



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:47 PM GMT

PDB ID : 3S29  
Title : The crystal structure of sucrose synthase-1 from Arabidopsis thaliana and its functional implications.  
Authors : Zheng, Yi; Garavito, R.Michael  
Deposited on : 2011-05-16  
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

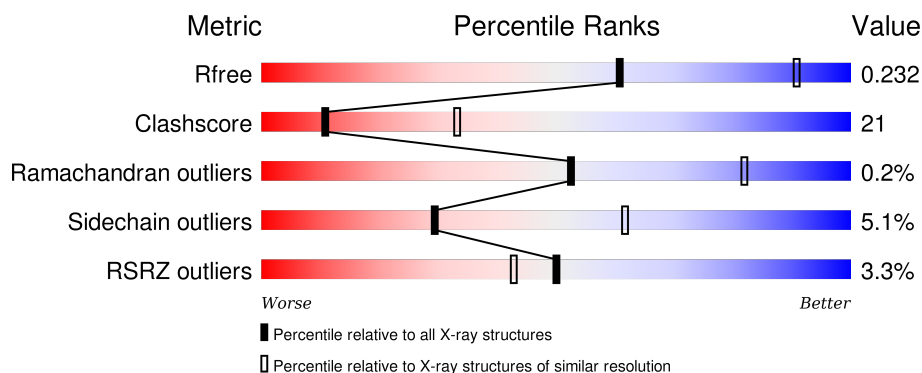
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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
3	FRU	A	902	-	-	X	X
3	FRU	B	902	-	-	X	-
3	FRU	E	902	-	-	X	-
4	SO4	A	911	-	-	-	X
4	SO4	B	911	-	-	-	X
4	SO4	B	913	-	-	X	X
4	SO4	C	911	-	-	-	X
4	SO4	C	913	-	-	-	X
4	SO4	D	911	-	-	-	X
4	SO4	D	913	-	-	-	X
4	SO4	E	913	-	-	X	-
4	SO4	F	911	-	-	-	X
4	SO4	G	913	-	-	-	X
4	SO4	H	911	-	-	-	X
4	SO4	H	913	-	-	-	X
5	MLA	A	921	-	-	-	X
5	MLA	B	921	-	-	-	X
5	MLA	C	921	-	-	-	X
5	MLA	D	921	-	-	-	X
5	MLA	E	921	-	-	-	X
5	MLA	F	921	-	-	-	X
5	MLA	F	922	-	-	-	X
5	MLA	G	921	-	-	-	X
5	MLA	H	921	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 51504 atoms, of which 24 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
			6280	4033	1066	1159	22			
1	B	791	Total	C	N	O	S	0	0	0
			6321	4056	1073	1170	22			
1	C	781	Total	C	N	O	S	0	0	0
			6294	4047	1065	1160	22			
1	D	781	Total	C	N	O	S	0	0	0
			6275	4032	1062	1159	22			
1	E	781	Total	C	N	O	S	0	0	0
			6275	4031	1063	1159	22			
1	F	781	Total	C	N	O	S	0	0	0
			6299	4047	1070	1160	22			
1	G	781	Total	C	N	O	S	0	0	0
			6301	4047	1070	1162	22			
1	H	797	Total	C	N	O	S	0	0	0
			6398	4101	1091	1184	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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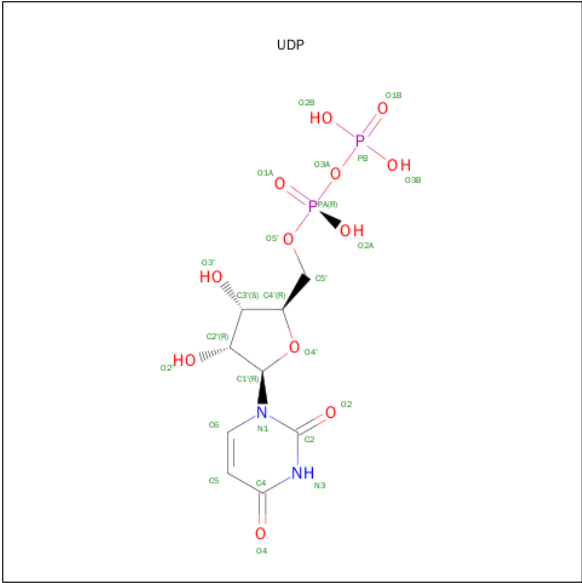
Chain	Residue	Modelled	Actual	Comment	Reference
B	814	HIS	-	EXPRESSION TAG	UNP P49040
B	815	HIS	-	EXPRESSION TAG	UNP P49040
B	816	HIS	-	EXPRESSION TAG	UNP P49040
C	809	VAL	-	EXPRESSION TAG	UNP P49040
C	810	GLU	-	EXPRESSION TAG	UNP P49040
C	811	HIS	-	EXPRESSION TAG	UNP P49040
C	812	HIS	-	EXPRESSION TAG	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 (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



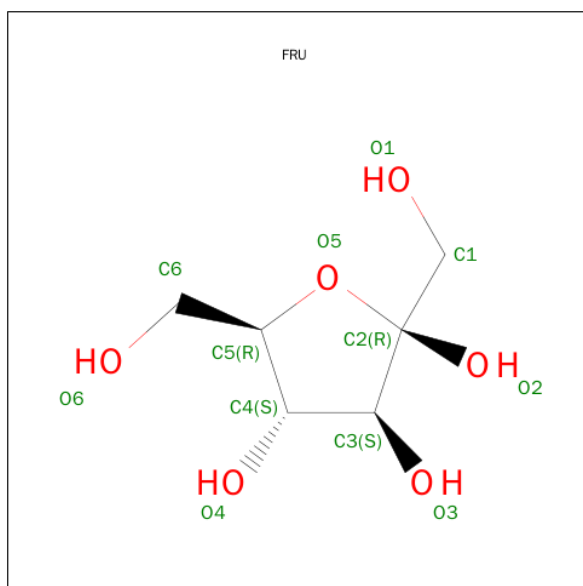
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	G	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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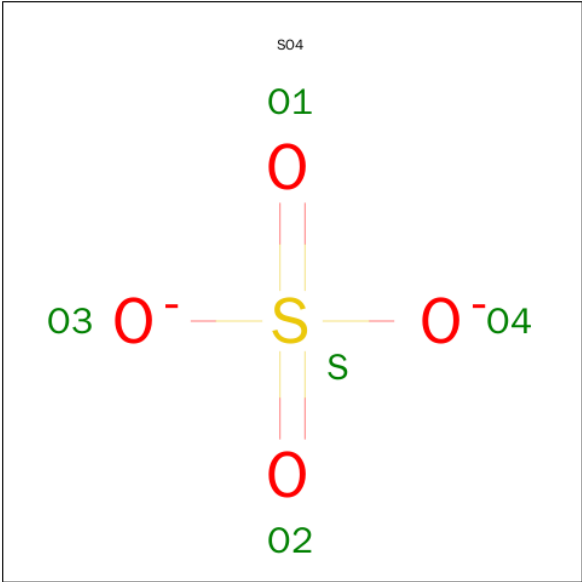
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is SUGAR (FRUCTOSE) (three-letter code: FRU) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			12	6	6		
3	G	1	Total	C	O	0	0
			12	6	6		
3	H	1	Total	C	O	0	0
			12	6	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	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

