



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:55 PM UTC

PDB ID : 3UYL / pdb_00003uyl
Title : Spinosyn Rhamnosyltransferase SpnG complexed with thymidine diphosphate
Authors : Isiorho, E.A.; Liu, H.-W.; Keatinge-Clay, A.T.
Deposited on : 2011-12-06
Resolution : 1.85 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

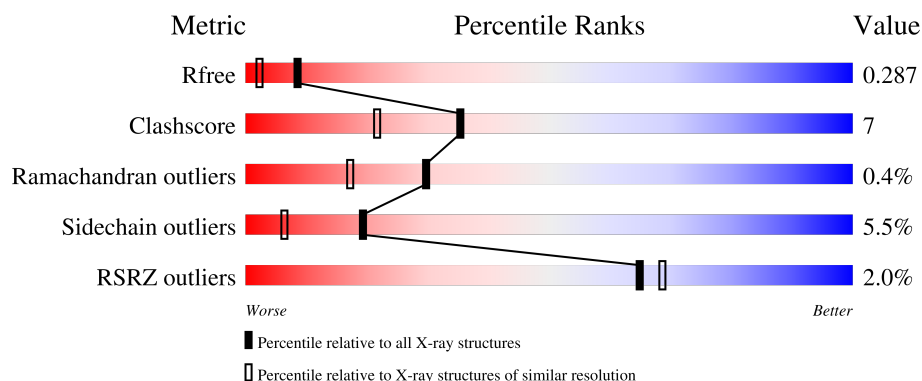
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	387	% 78% 17% ...
1	B	387	3% 80% 12% ...

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
2	TYD	A	401	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6014 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.

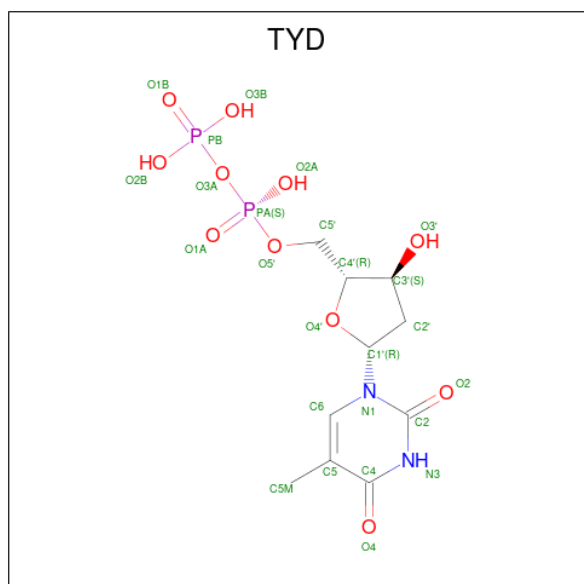
- Molecule 1 is a protein called NDP-rhamnosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2775	1760	490	510	15			
1	B	370	Total	C	N	O	S	0	0	0
			2758	1750	486	507	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q9ALM8
A	360	ALA	SER	SEE REMARK 999	UNP Q9ALM8
B	0	HIS	-	expression tag	UNP Q9ALM8
B	360	ALA	SER	SEE REMARK 999	UNP Q9ALM8

- Molecule 2 is THYMIDINE-5'-DIPHOSPHATE (CCD ID: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).

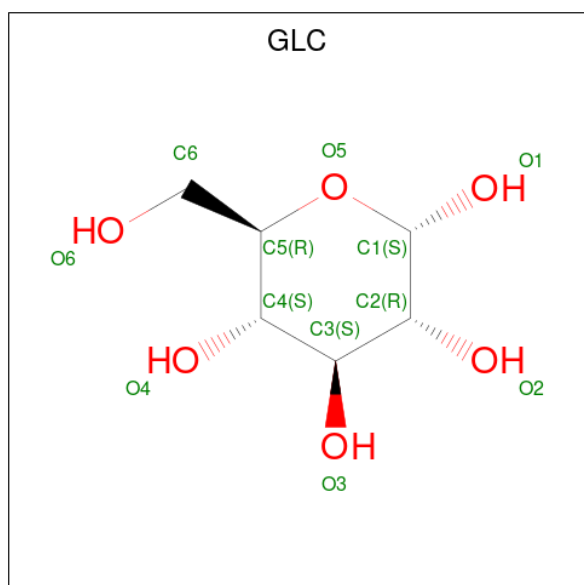


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
2	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		

