



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:32 AM UTC

PDB ID : 3OY7 / pdb_00003oy7
Title : Crystal structure of a virus encoded glycosyltransferase in complex with GDP-mannose
Authors : Xiang, Y.; Rossmann, M.G.
Deposited on : 2010-09-23
Resolution : 2.73 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

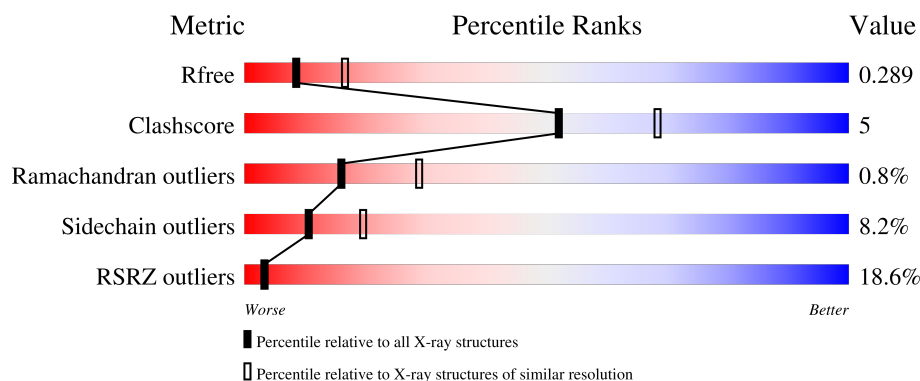
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	413	
1	B	413	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6289 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.

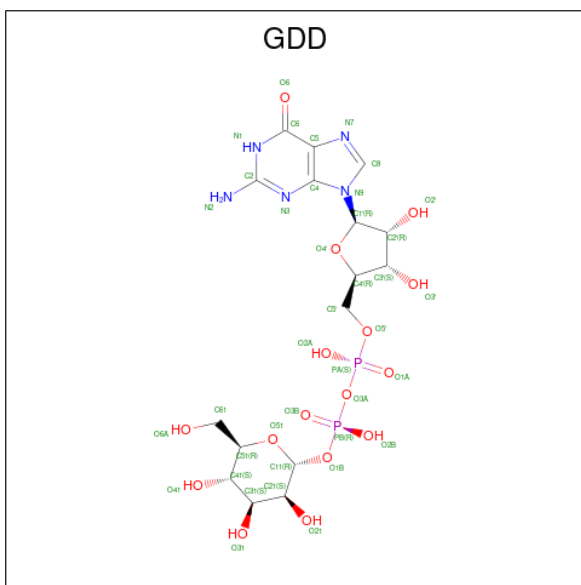
- Molecule 1 is a protein called Glycosyltransferase B736L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3101	1983	531	568	19			
1	B	392	Total	C	N	O	S	0	0	0
			3101	1983	531	568	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	LEU	-	expression tag	UNP A7IXR1
A	407	GLU	-	expression tag	UNP A7IXR1
A	408	HIS	-	expression tag	UNP A7IXR1
A	409	HIS	-	expression tag	UNP A7IXR1
A	410	HIS	-	expression tag	UNP A7IXR1
A	411	HIS	-	expression tag	UNP A7IXR1
A	412	HIS	-	expression tag	UNP A7IXR1
A	413	HIS	-	expression tag	UNP A7IXR1
B	406	LEU	-	expression tag	UNP A7IXR1
B	407	GLU	-	expression tag	UNP A7IXR1
B	408	HIS	-	expression tag	UNP A7IXR1
B	409	HIS	-	expression tag	UNP A7IXR1
B	410	HIS	-	expression tag	UNP A7IXR1
B	411	HIS	-	expression tag	UNP A7IXR1
B	412	HIS	-	expression tag	UNP A7IXR1
B	413	HIS	-	expression tag	UNP A7IXR1

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (CCD ID: GDD) (formula: $C_{16}H_{25}N_5O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 39	C 16	N 5	O 16	P 2	0	0
2	B	1	Total 39	C 16	N 5	O 16	P 2	0	0

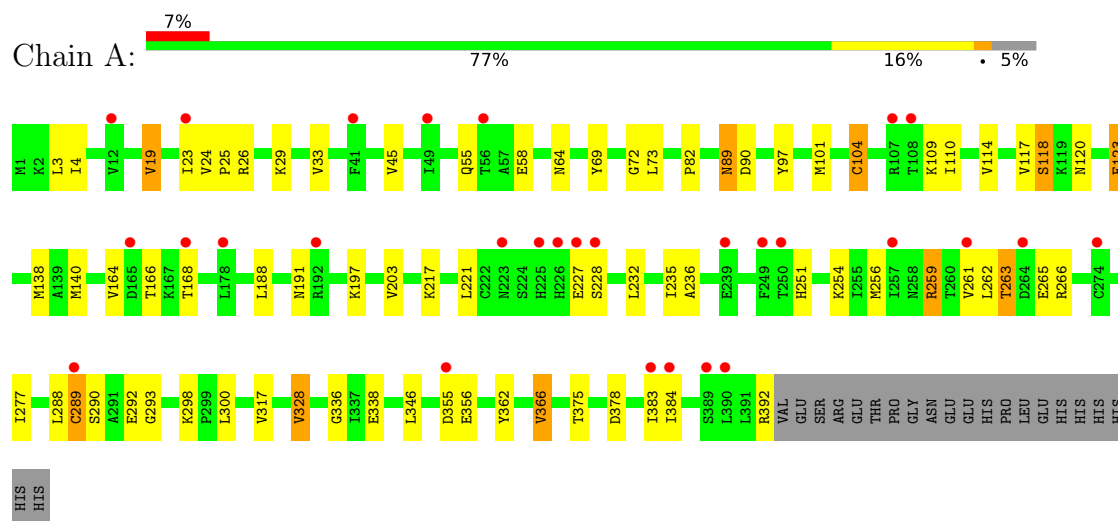
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	4	Total O 4 4	0	0

