



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 13, 2023 – 02:01 am GMT

PDB ID : 4D11  
Title : GalNAc-T2 crystal soaked with UDP-5SGalNAc, mEA2 peptide and manganese (Lower resolution dataset)  
Authors : Lira-Navarrete, E.; Iglesias-Fernandez, J.; Zandberg, W.F.; Companon, I.; Kong, Y.; Corzana, F.; Pinto, B.M.; Clausen, H.; Peregrina, J.M.; Vocadlo, D.; Rovira, C.; Hurtado-Guerrero, R.  
Deposited on : 2014-05-01  
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (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

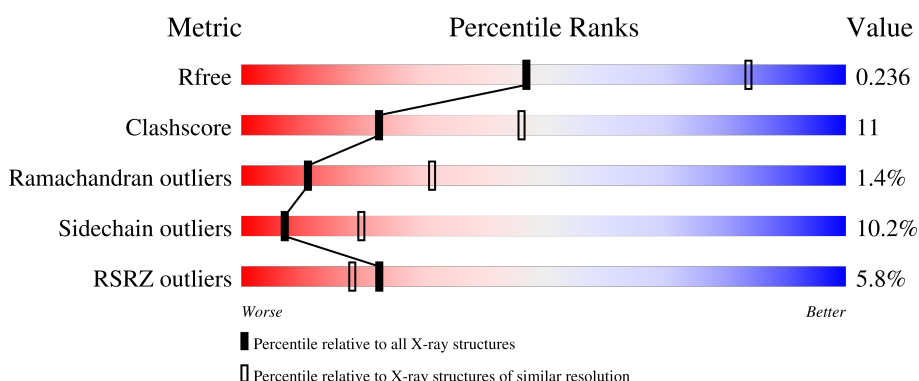
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	571	 2% 71% 11% • 14%
1	B	571	 2% 65% 16% • • 16%
1	D	571	 3% 65% 15% • • 15%
1	E	571	 3% 68% 14% • 15%
1	F	571	 7% 36% 10% • 52%

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Mol	Chain	Length	Quality of chain
2	C	571	<p>10% 56% 16% 24%</p>
3	L	6	<p>17% 50% 17% 33%</p>
3	O	6	<p>67% 17% 17%</p>
3	P	6	<p>67% 33%</p>
3	X	6	<p>67% 50% 33% 17%</p>
3	Z	6	<p>67% 17% 17%</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21829 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 GALNAC-TRANSFERASE T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	3938	2477	715	722	24	20	0	0
1	B	482	3877	2441	703	710	23	20	1	0
1	D	487	3916	2465	711	716	24	20	0	0
1	E	487	3917	2465	711	717	24	20	0	0
1	F	276	2246	1419	406	407	14	8	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	engineered mutation	UNP Q10471
B	516	ASP	ASN	engineered mutation	UNP Q10471
D	516	ASP	ASN	engineered mutation	UNP Q10471
E	516	ASP	ASN	engineered mutation	UNP Q10471
F	516	ASP	ASN	engineered mutation	UNP Q10471

- Molecule 2 is a protein called POLYPEPTIDE GALNAC-TRANSFERASE T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	436	3560	2249	646	644	21	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	74	SER	GLY	conflict	UNP Q10471
C	516	ASP	ASN	engineered mutation	UNP Q10471

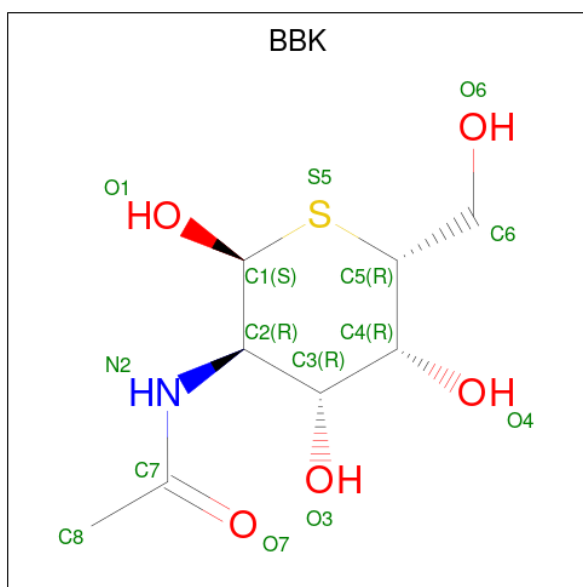
- Molecule 3 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	O	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	P	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	X	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	Z	5	Total	C	N	O	S	0	0	0
			31	18	5	7	1			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

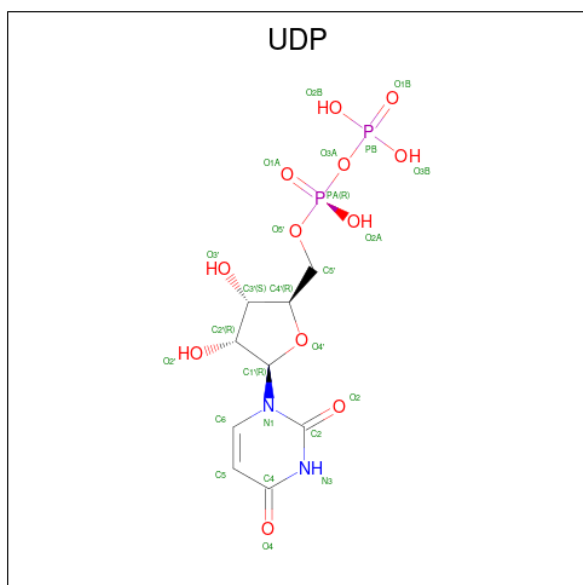
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		
4	E	1	Total	Mn	0	0
			1	1		
4	F	1	Total	Mn	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-5-thio-alpha-D-galactopyranose (three-letter code: BBK) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

