



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:54 PM UTC

PDB ID : 2E9B / pdb_00002e9b
Title : Crystal structure of pullulanase type I from *Bacillus subtilis* str. 168 complexed with maltose
Authors : Mikami, B.; Malle, D.; Utsumi, S.; Iwamoto, H.; Katsuya, Y.
Deposited on : 2007-01-24
Resolution : 2.30 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

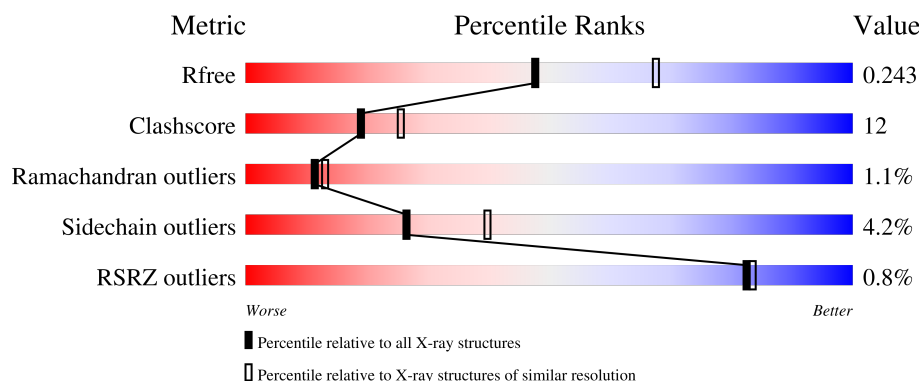
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	718	% 72% 25% ..
1	B	718	% 78% 19% ..
2	C	3	100%
3	D	2	50% 50%
4	E	3	67% 33%

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
7	GOL	A	761	-	X	-	-
7	GOL	B	762	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11961 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.

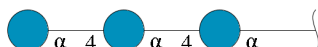
- Molecule 1 is a protein called AmyX protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	0
			5674	3617	975	1060	22			
1	B	712	Total	C	N	O	S	0	0	0
			5674	3617	975	1060	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LYS	MET	conflict	UNP O34587
B	365	LYS	MET	conflict	UNP O34587

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



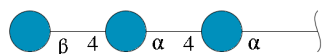
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



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

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

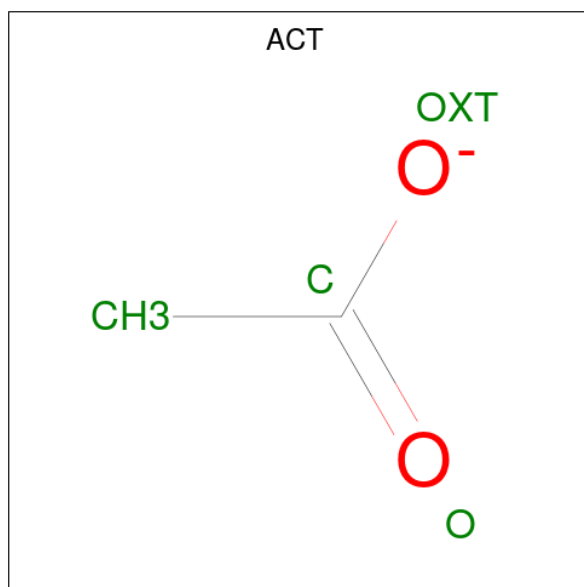


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

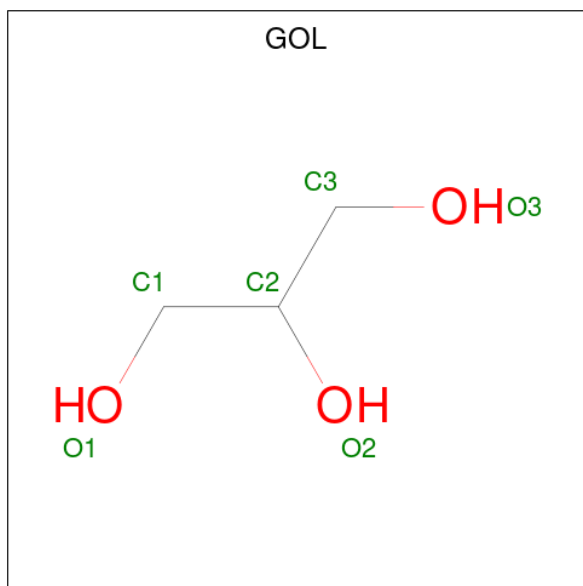
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

