



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:45 PM JST

PDB ID : 7VEL  
Title : Crystal structure of *Phytolacca americana* UGT3 with UDP-2fluoroglucose  
Authors : Maharjan, R.; Fukuda, Y.; Nakayama, T.; Nakayama, T.; Hamada, H.; Ozaki, S.; Inoue, T.  
Deposited on : 2021-09-09  
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

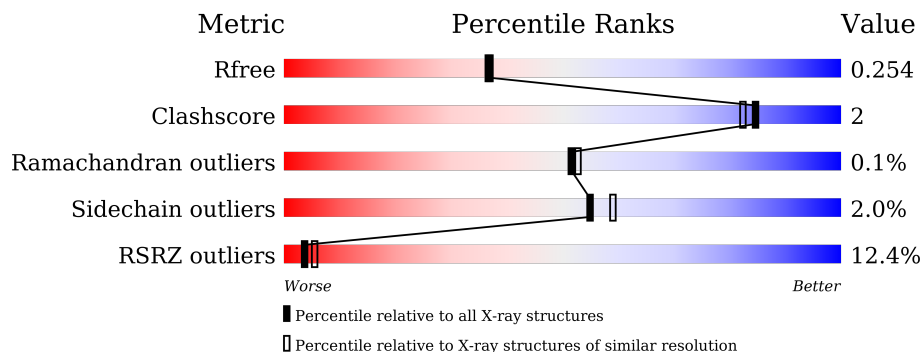
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	505	 13% 81% 8% 11%
1	B	505	 9% 82% 7% 11%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7458 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3593	2320	613	644	16	0	0	0
1	B	449	3606	2327	615	648	16	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

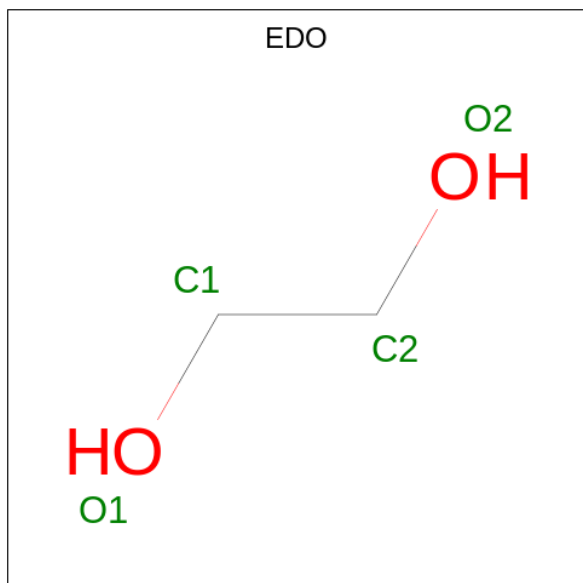
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B5MGN9
A	-18	ASN	-	expression tag	UNP B5MGN9
A	-17	HIS	-	expression tag	UNP B5MGN9
A	-16	LYS	-	expression tag	UNP B5MGN9
A	-15	VAL	-	expression tag	UNP B5MGN9
A	-14	HIS	-	expression tag	UNP B5MGN9
A	-13	HIS	-	expression tag	UNP B5MGN9
A	-12	HIS	-	expression tag	UNP B5MGN9
A	-11	HIS	-	expression tag	UNP B5MGN9
A	-10	HIS	-	expression tag	UNP B5MGN9
A	-9	HIS	-	expression tag	UNP B5MGN9
A	-8	LEU	-	expression tag	UNP B5MGN9
A	-7	GLN	-	expression tag	UNP B5MGN9
A	-6	GLU	-	expression tag	UNP B5MGN9
A	-5	ASN	-	expression tag	UNP B5MGN9
A	-4	LEU	-	expression tag	UNP B5MGN9
A	-3	TYR	-	expression tag	UNP B5MGN9
A	-2	PHE	-	expression tag	UNP B5MGN9
A	-1	GLN	-	expression tag	UNP B5MGN9
A	0	GLY	-	expression tag	UNP B5MGN9
B	-19	MET	-	initiating methionine	UNP B5MGN9
B	-18	ASN	-	expression tag	UNP B5MGN9
B	-17	HIS	-	expression tag	UNP B5MGN9
B	-16	LYS	-	expression tag	UNP B5MGN9
B	-15	VAL	-	expression tag	UNP B5MGN9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B5MGN9
B	-13	HIS	-	expression tag	UNP B5MGN9
B	-12	HIS	-	expression tag	UNP B5MGN9
B	-11	HIS	-	expression tag	UNP B5MGN9
B	-10	HIS	-	expression tag	UNP B5MGN9
B	-9	HIS	-	expression tag	UNP B5MGN9
B	-8	LEU	-	expression tag	UNP B5MGN9
B	-7	GLN	-	expression tag	UNP B5MGN9
B	-6	GLU	-	expression tag	UNP B5MGN9
B	-5	ASN	-	expression tag	UNP B5MGN9
B	-4	LEU	-	expression tag	UNP B5MGN9
B	-3	TYR	-	expression tag	UNP B5MGN9
B	-2	PHE	-	expression tag	UNP B5MGN9
B	-1	GLN	-	expression tag	UNP B5MGN9
B	0	GLY	-	expression tag	UNP B5MGN9