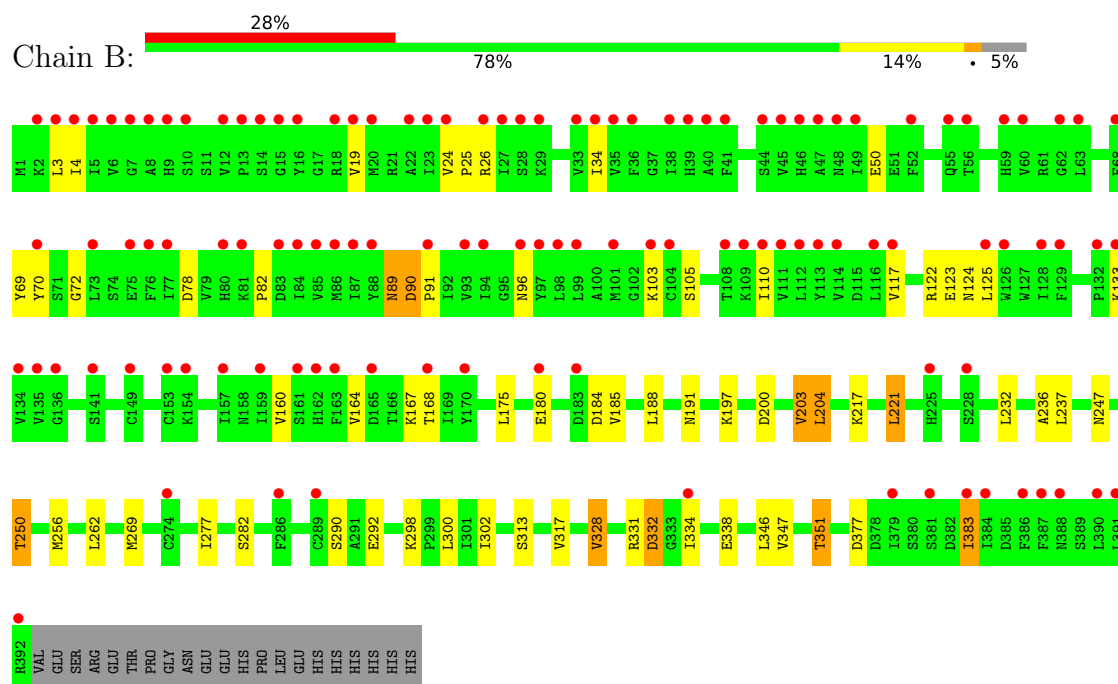
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glycosyltransferase B736L



• Molecule 1: Glycosyltransferase B736L



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.25Å 243.19Å 67.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.19 – 2.73 130.19 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.7 (130.19-2.73) 98.7 (130.19-2.73)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.73Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.290 (Not available) , 0.289	Depositor DCC
R_{free} test set	1701 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6289	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: GDD

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	0.45	0/3168	0.81	1/4284 (0.0%)
1	B	0.45	0/3168	0.81	2/4284 (0.0%)
All	All	0.45	0/6336	0.81	3/8568 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	VAL	CB-CA-C	5.96	116.60	110.70
1	B	90	ASP	CA-C-N	5.46	126.67	119.84
1	B	90	ASP	C-N-CA	5.46	126.67	119.84