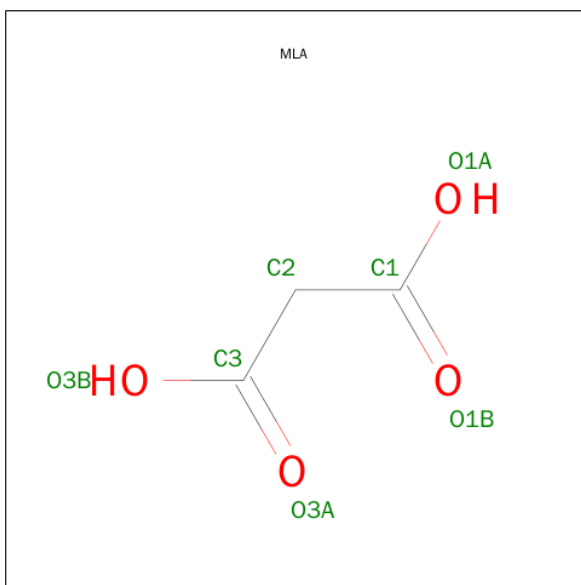
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0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

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	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	H	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	A	1	Total K 1 1	0	0
6	F	1	Total K 1 1	0	0

- Molecule 7 is water.

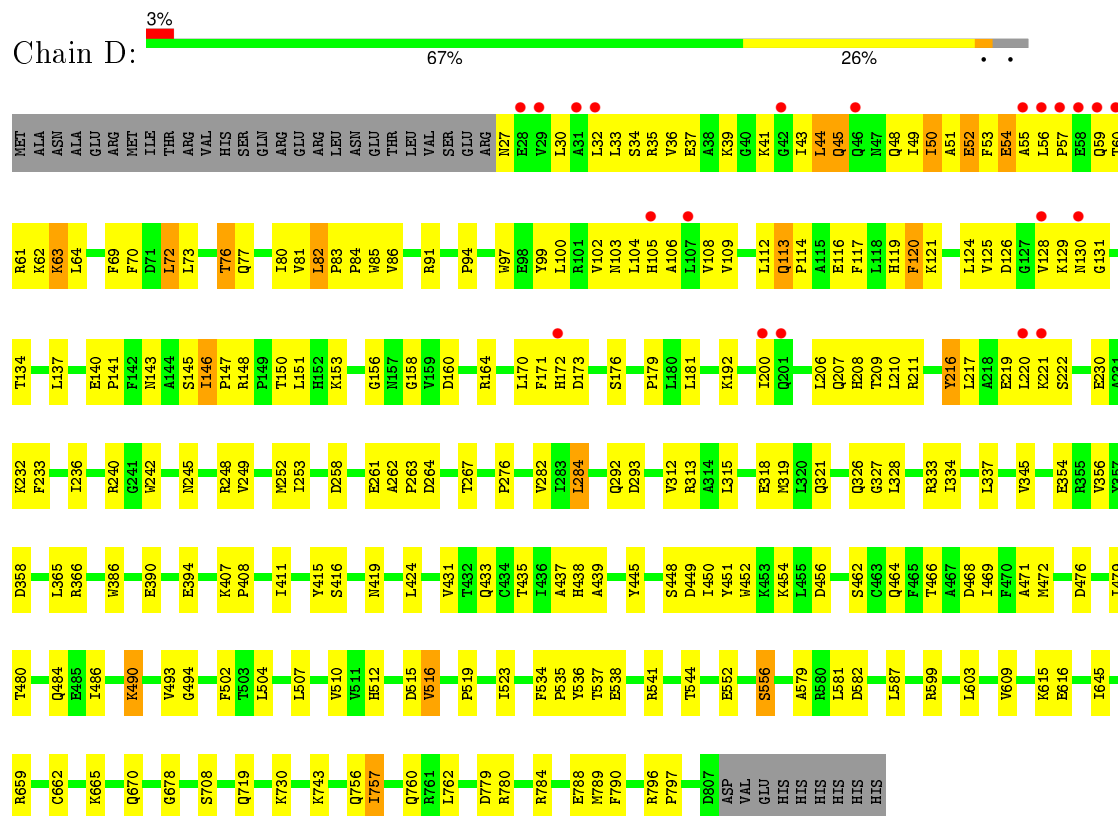
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	76	Total O 76 76	0	0
7	B	62	Total O 62 62	0	0
7	C	38	Total O 38 38	0	0
7	D	64	Total O 64 64	0	0
7	E	58	Total O 58 58	0	0
7	F	80	Total O 80 80	0	0
7	G	71	Total O 71 71	0	0
7	H	50	Total O 50 50	0	0



