



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 04:38 PM UTC

PDB ID : 3S28 / pdb_00003s28
Title : The crystal structure of sucrose synthase-1 in complex with a breakdown product of the UDP-glucose
Authors : Zheng, Y.; Garavito, R.M.
Deposited on : 2011-05-16
Resolution : 2.80 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

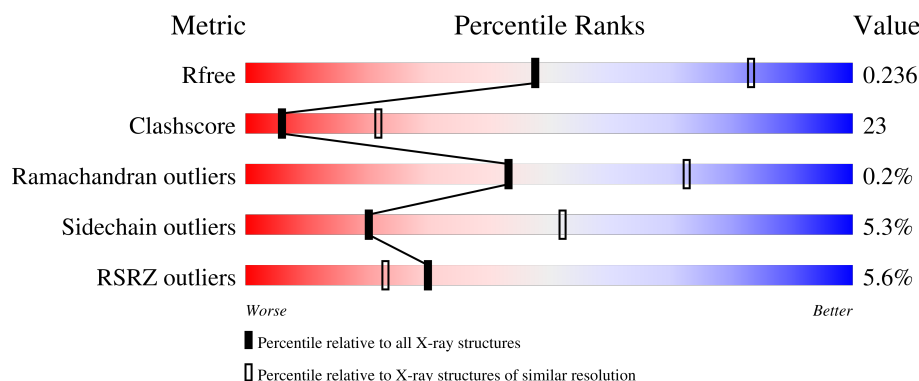
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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% 62% 31% • •
1	B	816	9% 61% 32% • •
1	C	816	4% 57% 35% • •
1	D	816	4% 64% 29% • •
1	E	816	5% 65% 27% • •

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Mol	Chain	Length	Quality of chain
1	F	816	
1	G	816	
1	H	816	

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	NHF	D	904[B]	-	-	X	-
5	SO4	A	912	-	-	X	-
5	SO4	B	913	-	-	X	-
5	SO4	D	913	-	-	X	-
5	SO4	F	912	-	-	X	-
5	SO4	F	913	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 51388 atoms, of which 264 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	0	0	0
			6289	4039	1069	1159	22			
1	B	780	Total	C	N	O	S	0	0	0
			6158	3949	1050	1137	22			
1	C	781	Total	C	N	O	S	0	0	0
			6290	4045	1066	1157	22			
1	D	781	Total	C	N	O	S	0	0	0
			6280	4035	1062	1161	22			
1	E	781	Total	C	N	O	S	0	0	0
			6271	4028	1062	1159	22			
1	F	781	Total	C	N	O	S	0	0	0
			6292	4042	1070	1158	22			
1	G	781	Total	C	N	O	S	0	0	0
			6299	4045	1070	1162	22			
1	H	780	Total	C	N	O	S	0	0	0
			6243	4007	1063	1151	22			

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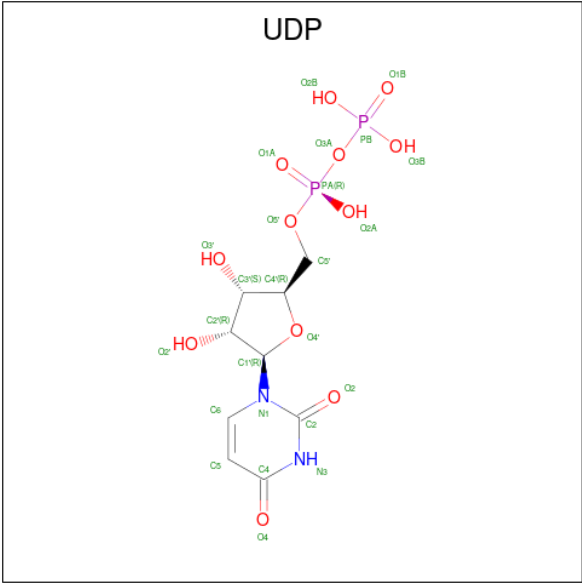
Chain	Residue	Modelled	Actual	Comment	Reference
B	814	HIS	-	expression tag	UNP P49040
B	815	HIS	-	expression tag	UNP P49040
B	816	HIS	-	expression tag	UNP P49040
C	809	VAL	-	expression tag	UNP P49040
C	810	GLU	-	expression tag	UNP P49040
C	811	HIS	-	expression tag	UNP P49040
C	812	HIS	-	expression tag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



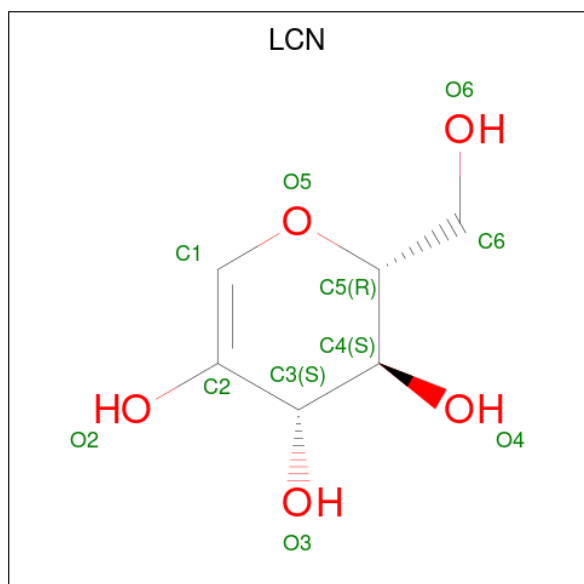
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	B	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	C	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	D	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	E	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	F	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	G	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		

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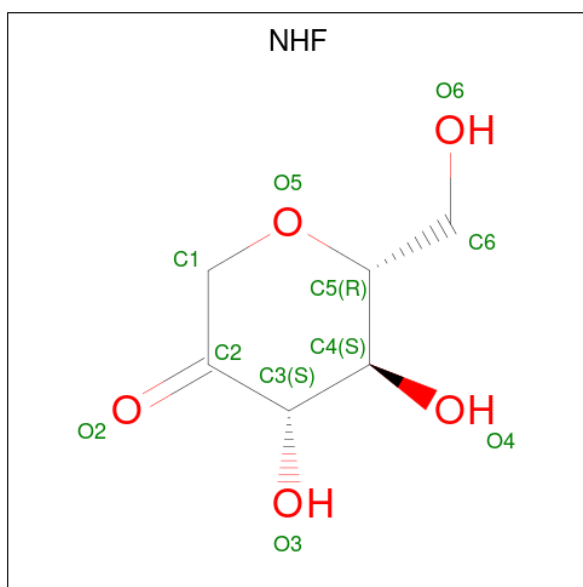
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	H	N	O	P	
			36	9	11	2	12	2	
								0	0

- Molecule 3 is 1,5-anhydro-D-arabino-hex-1-enitol (CCD ID: LCN) (formula: $C_6H_{10}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O		
			21	6	10	5	0	1
3	B	1	Total	C	H	O		
			21	6	10	5	0	1
3	C	1	Total	C	H	O		
			21	6	10	5	0	1
3	D	1	Total	C	H	O		
			21	6	10	5	0	1
3	E	1	Total	C	H	O		
			21	6	10	5	0	1
3	F	1	Total	C	H	O		
			21	6	10	5	0	1
3	G	1	Total	C	H	O		
			21	6	10	5	0	1
3	H	1	Total	C	H	O		
			21	6	10	5	0	1

- Molecule 4 is 1,5-anhydro-D-fructose (CCD ID: NHF) (formula: $C_6H_{10}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	1
			21	6	10	5		
4	B	1	Total	C	H	O	0	1
			21	6	10	5		
4	C	1	Total	C	H	O	0	1
			21	6	10	5		
4	D	1	Total	C	H	O	0	1
			21	6	10	5		
4	E	1	Total	C	H	O	0	1
			21	6	10	5		
4	F	1	Total	C	H	O	0	1
			21	6	10	5		
4	G	1	Total	C	H	O	0	1
			21	6	10	5		
4	H	1	Total	C	H	O	0	1
			21	6	10	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



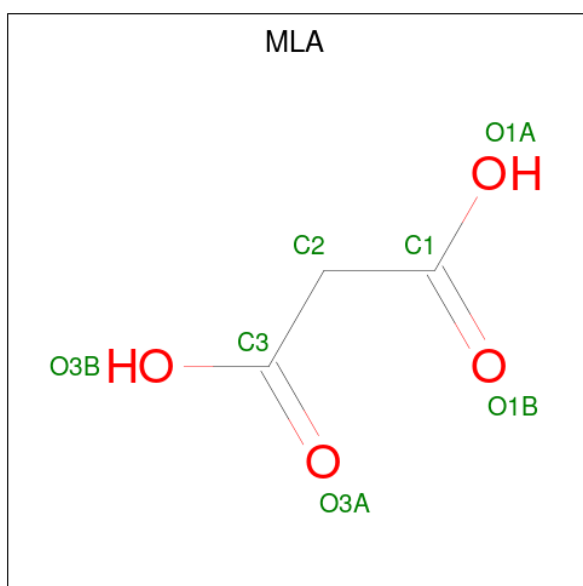
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total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

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

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



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

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

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 8 is water.

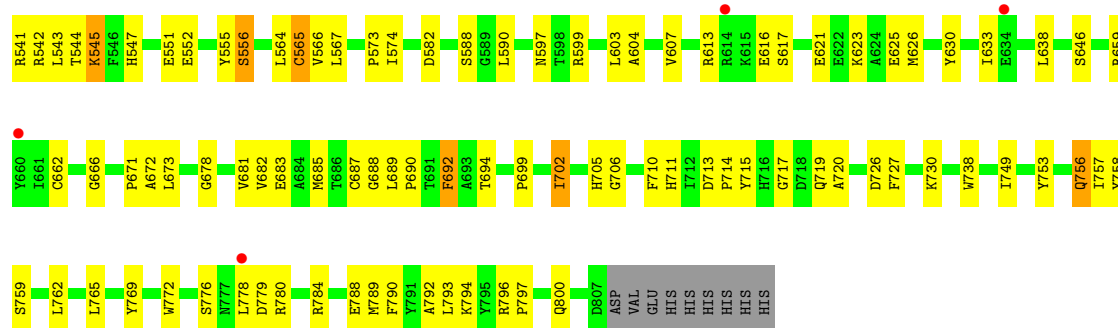
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	69	Total	O	0	0
			69	69		
8	B	55	Total	O	0	0
			55	55		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	24	Total 24	O 24	0	0
8	D	54	Total 54	O 54	0	0
8	E	50	Total 50	O 50	0	0
8	F	79	Total 79	O 79	0	0
8	G	62	Total 62	O 62	0	0
8	H	49	Total 49	O 49	0	0

