



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:02 AM UTC

PDB ID : 8P0O / pdb_00008p0o
Title : Crystal structure of AaNGT complexed to UDP-Gal
Authors : Pinello, B.; Macias-Leon, J.; Rovira, C.; Hurtado-Guerrero, R.
Deposited on : 2023-05-10
Resolution : 1.76 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

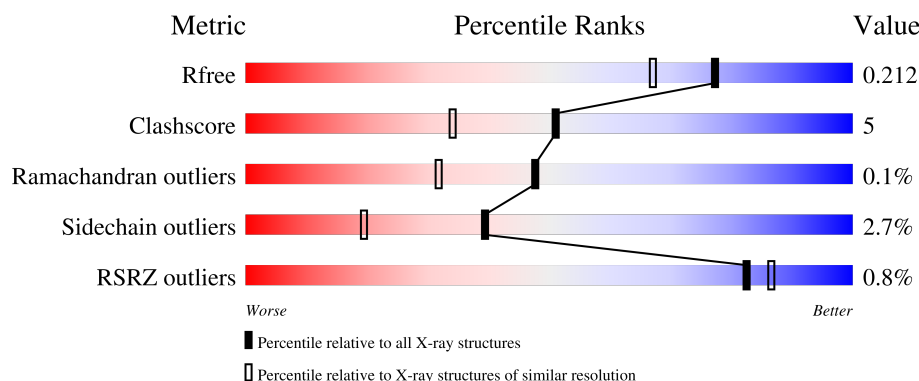
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	622	 89% 9% .
1	B	622	 % 91% 8% .

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	EDO	A	801	-	-	X	-
2	EDO	B	801	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10915 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.

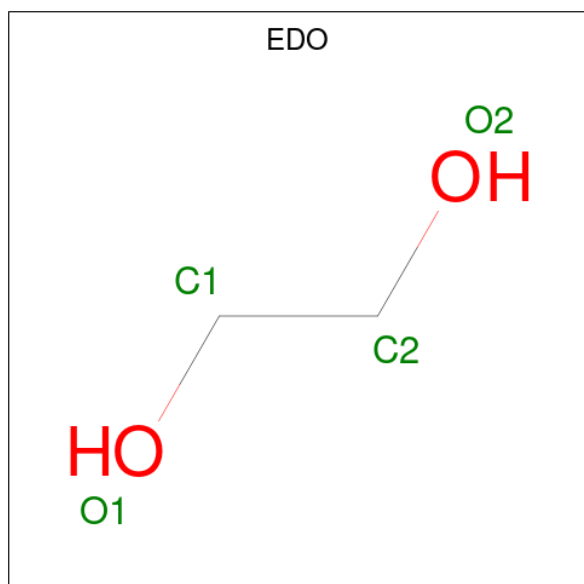
- Molecule 1 is a protein called Adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	0	0
			4983	3181	849	924	29			
1	B	621	Total	C	N	O	S	0	0	0
			4975	3175	848	923	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A3M6PNT1
A	3	ARG	GLU	conflict	UNP A0A3M6PNT1
B	0	GLY	-	expression tag	UNP A0A3M6PNT1
B	3	ARG	GLU	conflict	UNP A0A3M6PNT1

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



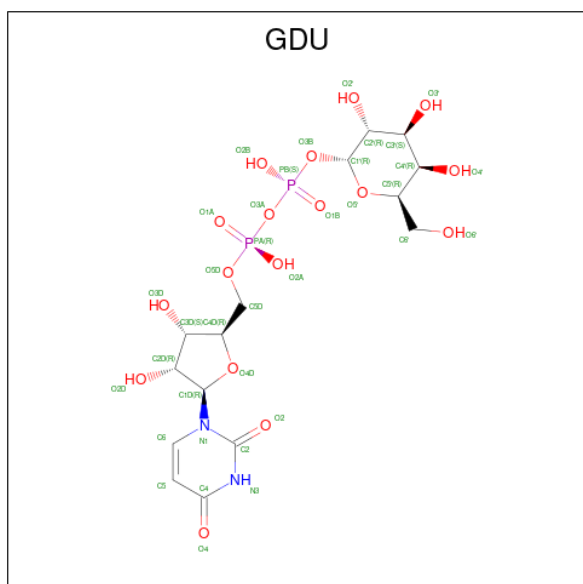
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0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

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

- Molecule 3 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (CCD ID: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

