



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:34 AM UTC

PDB ID : 5GTG / pdb_00005gtg
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

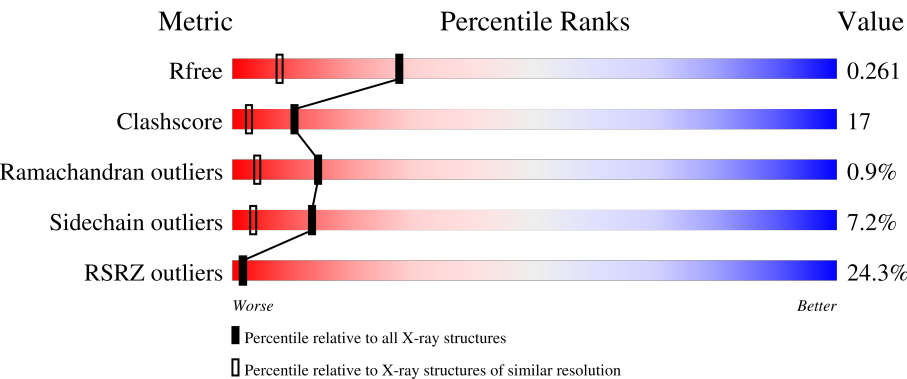
1 Overall quality at a glance i

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	175	
1	C	175	
1	D	175	
1	E	175	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	175	
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

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:

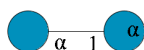
Chain	Residue	Modelled	Actual	Comment	Reference
A	170	HIS	-	expression tag	UNP P59082
A	171	HIS	-	expression tag	UNP P59082
A	172	HIS	-	expression tag	UNP P59082
A	173	HIS	-	expression tag	UNP P59082
A	174	HIS	-	expression tag	UNP P59082
A	175	HIS	-	expression tag	UNP P59082
B	170	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

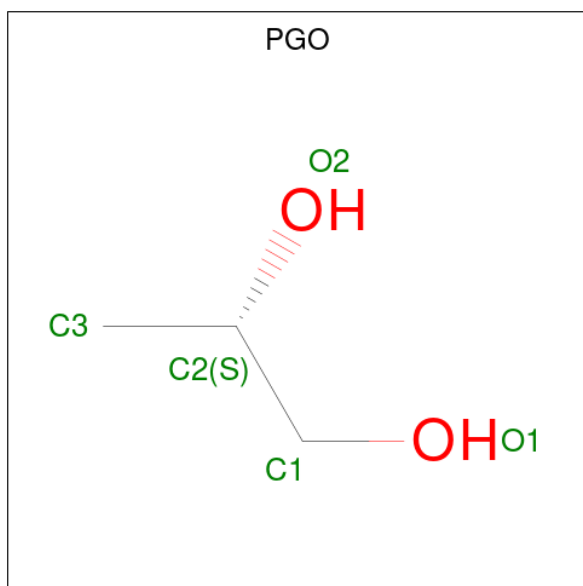
Chain	Residue	Modelled	Actual	Comment	Reference
C	171	HIS	-	expression tag	UNP P59082
C	172	HIS	-	expression tag	UNP P59082
C	173	HIS	-	expression tag	UNP P59082
C	174	HIS	-	expression tag	UNP P59082
C	175	HIS	-	expression tag	UNP P59082
D	170	HIS	-	expression tag	UNP P59082
D	171	HIS	-	expression tag	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 (CCD ID: PGO) (formula: $C_3H_8O_2$).



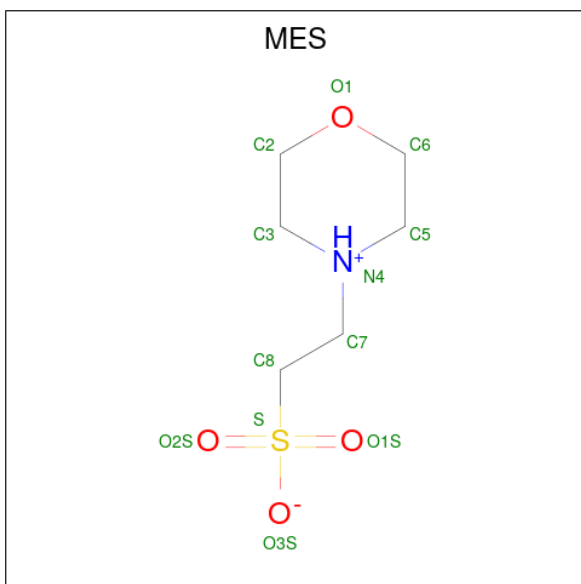
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	D	1	Total	C	O	0	0
			5	3	2		
3	G	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is SULFATE ION (CCD ID: 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 (CCD ID: 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		

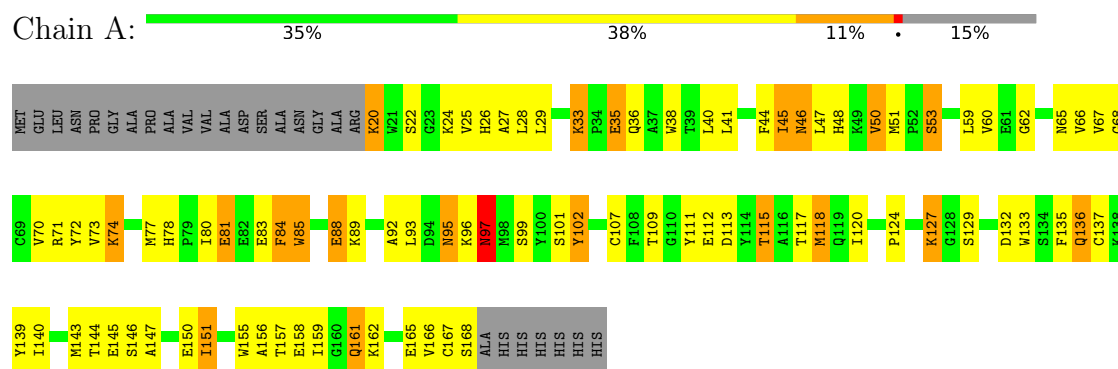
- Molecule 6 is water.

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

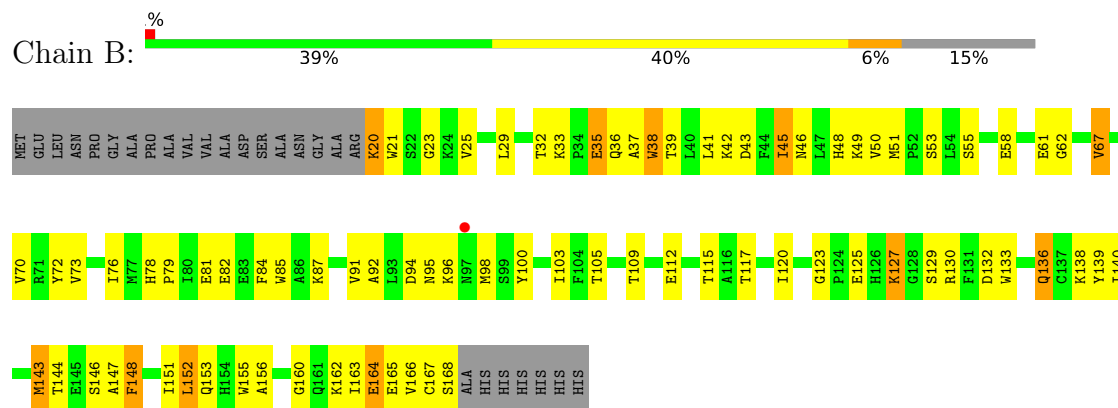
3 Residue-property plots

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.

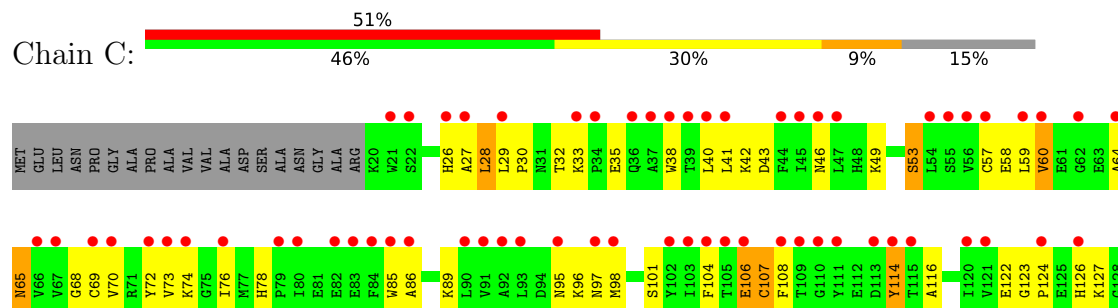
• Molecule 1: Lachrymatory-factor synthase

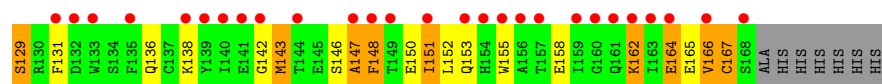


• Molecule 1: Lachrymatory-factor synthase

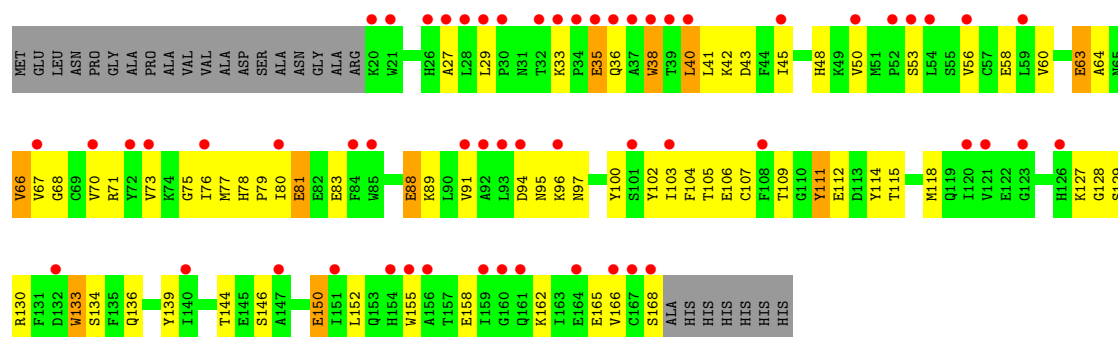
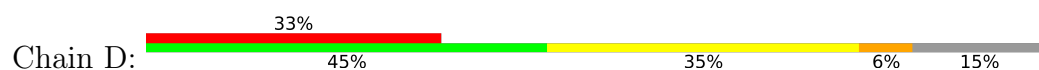