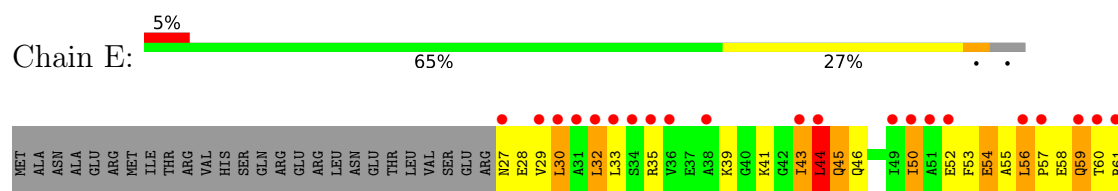


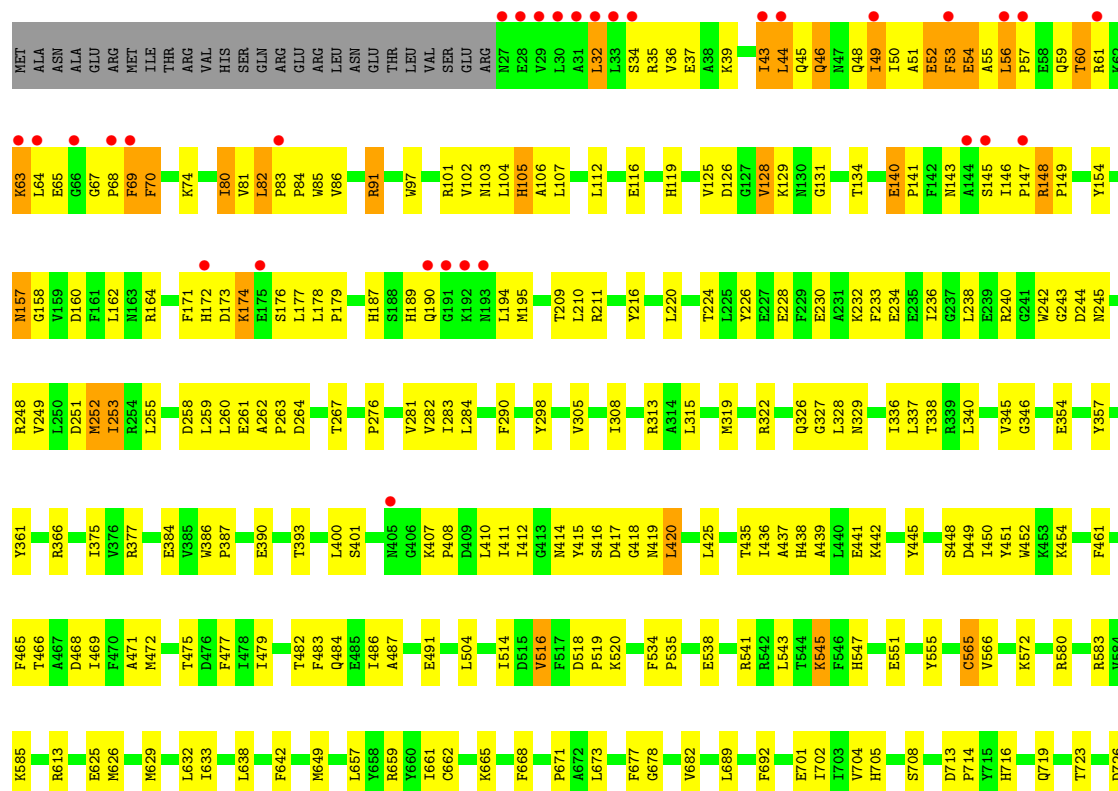


● Molecule 1: Sucrose synthase 1



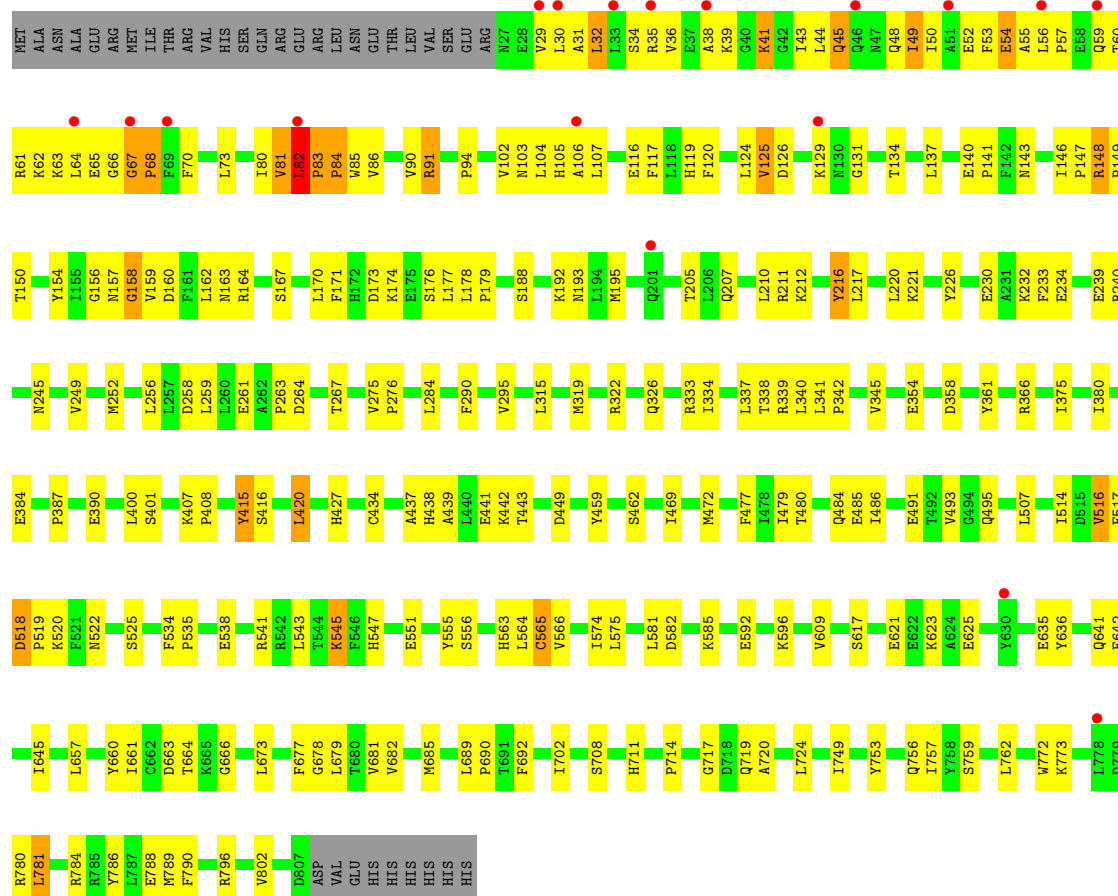
● Molecule 1: Sucrose synthase 1



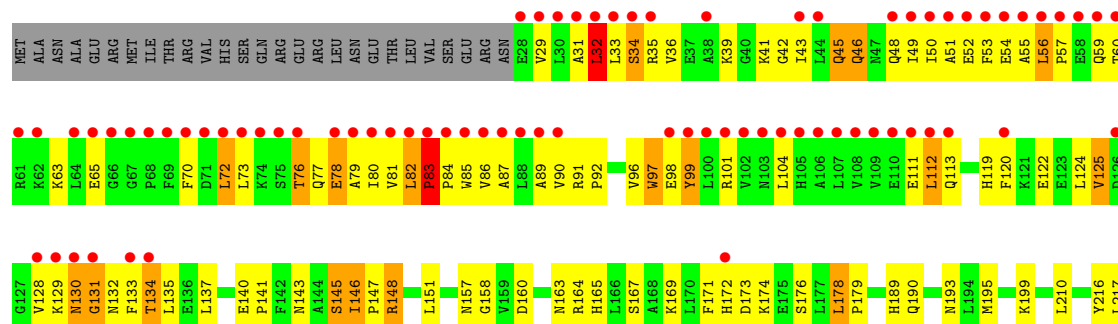




• Molecule 1: Sucrose synthase 1



• Molecule 1: Sucrose synthase 1



HIS	S708	H563	E441	I334	L220
	D713	L564	D447	L337	K221
	P714	V566	I450	T338	L224
	Q719	L567	D456	R339	L225
	D722	K572	P573	L340	E228
	K743	P578	Y459	L341	K232
	R748	A579	D468	P342	F233
	I749	D582	M472	T348	E234
	E750	L590	R352	E351	E239
	K752	L603	L353	L353	W242
	I757	A604	R354	E354	G243
	Y758	I605	V356	V357	V249
	S759	I606	D358	Y361	L250
	L762	R613	I479	L365	D251
	L763	E616	F483	R366	I253
	G770	E621	Q484	L375	R254
	F771	M626	E491	I375	L259
	K773	Y630	I492	I380	L260
	S776	I639	V493	W386	E261
	N777	G640	Q495	P387	A262
	L778	M649	G506	E390	P263
	D779	D650	I514	L400	L268
	L781	R651	V516	S401	F271
	R784	I654	F517	L404	V275
	E788	R659	D518	K407	P276
	M789	C662	P519	P408	M277
	F790	F668	K520	N414	V278
	L793	V669	F534	Y415	F279
	K794	P671	P535	S416	F290
	R796	F677	E538	D417	A291
	P797	G678	R541	G418	Q292
	Q800	L679	L543	N419	D293
	D807	C687	T544	L420	V295
	ASP	C688	K545	L425	G303
	VAL	L689	F546	L425	L315
	GLU	P690	H547	Q433	M319
	HIS	T691	E552	C434	R322
	HIS	F692	S556	T435	Q326
	HIS	K696	K561	T436	I330
	HIS		E562	A437	
				H438	
				A439	
				L440	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.75Å 261.88Å 160.19Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	24.98 – 2.80 24.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.98-2.80) 99.6 (24.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.188 , 0.236 0.188 , 0.236	Depositor DCC
R_{free} test set	13263 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51388	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 27.65 % 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 2.1188e-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: SO4, LCN, NHF, MLA, UDP, K

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	0.47	0/6436	0.86	9/8714 (0.1%)
1	B	0.45	0/6304	0.92	13/8549 (0.2%)
1	C	0.41	0/6437	0.86	16/8718 (0.2%)
1	D	0.45	0/6427	0.89	18/8707 (0.2%)
1	E	0.44	0/6417	0.94	18/8693 (0.2%)
1	F	0.48	0/6439	0.91	16/8719 (0.2%)
1	G	0.46	0/6446	0.92	22/8728 (0.3%)
1	H	0.45	0/6390	0.90	17/8655 (0.2%)
All	All	0.45	0/51296	0.90	129/69483 (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	B	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	3
All	All	0	8

There are no bond length outliers.