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	3101	0	3089	36	0
1	B	3101	0	3089	29	0
2	A	39	0	23	0	0
2	B	39	0	23	0	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6289	0	6224	64	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 (64) 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:191:ASN:HB3	1:A:197:LYS:HG2	1.42	1.01
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.41	0.84
1:B:200:ASP:O	1:B:204:LEU:HB2	1.92	0.70
1:A:259:ARG:HH11	1:A:259:ARG:CG	2.04	0.69
1:A:191:ASN:HB3	1:A:197:LYS:CG	2.23	0.64
1:A:288:LEU:O	1:A:289:CYS:HB2	1.99	0.63
1:A:101:MET:HE2	1:A:110:ILE:HD11	1.81	0.62
1:A:123:GLU:HG2	1:B:237:LEU:HD22	1.80	0.61
1:B:277:ILE:HB	1:B:300:LEU:HD23	1.83	0.60
1:B:89:ASN:HD22	1:B:90:ASP:H	1.48	0.60
1:B:160:VAL:HG13	1:B:383:ILE:HD11	1.85	0.58
1:A:138:MET:HE1	1:A:383:ILE:HG23	1.86	0.57
1:A:164:VAL:CG2	1:A:292:GLU:HG2	2.35	0.56
1:B:221:LEU:HD22	1:B:256:MET:HB2	1.87	0.56
1:A:4:ILE:HD12	1:A:82:PRO:HG3	1.87	0.56
1:B:203:VAL:HG13	1:B:236:ALA:HB2	1.87	0.55
1:B:26:ARG:HD3	1:B:377:ASP:OD1	2.06	0.54
1:A:89:ASN:HD22	1:A:90:ASP:H	1.54	0.54
1:B:191:ASN:HB3	1:B:197:LYS:HD3	1.90	0.54
1:B:347:VAL:O	1:B:351:THR:HG23	2.08	0.53
1:A:101:MET:O	1:A:104:CYS:HB2	2.10	0.52
1:B:282:SER:HB2	1:B:338:GLU:HB3	1.91	0.52
1:B:203:VAL:HG21	1:B:232:LEU:HB3	1.90	0.52
1:B:4:ILE:HG13	1:B:82:PRO:HB3	1.91	0.52
1:B:175:LEU:HB3	1:B:269:MET:HE3	1.90	0.52
1:B:69:TYR:CE2	1:B:72:GLY:HA3	2.46	0.50
1:A:19:VAL:HG23	1:A:23:ILE:HD12	1.94	0.50
1:A:263:THR:HG23	1:A:266:ARG:HG3	1.93	0.49
1:A:55:GLN:O	1:A:58:GLU:HB3	2.12	0.49
1:B:34:ILE:HG22	1:B:50:GLU:HB3	1.95	0.49
1:A:26:ARG:HA	1:A:29:LYS:HE2	1.95	0.48
1:A:277:ILE:HG13	1:A:293:GLY:HA3	1.95	0.48
1:B:4:ILE:HG12	1:B:34:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:VAL:O	1:B:328:VAL:CG1	2.63	0.46
1:A:375:THR:HG23	1:A:378:ASP:H	1.80	0.46
1:B:164:VAL:HG21	1:B:292:GLU:HG2	1.98	0.45
1:A:203:VAL:HG21	1:A:232:LEU:HB3	1.98	0.45
1:A:123:GLU:CD	1:A:123:GLU:H	2.23	0.45
1:A:164:VAL:HG21	1:A:292:GLU:HA	1.98	0.45
1:B:160:VAL:CG1	1:B:383:ILE:HD11	2.46	0.45
1:A:164:VAL:HG21	1:A:292:GLU:HG2	1.98	0.45
1:B:4:ILE:HD12	1:B:82:PRO:HG3	1.99	0.45
1:A:259:ARG:CG	1:A:259:ARG:NH1	2.70	0.44
1:A:290:SER:HB2	1:A:300:LEU:HD13	1.99	0.44
1:B:302:ILE:HG12	1:B:317:VAL:HG11	2.00	0.44
1:A:24:VAL:HB	1:A:25:PRO:HD3	2.00	0.44
1:A:73:LEU:HD22	1:A:97:TYR:CD2	2.53	0.43
1:A:118:SER:HB3	1:A:338:GLU:HG2	2.00	0.43
1:A:288:LEU:O	1:A:289:CYS:CB	2.65	0.43
1:A:392:ARG:HA	1:A:392:ARG:HE	1.83	0.43
1:A:140:MET:HE3	1:A:140:MET:HB2	1.93	0.43
1:A:203:VAL:HG13	1:A:236:ALA:HB2	2.01	0.43
1:B:122:ARG:NH2	1:B:332:ASP:O	2.51	0.43
1:B:110:ILE:HD12	1:B:133:LYS:HB2	2.01	0.43
1:B:70:TYR:CE2	1:B:96:ASN:HB2	2.54	0.42
1:B:78:ASP:CG	1:B:105:SER:HB2	2.44	0.42
1:B:123:GLU:C	1:B:125:LEU:H	2.27	0.42
1:A:120:ASN:O	1:A:336:GLY:HA2	2.20	0.42
1:A:362:TYR:O	1:A:366:VAL:HG22	2.20	0.41
1:A:221:LEU:HD22	1:A:256:MET:HB2	2.02	0.41
1:B:247:ASN:HB3	1:B:250:THR:HG23	2.02	0.41
1:A:251:HIS:HA	1:A:254:LYS:HE3	2.02	0.41
1:B:24:VAL:N	1:B:25:PRO:HD2	2.35	0.41
1:A:69:TYR:CE2	1:A:72:GLY:HA3	2.56	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	390/413 (94%)	374 (96%)	14 (4%)	2 (0%)	24	40
1	B	390/413 (94%)	368 (94%)	18 (5%)	4 (1%)	12	22
All	All	780/826 (94%)	742 (95%)	32 (4%)	6 (1%)	16	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	SER
1	B	290	SER
1	B	313	SER
1	A	289	CYS
1	B	124	ASN
1	B	91	PRO

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	341/361 (94%)	310 (91%)	31 (9%)	9	16
1	B	341/361 (94%)	316 (93%)	25 (7%)	13	24
All	All	682/722 (94%)	626 (92%)	56 (8%)	10	19

