



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AIC
Title : Crystal Structure of Glucansucrase from Streptococcus mutans
Authors : Ito, K.; Ito, S.; Shimamura, T.; Iwata, S.
Deposited on : 2010-05-12
Resolution : 3.11 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

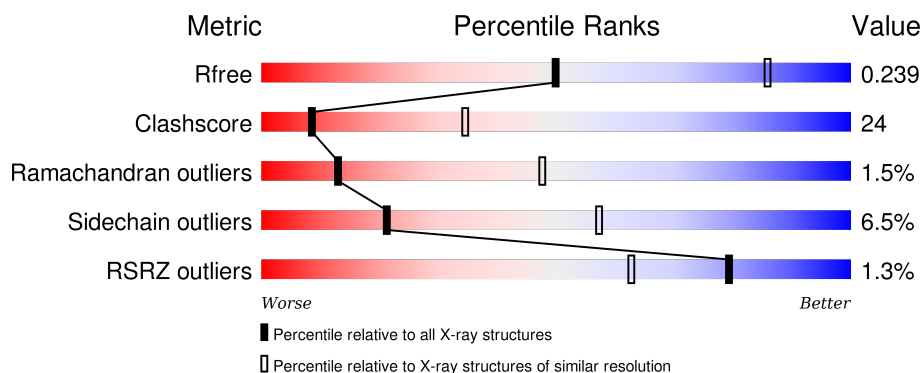
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	844	<div> <div>2%</div> <div>65% 31% .</div> </div>
1	B	844	<div> <div>2%</div> <div>57% 29% . 11%</div> </div>
1	C	844	<div> <div>66% 31% .</div> </div>
1	D	844	<div> <div>2%</div> <div>63% 32% 5%</div> </div>
1	E	844	<div> <div>2%</div> <div>66% 28% 5% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	844	
1	G	844	
1	H	844	

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	ACR	C	5044	-	-	-	X
4	ACR	E	5044	-	-	-	X
4	ACR	F	5044	-	-	-	X
4	ACR	G	5044	-	-	-	X
4	ACR	H	5044	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52865 atoms, of which 0 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 Glucosyltransferase-SI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	0	0
			6643	4184	1141	1302	16			
1	B	747	Total	C	N	O	S	0	0	0
			5854	3684	1005	1151	14			
1	C	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	D	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	E	843	Total	C	N	O	S	0	0	0
			6654	4193	1142	1303	16			
1	F	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	G	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	H	807	Total	C	N	O	S	0	0	0
			6372	4019	1093	1244	16			

There are 32 discrepancies between the modelled and reference sequences:

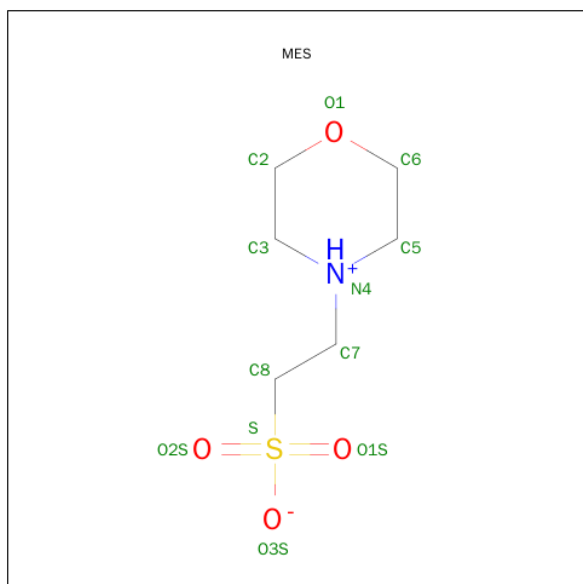
Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASP	ASN	SEE REMARK 999	UNP P13470
A	600	LYS	ARG	SEE REMARK 999	UNP P13470
A	727	ILE	THR	SEE REMARK 999	UNP P13470
A	734	VAL	ALA	SEE REMARK 999	UNP P13470
B	597	ASP	ASN	SEE REMARK 999	UNP P13470
B	600	LYS	ARG	SEE REMARK 999	UNP P13470
B	727	ILE	THR	SEE REMARK 999	UNP P13470
B	734	VAL	ALA	SEE REMARK 999	UNP P13470
C	597	ASP	ASN	SEE REMARK 999	UNP P13470
C	600	LYS	ARG	SEE REMARK 999	UNP P13470
C	727	ILE	THR	SEE REMARK 999	UNP P13470
C	734	VAL	ALA	SEE REMARK 999	UNP P13470
D	597	ASP	ASN	SEE REMARK 999	UNP P13470

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	600	LYS	ARG	SEE REMARK 999	UNP P13470
D	727	ILE	THR	SEE REMARK 999	UNP P13470
D	734	VAL	ALA	SEE REMARK 999	UNP P13470
E	597	ASP	ASN	SEE REMARK 999	UNP P13470
E	600	LYS	ARG	SEE REMARK 999	UNP P13470
E	727	ILE	THR	SEE REMARK 999	UNP P13470
E	734	VAL	ALA	SEE REMARK 999	UNP P13470
F	597	ASP	ASN	SEE REMARK 999	UNP P13470
F	600	LYS	ARG	SEE REMARK 999	UNP P13470
F	727	ILE	THR	SEE REMARK 999	UNP P13470
F	734	VAL	ALA	SEE REMARK 999	UNP P13470
G	597	ASP	ASN	SEE REMARK 999	UNP P13470
G	600	LYS	ARG	SEE REMARK 999	UNP P13470
G	727	ILE	THR	SEE REMARK 999	UNP P13470
G	734	VAL	ALA	SEE REMARK 999	UNP P13470
H	597	ASP	ASN	SEE REMARK 999	UNP P13470
H	600	LYS	ARG	SEE REMARK 999	UNP P13470
H	727	ILE	THR	SEE REMARK 999	UNP P13470
H	734	VAL	ALA	SEE REMARK 999	UNP P13470

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

Continued on next page...

