



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:15 PM BST

PDB ID : 5GTG  
Title : Crystal structure of onion lachrymatory factor synthase (LFS) containing 1,2-propanediol  
Authors : Arakawa, T.; Sato, Y.; Takabe, J.; Masamura, N.; Tsuge, N.; Imai, S.; Fushinobu, S.  
Deposited on : 2016-08-20  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

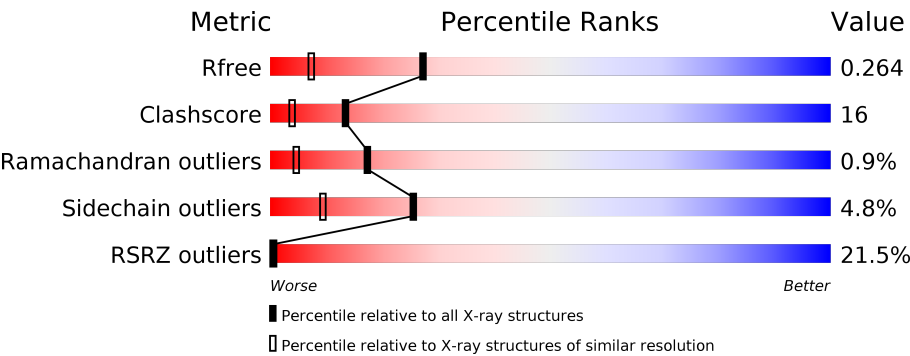
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	175	<div><div>5%</div><div><div></div><div>50%</div><div>30%</div><div>6%</div><div>15%</div></div></div>
1	B	175	<div><div></div><div><div>52%</div><div>29%</div><div>•</div><div>15%</div></div></div>
1	C	175	<div><div>47%</div><div><div>53%</div><div>29%</div><div>• •</div><div>15%</div></div></div>
1	D	175	<div><div>23%</div><div><div>53%</div><div>32%</div><div>•</div><div>15%</div></div></div>
1	E	175	<div><div>14%</div><div><div>55%</div><div>23%</div><div>6%</div><div>•</div><div>15%</div></div></div>
1	F	175	<div><div>9%</div><div><div>43%</div><div>32%</div><div>9%</div><div>•</div><div>15%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	175	
1	H	175	
2	I	2	

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
5	MES	B	204	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10289 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 Lachrymatory-factor synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1205	776	192	227	10			
1	B	149	Total	C	N	O	S	0	0	0
			1205	776	192	227	10			
1	C	149	Total	C	N	O	S	0	0	0
			1205	776	192	227	10			
1	D	149	Total	C	N	O	S	0	0	0
			1205	776	192	227	10			
1	E	149	Total	C	N	O	S	0	0	0
			1205	776	192	227	10			
1	F	149	Total	C	N	O	S	0	0	0
			1205	776	192	227	10			
1	G	149	Total	C	N	O	S	0	0	0
			1205	776	192	227	10			
1	H	149	Total	C	N	O	S	0	0	0
			1205	776	192	227	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	HIS	-	expression tag	UNP P59082
A	171	HIS	-	expression tag	UNP P59082
A	172	HIS	-	expression tag	UNP P59082
A	173	HIS	-	expression tag	UNP P59082
A	174	HIS	-	expression tag	UNP P59082
A	175	HIS	-	expression tag	UNP P59082
B	170	HIS	-	expression tag	UNP P59082
B	171	HIS	-	expression tag	UNP P59082
B	172	HIS	-	expression tag	UNP P59082
B	173	HIS	-	expression tag	UNP P59082
B	174	HIS	-	expression tag	UNP P59082
B	175	HIS	-	expression tag	UNP P59082
C	170	HIS	-	expression tag	UNP P59082

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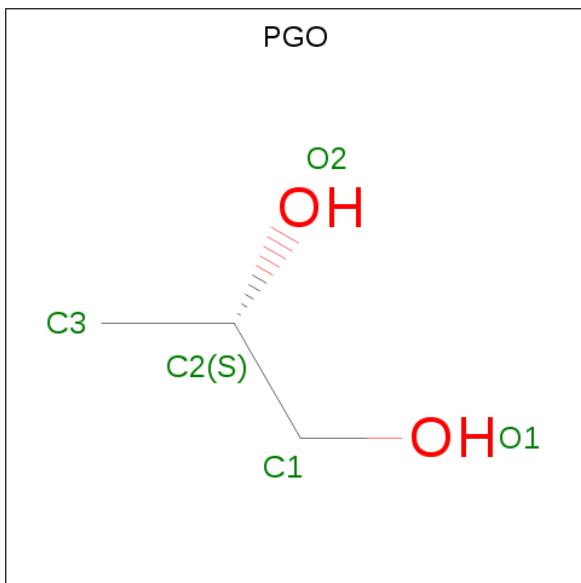
Chain	Residue	Modelled	Actual	Comment	Reference
C	171	HIS	-	expression tag	UNP P59082
C	172	HIS	-	expression tag	UNP P59082
C	173	HIS	-	expression tag	UNP P59082
C	174	HIS	-	expression tag	UNP P59082
C	175	HIS	-	expression tag	UNP P59082
D	170	HIS	-	expression tag	UNP P59082
D	171	HIS	-	expression tag	UNP P59082
D	172	HIS	-	expression tag	UNP P59082
D	173	HIS	-	expression tag	UNP P59082
D	174	HIS	-	expression tag	UNP P59082
D	175	HIS	-	expression tag	UNP P59082
E	170	HIS	-	expression tag	UNP P59082
E	171	HIS	-	expression tag	UNP P59082
E	172	HIS	-	expression tag	UNP P59082
E	173	HIS	-	expression tag	UNP P59082
E	174	HIS	-	expression tag	UNP P59082
E	175	HIS	-	expression tag	UNP P59082
F	170	HIS	-	expression tag	UNP P59082
F	171	HIS	-	expression tag	UNP P59082
F	172	HIS	-	expression tag	UNP P59082
F	173	HIS	-	expression tag	UNP P59082
F	174	HIS	-	expression tag	UNP P59082
F	175	HIS	-	expression tag	UNP P59082
G	170	HIS	-	expression tag	UNP P59082
G	171	HIS	-	expression tag	UNP P59082
G	172	HIS	-	expression tag	UNP P59082
G	173	HIS	-	expression tag	UNP P59082
G	174	HIS	-	expression tag	UNP P59082
G	175	HIS	-	expression tag	UNP P59082
H	170	HIS	-	expression tag	UNP P59082
H	171	HIS	-	expression tag	UNP P59082
H	172	HIS	-	expression tag	UNP P59082
H	173	HIS	-	expression tag	UNP P59082
H	174	HIS	-	expression tag	UNP P59082
H	175	HIS	-	expression tag	UNP P59082

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula:  $C_3H_8O_2$ ).



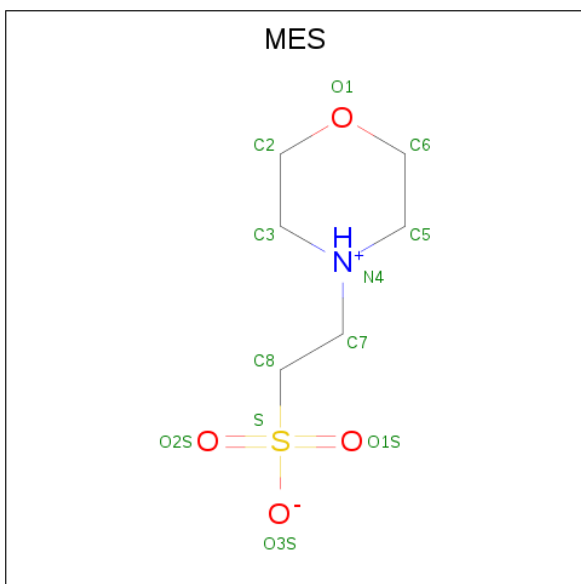
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	D	1	Total	C	O	0	0
			5	3	2		
3	G	1	Total	C	O	0	0
			5	3	2		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 6 is water.

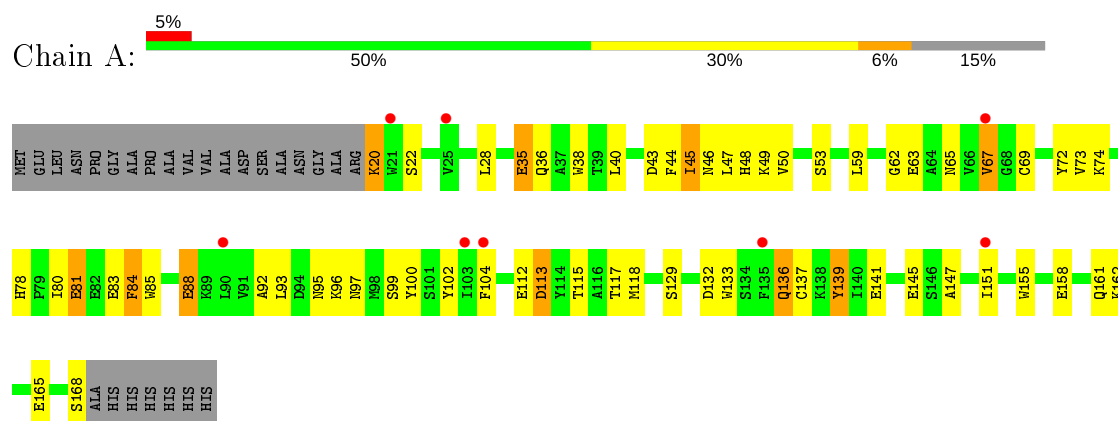
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total 147	O 147	0	0
6	B	111	Total 111	O 111	0	0
6	C	24	Total 24	O 24	0	0
6	D	42	Total 42	O 42	0	0
6	E	54	Total 54	O 54	0	0
6	F	86	Total 86	O 86	0	0
6	G	66	Total 66	O 66	0	0
6	H	54	Total 54	O 54	0	0



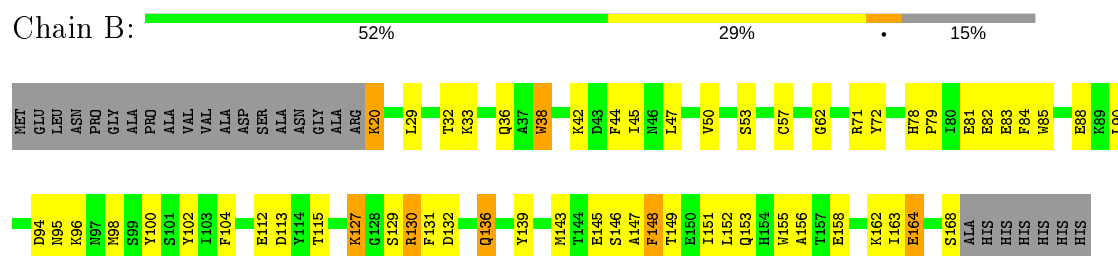
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

