



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:21 AM UTC

PDB ID : 8RZ3 / pdb_00008rz3
Title : Structures of Se- glycosyltransferase SenB from Variovorax paradoxus
Authors : Ma, Y.Y.; Gao, Y.; Xu, S.H.
Deposited on : 2024-02-12
Resolution : 2.15 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

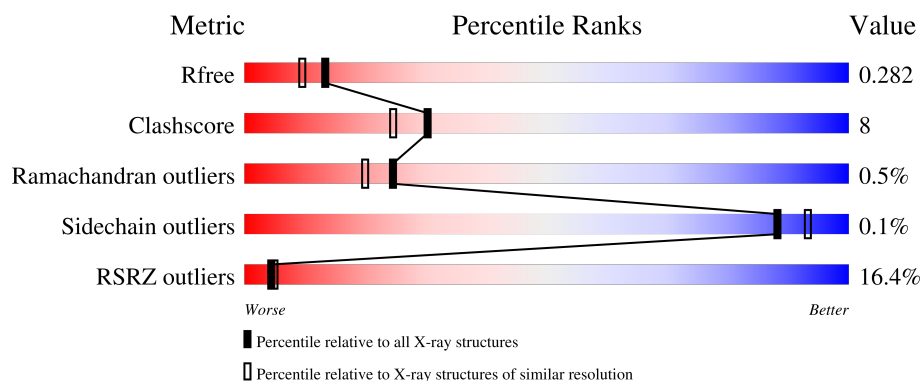
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	331	16% 79% 18% .
1	B	331	13% 85% 12% .
1	C	331	19% 85% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7536 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.

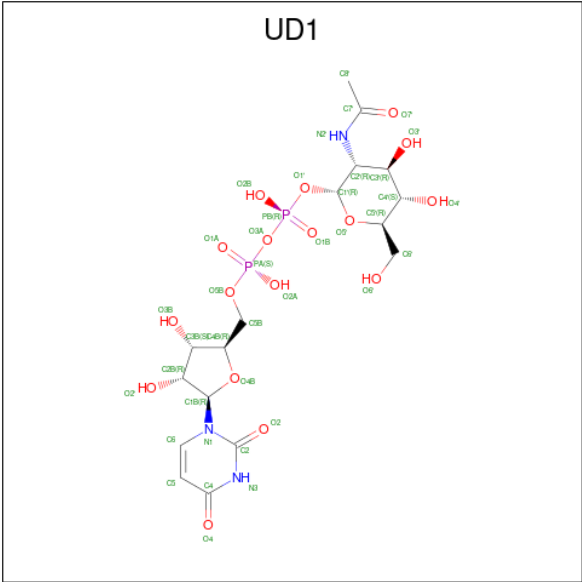
- Molecule 1 is a protein called TIGR04348 family glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2403	1493	464	436	10			
1	B	321	Total	C	N	O	S	0	0	0
			2402	1493	464	435	10			
1	C	325	Total	C	N	O	S	0	0	0
			2434	1510	472	442	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	VAL	ALA	conflict	UNP A0A952K6X5
A	47	ASP	GLY	conflict	UNP A0A952K6X5
A	134	SER	PRO	conflict	UNP A0A952K6X5
A	174	GLU	GLY	conflict	UNP A0A952K6X5
B	34	VAL	ALA	conflict	UNP A0A952K6X5
B	47	ASP	GLY	conflict	UNP A0A952K6X5
B	134	SER	PRO	conflict	UNP A0A952K6X5
B	174	GLU	GLY	conflict	UNP A0A952K6X5
C	34	VAL	ALA	conflict	UNP A0A952K6X5
C	47	ASP	GLY	conflict	UNP A0A952K6X5
C	134	SER	PRO	conflict	UNP A0A952K6X5
C	174	GLU	GLY	conflict	UNP A0A952K6X5

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

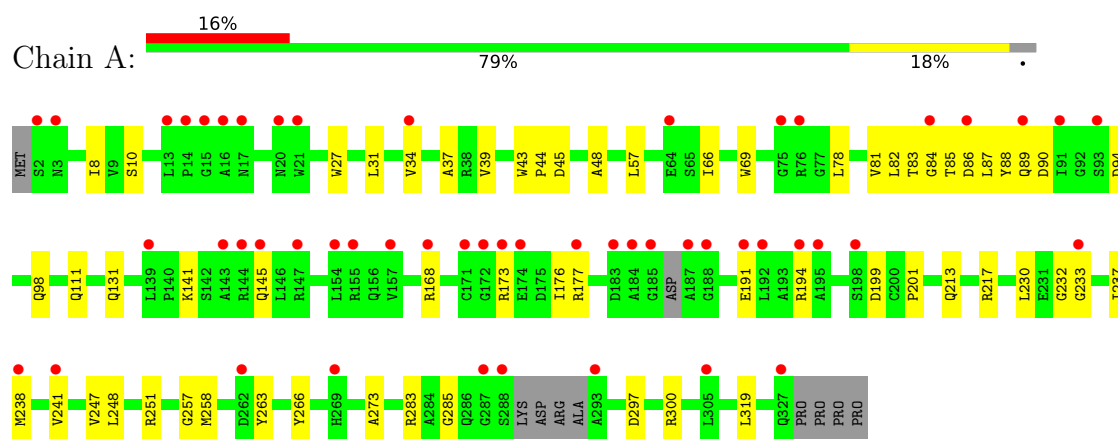
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	66	Total	O	0	0
			66	66		
3	C	52	Total	O	0	0
			52	52		

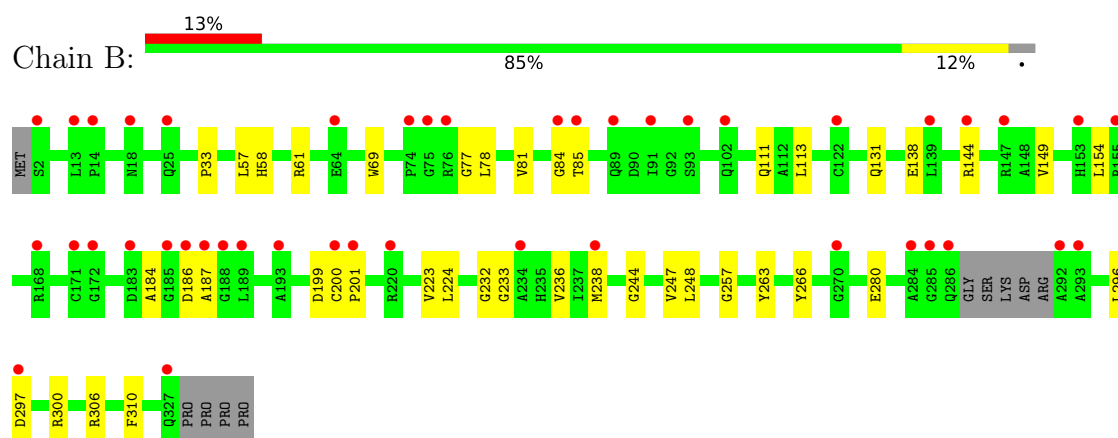
3 Residue-property plots [i](#)

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.

