



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2023 – 10:28 AM EDT

PDB ID : 3S28
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.

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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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

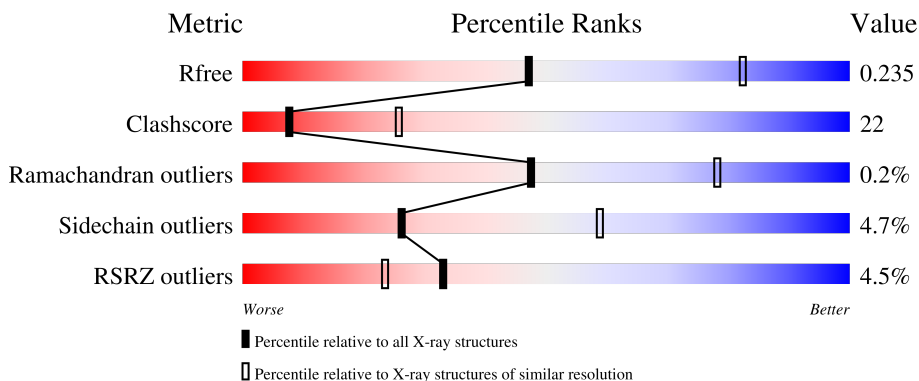
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	
1	B	816	
1	C	816	
1	D	816	
1	E	816	

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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
			Total	C	N	O	S			
1	A	781	6289	4039	1069	1159	22	0	0	0
1	B	780	6158	3949	1050	1137	22	0	0	0
1	C	781	6290	4045	1066	1157	22	0	0	0
1	D	781	6280	4035	1062	1161	22	0	0	0
1	E	781	6271	4028	1062	1159	22	0	0	0
1	F	781	6292	4042	1070	1158	22	0	0	0
1	G	781	6299	4045	1070	1162	22	0	0	0
1	H	780	6243	4007	1063	1151	22	0	0	0

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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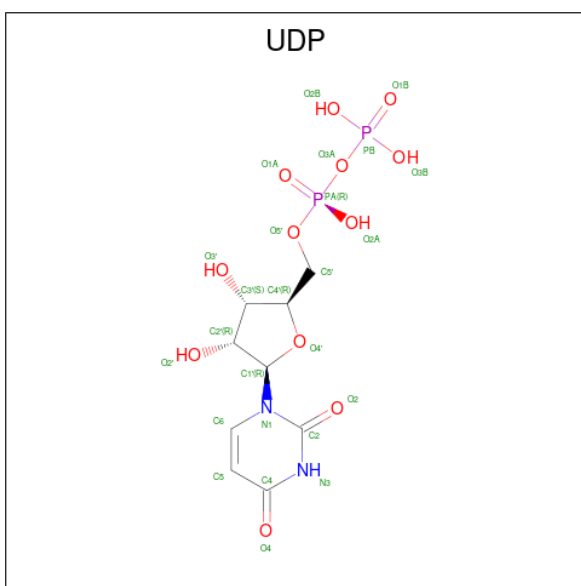
Chain	Residue	Modelled	Actual	Comment	Reference
B	814	HIS	-	expression tag	UNP P49040
B	815	HIS	-	expression tag	UNP P49040
B	816	HIS	-	expression tag	UNP P49040
C	809	VAL	-	expression tag	UNP P49040
C	810	GLU	-	expression tag	UNP P49040
C	811	HIS	-	expression tag	UNP P49040
C	812	HIS	-	expression tag	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 (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



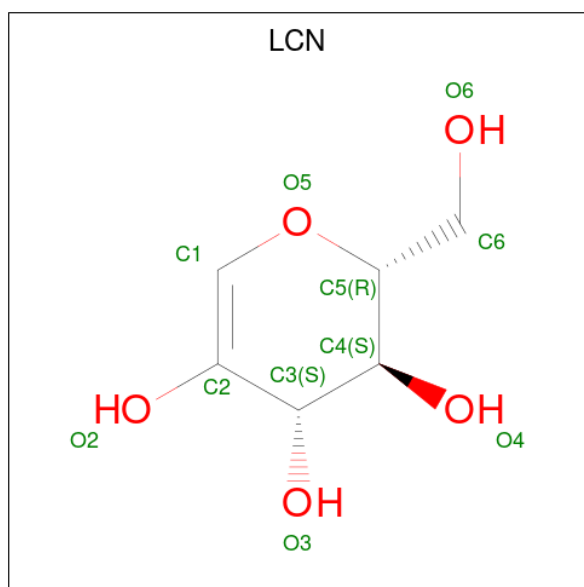
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	B	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	C	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	D	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	E	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
2	F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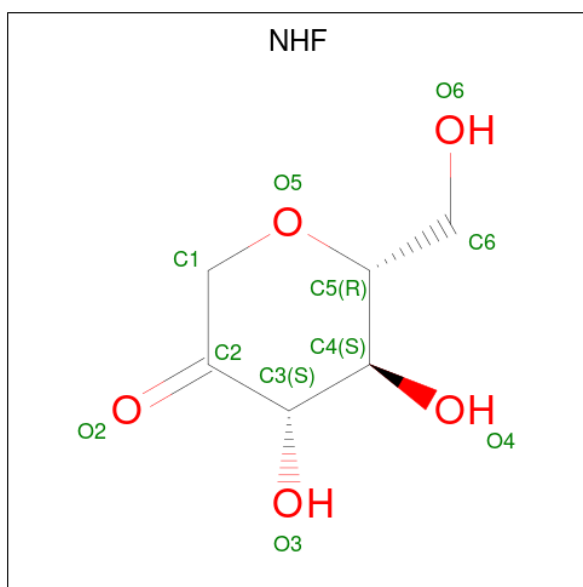
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	H	1	36	9	11	2	12	2	0	0

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



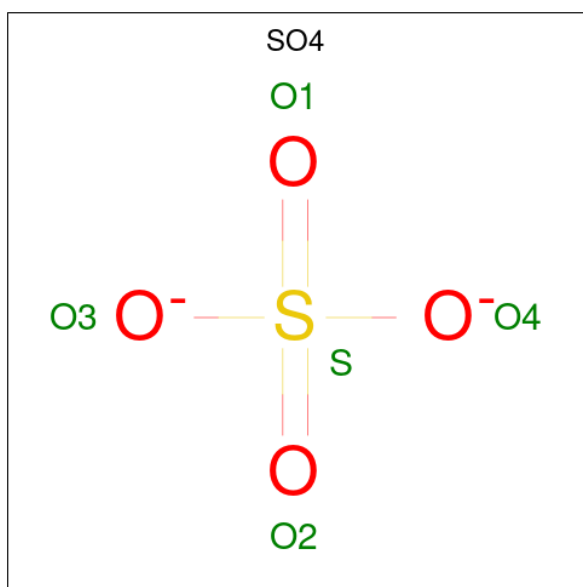
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	21	6	10	5	0	1
3	B	1	21	6	10	5	0	1
3	C	1	21	6	10	5	0	1
3	D	1	21	6	10	5	0	1
3	E	1	21	6	10	5	0	1
3	F	1	21	6	10	5	0	1
3	G	1	21	6	10	5	0	1
3	H	1	21	6	10	5	0	1

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



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



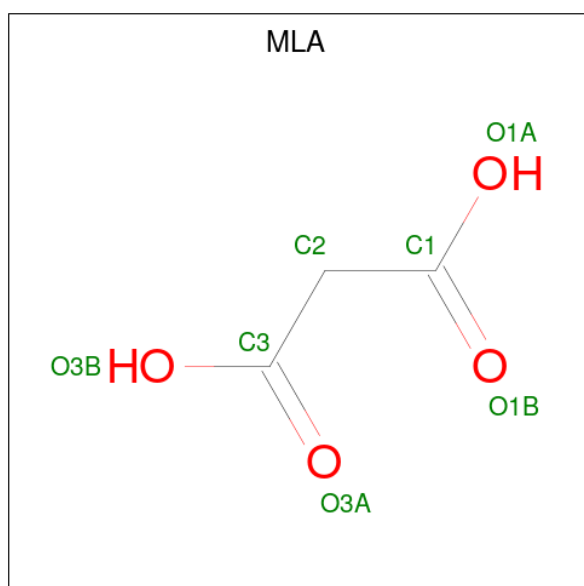
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	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 (three-letter code: MLA) (formula: C₃H₄O₄).



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 (three-letter code: 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		

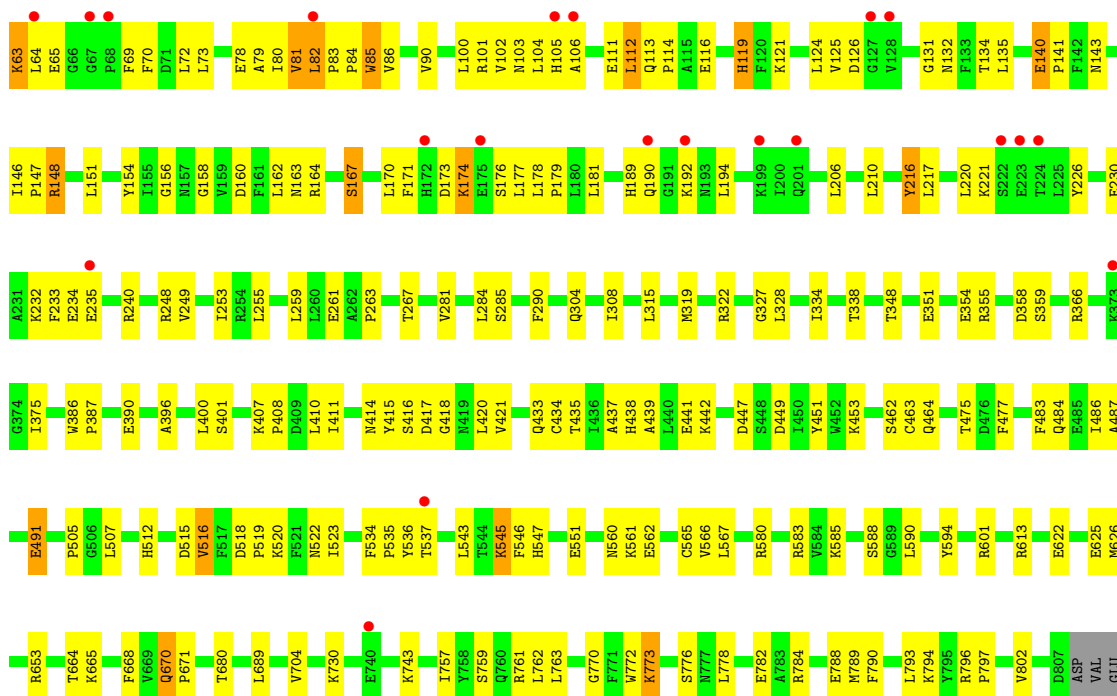
- Molecule 8 is water.