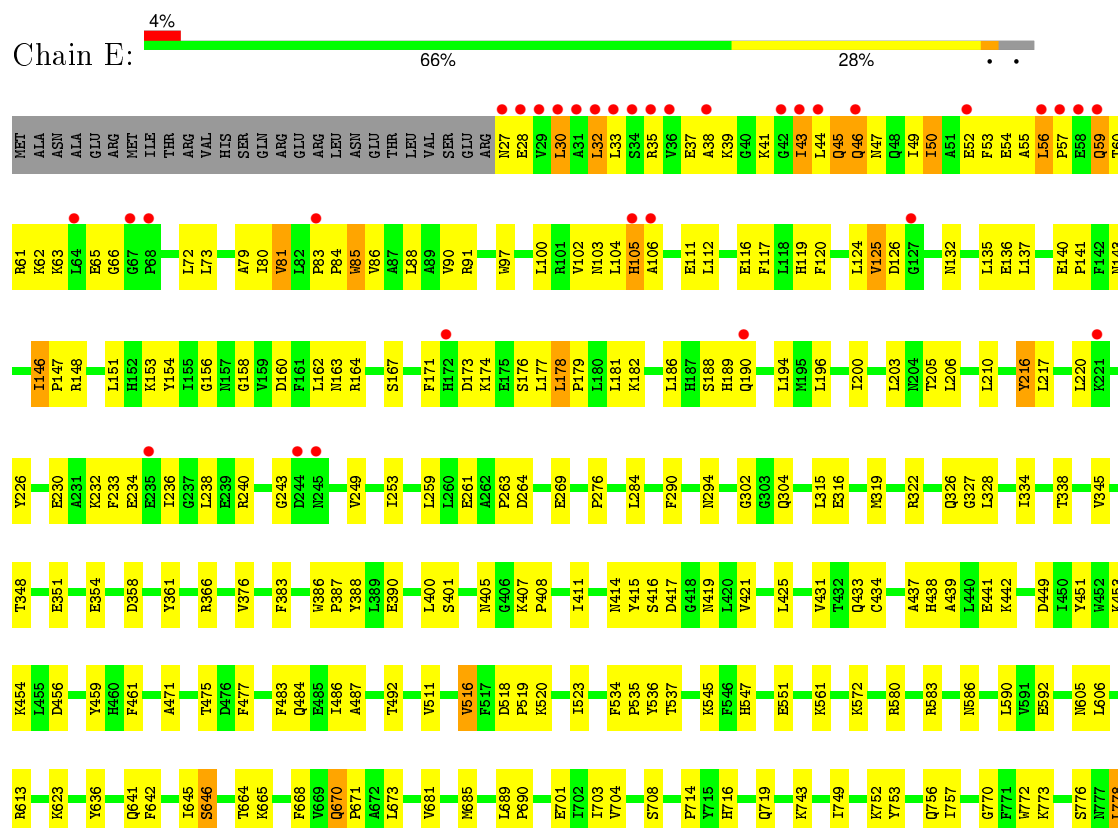


MET	L64	L135	F229	T338	T475	H605	G770	Y769
	B65	E136	E230	V345	F477	R613	F771	G770
	P68	L137	K232	F348	F483	R614	F772	G771
	F69	E140	F233	C349	Q484	R615	F773	G772
	F70	F141		G350	E485	R618	S776	G773
	D71	M143	R240	E351	E486	R621	S777	G774
	L72	M143	G241	E354	A487	R625	L778	G775
	L73	A144	V242			R628	D779	G776
	ARG	G243	G243	E354	K490	R629	R780	G777
	VAL	D244	D244	E360	E491	R630	L781	G778
HIS	A79	N245						G779
VAL	180							G780
VAL	181	L151	R248		I514	R633	R781	G781
GLN	ARG	L151	V249	R366	V616	R634	R782	G782
GLU	P83	Y154	D250					G783
ARG	P84	D251	H386					G784
LEU	H85	M157	M252	P387	D518	L638	F787	G785
GLU	A87	G158	L253		P519			G786
GLU	L88	D160		E390	K520	Q641		G787
LEU			D258		G527		K794	G788
VAL	R91	M163	L259	L400		L645	Y795	G789
SER	P92	R164	E261	M405	M530	S646	Y796	G790
GLU	V96	S167	P263	G406	F534			G791
GLU	P97	A168	D264	K407	P535			G792
THR	X99	K169	L268	D409	E538	P668	L804	G793
VAL	L100	F171		L410		P669		G794
ASP	H172	H172	L272	I411	E552	P671	D807	G795
GLU	V102	D173	P276	Y415	L553	V681	VAL	G796
HIS	N103	K174	P277	S416				G797
HIS	L104	H175	V277	L420	S556	V685	GLU	G798
HIS	H105	S176	V278					G799
HIS	A106	L177						G800
HIS	L107	L178	L284	Q433	M560	L689	HIS	G801
HIS	V108	P179	F290	G434	R561	F692	HIS	G802
HIS	E110	G190	G295	T436	L564	I702	HIS	G803
HIS	E111	V295	L296	H438	K572	F727	HIS	G804
HIS	L112	L202		A439				G805
HIS	E116	L203	T301	L440	R580	D739		G806
HIS	N47	N204	G302	E441	L581			G807
HIS	Q48	T205	G303	K442	D582	K743		G808
HIS	F120	F120	Q304	T443	M586			G809
HIS	K121	L210		K444	L587	Y753		G810
HIS	A51		I308	V445	L588	Y754		G811
HIS	E52	Y216	L315	S448	G589	W755		G812
HIS	F53	D126	M319	D449	L590	Q756		G813
HIS	A55	G127	L220	K458	Y594	I757		G814
HIS	L56	V128	K221	V459	N597	R761		G815
HIS	P57	K129	T224	D468	R601	L763		G816
HIS	E58	M130	L225			L764		G817
HIS	Q59	G131	Q326			L765		G818
HIS	T60	M132	L334	H472	E602			G819
HIS	F133	E227						G820
HIS	T124	E228						G821

