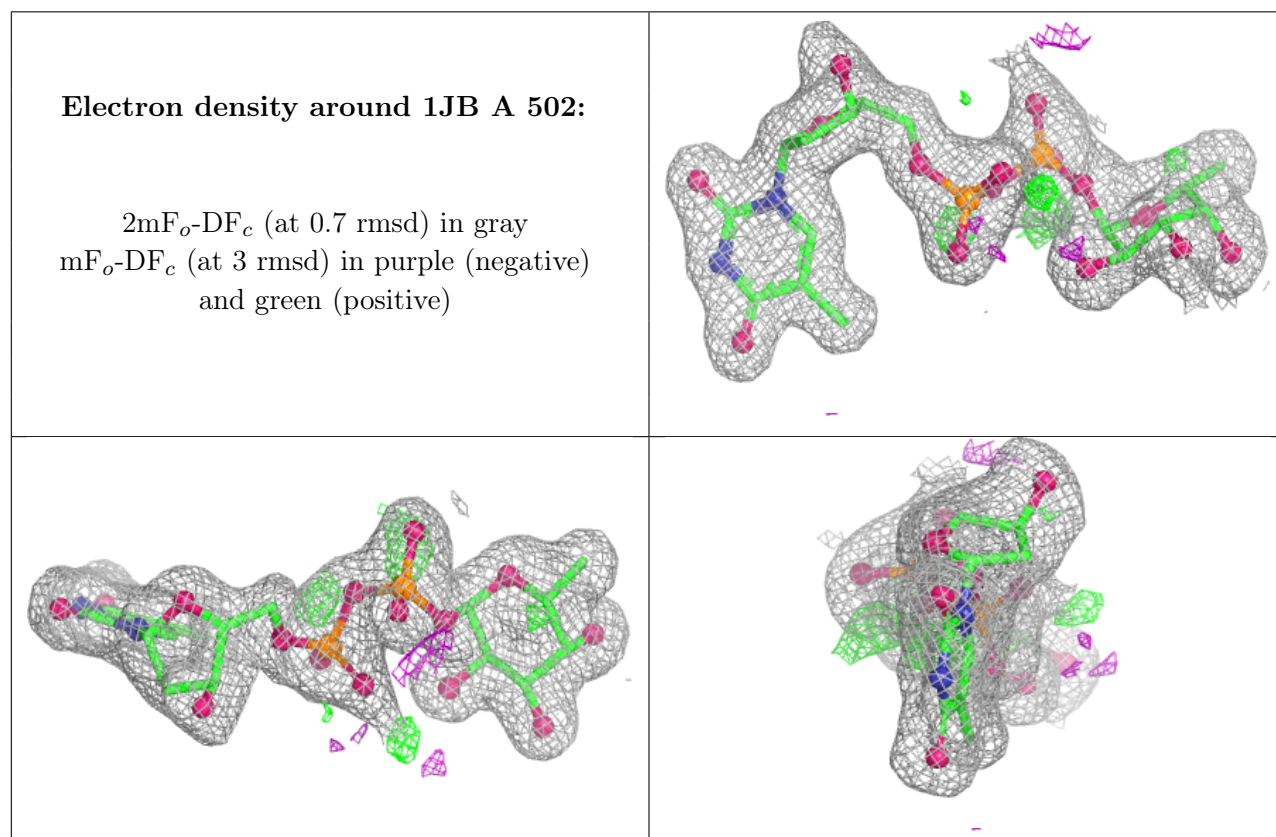
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

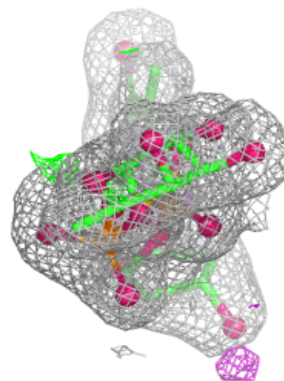
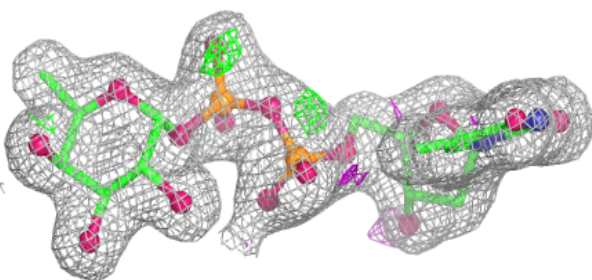
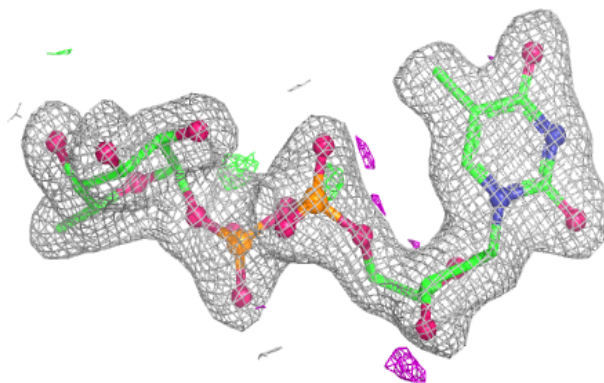
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	1JB	A	502	35/35	0.97	0.07	19,27,38,43	0
3	1JB	B	502	35/35	0.97	0.06	20,29,40,46	0
2	TRH	A	501	35/35	0.98	0.05	20,22,25,26	0
2	TRH	B	501	35/35	0.98	0.04	18,23,26,31	0

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.

