

Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 01:24 pm GMT

PDB ID	:	1W2T
Title	:	beta-fructosidase from Thermotoga maritima in complex with raffinose
Authors	:	Alberto, F.; Henrissat, B.; Czjzek, M.
Deposited on	:	2004-07-08
Resolution	:	1.87 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.87 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.



Motria	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	٨	490	5%		
1	А	432	86%	13%	•
			11%		
1	В	432	82%	16%	•
			9%		
1	С	432	85%	13%	•
			8%		
1	D	432	84%	14%	•
			10%		
1	E	432	88%	12%	•



Mol	Chain	Length	Quality of chain				
1	F	432	8%	87%	12% •		
2	G	3	33%	67%			
2	Н	3	33%	67%			
2	Ι	3	33%	67%			
2	J	3	33%	67%			
2	K	3	33%	67%			
2	L	3	33%	67%			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23234 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	429	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	432	3517	2250	589	665	13	0	0	0
1	р	429	Total	С	Ν	0	S	0	0	0
1	D	402	3519	2252	589	665	13	0	0	0
1	C	429	Total	С	Ν	0	S	0	0	0
		432	3519	2252	589	665	13	0	0	0
1	П	429	Total	С	Ν	0	S	0	0	0
	D	402	3518	2251	589	665	13	0	0	U
1	F	429	Total	С	Ν	0	S	0	0	0
		432	3518	2251	589	665	13	0	0	0
1	1	429	Total	С	Ν	0	S	0	0	0
	Г	432	3518	2252	588	665	13	0	U	

• Molecule 1 is a protein called BETA FRUCTOSIDASE.

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	190	ASP	GLU	engineered mutation	UNP 033833
А	108	VAL	ALA	cloning artifact	UNP O33833
А	179	ALA	VAL	cloning artifact	UNP 033833
В	190	ASP	GLU	engineered mutation	UNP 033833
В	108	VAL	ALA	cloning artifact	UNP O33833
В	179	ALA	VAL	cloning artifact	UNP O33833
С	190	ASP	GLU	engineered mutation	UNP 033833
С	108	VAL	ALA	cloning artifact	UNP O33833
С	179	ALA	VAL	cloning artifact	UNP 033833
D	190	ASP	GLU	engineered mutation	UNP 033833
D	108	VAL	ALA	cloning artifact	UNP O33833
D	179	ALA	VAL	cloning artifact	UNP O33833
Е	190	ASP	GLU	engineered mutation	UNP 033833
E	108	VAL	ALA	cloning artifact	UNP O33833
E	179	ALA	VAL	cloning artifact	UNP 033833
F	190	ASP	GLU	engineered mutation	UNP 033833
F	108	VAL	ALA	cloning artifact	UNP 033833



Chain	Residue	Modelled	Actual	Comment	Reference
F	179	ALA	VAL	cloning artifact	UNP 033833

• Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-[alpha-D-galactopyranos e-(1-6)]alpha-D-glucopyranose.



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf	Trace						
9		2	Total	С	0	0	0	0						
	G	5	34	18	16	0	0	0						
9	Ц	3	Total	С	0	0	0	0						
	11	5	34	18	16	0	0	U						
2	т	т	Т	Т	т	T	T	3	Total	С	0	0	0	0
2	I	0	34	18	16	0	0	0						
9	Т	3	Total	С	0	0	0	0						
	J	ა	34	18	16	0	0	U						
9	K	3	Total	С	0	0	0	0						
	IX	5	34	18	16	0	0	0						
2 L	т	3	Total	С	0	0	0	0						
		9	34	18	16	0	U	U						

• Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 13	С 6	O 7	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Ε	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	339	Total O 339 339	0	0
5	В	259	Total O 259 259	0	0
5	С	316	Total O 316 316	0	0
5	D	364	Total O 364 364	0	0
5	Е	296	Total O 296 296	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	314	Total O 314 314	0	0



3 Residue-property plots (i)

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: BETA FRUCTOSIDASE

• Molecule 1: BETA FRUCTOSIDASE



D357 L184 L1 R300 K197 F2 T372 K196 F2 F376 D201 H7 A377 L203 H2 A377 L203 H3 D386 T201 H3 A377 L203 H3 D386 T303 H3 A377 L203 H3 D386 T206 H4 A37 L203 Q33 D386 T206 H4 A37 L203 Q33 Q34 T206 H4 A41 N211 D62 A41 N211 D63 A421 N214 N14 A421 N214 D14 K421 N274 D116 K421 N274 D116 K421 N274 D13 K421 N274 D116 K421 N274 D13 K421 N287 H97 L433 L233 L236 K423 N286 H97 L336 L33 L336 L33 L336 L33 L336 L33 L336</t



• Molecule 2: e	beta-D-fructofu	iranose-(2-1)-[alpha	a-D-galactopyran	nose-(1-6)]alph	a-D-glucopyranos
Chain G:	33%		67%		
GLC1 FRU2 GLA3					
• Molecule 2: e	beta-D-fructofu	aranose-(2-1)-[alpha	a-D-galactopyran	nose-(1-6)]alph	a-D-glucopyranos
Chain H:	33%		67%		
GLC1 FRU2 GLA3					
• Molecule 2: e	beta-D-fructofu	aranose-(2-1)-[alpha	a-D-galactopyran	nose-(1-6)]alph	a-D-glucopyranos
Chain I:	33%		67%		
GLC1 FRU2 GLA3					
• Molecule 2: e	beta-D-fructofu	aranose-(2-1)-[alpha	a-D-galactopyran	nose-(1-6)]alph	a-D-glucopyranos
Chain J:	33%		67%		
GLC1 FRU2 GLA3					
• Molecule 2: e	beta-D-fructofu	uranose-(2-1)-[alpha	a-D-galactopyran	nose-(1-6)]alph	a-D-glucopyranos
Chain K:	33%		67%		
GLC1 FRU2 GLA3					
• Molecule 2: e	beta-D-fructofu	uranose-(2-1)-[alpha	a-D-galactopyran	nose-(1-6)]alph	a-D-glucopyranos
Chain L:	33%		67%		
GLC1 FRU2 GLA3					



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	94.50Å 114.70Å 130.00Å	Depositor
a, b, c, α , β , γ	90.00° 98.90° 90.00°	Depositor
Bosolution(A)	40.00 - 1.87	Depositor
Resolution (A)	32.11 - 1.87	EDS
% Data completeness	97.7 (40.00-1.87)	Depositor
(in resolution range)	97.7 (32.11-1.87)	EDS
R_{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.97 (at 1.87 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
B B.	0.198 , 0.229	Depositor
n, n_{free}	0.213 , 0.241	DCC
R_{free} test set	11055 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	17.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.38 , 52.2	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23234	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, GLC, CIT, SO4, FRU

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).