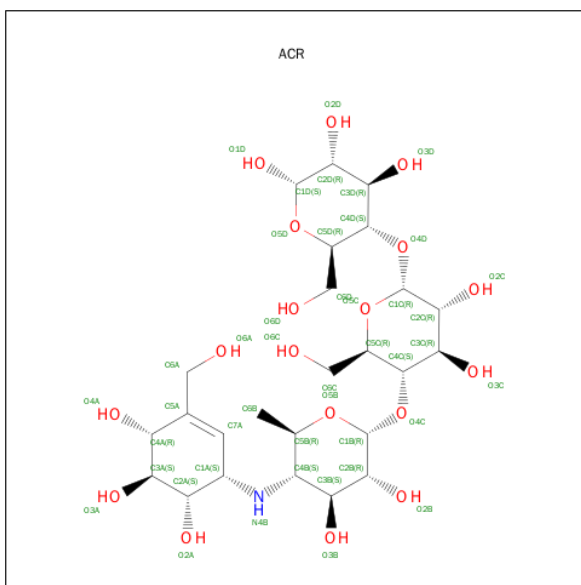
Continued from previous page...

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is SUGAR (ALPHA-ACARBOSE) (three-letter code: ACR) (formula: C₂₅H₄₃N₁O₁₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 44	C 25	N 1	O 18	0	0
4	B	1	Total 44	C 25	N 1	O 18	0	0
4	C	1	Total 44	C 25	N 1	O 18	0	0
4	D	1	Total 44	C 25	N 1	O 18	0	0
4	E	1	Total 44	C 25	N 1	O 18	0	0
4	F	1	Total 44	C 25	N 1	O 18	0	0
4	G	1	Total 44	C 25	N 1	O 18	0	0
4	H	1	Total 44	C 25	N 1	O 18	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	20	Total O 20 20	0	0
5	C	32	Total O 32 32	0	0
5	D	40	Total O 40 40	0	0

Continued on next page...

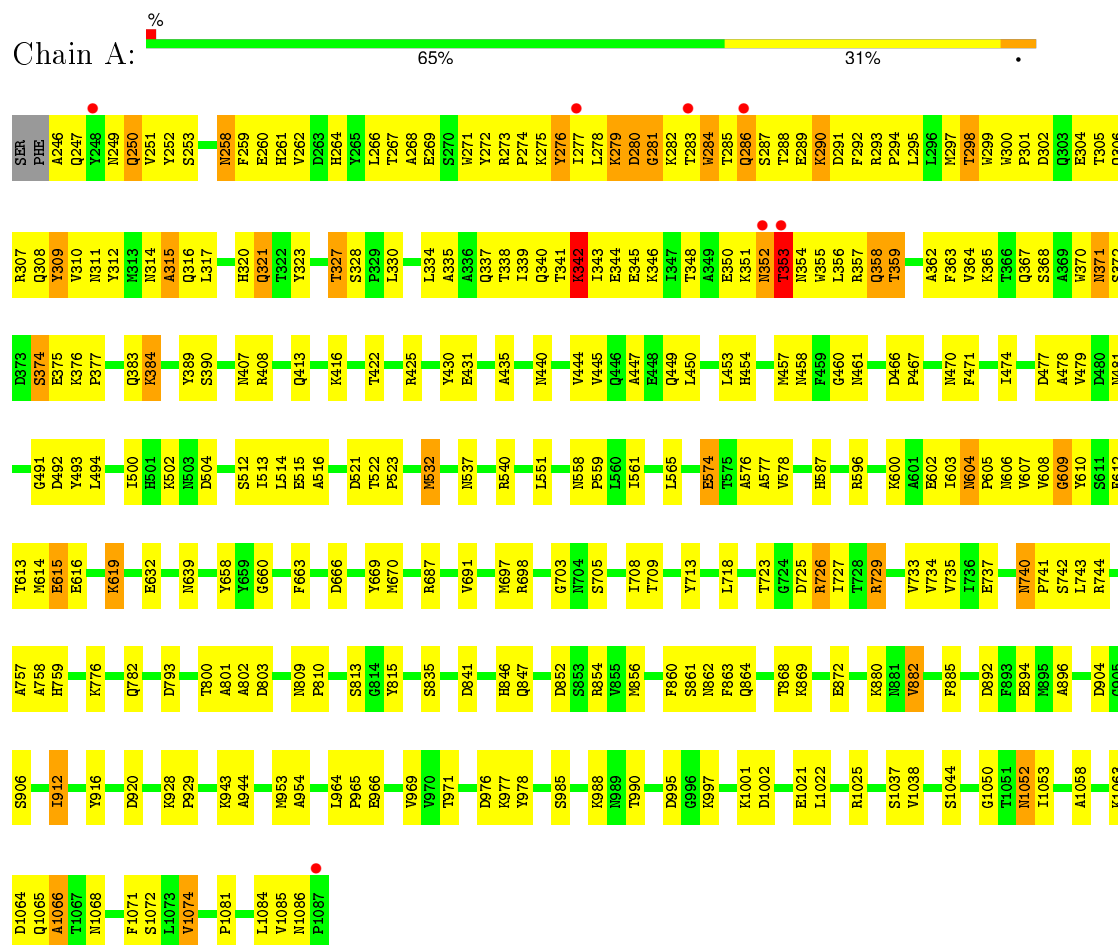
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	48	Total 48	O 48	0	0
5	F	15	Total 15	O 15	0	0
5	G	34	Total 34	O 34	0	0
5	H	24	Total 24	O 24	0	0