• Molecule 1: Lachrymatory-factor synthase

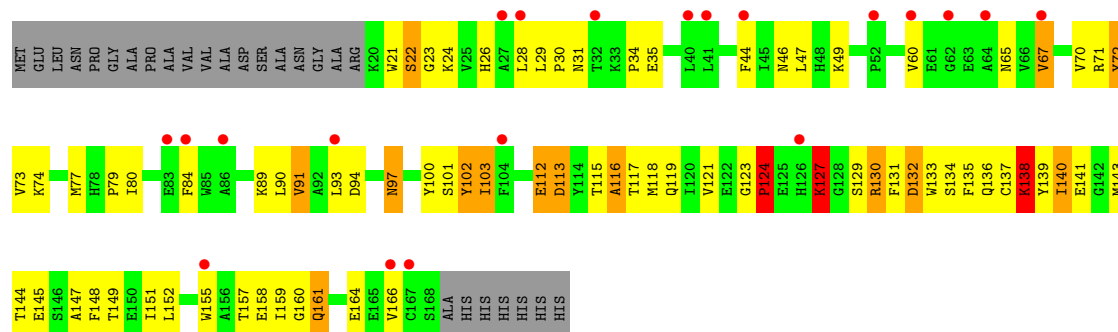




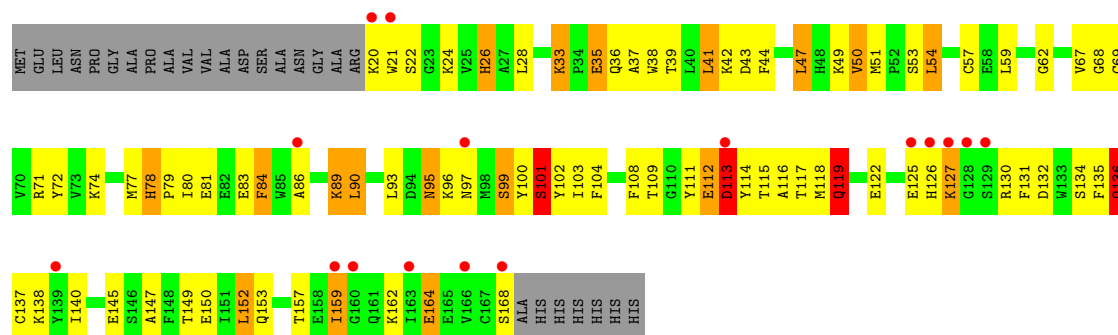
• Molecule 1: Lachrymatory-factor synthase



• Molecule 1: Lachrymatory-factor synthase

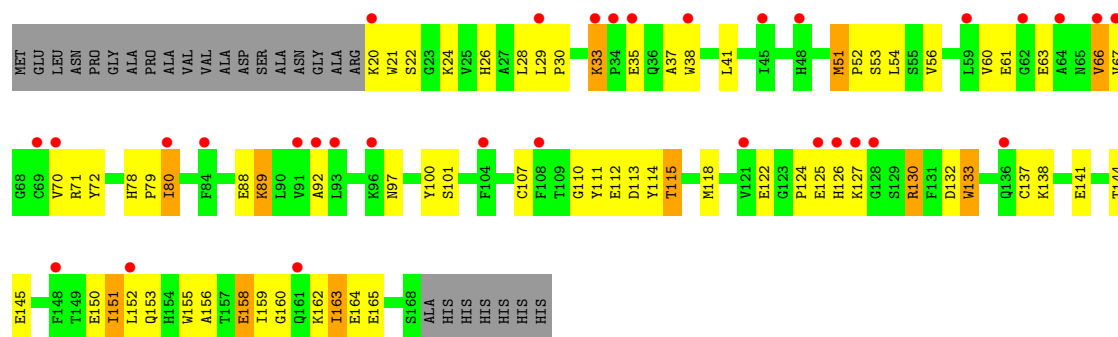


• Molecule 1: Lachrymatory-factor synthase

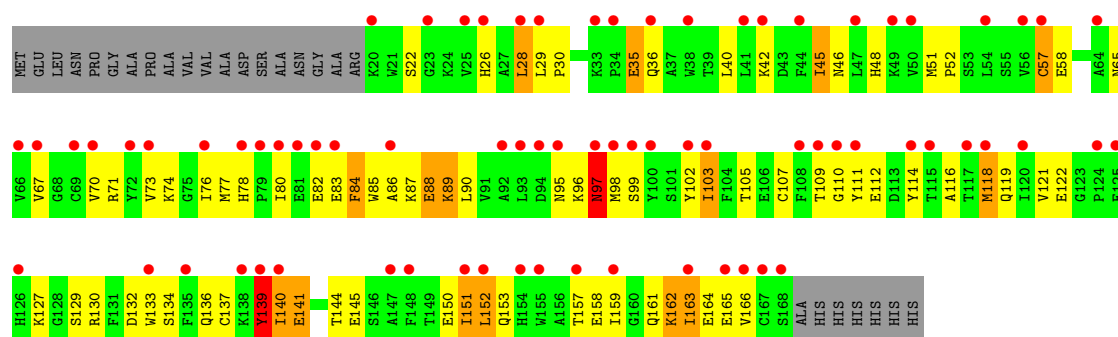
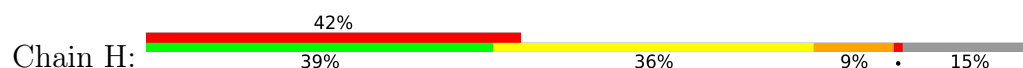


• Molecule 1: Lachrymatory-factor synthase





• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.230 , 0.260 0.236 , 0.261	Depositor DCC
R_{free} test set	15277 reflections (7.26%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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	0.91	EDS
Total number of atoms	10289	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GLC, SO4, PGO, 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	2.57	81/1237 (6.5%)	1.91	31/1674 (1.9%)
1	B	2.39	63/1237 (5.1%)	1.91	22/1674 (1.3%)
1	C	1.49	8/1237 (0.6%)	1.52	15/1674 (0.9%)
1	D	1.79	23/1237 (1.9%)	1.58	8/1674 (0.5%)
1	E	1.86	34/1237 (2.7%)	1.69	24/1674 (1.4%)
1	F	2.08	31/1237 (2.5%)	1.86	24/1674 (1.4%)
1	G	1.82	20/1237 (1.6%)	1.61	11/1674 (0.7%)
1	H	1.90	30/1237 (2.4%)	1.65	17/1674 (1.0%)
All	All	2.01	290/9896 (2.9%)	1.72	152/13392 (1.1%)