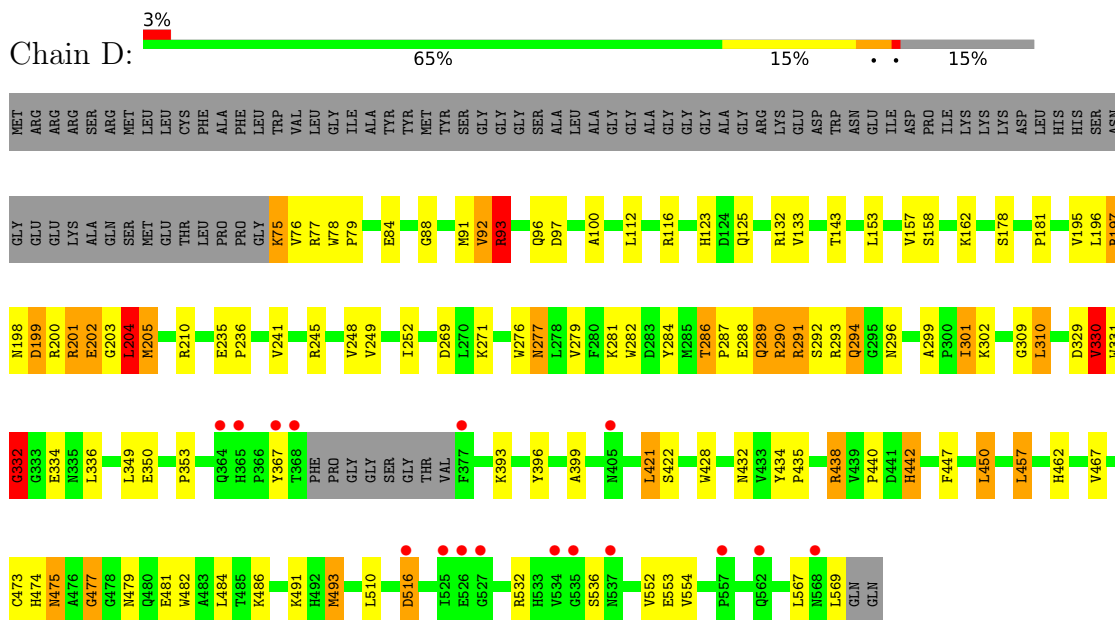
- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



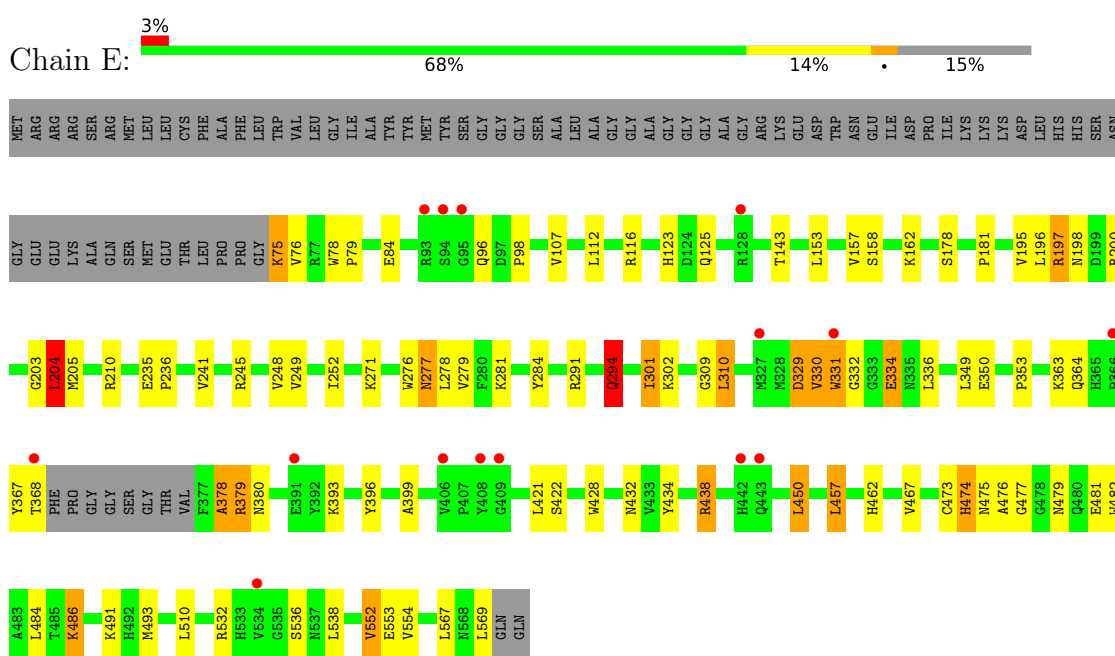
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		