Mal	Mol Chain		nd lengths	Bond angles		
	Unain	$RMSZ \qquad \# Z > 5$		RMSZ	# Z > 5	
1	А	0.34	1/3607~(0.0%)	0.73	13/4881~(0.3%)	
1	В	0.32	0/3610	0.71	8/4885~(0.2%)	
1	С	0.39	1/3610~(0.0%)	0.70	9/4885~(0.2%)	
1	D	0.32	0/3608	0.70	8/4883~(0.2%)	
1	Е	0.31	0/3609	0.70	4/4883~(0.1%)	
1	F	0.33	0/3609	0.74	14/4884~(0.3%)	
All	All	0.34	2/21653~(0.0%)	0.71	56/29301~(0.2%)	

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	В	0	1
1	С	0	1
1	F	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	80	GLU	C-N	12.95	1.63	1.34
1	А	2	PHE	C-N	-5.36	1.21	1.34

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	F	198	GLY	CA-C-N	8.66	136.25	117.20
1	F	198	GLY	CA-C-O	-8.53	105.24	120.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	F	198	GLY	O-C-N	-7.91	110.04	122.70
1	А	2	PHE	O-C-N	-7.81	110.21	122.70
1	А	1	LEU	CB-CA-C	-5.99	98.82	110.20
1	С	68	ASP	CB-CG-OD2	5.92	123.62	118.30
1	В	115	ASP	CB-CG-OD2	5.76	123.49	118.30
1	В	201	ASP	CB-CG-OD2	5.76	123.48	118.30
1	D	318	ASP	CB-CG-OD2	5.71	123.44	118.30
1	F	199	GLU	N-CA-C	5.71	126.41	111.00
1	D	115	ASP	CB-CG-OD2	5.63	123.37	118.30
1	А	318	ASP	CB-CG-OD2	5.60	123.34	118.30
1	С	115	ASP	CB-CG-OD2	5.60	123.34	118.30
1	F	357	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	183	ASP	CB-CG-OD2	5.58	123.32	118.30
1	Ε	68	ASP	CB-CG-OD2	5.57	123.31	118.30
1	F	183	ASP	CB-CG-OD2	5.54	123.28	118.30
1	Ε	183	ASP	CB-CG-OD2	5.52	123.27	118.30
1	А	115	ASP	CB-CG-OD2	5.51	123.26	118.30
1	Ε	201	ASP	CB-CG-OD2	5.50	123.25	118.30
1	А	169	ASP	CB-CG-OD2	5.49	123.24	118.30
1	А	249	ASP	CB-CG-OD2	5.49	123.24	118.30
1	F	68	ASP	CB-CG-OD2	5.46	123.22	118.30
1	А	82	ASP	CB-CG-OD2	5.46	123.21	118.30
1	А	2	PHE	CA-C-N	5.45	129.20	117.20
1	Ε	138	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	82	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	201	ASP	CB-CG-OD2	5.42	123.17	118.30
1	В	138	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	115	ASP	CB-CG-OD2	5.38	123.14	118.30
1	А	53	ASP	CB-CG-OD2	5.38	123.14	118.30
1	В	318	ASP	CB-CG-OD2	5.37	123.13	118.30
1	С	201	ASP	CB-CG-OD2	5.36	123.12	118.30
1	С	249	ASP	CB-CG-OD2	5.32	123.09	118.30
1	В	68	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	201	ASP	CB-CG-OD2	5.27	123.04	118.30
1	С	157	ASP	CB-CG-OD2	5.26	123.03	118.30
1	D	375	ASP	CB-CG-OD2	5.24	123.02	118.30
1	F	52	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	82	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	68	ASP	CB-CG-OD2	5.20	122.98	118.30
1	F	157	ASP	CB-CG-OD2	5.17	122.96	118.30
1	С	170	ASP	CB-CG-OD2	5.16	122.95	118.30
1	А	157	ASP	CB-CG-OD2	5.14	122.93	118.30



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	В	169	ASP	CB-CG-OD2	5.14	122.93	118.30
1	В	375	ASP	CB-CG-OD2	5.13	122.92	118.30
1	С	352	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	396	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	234	ASP	CB-CG-OD2	5.09	122.88	118.30
1	С	234	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	386	ASP	CB-CG-OD2	5.07	122.87	118.30
1	F	201	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	138	ASP	CB-CG-OD2	5.04	122.84	118.30
1	А	234	ASP	CB-CG-OD2	5.04	122.84	118.30
1	В	183	ASP	CB-CG-OD2	5.02	122.82	118.30
1	С	138	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	388	CYS	Mainchain
1	С	80	GLU	Mainchain
1	F	198	GLY	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3517	0	3398	31	0
1	В	3519	0	3411	33	0
1	С	3519	0	3411	42	0
1	D	3518	0	3404	35	0
1	Е	3518	0	3407	31	0
1	F	3518	0	3406	20	0
2	G	34	0	29	0	0
2	Н	34	0	29	0	0
2	Ι	34	0	29	0	0
2	J	34	0	29	0	0
2	Κ	34	0	29	0	0
2	L	34	0	29	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	13	0	5	5	0
4	В	5	0	0	0	0
4	С	10	0	0	0	0
4	Е	5	0	0	0	0
5	А	339	0	0	16	0
5	В	259	0	0	1	0
5	С	316	0	0	5	0
5	D	364	0	0	4	0
5	Е	296	0	0	4	0
5	F	314	0	0	6	0
All	All	23234	0	20616	191	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 5.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:211:ASN:OD1	5:A:2179:HOH:O	1.56	1.20
1:F:270:ARG:CZ	5:F:2203:HOH:O	1.88	1.18
1:B:267:PRO:HD2	1:B:405:HIS:CD2	1.87	1.08
3:A:1433:CIT:O2	5:A:2332:HOH:O	1.75	1.03
1:C:211:ASN:HD21	1:C:259:SER:HA	1.19	1.02
1:E:211:ASN:ND2	1:E:261:LEU:HG	1.89	0.88
1:C:31:PHE:CZ	1:C:48:HIS:CE1	2.65	0.85
1:F:270:ARG:NE	5:F:2203:HOH:O	2.04	0.83
3:A:1433:CIT:O3	5:A:2331:HOH:O	1.95	0.83
3:A:1433:CIT:C6	5:A:2336:HOH:O	2.27	0.82
3:A:1433:CIT:O5	5:A:2336:HOH:O	1.97	0.81
1:C:211:ASN:HD21	1:C:259:SER:CA	1.93	0.81
1:E:97:HIS:O	1:E:98:ASN:HB2	1.79	0.80
1:C:211:ASN:ND2	1:C:259:SER:HA	1.95	0.80
1:C:31:PHE:CE2	1:C:48:HIS:ND1	2.51	0.79
1:C:211:ASN:ND2	1:C:259:SER:CB	2.47	0.77
1:B:11:ILE:HG23	1:B:59:HIS:CE1	2.20	0.77
1:E:97:HIS:O	1:E:98:ASN:ND2	2.17	0.77
1:E:97:HIS:O	1:E:98:ASN:CB	2.36	0.74
1:C:96:THR:OG1	1:C:99:LYS:HB2	1.87	0.73
1:F:45:CYS:HB2	1:F:64:LEU:O	1.89	0.73
3:A:1433:CIT:O6	5:A:2333:HOH:O	2.06	0.73
1:E:262:ARG:NH2	5:E:2184:HOH:O	2.22	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:267:PRO:CD	1:B:405:HIS:CD2	2.70	0.71
1:F:48:HIS:CE1	1:F:60:LEU:HD23	2.26	0.70
1:A:3:LYS:NZ	5:A:2002:HOH:O	2.04	0.70
1:A:360:ARG:NE	5:A:2281:HOH:O	2.25	0.70
1:D:7:HIS:CE1	1:D:279:LEU:HD13	2.27	0.69
1:E:97:HIS:C	1:E:98:ASN:HD22	1.95	0.69
1:C:211:ASN:CG	5:C:2163:HOH:O	2.31	0.69
1:E:19:ASN:HD21	1:E:33:GLN:HE21	1.39	0.68
1:C:211:ASN:ND2	1:C:259:SER:CA	2.55	0.68
1:B:145:ASN:OD1	1:C:81:LYS:HA	1.94	0.68
1:F:7:HIS:CE1	1:F:279:LEU:HD13	2.29	0.68
1:C:45:CYS:HB2	1:C:64:LEU:O	1.94	0.67
1:D:208:THR:O	1:D:211:ASN:ND2	2.28	0.67
1:E:211:ASN:HD21	1:E:261:LEU:HG	1.58	0.67
1:B:267:PRO:HD2	1:B:405:HIS:HD2	1.60	0.65
1:D:19:ASN:HD21	1:D:33:GLN:HE21	1.45	0.65
1:F:19:ASN:HD21	1:F:33:GLN:HE21	1.45	0.65
1:E:336:LEU:HD11	1:E:413:LEU:HD11	1.77	0.65
1:D:79:VAL:HG11	1:D:148:TRP:CZ3	2.31	0.64
1:A:19:ASN:HD21	1:A:33:GLN:HE21	1.46	0.63
1:D:1:LEU:N	1:D:1:LEU:HD12	2.15	0.62
1:C:211:ASN:ND2	1:C:259:SER:OG	2.32	0.61
1:D:96:THR:OG1	1:D:99:LYS:HB2	2.01	0.60
1:A:360:ARG:CD	5:A:2281:HOH:O	2.48	0.60
1:A:360:ARG:CG	5:A:2280:HOH:O	2.50	0.60
1:F:1:LEU:CD1	1:F:2:PHE:CD1	2.86	0.59
1:C:211:ASN:ND2	5:C:2163:HOH:O	2.35	0.58
1:C:351:ARG:NH2	5:C:2258:HOH:O	2.36	0.58
1:E:335:GLU:OE1	1:E:337:ARG:NE	2.37	0.58
1:B:19:ASN:HD21	1:B:33:GLN:HE21	1.52	0.58
1:D:1:LEU:HD12	1:D:1:LEU:H3	1.67	0.58
1:E:211:ASN:HD21	1:E:261:LEU:H	1.52	0.57
1:C:211:ASN:HD22	1:C:259:SER:CB	2.13	0.57
1:E:302:ARG:HD3	1:E:325:GLU:OE1	2.04	0.57
1:C:411:ASN:HD22	1:C:411:ASN:H	1.53	0.57
1:E:19:ASN:ND2	1:E:33:GLN:HE21	2.02	0.57
1:B:31:PHE:CE2	1:B:48:HIS:CE1	2.92	0.57
1:B:31:PHE:CZ	1:B:48:HIS:CE1	2.93	0.56
1:D:302:ARG:HD3	1:D:325:GLU:OE1	2.06	0.56
1:B:7:HIS:HD2	1:B:386:ASP:OD2	1.88	0.56
1:A:336:LEU:HD11	1:A:413:LEU:HD11	1.88	0.56



