



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 11:50 PM EDT

PDB ID : 1NKH  
Title : Crystal structure of Lactose synthase complex with UDP and Manganese  
Authors : Ramakrishnan, B.; Qasba, P.K.  
Deposited on : 2003-01-03  
Resolution : 2.00 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)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

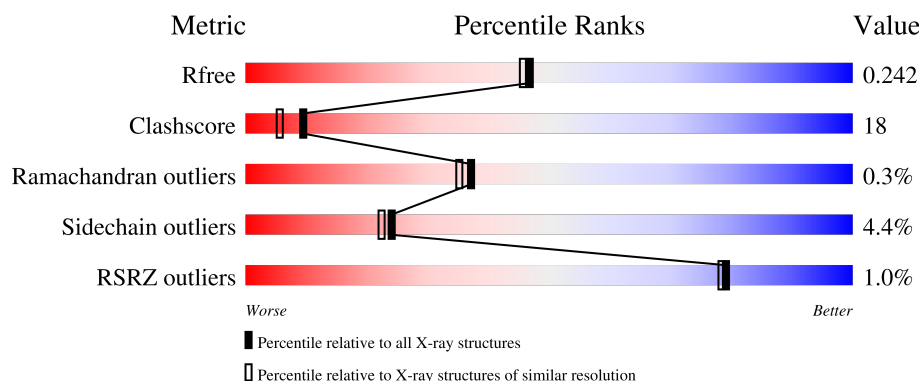
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	123	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>•</div> </div> </div>
1	C	123	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>26%</div> </div> </div>
2	B	286	<div> <div></div> <div> <div>70%</div> <div>22%</div> <div>• 5%</div> </div> </div>
2	D	286	<div> <div></div> <div> <div>67%</div> <div>24%</div> <div>• 5%</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
5	PG4	B	817	-	-	X	-
5	PG4	D	816	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7183 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 ALPHA-LACTALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			980	620	156	195	9			
1	C	123	Total	C	N	O	S	0	0	0
			980	620	156	195	9			

- Molecule 2 is a protein called BETA-1,4-GALACTOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	272	Total	C	N	O	S	0	0	0
			2218	1424	382	398	14			
2	D	272	Total	C	N	O	S	0	0	0
			2218	1424	382	398	14			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MET	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037
B	127	ARG	-	SEE REMARK 999	UNP P08037
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
D	117	ALA	-	SEE REMARK 999	UNP P08037
D	118	SER	-	SEE REMARK 999	UNP P08037
D	119	MET	-	SEE REMARK 999	UNP P08037

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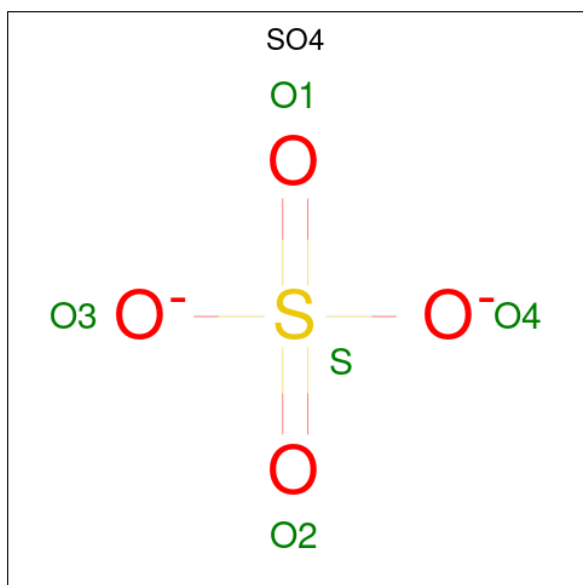
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Chain	Residue	Modelled	Actual	Comment	Reference
D	120	THR	-	SEE REMARK 999	UNP P08037
D	121	GLY	-	SEE REMARK 999	UNP P08037
D	122	GLY	-	SEE REMARK 999	UNP P08037
D	123	GLN	-	SEE REMARK 999	UNP P08037
D	124	GLN	-	SEE REMARK 999	UNP P08037
D	125	MET	-	SEE REMARK 999	UNP P08037
D	126	GLY	-	SEE REMARK 999	UNP P08037
D	127	ARG	-	SEE REMARK 999	UNP P08037
D	128	GLY	-	SEE REMARK 999	UNP P08037
D	129	SER	-	SEE REMARK 999	UNP P08037

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

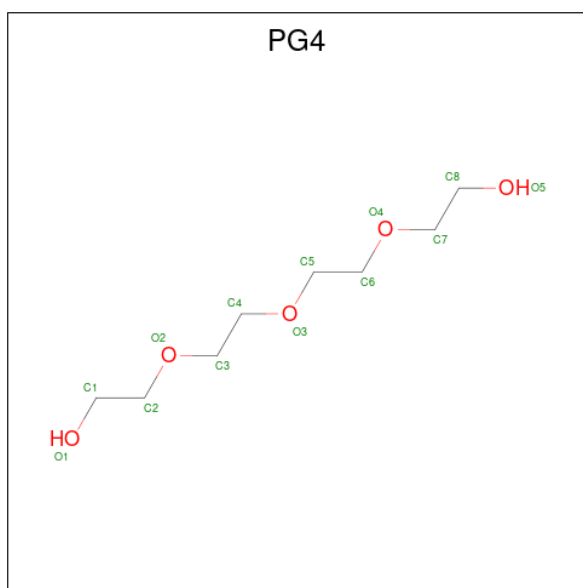
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).

