



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:59 pm BST

PDB ID : 5FV9  
Title : Crystal structure of GalNAc-T2 in complex with compound 16d  
Authors : Ghirardello, M.; Rivas, M.; Lacetera, A.; Delso, I.; Lira-Navarrete, E.; Tejero, T.; Martin-Santamaria, S.; Hurtado-Guerrero, R.; Merino, P.  
Deposited on : 2016-02-03  
Resolution : 2.07 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



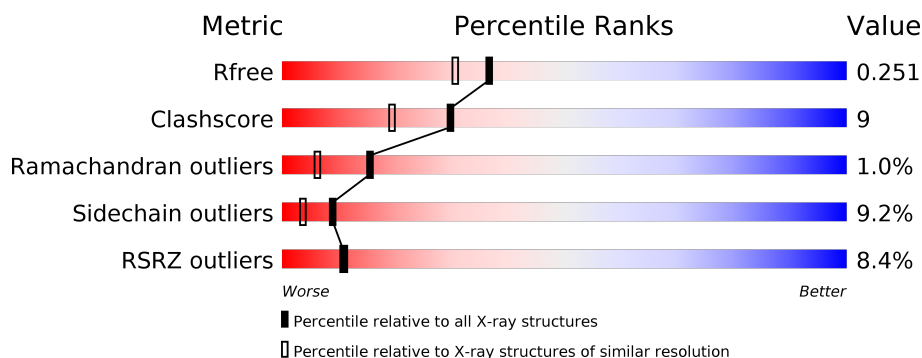
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	571	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>13%</div> <div>• •</div> <div>15%</div> </div> </div>
1	B	571	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>14%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	571	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	571	<div> <div>11%</div> <div> <div></div> <div>58%</div> <div>16%</div> <div>• •</div> <div>22%</div> </div> </div>
1	E	571	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>14%</div> <div>•</div> <div>15%</div> </div> </div>
1	F	571	<div> <div>9%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>• •</div> <div>16%</div> </div> </div>



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UDP	B	1572	-	-	X	-
4	EDO	A	1573	-	-	-	X



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24993 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 GALNAC-T2.

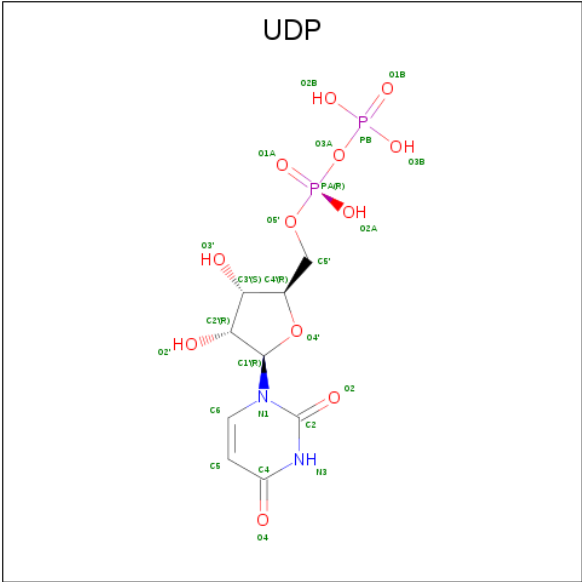
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	20	2	0
			3896	2451	709	712	24			
1	B	484	Total	C	N	O	S	20	1	0
			3894	2450	709	711	24			
1	C	482	Total	C	N	O	S	20	3	0
			3897	2451	712	710	24			
1	D	443	Total	C	N	O	S	20	0	0
			3575	2256	645	652	22			
1	E	483	Total	C	N	O	S	20	1	0
			3885	2445	705	711	24			
1	F	481	Total	C	N	O	S	20	1	0
			3869	2432	706	707	24			

There are 6 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
C	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 URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).





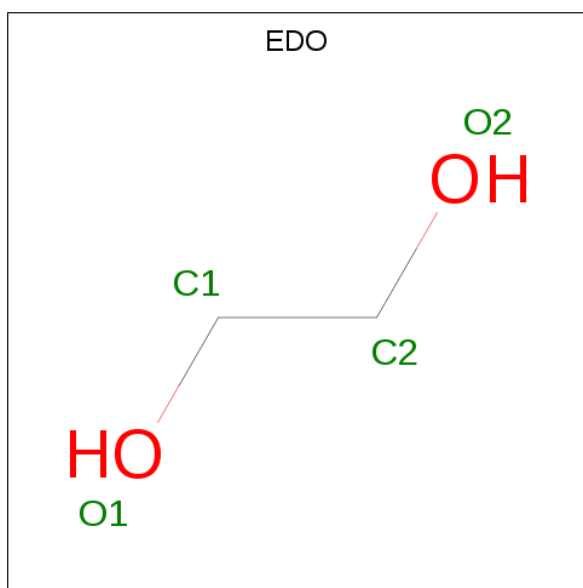
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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



- Molecule 4 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
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

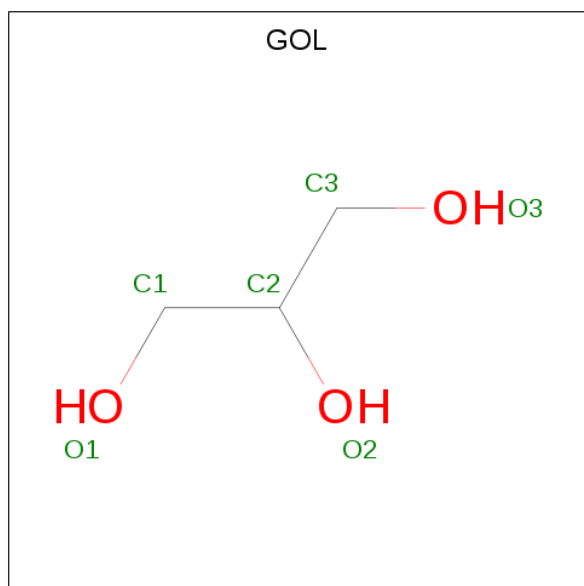
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			4	2	2		

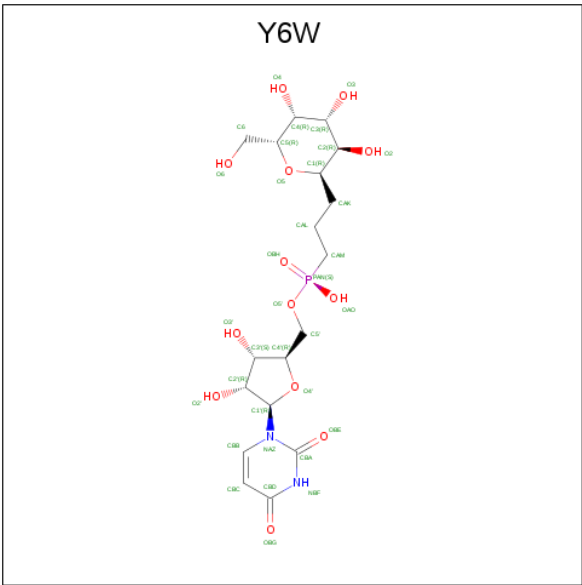
- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is [(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl hydrogen (S)-{3-[(2R,3R,4R,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]propyl}phosphonate (three-letter code: Y6W) (formula:  $C_{18}H_{29}N_2O_{13}P$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			34	18	2	13	1		
6	E	1	Total	C	N	O	P	0	0
			34	18	2	13	1		
6	F	1	Total	C	N	O	P	0	0
			34	18	2	13	1		

- Molecule 7 is water.

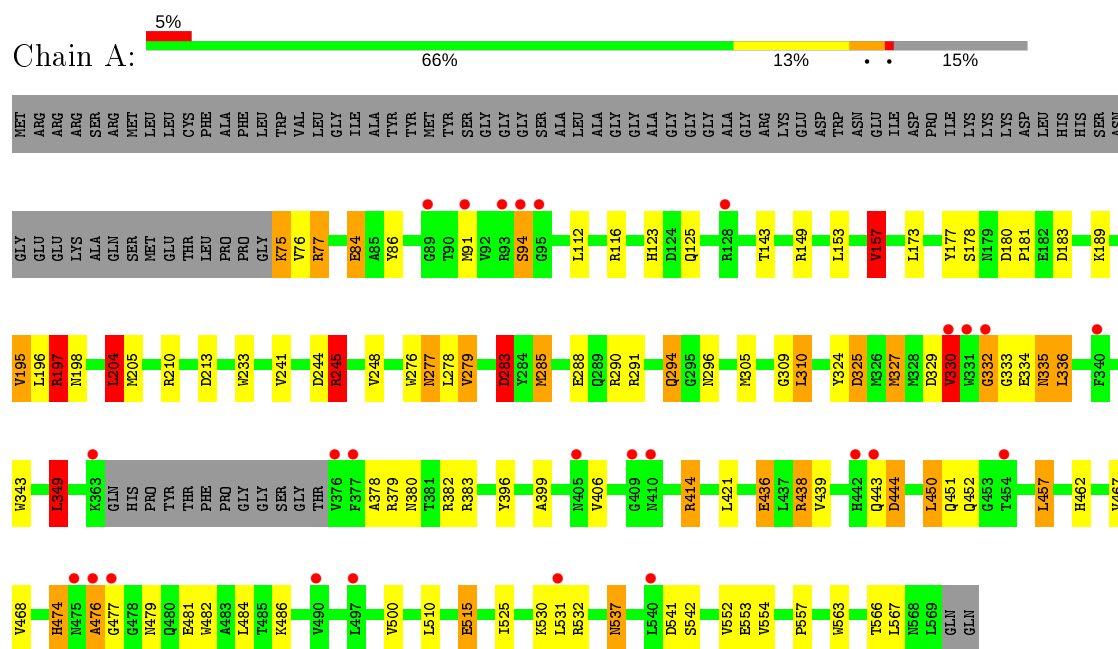
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	346	Total	O	0	0
			346	346		
7	B	299	Total	O	0	0
			299	299		
7	C	306	Total	O	0	0
			306	306		
7	D	184	Total	O	0	0
			184	184		
7	E	290	Total	O	0	0
			290	290		
7	F	208	Total	O	0	0
			208	208		



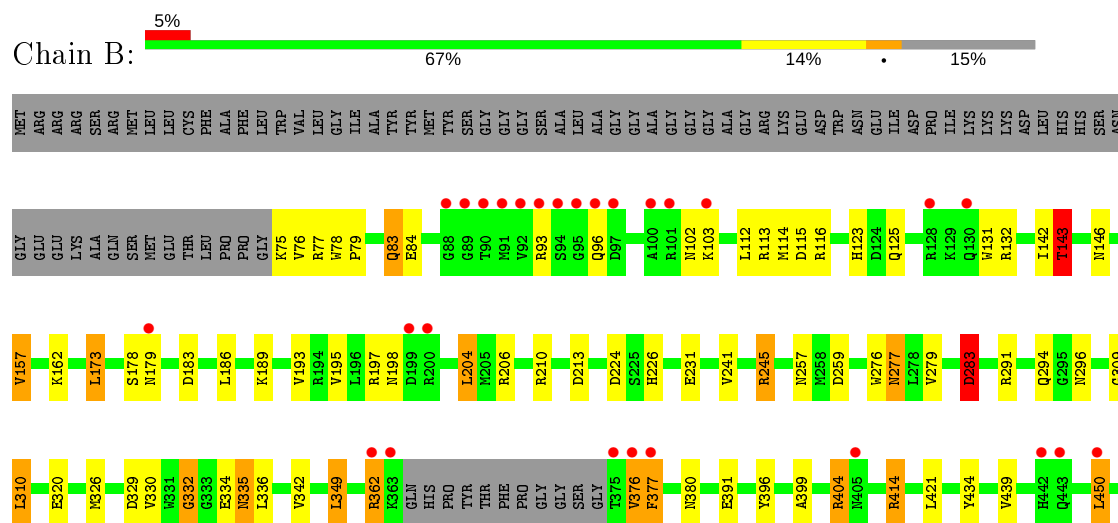
### 3 Residue-property plots [i](#)

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: GALNAC-T2



#### • Molecule 1: GALNAC-T2

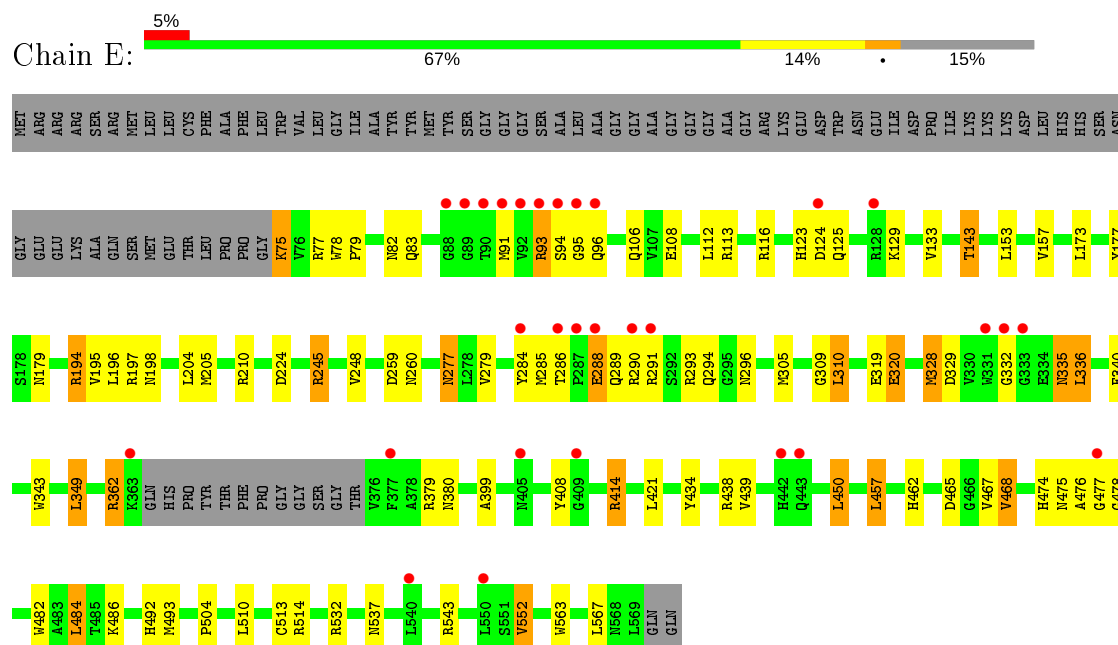




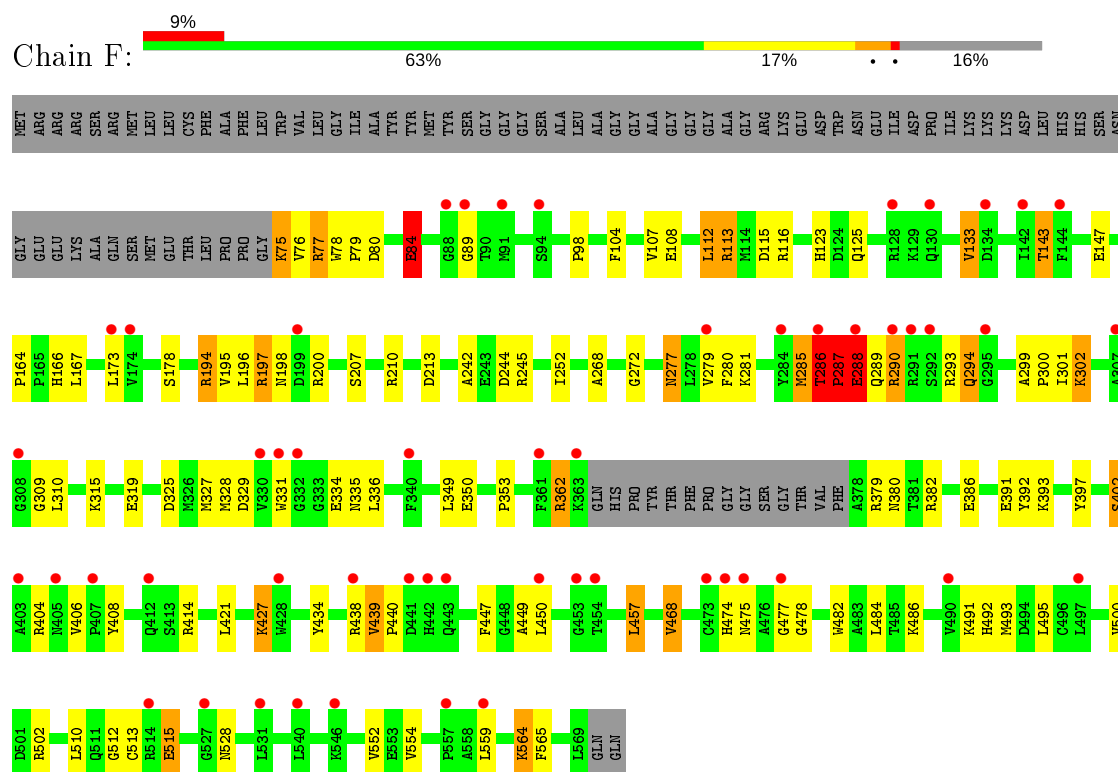




• Molecule 1: GALNAC-T2



• Molecule 1: GALNAC-T2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.49Å 121.75Å 250.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	250.15 – 2.07 19.99 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (250.15-2.07) 99.9 (19.99-2.07)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.190 , 0.247 0.198 , 0.251	Depositor DCC
$R_{free}$ test set	5938 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	24993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.06% 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: GOL, UDP, Y6W, EDO, 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	0.99	7/3982 (0.2%)	1.09	26/5380 (0.5%)
1	B	0.96	6/3980 (0.2%)	1.08	21/5378 (0.4%)
1	C	0.93	4/3986 (0.1%)	1.02	15/5384 (0.3%)
1	D	0.87	4/3653 (0.1%)	0.98	13/4935 (0.3%)
1	E	1.06	5/3971 (0.1%)	1.18	27/5366 (0.5%)
1	F	1.00	4/3954 (0.1%)	1.06	23/5342 (0.4%)
All	All	0.97	30/23526 (0.1%)	1.07	125/31785 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
1	D	0	4
1	E	0	1
1	F	0	4
All	All	0	14