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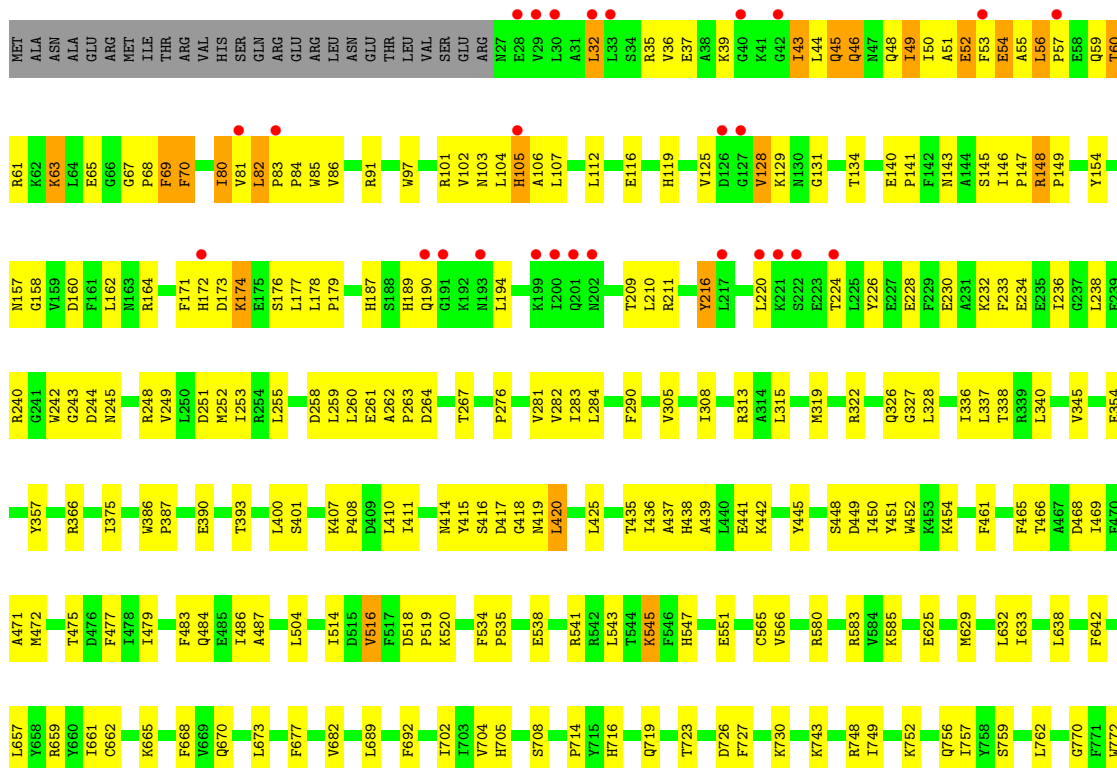
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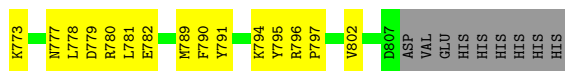
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	24	Total O 24 24	0	0
8	D	54	Total O 54 54	0	0
8	E	50	Total O 50 50	0	0
8	F	79	Total O 79 79	0	0
8	G	62	Total O 62 62	0	0
8	H	49	Total O 49 49	0	0



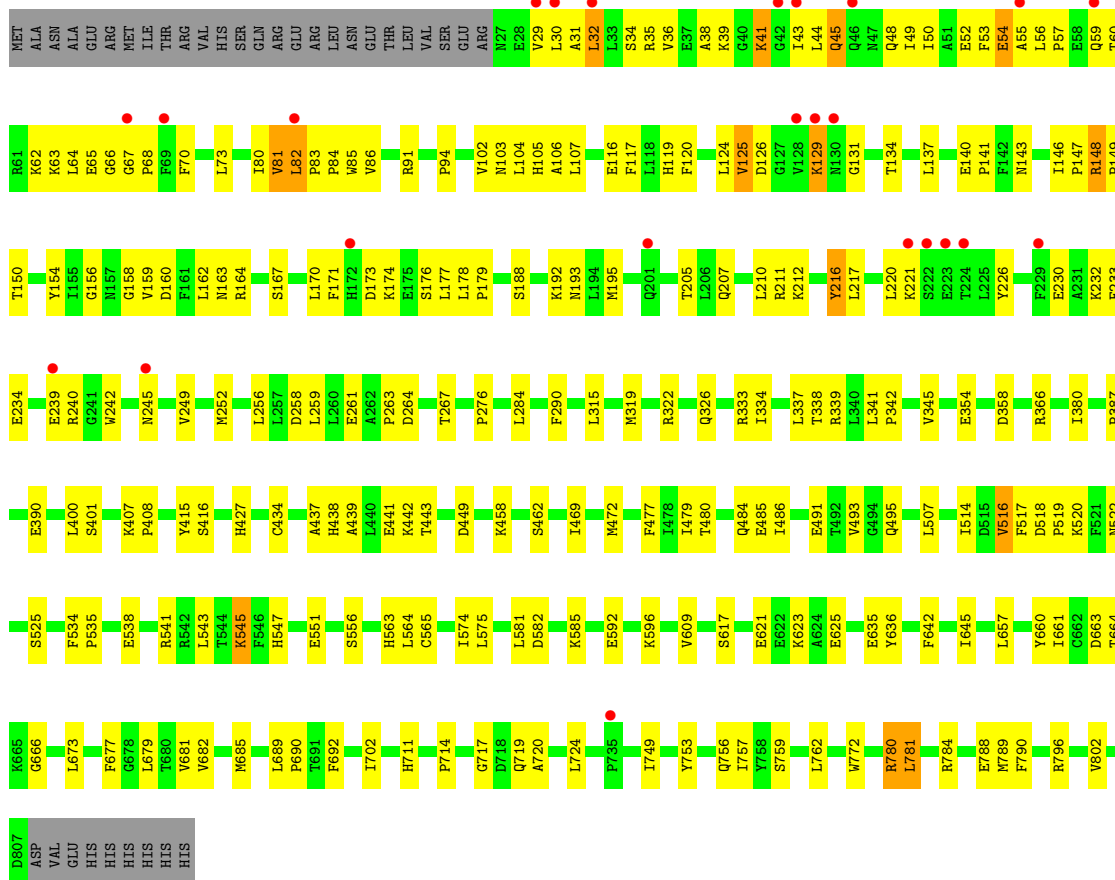
HIS
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● Molecule 1: Sucrose synthase 1

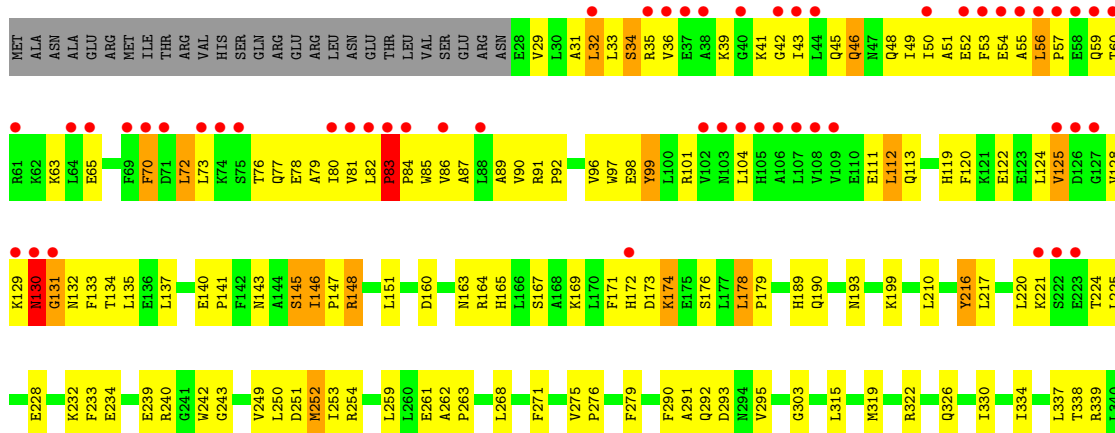


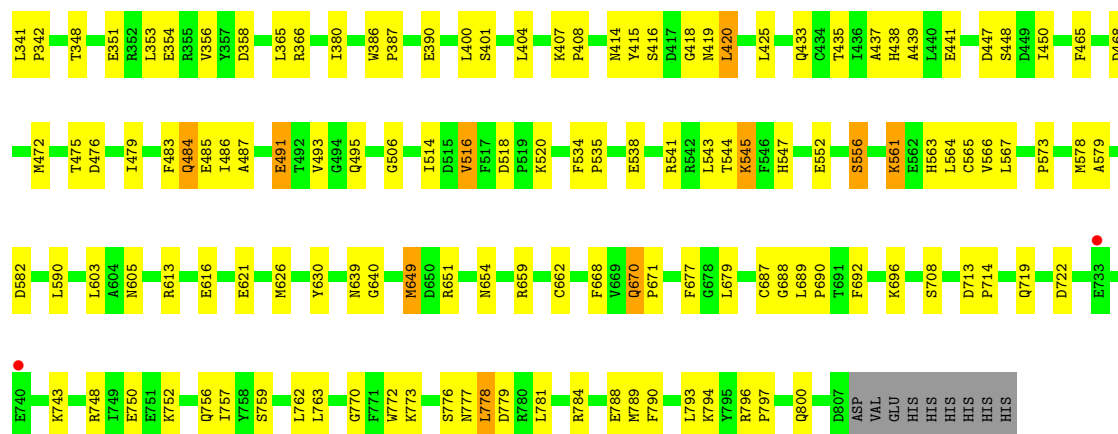


• Molecule 1: Sucrose synthase 1



• 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	276.75Å 261.88Å 160.19Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	24.98 – 2.80 50.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.98-2.80) 99.7 (50.06-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.188 , 0.236 0.186 , 0.235	Depositor DCC
R_{free} test set	13263 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NHF, SO4, UDP, MLA, LCN, 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	0.37	0/6436	0.56	1/8714 (0.0%)
1	B	0.35	0/6304	0.58	1/8549 (0.0%)
1	C	0.33	0/6437	0.53	0/8718
1	D	0.36	0/6427	0.56	1/8707 (0.0%)
1	E	0.35	0/6417	0.56	0/8693
1	F	0.38	0/6439	0.58	0/8719
1	G	0.36	0/6446	0.57	0/8728
1	H	0.35	0/6390	0.55	0/8655
All	All	0.36	0/51296	0.56	3/69483 (0.0%)

