



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:50 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

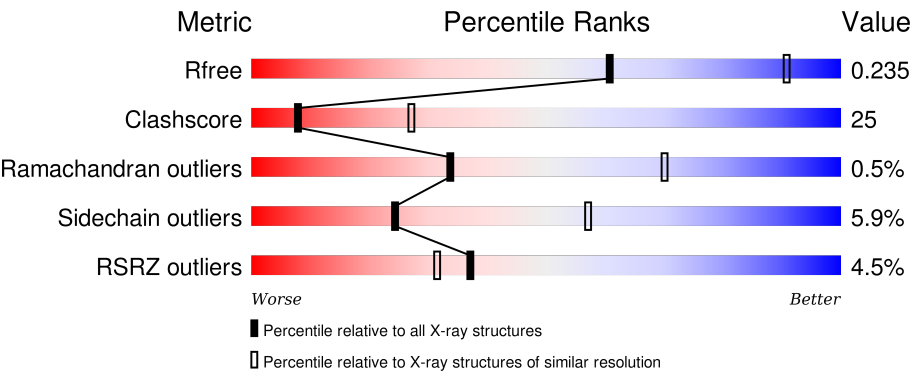
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance 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}	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div><div>4%</div><div>58%34%</div><div></div></div>
1	B	816	<div><div>7%</div><div>58%36%</div><div></div></div>
1	C	816	<div><div>3%</div><div>54%38%</div><div></div></div>
1	D	816	<div><div>3%</div><div>60%34%</div><div></div></div>
1	E	816	<div><div>4%</div><div>60%31%</div><div></div></div>

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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	SO4	A	911	-	-	-	X
4	SO4	B	913	-	-	X	X
4	SO4	D	911	-	-	-	X
4	SO4	E	913	-	-	-	X
4	SO4	F	911	-	-	-	X
4	SO4	F	913	-	-	X	-
4	SO4	G	911	-	-	-	X
4	SO4	H	913	-	-	-	X
5	MLA	B	921	-	-	-	X
5	MLA	C	921	-	-	-	X
5	MLA	D	921	-	-	-	X
5	MLA	E	921	-	-	X	X
5	MLA	F	921	-	-	-	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 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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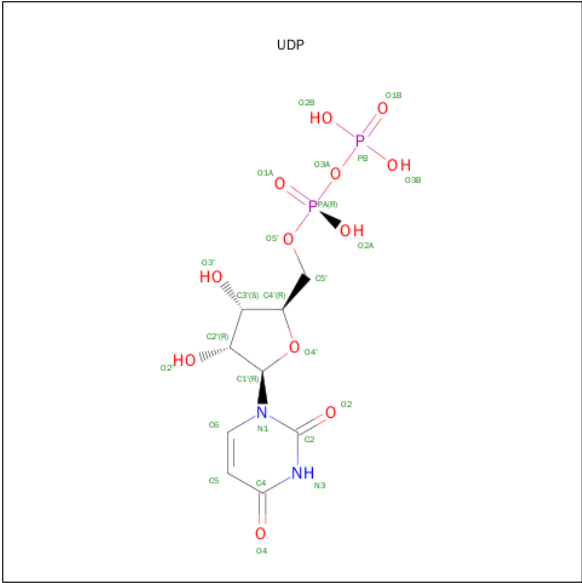
Chain	Residue	Modelled	Actual	Comment	Reference
B	814	HIS	-	EXPRESSION TAG	UNP P49040
B	815	HIS	-	EXPRESSION TAG	UNP P49040
B	816	HIS	-	EXPRESSION TAG	UNP P49040
C	809	VAL	-	EXPRESSION TAG	UNP P49040
C	810	GLU	-	EXPRESSION TAG	UNP P49040
C	811	HIS	-	EXPRESSION TAG	UNP P49040
C	812	HIS	-	EXPRESSION TAG	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

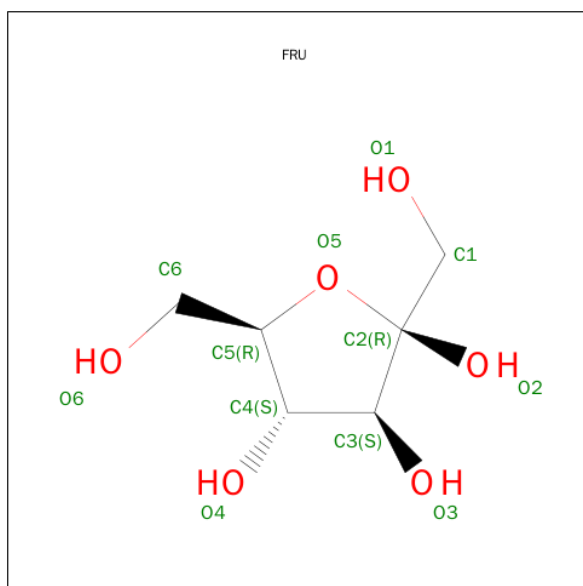
- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



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

- Molecule 3 is SUGAR (FRUCTOSE) (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).