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	83	PRO	CA-C-N	14.72	134.24	119.82
1	E	83	PRO	C-N-CA	14.72	134.24	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	82	LEU	CA-C-N	11.82	132.56	120.38
1	E	82	LEU	C-N-CA	11.82	132.56	120.38
1	G	82	LEU	CA-C-N	11.46	132.19	120.38

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	B	71	ASP	Peptide
1	E	81	VAL	Peptide
1	F	82	LEU	Peptide
1	G	81	VAL	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	6289	0	6220	296	0
1	B	6158	0	5959	306	0
1	C	6290	0	6242	330	0
1	D	6280	0	6206	285	0
1	E	6271	0	6194	276	0
1	F	6292	0	6234	302	0
1	G	6299	0	6240	274	0
1	H	6243	0	6130	327	0
2	A	25	11	11	3	0
2	B	25	11	11	1	0
2	C	25	11	11	1	0
2	D	25	11	11	4	0
2	E	25	11	11	1	0
2	F	25	11	11	1	0
2	G	25	11	11	4	0
2	H	25	11	11	4	0
3	A	11	10	10	1	0
3	B	11	10	10	0	0
3	C	11	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11	10	10	1	0
3	E	11	10	10	0	0
3	F	11	10	10	1	0
3	G	11	10	10	1	0
3	H	11	10	10	0	0
4	A	11	10	10	2	0
4	B	11	10	10	2	0
4	C	11	10	10	1	0
4	D	11	10	10	6	0
4	E	11	10	10	2	0
4	F	11	10	10	0	0
4	G	11	10	10	1	0
4	H	11	10	10	4	0
5	A	15	0	0	3	0
5	B	15	0	0	5	0
5	C	15	0	0	1	0
5	D	15	0	0	2	0
5	E	15	0	0	1	0
5	F	15	0	0	5	0
5	G	15	0	0	2	0
5	H	15	0	0	1	0
6	A	7	2	2	0	0
6	B	7	2	2	0	0
6	C	7	2	2	0	0
6	D	7	2	2	0	0
6	E	7	2	2	1	0
6	F	7	2	2	1	0
6	G	7	2	2	0	0
6	H	7	2	2	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	A	69	0	0	0	0
8	B	55	0	0	2	0
8	C	24	0	0	0	0
8	D	54	0	0	1	0
8	E	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	79	0	0	2	0
8	G	62	0	0	1	0
8	H	49	0	0	1	0
All	All	51124	264	49689	2283	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 23.

The worst 5 of 2283 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:B:46:GLN:HG2	1:B:50:ILE:CB	1.66	1.25
1:G:66:GLY:C	1:G:68:PRO:HD3	1.60	1.24
1:E:789:MET:HB3	1:H:789:MET:CE	1.68	1.22
1:F:789:MET:CE	1:G:789:MET:HB3	1.71	1.21
1:H:82:LEU:HB2	1:H:83:PRO:HD2	1.20	1.19

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%)	741 (95%)	37 (5%)	1 (0%)	48 77
1	B	778/816 (95%)	724 (93%)	52 (7%)	2 (0%)	36 66
1	C	779/816 (96%)	739 (95%)	40 (5%)	0	100 100
1	D	779/816 (96%)	741 (95%)	38 (5%)	0	100 100
1	E	779/816 (96%)	742 (95%)	35 (4%)	2 (0%)	36 66
1	F	779/816 (96%)	737 (95%)	39 (5%)	3 (0%)	30 60
1	G	779/816 (96%)	743 (95%)	36 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	778/816 (95%)	736 (95%)	40 (5%)	2 (0%)	36	66
All	All	6230/6528 (95%)	5903 (95%)	317 (5%)	10 (0%)	43	72

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	29	VAL
1	B	56	LEU
1	F	63	LYS
1	A	83	PRO
1	E	63	LYS

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	670/718 (93%)	636 (95%)	34 (5%)	21	54
1	B	635/718 (88%)	601 (95%)	34 (5%)	20	51
1	C	673/718 (94%)	641 (95%)	32 (5%)	23	56
1	D	671/718 (94%)	632 (94%)	39 (6%)	18	49
1	E	668/718 (93%)	634 (95%)	34 (5%)	21	54
1	F	672/718 (94%)	639 (95%)	33 (5%)	22	55
1	G	674/718 (94%)	642 (95%)	32 (5%)	23	57
1	H	658/718 (92%)	615 (94%)	43 (6%)	15	43
All	All	5321/5744 (93%)	5040 (95%)	281 (5%)	20	52

5 of 281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	556	SER
1	H	32	LEU
1	H	450	ILE
1	C	756	GLN

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Mol	Chain	Res	Type
1	C	646	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	119	HIS
1	G	105	HIS
1	F	190	GLN
1	F	711	HIS
1	G	165	HIS

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 64 ligands modelled in this entry, 8 are monoatomic - leaving 56 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	SO4	D	913	-	4,4,4	0.30	0	6,6,6	0.13	0
5	SO4	D	911	-	4,4,4	0.34	0	6,6,6	0.25	0
5	SO4	B	912	-	4,4,4	0.26	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MLA	C	921	-	6,6,6	1.25	0	7,7,7	1.41	1 (14%)
2	UDP	C	901	-	25,26,26	0.97	0	38,40,40	1.57	5 (13%)
6	MLA	G	921	-	6,6,6	1.20	0	7,7,7	1.26	0
5	SO4	D	912	-	4,4,4	0.26	0	6,6,6	0.23	0
6	MLA	F	921	-	6,6,6	1.12	0	7,7,7	1.51	1 (14%)
6	MLA	B	921	-	6,6,6	1.31	0	7,7,7	1.26	0
5	SO4	H	911	-	4,4,4	0.28	0	6,6,6	0.20	0
6	MLA	H	921	-	6,6,6	1.14	0	7,7,7	1.46	0
3	LCN	A	903[A]	-	11,11,11	2.08	2 (18%)	11,15,15	2.45	3 (27%)
4	NHF	C	904[B]	-	11,11,11	1.86	4 (36%)	11,15,15	0.70	0
2	UDP	D	901	-	25,26,26	1.04	0	38,40,40	1.94	8 (21%)
4	NHF	A	904[B]	-	11,11,11	1.70	4 (36%)	11,15,15	0.93	0
2	UDP	H	901	-	25,26,26	1.03	1 (4%)	38,40,40	1.82	6 (15%)
5	SO4	E	912	-	4,4,4	0.30	0	6,6,6	0.07	0
2	UDP	G	901	-	25,26,26	1.04	1 (4%)	38,40,40	1.52	6 (15%)
5	SO4	F	912	-	4,4,4	0.28	0	6,6,6	0.21	0
2	UDP	A	901	-	25,26,26	0.98	0	38,40,40	1.71	6 (15%)
4	NHF	F	904[B]	-	11,11,11	1.87	4 (36%)	11,15,15	0.74	0
5	SO4	C	913	-	4,4,4	0.30	0	6,6,6	0.06	0
6	MLA	E	921	-	6,6,6	1.33	0	7,7,7	0.95	0
3	LCN	D	903[A]	-	11,11,11	2.05	4 (36%)	11,15,15	2.32	3 (27%)
3	LCN	C	903[A]	-	11,11,11	2.08	3 (27%)	11,15,15	2.75	3 (27%)
3	LCN	B	903[A]	-	11,11,11	1.97	3 (27%)	11,15,15	2.79	2 (18%)
5	SO4	F	911	-	4,4,4	0.29	0	6,6,6	0.30	0
5	SO4	E	911	-	4,4,4	0.32	0	6,6,6	0.36	0
5	SO4	A	913	-	4,4,4	0.33	0	6,6,6	0.10	0
5	SO4	A	911	-	4,4,4	0.30	0	6,6,6	0.26	0
6	MLA	D	921	-	6,6,6	1.31	0	7,7,7	1.12	0
5	SO4	G	913	-	4,4,4	0.27	0	6,6,6	0.16	0
4	NHF	D	904[B]	-	11,11,11	1.80	4 (36%)	11,15,15	1.66	1 (9%)
5	SO4	F	913	-	4,4,4	0.31	0	6,6,6	0.17	0
5	SO4	H	912	-	4,4,4	0.33	0	6,6,6	0.06	0
5	SO4	E	913	-	4,4,4	0.30	0	6,6,6	0.13	0
3	LCN	F	903[A]	-	11,11,11	2.01	3 (27%)	11,15,15	2.93	3 (27%)
4	NHF	B	904[B]	-	11,11,11	1.90	5 (45%)	11,15,15	1.01	1 (9%)
5	SO4	G	912	-	4,4,4	0.30	0	6,6,6	0.16	0
4	NHF	G	904[B]	-	11,11,11	1.87	4 (36%)	11,15,15	0.62	0
5	SO4	G	911	-	4,4,4	0.36	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UDP	E	901	-	25,26,26	0.99	1 (4%)	38,40,40	1.67	7 (18%)
3	LCN	E	903[A]	-	11,11,11	1.98	1 (9%)	11,15,15	2.91	2 (18%)
5	SO4	A	912	-	4,4,4	0.29	0	6,6,6	0.20	0
2	UDP	B	901	-	25,26,26	0.99	1 (4%)	38,40,40	1.87	7 (18%)
4	NHF	E	904[B]	-	11,11,11	1.82	3 (27%)	11,15,15	0.68	0
2	UDP	F	901	-	25,26,26	1.03	1 (4%)	38,40,40	1.69	6 (15%)
5	SO4	H	913	-	4,4,4	0.32	0	6,6,6	0.10	0
6	MLA	A	921	-	6,6,6	1.15	0	7,7,7	1.32	0
3	LCN	H	903[A]	-	11,11,11	2.01	3 (27%)	11,15,15	2.53	2 (18%)
5	SO4	B	913	-	4,4,4	0.31	0	6,6,6	0.23	0
5	SO4	B	911	-	4,4,4	0.41	0	6,6,6	0.21	0
5	SO4	C	911	-	4,4,4	0.25	0	6,6,6	0.25	0
4	NHF	H	904[B]	-	11,11,11	1.76	3 (27%)	11,15,15	0.81	1 (9%)
5	SO4	C	912	-	4,4,4	0.28	0	6,6,6	0.13	0
3	LCN	G	903[A]	-	11,11,11	2.03	3 (27%)	11,15,15	2.78	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MLA	C	921	-	-	2/4/4/4	-
2	UDP	C	901	-	-	5/16/32/32	0/2/2/2
6	MLA	G	921	-	-	0/4/4/4	-
6	MLA	F	921	-	-	4/4/4/4	-
6	MLA	B	921	-	-	0/4/4/4	-
6	MLA	H	921	-	-	1/4/4/4	-
3	LCN	A	903[A]	-	-	0/2/19/19	0/1/1/1
4	NHF	C	904[B]	-	-	2/2/19/19	0/1/1/1
2	UDP	D	901	-	-	5/16/32/32	0/2/2/2
4	NHF	A	904[B]	-	-	2/2/19/19	0/1/1/1
2	UDP	H	901	-	-	2/16/32/32	0/2/2/2
2	UDP	G	901	-	-	1/16/32/32	0/2/2/2
2	UDP	A	901	-	-	5/16/32/32	0/2/2/2
4	NHF	F	904[B]	-	-	2/2/19/19	0/1/1/1
6	MLA	E	921	-	-	0/4/4/4	-
3	LCN	D	903[A]	-	-	2/2/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LCN	C	903[A]	-	-	1/2/19/19	0/1/1/1
3	LCN	B	903[A]	-	-	0/2/19/19	0/1/1/1
6	MLA	D	921	-	-	2/4/4/4	-
4	NHF	D	904[B]	-	-	1/2/19/19	0/1/1/1
3	LCN	F	903[A]	-	-	0/2/19/19	0/1/1/1
4	NHF	B	904[B]	-	-	1/2/19/19	0/1/1/1
4	NHF	G	904[B]	-	-	0/2/19/19	0/1/1/1
2	UDP	E	901	-	-	3/16/32/32	0/2/2/2
3	LCN	E	903[A]	-	-	1/2/19/19	0/1/1/1
2	UDP	B	901	-	-	4/16/32/32	0/2/2/2
4	NHF	E	904[B]	-	-	1/2/19/19	0/1/1/1
2	UDP	F	901	-	-	4/16/32/32	0/2/2/2
6	MLA	A	921	-	-	2/4/4/4	-
3	LCN	H	903[A]	-	-	0/2/19/19	0/1/1/1
4	NHF	H	904[B]	-	-	1/2/19/19	0/1/1/1
3	LCN	G	903[A]	-	-	0/2/19/19	0/1/1/1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903[A]	LCN	O5-C5	-5.12	1.39	1.44
3	C	903[A]	LCN	O5-C5	-4.98	1.39	1.44
3	E	903[A]	LCN	O5-C5	-4.96	1.39	1.44
3	G	903[A]	LCN	O5-C5	-4.93	1.39	1.44
3	H	903[A]	LCN	O5-C5	-4.90	1.39	1.44