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	515	GLU	CB-CG	-31.88	0.91	1.52
1	E	486	LYS	CB-CG	-28.54	0.75	1.52
1	A	515	GLU	CB-CG	-18.04	1.17	1.52
1	C	515	GLU	CB-CG	-16.08	1.21	1.52
1	C	84	GLU	CB-CG	-14.73	1.24	1.52
1	D	486	LYS	CB-CG	13.04	1.87	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	84	GLU	CB-CG	-12.77	1.27	1.52
1	D	84	GLU	CB-CG	-12.47	1.28	1.52
1	C	75	LYS	CB-CG	-12.07	1.20	1.52
1	B	486	LYS	CB-CG	-11.69	1.21	1.52
1	B	75	LYS	CB-CG	-10.86	1.23	1.52
1	B	84	GLU	CB-CG	-10.77	1.31	1.52
1	A	486	LYS	CB-CG	10.65	1.81	1.52
1	D	294	GLN	CB-CG	-9.85	1.25	1.52
1	A	75	LYS	CB-CG	-9.02	1.28	1.52
1	B	294	GLN	CB-CG	-9.02	1.28	1.52
1	E	513	CYS	C-N	-8.01	1.15	1.34
1	E	294	GLN	CB-CG	7.26	1.72	1.52
1	A	84	GLU	CB-CG	-7.25	1.38	1.52
1	E	332	GLY	N-CA	7.22	1.56	1.46
1	F	294	GLN	CB-CG	6.24	1.69	1.52
1	E	319	GLU	C-N	-6.24	1.19	1.34
1	D	515	GLU	CB-CG	-6.09	1.40	1.52
1	A	283	ASP	CB-CG	6.06	1.64	1.51
1	C	199	ASP	CB-CG	5.90	1.64	1.51
1	B	143	THR	CB-CG2	-5.81	1.33	1.52
1	B	283	ASP	CB-CG	5.78	1.63	1.51
1	F	147	GLU	CD-OE2	-5.73	1.19	1.25
1	A	332	GLY	N-CA	5.50	1.54	1.46
1	A	233	TRP	CB-CG	-5.10	1.41	1.50

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	197	ARG	NE-CZ-NH2	-23.21	108.69	120.30
1	E	197	ARG	NE-CZ-NH1	18.01	129.31	120.30
1	B	75	LYS	CA-CB-CG	13.77	143.68	113.40
1	F	75	LYS	CB-CG-CD	13.08	145.61	111.60
1	A	486	LYS	CB-CG-CD	-12.86	78.16	111.60
1	E	486	LYS	CA-CB-CG	12.21	140.27	113.40
1	B	532	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	C	75	LYS	CA-CB-CG	11.79	139.34	113.40
1	C	414	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	197	ARG	NE-CZ-NH2	-10.99	114.81	120.30
1	A	486	LYS	CA-CB-CG	-10.88	89.46	113.40
1	D	84	GLU	CA-CB-CG	10.75	137.06	113.40
1	B	414	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	C	414	ARG	NE-CZ-NH1	10.29	125.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	75	LYS	CB-CG-CD	9.61	136.59	111.60
1	F	294	GLN	CA-CB-CG	-9.57	92.34	113.40
1	A	414	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	D	486	LYS	CA-CB-CG	9.42	134.12	113.40
1	B	414	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	F	77	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	D	486	LYS	CB-CG-CD	8.99	134.98	111.60
1	B	224	ASP	CB-CG-OD1	-8.72	110.45	118.30
1	A	245	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	F	75	LYS	CA-CB-CG	-8.56	94.57	113.40
1	B	77	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	532	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	414	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	A	294	GLN	CA-CB-CG	8.20	131.43	113.40
1	F	515	GLU	CA-CB-CG	8.18	131.39	113.40
1	E	245	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	F	77	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	C	204	LEU	CA-CB-CG	7.62	132.84	115.30
1	D	75	LYS	CB-CG-CD	7.58	131.31	111.60
1	E	532	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	E	294	GLN	CA-CB-CG	-7.40	97.13	113.40
1	C	113	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	E	197	ARG	CD-NE-CZ	7.32	133.84	123.60
1	E	532	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	F	113	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	E	305	MET	CG-SD-CE	7.08	111.52	100.20
1	F	113	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	E	414	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	195	VAL	CG1-CB-CG2	6.95	122.01	110.90
1	F	84	GLU	CA-CB-CG	6.93	128.64	113.40
1	B	514[A]	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	514[B]	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	404	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	E	552	VAL	CG1-CB-CG2	6.84	121.84	110.90
1	D	204	LEU	CA-CB-CG	6.69	130.69	115.30
1	B	450	LEU	CB-CG-CD2	6.69	122.37	111.00
1	A	310	LEU	CA-CB-CG	6.66	130.60	115.30
1	A	75	LYS	CB-CG-CD	-6.64	94.34	111.60
1	A	197	ARG	CG-CD-NE	-6.64	97.86	111.80
1	B	519	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	E	194	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	E	197	ARG	CG-CD-NE	-6.31	98.55	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	GLU	CA-CB-CG	6.29	127.24	113.40
1	A	75	LYS	CA-CB-CG	6.28	127.22	113.40
1	F	362	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	E	362	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	D	224	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	A	244	ASP	CB-CG-OD1	6.09	123.79	118.30
1	B	486	LYS	CA-CB-CG	6.07	126.76	113.40
1	A	204	LEU	CA-CB-CG	6.06	129.25	115.30
1	E	414	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	F	414	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	328	MET	CG-SD-CE	5.90	109.65	100.20
1	B	484	LEU	CB-CG-CD2	5.90	121.03	111.00
1	B	162	LYS	CD-CE-NZ	5.89	125.25	111.70
1	F	197	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	F	194[A]	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	F	194[B]	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	75	LYS	CB-CG-CD	-5.85	96.39	111.60
1	C	113	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	E	362	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	404	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	515	GLU	CA-CB-CG	5.73	126.02	113.40
1	E	468	VAL	CG1-CB-CG2	5.73	120.08	110.90
1	F	493	MET	CG-SD-CE	5.71	109.34	100.20
1	F	294	GLN	CB-CG-CD	5.71	126.44	111.60
1	D	310	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	213	ASP	CB-CG-OD1	5.69	123.42	118.30
1	E	224	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	C	310	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	204	LEU	CA-CB-CG	5.67	128.33	115.30
1	E	514	ARG	O-C-N	-5.61	113.72	122.70
1	F	414	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	245	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	E	320	GLU	O-C-N	5.56	131.59	122.70
1	A	157	VAL	CG1-CB-CG2	5.55	119.77	110.90
1	E	543	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	77	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	478	GLY	N-CA-C	-5.50	99.34	113.10
1	A	532	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	465	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	205	MET	CB-CG-SD	5.46	128.77	112.40
1	D	474	HIS	N-CA-C	5.42	125.62	111.00
1	F	112	LEU	CB-CG-CD1	5.40	120.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	MET	CG-SD-CE	-5.38	91.59	100.20
1	E	514	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	245	ARG	CG-CD-NE	-5.32	100.63	111.80
1	D	154	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	F	244	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	349	LEU	CB-CG-CD1	5.27	119.95	111.00
1	C	310	LEU	CB-CG-CD2	5.26	119.95	111.00
1	A	532	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	E	484	LEU	CB-CG-CD2	5.20	119.84	111.00
1	F	290	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	127[A]	GLN	CB-CA-C	5.16	120.72	110.40
1	C	127[B]	GLN	CB-CA-C	5.16	120.72	110.40
1	B	501	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	F	197	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	F	468	VAL	N-CA-CB	-5.14	100.20	111.50
1	D	475	ASN	N-CA-C	5.11	124.80	111.00
1	A	197	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	444	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	110	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	501	ASP	CB-CG-OD1	5.07	122.86	118.30
1	F	213	ASP	CB-CG-OD1	5.06	122.86	118.30
1	D	362	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	438	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	E	510	LEU	CA-CB-CG	5.04	126.88	115.30
1	C	438	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	C	143	THR	N-CA-CB	-5.03	100.75	110.30
1	A	349	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	VAL	Peptide
1	A	476	ALA	Peptide
1	B	332	GLY	Peptide
1	C	129	LYS	Peptide
1	C	198	ASN	Peptide
1	D	329	ASP	Peptide
1	D	330	VAL	Peptide
1	D	452	GLN	Peptide
1	D	475	ASN	Peptide
1	E	476	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	F	285	MET	Peptide
1	F	286	THR	Peptide
1	F	288	GLU	Peptide
1	F	89	GLY	Peptide

## 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	3896	0	3829	79	0
1	B	3894	0	3831	77	0
1	C	3897	0	3835	61	0
1	D	3575	0	3512	75	0
1	E	3885	0	3815	56	1
1	F	3869	0	3806	69	1
2	A	25	0	11	3	0
2	B	25	0	4	8	0
2	C	25	0	11	1	0
2	D	25	0	11	3	0
2	E	25	0	8	2	0
2	F	25	0	4	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	12	0	18	2	0
4	B	8	0	12	0	0
4	C	8	0	12	0	0
4	E	16	0	24	2	0
4	F	12	0	18	0	0
5	A	12	0	16	0	0
5	C	6	0	8	0	0
5	F	12	0	16	0	0
6	B	34	0	0	15	0
6	E	34	0	0	5	0
6	F	34	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	346	0	0	16	0
7	B	299	0	0	16	0
7	C	306	0	0	10	0
7	D	184	0	0	6	0
7	E	290	0	0	14	1
7	F	208	0	0	9	1
All	All	24993	0	22801	431	2