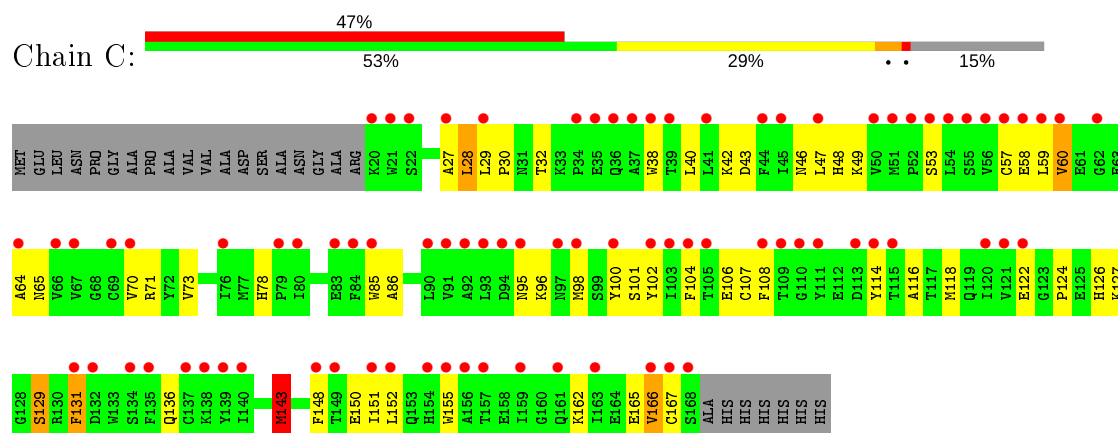
#### • Molecule 1: Lachrymatory-factor synthase



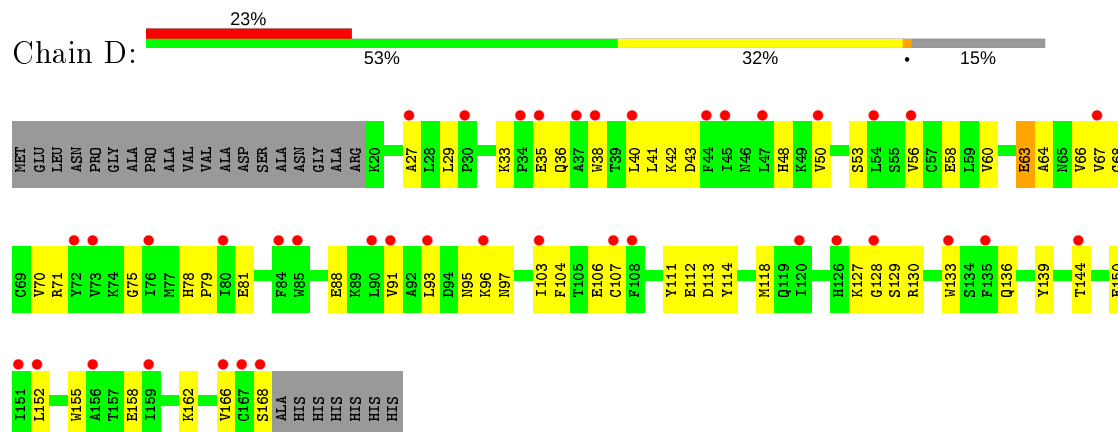
#### • Molecule 1: Lachrymatory-factor synthase



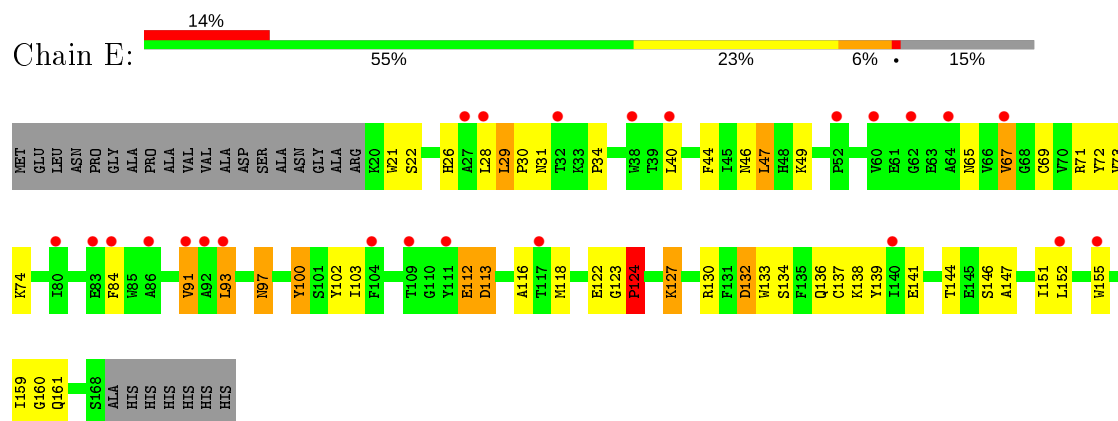
#### • Molecule 1: Lachrymatory-factor synthase



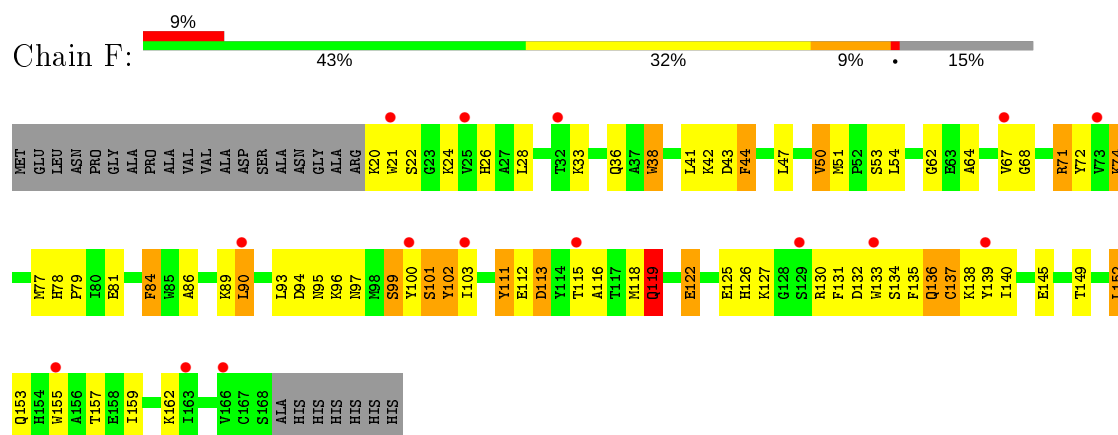
- Molecule 1: Lachrymatory-factor synthase



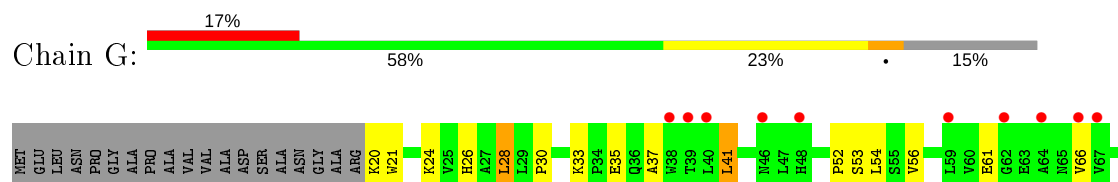
- Molecule 1: Lachrymatory-factor synthase

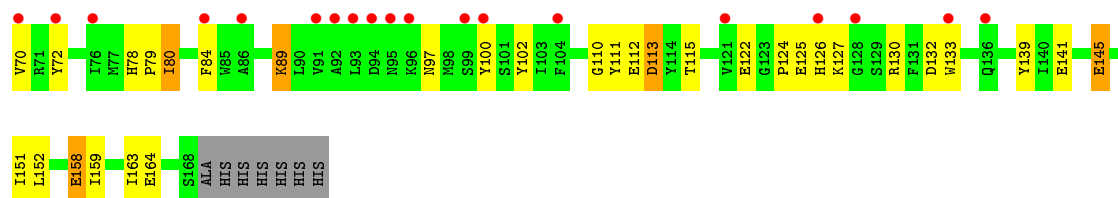


- Molecule 1: Lachrymatory-factor synthase

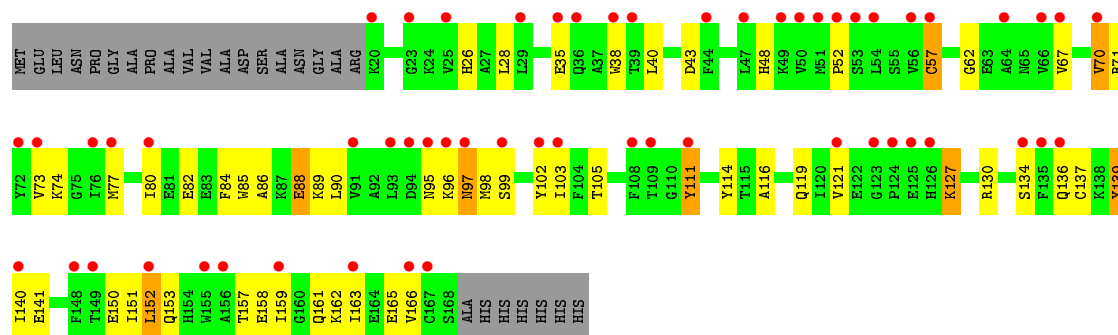


- Molecule 1: Lachrymatory-factor synthase





● Molecule 1: Lachrymatory-factor synthase



● Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.86Å 172.86Å 64.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 1.70 47.94 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.94-1.70) 97.5 (47.94-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.230 , 0.260 0.239 , 0.264	Depositor DCC
$R_{free}$ test set	10273 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
Reported twinning fraction	0.501 for H, K, L 0.499 for -H, K, -L	Depositor
Outliers	1 of 205386 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGO, GLC, SO4, 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	2.08	36/1237 (2.9%)	1.64	18/1674 (1.1%)
1	B	1.95	26/1237 (2.1%)	1.69	23/1674 (1.4%)
1	C	1.17	1/1237 (0.1%)	1.18	4/1674 (0.2%)
1	D	1.36	5/1237 (0.4%)	1.26	4/1674 (0.2%)
1	E	1.45	8/1237 (0.6%)	1.39	12/1674 (0.7%)
1	F	1.64	13/1237 (1.1%)	1.52	17/1674 (1.0%)
1	G	1.41	3/1237 (0.2%)	1.33	4/1674 (0.2%)
1	H	1.44	4/1237 (0.3%)	1.30	3/1674 (0.2%)
All	All	1.59	96/9896 (1.0%)	1.42	85/13392 (0.6%)

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	2
1	C	0	1
1	F	0	2
All	All	0	5