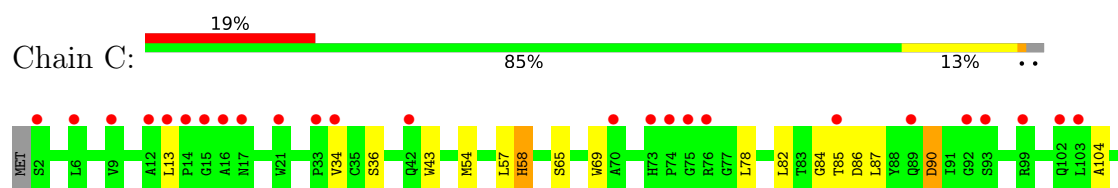
- Molecule 1: TIGR04348 family glycosyltransferase

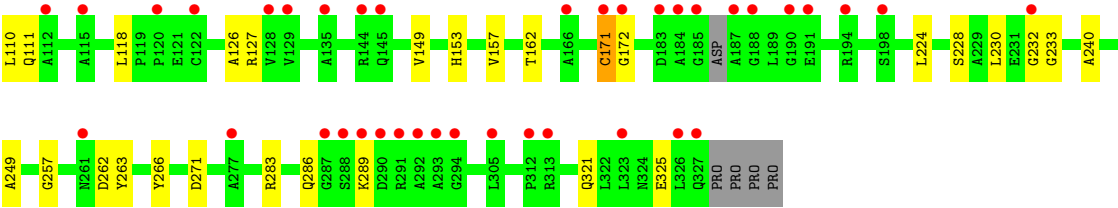


- Molecule 1: TIGR04348 family glycosyltransferase



- Molecule 1: TIGR04348 family glycosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 56.32Å 108.05Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	48.62 – 2.15 48.62 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.62-2.15) 99.5 (48.62-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.237 , 0.286 0.244 , 0.282	Depositor DCC
R_{free} test set	3883 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.000 for h,-k,-l 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7536	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: UD1

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	0.63	0/2448	0.70	3/3327 (0.1%)
1	B	0.57	0/2448	0.61	3/3330 (0.1%)
1	C	0.54	0/2479	0.65	4/3368 (0.1%)
All	All	0.58	0/7375	0.66	10/10025 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ASP	N-CA-C	7.91	120.80	111.71
1	C	90	ASP	N-CA-C	-6.21	106.24	113.88
1	C	228	SER	N-CA-C	6.04	118.80	110.35
1	C	36	SER	N-CA-C	-5.54	100.21	109.24
1	C	171	CYS	N-CA-C	5.42	122.35	110.80
1	B	199	ASP	CA-C-N	-5.42	115.87	122.64
1	B	199	ASP	C-N-CA	-5.42	115.87	122.64
1	A	34	VAL	N-CA-C	5.15	117.84	112.90
1	B	77	GLY	N-CA-C	5.13	125.35	113.18
1	A	37	ALA	N-CA-C	5.05	117.64	109.40

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	2403	0	2413	57	0
1	B	2402	0	2411	40	0
1	C	2434	0	2443	38	0
2	A	39	0	24	4	0
2	B	39	0	24	6	0
2	C	39	0	24	4	0
3	A	62	0	0	3	0
3	B	66	0	0	3	0
3	C	52	0	0	4	0
All	All	7536	0	7339	124	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 8.