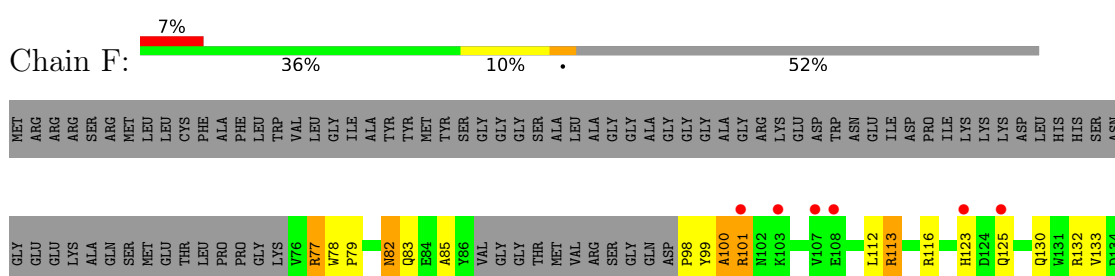




• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2



• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2





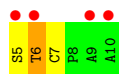
## ● Molecule 3: PEPTIDE

Chain O:  67% 17% 17%

## ● Molecule 3: PEPTIDE

Chain P:  67% 33%

## ● Molecule 3: PEPTIDE

Chain X:  67% 50% 33% 17%

## ● Molecule 3: PEPTIDE

Chain Z:  67% 17% 17%

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.77Å 120.90Å 249.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.61 – 2.85 46.14 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (249.61-2.85) 100.0 (46.14-2.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.216 , 0.235 0.219 , 0.236	Depositor DCC
$R_{free}$ test set	2285 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.9	Xtrriage
Anisotropy	0.339	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.018 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, BBK, 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	0.95	4/4027 (0.1%)	1.03	4/5443 (0.1%)
1	B	1.19	5/3967 (0.1%)	1.05	6/5361 (0.1%)
1	D	1.18	4/4005 (0.1%)	1.05	8/5413 (0.1%)
1	E	1.12	3/4006 (0.1%)	1.05	7/5415 (0.1%)
1	F	0.84	1/2297 (0.0%)	1.03	2/3104 (0.1%)
2	C	0.90	2/3639 (0.1%)	1.03	3/4909 (0.1%)
3	L	0.64	0/32	0.65	0/44
3	O	0.87	0/32	1.25	0/44
3	P	0.94	0/32	1.33	0/44
3	X	0.68	0/32	0.89	0/44
3	Z	0.90	0/31	0.93	0/42
All	All	1.05	19/22100 (0.1%)	1.04	30/29863 (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	D	0	1
2	C	0	1
All	All	0	2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	LYS	CB-CG	-34.06	0.60	1.52
1	D	202	GLU	C-N	-33.06	0.73	1.33
1	B	84	GLU	CB-CG	-32.47	0.90	1.52
1	E	84	GLU	CB-CG	-30.61	0.94	1.52
1	D	486	LYS	CB-CG	-25.67	0.83	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	LYS	CB-CG-CD	18.38	159.39	111.60
1	B	84	GLU	CA-CB-CG	13.47	143.04	113.40
1	A	294	GLN	CA-CB-CG	11.16	137.95	113.40
1	B	75	LYS	CA-CB-CG	11.01	137.63	113.40
2	C	75	LYS	CB-CG-CD	10.64	139.28	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	127	GLN	Peptide
1	D	332	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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	3938	0	3863	41	0
1	B	3877	0	3804	99	0
1	D	3916	0	3842	83	0
1	E	3917	0	3843	76	0
1	F	2246	0	2214	88	0
2	C	3560	0	3495	106	0
3	L	32	0	28	3	0
3	O	32	0	28	1	0
3	P	32	0	28	0	0
3	X	32	0	28	7	0
3	Z	31	0	28	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	15	0	14	4	0
5	B	15	0	15	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	15	0	15	1	0
5	E	15	0	15	1	0
6	A	25	0	11	0	0
6	B	25	0	11	0	0
6	C	25	0	11	0	0
6	D	25	0	11	0	0
6	E	25	0	11	1	0
6	F	25	0	11	0	0
All	All	21829	0	21326	492	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 11.

The worst 5 of 492 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:F:328:MET:SD	1:F:334:GLU:CB	2.07	1.42
1:D:202:GLU:C	1:D:203:GLY:CA	1.92	1.36
1:D:202:GLU:CA	1:D:203:GLY:N	1.92	1.30
1:F:328:MET:SD	1:F:334:GLU:HB2	1.68	1.29
1:B:329:ASP:HB2	1:B:379:ARG:NH2	1.47	1.28

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	487/571 (85%)	461 (95%)	24 (5%)	2 (0%)	34 62
1	B	477/571 (84%)	445 (93%)	26 (6%)	6 (1%)	12 33
1	D	483/571 (85%)	449 (93%)	28 (6%)	6 (1%)	13 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	483/571 (85%)	457 (95%)	21 (4%)	5 (1%)	15	40
1	F	272/571 (48%)	252 (93%)	15 (6%)	5 (2%)	8	25
2	C	422/571 (74%)	387 (92%)	27 (6%)	8 (2%)	8	24
3	L	4/6 (67%)	1 (25%)	1 (25%)	2 (50%)	0	0
3	O	4/6 (67%)	2 (50%)	2 (50%)	0	100	100
3	P	4/6 (67%)	3 (75%)	0	1 (25%)	0	0
3	X	4/6 (67%)	1 (25%)	2 (50%)	1 (25%)	0	0
3	Z	3/6 (50%)	3 (100%)	0	0	100	100
All	All	2643/3456 (76%)	2461 (93%)	146 (6%)	36 (1%)	11	31

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	A	477	GLY
1	B	132	ARG
1	B	477	GLY
2	C	365	HIS

### 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	425/485 (88%)	386 (91%)	39 (9%)	9	24
1	B	418/485 (86%)	379 (91%)	39 (9%)	9	24
1	D	423/485 (87%)	379 (90%)	44 (10%)	7	19
1	E	423/485 (87%)	384 (91%)	39 (9%)	9	24
1	F	244/485 (50%)	215 (88%)	29 (12%)	5	13
2	C	385/486 (79%)	340 (88%)	45 (12%)	5	14
3	L	4/4 (100%)	4 (100%)	0	100	100
3	O	4/4 (100%)	2 (50%)	2 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	4/4 (100%)	3 (75%)	1 (25%)	0	1
3	X	4/4 (100%)	4 (100%)	0	100	100
3	Z	4/4 (100%)	3 (75%)	1 (25%)	0	1
All	All	2338/2931 (80%)	2099 (90%)	239 (10%)	7	20

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	480	GLN
1	F	205	MET
1	D	291	ARG
1	F	201	ARG
3	O	7	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	405	ASN
1	F	123	HIS
1	D	296	ASN
1	F	82	ASN
1	F	277	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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
6	UDP	A	1572	4	24,26,26	1.29	3 (12%)	37,40,40	1.88	9 (24%)
5	BBK	B	1572	-	13,15,15	8.91	4 (30%)	15,21,21	1.65	2 (13%)
6	UDP	F	1364	4	24,26,26	1.22	2 (8%)	37,40,40	1.74	6 (16%)
6	UDP	B	1573	4	24,26,26	1.24	2 (8%)	37,40,40	1.86	7 (18%)
5	BBK	E	1571	-	13,15,15	9.33	4 (30%)	15,21,21	1.50	1 (6%)
6	UDP	D	1571	4	24,26,26	1.30	1 (4%)	37,40,40	1.83	7 (18%)
5	BBK	D	1572	-	13,15,15	9.07	4 (30%)	15,21,21	1.67	4 (26%)
6	UDP	E	1572	4	24,26,26	1.33	2 (8%)	37,40,40	1.89	6 (16%)
6	UDP	C	1571	4	24,26,26	1.23	2 (8%)	37,40,40	1.82	7 (18%)
5	BBK	A	1571	-	13,15,15	9.04	2 (15%)	15,21,21	1.42	4 (26%)