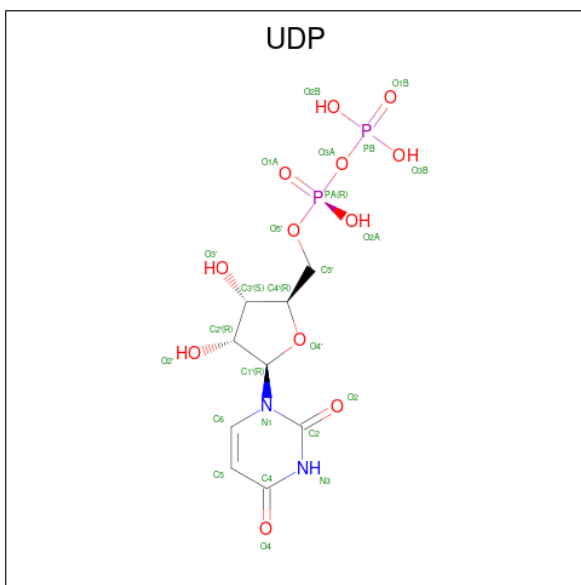


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			13	8	5		
5	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mn	0	0
			1	1		
6	D	1	Total	Mn	0	0
			1	1		

- Molecule 7 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



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

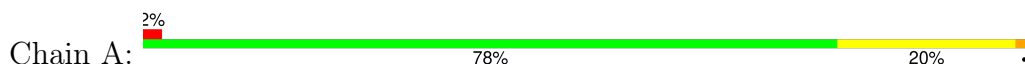
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	110	Total O 110 110	0	0
8	B	204	Total O 204 204	0	0
8	C	111	Total O 111 111	0	0
8	D	183	Total O 183 183	0	0

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

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

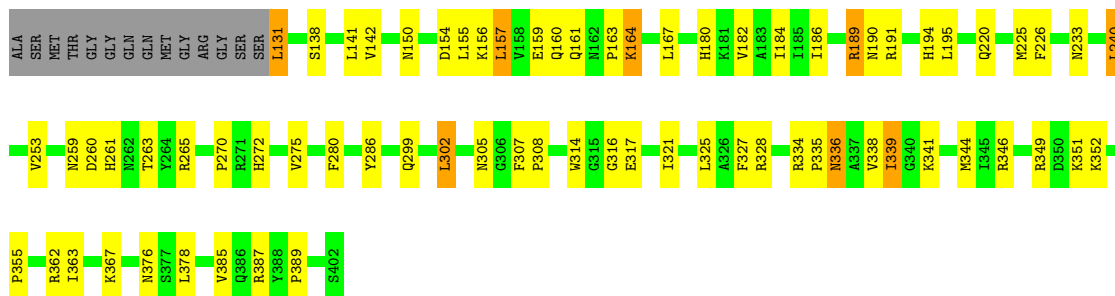
- Molecule 1: ALPHA-LACTALBUMIN



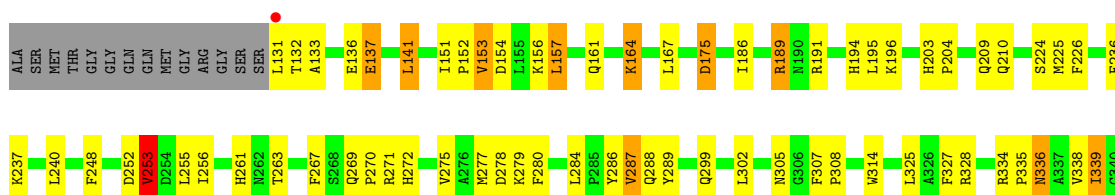
- Molecule 1: ALPHA-LACTALBUMIN



- Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE



- Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE





K341	
M344	
I345	
R346	
K351	
K352	
N353	
E354	
P357	
Q358	
R362	
K367	
L371	
N376	
R387	
S402	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.47Å 99.14Å 102.26Å 90.00° 104.14° 90.00°	Depositor
Resolution (Å)	24.71 – 2.00 24.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	79.5 (24.71-2.00) 79.5 (24.71-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.196 , 0.251 0.187 , 0.242	Depositor DCC
$R_{free}$ test set	5840 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: MN, UDP, SO4, CA, PG4