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	19	VAL
1	A	33	VAL
1	A	45	VAL
1	A	64	ASN
1	A	89	ASN
1	A	104	CYS

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Mol	Chain	Res	Type
1	A	109	LYS
1	A	114	VAL
1	A	117	VAL
1	A	118	SER
1	A	123	GLU
1	A	166	THR
1	A	168	THR
1	A	188	LEU
1	A	217	LYS
1	A	227	GLU
1	A	235	ILE
1	A	259	ARG
1	A	261	VAL
1	A	262	LEU
1	A	263	THR
1	A	265	GLU
1	A	298	LYS
1	A	317	VAL
1	A	328	VAL
1	A	346	LEU
1	A	355	ASP
1	A	356	GLU
1	A	366	VAL
1	A	384	ILE
1	B	3	LEU
1	B	19	VAL
1	B	89	ASN
1	B	103	LYS
1	B	117	VAL
1	B	167	LYS
1	B	168	THR
1	B	180	GLU
1	B	184	ASP
1	B	185	VAL
1	B	188	LEU
1	B	203	VAL
1	B	204	LEU
1	B	217	LYS
1	B	221	LEU
1	B	250	THR
1	B	262	LEU
1	B	298	LYS

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Mol	Chain	Res	Type
1	B	328	VAL
1	B	331	ARG
1	B	332	ASP
1	B	334	ILE
1	B	346	LEU
1	B	351	THR
1	B	383	ILE

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	80	HIS
1	A	89	ASN
1	A	106	HIS
1	A	158	ASN
1	A	191	ASN
1	A	226	HIS
1	A	367	GLN
1	B	39	HIS
1	B	55	GLN
1	B	89	ASN
1	B	158	ASN
1	B	388	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](#)

2 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	GDD	A	414	-	41,42,42	1.40	4 (9%)	62,65,65	1.79	13 (20%)
2	GDD	B	414	-	41,42,42	1.15	4 (9%)	62,65,65	1.65	12 (19%)

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	GDD	A	414	-	-	8/23/59/59	0/4/4/4
2	GDD	B	414	-	-	4/23/59/59	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	414	GDD	PA-O3A	4.64	1.64	1.59
2	A	414	GDD	PB-O3A	3.91	1.63	1.59
2	B	414	GDD	C5-N7	-2.82	1.33	1.39
2	B	414	GDD	PB-O3A	2.74	1.62	1.59
2	A	414	GDD	C5-N7	-2.69	1.33	1.39
2	A	414	GDD	O51-C11	2.45	1.48	1.41
2	B	414	GDD	O51-C11	2.13	1.47	1.41
2	B	414	GDD	PA-O3A	2.03	1.61	1.59

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	414	GDD	C2-N3-C4	5.24	121.33	112.30
2	A	414	GDD	O51-C51-C41	5.24	119.15	109.70
2	A	414	GDD	C2-N3-C4	5.18	121.22	112.30
2	B	414	GDD	C5-C4-N3	-4.90	120.59	128.39
2	A	414	GDD	C5-C4-N3	-4.83	120.70	128.39
2	A	414	GDD	O51-C11-O1B	4.10	116.72	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	414	GDD	O51-C51-C41	4.01	116.92	109.70
2	A	414	GDD	C11-O51-C51	3.85	121.25	113.72
2	B	414	GDD	C2-N1-C6	-3.30	119.12	125.11
2	B	414	GDD	C11-O51-C51	3.20	119.98	113.72
2	A	414	GDD	C2-N1-C6	-3.17	119.36	125.11
2	A	414	GDD	N9-C4-N3	3.17	132.28	125.95
2	B	414	GDD	N9-C4-N3	3.09	132.13	125.95
2	A	414	GDD	C4'-O4'-C1'	-2.93	102.99	109.47
2	B	414	GDD	O51-C11-C21	2.65	115.82	110.37
2	B	414	GDD	C8-N7-C5	2.34	108.43	104.26
2	B	414	GDD	C4-C5-N7	-2.32	107.00	110.67
2	B	414	GDD	N9-C8-N7	-2.29	109.15	113.40
2	B	414	GDD	C5-C6-N1	2.14	118.71	113.25
2	A	414	GDD	C4-C5-N7	-2.12	107.31	110.67
2	A	414	GDD	C5-C6-N1	2.10	118.60	113.25
2	A	414	GDD	C8-N7-C5	2.10	107.99	104.26
2	B	414	GDD	O6-C6-C5	-2.06	121.10	126.53
2	A	414	GDD	N9-C8-N7	-2.04	109.61	113.40
2	A	414	GDD	O6-C6-C5	-2.02	121.19	126.53

There are no chirality outliers.

