



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 05:58 PM UTC

PDB ID : 3S27 / pdb_00003s27
Title : The crystal structure of sucrose synthase-1 from Arabidopsis thaliana and its functional implications.
Authors : Zheng, Y.; Garavito, R.M.
Deposited on : 2011-05-16
Resolution : 2.91 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

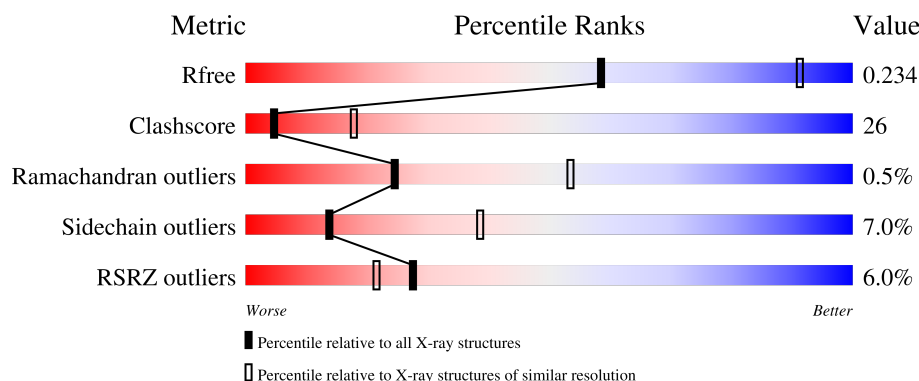
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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 ≥ 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	816	5% 56% 36% • •
1	B	816	10% 56% 37% • •
1	C	816	3% 53% 38% • •
1	D	816	4% 58% 34% • •
1	E	816	5% 59% 32% 5% •

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Mol	Chain	Length	Quality of chain
1	F	816	4% 57% 33% • • •
1	G	816	3% 58% 33% • •
1	H	816	10% 60% 33% 5% •

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
4	SO4	B	913	-	-	X	-
4	SO4	F	913	-	-	X	-
5	MLA	E	921	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 51483 atoms, of which 200 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 Sucrose synthase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	Se	0	0	0
			6277	4031	1065	1159	10	12			
1	B	793	Total	C	N	O	S	Se	0	0	0
			6313	4046	1074	1171	10	12			
1	C	781	Total	C	N	O	S	Se	0	0	0
			6268	4028	1064	1154	10	12			
1	D	781	Total	C	N	O	S	Se	0	0	0
			6243	4014	1059	1148	10	12			
1	E	781	Total	C	N	O	S	Se	0	0	0
			6249	4014	1061	1152	10	12			
1	F	781	Total	C	N	O	S	Se	0	0	0
			6275	4031	1064	1158	10	12			
1	G	781	Total	C	N	O	S	Se	0	0	0
			6279	4032	1068	1157	10	12			
1	H	797	Total	C	N	O	S	Se	0	0	0
			6336	4060	1087	1167	10	12			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	809	VAL	-	expression tag	UNP P49040
A	810	GLU	-	expression tag	UNP P49040
A	811	HIS	-	expression tag	UNP P49040
A	812	HIS	-	expression tag	UNP P49040
A	813	HIS	-	expression tag	UNP P49040
A	814	HIS	-	expression tag	UNP P49040
A	815	HIS	-	expression tag	UNP P49040
A	816	HIS	-	expression tag	UNP P49040
B	809	VAL	-	expression tag	UNP P49040
B	810	GLU	-	expression tag	UNP P49040
B	811	HIS	-	expression tag	UNP P49040
B	812	HIS	-	expression tag	UNP P49040
B	813	HIS	-	expression tag	UNP P49040

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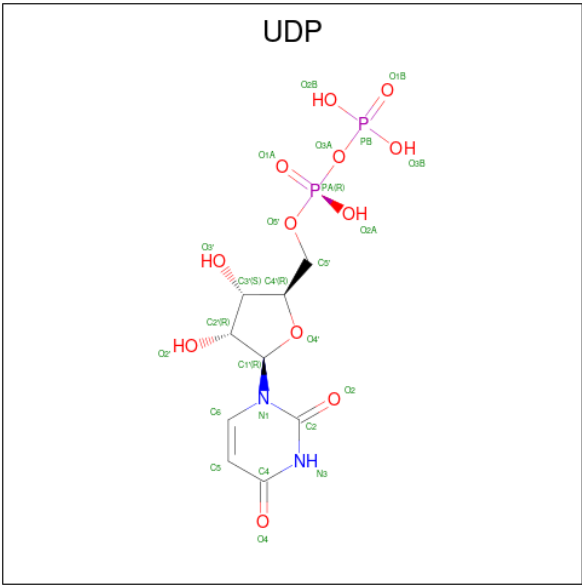
Chain	Residue	Modelled	Actual	Comment	Reference
B	814	HIS	-	expression tag	UNP P49040
B	815	HIS	-	expression tag	UNP P49040
B	816	HIS	-	expression tag	UNP P49040
C	809	VAL	-	expression tag	UNP P49040
C	810	GLU	-	expression tag	UNP P49040
C	811	HIS	-	expression tag	UNP P49040
C	812	HIS	-	expression tag	UNP P49040
C	813	HIS	-	expression tag	UNP P49040
C	814	HIS	-	expression tag	UNP P49040
C	815	HIS	-	expression tag	UNP P49040
C	816	HIS	-	expression tag	UNP P49040
D	809	VAL	-	expression tag	UNP P49040
D	810	GLU	-	expression tag	UNP P49040
D	811	HIS	-	expression tag	UNP P49040
D	812	HIS	-	expression tag	UNP P49040
D	813	HIS	-	expression tag	UNP P49040
D	814	HIS	-	expression tag	UNP P49040
D	815	HIS	-	expression tag	UNP P49040
D	816	HIS	-	expression tag	UNP P49040
E	809	VAL	-	expression tag	UNP P49040
E	810	GLU	-	expression tag	UNP P49040
E	811	HIS	-	expression tag	UNP P49040
E	812	HIS	-	expression tag	UNP P49040
E	813	HIS	-	expression tag	UNP P49040
E	814	HIS	-	expression tag	UNP P49040
E	815	HIS	-	expression tag	UNP P49040
E	816	HIS	-	expression tag	UNP P49040
F	809	VAL	-	expression tag	UNP P49040
F	810	GLU	-	expression tag	UNP P49040
F	811	HIS	-	expression tag	UNP P49040
F	812	HIS	-	expression tag	UNP P49040
F	813	HIS	-	expression tag	UNP P49040
F	814	HIS	-	expression tag	UNP P49040
F	815	HIS	-	expression tag	UNP P49040
F	816	HIS	-	expression tag	UNP P49040
G	809	VAL	-	expression tag	UNP P49040
G	810	GLU	-	expression tag	UNP P49040
G	811	HIS	-	expression tag	UNP P49040
G	812	HIS	-	expression tag	UNP P49040
G	813	HIS	-	expression tag	UNP P49040
G	814	HIS	-	expression tag	UNP P49040
G	815	HIS	-	expression tag	UNP P49040

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Chain	Residue	Modelled	Actual	Comment	Reference
G	816	HIS	-	expression tag	UNP P49040
H	809	VAL	-	expression tag	UNP P49040
H	810	GLU	-	expression tag	UNP P49040
H	811	HIS	-	expression tag	UNP P49040
H	812	HIS	-	expression tag	UNP P49040
H	813	HIS	-	expression tag	UNP P49040
H	814	HIS	-	expression tag	UNP P49040
H	815	HIS	-	expression tag	UNP P49040
H	816	HIS	-	expression tag	UNP P49040

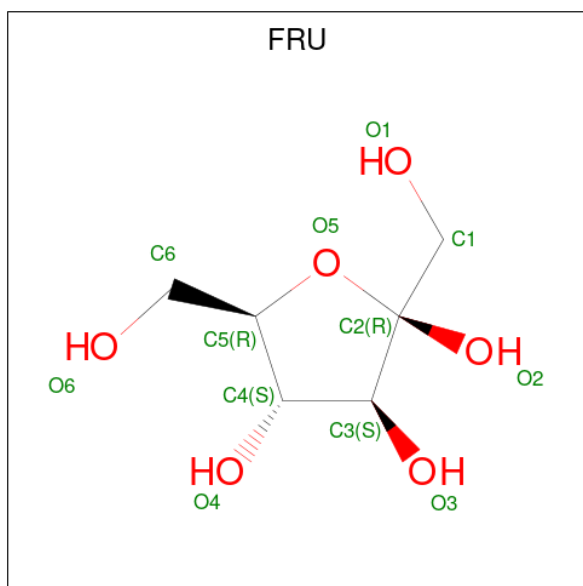
- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	H	N	O	P	
			36	9	11	2	12	2	
								0	0

- Molecule 3 is beta-D-fructofuranose (CCD ID: FRU) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O		
			24	6	12	6	0	0
3	B	1	Total	C	H	O		
			24	6	12	6	0	0
3	C	1	Total	C	H	O		
			24	6	12	6	0	0
3	D	1	Total	C	H	O		
			24	6	12	6	0	0
3	E	1	Total	C	H	O		
			24	6	12	6	0	0
3	F	1	Total	C	H	O		
			24	6	12	6	0	0
3	G	1	Total	C	H	O		
			24	6	12	6	0	0
3	H	1	Total	C	H	O		
			24	6	12	6	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



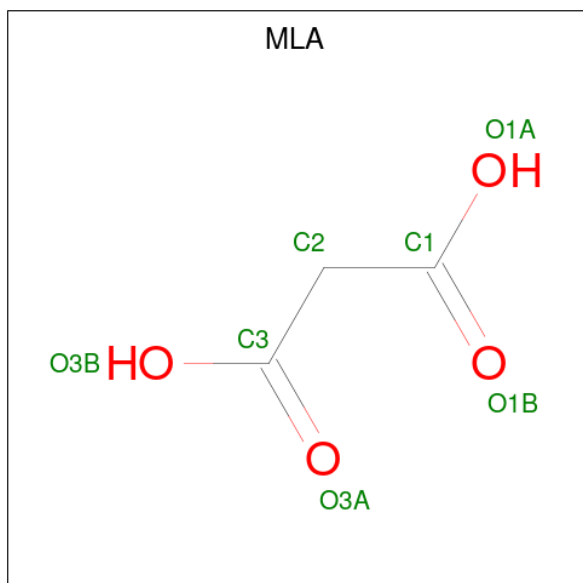
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			9	3	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			9	3	2	4		
5	C	1	Total	C	H	O	0	0
			9	3	2	4		
5	D	1	Total	C	H	O	0	0
			9	3	2	4		
5	E	1	Total	C	H	O	0	0
			9	3	2	4		
5	F	1	Total	C	H	O	0	0
			9	3	2	4		
5	G	1	Total	C	H	O	0	0
			9	3	2	4		
5	H	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		
6	B	1	Total	K	0	0
			1	1		
6	C	1	Total	K	0	0
			1	1		
6	D	1	Total	K	0	0
			1	1		
6	E	1	Total	K	0	0
			1	1		
6	F	1	Total	K	0	0
			1	1		
6	G	1	Total	K	0	0
			1	1		
6	H	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	82	Total	O	0	0
			82	82		
7	B	72	Total	O	0	0
			72	72		