All (124) 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:273:ALA:CB	1:C:289:LYS:HE3	1.72	1.20
2:B:401:UD1:O4B	2:B:401:UD1:C4B	1.65	1.20
2:A:401:UD1:O4B	2:A:401:UD1:C4B	1.65	1.16
2:C:401:UD1:O4B	2:C:401:UD1:C4B	1.65	1.15
1:A:201:PRO:HG3	1:B:144:ARG:CD	1.78	1.13
1:A:201:PRO:HG3	1:B:144:ARG:HD2	1.27	1.11
1:A:173:ARG:HE	1:A:176:ILE:HD12	1.09	1.07
1:A:201:PRO:HG3	1:B:144:ARG:NE	1.77	0.98
1:A:273:ALA:HB1	1:C:289:LYS:HE3	1.43	0.96
1:A:131:GLN:HB2	1:A:238:MET:HE1	1.50	0.94
1:B:186:ASP:OD1	1:B:187:ALA:N	2.01	0.92
1:A:111:GLN:HG3	1:A:257:GLY:HA3	1.51	0.92
1:A:273:ALA:HB1	1:C:289:LYS:CE	2.01	0.91
1:A:173:ARG:NE	1:A:176:ILE:HD12	1.86	0.89
1:B:111:GLN:HG3	1:B:257:GLY:HA3	1.59	0.84
1:B:85:THR:HG22	3:B:518:HOH:O	1.77	0.83
1:B:58:HIS:HE2	1:B:85:THR:HG23	1.45	0.80
1:B:238:MET:HG3	1:B:310:PHE:CG	2.16	0.80
1:A:201:PRO:HG3	1:B:144:ARG:HE	1.47	0.80
1:A:201:PRO:CG	1:B:144:ARG:HE	1.94	0.80
1:A:273:ALA:CB	1:C:289:LYS:CE	2.57	0.79
1:A:85:THR:HG22	1:A:230:LEU:HD11	1.63	0.78
1:C:162:THR:HG21	3:C:502:HOH:O	1.84	0.77
1:C:149:VAL:O	1:C:224:LEU:HD12	1.86	0.76
1:A:86:ASP:OD1	1:A:87:LEU:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PRO:CG	1:B:144:ARG:NE	2.48	0.75
1:B:138:GLU:HG3	1:B:244:GLY:HA3	1.69	0.74
1:A:273:ALA:HB2	1:C:289:LYS:HE3	1.68	0.74
1:A:201:PRO:CG	1:B:144:ARG:HD2	2.14	0.72
1:A:85:THR:O	1:A:89:GLN:HB3	1.96	0.66
1:B:186:ASP:CG	1:B:187:ALA:H	1.99	0.66
1:A:191:GLU:HG3	1:A:194:ARG:HH12	1.60	0.64
1:A:145:GLN:OE1	1:A:177:ARG:CZ	2.46	0.64
1:C:157:VAL:CG2	1:C:230:LEU:HG	2.28	0.64
1:A:173:ARG:HH21	1:A:283:ARG:HG2	1.63	0.63
1:B:57:LEU:HD23	1:B:81:VAL:HB	1.80	0.63
1:C:78:LEU:HD23	1:C:104:ALA:HA	1.78	0.63
1:A:173:ARG:HE	1:A:176:ILE:CD1	1.99	0.61
1:A:232:GLY:H	2:A:401:UD1:H8'2	1.64	0.60
1:B:297:ASP:OD1	1:B:300:ARG:NH2	2.36	0.58
1:A:94:ASP:O	1:A:98:GLN:HG3	2.04	0.58
1:C:111:GLN:HG3	1:C:257:GLY:HA3	1.84	0.58
1:A:82:LEU:HA	1:A:86:ASP:OD2	2.04	0.58
1:C:86:ASP:HA	1:C:90:ASP:HB2	1.86	0.58
1:B:58:HIS:NE2	1:B:85:THR:HG23	2.16	0.57
1:C:232:GLY:H	2:C:401:UD1:H8'2	1.69	0.57
1:A:84:GLY:HA3	2:A:401:UD1:C8'	2.36	0.56
2:C:401:UD1:O4B	2:C:401:UD1:C5B	2.50	0.56
1:A:238:MET:HE2	1:A:258:MET:HE1	1.87	0.56
1:A:273:ALA:HB1	1:C:289:LYS:HE2	1.85	0.56
1:A:82:LEU:HD23	1:A:86:ASP:OD2	2.05	0.55
1:A:57:LEU:HD23	1:A:81:VAL:HB	1.87	0.55
1:B:131:GLN:HG3	3:B:519:HOH:O	2.08	0.54
1:A:201:PRO:HG2	1:B:144:ARG:HE	1.70	0.54
1:A:168:ARG:NH2	1:A:199:ASP:OD2	2.42	0.53
1:A:217:ARG:HD3	3:A:511:HOH:O	2.08	0.53
1:A:141:LYS:NZ	3:A:504:HOH:O	2.42	0.53
1:C:58:HIS:HE2	1:C:85:THR:HG1	1.56	0.53
1:B:186:ASP:CG	1:B:187:ALA:N	2.61	0.51
1:C:249:ALA:O	1:C:266:TYR:HA	2.11	0.51
1:C:126:ALA:O	1:C:127:ARG:HD3	2.11	0.50
1:B:232:GLY:H	2:B:401:UD1:H8'2	1.76	0.50
1:C:82:LEU:HA	1:C:86:ASP:OD2	2.12	0.50
1:C:157:VAL:HG22	1:C:230:LEU:HG	1.94	0.50
1:C:110:LEU:HB2	1:C:232:GLY:O	2.12	0.49
2:B:401:UD1:O4B	2:B:401:UD1:C5B	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:VAL:O	1:C:34:VAL:HG22	2.13	0.49
1:B:58:HIS:CE1	1:B:61:ARG:HG3	2.47	0.49
1:A:297:ASP:OD1	1:A:300:ARG:NH1	2.46	0.48
1:C:263:TYR:HB3	1:C:266:TYR:CE2	2.49	0.48
1:C:262:ASP:OD1	1:C:262:ASP:N	2.45	0.48
1:C:82:LEU:HB3	1:C:87:LEU:HB2	1.95	0.47
1:B:263:TYR:HB3	1:B:266:TYR:CE2	2.49	0.47
1:A:87:LEU:HD23	1:A:88:TYR:CE2	2.50	0.46
1:B:238:MET:HG3	1:B:310:PHE:CB	2.45	0.46
1:B:149:VAL:HG13	1:B:224:LEU:HD12	1.98	0.45
1:A:173:ARG:NH2	1:A:283:ARG:HG2	2.30	0.45
1:B:200:CYS:HA	1:B:201:PRO:HD2	1.72	0.45
1:C:84:GLY:HA3	2:C:401:UD1:C8'	2.45	0.45
1:B:111:GLN:HG2	1:B:113:LEU:H	1.80	0.45
1:C:82:LEU:CD1	1:C:118:LEU:HD21	2.46	0.45
1:C:321:GLN:O	1:C:325:GLU:HG3	2.17	0.45
1:A:69:TRP:CD1	1:A:78:LEU:HB2	2.52	0.44
1:A:45:ASP:H	1:A:48:ALA:HB2	1.81	0.44
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.85	0.44
1:C:224:LEU:HD22	1:C:240:ALA:HB2	1.98	0.44
1:C:86:ASP:N	1:C:86:ASP:OD1	2.50	0.44
1:A:66:ILE:HG23	1:A:78:LEU:HD21	1.99	0.44
1:A:285:GLY:HA3	3:A:542:HOH:O	2.16	0.44
1:B:223:VAL:HG21	1:B:248:LEU:HG	1.99	0.44
1:B:280:GLU:CD	3:B:505:HOH:O	2.61	0.43
1:A:8:ILE:HB	1:A:39:VAL:HG22	2.01	0.43
1:B:236:VAL:HG13	2:B:401:UD1:O2A	2.19	0.43
1:C:43:TRP:N	1:C:65:SER:OG	2.41	0.43
1:C:172:GLY:HA3	3:C:535:HOH:O	2.19	0.42
1:C:283:ARG:HD2	1:C:286:GLN:OE1	2.19	0.42
1:C:54:MET:HE3	1:C:69:TRP:CE3	2.55	0.42
1:A:82:LEU:HD13	1:A:87:LEU:HD13	2.01	0.42
1:A:83:THR:HG22	2:A:401:UD1:H6'1	2.01	0.42
1:C:153:HIS:HD2	3:C:512:HOH:O	2.02	0.42
1:A:10:SER:HB2	1:A:57:LEU:HD12	2.01	0.42
1:B:84:GLY:HA3	2:B:401:UD1:C8'	2.50	0.42
1:B:33:PRO:HG3	1:C:271:ASP:HA	2.00	0.41
1:A:27:TRP:CD1	1:A:319:LEU:HD11	2.56	0.41
1:A:201:PRO:CG	1:B:144:ARG:CD	2.72	0.41
1:B:154:LEU:HD12	1:B:184:ALA:HA	2.02	0.41
1:A:145:GLN:OE1	1:A:177:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:HG12	1:A:248:LEU:N	2.36	0.41
1:A:263:TYR:HB3	1:A:266:TYR:CE2	2.56	0.41
1:A:213:GLN:O	1:A:217:ARG:HG3	2.21	0.41
1:B:69:TRP:CD1	1:B:78:LEU:HB2	2.56	0.41
1:C:111:GLN:CG	1:C:257:GLY:HA3	2.50	0.41
1:B:224:LEU:O	1:B:247:VAL:HA	2.20	0.41
1:A:43:TRP:CG	1:A:44:PRO:HA	2.56	0.40
1:A:145:GLN:HE22	1:A:177:ARG:NE	2.20	0.40
1:B:57:LEU:CD2	1:B:81:VAL:HB	2.50	0.40
1:C:162:THR:CB	3:C:502:HOH:O	2.68	0.40
1:C:13:LEU:H	1:C:13:LEU:HD12	1.86	0.40
1:A:237:ILE:O	1:A:241:VAL:HG23	2.21	0.40
1:B:306:ARG:HA	1:B:306:ARG:HD2	1.89	0.40
1:A:31:LEU:HD21	1:A:319:LEU:HB3	2.03	0.40
1:A:251:ARG:NH1	1:A:266:TYR:HD2	2.19	0.40
1:B:84:GLY:HA3	2:B:401:UD1:H8'2	2.01	0.40
1:C:34:VAL:O	1:C:34:VAL:CG2	2.69	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	315/331 (95%)	305 (97%)	9 (3%)	1 (0%)	36	34
1	B	317/331 (96%)	310 (98%)	6 (2%)	1 (0%)	36	34
1	C	321/331 (97%)	308 (96%)	10 (3%)	3 (1%)	14	9
All	All	953/993 (96%)	923 (97%)	25 (3%)	5 (0%)	24	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	171	CYS
1	B	233	GLY
1	C	58	HIS
1	C	233	GLY
1	A	233	GLY