All (12) torsion outliers are listed below:

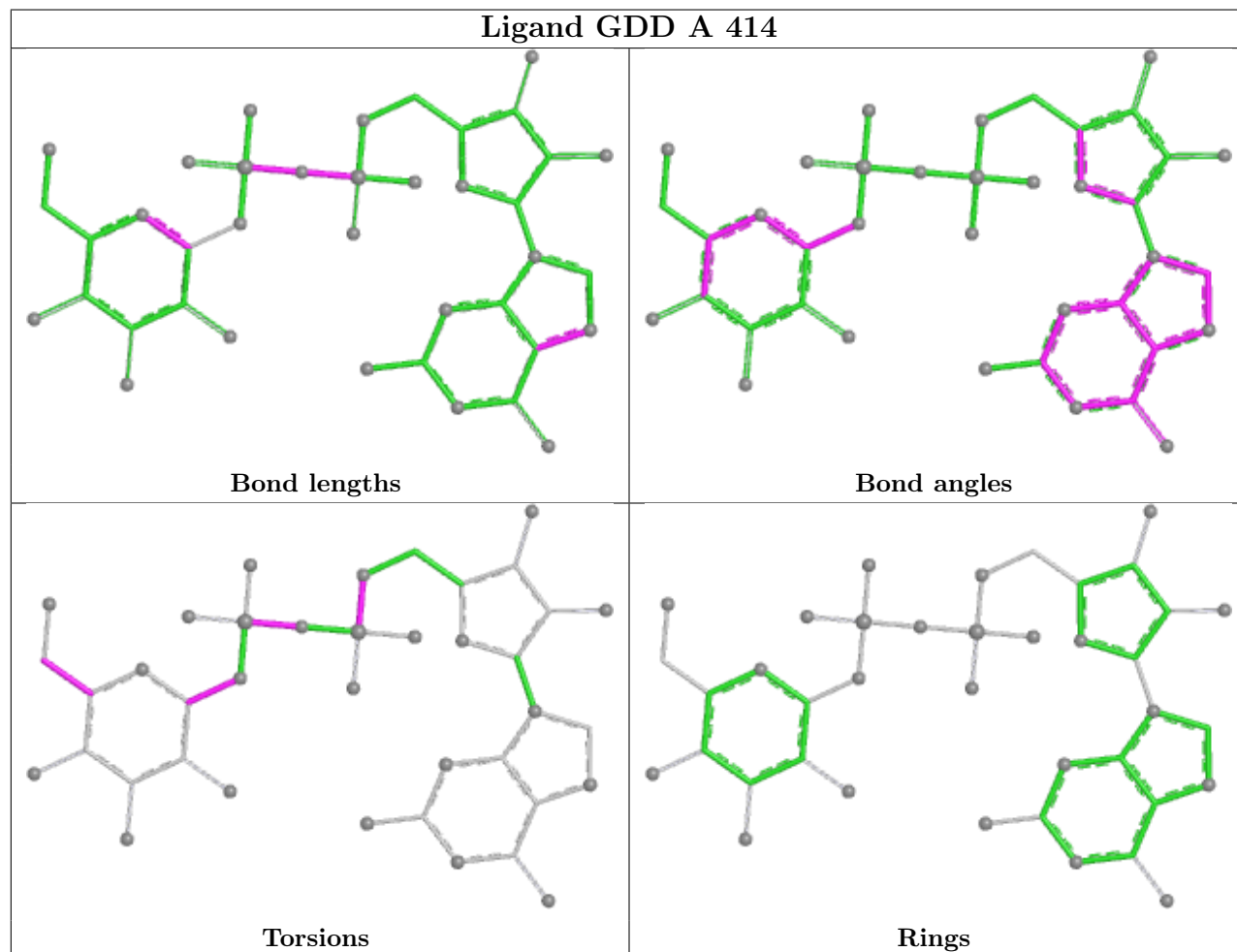
Mol	Chain	Res	Type	Atoms
2	A	414	GDD	C5'-O5'-PA-O1A
2	A	414	GDD	C5'-O5'-PA-O2A
2	A	414	GDD	C5'-O5'-PA-O3A
2	A	414	GDD	O51-C11-O1B-PB
2	B	414	GDD	C11-O1B-PB-O3A
2	A	414	GDD	O51-C51-C61-O6A
2	A	414	GDD	C41-C51-C61-O6A
2	B	414	GDD	O4'-C4'-C5'-O5'
2	B	414	GDD	C3'-C4'-C5'-O5'
2	A	414	GDD	PA-O3A-PB-O3B
2	B	414	GDD	C21-C11-O1B-PB
2	A	414	GDD	PA-O3A-PB-O2B