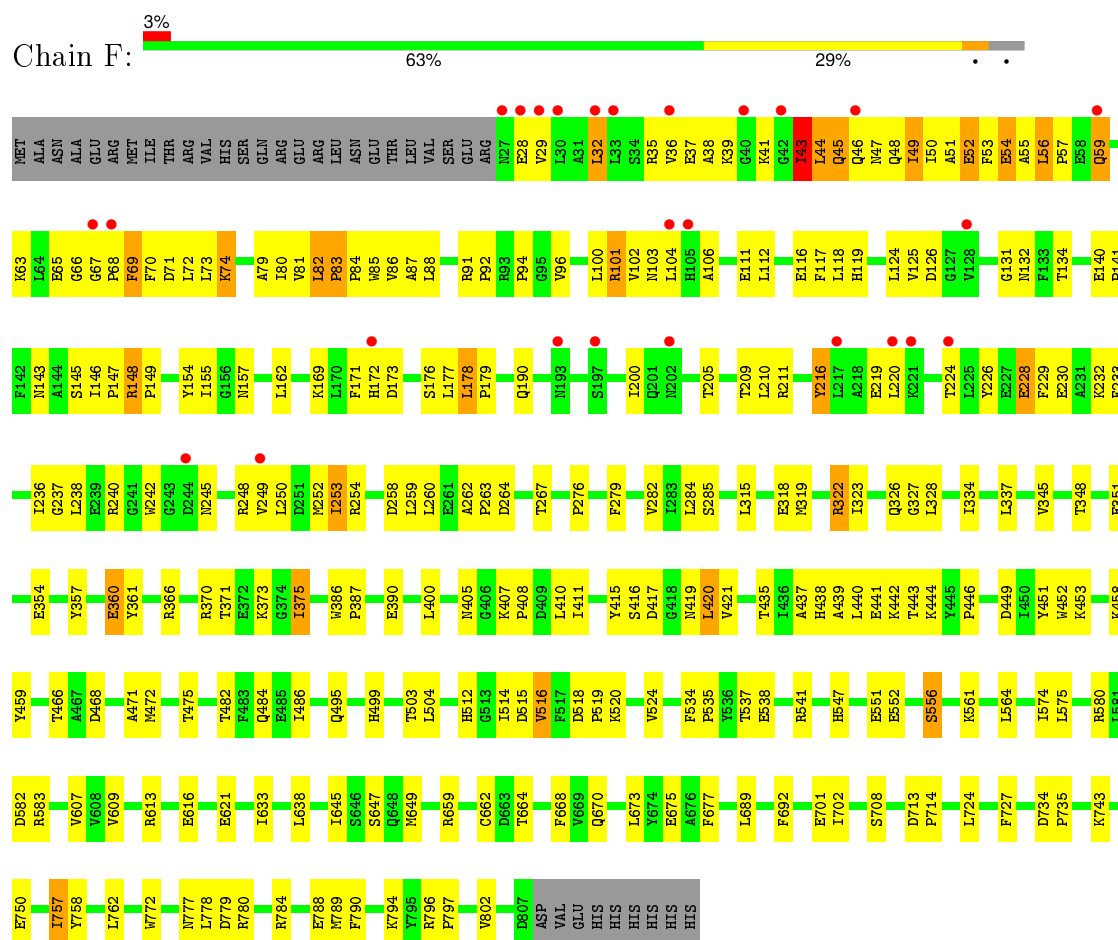
• Molecule 1: Sucrose synthase 1



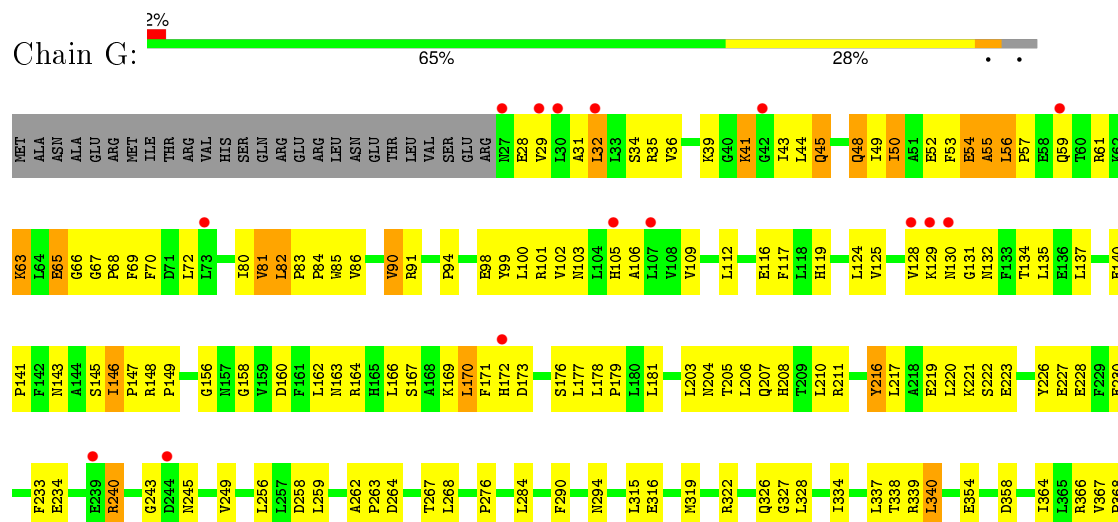
• Molecule 1: Sucrose synthase 1

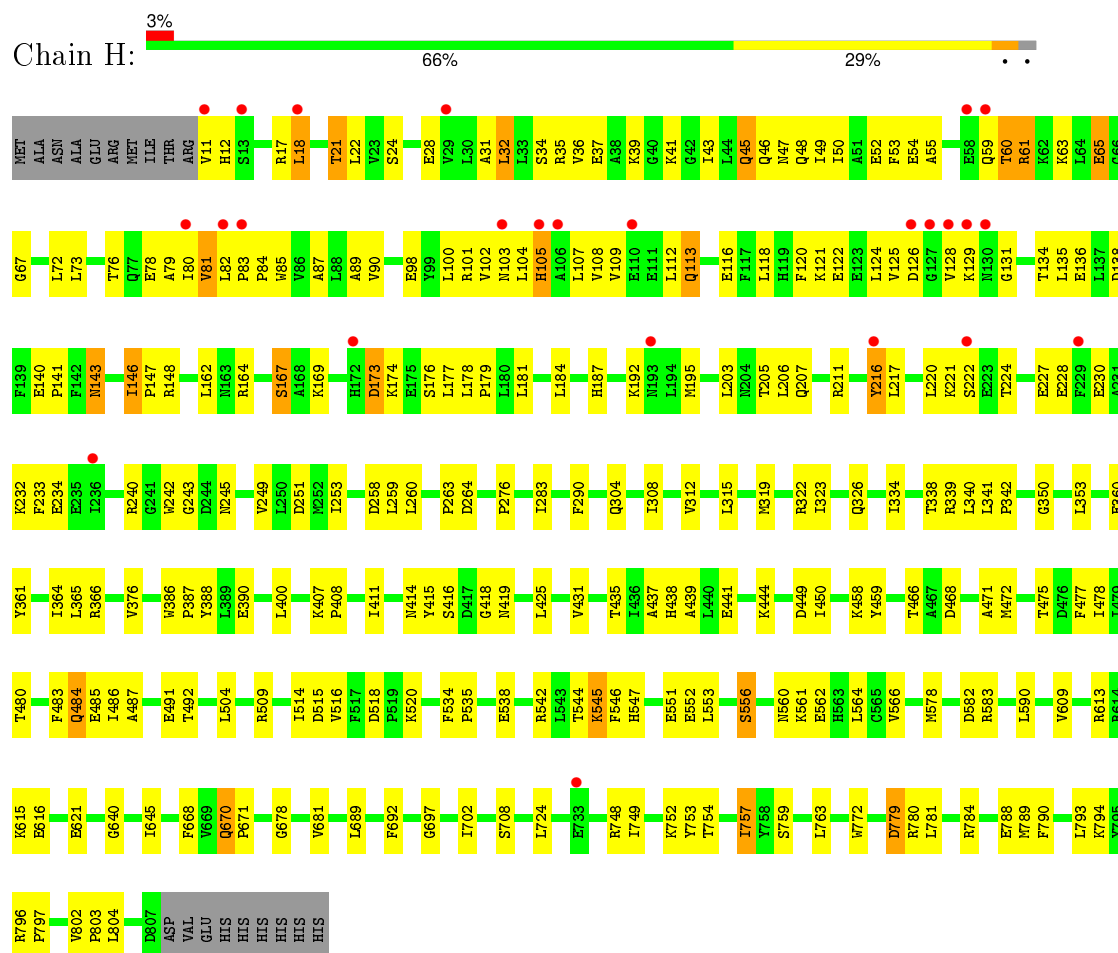


- Molecule 1: Sucrose synthase 1



- 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, $\alpha$ , $\beta$ , $\gamma$	277.16Å 261.50Å 161.10Å 90.00° 109.27° 90.00°	Depositor
Resolution (Å)	24.96 – 2.85 48.88 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.96-2.85) 99.3 (48.88-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.185 , 0.234 0.185 , 0.232	Depositor DCC
$R_{free}$ test set	11892 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	4 of 249728 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	51504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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 24.47 % 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 3.8124e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, MLA, K, FRU, 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	0.36	0/6427	0.54	0/8703
1	B	0.35	0/6467	0.54	0/8761
1	C	0.33	0/6441	0.52	0/8723
1	D	0.35	0/6422	0.55	0/8700
1	E	0.34	0/6421	0.54	0/8697
1	F	0.35	0/6446	0.54	0/8728
1	G	0.35	0/6448	0.53	0/8731
1	H	0.34	0/6546	0.54	0/8867
All	All	0.35	0/51618	0.54	0/69910

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	B	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	143	ASN	Peptide
1	F	83	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6280	0	6200	278	0
1	B	6321	0	6203	312	0
1	C	6294	0	6244	272	0
1	D	6275	0	6197	257	0
1	E	6275	0	6205	272	0
1	F	6299	0	6247	283	0
1	G	6301	0	6247	280	0