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	LYS	N-CA	11.98	1.70	1.46
1	B	112	GLU	CD-OE2	-10.85	1.13	1.25
1	A	83	GLU	CD-OE1	10.11	1.36	1.25
1	A	133	TRP	CG-CD1	9.77	1.50	1.36
1	A	62	GLY	C-O	8.37	1.37	1.23
1	A	102	TYR	CD1-CE1	-8.33	1.26	1.39
1	B	129	SER	CB-OG	-8.22	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	TRP	CB-CG	-8.11	1.35	1.50
1	A	84	PHE	CG-CD2	-8.04	1.26	1.38
1	A	99	SER	CA-CB	7.93	1.64	1.52
1	B	57	CYS	CB-SG	-7.65	1.69	1.82
1	F	153	GLN	C-O	-7.49	1.09	1.23
1	F	38	TRP	CB-CG	-6.88	1.37	1.50
1	F	155	TRP	CE3-CZ3	6.84	1.50	1.38
1	E	112	GLU	CD-OE1	-6.83	1.18	1.25
1	B	155	TRP	CZ3-CH2	-6.81	1.29	1.40
1	B	88	GLU	CD-OE1	-6.76	1.18	1.25
1	B	100	TYR	CG-CD2	6.75	1.48	1.39
1	F	122	GLU	CD-OE1	6.73	1.33	1.25
1	A	112	GLU	C-O	6.71	1.36	1.23
1	A	93	LEU	C-O	6.70	1.36	1.23
1	A	129	SER	CA-C	-6.63	1.35	1.52
1	B	84	PHE	CG-CD1	-6.62	1.28	1.38
1	D	91	VAL	N-CA	6.61	1.59	1.46
1	B	155	TRP	CE3-CZ3	6.49	1.49	1.38
1	G	102	TYR	CD1-CE1	-6.47	1.29	1.39
1	B	84	PHE	CG-CD2	6.46	1.48	1.38
1	A	100	TYR	CG-CD2	6.43	1.47	1.39
1	B	146	SER	CA-CB	6.41	1.62	1.52
1	G	133	TRP	CB-CG	6.38	1.61	1.50
1	A	117	THR	CB-CG2	-6.33	1.31	1.52
1	F	62	GLY	C-O	6.28	1.33	1.23
1	A	145	GLU	CD-OE2	-6.25	1.18	1.25
1	E	123	GLY	N-CA	-6.16	1.36	1.46
1	B	145	GLU	CD-OE1	6.15	1.32	1.25
1	B	72	TYR	CG-CD2	6.04	1.47	1.39
1	A	141	GLU	CD-OE1	6.02	1.32	1.25
1	A	63	GLU	CD-OE2	-5.98	1.19	1.25
1	E	124	PRO	N-CA	-5.96	1.37	1.47
1	B	148	PHE	CG-CD2	5.91	1.47	1.38
1	E	132	ASP	CB-CG	-5.90	1.39	1.51
1	A	136	GLN	CB-CG	-5.89	1.36	1.52
1	D	68	GLY	N-CA	5.85	1.54	1.46
1	A	147	ALA	C-O	5.84	1.34	1.23
1	A	155	TRP	CB-CG	-5.82	1.39	1.50
1	A	88	GLU	CD-OE2	5.76	1.31	1.25
1	H	62	GLY	N-CA	-5.74	1.37	1.46
1	B	163	ILE	C-O	5.69	1.34	1.23
1	B	62	GLY	C-O	5.65	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	CYS	CB-SG	-5.63	1.72	1.81
1	E	151	ILE	C-O	5.62	1.34	1.23
1	B	85	TRP	CZ3-CH2	5.61	1.49	1.40
1	B	20	LYS	N-CA	5.59	1.57	1.46
1	B	83	GLU	CD-OE2	5.58	1.31	1.25
1	H	38	TRP	CE3-CZ3	5.58	1.48	1.38
1	A	81	GLU	CD-OE1	5.56	1.31	1.25
1	F	44	PHE	CG-CD1	5.56	1.47	1.38
1	B	136	GLN	CA-C	-5.56	1.38	1.52
1	B	38	TRP	CG-CD1	-5.55	1.28	1.36
1	A	40	LEU	N-CA	5.53	1.57	1.46
1	D	113	ASP	CB-CG	5.51	1.63	1.51
1	A	141	GLU	CD-OE2	-5.46	1.19	1.25
1	B	158	GLU	CD-OE2	5.45	1.31	1.25
1	A	132	ASP	CB-CG	-5.44	1.40	1.51
1	A	102	TYR	C-O	-5.43	1.13	1.23
1	G	145	GLU	CD-OE1	5.41	1.31	1.25
1	A	158	GLU	CA-CB	-5.41	1.42	1.53
1	F	133	TRP	CE3-CZ3	5.36	1.47	1.38
1	D	75	GLY	N-CA	5.32	1.54	1.46
1	F	77	MET	C-O	5.32	1.33	1.23
1	F	113	ASP	CB-CG	-5.31	1.40	1.51
1	A	92	ALA	CA-CB	-5.29	1.41	1.52
1	B	156	ALA	C-O	5.29	1.33	1.23
1	A	155	TRP	CE2-CZ2	-5.26	1.30	1.39
1	C	102	TYR	CE1-CZ	5.26	1.45	1.38
1	A	137	CYS	C-O	5.25	1.33	1.23
1	B	153	GLN	N-CA	5.25	1.56	1.46
1	D	71	ARG	N-CA	5.24	1.56	1.46
1	B	164	GLU	CD-OE2	5.21	1.31	1.25
1	A	45	ILE	C-O	5.20	1.33	1.23
1	F	157	THR	C-O	5.19	1.33	1.23
1	B	113	ASP	CB-CG	5.18	1.62	1.51
1	B	36	GLN	CD-OE1	5.18	1.35	1.24
1	F	102	TYR	CE1-CZ	5.17	1.45	1.38
1	A	136	GLN	CA-CB	-5.15	1.42	1.53
1	E	146	SER	CB-OG	-5.15	1.35	1.42
1	F	102	TYR	CE2-CZ	-5.13	1.31	1.38
1	H	88	GLU	CD-OE1	-5.12	1.20	1.25
1	F	111	TYR	CB-CG	-5.09	1.44	1.51
1	H	111	TYR	CG-CD1	5.09	1.45	1.39
1	A	48	HIS	CA-CB	-5.07	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	147	ALA	C-O	5.05	1.32	1.23
1	A	22	SER	C-O	5.05	1.32	1.23
1	A	59	LEU	C-O	5.04	1.32	1.23
1	A	139	TYR	CG-CD1	5.02	1.45	1.39
1	E	91	VAL	N-CA	5.01	1.56	1.46

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ASP	CB-CG-OD1	10.98	128.18	118.30
1	B	127	LYS	CD-CE-NZ	9.58	133.72	111.70
1	F	152	LEU	CB-CG-CD1	9.11	126.48	111.00
1	F	71	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	B	113	ASP	CB-CG-OD1	8.21	125.69	118.30
1	E	127	LYS	CD-CE-NZ	8.15	130.44	111.70
1	F	43	ASP	CB-CG-OD1	8.13	125.62	118.30
1	A	113	ASP	CB-CG-OD2	-7.92	111.18	118.30
1	B	104	PHE	CB-CG-CD2	-7.74	115.38	120.80
1	B	83	GLU	OE1-CD-OE2	7.58	132.40	123.30
1	B	113	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	B	130	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	132	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	83	GLU	CG-CD-OE2	-6.93	104.44	118.30
1	A	93	LEU	CB-CA-C	6.88	123.27	110.20
1	H	43	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	B	132	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	G	28	LEU	CB-CG-CD2	6.84	122.63	111.00
1	G	41	LEU	CB-CG-CD2	-6.78	99.47	111.00
1	A	104	PHE	CB-CG-CD1	6.69	125.48	120.80
1	A	43	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	C	143	MET	CG-SD-CE	6.68	110.88	100.20
1	B	94	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	E	132	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	45	ILE	CG1-CB-CG2	6.31	125.27	111.40
1	D	93	LEU	CA-CB-CG	6.21	129.58	115.30
1	B	104	PHE	CB-CG-CD1	6.20	125.14	120.80
1	B	90	LEU	CB-CG-CD1	-6.19	100.47	111.00
1	B	139	TYR	CG-CD2-CE2	-6.19	116.35	121.30
1	C	71	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	F	90	LEU	CB-CG-CD2	-6.04	100.73	111.00
1	E	40	LEU	CB-CG-CD2	5.98	121.17	111.00
1	E	29	LEU	CA-CB-CG	5.98	129.05	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	ASP	CB-CG-OD1	5.93	123.64	118.30
1	F	74	LYS	CD-CE-NZ	5.90	125.28	111.70
1	E	47	LEU	CB-CG-CD1	5.89	121.02	111.00
1	B	32	THR	CA-CB-CG2	-5.86	104.19	112.40
1	F	97	ASN	CB-CA-C	5.85	122.10	110.40
1	E	93	LEU	CB-CG-CD1	5.83	120.90	111.00
1	F	43	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	47	LEU	CB-CG-CD2	-5.79	101.15	111.00
1	D	104	PHE	CB-CG-CD1	5.73	124.81	120.80
1	B	71	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	E	113	ASP	CB-CG-OD1	5.69	123.42	118.30
1	F	99	SER	N-CA-CB	5.67	119.01	110.50
1	F	100	TYR	CA-CB-CG	5.62	124.08	113.40
1	F	139	TYR	CB-CG-CD1	5.62	124.37	121.00
1	B	136	GLN	CA-CB-CG	5.59	125.70	113.40
1	E	100	TYR	CA-CB-CG	5.54	123.93	113.40
1	B	168	SER	CB-CA-C	5.53	120.60	110.10
1	A	132	ASP	OD1-CG-OD2	-5.53	112.80	123.30
1	F	113	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	A	83	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	F	149	THR	CA-CB-CG2	5.47	120.06	112.40
1	A	28	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	B	102	TYR	CZ-CE2-CD2	-5.41	114.93	119.80
1	B	44	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	B	139	TYR	CD1-CE1-CZ	-5.38	114.95	119.80
1	A	49	LYS	CD-CE-NZ	5.38	124.07	111.70
1	A	36	GLN	CA-CB-CG	5.36	125.18	113.40
1	G	113	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	131	PHE	CG-CD1-CE1	-5.33	114.94	120.80
1	D	93	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	C	150	GLU	CA-CB-CG	5.25	124.96	113.40
1	A	47	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	H	90	LEU	CB-CG-CD1	5.19	119.83	111.00
1	F	137	CYS	CA-CB-SG	5.19	123.34	114.00
1	A	44	PHE	CG-CD2-CE2	5.18	126.50	120.80
1	G	139	TYR	CD1-CE1-CZ	-5.17	115.15	119.80
1	A	59	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	F	130	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	F	119	GLN	CA-CB-CG	5.16	124.75	113.40
1	E	112	GLU	CA-CB-CG	5.14	124.72	113.40
1	A	44	PHE	CB-CG-CD1	5.13	124.39	120.80
1	E	122	GLU	OE1-CD-OE2	-5.12	117.15	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	69	CYS	CA-CB-SG	5.11	123.20	114.00
1	A	67	VAL	CA-CB-CG1	-5.08	103.27	110.90
1	B	102	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	C	131	PHE	CB-CG-CD1	-5.06	117.25	120.80
1	F	64	ALA	N-CA-CB	5.05	117.18	110.10
1	H	70	VAL	CA-CB-CG1	5.05	118.47	110.90
1	F	94	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	155	TRP	CA-CB-CG	5.02	123.23	113.70
1	A	118	MET	CB-CG-SD	-5.01	97.38	112.40
1	B	149	THR	CA-CB-CG2	-5.00	105.39	112.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Mainchain
1	A	97	ASN	Mainchain
1	C	58	GLU	Peptide
1	F	135	PHE	Peptide
1	F	86	ALA	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	1205	0	1165	26	0
1	B	1205	0	1165	26	0
1	C	1205	0	1165	33	0
1	D	1205	0	1165	46	0
1	E	1205	0	1165	49	0
1	F	1205	0	1165	56	0
1	G	1205	0	1165	31	0
1	H	1205	0	1165	54	0
2	I	23	0	20	3	0
3	A	5	0	8	2	0
3	B	5	0	7	0	0
3	D	5	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	5	0	8	1	0
4	B	10	0	0	1	0
5	B	12	0	13	4	0
6	A	147	0	0	11	0
6	B	111	0	0	7	0
6	C	24	0	0	5	0
6	D	42	0	0	16	0
6	E	54	0	0	17	0
6	F	86	0	0	18	0
6	G	66	0	0	8	0
6	H	54	0	0	19	0
All	All	10289	0	9384	308	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 16.