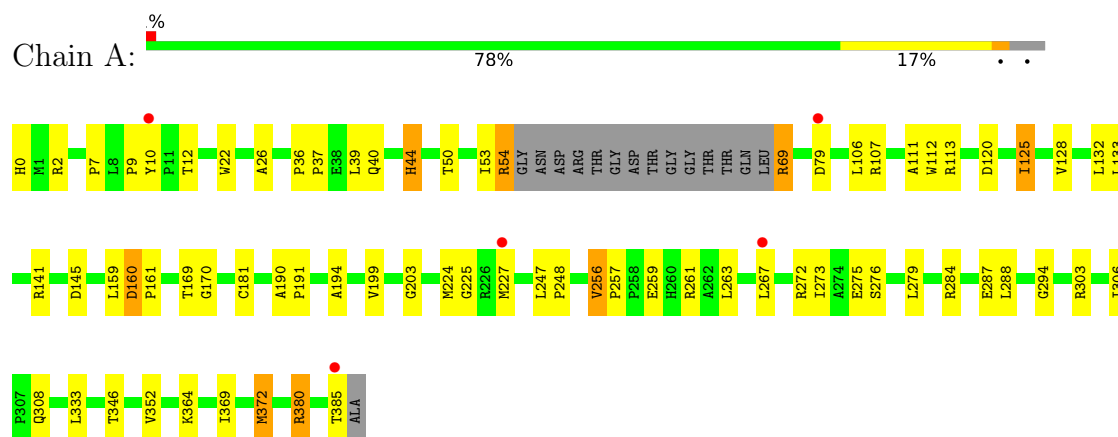
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	209	Total	O	0	0
			209	209		
5	B	208	Total	O	0	0
			208	208		

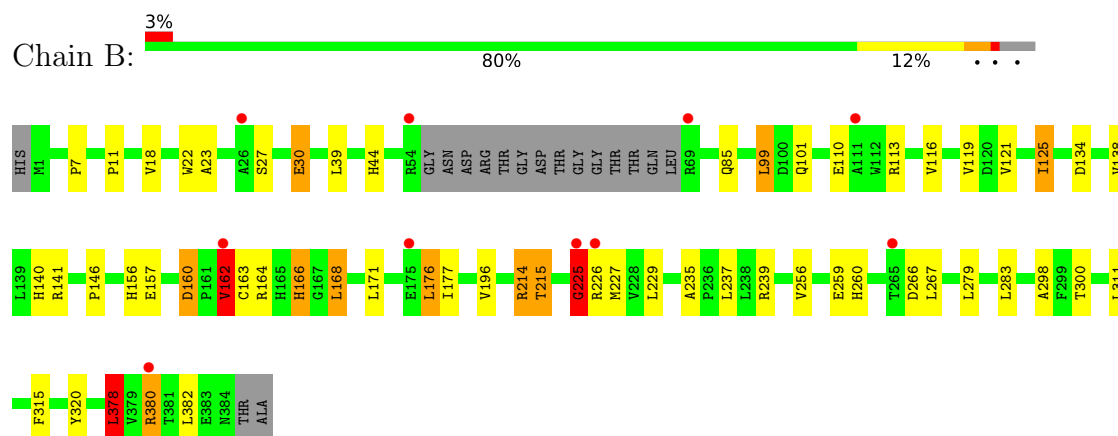
3 Residue-property plots [i](#)

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: NDP-rhamnosyltransferase



• Molecule 1: NDP-rhamnosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.15Å 57.63Å 68.20Å 81.63° 73.79° 85.74°	Depositor
Resolution (Å)	24.62 – 1.85 24.62 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.0 (24.62-1.85) 92.0 (24.62-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.85Å)	Xtriage
Refinement program	REFMAC version: 5.5.0072	Depositor
R, R_{free}	0.232 , 0.291 0.229 , 0.287	Depositor DCC
R_{free} test set	3104 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6014	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 6.52% 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: MG, TYD, GLC

