wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 05:10 PM EDT

PDB ID	:	3S27
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 (i) 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 (i)) were used in the production of this report:

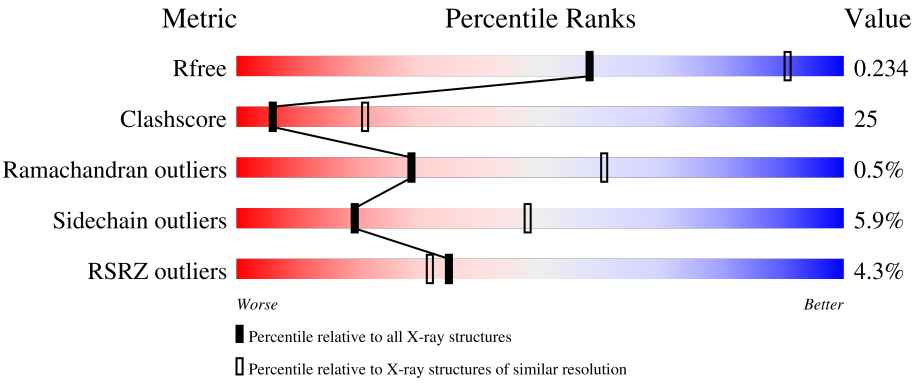
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (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 <=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	3% 58% 34%
1	B	816	7% 58% 36%
1	C	816	3% 54% 38%
1	D	816	3% 60% 34%
1	E	816	4% 60% 31%

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Mol	Chain	Length	Quality of chain
1	F	816	3% 59% 33%
1	G	816	2% 60% 32%
1	H	816	7% 61% 34%

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 (i)

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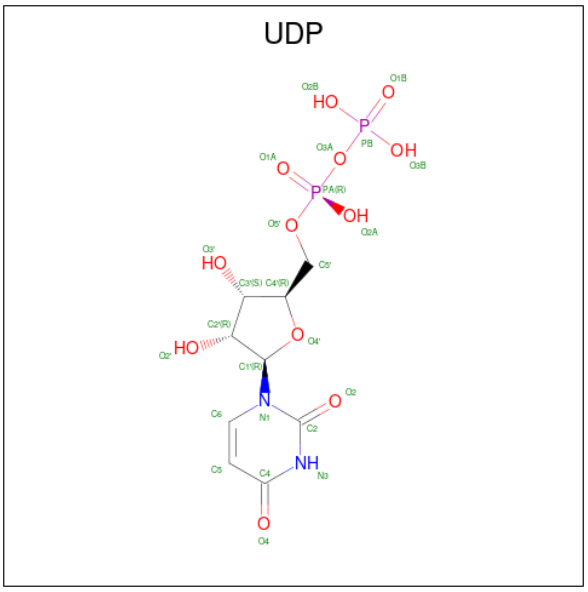
Chain	Residue	Modelled	Actual	Comment	Reference
G	816	HIS	-	expression tag	UNP P49040
H	809	VAL	-	expression tag	UNP P49040
H	810	GLU	-	expression tag	UNP P49040
H	811	HIS	-	expression tag	UNP P49040
H	812	HIS	-	expression tag	UNP P49040
H	813	HIS	-	expression tag	UNP P49040
H	814	HIS	-	expression tag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

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



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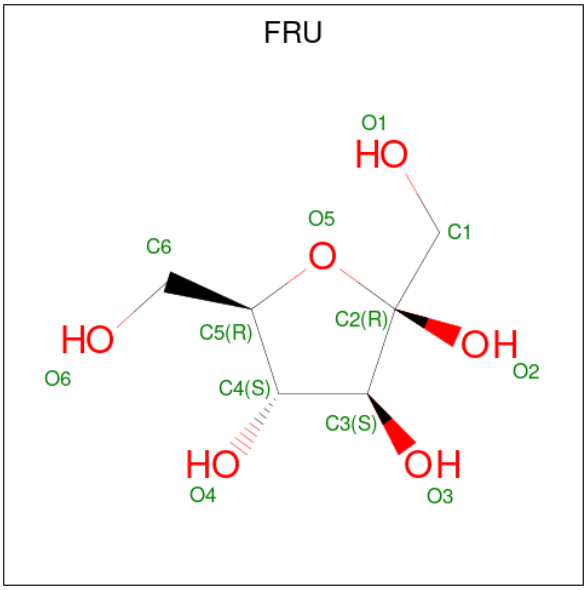
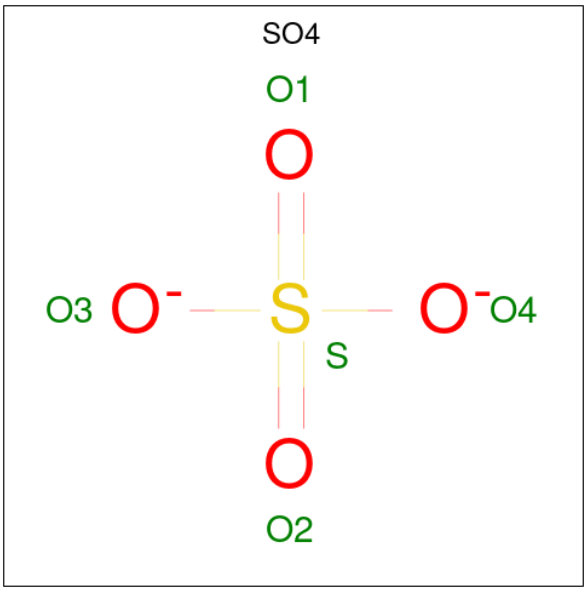
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	H	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		

- Molecule 3 is beta-D-fructofuranose (three-letter code: FRU) (formula: $C_6H_{12}O_6$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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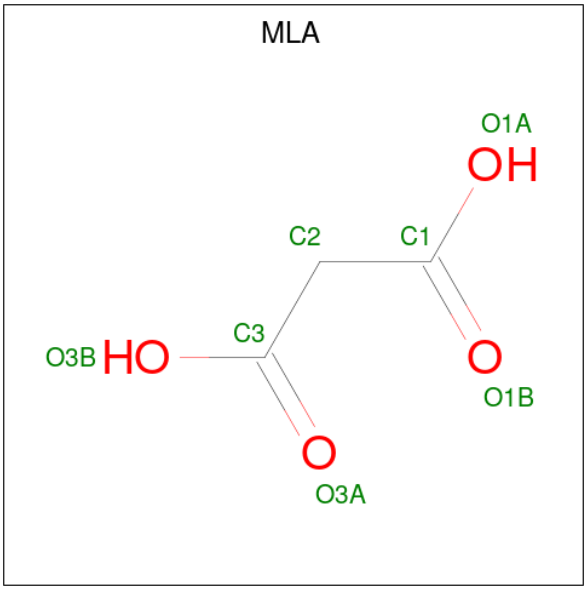
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



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

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 7 is water.

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

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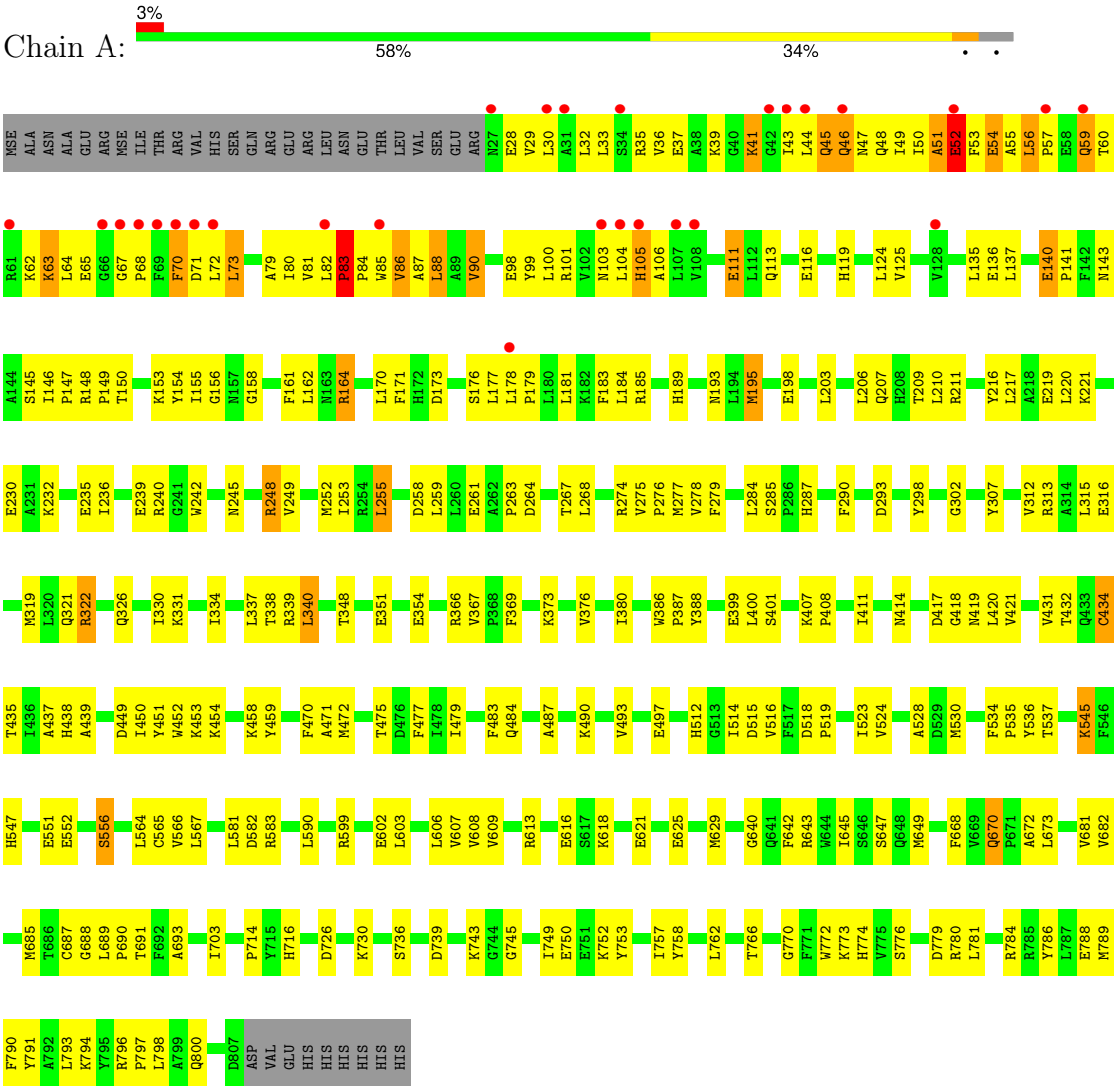
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	45	Total O 45 45	0	0
7	D	67	Total O 67 67	0	0
7	E	66	Total O 66 66	0	0
7	F	90	Total O 90 90	0	0
7	G	81	Total O 81 81	0	0
7	H	60	Total O 60 60	0	0

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.