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 3 is 1,4,7,10,13,16-HEXAOXACYCLOOCTADECANE (three-letter code: O4B) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			P
5	A	1	36	15	1	2	16	2	0	0
5	B	1	36	15	1	2	16	2	0	0

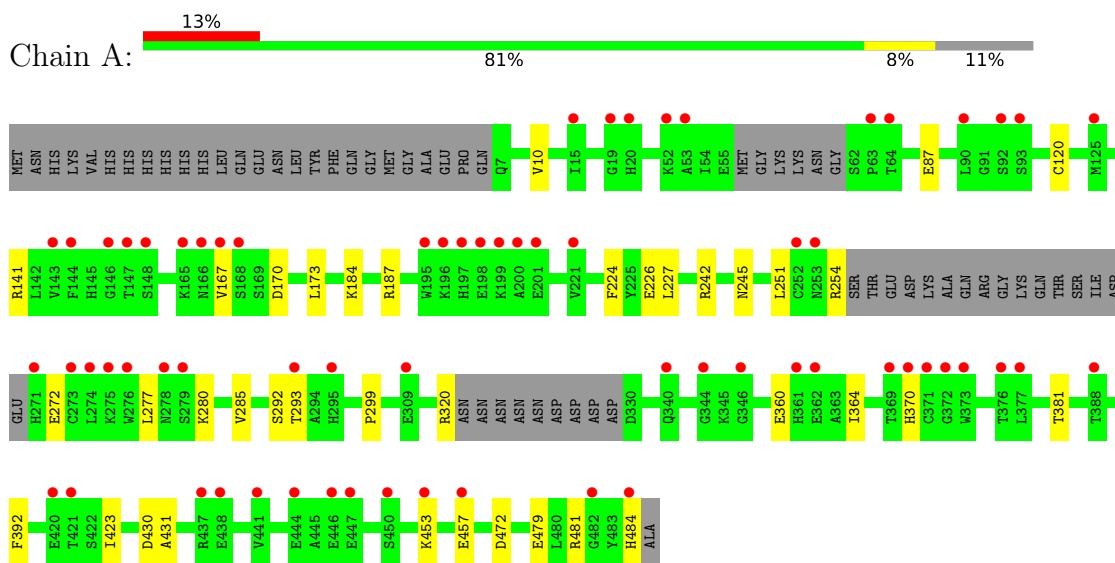
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		
6	B	97	Total	O	0	0
			97	97		

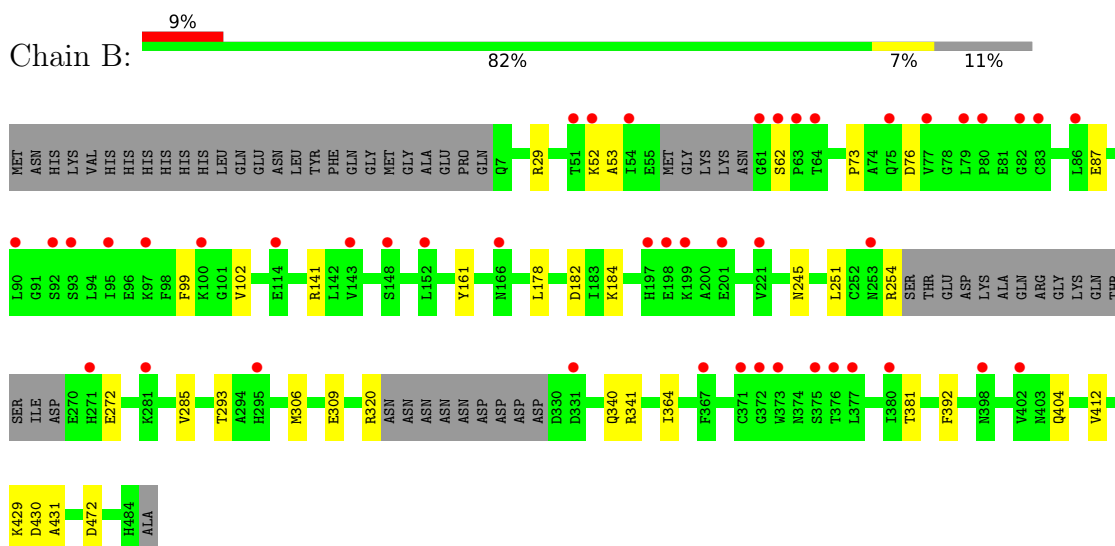
### 3 Residue-property plots [i](#)

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

- Molecule 1: Glycosyltransferase



- Molecule 1: Glycosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.22Å 103.85Å 110.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.05 – 2.15 35.05 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.05-2.15) 99.6 (35.05-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.16Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.213 , 0.254 0.213 , 0.254	Depositor DCC
$R_{free}$ test set	2977 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: K, EDO, O4B, U2F

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	0.31	0/3681	0.47	0/4976
1	B	0.31	0/3694	0.47	0/4993
All	All	0.31	0/7375	0.47	0/9969

There are no bond length outliers.

There are no bond angle outliers.