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	903[A]	LCN	O5-C1-C2	-8.53	117.21	125.57
2	D	901	UDP	C4-N3-C2	-7.20	117.67	126.61
3	F	903[A]	LCN	O5-C1-C2	-7.10	118.62	125.57
3	C	903[A]	LCN	O5-C1-C2	-6.81	118.90	125.57
3	G	903[A]	LCN	O5-C1-C2	-6.73	118.97	125.57

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	UDP	PA-O3A-PB-O2B

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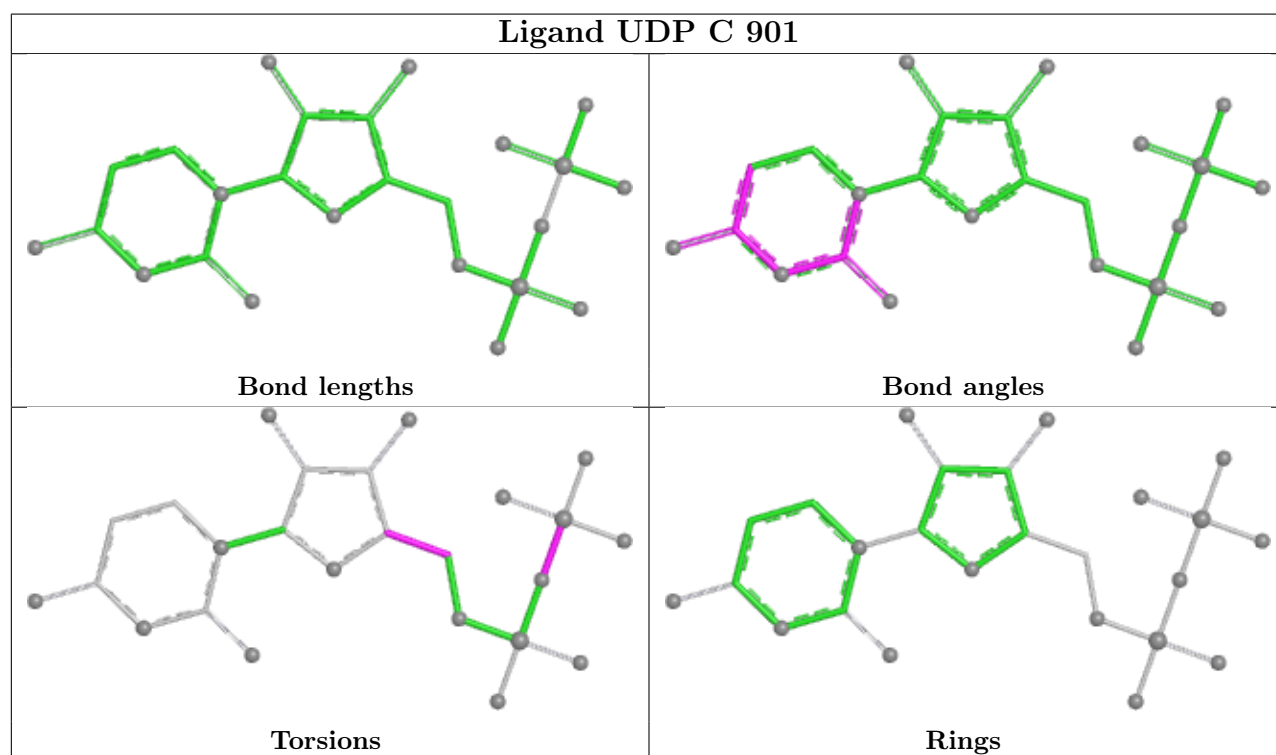
Mol	Chain	Res	Type	Atoms
2	A	901	UDP	PA-O3A-PB-O3B
2	D	901	UDP	PA-O3A-PB-O2B
3	D	903[A]	LCN	O5-C5-C6-O6
4	C	904[B]	NHF	O5-C5-C6-O6

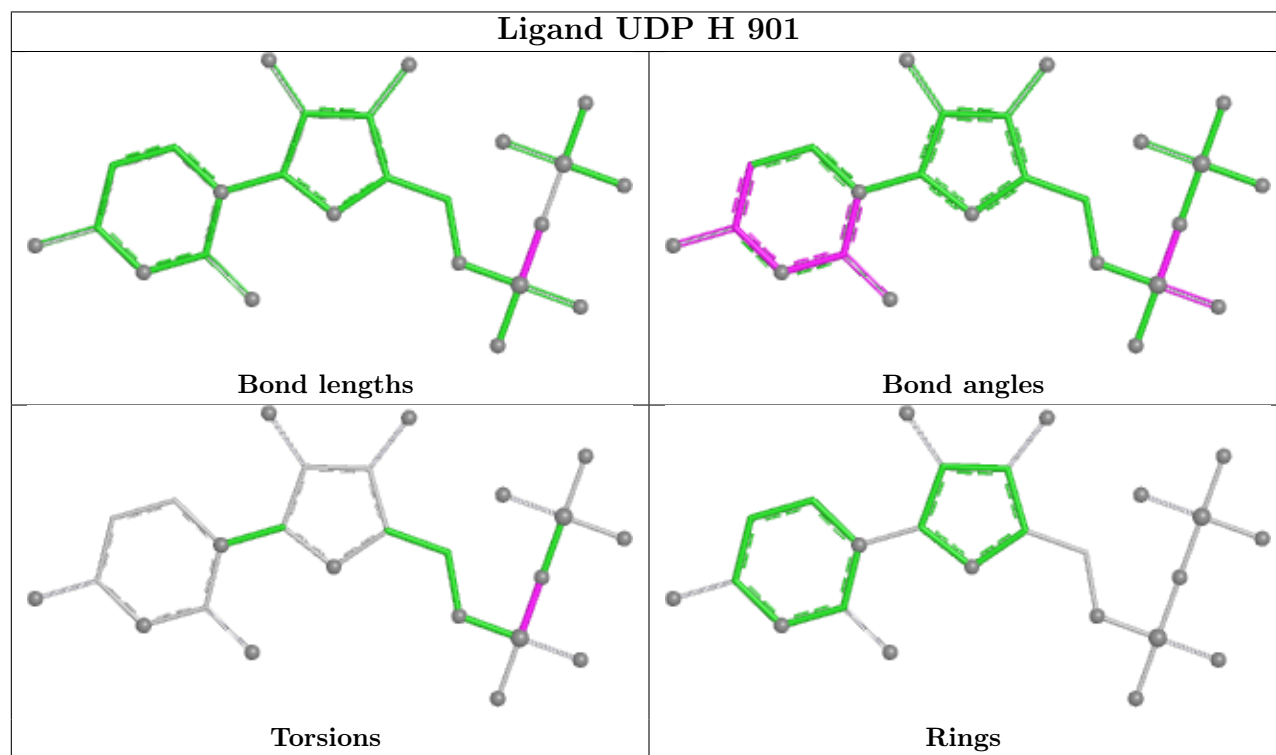
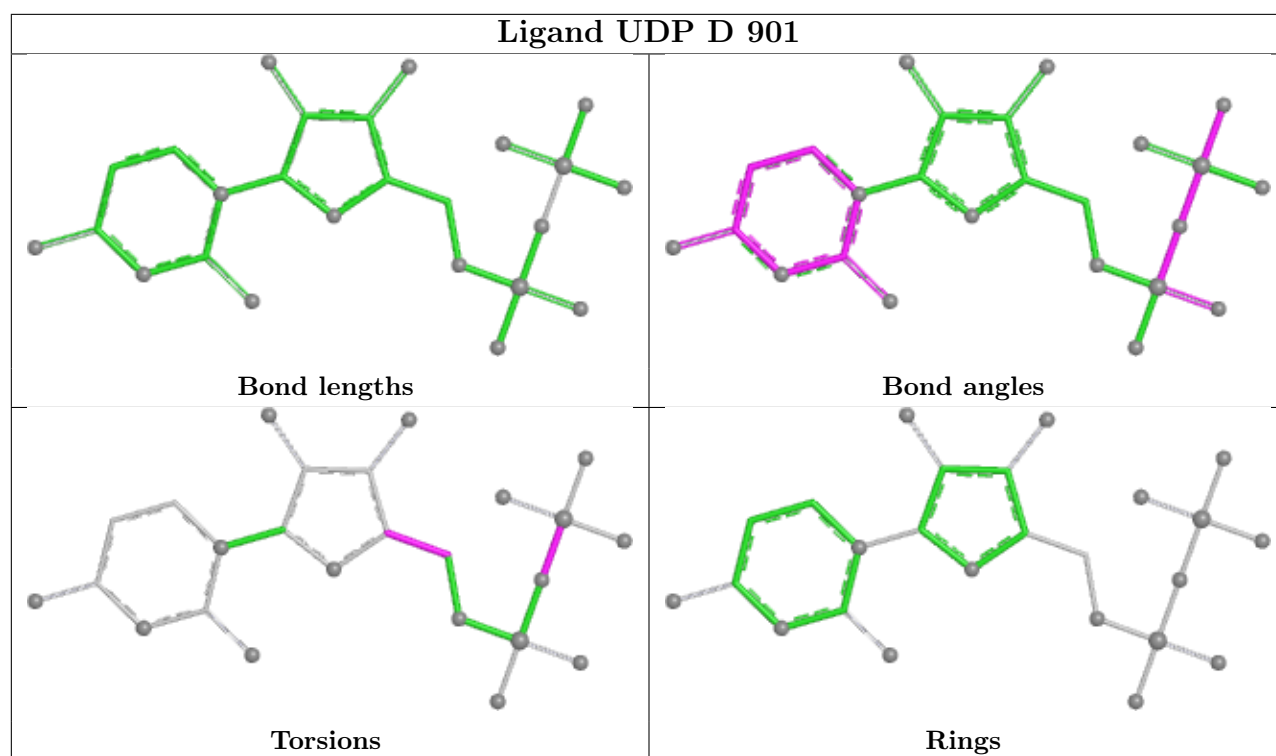
There are no ring outliers.