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 (431) 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:205:MET:SD	1:A:334:GLU:HB3	1.50	1.50
1:A:205:MET:SD	1:A:334:GLU:CB	2.24	1.23
1:C:291[B]:ARG:HG3	1:C:291[B]:ARG:HH11	1.10	1.13
1:B:362:ARG:HH21	6:B:1570:Y6W:CAL	1.66	1.08
1:D:329:ASP:O	1:D:330:VAL:HG12	1.51	1.08
1:A:438:ARG:HG2	1:A:481:GLU:OE1	1.52	1.08
1:D:475:ASN:N	1:D:476:ALA:HB2	1.69	1.05
1:A:334:GLU:OE1	7:A:2249:HOH:O	1.76	1.03
1:B:226:HIS:CE1	6:B:1570:Y6W:CAM	2.41	1.02
1:C:538:LEU:HB3	1:C:552:VAL:HG22	1.43	1.00
1:E:537:ASN:HB3	7:E:2277:HOH:O	1.57	1.00
1:C:291[B]:ARG:CG	1:C:291[B]:ARG:HH11	1.75	0.99
6:F:1572:Y6W:C4	6:F:1572:Y6W:OAO	2.10	0.99
1:B:362:ARG:NH2	6:B:1570:Y6W:CAM	2.28	0.97
1:F:287:PRO:HB3	1:F:288:GLU:HB2	1.45	0.95
1:C:291[B]:ARG:NH1	1:C:291[B]:ARG:HG3	1.68	0.93
6:E:1572:Y6W:OAO	6:E:1572:Y6W:C4	2.17	0.92
1:E:493:MET:HG2	7:E:2246:HOH:O	1.71	0.90
1:E:277:ASN:ND2	1:E:279:VAL:HG12	1.87	0.89
1:F:293:ARG:NH1	1:F:299:ALA:O	2.06	0.89
1:E:143:THR:HG23	2:E:1570:UDP:O4	1.71	0.89
1:D:455:ASN:O	1:D:473:CYS:SG	2.32	0.88
1:C:123:HIS:HD2	1:C:125:GLN:H	1.20	0.87
1:B:226:HIS:HE1	6:B:1570:Y6W:CAM	1.80	0.87
1:B:277:ASN:ND2	1:B:279:VAL:HG12	1.90	0.87
1:A:143:THR:HG22	7:A:2083:HOH:O	1.75	0.87
1:D:143:THR:HG23	2:D:1555:UDP:O4	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:ASN:CA	1:D:476:ALA:HB2	2.07	0.84
1:B:277:ASN:HD21	1:B:279:VAL:HG12	1.42	0.84
1:B:206:ARG:HH11	1:B:206:ARG:HG3	1.41	0.84
1:C:143:THR:HG23	2:C:1570:UDP:O4	1.76	0.84
1:B:143:THR:HG23	6:B:1570:Y6W:OBG	1.77	0.83
1:D:123:HIS:HD2	1:D:125:GLN:H	1.23	0.83
1:B:362:ARG:HH21	6:B:1570:Y6W:CAM	1.91	0.82
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.15	0.81
7:A:2052:HOH:O	1:B:514[B]:ARG:NH1	2.04	0.81
1:A:553[A]:GLU:OE2	1:A:554:VAL:HG12	1.80	0.81
1:A:329:ASP:O	1:A:330:VAL:HG12	1.81	0.81
1:C:128:ARG:HB3	1:C:129:LYS:HA	1.62	0.81
1:A:290:ARG:HD2	1:B:493:MET:HE1	1.63	0.80
1:B:329:ASP:H	1:B:380:ASN:HD21	1.24	0.80
1:A:205:MET:SD	1:A:334:GLU:HB2	2.21	0.80
1:A:123:HIS:HD2	1:A:125:GLN:H	1.27	0.79
1:B:206:ARG:HG2	7:B:2089:HOH:O	1.81	0.78
1:F:178:SER:O	1:F:197:ARG:NH2	2.16	0.78
1:C:329:ASP:H	1:C:380:ASN:HD21	1.32	0.78
1:F:457:LEU:HD13	1:F:482:TRP:CE2	2.18	0.78
1:E:329:ASP:H	1:E:380:ASN:HD21	1.30	0.77
1:D:329:ASP:O	1:D:330:VAL:CG1	2.32	0.77
1:C:457:LEU:HD13	1:C:482:TRP:CE2	2.19	0.77
1:D:162:LYS:NZ	7:D:2066:HOH:O	2.12	0.77
1:D:231:GLU:OE1	7:D:2091:HOH:O	2.02	0.76
1:B:362:ARG:NH2	6:B:1570:Y6W:CAL	2.46	0.76
1:F:287:PRO:HB2	1:F:289:GLN:N	2.00	0.76
1:C:291[B]:ARG:NH2	7:C:2180:HOH:O	2.18	0.76
1:F:287:PRO:CB	1:F:288:GLU:HB2	2.16	0.75
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.21	0.75
1:D:206:ARG:HD3	1:D:326:MET:O	1.87	0.75
1:F:287:PRO:HB2	1:F:289:GLN:H	1.51	0.74
1:F:123:HIS:HD2	1:F:125:GLN:H	1.35	0.74
1:E:399:ALA:HB2	1:E:567:LEU:HD22	1.70	0.74
1:C:178:SER:O	1:C:197:ARG:NH2	2.20	0.73
1:B:569:LEU:C	7:B:2296:HOH:O	2.25	0.73
1:F:329:ASP:H	1:F:380:ASN:HD21	1.36	0.73
1:E:277:ASN:HD21	1:E:279:VAL:HG12	1.52	0.73
1:A:189:LYS:HD3	7:A:2130:HOH:O	1.89	0.72
1:E:143:THR:HG23	6:E:1572:Y6W:OBG	1.88	0.72
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:VAL:HG13	7:B:2143:HOH:O	1.91	0.71
6:E:1572:Y6W:O5'	6:E:1572:Y6W:C6	2.38	0.71
1:A:537:ASN:ND2	7:A:2327:HOH:O	2.24	0.70
1:E:328:MET:HB2	7:E:2110:HOH:O	1.90	0.70
1:B:186:LEU:O	1:B:189:LYS:HE3	1.92	0.70
1:C:523:GLU:OE2	1:C:532:ARG:NH1	2.23	0.70
1:B:414:ARG:HD3	7:B:2183:HOH:O	1.91	0.70
1:B:178:SER:O	1:B:197:ARG:NH2	2.25	0.69
1:F:327:MET:O	1:F:379:ARG:NH2	2.25	0.69
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.38	0.69
1:B:213:ASP:HB3	7:B:2101:HOH:O	1.93	0.68
1:C:442:HIS:HB2	7:C:2248:HOH:O	1.92	0.68
1:F:319:GLU:OE1	7:F:2146:HOH:O	2.09	0.68
1:C:123:HIS:CD2	1:C:125:GLN:H	2.08	0.68
6:B:1570:Y6W:C4	2:B:1572:UDP:O1A	2.42	0.68
1:B:439:VAL:HG12	7:B:2212:HOH:O	1.93	0.68
1:A:205:MET:CE	1:A:334:GLU:HB3	2.23	0.68
1:E:286:THR:OG1	1:E:288:GLU:HG3	1.93	0.68
1:E:205:MET:HB3	7:E:2110:HOH:O	1.92	0.67
1:D:473:CYS:O	1:D:475:ASN:N	2.24	0.67
6:B:1570:Y6W:C5	2:B:1572:UDP:O1A	2.43	0.67
1:B:143:THR:HG23	2:B:1572:UDP:O4	1.94	0.67
1:D:202:GLU:OE1	1:D:206:ARG:NH2	2.28	0.67
1:D:475:ASN:CA	1:D:476:ALA:CB	2.73	0.67
1:F:113:ARG:CD	1:F:115:ASP:OD1	2.43	0.67
1:F:287:PRO:HB3	1:F:288:GLU:CB	2.23	0.66
1:D:476:ALA:HB3	7:D:2170:HOH:O	1.96	0.66
1:B:123:HIS:HD2	1:B:125:GLN:H	1.42	0.66
1:A:290:ARG:CD	1:B:493:MET:HE1	2.26	0.66
1:F:334:GLU:OE2	6:F:1572:Y6W:O3	2.11	0.66
1:B:186:LEU:O	1:B:189:LYS:CE	2.44	0.65
1:C:83:GLN:HE22	1:C:114:MET:H	1.44	0.65
1:B:206:ARG:HD3	1:B:326:MET:O	1.95	0.65
1:A:75:LYS:HA	1:A:189:LYS:O	1.96	0.65
1:B:113:ARG:NH1	1:B:115:ASP:OD1	2.29	0.65
1:A:285:MET:O	1:A:290:ARG:NH1	2.29	0.65
1:B:335:ASN:HD22	1:B:335:ASN:H	1.44	0.65
1:F:382:ARG:NE	1:F:397:TYR:OH	2.29	0.64
1:C:128:ARG:HB3	1:C:129:LYS:CA	2.27	0.64
1:F:362:ARG:HB2	7:F:2025:HOH:O	1.96	0.64
1:A:291[B]:ARG:NH2	7:A:2227:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ARG:HD3	7:E:2196:HOH:O	1.97	0.64
2:F:1570:UDP:O2'	6:F:1572:Y6W:OBE	2.15	0.64
1:A:343:TRP:CD1	1:A:349:LEU:HD22	2.33	0.63
1:C:335:ASN:HD22	1:C:335:ASN:H	1.46	0.63
1:B:309:GLY:C	1:B:310:LEU:HD23	2.18	0.63
1:F:285:MET:O	1:F:287:PRO:HD3	1.98	0.63
1:B:399:ALA:HB2	1:B:567:LEU:HD22	1.79	0.63
1:D:386:GLU:OE1	1:D:393:LYS:NZ	2.18	0.63
1:C:78:TRP:CG	1:C:79:PRO:HD3	2.35	0.62
1:F:285:MET:C	1:F:287:PRO:CD	2.68	0.62
1:A:245:ARG:HG2	7:A:2180:HOH:O	1.98	0.62
1:E:143:THR:CG2	2:E:1570:UDP:O4	2.46	0.62
2:F:1570:UDP:O3B	6:F:1572:Y6W:O5'	2.13	0.62
1:F:113:ARG:HD3	1:F:115:ASP:OD1	1.99	0.62
1:C:113:ARG:HD2	1:C:115:ASP:OD1	2.00	0.61
1:E:108:GLU:HG2	1:E:260:ASN:HA	1.82	0.61
1:B:143:THR:CG2	2:B:1572:UDP:O4	2.49	0.61
1:A:177:TYR:CE2	4:A:1573:EDO:H21	2.35	0.61
1:A:283:ASP:HB3	7:A:2214:HOH:O	1.99	0.61
1:C:538:LEU:HB3	1:C:552:VAL:CG2	2.23	0.61
1:F:335:ASN:H	1:F:335:ASN:HD22	1.49	0.60
1:B:462:HIS:HD2	1:B:467:VAL:O	1.83	0.60
1:C:245:ARG:NH2	1:C:320:GLU:OE1	2.28	0.60
1:B:83:GLN:HE22	1:B:114:MET:H	1.49	0.60
6:B:1570:Y6W:C5	2:B:1572:UDP:PA	2.90	0.60
1:D:147:GLU:HG2	1:D:225:SER:HB2	1.84	0.60
1:F:113:ARG:HD2	1:F:115:ASP:OD1	2.03	0.59
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.51	0.59
1:D:206:ARG:NE	7:D:2086:HOH:O	2.13	0.59
1:A:525:ILE:HG13	1:A:530:LYS:HB2	1.84	0.59
1:D:153:LEU:O	1:D:157:VAL:HG13	2.03	0.58
1:A:277:ASN:ND2	1:A:279:VAL:H	2.01	0.58
1:D:475:ASN:HA	1:D:476:ALA:HB2	1.84	0.58
1:F:78:TRP:CG	1:F:79:PRO:HD3	2.38	0.58
1:A:290:ARG:CD	1:B:493:MET:CE	2.81	0.58
1:C:258:MET:HE1	7:C:2214:HOH:O	2.03	0.58
1:D:383:ARG:O	1:D:387:VAL:HG23	2.02	0.58
1:A:329:ASP:H	1:A:380:ASN:HD21	1.52	0.58
1:C:335:ASN:ND2	1:C:335:ASN:H	2.02	0.58
1:B:143:THR:CG2	6:B:1570:Y6W:OBG	2.50	0.57
1:F:302:LYS:NZ	1:F:350:GLU:OE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:HG3	1:B:206:ARG:NH1	2.15	0.57
1:B:78:TRP:CG	1:B:79:PRO:HD3	2.40	0.57
1:F:290:ARG:HA	1:F:290:ARG:NH1	2.20	0.57
1:D:441:ASP:OD1	1:D:443:GLN:N	2.37	0.57
1:C:414:ARG:HD3	7:C:2207:HOH:O	2.04	0.56
1:C:568:ASN:HD22	1:C:568:ASN:C	2.08	0.56
1:D:469:GLY:HA2	1:D:550:LEU:HD23	1.87	0.56
1:F:76:VAL:CG2	1:F:80:ASP:HB2	2.36	0.56
1:C:128:ARG:CB	1:C:129:LYS:HA	2.31	0.56
1:C:218:LYS:HD2	1:E:82:ASN:HA	1.87	0.56
1:F:277:ASN:O	7:F:2138:HOH:O	2.18	0.56
1:D:475:ASN:H	1:D:476:ALA:HB2	1.64	0.55
1:B:362:ARG:HH22	6:B:1570:Y6W:CAM	2.16	0.55
1:C:414:ARG:CD	7:C:2207:HOH:O	2.55	0.55
1:F:143:THR:HG23	2:F:1570:UDP:O4	2.05	0.55
1:A:474:HIS:CD2	1:A:476:ALA:HB3	2.42	0.55
1:A:438:ARG:CG	1:A:481:GLU:OE1	2.42	0.55
1:A:541:ASP:CB	1:A:553[B]:GLU:HG3	2.37	0.55
1:F:252:ILE:HD12	1:F:353:PRO:HA	1.89	0.55
1:E:414:ARG:CD	7:E:2196:HOH:O	2.54	0.55
1:C:126:CYS:O	1:C:129:LYS:HB2	2.07	0.54
6:E:1572:Y6W:O5'	6:E:1572:Y6W:C5	2.55	0.54
1:D:336:LEU:CD1	1:D:340:PHE:CE2	2.90	0.54
1:F:528:ASN:O	1:F:564:LYS:HD2	2.06	0.54
1:A:481:GLU:HG2	1:A:482:TRP:N	2.23	0.54
1:F:335:ASN:ND2	1:F:335:ASN:H	2.05	0.54
1:F:286:THR:C	1:F:287:PRO:O	2.46	0.54
1:A:325:ASP:HB2	1:A:414:ARG:HD2	1.88	0.54
1:B:478:GLY:O	1:B:492:HIS:HE1	1.91	0.54
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.55	0.54
1:C:198:ASN:HD22	1:C:210:ARG:HH11	1.54	0.54
1:A:414:ARG:HD3	7:A:2251:HOH:O	2.07	0.53
1:D:252:ILE:HD12	1:D:353:PRO:HA	1.89	0.53
6:F:1572:Y6W:CAL	6:F:1572:Y6W:C5'	2.86	0.53
1:A:444:ASP:OD2	7:A:2277:HOH:O	2.19	0.53
1:E:177:TYR:O	4:E:1575:EDO:H11	2.08	0.53
1:F:143:THR:HG22	7:F:2062:HOH:O	2.08	0.53
1:D:445:ILE:HB	1:D:484:LEU:HD13	1.90	0.53
1:C:452:GLN:NE2	1:C:542:SER:OG	2.35	0.53
1:D:385:ALA:HA	1:D:389:MET:HE2	1.91	0.53
1:D:475:ASN:HA	1:D:476:ALA:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ARG:HH22	1:B:320:GLU:CD	2.12	0.53
1:B:142:ILE:HB	1:B:173:LEU:HD12	1.92	0.52
1:B:530:LYS:NZ	7:B:2271:HOH:O	2.42	0.52
1:A:177:TYR:CZ	4:A:1573:EDO:H21	2.44	0.52
1:A:378:ALA:HB3	1:A:406:VAL:HG21	1.89	0.52
1:D:183:ASP:HB2	7:D:2076:HOH:O	2.10	0.52
1:B:146:ASN:HD21	1:B:179:ASN:ND2	2.08	0.52
1:B:334:GLU:OE2	6:B:1570:Y6W:O3	2.27	0.52
1:F:194[B]:ARG:NH1	7:F:2093:HOH:O	2.42	0.52
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.58	0.52
1:E:279:VAL:HG13	7:E:2158:HOH:O	2.10	0.52
1:A:143:THR:CG2	1:A:204:LEU:HD22	2.40	0.52
1:A:414:ARG:CD	7:A:2251:HOH:O	2.58	0.52
1:D:330:VAL:HA	1:D:332:GLY:N	2.24	0.52
6:F:1572:Y6W:C3	6:F:1572:Y6W:OAO	2.58	0.51
1:E:77:ARG:HD3	7:E:2003:HOH:O	2.10	0.51
1:A:290:ARG:HD3	1:B:493:MET:HE2	1.92	0.51
1:D:382:ARG:NH1	1:D:406:VAL:O	2.31	0.51
6:E:1572:Y6W:PAN	6:E:1572:Y6W:C5	2.99	0.51
1:E:93:ARG:HB2	1:E:96:GLN:CD	2.31	0.51
1:D:474:HIS:CE1	1:D:476:ALA:HB1	2.46	0.51
1:F:491:LYS:HE2	1:F:513:CYS:SG	2.51	0.51
1:E:123:HIS:CD2	1:E:125:GLN:H	2.29	0.51
1:A:450:LEU:HD13	1:A:563:TRP:CE3	2.46	0.50
1:D:462:HIS:HD2	1:D:467:VAL:O	1.94	0.50
2:F:1570:UDP:O3B	6:F:1572:Y6W:C5'	2.59	0.50
1:A:143:THR:HG23	2:A:1570:UDP:C5	2.47	0.50
1:B:376:VAL:O	1:B:377:PHE:CB	2.60	0.50
1:A:329:ASP:O	1:A:330:VAL:CG1	2.57	0.50
1:C:462:HIS:HD2	1:C:467:VAL:O	1.94	0.50
1:D:331:TRP:CD1	1:D:331:TRP:N	2.80	0.50
1:E:205:MET:CB	7:E:2110:HOH:O	2.54	0.50
1:E:285:MET:O	1:E:290:ARG:NH1	2.44	0.50
6:F:1572:Y6W:C5	6:F:1572:Y6W:PAN	2.99	0.50
1:F:287:PRO:CB	1:F:288:GLU:CB	2.86	0.50
1:B:414:ARG:CD	7:B:2183:HOH:O	2.55	0.50
1:E:309:GLY:C	1:E:310:LEU:HD23	2.32	0.50
6:B:1570:Y6W:C3'	2:B:1572:UDP:O5'	2.60	0.49
1:B:276:TRP:O	1:B:396:TYR:HA	2.13	0.49
1:D:113:ARG:NH1	1:D:115:ASP:OD1	2.45	0.49
1:A:123:HIS:CD2	1:A:125:GLN:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LYS:NZ	1:B:556:GLY:O	2.44	0.49
1:F:457:LEU:HD13	1:F:482:TRP:CD2	2.48	0.49
1:A:333:GLY:HA3	1:A:380:ASN:HB3	1.94	0.49
2:F:1570:UDP:O2B	6:F:1572:Y6W:C3	2.52	0.49
1:F:272:GLY:HA2	1:F:280:PHE:CZ	2.48	0.49
1:D:452:GLN:HE21	1:D:452:GLN:C	2.16	0.49
1:C:162:LYS:HE2	7:C:2076:HOH:O	2.12	0.49
1:F:252:ILE:CD1	1:F:353:PRO:HA	2.42	0.49
1:B:310:LEU:HD23	1:B:310:LEU:N	2.27	0.49
1:C:290:ARG:HD3	1:D:493:MET:HE3	1.94	0.49
1:E:335:ASN:HD22	1:E:335:ASN:H	1.61	0.49
1:E:379:ARG:HG3	1:E:408:TYR:HA	1.95	0.48
1:D:143:THR:CG2	2:D:1555:UDP:O4	2.56	0.48
1:D:235:GLU:HB2	1:D:236:PRO:HD3	1.94	0.48
1:F:242:ALA:HA	7:F:2112:HOH:O	2.14	0.48
1:A:277:ASN:HD22	1:A:277:ASN:C	2.16	0.48
1:A:343:TRP:NE1	1:A:349:LEU:HD22	2.28	0.48
1:D:491:LYS:HB3	1:D:496:CYS:SG	2.54	0.48
1:D:83:GLN:HE22	1:D:114:MET:H	1.60	0.48
1:A:557:PRO:HB2	1:E:259:ASP:HB3	1.95	0.48
1:C:440:PRO:HG3	1:C:447:PHE:CG	2.49	0.48
1:E:179:ASN:HA	4:E:1575:EDO:H12	1.94	0.48
1:C:465:ASP:O	1:C:509:LYS:HE2	2.14	0.48
1:E:362:ARG:HB2	7:E:2009:HOH:O	2.13	0.48
1:A:452:GLN:NE2	1:A:542:SER:OG	2.38	0.48
1:E:343:TRP:CD1	1:E:349:LEU:HD22	2.49	0.48
1:A:462:HIS:HD2	1:A:467:VAL:O	1.96	0.48
2:F:1570:UDP:O1A	6:F:1572:Y6W:C4	2.47	0.48
1:A:86:TYR:CE2	1:A:149:ARG:HB3	2.49	0.48
1:C:248:VAL:HB	1:C:349:LEU:HD12	1.96	0.48
1:B:376:VAL:O	1:B:377:PHE:HB2	2.13	0.47
2:D:1555:UDP:O3B	2:D:1555:UDP:O1A	2.32	0.47
1:E:194:ARG:HG3	7:E:2091:HOH:O	2.13	0.47
1:F:382:ARG:NH1	1:F:406:VAL:O	2.46	0.47
1:D:281:LYS:NZ	7:D:2118:HOH:O	2.47	0.47
1:C:525:ILE:O	1:C:528:ASN:N	2.45	0.47
1:D:441:ASP:CG	1:D:443:GLN:N	2.68	0.47
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.63	0.47
1:E:143:THR:HG21	1:E:204:LEU:HD22	1.96	0.47
1:F:286:THR:O	1:F:287:PRO:O	2.32	0.47
1:F:309:GLY:C	1:F:310:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HG2	7:B:2037:HOH:O	2.14	0.47
1:F:315:LYS:CE	7:F:2102:HOH:O	2.62	0.47
1:D:252:ILE:CD1	1:D:353:PRO:HA	2.45	0.47
1:B:391:GLU:CD	1:B:391:GLU:H	2.18	0.46
1:E:336:LEU:HD13	1:E:340:PHE:CE2	2.50	0.46
1:F:478:GLY:O	1:F:492:HIS:HE1	1.97	0.46
1:A:183:ASP:HB2	7:A:2120:HOH:O	2.15	0.46
1:B:283:ASP:HA	7:B:2150:HOH:O	2.15	0.46
1:B:231:GLU:HG3	7:B:2107:HOH:O	2.15	0.46
1:E:277:ASN:HD21	1:E:279:VAL:CG1	2.23	0.46
1:E:478:GLY:O	1:E:492:HIS:HE1	1.98	0.46
7:A:2225:HOH:O	1:B:493:MET:HE1	2.14	0.46
7:A:2320:HOH:O	1:E:95:GLY:HA2	2.15	0.46
6:F:1572:Y6W:C6	6:F:1572:Y6W:O5'	2.64	0.46
1:F:285:MET:C	1:F:287:PRO:HD2	2.35	0.46
1:F:325:ASP:HB3	1:F:328:MET:HG3	1.97	0.46
1:D:455:ASN:HD22	1:D:455:ASN:HA	1.65	0.46
1:A:378:ALA:O	1:A:382:ARG:HG3	2.16	0.46
1:C:94:SER:HB3	7:C:2016:HOH:O	2.15	0.46
1:D:342:VAL:HG11	1:D:349:LEU:HD13	1.98	0.46
1:A:91:MET:CE	7:A:2010:HOH:O	2.63	0.46
1:B:330:VAL:HG22	1:B:330:VAL:O	2.14	0.46
1:D:198:ASN:HD22	1:D:210:ARG:NH1	2.14	0.46
1:E:83:GLN:NE2	7:E:2005:HOH:O	2.48	0.46
1:F:500:VAL:CG1	1:F:500:VAL:O	2.64	0.46
1:E:198:ASN:ND2	1:E:210:ARG:HH11	2.10	0.45
1:C:344:GLN:HE22	1:C:388:TRP:HB3	1.81	0.45
1:D:465:ASP:O	1:D:509:LYS:HE2	2.15	0.45
1:A:143:THR:HG21	1:A:204:LEU:HD22	1.97	0.45
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.12	0.45
1:B:532:ARG:HG2	1:B:533:HIS:N	2.31	0.45
1:C:94:SER:CB	7:C:2016:HOH:O	2.64	0.45
1:D:343:TRP:CD1	1:D:349:LEU:HD22	2.52	0.45
1:D:455:ASN:O	1:D:456:CYS:HB2	2.17	0.45
6:F:1572:Y6W:C5	6:F:1572:Y6W:OAO	2.62	0.45
1:A:330:VAL:HG13	1:A:330:VAL:O	2.16	0.45
1:D:329:ASP:H	1:D:380:ASN:HD21	1.63	0.45
1:D:330:VAL:CG2	1:D:331:TRP:HA	2.47	0.45
6:B:1570:Y6W:CAL	2:B:1572:UDP:O1B	0.47	0.45
1:F:164:PRO:HG2	1:F:167:LEU:HD12	1.98	0.45
1:F:439:VAL:HG13	7:F:2167:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:VAL:HG13	1:D:262:GLN:HE22	1.82	0.45
1:D:336:LEU:HD11	1:D:340:PHE:CE2	2.52	0.45
1:A:309:GLY:C	1:A:310:LEU:HD23	2.37	0.44
1:A:325:ASP:OD1	1:A:325:ASP:C	2.54	0.44
1:C:363:LYS:HG2	7:C:2214:HOH:O	2.16	0.44
1:E:77:ARG:CD	7:E:2003:HOH:O	2.64	0.44
1:E:124:ASP:HB2	7:E:2033:HOH:O	2.17	0.44
1:E:153:LEU:O	1:E:157:VAL:HG13	2.16	0.44
1:F:280:PHE:CD1	1:F:281:LYS:N	2.85	0.44
1:B:546:LYS:HA	7:B:2281:HOH:O	2.17	0.44
1:C:206:ARG:HG3	7:C:2111:HOH:O	2.17	0.44
1:F:285:MET:O	1:F:287:PRO:CD	2.64	0.44
1:F:98:PRO:HB3	1:F:107:VAL:HG23	1.99	0.44
1:A:178:SER:O	1:A:197:ARG:NH2	2.43	0.44
1:B:362:ARG:NH2	2:B:1572:UDP:O1B	2.35	0.44
1:D:484:LEU:HA	1:D:489:SER:O	2.18	0.44
1:A:332:GLY:HA2	1:A:380:ASN:HB2	2.00	0.44
1:D:335:ASN:HD22	1:D:335:ASN:H	1.66	0.44
1:B:114:MET:O	1:B:157:VAL:HG22	2.18	0.44
1:B:186:LEU:O	1:B:189:LYS:HE2	2.17	0.44
1:B:257:ASN:OD1	1:B:259:ASP:N	2.47	0.44
1:D:328:MET:HA	1:D:380:ASN:ND2	2.33	0.44
1:D:401:PRO:O	1:D:404:ARG:HG3	2.17	0.44
1:D:328:MET:HA	1:D:380:ASN:HD21	1.83	0.44
1:E:462:HIS:HD2	1:E:467:VAL:O	1.99	0.44
1:D:474:HIS:ND1	1:D:476:ALA:CB	2.80	0.44
1:F:564:LYS:HE3	1:F:565:PHE:N	2.33	0.44
1:B:404:ARG:HD2	7:B:2192:HOH:O	2.18	0.43
1:D:487:GLU:O	1:D:488:LYS:HB2	2.18	0.43
1:D:248:VAL:HB	1:D:349:LEU:HD12	1.99	0.43
1:F:379:ARG:HD3	1:F:408:TYR:HA	2.00	0.43
1:F:76:VAL:HG23	1:F:80:ASP:HB2	1.99	0.43
1:A:143:THR:HG23	2:A:1570:UDP:H5	1.82	0.43
1:D:178:SER:O	1:D:197:ARG:NH2	2.37	0.43
1:E:457:LEU:HD13	1:E:482:TRP:CD2	2.53	0.43
1:B:131:TRP:HZ2	7:B:2031:HOH:O	2.01	0.43
1:F:386:GLU:OE1	1:F:393:LYS:HD2	2.18	0.43
1:F:495:LEU:HD23	1:F:512:GLY:HA2	2.00	0.43
1:B:462:HIS:HE1	7:B:2105:HOH:O	2.01	0.43
1:C:424:LYS:HD2	1:C:428:TRP:CE2	2.53	0.43
1:B:198:ASN:ND2	1:B:210:ARG:HH11	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ARG:CD	1:D:326:MET:O	2.63	0.43
1:E:277:ASN:CG	1:E:279:VAL:HG12	2.36	0.43
1:A:334:GLU:HG2	1:A:335:ASN:N	2.34	0.43
1:C:379:ARG:HG2	1:C:408:TYR:HA	2.01	0.43
1:C:343:TRP:CD1	1:C:349:LEU:HD22	2.54	0.43
1:C:567:LEU:HD23	1:C:568:ASN:H	1.84	0.43
1:F:198:ASN:ND2	1:F:210:ARG:HH11	2.16	0.43
1:A:276:TRP:O	1:A:396:TYR:HA	2.19	0.43
1:B:342:VAL:CG1	1:B:349:LEU:HD13	2.49	0.43
1:C:198:ASN:ND2	1:C:210:ARG:HH11	2.17	0.43
1:C:440:PRO:HG3	1:C:447:PHE:CD2	2.54	0.43
1:F:76:VAL:HG22	1:F:77:ARG:O	2.19	0.43
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.88	0.42
1:C:86:TYR:CE2	1:C:149:ARG:HB3	2.54	0.42
1:E:289:GLN:O	1:E:293:ARG:HG3	2.18	0.42
1:A:197:ARG:HD3	7:A:2142:HOH:O	2.19	0.42
1:B:206:ARG:CD	1:B:326:MET:O	2.65	0.42
1:B:478:GLY:O	1:B:492:HIS:CE1	2.71	0.42
1:E:450:LEU:HD13	1:E:563:TRP:CE3	2.54	0.42
1:C:537:ASN:OD1	1:C:554:VAL:HG23	2.18	0.42
1:C:502:ARG:O	1:C:538:LEU:HD11	2.20	0.42
1:E:123:HIS:HD2	1:E:125:GLN:HB2	1.84	0.42
1:A:277:ASN:HD22	1:A:278:LEU:N	2.17	0.42
1:D:451:GLN:HG2	1:D:453:GLY:HA2	2.01	0.42
1:F:143:THR:OG1	1:F:207:SER:HB3	2.20	0.42
1:A:324:TYR:CE1	1:A:334:GLU:HG3	2.55	0.42
1:A:76:VAL:HG12	1:A:77:ARG:O	2.18	0.42
1:C:568:ASN:ND2	1:C:568:ASN:C	2.73	0.42
1:E:248:VAL:HB	1:E:349:LEU:HD12	2.02	0.42
1:E:291:ARG:CZ	1:E:291:ARG:HB3	2.50	0.42
1:C:377:PHE:CG	1:C:377:PHE:O	2.72	0.42
1:C:478:GLY:O	1:C:492:HIS:HE1	2.01	0.42
1:C:491:LYS:HD2	1:C:493:MET:O	2.19	0.42
1:E:78:TRP:N	1:E:79:PRO:CD	2.82	0.42
1:F:268:ALA:O	1:F:293:ARG:NH2	2.53	0.42
1:A:305:MET:HE2	1:A:336:LEU:HA	2.01	0.42
1:A:451:GLN:OE1	1:A:566:THR:CG2	2.67	0.42
1:D:330:VAL:HA	1:D:332:GLY:H	1.85	0.42
1:F:528:ASN:O	1:F:564:LYS:CD	2.68	0.42
1:A:248:VAL:HB	1:A:349:LEU:HD12	2.02	0.41
1:B:93:ARG:O	1:B:96:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:VAL:HG22	1:D:331:TRP:HA	2.02	0.41
1:E:78:TRP:CG	1:E:79:PRO:HD3	2.55	0.41
1:D:387:VAL:HB	1:D:388:TRP:CD1	2.55	0.41
1:E:335:ASN:ND2	1:E:335:ASN:H	2.18	0.41
1:D:362:ARG:C	1:D:363:LYS:HD3	2.40	0.41
1:D:385:ALA:HA	1:D:389:MET:HG3	2.00	0.41
6:F:1572:Y6W:O5'	6:F:1572:Y6W:C5	2.68	0.41
1:A:457:LEU:HD13	1:A:482:TRP:CD2	2.55	0.41
1:B:335:ASN:ND2	1:B:335:ASN:H	2.14	0.41
1:D:129:LYS:HB3	1:D:129:LYS:HE2	1.96	0.41
1:F:133:VAL:HG22	1:F:166:HIS:CE1	2.56	0.41
1:F:449:ALA:O	1:F:565:PHE:HA	2.20	0.41
1:A:283:ASP:N	1:A:283:ASP:OD1	2.53	0.41
1:E:94:SER:C	1:E:96:GLN:H	2.24	0.41
1:B:183:ASP:HB2	7:B:2077:HOH:O	2.21	0.41
1:E:106:GLN:O	1:E:106:GLN:HG2	2.19	0.41
1:B:173:LEU:HD22	1:B:193:VAL:HG13	2.02	0.41
1:C:134:ASP:OD1	1:C:134:ASP:N	2.48	0.41
1:F:392:TYR:OH	1:F:427:LYS:HD2	2.21	0.41
1:A:276:TRP:C	1:A:278:LEU:H	2.24	0.41
1:A:399:ALA:HB2	1:A:567:LEU:HD22	2.03	0.41
1:A:378:ALA:CB	1:A:406:VAL:HG21	2.51	0.41
1:D:380:ASN:HA	1:D:380:ASN:HD22	1.62	0.41
1:A:327:MET:HB2	1:A:383:ARG:CZ	2.51	0.40
1:C:532:ARG:HD3	1:C:536:SER:O	2.21	0.40
1:F:108:GLU:HG3	7:F:2028:HOH:O	2.20	0.40
1:F:299:ALA:HA	1:F:300:PRO:HD2	1.97	0.40
1:A:143:THR:HG23	2:A:1570:UDP:O4	2.21	0.40
1:D:176:ASP:OD1	1:D:198:ASN:OD1	2.37	0.40
1:F:440:PRO:HG3	1:F:447:PHE:CD2	2.56	0.40
1:A:153:LEU:O	1:A:157:VAL:HG13	2.21	0.40
1:B:342:VAL:HG11	1:B:349:LEU:CD1	2.52	0.40
1:C:164:PRO:HA	1:C:165:PRO:HD3	1.95	0.40
1:D:474:HIS:ND1	1:D:476:ALA:HA	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:2235:HOH:O	7:F:2129:HOH:O[1_655]	1.89	0.31
1:E:320:GLU:OE2	1:F:84:GLU:OE2[3_554]	2.15	0.05