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

All (290) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	SER	CA-C	-13.34	1.35	1.52
1	A	20	LYS	N-CA	12.66	1.70	1.46
1	F	153	GLN	C-O	-12.60	1.09	1.24
1	B	136	GLN	CA-C	-11.14	1.38	1.52
1	A	112	GLU	C-O	10.99	1.36	1.23
1	A	93	LEU	C-O	10.97	1.36	1.23
1	D	91	VAL	N-CA	10.58	1.59	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	91	VAL	N-CA	9.54	1.56	1.46
1	D	71	ARG	N-CA	9.36	1.56	1.45
1	A	147	ALA	C-O	9.00	1.34	1.24
1	A	62	GLY	C-O	8.91	1.37	1.23
1	A	40	LEU	N-CA	8.82	1.57	1.46
1	E	151	ILE	C-O	8.76	1.34	1.24
1	A	102	TYR	C-O	-8.68	1.13	1.23
1	H	51	MET	CA-C	8.64	1.61	1.52
1	F	37	ALA	C-O	-8.62	1.13	1.24
1	B	163	ILE	C-O	8.54	1.34	1.24
1	B	153	GLN	N-CA	8.53	1.56	1.46
1	A	118	MET	CA-C	-8.47	1.42	1.52
1	D	134	SER	CA-C	-8.37	1.42	1.52
1	A	111	TYR	C-O	-8.28	1.14	1.23
1	B	46	ASN	CA-CB	8.22	1.64	1.53
1	B	87	LYS	CA-C	-8.22	1.42	1.52
1	A	45	ILE	N-CA	8.14	1.55	1.46
1	D	75	GLY	N-CA	8.11	1.54	1.45
1	E	148	PHE	N-CA	8.02	1.56	1.46
1	E	124	PRO	N-CA	-7.97	1.37	1.47
1	F	95	ASN	N-CA	7.96	1.55	1.46
1	B	156	ALA	C-O	7.93	1.33	1.24
1	B	85	TRP	CA-C	-7.90	1.42	1.52
1	F	77	MET	C-O	7.83	1.33	1.23
1	A	137	CYS	C-O	7.78	1.33	1.23
1	B	62	GLY	C-O	7.75	1.32	1.23
1	G	107	CYS	CA-C	-7.70	1.43	1.52
1	H	58	GLU	N-CA	-7.68	1.36	1.46
1	G	162	LYS	C-O	-7.66	1.15	1.24
1	F	157	THR	C-O	7.64	1.33	1.24
1	A	92	ALA	CA-CB	-7.61	1.41	1.53
1	A	45	ILE	C-O	7.60	1.33	1.24
1	A	22	SER	C-O	7.60	1.32	1.23
1	A	47	LEU	C-O	-7.57	1.14	1.24
1	E	145	GLU	C-O	7.53	1.32	1.24
1	B	103	ILE	CA-C	-7.46	1.43	1.52
1	A	59	LEU	C-O	7.44	1.32	1.23
1	E	147	ALA	C-O	7.43	1.32	1.24
1	B	139	TYR	CA-C	-7.36	1.43	1.52
1	H	65	ASN	CA-C	7.34	1.63	1.52
1	A	158	GLU	CA-CB	-7.29	1.42	1.53
1	F	35	GLU	C-O	-7.25	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	88	GLU	N-CA	7.24	1.54	1.46
1	A	83	GLU	C-O	-7.16	1.14	1.23
1	E	70	VAL	CA-C	7.12	1.61	1.52
1	B	84	PHE	C-O	7.07	1.32	1.23
1	B	166	VAL	CA-CB	7.06	1.63	1.54
1	F	62	GLY	C-O	7.01	1.33	1.23
1	A	145	GLU	CA-C	-7.00	1.43	1.52
1	C	41	LEU	N-CA	6.96	1.54	1.46
1	B	138	LYS	C-O	-6.96	1.15	1.24
1	B	144	THR	C-O	6.94	1.32	1.23
1	H	87	LYS	C-O	6.93	1.32	1.24
1	A	157	THR	C-O	6.84	1.32	1.24
1	H	22	SER	N-CA	6.83	1.54	1.46
1	F	26	HIS	N-CA	-6.83	1.37	1.45
1	A	27	ALA	CA-C	-6.81	1.44	1.52
1	B	127	LYS	C-O	6.81	1.32	1.24
1	E	117	THR	N-CA	6.80	1.54	1.46
1	A	143	MET	N-CA	-6.79	1.36	1.45
1	F	108	PHE	N-CA	6.79	1.54	1.46
1	A	28	LEU	CA-CB	-6.78	1.43	1.53
1	D	165	GLU	N-CA	6.77	1.54	1.46
1	G	101	SER	CA-C	-6.73	1.44	1.52
1	H	46	ASN	C-O	6.73	1.32	1.23
1	D	109	THR	C-O	6.72	1.31	1.23
1	F	114	TYR	C-O	-6.70	1.16	1.24
1	B	55	SER	N-CA	6.65	1.54	1.46
1	A	89	LYS	CA-C	-6.62	1.44	1.52
1	H	103	ILE	C-O	6.62	1.31	1.23
1	A	161	GLN	N-CA	6.61	1.54	1.46
1	B	140	ILE	C-O	6.54	1.31	1.24
1	D	68	GLY	N-CA	6.52	1.54	1.45
1	H	141	GLU	C-O	-6.51	1.15	1.23
1	A	136	GLN	CA-CB	-6.49	1.42	1.53
1	H	78	HIS	CA-C	6.49	1.59	1.52
1	B	67	VAL	C-O	6.47	1.31	1.24
1	A	51	MET	C-O	-6.47	1.16	1.24
1	B	38	TRP	N-CA	6.40	1.54	1.46
1	A	47	LEU	CA-C	6.39	1.61	1.52
1	A	117	THR	CB-CG2	-6.39	1.31	1.52
1	F	47	LEU	CA-C	6.38	1.61	1.52
1	A	88	GLU	N-CA	6.35	1.53	1.46
1	H	109	THR	CA-C	6.34	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	THR	CA-C	-6.34	1.45	1.52
1	A	118	MET	SD-CE	-6.34	1.63	1.79
1	B	146	SER	N-CA	-6.34	1.38	1.46
1	F	104	PHE	C-O	6.33	1.31	1.23
1	C	146	SER	C-O	-6.32	1.16	1.24
1	A	60	VAL	N-CA	-6.32	1.40	1.46
1	B	91	VAL	CA-CB	6.30	1.61	1.54
1	A	48	HIS	CA-CB	-6.28	1.42	1.53
1	A	70	VAL	CA-CB	-6.27	1.46	1.54
1	A	29	LEU	CA-CB	6.27	1.60	1.53
1	D	43	ASP	N-CA	6.24	1.54	1.46
1	A	44	PHE	C-O	-6.23	1.16	1.24
1	B	36	GLN	CD-OE1	6.21	1.35	1.23
1	F	59	LEU	C-O	6.20	1.31	1.23
1	H	76	ILE	C-O	6.20	1.30	1.24
1	A	93	LEU	CA-C	6.19	1.59	1.52
1	B	129	SER	CA-C	-6.19	1.44	1.53
1	A	27	ALA	C-O	-6.18	1.17	1.23
1	F	153	GLN	CA-C	-6.17	1.44	1.52
1	H	78	HIS	N-CA	6.16	1.53	1.45
1	A	102	TYR	N-CA	-6.13	1.38	1.45
1	B	105	THR	N-CA	6.12	1.53	1.45
1	B	112	GLU	CD-OE2	-6.12	1.13	1.25
1	B	164	GLU	C-O	6.10	1.31	1.24
1	F	112	GLU	CA-C	6.08	1.59	1.52
1	A	74	LYS	N-CA	6.07	1.53	1.46
1	C	108	PHE	CA-C	-6.07	1.44	1.52
1	F	101	SER	C-O	6.05	1.31	1.23
1	E	151	ILE	CA-C	6.04	1.60	1.52
1	A	92	ALA	C-N	-6.03	1.25	1.33
1	F	54	LEU	CA-C	6.02	1.60	1.52
1	C	147	ALA	C-O	-6.02	1.16	1.24
1	A	77	MET	N-CA	6.01	1.53	1.46
1	A	83	GLU	CD-OE1	6.01	1.36	1.25
1	B	58	GLU	C-O	6.01	1.31	1.23
1	F	150	GLU	CA-C	6.01	1.60	1.52
1	A	101	SER	C-O	6.00	1.31	1.23
1	E	119	GLN	N-CA	5.99	1.53	1.45
1	C	151	ILE	C-O	5.96	1.31	1.24
1	D	76	ILE	N-CA	5.96	1.53	1.46
1	E	90	LEU	N-CA	5.95	1.53	1.46
1	B	72	TYR	N-CA	-5.95	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	SER	CA-CB	5.95	1.62	1.53
1	B	20	LYS	N-CA	5.94	1.57	1.46
1	C	26	HIS	N-CA	5.92	1.52	1.46
1	E	140	ILE	CA-CB	5.91	1.62	1.54
1	B	21	TRP	N-CA	-5.91	1.39	1.45
1	A	25	VAL	N-CA	5.90	1.52	1.46
1	G	133	TRP	N-CA	5.90	1.53	1.46
1	B	49	LYS	CA-C	-5.89	1.44	1.52
1	H	132	ASP	CA-C	5.88	1.60	1.52
1	E	121	VAL	CA-C	5.87	1.60	1.52