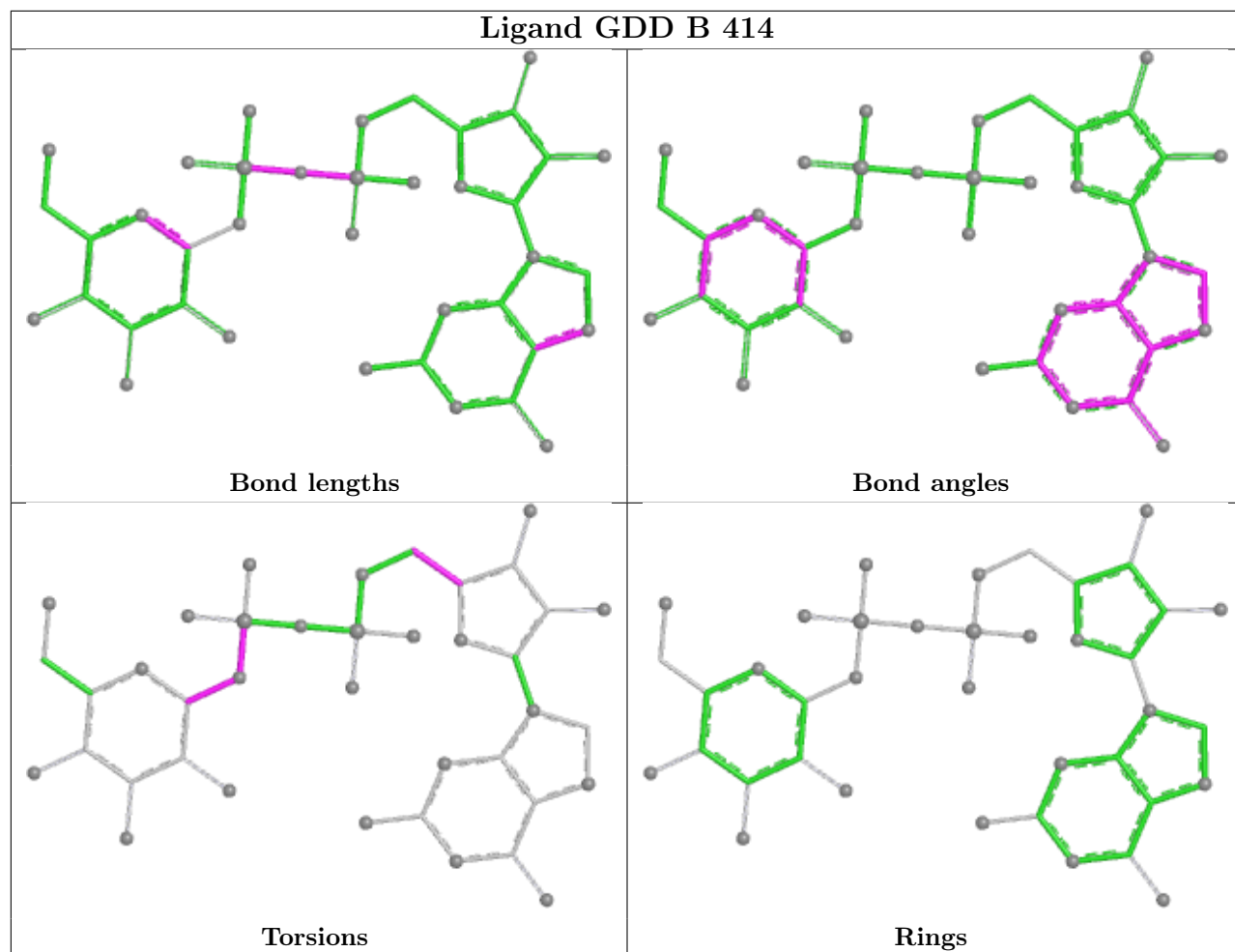
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	392/413 (94%)	0.56	29 (7%)	20 20	46, 68, 108, 136	0
1	B	392/413 (94%)	1.35	117 (29%)	1 1	47, 101, 214, 246	0
All	All	784/826 (94%)	0.95	146 (18%)	3 3	46, 79, 193, 246	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	97	TYR	7.6
1	B	27	ILE	6.5
1	B	86	MET	6.1
1	B	23	ILE	5.8
1	B	33	VAL	5.3
1	B	87	ILE	5.0
1	B	3	LEU	5.0
1	B	99	LEU	5.0
1	B	34	ILE	5.0
1	B	84	ILE	5.0
1	B	109	LYS	5.0
1	B	24	VAL	5.0
1	B	6	VAL	4.9
1	B	114	VAL	4.8
1	B	45	VAL	4.5
1	B	85	VAL	4.5
1	B	35	VAL	4.5
1	B	15	GLY	4.4
1	B	20	MET	4.3
1	B	98	LEU	4.2
1	A	226	HIS	4.1
1	B	49	ILE	4.0
1	B	387	PHE	4.0
1	B	39	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	391	LEU	3.8
1	B	59	HIS	3.7
1	B	384	ILE	3.7
1	B	8	ALA	3.6
1	B	108	THR	3.6
1	B	103	LYS	3.6
1	B	4	ILE	3.5
1	B	94	ILE	3.5
1	A	261	VAL	3.5
1	B	46	HIS	3.5
1	B	41	PHE	3.5
1	B	149	CYS	3.4
1	B	390	LEU	3.3
1	B	36	PHE	3.3
1	B	5	ILE	3.3
1	B	80	HIS	3.2
1	B	55	GLN	3.2
1	B	16	TYR	3.2
1	B	29	LYS	3.2
1	B	392	ARG	3.1
1	B	101	MET	3.1
1	B	125	LEU	3.1
1	B	183	ASP	3.1
1	A	23	ILE	3.1
1	A	274	CYS	3.1
1	B	44	SER	3.1
1	A	390	LEU	3.0
1	B	154	LYS	3.0
1	B	77	ILE	3.0
1	B	76	PHE	2.9
1	A	228	SER	2.9
1	B	22	ALA	2.9
1	B	7	GLY	2.9
1	B	110	ILE	2.9
1	B	52	PHE	2.8
1	B	383	ILE	2.8
1	B	60	VAL	2.7
1	B	274	CYS	2.7
1	A	41	PHE	2.7
1	B	12	VAL	2.7
1	B	135	VAL	2.7
1	B	116	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	129	PHE	2.7
1	B	165	ASP	2.7
1	B	132	PRO	2.7
1	B	38	ILE	2.7
1	B	379	ILE	2.7
1	B	10	SER	2.6
1	B	13	PRO	2.6
1	B	83	ASP	2.6
1	B	170	TYR	2.6
1	A	249	PHE	2.6
1	B	126	TRP	2.6
1	B	113	TYR	2.6
1	A	250	THR	2.5
1	B	162	HIS	2.5
1	B	117	VAL	2.5
1	B	28	SER	2.5
1	A	225	HIS	2.5
1	B	88	TYR	2.5
1	B	163	PHE	2.5
1	A	56	THR	2.5
1	A	289	CYS	2.5
1	B	96	ASN	2.5
1	B	73	LEU	2.5
1	B	91	PRO	2.4
1	A	12	VAL	2.4
1	B	128	ILE	2.4
1	B	18	ARG	2.4
1	B	56	THR	2.4
1	A	239	GLU	2.4
1	B	141	SER	2.4
1	B	2	LYS	2.4
1	B	40	ALA	2.4
1	B	68	PHE	2.4
1	B	63	LEU	2.3
1	A	49	ILE	2.3
1	B	136	GLY	2.3
1	B	14	SER	2.3
1	B	228	SER	2.3
1	B	112	LEU	2.3
1	B	75	GLU	2.3
1	A	355	ASP	2.3
1	B	26	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	257	ILE	2.3
1	B	168	THR	2.3
1	B	388	ASN	2.3
1	B	19	VAL	2.3
1	B	93	VAL	2.3
1	B	334	ILE	2.2
1	B	48	ASN	2.2
1	B	133	LYS	2.2
1	B	286	PHE	2.2
1	B	62	GLY	2.2
1	B	381	SER	2.2
1	A	107	ARG	2.2
1	A	192	ARG	2.2
1	B	9	HIS	2.2
1	B	70	TYR	2.2
1	A	389	SER	2.2
1	B	134	VAL	2.2
1	B	180	GLU	2.1
1	A	168	THR	2.1
1	B	81	LYS	2.1
1	B	289	CYS	2.1
1	B	161	SER	2.1
1	A	383	ILE	2.1
1	A	264	ASP	2.1
1	B	47	ALA	2.1
1	A	108	THR	2.1
1	B	104	CYS	2.1
1	B	159	ILE	2.1
1	B	111	VAL	2.1
1	B	386	PHE	2.1
1	A	227	GLU	2.0
1	B	153	CYS	2.0
1	A	165	ASP	2.0
1	A	178	LEU	2.0
1	B	225	HIS	2.0
1	A	223	ASN	2.0
1	A	384	ILE	2.0
1	B	157	ILE	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](#)

