



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:46 am BST

PDB ID : 6EGS  
Title : Crystal structure of the GalNAc-T2 F104S mutant in complex with UDP-GalNAc  
Authors : de las Rivas, M.; Coelho, H.; Diniz, A.; Lira-Navarrete, E.; Jimenez-Barbero, J.; Schjoldager, K.T.; Bennett, E.P.; Vakhrushev, S.Y.; Clausen, H.; Corzana, F.; Marcelo, F.; Hurtado-Guerrero, R.  
Deposited on : 2017-09-12  
Resolution : 2.70 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

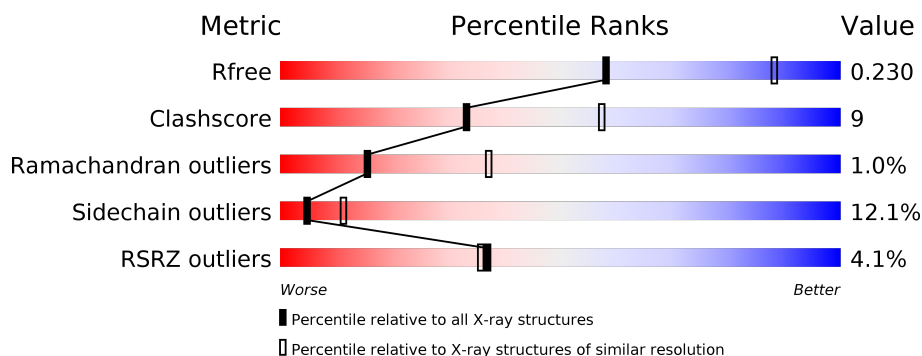
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	503	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	B	503	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>5%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7662 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 Polypeptide N-acetylgalactosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3806	2401	686	696	23			
1	B	467	Total	C	N	O	S	0	0	0
			3716	2343	672	678	23			

There are 14 discrepancies between the modelled and reference sequences:

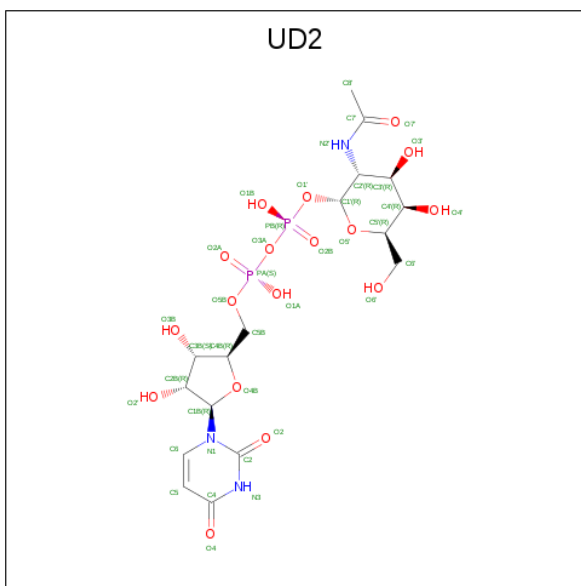
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LYS	-	expression tag	UNP Q10471
A	70	ARG	-	expression tag	UNP Q10471
A	71	GLU	-	expression tag	UNP Q10471
A	72	ALA	-	expression tag	UNP Q10471
A	73	GLU	-	expression tag	UNP Q10471
A	74	ALA	-	expression tag	UNP Q10471
A	104	SER	PHE	engineered mutation	UNP Q10471
B	69	LYS	-	expression tag	UNP Q10471
B	70	ARG	-	expression tag	UNP Q10471
B	71	GLU	-	expression tag	UNP Q10471
B	72	ALA	-	expression tag	UNP Q10471
B	73	GLU	-	expression tag	UNP Q10471
B	74	ALA	-	expression tag	UNP Q10471
B	104	SER	PHE	engineered mutation	UNP Q10471

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGALACTOSAMINE (three-letter

code: UD2) (formula:  $\text{C}_{17}\text{H}_{27}\text{N}_3\text{O}_{17}\text{P}_2$ ).