1	A	146	SER	N-CA	5.84	1.53	1.46
1	A	26	HIS	C-O	5.84	1.30	1.23
1	A	53	SER	CA-C	-5.83	1.44	1.52
1	A	135	PHE	CA-C	-5.83	1.45	1.52
1	H	144	THR	C-O	5.82	1.31	1.23
1	E	116	ALA	N-CA	-5.80	1.38	1.45
1	B	117	THR	N-CA	-5.80	1.38	1.46
1	F	147	ALA	C-O	5.80	1.30	1.24
1	A	84	PHE	CG-CD2	-5.79	1.26	1.38
1	H	22	SER	CA-C	-5.79	1.45	1.52
1	B	37	ALA	CA-CB	-5.77	1.44	1.53
1	E	123	GLY	N-CA	-5.76	1.36	1.44
1	G	71	ARG	N-CA	5.76	1.52	1.45
1	G	138	LYS	C-O	5.75	1.30	1.24
1	E	131	PHE	N-CA	5.75	1.53	1.46
1	H	139	TYR	CA-CB	5.74	1.63	1.53
1	B	39	THR	CA-C	5.72	1.61	1.52
1	H	129	SER	C-O	-5.72	1.17	1.23
1	F	69	CYS	N-CA	5.72	1.53	1.45
1	G	133	TRP	C-O	-5.72	1.17	1.24
1	B	156	ALA	CA-C	-5.72	1.45	1.52
1	F	130	ARG	C-O	5.71	1.30	1.23
1	B	120	ILE	C-O	-5.70	1.17	1.24
1	B	100	TYR	N-CA	5.68	1.53	1.45
1	H	88	GLU	C-O	5.68	1.30	1.24
1	A	46	ASN	N-CA	5.68	1.53	1.46
1	G	38	TRP	C-O	-5.67	1.17	1.24
1	D	76	ILE	C-O	5.65	1.30	1.24
1	D	115	THR	N-CA	5.64	1.52	1.45
1	B	48	HIS	CA-C	5.63	1.60	1.52
1	E	72	TYR	C-O	5.63	1.30	1.24
1	G	92	ALA	N-CA	5.63	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	115	THR	N-CA	-5.62	1.39	1.45
1	E	22	SER	C-O	-5.61	1.16	1.23
1	B	143	MET	SD-CE	-5.61	1.65	1.79
1	A	161	GLN	C-O	-5.61	1.17	1.24
1	F	90	LEU	N-CA	5.59	1.53	1.46
1	A	115	THR	C-N	-5.59	1.26	1.33
1	D	40	LEU	CA-C	5.59	1.60	1.52
1	D	104	PHE	CA-C	5.59	1.59	1.52
1	A	155	TRP	C-O	5.58	1.31	1.24
1	E	101	SER	N-CA	5.58	1.53	1.45
1	F	41	LEU	CA-CB	-5.58	1.44	1.53
1	B	148	PHE	C-N	-5.57	1.26	1.33
1	C	167	CYS	CA-C	5.57	1.60	1.52
1	G	151	ILE	C-O	-5.56	1.17	1.24
1	H	36	GLN	N-CA	5.56	1.53	1.46
1	B	36	GLN	N-CA	-5.55	1.39	1.46
1	E	103	ILE	C-O	-5.55	1.17	1.23
1	B	70	VAL	CA-CB	5.54	1.61	1.54
1	E	77	MET	C-O	5.54	1.30	1.24
1	A	81	GLU	CA-C	-5.53	1.47	1.53
1	B	105	THR	C-O	5.53	1.30	1.23
1	A	41	LEU	C-O	-5.53	1.17	1.24
1	A	118	MET	C-O	5.51	1.30	1.24
1	B	139	TYR	C-O	5.51	1.31	1.23
1	H	112	GLU	C-O	-5.51	1.17	1.24
1	A	66	VAL	CA-C	5.50	1.59	1.52
1	H	110	GLY	C-O	5.50	1.31	1.23
1	A	146	SER	CA-C	5.49	1.59	1.52
1	E	94	ASP	CA-C	5.49	1.60	1.53
1	E	157	THR	N-CA	5.49	1.52	1.46
1	B	92	ALA	CA-C	-5.48	1.45	1.52
1	A	166	VAL	CA-C	-5.46	1.46	1.52
1	H	122	GLU	N-CA	5.46	1.52	1.46
1	H	45	ILE	C-O	-5.45	1.17	1.24
1	E	149	THR	C-O	-5.45	1.17	1.24
1	B	76	ILE	CA-CB	5.44	1.60	1.54
1	B	160	GLY	N-CA	5.44	1.52	1.45
1	H	107	CYS	CA-C	5.44	1.59	1.52
1	B	25	VAL	CA-CB	-5.44	1.46	1.54
1	E	135	PHE	C-O	-5.44	1.17	1.23
1	F	113	ASP	N-CA	5.43	1.54	1.46
1	G	88	GLU	CA-C	-5.43	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	LYS	N-CA	5.41	1.52	1.46
1	G	115	THR	N-CA	-5.40	1.39	1.46
1	A	50	VAL	C-O	-5.40	1.16	1.24
1	A	133	TRP	CG-CD1	5.39	1.50	1.36
1	E	132	ASP	CG-OD2	-5.39	1.15	1.25
1	F	117	THR	C-O	-5.39	1.17	1.24
1	B	94	ASP	CA-C	-5.38	1.47	1.53
1	D	146	SER	CA-C	5.35	1.59	1.52
1	E	23	GLY	N-CA	5.35	1.53	1.45
1	G	66	VAL	CA-C	-5.34	1.45	1.52
1	G	130	ARG	CA-C	-5.32	1.46	1.52
1	D	94	ASP	N-CA	-5.32	1.40	1.46
1	F	57	CYS	CA-CB	-5.29	1.45	1.53
1	B	129	SER	CB-OG	-5.29	1.31	1.42
1	F	136	GLN	C-O	-5.28	1.17	1.23
1	A	136	GLN	CB-CG	-5.27	1.36	1.52
1	B	109	THR	N-CA	5.26	1.52	1.45
1	G	165	GLU	N-CA	5.26	1.52	1.46
1	B	155	TRP	CA-C	5.24	1.59	1.52
1	A	27	ALA	N-CA	-5.24	1.39	1.46
1	D	45	ILE	C-O	5.22	1.30	1.24
1	B	133	TRP	CA-C	5.22	1.58	1.52
1	G	60	VAL	CA-C	-5.21	1.44	1.52
1	D	91	VAL	CA-C	-5.21	1.46	1.52
1	A	48	HIS	C-O	-5.20	1.17	1.24
1	A	99	SER	CA-CB	5.20	1.64	1.54
1	F	150	GLU	C-O	5.20	1.30	1.24
1	D	111	TYR	C-O	-5.19	1.17	1.24
1	A	93	LEU	N-CA	5.18	1.52	1.46
1	B	32	THR	CA-C	-5.18	1.46	1.52
1	B	132	ASP	CA-CB	-5.17	1.46	1.53
1	B	61	GLU	CA-C	-5.17	1.46	1.52
1	A	85	TRP	C-O	5.17	1.30	1.23
1	A	143	MET	C-O	5.16	1.30	1.23
1	G	29	LEU	N-CA	5.15	1.52	1.46
1	A	157	THR	CA-CB	-5.14	1.45	1.53
1	H	42	LYS	CA-C	5.14	1.59	1.52
1	H	118	MET	N-CA	5.14	1.52	1.46
1	F	39	THR	CA-C	-5.14	1.45	1.52
1	B	100	TYR	C-O	5.13	1.30	1.23
1	A	71	ARG	C-O	5.13	1.30	1.23
1	B	23	GLY	N-CA	-5.13	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	127	LYS	C-O	5.12	1.30	1.24
1	A	45	ILE	CA-C	5.11	1.58	1.52
1	B	45	ILE	N-CA	-5.11	1.39	1.46
1	D	100	TYR	CA-C	5.11	1.58	1.52
1	E	166	VAL	C-O	5.10	1.29	1.24
1	G	63	GLU	CA-C	-5.10	1.46	1.52
1	E	91	VAL	C-O	-5.09	1.19	1.24
1	H	90	LEU	N-CA	5.09	1.52	1.46
1	E	102	TYR	C-O	5.09	1.30	1.23
1	A	71	ARG	CA-CB	-5.09	1.44	1.53
1	B	167	CYS	C-O	5.08	1.30	1.24
1	D	105	THR	C-O	5.08	1.30	1.24
1	E	132	ASP	CB-CG	-5.07	1.39	1.52
1	G	153	GLN	N-CA	5.07	1.52	1.46
1	D	89	LYS	N-CA	-5.06	1.40	1.46
1	D	133	TRP	N-CA	5.06	1.52	1.46
1	H	30	PRO	N-CA	5.06	1.54	1.47
1	H	145	GLU	N-CA	-5.05	1.40	1.46
1	A	107	CYS	C-O	5.04	1.29	1.23
1	A	156	ALA	CA-CB	-5.04	1.45	1.53
1	A	109	THR	CA-C	5.03	1.59	1.52
1	A	151	ILE	C-O	5.03	1.29	1.24
1	A	97	ASN	CA-CB	5.03	1.60	1.53
1	F	117	THR	N-CA	5.03	1.52	1.46
1	E	143	MET	C-O	5.02	1.29	1.24
1	E	158	GLU	N-CA	5.02	1.52	1.46
1	H	140	ILE	CA-C	5.02	1.59	1.52
1	B	152	LEU	CA-CB	-5.01	1.45	1.53
1	B	84	PHE	CA-CB	5.00	1.61	1.53
1	G	144	THR	CA-C	-5.00	1.46	1.53
1	A	124	PRO	CA-C	5.00	1.58	1.52