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	241/250 (96%)	241 (100%)	0	100	100
1	B	240/250 (96%)	240 (100%)	0	100	100
1	C	243/250 (97%)	242 (100%)	1 (0%)	84	89
All	All	724/750 (96%)	723 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	25	GLN
1	B	73	HIS
1	B	211	HIS
1	C	261	ASN
1	C	327	GLN

5.3.3 RNA [i](#)

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](#)

3 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	UD1	C	401	-	40,41,41	3.98	19 (47%)	59,62,62	1.62	13 (22%)
2	UD1	A	401	-	40,41,41	3.86	20 (50%)	59,62,62	1.35	4 (6%)
2	UD1	B	401	-	40,41,41	3.97	19 (47%)	59,62,62	1.51	9 (15%)

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	UD1	C	401	-	-	9/26/63/63	0/3/3/3
2	UD1	A	401	-	-	8/26/63/63	0/3/3/3
2	UD1	B	401	-	-	9/26/63/63	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	UD1	C2-N3	10.20	1.55	1.38
2	A	401	UD1	C2-N3	9.66	1.54	1.38
2	C	401	UD1	C2-N3	9.49	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	UD1	O4B-C4B	9.33	1.65	1.45
2	B	401	UD1	C3B-C4B	-9.26	1.29	1.53
2	C	401	UD1	C3B-C4B	-9.26	1.29	1.53
2	A	401	UD1	O4B-C4B	9.25	1.65	1.45
2	A	401	UD1	C3B-C4B	-9.17	1.29	1.53
2	B	401	UD1	O4B-C4B	9.16	1.65	1.45
2	C	401	UD1	PA-O3A	9.15	1.69	1.59
2	C	401	UD1	C2-N1	8.04	1.51	1.38
2	B	401	UD1	C2-N1	7.75	1.50	1.38
2	B	401	UD1	PA-O3A	7.75	1.67	1.59
2	A	401	UD1	C2-N1	7.62	1.50	1.38
2	C	401	UD1	PB-O3A	7.60	1.67	1.59
2	A	401	UD1	PA-O3A	7.33	1.67	1.59
2	B	401	UD1	PB-O3A	7.18	1.67	1.59
2	A	401	UD1	PB-O3A	6.73	1.66	1.59
2	B	401	UD1	O4B-C1B	-5.50	1.29	1.42
2	A	401	UD1	O4B-C1B	-5.14	1.30	1.42
2	B	401	UD1	C6-C5	4.97	1.46	1.35
2	A	401	UD1	C6-C5	4.92	1.46	1.35
2	C	401	UD1	O4B-C1B	-4.81	1.30	1.42
2	C	401	UD1	C6-C5	4.68	1.45	1.35
2	B	401	UD1	C4-N3	4.10	1.45	1.38
2	A	401	UD1	C7'-N2'	3.97	1.47	1.34
2	C	401	UD1	O4-C4	-3.89	1.16	1.24
2	B	401	UD1	C7'-N2'	3.75	1.46	1.34
2	B	401	UD1	O2'-C2B	-3.66	1.33	1.43
2	A	401	UD1	C4-N3	3.64	1.44	1.38
2	C	401	UD1	O2'-C2B	-3.64	1.34	1.43
2	A	401	UD1	O2'-C2B	-3.56	1.34	1.43
2	A	401	UD1	O4-C4	-3.48	1.17	1.24
2	C	401	UD1	C7'-N2'	3.45	1.45	1.34
2	C	401	UD1	C4-N3	3.36	1.44	1.38
2	A	401	UD1	C6-N1	3.36	1.46	1.38
2	A	401	UD1	PB-O1'	3.35	1.69	1.59
2	B	401	UD1	C6-N1	3.28	1.45	1.38
2	B	401	UD1	O4-C4	-3.27	1.18	1.24
2	C	401	UD1	C6-N1	3.25	1.45	1.38
2	C	401	UD1	PB-O1'	3.20	1.69	1.59
2	B	401	UD1	O2-C2	-3.12	1.17	1.23
2	B	401	UD1	PB-O1'	2.94	1.68	1.59
2	A	401	UD1	C2'-N2'	2.82	1.50	1.45
2	C	401	UD1	C2'-N2'	2.45	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	UD1	O3B-C3B	2.33	1.48	1.43
2	C	401	UD1	O3B-C3B	2.26	1.48	1.43
2	C	401	UD1	O5'-C5'	2.26	1.49	1.44
2	C	401	UD1	O2-C2	-2.23	1.19	1.23
2	B	401	UD1	O5'-C5'	2.22	1.49	1.44
2	C	401	UD1	O7'-C7'	-2.19	1.18	1.23
2	A	401	UD1	O2-C2	-2.19	1.19	1.23
2	A	401	UD1	C4'-C3'	-2.18	1.46	1.52
2	B	401	UD1	O7'-C7'	-2.07	1.18	1.23
2	A	401	UD1	O3B-C3B	2.07	1.48	1.43
2	B	401	UD1	C2'-N2'	2.04	1.49	1.45
2	A	401	UD1	C8'-C7'	2.02	1.54	1.50
2	A	401	UD1	C3'-C2'	-2.01	1.49	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	UD1	C5-C4-N3	5.06	121.89	114.80
2	A	401	UD1	C5-C4-N3	4.64	121.31	114.80
2	B	401	UD1	C4-N3-C2	-4.58	120.93	126.61
2	B	401	UD1	C5-C4-N3	4.28	120.80	114.80
2	C	401	UD1	C4-N3-C2	-4.15	121.47	126.61
2	A	401	UD1	C4-N3-C2	-3.95	121.72	126.61
2	C	401	UD1	C1'-C2'-N2'	-3.65	104.79	110.92
2	B	401	UD1	C1'-C2'-N2'	-3.53	105.00	110.92
2	B	401	UD1	O4-C4-C5	-3.28	119.50	125.16
2	C	401	UD1	C2'-N2'-C7'	-3.27	115.46	123.11
2	C	401	UD1	O4-C4-C5	-3.20	119.65	125.16
2	C	401	UD1	O5'-C1'-C2'	-3.17	104.60	110.59
2	A	401	UD1	O4-C4-C5	-3.14	119.75	125.16
2	B	401	UD1	O5'-C1'-O1'	-2.95	107.51	111.36
2	C	401	UD1	C3'-C2'-N2'	2.53	115.28	110.62
2	B	401	UD1	O2-C2-N1	-2.31	119.79	122.80
2	B	401	UD1	O2-C2-N3	2.18	125.50	121.49
2	C	401	UD1	O5'-C1'-O1'	-2.14	108.57	111.36
2	B	401	UD1	C8'-C7'-N2'	2.11	119.62	116.12
2	C	401	UD1	O3B-C3B-C2B	-2.06	105.23	111.82
2	A	401	UD1	O5'-C1'-C2'	-2.05	106.72	110.59
2	C	401	UD1	C3'-C4'-C5'	2.05	113.95	110.23
2	B	401	UD1	O5'-C1'-C2'	-2.05	106.73	110.59
2	C	401	UD1	O1'-C1'-C2'	2.04	112.09	108.40
2	C	401	UD1	C2B-C3B-C4B	2.02	106.52	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	UD1	C6-N1-C2	2.02	123.45	121.00