1	H	6398	0	6301	285	0
2	A	25	0	11	1	0
2	B	25	0	11	2	0
2	C	25	0	11	0	0
2	D	25	0	11	0	0
2	E	25	0	11	1	0
2	F	25	0	11	1	0
2	G	25	0	11	1	0
2	H	25	0	11	0	0
3	A	12	0	12	7	0
3	B	12	0	12	6	0
3	C	12	0	12	4	0
3	D	12	0	12	0	0
3	E	12	0	12	11	0
3	F	12	0	12	0	0
3	G	12	0	12	0	0
3	H	12	0	12	1	0
4	A	25	0	0	2	0
4	B	15	0	0	3	0
4	C	15	0	0	0	0
4	D	20	0	0	1	0
4	E	20	0	0	4	0
4	F	20	0	0	0	0
4	G	20	0	0	1	0
4	H	15	0	0	0	0
5	A	7	2	2	0	0
5	B	7	2	2	0	0
5	C	7	2	2	0	0
5	D	14	4	4	2	0
5	E	7	2	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	14	4	4	2	0
5	G	14	4	4	0	0
5	H	14	4	4	1	0
6	A	1	0	0	0	0
6	B	1	0	0	1	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	76	0	0	3	0
7	B	62	0	0	4	0
7	C	38	0	0	1	0
7	D	64	0	0	2	0
7	E	58	0	0	4	0
7	F	80	0	0	0	0
7	G	71	0	0	3	0
7	H	50	0	0	2	0
All	All	51480	24	50052	2131	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 21.

The worst 5 of 2131 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:D:145:SER:HB3	1:D:779:ASP:OD2	1.16	1.31
1:G:66:GLY:C	1:G:68:PRO:HD3	1.57	1.23
1:G:119:HIS:CE1	1:G:129:LYS:HD2	1.73	1.21
1:H:46:GLN:HB2	1:H:79:ALA:HB3	1.20	1.18
1:B:83:PRO:HB2	1:B:84:PRO:HD2	1.26	1.15

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	737 (95%)	38 (5%)	4 (0%)	34	67
1	B	787/816 (96%)	732 (93%)	51 (6%)	4 (0%)	34	67
1	C	779/816 (96%)	741 (95%)	38 (5%)	0	100	100
1	D	779/816 (96%)	739 (95%)	39 (5%)	1 (0%)	56	85
1	E	779/816 (96%)	740 (95%)	38 (5%)	1 (0%)	56	85
1	F	779/816 (96%)	736 (94%)	41 (5%)	2 (0%)	46	76
1	G	779/816 (96%)	741 (95%)	36 (5%)	2 (0%)	46	76
1	H	795/816 (97%)	751 (94%)	43 (5%)	1 (0%)	56	85
All	All	6256/6528 (96%)	5917 (95%)	324 (5%)	15 (0%)	52	82

