



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:12 PM UTC

PDB ID : 4WAD / pdb_00004wad
Title : Crystal Structure of TarM with UDP-GlcNAc
Authors : Koc, C.; Stehle, T.; Xia, G.; Peschel, A.
Deposited on : 2014-08-29
Resolution : 2.80 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

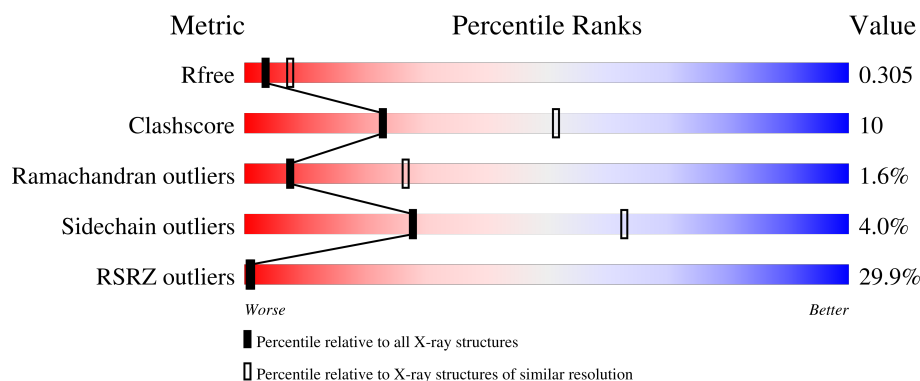
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	498	30% 72% 26% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4168 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.

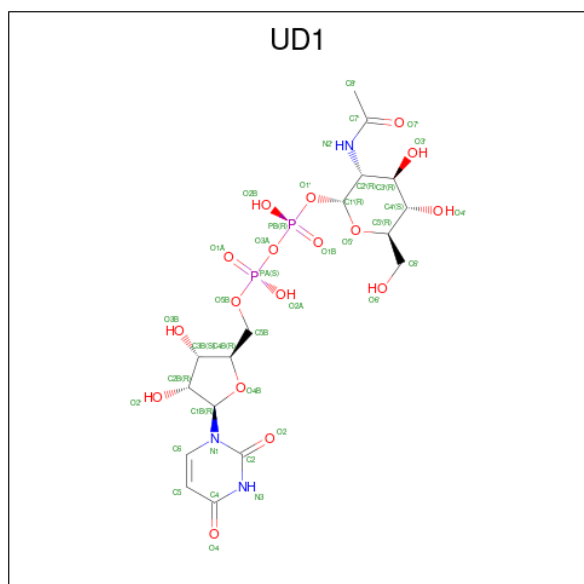
- Molecule 1 is a protein called Glycosyl transferase, group 1 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	4074	2609	686	760	19	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

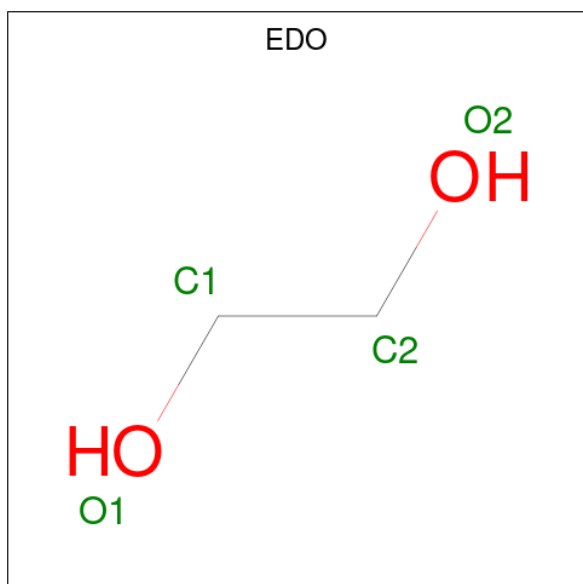
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ILE	-	expression tag	UNP Q2FI41
A	-3	ASP	-	expression tag	UNP Q2FI41
A	-2	PRO	-	expression tag	UNP Q2FI41
A	-1	PHE	-	expression tag	UNP Q2FI41
A	0	THR	-	expression tag	UNP Q2FI41