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	3593	0	3594	16	0
1	B	3606	0	3603	17	0
2	A	4	0	6	0	0
3	A	18	0	24	0	0
4	A	1	0	0	0	0
5	A	36	0	21	0	0
5	B	36	0	20	0	0
6	A	67	0	0	1	0
6	B	97	0	0	1	0
All	All	7458	0	7268	33	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 2.

All (33) 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:251:LEU:HD21	1:A:381:THR:HG21	1.65	0.78
1:B:182:ASP:O	1:B:404:GLN:NE2	2.27	0.67
1:B:182:ASP:OD2	1:B:184:LYS:NZ	2.28	0.66
1:A:430:ASP:OD1	1:A:431:ALA:N	2.32	0.62
1:A:254:ARG:NH1	1:A:360:GLU:OE1	2.34	0.61
1:B:73:PRO:HB2	1:B:76:ASP:HB3	1.83	0.60
1:A:292:SER:O	1:A:320:ARG:NH2	2.26	0.58
1:B:309:GLU:OE2	1:B:341:ARG:NE	2.32	0.56
1:B:87:GLU:HG2	1:B:293:THR:HG21	1.87	0.56
1:A:277:LEU:HA	1:A:280:LYS:HD3	1.90	0.54
1:B:254:ARG:NH1	6:B:602:HOH:O	2.41	0.53
1:B:306:MET:HE3	1:B:429:LYS:HD3	1.89	0.53
1:A:170:ASP:HA	1:A:187:ARG:HE	1.73	0.53
1:A:173:LEU:HD23	1:A:184:LYS:HB3	1.91	0.51
1:B:29:ARG:NH1	1:B:53:ALA:O	2.45	0.50
1:B:430:ASP:OD1	1:B:431:ALA:N	2.45	0.49
1:A:224:PHE:CZ	1:A:227:LEU:HB2	2.49	0.47
1:B:161:TYR:OH	1:B:178:LEU:HD11	2.15	0.47
1:A:481:ARG:NH1	6:A:702:HOH:O	2.40	0.47
1:B:272:GLU:OE1	1:B:272:GLU:N	2.44	0.46
1:A:285:VAL:HB	1:A:364:ILE:HD13	1.96	0.46
1:B:99:PHE:HA	1:B:102:VAL:HG22	1.97	0.46
1:A:453:LYS:O	1:A:457:GLU:HG2	2.19	0.42
1:B:52:LYS:HB3	1:B:52:LYS:HE2	1.83	0.42
1:A:226:GLU:OE1	1:A:226:GLU:N	2.49	0.42
1:A:10:VAL:HG22	1:A:120:CYS:HB3	2.02	0.41
1:A:242:ARG:NH1	1:A:479:GLU:OE1	2.48	0.41
1:A:299:PRO:HG2	1:A:423:ILE:HD12	2.01	0.41
1:A:272:GLU:OE2	1:A:272:GLU:N	2.43	0.41
1:B:251:LEU:HD21	1:B:381:THR:HG21	2.02	0.41
1:B:320:ARG:HD2	1:B:320:ARG:HA	1.89	0.41
1:B:306:MET:CE	1:B:429:LYS:HD3	2.51	0.41
1:B:285:VAL:HB	1:B:364:ILE:HD13	2.03	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	439/505 (87%)	428 (98%)	11 (2%)	0	100	100
1	B	441/505 (87%)	429 (97%)	11 (2%)	1 (0%)	47	46
All	All	880/1010 (87%)	857 (97%)	22 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/434 (88%)	375 (98%)	9 (2%)	50	53
1	B	385/434 (89%)	379 (98%)	6 (2%)	62	67
All	All	769/868 (89%)	754 (98%)	15 (2%)	55	59

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLU
1	A	141	ARG
1	A	167	VAL
1	A	245	ASN
1	A	293	THR

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Mol	Chain	Res	Type
1	A	370	HIS
1	A	392	PHE
1	A	472	ASP
1	A	484	HIS
1	B	141	ARG
1	B	245	ASN
1	B	340	GLN
1	B	392	PHE
1	B	412	VAL
1	B	472	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	O4B	A	602	4	18,18,18	0.55	0	18,18,18	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	U2F	B	501	-	35,38,38	3.35	15 (42%)	51,58,58	1.60	8 (15%)
2	EDO	A	601	-	3,3,3	0.51	0	2,2,2	0.20	0
5	U2F	A	604	-	35,38,38	3.34	16 (45%)	51,58,58	1.55	6 (11%)