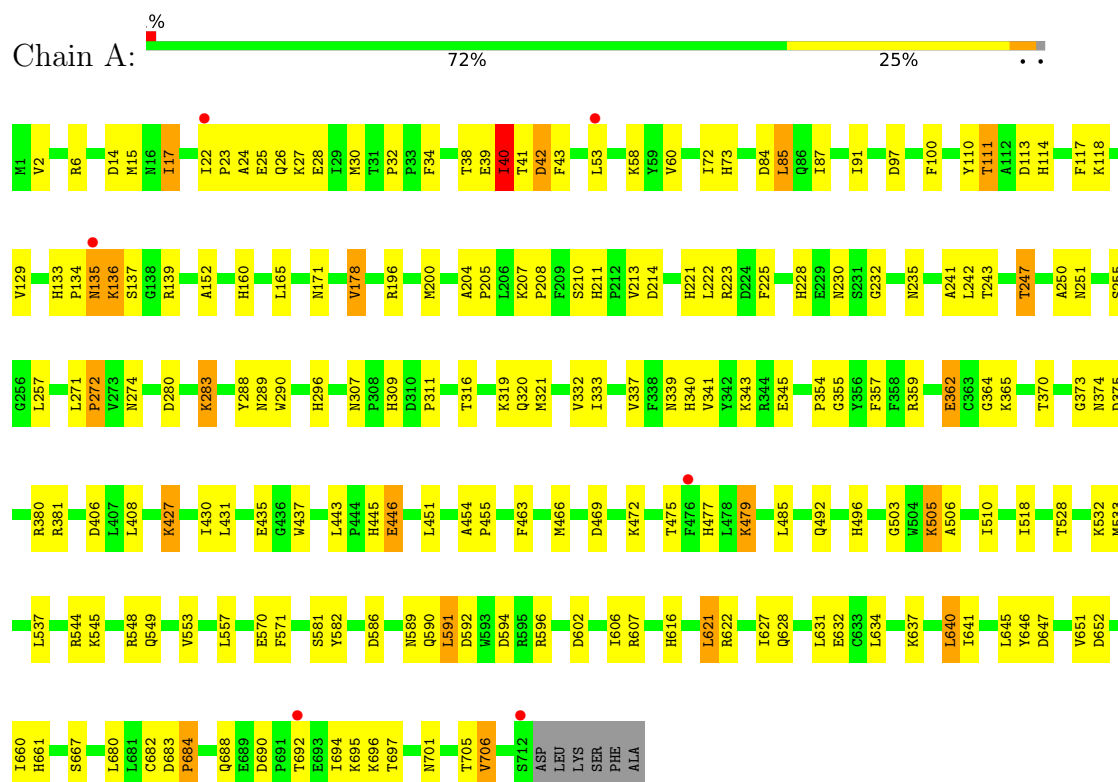
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	236	Total	O	0	0
			236	236		
8	B	260	Total	O	0	0
			260	260		