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

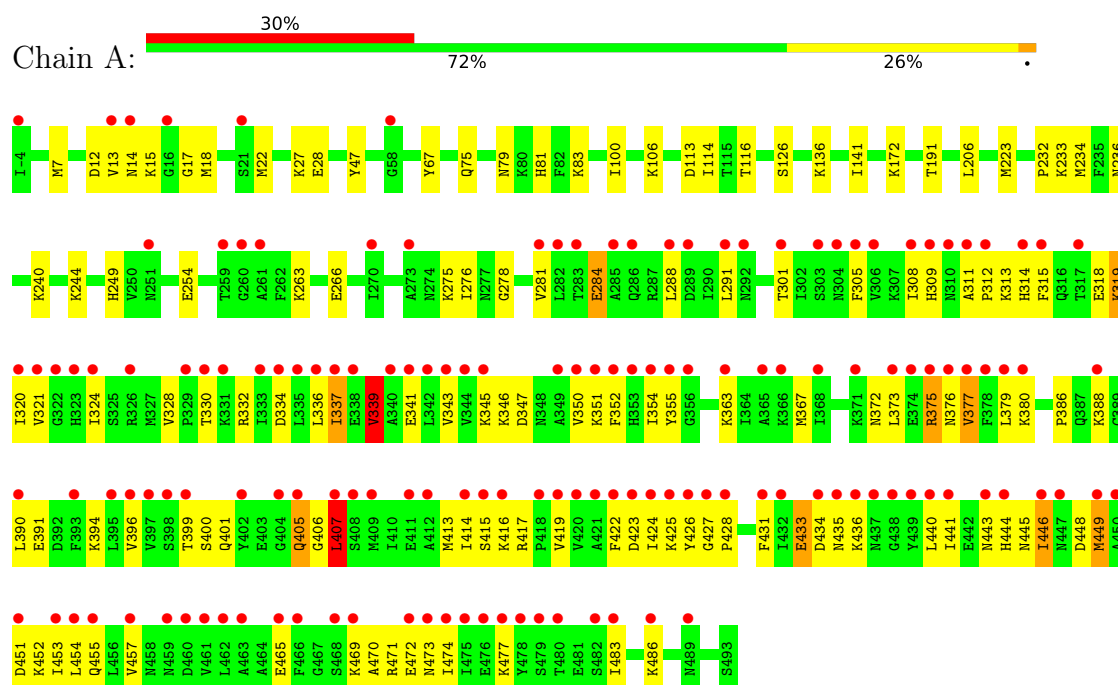
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	45	Total	O	0	0
			45	45		

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: Glycosyl transferase, group 1 family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.02Å 124.02Å 217.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.13 – 2.80 48.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.13-2.80) 99.3 (48.13-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.252 , 0.294 0.262 , 0.305	Depositor DCC
R_{free} test set	1246 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4168	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: CL, UD1, EDO

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	0.32	0/4153	0.74	1/5576 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	VAL	N-CA-C	-5.67	107.98	113.53

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	4074	0	4095	86	1
2	A	39	0	25	7	0
3	A	8	0	12	1	0
4	A	2	0	0	1	0
5	A	45	0	0	2	0
All	All	4168	0	4132	86	1

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 10.