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	1.33	7/2845 (0.2%)	1.30	18/3904 (0.5%)
1	B	1.35	9/2827 (0.3%)	1.31	15/3879 (0.4%)
All	All	1.34	16/5672 (0.3%)	1.30	33/7783 (0.4%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	ILE	CA-C	7.19	1.58	1.52
1	A	333	LEU	CA-C	6.67	1.60	1.52
1	A	257	PRO	CA-C	6.33	1.58	1.52
1	A	294	GLY	C-O	6.29	1.30	1.23
1	A	44	HIS	CE1-NE2	6.01	1.38	1.32
1	B	166	HIS	CG-CD2	5.88	1.42	1.35
1	B	215	THR	N-CA	-5.87	1.38	1.45
1	B	44	HIS	ND1-CE1	5.66	1.38	1.32
1	B	215	THR	CA-C	5.63	1.59	1.52
1	A	160	ASP	CA-C	5.53	1.59	1.52
1	B	260	HIS	CG-CD2	5.53	1.42	1.35
1	B	160	ASP	CA-C	5.50	1.59	1.52
1	B	225	GLY	C-O	5.48	1.31	1.23
1	B	121	VAL	C-O	-5.38	1.17	1.24
1	A	112	TRP	CD2-CE2	5.26	1.50	1.41
1	B	260	HIS	CE1-NE2	5.20	1.37	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	LEU	CA-C-N	-12.25	108.31	120.31
1	B	171	LEU	C-N-CA	-12.25	108.31	120.31
1	A	203	GLY	N-CA-C	-8.94	102.93	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	CYS	CA-C-N	-8.60	111.52	120.38
1	A	181	CYS	C-N-CA	-8.60	111.52	120.38
1	B	267	LEU	CA-C-N	7.66	128.12	119.92
1	B	267	LEU	C-N-CA	7.66	128.12	119.92
1	A	372	MET	CA-C-N	-7.33	112.23	119.78
1	A	372	MET	C-N-CA	-7.33	112.23	119.78
1	A	256	VAL	CA-C-N	-7.22	112.94	120.38
1	A	256	VAL	C-N-CA	-7.22	112.94	120.38
1	B	215	THR	N-CA-CB	-7.14	100.06	110.70
1	A	145	ASP	CA-C-N	7.00	128.58	119.84
1	A	145	ASP	C-N-CA	7.00	128.58	119.84
1	A	372	MET	CG-SD-CE	-6.92	85.68	100.90
1	A	159	LEU	N-CA-C	6.27	121.00	113.23
1	B	311	LEU	CA-C-N	-6.04	113.75	119.85
1	B	311	LEU	C-N-CA	-6.04	113.75	119.85
1	B	378	LEU	CA-CB-CG	-6.01	95.27	116.30
1	A	194	ALA	N-CA-C	-5.80	102.74	109.93
1	A	263	LEU	N-CA-C	5.71	118.44	111.82
1	B	177	ILE	CB-CA-C	-5.70	103.95	110.73
1	A	111	ALA	N-CA-C	5.64	117.12	110.97
1	A	333	LEU	CB-CA-C	5.33	115.45	110.17
1	A	170	GLY	N-CA-C	-5.28	100.66	113.18
1	B	18	VAL	CA-C-N	-5.22	113.66	119.19
1	B	18	VAL	C-N-CA	-5.22	113.66	119.19
1	B	119	VAL	N-CA-C	5.18	115.58	108.12
1	B	300	THR	N-CA-C	-5.18	105.71	111.36
1	A	199	VAL	CA-C-N	-5.18	113.37	119.84
1	A	199	VAL	C-N-CA	-5.18	113.37	119.84
1	B	162	VAL	CB-CA-C	-5.17	105.27	112.04
1	B	315	PHE	N-CA-C	5.05	115.99	108.31

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	2775	0	2769	55	0
1	B	2758	0	2755	31	0
2	A	25	0	13	10	0
2	B	25	0	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	12	0	12	0	0
5	A	209	0	0	10	3
5	B	208	0	0	2	3
All	All	6014	0	5562	83	3

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 7.