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	O4B	A	602	4	-	1/18/18/18	0/1/1/1
5	U2F	B	501	-	-	2/22/59/59	0/3/3/3
2	EDO	A	601	-	-	0/1/1/1	-
5	U2F	A	604	-	-	2/22/59/59	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	U2F	C3'-C4'	-8.94	1.30	1.53
5	A	604	U2F	C3'-C4'	-8.79	1.30	1.53
5	B	501	U2F	O4'-C4'	7.36	1.61	1.45
5	A	604	U2F	O4'-C4'	7.13	1.60	1.45
5	B	501	U2F	C6'-N1	6.81	1.49	1.38
5	A	604	U2F	C6'-N3	6.79	1.50	1.38
5	B	501	U2F	C6'-N3	6.78	1.50	1.38
5	A	604	U2F	C6'-N1	6.77	1.49	1.38
5	A	604	U2F	C9'-C8'	6.07	1.49	1.35
5	B	501	U2F	C9'-C8'	5.77	1.48	1.35
5	A	604	U2F	O4'-C1'	-4.98	1.30	1.42
5	B	501	U2F	O4'-C1'	-4.85	1.30	1.42
5	A	604	U2F	C2-C3	-4.77	1.48	1.52
5	B	501	U2F	C2-C3	-4.58	1.48	1.52
5	B	501	U2F	C7'-N3	4.18	1.46	1.38
5	A	604	U2F	C7'-N3	4.06	1.45	1.38
5	B	501	U2F	O5-C1	3.30	1.50	1.41
5	A	604	U2F	O3'-C3'	3.23	1.50	1.43
5	A	604	U2F	O5-C1	3.17	1.49	1.41
5	A	604	U2F	C9'-N1	3.05	1.45	1.38
5	B	501	U2F	C9'-N1	2.96	1.45	1.38
5	B	501	U2F	O3'-C3'	2.92	1.49	1.43
5	B	501	U2F	C8'-C7'	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	U2F	O2'-C2'	-2.68	1.36	1.43
5	A	604	U2F	C8'-C7'	2.66	1.49	1.43
5	B	501	U2F	O6'-C6'	-2.64	1.18	1.23
5	A	604	U2F	O7'-C7'	-2.57	1.19	1.24
5	B	501	U2F	O7'-C7'	-2.53	1.19	1.24
5	A	604	U2F	O6'-C6'	-2.43	1.18	1.23
5	A	604	U2F	PB-O1	2.39	1.66	1.60
5	A	604	U2F	O2'-C2'	-2.33	1.37	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	U2F	C7'-N3-C6'	-5.47	119.36	126.58
5	A	604	U2F	C7'-N3-C6'	-5.02	119.96	126.58
5	A	604	U2F	PA-O3A-PB	-4.38	117.79	132.83
5	B	501	U2F	O5-C1-O1	-3.89	106.28	111.36
5	B	501	U2F	N3-C6'-N1	3.68	119.78	114.89
5	A	604	U2F	N3-C6'-N1	3.67	119.77	114.89
5	B	501	U2F	C8'-C7'-N3	3.52	120.11	114.84
5	A	604	U2F	C8'-C7'-N3	3.32	119.81	114.84
5	B	501	U2F	PA-O3A-PB	-3.12	122.13	132.83
5	A	604	U2F	O6'-C6'-N1	-2.93	118.90	122.79
5	B	501	U2F	O6'-C6'-N1	-2.81	119.06	122.79
5	B	501	U2F	O7'-C7'-C8'	-2.69	120.44	125.16
5	A	604	U2F	O7'-C7'-C8'	-2.50	120.76	125.16
5	B	501	U2F	O1-C1-C2	-2.12	104.50	108.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

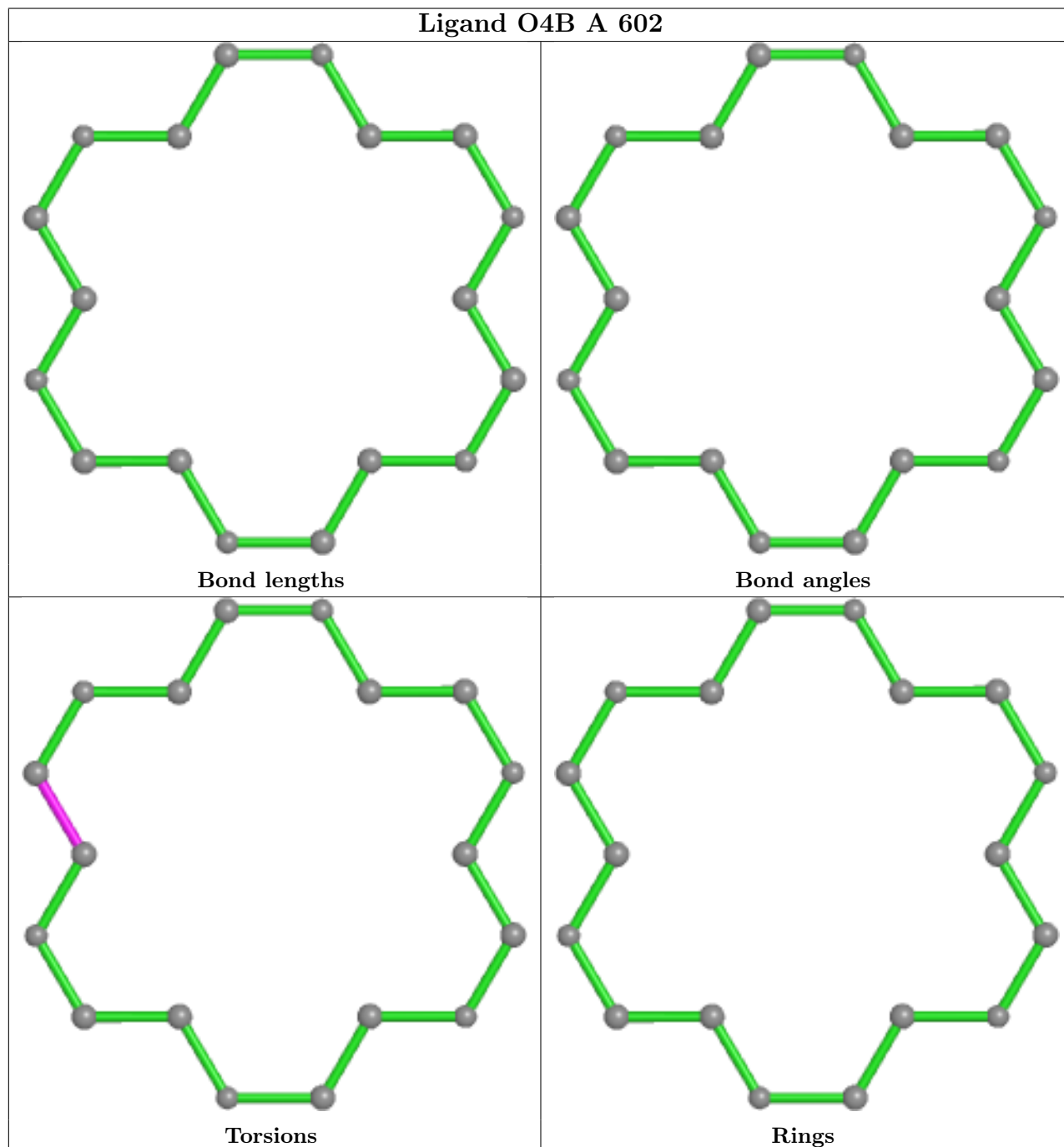
Mol	Chain	Res	Type	Atoms
5	A	604	U2F	O4'-C4'-C5'-O5'
5	B	501	U2F	O4'-C4'-C5'-O5'
5	B	501	U2F	C3'-C4'-C5'-O5'
5	A	604	U2F	C3'-C4'-C5'-O5'
3	A	602	O4B	OAQ-CAK-CAL-OAR