## 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	481/571 (84%)	462 (96%)	15 (3%)	4 (1%)	19	9
1	B	481/571 (84%)	459 (95%)	19 (4%)	3 (1%)	25	15
1	C	481/571 (84%)	453 (94%)	25 (5%)	3 (1%)	25	15
1	D	435/571 (76%)	402 (92%)	26 (6%)	7 (2%)	9	2
1	E	480/571 (84%)	460 (96%)	17 (4%)	3 (1%)	25	15
1	F	478/571 (84%)	447 (94%)	24 (5%)	7 (2%)	10	3
All	All	2836/3426 (83%)	2683 (95%)	126 (4%)	27 (1%)	15	6

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	B	332	GLY
1	B	477	GLY
1	C	199	ASP
1	D	440	PRO
1	D	456	CYS
1	D	474	HIS
1	D	476	ALA
1	F	286	THR
1	F	287	PRO
1	F	288	GLU
1	A	477	GLY
1	B	377	PHE
1	C	332	GLY
1	D	88	GLY
1	E	93	ARG
1	C	94	SER
1	E	477	GLY
1	F	331	TRP
1	F	475	ASN

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Mol	Chain	Res	Type
1	F	477	GLY
1	A	94	SER
1	D	330	VAL
1	E	475	ASN
1	F	402	SER
1	A	479	ASN
1	D	448	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	420/485 (87%)	379 (90%)	41 (10%)	8	3
1	B	420/485 (87%)	387 (92%)	33 (8%)	12	5
1	C	420/485 (87%)	380 (90%)	40 (10%)	8	3
1	D	385/485 (79%)	344 (89%)	41 (11%)	6	2
1	E	419/485 (86%)	388 (93%)	31 (7%)	13	6
1	F	417/485 (86%)	376 (90%)	41 (10%)	8	3
All	All	2481/2910 (85%)	2254 (91%)	227 (9%)	9	4

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	94	SER
1	A	112	LEU
1	A	116	ARG
1	A	157	VAL
1	A	173	LEU
1	A	195	VAL
1	A	196	LEU
1	A	197	ARG
1	A	204	LEU
1	A	241	VAL

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Mol	Chain	Res	Type
1	A	245	ARG
1	A	277	ASN
1	A	279	VAL
1	A	283	ASP
1	A	288	GLU
1	A	294	GLN
1	A	296	ASN
1	A	325	ASP
1	A	327	MET
1	A	330	VAL
1	A	335	ASN
1	A	336	LEU
1	A	349	LEU
1	A	379	ARG
1	A	421	LEU
1	A	436	GLU
1	A	438	ARG
1	A	439	VAL
1	A	443	GLN
1	A	450	LEU
1	A	457	LEU
1	A	468	VAL
1	A	474	HIS
1	A	484	LEU
1	A	500	VAL
1	A	510	LEU
1	A	515	GLU
1	A	531	LEU
1	A	537	ASN
1	A	552	VAL
1	B	76	VAL
1	B	83	GLN
1	B	102	ASN
1	B	103	LYS
1	B	112	LEU
1	B	116	ARG
1	B	143	THR
1	B	157	VAL
1	B	173	LEU
1	B	195	VAL
1	B	204	LEU
1	B	241	VAL

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Mol	Chain	Res	Type
1	B	277	ASN
1	B	283	ASP
1	B	291	ARG
1	B	296	ASN
1	B	310	LEU
1	B	335	ASN
1	B	336	LEU
1	B	349	LEU
1	B	362	ARG
1	B	376	VAL
1	B	421	LEU
1	B	434	TYR
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	484	LEU
1	B	488	LYS
1	B	508	ILE
1	B	510	LEU
1	B	515	GLU
1	B	546	LYS
1	C	83	GLN
1	C	84	GLU
1	C	112	LEU
1	C	116	ARG
1	C	130	GLN
1	C	132	ARG
1	C	143	THR
1	C	157	VAL
1	C	173	LEU
1	C	195	VAL
1	C	196	LEU
1	C	204	LEU
1	C	218	LYS
1	C	241	VAL
1	C	258	MET
1	C	277	ASN
1	C	288	GLU
1	C	296	ASN
1	C	310	LEU
1	C	335	ASN
1	C	349	LEU

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Mol	Chain	Res	Type
1	C	379	ARG
1	C	412	GLN
1	C	421	LEU
1	C	436	GLU
1	C	438	ARG
1	C	439	VAL
1	C	450	LEU
1	C	457	LEU
1	C	468	VAL
1	C	484	LEU
1	C	491	LYS
1	C	502	ARG
1	C	504	PRO
1	C	510	LEU
1	C	515	GLU
1	C	529	SER
1	C	567	LEU
1	C	568	ASN
1	C	569	LEU
1	D	75	LYS
1	D	93	ARG
1	D	112	LEU
1	D	116	ARG
1	D	129	LYS
1	D	143	THR
1	D	157	VAL
1	D	173	LEU
1	D	177	TYR
1	D	195	VAL
1	D	204	LEU
1	D	243	GLU
1	D	245	ARG
1	D	277	ASN
1	D	296	ASN
1	D	310	LEU
1	D	329	ASP
1	D	336	LEU
1	D	349	LEU
1	D	362	ARG
1	D	363	LYS
1	D	379	ARG
1	D	391	GLU

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Mol	Chain	Res	Type
1	D	402	SER
1	D	404	ARG
1	D	421	LEU
1	D	434	TYR
1	D	439	VAL
1	D	441	ASP
1	D	452	GLN
1	D	468	VAL
1	D	474	HIS
1	D	475	ASN
1	D	484	LEU
1	D	488	LYS
1	D	491	LYS
1	D	510	LEU
1	D	514	ARG
1	D	515	GLU
1	D	552	VAL
1	D	554	VAL
1	E	75	LYS
1	E	91	MET
1	E	112	LEU
1	E	113	ARG
1	E	116	ARG
1	E	129	LYS
1	E	133	VAL
1	E	143	THR
1	E	173	LEU
1	E	195	VAL
1	E	196	LEU
1	E	245	ARG
1	E	277	ASN
1	E	284	TYR
1	E	288	GLU
1	E	296	ASN
1	E	310	LEU
1	E	335	ASN
1	E	336	LEU
1	E	349	LEU
1	E	421	LEU
1	E	434	TYR
1	E	438	ARG
1	E	439	VAL

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Mol	Chain	Res	Type
1	E	450	LEU
1	E	457	LEU
1	E	468	VAL
1	E	474	HIS
1	E	484	LEU
1	E	504	PRO
1	E	552	VAL
1	F	75	LYS
1	F	84	GLU
1	F	104	PHE
1	F	112	LEU
1	F	116	ARG
1	F	133	VAL
1	F	143	THR
1	F	173	LEU
1	F	195	VAL
1	F	196	LEU
1	F	200	ARG
1	F	245	ARG
1	F	277	ASN
1	F	279	VAL
1	F	287	PRO
1	F	294	GLN
1	F	301	ILE
1	F	302	LYS
1	F	336	LEU
1	F	349	LEU
1	F	391	GLU
1	F	402	SER
1	F	404	ARG
1	F	421	LEU
1	F	427	LYS
1	F	434	TYR
1	F	438	ARG
1	F	439	VAL
1	F	450	LEU
1	F	457	LEU
1	F	468	VAL
1	F	474	HIS
1	F	484	LEU
1	F	486	LYS
1	F	502	ARG