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:29:HIS:HD2	1:D:48:HIS:NE2	2.04	0.56
1:E:1:LEU:HD23	5:E:2002:HOH:O	2.06	0.55
1:E:29:HIS:HD2	1:E:48:HIS:NE2	2.04	0.55
1:C:31:PHE:CZ	1:C:48:HIS:HE1	2.20	0.55
1:D:235:HIS:HD2	5:D:2308:HOH:O	1.90	0.55
1:D:19:ASN:ND2	1:D:33:GLN:HE21	2.05	0.55
1:F:411:ASN:H	1:F:411:ASN:HD22	1.54	0.55
1:C:31:PHE:CE2	1:C:48:HIS:CE1	2.94	0.54
1:C:134:HIS:CD2	1:C:135:ALA:H	2.25	0.54
1:B:11:ILE:HG23	1:B:59:HIS:ND1	2.22	0.54
1:C:19:ASN:HD21	1:C:33:GLN:HE21	1.53	0.54
1:C:29:HIS:HD2	1:C:48:HIS:NE2	2.06	0.54
1:A:360:ARG:HD3	5:A:2281:HOH:O	2.05	0.54
1:F:232:LEU:HB2	1:F:235:HIS:CE1	2.42	0.54
1:B:29:HIS:HD2	1:B:48:HIS:NE2	2.06	0.54
1:D:388:CYS:HB2	1:D:405:HIS:CE1	2.43	0.54
1:A:302:ARG:HD3	1:A:325:GLU:OE1	2.08	0.54
1:D:149:ARG:HD2	5:D:2130:HOH:O	2.08	0.54
1:A:360:ARG:HG2	5:A:2280:HOH:O	2.07	0.53
1:F:1:LEU:HD12	1:F:2:PHE:N	2.24	0.53
1:B:7:HIS:HE1	1:B:391:GLU:OE1	1.92	0.53
1:D:97:HIS:O	1:D:98:ASN:CG	2.46	0.53
1:A:208:THR:HG22	5:A:2165:HOH:O	2.08	0.53
1:F:7:HIS:ND1	1:F:279:LEU:HD13	2.25	0.52
1:F:19:ASN:ND2	1:F:33:GLN:HE21	2.07	0.52
1:A:304:ARG:NE	5:A:2319:HOH:O	2.42	0.52
1:B:411:ASN:H	1:B:411:ASN:HD22	1.57	0.52
1:B:145:ASN:HA	1:C:80:GLU:O	2.10	0.51
1:A:351:ARG:NH2	1:C:220:LEU:O	2.42	0.51
1:B:336:LEU:HD11	1:B:413:LEU:HD11	1.92	0.51
1:E:411:ASN:H	1:E:411:ASN:HD22	1.58	0.51
1:B:81:LYS:NZ	1:B:86:PHE:CZ	2.80	0.50
1:D:7:HIS:HD2	1:D:386:ASP:OD2	1.93	0.50
1:E:211:ASN:ND2	1:E:261:LEU:H	2.10	0.50
1:F:270:ARG:NH2	5:F:2203:HOH:O	2.21	0.50
1:A:403:ARG:HH21	1:A:405:HIS:HE1	1.58	0.50
1:F:1:LEU:HD22	5:F:2287:HOH:O	2.11	0.50
1:C:81:LYS:HB3	1:C:86:PHE:CE1	2.46	0.49
1:C:134:HIS:CD2	1:C:135:ALA:N	2.80	0.49
1:A:19:ASN:ND2	1:A:33:GLN:HE21	2.08	0.49
1:B:302:ARG:HD2	1:B:425:PHE:CG	2.47	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:D:336:LEU:HD11	1:D:413:LEU:HD11	1.94	0.49
1:B:11:ILE:CG2	1:B:59:HIS:CE1	2.95	0.49
1:F:29:HIS:HD2	1:F:48:HIS:NE2	2.11	0.49
1:C:19:ASN:ND2	1:C:33:GLN:HE21	2.12	0.48
1:C:336:LEU:HD11	1:C:413:LEU:HD11	1.94	0.48
1:A:375:ASP:OD2	1:C:200:LYS:NZ	2.46	0.48
1:E:1:LEU:HB3	5:E:2002:HOH:O	2.13	0.48
1:D:337:ARG:O	1:D:413:LEU:HD12	2.14	0.48
1:E:206:SER:HB3	1:E:240:TYR:CE1	2.49	0.48
1:B:29:HIS:HE1	5:B:2015:HOH:O	1.97	0.48
1:B:108:VAL:HG11	1:B:116:PHE:HB3	1.96	0.48
1:D:97:HIS:O	1:D:98:ASN:ND2	2.47	0.48
1:E:108:VAL:HG11	1:E:116:PHE:HB3	1.94	0.48
1:B:19:ASN:ND2	1:B:33:GLN:HE21	2.11	0.48
1:B:124:VAL:HG22	1:B:172:PHE:O	2.13	0.48
1:D:108:VAL:HG11	1:D:116:PHE:HB3	1.96	0.48
1:C:101:GLU:CD	1:C:134:HIS:CE1	2.87	0.47
1:E:211:ASN:ND2	1:E:261:LEU:CG	2.70	0.47
1:A:426:GLU:CD	5:A:2319:HOH:O	2.53	0.47
1:C:7:HIS:NE2	1:C:279:LEU:HD13	2.29	0.47
1:D:7:HIS:CD2	1:D:386:ASP:OD2	2.68	0.47
1:D:53:ASP:OD2	1:D:56:HIS:HD2	1.98	0.47
1:C:29:HIS:HE1	5:C:2020:HOH:O	1.98	0.47
1:F:1:LEU:HD13	1:F:2:PHE:CD1	2.49	0.47
1:E:108:VAL:CG1	1:E:116:PHE:HB3	2.45	0.47
1:A:421:LYS:NZ	1:E:318:ASP:HB3	2.29	0.47
1:A:421:LYS:HG2	1:E:306:VAL:HA	1.97	0.46
1:B:53:ASP:OD2	1:B:56:HIS:HD2	1.98	0.46
1:C:351:ARG:CZ	5:C:2258:HOH:O	2.62	0.46
1:E:19:ASN:HD21	1:E:33:GLN:NE2	2.11	0.46
1:D:411:ASN:HD22	1:D:411:ASN:H	1.63	0.46
1:B:388:CYS:O	1:B:389:SER:HB3	2.15	0.46
1:C:238:ASP:O	1:C:257:LEU:HD23	2.16	0.46
1:D:96:THR:HB	1:D:97:HIS:H	1.58	0.46
1:C:354:LEU:HB2	1:C:373:VAL:HG21	1.98	0.46
1:D:7:HIS:ND1	1:D:279:LEU:HD13	2.31	0.46
1:F:270:ARG:NH2	5:F:2204:HOH:O	2.49	0.46
1:B:302:ARG:HD3	1:B:325:GLU:OE1	2.16	0.45
1:F:1:LEU:HD12	1:F:2:PHE:H	1.81	0.45
1:B:267:PRO:HD2	1:B:405:HIS:NE2	2.25	0.45
1:A:29:HIS:HD2	1:A:48:HIS:NE2	2.15	0.45