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	153	GLN	N-CA-C	-9.77	100.71	111.36
1	F	95	ASN	N-CA-C	8.94	121.83	111.11
1	B	73	VAL	N-CA-C	8.56	121.90	108.89
1	C	148	PHE	N-CA-C	-8.24	101.55	111.69
1	C	153	GLN	N-CA-C	7.97	121.95	111.75
1	F	113	ASP	N-CA-C	7.88	120.87	111.02
1	A	93	LEU	CB-CA-C	7.79	123.27	109.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLY	N-CA-C	-7.74	104.40	114.85
1	A	95	ASN	N-CA-C	7.67	120.61	111.33
1	C	65	ASN	N-CA-C	7.60	122.14	112.86
1	A	150	GLU	CA-C-N	7.49	129.99	120.56
1	A	150	GLU	C-N-CA	7.49	129.99	120.56
1	H	51	MET	CA-C-N	7.41	127.77	119.32
1	H	51	MET	C-N-CA	7.41	127.77	119.32
1	D	165	GLU	N-CA-C	7.35	118.93	111.07
1	D	109	THR	N-CA-C	-6.97	99.11	108.74
1	F	150	GLU	N-CA-C	6.93	118.48	111.07
1	E	148	PHE	N-CA-C	6.92	118.90	111.36
1	B	152	LEU	CA-C-O	-6.91	112.29	120.10
1	B	123	GLY	CA-C-N	6.91	126.88	119.76
1	B	123	GLY	C-N-CA	6.91	126.88	119.76
1	B	163	ILE	N-CA-CB	6.87	119.89	110.54
1	A	66	VAL	N-CA-C	-6.87	98.49	108.11
1	H	151	ILE	CB-CA-C	-6.83	103.14	111.88
1	B	127	LYS	CD-CE-NZ	6.82	133.72	111.90
1	B	35	GLU	CA-C-N	6.79	129.67	120.44
1	B	35	GLU	C-N-CA	6.79	129.67	120.44
1	H	28	LEU	CA-C-N	6.79	130.31	122.85
1	H	28	LEU	C-N-CA	6.79	130.31	122.85
1	F	97	ASN	CB-CA-C	6.76	122.10	110.94
1	F	109	THR	CA-C-N	6.62	126.39	120.10
1	F	109	THR	C-N-CA	6.62	126.39	120.10
1	B	160	GLY	N-CA-C	-6.51	104.77	112.64
1	E	158	GLU	N-CA-C	6.45	120.01	111.75
1	D	102	TYR	N-CA-C	6.33	118.40	108.96
1	A	84	PHE	CA-CB-CG	6.32	120.12	113.80
1	B	165	GLU	N-CA-C	-6.32	103.69	111.40
1	G	67	VAL	N-CA-C	-6.30	100.58	108.89
1	C	142	GLY	N-CA-C	-6.28	106.45	114.37
1	E	147	ALA	N-CA-C	-6.24	104.56	111.36
1	F	33	LYS	N-CA-C	-6.21	101.51	110.08
1	F	54	LEU	N-CA-C	6.15	119.19	109.96
1	B	43	ASP	CA-C-N	6.13	130.01	120.82
1	B	43	ASP	C-N-CA	6.13	130.01	120.82
1	C	53	SER	N-CA-C	-6.10	105.32	112.89
1	H	76	ILE	CB-CG1-CD1	6.09	126.58	113.80
1	A	83	GLU	CG-CD-OE2	-6.07	104.44	118.40
1	E	138	LYS	N-CA-C	-6.04	104.39	110.97
1	G	156	ALA	N-CA-C	6.00	117.68	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	83	GLU	N-CA-C	5.96	118.91	109.96
1	E	166	VAL	CB-CA-C	5.94	119.81	112.02
1	D	38	TRP	N-CA-C	5.90	118.47	111.33
1	C	164	GLU	N-CA-C	5.90	118.47	111.33
1	C	72	TYR	N-CA-C	-5.86	101.33	110.42
1	D	81	GLU	N-CA-C	5.85	119.42	111.17
1	A	135	PHE	N-CA-C	5.83	118.56	109.52
1	E	164	GLU	N-CA-C	5.81	117.69	111.36
1	B	136	GLN	CA-CB-CG	5.80	125.70	114.10
1	E	127	LYS	CD-CE-NZ	5.79	130.44	111.90
1	G	150	GLU	N-CA-C	5.77	117.37	111.14
1	B	70	VAL	CA-C-O	5.76	126.47	120.36
1	H	89	LYS	N-CA-C	5.76	119.02	109.46
1	H	97	ASN	N-CA-C	5.75	119.99	112.92
1	A	40	LEU	N-CA-C	5.72	118.73	111.69
1	A	161	GLN	CA-C-O	-5.68	114.40	120.42
1	C	76	ILE	CA-C-N	5.68	129.54	121.42
1	C	76	ILE	C-N-CA	5.68	129.54	121.42
1	A	159	ILE	CA-C-O	-5.67	115.05	120.95
1	G	160	GLY	CA-C-N	5.67	127.89	120.28
1	G	160	GLY	C-N-CA	5.67	127.89	120.28
1	A	51	MET	CA-C-N	5.66	126.04	119.47
1	A	51	MET	C-N-CA	5.66	126.04	119.47
1	H	29	LEU	N-CA-C	-5.66	99.13	108.75
1	E	89	LYS	CG-CD-CE	5.65	124.30	111.30
1	F	100	TYR	CA-CB-CG	5.65	124.08	113.90
1	G	22	SER	N-CA-C	5.63	117.08	108.42
1	H	78	HIS	O-C-N	-5.63	117.89	121.88
1	A	120	ILE	N-CA-C	5.62	116.40	108.36
1	F	149	THR	CA-CB-CG2	5.62	120.06	110.50
1	G	163	ILE	CB-CA-C	-5.61	104.57	112.14
1	A	45	ILE	N-CA-C	-5.59	105.99	112.98
1	A	167	CYS	O-C-N	5.59	128.05	122.12
1	E	100	TYR	CA-CB-CG	5.57	123.93	113.90
1	A	36	GLN	CA-CB-CG	5.54	125.18	114.10
1	B	67	VAL	N-CA-C	-5.54	101.66	109.63
1	B	168	SER	CB-CA-C	5.53	120.60	110.10
1	B	36	GLN	O-C-N	5.52	128.05	122.09
1	E	24	LYS	CB-CG-CD	5.52	124.00	111.30
1	G	137	CYS	N-CA-C	5.52	116.92	108.42
1	H	139	TYR	CA-C-N	5.50	131.87	121.97
1	H	139	TYR	C-N-CA	5.50	131.87	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	43	ASP	N-CA-C	5.49	118.07	108.52
1	C	150	GLU	CA-CB-CG	5.43	124.96	114.10
1	A	136	GLN	N-CA-C	5.43	118.03	108.75
1	H	151	ILE	N-CA-C	5.41	116.05	110.36
1	F	49	LYS	CA-C-O	5.41	126.03	119.38
1	F	99	SER	N-CA-C	5.40	117.61	109.23
1	B	133	TRP	CB-CA-C	-5.39	102.75	110.62
1	E	123	GLY	CA-C-N	5.39	126.58	119.84
1	E	123	GLY	C-N-CA	5.39	126.58	119.84
1	E	161	GLN	N-CA-C	-5.37	105.51	111.36
1	H	84	PHE	CA-CB-CG	5.35	119.15	113.80
1	B	58	GLU	N-CA-C	5.33	118.14	109.24
1	F	119	GLN	CA-CB-CG	5.33	124.75	114.10
1	G	66	VAL	N-CA-C	-5.32	100.81	108.89
1	G	51	MET	CA-C-N	-5.32	114.61	119.82
1	G	51	MET	C-N-CA	-5.32	114.61	119.82
1	A	127	LYS	CG-CD-CE	5.31	123.52	111.30
1	E	113	ASP	CA-CB-CG	5.31	117.91	112.60
1	E	112	GLU	CA-CB-CG	5.31	124.72	114.10
1	A	44	PHE	N-CA-CB	-5.30	102.31	110.16
1	E	101	SER	N-CA-C	5.30	117.74	109.52
1	D	66	VAL	CB-CA-C	5.26	118.00	110.84
1	F	152	LEU	CB-CG-CD1	5.26	126.48	110.70
1	A	132	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	114	TYR	N-CA-C	-5.25	101.41	109.76
1	E	129	SER	N-CA-C	-5.24	101.11	109.07
1	H	162	LYS	N-CA-C	5.22	116.98	111.28
1	C	107	CYS	N-CA-C	5.22	116.14	107.73
1	F	33	LYS	CA-C-N	5.21	124.66	119.24
1	F	33	LYS	C-N-CA	5.21	124.66	119.24
1	A	24	LYS	CA-C-N	-5.21	115.53	122.77
1	A	24	LYS	C-N-CA	-5.21	115.53	122.77
1	C	41	LEU	CB-CA-C	-5.16	102.22	110.79
1	F	43	ASP	CA-C-N	5.15	127.50	120.54
1	F	43	ASP	C-N-CA	5.15	127.50	120.54
1	C	138	LYS	N-CA-C	-5.15	105.56	111.07
1	D	150	GLU	N-CA-C	5.15	117.79	111.82
1	E	130	ARG	CB-CA-C	5.15	119.02	109.70
1	F	80	ILE	N-CA-C	5.15	120.05	109.34
1	A	167	CYS	CA-C-O	-5.14	115.10	120.55
1	F	164	GLU	O-C-N	5.14	127.56	122.12
1	A	93	LEU	N-CA-C	-5.12	99.62	108.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	GLU	O-C-N	5.12	127.56	122.08
1	H	163	ILE	N-CA-CB	5.12	117.50	110.54
1	B	41	LEU	CA-C-N	5.11	128.78	120.60
1	B	41	LEU	C-N-CA	5.11	128.78	120.60
1	A	118	MET	CB-CG-SD	-5.11	97.38	112.70
1	A	33	LYS	N-CA-C	-5.11	103.60	109.93
1	H	78	HIS	N-CA-C	5.11	117.45	108.82
1	F	78	HIS	CB-CA-C	5.10	116.41	108.61
1	E	79	PRO	CA-C-N	5.09	128.64	120.30
1	E	79	PRO	C-N-CA	5.09	128.64	120.30
1	B	125	GLU	CA-CB-CG	-5.09	103.93	114.10
1	A	155	TRP	CA-CB-CG	5.07	123.23	113.60
1	A	102	TYR	N-CA-C	5.05	116.86	109.24
1	A	140	ILE	CA-C-O	-5.04	115.26	120.25
1	C	123	GLY	CA-C-O	-5.02	117.21	122.38
1	E	164	GLU	CA-C-N	5.02	127.42	120.29
1	E	164	GLU	C-N-CA	5.02	127.42	120.29
1	D	83	GLU	CB-CG-CD	-5.01	104.09	112.60
1	E	117	THR	CB-CA-C	-5.00	100.64	109.70