All (86) 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:465:GLU:HG3	1:A:469:LYS:HE2	1.46	0.98
1:A:405:GLN:HA	1:A:427:GLY:HA2	1.63	0.80
1:A:473:ASN:OD1	1:A:477:LYS:NZ	2.15	0.78
1:A:284:GLU:HG2	1:A:301:THR:HG21	1.70	0.73
1:A:249:HIS:O	2:A:501:UD1:O3'	2.07	0.72
1:A:434:ASP:HB2	1:A:440:LEU:HG	1.73	0.71
1:A:350:VAL:O	1:A:376:ASN:ND2	2.24	0.69
1:A:352:PHE:HB2	1:A:377:VAL:HG22	1.78	0.66
1:A:312:PRO:HG3	1:A:391:GLU:HB2	1.79	0.64
1:A:81:HIS:O	1:A:172:LYS:NZ	2.28	0.63
1:A:67:TYR:OH	4:A:504:CL:CL	2.52	0.62
1:A:311:ALA:H	1:A:471:ARG:HH12	1.46	0.62
1:A:343:VAL:HG13	1:A:454:LEU:HD11	1.84	0.60
1:A:339:VAL:HG12	1:A:446:ILE:HG12	1.82	0.59
1:A:191:THR:HG21	1:A:206:LEU:HD22	1.85	0.59
1:A:337:ILE:HD11	1:A:367:MET:HE2	1.85	0.59
1:A:12:ASP:HB3	1:A:15:LYS:HE3	1.84	0.58
1:A:332:ARG:HG3	1:A:401:GLN:HG3	1.86	0.57
1:A:223:MET:HE3	1:A:244:LYS:HG2	1.86	0.57
1:A:12:ASP:HB3	1:A:15:LYS:CE	2.36	0.56
1:A:415:SER:O	1:A:417:ARG:NH1	2.39	0.55
1:A:18:MET:HG3	1:A:249:HIS:CE1	2.41	0.55
1:A:413:MET:CB	1:A:474:ILE:HD11	2.37	0.55
1:A:470:ALA:O	1:A:474:ILE:HD12	2.07	0.54
1:A:318:GLU:O	1:A:320:ILE:N	2.40	0.54
1:A:413:MET:HB2	1:A:474:ILE:HD11	1.88	0.54
1:A:232:PRO:O	1:A:236:ASN:ND2	2.28	0.54
1:A:422:PHE:CG	1:A:443:ASN:HA	2.43	0.53
1:A:311:ALA:H	1:A:471:ARG:NH1	2.07	0.52
1:A:313:LYS:HE2	1:A:314:HIS:NE2	2.23	0.52
1:A:424:ILE:HG22	1:A:425:LYS:N	2.24	0.52
1:A:14:ASN:C	1:A:15:LYS:HD3	2.34	0.52
1:A:319:LYS:NZ	1:A:347:ASP:OD2	2.35	0.51
1:A:321:VAL:O	1:A:352:PHE:HA	2.10	0.51
1:A:394:LYS:NZ	1:A:457:VAL:O	2.39	0.50
1:A:396:VAL:HB	1:A:419:VAL:HG12	1.94	0.50
1:A:136:LYS:HB2	1:A:141:ILE:HD13	1.94	0.49
1:A:406:GLY:HA3	1:A:431:PHE:CE2	2.47	0.49
1:A:407:LEU:HD21	2:A:501:UD1:H8'2	1.94	0.49
1:A:388:LYS:HA	1:A:391:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ILE:O	1:A:486:LYS:HB2	2.13	0.49
1:A:433:GLU:HB2	1:A:436:LYS:HD2	1.95	0.48