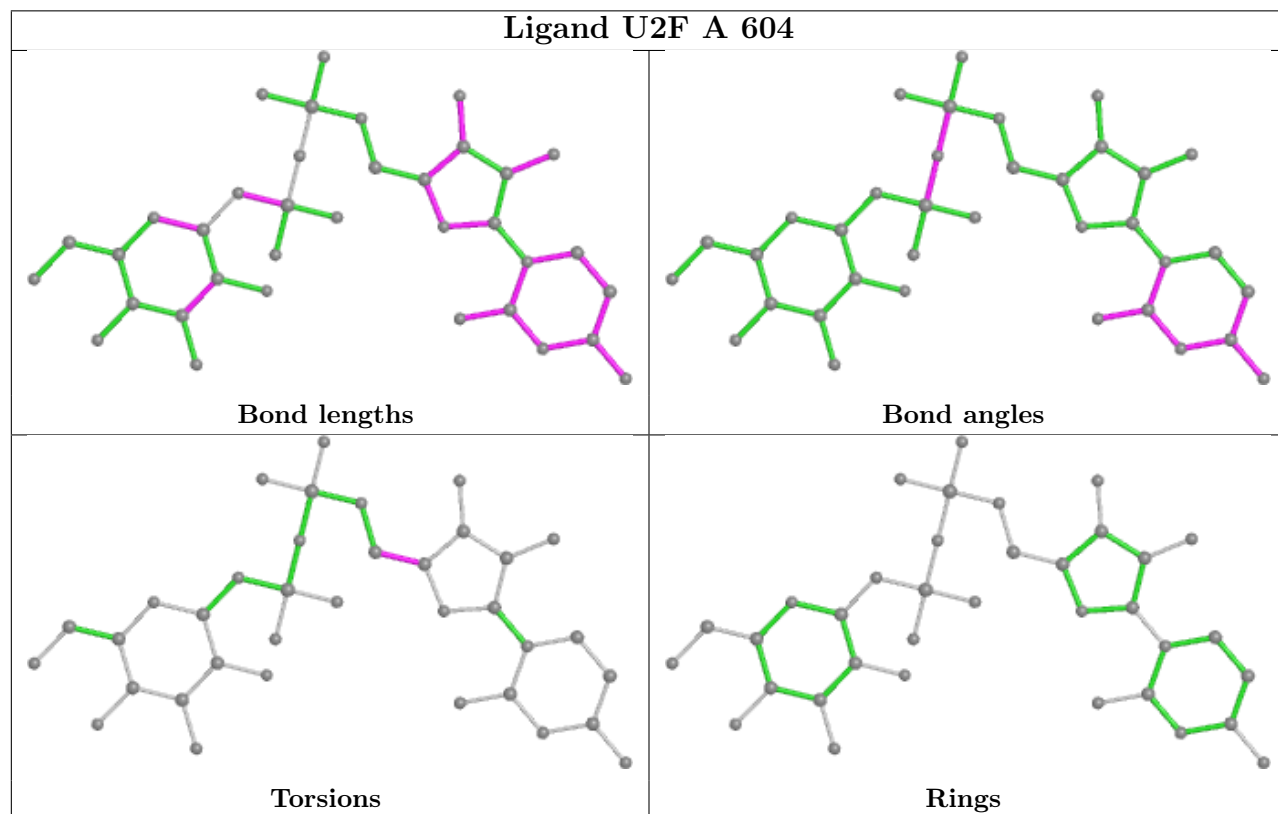
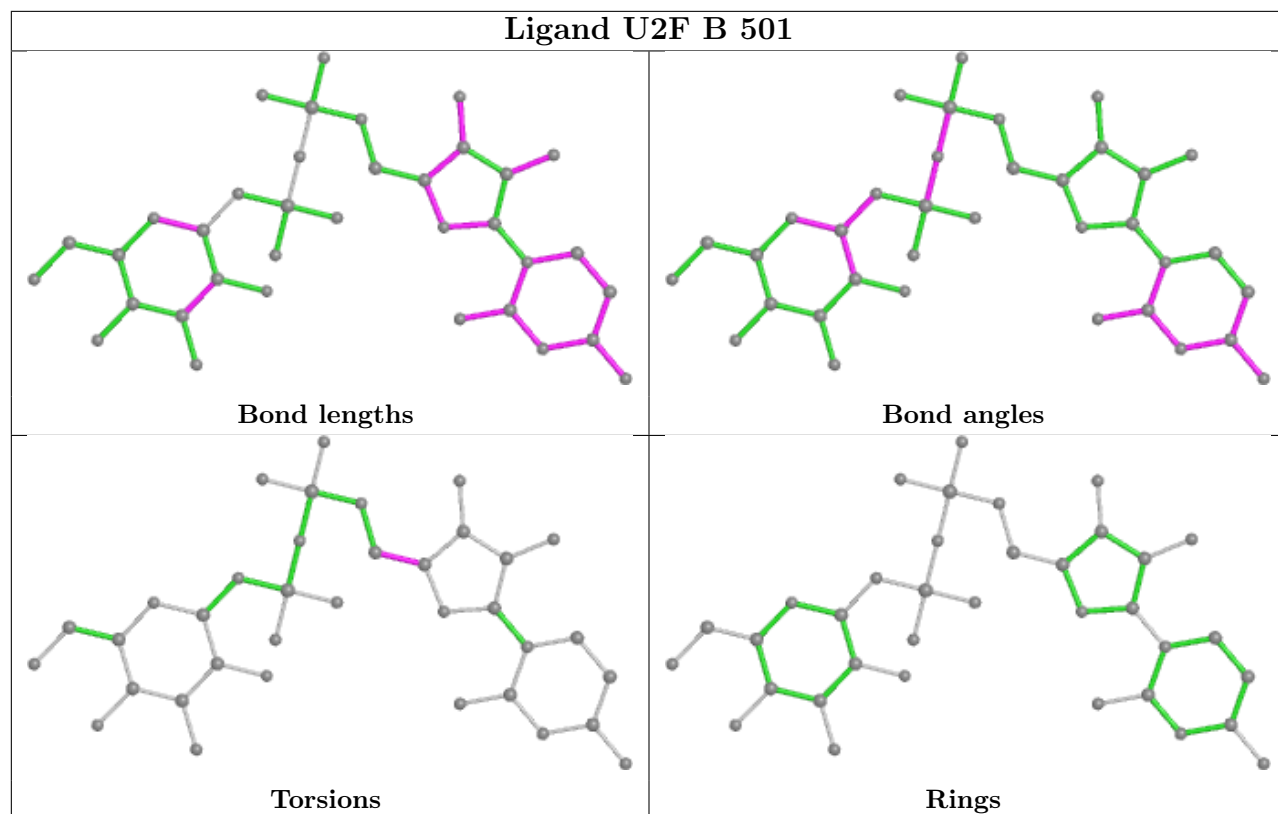
There are no ring outliers.