	Interstomic Clash				
Atom-1	Atom-2	distance $(Å)$	overlan (Å)		
1.C.211.ASN.OD1	1.C.240.TYB.HB2	2.16	0.45		
1.A.388.CVS.HB2	1:A:405:HIS:CE1	2.52	0.45		
1.D.1.LEU.HD13	1.D.271.GLU.OE1	2.02	0.15		
1.D.108.VAL:CG1	1.D.116.PHE.HB3	2.10	0.15		
1.C.48.HIS.CD2	$1 \cdot C \cdot 49 \cdot ALA \cdot N$	2.10	0.19		
1.0.40.III.0.02	1.0.49.11LH.10	2.00	0.44		
1.Λ.300. VAL.HO12 1.Δ.45.CVS·HB3	1.A.64.LEU.O	2.00	0.44		
1:C:48:HIS:CD2	1.R.04.EE0.0	2.10	0.44		
1.E.124.VAL.:HG22	1.C.00.LLC.IID12	2.00	0.44		
1.E.124. VILLII022	1.E.112.1 IIE.O	2.10	0.44		
1:D:1/0:ABC:CC	1.D.415.LEU.HD11	2.41	0.43		
1.4.306.VAL.HC21	1.D.100.LE0.IID11 $1.A.310.VAI.HC13$	2.40	0.43		
1.A.300.VAL.IIG21	1.A.319.VAL.IIG13	2.00	0.43		
1.A.350. VAL.IIG11	1.A.402.1 IIE.OE2	2.54	0.43		
1.D.100.VAL.UG1	1.D.110.1 IIE.IID3	2.40	0.43		
$1:D:207:LEU:\Pi D20$	1:D:403:ARG:IIG2	1.99	0.45		
1:D:1:LEU:U	1:D:387:5ER:HB3	2.18	0.43		
1:D:300:ARG:HG2	5:D:2295:HUH:U	2.18	0.43		
1:D:226:ASN:HD22	1:D:220:ASN:N	2.17	0.43		
1:D:250:TRP:CE2	1:D:258:GLN:HB3	2.53	0.43		
1:A:124:VAL:HG22	1:A:172:PHE:O	2.18	0.42		
1:C:7:HIS:CD2	1:C:279:LEU:HD13	2.54	0.42		
1:F:206:SER:HB3	1:F:240:TYR:CE1	2.53	0.42		
1:B:170:ASP:OD2	1:B:173:HIS:HD2	2.01	0.42		
1:C:373:VAL:HG11	1:C:394:PHE:CD2	2.55	0.42		
1:E:256:TRP:CE2	1:E:258:GLN:HB3	2.54	0.42		
1:C:101:GLU:OE2	1:C:134:HIS:CE1	2.72	0.42		
1:E:29:HIS:CD2	1:E:48:HIS:NE2	2.87	0.42		
1:A:360:ARG:HG3	5:A:2280:HOH:O	2.15	0.42		
1:A:411:ASN:H	1:A:411:ASN:HD22	1.66	0.42		
1:A:124:VAL:CG2	1:A:172:PHE:HA	2.49	0.42		
1:C:350:SER:O	1:C:351:ARG:C	2.58	0.42		
1:B:206:SER:HB3	1:B:240:TYR:CE1	2.55	0.42		
1:D:206:SER:HB3	1:D:240:TYR:CE1	2.55	0.41		
1:B:19:ASN:HD21	1:B:33:GLN:NE2	2.16	0.41		
1:B:11:ILE:CG2	1:B:59:HIS:ND1	2.83	0.41		
1:B:417:SER:HB3	1:B:420:VAL:CG1	2.50	0.41		
1:E:97:HIS:C	1:E:98:ASN:ND2	2.67	0.41		
1:E:145:ASN:ND2	5:E:2128:HOH:O	2.48	0.41		
1:A:364:SER:OG	1:A:405:HIS:HD2	2.04	0.41		
1:C:89:TYR:HE1	1:C:108:VAL:HG22	1.85	0.41		
1:D:29:HIS:HE1	5:D:2018:HOH:O	2.04	0.41		



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:LYS:NZ	5:F:2244:HOH:O	2.37	0.40
1:D:403:ARG:HH21	1:D:405:HIS:HE1	1.68	0.40
1:A:256:TRP:CE2	1:A:258:GLN:HB3	2.56	0.40
1:D:71:HIS:ND1	1:D:93:ARG:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	430/432~(100%)	411 (96%)	18 (4%)	1 (0%)	47	37
1	В	430/432~(100%)	412 (96%)	17 (4%)	1 (0%)	47	37
1	С	430/432~(100%)	414 (96%)	15 (4%)	1 (0%)	47	37
1	D	430/432~(100%)	414 (96%)	15 (4%)	1 (0%)	47	37
1	Е	430/432~(100%)	414 (96%)	15 (4%)	1 (0%)	47	37
1	F	430/432~(100%)	412 (96%)	16 (4%)	2 (0%)	29	17
All	All	2580/2592~(100%)	2477 (96%)	96 (4%)	7 (0%)	41	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	351	ARG
1	F	199	GLU
1	D	98	ASN
1	Е	98	ASN
1	В	389	SER
1	А	198	GLY
1	F	198	GLY



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	385/387~(100%)	363~(94%)	22~(6%)	20 9
1	В	387/387~(100%)	352~(91%)	35~(9%)	9 3
1	С	387/387~(100%)	359~(93%)	28~(7%)	14 5
1	D	386/387~(100%)	358~(93%)	28 (7%)	14 5
1	Ε	387/387~(100%)	362~(94%)	25~(6%)	17 7
1	F	386/387~(100%)	355~(92%)	31 (8%)	12 4
All	All	2318/2322~(100%)	2149~(93%)	169 (7%)	14 5