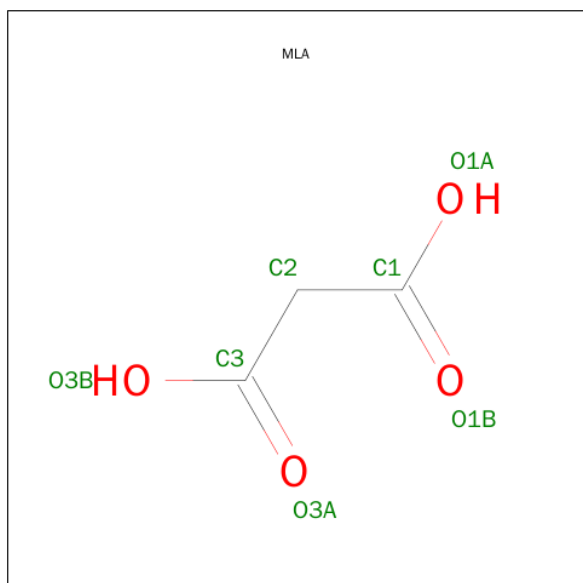
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

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

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



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

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

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

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

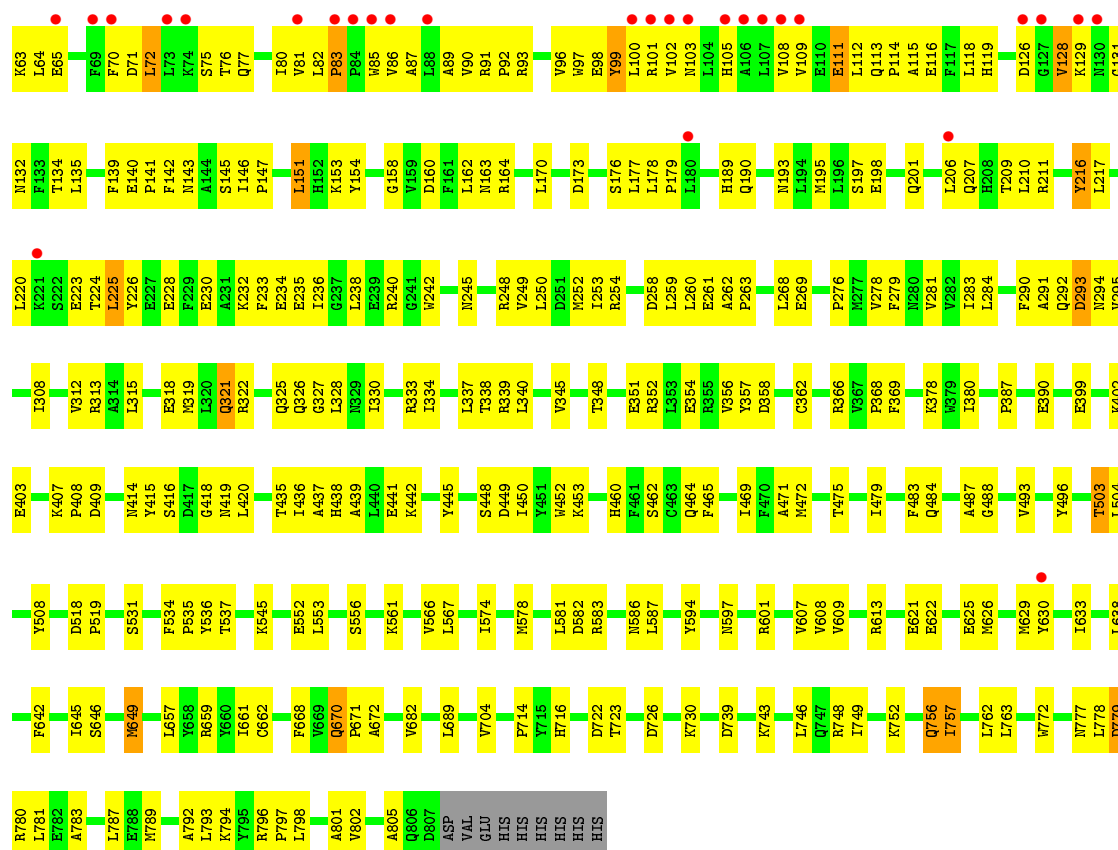
- Molecule 7 is water.