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

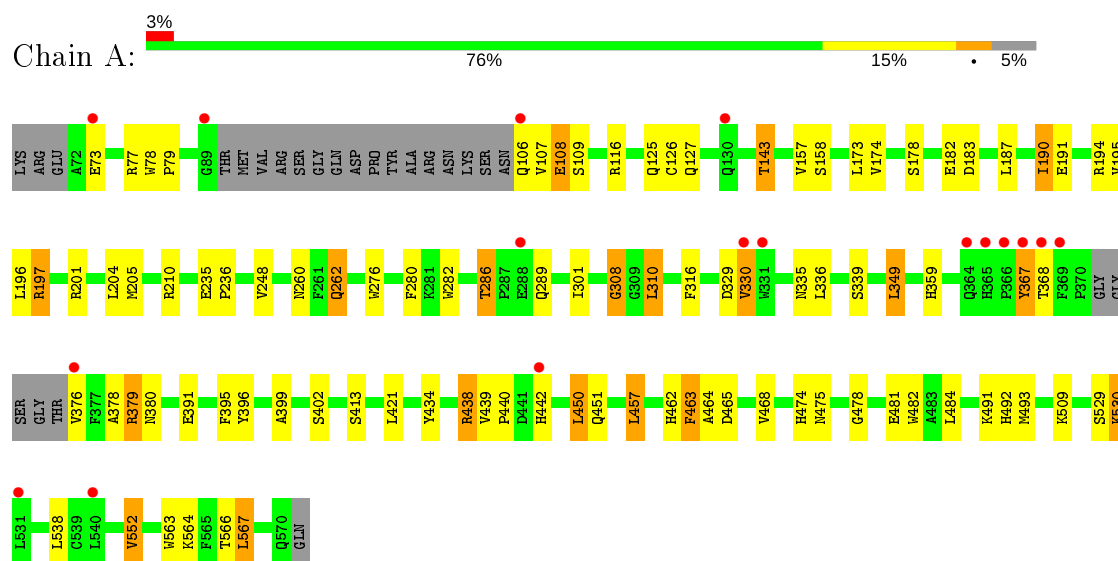
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	B	34	Total O 34 34	0	0

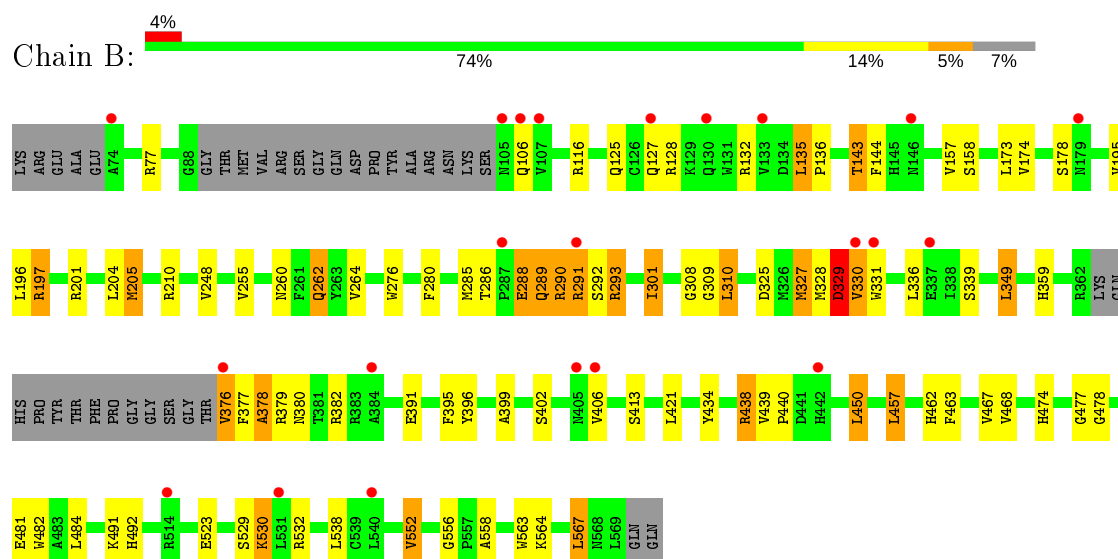
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Polypeptide N-acetylgalactosaminyltransferase 2



- Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.04Å 154.04Å 109.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.04 – 2.70 19.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (154.04-2.70) 100.0 (19.91-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.206 , 0.221 0.216 , 0.230	Depositor DCC
$R_{free}$ test set	1952 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: UD2, MN

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	0.60	0/3893	0.76	1/5270 (0.0%)
1	B	0.60	0/3798	0.75	3/5139 (0.1%)
All	All	0.60	0/7691	0.76	4/10409 (0.0%)

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	1	0
1	B	1	0
All	All	2	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	PHE	N-CA-C	7.15	130.31	111.00
1	B	331	TRP	N-CA-C	-6.19	94.30	111.00
1	B	463	PHE	N-CA-C	5.21	125.06	111.00
1	B	329	ASP	N-CA-C	5.18	124.99	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	143	THR	CB
1	B	143	THR	CB

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	3806	0	3705	55	0
1	B	3716	0	3631	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	39	0	25	5	0
3	B	39	0	25	16	0
4	A	26	0	0	1	0
4	B	34	0	0	1	0
All	All	7662	0	7386	129	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 9.