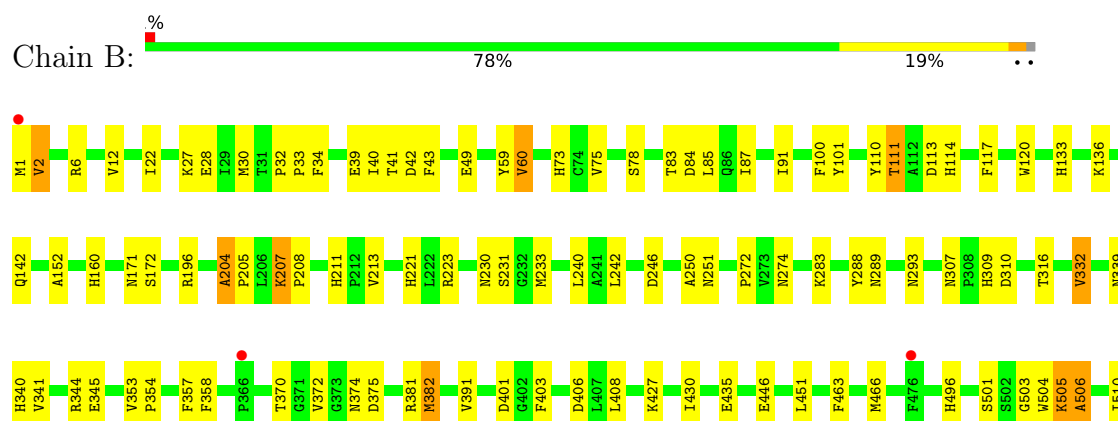
3 Residue-property plots

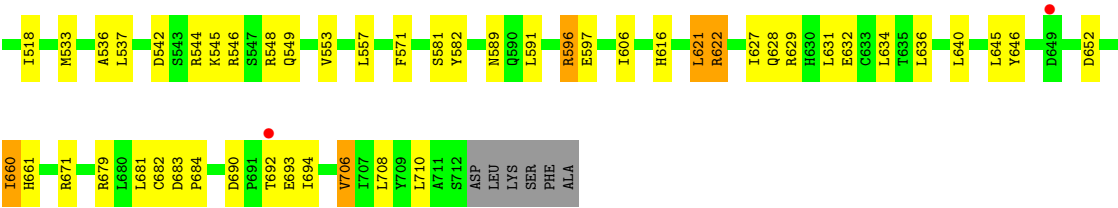
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: AmyX protein



• Molecule 1: AmyX protein





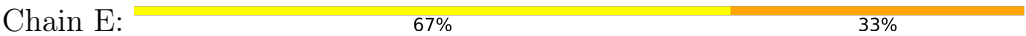
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranos e



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



• Molecule 4: beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranos e



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.03Å 129.18Å 192.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.30 14.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.1 (14.97-2.30) 84.7 (14.97-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.242 0.196 , 0.243	Depositor DCC
R_{free} test set	6750 reflections (8.29%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11961	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.61% 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: ACT, GOL, CA, GLC, BGC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/5822	0.93	18/7905 (0.2%)
1	B	0.45	1/5822 (0.0%)	0.94	23/7905 (0.3%)
All	All	0.44	1/11644 (0.0%)	0.93	41/15810 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	MET	SD-CE	-6.09	1.64	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	GLY	N-CA-C	8.01	122.16	113.58
1	A	2	VAL	N-CA-C	-7.34	102.05	110.05
1	A	357	PHE	N-CA-C	6.98	121.65	113.20
1	A	225	PHE	N-CA-C	6.90	119.68	111.33