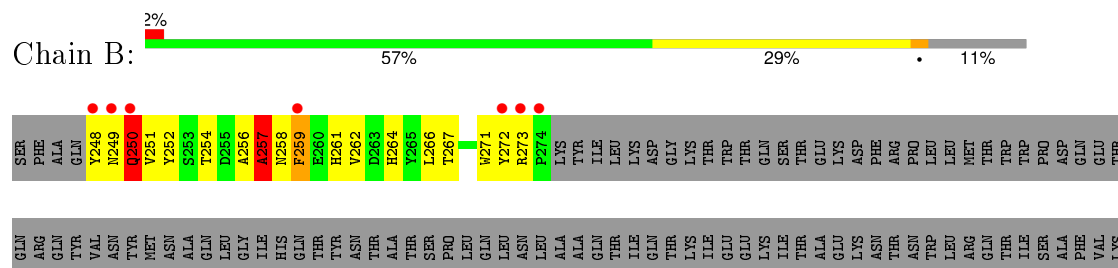
3 Residue-property plots

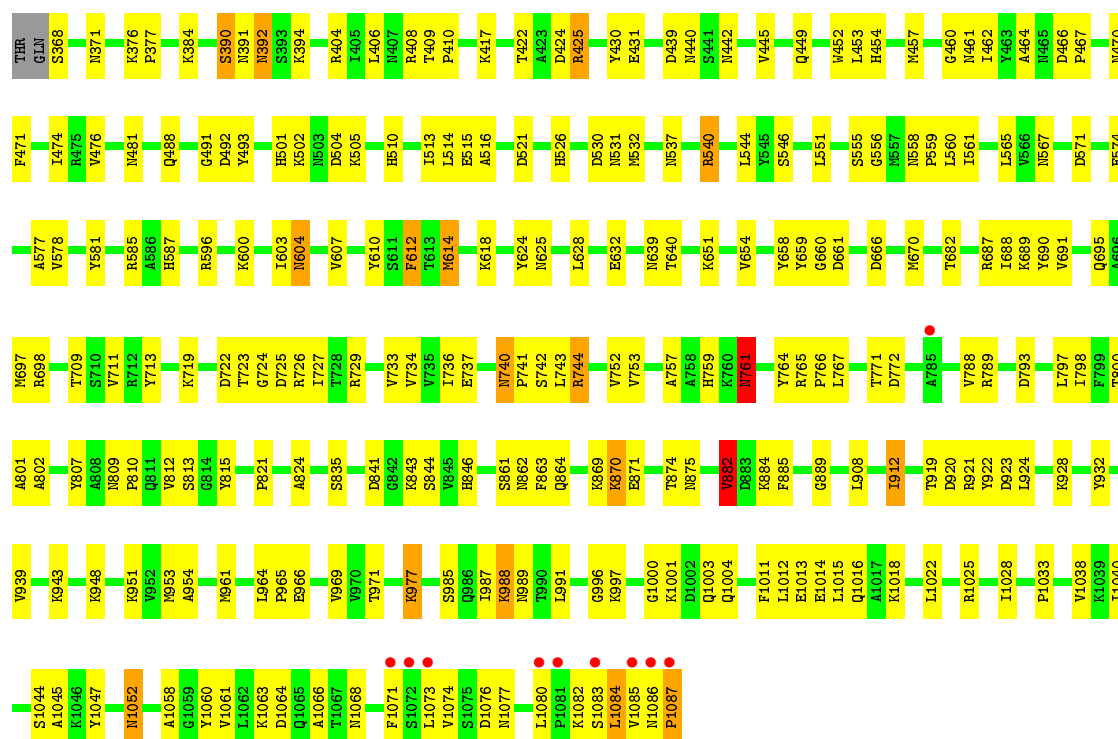
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Glucosyltransferase-SI