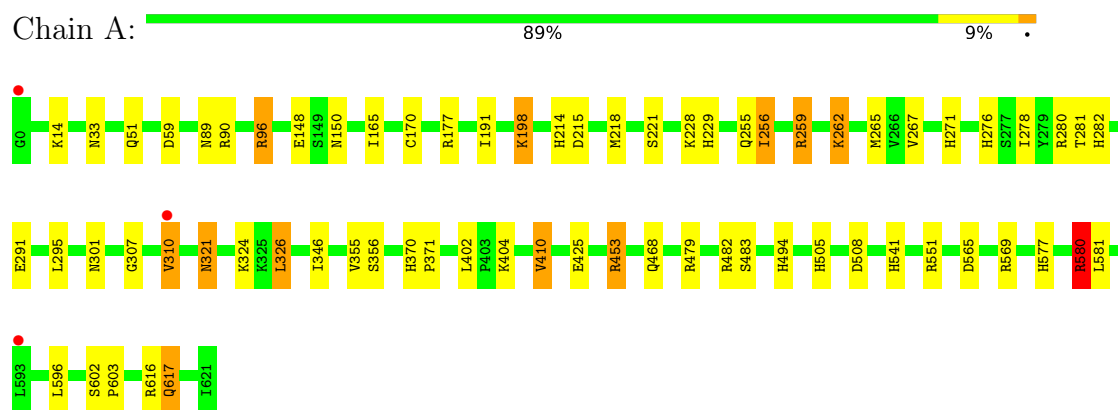
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	441	Total	O	0	0
			441	441		
4	B	340	Total	O	0	0
			340	340		

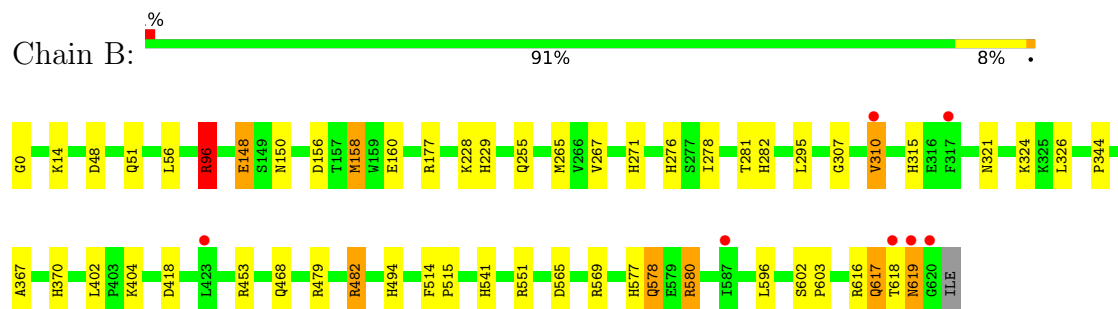
3 Residue-property plots

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: Adhesin



• Molecule 1: Adhesin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.34Å 113.33Å 260.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.76 20.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.76) 99.9 (20.00-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.174 , 0.207 0.184 , 0.212	Depositor DCC
R_{free} test set	5584 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10915	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: GDU, 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	0.62	1/5104 (0.0%)	0.98	5/6927 (0.1%)
1	B	0.60	0/5096	0.93	3/6916 (0.0%)
All	All	0.61	1/10200 (0.0%)	0.96	8/13843 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ARG	CD-NE	-5.61	1.38	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	MET	CG-SD-CE	-6.75	86.04	100.90
1	A	479	ARG	NE-CZ-NH2	-6.55	113.30	119.20
1	A	301	ASN	CB-CA-C	-6.13	99.29	110.63
1	A	617	GLN	CB-CA-C	6.05	121.99	109.95
1	A	453	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	A	580	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	B	479	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	B	148	GLU	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	ARG	Sidechain
1	A	551	ARG	Sidechain
1	A	580	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	482	ARG	Sidechain
1	B	551	ARG	Sidechain
1	B	580	ARG	Sidechain
1	B	96	ARG	Sidechain

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	4983	0	4903	55	0
1	B	4975	0	4892	48	0
2	A	52	0	78	8	0
2	B	52	0	78	6	0
3	A	36	0	22	0	0
3	B	36	0	22	0	0
4	A	441	0	0	16	0
4	B	340	0	0	12	0
All	All	10915	0	9995	105	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 5.