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, 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	447/505 (88%)	0.80	66 (14%) <b>2</b> <b>3</b>	30, 54, 87, 109	0
1	B	449/505 (88%)	0.64	45 (10%) <b>7</b> <b>11</b>	30, 52, 91, 115	0
All	All	896/1010 (88%)	0.72	111 (12%) <b>4</b> <b>5</b>	30, 53, 90, 115	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	LEU	8.2
1	A	197	HIS	7.0
1	B	62	SER	6.6
1	B	61	GLY	6.3
1	B	295	HIS	6.0
1	A	484	HIS	5.5
1	A	64	THR	5.1
1	B	199	LYS	4.9
1	A	295	HIS	4.9
1	B	63	PRO	4.7
1	A	90	LEU	4.6
1	A	274	LEU	4.6
1	A	195	TRP	4.6
1	A	420	GLU	4.5
1	B	64	THR	4.2
1	A	92	SER	4.2
1	A	199	LYS	4.1
1	A	279	SER	4.1
1	A	450	SER	4.1
1	B	331	ASP	3.9
1	A	253	ASN	3.8
1	B	95	ILE	3.7
1	B	77	VAL	3.6
1	A	444	GLU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	373	TRP	3.6
1	A	52	LYS	3.6
1	A	166	ASN	3.6
1	A	93	SER	3.5
1	B	82	GLY	3.5
1	A	147	THR	3.5
1	B	75	GLN	3.4
1	A	373	TRP	3.4
1	B	51	THR	3.3
1	B	201	GLU	3.3
1	B	197	HIS	3.3
1	A	453	LYS	3.2
1	A	438	GLU	3.2
1	A	446	GLU	3.1
1	A	441	VAL	3.1
1	A	63	PRO	3.1
1	B	253	ASN	3.1
1	A	362	GLU	3.0
1	B	93	SER	3.0
1	A	372	GLY	3.0
1	A	168	SER	3.0
1	A	221	VAL	2.9
1	A	273	CYS	2.9
1	A	482	GLY	2.9
1	B	54	ILE	2.8
1	A	437	ARG	2.8
1	A	143	VAL	2.8
1	A	271	HIS	2.8
1	B	198	GLU	2.8
1	B	371	CYS	2.8
1	A	201	GLU	2.7
1	A	20	HIS	2.7
1	A	165	LYS	2.7
1	A	53	ALA	2.6
1	B	380	ILE	2.6
1	A	146	GLY	2.6
1	B	52	LYS	2.6
1	A	421	THR	2.6
1	A	198	GLU	2.6
1	B	92	SER	2.5
1	A	200	ALA	2.5
1	A	15	ILE	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	377	LEU	2.5
1	A	19	GLY	2.5
1	A	144	PHE	2.5
1	A	344	GLY	2.4
1	A	309	GLU	2.4
1	B	152	LEU	2.4
1	A	196	LYS	2.4
1	A	293	THR	2.4
1	B	143	VAL	2.4
1	A	340	GLN	2.4
1	B	367	PHE	2.3
1	A	252	CYS	2.3
1	B	79	LEU	2.3
1	A	346	GLY	2.3
1	B	80	PRO	2.3
1	B	221	VAL	2.3
1	B	372	GLY	2.3
1	B	402	VAL	2.3
1	A	377	LEU	2.3
1	B	97	LYS	2.3
1	B	100	LYS	2.3
1	A	278	ASN	2.3
1	B	83	CYS	2.3
1	A	276	TRP	2.2
1	B	114	GLU	2.2
1	A	371	CYS	2.2
1	A	369	THR	2.2
1	B	148	SER	2.2
1	A	361	HIS	2.2
1	B	166	ASN	2.2
1	A	125	MET	2.2
1	A	275	LYS	2.2
1	B	281	LYS	2.2
1	B	86	LEU	2.1
1	B	398	ASN	2.1
1	A	167	VAL	2.1
1	A	457	GLU	2.1
1	B	376	THR	2.1
1	A	148	SER	2.0
1	B	375	SER	2.0
1	A	370	HIS	2.0
1	B	271	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	376	THR	2.0
1	A	388	THR	2.0
1	A	447	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