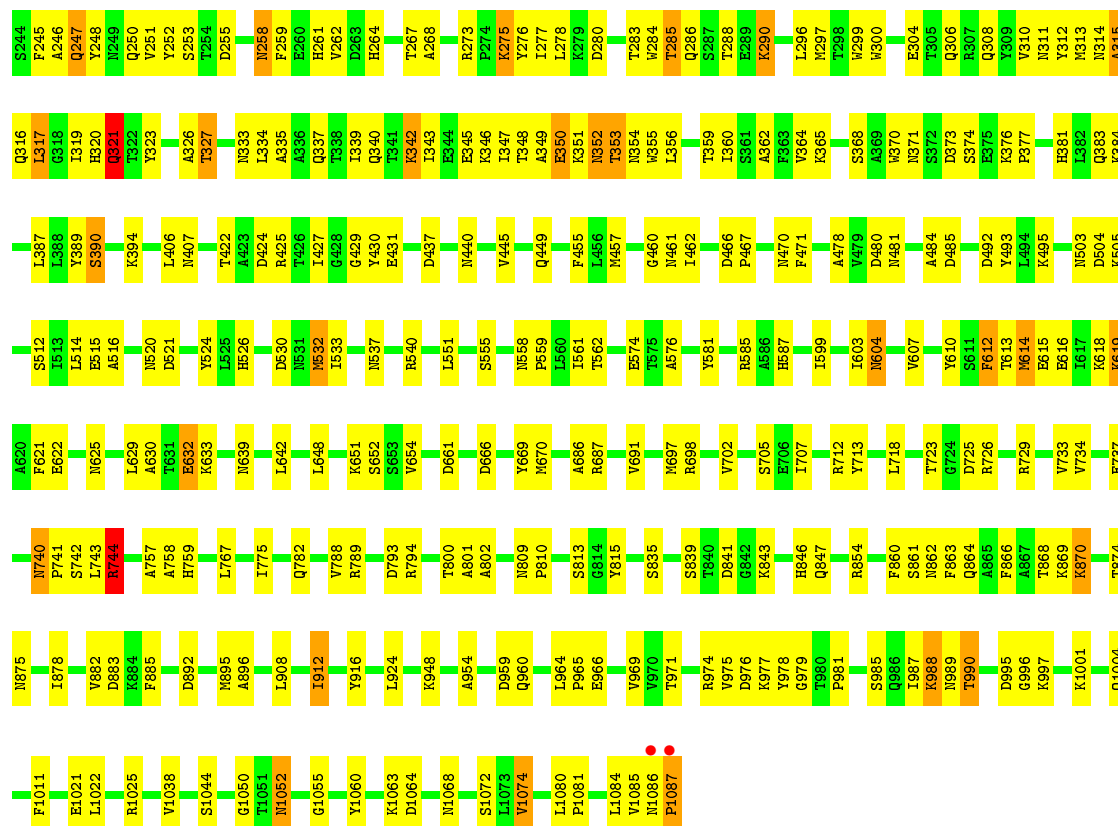
• Molecule 1: Glucosyltransferase-SI





• Molecule 1: Glucosyltransferase-SI

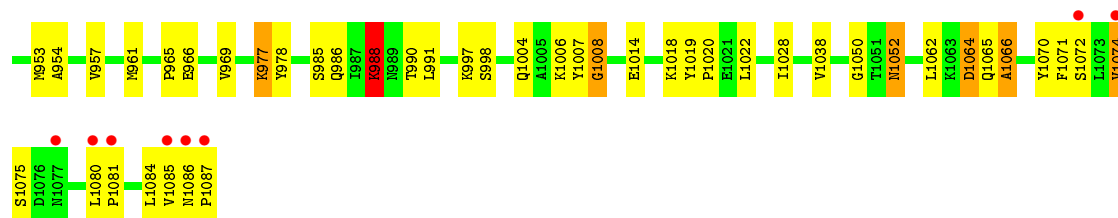
Chain C: 66% 31% •



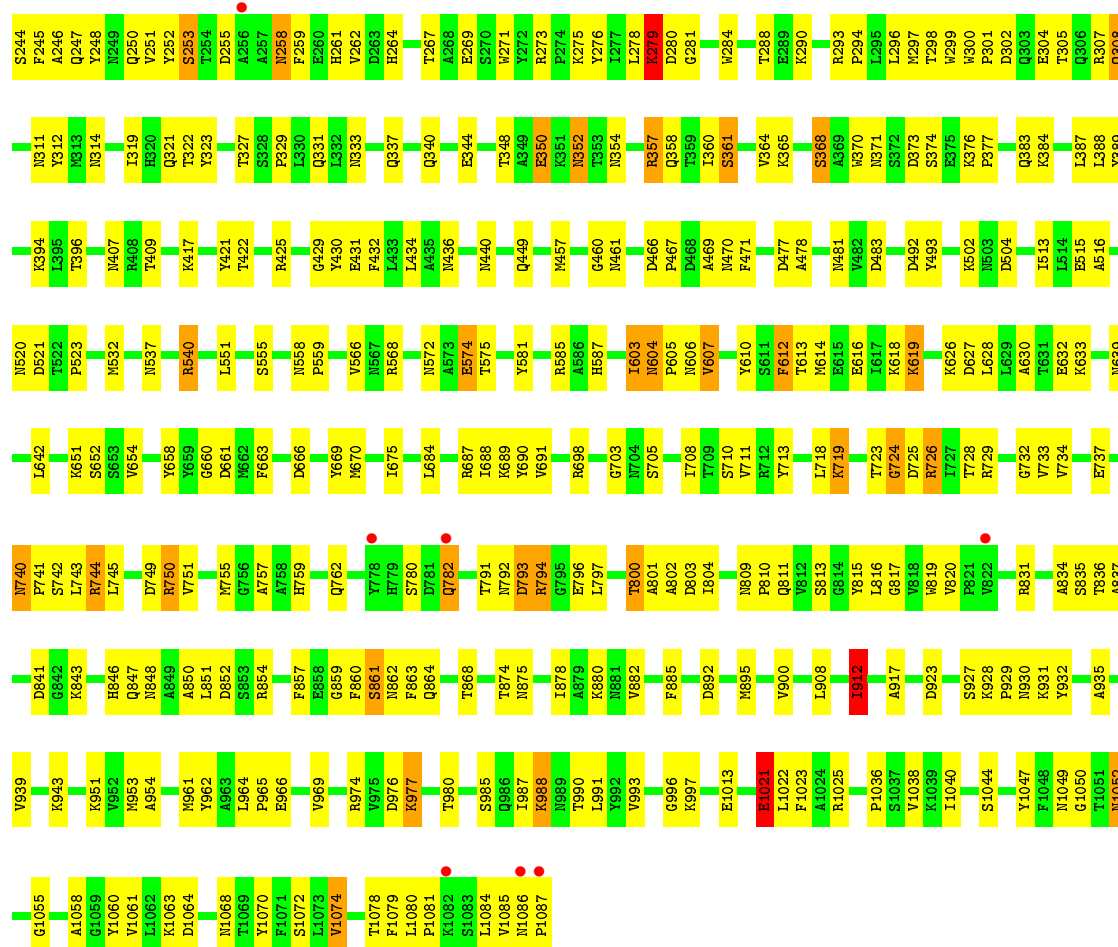
Chain D: ■ 63% ■ 32% ■ 5%

Category	Sub-Category	Value
63%	K997	Y764
	S998	R765
	S999	F766
	K1000	F967
	K1001	L768
	D1002	A777
	A1005	L908
	E1013	I912
	K1021	Y916
	L1022	T919
32%	V1038	D920
	K1041	L924
	Q1042	T800
	W1043	K928
	G1050	P929
	T1051	D803