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

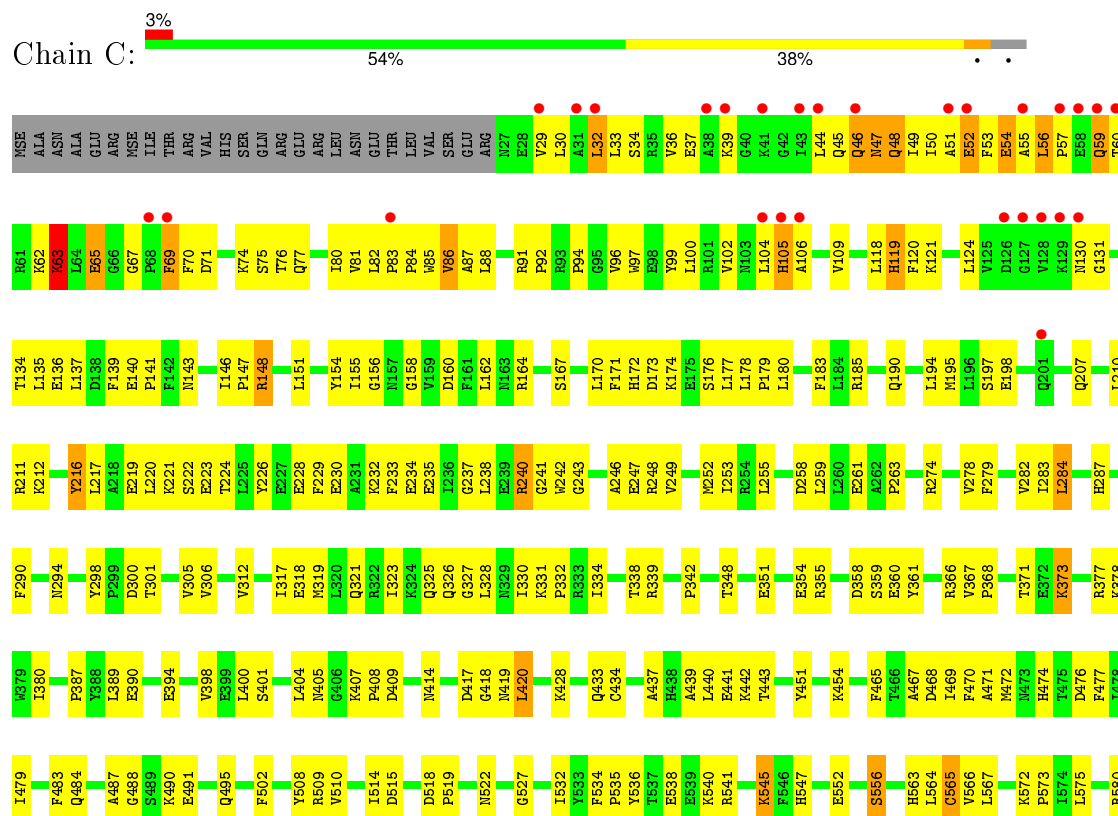
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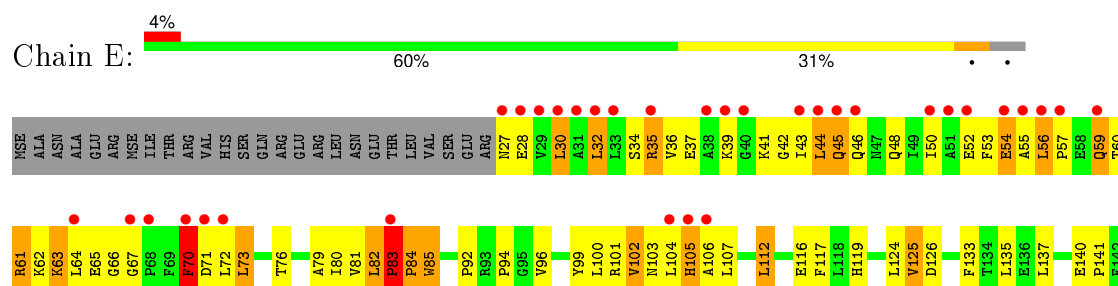
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	45	Total 45	O 45	0	0
7	D	67	Total 67	O 67	0	0
7	E	66	Total 66	O 66	0	0
7	F	90	Total 90	O 90	0	0
7	G	81	Total 81	O 81	0	0
7	H	60	Total 60	O 60	0	0