All (105) 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)
2:A:801:EDO:H22	4:A:1173:HOH:O	1.35	1.26
1:B:468:GLN:H	1:B:494:HIS:HD2	1.13	0.95
1:A:468:GLN:H	1:A:494:HIS:HD2	1.14	0.94
1:B:617:GLN:C	1:B:617:GLN:HE21	1.75	0.93
1:B:265:MET:HE2	1:B:295:LEU:HG	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:MET:HE3	1:B:267:VAL:HG22	1.65	0.78
2:B:801:EDO:C2	4:B:1081:HOH:O	2.32	0.77
1:B:14:LYS:HG3	4:B:1103:HOH:O	1.85	0.74
1:A:214:HIS:NE2	2:A:801:EDO:H21	2.02	0.74
1:A:265:MET:HE2	1:A:295:LEU:CG	2.18	0.73
1:B:271:HIS:O	1:B:278:ILE:HG21	1.89	0.72
1:A:265:MET:HE2	1:A:295:LEU:HG	1.72	0.71
1:A:468:GLN:H	1:A:494:HIS:CD2	2.05	0.71
1:A:577:HIS:HD2	1:A:580:ARG:HH12	1.37	0.70
1:B:577:HIS:HD2	1:B:580:ARG:HH12	1.39	0.69
1:B:265:MET:HE3	1:B:267:VAL:CG2	2.22	0.69
1:A:271:HIS:O	1:A:278:ILE:HG21	1.92	0.69
1:B:578:GLN:H	1:B:578:GLN:CD	2.01	0.69
2:A:802:EDO:H12	4:A:1218:HOH:O	1.93	0.68
1:A:265:MET:HE3	1:A:267:VAL:CG2	2.25	0.67
2:B:801:EDO:H22	4:B:1081:HOH:O	1.93	0.66
2:A:801:EDO:H21	4:A:1190:HOH:O	1.95	0.66
1:A:89:ASN:ND2	4:A:901:HOH:O	2.21	0.65
1:B:156:ASP:O	1:B:160:GLU:HG3	1.97	0.65
1:A:265:MET:HE3	1:A:267:VAL:HG22	1.79	0.65
2:A:802:EDO:C1	4:A:1218:HOH:O	2.45	0.64
1:B:617:GLN:C	1:B:617:GLN:NE2	2.53	0.64
1:A:150:ASN:HD21	1:B:51:GLN:HE21	1.46	0.64
1:B:580:ARG:HD3	4:B:957:HOH:O	1.98	0.63
1:B:468:GLN:H	1:B:494:HIS:CD2	2.05	0.63
1:B:370:HIS:HD2	4:B:1210:HOH:O	1.81	0.62
1:A:89:ASN:HB2	4:A:1244:HOH:O	1.98	0.62
1:B:229:HIS:HD2	4:B:941:HOH:O	1.83	0.62
1:B:321:ASN:HD22	1:B:324:LYS:H	1.44	0.62
1:A:215:ASP:OD1	2:A:801:EDO:H11	2.00	0.61
1:A:259:ARG:HB2	1:A:259:ARG:HH11	1.65	0.61
1:A:214:HIS:CE1	2:A:801:EDO:H21	2.37	0.60
1:A:281:THR:OG1	1:A:282:HIS:HD2	1.84	0.60
1:B:281:THR:OG1	1:B:282:HIS:HD2	1.85	0.60
1:B:265:MET:HE2	1:B:295:LEU:CG	2.32	0.59
1:A:150:ASN:ND2	1:B:51:GLN:HE21	2.01	0.59
1:B:96:ARG:HH12	2:B:801:EDO:H12	1.67	0.59
1:A:51:GLN:HE21	1:B:150:ASN:HD21	1.52	0.58
1:A:265:MET:HE2	1:A:295:LEU:CD1	2.33	0.58
1:A:265:MET:HE2	1:A:295:LEU:HD11	1.85	0.58
2:A:801:EDO:C2	4:A:1190:HOH:O	2.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:MET:HE3	1:A:370:HIS:CG	2.38	0.57
2:B:801:EDO:H21	4:B:1081:HOH:O	1.97	0.56
1:A:602:SER:N	1:A:603:PRO:CD	2.69	0.55
1:B:177:ARG:HH21	1:B:468:GLN:NE2	2.04	0.55
1:B:617:GLN:HE21	1:B:618:THR:N	2.03	0.54
1:A:177:ARG:HH21	1:A:468:GLN:NE2	2.05	0.54
1:B:602:SER:N	1:B:603:PRO:CD	2.70	0.54
1:A:262:LYS:HE2	1:A:291:GLU:O	2.07	0.54
1:A:280:ARG:HA	1:A:410:VAL:HG13	1.89	0.54
1:A:565:ASP:O	1:A:569:ARG:HG2	2.08	0.54
1:B:618:THR:O	1:B:619:ASN:HB2	2.09	0.53
1:A:90:ARG:HD2	4:A:1195:HOH:O	2.09	0.53
1:B:580:ARG:CD	4:B:957:HOH:O	2.55	0.53
1:B:276:HIS:ND1	1:B:278:ILE:HG22	2.25	0.52
1:A:198:LYS:N	1:A:198:LYS:HD2	2.25	0.52
1:A:321:ASN:HD22	1:A:324:LYS:H	1.56	0.52
1:B:228:LYS:HZ1	1:B:541:HIS:HE1	1.58	0.51
1:A:259:ARG:HB2	1:A:259:ARG:NH1	2.25	0.51
1:A:326:LEU:HD22	1:A:355:VAL:HG22	1.92	0.51
1:B:96:ARG:HH12	2:B:801:EDO:C1	2.25	0.50
1:B:565:ASP:O	1:B:569:ARG:HG2	2.12	0.49
1:A:33:ASN:ND2	4:A:910:HOH:O	2.45	0.49
1:B:315:HIS:ND1	4:B:901:HOH:O	2.35	0.48
1:B:578:GLN:CD	1:B:578:GLN:N	2.70	0.48
1:B:228:LYS:NZ	1:B:541:HIS:HE1	2.11	0.48
1:A:228:LYS:NZ	1:A:541:HIS:HE1	2.10	0.48
1:A:59:ASP:OD2	1:B:482:ARG:NH1	2.47	0.48
1:A:51:GLN:HE21	1:B:150:ASN:ND2	2.11	0.48
1:A:14:LYS:HG3	4:A:1237:HOH:O	2.14	0.47
1:A:255:GLN:C	1:A:256:ILE:HD12	2.39	0.47
1:B:271:HIS:O	1:B:278:ILE:CG2	2.61	0.47
1:A:276:HIS:HB2	4:A:1305:HOH:O	2.14	0.47
1:A:580:ARG:CD	4:A:1042:HOH:O	2.61	0.47
1:A:170:CYS:SG	1:A:191:ILE:HD12	2.55	0.46
1:A:425:GLU:HA	1:A:581:LEU:HD21	1.97	0.46
1:A:580:ARG:HD3	4:A:1042:HOH:O	2.16	0.46
1:B:482:ARG:NH2	4:B:909:HOH:O	2.48	0.46
1:B:0:GLY:N	4:B:907:HOH:O	2.48	0.46
1:A:276:HIS:ND1	1:A:278:ILE:HG22	2.30	0.46
1:A:218:MET:CE	1:A:370:HIS:ND1	2.79	0.46
1:B:48:ASP:OD2	2:B:804:EDO:H21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:GLY:O	1:B:310:VAL:HG13	2.16	0.45
1:B:617:GLN:HG2	1:B:617:GLN:O	2.15	0.45
1:A:229:HIS:HD2	4:A:956:HOH:O	2.00	0.45
1:A:482:ARG:HD3	4:A:1247:HOH:O	2.18	0.44
1:A:321:ASN:ND2	1:A:324:LYS:H	2.15	0.44
1:B:321:ASN:ND2	1:B:324:LYS:H	2.14	0.44
1:B:418:ASP:OD1	1:B:418:ASP:N	2.51	0.43
1:A:508:ASP:O	1:A:580:ARG:HD3	2.19	0.43
1:B:276:HIS:HB2	4:B:1226:HOH:O	2.19	0.43
1:A:221:SER:OG	1:A:229:HIS:HE1	2.01	0.43
1:A:577:HIS:CD2	1:A:580:ARG:HH12	2.27	0.43
1:B:514:PHE:HB2	1:B:515:PRO:HA	2.01	0.42
1:A:483:SER:HA	1:B:56:LEU:HD21	2.00	0.42
1:B:344:PRO:HA	1:B:367:ALA:HB3	2.00	0.42
1:A:307:GLY:O	1:A:310:VAL:HG13	2.18	0.42
1:A:577:HIS:HE1	4:A:1280:HOH:O	2.02	0.41
1:A:371:PRO:O	1:A:541:HIS:HD2	2.03	0.41
1:A:346:ILE:CD1	1:A:356:SER:HB3	2.52	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	620/622 (100%)	609 (98%)	11 (2%)	0	100	100
1	B	619/622 (100%)	606 (98%)	12 (2%)	1 (0%)	43	27
All	All	1239/1244 (100%)	1215 (98%)	23 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	619	ASN