	M1052	I804
	I1053	K805
	R1056	K948
	G1057	M953
5%	A1058	A954
	D1064	V957
	K1065	P958
	A1066	D959
	T1067	Q960
	M1068	V818
	T1069	W820
	S1072	V832
	L1073	D841
	V1074	K842
2%	S1075	V969
	D1076	V970
	M1077	T971
	T1078	A972
	L1079	T973
	L1080	R974
	P1081	V975
	K1082	D976
	S1083	K977
	L1084	T978
5%	V1085	G979
	M1086	Q986
	P1087	I987
	K1088	K988
	L1089	I991
	V1090	Y992
	P1091	V993
	D1092	D994
	S1093	C995
	L1094	T996

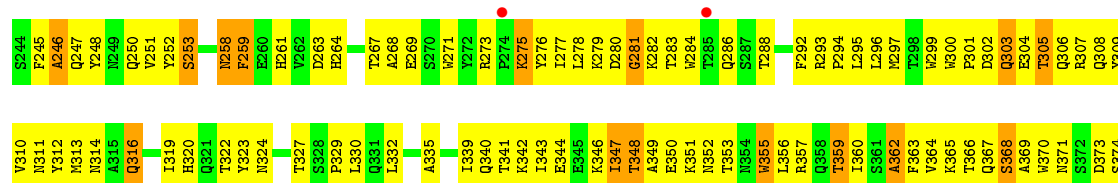
[illegible]