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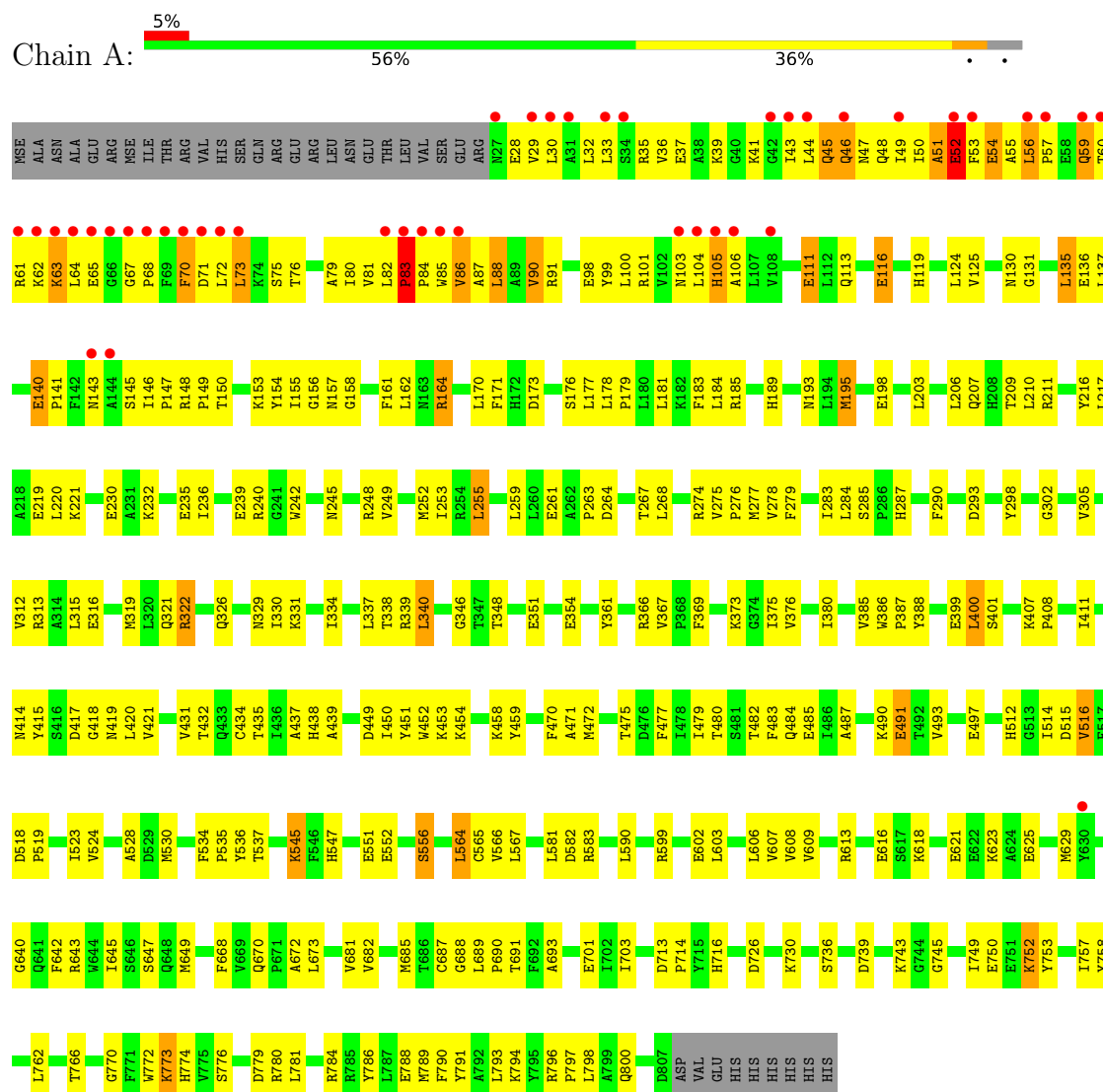
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	45	Total 45	O 45	0	0
7	D	67	Total 67	O 67	0	0
7	E	66	Total 66	O 66	0	0
7	F	90	Total 90	O 90	0	0
7	G	81	Total 81	O 81	0	0
7	H	60	Total 60	O 60	0	0

3 Residue-property plots [i](#)

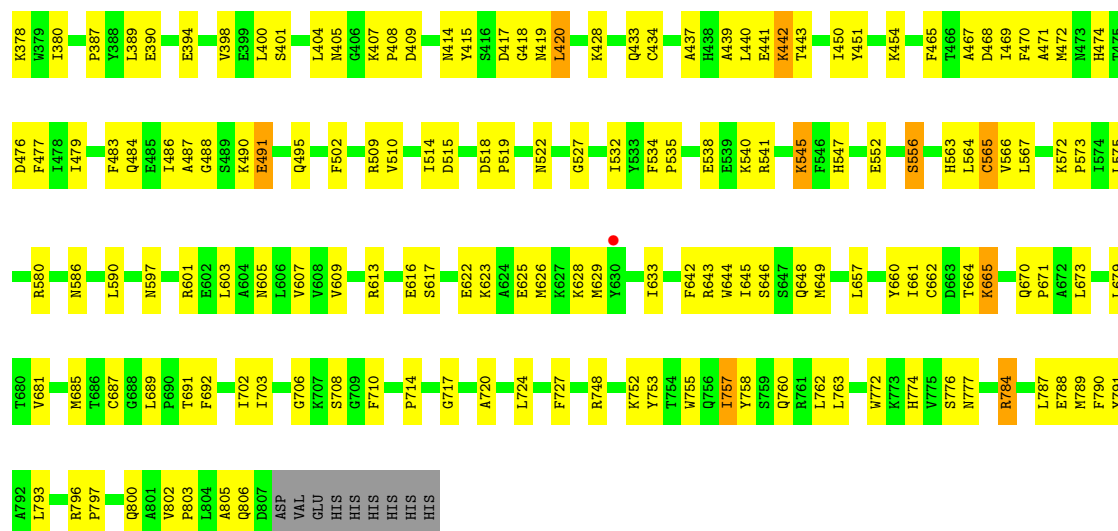
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sucrose synthase 1