All (308) 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:A:20:LYS:N	1:A:20:LYS:CA	1.70	1.52
1:C:155:TRP:HD1	6:C:201:HOH:O	1.27	1.16
1:B:127:LYS:HE2	6:B:346:HOH:O	1.49	1.11
1:H:151:ILE:HG12	6:H:205:HOH:O	1.51	1.08
1:A:46:ASN:HD21	2:I:1:GLC:H61	1.19	1.07
6:F:268:HOH:O	1:G:28:LEU:HD11	1.55	1.06
1:A:113:ASP:HB3	6:A:353:HOH:O	1.54	1.06
1:F:131:PHE:HE1	6:F:219:HOH:O	1.40	1.02
1:F:41:LEU:HD21	6:F:219:HOH:O	1.61	1.01
1:H:105:THR:HG21	6:H:241:HOH:O	1.58	1.00
1:A:80:ILE:HD13	6:A:423:HOH:O	1.61	0.99
1:D:130:ARG:HG3	6:D:302:HOH:O	1.63	0.97
1:H:151:ILE:CG1	6:H:205:HOH:O	2.10	0.96
1:A:73:VAL:HG21	3:A:201:PGO:H33	1.46	0.95
1:G:115:THR:HG22	6:G:327:HOH:O	1.65	0.94
1:A:96:LYS:HE3	6:A:395:HOH:O	1.68	0.93
1:F:21:TRP:HB3	1:F:145:GLU:HG3	1.51	0.92
1:F:26:HIS:HB3	6:F:268:HOH:O	1.70	0.92
1:E:73:VAL:HG22	6:E:214:HOH:O	1.69	0.92
1:E:124:PRO:HA	1:H:26:HIS:CD2	2.05	0.92
1:F:140:ILE:HA	6:F:223:HOH:O	1.69	0.91
1:D:66:VAL:HG12	1:E:136:GLN:HE22	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:GLU:HG2	6:G:301:HOH:O	1.70	0.90
1:D:60:VAL:CG2	6:D:324:HOH:O	2.20	0.89
1:B:20:LYS:N	5:B:204:MES:H21	1.87	0.89
1:D:70:VAL:HG12	6:D:324:HOH:O	1.73	0.88
1:F:28:LEU:HD12	6:G:340:HOH:O	1.73	0.88
1:B:127:LYS:HB2	6:B:371:HOH:O	1.75	0.87
1:F:111:TYR:CB	6:F:223:HOH:O	2.23	0.86
1:F:131:PHE:CE1	6:F:219:HOH:O	2.21	0.83
6:A:355:HOH:O	1:F:67:VAL:HG12	1.80	0.81
1:G:79:PRO:HD2	6:G:314:HOH:O	1.80	0.81
1:E:160:GLY:CA	6:E:243:HOH:O	2.28	0.81
1:A:67:VAL:O	1:F:136:GLN:NE2	2.14	0.80
1:E:160:GLY:HA2	6:E:243:HOH:O	1.81	0.79
6:A:368:HOH:O	1:B:127:LYS:HD3	1.83	0.79
1:C:29:LEU:N	1:C:29:LEU:HD12	1.99	0.78
1:H:40:LEU:HD11	1:H:166:VAL:HG11	1.66	0.77
1:A:168:SER:HA	6:A:347:HOH:O	1.85	0.76
6:F:268:HOH:O	1:G:28:LEU:CD1	2.23	0.76
1:F:111:TYR:HB3	6:F:223:HOH:O	1.85	0.76
1:E:112:GLU:HB3	6:E:203:HOH:O	1.86	0.76
1:E:112:GLU:CB	6:E:203:HOH:O	2.33	0.76
1:H:52:PRO:HD3	6:H:208:HOH:O	1.85	0.75
1:F:26:HIS:CB	6:F:268:HOH:O	2.31	0.75
1:C:32:THR:O	1:C:129:SER:OG	2.05	0.74
1:E:112:GLU:HG2	6:E:203:HOH:O	1.87	0.74
1:D:106:GLU:HB3	6:D:308:HOH:O	1.87	0.74
1:E:124:PRO:HA	1:H:26:HIS:HD2	1.53	0.74
1:F:44:PHE:CZ	1:F:71:ARG:HD3	2.23	0.73
1:A:151:ILE:HD11	6:A:423:HOH:O	1.87	0.73
1:H:40:LEU:HD11	1:H:166:VAL:CG1	2.19	0.72
1:C:28:LEU:C	1:C:29:LEU:HD12	2.11	0.71
1:F:24:LYS:NZ	1:G:125:GLU:OE2	2.24	0.70
1:D:66:VAL:CG1	1:E:136:GLN:HE22	2.04	0.70
6:A:355:HOH:O	1:F:67:VAL:CG1	2.37	0.70
1:E:112:GLU:CG	6:E:203:HOH:O	2.38	0.69
1:E:124:PRO:CA	1:H:26:HIS:HD2	2.04	0.69
1:C:148:PHE:HA	1:C:151:ILE:HD12	1.73	0.69
1:D:67:VAL:O	1:E:136:GLN:NE2	2.25	0.68
1:H:111:TYR:HE2	6:H:238:HOH:O	1.75	0.67
1:F:111:TYR:HB2	6:F:223:HOH:O	1.91	0.67
1:B:82:GLU:OE2	6:B:301:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:LEU:HD23	1:E:93:LEU:C	2.16	0.66
1:D:96:LYS:HE2	6:E:239:HOH:O	1.94	0.66
1:H:162:LYS:HB2	6:H:208:HOH:O	1.95	0.66
1:F:78:HIS:HD2	1:F:81:GLU:OE2	1.78	0.66
1:D:112:GLU:HG3	1:D:139:TYR:CZ	2.31	0.66
1:A:88:GLU:OE1	3:A:201:PGO:H32	1.95	0.66
1:C:30:PRO:HB2	1:C:127:LYS:HE3	1.78	0.65
1:H:73:VAL:HG22	1:H:86:ALA:O	1.96	0.65
1:E:29:LEU:CD1	6:E:243:HOH:O	2.44	0.65
1:D:106:GLU:HG2	6:D:333:HOH:O	1.97	0.64
1:H:152:LEU:HD23	6:H:212:HOH:O	1.97	0.64
1:D:78:HIS:HD2	1:D:81:GLU:OE2	1.80	0.64
1:G:24:LYS:HE2	1:G:132:ASP:HB3	1.78	0.64
1:F:68:GLY:HA2	1:F:89:LYS:NZ	2.12	0.64
1:H:161:GLN:HG2	1:H:165:GLU:OE2	1.97	0.64
1:H:134:SER:C	6:H:212:HOH:O	2.36	0.63
1:F:28:LEU:CD1	6:G:340:HOH:O	2.36	0.63
1:E:93:LEU:HD23	1:E:93:LEU:O	1.98	0.63
1:H:97:ASN:C	1:H:97:ASN:OD1	2.37	0.63
1:D:60:VAL:HG22	6:D:324:HOH:O	1.91	0.63
6:D:311:HOH:O	1:E:67:VAL:HB	1.98	0.62
1:A:46:ASN:ND2	2:I:1:GLC:H61	2.04	0.62
1:E:160:GLY:HA3	6:E:243:HOH:O	1.98	0.62
1:E:118:MET:CE	1:E:133:TRP:CZ2	2.83	0.61
1:G:110:GLY:HA3	1:G:141:GLU:OE1	2.00	0.61
1:F:41:LEU:CD2	6:F:219:HOH:O	2.33	0.61
1:C:28:LEU:HD21	1:C:124:PRO:HD3	1.81	0.61
1:D:38:TRP:HE1	1:D:95:ASN:HD22	1.49	0.61
1:H:127:LYS:CG	6:H:237:HOH:O	2.50	0.60
1:F:140:ILE:HG23	6:F:223:HOH:O	1.99	0.60
1:E:71:ARG:HG3	6:E:214:HOH:O	2.01	0.60
1:B:20:LYS:HE3	6:B:377:HOH:O	2.01	0.60
1:C:155:TRP:CD1	6:C:201:HOH:O	2.16	0.60
1:F:93:LEU:HD23	1:F:93:LEU:C	2.22	0.60
1:F:102:TYR:CE1	1:F:116:ALA:HB3	2.37	0.59
1:C:155:TRP:HA	6:C:201:HOH:O	2.03	0.59
1:E:155:TRP:O	1:E:159:ILE:HG13	2.02	0.59
1:H:127:LYS:HG2	6:H:237:HOH:O	2.02	0.59
1:G:122:GLU:OE1	1:G:126:HIS:ND1	2.35	0.58
1:C:29:LEU:N	1:C:29:LEU:CD1	2.65	0.58
1:E:118:MET:HE3	1:E:133:TRP:CZ2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LEU:HB2	1:D:129:SER:HB2	1.85	0.58
1:D:66:VAL:HG12	1:E:136:GLN:NE2	2.15	0.58
1:E:112:GLU:HA	6:E:221:HOH:O	2.02	0.58
1:G:52:PRO:HD2	1:G:158:GLU:HG3	1.86	0.58
1:H:40:LEU:CD1	1:H:166:VAL:HG11	2.33	0.58
1:A:38:TRP:HE1	1:A:95:ASN:HD22	1.52	0.58
1:H:74:LYS:HG3	1:H:85:TRP:HB3	1.86	0.57
1:B:53:SER:OG	1:B:78:HIS:HE1	1.87	0.57
1:C:27:ALA:HB3	1:C:131:PHE:HB3	1.87	0.57
1:F:99:SER:HB3	1:F:119:GLN:HB2	1.86	0.57
1:E:97:ASN:C	1:E:97:ASN:OD1	2.43	0.57
1:B:38:TRP:HE1	1:B:95:ASN:HD22	1.52	0.57
1:D:42:LYS:HE3	1:D:95:ASN:HD21	1.70	0.56
1:H:95:ASN:O	1:H:96:LYS:C	2.44	0.56
1:E:28:LEU:HD23	1:E:130:ARG:HG3	1.87	0.56
1:A:53:SER:OG	1:A:78:HIS:HE1	1.88	0.56
1:B:130:ARG:NH1	4:B:202:SO4:O2	2.30	0.56
1:D:144:THR:HG23	6:D:305:HOH:O	2.05	0.56
1:E:113:ASP:O	1:E:137:CYS:HA	2.06	0.56
1:F:21:TRP:HA	1:F:145:GLU:OE2	2.05	0.56
1:B:50:VAL:HA	1:B:162:LYS:HG2	1.88	0.56
1:C:53:SER:OG	1:C:78:HIS:HE1	1.88	0.56
1:A:46:ASN:HD21	2:I:1:GLC:C6	2.07	0.55
1:D:130:ARG:CG	6:D:302:HOH:O	2.38	0.55
1:H:152:LEU:CD2	6:H:212:HOH:O	2.55	0.55
1:E:124:PRO:CA	1:H:26:HIS:CD2	2.80	0.55
1:H:82:GLU:C	6:H:201:HOH:O	2.44	0.55
1:B:20:LYS:CE	6:B:377:HOH:O	2.54	0.55
1:C:38:TRP:HE1	1:C:95:ASN:HD22	1.54	0.55
1:C:143:MET:HA	1:C:143:MET:CE	2.37	0.54
1:F:22:SER:HB3	6:F:222:HOH:O	2.07	0.54
1:A:78:HIS:HD2	1:A:81:GLU:OE2	1.89	0.54
1:G:53:SER:OG	1:G:78:HIS:HE1	1.90	0.54
1:H:71:ARG:HG3	1:H:73:VAL:CG1	2.38	0.54
1:F:44:PHE:CE2	1:F:71:ARG:HD3	2.42	0.54
1:H:80:ILE:HG12	6:H:205:HOH:O	2.06	0.54
1:D:33:LYS:HB2	1:D:36:GLN:OE1	2.08	0.54
1:G:56:VAL:HG11	1:G:72:TYR:CE1	2.43	0.54
1:F:78:HIS:CD2	1:F:81:GLU:OE2	2.61	0.53
1:H:97:ASN:O	1:H:97:ASN:OD1	2.26	0.53
1:H:102:TYR:CZ	1:H:116:ALA:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:CG2	1:B:136:GLN:HG2	2.38	0.53
1:H:52:PRO:HD2	1:H:158:GLU:CG	2.39	0.53
1:D:50:VAL:HA	1:D:162:LYS:HG2	1.90	0.52
1:F:38:TRP:HE1	1:F:95:ASN:HD22	1.57	0.52
1:D:118:MET:HB3	6:D:318:HOH:O	2.10	0.52
1:D:128:GLY:N	6:D:301:HOH:O	2.41	0.52
1:A:80:ILE:HG21	6:A:423:HOH:O	2.08	0.52
1:F:99:SER:CB	1:F:119:GLN:HB2	2.40	0.52