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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	678	GLY	N-CA-C	5.35	126.48	113.10
1	B	678	GLY	N-CA-C	5.33	126.43	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	678	GLY	N-CA-C	5.11	125.88	113.10

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6289	0	6220	285	0
1	B	6158	0	5959	298	0
1	C	6290	0	6242	314	0
1	D	6280	0	6206	274	0
1	E	6271	0	6194	266	0
1	F	6292	0	6234	285	0
1	G	6299	0	6240	268	0
1	H	6243	0	6130	322	0
2	A	25	11	11	3	0
2	B	25	11	11	1	0
2	C	25	11	11	0	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
3	D	11	10	10	1	0
3	E	11	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
8	F	79	0	0	2	0
8	G	62	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	49	0	0	1	0
All	All	51124	264	49689	2198	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 22.

The worst 5 of 2198 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: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:G:66:GLY:C	1:G:68:PRO:HD3	1.60	1.19
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%)	51	81
1	B	778/816 (95%)	724 (93%)	52 (7%)	2 (0%)	41	72
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%)	41	72
1	F	779/816 (96%)	737 (95%)	39 (5%)	3 (0%)	34	66
1	G	779/816 (96%)	743 (95%)	36 (5%)	0	100	100
1	H	778/816 (95%)	736 (95%)	40 (5%)	2 (0%)	41	72
All	All	6230/6528 (95%)	5903 (95%)	317 (5%)	10 (0%)	47	78

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 [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	670/718 (93%)	644 (96%)	26 (4%)	32	66
1	B	635/718 (88%)	600 (94%)	35 (6%)	21	52
1	C	673/718 (94%)	649 (96%)	24 (4%)	35	69
1	D	671/718 (94%)	640 (95%)	31 (5%)	27	60
1	E	668/718 (93%)	633 (95%)	35 (5%)	23	55
1	F	672/718 (94%)	641 (95%)	31 (5%)	27	60
1	G	674/718 (94%)	647 (96%)	27 (4%)	31	65
1	H	658/718 (92%)	615 (94%)	43 (6%)	17	44
All	All	5321/5744 (93%)	5069 (95%)	252 (5%)	26	59

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	778	LEU
1	H	146	ILE
1	E	516	VAL
1	H	130	ASN
1	H	545	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	143	ASN
1	F	512	HIS
1	H	119	HIS
1	E	190	GLN
1	F	48	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	A	911	-	4,4,4	0.19	0	6,6,6	0.27	0
3	LCN	G	903[A]	-	11,11,11	2.01	3 (27%)	9,15,15	0.99	0
5	SO4	E	912	-	4,4,4	0.18	0	6,6,6	0.08	0
4	NHF	D	904[B]	-	11,11,11	1.73	4 (36%)	12,15,15	1.65	1 (8%)
5	SO4	F	911	-	4,4,4	0.18	0	6,6,6	0.30	0
6	MLA	A	921	-	6,6,6	1.12	0	7,7,7	1.31	0
6	MLA	H	921	-	6,6,6	1.11	0	7,7,7	1.44	0
2	UDP	F	901	-	24,26,26	0.99	1 (4%)	37,40,40	1.69	6 (16%)
4	NHF	C	904[B]	-	11,11,11	1.79	4 (36%)	12,15,15	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NHF	H	904[B]	-	11,11,11	1.70	3 (27%)	12,15,15	0.79	0
3	LCN	F	903[A]	-	11,11,11	2.00	3 (27%)	9,15,15	1.23	2 (22%)
5	SO4	B	912	-	4,4,4	0.14	0	6,6,6	0.14	0
5	SO4	D	911	-	4,4,4	0.23	0	6,6,6	0.30	0
5	SO4	B	913	-	4,4,4	0.19	0	6,6,6	0.21	0
3	LCN	D	903[A]	-	11,11,11	2.04	4 (36%)	9,15,15	1.18	1 (11%)
5	SO4	F	912	-	4,4,4	0.16	0	6,6,6	0.22	0
5	SO4	G	913	-	4,4,4	0.16	0	6,6,6	0.15	0
5	SO4	A	913	-	4,4,4	0.22	0	6,6,6	0.08	0
2	UDP	A	901	-	24,26,26	0.99	1 (4%)	37,40,40	1.71	7 (18%)
5	SO4	H	912	-	4,4,4	0.21	0	6,6,6	0.09	0
6	MLA	F	921	-	6,6,6	1.10	0	7,7,7	1.49	0
2	UDP	D	901	-	24,26,26	1.02	0	37,40,40	1.88	8 (21%)
5	SO4	F	913	-	4,4,4	0.20	0	6,6,6	0.20	0
6	MLA	B	921	-	6,6,6	1.29	0	7,7,7	1.23	0
5	SO4	G	912	-	4,4,4	0.19	0	6,6,6	0.12	0
6	MLA	E	921	-	6,6,6	1.32	0	7,7,7	0.92	0
3	LCN	H	903[A]	-	11,11,11	2.00	3 (27%)	9,15,15	1.08	0
5	SO4	D	912	-	4,4,4	0.14	0	6,6,6	0.23	0
3	LCN	B	903[A]	-	11,11,11	1.95	3 (27%)	9,15,15	1.12	1 (11%)
4	NHF	B	904[B]	-	11,11,11	1.83	4 (36%)	12,15,15	0.99	1 (8%)
5	SO4	E	911	-	4,4,4	0.20	0	6,6,6	0.40	0
5	SO4	A	912	-	4,4,4	0.17	0	6,6,6	0.21	0
6	MLA	G	921	-	6,6,6	1.17	0	7,7,7	1.24	0
5	SO4	E	913	-	4,4,4	0.18	0	6,6,6	0.16	0
6	MLA	D	921	-	6,6,6	1.30	0	7,7,7	1.10	0
3	LCN	A	903[A]	-	11,11,11	2.07	2 (18%)	9,15,15	0.91	1 (11%)
6	MLA	C	921	-	6,6,6	1.23	0	7,7,7	1.38	1 (14%)
2	UDP	E	901	-	24,26,26	0.99	1 (4%)	37,40,40	1.71	7 (18%)
4	NHF	A	904[B]	-	11,11,11	1.65	3 (27%)	12,15,15	1.09	1 (8%)
4	NHF	G	904[B]	-	11,11,11	1.80	3 (27%)	12,15,15	0.66	0
5	SO4	B	911	-	4,4,4	0.30	0	6,6,6	0.28	0
5	SO4	H	911	-	4,4,4	0.16	0	6,6,6	0.21	0
3	LCN	E	903[A]	-	11,11,11	1.96	1 (9%)	9,15,15	1.01	0
5	SO4	G	911	-	4,4,4	0.25	0	6,6,6	0.18	0
5	SO4	C	912	-	4,4,4	0.17	0	6,6,6	0.11	0
5	SO4	C	913	-	4,4,4	0.18	0	6,6,6	0.09	0
4	NHF	F	904[B]	-	11,11,11	1.81	4 (36%)	12,15,15	0.83	0
5	SO4	H	913	-	4,4,4	0.20	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UDP	B	901	-	24,26,26	0.97	0	37,40,40	1.85	8 (21%)
2	UDP	H	901	-	24,26,26	0.95	0	37,40,40	1.75	5 (13%)
5	SO4	D	913	-	4,4,4	0.18	0	6,6,6	0.12	0
5	SO4	C	911	-	4,4,4	0.13	0	6,6,6	0.25	0
3	LCN	C	903[A]	-	11,11,11	2.07	2 (18%)	9,15,15	0.98	1 (11%)
4	NHF	E	904[B]	-	11,11,11	1.75	3 (27%)	12,15,15	0.70	0
2	UDP	G	901	-	24,26,26	1.03	1 (4%)	37,40,40	1.52	7 (18%)
2	UDP	C	901	-	24,26,26	0.92	0	37,40,40	1.56	6 (16%)

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

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903[A]	LCN	O5-C5	-5.04	1.39	1.45
3	C	903[A]	LCN	O5-C5	-4.90	1.39	1.45
3	E	903[A]	LCN	O5-C5	-4.88	1.39	1.45
3	G	903[A]	LCN	O5-C5	-4.86	1.39	1.45
3	H	903[A]	LCN	O5-C5	-4.83	1.39	1.45

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	UDP	C4-N3-C2	-6.75	117.67	126.58
2	B	901	UDP	C4-N3-C2	-6.27	118.31	126.58
2	H	901	UDP	C4-N3-C2	-6.22	118.37	126.58
2	A	901	UDP	C4-N3-C2	-5.89	118.81	126.58
2	F	901	UDP	C4-N3-C2	-5.84	118.87	126.58

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	UDP	O4'-C4'-C5'-O5'
2	A	901	UDP	PA-O3A-PB-O2B
2	A	901	UDP	PA-O3A-PB-O3B
2	B	901	UDP	O4'-C4'-C5'-O5'
2	D	901	UDP	PA-O3A-PB-O2B