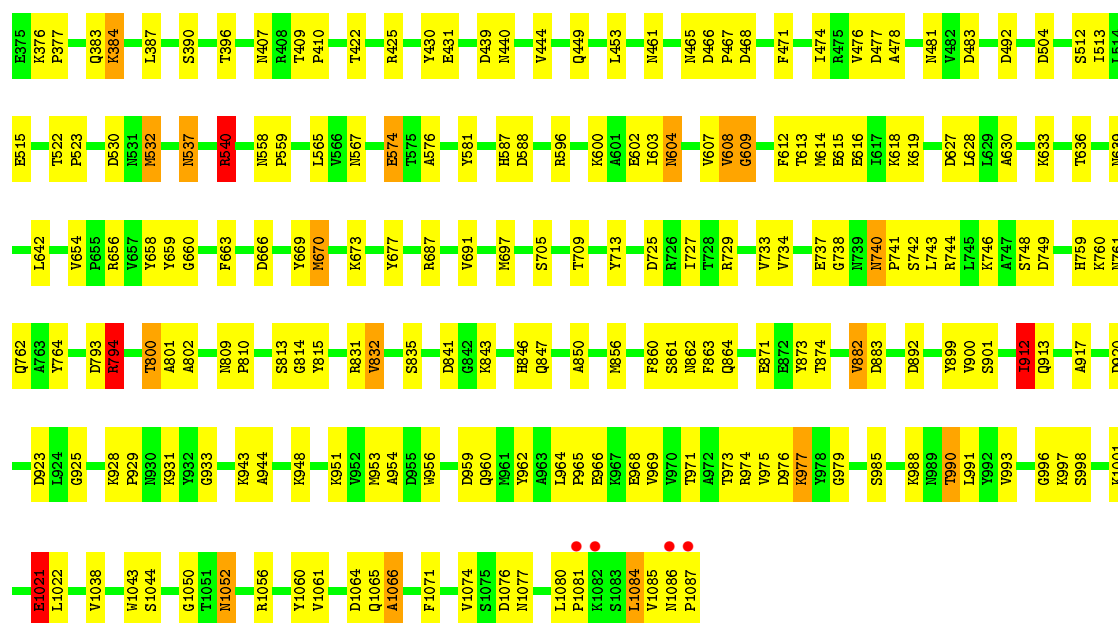


• Molecule 1: Glucosyltransferase-SI

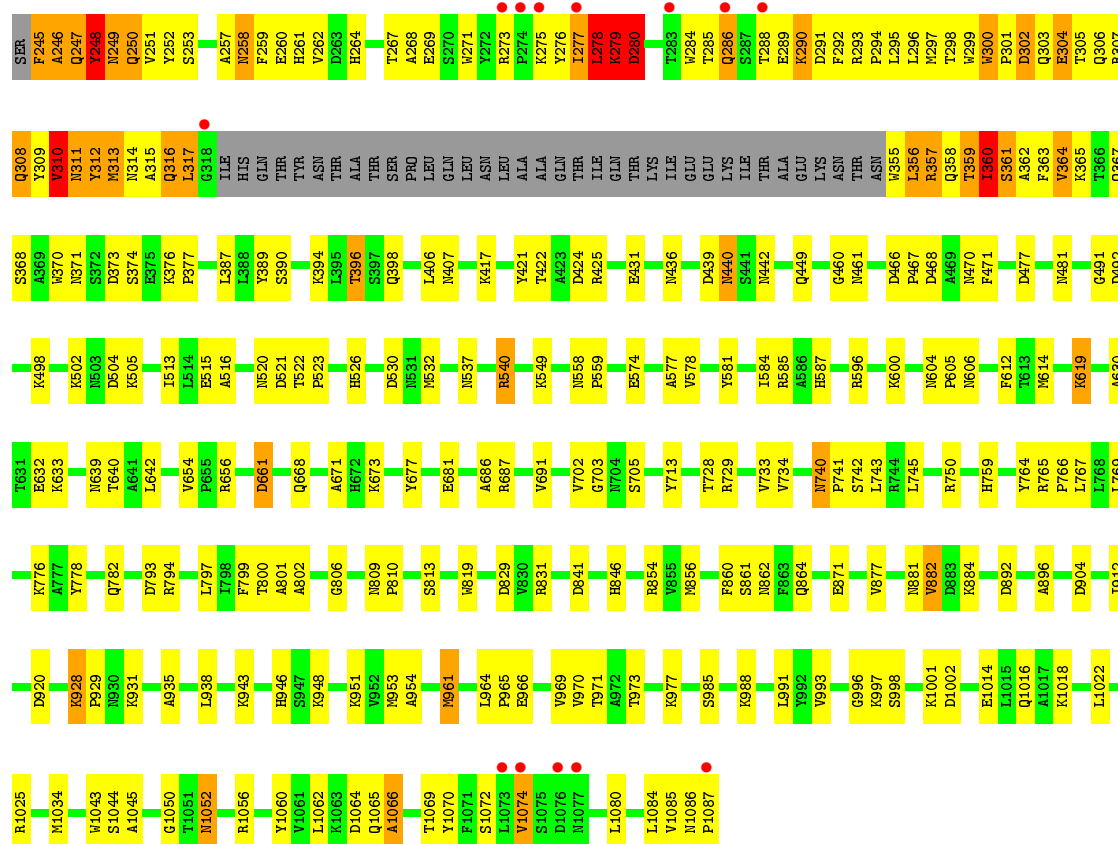


• Molecule 1: Glucosyltransferase-SI





Molecule 1: Glucosyltransferase-SI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	295.52Å 214.41Å 220.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.77 – 3.11 61.77 – 3.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.77-3.11) 95.3 (61.77-3.11)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.211 , 0.244 0.208 , 0.239	Depositor DCC
R_{free} test set	12026 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.0	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 238566 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52865	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 32.08 % 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 9.9554e-04. 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: ACR, CA, MES

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	0.99	9/6784 (0.1%)	0.95	3/9213 (0.0%)
1	B	0.88	12/5976 (0.2%)	0.88	7/8113 (0.1%)
1	C	0.94	1/6802 (0.0%)	0.94	8/9237 (0.1%)
1	D	0.95	4/6802 (0.1%)	0.92	11/9237 (0.1%)
1	E	1.04	14/6796 (0.2%)	0.95	10/9229 (0.1%)
1	F	0.81	1/6802 (0.0%)	0.85	3/9237 (0.0%)
1	G	0.97	6/6802 (0.1%)	0.95	7/9237 (0.1%)
1	H	0.91	4/6510 (0.1%)	0.93	9/8837 (0.1%)
All	All	0.94	51/53274 (0.1%)	0.92	58/72340 (0.1%)

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	H	0	1
All	All	0	2

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	HIS	CE1-NE2	14.48	1.66	1.32
1	E	245	PHE	N-CA	12.06	1.70	1.46
1	E	245	PHE	CE2-CZ	11.00	1.58	1.37
1	E	273	ARG	CZ-NH1	10.60	1.46	1.33
1	H	249	ASN	CG-OD1	10.12	1.46	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	245	PHE	CB-CG-CD1	-11.95	112.44	120.80
1	H	245	PHE	CG-CD2-CE2	-10.93	108.77	120.80
1	E	273	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	D	793	ASP	CB-CA-C	-8.51	93.38	110.40
1	E	727	ILE	CG1-CB-CG2	-8.07	93.64	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	TRP	Peptide
1	H	245	PHE	Sidechain

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	6643	0	6475	332	0
1	B	5854	0	5691	243	0
1	C	6660	0	6489	258	0
1	D	6660	0	6489	324	0
1	E	6654	0	6484	338	0
1	F	6660	0	6489	318	0
1	G	6660	0	6489	287	0
1	H	6372	0	6196	335	0
2	A	12	0	12	2	0
2	B	12	0	12	0	0
2	C	12	0	12	2	0
2	D	12	0	12	2	0
2	E	12	0	12	1	0
2	F	12	0	12	0	0
2	G	12	0	12	1	0
2	H	12	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	44	0	43	12	0
4	B	44	0	43	9	0
4	C	44	0	43	10	0
4	D	44	0	43	9	0
4	E	44	0	43	12	0
4	F	44	0	43	8	0
4	G	44	0	43	8	0
4	H	44	0	43	9	0
5	A	33	0	0	6	0
5	B	20	0	0	6	0
5	C	32	0	0	2	0
5	D	40	0	0	2	0
5	E	48	0	0	2	0
5	F	15	0	0	10	0
5	G	34	0	0	2	0
5	H	24	0	0	5	0
All	All	52865	0	51242	2480	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 24.