1	A	283	LYS	CA-C-N	6.66	127.19	119.47
1	A	283	LYS	C-N-CA	6.66	127.19	119.47
1	B	100	PHE	N-CA-C	6.57	121.00	112.92
1	A	381	ARG	N-CA-C	6.49	118.35	111.28
1	A	274	ASN	N-CA-C	-6.26	102.09	110.55
1	B	581	SER	N-CA-C	6.23	119.90	112.93
1	A	210	SER	N-CA-C	6.12	118.48	111.02
1	B	283	LYS	CA-C-N	6.04	125.72	119.56
1	B	283	LYS	C-N-CA	6.04	125.72	119.56
1	B	510	ILE	N-CA-C	-6.01	105.20	111.58
1	B	310	ASP	CA-C-N	5.87	126.02	119.32
1	B	310	ASP	C-N-CA	5.87	126.02	119.32
1	B	353	VAL	CA-C-N	5.81	126.15	119.93
1	B	353	VAL	C-N-CA	5.81	126.15	119.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ASN	N-CA-C	-5.80	102.72	110.55
1	B	332	VAL	N-CA-C	5.74	117.01	108.46
1	B	110	TYR	N-CA-C	5.62	118.97	109.76
1	B	204	ALA	CA-C-N	5.61	125.54	119.76
1	B	204	ALA	C-N-CA	5.61	125.54	119.76
1	B	246	ASP	N-CA-C	5.61	119.16	111.54
1	B	293	ASN	CA-C-N	5.53	125.85	119.93
1	B	293	ASN	C-N-CA	5.53	125.85	119.93
1	B	589	ASN	N-CA-C	5.52	120.17	113.38
1	B	622	ARG	N-CA-C	5.46	119.67	112.89
1	B	401	ASP	N-CA-C	5.43	119.46	112.41
1	A	332	VAL	N-CA-C	5.38	116.23	108.48
1	B	646	TYR	N-CA-C	5.32	116.74	109.18
1	B	381	ARG	N-CA-C	5.32	117.82	111.71
1	A	510	ILE	N-CA-C	-5.31	105.95	111.58
1	A	100	PHE	N-CA-C	5.23	120.31	113.30
1	A	581	SER	N-CA-C	5.22	118.78	112.93
1	A	589	ASN	N-CA-C	5.21	119.69	113.23
1	A	58	LYS	N-CA-C	5.18	118.00	109.72
1	B	357	PHE	N-CA-C	5.14	119.42	113.20
1	A	528	THR	N-CA-C	-5.11	104.12	110.41
1	A	505	LYS	CB-CA-C	-5.08	110.74	116.63
1	A	222	LEU	N-CA-C	5.06	118.22	111.75