All (169) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	60	LEU
1	А	114	LEU
1	А	124	VAL
1	А	127	LYS
1	А	147	GLU
1	А	203	LEU
1	А	226	ASN
1	А	233	LEU
1	А	274	ASN
1	А	279	LEU
1	А	283	LEU
1	А	290	LEU
1	А	298	LEU
1	А	306	VAL
1	А	321	GLU
1	А	349	LYS
1	А	354	LEU
1	A	373	VAL
1	А	375	ASP
1	А	378	THR
1	А	411	ASN
1	А	421	LYS



Mol	Chain	Res	Type
1	В	1	LEU
1	В	38	LYS
1	В	60	LEU
1	В	96	THR
1	В	97	HIS
1	В	114	LEU
1	В	124	VAL
1	В	134	HIS
1	В	159	LYS
1	В	162	ARG
1	В	199	GLU
1	В	211	ASN
1	В	220	LEU
1	В	233	LEU
1	В	257	LEU
1	В	269	LYS
1	В	274	ASN
1	В	279	LEU
1	В	283	LEU
1	В	290	LEU
1	В	298	LEU
1	В	303	LYS
1	В	304	ARG
1	В	316	LEU
1	В	320	LYS
1	В	349	LYS
1	В	352	ASP
1	В	354	LEU
1	В	370	LYS
1	В	373	VAL
1	В	375	ASP
1	В	376	GLU
1	В	397	SER
1	В	411	ASN
1	В	421	LYS
1	C	1	LEU
1	С	108	VAL
1	С	114	LEU
1	С	131	GLU
1	С	145	ASN
1	C	199	GLU
1	С	200	LYS



Mol	Chain	Res	Type
1	С	203	LEU
1	С	226	ASN
1	С	233	LEU
1	С	257	LEU
1	С	274	ASN
1	С	279	LEU
1	С	283	LEU
1	С	290	LEU
1	С	298	LEU
1	С	303	LYS
1	С	304	ARG
1	С	320	LYS
1	С	331	SER
1	С	349	LYS
1	С	354	LEU
1	С	373	VAL
1	С	376	GLU
1	С	411	ASN
1	С	419	GLN
1	С	420	VAL
1	С	421	LYS
1	D	1	LEU
1	D	79	VAL
1	D	96	THR
1	D	114	LEU
1	D	131	GLU
1	D	133	THR
1	D	200	LYS
1	D	208	THR
1	D	220	LEU
1	D	226	ASN
1	D	233	LEU
1	D	257	LEU
1	D	259	SER
1	D	274	ASN
1	D	279	LEU
1	D	283	LEU
1	D	290	LEU
1	D	298	LEU
1	D	321	GLU
1	D	352	ASP
1	D	354	LEU



Mol	Chain	Res	Type
1	D	355	ILE
1	D	373	VAL
1	D	376	GLU
1	D	378	THR
1	D	411	ASN
1	D	421	LYS
1	D	423	GLU
1	Е	60	LEU
1	Е	96	THR
1	Е	97	HIS
1	Е	114	LEU
1	Е	124	VAL
1	Е	127	LYS
1	Е	133	THR
1	Е	159	LYS
1	Е	199	GLU
1	Е	200	LYS
1	Е	203	LEU
1	Е	220	LEU
1	Е	274	ASN
1	Е	290	LEU
1	Е	298	LEU
1	Е	304	ARG
1	Е	320	LYS
1	Е	349	LYS
1	Е	354	LEU
1	Е	355	ILE
1	Ε	373	VAL
1	Ε	378	THR
1	E	411	ASN
1	E	420	VAL
1	E	421	LYS
1	F	1	LEU
1	F	60	LEU
1	F	96	THR
1	F	108	VAL
1	F	109	MET
1	F	114	LEU
1	F	127	LYS
1	F	142	ASN
1	F	169	ASP
1	F	199	GLU



Mol	Chain	Res	Type
1	F	203	LEU
1	F	208	THR
1	F	211	ASN
1	F	220	LEU
1	F	226	ASN
1	F	229	LYS
1	F	257	LEU
1	F	259	SER
1	F	274	ASN
1	F	279	LEU
1	F	283	LEU
1	F	290	LEU
1	F	298	LEU
1	F	321	GLU
1	F	336	LEU
1	F	354	LEU
1	F	372	THR
1	F	376	GLU
1	F	378	THR
1	F	411	ASN
1	F	414	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	19	ASN
1	А	29	HIS
1	А	98	ASN
1	А	211	ASN
1	А	235	HIS
1	А	243	GLN
1	А	274	ASN
1	А	405	HIS
1	А	411	ASN
1	В	7	HIS
1	В	19	ASN
1	В	29	HIS
1	В	56	HIS
1	В	59	HIS
1	В	211	ASN
1	В	235	HIS
1	В	243	GLN