All (83) 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:113:ARG:HD2	5:A:688:HOH:O	1.35	1.26
1:A:107:ARG:HD3	5:A:670:HOH:O	1.54	1.06
1:A:225:GLY:HA3	2:A:401:TYD:O3B	1.67	0.95
1:A:380:ARG:HG2	1:A:380:ARG:HH21	1.30	0.93
1:A:279:LEU:HD12	2:A:401:TYD:O2	1.71	0.90
1:A:54:ARG:HH11	1:A:54:ARG:HG3	1.36	0.90
1:A:0:HIS:HD2	5:A:666:HOH:O	1.56	0.87
1:B:138:VAL:HG13	1:B:176:LEU:HD23	1.56	0.87
1:A:0:HIS:CD2	5:A:666:HOH:O	2.33	0.81
1:B:99:LEU:HD11	1:B:162:VAL:HG21	1.62	0.80
1:A:225:GLY:HA3	2:A:401:TYD:PB	2.22	0.78
1:B:7:PRO:HG2	1:B:39:LEU:CD1	2.15	0.76
1:A:380:ARG:HG2	1:A:380:ARG:NH2	2.00	0.75
1:B:110:GLU:O	1:B:113:ARG:HD3	1.87	0.75
1:B:214:ARG:HD3	1:B:215:THR:O	1.89	0.72
1:A:225:GLY:CA	2:A:401:TYD:O3B	2.38	0.72
1:A:369:ILE:HA	1:A:372:MET:HE3	1.72	0.72
1:B:226:ARG:NE	1:B:259:GLU:OE2	2.23	0.72
1:B:138:VAL:CG1	1:B:176:LEU:HD23	2.25	0.66
1:A:279:LEU:HD12	2:A:401:TYD:C2	2.26	0.65
1:A:7:PRO:HG2	1:A:39:LEU:CD1	2.29	0.62
1:B:101:GLN:HG2	5:B:644:HOH:O	1.99	0.61
1:A:279:LEU:HD13	2:A:401:TYD:H2'1	1.81	0.61
1:A:279:LEU:CD1	2:A:401:TYD:O2	2.44	0.61
1:A:37:PRO:HD2	1:A:54:ARG:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLY:HA3	2:B:401:TYD:O1B	2.00	0.61
1:A:54:ARG:HH11	1:A:54:ARG:CG	2.13	0.61
1:B:196:VAL:HG23	1:B:378:LEU:HD13	1.81	0.60
1:A:284:ARG:NH2	1:B:30:GLU:OE1	2.34	0.60
1:A:40:GLN:NE2	1:A:50:THR:OG1	2.36	0.59
1:A:279:LEU:CD1	2:A:401:TYD:C2	2.81	0.57
1:A:261:ARG:HD2	1:A:275:GLU:OE2	2.05	0.57
1:B:196:VAL:CG2	1:B:378:LEU:HD13	2.36	0.54
1:A:22:TRP:HB3	1:B:22:TRP:HB3	1.90	0.53
1:A:225:GLY:N	2:A:401:TYD:O3B	2.41	0.53
1:A:40:GLN:HE21	1:A:44:HIS:CE1	2.27	0.52
1:A:190:ALA:HB3	5:A:709:HOH:O	2.08	0.52
1:B:156:HIS:O	1:B:160:ASP:HB2	2.10	0.52
1:A:279:LEU:HD12	1:A:279:LEU:H	1.75	0.52
1:A:125:ILE:HG22	5:A:611:HOH:O	2.10	0.51
1:A:380:ARG:HH21	1:A:380:ARG:CG	2.13	0.50
1:A:26:ALA:HB1	1:B:23:ALA:HB2	1.93	0.50
1:A:287:GLU:OE1	5:A:656:HOH:O	2.19	0.49
1:B:163:CYS:HB3	1:B:168:LEU:HD12	1.95	0.49
1:A:69:ARG:HB3	1:A:69:ARG:NH1	2.27	0.49
1:A:128:VAL:O	1:A:132:LEU:HD13	2.13	0.49
1:A:2:ARG:NH2	1:A:2:ARG:HG2	2.26	0.49
1:A:247:LEU:HD13	1:A:346:THR:HG22	1.94	0.49
1:A:54:ARG:HG3	5:A:698:HOH:O	2.13	0.48
1:B:164:ARG:HA	1:B:168:LEU:O	2.13	0.48
1:A:36:PRO:HA	1:A:53:ILE:O	2.14	0.48
1:A:2:ARG:HG2	1:A:2:ARG:HH21	1.78	0.48
1:B:227:MET:HB2	2:B:401:TYD:O2B	2.13	0.48
1:A:106:LEU:HD23	1:A:133:LEU:HD21	1.97	0.47
1:A:141:ARG:NH2	1:A:191:PRO:HD2	2.30	0.47
1:B:235:ALA:O	1:B:239:ARG:HG3	2.13	0.47
1:A:53:ILE:O	1:A:54:ARG:HB3	2.15	0.47
1:A:190:ALA:CB	5:A:709:HOH:O	2.62	0.47
1:B:229:LEU:HD11	1:B:237:LEU:HB2	1.97	0.47
1:B:110:GLU:HA	1:B:110:GLU:OE1	2.15	0.46
1:B:380:ARG:CG	1:B:380:ARG:HH11	2.28	0.46
1:A:7:PRO:CG	1:A:39:LEU:CD1	2.94	0.46
1:A:9:PRO:HB3	1:A:36:PRO:HG2	1.98	0.46
1:B:140:HIS:CD2	1:B:141:ARG:O	2.69	0.46
1:B:298:ALA:HB1	1:B:320:TYR:CZ	2.50	0.46
1:B:138:VAL:HG21	1:B:382:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PRO:HG2	1:B:39:LEU:HD11	1.96	0.45
1:A:12:THR:HG21	2:A:401:TYD:O5'	2.17	0.44
1:B:85:GLN:NE2	5:B:693:HOH:O	2.40	0.44
1:B:196:VAL:HB	1:B:378:LEU:HD13	1.99	0.44
1:A:267:LEU:HD22	1:A:273:ILE:HD11	1.99	0.44
1:A:37:PRO:HD3	1:A:53:ILE:O	2.18	0.44
1:B:162:VAL:O	1:B:166:HIS:HD2	2.02	0.43
1:A:10:TYR:CD1	1:A:227:MET:HE2	2.54	0.42
1:B:138:VAL:HG13	1:B:176:LEU:CD2	2.39	0.42
1:B:298:ALA:HB1	1:B:320:TYR:CE1	2.54	0.42
1:A:7:PRO:HA	1:A:120:ASP:HB2	2.00	0.42
1:A:247:LEU:HG	1:A:248:PRO:HD2	2.01	0.42
1:A:288:LEU:HD13	1:A:352:VAL:HG11	2.01	0.42
1:A:364:LYS:HE3	5:A:662:HOH:O	2.19	0.41
1:A:247:LEU:HD13	1:A:346:THR:CG2	2.51	0.41
1:A:54:ARG:CG	1:A:54:ARG:NH1	2.80	0.41
1:A:160:ASP:N	1:A:161:PRO:HD2	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:597:HOH:O	5:B:708:HOH:O[1_556]	1.57	0.63
5:A:703:HOH:O	5:B:704:HOH:O[1_556]	1.80	0.40
5:A:703:HOH:O	5:B:705:HOH:O[1_556]	1.94	0.26

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	368/387 (95%)	356 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	366/387 (95%)	353 (96%)	10 (3%)	3 (1%)	16	6
All	All	734/774 (95%)	709 (97%)	22 (3%)	3 (0%)	30	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	225	GLY
1	B	146	PRO
1	B	125	ILE