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	ALA
1	B	83	PRO
1	A	63	LYS
1	D	63	LYS
1	A	55	ALA

### 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	668/718 (93%)	626 (94%)	42 (6%)	22	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	668/718 (93%)	631 (94%)	37 (6%)	27	58
1	C	674/718 (94%)	646 (96%)	28 (4%)	36	70
1	D	669/718 (93%)	639 (96%)	30 (4%)	34	67
1	E	669/718 (93%)	639 (96%)	30 (4%)	34	67
1	F	674/718 (94%)	633 (94%)	41 (6%)	23	52
1	G	675/718 (94%)	641 (95%)	34 (5%)	30	62
1	H	681/718 (95%)	649 (95%)	32 (5%)	32	66
All	All	5378/5744 (94%)	5104 (95%)	274 (5%)	29	62

5 of 274 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	284	LEU
1	E	216	TYR
1	H	113	GLN
1	D	358	ASP
1	E	45	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	189	HIS
1	E	405	ASN
1	H	201	GLN
1	D	304	GLN
1	D	427	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 66 ligands modelled in this entry, 8 are monoatomic - leaving 58 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	UDP	A	901	-	18,26,26	1.18	1 (5%)	26,40,40	1.46	2 (7%)
3	FRU	A	902	-	11,12,12	0.63	0	10,18,18	1.11	0
4	SO4	A	911	-	4,4,4	0.11	0	6,6,6	0.31	0
4	SO4	A	912	-	4,4,4	0.05	0	6,6,6	0.08	0
4	SO4	A	913	-	4,4,4	0.12	0	6,6,6	0.17	0
4	SO4	A	914	-	4,4,4	0.05	0	6,6,6	0.15	0
4	SO4	A	915	-	4,4,4	0.17	0	6,6,6	0.08	0
5	MLA	A	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	B	901	-	18,26,26	1.15	1 (5%)	26,40,40	1.67	2 (7%)
3	FRU	B	902	-	11,12,12	0.65	0	10,18,18	1.16	1 (10%)
4	SO4	B	911	-	4,4,4	0.19	0	6,6,6	0.18	0
4	SO4	B	912	-	4,4,4	0.11	0	6,6,6	0.13	0
4	SO4	B	913	-	4,4,4	0.13	0	6,6,6	0.19	0
5	MLA	B	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	C	901	-	18,26,26	1.09	1 (5%)	26,40,40	1.42	2 (7%)
3	FRU	C	902	-	11,12,12	0.63	0	10,18,18	1.08	0
4	SO4	C	911	-	4,4,4	0.06	0	6,6,6	0.21	0
4	SO4	C	912	-	4,4,4	0.06	0	6,6,6	0.09	0
4	SO4	C	913	-	4,4,4	0.05	0	6,6,6	0.11	0
5	MLA	C	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	D	901	-	18,26,26	1.18	1 (5%)	26,40,40	1.48	2 (7%)
3	FRU	D	902	-	11,12,12	0.66	0	10,18,18	0.97	0
4	SO4	D	911	-	4,4,4	0.09	0	6,6,6	0.23	0
4	SO4	D	912	-	4,4,4	0.05	0	6,6,6	0.12	0
4	SO4	D	913	-	4,4,4	0.11	0	6,6,6	0.09	0
4	SO4	D	914	-	4,4,4	0.06	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MLA	D	921	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	D	922	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	E	901	-	18,26,26	1.10	1 (5%)	26,40,40	1.53	2 (7%)
3	FRU	E	902	-	11,12,12	0.77	1 (9%)	10,18,18	0.97	0
4	SO4	E	911	-	4,4,4	0.15	0	6,6,6	0.22	0
4	SO4	E	912	-	4,4,4	0.06	0	6,6,6	0.08	0
4	SO4	E	913	-	4,4,4	0.06	0	6,6,6	0.17	0
4	SO4	E	914	-	4,4,4	0.06	0	6,6,6	0.13	0
5	MLA	E	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	F	901	-	18,26,26	1.12	1 (5%)	26,40,40	1.38	1 (3%)
3	FRU	F	902	-	11,12,12	0.56	0	10,18,18	1.02	0
4	SO4	F	911	-	4,4,4	0.16	0	6,6,6	0.18	0
4	SO4	F	912	-	4,4,4	0.06	0	6,6,6	0.09	0
4	SO4	F	913	-	4,4,4	0.11	0	6,6,6	0.25	0
4	SO4	F	914	-	4,4,4	0.09	0	6,6,6	0.12	0
5	MLA	F	921	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	F	922	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	G	901	-	18,26,26	1.15	1 (5%)	26,40,40	1.38	2 (7%)
3	FRU	G	902	-	11,12,12	1.04	1 (9%)	10,18,18	1.19	0
4	SO4	G	911	-	4,4,4	0.09	0	6,6,6	0.18	0
4	SO4	G	912	-	4,4,4	0.06	0	6,6,6	0.12	0
4	SO4	G	913	-	4,4,4	0.10	0	6,6,6	0.15	0
4	SO4	G	914	-	4,4,4	0.05	0	6,6,6	0.15	0
5	MLA	G	921	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	G	922	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	H	901	-	18,26,26	1.19	1 (5%)	26,40,40	1.47	2 (7%)
3	FRU	H	902	-	11,12,12	1.07	1 (9%)	10,18,18	1.20	0
4	SO4	H	911	-	4,4,4	0.18	0	6,6,6	0.21	0
4	SO4	H	912	-	4,4,4	0.03	0	6,6,6	0.10	0