1:A:315:PHE:CZ	1:A:416:LYS:HD3	2.48	0.48
1:A:328:VAL:HG12	1:A:330:THR:H	1.78	0.48
1:A:424:ILE:HG22	1:A:425:LYS:H	1.79	0.47
1:A:309:HIS:O	1:A:471:ARG:NH2	2.47	0.47
1:A:407:LEU:HD11	2:A:501:UD1:C7'	2.44	0.47
1:A:451:ASP:O	1:A:455:GLN:HG3	2.13	0.47
1:A:406:GLY:HA3	1:A:431:PHE:CZ	2.50	0.47
1:A:354:ILE:O	1:A:380:LYS:N	2.48	0.47
1:A:341:GLU:O	1:A:345:LYS:HG2	2.14	0.47
1:A:427:GLY:HA3	1:A:428:PRO:HD3	1.63	0.46
1:A:83:LYS:NZ	5:A:603:HOH:O	2.43	0.46
1:A:434:ASP:OD1	1:A:435:ASN:N	2.49	0.46
1:A:341:GLU:HG3	1:A:373:LEU:HD11	1.98	0.46
1:A:386:PRO:O	1:A:390:LEU:HB2	2.16	0.46
1:A:81:HIS:HE1	3:A:503:EDO:H12	1.81	0.46
1:A:263:LYS:HB2	1:A:266:GLU:HB2	1.98	0.46
1:A:7:MET:HE1	1:A:234:MET:HB2	1.98	0.45
1:A:75:GLN:O	1:A:79:ASN:ND2	2.49	0.45
1:A:441:ILE:HD13	1:A:449:MET:HB2	1.98	0.45
1:A:12:ASP:OD1	1:A:13:VAL:N	2.46	0.45
1:A:423:ASP:C	1:A:424:ILE:HG13	2.40	0.45
1:A:399:THR:OG1	1:A:400:SER:N	2.49	0.44
1:A:288:LEU:HA	1:A:291:LEU:HG	1.98	0.44
1:A:113:ASP:OD2	1:A:116:THR:N	2.45	0.44
1:A:276:ILE:HG13	1:A:278:GLY:H	1.82	0.43
1:A:444:HIS:O	1:A:446:ILE:N	2.51	0.43
1:A:17:GLY:HA3	2:A:501:UD1:O2B	2.18	0.43
1:A:308:ILE:HA	1:A:414:ILE:HD13	2.00	0.43
1:A:453:ILE:O	1:A:457:VAL:HG22	2.19	0.43
1:A:390:LEU:HD22	1:A:415:SER:HB2	2.01	0.42
1:A:249:HIS:ND1	2:A:501:UD1:H8'3	2.35	0.42
1:A:324:ILE:HG12	1:A:355:TYR:HB2	2.01	0.42
1:A:346:LYS:HB2	1:A:454:LEU:HD21	2.01	0.42
1:A:18:MET:O	1:A:22:MET:HG3	2.20	0.41
1:A:100:ILE:HB	1:A:114:ILE:HG22	2.02	0.41
1:A:448:ASP:O	1:A:452:LYS:HG2	2.20	0.41
1:A:469:LYS:O	1:A:473:ASN:HB2	2.20	0.41
1:A:407:LEU:HD11	2:A:501:UD1:O7'	2.19	0.41
1:A:27:LYS:NZ	1:A:28:GLU:OE2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ILE:HB	1:A:379:LEU:HA	2.03	0.41
1:A:332:ARG:NH2	1:A:334:ASP:OD1	2.54	0.40
1:A:28:GLU:HG3	1:A:305:PHE:CG	2.56	0.40
1:A:407:LEU:HD21	2:A:501:UD1:C7'	2.51	0.40
1:A:233:LYS:NZ	5:A:605:HOH:O	2.50	0.40