There are no chirality outliers.

All (26) torsion outliers are listed below:

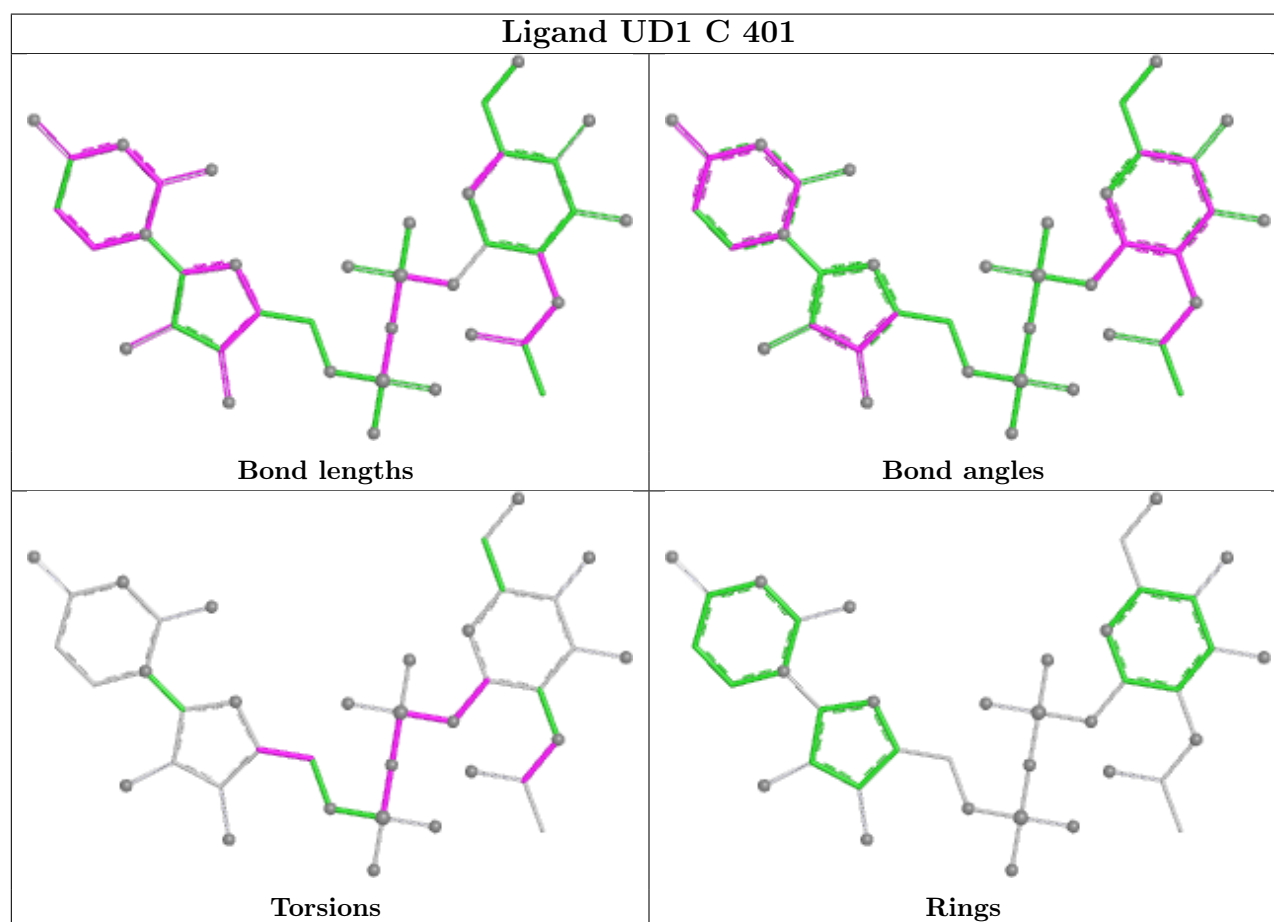
Mol	Chain	Res	Type	Atoms
2	A	401	UD1	O5'-C1'-O1'-PB
2	A	401	UD1	C1'-O1'-PB-O3A
2	B	401	UD1	O5'-C1'-O1'-PB
2	B	401	UD1	C1'-O1'-PB-O3A
2	B	401	UD1	C1'-O1'-PB-O2B
2	C	401	UD1	O5'-C1'-O1'-PB
2	C	401	UD1	C1'-O1'-PB-O3A
2	C	401	UD1	C1'-O1'-PB-O2B
2	C	401	UD1	PB-O3A-PA-O5B
2	C	401	UD1	PA-O3A-PB-O1'
2	A	401	UD1	C8'-C7'-N2'-C2'
2	A	401	UD1	O7'-C7'-N2'-C2'
2	B	401	UD1	C8'-C7'-N2'-C2'
2	B	401	UD1	O7'-C7'-N2'-C2'
2	C	401	UD1	C8'-C7'-N2'-C2'
2	C	401	UD1	O7'-C7'-N2'-C2'
2	C	401	UD1	C3B-C4B-C5B-O5B
2	C	401	UD1	O4B-C4B-C5B-O5B
2	A	401	UD1	C3B-C4B-C5B-O5B
2	A	401	UD1	O4B-C4B-C5B-O5B
2	A	401	UD1	PA-O3A-PB-O1'
2	B	401	UD1	PB-O3A-PA-O5B
2	B	401	UD1	PA-O3A-PB-O1'
2	B	401	UD1	C3B-C4B-C5B-O5B
2	A	401	UD1	C1'-O1'-PB-O2B
2	B	401	UD1	O4B-C4B-C5B-O5B