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	0.48	0/1001	0.74	0/1350
1	C	0.53	0/1001	0.75	0/1350
2	B	0.52	0/2278	0.73	0/3085
2	D	0.51	0/2278	0.78	3/3085 (0.1%)
All	All	0.51	0/6558	0.75	3/8870 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	VAL	CB-CA-C	-6.42	99.19	111.40
2	D	278	ASP	CB-CG-OD1	5.34	123.10	118.30
2	D	284	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	980	0	936	23	0
1	C	980	0	936	27	0
2	B	2218	0	2185	83	0
2	D	2218	0	2185	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	13	0	18	1	0
5	B	26	0	36	18	0
5	C	13	0	18	6	0
5	D	13	0	18	9	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	50	0	22	3	0
7	D	50	0	22	3	0
8	A	110	0	0	2	0
8	B	204	0	0	11	0
8	C	111	0	0	4	0
8	D	183	0	0	6	0
All	All	7183	0	6376	228	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 18.

The worst 5 of 228 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)
2:B:387:ARG:HH21	5:B:815:PG4:H62	1.31	0.95
1:C:10:HIS:HA	1:C:13:LYS:HE2	1.49	0.95
2:B:275:VAL:HG11	8:B:951:HOH:O	1.70	0.88
2:D:336:ASN:ND2	2:D:338:VAL:HG12	1.92	0.84
2:D:336:ASN:ND2	2:D:339:ILE:H	1.77	0.83

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	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	16	12
1	C	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
2	B	270/286 (94%)	261 (97%)	9 (3%)	0	100	100
2	D	270/286 (94%)	259 (96%)	10 (4%)	1 (0%)	30	27
All	All	782/818 (96%)	746 (95%)	34 (4%)	2 (0%)	37	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
2	D	189	ARG

### 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	109/109 (100%)	106 (97%)	3 (3%)	38	40
1	C	109/109 (100%)	108 (99%)	1 (1%)	75	81
2	B	245/254 (96%)	232 (95%)	13 (5%)	19	16
2	D	245/254 (96%)	231 (94%)	14 (6%)	17	14
All	All	708/726 (98%)	677 (96%)	31 (4%)	24	22

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	336	ASN
2	D	302	LEU
2	D	136	GLU
2	D	339	ILE
2	D	195	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	190	ASN
2	D	261	HIS
2	D	210	GLN
2	D	269	GLN
2	B	336	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	PG4	B	817	-	12,12,12	0.59	0	11,11,11	0.35	0
7	UDP	B	809	6	25,26,26	1.81	4 (16%)	38,40,40	1.53	7 (18%)
4	SO4	A	819	-	4,4,4	1.93	2 (50%)	6,6,6	0.89	0
7	UDP	B	811	-	25,26,26	1.78	3 (12%)	38,40,40	1.47	6 (15%)
7	UDP	D	812	-	25,26,26	1.71	4 (16%)	38,40,40	1.47	7 (18%)
7	UDP	D	810	6	25,26,26	1.83	4 (16%)	38,40,40	1.47	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PG4	D	816	-	12,12,12	0.43	0	11,11,11	0.40	0
5	PG4	B	815	-	12,12,12	0.55	0	11,11,11	0.24	0
5	PG4	C	814	-	12,12,12	0.63	0	11,11,11	0.13	0
5	PG4	A	813	-	12,12,12	0.55	0	11,11,11	0.33	0
4	SO4	D	818	-	4,4,4	1.90	2 (50%)	6,6,6	0.79	0

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	PG4	B	817	-	-	7/10/10/10	-
7	UDP	B	809	6	-	1/16/32/32	0/2/2/2
7	UDP	B	811	-	-	2/16/32/32	0/2/2/2
7	UDP	D	812	-	-	1/16/32/32	0/2/2/2
7	UDP	D	810	6	-	1/16/32/32	0/2/2/2
5	PG4	D	816	-	-	6/10/10/10	-
5	PG4	B	815	-	-	5/10/10/10	-
5	PG4	C	814	-	-	3/10/10/10	-
5	PG4	A	813	-	-	5/10/10/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	810	UDP	PA-O3A	6.80	1.66	1.59
7	B	811	UDP	PA-O3A	6.32	1.66	1.59
7	B	809	UDP	PA-O3A	6.20	1.66	1.59
7	D	812	UDP	PA-O3A	5.44	1.65	1.59
7	D	812	UDP	PB-O1B	3.69	1.61	1.50

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	810	UDP	O3B-PB-O1B	4.00	126.41	110.83
7	D	812	UDP	O3B-PB-O1B	3.90	126.04	110.83
7	B	811	UDP	O3B-PB-O1B	3.88	125.95	110.83
7	B	809	UDP	O3B-PB-O1B	3.78	125.57	110.83
7	D	810	UDP	O4'-C4'-C3'	-3.63	97.96	105.15