All (129) 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:B:135:LEU:HB3	1:B:136:PRO:HD2	1.31	1.13
1:B:359:HIS:CE1	3:B:602:UD2:H8'2	1.88	1.07
1:B:359:HIS:NE2	3:B:602:UD2:C8'	2.19	1.06
1:A:329:ASP:OD2	1:A:380:ASN:ND2	1.93	1.01
1:B:359:HIS:NE2	3:B:602:UD2:H8'3	1.75	1.00
1:B:289:GLN:HA	1:B:289:GLN:HE21	1.32	0.93
1:B:309:GLY:HA3	3:B:602:UD2:O3'	1.70	0.92
1:B:359:HIS:CD2	3:B:602:UD2:H8'3	2.05	0.91
1:B:359:HIS:CD2	3:B:602:UD2:C8'	2.54	0.91
1:A:286:THR:HB	1:A:289:GLN:H	1.40	0.86
1:B:329:ASP:H	1:B:380:ASN:HD21	1.24	0.83
1:B:359:HIS:CE1	3:B:602:UD2:C8'	2.60	0.83
1:B:330:VAL:HG23	3:B:602:UD2:O4	1.82	0.79
1:B:285:MET:HB3	1:B:289:GLN:CG	2.13	0.78
1:B:359:HIS:NE2	3:B:602:UD2:H8'2	1.94	0.78
1:B:135:LEU:HB3	1:B:136:PRO:CD	2.13	0.77
1:B:135:LEU:CB	1:B:136:PRO:HD2	2.13	0.76
1:A:493:MET:CE	1:B:290:ARG:NH2	2.50	0.75
3:B:602:UD2:O2B	3:B:602:UD2:N2'	2.13	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:OG1	1:A:289:GLN:HB2	1.87	0.75
1:A:376:VAL:HG11	4:A:704:HOH:O	1.87	0.74
1:B:289:GLN:HE21	1:B:289:GLN:CA	2.01	0.74
1:B:558:ALA:O	4:B:701:HOH:O	2.07	0.73
1:A:493:MET:HE1	1:B:290:ARG:NH2	2.07	0.70
1:A:464:ALA:HB1	1:B:255:VAL:HG21	1.74	0.69
1:A:178:SER:O	1:A:197:ARG:NH2	2.29	0.66
1:A:260:ASN:OD1	1:A:262:GLN:HB2	1.96	0.65
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.31	0.65
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.32	0.65
1:B:285:MET:HB3	1:B:289:GLN:HB3	1.78	0.65
1:B:178:SER:O	1:B:197:ARG:NH2	2.30	0.65
1:B:530:LYS:NZ	1:B:556:GLY:O	2.30	0.65
1:B:286:THR:O	1:B:289:GLN:HB2	1.98	0.64
3:B:602:UD2:PA	3:B:602:UD2:H3B	2.39	0.62
1:A:108:GLU:HG3	1:A:108:GLU:O	1.98	0.62
1:B:310:LEU:HD23	1:B:310:LEU:N	2.15	0.61
1:A:438:ARG:NH1	1:A:481:GLU:OE2	2.33	0.61
1:B:286:THR:N	1:B:289:GLN:HB2	2.17	0.60
1:B:329:ASP:N	1:B:380:ASN:HD21	1.98	0.60
1:B:260:ASN:OD1	1:B:262:GLN:HB2	2.00	0.60
1:B:309:GLY:HA3	3:B:602:UD2:HO3'	1.67	0.59
3:B:602:UD2:HN2'	3:B:602:UD2:PB	2.25	0.59
1:B:285:MET:HB3	1:B:289:GLN:CB	2.33	0.59
1:A:330:VAL:O	1:A:330:VAL:HG22	2.03	0.58
1:B:438:ARG:NH1	1:B:481:GLU:OE2	2.36	0.58
1:A:330:VAL:HG13	1:A:330:VAL:O	2.04	0.58
1:B:285:MET:HB3	1:B:289:GLN:HG2	1.85	0.58
1:A:493:MET:HE2	1:B:290:ARG:NH2	2.18	0.57
1:A:329:ASP:H	1:A:380:ASN:HD21	1.53	0.56
1:A:464:ALA:HB1	1:B:255:VAL:CG2	2.36	0.56
1:A:329:ASP:N	1:A:329:ASP:OD2	2.39	0.56
1:A:330:VAL:HG22	3:A:602:UD2:O2'	2.07	0.55
1:B:144:PHE:HA	3:B:602:UD2:O2'	2.06	0.55
1:B:289:GLN:HA	1:B:289:GLN:NE2	2.13	0.55
1:A:464:ALA:CB	1:B:255:VAL:HG21	2.36	0.54
1:B:376:VAL:O	1:B:376:VAL:HG23	2.08	0.54
1:B:280:PHE:CD2	1:B:280:PHE:C	2.82	0.53
1:B:538:LEU:HB3	1:B:552:VAL:HG22	1.89	0.53
1:A:538:LEU:HB3	1:A:552:VAL:HG22	1.90	0.52
1:A:310:LEU:HD23	1:A:310:LEU:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLY:CA	3:B:602:UD2:O3'	2.52	0.52
3:B:602:UD2:N2'	3:B:602:UD2:PB	2.84	0.51
1:B:293:ARG:HH12	1:B:301:ILE:HG22	1.76	0.51
1:B:286:THR:O	1:B:289:GLN:CB	2.58	0.51
1:B:285:MET:CA	1:B:289:GLN:HG2	2.42	0.50
1:B:143:THR:HG22	1:B:174:VAL:HB	1.94	0.50