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	29	0
1	B	1205	0	1165	27	0
1	C	1205	0	1165	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1205	0	1165	48	0
1	E	1205	0	1165	49	0
1	F	1205	0	1165	56	0
1	G	1205	0	1165	37	0
1	H	1205	0	1165	57	0
2	I	23	0	20	3	0
3	A	5	0	8	2	0
3	B	5	0	7	2	0
3	D	5	0	8	1	0
3	G	5	0	8	3	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	6	0
6	C	24	0	0	5	0
6	D	42	0	0	16	0
6	E	54	0	0	18	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	327	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 17.

All (327) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:118:MET:HE3	1:E:133:TRP:CZ2	2.09	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:C:28:LEU:C	1:C:29:LEU:HD12	2.11	0.75
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:35:GLU:HB3	1:H:98:MET:HE1	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:LEU:HD11	1:H:166:VAL:CG1	2.19	0.72
1:E:93:LEU:HD23	1:E:93:LEU:C	2.16	0.71
1:F:24:LYS:NZ	1:G:125:GLU:OE2	2.24	0.70
6:A:355:HOH:O	1:F:67:VAL:CG1	2.37	0.70
1:D:66:VAL:CG1	1:E:136:GLN:HE22	2.04	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:134:SER:C	6:H:212:HOH:O	2.36	0.68
1:H:97:ASN:C	1:H:97:ASN:OD1	2.37	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
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:A:102:TYR:CE1	1:A:118:MET:HE3	2.30	0.65
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:B:51:MET:HE1	3:B:203:PGO:C3	2.26	0.65
1:D:77:MET:HE3	1:D:80:ILE:HD11	1.79	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:F:93:LEU:C	1:F:93:LEU:HD23	2.22	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: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:G:110:GLY:HA3	1:G:141:GLU:OE1	2.00	0.61
1:E:97:ASN:C	1:E:97:ASN:OD1	2.43	0.61
1:E:118:MET:CE	1:E:133:TRP:CZ2	2.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:95:ASN:O	1:H:96:LYS:C	2.44	0.61
1:H:118:MET:HE2	1:H:133:TRP:CZ2	2.34	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:H:82:GLU:C	6:H:201:HOH:O	2.44	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: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: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:51:MET:HE1	3:B:203:PGO:H32	1.84	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: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: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:C:143:MET:HE3	1:C:143:MET:HA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:PRO:CA	1:H:26:HIS:CD2	2.80	0.55
1:H:152:LEU:CD2	6:H:212:HOH:O	2.55	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:C:143:MET:HE2	1:C:147:ALA:HB3	1.89	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:A:35:GLU:CD	1:A:35:GLU:H	2.16	0.53
1:F:51:MET:HE2	1:F:54:LEU:HG	1.90	0.53
1:F:78:HIS:CD2	1:F:81:GLU:OE2	2.61	0.53
1:H:97:ASN:OD1	1:H:97:ASN:O	2.26	0.53
1:H:102:TYR:CZ	1:H:116:ALA:HB3	2.43	0.53
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:E:118:MET:HE3	1:E:133:TRP:CE2	2.44	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:G:51:MET:HE1	3:G:201:PGO:C3	2.40	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:G:51:MET:HE3	1:G:155:TRP:CD1	2.45	0.52
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:F:68:GLY:HA2	1:F:89:LYS:HZ2	1.75	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:D:63:GLU:O	1:D:64:ALA:C	2.55	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:112:GLU:C	6:E:203:HOH:O	2.55	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:B:143:MET:HE2	1:B:148:PHE:CA	2.41	0.50
1:G:24:LYS:CE	1:G:132:ASP:HB3	2.41	0.50
1:B:143:MET:HE2	1:B:148:PHE:HA	1.94	0.50
1:H:114:TYR:CE1	1:H:116:ALA:HB2	2.47	0.50
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: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:102:TYR:HE1	1:A:118:MET:HE3	1.72	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:D:27:ALA:C	6:D:302:HOH:O	2.55	0.49
1:G:37:ALA:CB	1:G:163:ILE:HG21	2.43	0.49
1:H:139:TYR:CD1	1:H:139:TYR:C	2.91	0.48
1:D:133:TRP:CZ2	1:D:152:LEU:HD11	2.48	0.48
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: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: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:F:84:PHE:CD1	1:F:84:PHE:C	2.92	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:GLN:HG2	6:F:269:HOH:O	2.14	0.47
1:C:165:GLU:CD	6:C:202:HOH:O	2.58	0.47
1:D:112:GLU:HG3	1:D:139:TYR:OH	2.15	0.47
1:A:115:THR:CG2	1:F:67:VAL:HG11	2.45	0.47
1:F:33:LYS:HB2	1:F:36:GLN:HG3	1.96	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:143:MET:HE3	1:B:147:ALA:HB3	1.96	0.46
1:C:40:LEU:HD11	1:C:167:CYS:SG	2.56	0.46
1:D:97:ASN:OD1	1:D:97:ASN:C	2.59	0.46
1:H:82:GLU:CB	6:H:201:HOH:O	2.64	0.46
1:G:111:TYR:O	1:G:112:GLU:HG3	2.16	0.45
1:C:42:LYS:HE3	1:C:95:ASN:HD21	1.81	0.45
1:F:113:ASP:O	1:F:137:CYS:HA	2.16	0.45
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:D:118:MET:HE3	1:D:133:TRP:CZ2	2.51	0.45
1:D:139:TYR:CD1	1:D:139:TYR:C	2.94	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:B:78:HIS:HD2	1:B:81:GLU:CD	2.25	0.45
1:G:118:MET:HE2	1:G:133:TRP:CE2	2.52	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:114:TYR:CD1	1:G:114:TYR:C	2.95	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:G:51:MET:HE1	3:G:201:PGO:H32	1.99	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: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:E:44:PHE:HB3	1:E:65:ASN:OD1	2.19	0.42
1:D:66:VAL:O	1:D:67:VAL:C	2.60	0.42
1:E:47:LEU:HD22	1:E:71:ARG:HH12	1.84	0.42
1:G:80:ILE:HD11	1:G:151:ILE:HD11	2.01	0.42
1:H:70:VAL:HG22	1:H:89:LYS:HB2	2.01	0.42
1:H:139:TYR:CD1	1:H:140:ILE:N	2.87	0.42
1:B:78:HIS:HD2	1:B:81:GLU:OE2	2.03	0.42
1:C:165:GLU:O	1:C:166:VAL:C	2.60	0.42
1:H:77:MET:CE	6:H:201:HOH:O	2.67	0.42
1:H:121:VAL:HG23	1:H:130:ARG:HB3	2.01	0.42
5:B:204:MES:H32	5:B:204:MES:S	2.59	0.42
1:H:35:GLU:CD	1:H:35:GLU:H	2.27	0.42
1:H:118:MET:HE2	1:H:133:TRP:CE2	2.54	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:A:97:ASN:C	1:A:97:ASN:OD1	2.62	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:N	1:G:113:ASP:OD1	2.53	0.42
1:F:79:PRO:O	1:F:81:GLU:HG2	2.19	0.42
1:G:118:MET:HE2	1:G:133:TRP:CZ2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:F:115:THR:HG23	2.20	0.41
1:D:103:ILE:HB	6:D:312:HOH:O	2.20	0.41
1:G:33:LYS:NZ	1:G:35:GLU:OE1	2.45	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:E:113:ASP:CG	6:E:203:HOH:O	2.63	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:F:118:MET:HB3	6:F:219:HOH:O	2.19	0.41
1:C:68:GLY:O	1:C:69:CYS:C	2.61	0.41
1:C:97:ASN:O	1:C:98:MET:C	2.64	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: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: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:H:35:GLU:CD	1:H:35:GLU:N	2.80	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:89:LYS:NZ	6:G:309:HOH:O	2.54	0.40
1:G:159:ILE:HG22	1:G:163:ILE:HD12	2.03	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%)	4	0
1	D	147/175 (84%)	137 (93%)	9 (6%)	1 (1%)	18	7
1	E	147/175 (84%)	137 (93%)	8 (5%)	2 (1%)	9	2
1	F	147/175 (84%)	142 (97%)	4 (3%)	1 (1%)	18	7
1	G	147/175 (84%)	143 (97%)	4 (3%)	0	100	100
1	H	147/175 (84%)	136 (92%)	8 (5%)	3 (2%)	6	1
All	All	1176/1400 (84%)	1120 (95%)	45 (4%)	11 (1%)	14	4

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%)	128 (97%)	4 (3%)	36	19
1	B	132/150 (88%)	126 (96%)	6 (4%)	24	9
1	C	132/150 (88%)	118 (89%)	14 (11%)	6	1
1	D	132/150 (88%)	127 (96%)	5 (4%)	29	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	132/150 (88%)	118 (89%)	14 (11%)	6	1
1	F	132/150 (88%)	116 (88%)	16 (12%)	5	1
1	G	132/150 (88%)	124 (94%)	8 (6%)	17	5
1	H	132/150 (88%)	123 (93%)	9 (7%)	14	4
All	All	1056/1200 (88%)	980 (93%)	76 (7%)	13	3

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	35	GLU
1	A	84	PHE
1	A	127	LYS
1	B	33	LYS
1	B	35	GLU
1	B	45	ILE
1	B	67	VAL
1	B	96	LYS
1	B	152	LEU
1	C	28	LEU
1	C	33	LYS
1	C	35	GLU
1	C	60	VAL
1	C	74	LYS
1	C	89	LYS
1	C	96	LYS
1	C	106	GLU
1	C	129	SER
1	C	136	GLN
1	C	143	MET
1	C	152	LEU
1	C	158	GLU
1	C	164	GLU
1	D	35	GLU
1	D	63	GLU
1	D	73	VAL
1	D	127	LYS
1	D	168	SER
1	E	22	SER
1	E	34	PRO
1	E	35	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	60	VAL
1	E	80	ILE
1	E	84	PHE
1	E	97	ASN
1	E	103	ILE
1	E	127	LYS
1	E	134	SER
1	E	138	LYS
1	E	140	ILE
1	E	152	LEU
1	E	161	GLN
1	F	35	GLU
1	F	50	VAL
1	F	53	SER
1	F	84	PHE
1	F	89	LYS
1	F	101	SER
1	F	113	ASP
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	F	159	ILE
1	F	164	GLU
1	F	168	SER
1	G	20	LYS
1	G	33	LYS
1	G	66	VAL
1	G	80	ILE
1	G	89	LYS
1	G	97	ASN
1	G	152	LEU
1	G	158	GLU
1	H	28	LEU
1	H	35	GLU
1	H	45	ILE
1	H	83	GLU
1	H	84	PHE
1	H	97	ASN
1	H	152	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	157	THR
1	H	164	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) 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	B	78	HIS
1	B	95	ASN
1	B	154	HIS
1	C	48	HIS
1	C	78	HIS
1	C	95	ASN
1	C	97	ASN
1	C	119	GLN
1	D	26	HIS
1	D	78	HIS
1	D	95	ASN
1	D	136	GLN
1	D	153	GLN
1	D	154	HIS
1	D	161	GLN
1	E	31	ASN
1	E	36	GLN
1	E	78	HIS
1	E	136	GLN
1	E	161	GLN
1	F	26	HIS
1	F	46	ASN
1	F	48	HIS
1	F	78	HIS
1	F	95	ASN
1	G	36	GLN
1	G	78	HIS
1	G	119	GLN
1	G	154	HIS
1	H	78	HIS
1	H	95	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	136	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 ⓘ

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	1.52	2 (18%)	15,15,17	2.16	6 (40%)
2	GLC	I	2	2	12,12,12	1.44	2 (16%)	17,17,17	2.28	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	GLC	O5-C1	3.51	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	GLC	O5-C5	-2.92	1.37	1.44
2	I	1	GLC	C6-C5	2.09	1.58	1.51
2	I	2	GLC	O5-C1	2.02	1.47	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	GLC	C3-C4-C5	4.54	118.47	110.23
2	I	1	GLC	O5-C5-C4	4.30	121.30	110.83
2	I	2	GLC	C4-C3-C2	4.15	118.11	110.83
2	I	2	GLC	O4-C4-C5	-4.13	99.16	109.32
2	I	1	GLC	C6-C5-C4	-4.06	103.05	113.02
2	I	1	GLC	O6-C6-C5	-3.12	100.70	111.33
2	I	2	GLC	O3-C3-C2	-2.85	103.65	110.38
2	I	2	GLC	C1-C2-C3	2.53	115.51	110.36
2	I	1	GLC	O4-C4-C5	-2.42	103.35	109.32
2	I	2	GLC	C1-O5-C5	2.38	118.27	113.65
2	I	1	GLC	C3-C4-C5	2.37	114.53	110.23
2	I	1	GLC	C1-O5-C5	2.12	115.02	112.19
2	I	2	GLC	O2-C2-C1	2.04	113.95	109.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