1 B 274 ASN 1 B 411 ASN 1 C 19 ASN 1 C 29 HIS 1 C 56 HIS 1 C 211 ASN 1 C 235 HIS 1 C 243 GLN 1 C 243 GLN 1 C 243 GLN 1 C 411 ASN 1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 29 HIS 1 D 26 ASN 1 D 285 HIS 1 D 243 GLN 1 D 243 GLN 1 D 405 HIS 1 E 29	Mol	Chain	Res	Type
1 B 411 ASN 1 C 19 ASN 1 C 29 HIS 1 C 56 HIS 1 C 134 HIS 1 C 211 ASN 1 C 235 HIS 1 C 243 GLN 1 C 243 GLN 1 C 411 ASN 1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 59 HIS 1 D 266 ASN 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 411 ASN 1 E 19 ASN 1 E 19	1	В	274	ASN
1 C 19 ASN 1 C 29 HIS 1 C 56 HIS 1 C 134 HIS 1 C 211 ASN 1 C 235 HIS 1 C 243 GLN 1 C 243 GLN 1 C 243 GLN 1 C 411 ASN 1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 29 HIS 1 D 26 ASN 1 D 235 HIS 1 D 243 GLN 1 D 243 GLN 1 D 405 HIS 1 D 411 ASN 1 E 29	1	В	411	ASN
1 C 29 HIS 1 C 56 HIS 1 C 134 HIS 1 C 211 ASN 1 C 235 HIS 1 C 243 GLN 1 C 243 GLN 1 C 244 ASN 1 C 244 ASN 1 C 411 ASN 1 D 7 HIS 1 D 29 HIS 1 D 29 HIS 1 D 29 HIS 1 D 26 ASN 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 405 HIS 1 E 29 HIS 1 E 29	1	С	19	ASN
1 C 56 HIS 1 C 134 HIS 1 C 211 ASN 1 C 235 HIS 1 C 243 GLN 1 C 243 GLN 1 C 243 GLN 1 C 411 ASN 1 D 7 HIS 1 D 29 HIS 1 D 56 HIS 1 D 59 HIS 1 D 226 ASN 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 405 HIS 1 D 411 ASN 1 E 29 HIS 1 E 59 HIS 1 E 211	1	С	29	HIS
1 C 134 HIS 1 C 211 ASN 1 C 235 HIS 1 C 243 GLN 1 C 243 GLN 1 C 243 GLN 1 C 411 ASN 1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 56 HIS 1 D 59 HIS 1 D 226 ASN 1 D 235 HIS 1 D 243 GLN 1 D 243 GLN 1 D 405 HIS 1 D 411 ASN 1 E 19 ASN 1 E 59 HIS 1 E 211	1	С	56	HIS
1 C 211 ASN 1 C 235 HIS 1 C 243 GLN 1 C 274 ASN 1 C 411 ASN 1 D 7 HIS 1 D 7 HIS 1 D 29 HIS 1 D 56 HIS 1 D 59 HIS 1 D 226 ASN 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 243 GLN 1 D 405 HIS 1 D 411 ASN 1 E 19 ASN 1 E 19 HIS 1 E 59 HIS 1 E 235	1	С	134	HIS
1 C 235 HIS 1 C 243 GLN 1 C 274 ASN 1 C 411 ASN 1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 56 HIS 1 D 59 HIS 1 D 226 ASN 1 D 235 HIS 1 D 243 GLN 1 D 243 GLN 1 D 243 GLN 1 D 411 ASN 1 D 411 ASN 1 E 19 ASN 1 E 29 HIS 1 E 56 HIS 1 E 211 ASN 1 E 235	1	С	211	ASN
1 C 243 GLN 1 C 274 ASN 1 C 411 ASN 1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 56 HIS 1 D 59 HIS 1 D 226 ASN 1 D 235 HIS 1 D 243 GLN 1 D 243 GLN 1 D 243 GLN 1 D 274 ASN 1 D 405 HIS 1 D 411 ASN 1 E 19 ASN 1 E 19 HIS 1 E 56 HIS 1 E 211 ASN 1 E 235 <th>1</th> <th>С</th> <th>235</th> <th>HIS</th>	1	С	235	HIS
1 C 274 ASN 1 C 411 ASN 1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 56 HIS 1 D 56 HIS 1 D 98 ASN 1 D 226 ASN 1 D 235 HIS 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 405 HIS 1 D 411 ASN 1 E 19 ASN 1 E 19 HIS 1 E 59 HIS 1 E 211 ASN 1 E 235 HIS 1 E 243	1	С	243	GLN
1 C 411 ASN 1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 56 HIS 1 D 56 HIS 1 D 98 ASN 1 D 226 ASN 1 D 235 HIS 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 405 HIS 1 D 411 ASN 1 D 405 HIS 1 E 19 ASN 1 E 29 HIS 1 E 56 HIS 1 E 98 ASN 1 E 235 HIS 1 E 211 ASN 1 E 235 HIS 1 E	1	С	274	ASN
1 D 7 HIS 1 D 19 ASN 1 D 29 HIS 1 D 56 HIS 1 D 59 HIS 1 D 98 ASN 1 D 226 ASN 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 274 ASN 1 D 405 HIS 1 D 405 HIS 1 D 411 ASN 1 E 19 ASN 1 E 19 HIS 1 E 59 HIS 1 E 59 HIS 1 E 235 HIS 1 E 235 HIS 1 E 274 ASN 1 E 405 HIS 1 F	1	С	411	ASN
1 D 19 ASN 1 D 29 HIS 1 D 56 HIS 1 D 59 HIS 1 D 98 ASN 1 D 226 ASN 1 D 235 HIS 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 405 HIS 1 D 405 HIS 1 D 405 HIS 1 E 19 ASN 1 E 19 HIS 1 E 19 HIS 1 E 10 HIS 1 E 59 HIS 1 E 235 HIS 1 E 243 GLN 1 E 274 ASN 1 E 405 HIS 1 F <th>1</th> <th>D</th> <th>7</th> <th>HIS</th>	1	D	7	HIS
1 D 29 HIS 1 D 56 HIS 1 D 59 HIS 1 D 98 ASN 1 D 226 ASN 1 D 235 HIS 1 D 235 HIS 1 D 243 GLN 1 D 243 GLN 1 D 274 ASN 1 D 405 HIS 1 D 405 HIS 1 D 405 HIS 1 E 19 ASN 1 E 29 HIS 1 E 56 HIS 1 E 59 HIS 1 E 235 HIS 1 E 235 HIS 1 E 243 GLN 1 E 405 HIS 1 F 29 HIS 1 F <th>1</th> <th>D</th> <th>19</th> <th>ASN</th>	1	D	19	ASN
1 D 56 HIS 1 D 59 HIS 1 D 98 ASN 1 D 226 ASN 1 D 235 HIS 1 D 235 HIS 1 D 243 GLN 1 D 274 ASN 1 D 405 HIS 1 D 405 HIS 1 D 405 HIS 1 E 19 ASN 1 E 29 HIS 1 E 56 HIS 1 E 59 HIS 1 E 98 ASN 1 E 211 ASN 1 E 235 HIS 1 E 243 GLN 1 E 405 HIS 1 E 405 HIS 1 F 29 HIS 1 F <th>1</th> <th>D</th> <th>29</th> <th>HIS</th>	1	D	29	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	56	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	59	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	98	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	226	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	235	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	243	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	274	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	405	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	411	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	19	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	29	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	56	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	59	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	98	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	211	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	235	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	243	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	274	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	405	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	E	411	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	F	19	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	F	29	HIS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	F	56	HIS
1 F 235 HIS 1 F 243 GLN 1 F 274 ASN	1	F	59	HIS
$\begin{array}{c cccc} 1 & F & 243 & \text{GLN} \\ \hline 1 & F & 274 & \text{ASN} \end{array}$	1	F	235	HIS
1 F 274 ASN	1	F	243	GLN
	1	F	274	ASN
1 F 405 HIS	1	F	405	HIS



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type
1	F	411	ASN

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)

18 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).

Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	ths	B	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	G	1	2	11,11,12	0.82	0	15,15,17	1.56	2 (13%)
2	FRU	G	2	2	11,12,12	2.00	1 (9%)	10,18,18	0.70	0
2	GLA	G	3	2	11,11,12	0.63	0	15,15,17	0.59	0
2	GLC	Н	1	2	11,11,12	0.67	0	15,15,17	0.86	0
2	FRU	Н	2	2	11,12,12	2.02	1 (9%)	10,18,18	0.47	0
2	GLA	Н	3	2	11,11,12	0.55	0	15,15,17	0.74	1 (6%)
2	GLC	Ι	1	2	11,11,12	0.63	0	15,15,17	0.87	1 (6%)
2	FRU	Ι	2	2	11,12,12	2.04	1 (9%)	10,18,18	0.61	0
2	GLA	Ι	3	2	11,11,12	0.58	0	15,15,17	0.62	0
2	GLC	J	1	2	11,11,12	0.99	1 (9%)	15,15,17	2.13	3 (20%)
2	FRU	J	2	2	11,12,12	1.95	1 (9%)	10,18,18	0.56	0
2	GLA	J	3	2	11,11,12	0.61	0	15,15,17	0.55	0
2	GLC	K	1	2	11,11,12	0.83	0	15,15,17	1.30	2 (13%)
2	FRU	K	2	2	11,12,12	2.01	1 (9%)	10,18,18	0.66	0
2	GLA	K	3	2	11,11,12	0.55	0	15,15,17	0.54	0



Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	L	1	2	11,11,12	0.68	0	15,15,17	1.49	2 (13%)
2	FRU	L	2	2	11,12,12	2.02	1 (9%)	10,18,18	0.46	0
2	GLA	L	3	2	11,11,12	0.56	0	15,15,17	0.68	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
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	FRU	G	2	2	-	3/5/24/24	0/1/1/1
2	GLA	G	3	2	-	2/2/19/22	0/1/1/1
2	GLC	Н	1	2	-	0/2/19/22	0/1/1/1
2	FRU	Н	2	2	-	3/5/24/24	0/1/1/1
2	GLA	Н	3	2	-	2/2/19/22	0/1/1/1
2	GLC	Ι	1	2	-	0/2/19/22	0/1/1/1
2	FRU	Ι	2	2	-	3/5/24/24	0/1/1/1
2	GLA	Ι	3	2	-	1/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/19/22	0/1/1/1
2	FRU	J	2	2	-	3/5/24/24	0/1/1/1
2	GLA	J	3	2	-	2/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/19/22	0/1/1/1
2	FRU	K	2	2	-	3/5/24/24	0/1/1/1
2	GLA	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/19/22	0/1/1/1
2	FRU	L	2	2	-	3/5/24/24	0/1/1/1
2	GLA	L	3	2	-	1/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Κ	2	FRU	O6-C6	-6.52	1.14	1.42
2	Ι	2	FRU	O6-C6	-6.49	1.15	1.42
2	Н	2	FRU	O6-C6	-6.42	1.15	1.42
2	G	2	FRU	O6-C6	-6.40	1.15	1.42
2	L	2	FRU	O6-C6	-6.37	1.15	1.42
2	J	2	FRU	O6-C6	-6.24	1.16	1.42
2	J	1	GLC	C4-C5	2.04	1.57	1.53