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	290/300 (97%)	276 (95%)	14 (5%)	23	8
1	B	288/300 (96%)	270 (94%)	18 (6%)	16	4
All	All	578/600 (96%)	546 (94%)	32 (6%)	19	6

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	69	ARG
1	A	79	ASP
1	A	125	ILE
1	A	169	THR
1	A	224	MET
1	A	256	VAL
1	A	259	GLU
1	A	272	ARG
1	A	276	SER
1	A	303	ARG
1	A	308	GLN
1	A	380	ARG

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Mol	Chain	Res	Type
1	A	385	THR
1	B	11	PRO
1	B	27	SER
1	B	30	GLU
1	B	99	LEU
1	B	116	VAL
1	B	125	ILE
1	B	134	ASP
1	B	157	GLU
1	B	162	VAL
1	B	168	LEU
1	B	176	LEU
1	B	214	ARG
1	B	256	VAL
1	B	266	ASP
1	B	279	LEU
1	B	283	LEU
1	B	378	LEU
1	B	380	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	40	GLN
1	A	85	GLN
1	A	89	GLN
1	A	166	HIS
1	A	197	GLN
1	A	260	HIS
1	B	40	GLN
1	B	85	GLN
1	B	140	HIS
1	B	202	ASN
1	B	313	GLN

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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	TYD	A	401	-	25,26,26	1.57	4 (16%)	38,40,40	2.49	13 (34%)
2	TYD	B	401	-	25,26,26	1.43	4 (16%)	38,40,40	1.88	12 (31%)
4	GLC	B	402	-	12,12,12	0.80	0	17,17,17	2.50	5 (29%)

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	TYD	A	401	-	-	1/16/28/28	0/2/2/2
2	TYD	B	401	-	-	1/16/28/28	0/2/2/2
4	GLC	B	402	-	-	2/2/22/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	TYD	PA-O3A	5.06	1.65	1.59
2	B	401	TYD	PA-O3A	4.19	1.64	1.59
2	A	401	TYD	C4-C5	3.06	1.49	1.44
2	B	401	TYD	C6-C5	2.92	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	TYD	C2-N1	2.50	1.42	1.38
2	A	401	TYD	C2-N3	-2.28	1.34	1.38
2	B	401	TYD	C2-N3	-2.16	1.34	1.38
2	B	401	TYD	O2-C2	2.08	1.26	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	TYD	C5-C4-N3	7.45	121.80	115.32
2	A	401	TYD	C4-N3-C2	-6.67	118.59	127.34
4	B	402	GLC	O5-C1-C2	6.15	121.11	110.30
2	B	401	TYD	O4-C4-C5	-5.21	118.95	124.92
2	A	401	TYD	O4-C4-C5	-4.81	119.42	124.92
2	A	401	TYD	N3-C2-N1	4.74	121.06	114.89
4	B	402	GLC	O2-C2-C1	4.16	118.85	109.25
2	A	401	TYD	C5-C6-N1	-4.07	118.89	123.31
4	B	402	GLC	O3-C3-C4	-4.03	100.87	110.38
4	B	402	GLC	O3-C3-C2	-3.86	101.28	110.38
2	B	401	TYD	O3B-PB-O2B	3.84	122.21	107.80
2	A	401	TYD	O3B-PB-O3A	-3.68	92.28	104.64
2	B	401	TYD	O3A-PB-O1B	-3.60	92.09	111.04
2	B	401	TYD	C5-C4-N3	3.49	118.35	115.32
2	B	401	TYD	O3A-PA-O1A	2.98	119.65	110.70
4	B	402	GLC	C1-O5-C5	2.90	119.27	113.65
2	B	401	TYD	O2-C2-N1	-2.76	119.20	122.80
2	A	401	TYD	O3B-PB-O1B	2.69	121.33	110.83
2	A	401	TYD	O2B-PB-O3A	2.66	113.56	104.64
2	B	401	TYD	O2A-PA-O3A	-2.63	100.17	107.27
2	A	401	TYD	O3'-C3'-C2'	-2.61	101.80	110.88
2	B	401	TYD	N3-C2-N1	2.35	117.95	114.89
2	A	401	TYD	C5M-C5-C4	2.33	121.27	118.78
2	B	401	TYD	O3B-PB-O3A	2.32	112.42	104.64
2	A	401	TYD	O3A-PA-O1A	-2.29	103.82	110.70
2	B	401	TYD	O2B-PB-O1B	-2.26	102.03	110.83
2	B	401	TYD	C4-N3-C2	-2.25	124.39	127.34
2	A	401	TYD	O2-C2-N1	-2.22	119.91	122.80
2	B	401	TYD	O2B-PB-O3A	2.14	111.82	104.64
2	A	401	TYD	C2'-C1'-N1	2.01	118.84	113.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