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
6	UDP	A	1572	4	-	9/16/32/32	0/2/2/2
5	BBK	B	1572	-	-	5/6/26/26	0/1/1/1
6	UDP	F	1364	4	-	10/16/32/32	0/2/2/2
6	UDP	B	1573	4	-	9/16/32/32	0/2/2/2
5	BBK	E	1571	-	-	0/6/26/26	0/1/1/1
6	UDP	D	1571	4	-	9/16/32/32	0/2/2/2
5	BBK	D	1572	-	-	2/6/26/26	0/1/1/1
6	UDP	E	1572	4	-	12/16/32/32	0/2/2/2
6	UDP	C	1571	4	-	10/16/32/32	0/2/2/2
5	BBK	A	1571	-	-	2/6/26/26	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1571	BBK	C5-S5	-26.28	1.43	1.82
5	A	1571	BBK	C5-S5	-25.58	1.44	1.82
5	D	1572	BBK	C5-S5	-25.45	1.44	1.82
5	B	1572	BBK	C5-S5	-24.98	1.45	1.82
5	E	1571	BBK	C1-S5	-20.58	1.43	1.83

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1572	UDP	C4-N3-C2	-5.58	119.22	126.58
6	D	1571	UDP	C4-N3-C2	-5.31	119.57	126.58
6	C	1571	UDP	C4-N3-C2	-5.24	119.66	126.58
6	A	1572	UDP	C4-N3-C2	-5.08	119.88	126.58
6	B	1573	UDP	C4-N3-C2	-4.95	120.05	126.58

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1571	BBK	C4-C5-C6-O6
5	A	1571	BBK	S5-C5-C6-O6
5	B	1572	BBK	C4-C5-C6-O6
5	B	1572	BBK	S5-C5-C6-O6
5	D	1572	BBK	C4-C5-C6-O6

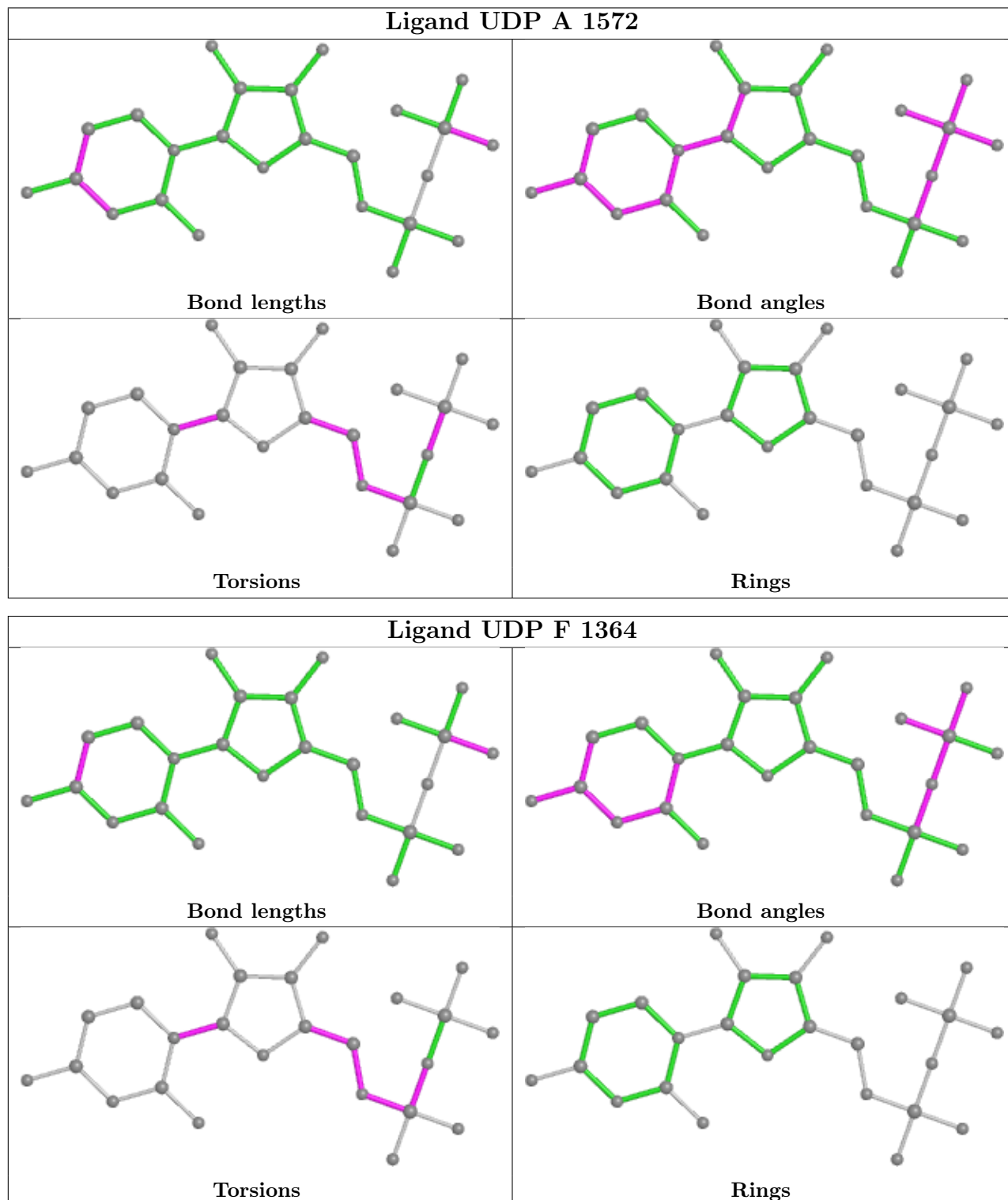
There are no ring outliers.