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	551/551 (100%)	534 (97%)	17 (3%)	35	15
1	B	550/551 (100%)	537 (98%)	13 (2%)	43	23
All	All	1101/1102 (100%)	1071 (97%)	30 (3%)	39	19

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	148	GLU
1	A	165	ILE
1	A	198	LYS
1	A	256	ILE
1	A	259	ARG
1	A	262	LYS
1	A	310	VAL
1	A	321	ASN
1	A	326	LEU
1	A	402	LEU
1	A	404	LYS
1	A	410	VAL
1	A	505	HIS
1	A	596	LEU
1	A	616	ARG
1	A	617	GLN
1	B	96	ARG
1	B	148	GLU
1	B	158	MET
1	B	255	GLN
1	B	310	VAL
1	B	326	LEU

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Mol	Chain	Res	Type
1	B	402	LEU
1	B	404	LYS
1	B	453	ARG
1	B	578	GLN
1	B	596	LEU
1	B	616	ARG
1	B	617	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	70	ASN
1	A	150	ASN
1	A	154	ASN
1	A	219	HIS
1	A	229	HIS
1	A	282	HIS
1	A	292	GLN
1	A	321	ASN
1	A	357	ASN
1	A	468	GLN
1	A	494	HIS
1	A	506	ASN
1	A	512	ASN
1	A	541	HIS
1	A	576	ASN
1	A	577	HIS
1	B	33	ASN
1	B	70	ASN
1	B	150	ASN
1	B	203	HIS
1	B	219	HIS
1	B	229	HIS
1	B	282	HIS
1	B	321	ASN
1	B	357	ASN
1	B	468	GLN
1	B	494	HIS
1	B	506	ASN
1	B	512	ASN
1	B	541	HIS