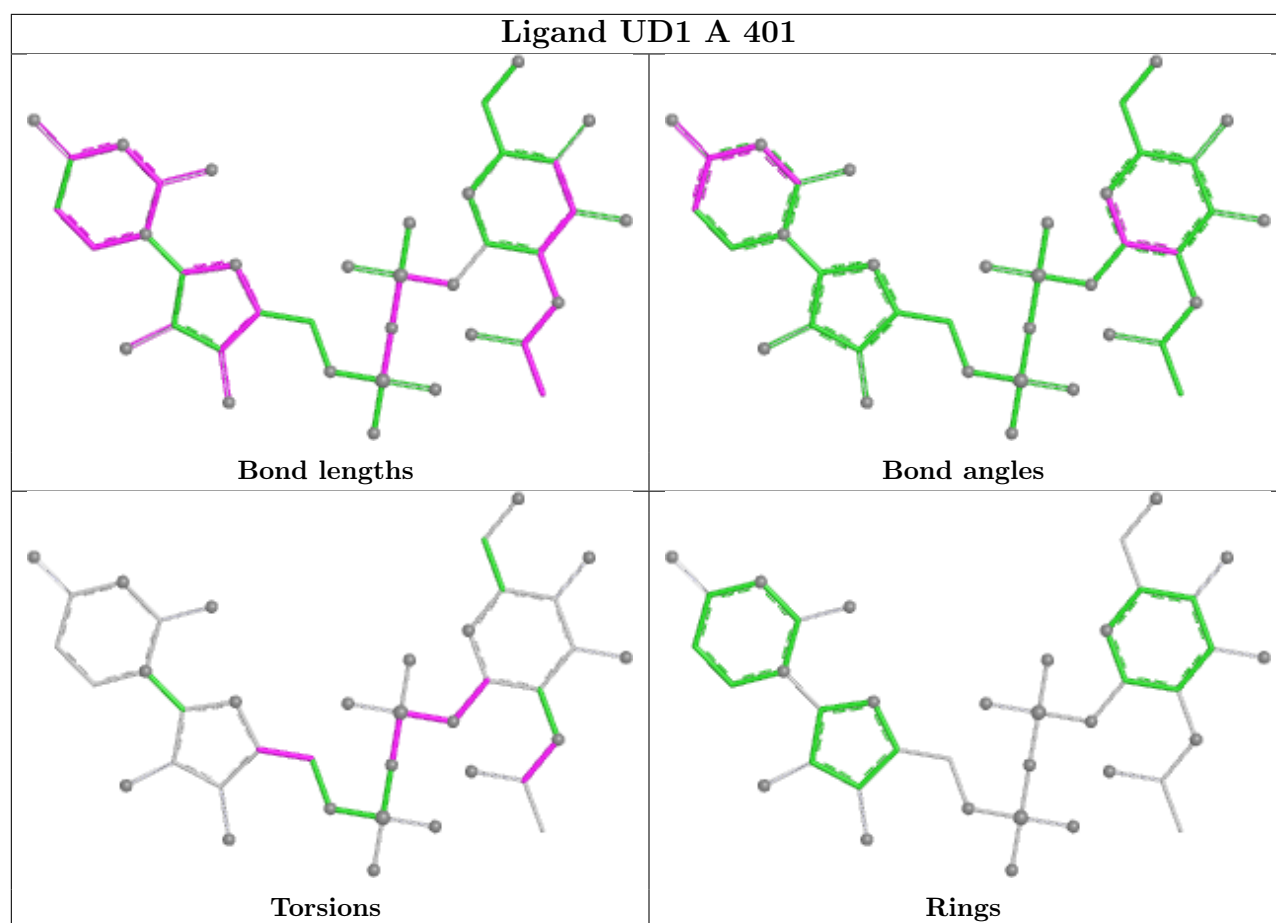
There are no ring outliers.