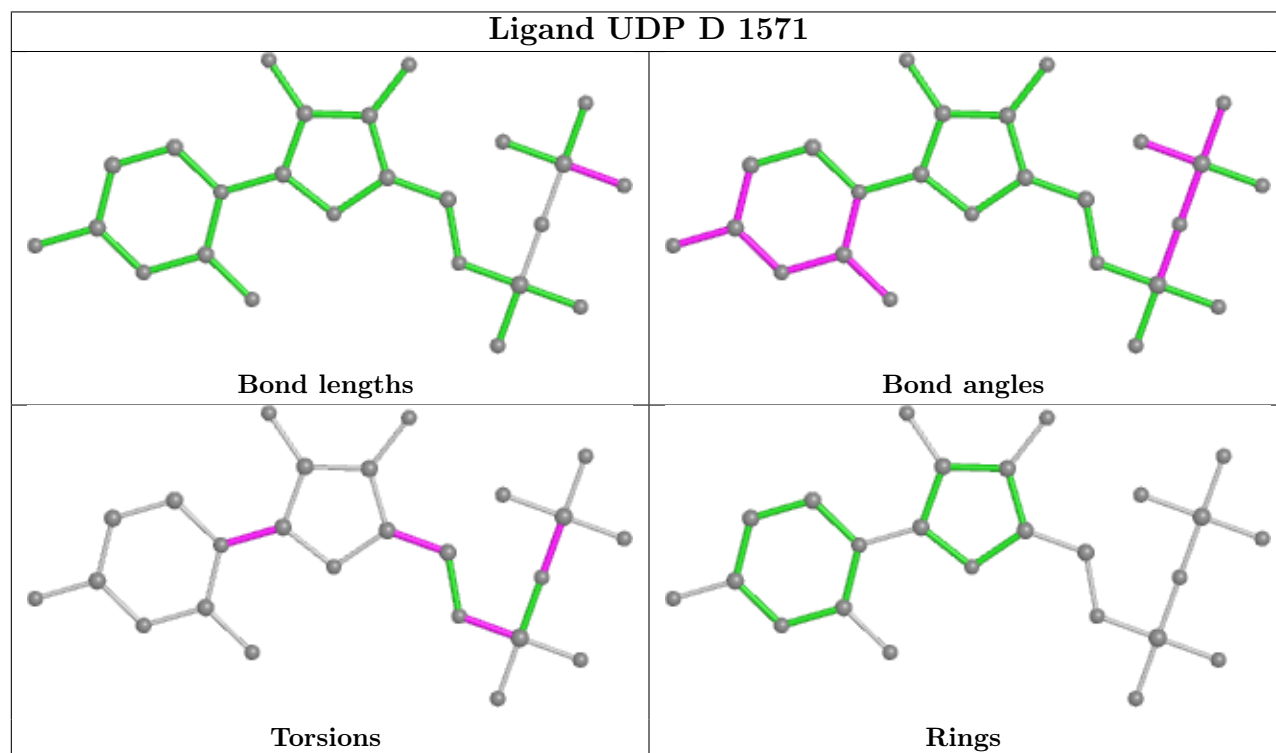
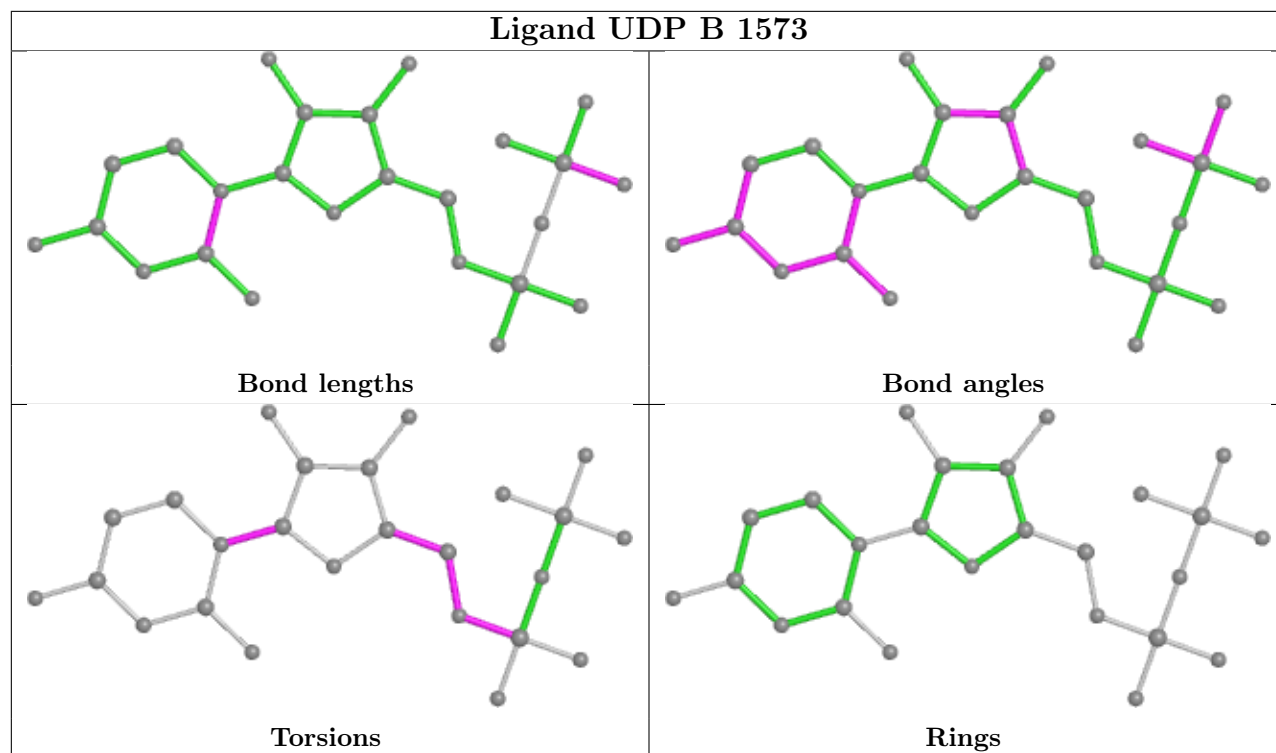
5 monomers are involved in 11 short contacts:

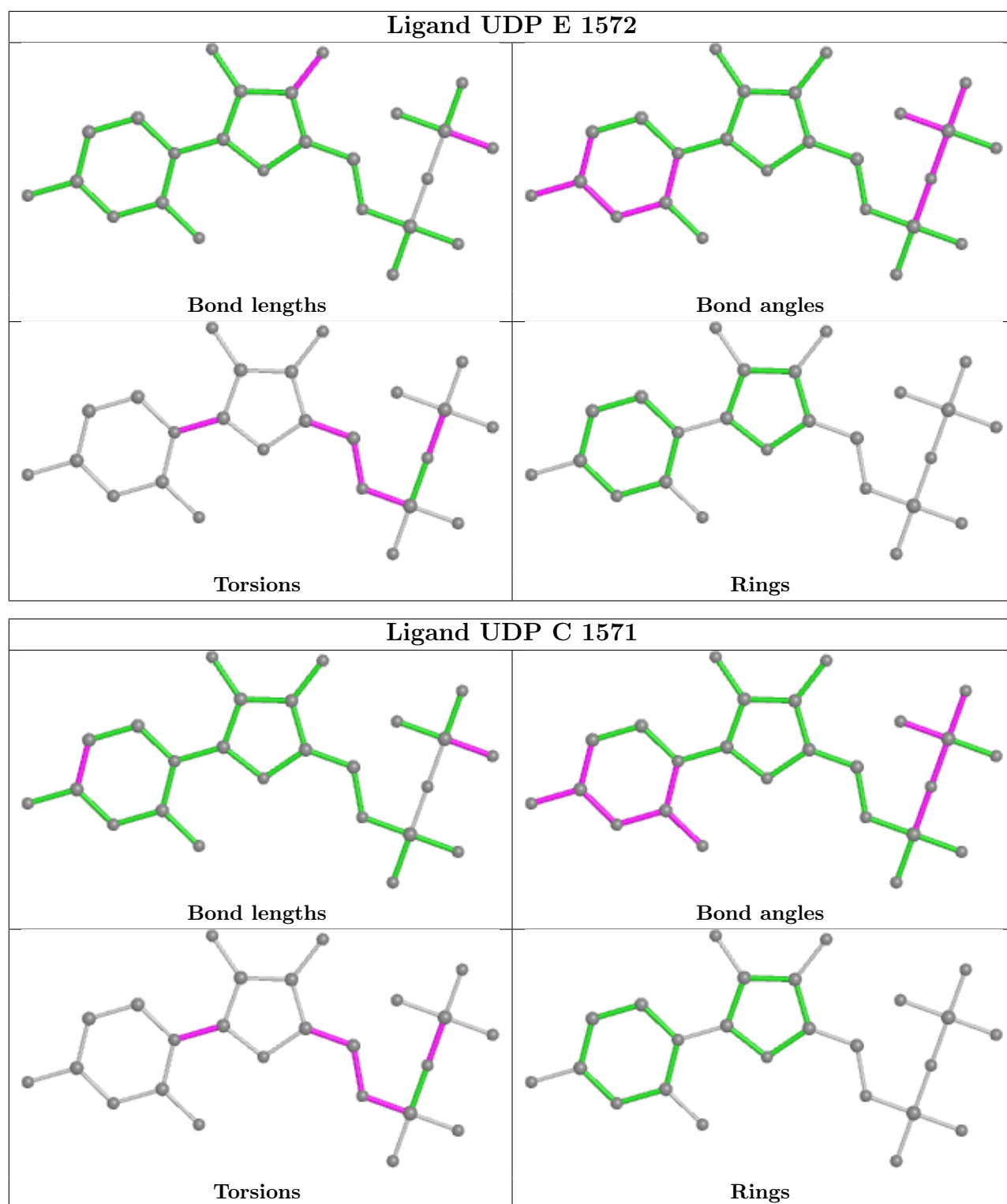
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1572	BBK	5	0
5	E	1571	BBK	1	0
5	D	1572	BBK	1	0
6	E	1572	UDP	1	0
5	A	1571	BBK	4	0

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	202:GLU	C	203:GLY	N	0.73



## 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, 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	491/571 (85%)	-0.03	11 (2%) 62 59	28, 56, 96, 129	5 (1%)
1	B	482/571 (84%)	0.08	14 (2%) 51 47	32, 65, 115, 151	5 (1%)
1	D	487/571 (85%)	0.11	16 (3%) 46 41	29, 64, 110, 144	5 (1%)
1	E	487/571 (85%)	0.09	15 (3%) 49 44	31, 58, 105, 159	5 (1%)
1	F	276/571 (48%)	0.87	41 (14%) 2 1	59, 112, 167, 187	2 (0%)
2	C	436/571 (76%)	0.53	55 (12%) 3 2	35, 89, 149, 182	5 (1%)
3	L	6/6 (100%)	1.47	1 (16%) 1 1	86, 109, 116, 126	0
3	O	6/6 (100%)	0.74	0 100 100	72, 94, 105, 110	0
3	P	6/6 (100%)	0.35	0 100 100	44, 72, 78, 90	0
3	X	6/6 (100%)	2.86	4 (66%) 0 0	91, 106, 118, 123	0
3	Z	5/6 (83%)	0.48	0 100 100	72, 73, 88, 92	0
All	All	2688/3456 (77%)	0.23	157 (5%) 23 18	28, 67, 136, 187	27 (1%)

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	10	ALA	7.5
1	F	264	VAL	7.1
2	C	500	VAL	6.2
1	F	276	TRP	6.1
2	C	511	GLN	5.7

### 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](#)

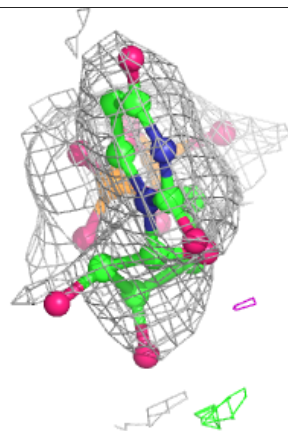
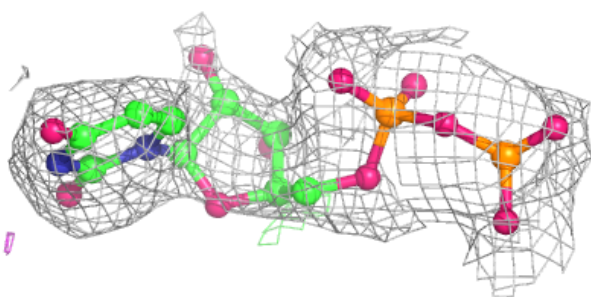
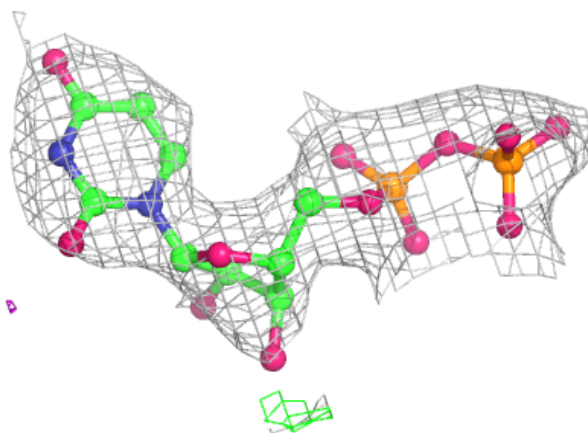
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BBK	D	1572	15/15	0.81	0.27	97,106,117,122	0
5	BBK	B	1572	15/15	0.82	0.26	66,81,110,110	0
5	BBK	E	1571	15/15	0.82	0.30	67,86,120,144	0
5	BBK	A	1571	15/15	0.87	0.22	52,76,82,88	0
6	UDP	C	1571	25/25	0.92	0.18	83,96,111,114	0
6	UDP	D	1571	25/25	0.92	0.21	64,98,118,128	0
6	UDP	B	1573	25/25	0.94	0.16	77,89,97,106	0
6	UDP	F	1364	25/25	0.94	0.16	107,134,151,177	0
6	UDP	E	1572	25/25	0.96	0.17	69,78,89,97	0
6	UDP	A	1572	25/25	0.97	0.16	54,74,89,97	0
4	MN	E	1570	1/1	0.97	0.13	46,46,46,46	0
4	MN	B	1571	1/1	0.98	0.15	63,63,63,63	0
4	MN	F	1363	1/1	0.98	0.10	93,93,93,93	0
4	MN	D	1570	1/1	0.98	0.13	58,58,58,58	0
4	MN	C	1570	1/1	0.99	0.13	67,67,67,67	0
4	MN	A	1570	1/1	0.99	0.10	46,46,46,46	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.