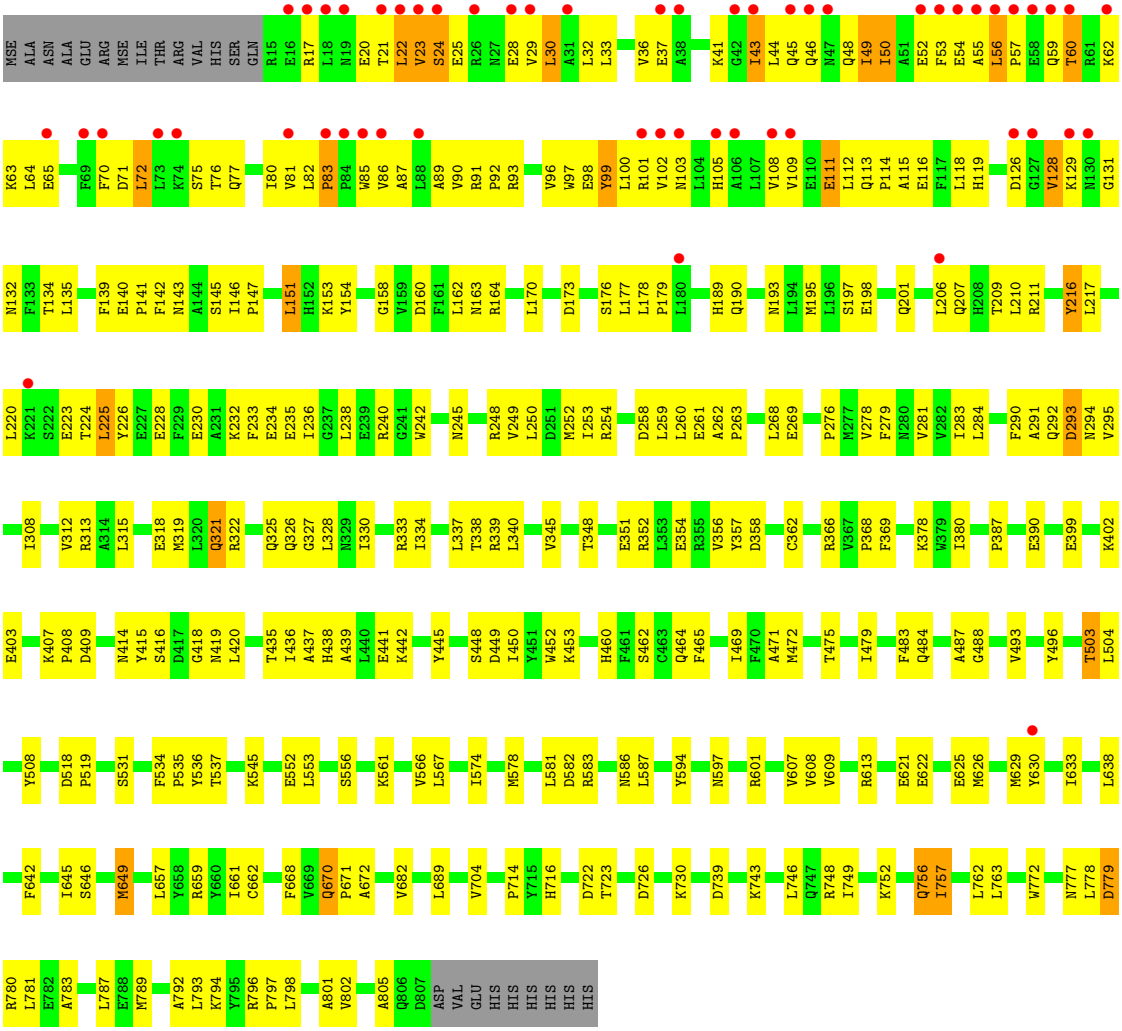
• Molecule 1: Sucrose synthase 1

Chain A:



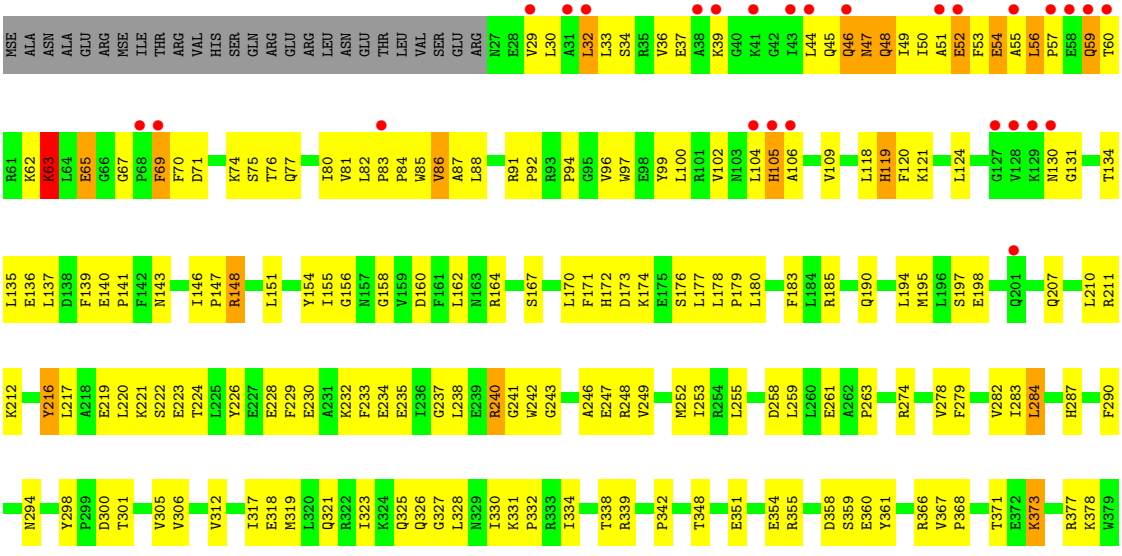
• Molecule 1: Sucrose synthase 1

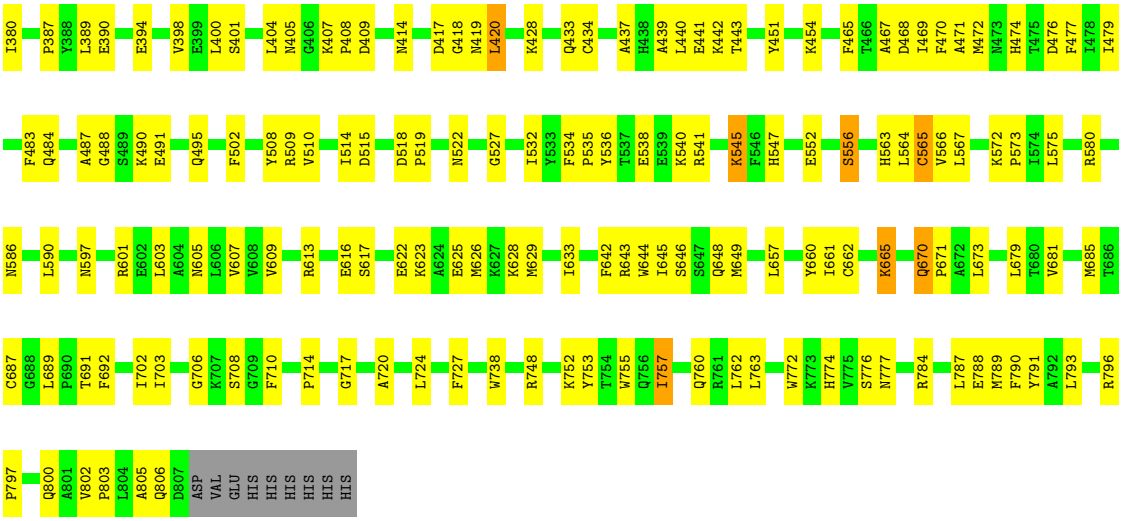
Chain B:



• Molecule 1: Sucrose synthase 1

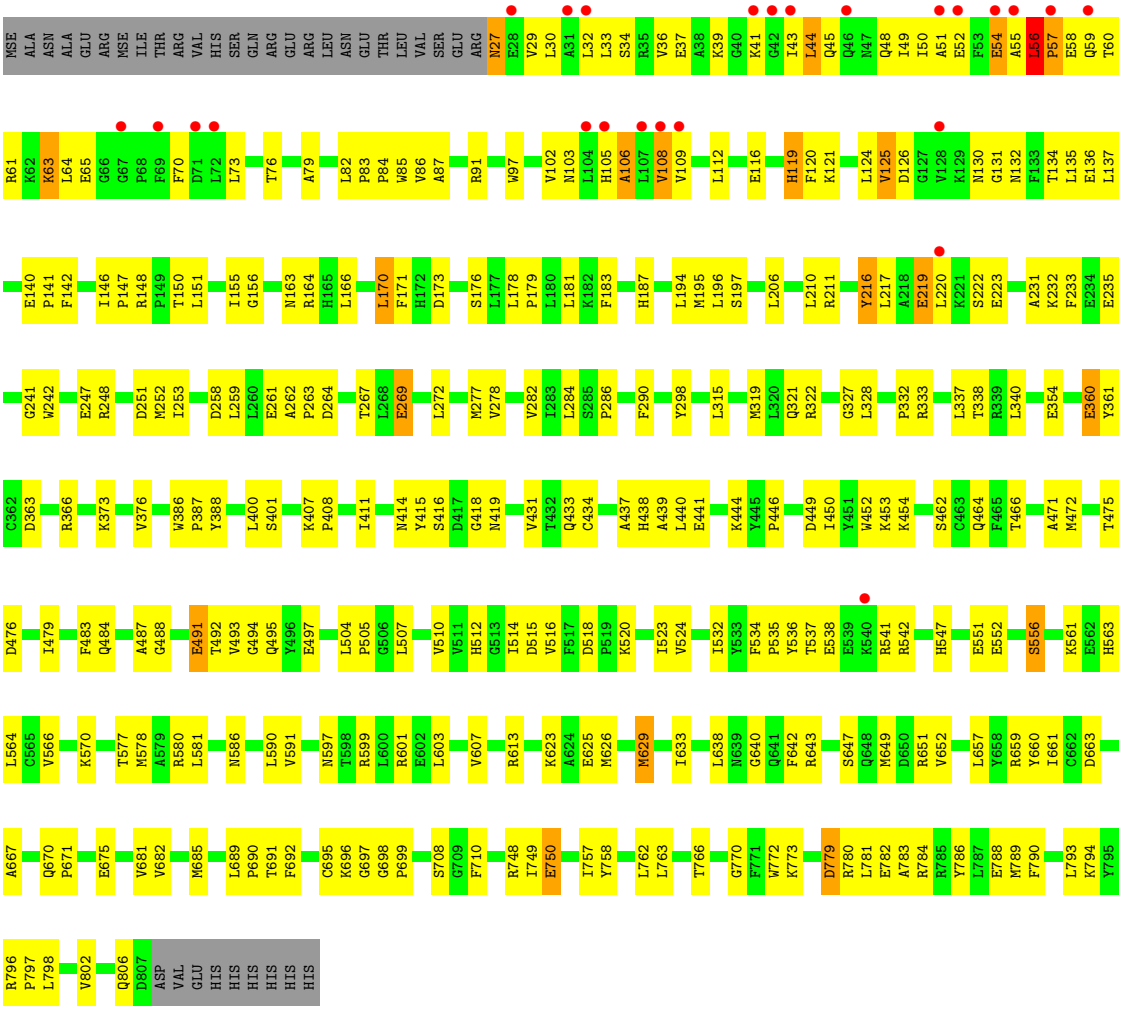
Chain C:





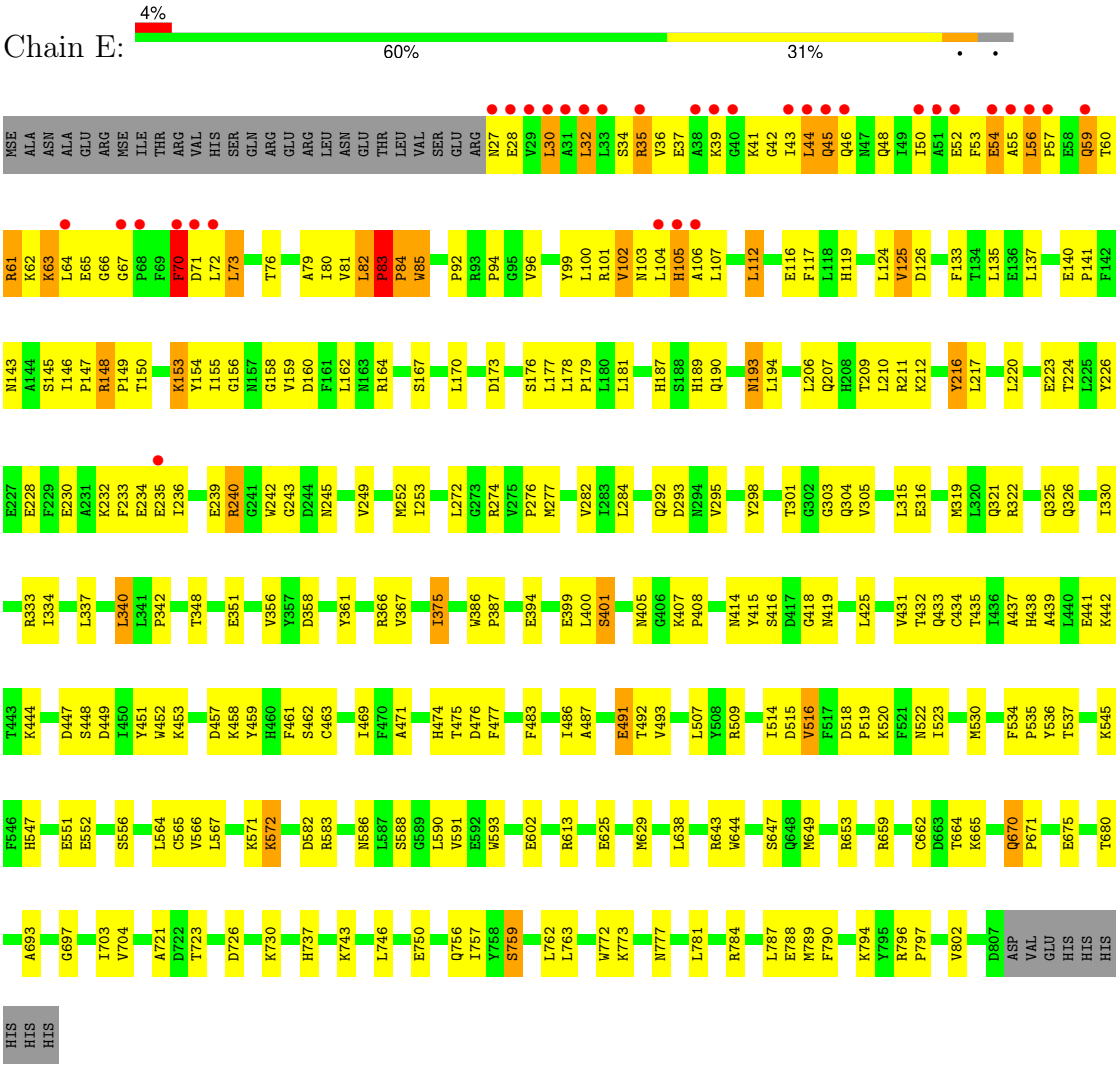
• Molecule 1: Sucrose synthase 1

Chain D:



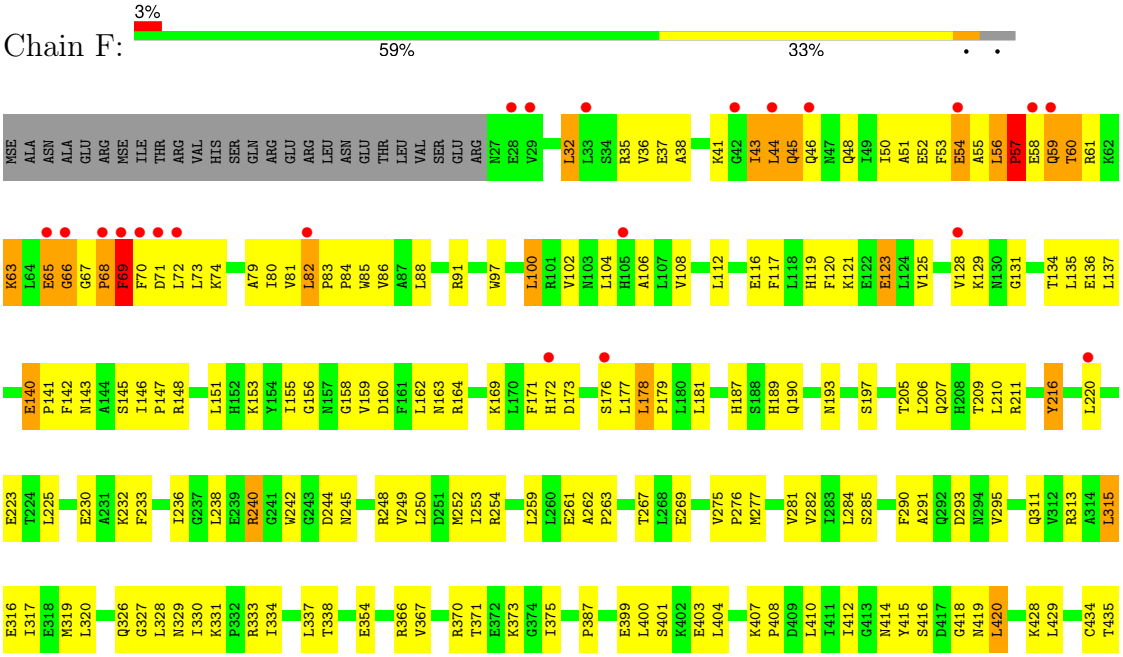
• Molecule 1: Sucrose synthase 1

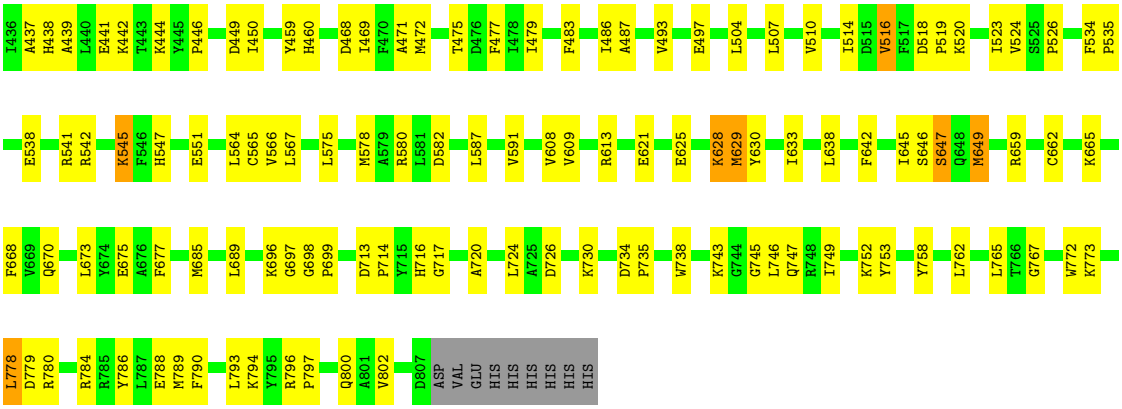
Chain E:



• Molecule 1: Sucrose synthase 1

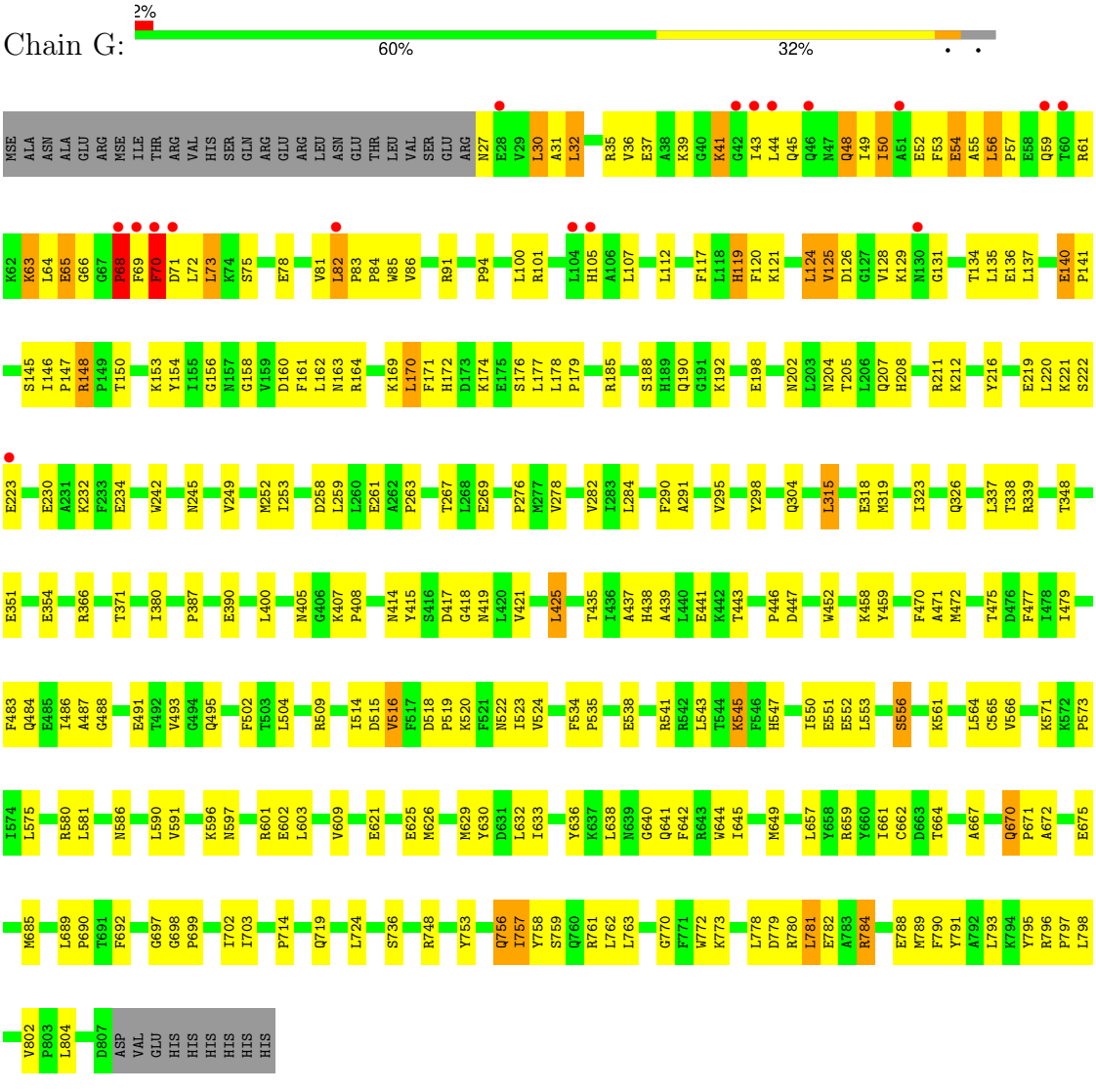
Chain F:





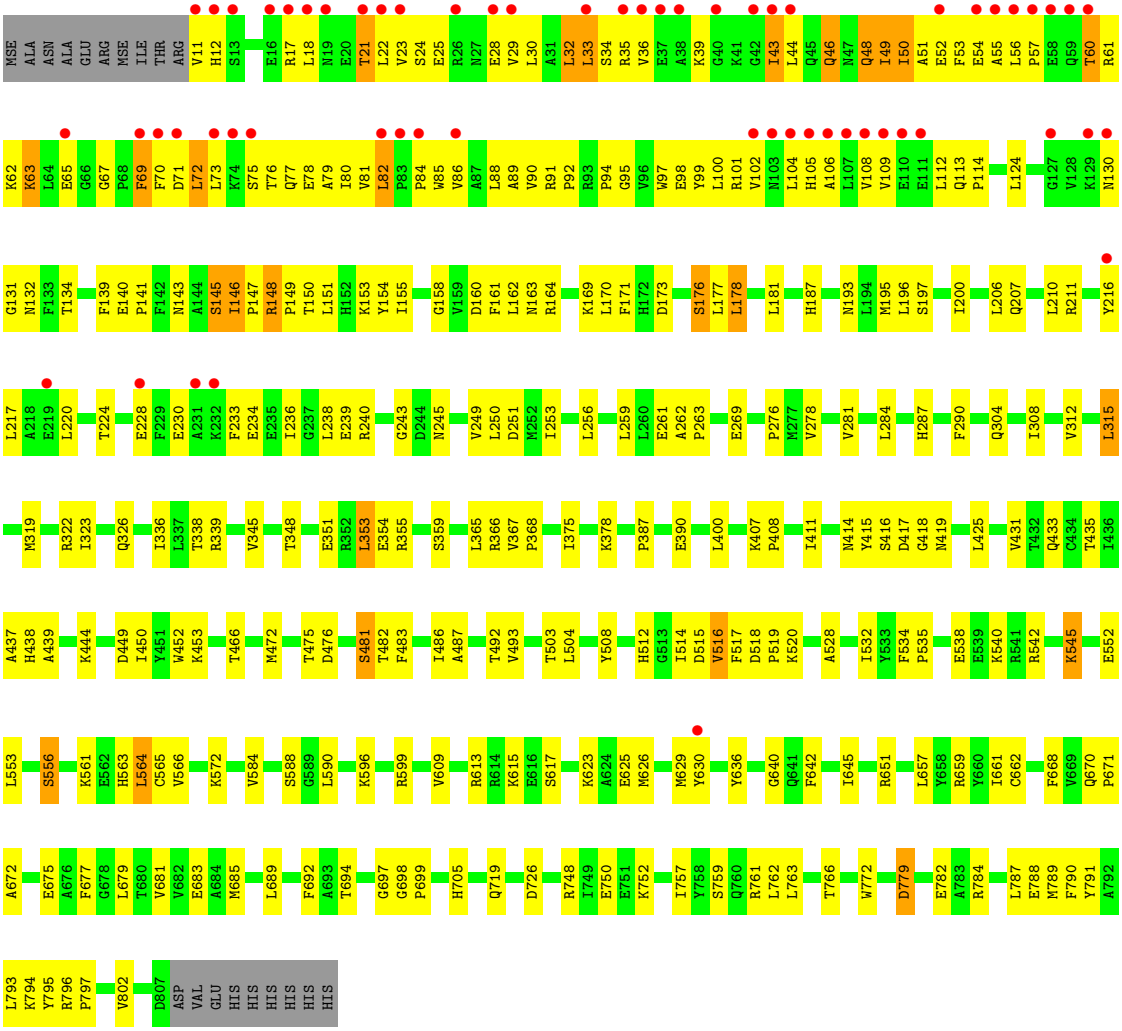
• Molecule 1: Sucrose synthase 1

Chain G:



• Molecule 1: Sucrose synthase 1

Chain H:


MSE ALA ASN ALA GLU ARG MSE ILE THR ARG V11 H12 S13 E16 R17 L18 N19 E20 T21 L22 V23 S24 E25 R26 N27 E28 V29 L30 A31 L32 L33 S34 R35 V36 E37 A38 K39 G40 K41 G42 I43 L44 Q45 Q46 N47 Q48 I49 I50 A51 E52 F53 E54 A55 L56 P57 E58 Q59 T60 R61
K62 K63 L64 E65 G66 G67 P68 F69 F70 D71 L72 L73 K74 S75 T76 Q77 E78 A79 I80 V81 L82 P83 P84 W85 V86 A87 L88 A89 V90 R91 P92 R93 P94 G95 V96 W97 E98 Y99 L100 R101 V102 N103 L104 H105 A106 L107 V108 V109 E110 E111 L112 Q113 P114 L124 G127 V128 K129 N130
G131 N132 F133 T134 F139 E140 P141 F142 N143 A144 S145 I146 P147 R148 P149 T150 L151 H152 K153 Y154 I155 G158 V159 D160 F161 L162 N163 R164 K169 L170 F171 H172 D173 S176 L177 L178 L181 H187 N193 L194 M195 L196 S197 I200 L206 Q207 L210 R211 Y216
L217 A218 E219 L220 T224 E228 F229 E230 A231 K232 F233 E234 E235 I236 G237 L238 E239 R240 G243 D244 N245 V249 L250 D251 M252 I253 L256 L259 L260 E261 A262 P263 E269 P276 M277 V278 V281 L284 H287 F290 Q304 I308 V312 L315
M319 R322 I323 Q326 I336 L337 T338 R339 V345 T348 E351 R352 L353 E354 R355 S359 L365 R366 V367 P368 I375 K378 P387 E390 L400 K407 P408 I411 N414 Y415 S416 D417 G418 N419 L425 V431 T432 Q433 C434 T435 I436
A437 H438 A439 K444 D449 I450 Y451 W452 K453 T466 M472 T475 D476 S481 T482 F483 I486 A487 T492 V493 T503 L504 Y508 H512 G513 I514 D515 V516 F517 D518 P519 K520 A528 I532 Y533 F534 P535 E538 E539 K540 R541 R542 K545 E552
L553 S556 K561 E562 H563 L564 C565 V566 K572 V584 S588 G589 L590 K596 R599 V609 R613 R614 K615 E616 S617 K623 A624 E625 M626 M629 Y630 Y636 G640 Q641 F642 I645 R651 L657 Y658 R659 Y660 I661 C662 F668 V669 Q670 P671
A672 E675 A676 F677 G678 L679 T680 V681 V682 E683 A684 M685 L689 F692 A693 T694 G697 G698 P699 H705 Q719 D726 R748 I749 E750 E751 K752 I757 Y758 S759 Q760 R761 L762 L763 T766 W772 D779 E782 A783 R784 L787 E788 M789 F790 Y791 A792
L793 K794 Y795 R796 P797 V802 D807 ASP VAL GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 49.68 – 2.91	Depositor EDS
% Data completeness (in resolution range)	91.0 (25.00-2.91) 90.8 (49.68-2.91)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.33 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FRU, K, UDP, MLA, SO4

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	0.40	0/6412	0.56	0/8664
1	B	0.37	0/6447	0.55	0/8717
1	C	0.36	0/6403	0.55	0/8654
1	D	0.39	0/6378	0.57	0/8624
1	E	0.39	0/6383	0.56	0/8629
1	F	0.41	0/6410	0.59	0/8663
1	G	0.38	0/6414	0.56	0/8667
1	H	0.37	0/6471	0.55	0/8749
All	All	0.38	0/51318	0.56	0/69367

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.

There are no bond angle outliers.

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 (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	6277	0	6191	319	0
1	B	6313	0	6170	321	0
1	C	6268	0	6189	314	0
1	D	6243	0	6143	311	0
1	E	6249	0	6158	348	0
1	F	6275	0	6195	360	0
1	G	6279	0	6201	329	0
1	H	6336	0	6196	308	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2497	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 25.

The worst 5 of 2497 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%)	29	60
1	B	791/816 (97%)	734 (93%)	56 (7%)	1 (0%)	51	81
1	C	779/816 (96%)	734 (94%)	42 (5%)	3 (0%)	34	65
1	D	779/816 (96%)	736 (94%)	38 (5%)	5 (1%)	25	57
1	E	779/816 (96%)	737 (95%)	38 (5%)	4 (0%)	29	60
1	F	779/816 (96%)	734 (94%)	39 (5%)	6 (1%)	19	49
1	G	779/816 (96%)	736 (94%)	39 (5%)	4 (0%)	29	60
1	H	795/816 (97%)	750 (94%)	42 (5%)	3 (0%)	34	65
All	All	6260/6528 (96%)	5891 (94%)	339 (5%)	30 (0%)	29	60

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 (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	667/704 (95%)	626 (94%)	41 (6%)	18	46
1	B	663/704 (94%)	626 (94%)	37 (6%)	21	50
1	C	666/704 (95%)	622 (93%)	44 (7%)	16	42
1	D	659/704 (94%)	624 (95%)	35 (5%)	22	53
1	E	662/704 (94%)	620 (94%)	42 (6%)	18	44
1	F	668/704 (95%)	635 (95%)	33 (5%)	25	56
1	G	668/704 (95%)	626 (94%)	42 (6%)	18	44
1	H	663/704 (94%)	623 (94%)	40 (6%)	19	47
All	All	5316/5632 (94%)	5002 (94%)	314 (6%)	19	48

5 of 314 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	778	LEU
1	H	61	ARG
1	G	56	LEU
1	G	516	VAL
1	H	417	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	806	GLN
1	H	204	ASN
1	F	59	GLN
1	H	189	HIS
1	H	705	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 monosaccharides 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	$\#\|Z\| > 2$
4	SO4	H	911	-	4,4,4	0.36	0	6,6,6	0.25	0
4	SO4	C	912	-	4,4,4	0.27	0	6,6,6	0.15	0
5	MLA	G	921	-	6,6,6	1.08	0	7,7,7	1.52	1 (14%)
4	SO4	G	913	-	4,4,4	0.29	0	6,6,6	0.13	0
4	SO4	F	911	-	4,4,4	0.37	0	6,6,6	0.41	0
4	SO4	E	911	-	4,4,4	0.33	0	6,6,6	0.41	0
5	MLA	C	921	-	6,6,6	1.15	0	7,7,7	1.42	1 (14%)
4	SO4	A	913	-	4,4,4	0.30	0	6,6,6	0.31	0
4	SO4	B	913	-	4,4,4	0.36	0	6,6,6	0.29	0
3	FRU	H	902	-	11,12,12	0.85	1 (9%)	10,18,18	1.06	0
4	SO4	D	911	-	4,4,4	0.32	0	6,6,6	0.28	0
4	SO4	D	912	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	A	911	-	4,4,4	0.33	0	6,6,6	0.19	0
4	SO4	G	912	-	4,4,4	0.29	0	6,6,6	0.08	0
5	MLA	F	921	-	6,6,6	1.34	0	7,7,7	1.11	0
5	MLA	H	921	-	6,6,6	1.14	0	7,7,7	1.32	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	B	911	-	4,4,4	0.39	0	6,6,6	0.25	0
4	SO4	B	912	-	4,4,4	0.33	0	6,6,6	0.24	0
3	FRU	C	902	-	11,12,12	0.70	1 (9%)	10,18,18	0.91	0
2	UDP	A	901	-	25,26,26	1.04	0	38,40,40	1.71	6 (15%)
5	MLA	A	921	-	6,6,6	1.14	0	7,7,7	1.38	1 (14%)
3	FRU	D	902	-	11,12,12	0.91	0	10,18,18	1.19	2 (20%)
2	UDP	B	901	-	25,26,26	1.02	1 (4%)	38,40,40	1.82	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MLA	B	921	-	6,6,6	1.31	0	7,7,7	1.06	0
3	FRU	F	902	-	11,12,12	0.73	0	10,18,18	0.75	0
5	MLA	E	921	-	6,6,6	1.27	0	7,7,7	0.94	0
3	FRU	G	902	-	11,12,12	0.70	0	10,18,18	0.76	0
4	SO4	C	911	-	4,4,4	0.26	0	6,6,6	0.22	0
4	SO4	E	912	-	4,4,4	0.33	0	6,6,6	0.14	0
4	SO4	C	913	-	4,4,4	0.30	0	6,6,6	0.14	0
4	SO4	H	913	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	G	911	-	4,4,4	0.36	0	6,6,6	0.17	0
3	FRU	A	902	-	11,12,12	0.74	0	10,18,18	0.79	0
5	MLA	D	921	-	6,6,6	1.12	0	7,7,7	1.23	0
2	UDP	E	901	-	25,26,26	1.03	1 (4%)	38,40,40	1.56	6 (15%)
3	FRU	B	902	-	11,12,12	0.79	1 (9%)	10,18,18	0.86	0
2	UDP	H	901	-	25,26,26	1.02	0	38,40,40	1.75	6 (15%)
2	UDP	G	901	-	25,26,26	0.97	0	38,40,40	1.57	6 (15%)
2	UDP	C	901	-	25,26,26	1.06	1 (4%)	38,40,40	1.63	7 (18%)
3	FRU	E	902	-	11,12,12	0.73	0	10,18,18	0.84	0
4	SO4	D	913	-	4,4,4	0.33	0	6,6,6	0.10	0
2	UDP	F	901	-	25,26,26	1.00	1 (4%)	38,40,40	1.81	8 (21%)
4	SO4	E	913	-	4,4,4	0.36	0	6,6,6	0.19	0
4	SO4	F	913	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	H	912	-	4,4,4	0.30	0	6,6,6	0.13	0
4	SO4	F	912	-	4,4,4	0.31	0	6,6,6	0.30	0

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

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

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

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(^{o})	Ideal(^{o})
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

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

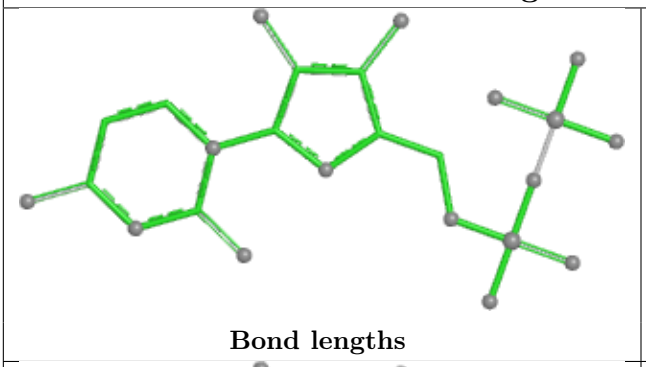
There are no ring outliers.