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Mol	Chain	Res	Type
1	B	576	ASN
1	B	577	HIS
1	B	617	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](#)

28 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	EDO	B	804	-	3,3,3	0.26	0	2,2,2	0.10	0
2	EDO	B	812	-	3,3,3	0.19	0	2,2,2	0.26	0
2	EDO	A	811	-	3,3,3	0.08	0	2,2,2	0.13	0
2	EDO	B	803	-	3,3,3	0.08	0	2,2,2	0.23	0
2	EDO	A	804	-	3,3,3	0.21	0	2,2,2	0.33	0
2	EDO	A	807	-	3,3,3	0.16	0	2,2,2	0.20	0
2	EDO	B	805	-	3,3,3	0.11	0	2,2,2	0.36	0
2	EDO	B	813	-	3,3,3	0.14	0	2,2,2	0.28	0
2	EDO	A	808	-	3,3,3	0.40	0	2,2,2	0.51	0
2	EDO	A	801	-	3,3,3	0.73	0	2,2,2	0.67	0
2	EDO	B	811	-	3,3,3	0.15	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	802	-	3,3,3	0.12	0	2,2,2	0.23	0
3	GDU	B	814	-	37,38,38	0.48	0	55,58,58	0.71	0
2	EDO	A	805	-	3,3,3	0.22	0	2,2,2	0.27	0
2	EDO	B	807	-	3,3,3	0.31	0	2,2,2	0.51	0
2	EDO	B	801	-	3,3,3	0.25	0	2,2,2	0.24	0
2	EDO	B	806	-	3,3,3	0.24	0	2,2,2	0.11	0
2	EDO	B	808	-	3,3,3	0.18	0	2,2,2	0.30	0
2	EDO	A	812	-	3,3,3	0.12	0	2,2,2	0.17	0
2	EDO	B	809	-	3,3,3	0.18	0	2,2,2	0.14	0
2	EDO	A	802	-	3,3,3	0.28	0	2,2,2	0.34	0
2	EDO	A	813	-	3,3,3	0.10	0	2,2,2	0.11	0
2	EDO	A	810	-	3,3,3	0.18	0	2,2,2	0.16	0
2	EDO	B	810	-	3,3,3	0.34	0	2,2,2	0.38	0
2	EDO	A	803	-	3,3,3	0.14	0	2,2,2	0.07	0
2	EDO	A	809	-	3,3,3	0.07	0	2,2,2	0.14	0
2	EDO	A	806	-	3,3,3	0.08	0	2,2,2	0.04	0
3	GDU	A	814	-	37,38,38	0.85	1 (2%)	55,58,58	0.77	1 (1%)

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	EDO	B	804	-	-	1/1/1/1	-
2	EDO	B	812	-	-	1/1/1/1	-
2	EDO	A	811	-	-	0/1/1/1	-
2	EDO	B	803	-	-	1/1/1/1	-
2	EDO	A	804	-	-	0/1/1/1	-
2	EDO	A	807	-	-	1/1/1/1	-
2	EDO	B	805	-	-	1/1/1/1	-
2	EDO	B	813	-	-	0/1/1/1	-
2	EDO	A	808	-	-	1/1/1/1	-
2	EDO	A	801	-	-	1/1/1/1	-
2	EDO	B	811	-	-	1/1/1/1	-
2	EDO	B	802	-	-	1/1/1/1	-
3	GDU	B	814	-	-	3/23/59/59	0/3/3/3
2	EDO	A	805	-	-	0/1/1/1	-
2	EDO	B	807	-	-	1/1/1/1	-
2	EDO	B	801	-	-	0/1/1/1	-
2	EDO	B	806	-	-	1/1/1/1	-
2	EDO	B	808	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	812	-	-	1/1/1/1	-
2	EDO	B	809	-	-	1/1/1/1	-
2	EDO	A	802	-	-	1/1/1/1	-
2	EDO	A	813	-	-	1/1/1/1	-
2	EDO	A	810	-	-	0/1/1/1	-
2	EDO	B	810	-	-	1/1/1/1	-
2	EDO	A	803	-	-	0/1/1/1	-
2	EDO	A	809	-	-	1/1/1/1	-
2	EDO	A	806	-	-	0/1/1/1	-
3	GDU	A	814	-	-	4/23/59/59	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	814	GDU	PA-O3A	4.35	1.64	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	814	GDU	O2A-PA-O3A	2.32	113.55	107.27

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	814	GDU	PA-O3A-PB-O3B
3	B	814	GDU	PA-O3A-PB-O3B
3	B	814	GDU	C1'-O3B-PB-O3A
2	B	805	EDO	O1-C1-C2-O2
2	A	801	EDO	O1-C1-C2-O2
2	A	809	EDO	O1-C1-C2-O2
2	B	812	EDO	O1-C1-C2-O2
2	B	802	EDO	O1-C1-C2-O2
2	B	803	EDO	O1-C1-C2-O2
2	B	810	EDO	O1-C1-C2-O2
2	B	806	EDO	O1-C1-C2-O2
3	A	814	GDU	PB-O3A-PA-O5D
2	B	809	EDO	O1-C1-C2-O2
3	A	814	GDU	C1'-O3B-PB-O3A
2	B	804	EDO	O1-C1-C2-O2
2	A	807	EDO	O1-C1-C2-O2