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Mol	Chain	Res	Type
1	F	510	LEU
1	F	515	GLU
1	F	552	VAL
1	F	554	VAL
1	F	559	LEU
1	F	564	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	106	GLN
1	A	123	HIS
1	A	125	GLN
1	A	127	GLN
1	A	198	ASN
1	A	277	ASN
1	A	296	ASN
1	A	335	ASN
1	A	344	GLN
1	A	405	ASN
1	A	452	GLN
1	A	462	HIS
1	A	474	HIS
1	A	524	GLN
1	A	537	ASN
1	A	568	ASN
1	B	83	GLN
1	B	96	GLN
1	B	106	GLN
1	B	123	HIS
1	B	125	GLN
1	B	179	ASN
1	B	198	ASN
1	B	216	GLN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN
1	B	380	ASN
1	B	452	GLN
1	B	462	HIS

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Mol	Chain	Res	Type
1	B	474	HIS
1	B	475	ASN
1	B	524	GLN
1	B	537	ASN
1	B	568	ASN
1	C	83	GLN
1	C	96	GLN
1	C	106	GLN
1	C	123	HIS
1	C	125	GLN
1	C	198	ASN
1	C	262	GLN
1	C	277	ASN
1	C	296	ASN
1	C	335	ASN
1	C	344	GLN
1	C	380	ASN
1	C	451	GLN
1	C	452	GLN
1	C	462	HIS
1	C	474	HIS
1	C	528	ASN
1	C	568	ASN
1	D	83	GLN
1	D	106	GLN
1	D	123	HIS
1	D	198	ASN
1	D	262	GLN
1	D	277	ASN
1	D	296	ASN
1	D	335	ASN
1	D	344	GLN
1	D	380	ASN
1	D	452	GLN
1	D	455	ASN
1	D	462	HIS
1	E	83	GLN
1	E	123	HIS
1	E	125	GLN
1	E	127	GLN
1	E	198	ASN
1	E	277	ASN

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Mol	Chain	Res	Type
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	380	ASN
1	E	451	GLN
1	E	452	GLN
1	E	462	HIS
1	E	474	HIS
1	E	537	ASN
1	F	83	GLN
1	F	123	HIS
1	F	127	GLN
1	F	130	GLN
1	F	198	ASN
1	F	216	GLN
1	F	262	GLN
1	F	277	ASN
1	F	296	ASN
1	F	335	ASN
1	F	344	GLN
1	F	380	ASN
1	F	452	GLN
1	F	462	HIS
1	F	474	HIS
1	F	492	HIS

### 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 ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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$
5	GOL	F	1577	-	5,5,5	0.56	0	5,5,5	0.79	0
2	UDP	B	1572	3	20,26,26	1.05	1 (5%)	25,40,40	1.09	2 (8%)
2	UDP	C	1570	3	20,26,26	1.27	2 (10%)	25,40,40	1.32	2 (8%)
5	GOL	C	1574	-	5,5,5	0.57	0	5,5,5	0.47	0
4	EDO	A	1574	-	3,3,3	0.44	0	2,2,2	0.58	0
2	UDP	D	1555	3	20,26,26	1.05	2 (10%)	25,40,40	1.38	3 (12%)
4	EDO	B	1574	-	3,3,3	0.40	0	2,2,2	0.38	0
4	EDO	F	1575	-	3,3,3	0.53	0	2,2,2	0.25	0
4	EDO	E	1575	-	3,3,3	0.65	0	2,2,2	1.05	0
4	EDO	F	1574	-	3,3,3	0.61	0	2,2,2	0.17	0
4	EDO	A	1572	-	3,3,3	0.41	0	2,2,2	0.29	0
4	EDO	A	1573	-	3,3,3	0.60	0	2,2,2	0.51	0
6	Y6W	E	1572	-	32,36,36	1.89	7 (21%)	37,53,53	1.98	10 (27%)
4	EDO	C	1573	-	3,3,3	0.51	0	2,2,2	0.33	0
4	EDO	E	1574	-	3,3,3	0.52	0	2,2,2	0.05	0
5	GOL	A	1575	-	5,5,5	0.33	0	5,5,5	1.18	0
2	UDP	F	1570	3	20,26,26	1.22	2 (10%)	25,40,40	1.18	1 (4%)
6	Y6W	B	1570	3	32,36,36	1.46	4 (12%)	37,53,53	1.13	3 (8%)
4	EDO	C	1572	-	3,3,3	0.51	0	2,2,2	0.38	0
4	EDO	E	1573	-	3,3,3	0.88	0	2,2,2	0.72	0
4	EDO	E	1576	-	3,3,3	0.23	0	2,2,2	0.65	0
2	UDP	E	1570	3	20,26,26	1.13	2 (10%)	25,40,40	1.16	2 (8%)
4	EDO	F	1573	-	3,3,3	0.45	0	2,2,2	0.18	0
4	EDO	B	1573	-	3,3,3	0.48	0	2,2,2	0.35	0
6	Y6W	F	1572	-	32,36,36	1.74	8 (25%)	37,53,53	1.66	9 (24%)
5	GOL	A	1576	-	5,5,5	0.41	0	5,5,5	0.31	0
5	GOL	F	1576	-	5,5,5	0.41	0	5,5,5	0.75	0
2	UDP	A	1570	3	20,26,26	1.28	3 (15%)	25,40,40	1.43	4 (16%)

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
5	GOL	F	1577	-	-	2/4/4/4	-
2	UDP	B	1572	3	-	2/14/32/32	0/2/2/2
2	UDP	C	1570	3	-	3/14/32/32	0/2/2/2
5	GOL	C	1574	-	-	2/4/4/4	-
4	EDO	A	1574	-	-	1/1/1/1	-
2	UDP	D	1555	3	-	3/14/32/32	0/2/2/2
4	EDO	B	1574	-	-	0/1/1/1	-
4	EDO	F	1575	-	-	0/1/1/1	-
4	EDO	E	1575	-	-	1/1/1/1	-
4	EDO	F	1574	-	-	1/1/1/1	-
4	EDO	A	1572	-	-	1/1/1/1	-
4	EDO	A	1573	-	-	0/1/1/1	-
6	Y6W	E	1572	-	-	8/17/55/55	0/3/3/3
4	EDO	C	1573	-	-	1/1/1/1	-
4	EDO	E	1574	-	-	0/1/1/1	-
5	GOL	A	1575	-	-	2/4/4/4	-
2	UDP	F	1570	3	-	3/14/32/32	0/2/2/2
6	Y6W	B	1570	3	-	7/17/55/55	0/3/3/3
4	EDO	C	1572	-	-	0/1/1/1	-
4	EDO	E	1573	-	-	1/1/1/1	-
4	EDO	E	1576	-	-	0/1/1/1	-
2	UDP	E	1570	3	-	2/14/32/32	0/2/2/2
4	EDO	F	1573	-	-	0/1/1/1	-
4	EDO	B	1573	-	-	1/1/1/1	-
6	Y6W	F	1572	-	-	10/17/55/55	0/3/3/3
5	GOL	A	1576	-	-	2/4/4/4	-
5	GOL	F	1576	-	-	0/4/4/4	-
2	UDP	A	1570	3	-	0/14/32/32	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1572	Y6W	O4'-C1'	5.19	1.48	1.41
6	B	1570	Y6W	OBG-CBD	4.76	1.36	1.24
6	E	1572	Y6W	OBG-CBD	4.56	1.36	1.24
2	C	1570	UDP	O4'-C1'	4.43	1.47	1.41
6	F	1572	Y6W	O4'-C1'	4.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1572	Y6W	OBG-CBD	4.06	1.34	1.24
6	F	1572	Y6W	CBB-NAZ	3.84	1.40	1.35
6	E	1572	Y6W	CBB-NAZ	3.75	1.40	1.35
6	B	1570	Y6W	CBB-NAZ	3.60	1.40	1.35
6	E	1572	Y6W	PAN-O5'	3.50	1.62	1.57
6	F	1572	Y6W	PAN-OAO	-3.47	1.48	1.56
6	B	1570	Y6W	PAN-OAO	-3.40	1.48	1.56
2	B	1572	UDP	O4'-C1'	3.23	1.45	1.41
6	E	1572	Y6W	PAN-OAO	-3.18	1.48	1.56
2	D	1555	UDP	O4'-C1'	3.08	1.45	1.41
2	F	1570	UDP	O4'-C1'	2.95	1.45	1.41
2	F	1570	UDP	C2-N3	-2.91	1.32	1.38
2	E	1570	UDP	O4'-C1'	2.79	1.45	1.41
6	B	1570	Y6W	PAN-O5'	2.75	1.61	1.57
2	A	1570	UDP	O4'-C1'	2.67	1.44	1.41
2	E	1570	UDP	C2-N3	-2.61	1.33	1.38
2	D	1555	UDP	C2-N3	-2.49	1.33	1.38
2	A	1570	UDP	C2-N3	-2.38	1.33	1.38
2	A	1570	UDP	C4-N3	2.36	1.37	1.33
6	E	1572	Y6W	CBA-NBF	-2.28	1.33	1.38
6	F	1572	Y6W	CAK-C1	2.27	1.57	1.52
6	F	1572	Y6W	C4-C5	-2.26	1.48	1.53
6	F	1572	Y6W	PAN-O5'	2.23	1.60	1.57
6	E	1572	Y6W	O4'-C4'	2.23	1.50	1.45
6	F	1572	Y6W	CBA-NBF	-2.11	1.34	1.38
2	C	1570	UDP	C2-N3	-2.01	1.34	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1572	Y6W	O5'-PAN-CAM	-4.63	91.88	104.11
6	E	1572	Y6W	C5-O5-C1	-4.59	105.14	113.16
2	A	1570	UDP	O3B-PB-O3A	4.30	119.04	104.64
2	D	1555	UDP	O3B-PB-O1B	3.87	125.82	110.68
6	F	1572	Y6W	O4'-C1'-C2'	-3.73	101.48	106.93
6	E	1572	Y6W	CAK-C1-C2	-3.65	108.17	114.02
2	A	1570	UDP	O3A-PB-O1B	-3.57	91.39	111.19
6	F	1572	Y6W	O5-C1-C2	-3.43	103.47	109.69
6	E	1572	Y6W	C4-C3-C2	3.29	116.56	110.82
6	E	1572	Y6W	O4'-C1'-C2'	-3.23	102.20	106.93
6	E	1572	Y6W	O6-C6-C5	-3.08	100.72	111.29
6	F	1572	Y6W	O6-C6-C5	-2.99	101.04	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1555	UDP	O2A-PA-O1A	2.96	126.89	112.24
6	F	1572	Y6W	OAO-PAN-OBH	2.90	119.74	110.07
6	B	1570	Y6W	OAO-PAN-OBH	2.87	119.67	110.07
6	E	1572	Y6W	CAK-CAL-CAM	-2.87	106.46	112.61
6	F	1572	Y6W	O5-C1-CAK	2.85	116.04	108.33
6	E	1572	Y6W	OAO-PAN-OBH	2.84	119.53	110.07
2	E	1570	UDP	O5'-C5'-C4'	2.83	118.72	108.99
6	F	1572	Y6W	O5'-PAN-CAM	-2.76	96.83	104.11
6	B	1570	Y6W	CAK-C1-C2	-2.75	109.61	114.02
6	E	1572	Y6W	OAO-PAN-CAM	2.71	111.88	105.63
2	C	1570	UDP	C2'-C3'-C4'	2.70	107.90	102.64
2	D	1555	UDP	PA-O3A-PB	-2.61	123.86	132.83
2	C	1570	UDP	O3B-PB-O1B	2.59	120.82	110.68
6	E	1572	Y6W	O3-C3-C2	-2.55	104.46	110.35
2	F	1570	UDP	O3B-PB-O2B	2.54	117.36	107.64
2	A	1570	UDP	O2A-PA-O1A	2.43	124.25	112.24
6	F	1572	Y6W	CAK-C1-C2	-2.39	110.19	114.02
6	F	1572	Y6W	C5-O5-C1	-2.21	109.29	113.16
2	A	1570	UDP	O3B-PB-O1B	2.13	119.02	110.68
6	B	1570	Y6W	C3'-C2'-C1'	2.07	104.09	100.98
2	E	1570	UDP	O3A-PB-O1B	-2.06	99.75	111.19
2	B	1572	UDP	O5'-C5'-C4'	2.04	116.00	108.99
2	B	1572	UDP	PA-O3A-PB	-2.03	125.86	132.83
6	F	1572	Y6W	CAK-CAL-CAM	-2.02	108.27	112.61

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1577	GOL	O1-C1-C2-C3
2	B	1572	UDP	PA-O3A-PB-O2B
2	B	1572	UDP	PA-O3A-PB-O3B
2	C	1570	UDP	PA-O3A-PB-O3B
5	C	1574	GOL	O1-C1-C2-C3
2	D	1555	UDP	PA-O3A-PB-O3B
6	E	1572	Y6W	O5-C1-CAK-CAL
6	E	1572	Y6W	CAK-CAL-CAM-PAN
5	A	1575	GOL	O1-C1-C2-C3
2	F	1570	UDP	PA-O3A-PB-O3B
6	B	1570	Y6W	O5-C1-CAK-CAL
5	A	1576	GOL	C1-C2-C3-O3
6	F	1572	Y6W	O5-C1-CAK-CAL

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Mol	Chain	Res	Type	Atoms
6	F	1572	Y6W	C1-CAK-CAL-CAM
6	F	1572	Y6W	CAK-CAL-CAM-PAN
6	E	1572	Y6W	O5-C5-C6-O6
6	E	1572	Y6W	C4-C5-C6-O6
4	E	1575	EDO	O1-C1-C2-O2
6	F	1572	Y6W	C5'-O5'-PAN-CAM
6	F	1572	Y6W	O5-C5-C6-O6
5	A	1575	GOL	O1-C1-C2-O2
5	A	1576	GOL	O2-C2-C3-O3
4	A	1572	EDO	O1-C1-C2-O2
4	B	1573	EDO	O1-C1-C2-O2
6	F	1572	Y6W	C4-C5-C6-O6
5	F	1577	GOL	O1-C1-C2-O2
5	C	1574	GOL	O1-C1-C2-O2
2	E	1570	UDP	PA-O3A-PB-O1B
6	F	1572	Y6W	CAL-CAM-PAN-OBH
2	C	1570	UDP	PA-O3A-PB-O1B
6	B	1570	Y6W	C4-C5-C6-O6
6	B	1570	Y6W	O5-C5-C6-O6
2	E	1570	UDP	PA-O3A-PB-O3B
2	D	1555	UDP	C5'-O5'-PA-O3A
6	E	1572	Y6W	C2-C1-CAK-CAL
6	F	1572	Y6W	C2-C1-CAK-CAL
6	B	1570	Y6W	CAK-CAL-CAM-PAN
6	F	1572	Y6W	C4'-C5'-O5'-PAN
4	F	1574	EDO	O1-C1-C2-O2
6	B	1570	Y6W	C4'-C5'-O5'-PAN
6	E	1572	Y6W	C5'-O5'-PAN-CAM
4	A	1574	EDO	O1-C1-C2-O2
4	E	1573	EDO	O1-C1-C2-O2
4	C	1573	EDO	O1-C1-C2-O2
2	F	1570	UDP	PA-O3A-PB-O1B
2	D	1555	UDP	PA-O3A-PB-O2B
2	F	1570	UDP	PA-O3A-PB-O2B
2	C	1570	UDP	C5'-O5'-PA-O3A
6	B	1570	Y6W	C2-C1-CAK-CAL
6	E	1572	Y6W	C4'-C5'-O5'-PAN
6	E	1572	Y6W	C1-CAK-CAL-CAM
6	B	1570	Y6W	C1-CAK-CAL-CAM
6	F	1572	Y6W	CAL-CAM-PAN-O5'

There are no ring outliers.