1:B:450:LEU:HD13	1:B:563:TRP:CE3	2.47	0.49
1:A:359:HIS:CD2	3:A:602:UD2:H8'2	2.48	0.49
1:B:289:GLN:NE2	1:B:289:GLN:CA	2.72	0.49
1:A:282:TRP:HZ2	1:A:367:TYR:CE1	2.30	0.49
1:A:280:PHE:CD2	1:A:280:PHE:C	2.86	0.49
1:A:329:ASP:OD2	1:A:380:ASN:CG	2.51	0.49
1:B:378:ALA:HB1	1:B:406:VAL:HG11	1.95	0.48
1:A:395:PHE:CE2	1:A:440:PRO:HG2	2.48	0.48
1:A:286:THR:CB	1:A:289:GLN:HB2	2.44	0.48
1:A:143:THR:HG22	1:A:174:VAL:HB	1.95	0.47
1:B:395:PHE:CE2	1:B:440:PRO:HG2	2.49	0.47
1:A:399:ALA:HB2	1:A:567:LEU:HD22	1.95	0.47
1:A:359:HIS:CD2	3:A:602:UD2:C8'	2.98	0.47
1:A:478:GLY:O	1:A:492:HIS:HE1	1.98	0.47
1:A:450:LEU:HD13	1:A:563:TRP:CE3	2.50	0.46
1:A:330:VAL:CG2	3:A:602:UD2:O2'	2.63	0.46
1:B:286:THR:N	1:B:289:GLN:CB	2.79	0.46
1:A:308:GLY:HA2	1:A:335:ASN:ND2	2.31	0.46
1:B:291:ARG:CZ	1:B:291:ARG:HB3	2.44	0.46
1:A:107:VAL:C	1:A:109:SER:N	2.70	0.45
1:A:276:TRP:O	1:A:396:TYR:HA	2.16	0.45
1:B:399:ALA:HB2	1:B:567:LEU:HD22	1.98	0.45
1:B:478:GLY:O	1:B:492:HIS:HE1	2.00	0.45
1:B:325:ASP:O	1:B:328:MET:HB2	2.17	0.45
1:B:377:PHE:CD1	1:B:377:PHE:O	2.70	0.45
1:A:493:MET:HE1	1:B:290:ARG:HH21	1.81	0.45
1:B:286:THR:H	1:B:289:GLN:HG2	1.81	0.45
1:B:293:ARG:NH1	1:B:301:ILE:HG22	2.31	0.44
1:A:107:VAL:C	1:A:109:SER:H	2.20	0.44
1:B:248:VAL:HB	1:B:349:LEU:HD12	1.98	0.44
1:A:465:ASP:O	1:A:509:LYS:CE	2.66	0.44
1:B:288:GLU:HG2	1:B:288:GLU:H	1.55	0.44
1:B:285:MET:HA	1:B:289:GLN:HG2	2.00	0.44
1:B:378:ALA:O	1:B:382:ARG:N	2.40	0.44
1:B:276:TRP:O	1:B:396:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:MET:CB	1:B:289:GLN:HG2	2.46	0.43
1:B:529:SER:C	1:B:530:LYS:HG2	2.39	0.43
1:A:248:VAL:HB	1:A:349:LEU:HD12	2.00	0.43
1:B:328:MET:HG2	1:B:380:ASN:ND2	2.33	0.43
1:A:359:HIS:NE2	3:A:602:UD2:H8'2	2.34	0.42
1:B:462:HIS:HD2	1:B:467:VAL:O	2.02	0.42
1:B:378:ALA:CB	1:B:406:VAL:HG11	2.50	0.42
1:A:378:ALA:O	1:A:379:ARG:C	2.58	0.42
1:B:327:MET:HE2	1:B:327:MET:HB3	1.65	0.42
1:A:529:SER:C	1:A:530:LYS:HG2	2.40	0.42
1:B:290:ARG:HA	1:B:293:ARG:HG3	2.02	0.42
1:B:135:LEU:CB	1:B:136:PRO:CD	2.76	0.41
1:B:523:GLU:OE1	1:B:532:ARG:NH2	2.53	0.41
1:A:194:ARG:HB3	1:A:194:ARG:HE	1.69	0.41
1:B:301:ILE:HD13	1:B:301:ILE:HG21	1.84	0.41
1:B:339:SER:HA	1:B:349:LEU:HD21	2.03	0.41
1:A:235:GLU:N	1:A:236:PRO:CD	2.84	0.41
1:A:451:GLN:OE1	1:A:566:THR:HG22	2.21	0.41
1:A:78:TRP:CG	1:A:79:PRO:HD3	2.56	0.41
1:A:339:SER:HA	1:A:349:LEU:HD21	2.03	0.41
1:A:465:ASP:HB2	1:B:264:VAL:HG11	2.02	0.41
1:A:191:GLU:O	1:A:191:GLU:HG3	2.21	0.40
1:A:182:GLU:O	1:A:183:ASP:C	2.60	0.40
1:A:126:CYS:O	1:A:127:GLN:C	2.60	0.40
1:A:493:MET:CE	1:B:290:ARG:HH21	2.28	0.40
1:B:205:MET:HE3	1:B:328:MET:O	2.20	0.40
1:B:286:THR:H	1:B:289:GLN:CG	2.35	0.40
1:A:187:LEU:O	1:A:190:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	472/503 (94%)	445 (94%)	22 (5%)	5 (1%)	14	34
1	B	461/503 (92%)	435 (94%)	22 (5%)	4 (1%)	17	40
All	All	933/1006 (93%)	880 (94%)	44 (5%)	9 (1%)	15	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	ASP
1	B	378	ALA
1	A	73	GLU
1	A	330	VAL
1	A	463	PHE
1	A	108	GLU
1	B	477	GLY
1	B	308	GLY
1	A	308	GLY