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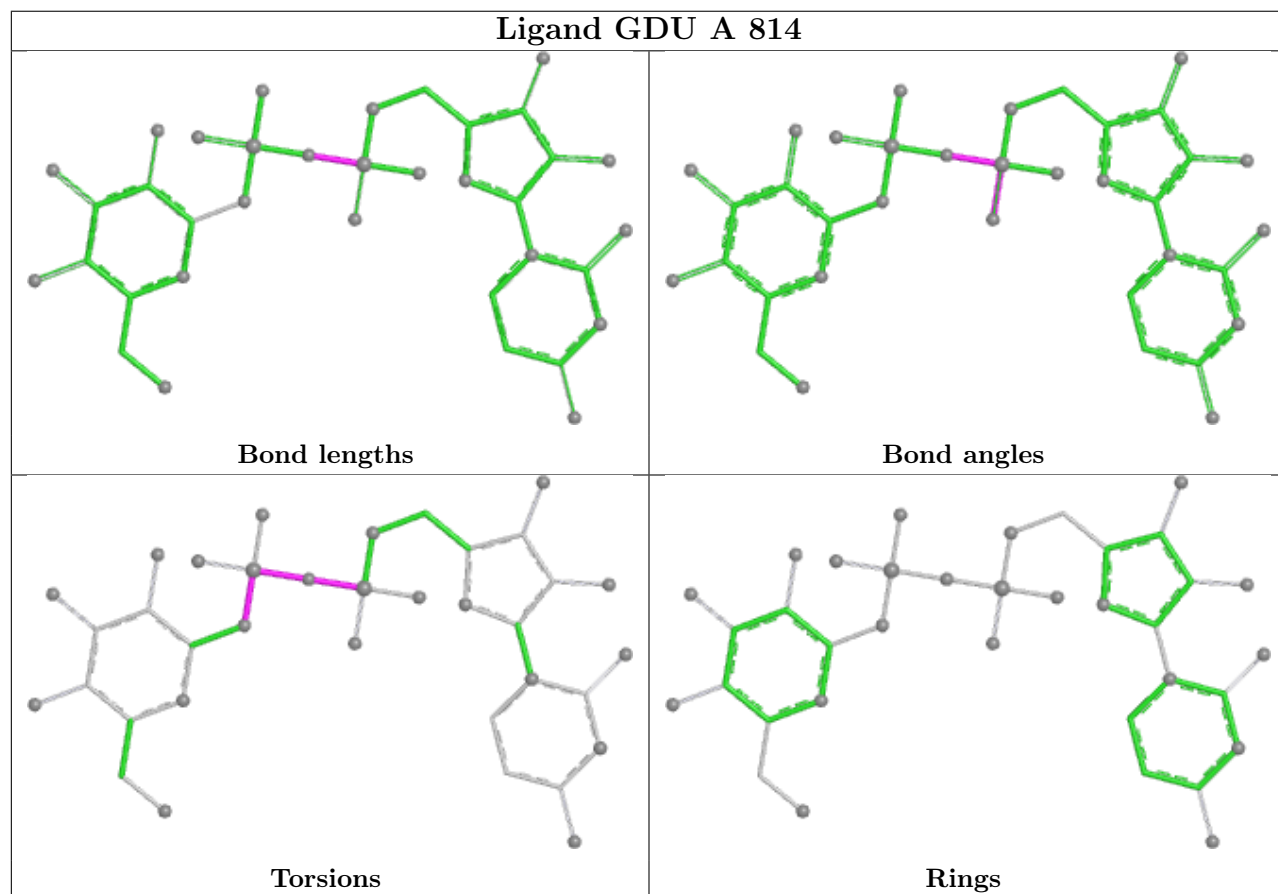
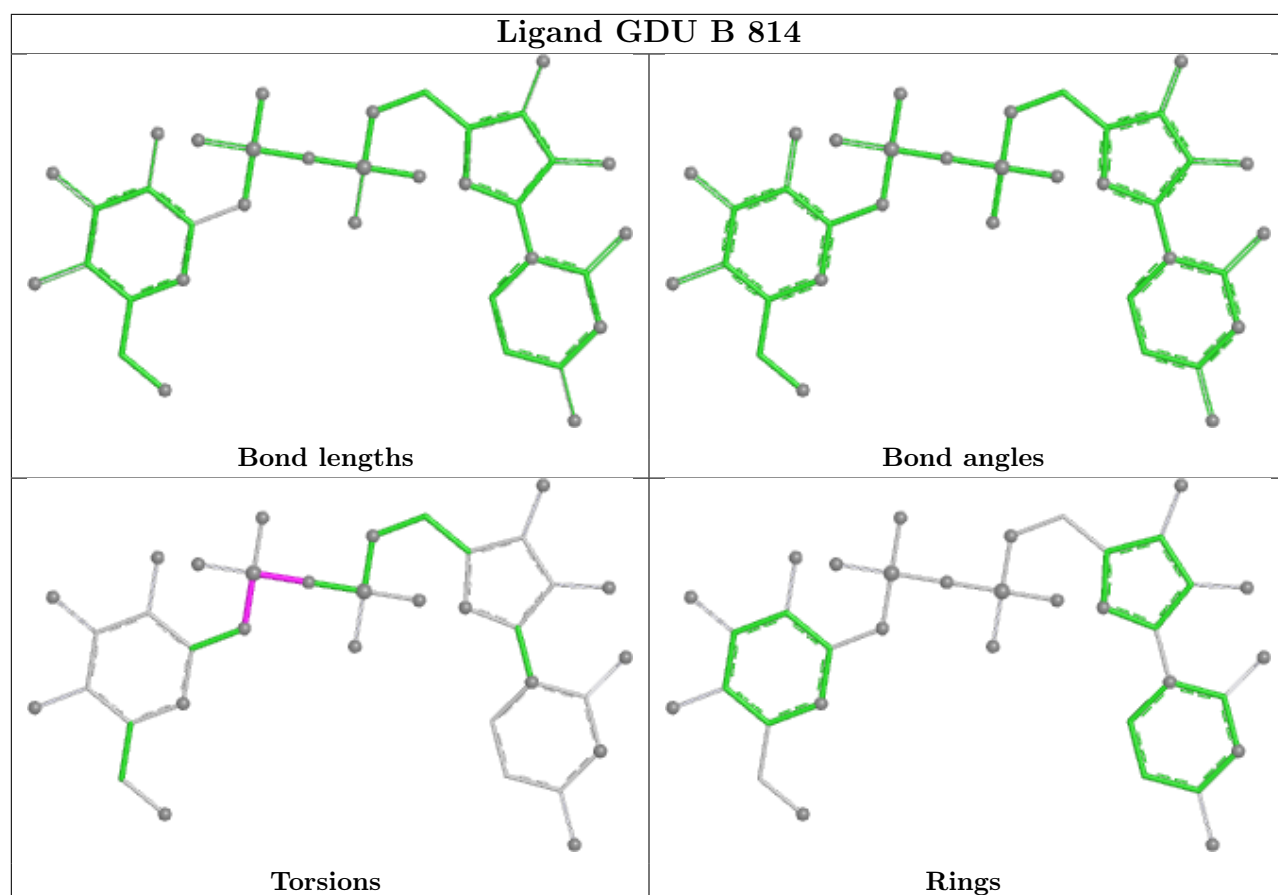
Mol	Chain	Res	Type	Atoms
2	A	802	EDO	O1-C1-C2-O2
2	A	808	EDO	O1-C1-C2-O2
2	A	812	EDO	O1-C1-C2-O2
2	A	813	EDO	O1-C1-C2-O2
2	B	807	EDO	O1-C1-C2-O2
3	A	814	GDU	C1'-O3B-PB-O1B
3	B	814	GDU	C1'-O3B-PB-O2B
2	B	811	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	804	EDO	1	0
2	A	801	EDO	6	0
2	B	801	EDO	5	0
2	A	802	EDO	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	622/622 (100%)	-0.03	3 (0%) 87 90	23, 35, 56, 86	0
1	B	621/622 (99%)	0.03	7 (1%) 78 83	23, 41, 66, 108	0
All	All	1243/1244 (99%)	-0.00	10 (0%) 82 86	23, 38, 62, 108	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	620	GLY	3.6
1	B	317	PHE	3.5
1	B	618	THR	3.2
1	A	0	GLY	2.5
1	B	310	VAL	2.5
1	B	423	LEU	2.3
1	B	619	ASN	2.2
1	B	587	ILE	2.2
1	A	593	LEU	2.2
1	A	310	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