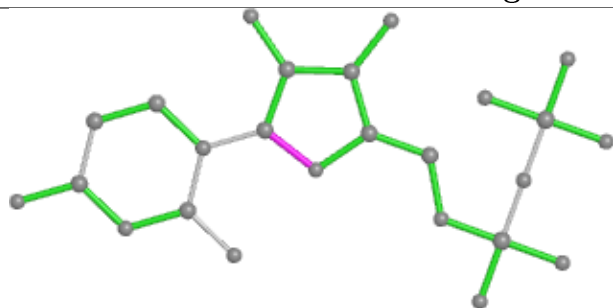
11 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1572	UDP	8	0
2	C	1570	UDP	1	0
2	D	1555	UDP	3	0
4	E	1575	EDO	2	0
4	A	1573	EDO	2	0
6	E	1572	Y6W	5	0
2	F	1570	UDP	6	0
6	B	1570	Y6W	15	0
2	E	1570	UDP	2	0
6	F	1572	Y6W	13	0
2	A	1570	UDP	3	0

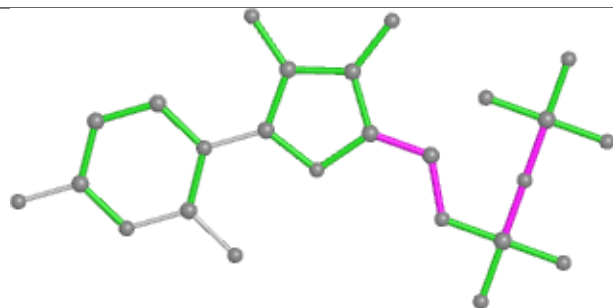
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



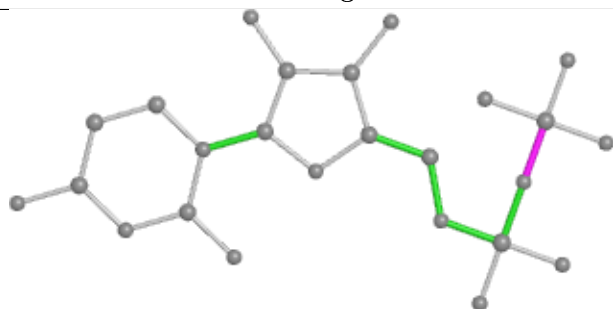
## Ligand UDP B 1572



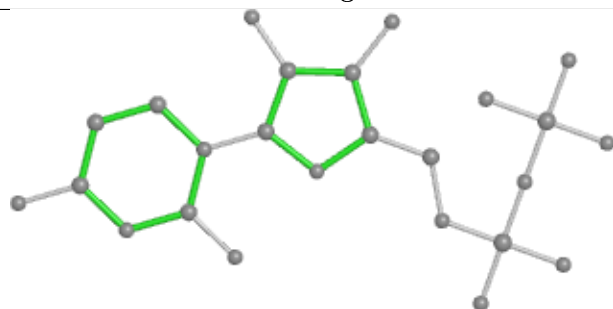
Bond lengths



Bond angles

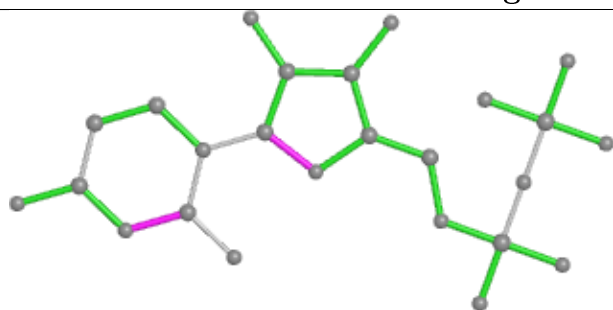


Torsions

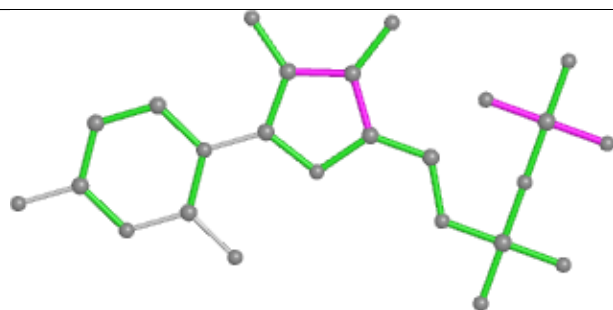


Rings

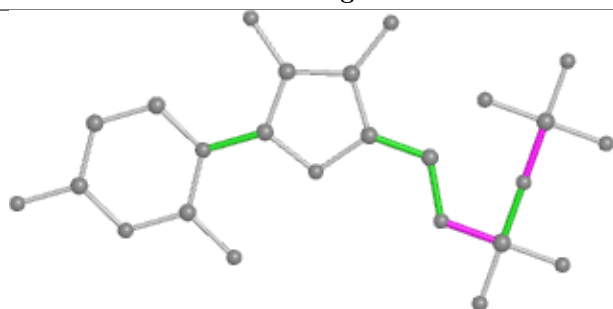
## Ligand UDP C 1570



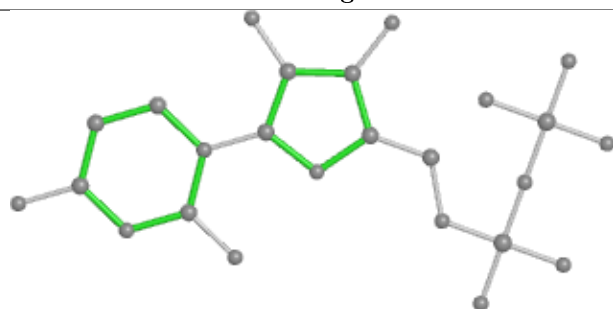
Bond lengths



Bond angles

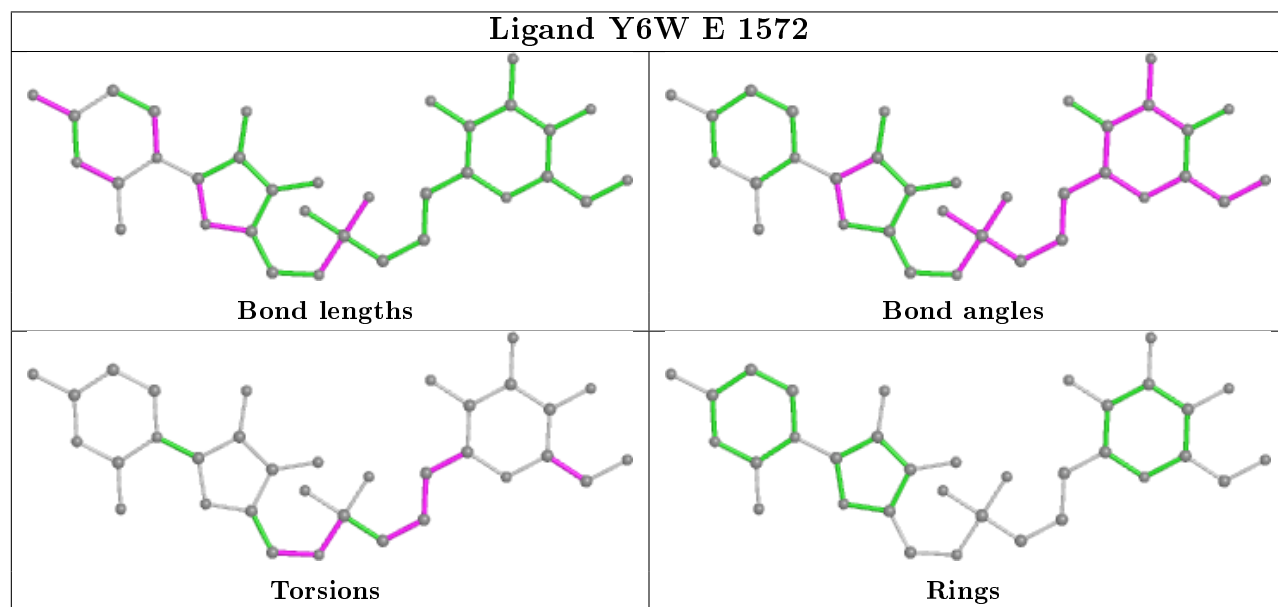
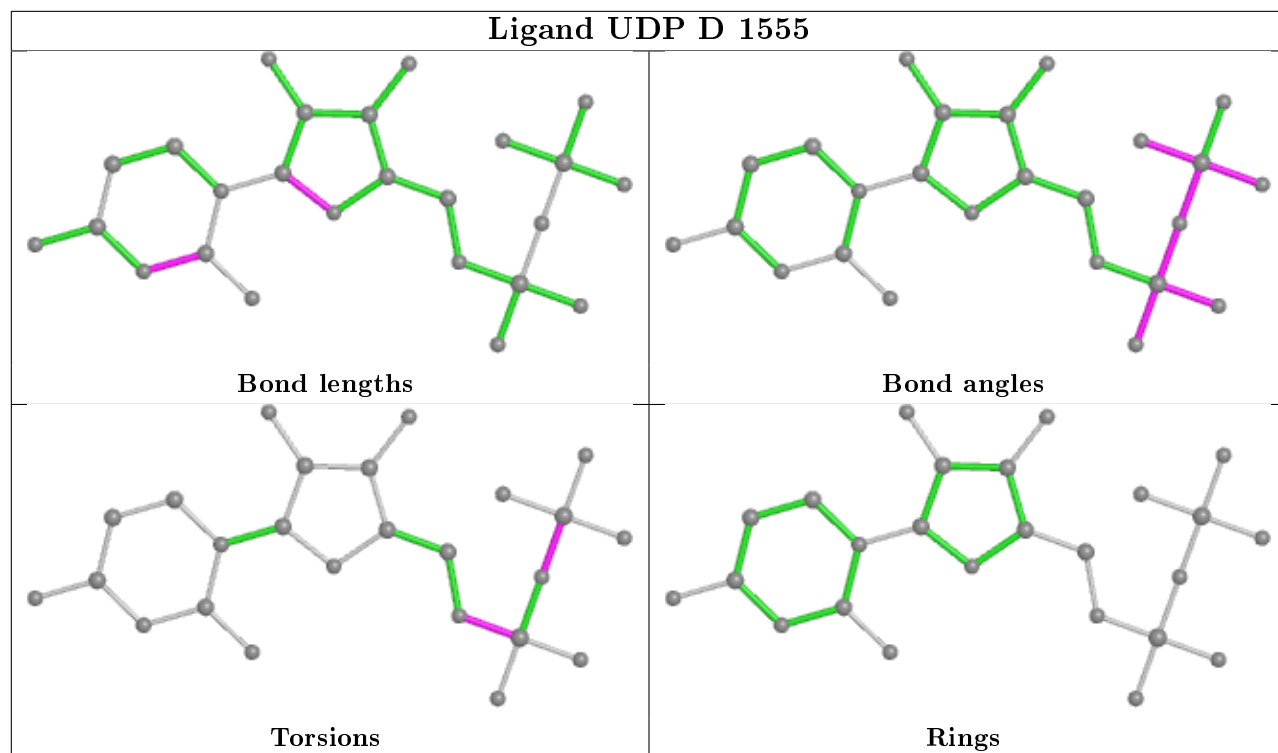


Torsions

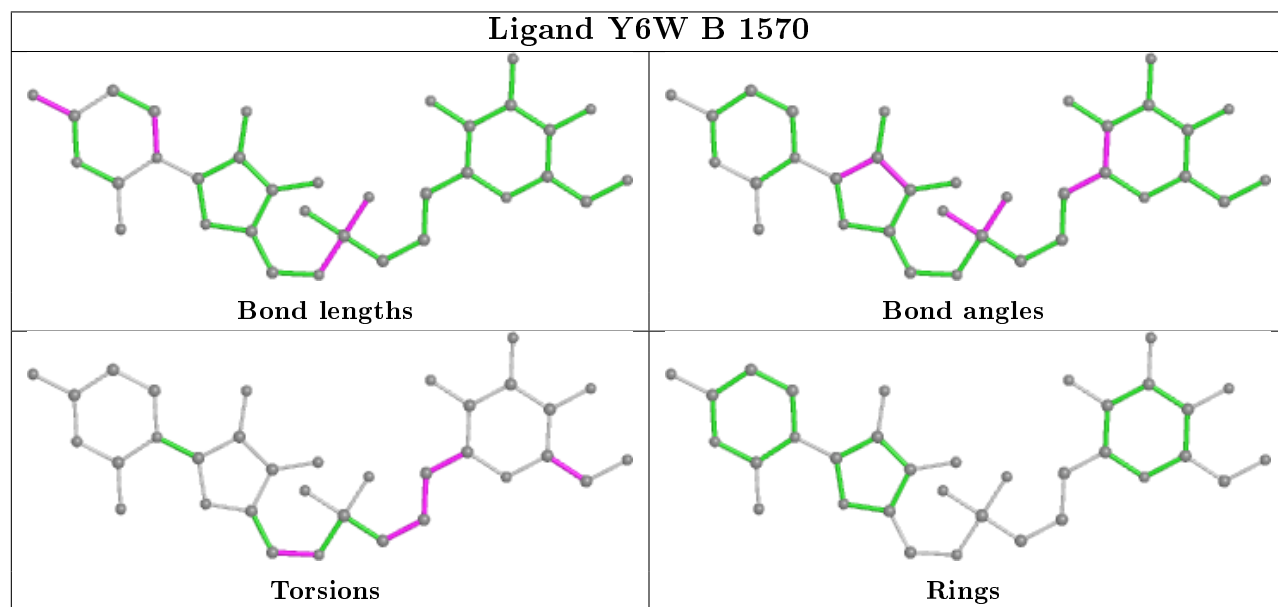
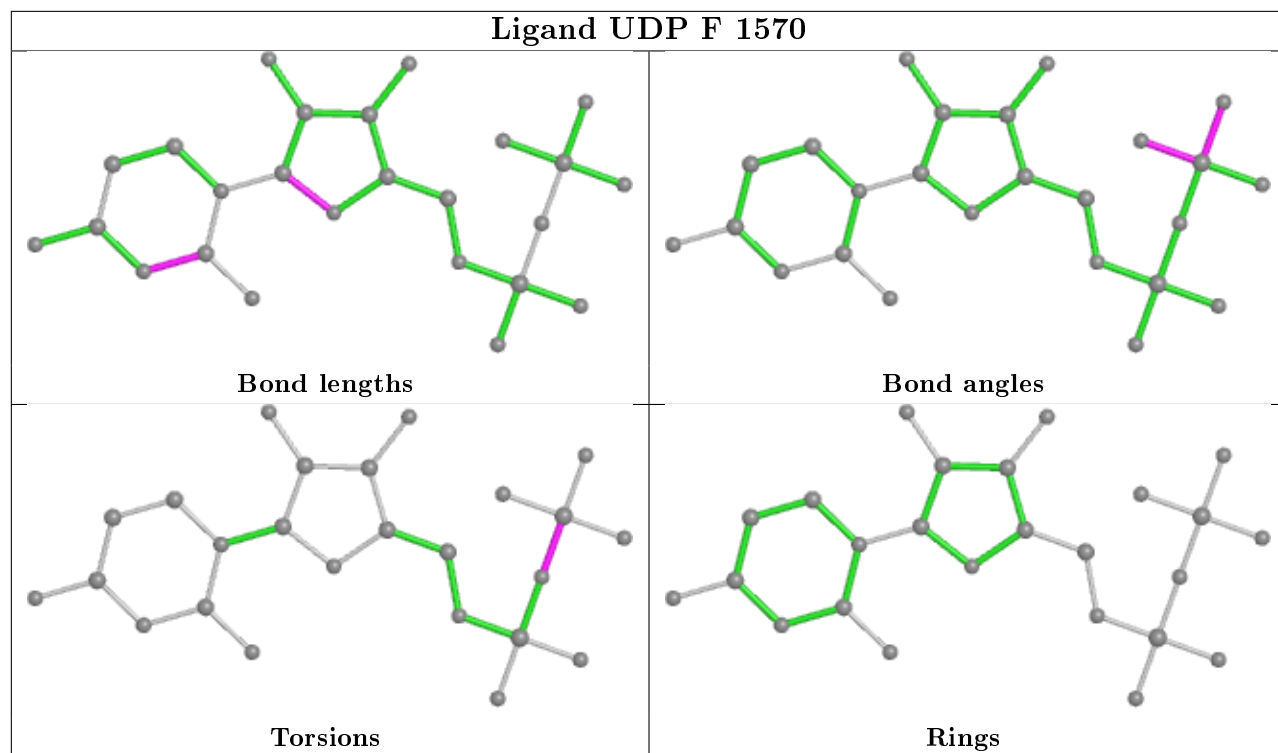


Rings

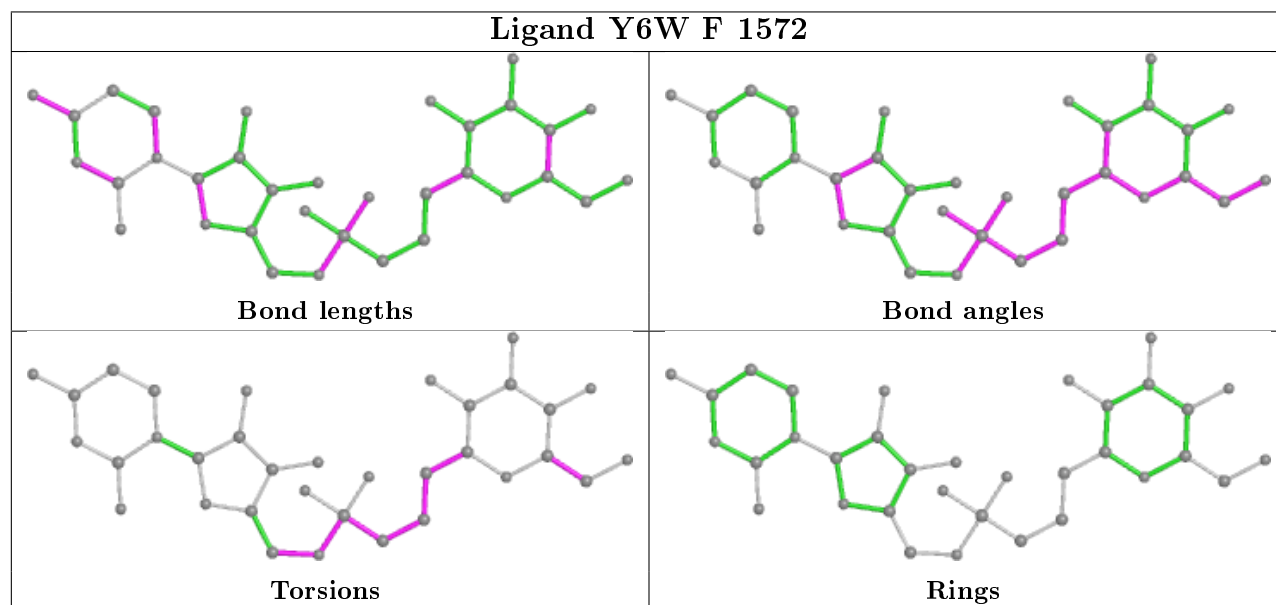
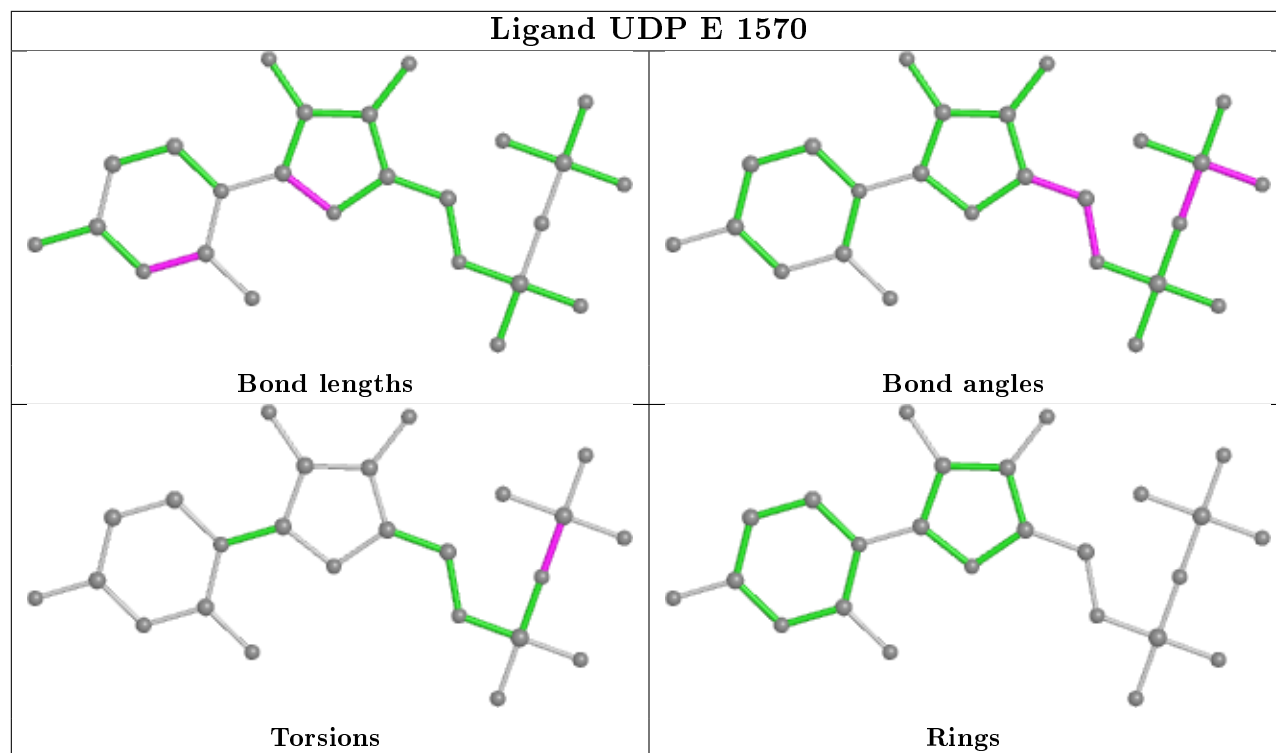