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	811	UDP	C5'-O5'-PA-O3A
5	D	816	PG4	C4-C3-O2-C2
5	D	816	PG4	O2-C3-C4-O3
5	A	813	PG4	O2-C3-C4-O3
5	A	813	PG4	O1-C1-C2-O2

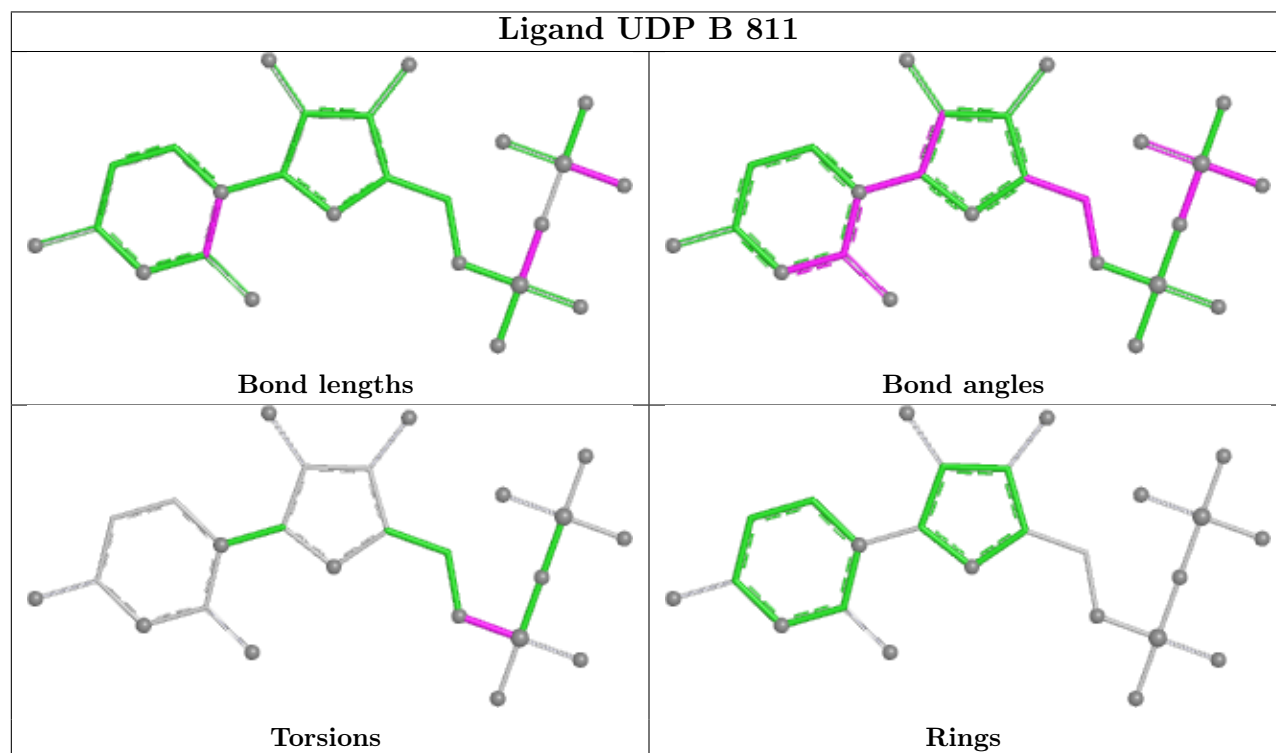
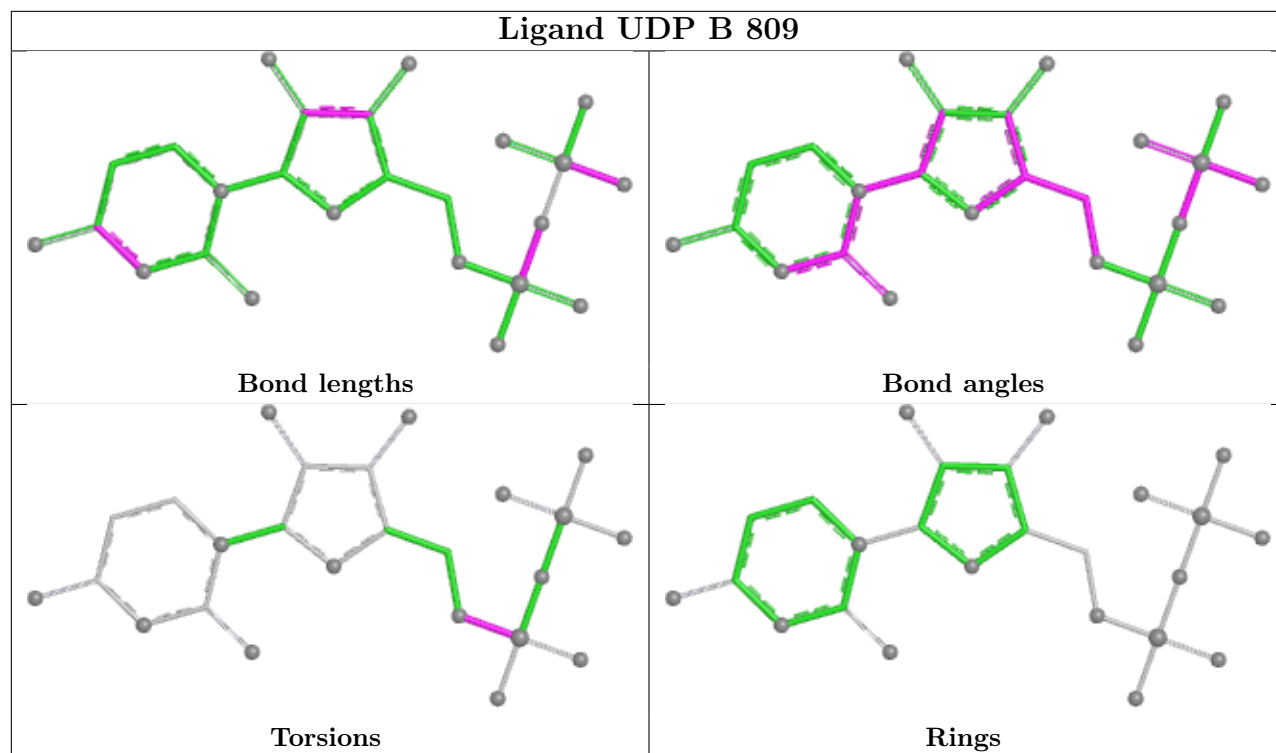
There are no ring outliers.