All (1) 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)
1:A:341:GLU:OE1	1:A:372:ASN:ND2[11_554]	1.97	0.23

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	496/498 (100%)	445 (90%)	43 (9%)	8 (2%)	7 27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	407	LEU
1	A	126	SER
1	A	445	ASN
1	A	405	GLN
1	A	426	TYR
1	A	375	ARG
1	A	281	VAL

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	454/454 (100%)	436 (96%)	18 (4%)	28	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	TYR
1	A	106	LYS
1	A	240	LYS
1	A	254	GLU
1	A	275	LYS
1	A	284	GLU
1	A	336	LEU
1	A	337	ILE
1	A	339	VAL
1	A	351	LYS
1	A	363	LYS
1	A	375	ARG
1	A	377	VAL
1	A	407	LEU
1	A	433	GLU
1	A	446	ILE
1	A	449	MET
1	A	472	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	68	ASN
1	A	81	HIS
1	A	138	ASN
1	A	286	GLN
1	A	387	GLN
1	A	458	ASN

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](#)

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	$\# Z > 2$
3	EDO	A	502	-	3,3,3	0.40	0	2,2,2	0.41	0
3	EDO	A	503	-	3,3,3	0.41	0	2,2,2	0.40	0
2	UD1	A	501	-	40,41,41	1.06	5 (12%)	59,62,62	1.37	6 (10%)

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	EDO	A	502	-	-	0/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
2	UD1	A	501	-	-	14/26/63/63	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UD1	C4-N3	-2.63	1.34	1.38
2	A	501	UD1	PB-O3A	2.37	1.62	1.59
2	A	501	UD1	PA-O3A	2.34	1.62	1.59
2	A	501	UD1	C2-N1	2.13	1.41	1.38
2	A	501	UD1	C2-N3	-2.09	1.34	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	UD1	C4-N3-C2	-4.75	120.72	126.61
2	A	501	UD1	N3-C2-N1	4.21	120.37	114.89
2	A	501	UD1	C5-C4-N3	3.71	120.00	114.80
2	A	501	UD1	O4-C4-C5	-2.98	120.03	125.16
2	A	501	UD1	O2-C2-N1	-2.11	120.05	122.80
2	A	501	UD1	O1'-C1'-C2'	2.05	112.11	108.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