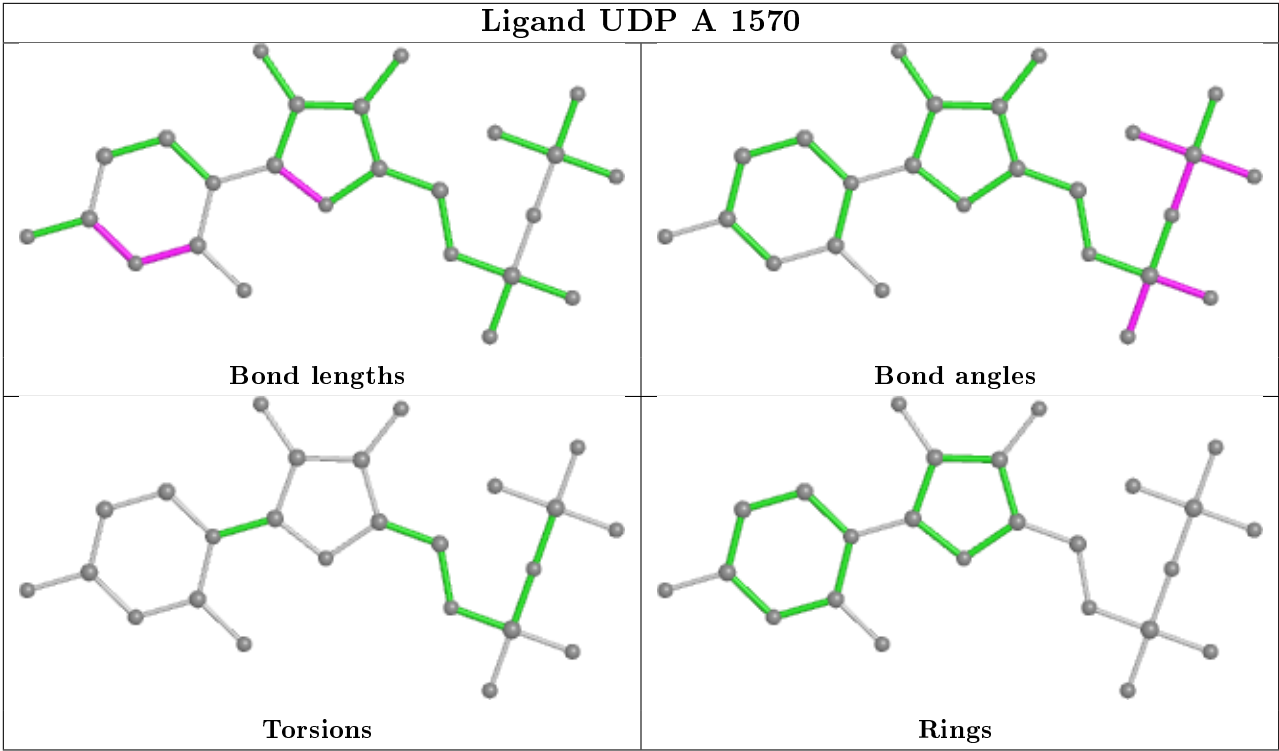












5.7 Other polymers ⓘ

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	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	319:GLU	C	320:GLU	N	1.19
1	E	513:CYS	C	514:ARG	N	1.15



## 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	483/571 (84%)	0.22	26 (5%)	25 26	23, 42, 67, 107	5 (1%)
1	B	484/571 (84%)	0.27	30 (6%)	20 21	26, 41, 73, 147	5 (1%)
1	C	482/571 (84%)	0.34	39 (8%)	12 12	26, 45, 70, 110	5 (1%)
1	D	443/571 (77%)	0.67	63 (14%)	2 2	27, 52, 87, 107	5 (1%)
1	E	483/571 (84%)	0.31	29 (6%)	21 22	26, 40, 67, 105	5 (1%)
1	F	481/571 (84%)	0.65	53 (11%)	5 5	29, 55, 82, 96	5 (1%)
All	All	2856/3426 (83%)	0.41	240 (8%)	11 11	23, 45, 79, 147	30 (1%)

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	525	ILE	10.2
1	B	93	ARG	10.1
1	D	331	TRP	9.0
1	A	377	PHE	7.3
1	B	92	VAL	7.0
1	C	377	PHE	6.9
1	E	95	GLY	6.9
1	B	95	GLY	6.9
1	C	133	VAL	6.6
1	C	95	GLY	5.8
1	D	88	GLY	5.7
1	F	531	LEU	5.7
1	B	94	SER	5.5
1	B	103	LYS	5.4
1	D	505	GLY	5.4
1	F	540	LEU	5.3
1	B	405	ASN	5.1
1	E	94	SER	5.0
1	E	442	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	93	ARG	5.0
1	D	554	VAL	4.9
1	D	447	PHE	4.8
1	D	506	SER	4.8
1	F	332	GLY	4.8
1	B	377	PHE	4.8
1	B	90	THR	4.8
1	D	453	GLY	4.7
1	F	331	TRP	4.6
1	B	101	ARG	4.6
1	D	552	VAL	4.6
1	F	330	VAL	4.6
1	E	287	PRO	4.6
1	A	93	ARG	4.5
1	A	363	LYS	4.5
1	B	96	GLN	4.3
1	D	377	PHE	4.3
1	A	540	LEU	4.3
1	D	401	PRO	4.3
1	B	376	VAL	4.2
1	E	284	TYR	4.2
1	C	96	GLN	4.2
1	B	91	MET	4.1
1	C	94	SER	4.1
1	D	504	PRO	4.1
1	F	514	ARG	4.1
1	B	89	GLY	4.1
1	E	333	GLY	4.1
1	F	284	TYR	4.1
1	C	363	LYS	4.1
1	D	502	ARG	4.1
1	F	557	PRO	4.0
1	B	442	HIS	3.9
1	D	95	GLY	3.9
1	E	291	ARG	3.9
1	F	286	THR	3.9
1	E	540	LEU	3.9
1	F	442	HIS	3.9
1	F	291	ARG	3.9
1	C	556	GLY	3.9
1	B	130	GLN	3.8
1	D	405	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	291	ARG	3.8
1	C	442	HIS	3.8
1	A	442	HIS	3.7
1	D	93	ARG	3.7
1	D	475	ASN	3.7
1	D	376	VAL	3.7
1	B	540	LEU	3.6
1	C	540	LEU	3.6
1	C	92	VAL	3.6
1	D	363	LYS	3.6
1	C	89	GLY	3.6
1	C	128	ARG	3.5
1	D	443	GLN	3.5
1	E	443	GLN	3.5
1	F	475	ASN	3.5
1	D	438	ARG	3.5
1	F	454	THR	3.5
1	B	100	ALA	3.5
1	A	405	ASN	3.4
1	D	553	GLU	3.4
1	A	331	TRP	3.4
1	C	331	TRP	3.4
1	C	93	ARG	3.4
1	C	130	GLN	3.3
1	C	525	ILE	3.3
1	D	419	LYS	3.3
1	E	363	LYS	3.3
1	F	91	MET	3.3
1	D	409	GLY	3.3
1	D	130	GLN	3.3
1	D	445	ILE	3.3
1	E	90	THR	3.2
1	F	438	ARG	3.2
1	F	407	PRO	3.2
1	E	96	GLN	3.2
1	F	174	VAL	3.2
1	C	200	ARG	3.1
1	A	332	GLY	3.1
1	C	503	ALA	3.1
1	B	450	LEU	3.1
1	C	557	PRO	3.1
1	F	474	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	199	ASP	3.1
1	E	89	GLY	3.1
1	F	363	LYS	3.1
1	E	91	MET	3.1
1	C	476	ALA	3.0
1	D	177	TYR	3.0
1	F	477	GLY	3.0
1	E	377	PHE	3.0
1	D	450	LEU	3.0
1	A	94	SER	3.0
1	F	295	GLY	3.0
1	B	97	ASP	2.9
1	F	405	ASN	2.9
1	C	497	LEU	2.9
1	F	199	ASP	2.9
1	F	94	SER	2.9
1	D	330	VAL	2.9
1	C	527	GLY	2.9
1	F	307	ALA	2.9
1	D	96	GLN	2.9
1	A	477	GLY	2.9
1	F	142	ILE	2.8
1	F	428	TRP	2.8
1	D	406	VAL	2.8
1	E	405	ASN	2.8
1	D	89	GLY	2.8
1	D	400	VAL	2.8
1	F	89	GLY	2.8
1	A	330	VAL	2.8
1	A	376	VAL	2.8
1	B	88	GLY	2.7
1	F	559	LEU	2.7
1	C	405	ASN	2.7
1	F	443	GLN	2.7
1	B	128	ARG	2.7
1	D	94	SER	2.7
1	D	410	ASN	2.7
1	F	546	LYS	2.7
1	F	128	ARG	2.7
1	F	527	GLY	2.7
1	B	375	THR	2.6
1	D	473	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	288	GLU	2.6
1	F	361	PHE	2.6
1	E	124	ASP	2.6
1	A	443	GLN	2.6
1	A	497	LEU	2.6
1	C	559	LEU	2.6
1	D	524	GLN	2.6
1	C	548	GLY	2.6
1	D	476	ALA	2.6
1	E	92	VAL	2.5
1	B	200	ARG	2.5
1	B	363	LYS	2.5
1	F	292	SER	2.5
1	B	179	ASN	2.5
1	D	407	PRO	2.5
1	D	441	ASP	2.5
1	D	361	PHE	2.5
1	C	531	LEU	2.5
1	E	88	GLY	2.5
1	D	477	GLY	2.5
1	C	547	SER	2.5
1	A	454	THR	2.4
1	F	497	LEU	2.4
1	A	410	ASN	2.4
1	C	522	TRP	2.4
1	B	443	GLN	2.4
1	A	95	GLY	2.4
1	C	537	ASN	2.4
1	F	173	LEU	2.4
1	D	100	ALA	2.4
1	D	408	TYR	2.4
1	E	290	ARG	2.4
1	A	476	ALA	2.4
1	B	475	ASN	2.4
1	C	101	ARG	2.4
1	F	290	ARG	2.4
1	A	409	GLY	2.4
1	C	295	GLY	2.4
1	E	477	GLY	2.4
1	F	308	GLY	2.4
1	A	531	LEU	2.3
1	F	279	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	409	GLY	2.3
1	D	152	LEU	2.3
1	D	507	LEU	2.3
1	F	88	GLY	2.3
1	E	331	TRP	2.3
1	B	362	ARG	2.3
1	F	412	GLN	2.3
1	E	288	GLU	2.3
1	B	457	LEU	2.3
1	C	569	LEU	2.3
1	D	288	GLU	2.3
1	D	92	VAL	2.3
1	E	286	THR	2.3
1	A	475	ASN	2.3
1	A	340	PHE	2.2
1	F	144	PHE	2.2
1	F	453	GLY	2.2
1	C	100	ALA	2.2
1	F	450	LEU	2.2
1	C	77[A]	ARG	2.2
1	D	446	ALA	2.2
1	D	454	THR	2.2
1	E	550	LEU	2.2
1	D	384	ALA	2.2
1	C	174	VAL	2.2
1	D	199	ASP	2.2
1	D	411	ILE	2.2
1	A	490	VAL	2.2
1	D	518	SER	2.2
1	D	415	LEU	2.1
1	F	473	CYS	2.1
1	C	384	ALA	2.1
1	D	381	THR	2.1
1	D	451	GLN	2.1
1	A	89	GLY	2.1
1	D	103	LYS	2.1
1	D	87	VAL	2.1
1	E	332	GLY	2.1
1	A	91	MET	2.1
1	F	340	PHE	2.1
1	E	128	ARG	2.1
1	F	130	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	490	VAL	2.1
1	C	291[A]	ARG	2.1
1	D	515	GLU	2.1
1	D	412	GLN	2.1
1	C	555	CYS	2.1
1	A	128	ARG	2.0
1	F	134	ASP	2.0
1	C	475	ASN	2.0
1	D	379	ARG	2.0
1	F	441	ASP	2.0
1	F	403	ALA	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(Å <sup>2</sup> )	Q<0.9
4	EDO	A	1574	4/4	0.57	0.35	72,75,80,80	0
5	GOL	A	1576	6/6	0.64	0.34	74,80,86,89	0
4	EDO	E	1574	4/4	0.72	0.22	63,65,72,73	0
4	EDO	C	1573	4/4	0.72	0.29	65,72,73,77	0
4	EDO	F	1574	4/4	0.75	0.23	72,73,76,78	0
4	EDO	F	1573	4/4	0.77	0.27	72,74,76,79	0
4	EDO	E	1575	4/4	0.78	0.16	44,47,51,62	0
4	EDO	F	1575	4/4	0.79	0.24	66,69,69,71	0
4	EDO	A	1573	4/4	0.79	0.41	64,65,66,67	0
4	EDO	B	1573	4/4	0.79	0.16	55,64,67,70	0
5	GOL	C	1574	6/6	0.79	0.14	50,60,63,65	0
4	EDO	A	1572	4/4	0.80	0.33	78,80,81,84	0

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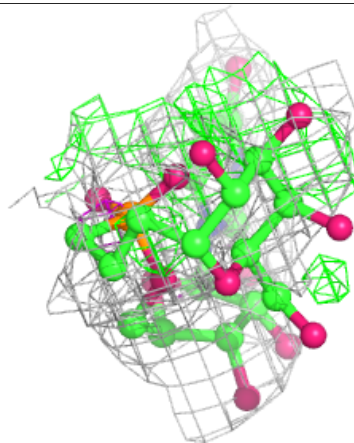
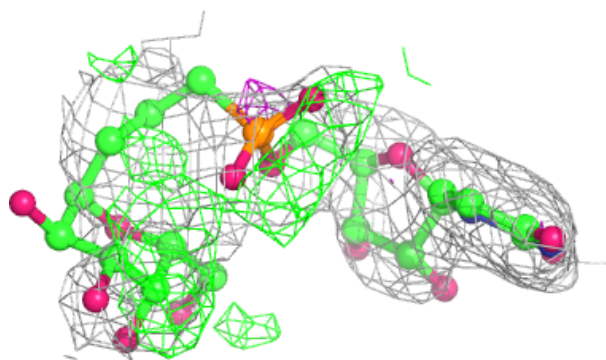
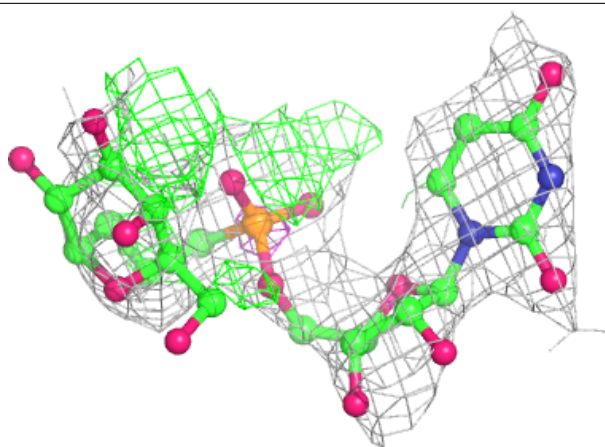
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	F	1577	6/6	0.81	0.14	66,67,69,72	0
5	GOL	A	1575	6/6	0.83	0.24	56,65,73,78	0
4	EDO	C	1572	4/4	0.85	0.22	52,55,56,60	0
5	GOL	F	1576	6/6	0.87	0.14	68,73,81,87	0
6	Y6W	B	1570	34/34	0.88	0.22	40,53,57,58	34
2	UDP	B	1572	25/25	0.89	0.18	35,53,57,58	25
2	UDP	F	1570	25/25	0.90	0.17	37,44,46,49	25
6	Y6W	F	1572	34/34	0.90	0.24	61,78,100,105	34
6	Y6W	E	1572	34/34	0.93	0.19	48,56,73,74	34
4	EDO	B	1574	4/4	0.94	0.15	50,54,55,56	0
4	EDO	E	1573	4/4	0.94	0.14	30,31,37,40	0
2	UDP	E	1570	25/25	0.94	0.15	29,35,42,42	25
2	UDP	D	1555	25/25	0.94	0.16	51,60,70,76	0
2	UDP	C	1570	25/25	0.95	0.15	40,49,55,59	0
4	EDO	E	1576	4/4	0.96	0.16	44,50,51,60	0
2	UDP	A	1570	25/25	0.97	0.13	37,44,50,51	0
3	MN	F	1571	1/1	0.99	0.09	34,34,34,34	0
3	MN	B	1571	1/1	0.99	0.10	35,35,35,35	0
3	MN	A	1571	1/1	0.99	0.07	27,27,27,27	0
3	MN	D	1556	1/1	0.99	0.08	41,41,41,41	0
3	MN	E	1571	1/1	1.00	0.10	29,29,29,29	0
3	MN	C	1571	1/1	1.00	0.08	30,30,30,30	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 Y6W B 1570:**