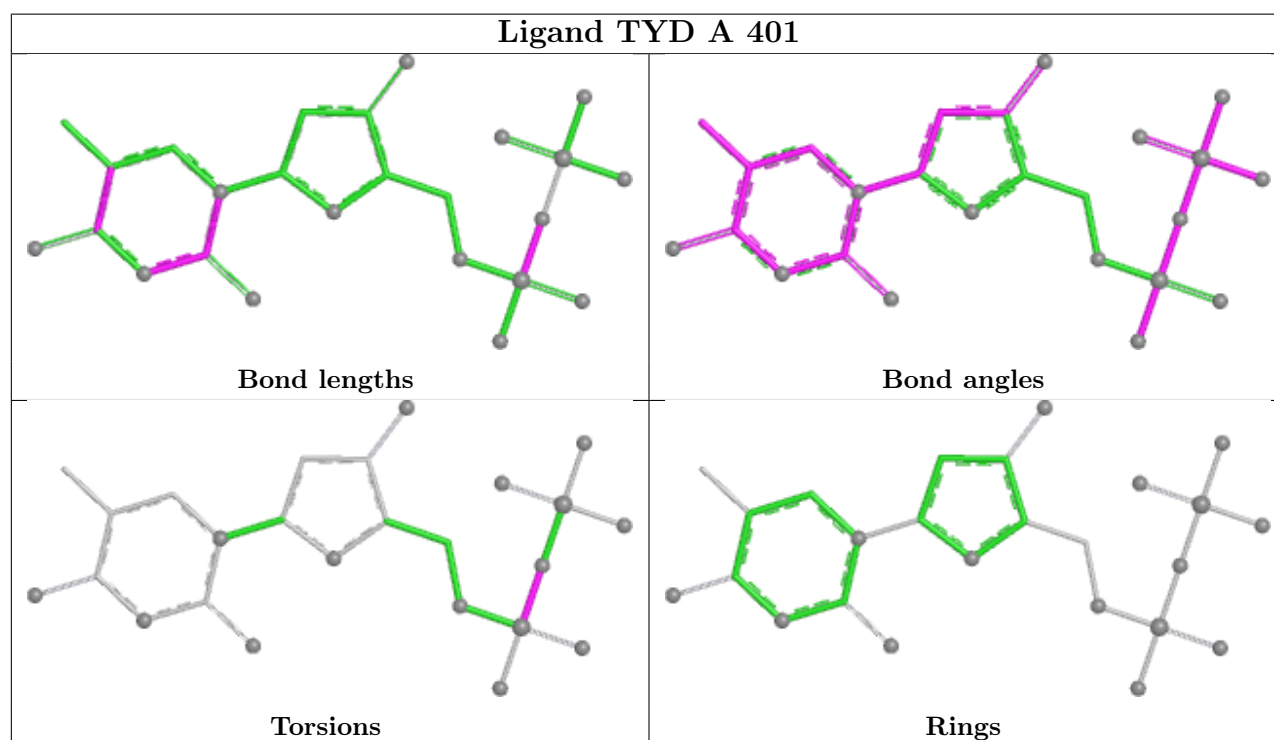
Mol	Chain	Res	Type	Atoms
2	B	401	TYD	PB-O3A-PA-O5'
4	B	402	GLC	O5-C5-C6-O6
4	B	402	GLC	C4-C5-C6-O6
2	A	401	TYD	PB-O3A-PA-O5'

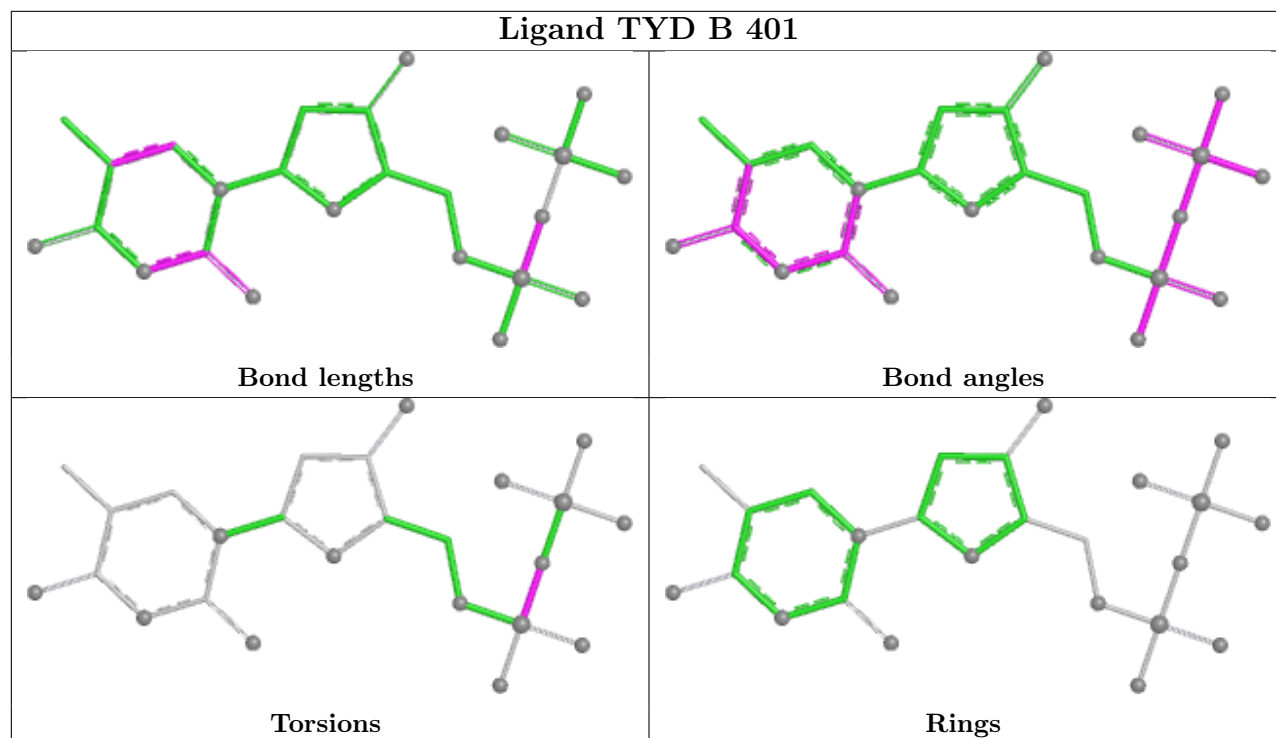
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TYD	10	0
2	B	401	TYD	2	0