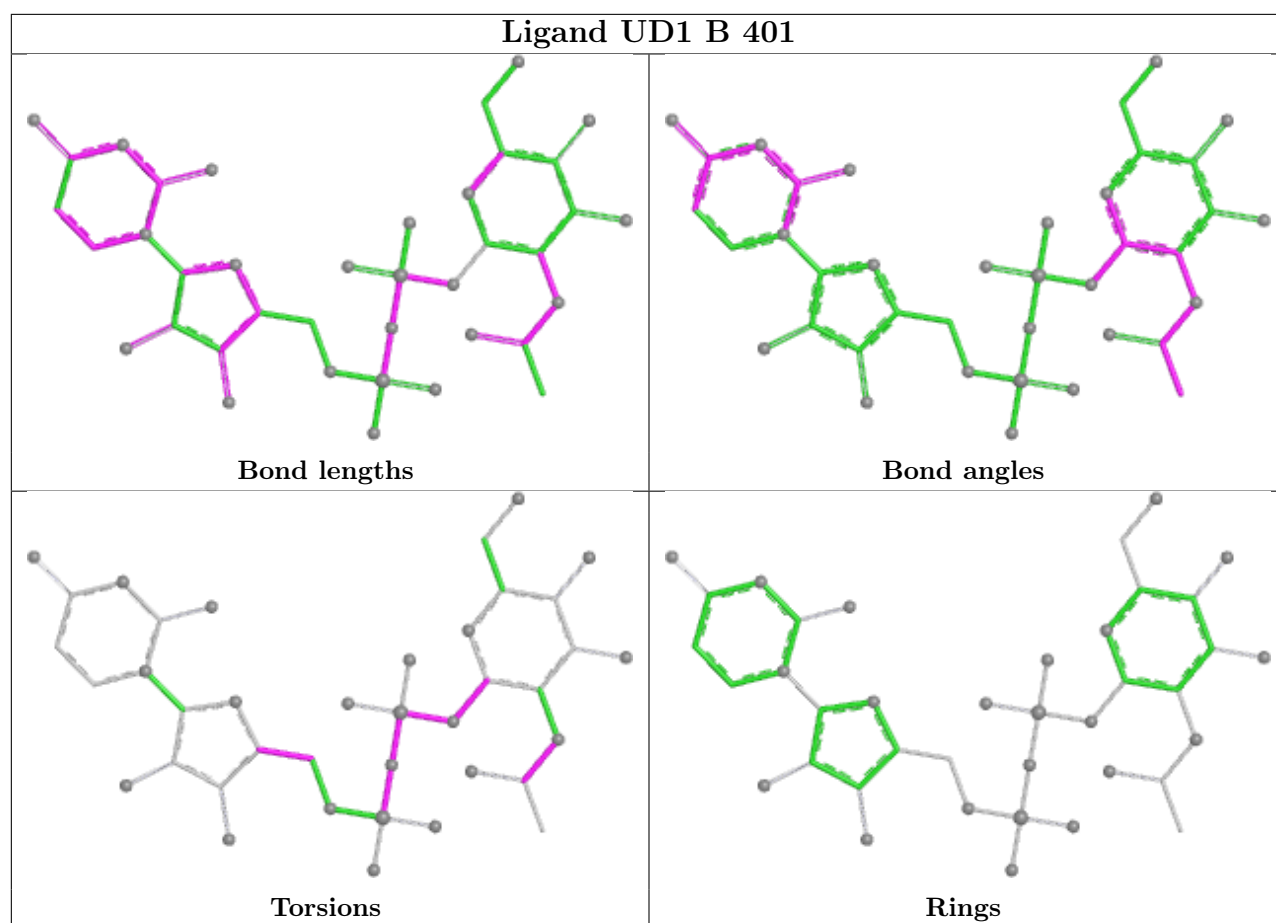
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	UD1	4	0
2	A	401	UD1	4	0
2	B	401	UD1	6	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 ⓘ

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	321/331 (96%)	1.27	52 (16%) 4 5	30, 45, 61, 79	0
1	B	321/331 (96%)	1.09	44 (13%) 6 7	30, 43, 58, 77	0
1	C	325/331 (98%)	1.31	63 (19%) 3 4	30, 46, 61, 90	0
All	All	967/993 (97%)	1.22	159 (16%) 4 5	30, 45, 60, 90	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	GLY	6.7
1	A	187	ALA	6.3
1	A	293	ALA	5.6
1	A	13	LEU	5.5
1	B	292	ALA	5.4
1	C	187	ALA	5.2
1	C	185	GLY	5.2
1	A	171	CYS	5.2
1	C	13	LEU	5.2
1	B	144	ARG	5.0
1	C	42	GLN	4.8
1	C	292	ALA	4.8
1	C	289	LYS	4.6
1	B	293	ALA	4.5
1	A	144	ARG	4.3
1	C	184	ALA	4.3
1	A	288	SER	4.3
1	B	186	ASP	4.2
1	A	89	GLN	4.2
1	A	173	ARG	4.2
1	C	73	HIS	4.2
1	C	172	GLY	4.1
1	A	184	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	16	ALA	4.0
1	B	200	CYS	3.9
1	A	327	GLN	3.9
1	B	168	ARG	3.8
1	C	14	PRO	3.8
1	B	25	GLN	3.8
1	C	15	GLY	3.8
1	C	171	CYS	3.7
1	A	86	ASP	3.6
1	A	177	ARG	3.5
1	A	14	PRO	3.5
1	C	291	ARG	3.5
1	C	305	LEU	3.4
1	C	21	TRP	3.4
1	B	139	LEU	3.4
1	B	188	GLY	3.3
1	C	198	SER	3.2
1	B	187	ALA	3.2
1	A	76	ARG	3.2
1	C	293	ALA	3.2
1	A	195	ALA	3.1
1	A	287	GLY	3.1
1	B	2	SER	3.1
1	A	3	ASN	3.1
1	C	102	GLN	3.0
1	A	192	LEU	3.0
1	B	64	GLU	3.0
1	C	145	GLN	3.0
1	A	2	SER	3.0
1	B	238	MET	3.0
1	A	155	ARG	2.9
1	C	294	GLY	2.9
1	C	290	ASP	2.9
1	B	185	GLY	2.9
1	A	21	TRP	2.9
1	A	34	VAL	2.9
1	C	183	ASP	2.9
1	A	93	SER	2.9
1	A	15	GLY	2.9
1	A	147	ARG	2.8
1	B	327	GLN	2.8
1	B	171	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	288	SER	2.8
1	B	85	THR	2.8
1	C	34	VAL	2.8
1	C	76	ARG	2.8
1	A	188	GLY	2.8
1	B	13	LEU	2.8
1	A	174	GLU	2.7
1	C	12	ALA	2.7
1	A	191	GLU	2.7
1	C	188	GLY	2.7
1	A	143	ALA	2.7
1	B	89	GLN	2.7
1	B	285	GLY	2.7
1	B	284	ALA	2.6
1	A	139	LEU	2.6
1	A	194	ARG	2.6
1	B	270	GLY	2.6
1	C	99	ARG	2.6
1	B	91	ILE	2.6
1	C	9	VAL	2.6
1	A	84	GLY	2.6
1	C	122	CYS	2.5
1	A	168	ARG	2.5
1	A	183	ASP	2.5
1	C	89	GLN	2.5
1	C	129	VAL	2.5
1	B	297	ASP	2.5
1	B	93	SER	2.5
1	C	85	THR	2.5
1	A	145	GLN	2.4
1	C	327	GLN	2.4
1	A	157	VAL	2.4
1	C	2	SER	2.4
1	C	70	ALA	2.4
1	B	189	LEU	2.4
1	B	76	ARG	2.4
1	C	191	GLU	2.4
1	C	166	ALA	2.3
1	A	154	LEU	2.3
1	A	198	SER	2.3
1	A	305	LEU	2.3
1	C	287	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	183	ASP	2.3
1	A	20	ASN	2.3
1	B	122	CYS	2.3
1	C	16	ALA	2.3
1	C	144	ARG	2.3
1	C	313	ARG	2.3
1	B	201	PRO	2.2
1	C	33	PRO	2.2
1	A	262	ASP	2.2
1	C	323	LEU	2.2
1	B	155	ARG	2.2
1	A	17	ASN	2.2
1	B	153	HIS	2.2
1	B	18	ASN	2.2
1	C	312	PRO	2.2
1	B	84	GLY	2.2
1	C	326	LEU	2.2
1	C	93	SER	2.2
1	C	261	ASN	2.2
1	B	74	PRO	2.1
1	C	120	PRO	2.1
1	B	75	GLY	2.1
1	B	172	GLY	2.1
1	A	64	GLU	2.1
1	A	172	GLY	2.1
1	C	92	GLY	2.1
1	C	232	GLY	2.1
1	C	194	ARG	2.1
1	C	277	ALA	2.1
1	B	14	PRO	2.1
1	A	269	HIS	2.1
1	A	233	GLY	2.1
1	C	190	GLY	2.1
1	C	6	LEU	2.1
1	B	102	GLN	2.1
1	B	147	ARG	2.1
1	A	75	GLY	2.1
1	A	91	ILE	2.1
1	C	128	VAL	2.1
1	B	193	ALA	2.1
1	C	115	ALA	2.1
1	C	135	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	238	MET	2.0
1	C	103	LEU	2.0
1	C	74	PRO	2.0
1	A	241	VAL	2.0
1	B	234	ALA	2.0
1	C	112	ALA	2.0
1	C	17	ASN	2.0
1	B	286	GLN	2.0
1	B	220	ARG	2.0
1	C	75	GLY	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](#)