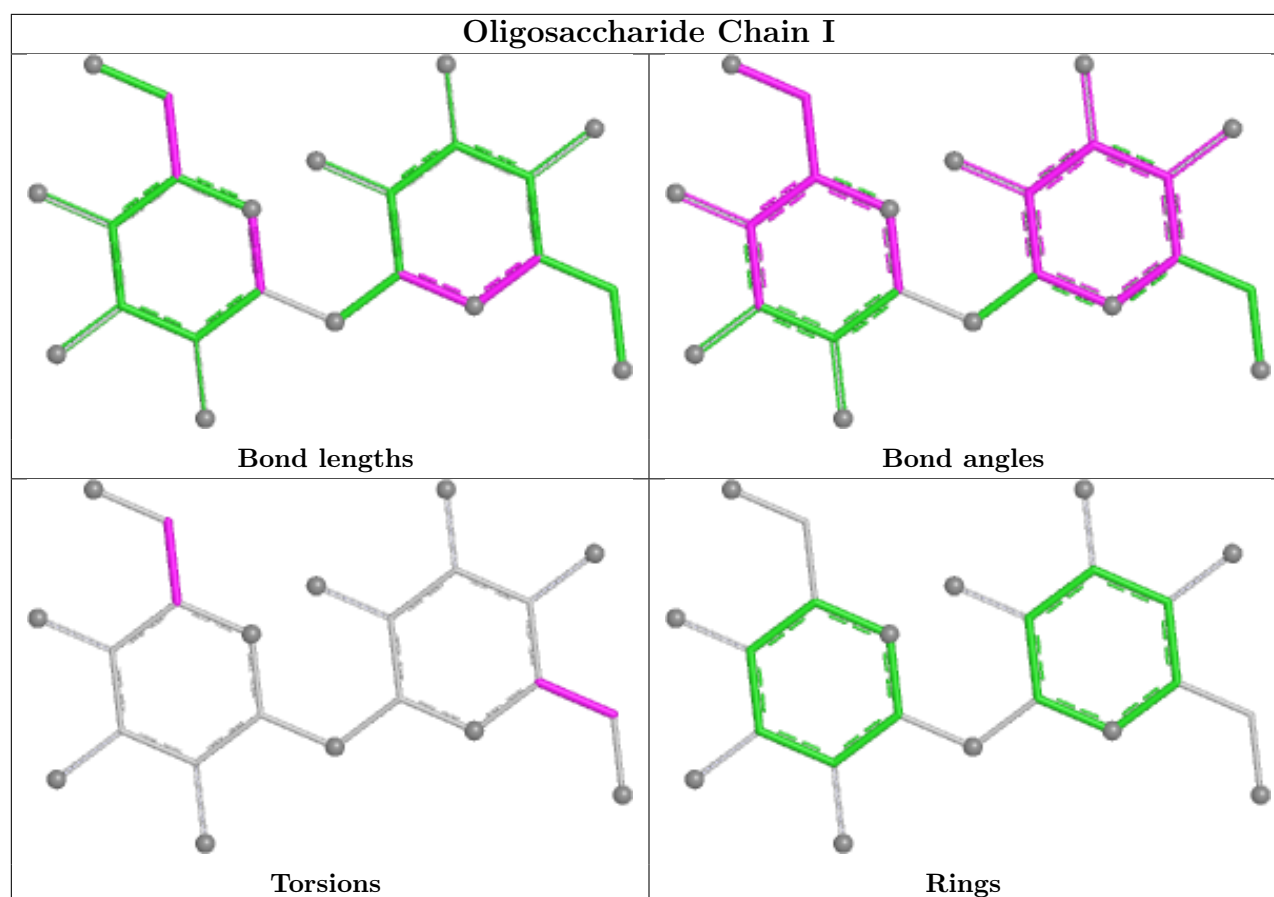
Mol	Chain	Res	Type	Atoms
2	I	1	GLC	C4-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6

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	$\# Z > 2$
4	SO4	B	202	-	4,4,4	0.53	0	6,6,6	1.07	0
3	PGO	D	201	-	4,4,4	0.31	0	4,4,4	1.16	1 (25%)
3	PGO	B	203	-	4,4,4	0.50	0	4,4,4	1.24	0
5	MES	B	204	-	12,12,12	2.42	5 (41%)	15,16,16	3.55	9 (60%)
4	SO4	B	201	-	4,4,4	0.95	0	6,6,6	0.59	0
3	PGO	A	201	-	4,4,4	0.87	0	4,4,4	2.09	2 (50%)
3	PGO	G	201	-	4,4,4	0.65	0	4,4,4	0.92	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	D	201	-	-	1/2/2/2	-
5	MES	B	204	-	-	5/6/14/14	0/1/1/1
3	PGO	B	203	-	-	2/2/2/2	-
3	PGO	A	201	-	-	1/2/2/2	-
3	PGO	G	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	-6.55	1.68	1.77
5	B	204	MES	C7-N4	2.51	1.53	1.47
5	B	204	MES	O2S-S	2.49	1.52	1.45
5	B	204	MES	O1S-S	2.25	1.51	1.45
5	B	204	MES	C5-C6	2.15	1.58	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	204	MES	O1S-S-C8	10.00	121.83	106.73
5	B	204	MES	C5-N4-C3	-3.98	100.28	108.84
5	B	204	MES	O1-C2-C3	3.78	119.91	111.77
5	B	204	MES	O3S-S-O1S	-3.67	102.23	111.40
5	B	204	MES	C2-C3-N4	3.41	115.30	110.12
5	B	204	MES	C8-C7-N4	2.84	123.10	112.36
3	A	201	PGO	C3-C2-C1	2.63	121.63	110.80
3	A	201	PGO	O2-C2-C1	-2.37	103.35	114.99
5	B	204	MES	O1-C6-C5	2.32	116.76	111.77
5	B	204	MES	O3S-S-C8	2.32	110.53	106.00
3	D	201	PGO	O2-C2-C1	-2.30	103.69	114.99
5	B	204	MES	C6-C5-N4	-2.29	106.64	110.12

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	203	PGO	O1-C1-C2-O2
3	G	201	PGO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	SO4	1	0
3	D	201	PGO	1	0
3	B	203	PGO	2	0
5	B	204	MES	4	0
3	A	201	PGO	2	0
3	G	201	PGO	3	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	149/175 (85%)	-0.26	0 100 100	4, 10, 19, 28	0
1	B	149/175 (85%)	-0.23	1 (0%) 84 86	5, 11, 21, 25	0
1	C	149/175 (85%)	2.63	90 (60%) 0 0	16, 23, 31, 34	149 (100%)
1	D	149/175 (85%)	1.77	57 (38%) 1 0	12, 18, 26, 34	149 (100%)
1	E	149/175 (85%)	1.18	20 (13%) 7 6	10, 16, 22, 28	149 (100%)
1	F	149/175 (85%)	1.07	16 (10%) 11 11	8, 14, 22, 26	149 (100%)
1	G	149/175 (85%)	1.39	32 (21%) 2 2	10, 17, 25, 32	149 (100%)
1	H	149/175 (85%)	1.97	74 (49%) 0 0	11, 18, 26, 34	149 (100%)
All	All	1192/1400 (85%)	1.19	290 (24%) 2 2	4, 16, 26, 34	894 (75%)