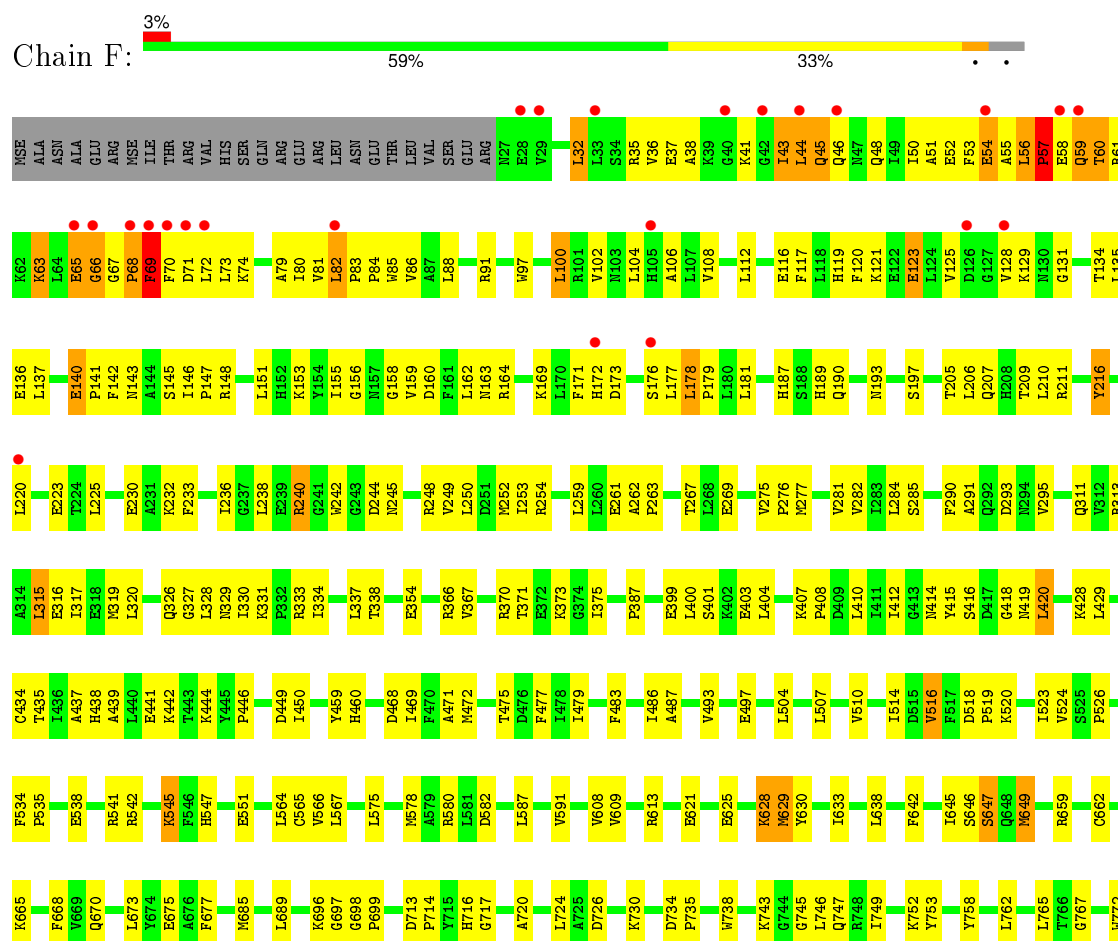


• Molecule 1: Sucrose synthase 1



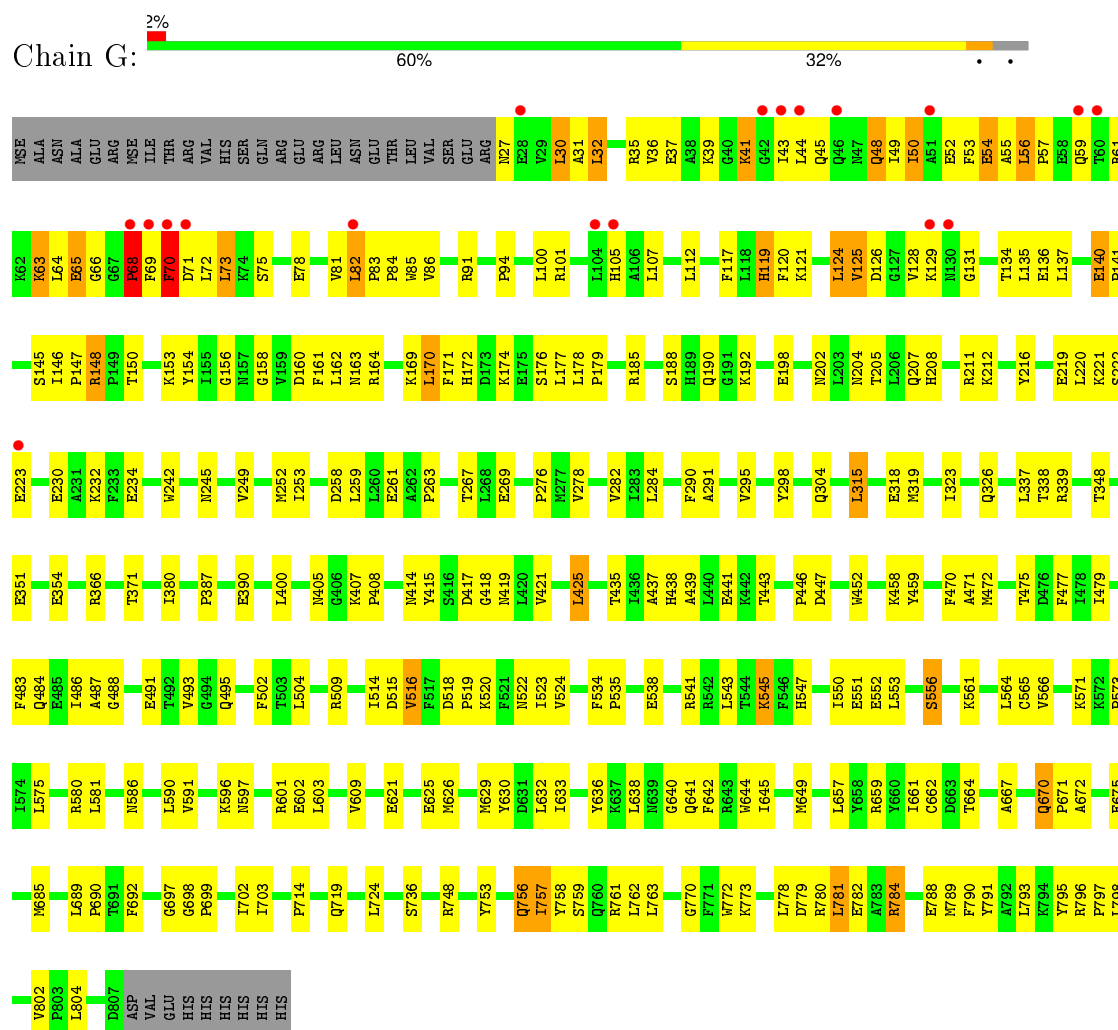


- Molecule 1: Sucrose synthase 1

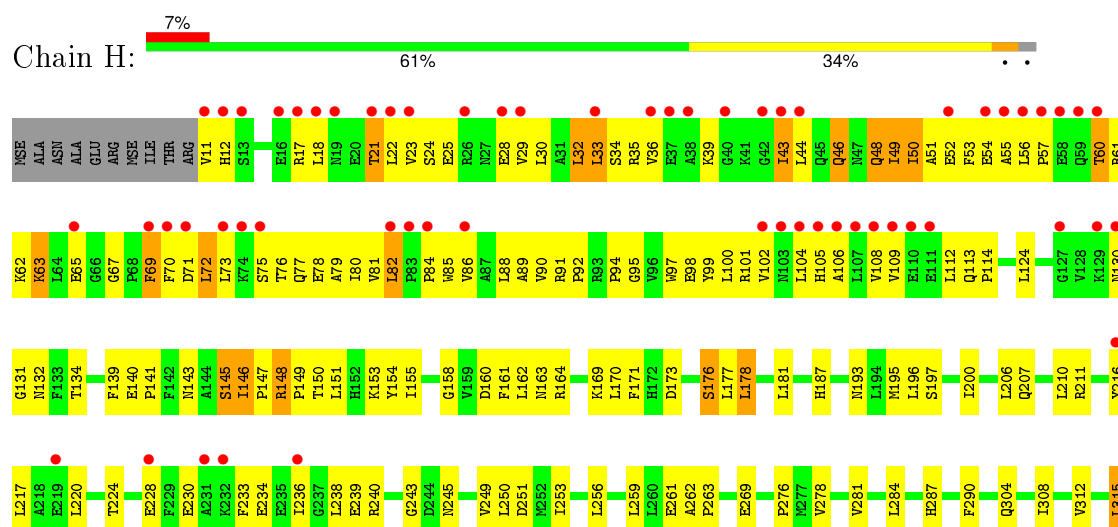




• Molecule 1: Sucrose synthase 1



• Molecule 1: Sucrose synthase 1



Y791	A672	L553	A437	K319
A792	E675	S556	H438	R322
L793	A676	K561	A439	I323
K794	F677	E562	K444	Q326
Y795	G678	H563	D449	I336
R796	L679	L564	I450	L337
P797	T680	C565	Y451	T338
V802	V681	V566	K453	R339
D807	V682	K572	T466	Y345
ASP	A684	V584	M472	T348
VAL	H685	S588	T475	E351
GLU	I689	G589	D476	R352
HIS	F692	L590	S481	L353
HIS	A693	K596	E354	R355
HIS	T694	R599	F483	S359
HIS	G697	V609	I486	L365
HIS	G698	R613	A487	R366
HIS	P699	K614	T492	V367
	H705	K615	V493	P368
	Q719	E616	T503	I375
	D726	S617	L504	K378
	E743	K623	Y508	P387
	R748	A624	H512	E390
	I749	E525	G513	L400
	E750	M626	I514	K407