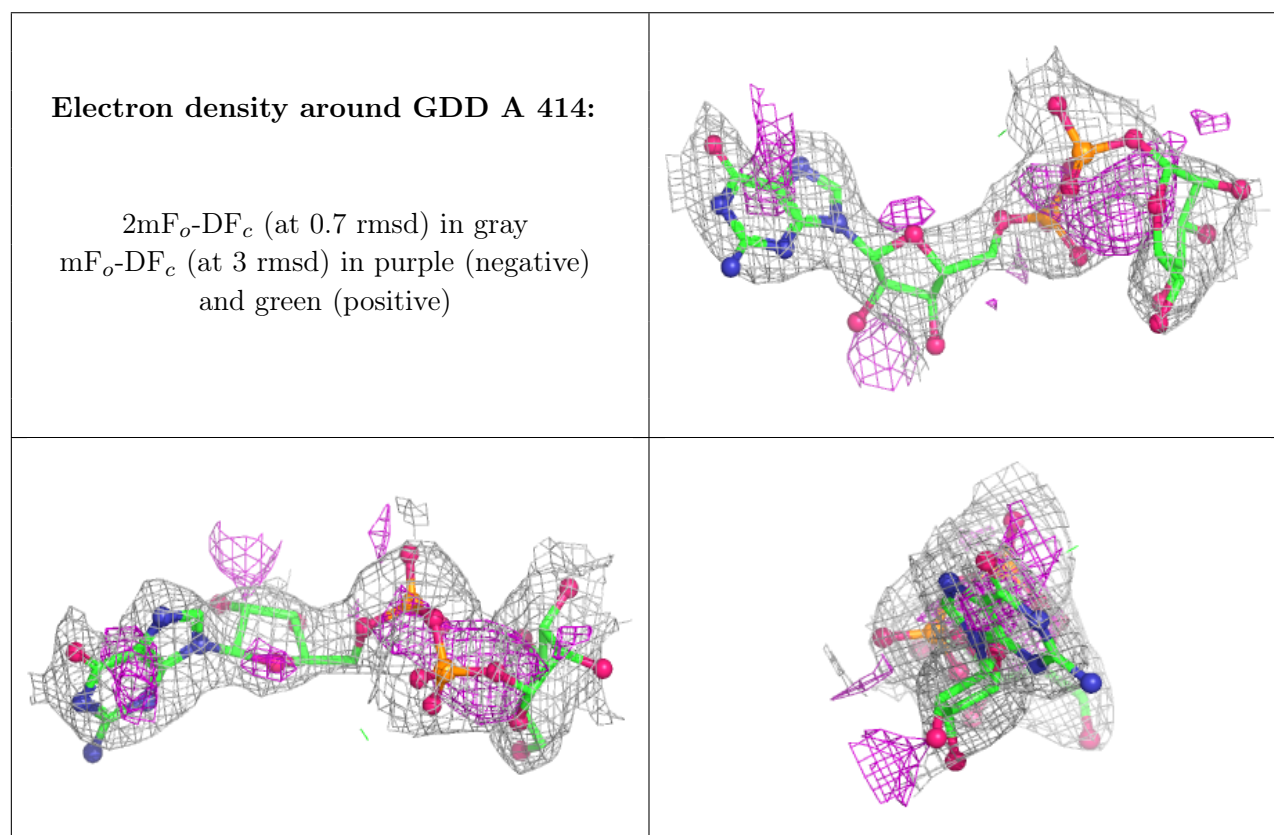
There are no oligosaccharides in this entry.