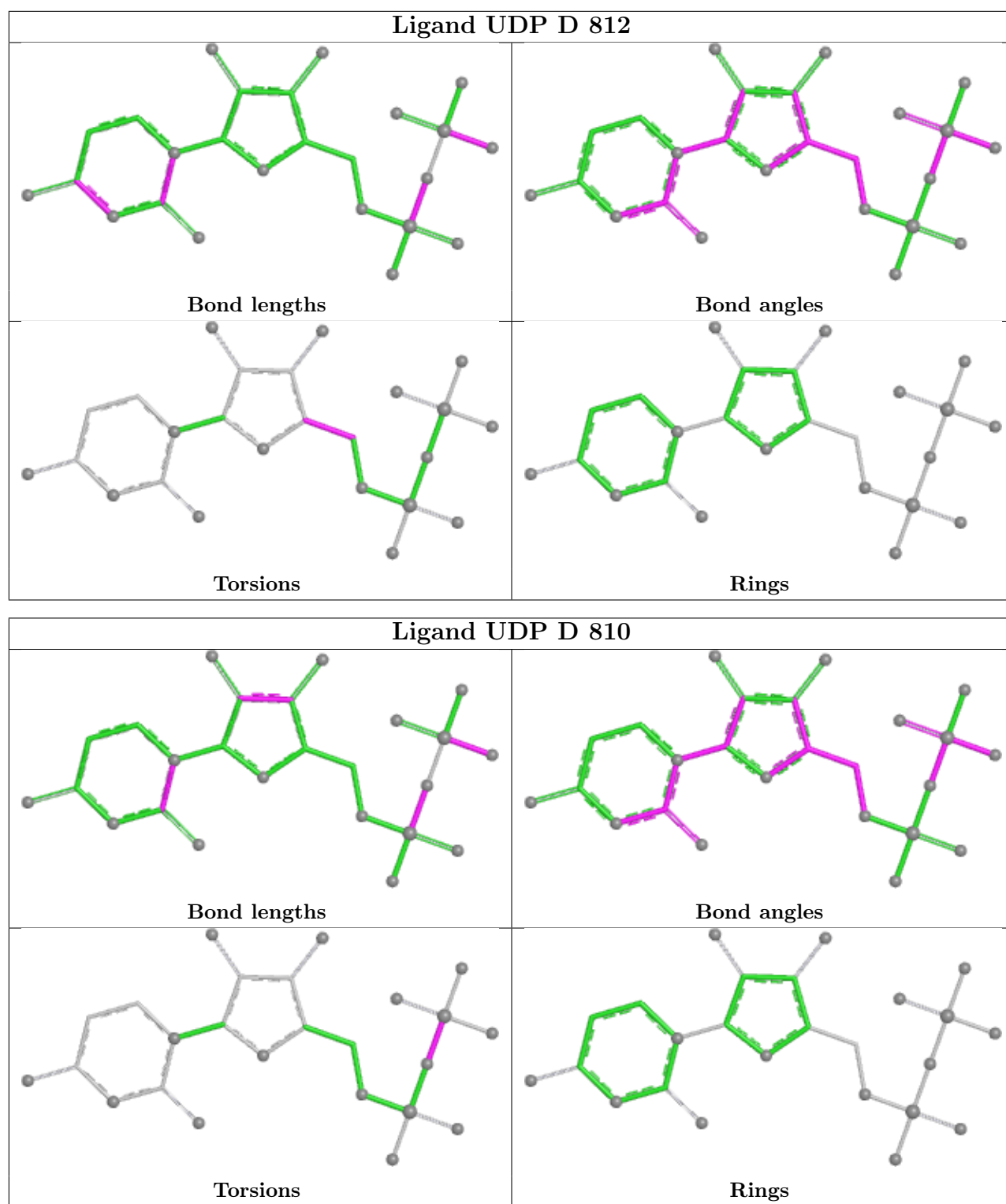
8 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	817	PG4	13	0
7	B	809	UDP	1	0
7	B	811	UDP	2	0
7	D	810	UDP	3	0
5	D	816	PG4	9	0
5	B	815	PG4	5	0
5	C	814	PG4	6	0
5	A	813	PG4	1	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 ⓘ