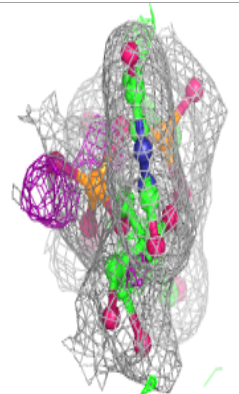
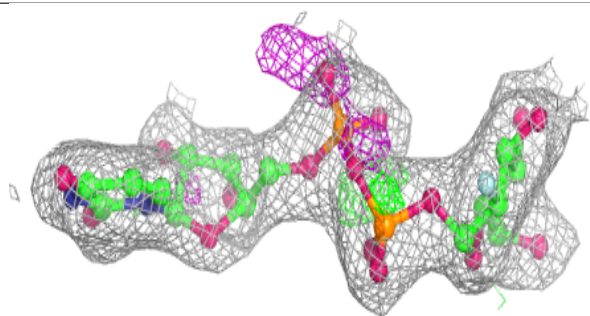
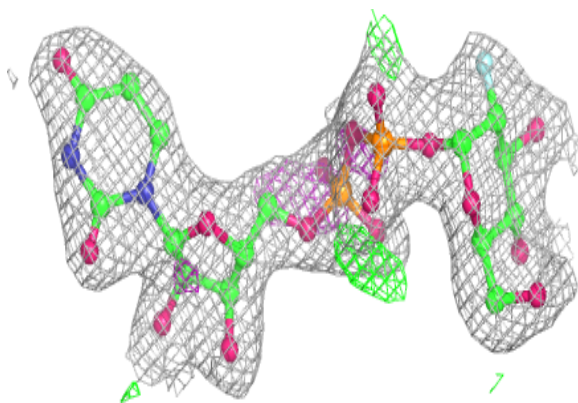
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	A	601	4/4	0.66	0.39	49,58,64,68	0
5	U2F	A	604	36/36	0.92	0.17	31,46,58,59	0
3	O4B	A	602	18/18	0.94	0.11	35,45,50,52	0
5	U2F	B	501	36/36	0.94	0.18	36,47,54,69	0
4	K	A	603	1/1	0.98	0.07	43,43,43,43	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.