20 monomers are involved in 33 short contacts:

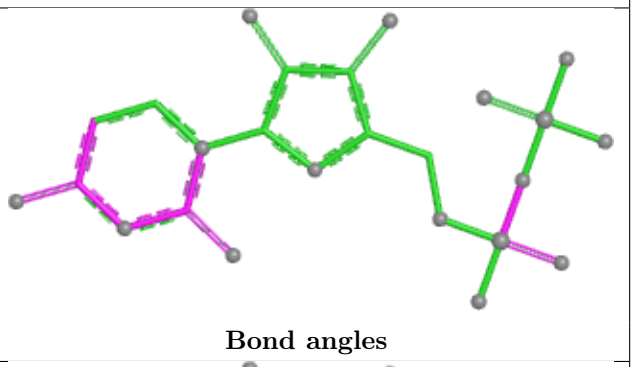
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	913	SO4	1	0
4	A	913	SO4	1	0
4	B	913	SO4	2	0
3	H	902	FRU	1	0
2	D	901	UDP	2	0
4	B	912	SO4	1	0
3	C	902	FRU	1	0
5	B	921	MLA	1	0
3	F	902	FRU	1	0
5	E	921	MLA	5	0
3	G	902	FRU	4	0
4	E	912	SO4	1	0
4	H	913	SO4	1	0
3	A	902	FRU	1	0
2	E	901	UDP	4	0
2	G	901	UDP	1	0
2	C	901	UDP	1	0
3	E	902	FRU	1	0
2	F	901	UDP	1	0
4	F	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