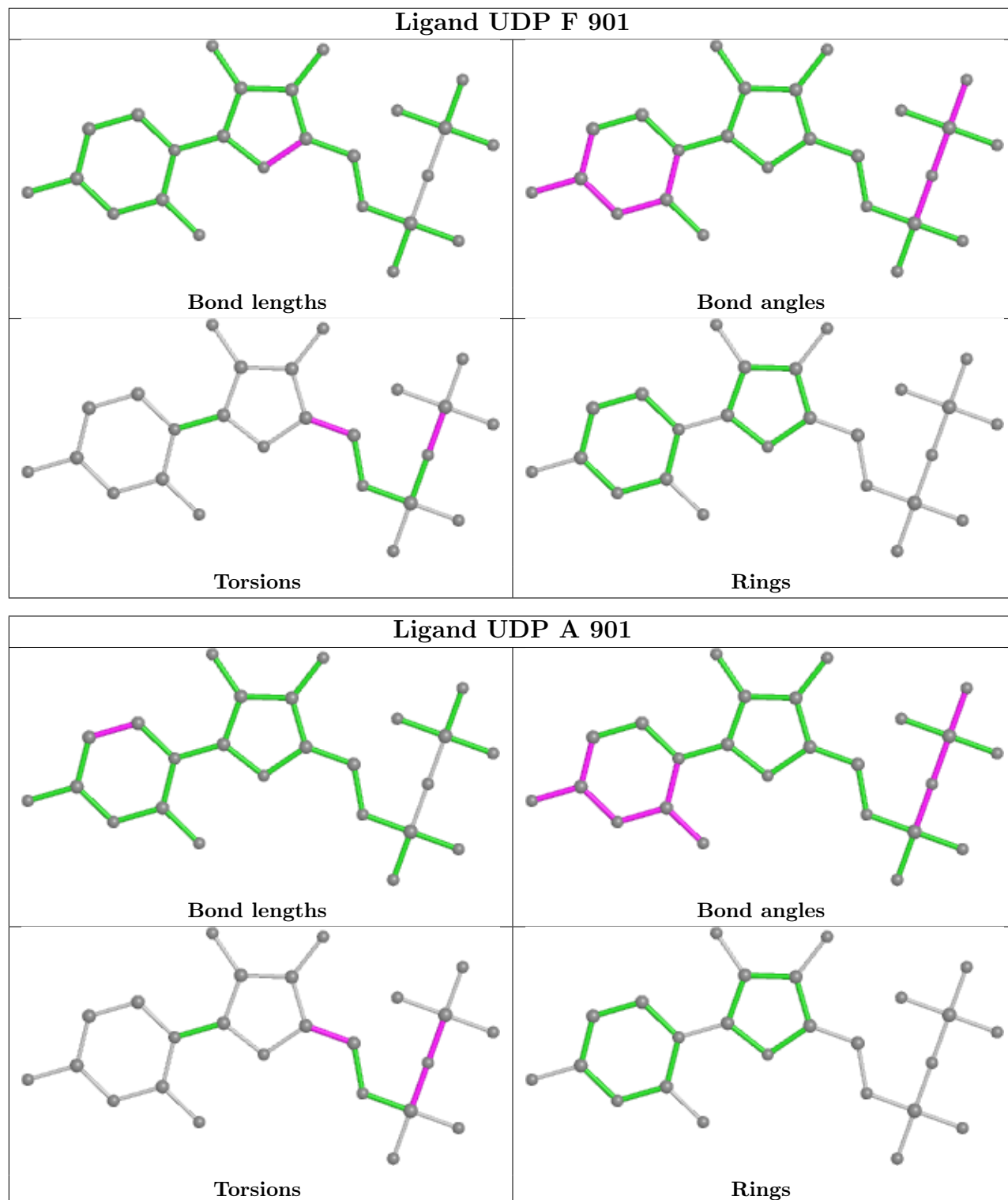
There are no ring outliers.

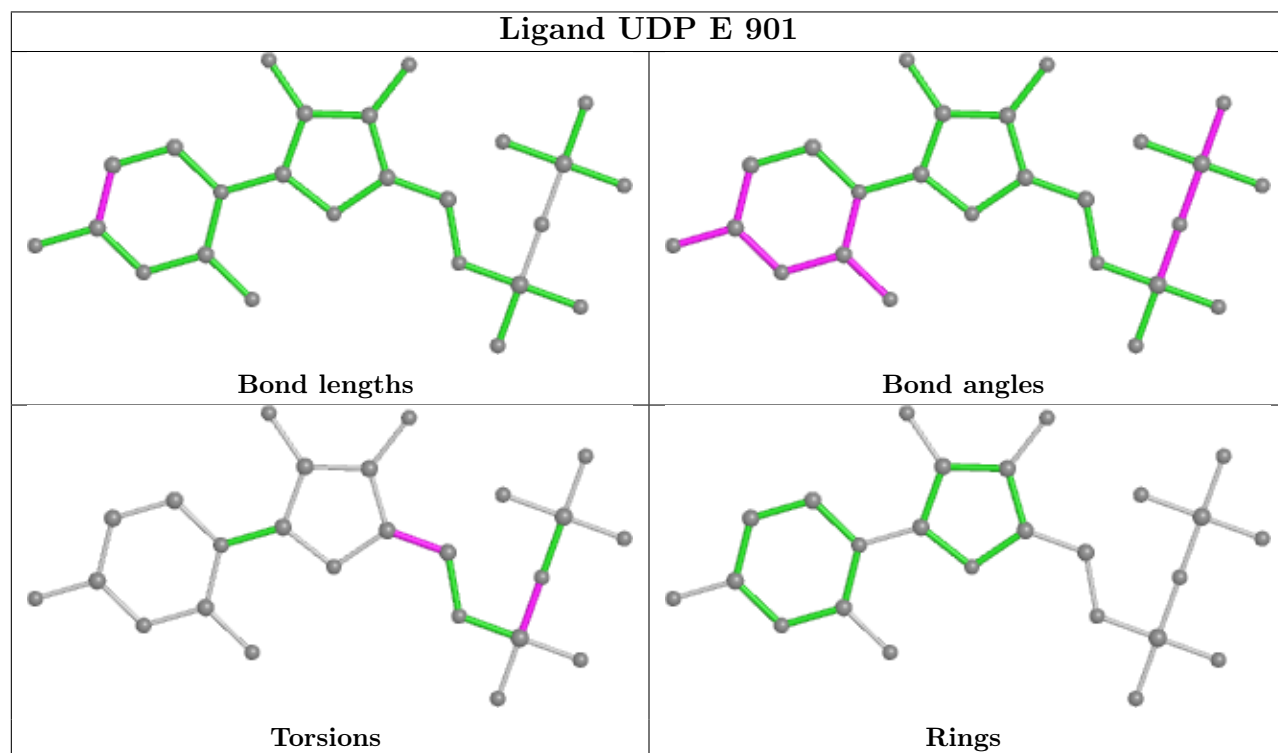
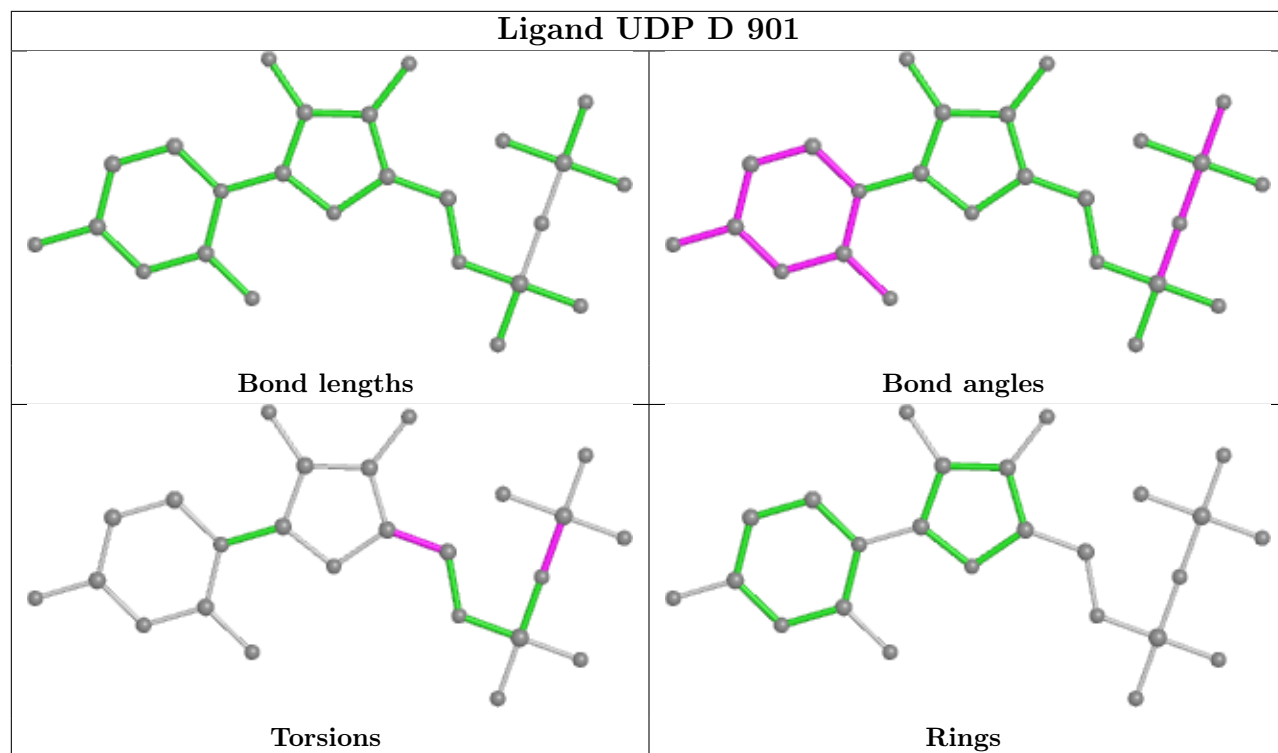
32 monomers are involved in 56 short contacts:

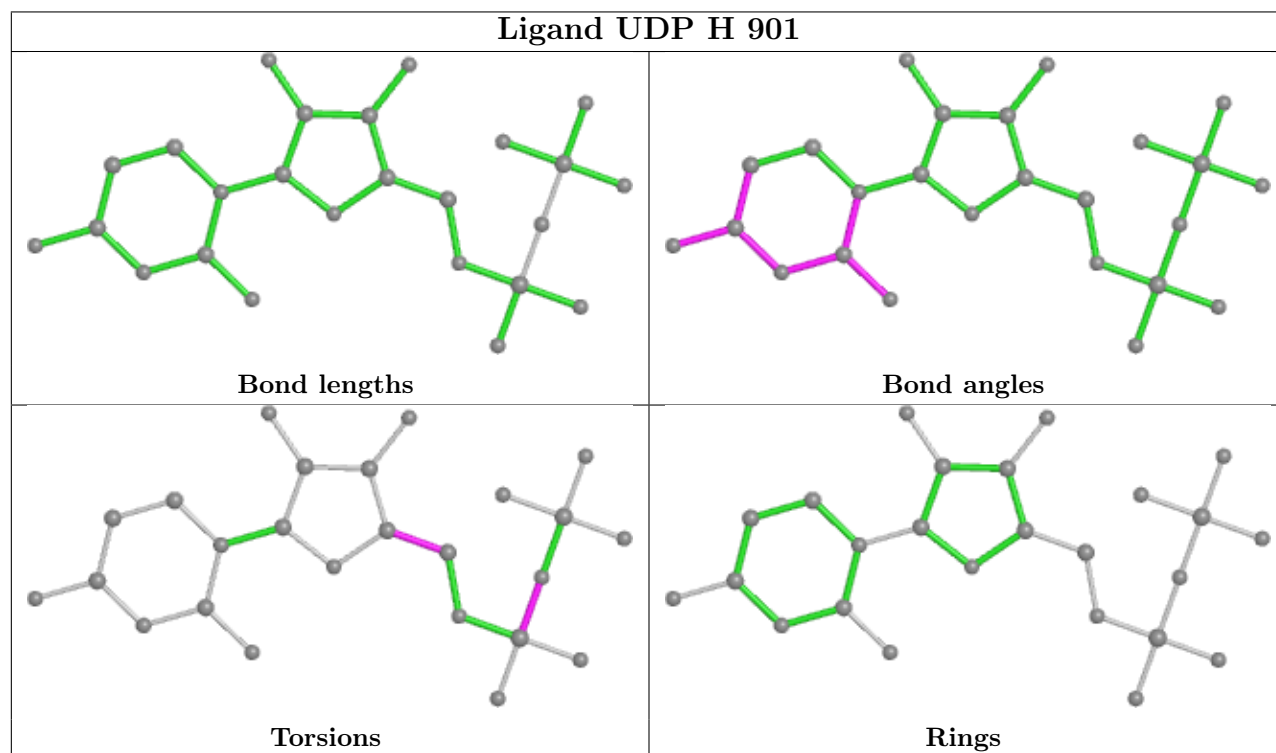
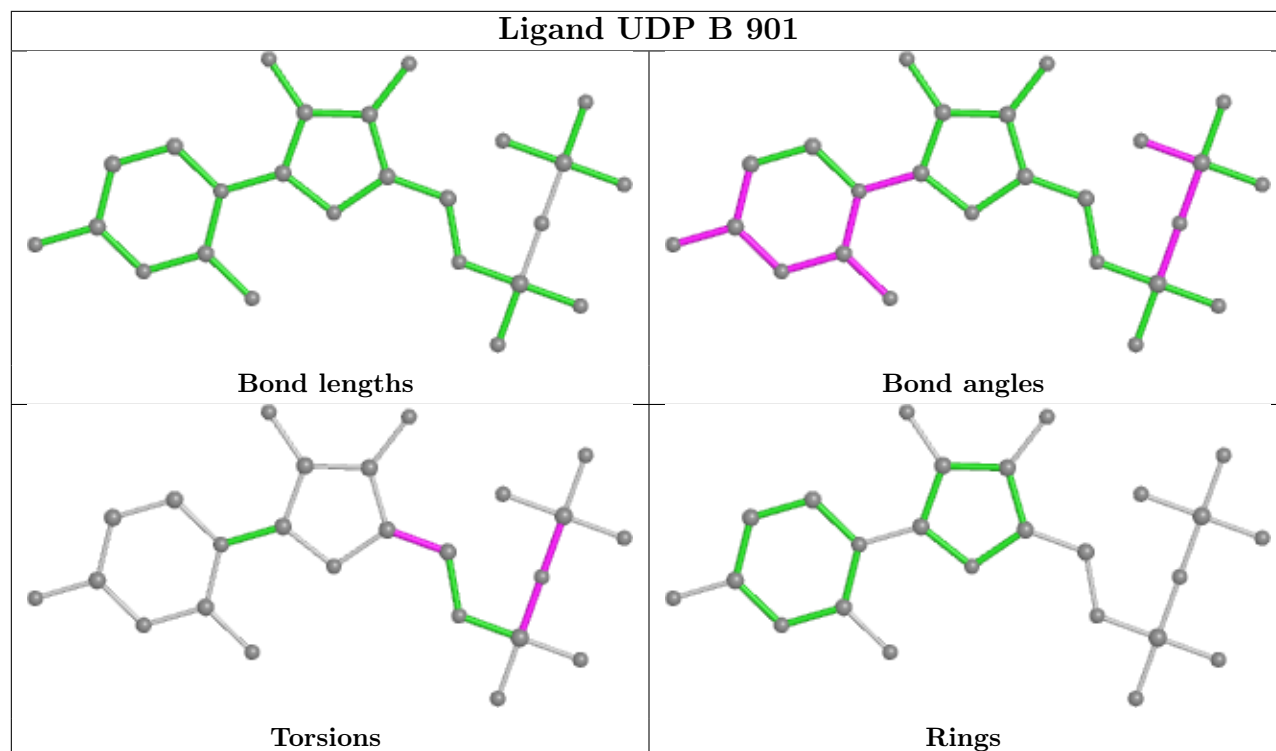
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	903[A]	LCN	1	0
5	E	912	SO4	1	0
4	D	904[B]	NHF	6	0
2	F	901	UDP	1	0
4	C	904[B]	NHF	1	0
4	H	904[B]	NHF	4	0
3	F	903[A]	LCN	1	0
5	B	912	SO4	1	0
5	B	913	SO4	4	0
3	D	903[A]	LCN	1	0
5	F	912	SO4	2	0
5	G	913	SO4	1	0
5	A	913	SO4	1	0
2	A	901	UDP	3	0
6	F	921	MLA	1	0
2	D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

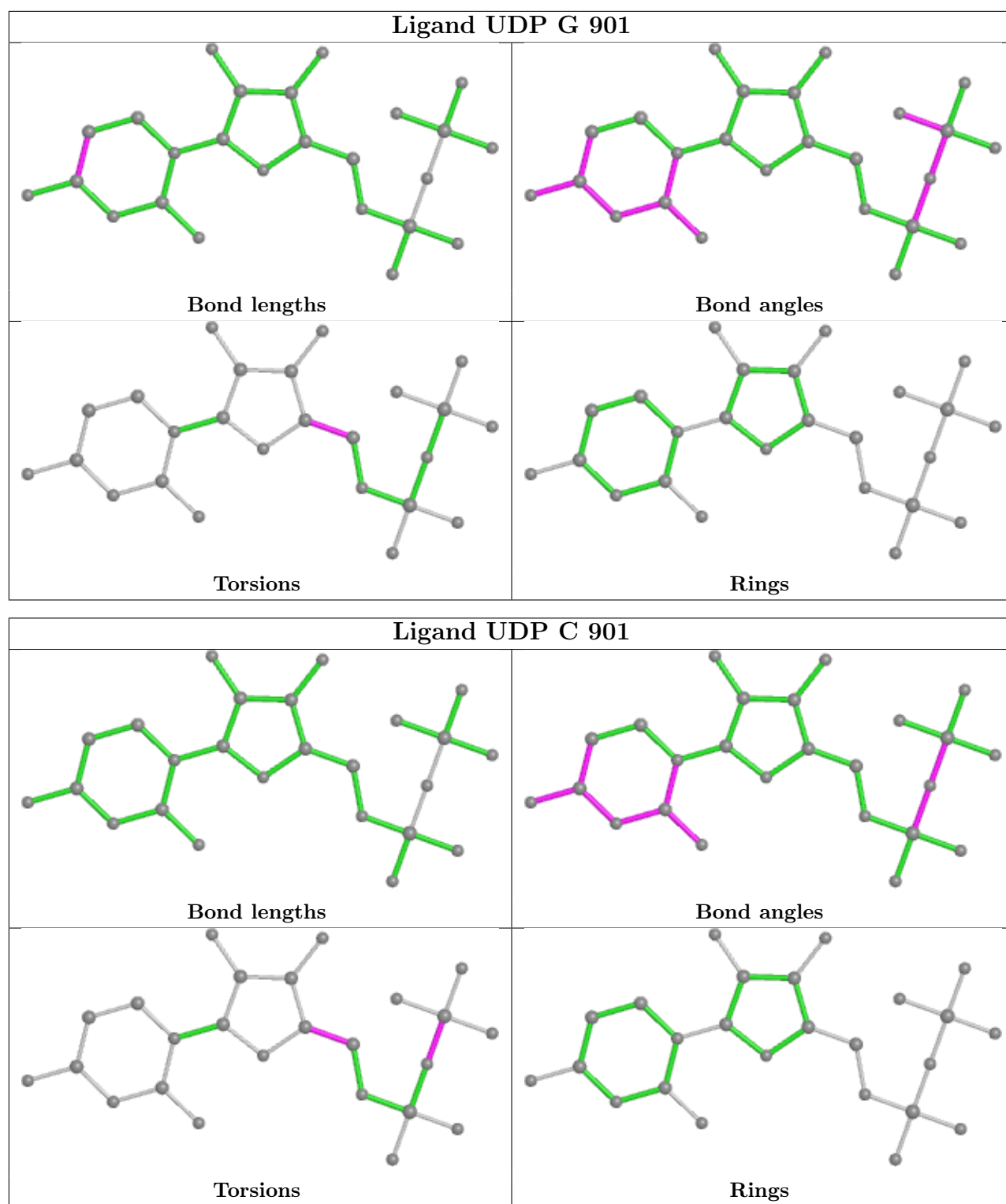
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.29	21 (2%) 54 44	19, 34, 105, 147	0
1	B	780/816 (95%)	-0.04	54 (6%) 16 10	23, 43, 130, 171	0
1	C	781/816 (95%)	-0.09	35 (4%) 33 23	30, 52, 101, 141	0
1	D	781/816 (95%)	-0.32	21 (2%) 54 44	22, 35, 92, 136	0
1	E	781/816 (95%)	-0.17	42 (5%) 25 17	23, 39, 116, 147	0
1	F	781/816 (95%)	-0.30	27 (3%) 44 34	17, 33, 84, 128	0
1	G	781/816 (95%)	-0.28	24 (3%) 49 39	22, 39, 81, 126	0
1	H	780/816 (95%)	-0.05	55 (7%) 16 9	26, 43, 127, 156	0
All	All	6246/6528 (95%)	-0.19	279 (4%) 33 23	17, 41, 105, 171	0