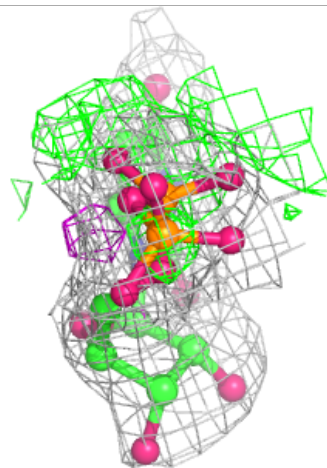
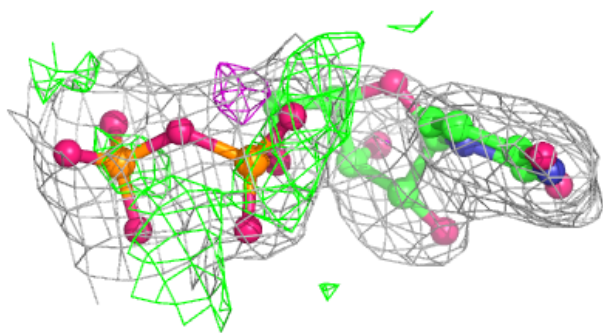
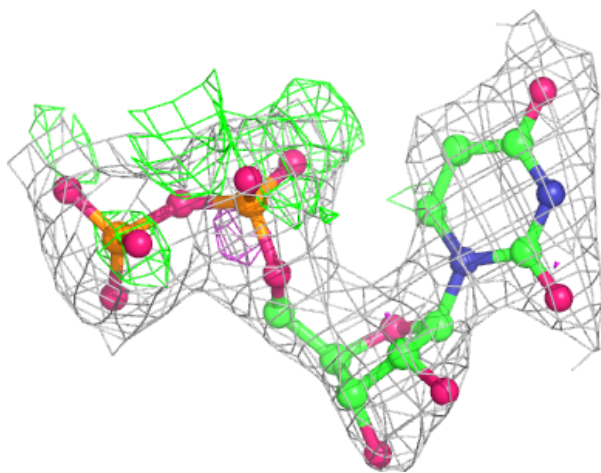
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around UDP B 1572:**

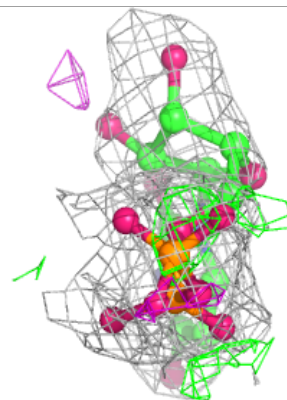
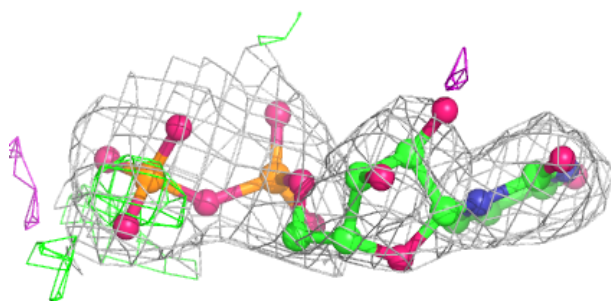
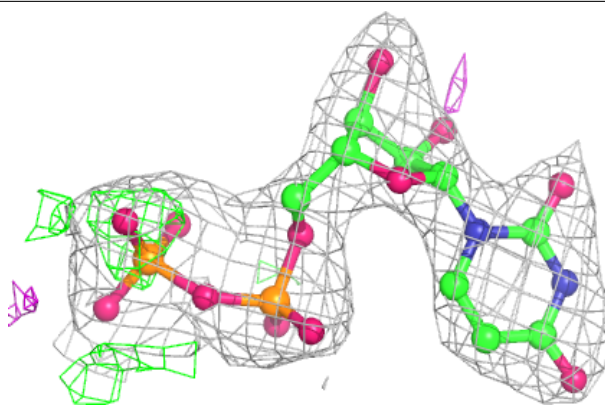
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



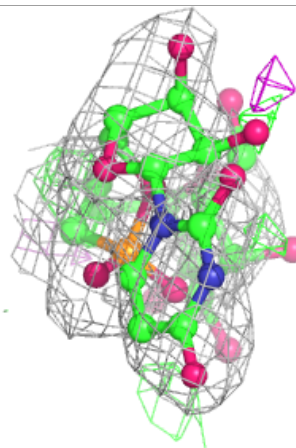
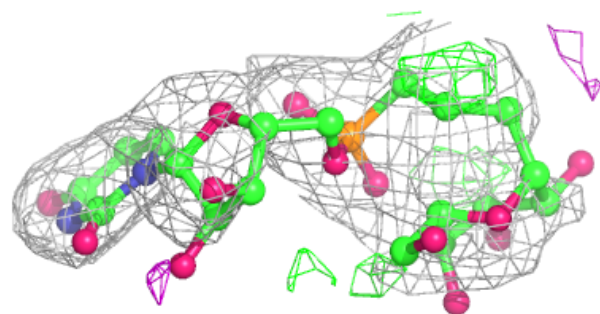
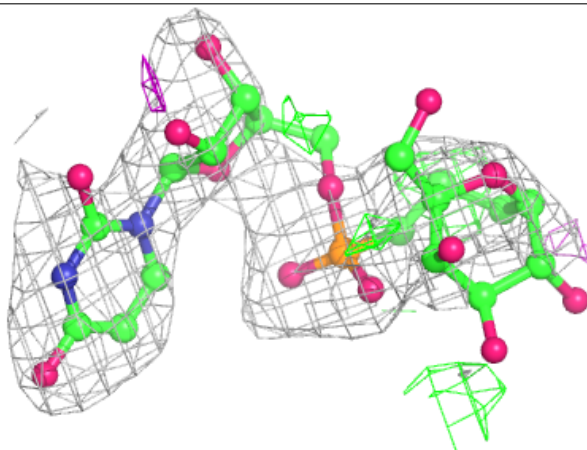


**Electron density around UDP F 1570:**

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

**Electron density around Y6W F 1572:**

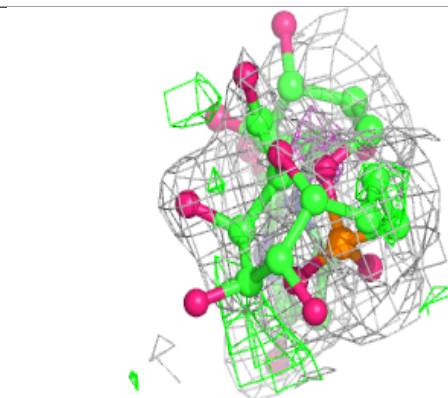
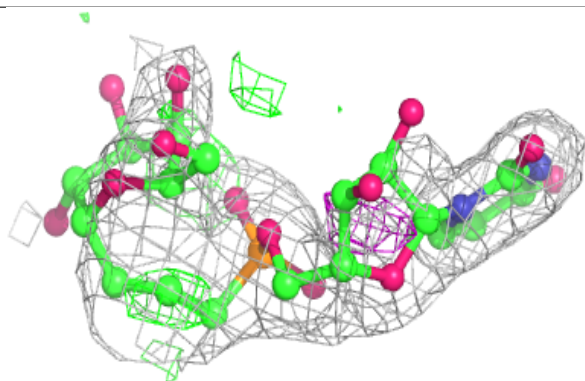
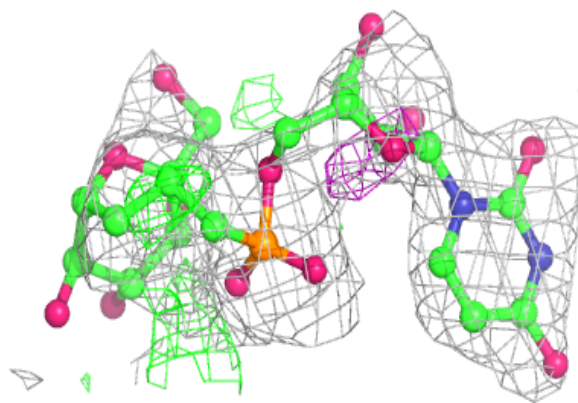
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



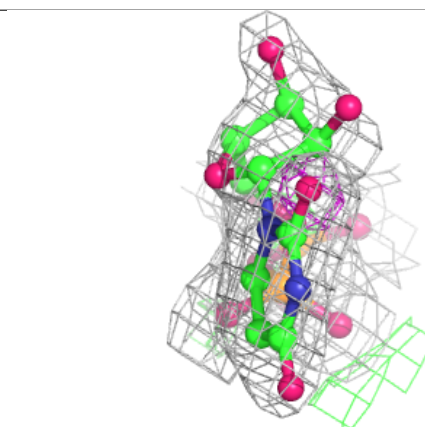
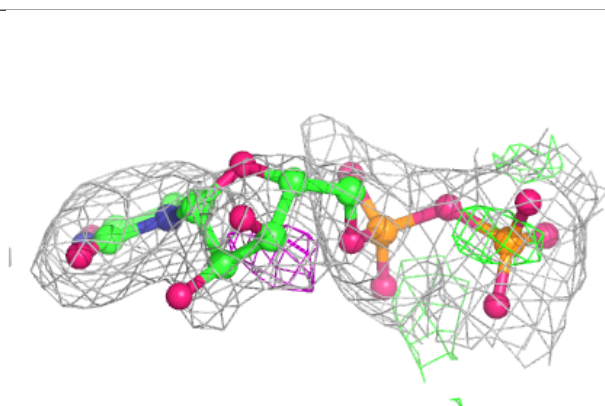
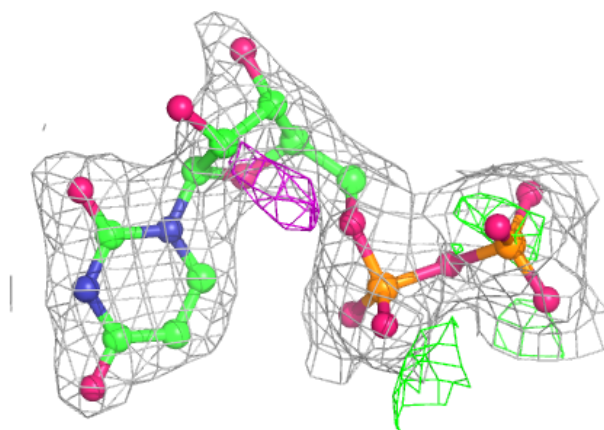


**Electron density around Y6W E 1572:**

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

**Electron density around UDP E 1570:**

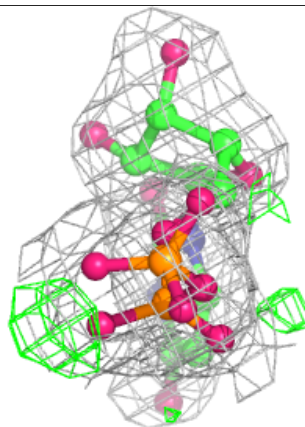
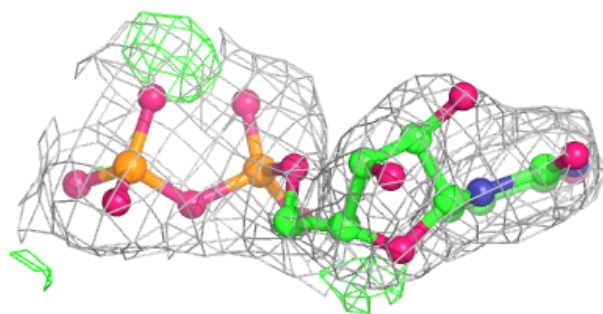
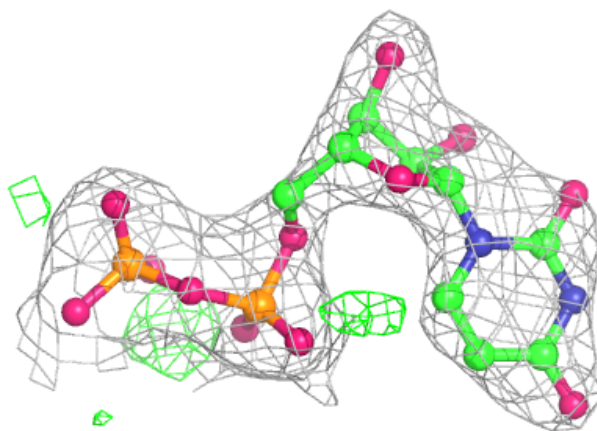
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around UDP D 1555:**

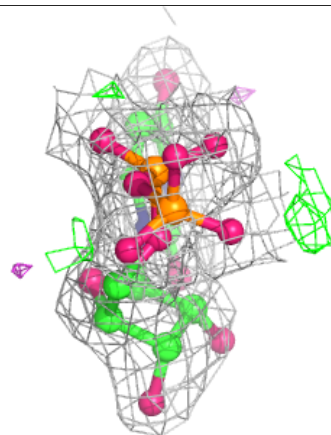
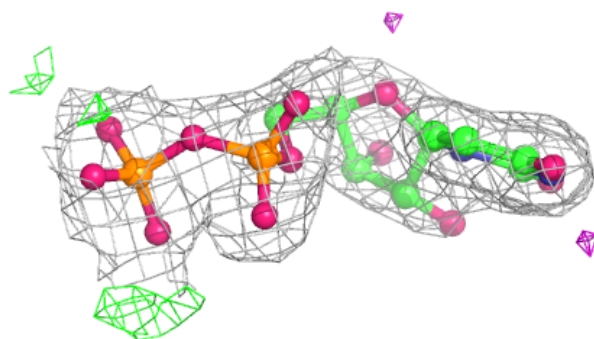
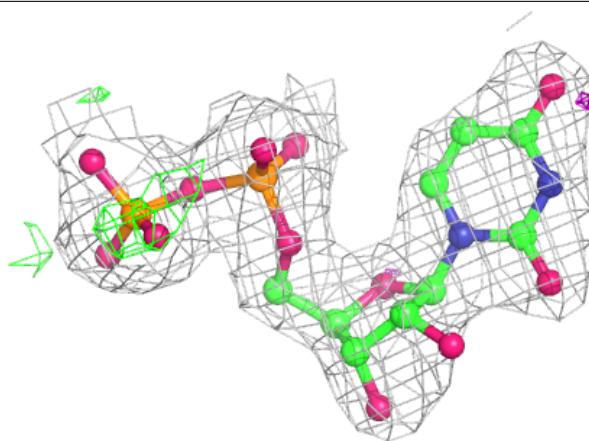
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around UDP C 1570:**

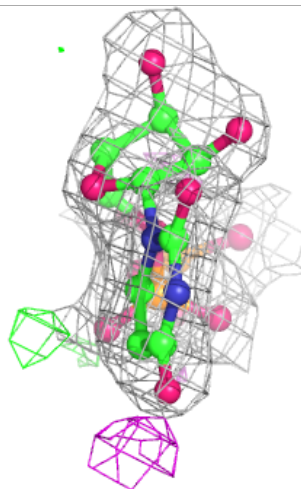
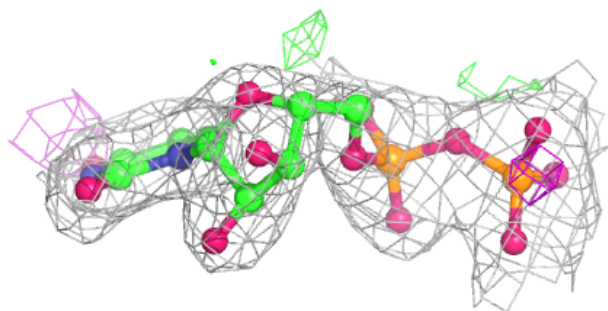
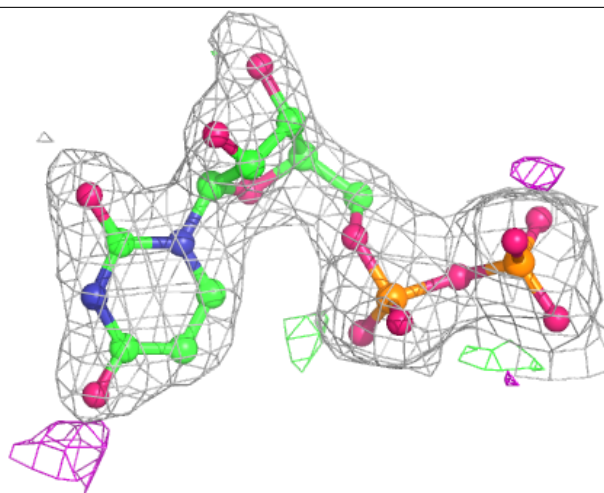
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around UDP A 1570:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.