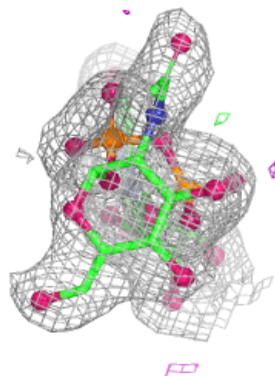
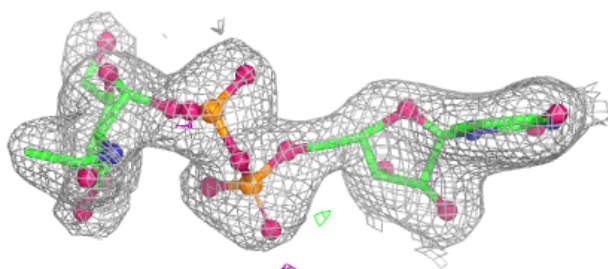
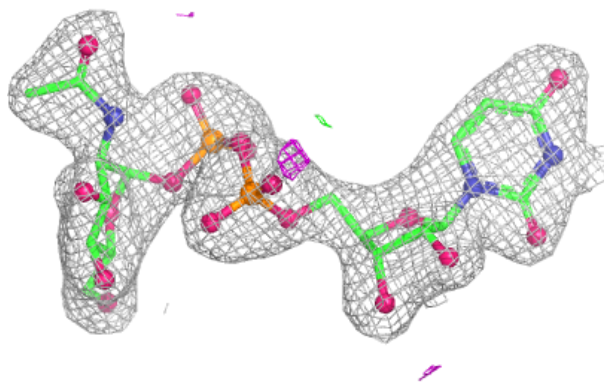
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	UD1	A	401	39/39	0.94	0.11	43,49,56,58	0
2	UD1	C	401	39/39	0.94	0.11	44,48,52,54	0
2	UD1	B	401	39/39	0.95	0.10	42,46,51,52	0

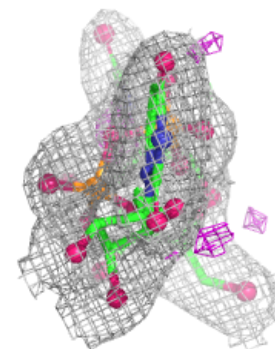
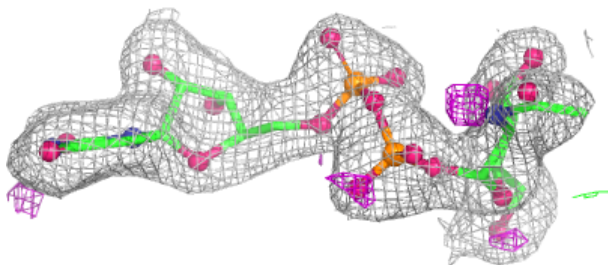
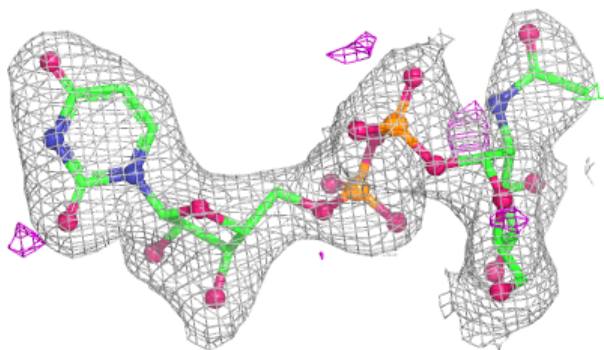
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UD1 A 401:

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

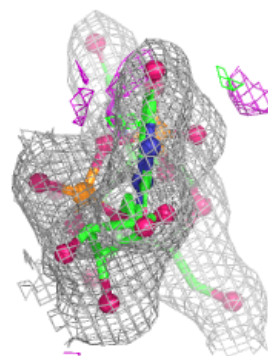
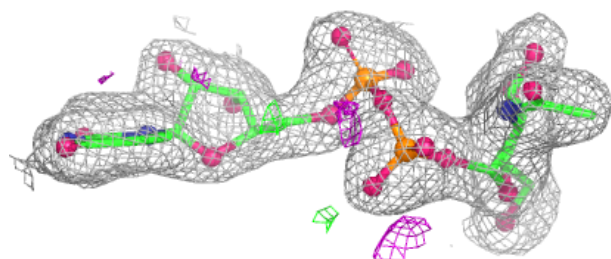
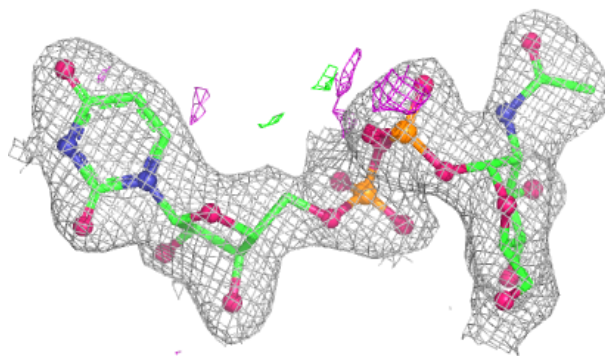
**Electron density around UD1 C 401:**

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



Electron density around UD1 B 401:

$2mF_o-DF_c$ (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.