The worst 5 of 279 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	THR	11.7
1	B	106	ALA	8.8
1	H	83	PRO	8.6
1	C	106	ALA	7.7
1	B	58	GLU	7.4

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, 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
7	K	E	931	1/1	0.70	0.12	73,73,73,73	0
7	K	F	931	1/1	0.76	0.21	82,82,82,82	0
7	K	B	931	1/1	0.81	0.25	83,83,83,83	0
5	SO4	C	912	5/5	0.82	0.36	84,89,106,115	0
7	K	G	931	1/1	0.82	0.20	74,74,74,74	0
5	SO4	H	913	5/5	0.87	0.47	81,87,102,115	0
5	SO4	C	913	5/5	0.88	0.30	81,84,103,107	0
5	SO4	D	912	5/5	0.90	0.22	59,77,86,101	0
7	K	D	931	1/1	0.91	0.24	72,72,72,72	0
6	MLA	H	921	7/7	0.91	0.27	52,61,68,70	0
5	SO4	B	912	5/5	0.92	0.17	70,76,90,106	0
6	MLA	B	921	7/7	0.92	0.21	51,58,61,61	0
5	SO4	A	912	5/5	0.92	0.15	51,56,69,85	0
5	SO4	H	912	5/5	0.92	0.23	70,77,86,105	0
5	SO4	G	913	5/5	0.93	0.21	59,63,84,96	0
5	SO4	B	911	5/5	0.93	0.17	45,47,65,81	0
6	MLA	C	921	7/7	0.93	0.31	70,73,87,91	0
5	SO4	B	913	5/5	0.94	0.38	68,71,80,95	0
6	MLA	G	921	7/7	0.94	0.31	58,62,74,74	0
6	MLA	E	921	7/7	0.95	0.28	42,50,55,56	0
5	SO4	F	911	5/5	0.95	0.18	42,42,63,71	0
5	SO4	G	912	5/5	0.95	0.23	59,69,86,94	0
7	K	A	931	1/1	0.95	0.15	61,61,61,61	0
3	LCN	H	903[A]	11/11	0.95	0.13	32,34,41,41	21
7	K	C	931	1/1	0.95	0.25	81,81,81,81	0
5	SO4	A	911	5/5	0.95	0.20	35,43,59,63	0
3	LCN	D	903[A]	11/11	0.95	0.16	24,27,32,32	21
5	SO4	D	913	5/5	0.95	0.22	46,47,69,73	0
5	SO4	E	913	5/5	0.95	0.28	56,63,79,86	0
7	K	H	931	1/1	0.95	0.13	69,69,69,69	0
5	SO4	F	912	5/5	0.96	0.15	55,58,68,85	0
3	LCN	A	903[A]	11/11	0.96	0.14	23,25,29,30	21
5	SO4	E	911	5/5	0.96	0.21	44,48,60,65	0
5	SO4	E	912	5/5	0.96	0.16	57,62,70,86	0
5	SO4	D	911	5/5	0.96	0.22	43,47,64,77	0
4	NHF	E	904[B]	11/11	0.96	0.15	27,29,34,35	21
4	NHF	H	904[B]	11/11	0.97	0.13	32,34,40,41	21

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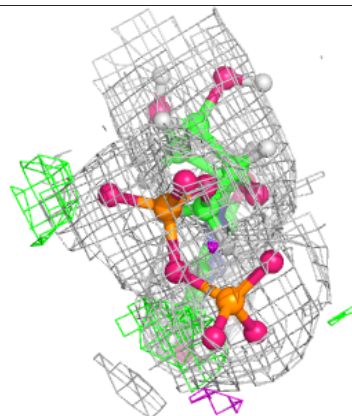
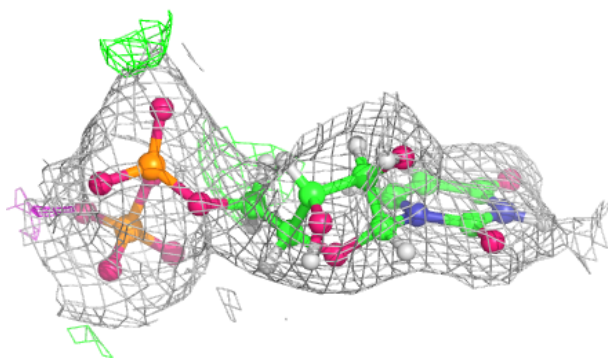
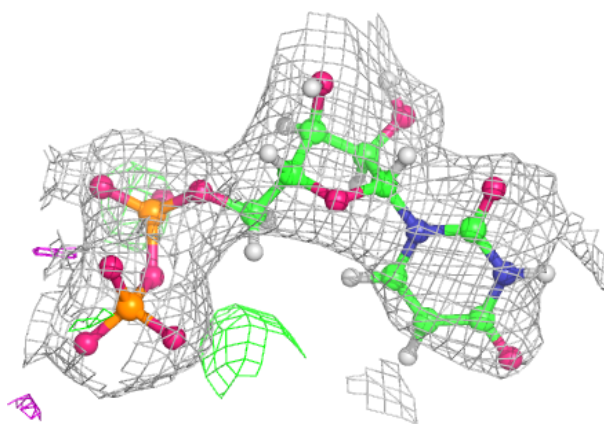
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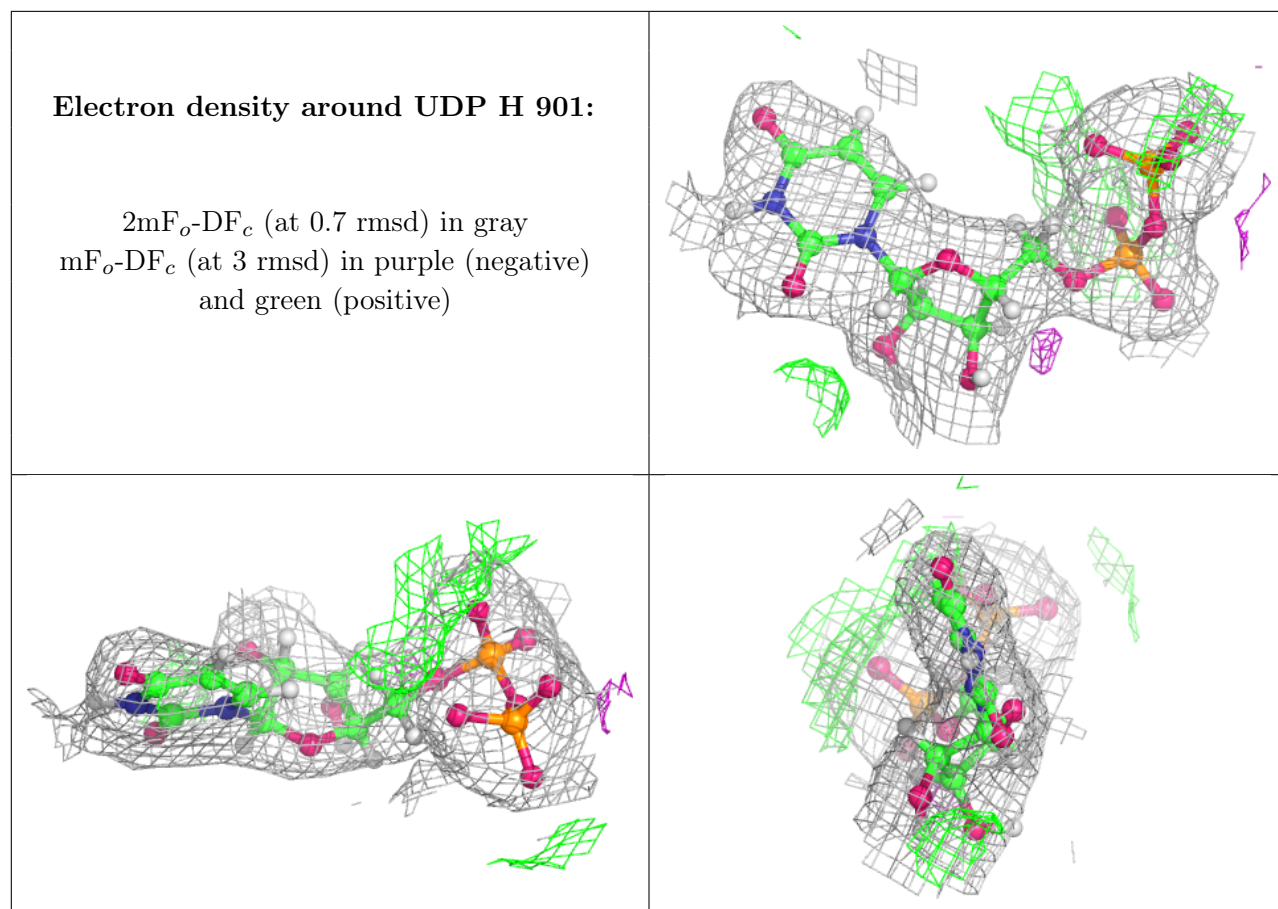
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	C	911	5/5	0.97	0.14	48,51,70,71	0
5	SO4	H	911	5/5	0.97	0.17	44,47,65,70	0
3	LCN	C	903[A]	11/11	0.97	0.13	36,39,46,48	21
4	NHF	D	904[B]	11/11	0.97	0.14	24,27,32,32	21
3	LCN	G	903[A]	11/11	0.97	0.16	25,28,33,34	21
4	NHF	G	904[B]	11/11	0.97	0.16	26,27,32,33	21
6	MLA	D	921	7/7	0.97	0.22	33,40,44,46	0
5	SO4	F	913	5/5	0.97	0.18	49,51,53,70	0
6	MLA	F	921	7/7	0.97	0.22	33,38,42,43	0
4	NHF	C	904[B]	11/11	0.98	0.13	37,38,45,47	21
2	UDP	C	901	25/25	0.98	0.17	32,41,49,54	0
3	LCN	E	903[A]	11/11	0.98	0.14	26,30,35,36	21
3	LCN	F	903[A]	11/11	0.98	0.13	23,27,31,33	21
6	MLA	A	921	7/7	0.98	0.24	31,38,42,42	0
3	LCN	B	903[A]	11/11	0.98	0.15	29,32,37,39	21
2	UDP	H	901	25/25	0.98	0.18	28,34,41,44	0
4	NHF	B	904[B]	11/11	0.98	0.15	29,32,37,38	21
5	SO4	G	911	5/5	0.98	0.13	35,41,56,61	0
5	SO4	A	913	5/5	0.98	0.19	44,50,74,74	0
4	NHF	A	904[B]	11/11	0.99	0.10	23,25,29,30	21
2	UDP	E	901	25/25	0.99	0.17	21,27,35,38	0
2	UDP	F	901	25/25	0.99	0.15	16,23,29,34	0
2	UDP	G	901	25/25	0.99	0.15	20,28,34,41	0
2	UDP	B	901	25/25	0.99	0.14	23,31,37,43	0
4	NHF	F	904[B]	11/11	0.99	0.14	24,25,30,32	21
2	UDP	A	901	25/25	0.99	0.14	18,23,29,32	0
2	UDP	D	901	25/25	0.99	0.15	22,28,34,39	0