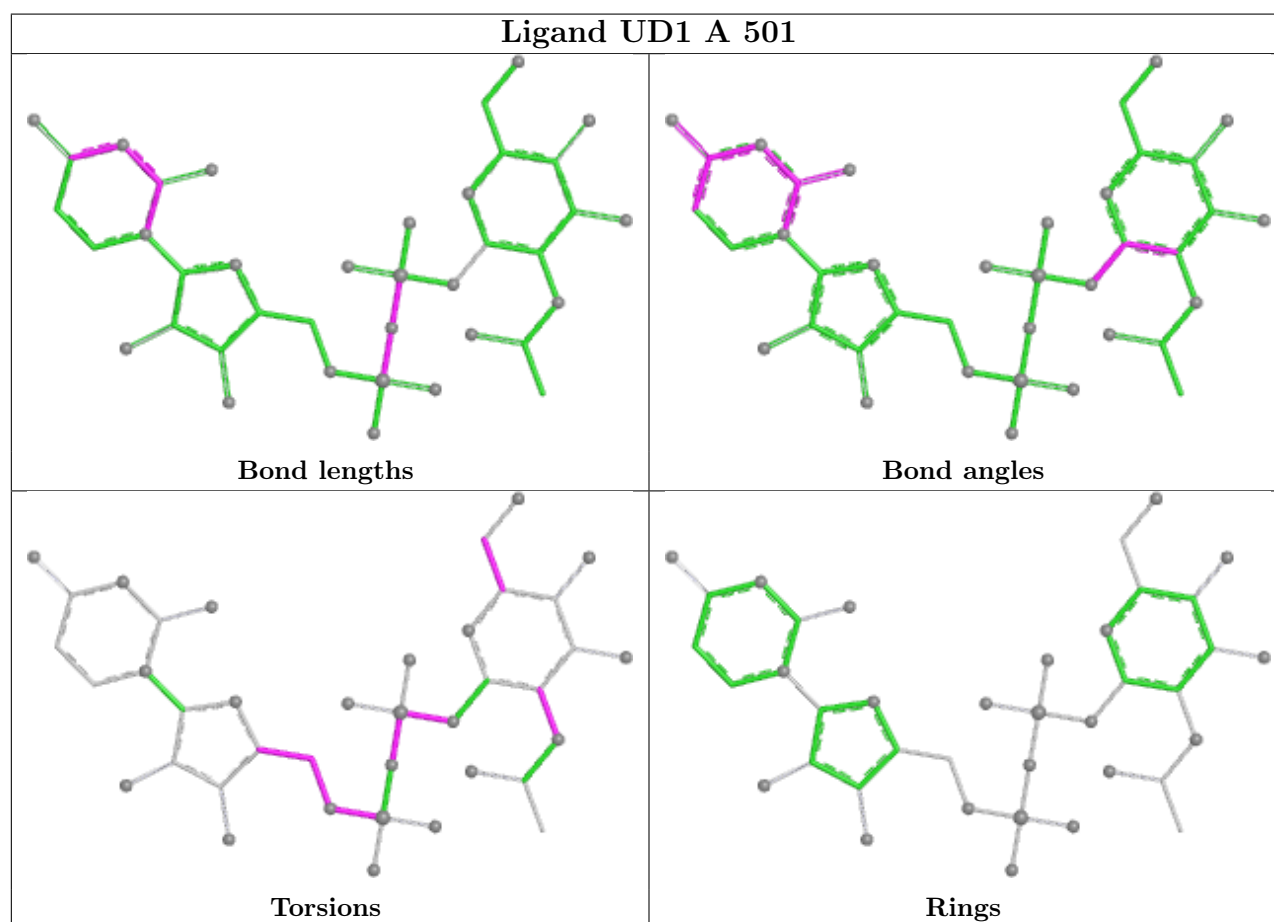
Mol	Chain	Res	Type	Atoms
2	A	501	UD1	C1'-O1'-PB-O3A
2	A	501	UD1	C5B-O5B-PA-O1A
2	A	501	UD1	C5B-O5B-PA-O2A
2	A	501	UD1	C5B-O5B-PA-O3A
2	A	501	UD1	O5'-C5'-C6'-O6'
2	A	501	UD1	O4B-C4B-C5B-O5B
2	A	501	UD1	C3B-C4B-C5B-O5B
2	A	501	UD1	C4'-C5'-C6'-O6'
2	A	501	UD1	C1'-O1'-PB-O1B
2	A	501	UD1	C4B-C5B-O5B-PA
2	A	501	UD1	C1'-C2'-N2'-C7'
2	A	501	UD1	PA-O3A-PB-O1B
2	A	501	UD1	C3'-C2'-N2'-C7'
2	A	501	UD1	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	EDO	1	0
2	A	501	UD1	7	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	498/498 (100%)	1.36	149 (29%) 1 1	25, 73, 104, 114	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	MET	8.6
1	A	454	LEU	7.9
1	A	397	VAL	7.0
1	A	439	TYR	6.8
1	A	438	GLY	6.7
1	A	462	LEU	6.4
1	A	338	GLU	6.3
1	A	453	ILE	6.3
1	A	440	LEU	6.3
1	A	379	LEU	6.1
1	A	411	GLU	5.7
1	A	432	ILE	5.5
1	A	441	ILE	5.4
1	A	398	SER	5.3
1	A	447	ASN	5.2
1	A	463	ALA	5.2
1	A	341	GLU	5.1
1	A	450	ALA	5.1
1	A	474	ILE	5.0
1	A	399	THR	4.7
1	A	428	PRO	4.6
1	A	405	GLN	4.5
1	A	419	VAL	4.5
1	A	352	PHE	4.5
1	A	373	LEU	4.4
1	A	342	LEU	4.4
1	A	321	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	409	MET	4.4
1	A	408	SER	4.3
1	A	322	GLY	4.3
1	A	418	PRO	4.2
1	A	378	PHE	4.2
1	A	353	HIS	4.1
1	A	377	VAL	4.1
1	A	336	LEU	4.1
1	A	396	VAL	4.1
1	A	350	VAL	4.0
1	A	461	VAL	4.0
1	A	402	TYR	3.9
1	A	446	ILE	3.9
1	A	309	HIS	3.8
1	A	393	PHE	3.7
1	A	422	PHE	3.6
1	A	475	ILE	3.6
1	A	335	LEU	3.6
1	A	457	VAL	3.5
1	A	306	VAL	3.5
1	A	427	GLY	3.5
1	A	395	LEU	3.5
1	A	333	ILE	3.4
1	A	320	ILE	3.3
1	A	281	VAL	3.3
1	A	16	GLY	3.3
1	A	468	SER	3.3
1	A	407	LEU	3.2
1	A	260	GLY	3.2
1	A	479	SER	3.1