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	J	1	GLC	C1-O5-C5	-4.70	105.82	112.19
2	L	1	GLC	O5-C1-C2	-4.53	103.77	110.77
2	J	1	GLC	C1-C2-C3	-4.11	104.62	109.67
2	J	1	GLC	O5-C1-C2	4.10	117.11	110.77
2	G	1	GLC	C1-O5-C5	-3.71	107.17	112.19
2	G	1	GLC	C1-C2-C3	-3.26	105.66	109.67
2	Κ	1	GLC	C1-O5-C5	-2.79	108.41	112.19
2	Κ	1	GLC	C1-C2-C3	-2.72	106.33	109.67
2	Ι	1	GLC	C1-O5-C5	2.53	115.62	112.19
2	Н	3	GLA	O5-C5-C6	2.43	111.01	107.20
2	L	1	GLC	C1-O5-C5	2.18	115.14	112.19

All (11) bond angle outliers are listed below:

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	FRU	O1-C1-C2-O2
2	Н	2	FRU	O1-C1-C2-O2
2	Ι	2	FRU	O1-C1-C2-O2
2	J	2	FRU	O1-C1-C2-O2
2	Κ	2	FRU	O1-C1-C2-O2
2	L	2	FRU	O1-C1-C2-C3
2	L	2	FRU	O1-C1-C2-O2
2	G	3	GLA	O5-C5-C6-O6
2	J	3	GLA	O5-C5-C6-O6
2	L	2	FRU	O1-C1-C2-O5
2	Н	3	GLA	O5-C5-C6-O6
2	Н	2	FRU	O1-C1-C2-C3
2	Ι	2	FRU	O1-C1-C2-C3
2	Н	2	FRU	O1-C1-C2-O5
2	Ι	2	FRU	O1-C1-C2-O5
2	J	2	FRU	O1-C1-C2-O5
2	Κ	2	FRU	O1-C1-C2-O5
2	L	3	GLA	O5-C5-C6-O6
2	G	2	FRU	O1-C1-C2-O5
2	G	2	FRU	O1-C1-C2-C3
2	J	2	FRU	O1-C1-C2-C3
2	К	2	FRU	O1-C1-C2-C3
2	Ι	3	GLA	C4-C5-C6-O6
2	G	3	GLA	C4-C5-C6-O6
2	Н	3	GLA	C4-C5-C6-O6



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Mol	Chain	Res	Type	Atoms
2	J	3	GLA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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)

5 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 Tuno Chain I		Dog	Pog Link	Bond lengths			Bond angles			
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	В	1433	-	4,4,4	0.16	0	6,6,6	0.17	0
4	SO4	Е	1433	-	4,4,4	0.55	0	$6,\!6,\!6$	0.88	0



Mal	Mol Type Chain Rea		Tink	Bo	Bond lengths			Bond angles		
INIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CIT	А	1433	-	12,12,12	1.04	0	17,17,17	1.76	4 (23%)
4	SO4	С	1434	-	4,4,4	0.14	0	6,6,6	0.12	0
4	SO4	С	1433	-	4,4,4	0.23	0	$6,\!6,\!6$	0.35	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	CIT	А	1433	-	-	4/16/16/16	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	1433	CIT	O6-C6-C3	3.63	119.35	113.05
3	А	1433	CIT	C4-C3-C2	3.18	117.45	109.16
3	А	1433	CIT	C2-C3-C6	-2.73	104.23	110.11
3	А	1433	CIT	C4-C3-C6	-2.14	105.50	110.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	1433	CIT	C1-C2-C3-O7
3	А	1433	CIT	C1-C2-C3-C6
3	А	1433	CIT	C1-C2-C3-C4
3	А	1433	CIT	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1433	CIT	5	0

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	С	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	С	80:GLU	С	81:LYS	N	1.63



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	А	432/432~(100%)	0.32	22 (5%) 28 29	7, 16, 28, 33	4 (0%)
1	В	432/432~(100%)	0.63	48 (11%) 5 5	8, 17, 28, 34	6 (1%)
1	С	432/432~(100%)	0.50	40 (9%) 8 9	7, 17, 28, 34	8 (1%)
1	D	432/432~(100%)	0.52	34 (7%) 12 13	8, 16, 28, 34	8 (1%)
1	Ε	432/432~(100%)	0.50	44 (10%) 6 7	8, 16, 28, 34	9 (2%)
1	F	432/432~(100%)	0.51	35 (8%) 12 13	7, 16, 28, 34	10 (2%)
All	All	2592/2592~(100%)	0.50	223 (8%) 10 11	7, 16, 28, 34	45 (1%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	98	ASN	11.9
1	D	98	ASN	10.9
1	Е	97	HIS	10.5
1	В	97	HIS	10.3
1	С	97	HIS	10.2
1	Е	96	THR	9.3
1	В	98	ASN	9.2
1	F	97	HIS	8.6
1	Е	99	LYS	8.2
1	D	97	HIS	8.1
1	F	96	THR	7.7
1	В	99	LYS	7.5
1	F	98	ASN	6.3
1	В	96	THR	5.9
1	С	132	GLY	5.7
1	В	134	HIS	5.6
1	Е	131	GLU	5.6
1	Е	198	GLY	5.6
1	В	351	ARG	5.5



Mol	Chain	Res	Type	RSRZ
1	D	96	THR	5.4
1	D	134	HIS	5.4
1	Е	134	HIS	5.3
1	С	134	HIS	5.2
1	В	287	ASN	5.2
1	С	131	GLU	5.2
1	А	418	ASN	5.1
1	F	287	ASN	5.1
1	Е	95	PRO	5.0
1	D	418	ASN	5.0
1	F	134	HIS	5.0
1	С	351	ARG	4.9
1	С	270	ARG	4.8
1	В	352	ASP	4.7
1	D	199	GLU	4.7
1	В	131	GLU	4.6
1	Е	100	GLY	4.5
1	В	350	SER	4.5
1	В	288	ASN	4.4
1	Е	158	GLU	4.3
1	Е	159	LYS	4.3
1	F	1	LEU	4.3
1	Е	377	ALA	4.3
1	А	159	LYS	4.2
1	В	418	ASN	4.2
1	В	372	THR	4.2
1	В	230	ARG	4.0
1	Е	157	ASP	4.0
1	В	1	LEU	3.9
1	F	159	LYS	3.9
1	С	99	LYS	3.9
1	В	332	GLY	3.8
1	А	419	GLN	3.8
1	Е	351	ARG	3.8
1	С	377	ALA	3.7
1	F	288	ASN	3.7
1	Е	101	GLU	3.7
1	Е	352	ASP	3.7
1	F	352	ASP	3.7
1	F	158	GLU	3.7
1	С	352	ASP	3.7
1	D	287	ASN	3.6