### 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	406/434 (94%)	360 (89%)	46 (11%)	6	13
1	B	397/434 (92%)	346 (87%)	51 (13%)	4	10
All	All	803/868 (92%)	706 (88%)	97 (12%)	5	11

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	106	GLN
1	A	116	ARG
1	A	125	GLN
1	A	143	THR
1	A	157	VAL
1	A	158	SER

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Mol	Chain	Res	Type
1	A	173	LEU
1	A	190	ILE
1	A	195	VAL
1	A	196	LEU
1	A	197	ARG
1	A	201	ARG
1	A	204	LEU
1	A	205	MET
1	A	210	ARG
1	A	262	GLN
1	A	286	THR
1	A	301	ILE
1	A	310	LEU
1	A	316	PHE
1	A	336	LEU
1	A	349	LEU
1	A	367	TYR
1	A	368	THR
1	A	379	ARG
1	A	391	GLU
1	A	402	SER
1	A	413	SER
1	A	421	LEU
1	A	434	TYR
1	A	438	ARG
1	A	439	VAL
1	A	442	HIS
1	A	450	LEU
1	A	457	LEU
1	A	462	HIS
1	A	468	VAL
1	A	474	HIS
1	A	475	ASN
1	A	484	LEU
1	A	491	LYS
1	A	530	LYS
1	A	552	VAL
1	A	564	LYS
1	A	567	LEU
1	B	77	ARG
1	B	106	GLN
1	B	116	ARG

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Mol	Chain	Res	Type
1	B	125	GLN
1	B	127	GLN
1	B	128	ARG
1	B	132	ARG
1	B	135	LEU
1	B	143	THR
1	B	157	VAL
1	B	158	SER
1	B	173	LEU
1	B	195	VAL
1	B	196	LEU
1	B	197	ARG
1	B	201	ARG
1	B	204	LEU
1	B	205	MET
1	B	210	ARG
1	B	262	GLN
1	B	288	GLU
1	B	289	GLN
1	B	290	ARG
1	B	291	ARG
1	B	292	SER
1	B	293	ARG
1	B	301	ILE
1	B	310	LEU
1	B	327	MET
1	B	330	VAL
1	B	336	LEU
1	B	349	LEU
1	B	376	VAL
1	B	379	ARG
1	B	391	GLU
1	B	402	SER
1	B	413	SER
1	B	421	LEU
1	B	434	TYR
1	B	438	ARG
1	B	439	VAL
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	474	HIS

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Mol	Chain	Res	Type
1	B	484	LEU
1	B	491	LYS
1	B	530	LYS
1	B	552	VAL
1	B	564	LYS
1	B	567	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	198	ASN
1	A	296	ASN
1	A	344	GLN
1	A	364	GLN
1	A	380	ASN
1	A	410	ASN
1	A	452	GLN
1	A	524	GLN
1	A	568	ASN
1	B	106	GLN
1	B	123	HIS
1	B	198	ASN
1	B	289	GLN
1	B	296	ASN
1	B	344	GLN
1	B	380	ASN
1	B	410	ASN
1	B	452	GLN
1	B	462	HIS
1	B	524	GLN
1	B	568	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	UD2	A	602	2	34,41,41	0.98	2 (5%)	45,62,62	1.39	7 (15%)
3	UD2	B	602	2	34,41,41	0.66	0	45,62,62	1.05	2 (4%)