1	A	368	ILE	3.1
1	A	324	ILE	3.1
1	A	261	ALA	3.1
1	A	478	TYR	3.1
1	A	334	ASP	3.1
1	A	414	ILE	3.1
1	A	420	VAL	3.0
1	A	259	THR	3.0
1	A	443	ASN	3.0
1	A	270	ILE	2.9
1	A	291	LEU	2.9
1	A	472	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	331	LYS	2.9
1	A	337	ILE	2.9
1	A	374	GLU	2.9
1	A	465	GLU	2.9
1	A	340	ALA	2.9
1	A	412	ALA	2.9
1	A	437	ASN	2.9
1	A	473	ASN	2.9
1	A	482	SER	2.9
1	A	477	LYS	2.8
1	A	388	LYS	2.8
1	A	431	PHE	2.8
1	A	404	GLY	2.8
1	A	-4	ILE	2.7
1	A	435	ASN	2.7
1	A	308	ILE	2.7
1	A	329	PRO	2.7
1	A	288	LEU	2.7
1	A	305	PHE	2.7
1	A	366	LYS	2.7
1	A	444	HIS	2.7
1	A	415	SER	2.7
1	A	423	ASP	2.7
1	A	285	ALA	2.6
1	A	451	ASP	2.6
1	A	311	ALA	2.6
1	A	349	ALA	2.6
1	A	323	HIS	2.6
1	A	355	TYR	2.6
1	A	14	ASN	2.6
1	A	466	PHE	2.6
1	A	371	LYS	2.6
1	A	282	LEU	2.6
1	A	459	ASN	2.6
1	A	489	ASN	2.6
1	A	58	GLY	2.5
1	A	315	PHE	2.5
1	A	455	GLN	2.5
1	A	310	ASN	2.5
1	A	273	ALA	2.5
1	A	351	LYS	2.5
1	A	416	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	312	PRO	2.5
1	A	356	GLY	2.5
1	A	344	VAL	2.5
1	A	469	LYS	2.4
1	A	304	ASN	2.4
1	A	486	LYS	2.4
1	A	286	GLN	2.4
1	A	343	VAL	2.3
1	A	345	LYS	2.3
1	A	289	ASP	2.3
1	A	21	SER	2.3
1	A	363	LYS	2.3
1	A	460	ASP	2.3
1	A	317	THR	2.3
1	A	375	ARG	2.3
1	A	376	ASN	2.3
1	A	326	ARG	2.3
1	A	380	LYS	2.2
1	A	483	ILE	2.2
1	A	480	THR	2.2
1	A	303	SER	2.2
1	A	425	LYS	2.2
1	A	251	ASN	2.2
1	A	13	VAL	2.2
1	A	365	ALA	2.2
1	A	283	THR	2.2
1	A	390	LEU	2.1
1	A	424	ILE	2.1
1	A	476	GLU	2.1
1	A	330	THR	2.1
1	A	354	ILE	2.1
1	A	421	ALA	2.1
1	A	301	THR	2.1
1	A	434	ASP	2.1
1	A	292	ASN	2.0
1	A	426	TYR	2.0
1	A	436	LYS	2.0
1	A	314	HIS	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 [i](#)