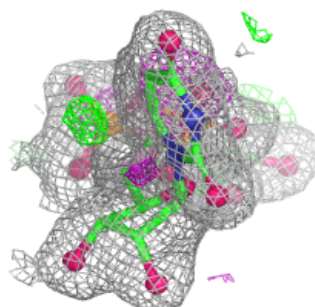
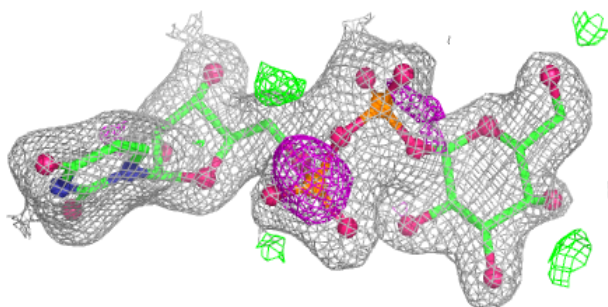
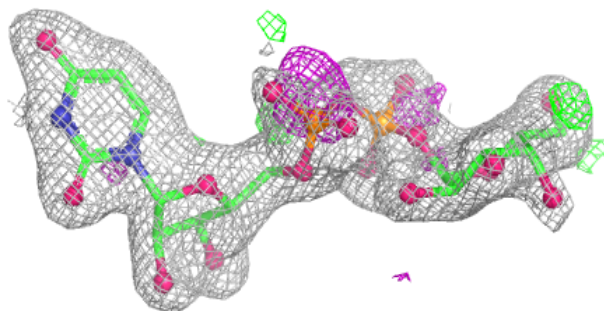
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	B	801	4/4	0.60	0.17	51,61,62,68	0
2	EDO	B	805	4/4	0.66	0.18	61,61,62,63	0
2	EDO	B	809	4/4	0.72	0.20	79,89,91,91	0
2	EDO	A	810	4/4	0.76	0.15	53,57,58,67	0
2	EDO	A	801	4/4	0.77	0.20	44,47,48,63	0
2	EDO	B	808	4/4	0.79	0.13	56,62,63,67	0
2	EDO	B	813	4/4	0.79	0.15	55,59,59,66	0
2	EDO	B	802	4/4	0.80	0.15	57,64,68,76	0
2	EDO	B	807	4/4	0.82	0.15	57,65,67,67	0
2	EDO	A	802	4/4	0.82	0.12	57,72,73,77	0
2	EDO	A	812	4/4	0.82	0.12	59,68,70,72	0
2	EDO	B	811	4/4	0.82	0.15	60,72,74,75	0
2	EDO	A	813	4/4	0.82	0.15	72,73,73,75	0
2	EDO	A	806	4/4	0.83	0.13	47,49,51,53	0
2	EDO	B	803	4/4	0.83	0.14	69,74,74,75	0
2	EDO	A	807	4/4	0.84	0.12	54,55,59,62	0
2	EDO	A	809	4/4	0.84	0.15	81,82,82,86	0
2	EDO	A	808	4/4	0.86	0.15	66,70,72,73	0
2	EDO	A	811	4/4	0.88	0.12	61,64,68,71	0
2	EDO	B	812	4/4	0.88	0.15	58,64,69,71	0
2	EDO	B	810	4/4	0.88	0.12	52,57,60,62	0
2	EDO	A	805	4/4	0.89	0.11	36,47,48,51	0
2	EDO	A	803	4/4	0.90	0.10	48,48,54,57	0
2	EDO	B	806	4/4	0.90	0.15	59,60,61,67	0
2	EDO	B	804	4/4	0.90	0.12	49,56,58,61	0
2	EDO	A	804	4/4	0.91	0.10	52,55,56,56	0
3	GDU	A	814	36/36	0.91	0.08	33,46,59,62	0
3	GDU	B	814	36/36	0.92	0.08	47,54,60,61	0