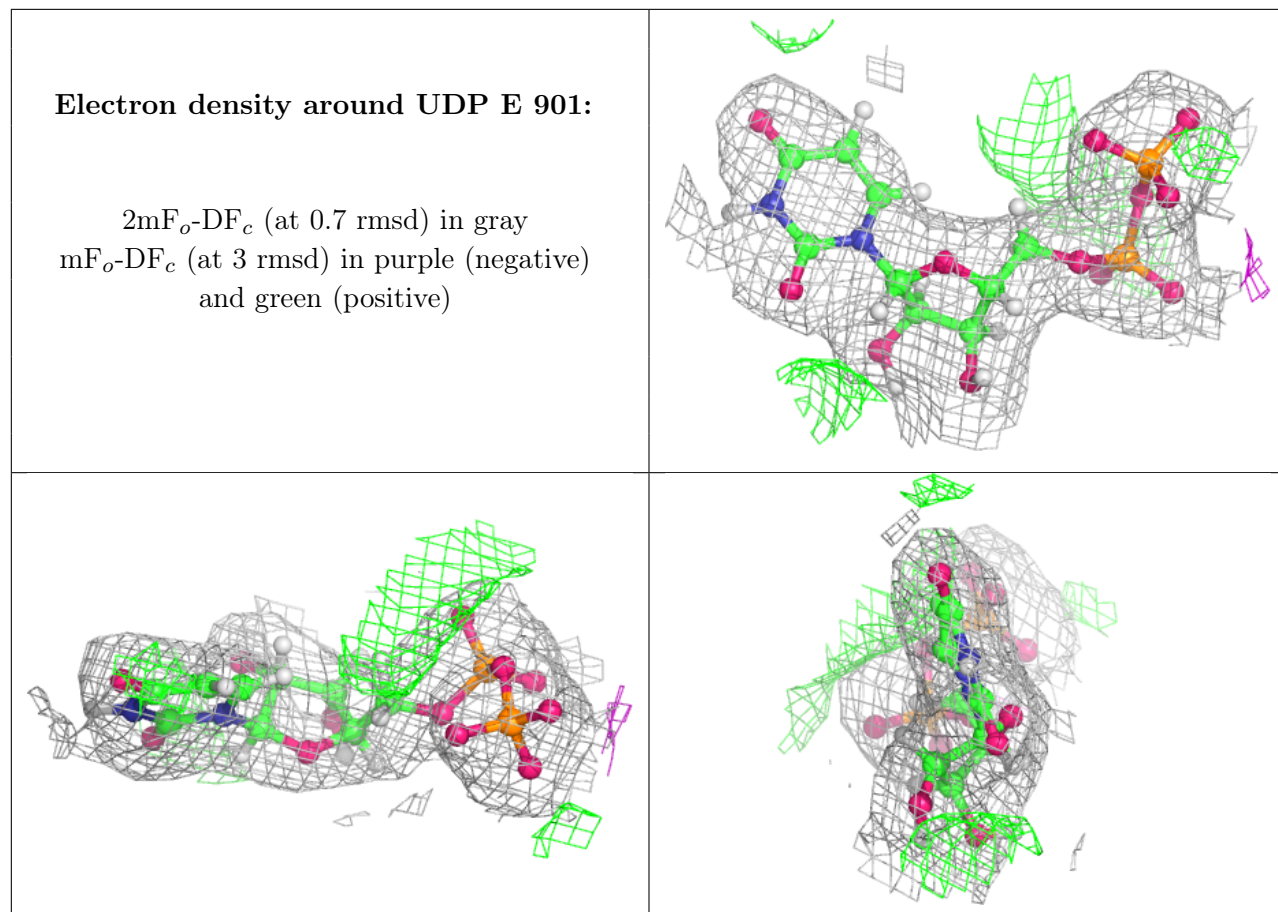
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

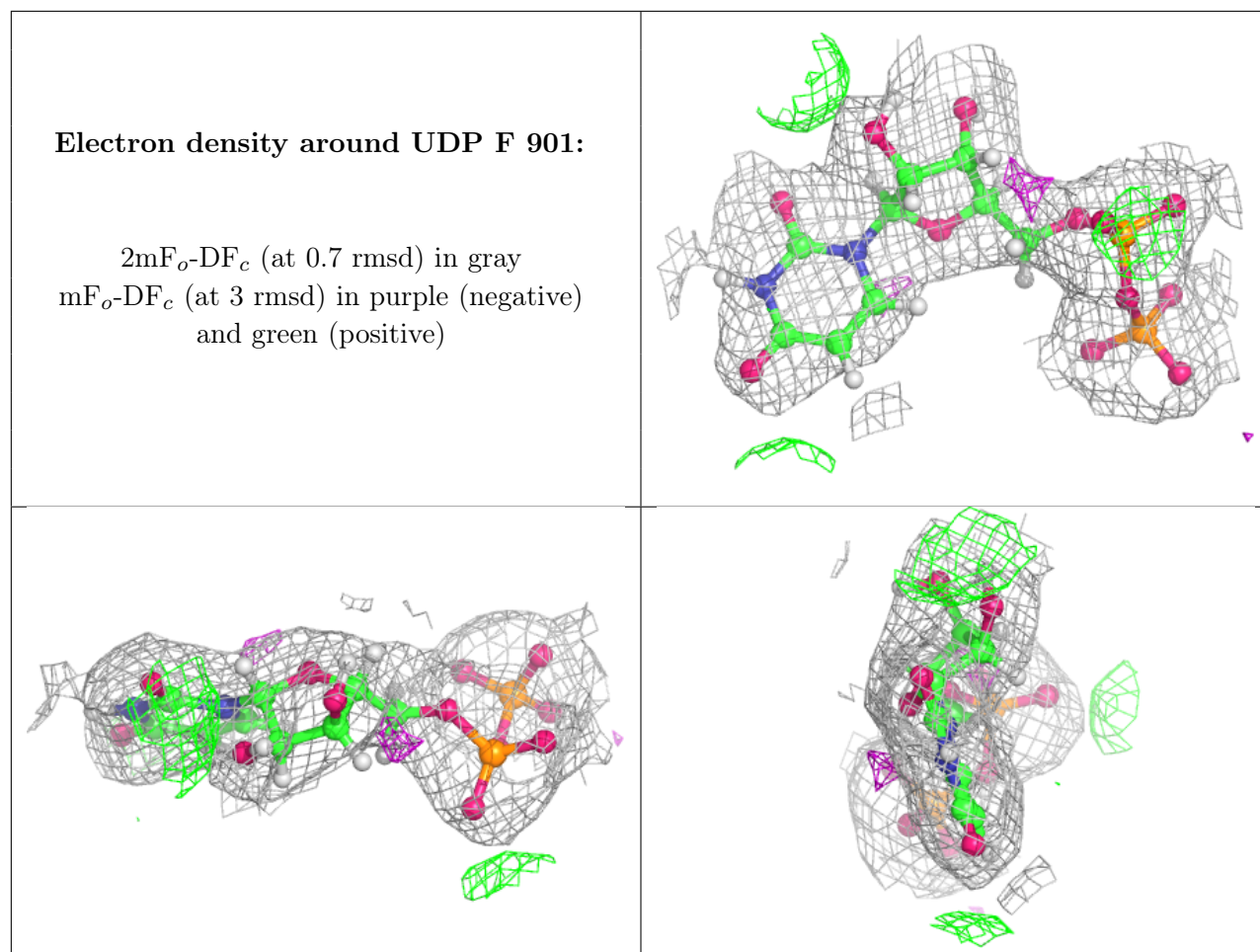
Electron density around UDP C 901:

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



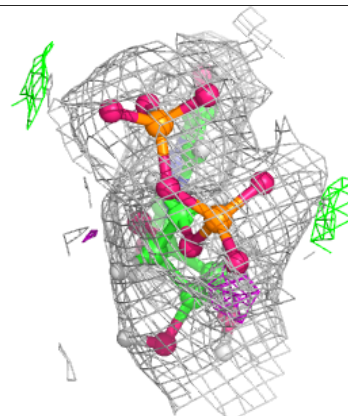
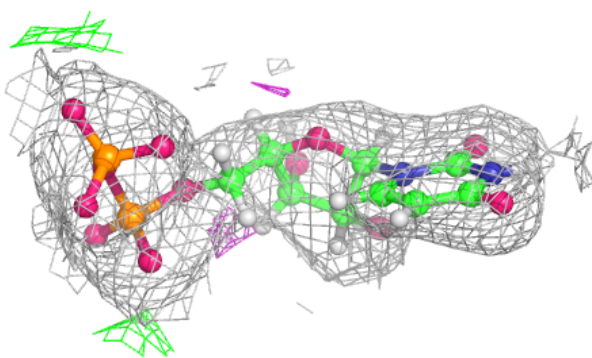
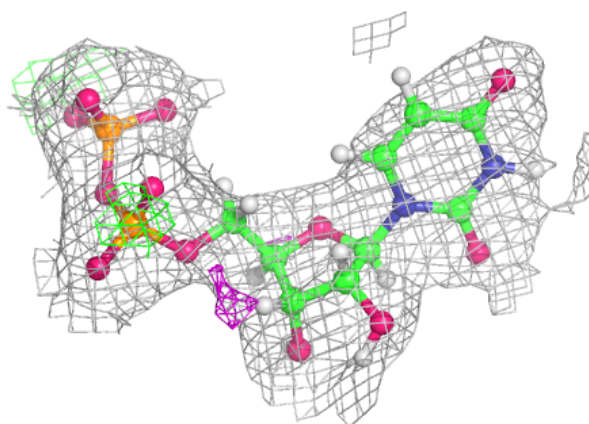