Mol	Chain	Res	Type	RSRZ
1	С	159	LYS	3.6
1	D	352	ASP	3.5
1	С	155	GLY	3.4
1	Е	155	GLY	3.4
1	В	132	GLY	3.4
1	D	419	GLN	3.4
1	F	208	THR	3.4
1	Е	156	LYS	3.4
1	D	131	GLU	3.4
1	F	131	GLU	3.4
1	F	351	ARG	3.3
1	Е	1	LEU	3.3
1	F	184	GLU	3.3
1	F	289	GLU	3.3
1	F	99	LYS	3.2
1	F	157	ASP	3.2
1	В	159	LYS	3.2
1	С	378	THR	3.2
1	D	377	ALA	3.2
1	В	341	GLU	3.1
1	В	374	GLU	3.1
1	С	375	ASP	3.1
1	С	96	THR	3.1
1	D	351	ARG	3.1
1	F	222	GLU	3.1
1	D	198	GLY	3.1
1	Е	132	GLY	3.1
1	А	134	HIS	3.1
1	С	333	GLU	3.1
1	А	208	THR	3.0
1	Е	288	ASN	3.0
1	F	418	ASN	3.0
1	В	375	ASP	3.0
1	D	1	LEU	3.0
1	А	145	ASN	3.0
1	F	187	LYS	3.0
1	С	350	SER	3.0
1	F	419	GLN	3.0
1	А	287	ASN	3.0
1	Е	129	PRO	3.0
1	D	145	ASN	3.0
1	F	360	ARG	2.9



1W2T	
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Mol	Chain	Res	Type	RSRZ
1	С	198	GLY	2.9
1	Е	184	GLU	2.9
1	С	157	ASP	2.9
1	F	199	GLU	2.9
1	D	157	ASP	2.9
1	Е	133	THR	2.9
1	F	133	THR	2.9
1	F	95	PRO	2.9
1	D	374	GLU	2.9
1	Е	199	GLU	2.9
1	D	95	PRO	2.8
1	С	376	GLU	2.8
1	Е	332	GLY	2.8
1	А	222	GLU	2.8
1	Е	375	ASP	2.8
1	С	133	THR	2.7
1	Е	350	SER	2.7
1	А	184	GLU	2.7
1	А	198	GLY	2.7
1	Е	130	GLU	2.7
1	D	360	ARG	2.7
1	D	249	ASP	2.7
1	В	158	GLU	2.7
1	D	99	LYS	2.7
1	В	157	ASP	2.7
1	В	184	GLU	2.7
1	С	100	GLY	2.7
1	В	419	GLN	2.7
1	С	265	LEU	2.7
1	В	82	ASP	2.6
1	В	355	ILE	2.6
1	C	419	GLN	2.6
1	В	376	GLU	2.6
1	F	221	LYS	2.6
1	С	374	GLU	2.6
1	F	421	LYS	2.6
1	C	158	GLU	2.5
1	В	187	LYS	2.5
1	C	127	LYS	2.5
1	Е	254	ILE	2.5
1	D	158	GLU	2.5
1	А	374	GLU	2.5



Mol	Chain	Res	Type	RSRZ
1	F	142	ASN	2.5
1	F	350	SER	2.5
1	С	101	GLU	2.5
1	А	249	ASP	2.5
1	Е	421	LYS	2.5
1	В	95	PRO	2.4
1	С	222	GLU	2.4
1	А	1	LEU	2.4
1	Ε	419	GLN	2.4
1	А	131	GLU	2.4
1	С	187	LYS	2.4
1	Е	230	ARG	2.4
1	В	328	CYS	2.4
1	В	333	GLU	2.4
1	В	416	LYS	2.4
1	F	101	GLU	2.4
1	Е	418	ASN	2.4
1	А	221	LYS	2.4
1	D	311	LYS	2.4
1	Е	222	GLU	2.4
1	В	377	ALA	2.4
1	В	421	LYS	2.4
1	Е	374	GLU	2.4
1	Е	160	ILE	2.4
1	D	209	SER	2.3
1	D	221	LYS	2.3
1	С	254	ILE	2.3
1	С	129	PRO	2.3
1	F	120	ASP	2.3
1	С	355	ILE	2.3
1	F	132	GLY	2.3
1	Е	303	LYS	2.3
1	С	184	GLU	2.3
1	А	304	ARG	2.3
1	A	288	ASN	2.3
1	С	287	ASN	2.3
1	В	318	ASP	2.3
1	В	337	ARG	2.3
1	D	132	GLY	2.3
1	В	185	THR	2.2
1	А	254	ILE	2.2
1	А	169	ASP	2.2



Mol	Chain	Res	Type	RSRZ
1	С	98	ASN	2.2
1	В	198	GLY	2.2
1	С	304	ARG	2.2
1	В	311	LYS	2.2
1	D	133	THR	2.2
1	С	173	HIS	2.2
1	D	213	VAL	2.2
1	D	230	ARG	2.2
1	Е	221	LYS	2.2
1	В	173	HIS	2.2
1	А	375	ASP	2.2
1	А	97	HIS	2.1
1	В	316	LEU	2.1
1	F	127	LYS	2.1
1	С	253	VAL	2.1
1	А	226	ASN	2.1
1	D	130	GLU	2.1
1	Е	226	ASN	2.1
1	D	375	ASP	2.1
1	Е	287	ASN	2.1
1	D	390	VAL	2.1
1	F	378	THR	2.1
1	В	208	THR	2.1
1	Е	127	LYS	2.1
1	В	142	ASN	2.1
1	D	288	ASN	2.1
1	Е	341	GLU	2.1
1	В	320	LYS	2.1
1	В	303	LYS	2.0
1	Е	224	LYS	2.0
1	В	270	ARG	2.0
1	F	160	ILE	2.0
1	С	45	CYS	2.0
1	В	378	THR	2.0
1	С	48	HIS	2.0
1	D	276	VAL	2.0

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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, 95^{th} 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	FRU	Ι	2	12/12	0.65	0.23	24,28,29,31	0
2	GLA	Н	3	11/12	0.68	0.22	41,42,42,43	0
2	GLA	Ι	3	11/12	0.72	0.27	43,44,45,45	0
2	GLC	Н	1	11/12	0.75	0.16	31,33,34,36	0
2	FRU	Н	2	12/12	0.76	0.17	25,27,27,29	0
2	GLC	Ι	1	11/12	0.76	0.15	33,34,36,37	0
2	GLA	G	3	11/12	0.80	0.17	29,30,31,31	0
2	FRU	K	2	12/12	0.81	0.16	21,23,25,25	0
2	GLA	K	3	11/12	0.81	0.17	35,36,37,38	0
2	GLA	L	3	11/12	0.85	0.27	33,35,36,36	0
2	FRU	L	2	12/12	0.88	0.14	18,19,20,21	0
2	GLA	J	3	11/12	0.89	0.17	29,31,32,32	0
2	GLC	K	1	11/12	0.89	0.11	27,28,29,30	0
2	GLC	L	1	11/12	0.90	0.12	23,24,25,26	0
2	FRU	G	2	12/12	0.90	0.14	17,19,20,21	0
2	FRU	J	2	12/12	0.90	0.14	16,17,18,19	0
2	GLC	J	1	11/12	0.91	0.12	20,21,22,24	0
2	GLC	G	1	11/12	0.92	0.09	23,24,25,27	0

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	CIT	А	1433	13/13	0.75	0.23	$50,\!51,\!51,\!52$	0
4	SO4	С	1434	5/5	0.82	0.24	44,45,45,46	0
4	SO4	В	1433	5/5	0.85	0.19	43,44,44,45	0
4	SO4	С	1433	5/5	0.89	0.44	2,2,13,14	0
4	SO4	Е	1433	5/5	0.94	0.39	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.