The worst 5 of 2480 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:E:245:PHE:N	1:E:245:PHE:CA	1.70	1.54
1:E:277:ILE:CD1	1:E:291:ASP:HB3	1.38	1.54
1:A:290:LYS:NZ	1:A:290:LYS:CE	1.71	1.53
1:E:279:LYS:CE	1:E:279:LYS:NZ	1.73	1.51
1:E:273:ARG:CD	1:E:287:SER:HB2	1.40	1.49

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	840/844 (100%)	772 (92%)	57 (7%)	11 (1%)	15	51
1	B	743/844 (88%)	678 (91%)	53 (7%)	12 (2%)	12	45
1	C	842/844 (100%)	777 (92%)	57 (7%)	8 (1%)	19	59
1	D	842/844 (100%)	763 (91%)	66 (8%)	13 (2%)	13	47
1	E	841/844 (100%)	758 (90%)	70 (8%)	13 (2%)	13	47
1	F	842/844 (100%)	771 (92%)	65 (8%)	6 (1%)	26	67
1	G	842/844 (100%)	776 (92%)	56 (7%)	10 (1%)	16	53
1	H	803/844 (95%)	717 (89%)	62 (8%)	24 (3%)	5	29
All	All	6595/6752 (98%)	6012 (91%)	486 (7%)	97 (2%)	13	47

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	GLN
1	C	321	GLN
1	C	327	THR
1	C	351	LYS
1	D	278	LEU

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	713/715 (100%)	669 (94%)	44 (6%)	23	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	627/715 (88%)	596 (95%)	31 (5%)	31	69
1	C	715/715 (100%)	671 (94%)	44 (6%)	23	59
1	D	715/715 (100%)	671 (94%)	44 (6%)	23	59
1	E	714/715 (100%)	658 (92%)	56 (8%)	16	50
1	F	715/715 (100%)	662 (93%)	53 (7%)	17	51
1	G	715/715 (100%)	666 (93%)	49 (7%)	19	55
1	H	682/715 (95%)	640 (94%)	42 (6%)	23	59
All	All	5596/5720 (98%)	5233 (94%)	363 (6%)	21	57

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	247	GLN
1	E	740	ASN
1	H	368	SER
1	E	286	GLN
1	E	332	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 178 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	700	GLN
1	E	440	ASN
1	H	407	ASN
1	D	759	HIS
1	E	258	ASN

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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	MES	A	5001	-	11,12,12	1.55	2 (18%)	14,16,16	11.49	9 (64%)
4	ACR	A	5044	-	46,47,47	1.03	4 (8%)	58,70,70	2.00	17 (29%)
2	MES	B	5001	-	11,12,12	1.55	3 (27%)	14,16,16	10.69	10 (71%)
4	ACR	B	5044	-	46,47,47	0.98	2 (4%)	58,70,70	1.96	18 (31%)
2	MES	C	5001	-	11,12,12	1.71	2 (18%)	14,16,16	9.25	8 (57%)
4	ACR	C	5044	-	46,47,47	0.98	2 (4%)	58,70,70	1.96	17 (29%)
2	MES	D	5001	-	11,12,12	1.36	1 (9%)	14,16,16	6.48	8 (57%)
4	ACR	D	5044	-	46,47,47	0.98	2 (4%)	58,70,70	1.96	17 (29%)
2	MES	E	5001	-	11,12,12	1.37	1 (9%)	14,16,16	9.84	10 (71%)
4	ACR	E	5044	-	46,47,47	0.98	2 (4%)	58,70,70	1.96	17 (29%)
2	MES	F	5001	-	11,12,12	1.55	3 (27%)	14,16,16	9.26	10 (71%)
4	ACR	F	5044	-	46,47,47	0.98	2 (4%)	58,70,70	1.96	17 (29%)
2	MES	G	5001	-	11,12,12	1.44	2 (18%)	14,16,16	8.31	9 (64%)
4	ACR	G	5044	-	46,47,47	0.98	2 (4%)	58,70,70	1.96	17 (29%)
2	MES	H	5001	-	11,12,12	0.98	0	14,16,16	9.23	10 (71%)
4	ACR	H	5044	-	46,47,47	0.98	2 (4%)	58,70,70	1.96	17 (29%)