	E761	M629	D515	P408
	K762	Y630	F517	I411
	L763	Y636	D518	M414
	T766	G640	P519	Y415
	H772	Q641	K520	S416
	D779	F642	A528	D417
	E782	I645	I532	O418
	A783	R651	Y533	M419
	R784	L657	F534	L425
	L787	Y658	P535	V431
	E788	R659	E538	T432
	M789	Y660	E539	Q433
	F790	I661	K540	C434
		C662	R541	T435
		F668	R542	I436
		V669	K545	
		Q670	E552	
		P671		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.21Å 263.70Å 159.66Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	25.00 – 2.91 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
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, R_{free}	0.186 , 0.237 0.186 , 0.235	Depositor DCC
R_{free} test set	11567 reflections (5.68%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	5 of 231037 reflections (0.002%)	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.40	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

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%)	34	70
1	B	791/816 (97%)	734 (93%)	56 (7%)	1 (0%)	56	86
1	C	779/816 (96%)	734 (94%)	42 (5%)	3 (0%)	39	74
1	D	779/816 (96%)	736 (94%)	38 (5%)	5 (1%)	30	66
1	E	779/816 (96%)	737 (95%)	38 (5%)	4 (0%)	34	70
1	F	779/816 (96%)	734 (94%)	39 (5%)	6 (1%)	24	58
1	G	779/816 (96%)	736 (94%)	39 (5%)	4 (0%)	34	70
1	H	795/816 (97%)	750 (94%)	42 (5%)	3 (0%)	39	74
All	All	6260/6528 (96%)	5891 (94%)	339 (5%)	30 (0%)	34	70

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%)	23	55
1	B	663/704 (94%)	626 (94%)	37 (6%)	26	59
1	C	666/704 (95%)	622 (93%)	44 (7%)	21	50
1	D	659/704 (94%)	624 (95%)	35 (5%)	28	62
1	E	662/704 (94%)	620 (94%)	42 (6%)	22	53
1	F	668/704 (95%)	635 (95%)	33 (5%)	31	66
1	G	668/704 (95%)	626 (94%)	42 (6%)	22	53
1	H	663/704 (94%)	623 (94%)	40 (6%)	24	56
All	All	5316/5632 (94%)	5002 (94%)	314 (6%)	24	57