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	UD2	A	602	2	-	7/24/63/63	0/3/3/3
3	UD2	B	602	2	-	11/24/63/63	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	UD2	C2-N3	-3.15	1.31	1.38
3	A	602	UD2	O4B-C1B	3.13	1.45	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	UD2	O3'-C3'-C2'	3.85	117.43	109.66
3	B	602	UD2	PB-O3A-PA	-3.59	120.50	132.83
3	B	602	UD2	C3B-C2B-C1B	3.55	106.32	100.98
3	A	602	UD2	PB-O3A-PA	-3.09	122.24	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	UD2	C4'-C3'-C2'	-2.86	106.16	110.34
3	A	602	UD2	C3B-C2B-C1B	2.78	105.17	100.98
3	A	602	UD2	C3'-C2'-N2'	2.73	115.77	110.62
3	A	602	UD2	O5'-C5'-C6'	2.64	112.99	106.44
3	A	602	UD2	C3'-C4'-C5'	-2.17	106.38	110.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	UD2	O5'-C1'-O1'-PB
3	B	602	UD2	C2B-C1B-N1-C6
3	B	602	UD2	O4B-C1B-N1-C6
3	B	602	UD2	C5B-O5B-PA-O1A
3	B	602	UD2	C5B-O5B-PA-O2A
3	A	602	UD2	O5'-C5'-C6'-O6'
3	B	602	UD2	O5'-C5'-C6'-O6'
3	A	602	UD2	C4'-C5'-C6'-O6'
3	A	602	UD2	C1'-O1'-PB-O3A
3	B	602	UD2	C4'-C5'-C6'-O6'
3	A	602	UD2	C1'-O1'-PB-O1B
3	A	602	UD2	PA-O3A-PB-O1'
3	B	602	UD2	PB-O3A-PA-O5B
3	A	602	UD2	C1'-O1'-PB-O2B
3	B	602	UD2	C4B-C5B-O5B-PA
3	B	602	UD2	C5B-O5B-PA-O3A
3	B	602	UD2	O4B-C4B-C5B-O5B
3	A	602	UD2	C5B-O5B-PA-O2A

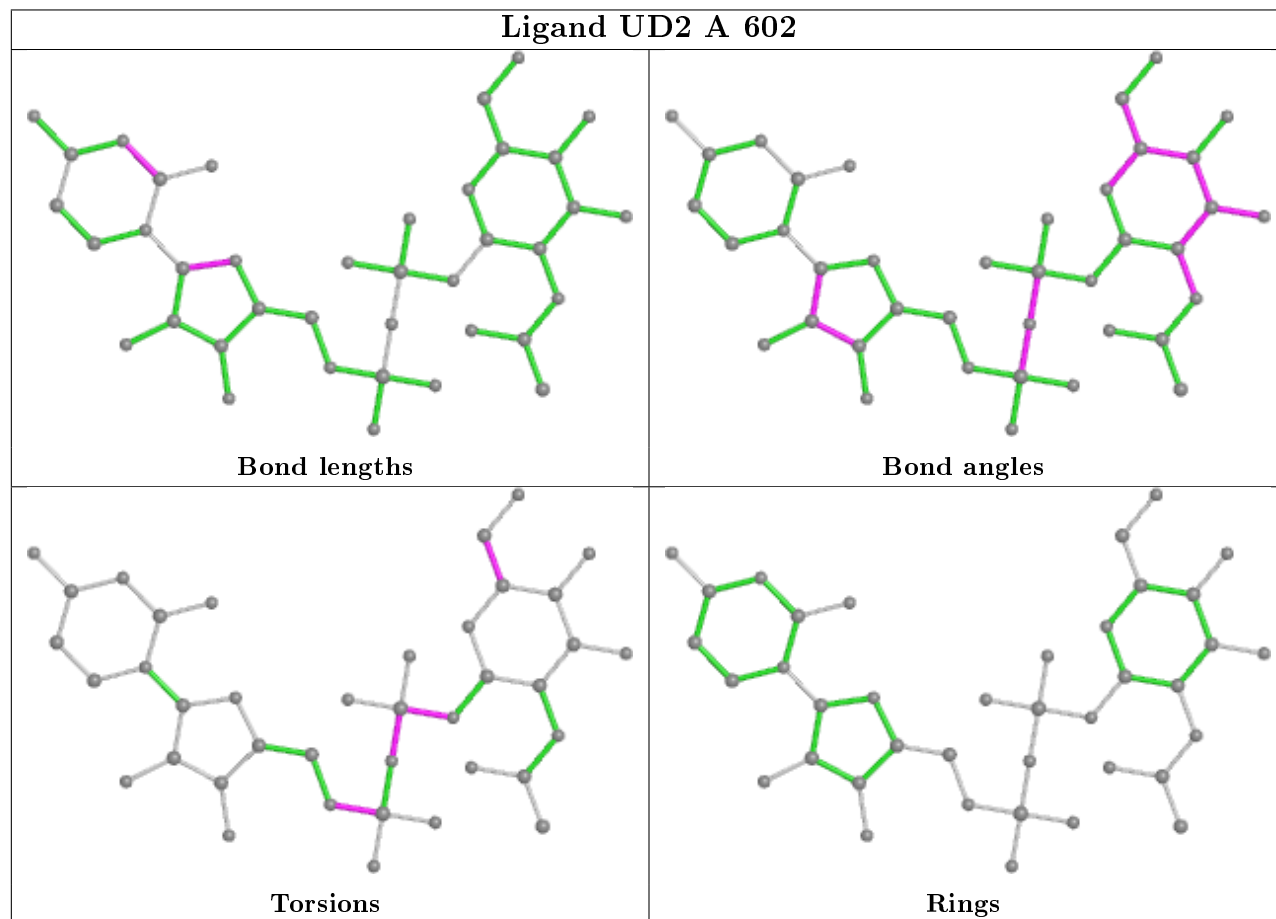
There are no ring outliers.