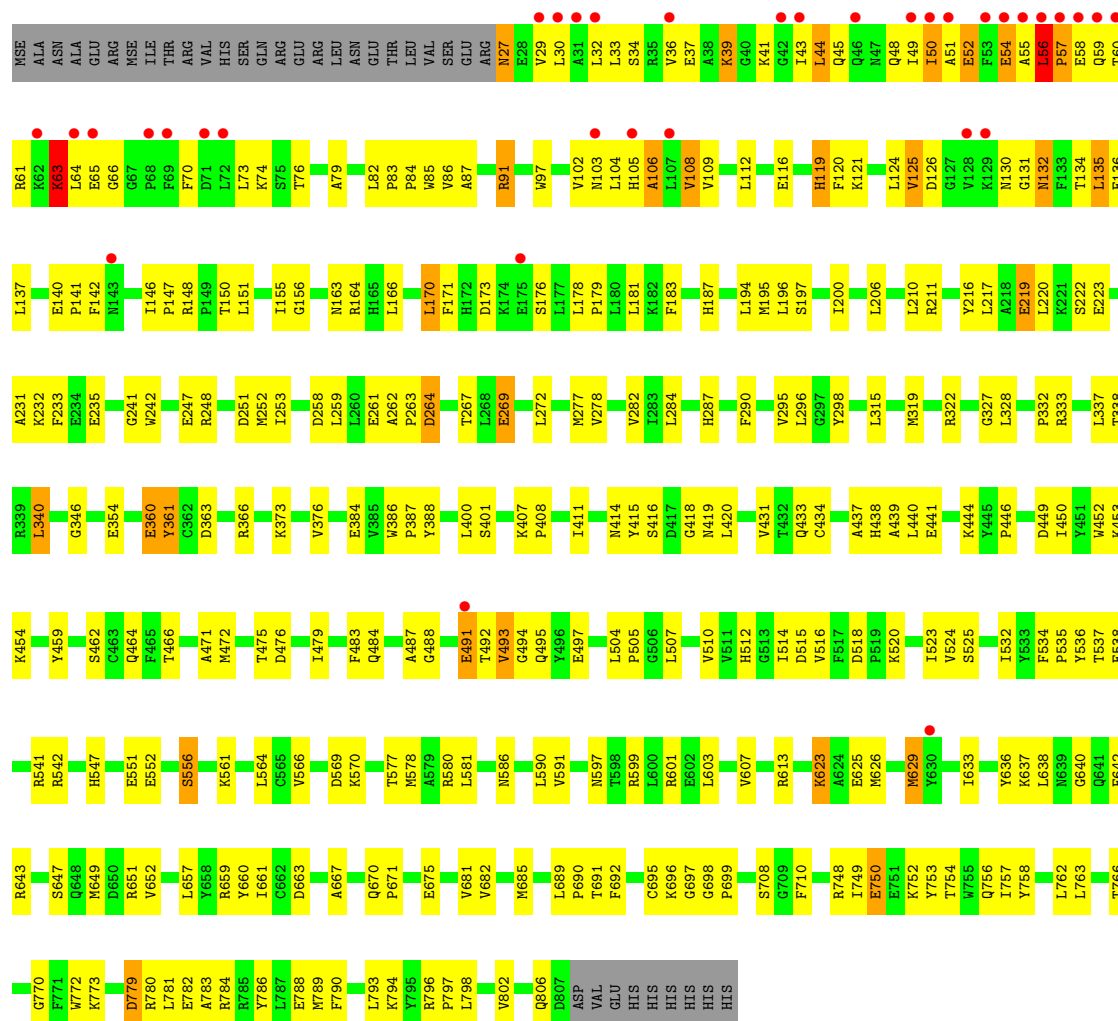


• Molecule 1: Sucrose synthase 1



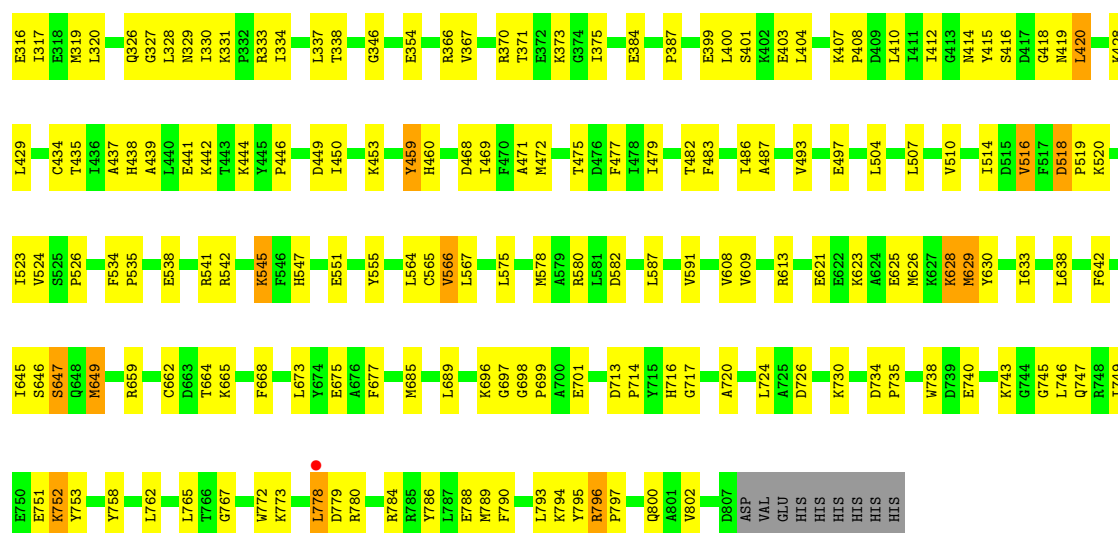


● Molecule 1: Sucrose synthase 1

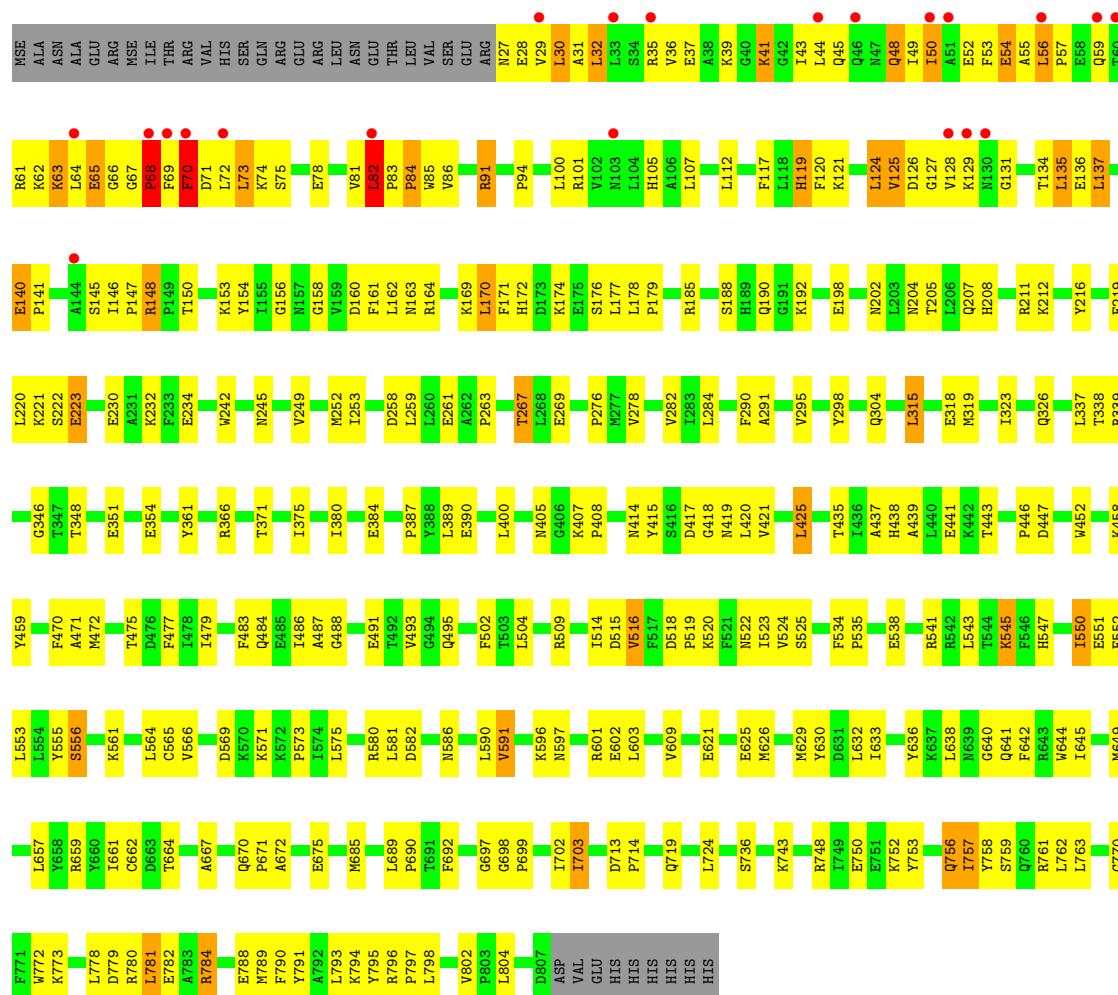


Chain E: 5% 59% 32% 5%

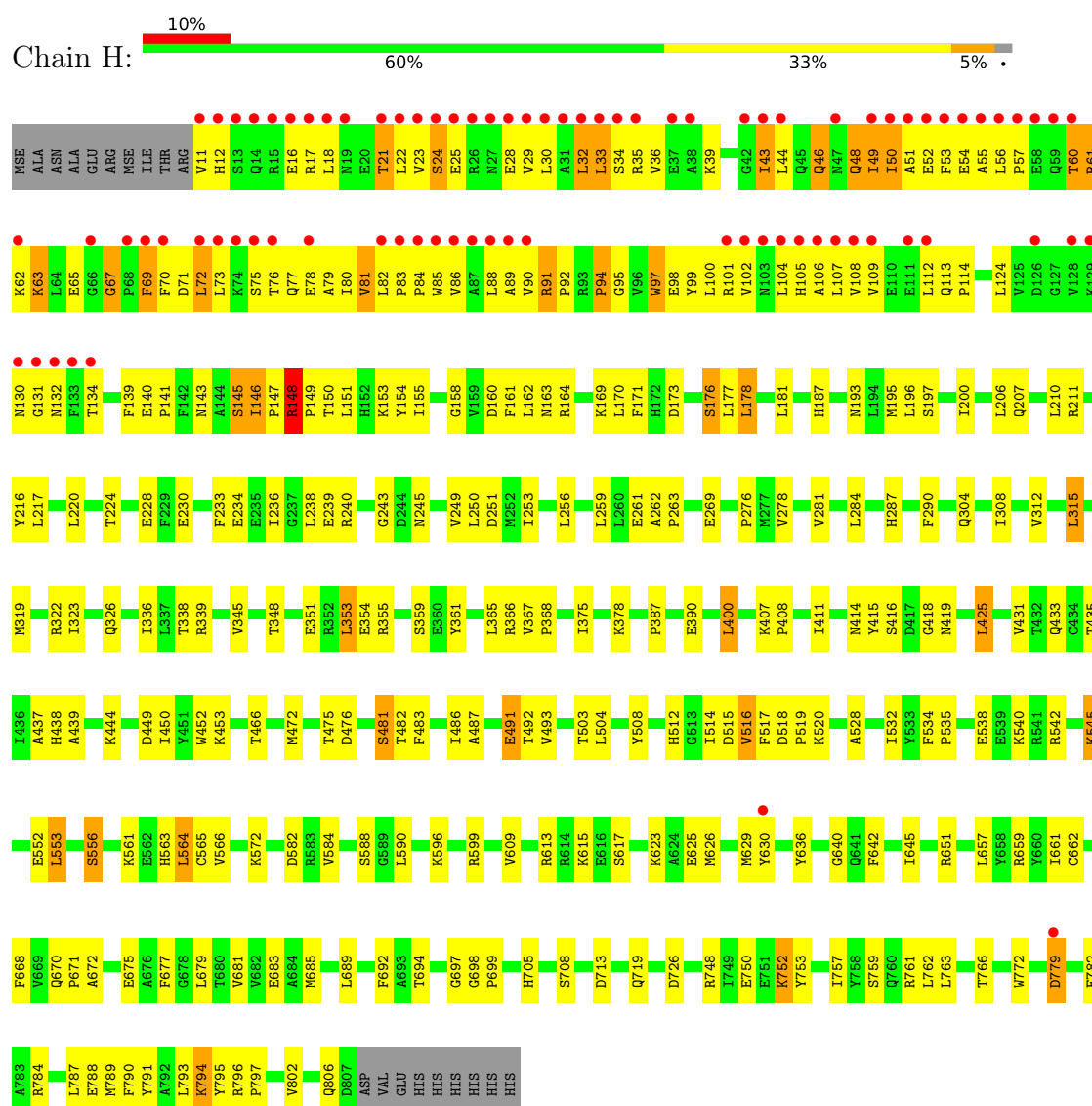




• Molecule 1: Sucrose synthase 1



• Molecule 1: Sucrose synthase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.21Å 263.70Å 159.66Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	25.00 – 2.91 25.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	91.0 (25.00-2.91) 90.9 (25.00-2.91)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.186 , 0.237 0.183 , 0.234	Depositor DCC
R_{free} test set	11586 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	51483	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7500e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: UDP, SO4, MLA, K, FRU

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	0.50	0/6412	0.86	10/8664 (0.1%)
1	B	0.47	0/6447	0.86	11/8717 (0.1%)
1	C	0.45	0/6403	0.88	10/8654 (0.1%)
1	D	0.48	0/6378	0.89	14/8624 (0.2%)
1	E	0.47	0/6383	0.89	14/8629 (0.2%)
1	F	0.51	0/6410	0.95	21/8663 (0.2%)
1	G	0.48	0/6414	0.90	18/8667 (0.2%)
1	H	0.47	0/6471	0.88	17/8749 (0.2%)
All	All	0.48	0/51318	0.89	115/69367 (0.2%)

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	1
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	3
1	G	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	GLY	CA-C-N	11.33	134.00	119.84
1	F	67	GLY	C-N-CA	11.33	134.00	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	82	LEU	CA-C-N	11.22	131.94	120.38
1	G	82	LEU	C-N-CA	11.22	131.94	120.38
1	F	82	LEU	CA-C-N	9.92	130.60	120.38

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	C	47	ASN	Peptide
1	D	56	LEU	Peptide
1	E	70	PHE	Peptide
1	E	83	PRO	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	6277	0	6191	337	0
1	B	6313	0	6170	330	0
1	C	6268	0	6189	320	0
1	D	6243	0	6143	324	0
1	E	6249	0	6158	360	0
1	F	6275	0	6195	365	0
1	G	6279	0	6201	347	0
1	H	6336	0	6196	320	0
2	A	25	11	11	0	0
2	B	25	11	11	0	0
2	C	25	11	11	1	0
2	D	25	11	11	2	0
2	E	25	11	11	4	0
2	F	25	11	11	1	0
2	G	25	11	11	1	0
2	H	25	11	11	0	0
3	A	12	12	12	1	0
3	B	12	12	12	0	0
3	C	12	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	12	12	0	0
3	E	12	12	12	1	0
3	F	12	12	12	1	0
3	G	12	12	12	4	0
3	H	12	12	12	1	0
4	A	15	0	0	1	0
4	B	15	0	0	3	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
4	E	15	0	0	1	0
4	F	15	0	0	2	0
4	G	15	0	0	1	0
4	H	15	0	0	1	0
5	A	7	2	2	0	0
5	B	7	2	2	1	0
5	C	7	2	2	0	0
5	D	7	2	2	0	0
5	E	7	2	2	5	0
5	F	7	2	2	0	0
5	G	7	2	2	0	0
5	H	7	2	2	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	82	0	0	5	0
7	B	72	0	0	7	0
7	C	45	0	0	3	0
7	D	67	0	0	3	0
7	E	66	0	0	2	0
7	F	90	0	0	10	0
7	G	81	0	0	5	0
7	H	60	0	0	6	0
All	All	51283	200	49643	2588	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 26.