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





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	372/387 (96%)	0.25	5 (1%) 75 79	11, 19, 35, 46	0
1	B	370/387 (95%)	0.37	10 (2%) 56 59	11, 20, 35, 56	0
All	All	742/774 (95%)	0.31	15 (2%) 65 68	11, 19, 35, 56	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	ALA	3.8
1	B	265	THR	3.1
1	B	69	ARG	3.0
1	B	380	ARG	2.9
1	B	175	GLU	2.8
1	A	10	TYR	2.8
1	A	267	LEU	2.5
1	A	227	MET	2.4
1	B	226	ARG	2.4
1	A	79	ASP	2.3
1	B	26	ALA	2.3
1	B	162	VAL	2.2
1	B	225	GLY	2.2
1	B	54	ARG	2.1
1	A	385	THR	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](#)

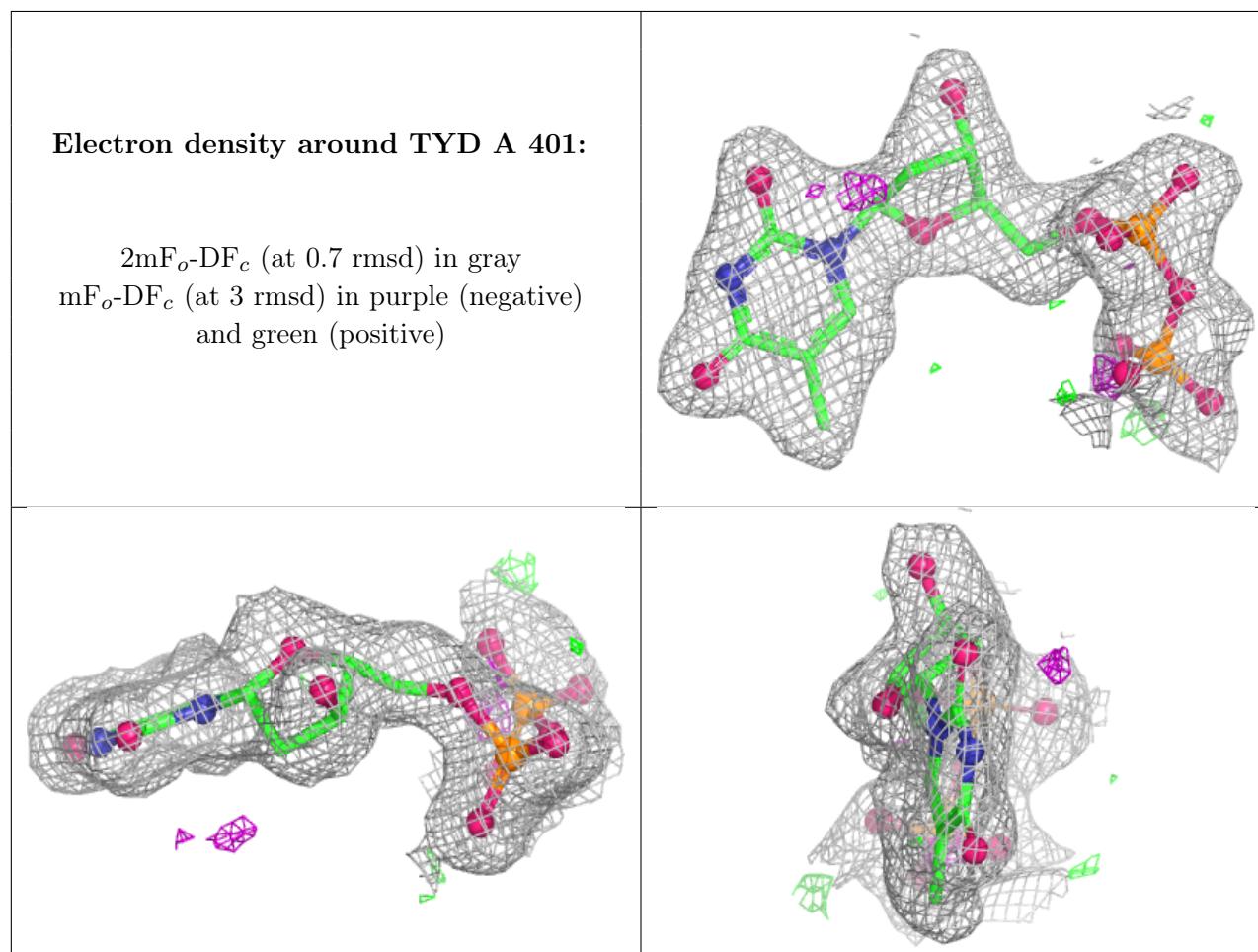
There are no oligosaccharides in this entry.