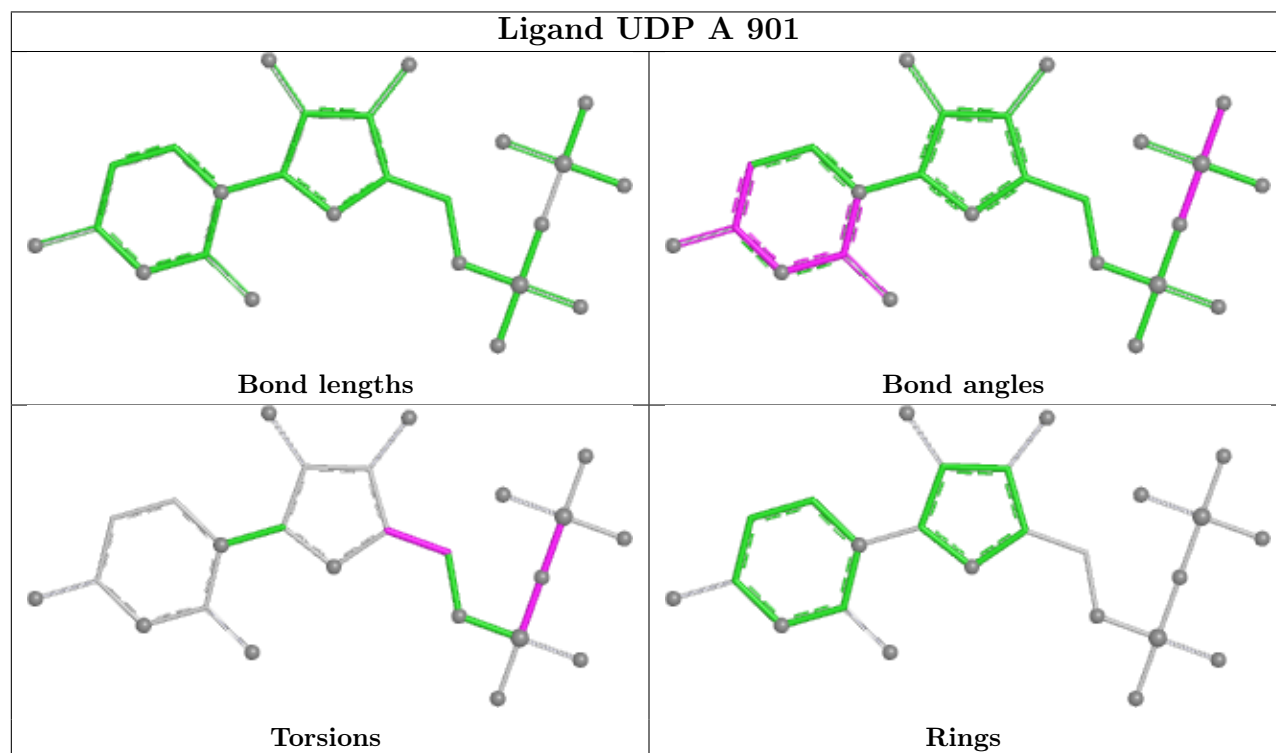
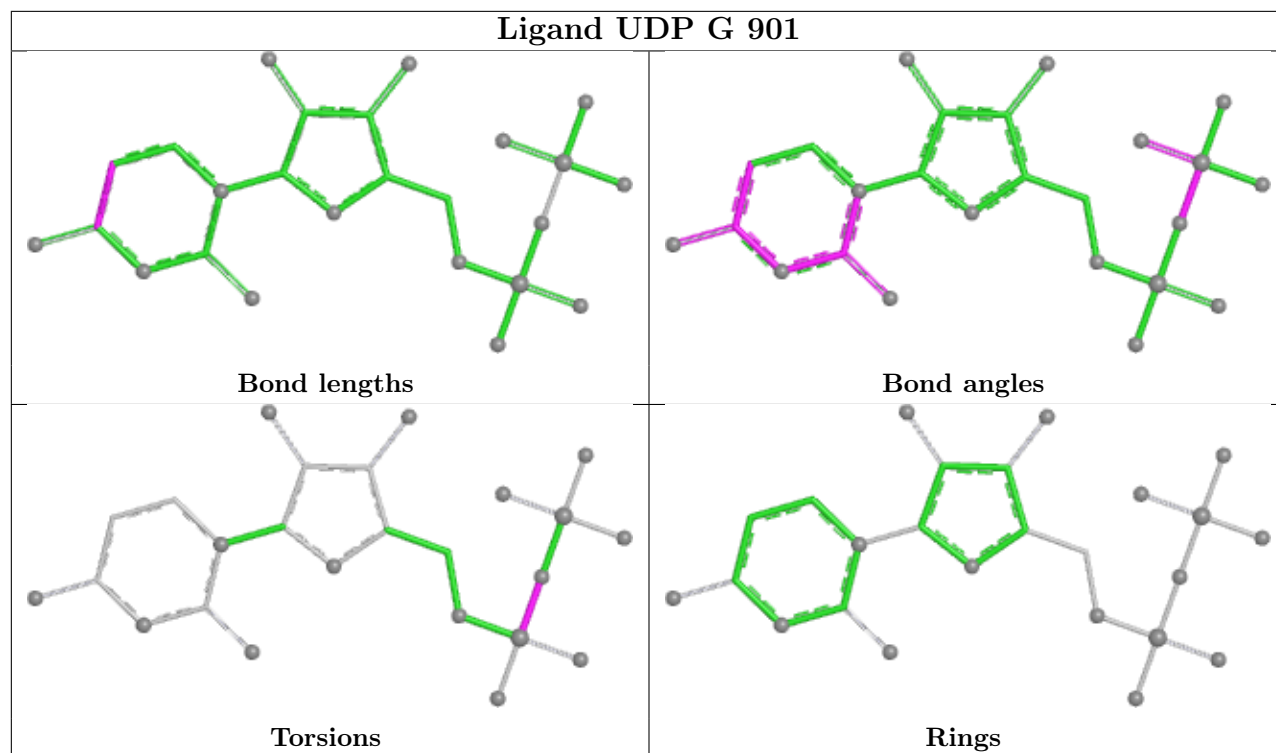
33 monomers are involved in 57 short contacts:

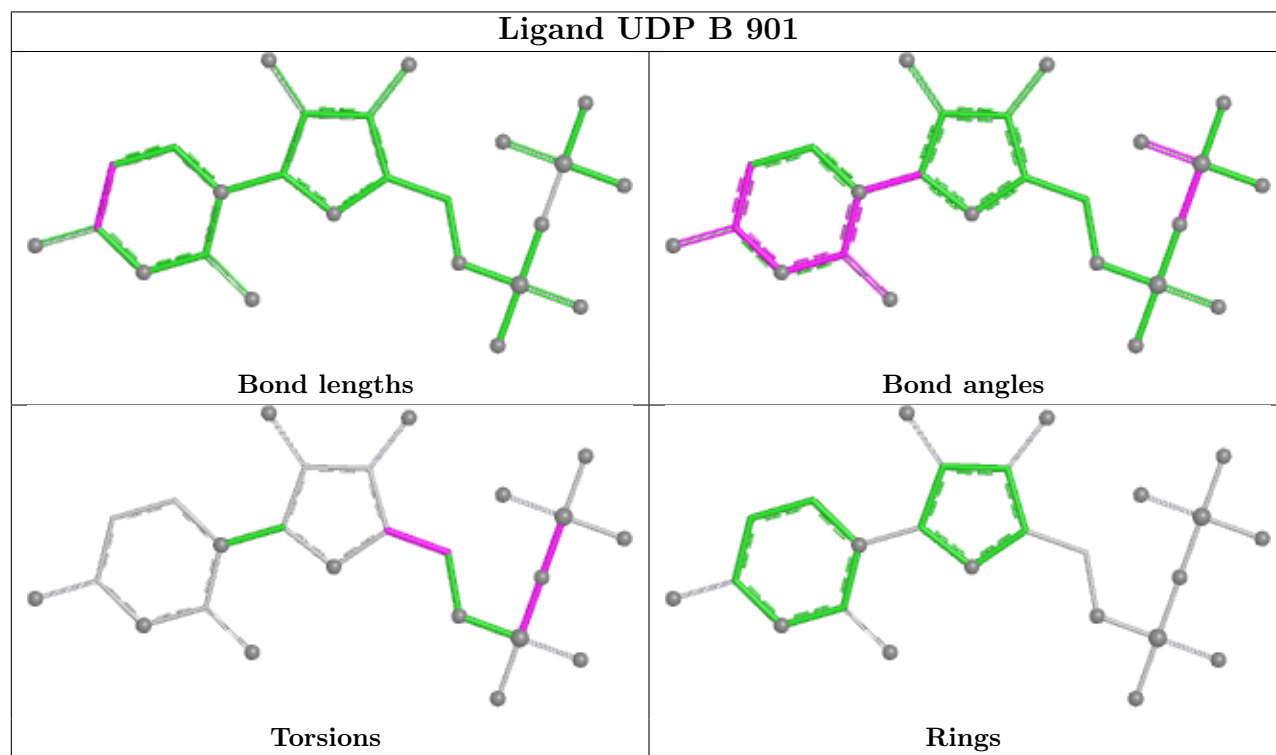
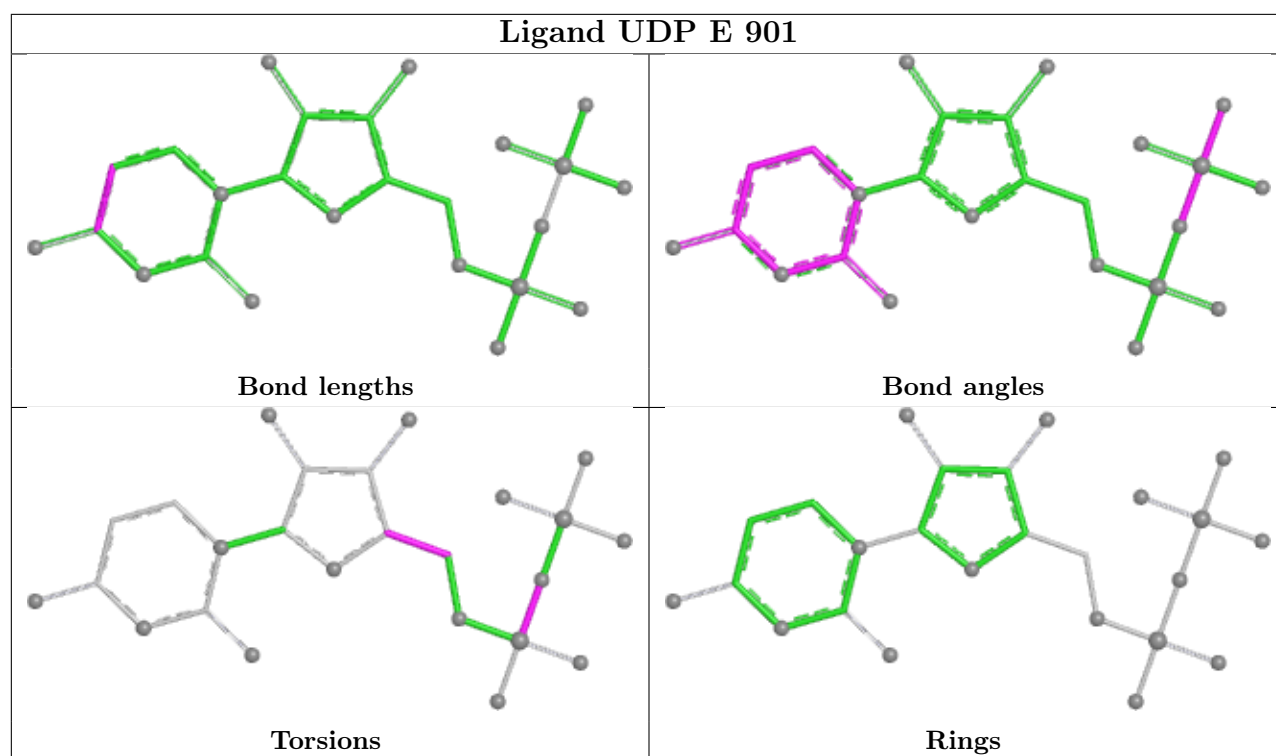
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	913	SO4	2	0
5	B	912	SO4	1	0
2	C	901	UDP	1	0
6	F	921	MLA	1	0
3	A	903[A]	LCN	1	0
4	C	904[B]	NHF	1	0
2	D	901	UDP	4	0
4	A	904[B]	NHF	2	0
2	H	901	UDP	4	0
5	E	912	SO4	1	0
2	G	901	UDP	4	0
5	F	912	SO4	2	0
2	A	901	UDP	3	0
5	C	913	SO4	1	0
6	E	921	MLA	1	0
3	D	903[A]	LCN	1	0
5	A	913	SO4	1	0
5	G	913	SO4	1	0
4	D	904[B]	NHF	6	0
5	F	913	SO4	3	0
3	F	903[A]	LCN	1	0
4	B	904[B]	NHF	2	0
5	G	912	SO4	1	0
4	G	904[B]	NHF	1	0
2	E	901	UDP	1	0
5	A	912	SO4	2	0
2	B	901	UDP	1	0
4	E	904[B]	NHF	2	0
2	F	901	UDP	1	0
5	H	913	SO4	1	0
5	B	913	SO4	4	0
4	H	904[B]	NHF	4	0
3	G	903[A]	LCN	1	0