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

Mol	Chain	Res	Type
1	D	286	PRO
1	E	167	SER
1	H	146	ILE
1	D	491	GLU
1	E	35	ARG

Some 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	719	GLN
1	E	737	HIS
1	H	204	ASN
1	E	193	ASN
1	F	59	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UDP	A	901	-	18,26,26	1.00	0	23,40,40	1.02	1 (4%)
3	FRU	A	902	-	11,12,12	0.77	0	10,18,18	0.80	0
4	SO4	A	911	-	4,4,4	0.19	0	6,6,6	0.26	0
4	SO4	A	912	-	4,4,4	0.09	0	6,6,6	0.17	0
4	SO4	A	913	-	4,4,4	0.09	0	6,6,6	0.33	0
5	MLA	A	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	B	901	-	18,26,26	0.90	0	23,40,40	1.09	1 (4%)
3	FRU	B	902	-	11,12,12	0.78	1 (9%)	10,18,18	0.83	0
4	SO4	B	911	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	B	912	-	4,4,4	0.09	0	6,6,6	0.32	0
4	SO4	B	913	-	4,4,4	0.17	0	6,6,6	0.24	0
5	MLA	B	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	C	901	-	18,26,26	0.94	0	23,40,40	0.99	1 (4%)
3	FRU	C	902	-	11,12,12	0.67	0	10,18,18	0.84	0
4	SO4	C	911	-	4,4,4	0.10	0	6,6,6	0.25	0
4	SO4	C	912	-	4,4,4	0.04	0	6,6,6	0.16	0
4	SO4	C	913	-	4,4,4	0.09	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	1.06	0	23,40,40	1.08	1 (4%)
3	FRU	D	902	-	11,12,12	1.02	1 (9%)	10,18,18	1.23	2 (20%)
4	SO4	D	911	-	4,4,4	0.17	0	6,6,6	0.26	0
4	SO4	D	912	-	4,4,4	0.03	0	6,6,6	0.10	0
4	SO4	D	913	-	4,4,4	0.11	0	6,6,6	0.17	0
5	MLA	D	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	E	901	-	18,26,26	0.98	0	23,40,40	1.09	1 (4%)
3	FRU	E	902	-	11,12,12	0.70	0	10,18,18	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	E	911	-	4,4,4	0.17	0	6,6,6	0.32	0
4	SO4	E	912	-	4,4,4	0.12	0	6,6,6	0.12	0
4	SO4	E	913	-	4,4,4	0.15	0	6,6,6	0.23	0
5	MLA	E	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	F	901	-	18,26,26	0.91	0	23,40,40	0.98	1 (4%)
3	FRU	F	902	-	11,12,12	0.71	0	10,18,18	0.71	0
4	SO4	F	911	-	4,4,4	0.24	0	6,6,6	0.38	0
4	SO4	F	912	-	4,4,4	0.09	0	6,6,6	0.20	0
4	SO4	F	913	-	4,4,4	0.13	0	6,6,6	0.20	0
5	MLA	F	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	G	901	-	18,26,26	0.99	0	23,40,40	0.97	1 (4%)
3	FRU	G	902	-	11,12,12	0.72	0	10,18,18	0.76	0
4	SO4	G	911	-	4,4,4	0.19	0	6,6,6	0.13	0
4	SO4	G	912	-	4,4,4	0.06	0	6,6,6	0.07	0
4	SO4	G	913	-	4,4,4	0.04	0	6,6,6	0.09	0
5	MLA	G	921	-	0,6,6	0.00	-	0,7,7	0.00	-
2	UDP	H	901	-	18,26,26	1.02	0	23,40,40	1.02	1 (4%)
3	FRU	H	902	-	11,12,12	0.89	1 (9%)	10,18,18	1.06	0
4	SO4	H	911	-	4,4,4	0.20	0	6,6,6	0.23	0
4	SO4	H	912	-	4,4,4	0.05	0	6,6,6	0.13	0
4	SO4	H	913	-	4,4,4	0.13	0	6,6,6	0.18	0
5	MLA	H	921	-	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
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
5	MLA	D	921	-	-	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
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
5	MLA	F	921	-	-	0/0/4/4	0/0/0/0
2	UDP	G	901	-	-	0/12/32/32	0/2/2/2
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
5	MLA	G	921	-	-	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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	902	FRU	O2-C2	2.19	1.44	1.41
3	B	902	FRU	O2-C2	2.30	1.44	1.41
3	D	902	FRU	C1-C2	2.35	1.56	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	UDP	PA-O3A-PB	-3.84	119.78	132.67
2	B	901	UDP	PA-O3A-PB	-3.69	120.30	132.67
2	A	901	UDP	PA-O3A-PB	-3.55	120.76	132.67
2	D	901	UDP	PA-O3A-PB	-3.48	121.02	132.67
2	G	901	UDP	PA-O3A-PB	-2.89	122.99	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 33 short contacts:

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

5.7 Other polymers

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	769/816 (94%)	-0.23	29 (3%)	44	38	13, 27, 90, 116	0
1	B	781/816 (95%)	0.09	57 (7%)	18	12	16, 33, 98, 131	0
1	C	769/816 (94%)	-0.11	28 (3%)	46	39	20, 38, 83, 122	0
1	D	769/816 (94%)	-0.23	26 (3%)	49	42	14, 28, 80, 111	0
1	E	769/816 (94%)	-0.15	35 (4%)	36	31	14, 30, 95, 118	0
1	F	769/816 (94%)	-0.24	24 (3%)	52	46	10, 26, 73, 111	0
1	G	769/816 (94%)	-0.27	18 (2%)	64	59	14, 30, 70, 108	0
1	H	785/816 (96%)	0.04	61 (7%)	16	11	17, 35, 92, 117	0
All	All	6180/6528 (94%)	-0.14	278 (4%)	37	31	10, 31, 87, 131	0

The worst 5 of 278 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	VAL	8.3
1	B	105	HIS	7.9
1	H	83	PRO	7.8
1	B	102	VAL	7.6
1	H	18	LEU	7.1