The worst 5 of 2588 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:C:83:PRO:HG2	1:C:84:PRO:HD3	1.22	1.19
1:G:82:LEU:HD12	1:G:83:PRO:CG	1.72	1.18
1:B:83:PRO:HG2	1:B:85:TRP:HB2	1.19	1.16
1:G:65:GLU:HB3	1:G:70:PHE:CD1	1.79	1.16
1:A:789:MSE:CE	1:D:789:MSE:HB3	1.76	1.14

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	779/816 (96%)	730 (94%)	45 (6%)	4 (0%)	24	53
1	B	791/816 (97%)	734 (93%)	56 (7%)	1 (0%)	48	76
1	C	779/816 (96%)	734 (94%)	42 (5%)	3 (0%)	30	58
1	D	779/816 (96%)	736 (94%)	38 (5%)	5 (1%)	21	50
1	E	779/816 (96%)	737 (95%)	38 (5%)	4 (0%)	24	53
1	F	779/816 (96%)	734 (94%)	39 (5%)	6 (1%)	16	43
1	G	779/816 (96%)	736 (94%)	39 (5%)	4 (0%)	24	53
1	H	795/816 (97%)	750 (94%)	42 (5%)	3 (0%)	30	58
All	All	6260/6528 (96%)	5891 (94%)	339 (5%)	30 (0%)	24	53

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	GLN
1	D	106	ALA
1	E	83	PRO
1	A	52	GLU
1	A	83	PRO

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	667/704 (95%)	623 (93%)	44 (7%)	15	41
1	B	663/704 (94%)	613 (92%)	50 (8%)	12	35
1	C	666/704 (95%)	614 (92%)	52 (8%)	11	33
1	D	659/704 (94%)	620 (94%)	39 (6%)	18	46
1	E	662/704 (94%)	614 (93%)	48 (7%)	13	37
1	F	668/704 (95%)	629 (94%)	39 (6%)	18	47
1	G	668/704 (95%)	616 (92%)	52 (8%)	11	33
1	H	663/704 (94%)	616 (93%)	47 (7%)	13	38
All	All	5316/5632 (94%)	4945 (93%)	371 (7%)	14	38

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	777	ASN
1	G	100	LEU
1	F	56	LEU
1	F	626	MSE
1	G	267	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	639	ASN
1	G	563	HIS
1	G	27	ASN
1	G	190	GLN
1	H	45	GLN

5.3.3 RNA ⓘ

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 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 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	$\# Z > 2$
2	UDP	F	901	-	25,26,26	1.00	1 (4%)	38,40,40	1.81	8 (21%)
4	SO4	A	913	-	4,4,4	0.30	0	6,6,6	0.31	0
5	MLA	F	921	-	6,6,6	1.34	0	7,7,7	1.11	0
4	SO4	A	911	-	4,4,4	0.33	0	6,6,6	0.19	0
3	FRU	A	902	-	11,12,12	0.74	0	10,18,18	0.79	0
4	SO4	H	912	-	4,4,4	0.30	0	6,6,6	0.13	0
2	UDP	C	901	-	25,26,26	1.06	1 (4%)	38,40,40	1.63	7 (18%)
2	UDP	E	901	-	25,26,26	1.03	1 (4%)	38,40,40	1.56	6 (15%)
4	SO4	H	911	-	4,4,4	0.36	0	6,6,6	0.25	0
5	MLA	E	921	-	6,6,6	1.27	0	7,7,7	0.94	0
4	SO4	D	912	-	4,4,4	0.28	0	6,6,6	0.09	0
3	FRU	C	902	-	11,12,12	0.70	1 (9%)	10,18,18	0.91	0
4	SO4	B	912	-	4,4,4	0.33	0	6,6,6	0.24	0
2	UDP	G	901	-	25,26,26	0.97	0	38,40,40	1.57	6 (15%)
5	MLA	A	921	-	6,6,6	1.14	0	7,7,7	1.38	1 (14%)
2	UDP	H	901	-	25,26,26	1.02	0	38,40,40	1.75	6 (15%)
5	MLA	G	921	-	6,6,6	1.08	0	7,7,7	1.52	1 (14%)
3	FRU	H	902	-	11,12,12	0.85	1 (9%)	10,18,18	1.06	0
4	SO4	F	912	-	4,4,4	0.31	0	6,6,6	0.30	0
4	SO4	E	913	-	4,4,4	0.36	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	G	911	-	4,4,4	0.36	0	6,6,6	0.17	0
3	FRU	B	902	-	11,12,12	0.79	1 (9%)	10,18,18	0.86	0
4	SO4	C	911	-	4,4,4	0.26	0	6,6,6	0.22	0
4	SO4	F	913	-	4,4,4	0.34	0	6,6,6	0.16	0
5	MLA	D	921	-	6,6,6	1.12	0	7,7,7	1.23	0
4	SO4	C	913	-	4,4,4	0.30	0	6,6,6	0.14	0
4	SO4	D	911	-	4,4,4	0.32	0	6,6,6	0.28	0
4	SO4	B	911	-	4,4,4	0.39	0	6,6,6	0.25	0
5	MLA	C	921	-	6,6,6	1.15	0	7,7,7	1.42	1 (14%)
3	FRU	F	902	-	11,12,12	0.73	0	10,18,18	0.75	0
2	UDP	D	901	-	25,26,26	1.03	0	38,40,40	1.81	6 (15%)
4	SO4	A	912	-	4,4,4	0.31	0	6,6,6	0.18	0
4	SO4	H	913	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	D	913	-	4,4,4	0.33	0	6,6,6	0.10	0
4	SO4	F	911	-	4,4,4	0.37	0	6,6,6	0.41	0
4	SO4	G	912	-	4,4,4	0.29	0	6,6,6	0.08	0
4	SO4	E	912	-	4,4,4	0.33	0	6,6,6	0.14	0
2	UDP	B	901	-	25,26,26	1.02	1 (4%)	38,40,40	1.82	7 (18%)
5	MLA	B	921	-	6,6,6	1.31	0	7,7,7	1.06	0
4	SO4	G	913	-	4,4,4	0.29	0	6,6,6	0.13	0
2	UDP	A	901	-	25,26,26	1.04	0	38,40,40	1.71	6 (15%)
5	MLA	H	921	-	6,6,6	1.14	0	7,7,7	1.32	0
3	FRU	G	902	-	11,12,12	0.70	0	10,18,18	0.76	0
4	SO4	C	912	-	4,4,4	0.27	0	6,6,6	0.15	0
3	FRU	E	902	-	11,12,12	0.73	0	10,18,18	0.84	0
3	FRU	D	902	-	11,12,12	0.91	0	10,18,18	1.19	2 (20%)
4	SO4	E	911	-	4,4,4	0.33	0	6,6,6	0.41	0
4	SO4	B	913	-	4,4,4	0.36	0	6,6,6	0.29	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
2	UDP	F	901	-	-	4/16/32/32	0/2/2/2
5	MLA	F	921	-	-	0/4/4/4	-
3	FRU	A	902	-	-	2/5/24/24	0/1/1/1
2	UDP	C	901	-	-	6/16/32/32	0/2/2/2
2	UDP	E	901	-	-	5/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLA	E	921	-	-	0/4/4/4	-
3	FRU	C	902	-	-	2/5/24/24	0/1/1/1
2	UDP	G	901	-	-	7/16/32/32	0/2/2/2
5	MLA	A	921	-	-	2/4/4/4	-
2	UDP	H	901	-	-	6/16/32/32	0/2/2/2
5	MLA	G	921	-	-	0/4/4/4	-
3	FRU	H	902	-	-	5/5/24/24	0/1/1/1
3	FRU	B	902	-	-	2/5/24/24	0/1/1/1
5	MLA	D	921	-	-	2/4/4/4	-
5	MLA	C	921	-	-	2/4/4/4	-
3	FRU	F	902	-	-	5/5/24/24	0/1/1/1
2	UDP	D	901	-	-	3/16/32/32	0/2/2/2
2	UDP	B	901	-	-	5/16/32/32	0/2/2/2
5	MLA	B	921	-	-	0/4/4/4	-
5	MLA	H	921	-	-	0/4/4/4	-
2	UDP	A	901	-	-	3/16/32/32	0/2/2/2
3	FRU	G	902	-	-	3/5/24/24	0/1/1/1
3	FRU	E	902	-	-	1/5/24/24	0/1/1/1
3	FRU	D	902	-	-	5/5/24/24	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	UDP	PA-O3A	2.90	1.62	1.59
2	B	901	UDP	PA-O3A	2.59	1.62	1.59
3	B	902	FRU	O2-C2	2.35	1.44	1.40
3	H	902	FRU	O2-C2	2.24	1.44	1.40
2	F	901	UDP	PA-O3A	2.11	1.61	1.59

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	UDP	C4-N3-C2	-7.01	117.90	126.61
2	F	901	UDP	C4-N3-C2	-6.77	118.20	126.61
2	D	901	UDP	C4-N3-C2	-6.74	118.25	126.61
2	H	901	UDP	C4-N3-C2	-6.47	118.58	126.61
2	A	901	UDP	C4-N3-C2	-6.41	118.65	126.61

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	UDP	PA-O3A-PB-O3B
2	C	901	UDP	PA-O3A-PB-O3B
2	F	901	UDP	PA-O3A-PB-O2B
2	G	901	UDP	C5'-O5'-PA-O1A
2	H	901	UDP	PA-O3A-PB-O3B