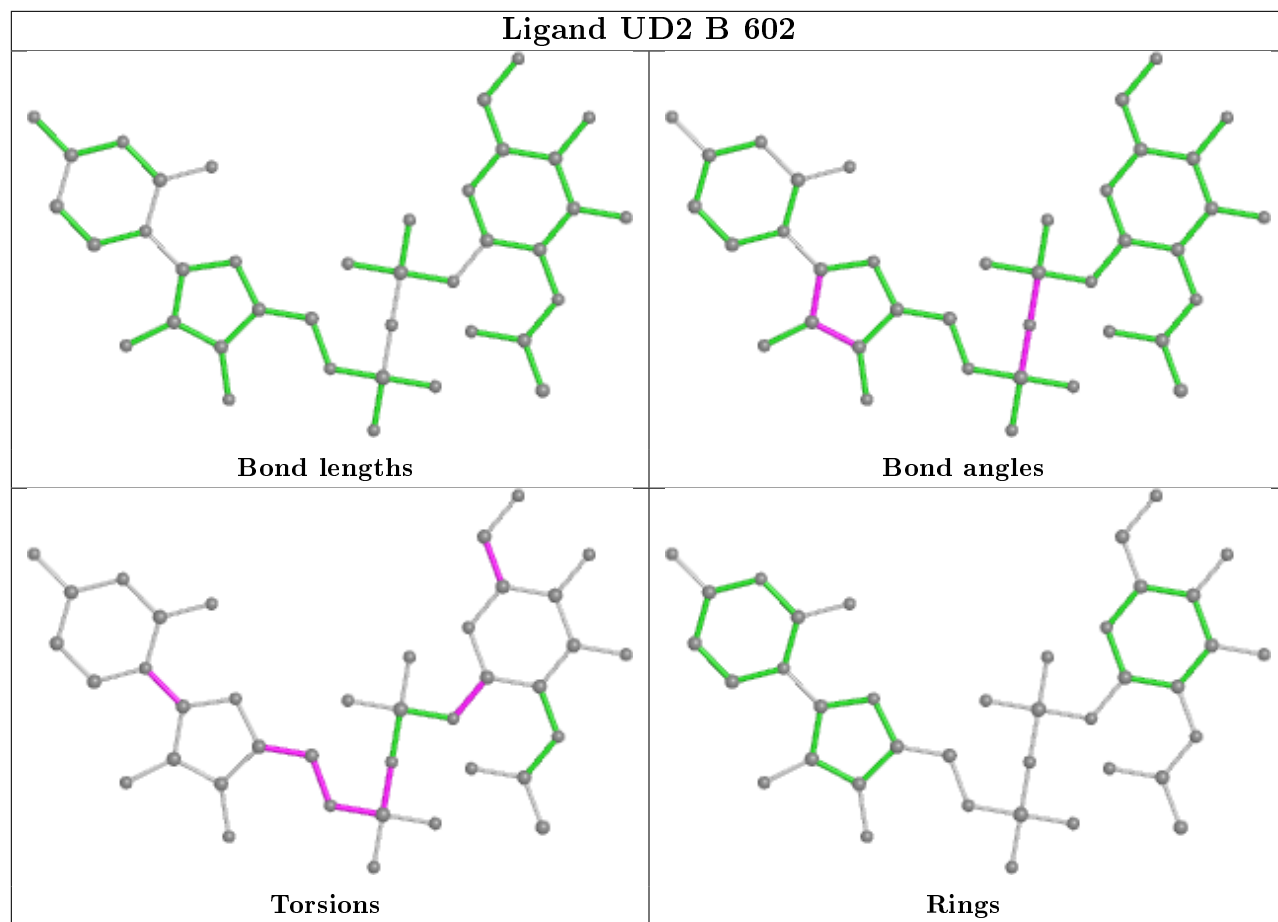
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	UD2	5	0
3	B	602	UD2	16	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	478/503 (95%)	-0.05	17 (3%) 42 42	45, 67, 114, 165	0
1	B	467/503 (92%)	0.04	22 (4%) 31 30	51, 72, 107, 147	0
All	All	945/1006 (93%)	-0.01	39 (4%) 37 36	45, 69, 111, 165	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	PRO	7.0
1	A	365	HIS	5.5
1	B	331	TRP	4.7
1	B	376	VAL	4.7
1	A	331	TRP	4.4
1	A	368	THR	3.8
1	A	376	VAL	3.8
1	B	133	VAL	3.8
1	B	105	ASN	3.7
1	A	106	GLN	3.5
1	B	384	ALA	3.2
1	A	369	PHE	3.0
1	B	405	ASN	2.9
1	B	514	ARG	2.9
1	B	74	ALA	2.9
1	B	287	PRO	2.8
1	B	540	LEU	2.8
1	A	364	GLN	2.8
1	B	106	GLN	2.7
1	B	442	HIS	2.7
1	A	288	GLU	2.7
1	B	531	LEU	2.7
1	A	531	LEU	2.6
1	A	330	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	107	VAL	2.5
1	B	406	VAL	2.4
1	B	291	ARG	2.4
1	B	146	ASN	2.4
1	A	73	GLU	2.4
1	B	337	GLU	2.4
1	B	130	GLN	2.3
1	A	367	TYR	2.3
1	A	89	GLY	2.3
1	B	179	ASN	2.3
1	A	540	LEU	2.2
1	B	330	VAL	2.0
1	A	130	GLN	2.0
1	B	127	GLN	2.0
1	A	442	HIS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