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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	H	913	5/5	0.89	0.42	15.97	64,70,86,101	0
5	MLA	D	921	7/7	0.94	0.33	6.76	33,40,44,47	0
5	MLA	H	921	7/7	0.89	0.41	6.27	53,58,69,69	0
5	MLA	E	921	7/7	0.95	0.37	5.04	34,38,43,43	0
4	SO4	B	913	5/5	0.91	0.28	4.78	53,54,65,78	0
5	MLA	C	921	7/7	0.89	0.41	4.14	56,60,68,77	0
4	SO4	A	911	5/5	0.97	0.22	4.01	31,35,46,58	0
4	SO4	G	911	5/5	0.96	0.24	3.52	32,40,56,64	0
4	SO4	E	913	5/5	0.95	0.21	3.22	44,47,62,71	0
5	MLA	F	921	7/7	0.93	0.23	2.60	30,35,36,36	0
5	MLA	B	921	7/7	0.94	0.26	2.54	38,45,50,53	0
4	SO4	D	911	5/5	0.95	0.20	2.42	38,41,56,67	0
5	MLA	G	921	7/7	0.92	0.27	2.21	46,49,59,59	0
4	SO4	F	911	5/5	0.95	0.20	2.09	32,36,45,64	0
4	SO4	E	911	5/5	0.94	0.17	1.41	31,35,59,60	0
5	MLA	A	921	7/7	0.93	0.19	1.21	27,31,34,36	0
2	UDP	F	901	25/25	0.99	0.18	1.04	14,18,23,25	0
3	FRU	C	902	12/12	0.93	0.21	1.00	30,36,44,50	0
4	SO4	D	913	5/5	0.96	0.16	0.90	44,46,53,63	0
6	K	C	931	1/1	0.95	0.25	0.79	69,69,69,69	0
2	UDP	B	901	25/25	0.98	0.18	0.61	19,25,30,34	0
4	SO4	C	911	5/5	0.96	0.16	0.53	44,46,57,63	0
3	FRU	B	902	12/12	0.96	0.17	0.48	25,30,35,35	0
4	SO4	H	911	5/5	0.95	0.15	0.37	37,38,69,70	0
4	SO4	F	913	5/5	0.97	0.15	0.25	40,44,61,64	0
2	UDP	H	901	25/25	0.98	0.17	0.18	22,28,36,38	0
2	UDP	G	901	25/25	0.99	0.17	0.15	14,21,25,35	0
3	FRU	H	902	12/12	0.94	0.17	0.09	22,29,34,37	0
4	SO4	G	913	5/5	0.95	0.17	0.08	52,58,68,74	0
4	SO4	B	911	5/5	0.95	0.14	-0.07	37,42,50,70	0
3	FRU	E	902	12/12	0.97	0.17	-0.14	18,25,30,32	0
6	K	F	931	1/1	0.82	0.21	-0.24	69,69,69,69	0
2	UDP	E	901	25/25	0.99	0.17	-0.28	17,21,27,29	0
6	K	B	931	1/1	0.91	0.22	-0.29	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FRU	D	902	12/12	0.96	0.15	-0.39	18,25,31,32	0
2	UDP	D	901	25/25	0.99	0.15	-0.43	17,21,25,30	0
6	K	D	931	1/1	0.93	0.17	-0.44	61,61,61,61	0
2	UDP	A	901	25/25	0.99	0.16	-0.44	14,17,21,24	0
3	FRU	F	902	12/12	0.97	0.15	-0.46	17,22,28,35	0
3	FRU	G	902	12/12	0.96	0.15	-0.46	18,25,34,34	0
2	UDP	C	901	25/25	0.98	0.15	-0.52	21,31,40,42	0
6	K	H	931	1/1	0.96	0.17	-0.62	61,61,61,61	0
6	K	E	931	1/1	0.90	0.16	-1.02	64,64,64,64	0
3	FRU	A	902	12/12	0.97	0.13	-1.62	16,22,27,28	0
6	K	A	931	1/1	0.94	0.09	-1.91	61,61,61,61	0
6	K	G	931	1/1	0.93	0.10	-2.49	57,57,57,57	0
4	SO4	F	912	5/5	0.93	0.19	-	46,50,62,76	0
4	SO4	E	912	5/5	0.91	0.32	-	47,55,63,84	0
4	SO4	D	912	5/5	0.92	0.28	-	54,74,96,98	0
4	SO4	H	912	5/5	0.93	0.30	-	63,66,76,94	0
4	SO4	B	912	5/5	0.94	0.24	-	49,67,79,88	0
4	SO4	A	912	5/5	0.93	0.21	-	47,55,59,81	0
4	SO4	C	913	5/5	0.92	0.36	-	63,74,75,89	0
4	SO4	A	913	5/5	0.96	0.19	-	42,44,52,59	0
4	SO4	C	912	5/5	0.90	0.38	-	71,74,96,104	0
4	SO4	G	912	5/5	0.95	0.30	-	48,67,72,86	0

6.5 Other polymers

There are no such residues in this entry.