There are no chain breaks in this entry.

## 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	123/123 (100%)	-0.19	3 (2%) 59 58	26, 39, 60, 76	0
1	C	123/123 (100%)	-0.35	4 (3%) 49 47	24, 34, 60, 93	0
2	B	272/286 (95%)	-0.41	0 100 100	21, 35, 56, 65	0
2	D	272/286 (95%)	-0.35	1 (0%) 89 88	25, 38, 57, 76	0
All	All	790/818 (96%)	-0.34	8 (1%) 79 78	21, 37, 57, 93	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	PRO	6.3
1	C	122	LYS	4.2
1	C	68	GLU	3.1
1	C	66	PHE	2.4
2	D	131	LEU	2.2

### 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](#)

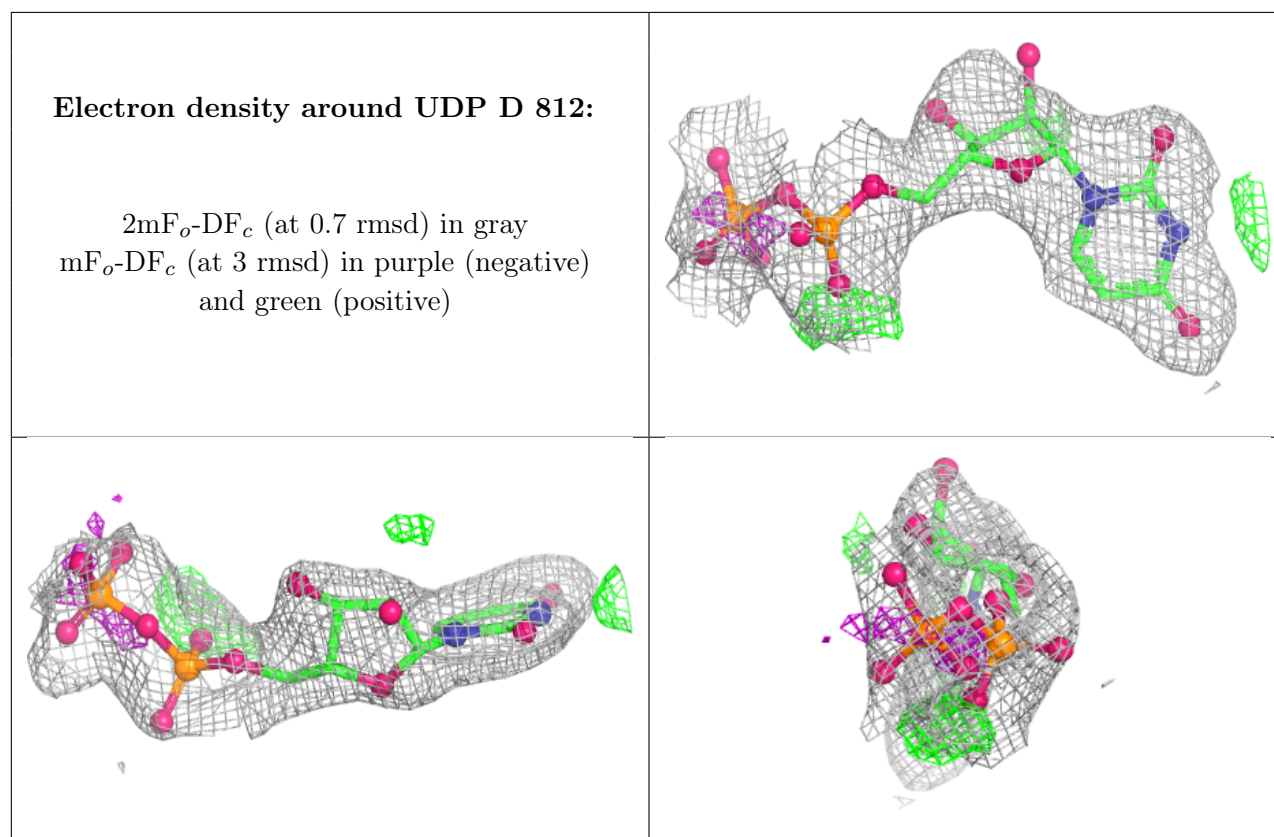
There are no monosaccharides in this entry.