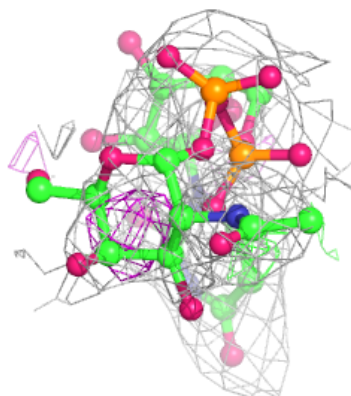
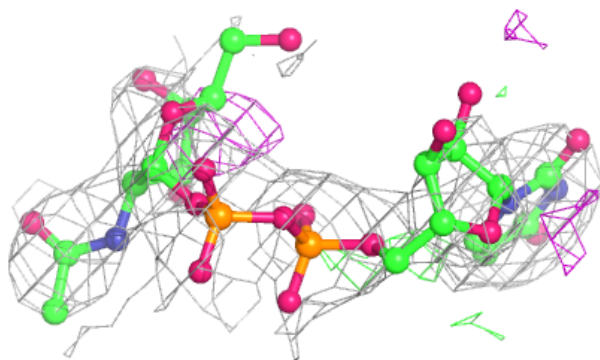
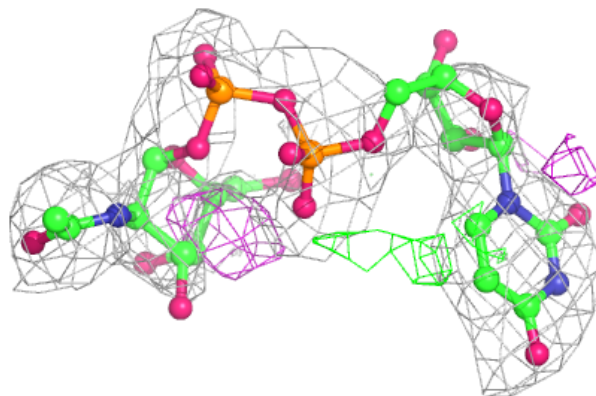
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MN	B	601	1/1	0.82	0.06	63,63,63,63	0
3	UD2	A	602	39/39	0.90	0.25	68,96,127,129	0
3	UD2	B	602	39/39	0.90	0.21	73,82,95,96	0
2	MN	A	601	1/1	0.98	0.08	55,55,55,55	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.

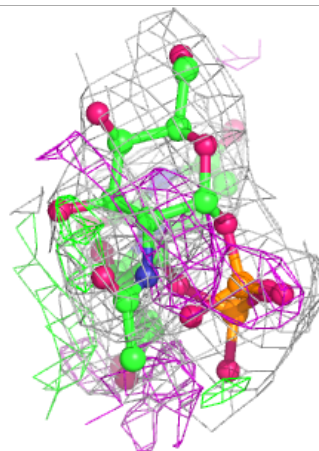
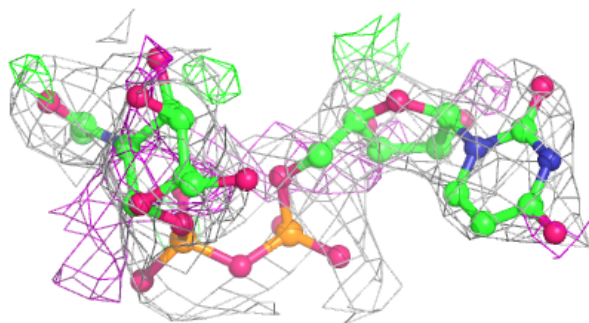
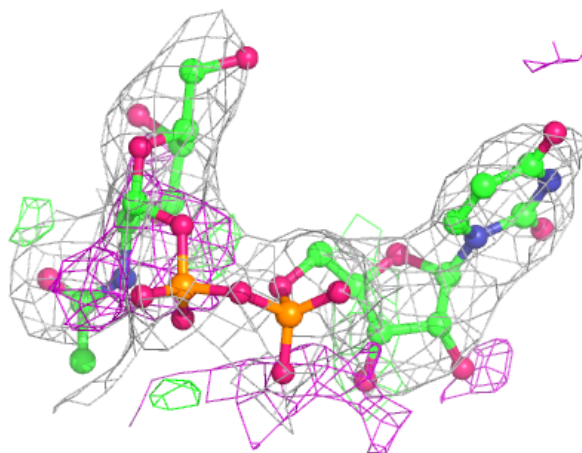
**Electron density around UD2 A 602:**

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



**Electron density around UD2 B 602:**

$2mF_o-DF_c$  (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.