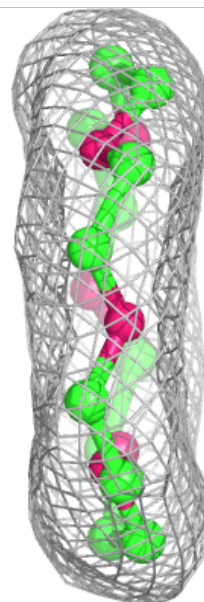
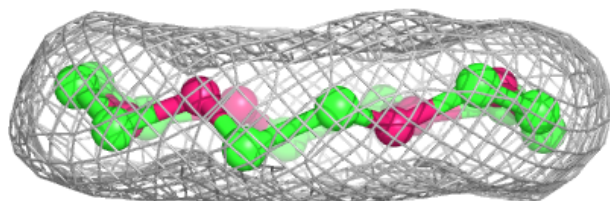
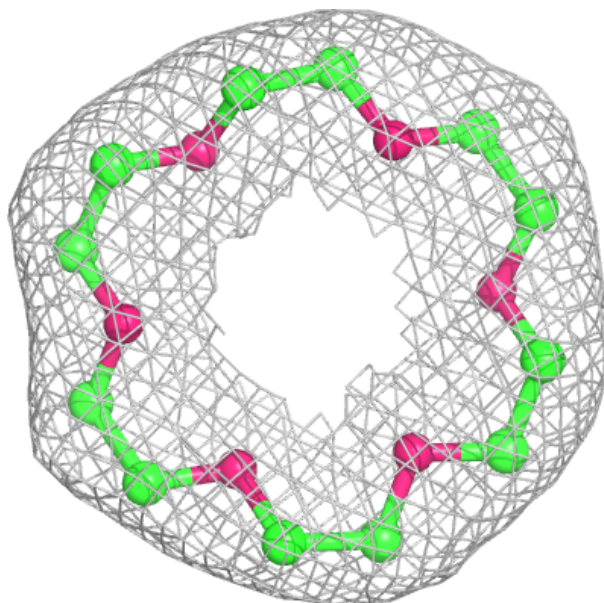
**Electron density around U2F A 604:**

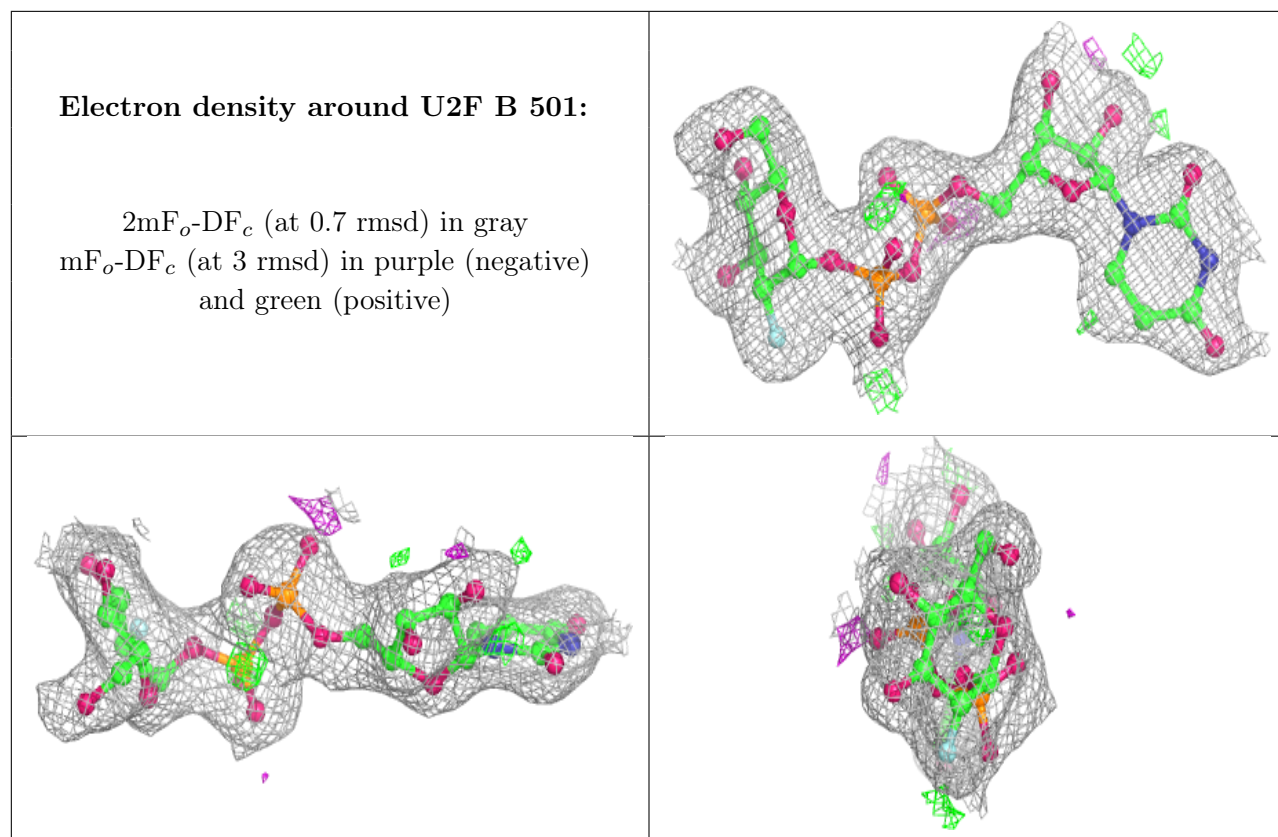
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around O4B 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.