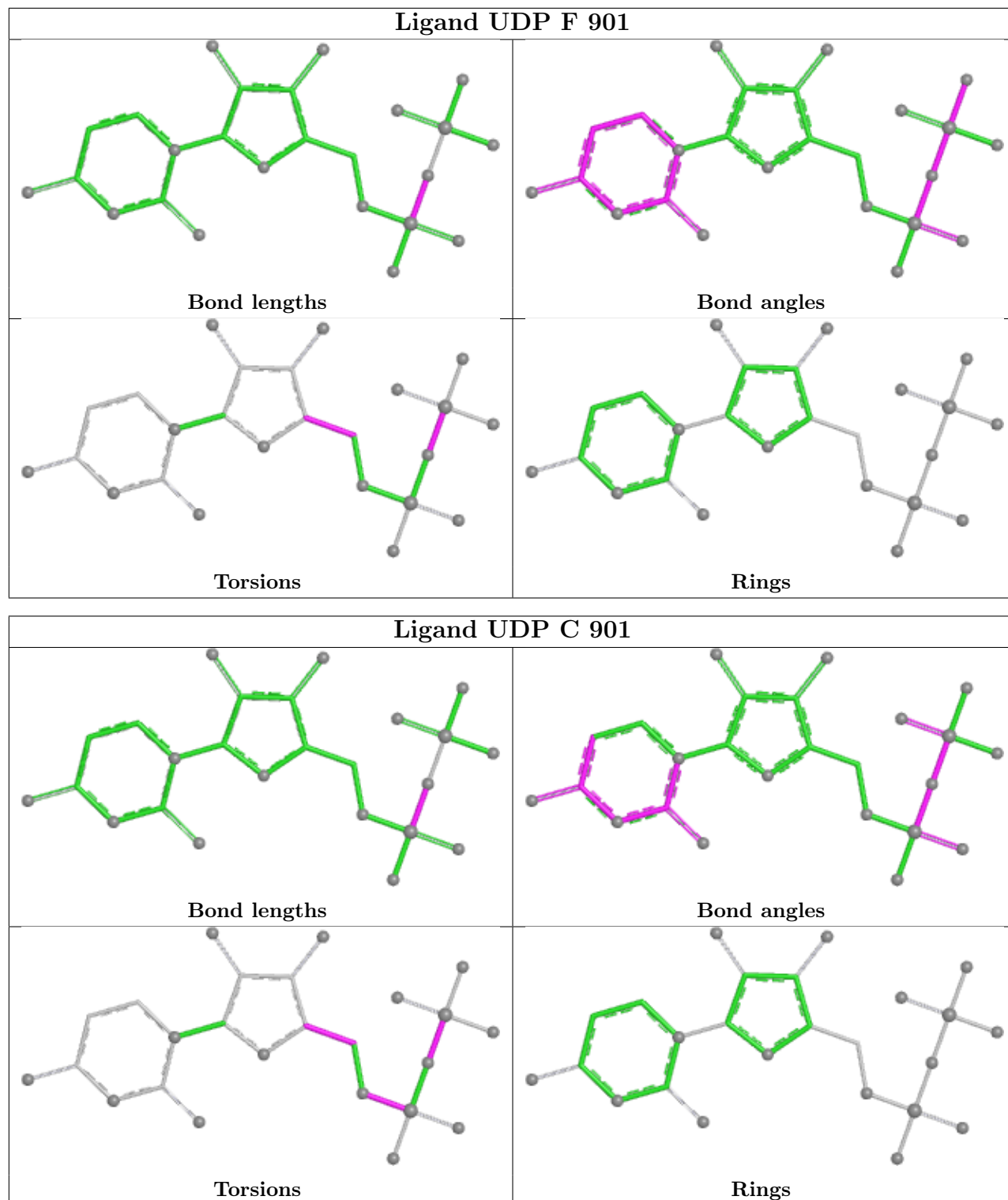
There are no ring outliers.

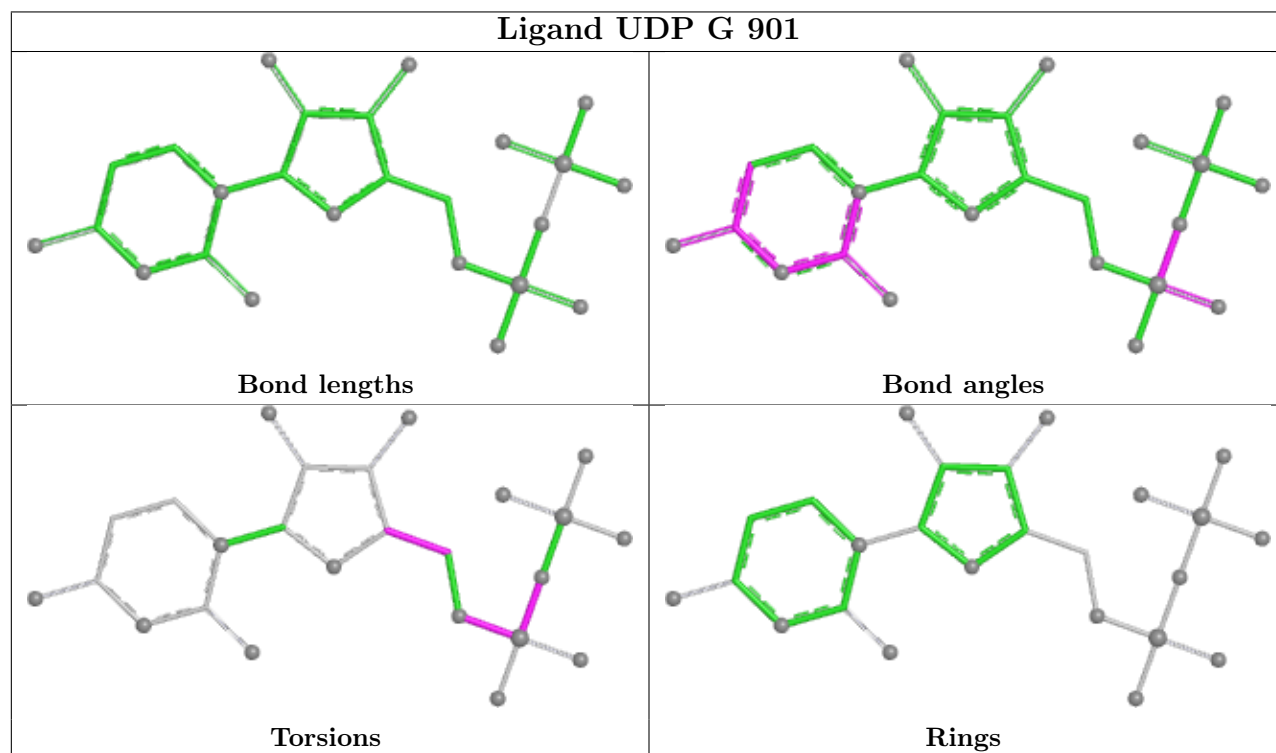
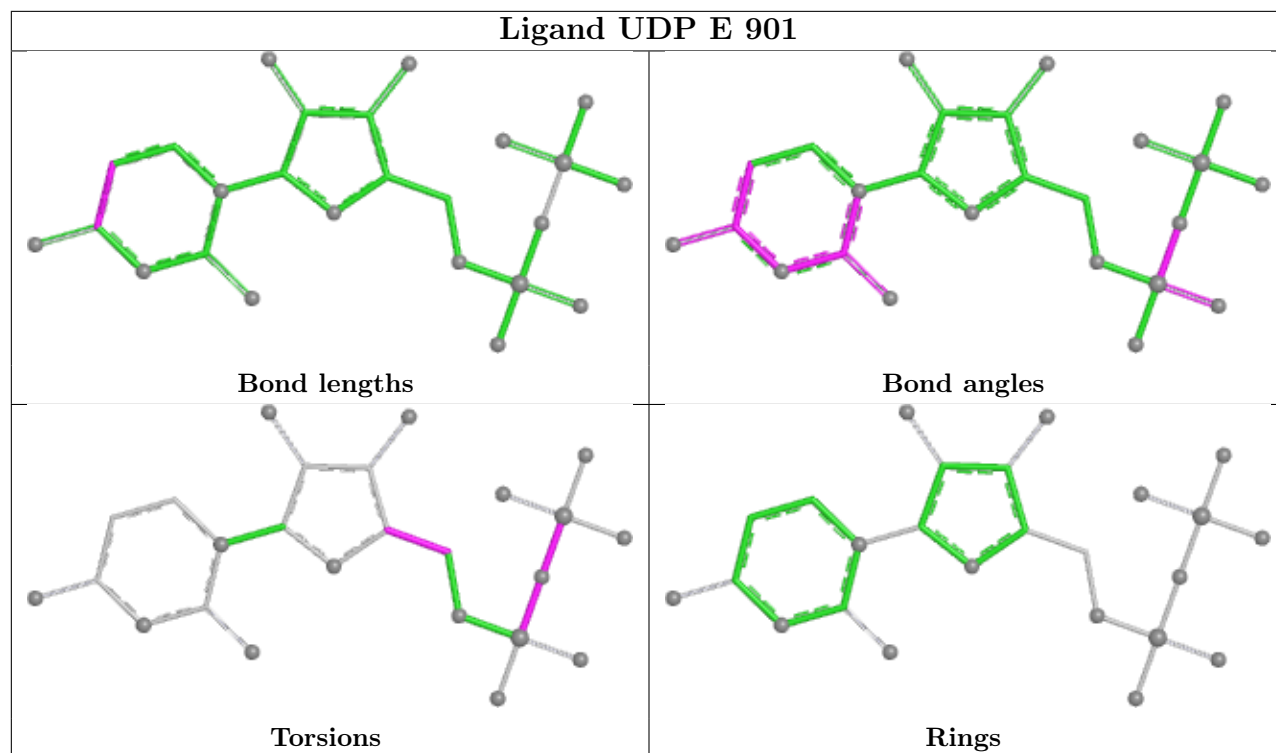
20 monomers are involved in 33 short contacts:

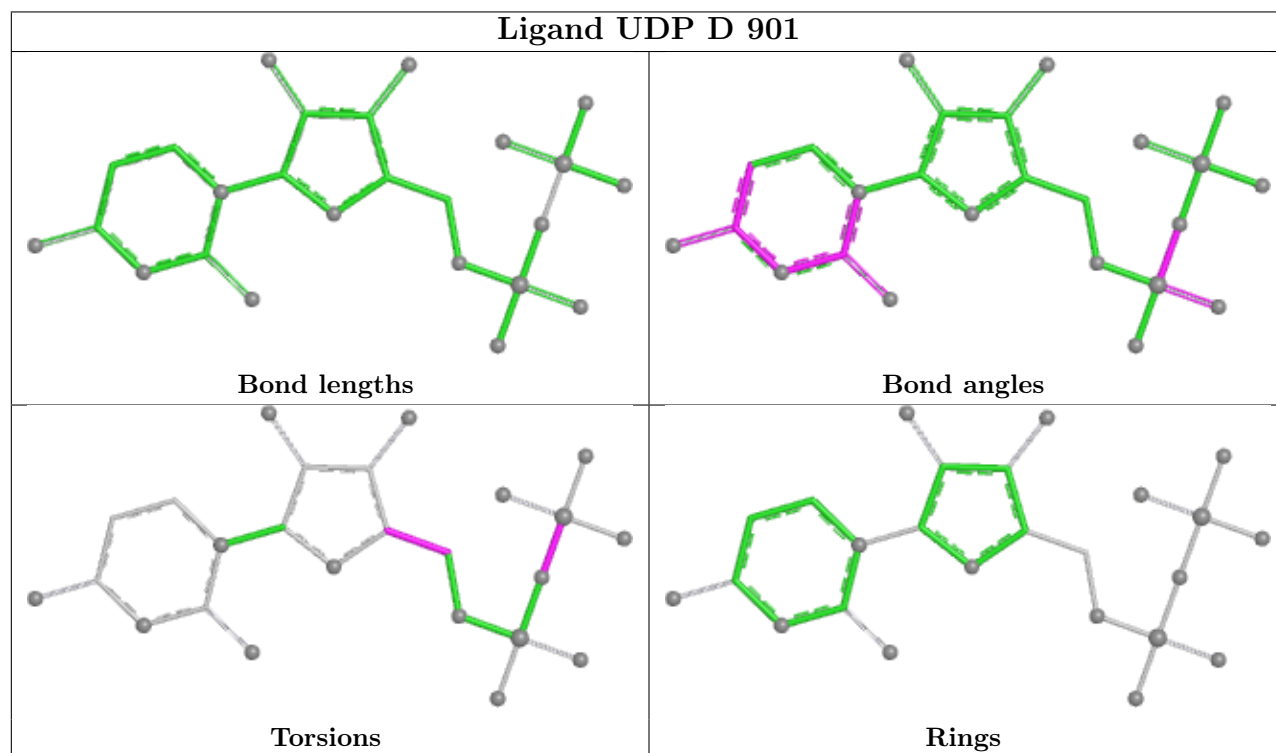
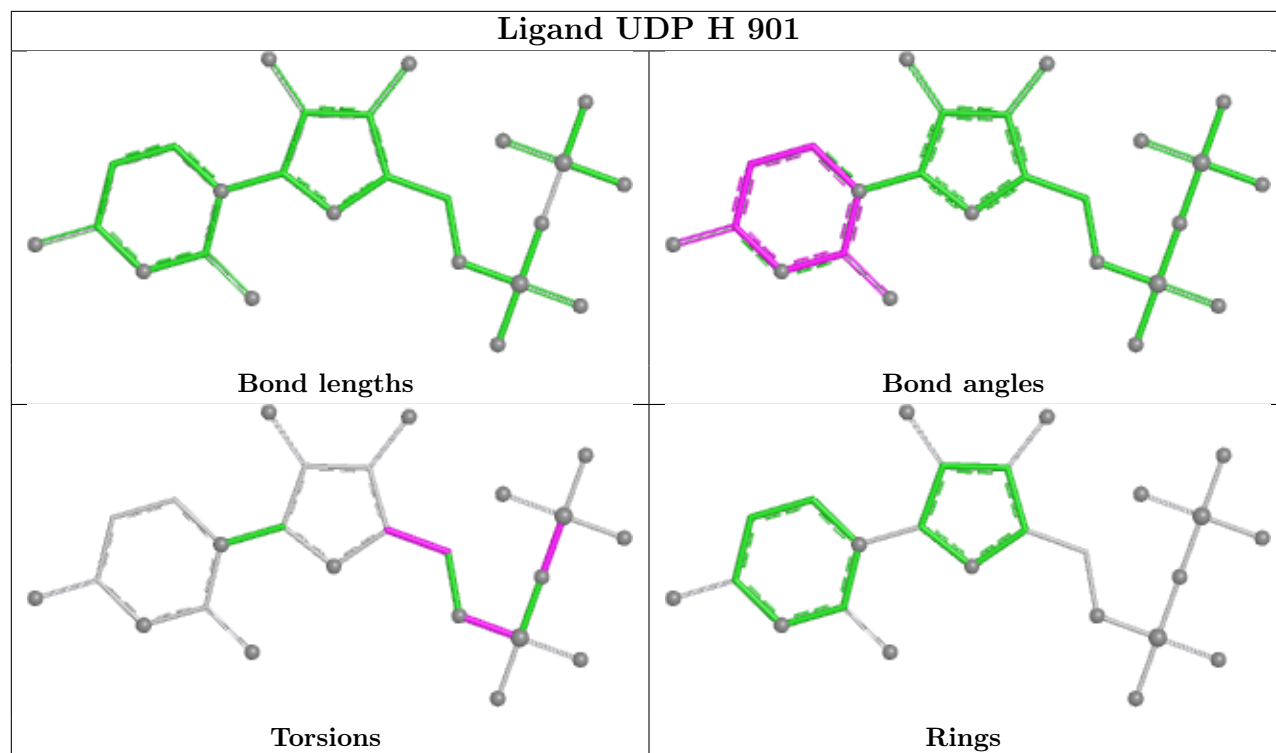
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	901	UDP	1	0
4	A	913	SO4	1	0
3	A	902	FRU	1	0
2	C	901	UDP	1	0
2	E	901	UDP	4	0
5	E	921	MLA	5	0
3	C	902	FRU	1	0
4	B	912	SO4	1	0
2	G	901	UDP	1	0
3	H	902	FRU	1	0
4	F	913	SO4	2	0
3	F	902	FRU	1	0
2	D	901	UDP	2	0
4	H	913	SO4	1	0
4	E	912	SO4	1	0
5	B	921	MLA	1	0
4	G	913	SO4	1	0
3	G	902	FRU	4	0
3	E	902	FRU	1	0
4	B	913	SO4	2	0

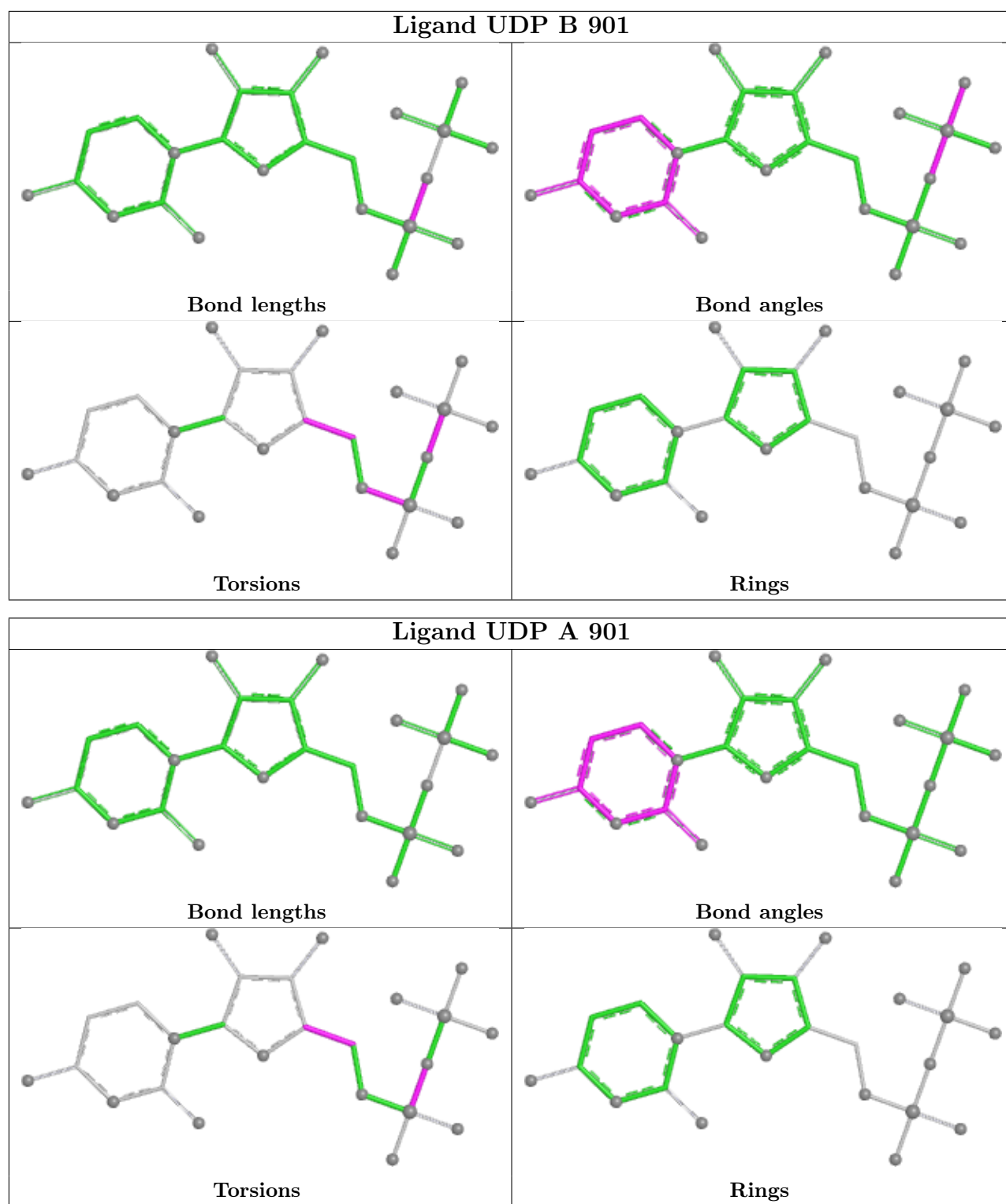
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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, 95th 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 ²)	Q<0.9
1	A	769/816 (94%)	-0.19	43 (5%) 30 23	13, 27, 90, 116	0
1	B	781/816 (95%)	0.15	84 (10%) 11 9	16, 33, 98, 131	0
1	C	769/816 (94%)	-0.05	28 (3%) 46 37	20, 38, 83, 122	0
1	D	769/816 (94%)	-0.21	35 (4%) 37 29	14, 28, 80, 111	0
1	E	769/816 (94%)	-0.13	43 (5%) 30 23	14, 30, 95, 118	0
1	F	769/816 (94%)	-0.22	31 (4%) 42 33	10, 26, 73, 111	0
1	G	769/816 (94%)	-0.24	21 (2%) 56 46	14, 30, 70, 108	0
1	H	785/816 (96%)	0.11	83 (10%) 11 9	17, 35, 92, 117	0
All	All	6180/6528 (94%)	-0.10	368 (5%) 27 21	10, 31, 87, 131	0