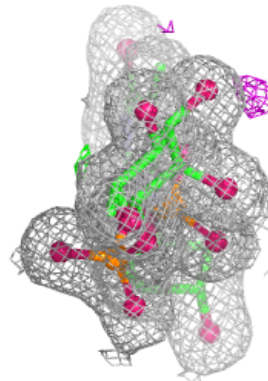
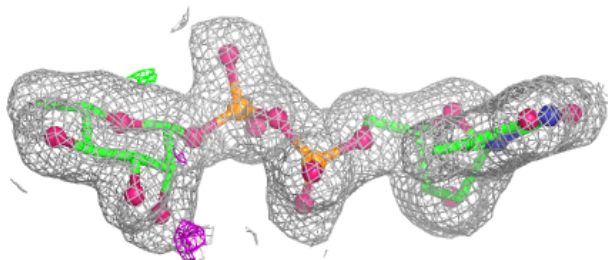
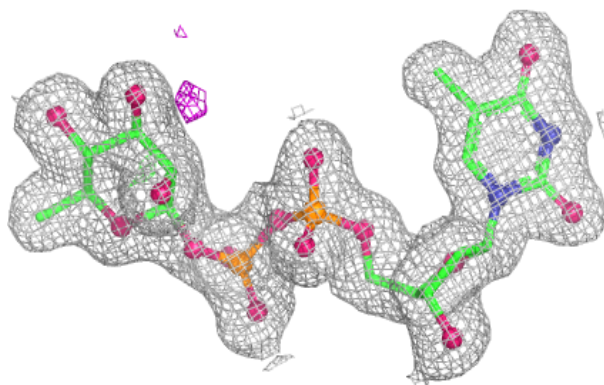


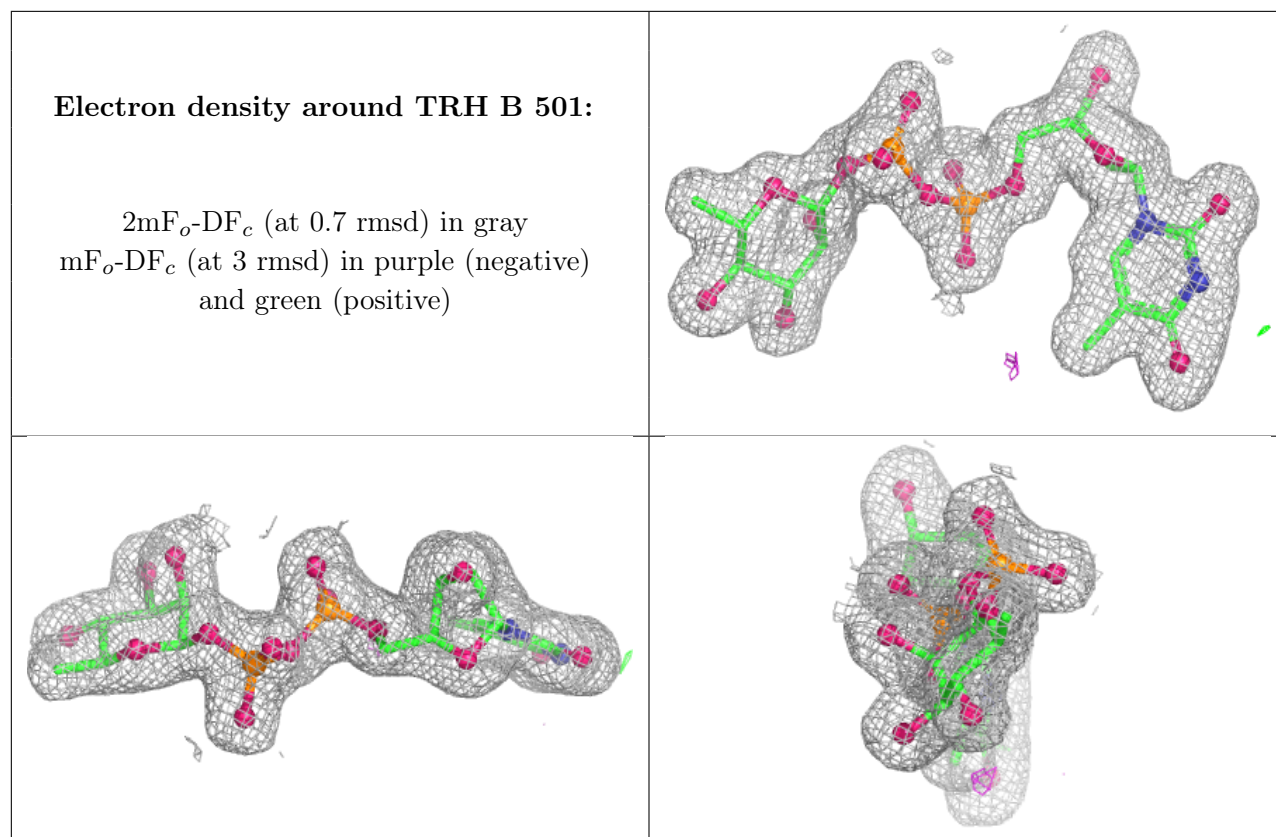
Electron density around 1JB B 502:

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

**Electron density around TRH A 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.