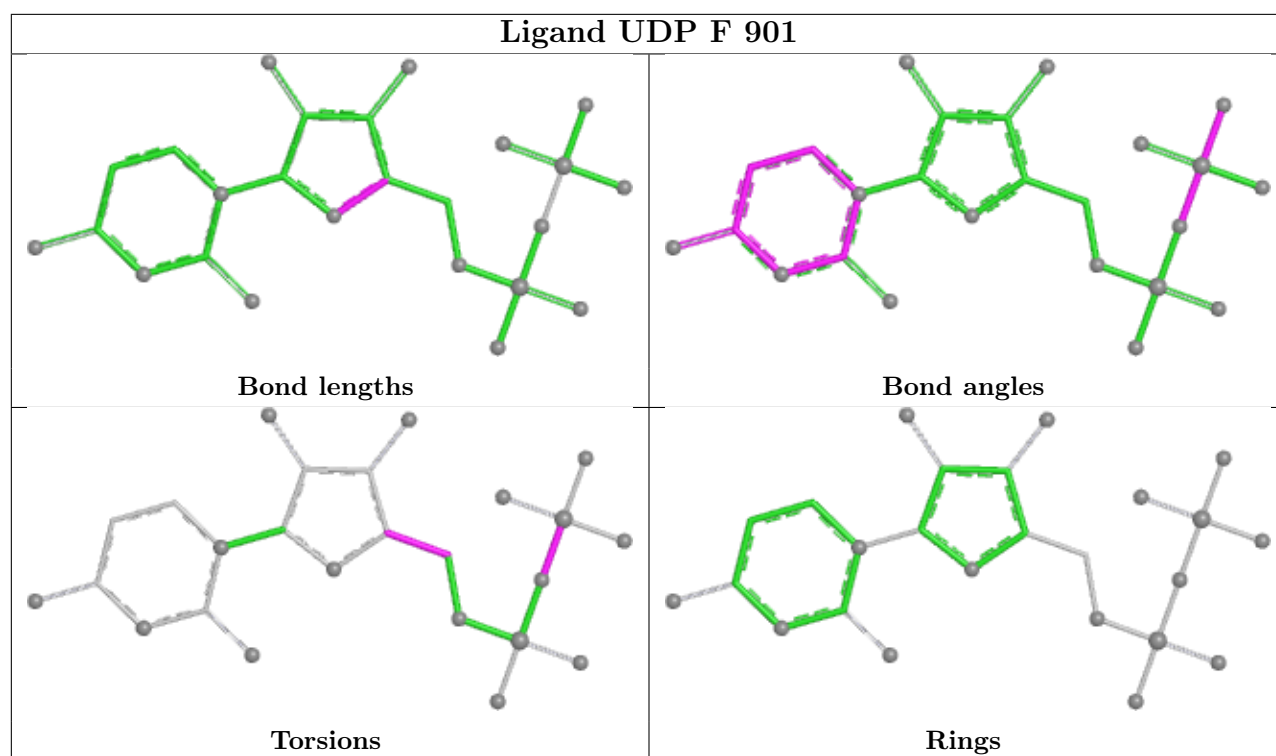
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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, 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	781/816 (95%)	-0.32	41 (5%)	33	25	19, 34, 105, 147	0
1	B	780/816 (95%)	0.04	74 (9%)	14	10	23, 43, 130, 171	0
1	C	781/816 (95%)	0.01	35 (4%)	38	30	30, 52, 101, 141	0
1	D	781/816 (95%)	-0.36	30 (3%)	44	35	22, 35, 92, 136	0
1	E	781/816 (95%)	-0.21	43 (5%)	30	23	23, 39, 116, 147	0
1	F	781/816 (95%)	-0.38	32 (4%)	41	33	17, 33, 84, 128	0
1	G	781/816 (95%)	-0.32	18 (2%)	61	51	22, 39, 81, 126	0
1	H	780/816 (95%)	0.02	78 (10%)	12	9	26, 43, 127, 156	0
All	All	6246/6528 (95%)	-0.19	351 (5%)	30	23	17, 41, 105, 171	0

The worst 5 of 351 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	103	ASN	7.1
1	H	51	ALA	7.0
1	B	57	PRO	6.7
1	H	73	LEU	6.4
1	H	56	LEU	6.2

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 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
5	SO4	C	912	5/5	0.65	0.25	84,89,106,115	0
5	SO4	H	912	5/5	0.78	0.22	70,77,86,105	0
5	SO4	H	913	5/5	0.79	0.29	81,87,102,115	0
5	SO4	D	912	5/5	0.81	0.18	59,77,86,101	0
5	SO4	C	913	5/5	0.83	0.19	81,84,103,107	0
7	K	E	931	1/1	0.83	0.10	73,73,73,73	0
3	LCN	D	903[A]	11/11	0.84	0.16	24,27,32,32	21
5	SO4	B	913	5/5	0.84	0.26	68,71,80,95	0
5	SO4	B	912	5/5	0.85	0.16	70,76,90,106	0
5	SO4	G	912	5/5	0.88	0.20	59,69,86,94	0
5	SO4	A	912	5/5	0.88	0.17	51,56,69,85	0
6	MLA	C	921	7/7	0.89	0.13	70,73,87,91	0
6	MLA	G	921	7/7	0.89	0.13	58,62,74,74	0
4	NHF	C	904[B]	11/11	0.89	0.16	37,38,45,47	21
5	SO4	B	911	5/5	0.90	0.17	45,47,65,81	0
4	NHF	F	904[B]	11/11	0.91	0.15	24,25,30,32	21
5	SO4	E	913	5/5	0.91	0.20	56,63,79,86	0
7	K	F	931	1/1	0.91	0.11	82,82,82,82	0
4	NHF	H	904[B]	11/11	0.92	0.18	32,34,40,41	21
5	SO4	F	912	5/5	0.92	0.17	55,58,68,85	0
6	MLA	E	921	7/7	0.92	0.12	42,50,55,56	0
4	NHF	E	904[B]	11/11	0.92	0.17	27,29,34,35	21
5	SO4	G	913	5/5	0.92	0.16	59,63,84,96	0
5	SO4	E	911	5/5	0.92	0.19	44,48,60,65	0
7	K	G	931	1/1	0.92	0.14	74,74,74,74	0
4	NHF	B	904[B]	11/11	0.93	0.10	29,32,37,38	21
5	SO4	E	912	5/5	0.93	0.17	57,62,70,86	0
6	MLA	H	921	7/7	0.93	0.12	52,61,68,70	0
7	K	B	931	1/1	0.93	0.11	83,83,83,83	0
5	SO4	D	911	5/5	0.93	0.22	43,47,64,77	0
5	SO4	F	911	5/5	0.93	0.19	42,42,63,71	0
4	NHF	G	904[B]	11/11	0.93	0.09	26,27,32,33	21
5	SO4	D	913	5/5	0.94	0.17	46,47,69,73	0
3	LCN	E	903[A]	11/11	0.94	0.14	26,30,35,36	21
7	K	D	931	1/1	0.94	0.15	72,72,72,72	0
3	LCN	H	903[A]	11/11	0.94	0.16	32,34,41,41	21
4	NHF	D	904[B]	11/11	0.94	0.10	24,27,32,32	21