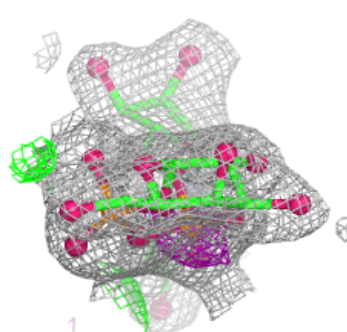
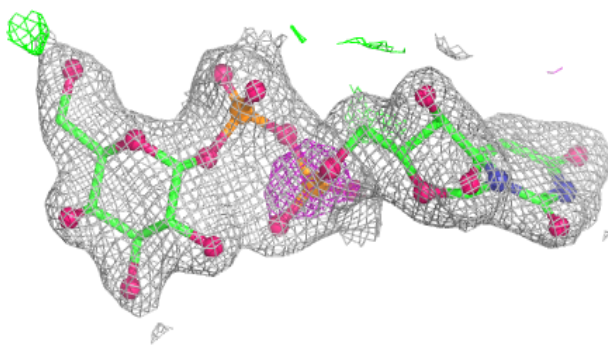
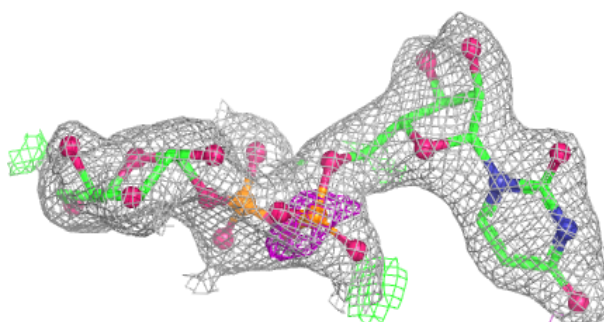
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDU A 814:

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

**Electron density around GDU B 814:**

$2mF_o-DF_c$ (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.