4	SO4	H	913	-	4,4,4	0.08	0	6,6,6	0.14	0
5	MLA	H	921	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	H	922	-	0,6,6	0.00	-	0,7,7	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	A	901	-	-	0/12/32/32	0/2/2/2
3	FRU	A	902	-	-	0/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	911	-	-	0/0/0/0	0/0/0/0
4	SO4	A	912	-	-	0/0/0/0	0/0/0/0
4	SO4	A	913	-	-	0/0/0/0	0/0/0/0
4	SO4	A	914	-	-	0/0/0/0	0/0/0/0
4	SO4	A	915	-	-	0/0/0/0	0/0/0/0
5	MLA	A	921	-	-	0/0/4/4	0/0/0/0
2	UDP	B	901	-	-	0/12/32/32	0/2/2/2
3	FRU	B	902	-	-	0/5/24/24	0/1/1/1
4	SO4	B	911	-	-	0/0/0/0	0/0/0/0
4	SO4	B	912	-	-	0/0/0/0	0/0/0/0
4	SO4	B	913	-	-	0/0/0/0	0/0/0/0
5	MLA	B	921	-	-	0/0/4/4	0/0/0/0
2	UDP	C	901	-	-	0/12/32/32	0/2/2/2
3	FRU	C	902	-	-	0/5/24/24	0/1/1/1
4	SO4	C	911	-	-	0/0/0/0	0/0/0/0
4	SO4	C	912	-	-	0/0/0/0	0/0/0/0
4	SO4	C	913	-	-	0/0/0/0	0/0/0/0
5	MLA	C	921	-	-	0/0/4/4	0/0/0/0
2	UDP	D	901	-	-	0/12/32/32	0/2/2/2
3	FRU	D	902	-	-	0/5/24/24	0/1/1/1
4	SO4	D	911	-	-	0/0/0/0	0/0/0/0
4	SO4	D	912	-	-	0/0/0/0	0/0/0/0
4	SO4	D	913	-	-	0/0/0/0	0/0/0/0
4	SO4	D	914	-	-	0/0/0/0	0/0/0/0
5	MLA	D	921	-	-	0/0/4/4	0/0/0/0
5	MLA	D	922	-	-	0/0/4/4	0/0/0/0
2	UDP	E	901	-	-	0/12/32/32	0/2/2/2
3	FRU	E	902	-	-	0/5/24/24	0/1/1/1
4	SO4	E	911	-	-	0/0/0/0	0/0/0/0
4	SO4	E	912	-	-	0/0/0/0	0/0/0/0
4	SO4	E	913	-	-	0/0/0/0	0/0/0/0
4	SO4	E	914	-	-	0/0/0/0	0/0/0/0
5	MLA	E	921	-	-	0/0/4/4	0/0/0/0
2	UDP	F	901	-	-	0/12/32/32	0/2/2/2
3	FRU	F	902	-	-	0/5/24/24	0/1/1/1
4	SO4	F	911	-	-	0/0/0/0	0/0/0/0
4	SO4	F	912	-	-	0/0/0/0	0/0/0/0
4	SO4	F	913	-	-	0/0/0/0	0/0/0/0
4	SO4	F	914	-	-	0/0/0/0	0/0/0/0
5	MLA	F	921	-	-	0/0/4/4	0/0/0/0
5	MLA	F	922	-	-	0/0/4/4	0/0/0/0
2	UDP	G	901	-	-	0/12/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	G	902	-	-	0/5/24/24	0/1/1/1
4	SO4	G	911	-	-	0/0/0/0	0/0/0/0
4	SO4	G	912	-	-	0/0/0/0	0/0/0/0
4	SO4	G	913	-	-	0/0/0/0	0/0/0/0
4	SO4	G	914	-	-	0/0/0/0	0/0/0/0
5	MLA	G	921	-	-	0/0/4/4	0/0/0/0
5	MLA	G	922	-	-	0/0/4/4	0/0/0/0
2	UDP	H	901	-	-	0/12/32/32	0/2/2/2
3	FRU	H	902	-	-	0/5/24/24	0/1/1/1
4	SO4	H	911	-	-	0/0/0/0	0/0/0/0
4	SO4	H	912	-	-	0/0/0/0	0/0/0/0
4	SO4	H	913	-	-	0/0/0/0	0/0/0/0
5	MLA	H	921	-	-	0/0/4/4	0/0/0/0
5	MLA	H	922	-	-	0/0/4/4	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	902	FRU	O5-C2	-2.51	1.39	1.43
3	H	902	FRU	O5-C2	-2.04	1.40	1.43
3	E	902	FRU	O2-C2	2.26	1.44	1.41
2	D	901	UDP	C4-N3	2.34	1.37	1.33
2	E	901	UDP	C4-N3	2.54	1.37	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	UDP	PA-O3A-PB	-4.06	119.06	132.67
2	B	901	UDP	PA-O3A-PB	-3.35	121.43	132.67
2	E	901	UDP	PA-O3A-PB	-3.23	121.84	132.67
2	G	901	UDP	PA-O3A-PB	-3.20	121.93	132.67
2	H	901	UDP	PA-O3A-PB	-3.16	122.09	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	UDP	1	0
3	A	902	FRU	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	912	SO4	1	0
4	A	913	SO4	1	0
2	B	901	UDP	2	0
3	B	902	FRU	6	0
4	B	913	SO4	3	0
3	C	902	FRU	4	0
4	D	913	SO4	1	0
5	D	921	MLA	1	0
5	D	922	MLA	1	0
2	E	901	UDP	1	0
3	E	902	FRU	11	0
4	E	912	SO4	1	0
4	E	913	SO4	2	0
4	E	914	SO4	1	0
2	F	901	UDP	1	0
5	F	922	MLA	2	0
2	G	901	UDP	1	0
4	G	913	SO4	1	0
3	H	902	FRU	1	0
5	H	922	MLA	1	0

## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	781/816 (95%)	-0.26	25 (3%)	51	44	21, 36, 99, 130	0
1	B	791/816 (96%)	-0.14	36 (4%)	36	30	24, 40, 108, 139	0
1	C	781/816 (95%)	-0.21	28 (3%)	46	39	27, 42, 89, 121	0
1	D	781/816 (95%)	-0.27	21 (2%)	58	52	23, 36, 89, 123	0
1	E	781/816 (95%)	-0.20	33 (4%)	40	33	22, 38, 109, 142	0
1	F	781/816 (95%)	-0.25	26 (3%)	50	43	21, 36, 85, 126	0
1	G	781/816 (95%)	-0.31	15 (1%)	70	66	22, 38, 83, 115	0
1	H	797/816 (97%)	-0.21	25 (3%)	52	46	24, 41, 94, 137	0
All	All	6274/6528 (96%)	-0.23	209 (3%)	50	43	21, 39, 94, 142	0