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	MES	A	5001	-	-	0/6/14/14	0/1/1/1
4	ACR	A	5044	-	-	0/18/98/98	0/4/4/4
2	MES	B	5001	-	-	0/6/14/14	0/1/1/1
4	ACR	B	5044	-	-	0/18/98/98	0/4/4/4
2	MES	C	5001	-	-	0/6/14/14	0/1/1/1
4	ACR	C	5044	-	-	0/18/98/98	0/4/4/4
2	MES	D	5001	-	-	0/6/14/14	0/1/1/1
4	ACR	D	5044	-	-	0/18/98/98	0/4/4/4
2	MES	E	5001	-	-	0/6/14/14	0/1/1/1
4	ACR	E	5044	-	-	0/18/98/98	0/4/4/4
2	MES	F	5001	-	-	0/6/14/14	1/1/1/1
4	ACR	F	5044	-	-	0/18/98/98	0/4/4/4
2	MES	G	5001	-	-	0/6/14/14	0/1/1/1
4	ACR	G	5044	-	-	0/18/98/98	0/4/4/4
2	MES	H	5001	-	-	0/6/14/14	0/1/1/1
4	ACR	H	5044	-	-	0/18/98/98	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5044	ACR	C2A-C1A	-2.42	1.49	1.53
4	F	5044	ACR	C3B-C4B	-2.39	1.48	1.53
4	E	5044	ACR	C3B-C4B	-2.37	1.48	1.53
4	G	5044	ACR	C3B-C4B	-2.37	1.48	1.53
4	H	5044	ACR	C3B-C4B	-2.37	1.48	1.53

The worst 5 of 211 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	MES	O2S-S-C8	-36.84	75.47	106.91
2	B	5001	MES	O1S-S-C8	-30.72	80.69	106.91
2	F	5001	MES	O2S-S-C8	-26.12	84.62	106.91
2	C	5001	MES	O1S-S-C8	-26.04	84.69	106.91
2	E	5001	MES	O2S-S-C8	-25.76	84.93	106.91

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	5001	MES	C2-C3-C5-C6-N4-O1

13 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	MES	2	0
4	A	5044	ACR	12	0
4	B	5044	ACR	9	0
2	C	5001	MES	2	0
4	C	5044	ACR	10	0
2	D	5001	MES	2	0
4	D	5044	ACR	9	0
2	E	5001	MES	1	0
4	E	5044	ACR	12	0
4	F	5044	ACR	8	0
2	G	5001	MES	1	0
4	G	5044	ACR	8	0
4	H	5044	ACR	9	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, 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	842/844 (99%)	-0.17	7 (0%) 87 75	23, 38, 90, 113	0
1	B	747/844 (88%)	-0.09	17 (2%) 64 41	31, 50, 88, 136	0
1	C	844/844 (100%)	-0.30	2 (0%) 95 91	24, 35, 60, 70	0
1	D	844/844 (100%)	-0.21	13 (1%) 76 58	26, 39, 83, 101	0
1	E	843/844 (99%)	-0.16	18 (2%) 67 45	22, 36, 101, 126	0
1	F	844/844 (100%)	-0.15	7 (0%) 87 75	37, 53, 73, 89	0
1	G	844/844 (100%)	-0.24	6 (0%) 89 79	24, 35, 68, 79	0
1	H	807/844 (95%)	-0.17	13 (1%) 74 55	24, 42, 95, 139	0
All	All	6615/6752 (97%)	-0.19	83 (1%) 79 63	22, 41, 83, 139	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1087	PRO	5.9
1	A	1087	PRO	5.5
1	G	1087	PRO	5.3
1	E	285	THR	4.8
1	H	1087	PRO	4.2

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, 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	ACR	E	5044	44/44	0.84	0.30	4.73	35,49,53,53	0
4	ACR	F	5044	44/44	0.85	0.28	4.26	35,49,53,53	0
4	ACR	G	5044	44/44	0.88	0.26	3.54	35,49,53,53	0
4	ACR	C	5044	44/44	0.88	0.26	3.30	35,49,53,53	0
4	ACR	H	5044	44/44	0.89	0.24	2.34	35,49,53,53	0
4	ACR	A	5044	44/44	0.90	0.23	1.99	35,49,53,53	0
4	ACR	D	5044	44/44	0.88	0.26	1.82	35,49,53,53	0
4	ACR	B	5044	44/44	0.90	0.23	1.47	35,49,53,53	0
2	MES	A	5001	12/12	0.94	0.20	0.39	29,31,33,33	0
2	MES	F	5001	12/12	0.94	0.17	0.22	36,37,37,37	0
2	MES	E	5001	12/12	0.96	0.18	0.20	30,33,35,36	0
2	MES	B	5001	12/12	0.94	0.18	0.10	39,41,43,44	0
2	MES	H	5001	12/12	0.97	0.17	0.07	28,30,32,32	0
3	CA	E	4001	1/1	0.98	0.18	-0.13	32,32,32,32	0
2	MES	D	5001	12/12	0.96	0.16	-0.22	31,33,35,35	0
3	CA	H	4001	1/1	0.99	0.16	-0.48	32,32,32,32	0
3	CA	D	4001	1/1	0.98	0.16	-0.59	32,32,32,32	0
2	MES	C	5001	12/12	0.95	0.16	-0.68	29,31,32,32	0
3	CA	B	4001	1/1	0.97	0.14	-0.84	33,33,33,33	0
3	CA	A	4001	1/1	0.96	0.16	-1.11	28,28,28,28	0
3	CA	G	4001	1/1	0.98	0.13	-1.34	28,28,28,28	0
3	CA	F	4001	1/1	0.94	0.15	-1.47	38,38,38,38	0
2	MES	G	5001	12/12	0.96	0.15	-1.68	30,31,33,33	0
3	CA	C	4001	1/1	0.98	0.13	-1.98	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.