1:D:41:LEU:HD21	6:D:318:HOH:O	2.09	0.52
1:F:50:VAL:O	1:F:159:ILE:HA	2.10	0.52
1:C:46:ASN:HB3	1:C:49:LYS:HG3	1.92	0.52
1:D:56:VAL:HG12	1:D:58:GLU:HG2	1.92	0.52
1:E:141:GLU:HA	6:E:231:HOH:O	2.09	0.52
1:E:118:MET:HE2	1:E:133:TRP:CZ2	2.46	0.51
1:E:47:LEU:HD22	1:E:71:ARG:NH1	2.25	0.51
1:D:53:SER:OG	1:D:158:GLU:OE1	2.29	0.51
1:E:26:HIS:ND1	1:E:132:ASP:OD1	2.40	0.51
1:F:122:GLU:OE1	1:F:126:HIS:ND1	2.39	0.51
1:H:35:GLU:HB3	1:H:98:MET:HE1	1.92	0.50
1:D:118:MET:CB	6:D:318:HOH:O	2.59	0.50
1:C:43:ASP:OD1	1:C:65:ASN:ND2	2.44	0.50
1:C:86:ALA:HA	1:C:107:CYS:HA	1.93	0.50
1:D:103:ILE:HG21	1:E:91:VAL:HB	1.94	0.50
1:H:162:LYS:O	1:H:166:VAL:HG23	2.11	0.50
1:F:68:GLY:HA2	1:F:89:LYS:HZ2	1.77	0.50
1:G:24:LYS:CE	1:G:132:ASP:HB3	2.41	0.50
1:H:114:TYR:CE1	1:H:116:ALA:HB2	2.47	0.50
1:B:143:MET:HE2	1:B:148:PHE:CA	2.41	0.49
1:C:101:SER:HA	1:C:116:ALA:O	2.12	0.49
1:C:106:GLU:O	1:C:107:CYS:HB2	2.13	0.49
1:D:50:VAL:HA	1:D:162:LYS:CG	2.41	0.49
1:C:47:LEU:HD21	1:C:118:MET:HE1	1.94	0.49
1:A:45:ILE:HG23	1:A:65:ASN:OD1	2.13	0.49
1:C:60:VAL:HG23	1:C:70:VAL:HB	1.93	0.49
1:E:30:PRO:HB3	1:H:153:GLN:HG2	1.95	0.49
1:C:104:PHE:CD1	1:C:114:TYR:CD1	3.01	0.49
1:A:72:TYR:OH	1:A:74:LYS:HE3	2.13	0.49
1:A:115:THR:HG21	1:F:67:VAL:HG11	1.95	0.49
1:G:37:ALA:CB	1:G:163:ILE:HG21	2.43	0.49
1:A:35:GLU:H	1:A:35:GLU:CD	2.16	0.49
1:D:133:TRP:CZ2	1:D:152:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:TRP:CB	1:F:145:GLU:HG3	2.34	0.48
1:G:127:LYS:HD2	6:G:364:HOH:O	2.13	0.48
1:E:138:LYS:HG2	1:E:139:TYR:CD2	2.48	0.48
1:B:79:PRO:O	1:B:81:GLU:HG2	2.14	0.48
6:A:333:HOH:O	1:F:96:LYS:HE3	2.13	0.48
1:B:143:MET:HE3	1:B:147:ALA:HB3	1.94	0.48
1:B:29:LEU:HD23	1:B:164:GLU:HG2	1.95	0.48
1:E:30:PRO:O	1:E:127:LYS:HE2	2.13	0.48
1:E:29:LEU:HD12	6:E:243:HOH:O	2.12	0.48
1:B:143:MET:HE2	1:B:148:PHE:HA	1.96	0.48
1:D:133:TRP:CE2	1:D:152:LEU:HD11	2.49	0.48
1:E:46:ASN:HB3	1:E:49:LYS:HE3	1.96	0.48
1:A:115:THR:HG22	1:A:136:GLN:HG3	1.94	0.48
1:C:122:GLU:OE1	1:C:126:HIS:ND1	2.28	0.48
1:H:127:LYS:HG3	6:H:237:HOH:O	2.13	0.48
1:C:73:VAL:O	1:C:85:TRP:HA	2.14	0.47
1:B:42:LYS:HE3	1:B:95:ASN:HD21	1.80	0.47
1:G:30:PRO:HD2	1:G:164:GLU:OE1	2.15	0.47
1:F:36:GLN:HG2	6:F:269:HOH:O	2.14	0.47
1:D:112:GLU:HG3	1:D:139:TYR:OH	2.15	0.47
1:F:33:LYS:HB2	1:F:36:GLN:HG3	1.96	0.47
1:A:115:THR:CG2	1:F:67:VAL:HG11	2.45	0.47
1:H:151:ILE:HG13	6:H:205:HOH:O	1.94	0.47
1:D:70:VAL:CG1	6:D:324:HOH:O	2.46	0.47
1:G:130:ARG:NH1	6:G:303:HOH:O	2.48	0.47
1:F:47:LEU:HD23	1:F:54:LEU:HD11	1.96	0.47
1:A:80:ILE:CG2	6:A:423:HOH:O	2.63	0.46
1:D:40:LEU:HD11	1:D:166:VAL:CG1	2.45	0.46
1:F:20:LYS:HD3	6:F:250:HOH:O	2.15	0.46
1:B:20:LYS:CB	5:B:204:MES:H21	2.46	0.46
1:H:71:ARG:HG3	1:H:73:VAL:HG13	1.98	0.46
1:C:162:LYS:O	1:C:166:VAL:HG23	2.15	0.46
1:B:127:LYS:NZ	6:B:304:HOH:O	2.44	0.46
1:C:40:LEU:HD11	1:C:167:CYS:SG	2.56	0.46
1:H:82:GLU:CB	6:H:201:HOH:O	2.64	0.46
1:D:63:GLU:O	1:D:64:ALA:C	2.55	0.45
1:G:111:TYR:O	1:G:112:GLU:HG3	2.16	0.45
1:H:35:GLU:HB3	1:H:98:MET:CE	2.45	0.45
1:C:42:LYS:HE3	1:C:95:ASN:HD21	1.81	0.45
1:E:112:GLU:C	6:E:203:HOH:O	2.55	0.45
1:F:113:ASP:O	1:F:137:CYS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:ILE:HG22	1:H:163:ILE:HD12	1.97	0.45
5:B:204:MES:O1S	5:B:204:MES:H32	2.15	0.45
1:E:31:ASN:ND2	1:H:150:GLU:OE2	2.50	0.45
1:G:21:TRP:HB3	1:G:145:GLU:HG3	1.97	0.45
1:H:162:LYS:CB	6:H:208:HOH:O	2.57	0.45
1:F:140:ILE:CB	6:F:223:HOH:O	2.65	0.45
1:H:136:GLN:NE2	6:H:207:HOH:O	2.47	0.45
1:G:33:LYS:NZ	1:G:35:GLU:OE1	2.45	0.45
1:C:38:TRP:CE2	1:C:98:MET:HA	2.52	0.44
1:E:97:ASN:OD1	1:E:97:ASN:O	2.35	0.44
1:G:24:LYS:HG2	1:G:26:HIS:CE1	2.52	0.44
1:D:107:CYS:HB3	1:D:111:TYR:CD1	2.52	0.44
1:H:40:LEU:HD11	1:H:166:VAL:CB	2.48	0.44
1:D:27:ALA:C	6:D:302:HOH:O	2.55	0.44
1:F:119:GLN:HG2	1:F:132:ASP:HB2	2.00	0.44
1:G:24:LYS:HE2	1:G:132:ASP:CB	2.45	0.44
1:H:88:GLU:HA	1:H:103:ILE:O	2.17	0.44
1:D:40:LEU:HD11	1:D:166:VAL:HG12	2.00	0.44
1:G:124:PRO:O	1:G:127:LYS:HB3	2.18	0.44
1:H:139:TYR:C	1:H:139:TYR:CD1	2.91	0.44
1:D:33:LYS:HE2	1:D:35:GLU:HG2	1.99	0.44
1:F:90:LEU:HD12	1:F:101:SER:O	2.18	0.44
1:H:48:HIS:ND1	1:H:57:CYS:HB3	2.33	0.44
1:C:28:LEU:HB3	6:C:203:HOH:O	2.18	0.43
1:G:54:LEU:HD21	3:G:201:PGO:H31	2.00	0.43
1:H:139:TYR:HE1	1:H:141:GLU:HG3	1.83	0.43
1:F:102:TYR:CZ	1:F:116:ALA:HB3	2.53	0.43
1:C:30:PRO:CB	1:C:127:LYS:HE3	2.47	0.43
1:G:37:ALA:HB1	1:G:163:ILE:HG21	2.01	0.43
1:G:61:GLU:HB3	1:G:70:VAL:HB	1.99	0.43
1:C:40:LEU:CD2	1:C:166:VAL:HG11	2.49	0.43
1:E:102:TYR:CZ	1:E:116:ALA:HB3	2.54	0.43
1:E:72:TYR:OH	1:E:74:LYS:HE3	2.18	0.43
1:B:38:TRP:CG	1:B:98:MET:HG2	2.53	0.43
1:F:84:PHE:CD1	1:F:84:PHE:C	2.92	0.43
1:A:50:VAL:HA	1:A:162:LYS:HG2	2.01	0.43
1:B:127:LYS:CE	6:B:304:HOH:O	2.67	0.42
1:C:165:GLU:CD	6:C:202:HOH:O	2.58	0.42
1:E:44:PHE:HB3	1:E:65:ASN:OD1	2.19	0.42
1:E:118:MET:HE2	1:E:133:TRP:CE2	2.54	0.42
1:E:47:LEU:HD22	1:E:71:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ILE:HD11	1:G:151:ILE:HD11	2.01	0.42
1:H:139:TYR:CD1	1:H:140:ILE:N	2.87	0.42
1:H:70:VAL:HG22	1:H:89:LYS:HB2	2.01	0.42
1:B:78:HIS:HD2	1:B:81:GLU:OE2	2.03	0.42
1:H:121:VAL:HG23	1:H:130:ARG:HB3	2.01	0.42
1:H:77:MET:CE	6:H:201:HOH:O	2.67	0.42
5:B:204:MES:S	5:B:204:MES:H32	2.59	0.42
1:B:147:ALA:O	1:B:151:ILE:HG13	2.19	0.42
1:E:21:TRP:CZ2	1:E:144:THR:HA	2.54	0.42
1:C:53:SER:OG	1:C:78:HIS:CE1	2.69	0.42
1:E:29:LEU:HG	6:E:243:HOH:O	2.20	0.42
1:G:113:ASP:OD1	1:G:113:ASP:N	2.53	0.42
1:D:103:ILE:HG13	1:D:103:ILE:O	2.20	0.42
1:F:79:PRO:O	1:F:81:GLU:HG2	2.19	0.42
1:H:73:VAL:O	1:H:85:TRP:HA	2.20	0.42
1:E:73:VAL:HG13	6:E:214:HOH:O	2.20	0.42
1:F:115:THR:HG23	1:F:115:THR:O	2.20	0.41
1:D:103:ILE:HB	6:D:312:HOH:O	2.20	0.41
1:H:99:SER:HB3	1:H:119:GLN:HG3	2.03	0.41
1:H:114:TYR:HA	1:H:137:CYS:HB3	2.03	0.41
1:F:89:LYS:HB3	1:F:103:ILE:HG12	2.02	0.41
1:G:41:LEU:O	1:G:100:TYR:HE2	2.04	0.41
1:B:78:HIS:HD2	1:B:81:GLU:OE1	2.04	0.41
1:D:97:ASN:C	1:D:97:ASN:OD1	2.59	0.41
1:F:118:MET:HB3	6:F:219:HOH:O	2.19	0.41
1:F:51:MET:HE2	1:F:54:LEU:HG	2.02	0.41
1:F:90:LEU:HD12	1:F:90:LEU:HA	1.79	0.41
1:F:72:TYR:OH	1:F:74:LYS:HE2	2.20	0.41
1:D:139:TYR:C	1:D:139:TYR:CD1	2.94	0.40
1:D:79:PRO:HD3	1:D:150:GLU:HG2	2.02	0.40
1:A:73:VAL:O	1:A:85:TRP:HA	2.21	0.40
1:F:112:GLU:HB3	1:F:138:LYS:HB3	2.03	0.40
1:B:78:HIS:HD2	1:B:81:GLU:CD	2.25	0.40
1:D:88:GLU:OE2	3:D:201:PGO:O2	2.37	0.40
1:F:50:VAL:HA	1:F:162:LYS:HG2	2.03	0.40
1:A:161:GLN:O	1:A:165:GLU:HG3	2.22	0.40
1:D:114:TYR:HA	1:D:136:GLN:O	2.21	0.40
1:D:155:TRP:HA	1:D:158:GLU:HG2	2.03	0.40
1:G:159:ILE:HG22	1:G:163:ILE:HD12	2.03	0.40
1:G:89:LYS:NZ	6:G:309:HOH:O	2.54	0.40