The worst 5 of 209 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	106	ALA	6.1
1	E	32	LEU	5.6
1	E	31	ALA	5.5
1	D	57	PRO	5.1
1	H	128	VAL	4.9

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	B	913	5/5	0.93	0.45	14.93	63,74,83,102	0
4	SO4	H	913	5/5	0.84	0.34	8.69	70,78,93,114	0
4	SO4	A	911	5/5	0.93	0.24	7.37	46,48,79,82	0
4	SO4	D	911	5/5	0.91	0.27	6.65	47,64,79,95	0
4	SO4	F	911	5/5	0.92	0.34	6.58	51,51,80,90	0
4	SO4	G	913	5/5	0.97	0.30	4.96	58,62,82,92	0
5	MLA	G	921	7/7	0.94	0.36	4.69	52,59,71,71	0
5	MLA	F	921	7/7	0.96	0.29	4.49	32,38,40,45	0
4	SO4	C	913	5/5	0.94	0.31	4.28	64,68,88,94	0
4	SO4	D	913	5/5	0.96	0.31	4.10	58,60,73,85	0
4	SO4	C	911	5/5	0.95	0.21	3.92	51,51,71,82	0
5	MLA	F	922	7/7	0.87	0.26	3.57	49,58,70,70	0
5	MLA	B	921	7/7	0.95	0.19	3.32	45,48,58,58	0
4	SO4	B	911	5/5	0.90	0.22	3.16	53,57,72,97	0
5	MLA	C	921	7/7	0.92	0.27	3.09	58,61,72,72	0
5	MLA	E	921	7/7	0.96	0.25	3.08	36,45,50,54	0
3	FRU	A	902	12/12	0.97	0.21	2.82	28,29,32,34	0
4	SO4	H	911	5/5	0.95	0.23	2.77	47,48,81,82	0
5	MLA	D	921	7/7	0.97	0.24	2.71	37,44,46,48	0
5	MLA	H	921	7/7	0.94	0.28	2.35	47,56,67,67	0
5	MLA	A	921	7/7	0.98	0.20	2.01	38,41,49,49	0
4	SO4	G	911	5/5	0.95	0.18	1.79	41,44,65,67	0
5	MLA	D	922	7/7	0.96	0.19	1.50	45,49,54,55	0
4	SO4	F	913	5/5	0.95	0.20	1.36	53,56,74,79	0
4	SO4	E	911	5/5	0.95	0.17	1.33	44,44,71,79	0
4	SO4	D	914	5/5	0.89	0.27	1.20	64,90,95,108	0
4	SO4	G	914	5/5	0.88	0.27	1.15	62,88,97,108	0
2	UDP	B	901	25/25	0.99	0.18	0.98	25,29,32,32	0
6	K	D	931	1/1	0.94	0.30	0.95	81,81,81,81	0
6	K	G	931	1/1	0.93	0.25	0.86	76,76,76,76	0
3	FRU	G	902	12/12	0.95	0.18	0.69	24,33,34,39	0
3	FRU	H	902	12/12	0.96	0.18	0.68	23,29,34,36	0
2	UDP	D	901	25/25	0.99	0.17	0.63	22,25,32,35	0
2	UDP	H	901	25/25	0.98	0.18	0.59	25,28,34,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FRU	B	902	12/12	0.97	0.17	0.46	27,30,33,33	0
3	FRU	D	902	12/12	0.98	0.17	0.45	25,28,32,32	0
5	MLA	H	922	7/7	0.88	0.23	0.43	70,79,84,85	0
2	UDP	E	901	25/25	0.99	0.18	0.43	23,26,31,33	0
2	UDP	F	901	25/25	0.99	0.17	0.35	18,25,29,33	0
6	K	F	931	1/1	0.89	0.26	0.26	89,89,89,89	0
2	UDP	G	901	25/25	0.99	0.16	0.23	19,26,29,31	0
2	UDP	A	901	25/25	0.99	0.16	0.13	20,26,29,33	0
3	FRU	F	902	12/12	0.98	0.17	0.06	23,26,28,28	0
2	UDP	C	901	25/25	0.99	0.16	0.04	25,31,35,39	0
3	FRU	C	902	12/12	0.96	0.17	0.03	31,38,43,46	0
6	K	B	931	1/1	0.82	0.22	-0.24	99,99,99,99	0
6	K	H	931	1/1	0.94	0.26	-0.29	74,74,74,74	0
3	FRU	E	902	12/12	0.98	0.16	-0.75	28,30,33,33	0
6	K	C	931	1/1	0.93	0.18	-0.97	75,75,75,75	0
6	K	E	931	1/1	0.80	0.18	-0.97	79,79,79,79	0
6	K	A	931	1/1	0.96	0.16	-1.02	72,72,72,72	0
4	SO4	E	912	5/5	0.93	0.22	-	65,77,86,100	0
4	SO4	H	912	5/5	0.89	0.32	-	66,89,99,112	0
4	SO4	D	912	5/5	0.90	0.24	-	57,71,94,108	0
4	SO4	B	912	5/5	0.93	0.19	-	76,85,96,114	0
5	MLA	G	922	7/7	0.85	0.15	-	69,86,100,100	0
4	SO4	A	913	5/5	0.93	0.28	-	49,66,79,86	0
4	SO4	E	913	5/5	0.93	0.29	-	54,57,84,92	0
4	SO4	F	914	5/5	0.94	0.21	-	59,81,101,102	0
4	SO4	A	914	5/5	0.89	0.20	-	59,91,102,108	0
4	SO4	F	912	5/5	0.94	0.19	-	57,71,79,92	0
4	SO4	A	912	5/5	0.93	0.23	-	62,72,79,100	0
4	SO4	C	912	5/5	0.93	0.23	-	73,82,95,107	0
4	SO4	A	915	5/5	0.87	0.24	-	120,122,135,138	0
4	SO4	G	912	5/5	0.97	0.20	-	57,74,84,97	0
4	SO4	E	914	5/5	0.93	0.27	-	65,88,93,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.