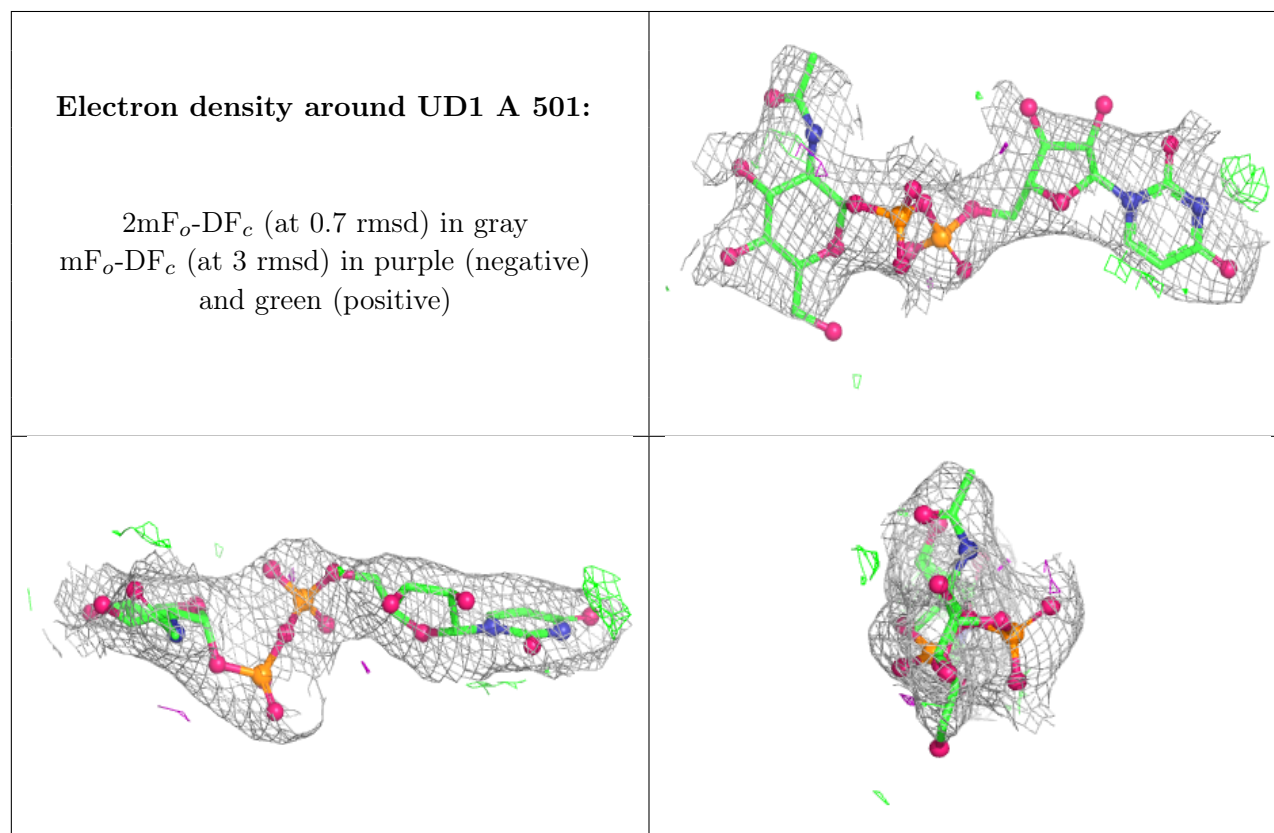
There are no oligosaccharides in this entry.

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	501	39/39	0.81	0.16	55,92,109,125	0
3	EDO	A	503	4/4	0.84	0.18	56,56,61,62	0
4	CL	A	504	1/1	0.84	0.21	82,82,82,82	0
3	EDO	A	502	4/4	0.89	0.20	48,50,57,69	0
4	CL	A	505	1/1	0.99	0.06	52,52,52,52	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.