The worst 5 of 368 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	VAL	7.0
1	B	86	VAL	6.7
1	H	23	VAL	6.5
1	H	103	ASN	6.3
1	H	86	VAL	6.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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, 95th 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 ²)	Q<0.9
6	K	F	931	1/1	0.78	0.11	69,69,69,69	0
4	SO4	C	913	5/5	0.80	0.24	63,74,75,89	0
4	SO4	C	912	5/5	0.81	0.26	71,74,96,104	0
4	SO4	B	913	5/5	0.83	0.28	53,54,65,78	0
4	SO4	H	913	5/5	0.83	0.33	64,70,86,101	0
4	SO4	B	912	5/5	0.83	0.24	49,67,79,88	0
4	SO4	H	912	5/5	0.85	0.25	63,66,76,94	0
6	K	E	931	1/1	0.86	0.11	64,64,64,64	0
5	MLA	G	921	7/7	0.86	0.14	46,49,59,59	0
5	MLA	C	921	7/7	0.87	0.19	56,60,68,77	0
6	K	C	931	1/1	0.88	0.10	69,69,69,69	0
4	SO4	D	912	5/5	0.88	0.20	54,74,96,98	0
4	SO4	E	912	5/5	0.88	0.23	47,55,63,84	0
4	SO4	G	913	5/5	0.89	0.16	52,58,68,74	0
4	SO4	G	912	5/5	0.89	0.24	48,67,72,86	0
6	K	B	931	1/1	0.90	0.09	74,74,74,74	0
3	FRU	C	902	12/12	0.90	0.18	30,36,44,50	0
4	SO4	F	911	5/5	0.91	0.21	32,36,45,64	0
4	SO4	F	912	5/5	0.91	0.16	46,50,62,76	0
4	SO4	A	912	5/5	0.92	0.15	47,55,59,81	0
5	MLA	H	921	7/7	0.92	0.17	53,58,69,69	0
3	FRU	H	902	12/12	0.92	0.12	22,29,34,37	0
5	MLA	D	921	7/7	0.92	0.18	33,40,44,47	0
5	MLA	E	921	7/7	0.92	0.17	34,38,43,43	0
5	MLA	F	921	7/7	0.92	0.13	30,35,36,36	0
4	SO4	E	911	5/5	0.93	0.17	31,35,59,60	0
6	K	A	931	1/1	0.93	0.08	61,61,61,61	0
4	SO4	B	911	5/5	0.93	0.15	37,42,50,70	0
3	FRU	B	902	12/12	0.93	0.12	25,30,35,35	0
3	FRU	D	902	12/12	0.93	0.10	18,25,31,32	0
5	MLA	A	921	7/7	0.93	0.12	27,31,34,36	0
4	SO4	A	913	5/5	0.94	0.20	42,44,52,59	0
3	FRU	E	902	12/12	0.94	0.10	18,25,30,32	0
4	SO4	F	913	5/5	0.94	0.20	40,44,61,64	0
4	SO4	D	911	5/5	0.94	0.17	38,41,56,67	0
4	SO4	A	911	5/5	0.94	0.20	31,35,46,58	0
4	SO4	D	913	5/5	0.94	0.16	44,46,53,63	0

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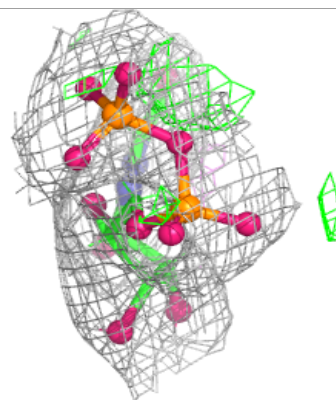
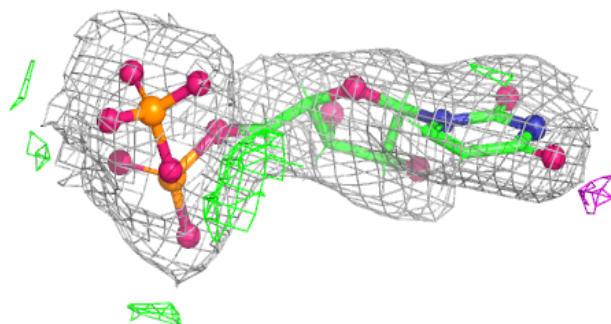
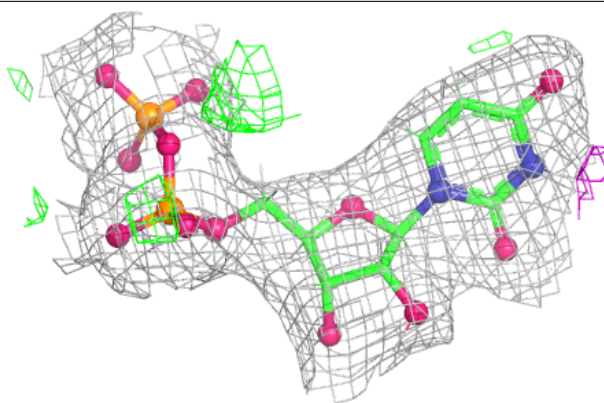
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FRU	G	902	12/12	0.94	0.11	18,25,34,34	0
4	SO4	C	911	5/5	0.94	0.16	44,46,57,63	0
6	K	D	931	1/1	0.94	0.10	61,61,61,61	0
5	MLA	B	921	7/7	0.94	0.12	38,45,50,53	0
4	SO4	E	913	5/5	0.94	0.20	44,47,62,71	0
4	SO4	G	911	5/5	0.95	0.20	32,40,56,64	0
4	SO4	H	911	5/5	0.95	0.16	37,38,69,70	0
6	K	H	931	1/1	0.95	0.07	61,61,61,61	0
3	FRU	F	902	12/12	0.96	0.12	17,22,28,35	0
6	K	G	931	1/1	0.96	0.08	57,57,57,57	0
3	FRU	A	902	12/12	0.96	0.10	16,22,27,28	0
2	UDP	B	901	25/25	0.98	0.06	19,25,30,34	0
2	UDP	C	901	25/25	0.98	0.05	21,31,40,42	0
2	UDP	F	901	25/25	0.98	0.05	14,18,23,25	0
2	UDP	H	901	25/25	0.98	0.06	22,28,36,38	0
2	UDP	E	901	25/25	0.99	0.04	17,21,27,29	0
2	UDP	A	901	25/25	0.99	0.04	14,17,21,24	0
2	UDP	G	901	25/25	0.99	0.05	14,21,25,35	0
2	UDP	D	901	25/25	0.99	0.04	17,21,25,30	0

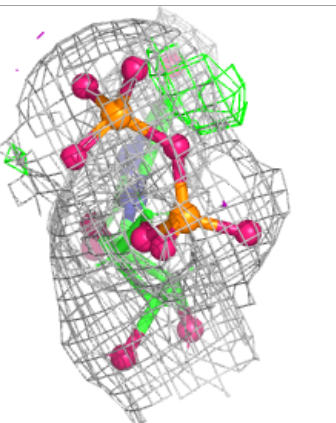
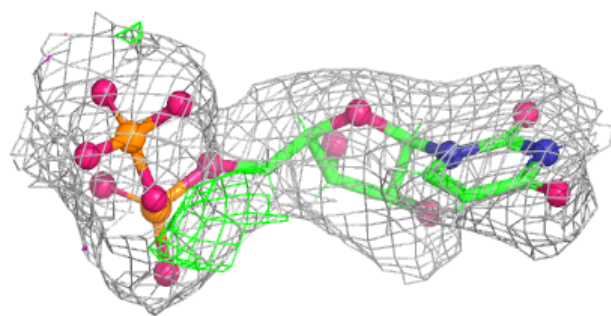
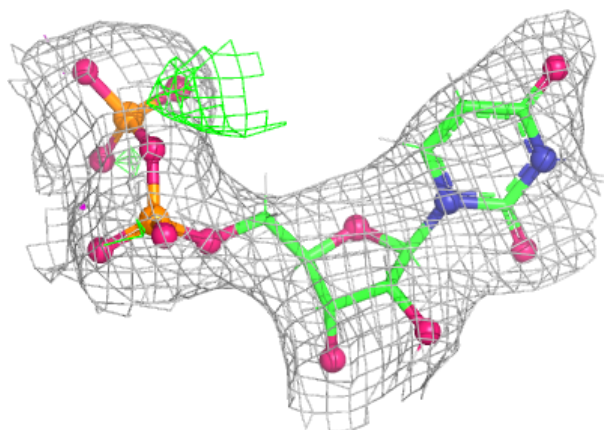
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDP B 901:

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

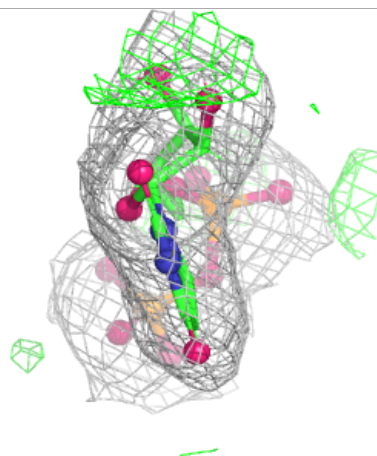
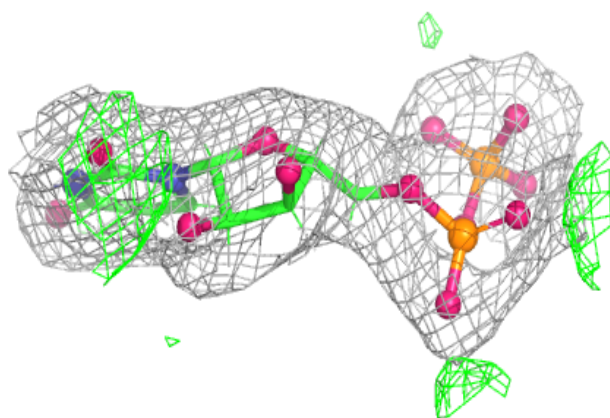
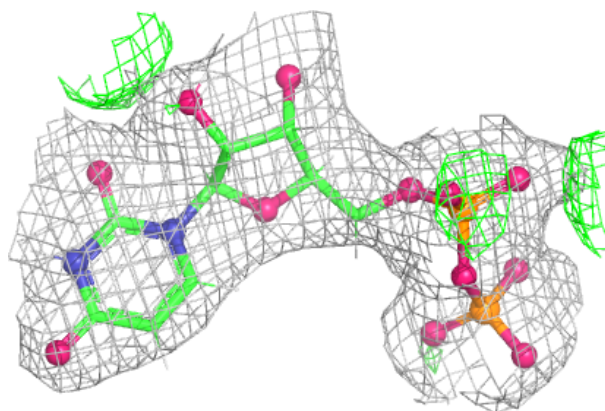
**Electron density around UDP C 901:**