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	147/175 (84%)	144 (98%)	3 (2%)	0	100	100
1	B	147/175 (84%)	146 (99%)	1 (1%)	0	100	100
1	C	147/175 (84%)	135 (92%)	8 (5%)	4 (3%)	5	0
1	D	147/175 (84%)	137 (93%)	9 (6%)	1 (1%)	22	8
1	E	147/175 (84%)	137 (93%)	8 (5%)	2 (1%)	11	2
1	F	147/175 (84%)	142 (97%)	4 (3%)	1 (1%)	22	8
1	G	147/175 (84%)	143 (97%)	4 (3%)	0	100	100
1	H	147/175 (84%)	136 (92%)	8 (5%)	3 (2%)	7	1
All	All	1176/1400 (84%)	1120 (95%)	45 (4%)	11 (1%)	17	5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	139	TYR
1	E	124	PRO
1	F	42	LYS
1	C	59	LEU
1	C	64	ALA
1	D	48	HIS
1	C	57	CYS
1	C	166	VAL
1	H	57	CYS
1	E	67	VAL
1	H	67	VAL

### 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	132/150 (88%)	130 (98%)	2 (2%)	65	51
1	B	132/150 (88%)	129 (98%)	3 (2%)	50	33
1	C	132/150 (88%)	122 (92%)	10 (8%)	13	3
1	D	132/150 (88%)	129 (98%)	3 (2%)	50	33
1	E	132/150 (88%)	123 (93%)	9 (7%)	16	4
1	F	132/150 (88%)	122 (92%)	10 (8%)	13	3
1	G	132/150 (88%)	124 (94%)	8 (6%)	18	5
1	H	132/150 (88%)	126 (96%)	6 (4%)	27	10
All	All	1056/1200 (88%)	1005 (95%)	51 (5%)	25	9

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	84	PHE
1	B	33	LYS
1	B	96	LYS
1	B	152	LEU
1	C	28	LEU
1	C	48	HIS
1	C	60	VAL
1	C	96	LYS
1	C	100	TYR
1	C	108	PHE
1	C	129	SER
1	C	136	GLN
1	C	143	MET
1	C	152	LEU
1	D	63	GLU
1	D	127	LYS
1	D	168	SER
1	E	22	SER
1	E	34	PRO
1	E	84	PHE
1	E	97	ASN
1	E	100	TYR
1	E	103	ILE

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Mol	Chain	Res	Type
1	E	134	SER
1	E	152	LEU
1	E	161	GLN
1	F	50	VAL
1	F	53	SER
1	F	84	PHE
1	F	101	SER
1	F	119	GLN
1	F	125	GLU
1	F	127	LYS
1	F	134	SER
1	F	136	GLN
1	F	152	LEU
1	G	20	LYS
1	G	66	VAL
1	G	80	ILE
1	G	84	PHE
1	G	89	LYS
1	G	97	ASN
1	G	152	LEU
1	G	158	GLU
1	H	28	LEU
1	H	84	PHE
1	H	97	ASN
1	H	127	LYS
1	H	152	LEU
1	H	157	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	48	HIS
1	A	78	HIS
1	A	95	ASN
1	A	136	GLN
1	A	153	GLN
1	A	161	GLN
1	B	78	HIS
1	B	95	ASN
1	B	154	HIS
1	C	78	HIS

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Mol	Chain	Res	Type
1	C	95	ASN
1	D	78	HIS
1	D	95	ASN
1	D	136	GLN
1	D	154	HIS
1	D	161	GLN
1	E	31	ASN
1	E	78	HIS
1	E	136	GLN
1	E	153	GLN
1	E	161	GLN
1	F	26	HIS
1	F	78	HIS
1	F	95	ASN
1	G	78	HIS
1	G	95	ASN
1	G	153	GLN
1	G	154	HIS
1	H	31	ASN
1	H	78	HIS
1	H	95	ASN
1	H	136	GLN
1	H	153	GLN
1	H	161	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

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	GLC	I	1	2	11,11,12	1.55	2 (18%)	15,15,17	2.27	7 (46%)
2	GLC	I	2	2	12,12,12	1.45	1 (8%)	17,17,17	2.29	7 (41%)