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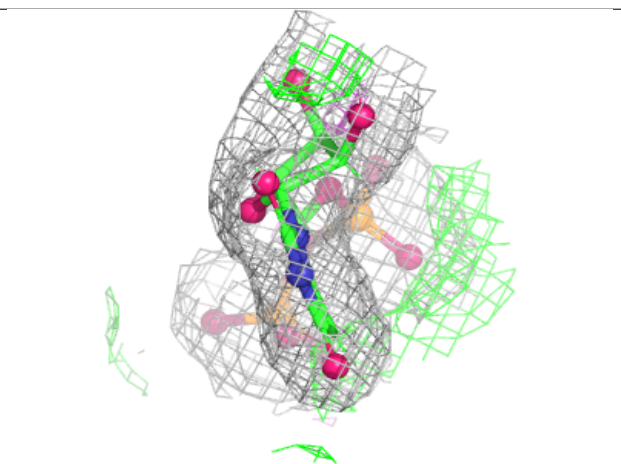
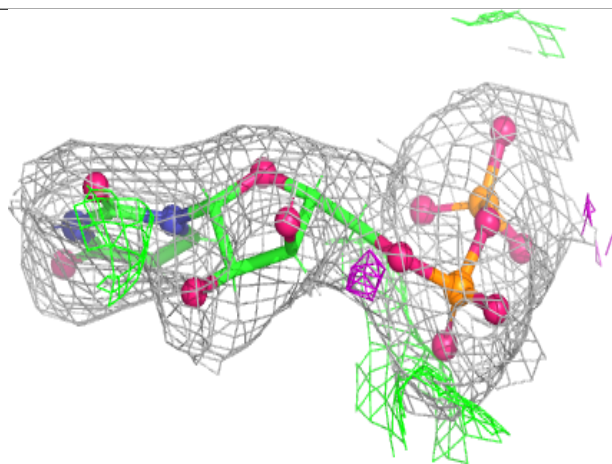
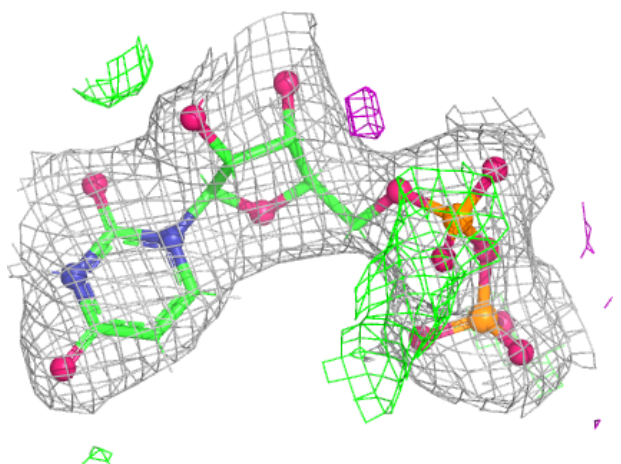
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	H	911	5/5	0.94	0.19	44,47,65,70	0
7	K	H	931	1/1	0.94	0.07	69,69,69,69	0
5	SO4	F	913	5/5	0.95	0.18	49,51,53,70	0
5	SO4	A	911	5/5	0.95	0.19	35,43,59,63	0
5	SO4	C	911	5/5	0.95	0.14	48,51,70,71	0
3	LCN	G	903[A]	11/11	0.95	0.08	25,28,33,34	21
5	SO4	A	913	5/5	0.95	0.20	44,50,74,74	0
3	LCN	A	903[A]	11/11	0.95	0.13	23,25,29,30	21
6	MLA	B	921	7/7	0.95	0.10	51,58,61,61	0
3	LCN	B	903[A]	11/11	0.95	0.09	29,32,37,39	21
6	MLA	D	921	7/7	0.95	0.10	33,40,44,46	0
5	SO4	G	911	5/5	0.96	0.14	35,41,56,61	0
3	LCN	F	903[A]	11/11	0.96	0.09	23,27,31,33	21
3	LCN	C	903[A]	11/11	0.97	0.10	36,39,46,48	21
7	K	C	931	1/1	0.97	0.12	81,81,81,81	0
6	MLA	A	921	7/7	0.97	0.09	31,38,42,42	0
6	MLA	F	921	7/7	0.97	0.09	33,38,42,43	0
2	UDP	H	901	25/25	0.97	0.06	28,34,41,44	0
4	NHF	A	904[B]	11/11	0.97	0.10	23,25,29,30	21
7	K	A	931	1/1	0.97	0.07	61,61,61,61	0
2	UDP	D	901	25/25	0.98	0.05	22,28,34,39	0
2	UDP	E	901	25/25	0.98	0.05	21,27,35,38	0
2	UDP	G	901	25/25	0.98	0.05	20,28,34,41	0
2	UDP	B	901	25/25	0.98	0.04	23,31,37,43	0
2	UDP	C	901	25/25	0.98	0.06	32,41,49,54	0
2	UDP	A	901	25/25	0.99	0.04	18,23,29,32	0
2	UDP	F	901	25/25	0.99	0.04	16,23,29,34	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.

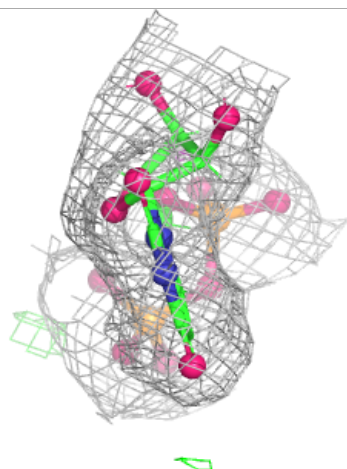
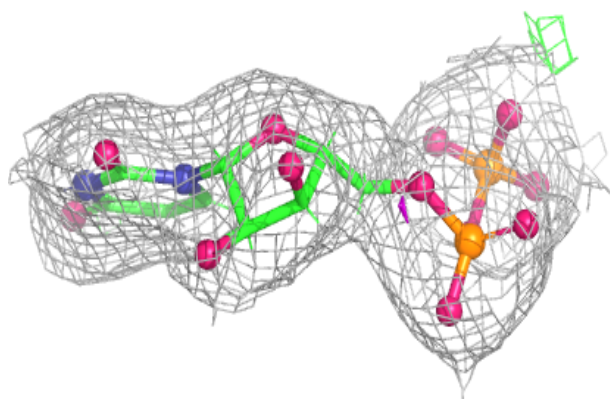
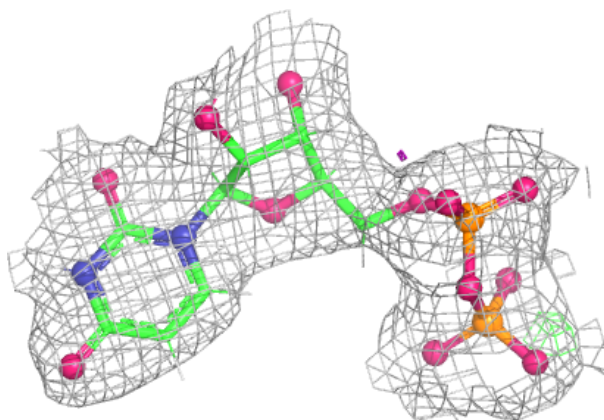
Electron density around UDP H 901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



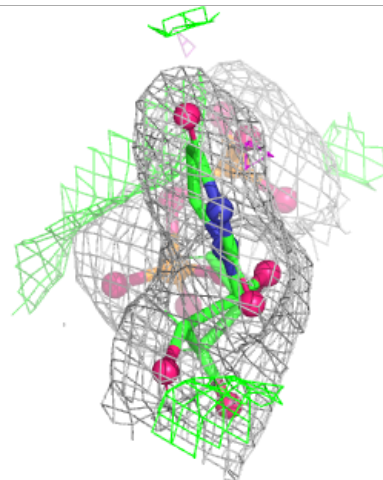
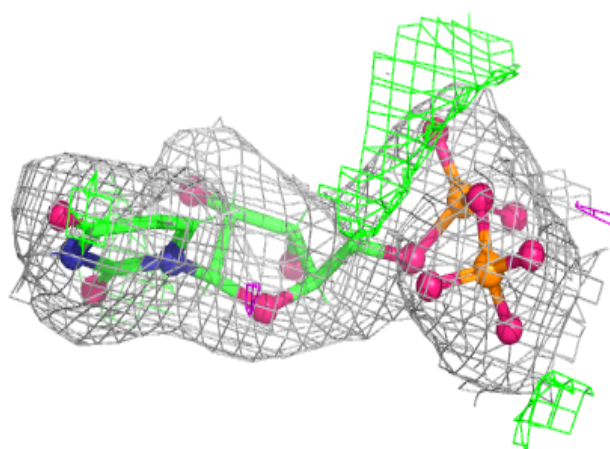
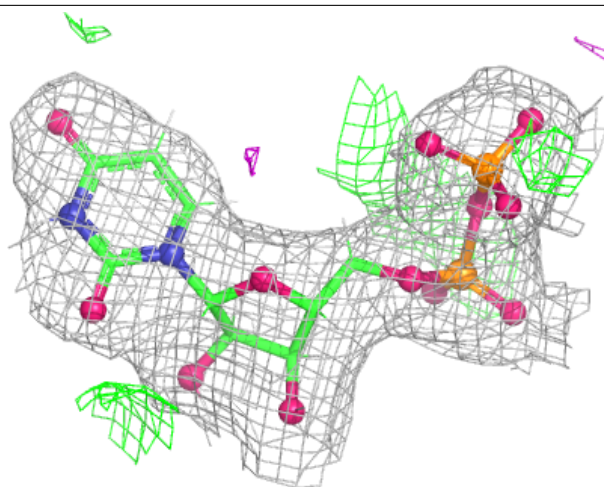
Electron density around UDP D 901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



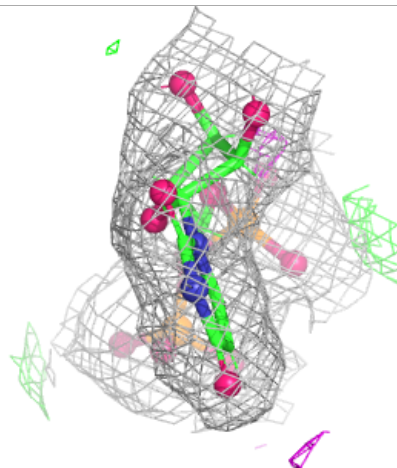
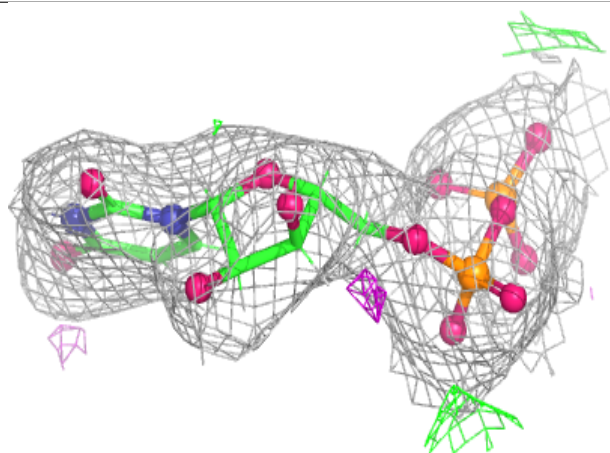
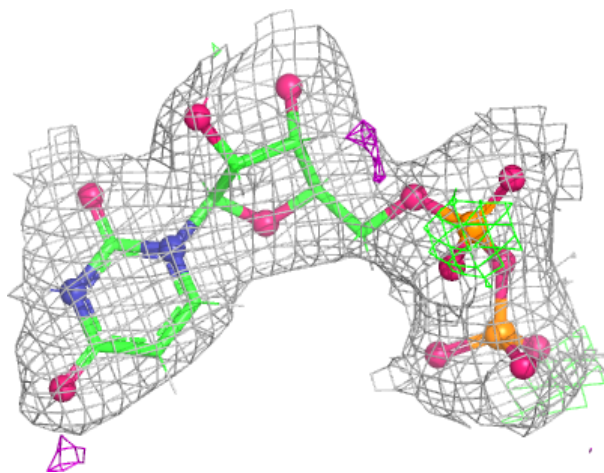
Electron density around UDP E 901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