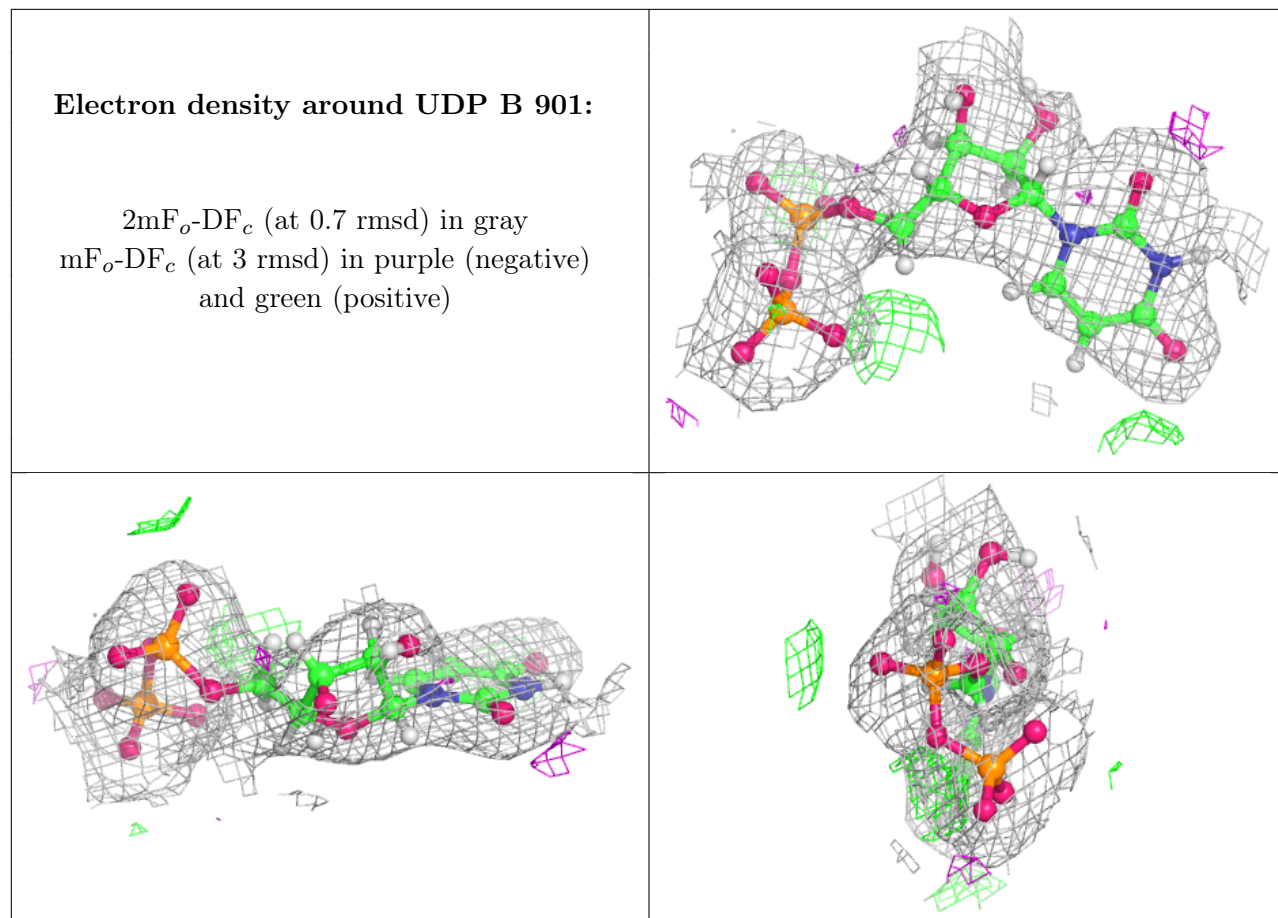




Electron density around UDP G 901:

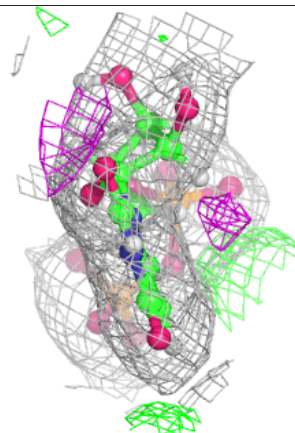
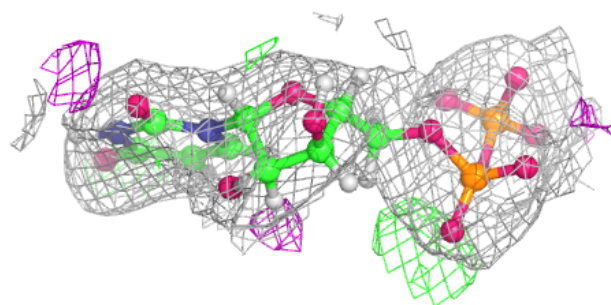
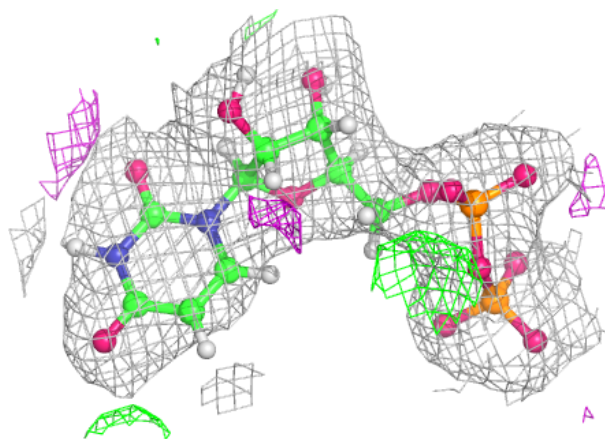
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

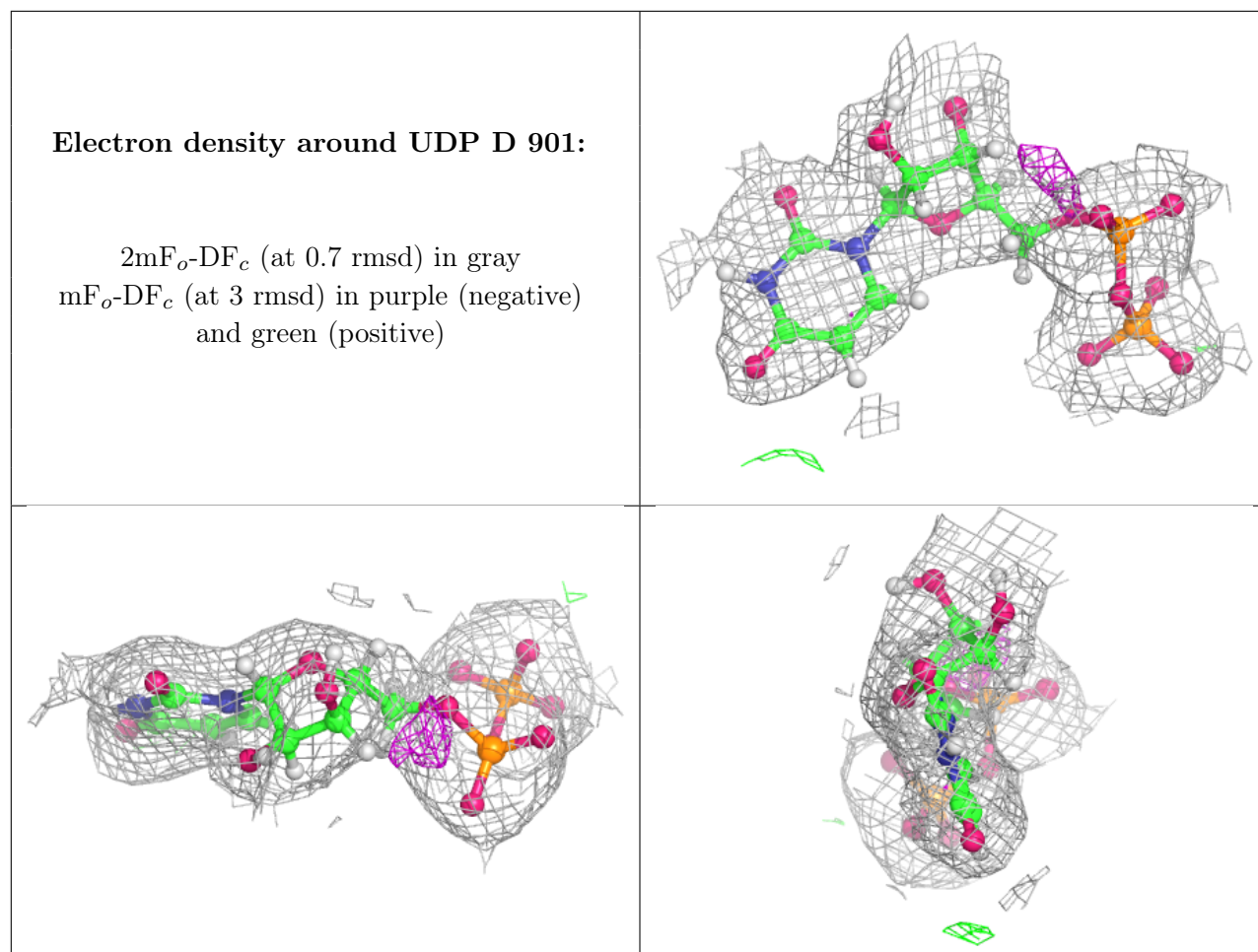




Electron density around UDP A 901:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.