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	GLC	I	1	2	-	2/2/19/22	0/1/1/1
2	GLC	I	2	2	-	1/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	GLC	O5-C1	3.68	1.49	1.43
2	I	2	GLC	O5-C5	-2.93	1.37	1.44
2	I	1	GLC	C6-C5	2.08	1.58	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	GLC	C3-C4-C5	4.61	118.47	110.24
2	I	1	GLC	O5-C5-C4	4.30	121.30	110.83
2	I	1	GLC	C6-C5-C4	-4.25	103.05	113.00
2	I	2	GLC	C4-C3-C2	4.17	118.11	110.82
2	I	2	GLC	O4-C4-C5	-4.08	99.16	109.30
2	I	1	GLC	O6-C6-C5	-3.09	100.70	111.29
2	I	2	GLC	O3-C3-C2	-2.90	103.65	110.35
2	I	1	GLC	O5-C1-C2	2.84	115.16	110.77
2	I	2	GLC	C1-C2-C3	2.50	115.51	110.31
2	I	2	GLC	C1-O5-C5	2.44	118.27	113.66
2	I	1	GLC	C3-C4-C5	2.41	114.53	110.24
2	I	1	GLC	O4-C4-C5	-2.39	103.35	109.30
2	I	1	GLC	C1-O5-C5	2.09	115.02	112.19
2	I	2	GLC	O2-C2-C1	2.07	113.95	109.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

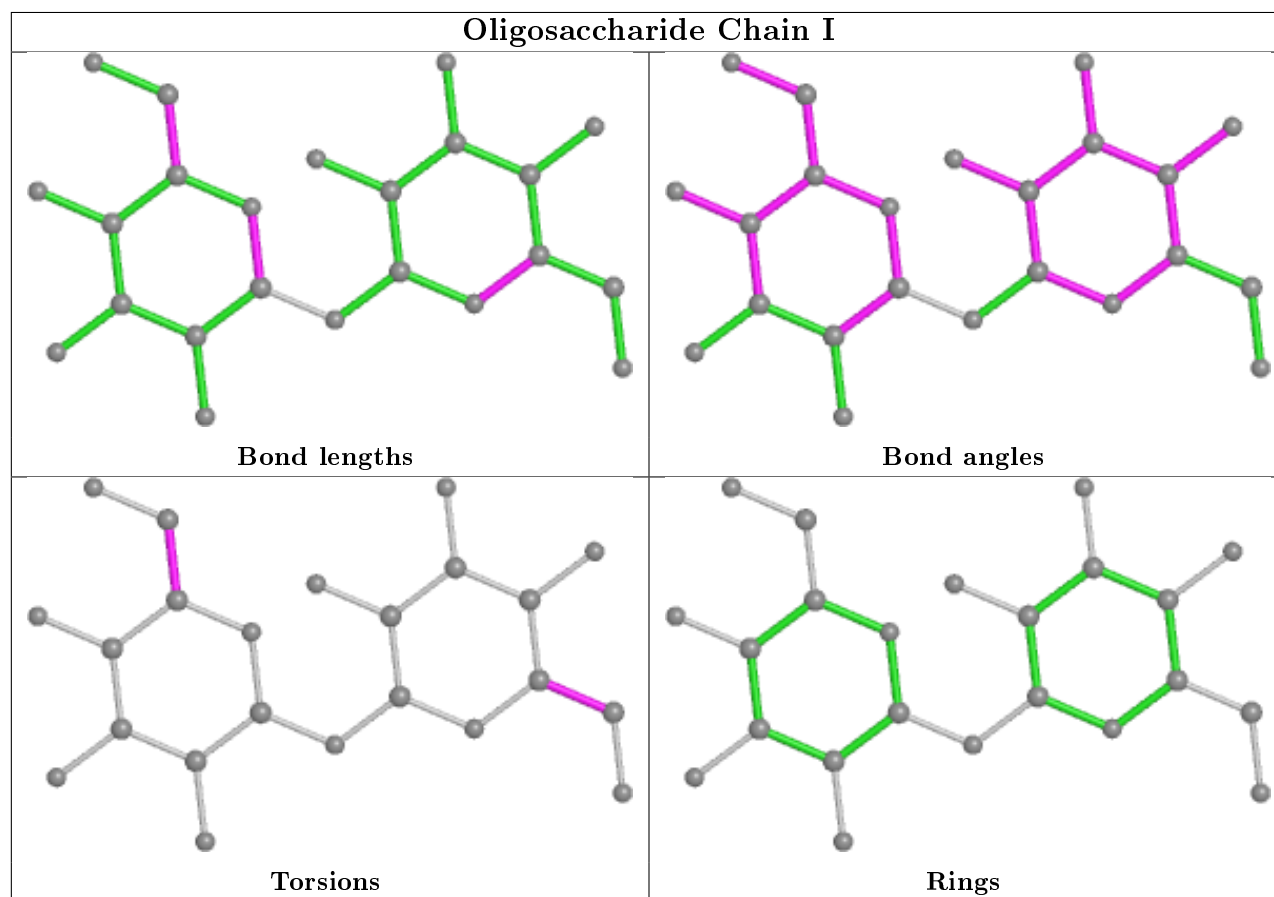
Mol	Chain	Res	Type	Atoms
2	I	1	GLC	C4-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	GLC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MES	B	204	-	12,12,12	2.36	5 (41%)	14,16,16	4.11	9 (64%)
3	PGO	A	201	-	3,4,4	0.45	0	1,4,4	1.52	0
3	PGO	G	201	-	3,4,4	0.43	0	1,4,4	0.93	0
3	PGO	B	203	-	3,4,4	0.54	0	1,4,4	1.46	0
3	PGO	D	201	-	3,4,4	0.20	0	1,4,4	0.27	0
4	SO4	B	201	-	4,4,4	0.90	0	6,6,6	0.60	0
4	SO4	B	202	-	4,4,4	0.44	0	6,6,6	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGO	A	201	-	-	2/2/2/2	-
5	MES	B	204	-	-	5/6/14/14	0/1/1/1
3	PGO	G	201	-	-	2/2/2/2	-
3	PGO	B	203	-	-	2/2/2/2	-
3	PGO	D	201	-	-	2/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	204	MES	C8-S	-6.40	1.68	1.77
5	B	204	MES	C7-N4	2.48	1.53	1.47
5	B	204	MES	O2S-S	2.41	1.52	1.45
5	B	204	MES	O1S-S	2.18	1.51	1.45
5	B	204	MES	C5-C6	2.09	1.58	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	204	MES	O1S-S-C8	12.39	121.83	106.92
5	B	204	MES	C5-N4-C3	-3.80	100.28	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	204	MES	O3S-S-O1S	-3.70	102.23	111.27
5	B	204	MES	O1-C2-C3	3.69	119.91	111.80
5	B	204	MES	C2-C3-N4	3.43	115.30	110.10
5	B	204	MES	O3S-S-C8	2.95	110.53	105.77
5	B	204	MES	C6-C5-N4	-2.28	106.64	110.10
5	B	204	MES	O1-C6-C5	2.25	116.76	111.80
5	B	204	MES	C7-N4-C3	2.02	116.41	111.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	204	MES	C8-C7-N4-C3
5	B	204	MES	C7-C8-S-O2S
3	G	201	PGO	O1-C1-C2-O2
3	B	203	PGO	O1-C1-C2-O2
5	B	204	MES	C7-C8-S-O3S
5	B	204	MES	C8-C7-N4-C5
3	G	201	PGO	O1-C1-C2-C3
3	B	203	PGO	O1-C1-C2-C3
5	B	204	MES	C7-C8-S-O1S
3	A	201	PGO	O1-C1-C2-O2
3	A	201	PGO	O1-C1-C2-C3
3	D	201	PGO	O1-C1-C2-C3
3	D	201	PGO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	204	MES	4	0
3	A	201	PGO	2	0
3	G	201	PGO	1	0
3	D	201	PGO	1	0
4	B	202	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	149/175 (85%)	0.84	8 (5%) 25 28	4, 10, 19, 28	0
1	B	149/175 (85%)	0.59	0 100 100	5, 11, 21, 25	0
1	C	149/175 (85%)	2.53	83 (55%) 0 0	19, 29, 38, 42	149 (100%)
1	D	149/175 (85%)	1.52	40 (26%) 0 0	15, 23, 33, 43	149 (100%)
1	E	149/175 (85%)	1.21	24 (16%) 1 1	12, 20, 28, 36	149 (100%)
1	F	149/175 (85%)	1.19	15 (10%) 7 8	10, 18, 27, 33	149 (100%)
1	G	149/175 (85%)	1.28	29 (19%) 1 1	13, 22, 31, 40	149 (100%)
1	H	149/175 (85%)	1.86	57 (38%) 0 0	13, 23, 33, 43	149 (100%)
All	All	1192/1400 (85%)	1.38	256 (21%) 0 0	4, 20, 33, 43	894 (75%)