### 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.

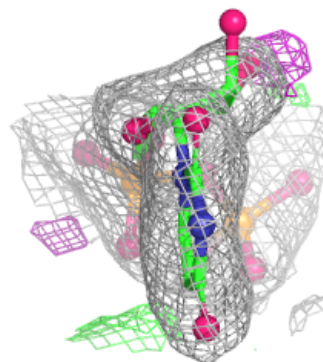
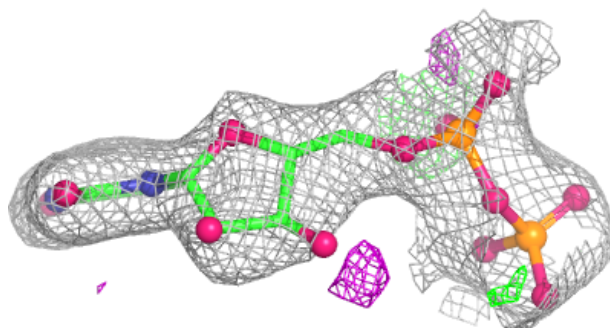
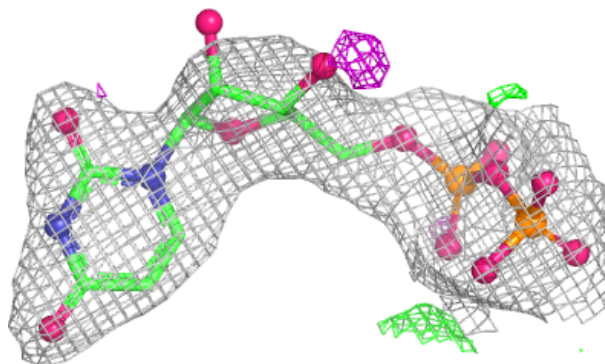
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PG4	B	815	13/13	0.73	0.15	64,66,73,75	0
4	SO4	A	819	5/5	0.74	0.11	88,89,89,89	0
7	UDP	D	812	25/25	0.77	0.12	58,76,100,100	0
5	PG4	B	817	13/13	0.79	0.20	64,66,73,75	0
7	UDP	B	811	25/25	0.80	0.12	69,82,98,99	0
4	SO4	D	818	5/5	0.82	0.11	82,83,83,84	0
5	PG4	D	816	13/13	0.84	0.17	64,66,70,70	0
5	PG4	C	814	13/13	0.89	0.12	52,55,64,66	0
5	PG4	A	813	13/13	0.89	0.11	46,48,49,50	0
7	UDP	B	809	25/25	0.97	0.05	30,34,38,40	0
7	UDP	D	810	25/25	0.98	0.04	26,30,34,36	0
3	CA	C	806	1/1	0.99	0.02	33,33,33,33	0
3	CA	A	805	1/1	0.99	0.02	34,34,34,34	0
6	MN	B	807	1/1	1.00	0.02	35,35,35,35	0
6	MN	D	808	1/1	1.00	0.03	35,35,35,35	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.



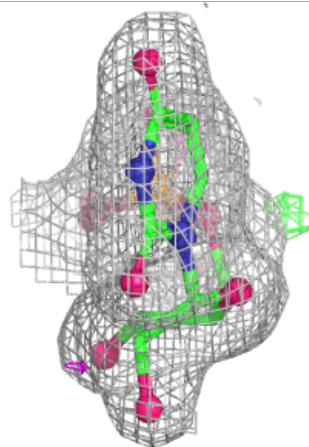
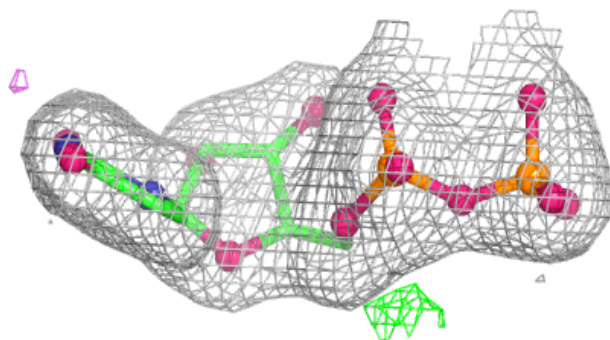
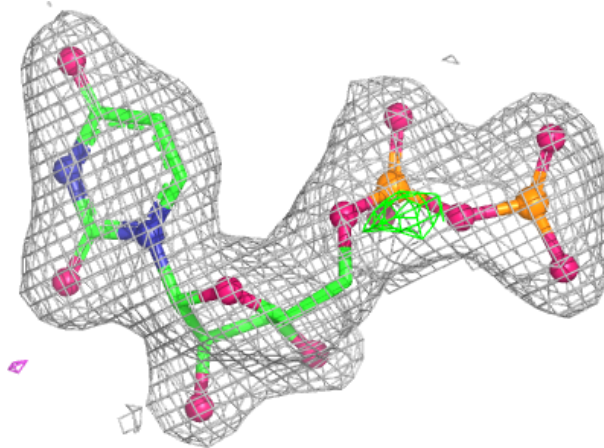
**Electron density around UDP B 811:**