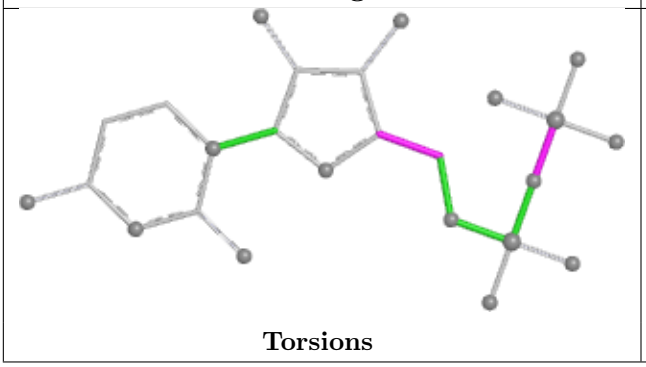
Ligand UDP D 901



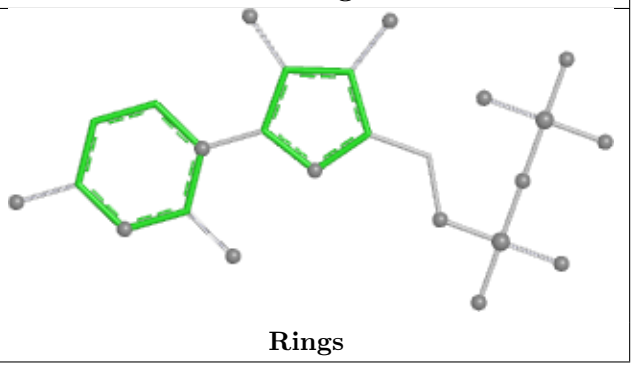
Bond lengths



Bond angles

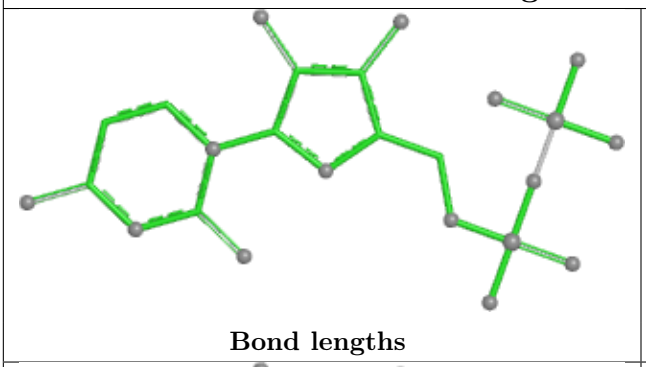


Torsions

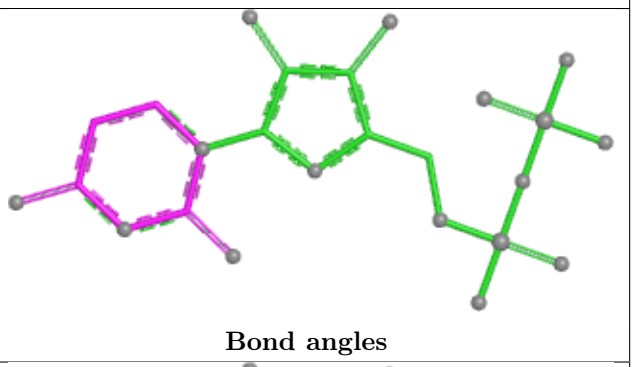


Rings

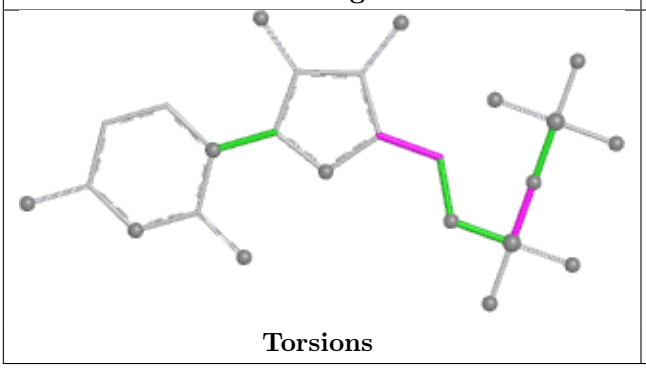
Ligand UDP A 901



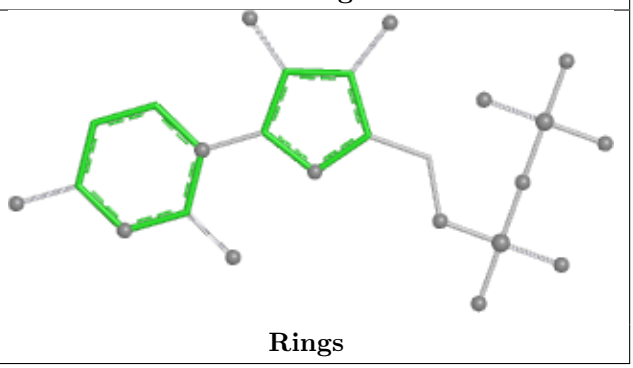
Bond lengths



Bond angles

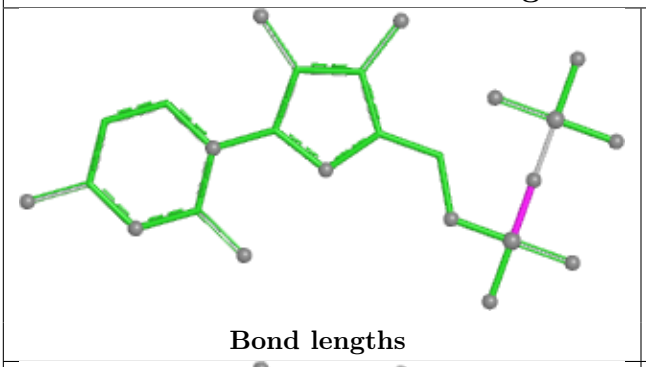


Torsions

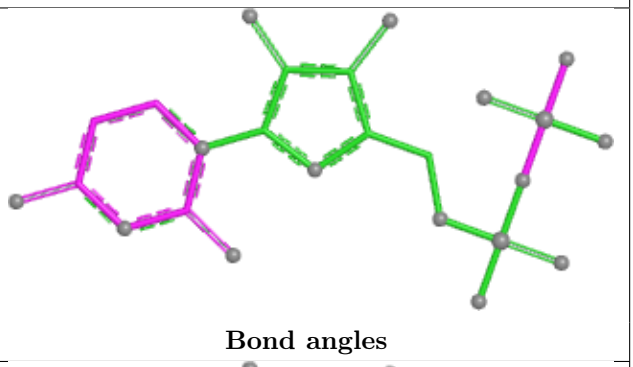


Rings

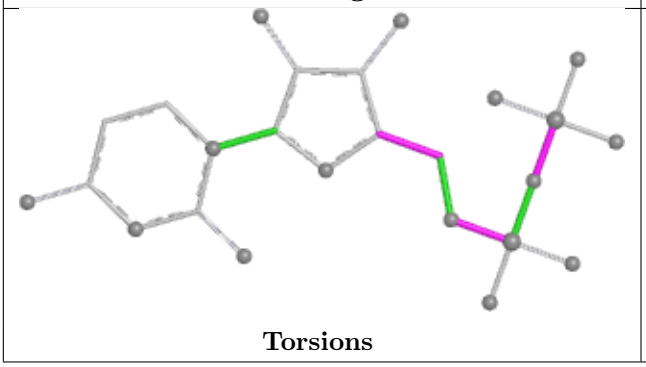
Ligand UDP B 901



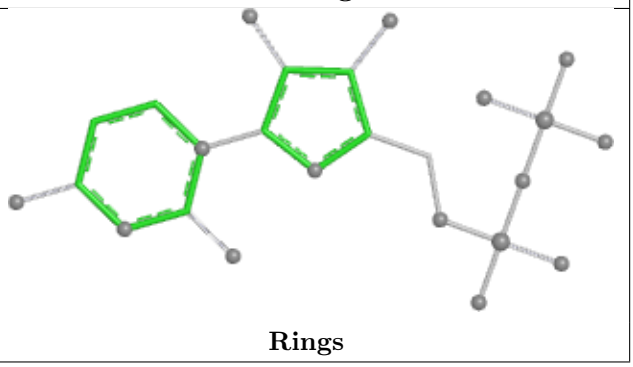
Bond lengths



Bond angles

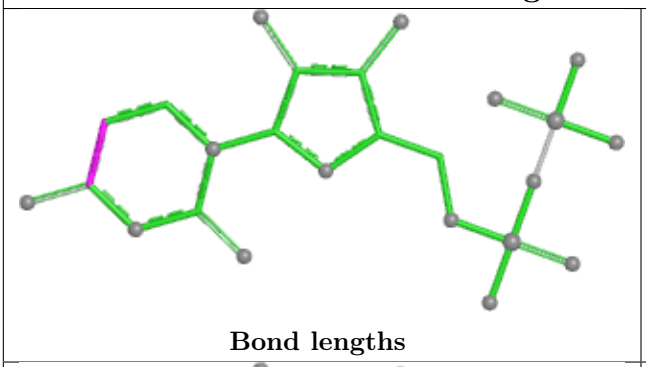


Torsions

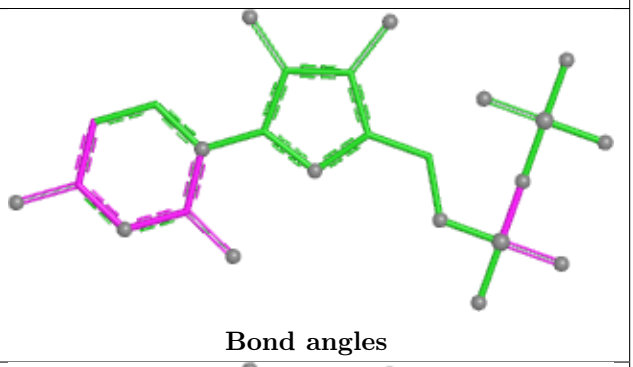


Rings

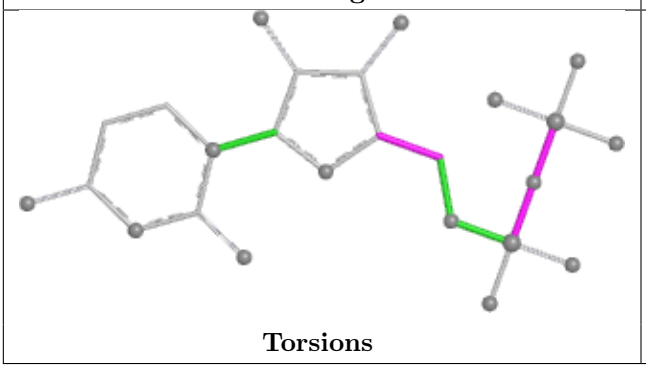
Ligand UDP E 901



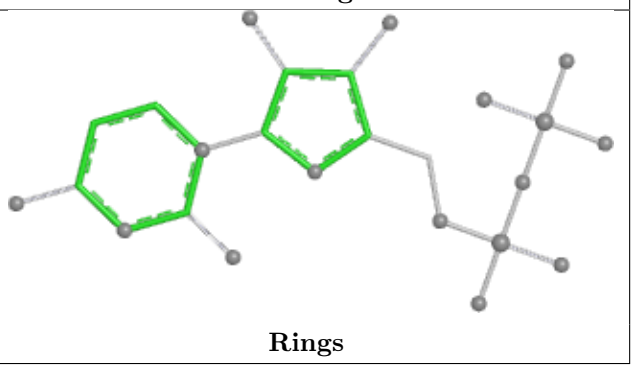
Bond lengths



Bond angles

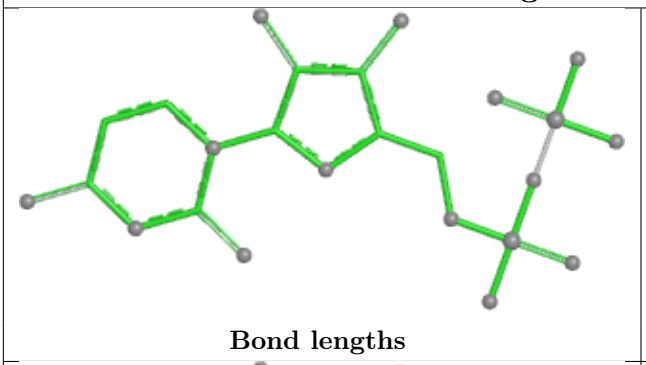


Torsions

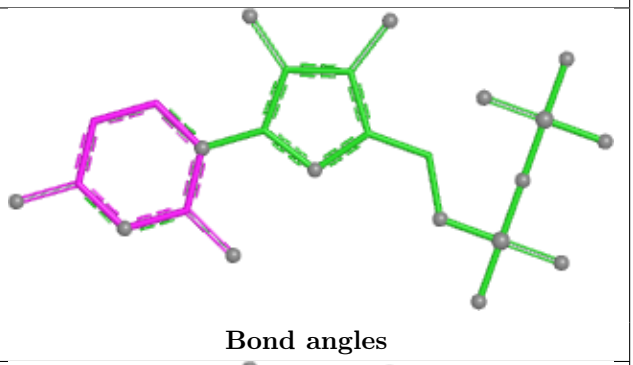


Rings

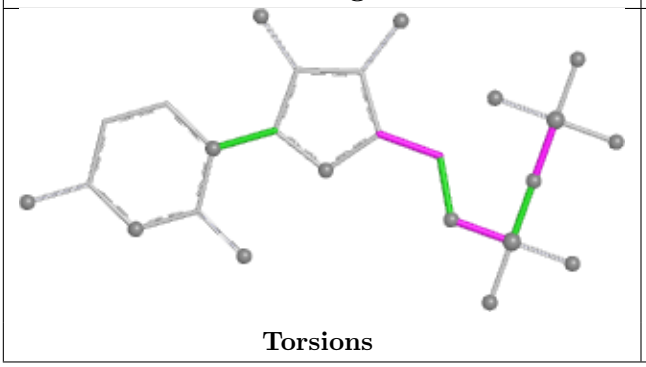
Ligand UDP H 901



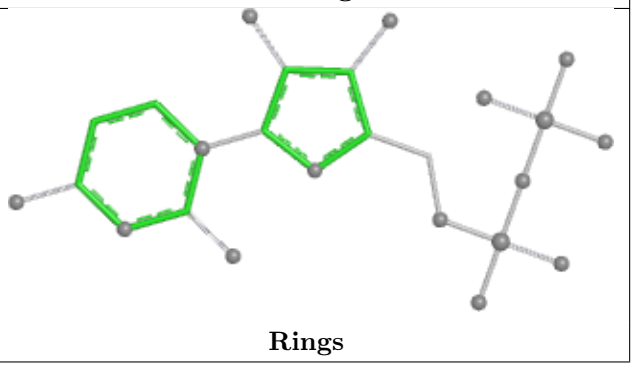
Bond lengths



Bond angles

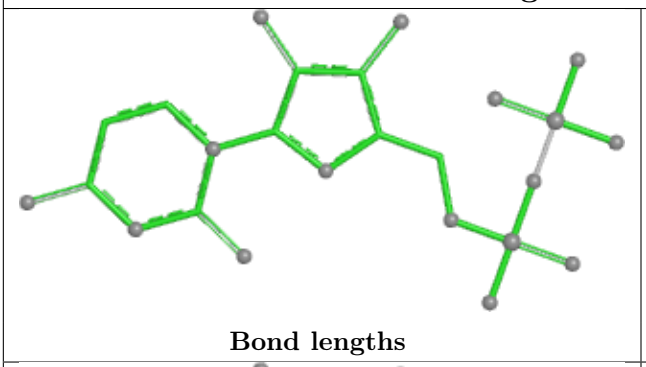


Torsions

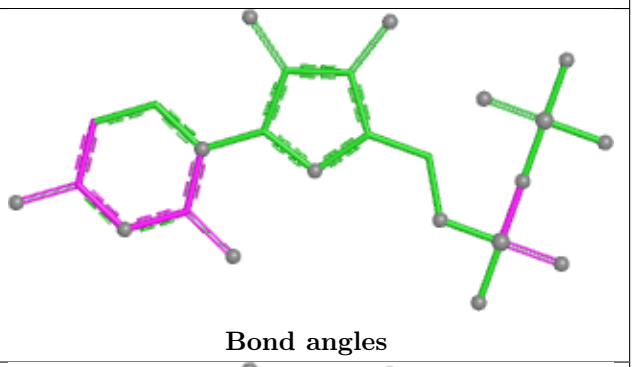


Rings

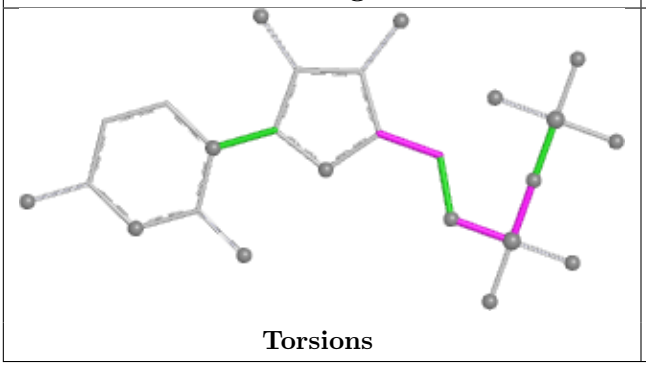
Ligand UDP G 901



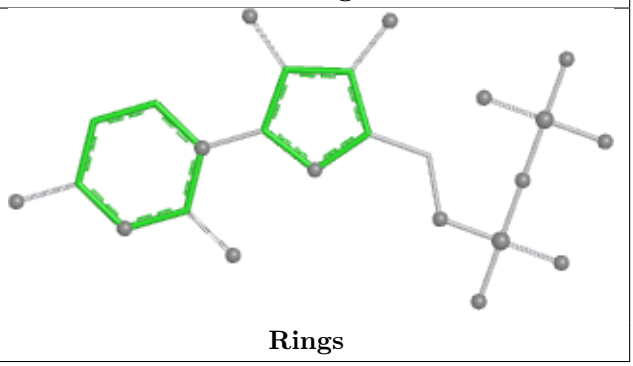
Bond lengths



Bond angles

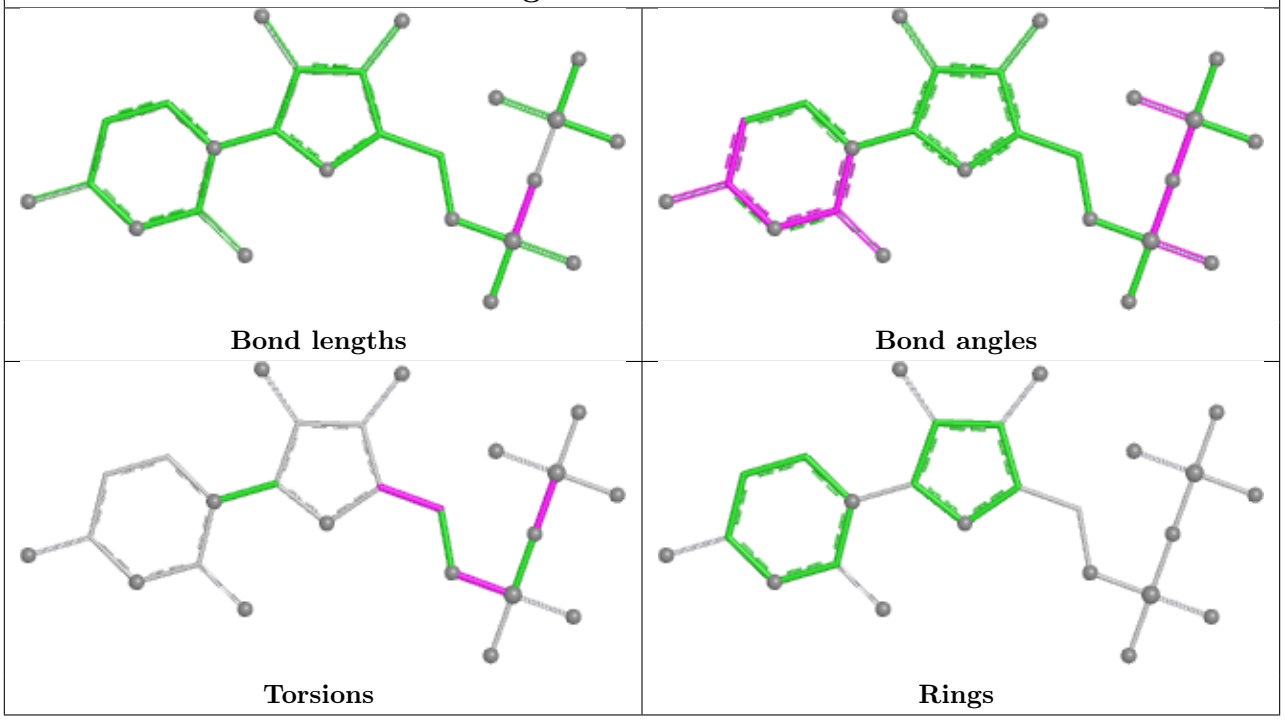


Torsions

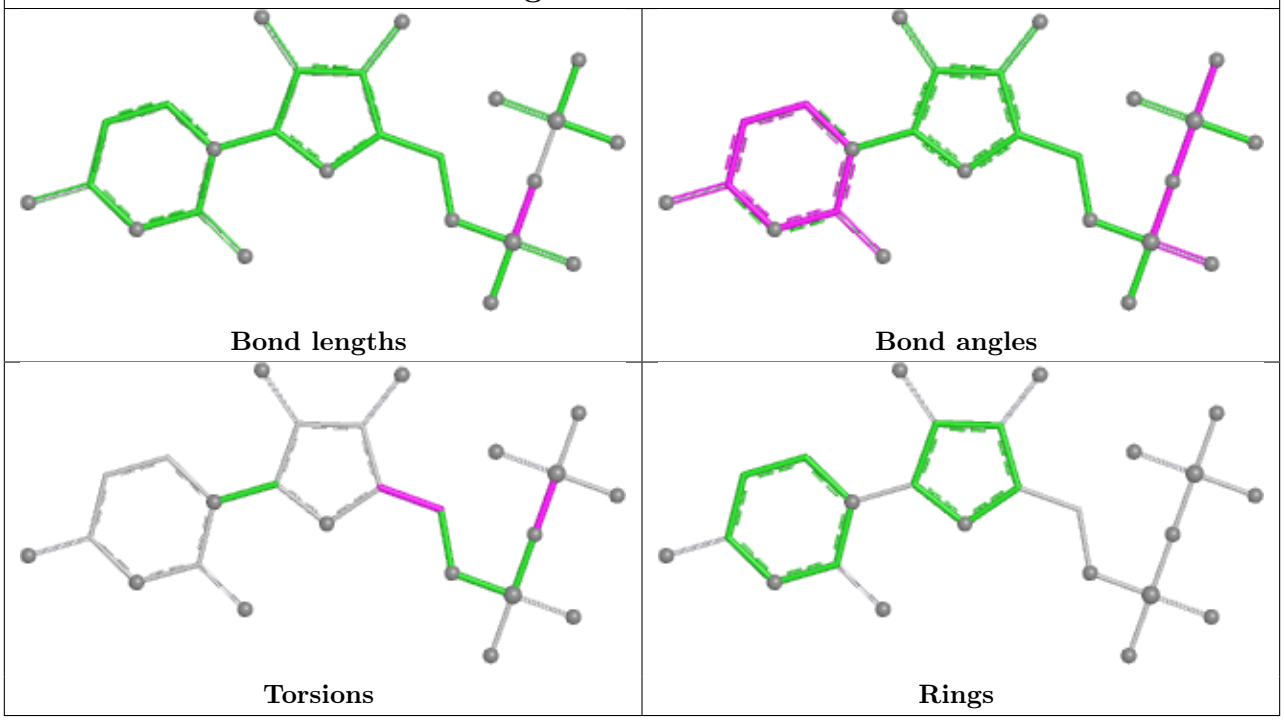


Rings

Ligand UDP C 901



Ligand UDP F 901



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.24	28 (3%)	42	39	13, 27, 90, 116	0
1	B	781/816 (95%)	0.07	55 (7%)	16	13	16, 33, 98, 131	0
1	C	769/816 (94%)	-0.13	27 (3%)	44	40	20, 38, 83, 122	0
1	D	769/816 (94%)	-0.24	25 (3%)	46	42	14, 28, 80, 111	0
1	E	769/816 (94%)	-0.16	33 (4%)	35	32	14, 30, 95, 118	0
1	F	769/816 (94%)	-0.25	22 (2%)	51	48	10, 26, 73, 111	0
1	G	769/816 (94%)	-0.28	17 (2%)	62	60	14, 30, 70, 108	0
1	H	785/816 (96%)	0.02	60 (7%)	13	11	17, 35, 92, 117	0
All	All	6180/6528 (94%)	-0.15	267 (4%)	35	32	10, 31, 87, 131	0