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	5.8
1	C	85	TRP	5.8
1	C	135	PHE	5.7
1	C	38	TRP	5.6
1	C	40	LEU	5.5
1	C	91	VAL	5.4
1	C	103	ILE	5.4
1	D	56	VAL	5.3
1	C	110	GLY	5.3
1	G	80	ILE	5.2
1	C	166	VAL	5.2
1	H	155	TRP	5.1
1	C	108	PHE	5.1
1	C	76	ILE	5.0
1	H	108	PHE	4.9
1	C	80	ILE	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	33	LYS	4.9
1	G	84	PHE	4.9
1	C	92	ALA	4.7
1	G	128	GLY	4.7
1	C	67	VAL	4.7
1	C	104	PHE	4.7
1	C	39	THR	4.6
1	H	148	PHE	4.6
1	C	109	THR	4.5
1	D	126	HIS	4.5
1	H	124	PRO	4.4
1	H	36	GLN	4.3
1	D	84	PHE	4.2
1	C	66	VAL	4.2
1	C	154	HIS	4.2
1	G	93	LEU	4.1
1	G	66	VAL	4.1
1	C	155	TRP	4.0
1	C	140	ILE	3.9
1	C	79	PRO	3.9
1	C	141	GLU	3.9
1	D	30	PRO	3.9
1	C	159	ILE	3.9
1	C	97	ASN	3.8
1	C	36	GLN	3.8
1	D	80	ILE	3.8
1	H	38	TRP	3.8
1	C	47	LEU	3.8
1	D	38	TRP	3.8
1	F	160	GLY	3.8
1	H	163	ILE	3.7
1	C	45	ILE	3.7
1	C	41	LEU	3.7
1	C	139	TYR	3.7
1	C	163	ILE	3.7
1	D	159	ILE	3.7
1	F	166	VAL	3.7
1	H	168	SER	3.7
1	D	20	LYS	3.6
1	C	111	TYR	3.6
1	H	72	TYR	3.6
1	C	149	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	166	VAL	3.6
1	G	20	LYS	3.6
1	H	167	CYS	3.6
1	F	21	TRP	3.6
1	D	27	ALA	3.6
1	H	95	ASN	3.6
1	C	56	VAL	3.6
1	D	40	LEU	3.6
1	H	140	ILE	3.5
1	C	157	THR	3.5
1	H	49	LYS	3.5
1	C	156	ALA	3.5
1	H	147	ALA	3.5
1	C	113	ASP	3.5
1	C	138	LYS	3.5
1	D	151	ILE	3.4
1	F	168	SER	3.4
1	D	29	LEU	3.4
1	C	70	VAL	3.4
1	C	34	PRO	3.4
1	D	72	TYR	3.4
1	H	115	THR	3.4
1	H	73	VAL	3.4
1	G	126	HIS	3.3
1	D	93	LEU	3.3
1	H	93	LEU	3.3
1	G	34	PRO	3.3
1	H	166	VAL	3.3
1	H	126	HIS	3.3
1	H	56	VAL	3.3
1	G	64	ALA	3.3
1	H	102	TYR	3.3
1	F	20	LYS	3.3
1	C	121	VAL	3.3
1	D	37	ALA	3.3
1	C	93	LEU	3.2
1	C	60	VAL	3.2
1	E	64	ALA	3.2
1	D	91	VAL	3.2
1	H	34	PRO	3.2
1	C	69	CYS	3.2
1	D	168	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	62	GLY	3.1
1	H	57	CYS	3.1
1	C	115	THR	3.1
1	D	103	ILE	3.1
1	D	160	GLY	3.1
1	C	168	SER	3.1
1	C	64	ALA	3.1
1	C	144	THR	3.1
1	C	55	SER	3.1
1	C	21	TRP	3.0
1	D	52	PRO	3.0
1	C	120	ILE	3.0
1	H	99	SER	3.0
1	D	96	LYS	3.0
1	H	25	VAL	3.0
1	C	72	TYR	3.0
1	E	86	ALA	3.0
1	G	92	ALA	3.0
1	G	35	GLU	2.9
1	E	28	LEU	2.9
1	C	95	ASN	2.9
1	G	67	VAL	2.9
1	C	102	TYR	2.9
1	D	59	LEU	2.9
1	C	151	ILE	2.9
1	D	123	GLY	2.9
1	F	163	ILE	2.9
1	D	36	GLN	2.9
1	C	98	MET	2.9
1	D	121	VAL	2.9
1	C	86	ALA	2.9
1	H	92	ALA	2.9
1	H	54	LEU	2.9
1	H	152	LEU	2.9
1	C	73	VAL	2.8
1	H	66	VAL	2.8
1	H	67	VAL	2.8
1	C	162	LYS	2.8
1	D	76	ILE	2.8
1	C	46	ASN	2.8
1	H	50	VAL	2.8
1	H	154	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	37	ALA	2.8
1	H	135	PHE	2.8
1	D	73	VAL	2.8
1	E	166	VAL	2.8
1	C	114	TYR	2.8
1	C	153	GLN	2.8
1	C	29	LEU	2.8
1	C	74	LYS	2.8
1	G	127	LYS	2.8
1	H	103	ILE	2.8
1	H	118	MET	2.8
1	E	62	GLY	2.8
1	H	23	GLY	2.8
1	E	84	PHE	2.7
1	E	93	LEU	2.7
1	G	59	LEU	2.7
1	H	28	LEU	2.7
1	D	67	VAL	2.7
1	H	151	ILE	2.7
1	H	138	LYS	2.7
1	D	92	ALA	2.7
1	C	132	ASP	2.7
1	G	148	PHE	2.7
1	E	167	CYS	2.7
1	H	70	VAL	2.7
1	D	45	ILE	2.7
1	D	120	ILE	2.7
1	E	52	PRO	2.6
1	C	148	PHE	2.6
1	G	62	GLY	2.6
1	E	67	VAL	2.6
1	D	164	GLU	2.6
1	G	125	GLU	2.6
1	E	104	PHE	2.6
1	C	124	PRO	2.6
1	C	131	PHE	2.6
1	H	29	LEU	2.6
1	G	70	VAL	2.6
1	G	91	VAL	2.6
1	D	155	TRP	2.6
1	H	94	ASP	2.5
1	D	26	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	154	HIS	2.5
1	G	96	LYS	2.5
1	H	20	LYS	2.5
1	E	155	TRP	2.5
1	G	38	TRP	2.5
1	G	33	LYS	2.5
1	E	40	LEU	2.5
1	D	156	ALA	2.5
1	H	139	TYR	2.5
1	G	161	GLN	2.4
1	D	85	TRP	2.4
1	C	54	LEU	2.4
1	E	126	HIS	2.4
1	E	27	ALA	2.4
1	H	80	ILE	2.4
1	C	59	LEU	2.4
1	C	142	GLY	2.4
1	C	84	PHE	2.4
1	G	104	PHE	2.4
1	H	86	ALA	2.4
1	F	97	ASN	2.4
1	E	60	VAL	2.4
1	C	83	GLU	2.4
1	G	29	LEU	2.4
1	G	152	LEU	2.4
1	H	64	ALA	2.4
1	C	44	PHE	2.4
1	E	32	THR	2.4
1	H	120	ILE	2.4
1	H	159	ILE	2.4
1	F	129	SER	2.3
1	C	126	HIS	2.3
1	H	133	TRP	2.3
1	H	76	ILE	2.3
1	G	121	VAL	2.3
1	D	35	GLU	2.3
1	H	81	GLU	2.3
1	F	113	ASP	2.3
1	D	33	LYS	2.3
1	H	157	THR	2.3
1	E	44	PHE	2.3
1	H	111	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	114	TYR	2.3
1	H	97	ASN	2.3
1	D	39	THR	2.3
1	D	161	GLN	2.3
1	D	54	LEU	2.3
1	C	82	GLU	2.2
1	E	83	GLU	2.2
1	F	125	GLU	2.2
1	H	47	LEU	2.2
1	H	33	LYS	2.2
1	D	94	ASP	2.2
1	C	160	GLY	2.2
1	D	108	PHE	2.2
1	F	128	GLY	2.2
1	H	100	TYR	2.2
1	G	136	GLN	2.2
1	C	147	ALA	2.2
1	H	69	CYS	2.2
1	H	125	GLU	2.2
1	H	165	GLU	2.2
1	G	48	HIS	2.2
1	G	108	PHE	2.2
1	H	78	HIS	2.2
1	F	159	ILE	2.2
1	G	45	ILE	2.2
1	F	127	LYS	2.2
1	H	98	MET	2.2
1	D	21	TRP	2.2
1	C	106	GLU	2.2
1	D	28	LEU	2.2
1	H	79	PRO	2.2
1	C	27	ALA	2.1
1	G	69	CYS	2.1
1	F	126	HIS	2.1
1	C	133	TRP	2.1
1	E	41	LEU	2.1
1	H	42	LYS	2.1
1	D	34	PRO	2.1
1	C	161	GLN	2.1
1	H	82	GLU	2.1
1	D	167	CYS	2.1
1	B	97	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	132	ASP	2.1
1	D	32	THR	2.1
1	F	139	TYR	2.1
1	C	26	HIS	2.1
1	D	147	ALA	2.1
1	C	57	CYS	2.1
1	C	164	GLU	2.1
1	D	53	SER	2.1
1	D	101	SER	2.1
1	H	41	LEU	2.1
1	C	105	THR	2.1
1	H	109	THR	2.1
1	H	117	THR	2.1
1	H	26	HIS	2.1
1	D	140	ILE	2.1
1	H	110	GLY	2.0
1	C	22	SER	2.0
1	D	70	VAL	2.0
1	H	83	GLU	2.0
1	H	44	PHE	2.0
1	F	86	ALA	2.0
1	D	50	VAL	2.0

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

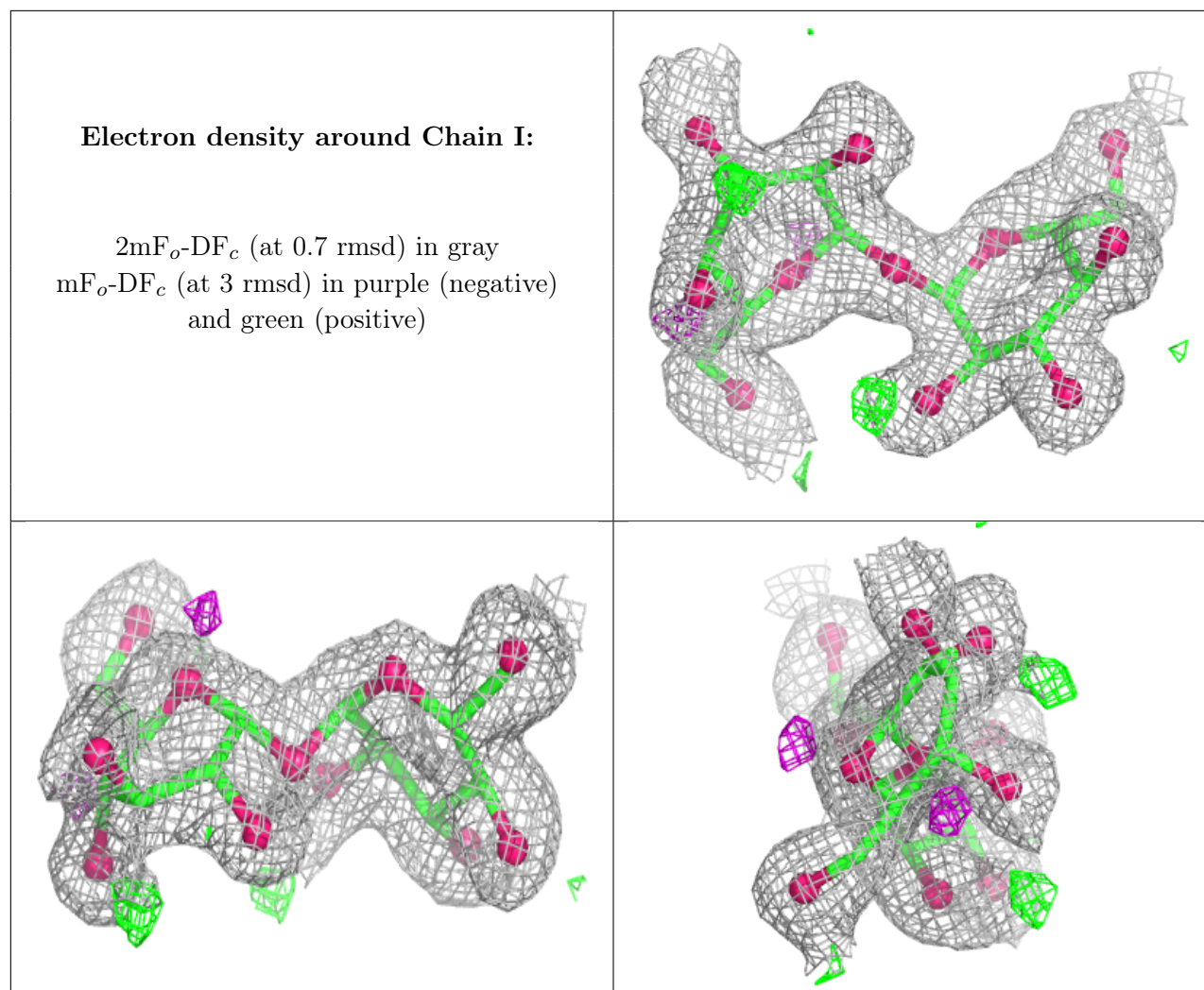
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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, 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	B-factors(Å ²)	Q<0.9
2	GLC	I	1	11/12	0.90	0.10	17,18,20,20	11
2	GLC	I	2	12/12	0.90	0.12	20,22,25,26	12

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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
5	MES	B	204	12/12	0.86	0.18	21,24,27,27	12
3	PGO	D	201	5/5	0.91	0.13	23,26,27,28	5
3	PGO	B	203	5/5	0.92	0.16	15,15,18,23	5
3	PGO	G	201	5/5	0.93	0.11	23,25,25,31	5
3	PGO	A	201	5/5	0.97	0.11	14,14,15,17	5
4	SO4	B	202	5/5	0.98	0.07	23,24,28,28	5
4	SO4	B	201	5/5	0.98	0.12	18,18,20,20	5

6.5 Other polymers [i](#)

There are no such residues in this entry.