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



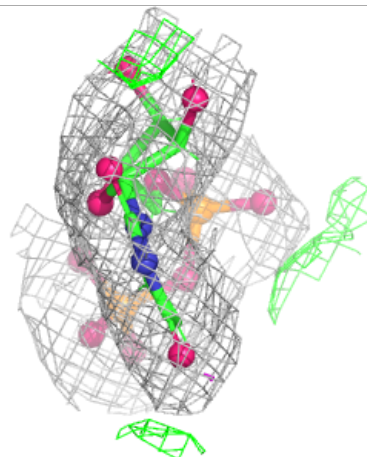
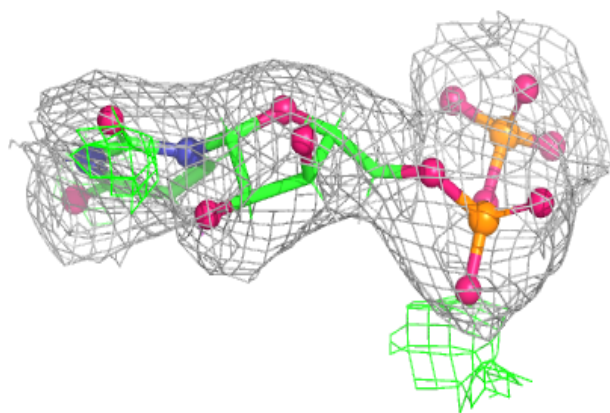
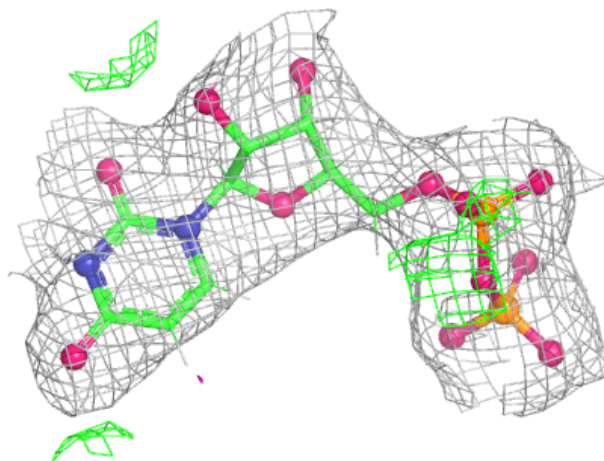
Electron density around UDP F 901:

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



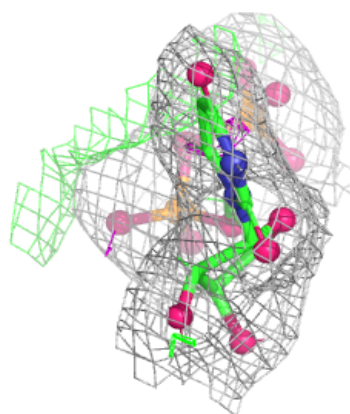
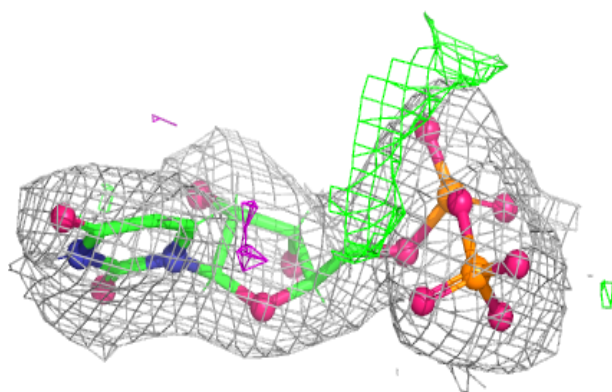
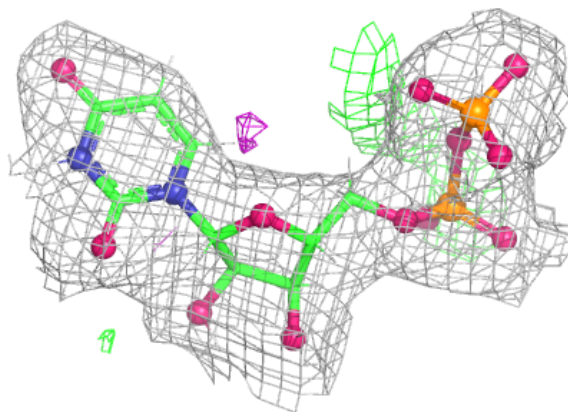
Electron density around UDP H 901:

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



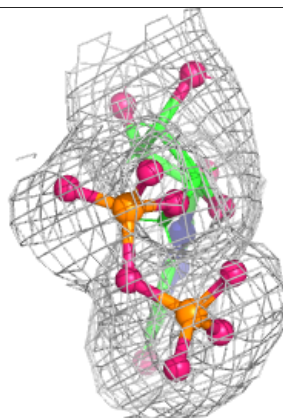
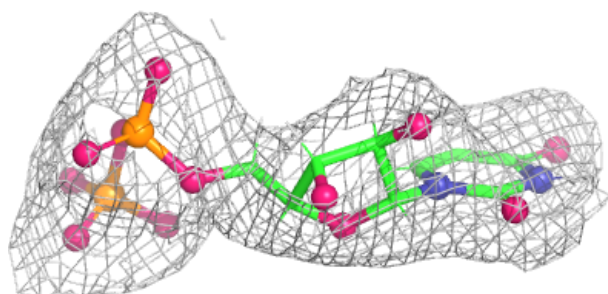
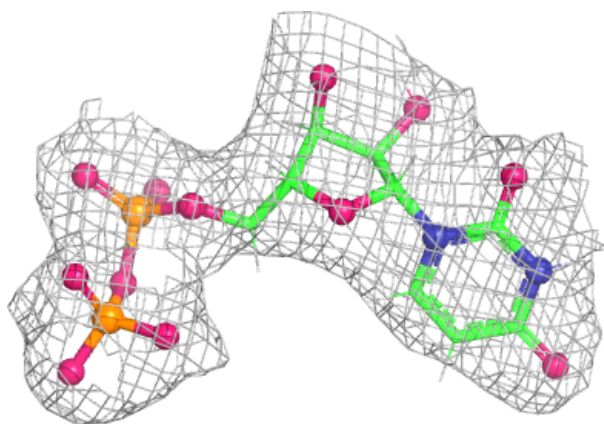
Electron density around UDP E 901:

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



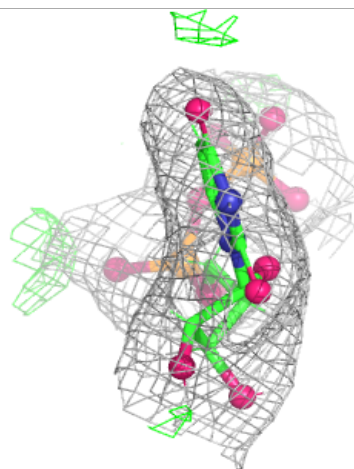
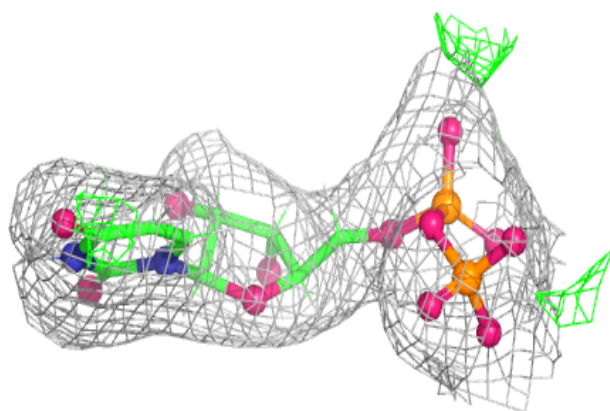
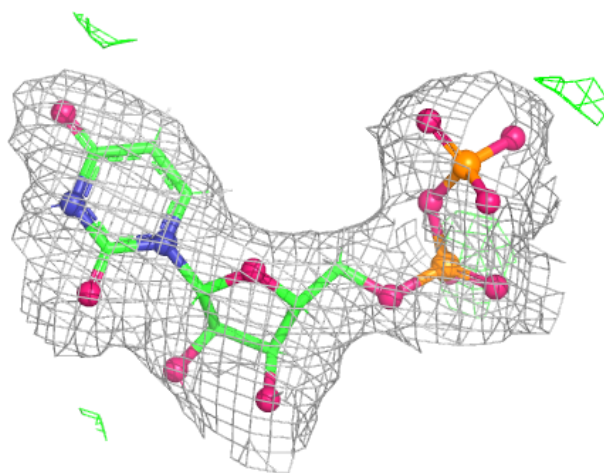
Electron density around UDP A 901:

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



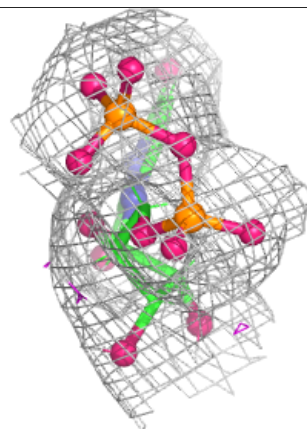
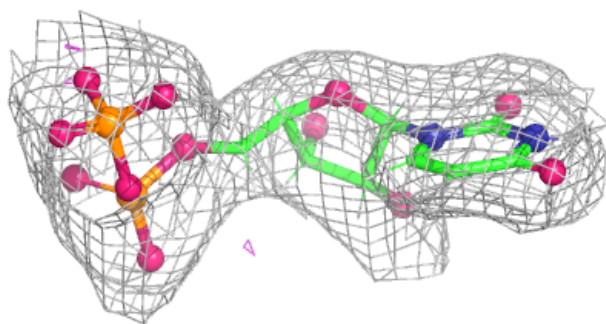
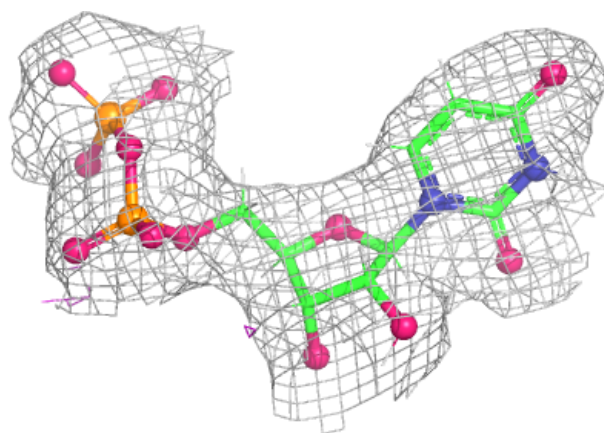
Electron density around UDP G 901:

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



Electron density around UDP D 901:

$2mF_o-DF_c$ (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.