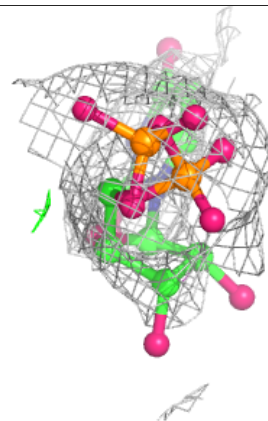
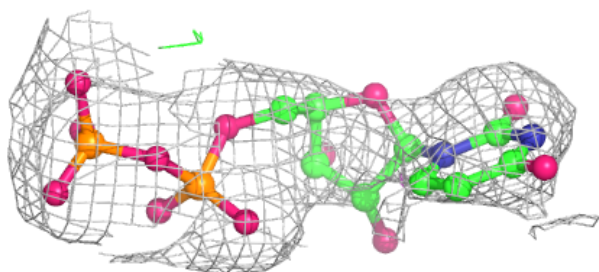
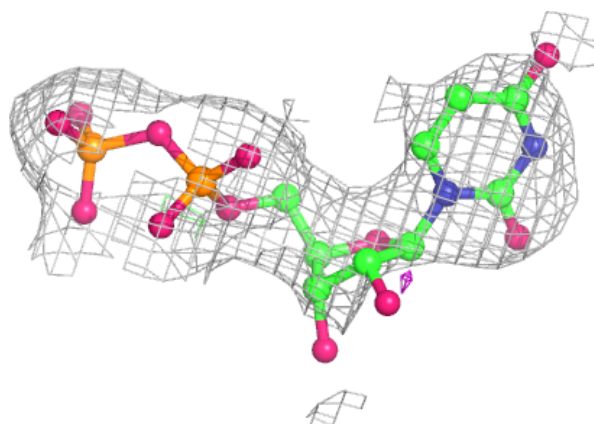
**Electron density around UDP C 1571:**

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

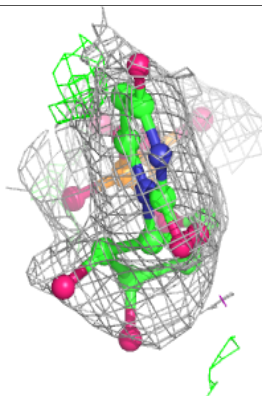
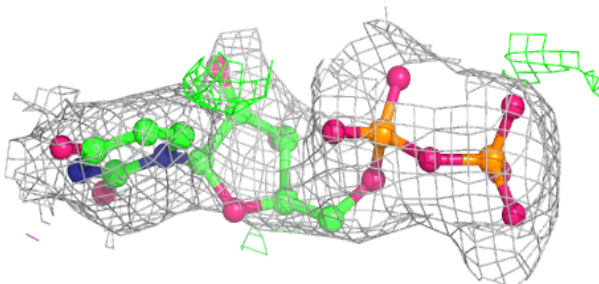
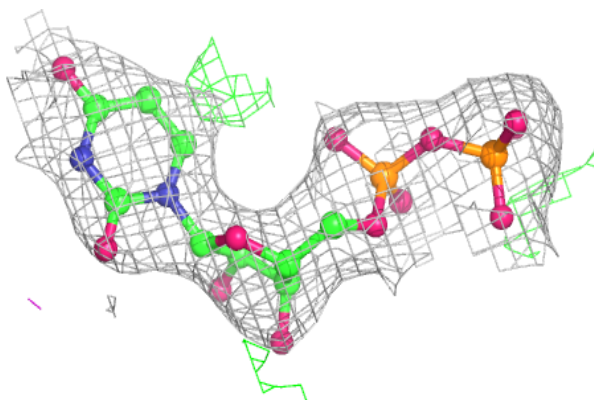


**Electron density around UDP D 1571:**

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

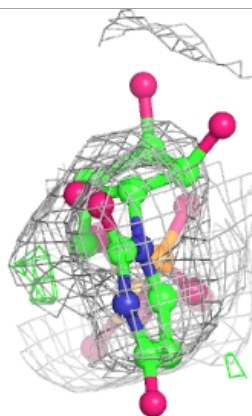
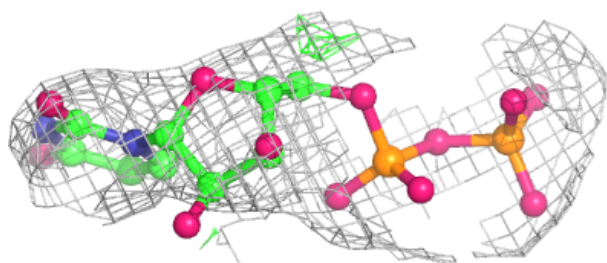
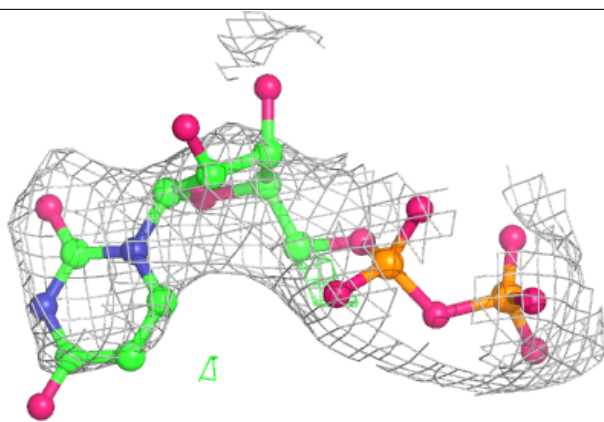
**Electron density around UDP B 1573:**