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

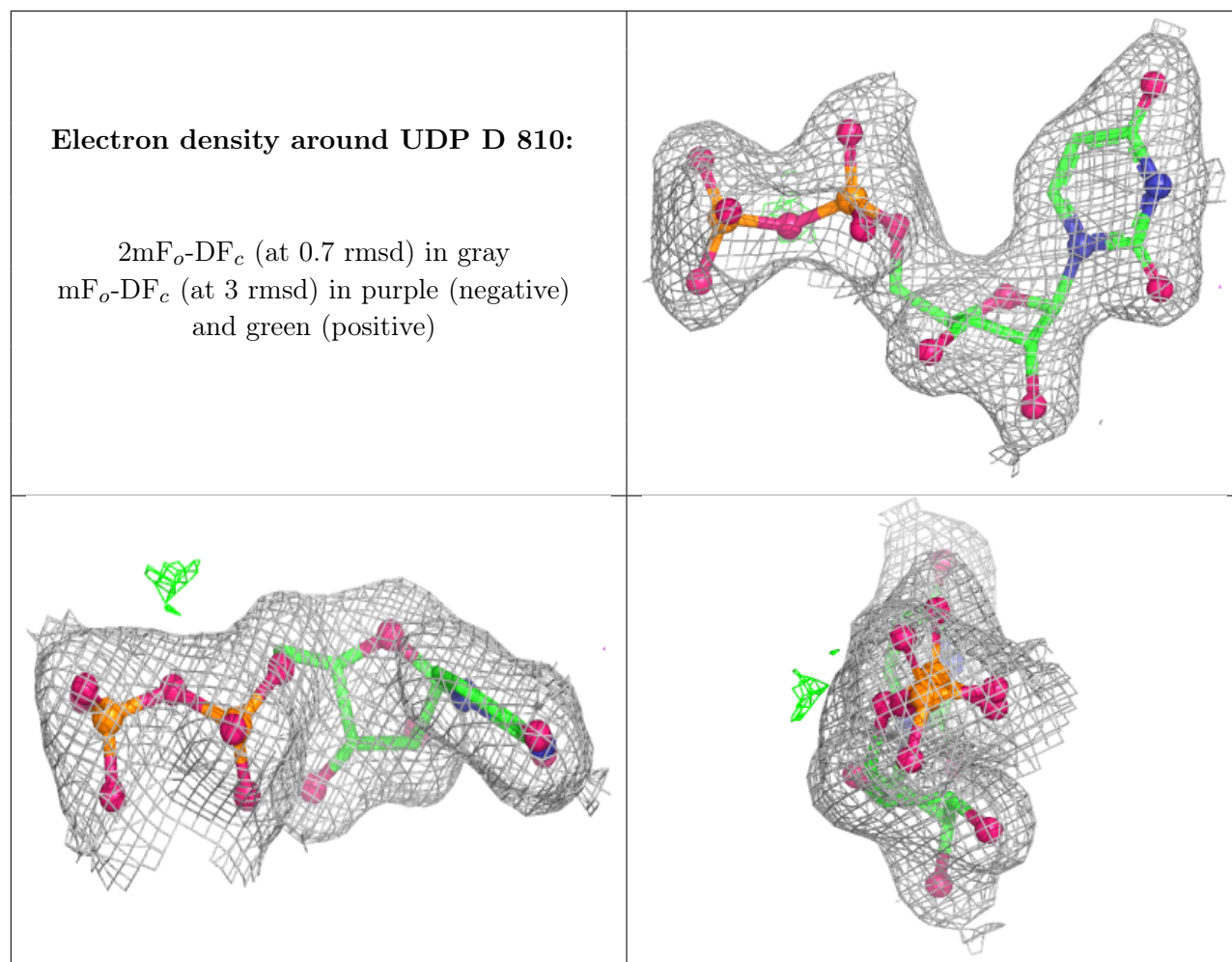


**Electron density around UDP B 809:**

$2mF_o-DF_c$  (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.