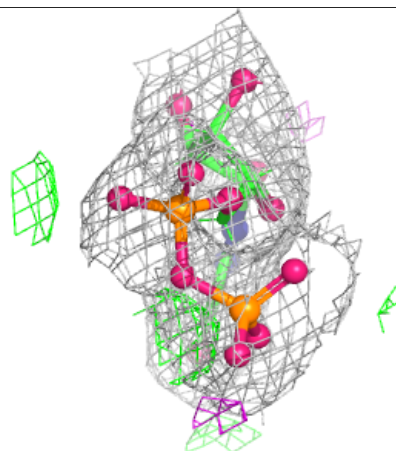
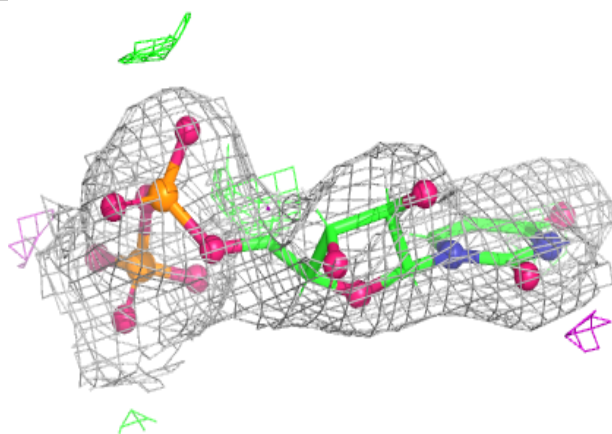
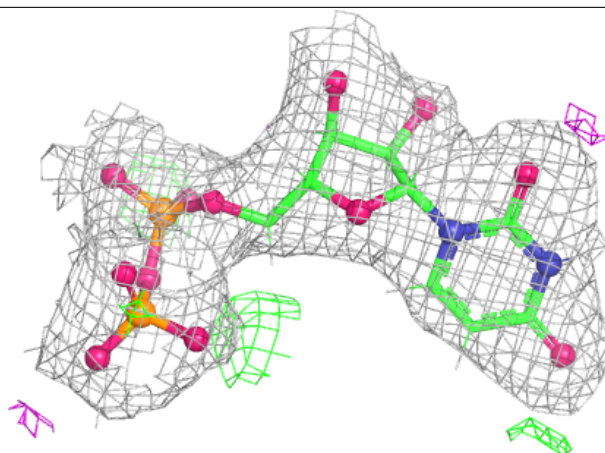
Electron density around UDP G 901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



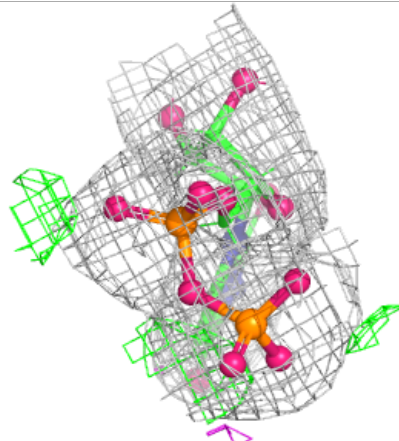
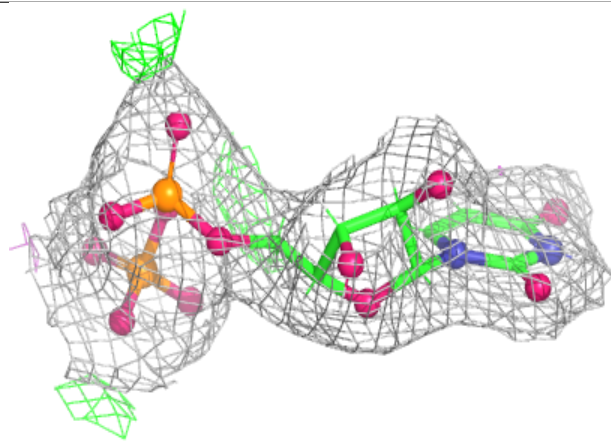
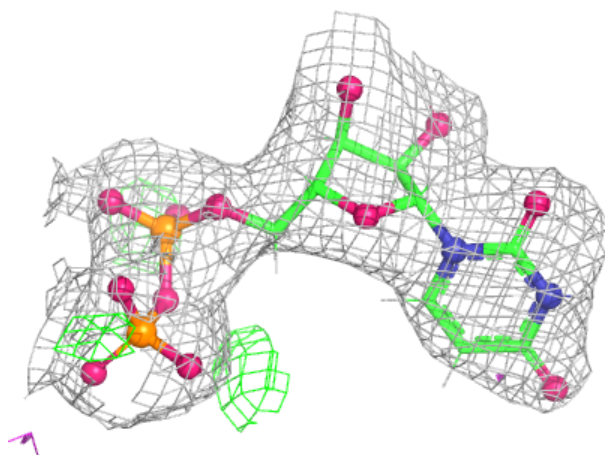
Electron density around UDP B 901:

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and green (positive)



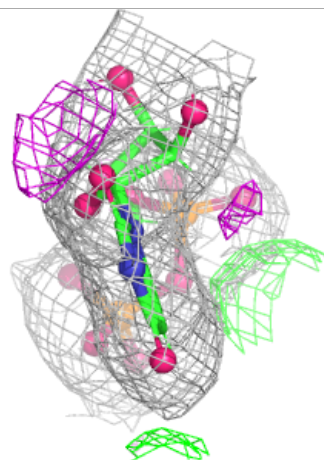
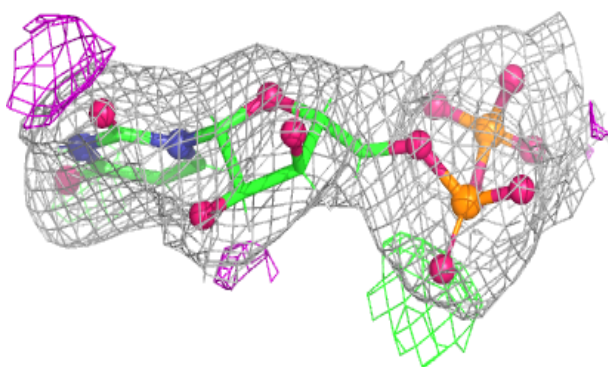
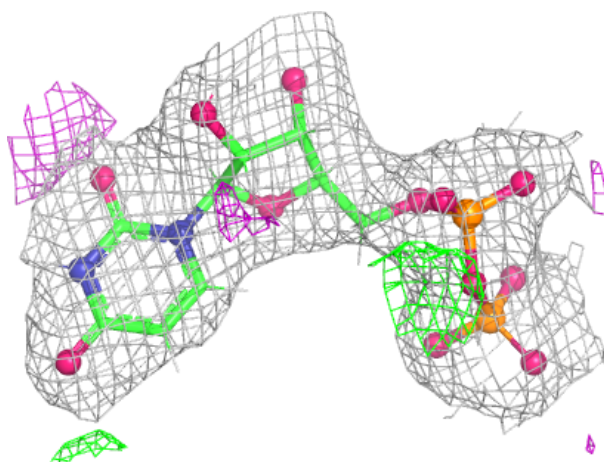
Electron density around UDP C 901:

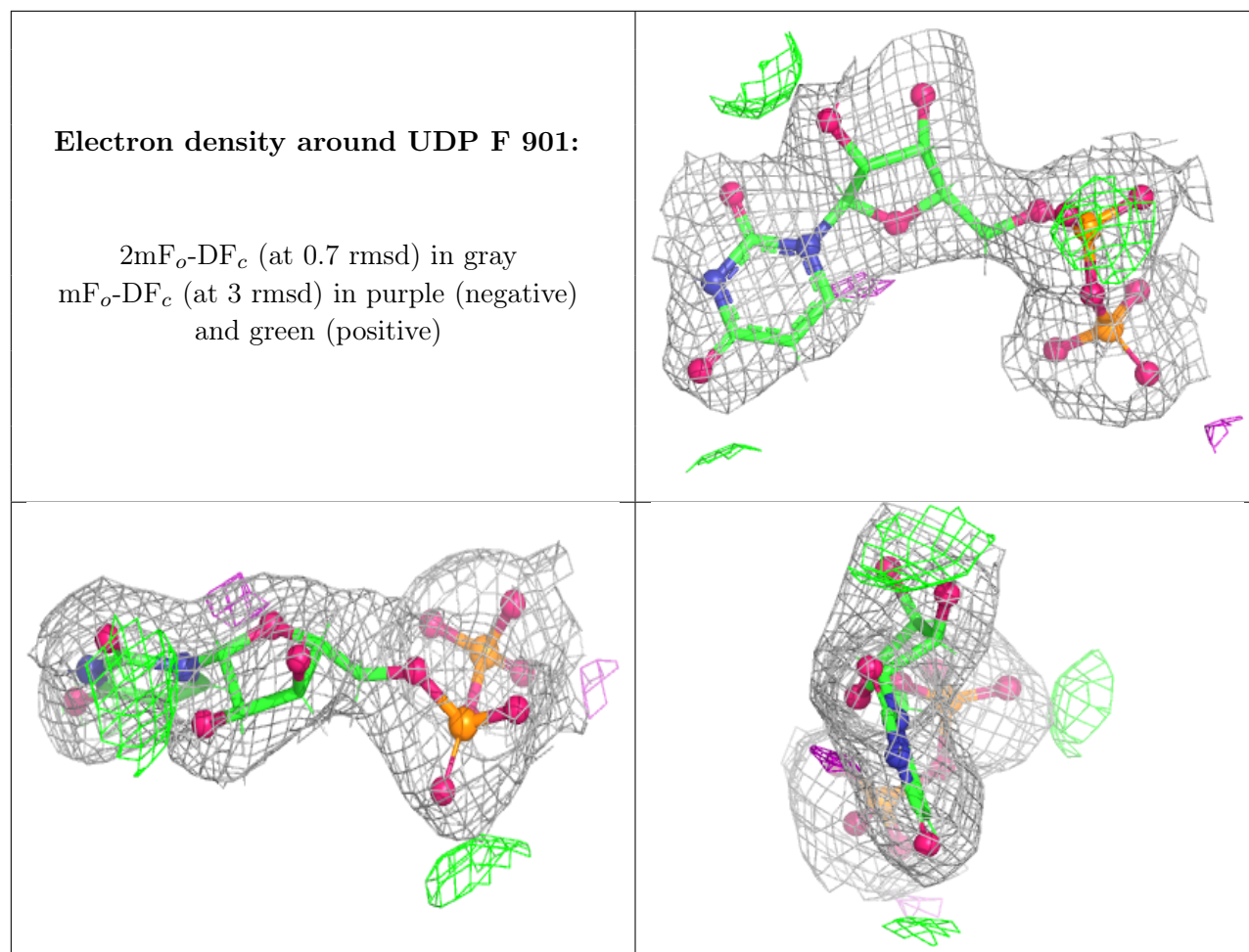
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UDP 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.