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

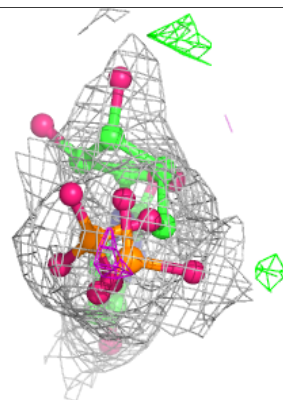
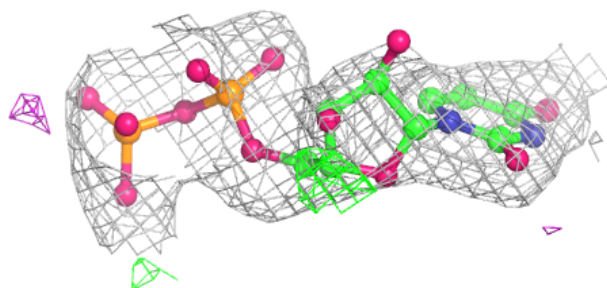
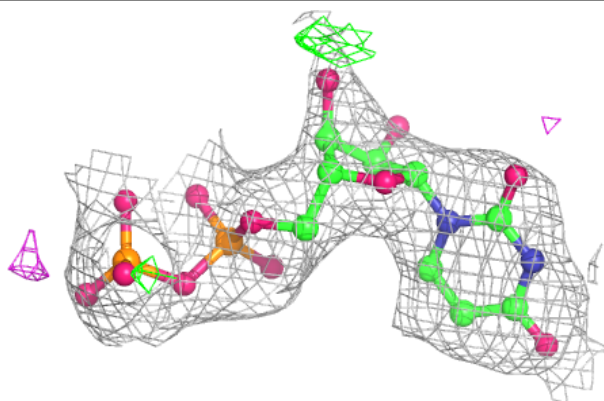


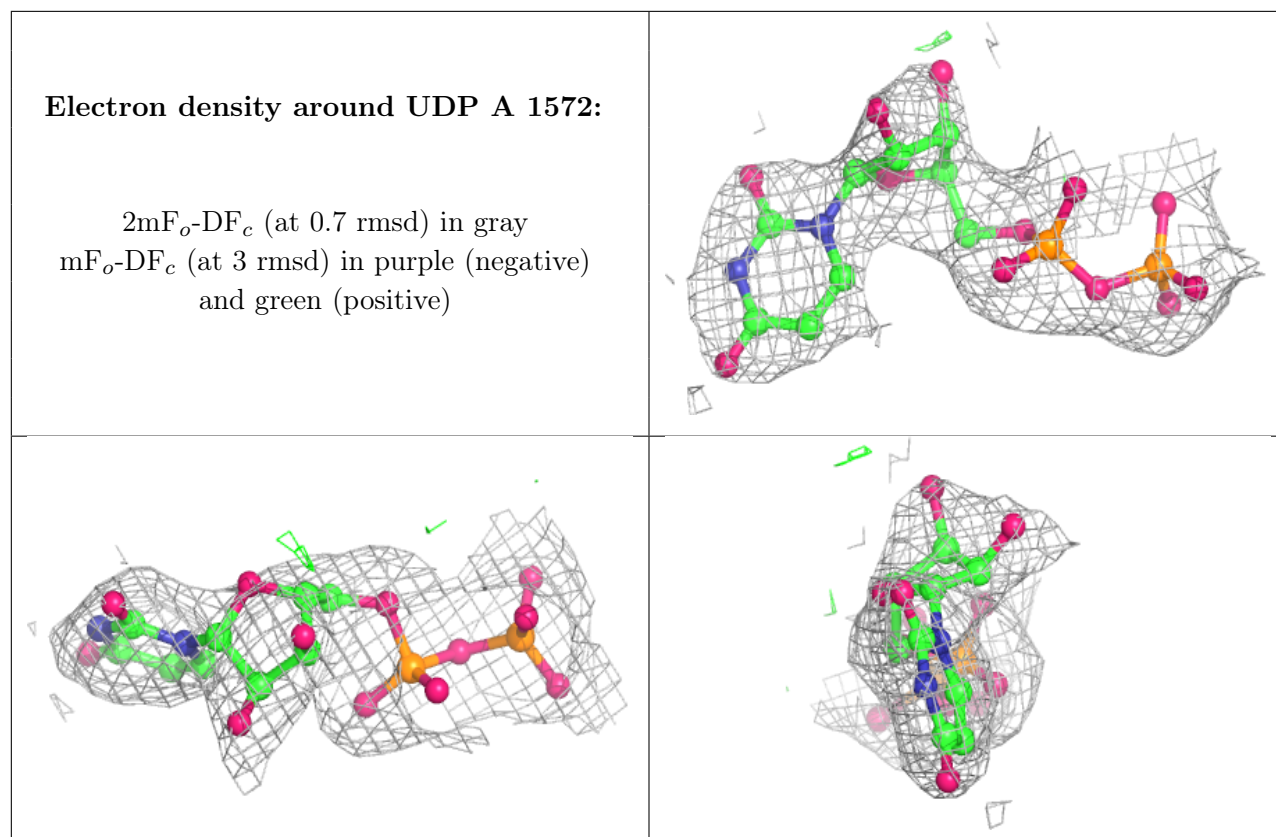
**Electron density around UDP F 1364:**

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

**Electron density around UDP E 1572:**

$2mF_o-DF_c$  (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.