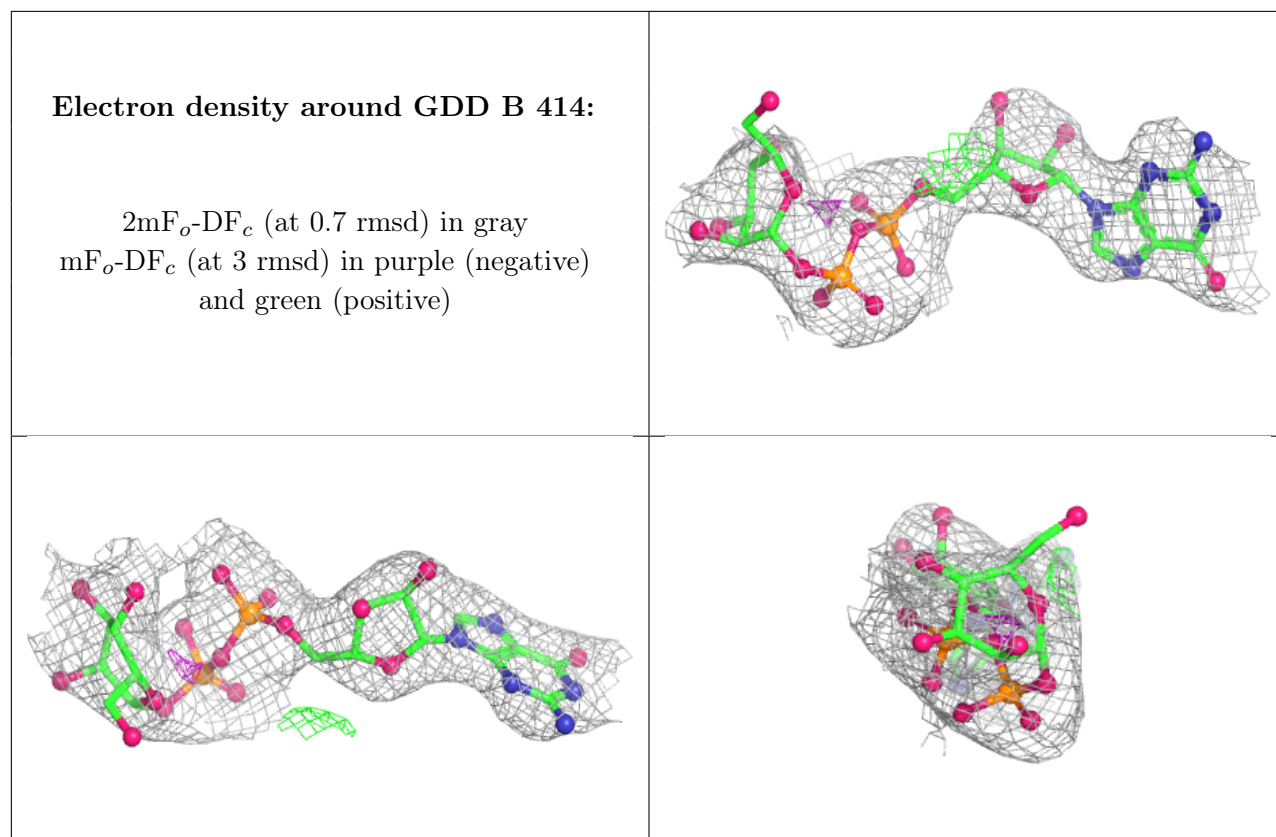
6.4 Ligands [i](#)

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	GDD	A	414	39/39	0.81	0.14	86,88,90,90	0
2	GDD	B	414	39/39	0.84	0.12	99,101,101,101	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.