The worst 5 of 267 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	VAL	7.9
1	H	83	PRO	7.6
1	B	105	HIS	7.6
1	B	102	VAL	7.4
1	H	18	LEU	7.1

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.82	0.20	69,69,69,69	0
5	MLA	C	921	7/7	0.89	0.41	56,60,68,77	0
5	MLA	H	921	7/7	0.89	0.41	53,58,69,69	0
4	SO4	H	913	5/5	0.89	0.41	64,70,86,101	0
6	K	E	931	1/1	0.90	0.15	64,64,64,64	0
4	SO4	C	912	5/5	0.90	0.38	71,74,96,104	0
6	K	B	931	1/1	0.91	0.21	74,74,74,74	0
4	SO4	E	912	5/5	0.91	0.32	47,55,63,84	0
4	SO4	B	913	5/5	0.91	0.27	53,54,65,78	0
4	SO4	C	913	5/5	0.92	0.35	63,74,75,89	0
5	MLA	G	921	7/7	0.92	0.28	46,49,59,59	0
4	SO4	D	912	5/5	0.92	0.28	54,74,96,98	0
5	MLA	F	921	7/7	0.93	0.23	30,35,36,36	0
4	SO4	F	912	5/5	0.93	0.19	46,50,62,76	0
4	SO4	H	912	5/5	0.93	0.30	63,66,76,94	0
4	SO4	A	912	5/5	0.93	0.21	47,55,59,81	0
6	K	D	931	1/1	0.93	0.17	61,61,61,61	0
5	MLA	A	921	7/7	0.93	0.20	27,31,34,36	0
3	FRU	C	902	12/12	0.93	0.21	30,36,44,50	0
6	K	G	931	1/1	0.93	0.09	57,57,57,57	0
6	K	A	931	1/1	0.94	0.09	61,61,61,61	0
4	SO4	E	911	5/5	0.94	0.17	31,35,59,60	0
5	MLA	D	921	7/7	0.94	0.33	33,40,44,47	0
3	FRU	H	902	12/12	0.94	0.17	22,29,34,37	0
4	SO4	B	912	5/5	0.94	0.24	49,67,79,88	0
5	MLA	B	921	7/7	0.94	0.26	38,45,50,53	0
4	SO4	B	911	5/5	0.95	0.14	37,42,50,70	0
4	SO4	E	913	5/5	0.95	0.21	44,47,62,71	0
4	SO4	F	911	5/5	0.95	0.20	32,36,45,64	0
4	SO4	D	911	5/5	0.95	0.19	38,41,56,67	0
6	K	C	931	1/1	0.95	0.24	69,69,69,69	0
4	SO4	G	912	5/5	0.95	0.30	48,67,72,86	0
4	SO4	G	913	5/5	0.95	0.16	52,58,68,74	0
5	MLA	E	921	7/7	0.95	0.37	34,38,43,43	0
4	SO4	H	911	5/5	0.95	0.15	37,38,69,70	0
6	K	H	931	1/1	0.95	0.15	61,61,61,61	0
4	SO4	D	913	5/5	0.96	0.16	44,46,53,63	0

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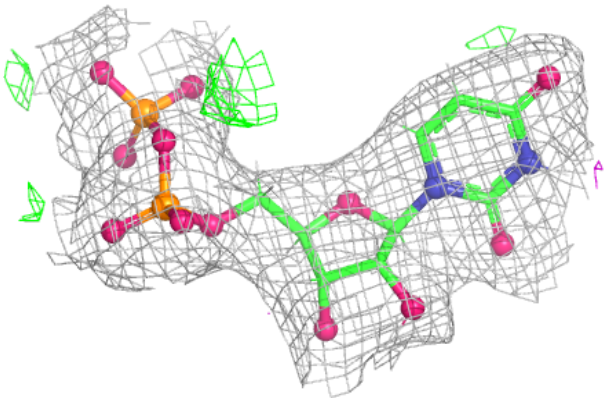
Continued from previous page...

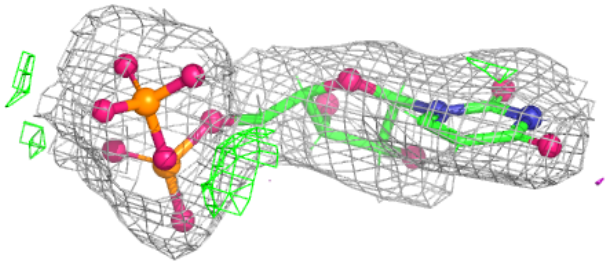
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	911	5/5	0.96	0.16	44,46,57,63	0
4	SO4	A	913	5/5	0.96	0.19	42,44,52,59	0
3	FRU	G	902	12/12	0.96	0.15	18,25,34,34	0
3	FRU	B	902	12/12	0.96	0.17	25,30,35,35	0
3	FRU	D	902	12/12	0.96	0.15	18,25,31,32	0
4	SO4	G	911	5/5	0.96	0.24	32,40,56,64	0
3	FRU	E	902	12/12	0.97	0.17	18,25,30,32	0
4	SO4	A	911	5/5	0.97	0.21	31,35,46,58	0
4	SO4	F	913	5/5	0.97	0.15	40,44,61,64	0
3	FRU	F	902	12/12	0.97	0.15	17,22,28,35	0
3	FRU	A	902	12/12	0.97	0.13	16,22,27,28	0
2	UDP	B	901	25/25	0.98	0.18	19,25,30,34	0
2	UDP	C	901	25/25	0.98	0.15	21,31,40,42	0
2	UDP	H	901	25/25	0.98	0.16	22,28,36,38	0
2	UDP	G	901	25/25	0.99	0.17	14,21,25,35	0
2	UDP	A	901	25/25	0.99	0.16	14,17,21,24	0
2	UDP	D	901	25/25	0.99	0.15	17,21,25,30	0
2	UDP	E	901	25/25	0.99	0.17	17,21,27,29	0
2	UDP	F	901	25/25	0.99	0.18	14,18,23,25	0

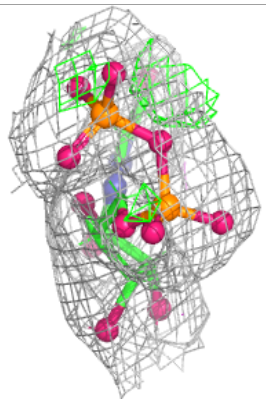
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

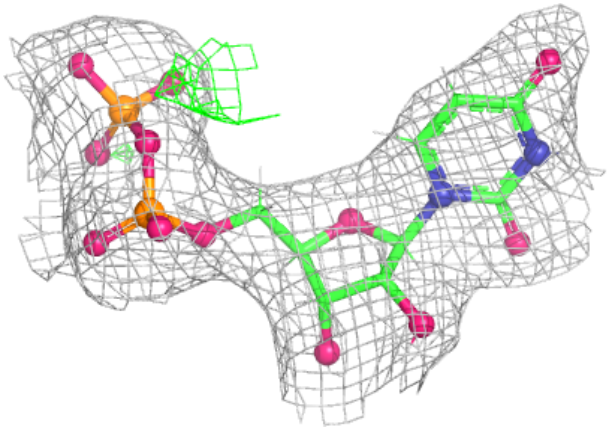


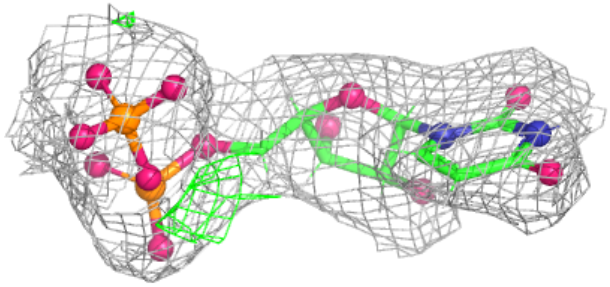


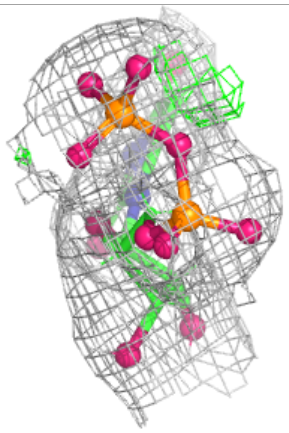


Electron density around UDP C 901:

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

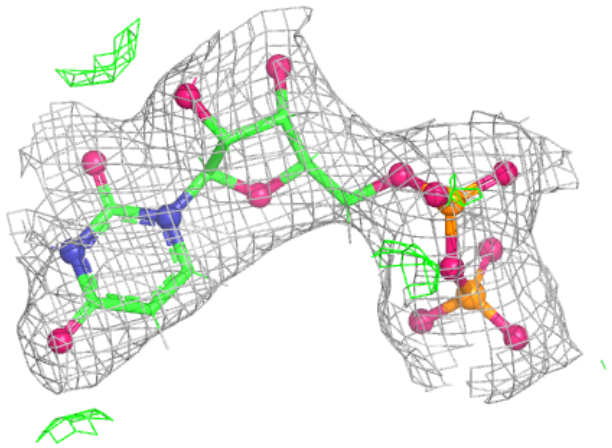


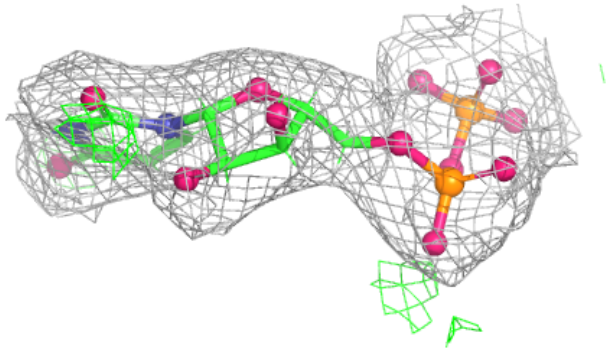


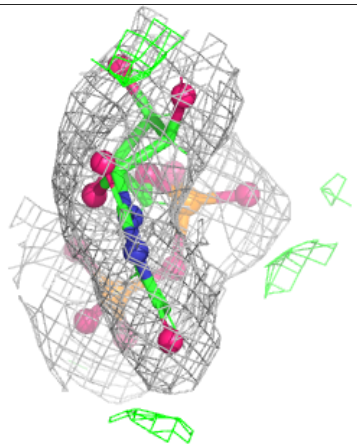


Electron density around UDP H 901:

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

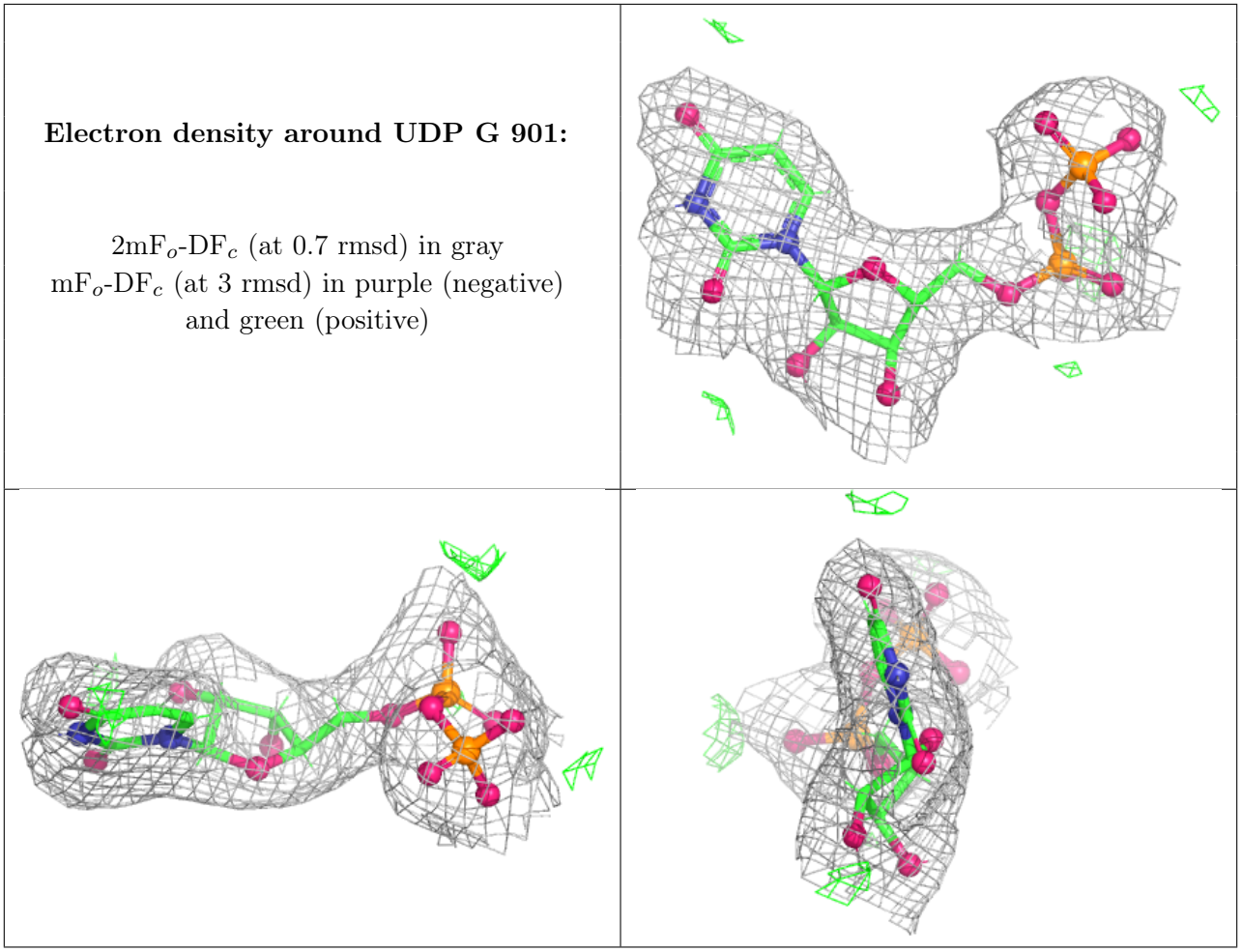






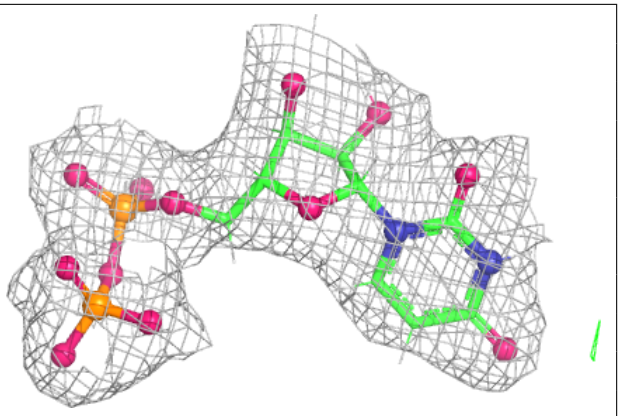
Electron density around UDP G 901:

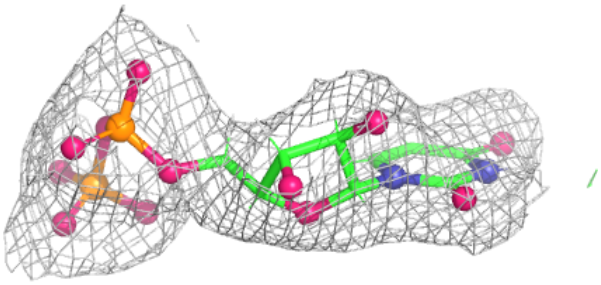
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

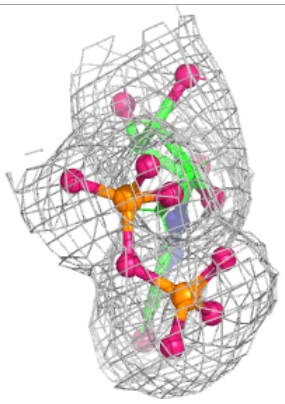


Electron density around UDP A 901:

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

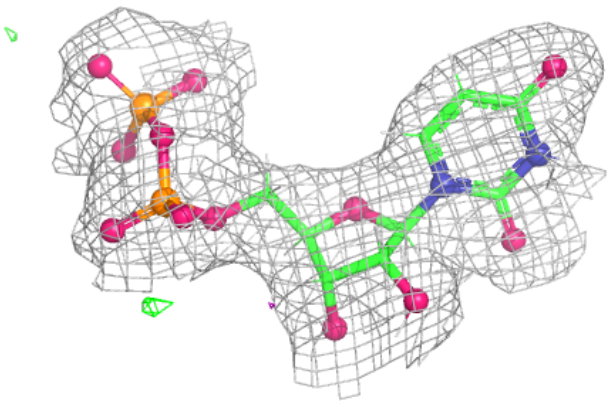


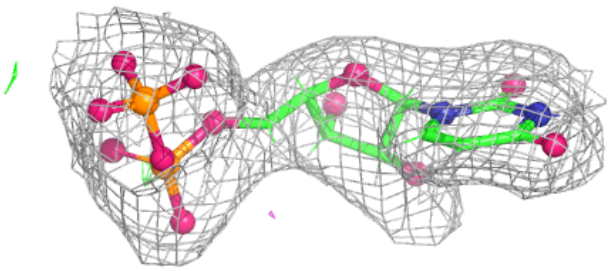


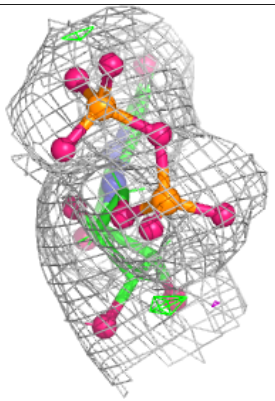


Electron density around UDP D 901:

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

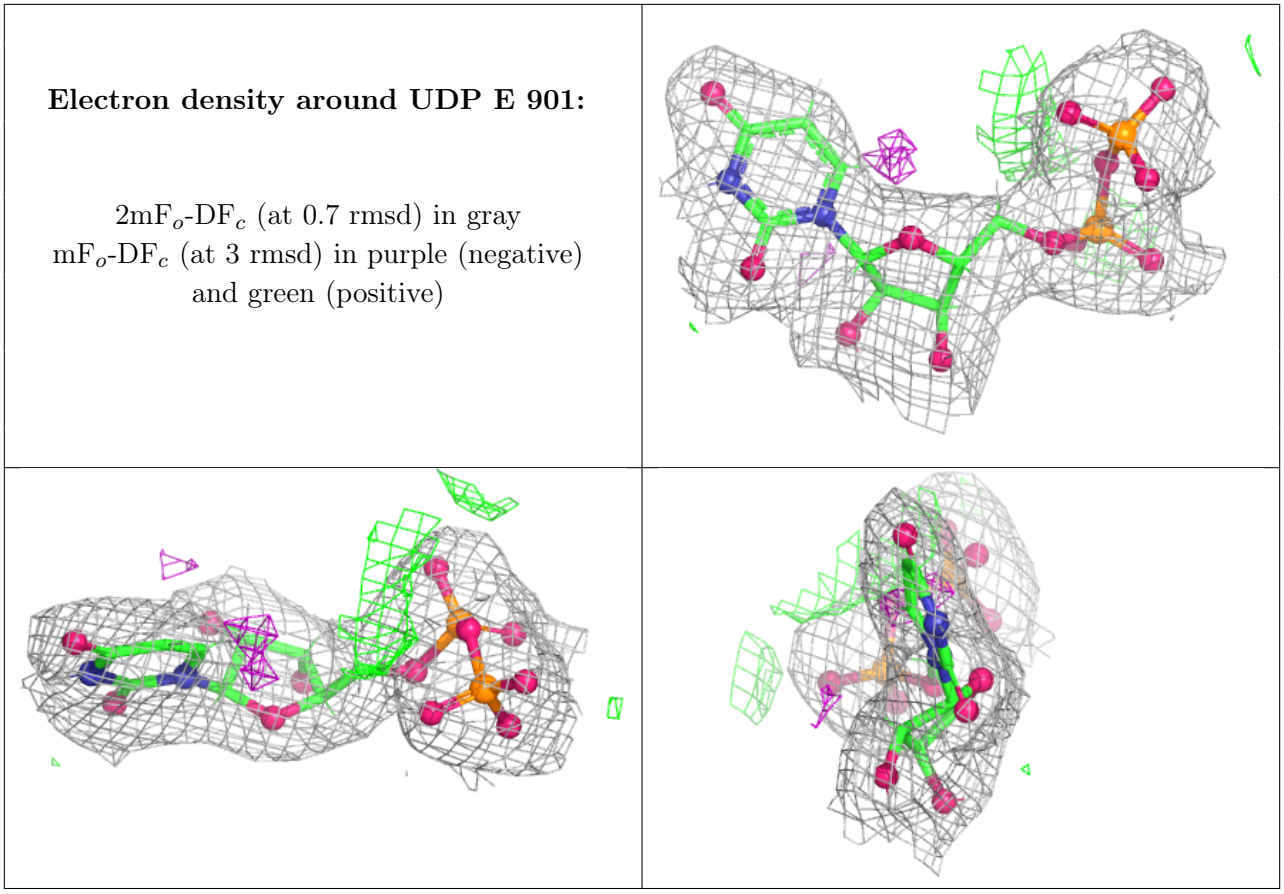






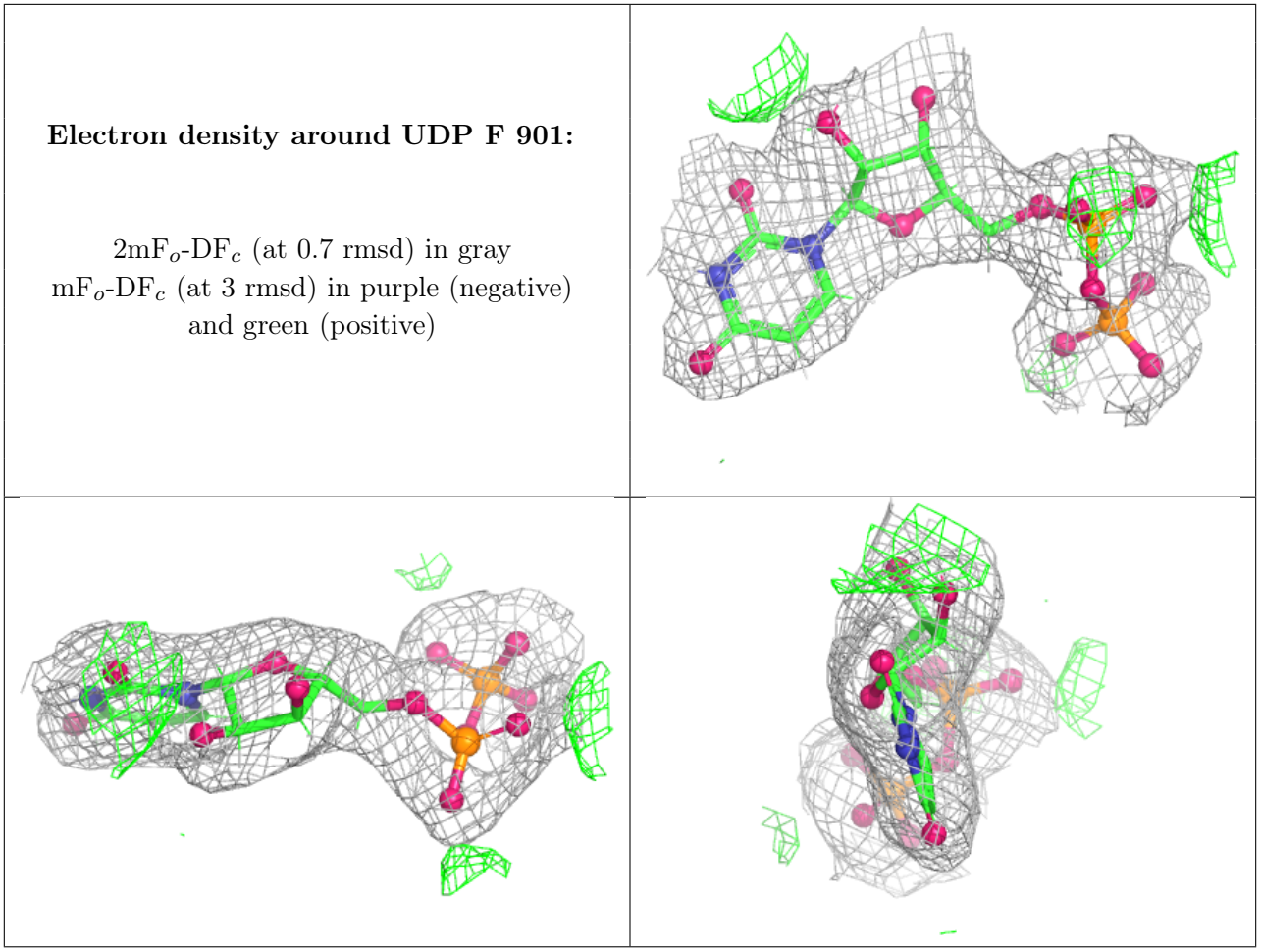
Electron density around UDP E 901:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.