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	VAL	8.3
1	C	155	TRP	7.9
1	C	47	LEU	6.8
1	C	92	ALA	6.3
1	C	45	ILE	6.3
1	C	93	LEU	6.1
1	C	121	VAL	5.8
1	C	103	ILE	5.3
1	D	56	VAL	5.2
1	C	44	PHE	5.1
1	C	38	TRP	5.1
1	C	80	ILE	5.0
1	C	135	PHE	5.0
1	H	148	PHE	5.0
1	H	64	ALA	5.0
1	C	149	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	G	93	LEU	4.9
1	H	67	VAL	4.9
1	H	163	ILE	4.9
1	C	120	ILE	4.8
1	C	97	ASN	4.7
1	H	155	TRP	4.6
1	D	45	ILE	4.4
1	C	156	ALA	4.4
1	C	39	THR	4.3
1	G	92	ALA	4.3
1	H	103	ILE	4.3
1	C	109	THR	4.3
1	C	50	VAL	4.2
1	C	159	ILE	4.2
1	C	56	VAL	4.2
1	H	95	ASN	4.1
1	C	41	LEU	4.1
1	H	93	LEU	4.1
1	C	166	VAL	4.1
1	E	93	LEU	4.0
1	C	85	TRP	4.0
1	C	90	LEU	4.0
1	C	113	ASP	4.0
1	C	163	ILE	4.0
1	H	94	ASP	4.0
1	G	67	VAL	3.9
1	D	84	PHE	3.9
1	H	108	PHE	3.9
1	F	166	VAL	3.8
1	G	100	TYR	3.8
1	H	124	PRO	3.8
1	C	108	PHE	3.7
1	C	55	SER	3.7
1	D	167	CYS	3.7
1	C	154	HIS	3.7
1	D	93	LEU	3.7
1	C	79	PRO	3.7
1	E	52	PRO	3.7
1	C	167	CYS	3.7
1	C	115	THR	3.7
1	F	67	VAL	3.7
1	G	96	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	36	GLN	3.6
1	G	59	LEU	3.6
1	C	131	PHE	3.5
1	C	69	CYS	3.5
1	F	163	ILE	3.5
1	C	34	PRO	3.5
1	F	21	TRP	3.5
1	C	22	SER	3.5
1	C	95	ASN	3.4
1	F	90	LEU	3.4
1	H	25	VAL	3.4
1	H	99	SER	3.4
1	C	157	THR	3.4
1	E	67	VAL	3.4
1	C	98	MET	3.4
1	D	156	ALA	3.4
1	H	56	VAL	3.4
1	H	39	THR	3.4
1	H	49	LYS	3.3
1	C	57	CYS	3.3
1	E	86	ALA	3.3
1	C	122	GLU	3.3
1	H	36	GLN	3.3
1	G	104	PHE	3.3
1	H	121	VAL	3.3
1	C	100	TYR	3.3
1	D	67	VAL	3.2
1	H	152	LEU	3.2
1	C	66	VAL	3.2
1	C	102	TYR	3.2
1	C	111	TYR	3.2
1	H	38	TRP	3.2
1	D	73	VAL	3.2
1	H	47	LEU	3.2
1	C	52	PRO	3.2
1	D	126	HIS	3.2
1	C	54	LEU	3.2
1	C	67	VAL	3.2
1	E	62	GLY	3.2
1	D	80	ILE	3.1
1	D	159	ILE	3.1
1	C	37	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	111	TYR	3.1
1	H	167	CYS	3.1
1	H	66	VAL	3.1
1	C	168	SER	3.1
1	D	72	TYR	3.1
1	H	72	TYR	3.1
1	D	54	LEU	3.1
1	H	54	LEU	3.1
1	C	83	GLU	3.0
1	C	148	PHE	3.0
1	C	59	LEU	3.0
1	G	72	TYR	3.0
1	C	161	GLN	3.0
1	G	64	ALA	3.0
1	H	156	ALA	3.0
1	E	104	PHE	3.0
1	E	27	ALA	2.9
1	D	128	GLY	2.9
1	C	84	PHE	2.9
1	C	132	ASP	2.9
1	H	166	VAL	2.9
1	D	107	CYS	2.9
1	C	152	LEU	2.9
1	D	40	LEU	2.9
1	F	25	VAL	2.9
1	H	91	VAL	2.9
1	H	140	ILE	2.9
1	D	38	TRP	2.8
1	G	99	SER	2.8
1	H	70	VAL	2.8
1	D	103	ILE	2.8
1	H	76	ILE	2.8
1	G	84	PHE	2.8
1	F	155	TRP	2.8
1	C	29	LEU	2.8
1	E	60	VAL	2.8
1	E	91	VAL	2.8
1	H	57	CYS	2.8
1	C	139	TYR	2.7
1	C	60	VAL	2.7
1	H	44	PHE	2.7
1	C	76	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	151	ILE	2.7
1	H	73	VAL	2.7
1	H	52	PRO	2.7
1	G	91	VAL	2.7
1	F	32	THR	2.7
1	H	149	THR	2.7
1	E	64	ALA	2.6
1	F	73	VAL	2.6
1	C	105	THR	2.6
1	F	115	THR	2.6
1	C	27	ALA	2.6
1	E	84	PHE	2.6
1	A	90	LEU	2.6
1	G	128	GLY	2.6
1	H	134	SER	2.6
1	C	62	GLY	2.6
1	D	37	ALA	2.6
1	H	96	LYS	2.6
1	D	35	GLU	2.6
1	D	168	SER	2.6
1	H	35	GLU	2.6
1	F	133	TRP	2.6
1	H	135	PHE	2.6
1	D	166	VAL	2.6
1	H	126	HIS	2.6
1	H	97	ASN	2.5
1	C	53	SER	2.5
1	C	51	MET	2.5
1	F	129	SER	2.5
1	C	94	ASP	2.5
1	H	50	VAL	2.5
1	F	139	TYR	2.5
1	E	109	THR	2.5
1	D	96	LYS	2.4
1	E	32	THR	2.4
1	D	47	LEU	2.4
1	E	155	TRP	2.4
1	C	104	PHE	2.4
1	G	95	ASN	2.4
1	E	140	ILE	2.4
1	D	85	TRP	2.4
1	C	138	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	23	GLY	2.4
1	C	35	GLU	2.4
1	C	140	ILE	2.3
1	G	40	LEU	2.3
1	C	110	GLY	2.3
1	D	133	TRP	2.3
1	D	108	PHE	2.3
1	E	38	TRP	2.3
1	H	136	GLN	2.3
1	G	121	VAL	2.3
1	H	159	ILE	2.3
1	H	109	THR	2.3
1	H	125	GLU	2.3
1	H	123	GLY	2.3
1	G	94	ASP	2.3
1	G	66	VAL	2.3
1	A	67	VAL	2.2
1	C	64	ALA	2.2
1	D	90	LEU	2.2
1	E	92	ALA	2.2
1	H	29	LEU	2.2
1	H	77	MET	2.2
1	E	111	TYR	2.2
1	C	134	SER	2.2
1	G	126	HIS	2.2
1	E	152	LEU	2.2
1	A	103	ILE	2.2
1	D	76	ILE	2.2
1	H	80	ILE	2.2
1	A	135	PHE	2.2
1	E	83	GLU	2.2
1	C	21	TRP	2.2
1	G	39	THR	2.2
1	A	104	PHE	2.2
1	D	44	PHE	2.2
1	H	53	SER	2.2
1	A	25	VAL	2.2
1	D	34	PRO	2.2
1	D	152	LEU	2.2
1	G	46	ASN	2.2
1	H	102	TYR	2.1
1	D	151	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	80	ILE	2.1
1	G	136	GLN	2.1
1	G	86	ALA	2.1
1	F	100	TYR	2.1
1	D	135	PHE	2.1
1	G	62	GLY	2.1
1	C	137	CYS	2.1
1	D	144	THR	2.1
1	E	40	LEU	2.1
1	C	20	LYS	2.1
1	F	103	ILE	2.1
1	C	58	GLU	2.1
1	E	117	THR	2.1
1	G	70	VAL	2.1
1	D	27	ALA	2.1
1	A	151	ILE	2.1
1	D	30	PRO	2.1
1	D	91	VAL	2.1
1	G	133	TRP	2.1
1	H	20	LYS	2.1
1	D	120	ILE	2.1
1	G	48	HIS	2.1
1	C	114	TYR	2.0
1	D	50	VAL	2.0
1	A	21	TRP	2.0
1	G	76	ILE	2.0
1	H	51	MET	2.0
1	C	70	VAL	2.0
1	E	28	LEU	2.0
1	G	38	TRP	2.0

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

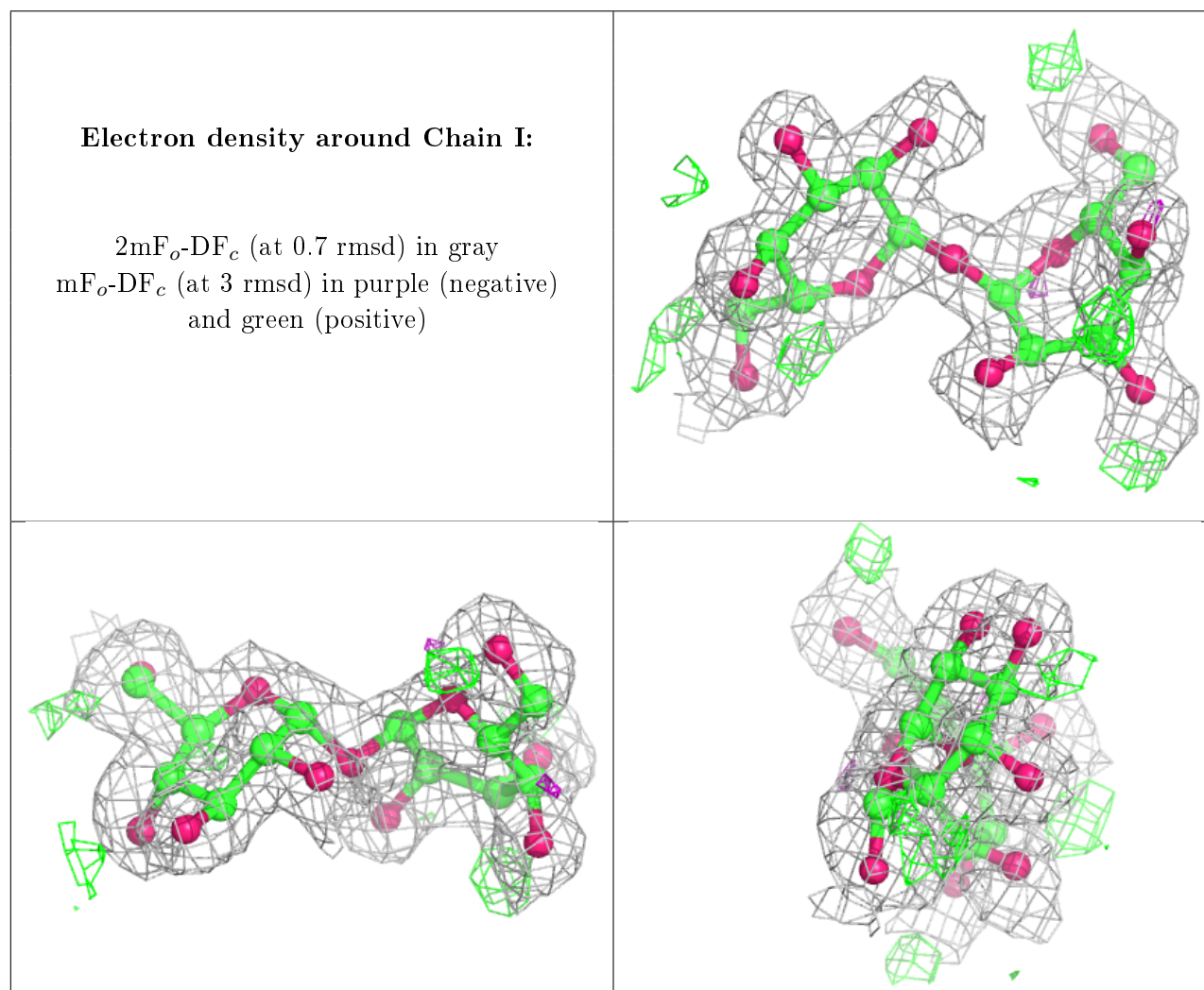
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	I	2	12/12	0.86	0.17	20,22,25,26	12
2	GLC	I	1	11/12	0.90	0.13	17,18,20,20	11

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MES	B	204	12/12	0.76	0.22	21,24,27,27	12
3	PGO	D	201	5/5	0.89	0.11	23,26,27,28	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PGO	B	203	5/5	0.92	0.21	15,15,18,23	5
3	PGO	G	201	5/5	0.92	0.11	23,25,25,31	5
3	PGO	A	201	5/5	0.97	0.25	14,14,15,17	5
4	SO4	B	201	5/5	0.98	0.15	18,18,20,20	5
4	SO4	B	202	5/5	0.98	0.12	23,24,28,28	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.