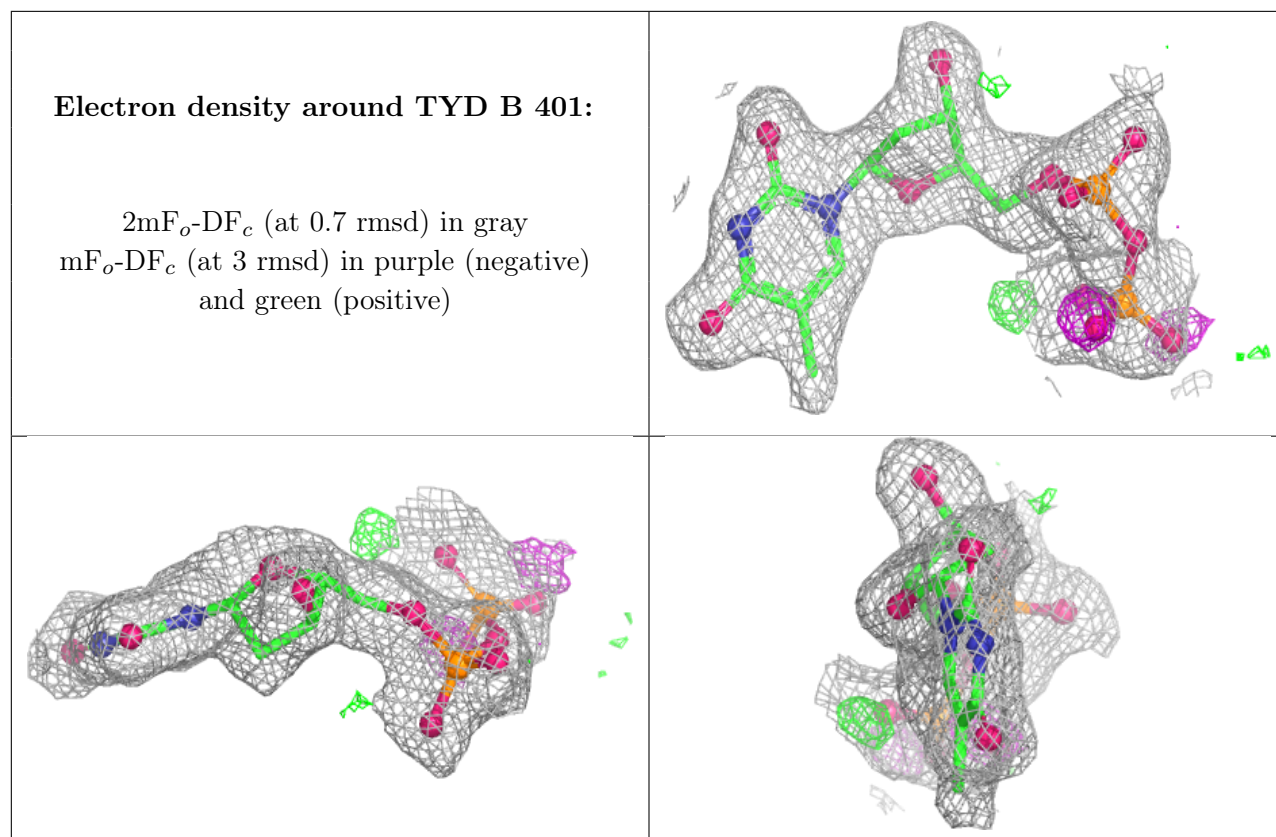
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	B	402	12/12	0.88	0.12	22,26,34,37	0
2	TYD	A	401	25/25	0.89	0.10	20,23,57,66	0
2	TYD	B	401	25/25	0.90	0.10	17,21,44,69	0
3	MG	B	403	1/1	0.94	0.19	451,451,451,451	0
3	MG	A	402	1/1	0.97	0.04	26,26,26,26	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.