There are no chirality outliers.

There are no planarity outliers.

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	5674	0	5528	153	0
1	B	5674	0	5528	114	0
2	C	34	0	30	2	0
3	D	23	0	21	0	0
4	E	34	0	30	6	0
5	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	8	0	6	0	0
6	B	4	0	3	0	0
7	A	6	0	3	1	0
7	B	6	0	3	1	0
8	A	236	0	0	9	0
8	B	260	0	0	10	0
All	All	11961	0	11152	267	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 12.

All (267) 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:B:207:LYS:H	1:B:207:LYS:HE2	0.93	1.09
1:A:111:THR:HG22	1:A:114:HIS:H	1.12	1.08
1:B:111:THR:HG22	1:B:114:HIS:H	1.14	1.04
1:B:660:ILE:HG23	1:B:706:VAL:HG13	1.42	1.01
1:B:207:LYS:HE2	1:B:207:LYS:N	1.76	1.01
1:A:247:THR:HG22	1:A:255:SER:OG	1.64	0.95
1:A:14:ASP:HB3	1:A:17:ILE:HG23	1.49	0.94
1:A:87:ILE:H	1:A:171:ASN:HD21	1.05	0.92
1:B:553:VAL:HG11	1:B:606:ILE:HD12	1.52	0.91
1:B:207:LYS:H	1:B:207:LYS:CE	1.84	0.90
1:A:505:LYS:HG2	1:A:506:ALA:H	1.38	0.87
1:A:570:GLU:HB2	1:A:606:ILE:HD13	1.57	0.86
1:B:230:ASN:HD21	1:B:250:ALA:H	1.23	0.84
1:A:505:LYS:CG	1:A:506:ALA:H	1.90	0.84
1:B:87:ILE:H	1:B:171:ASN:HD21	1.25	0.84
1:A:505:LYS:HG2	1:A:506:ALA:N	1.92	0.83
1:A:406:ASP:OD1	2:C:1:GLC:H1	1.79	0.82
1:B:160:HIS:HD2	1:B:196:ARG:H	1.27	0.82
1:B:382:MET:HA	1:B:382:MET:HE2	1.64	0.79
1:A:316:THR:O	1:A:320:GLN:HG3	1.83	0.79
1:B:101:TYR:CD1	1:B:382:MET:HE3	2.19	0.77
1:B:142:GLN:HG3	8:B:963:HOH:O	1.84	0.77
1:A:87:ILE:H	1:A:171:ASN:ND2	1.82	0.75
1:A:23:PRO:HG2	1:A:26:GLN:HG3	1.67	0.75
1:A:87:ILE:N	1:A:171:ASN:HD21	1.83	0.75
1:A:606:ILE:HG13	8:A:1146:HOH:O	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ILE:HB	1:A:706:VAL:HG13	1.70	0.74
1:A:479:LYS:H	1:A:479:LYS:HD2	1.52	0.73
1:B:640:LEU:HD21	1:B:660:ILE:HD11	1.71	0.72
1:A:230:ASN:HD21	1:A:250:ALA:H	1.36	0.72
1:A:341:VAL:H	1:A:374:ASN:HD21	1.37	0.72
1:A:496:HIS:HE1	1:A:503:GLY:H	1.38	0.72
1:B:339:ASN:ND2	1:B:340:HIS:HD2	1.88	0.71
1:B:496:HIS:HE1	1:B:503:GLY:H	1.38	0.71
1:A:247:THR:HG22	1:A:255:SER:HG	1.55	0.70
4:E:2:GLC:H62	4:E:3:BGC:O5	1.91	0.70
1:A:200:MET:HE2	1:A:319:LYS:HB3	1.74	0.70
1:B:111:THR:HG22	1:B:114:HIS:N	1.99	0.69
1:A:135:ASN:N	1:A:135:ASN:HD22	1.90	0.69
1:B:505:LYS:H	1:B:505:LYS:HD2	1.55	0.69
1:A:160:HIS:HD2	1:A:196:ARG:H	1.40	0.69
1:B:87:ILE:H	1:B:171:ASN:ND2	1.92	0.68
1:A:307:ASN:ND2	1:A:309:HIS:H	1.91	0.68
1:A:111:THR:CG2	1:A:114:HIS:H	1.99	0.67
1:A:211:HIS:HD2	1:A:213:VAL:HG22	1.60	0.67
1:B:339:ASN:HD21	1:B:340:HIS:HD2	1.41	0.67
1:B:553:VAL:HG22	8:B:1223:HOH:O	1.95	0.67
1:A:472:LYS:HE3	1:A:475:THR:HG22	1.77	0.67
1:A:39:GLU:O	1:A:40:ILE:HG13	1.95	0.66
1:A:479:LYS:H	1:A:479:LYS:CD	2.07	0.66
1:A:660:ILE:HB	1:A:706:VAL:CG1	2.26	0.66
1:B:22:ILE:HD13	1:B:30:MET:O	1.96	0.66
1:A:111:THR:HG23	1:A:113:ASP:H	1.61	0.66
1:A:40:ILE:HD12	1:A:40:ILE:O	1.97	0.65
1:B:596:ARG:HD2	1:B:596:ARG:O	1.97	0.64
1:A:586:ASP:O	1:A:590:GLN:HG2	1.97	0.64
1:B:370:THR:HG23	1:B:375:ASP:OD2	1.97	0.64
1:B:307:ASN:ND2	1:B:309:HIS:H	1.96	0.64
1:A:505:LYS:HE2	1:A:506:ALA:HB3	1.79	0.64
1:A:602:ASP:O	1:A:606:ILE:HD12	1.97	0.64
1:A:38:THR:HG22	1:A:73:HIS:HA	1.78	0.64
1:B:544:ARG:O	1:B:548:ARG:HG3	1.98	0.64
1:B:211:HIS:HD2	1:B:213:VAL:H	1.46	0.63
1:B:230:ASN:HD21	1:B:250:ALA:N	1.95	0.63
1:A:339:ASN:HD21	1:A:340:HIS:HD2	1.46	0.63
1:A:479:LYS:HD2	1:A:479:LYS:N	2.15	0.62
1:B:211:HIS:CD2	1:B:213:VAL:HG22	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LYS:CG	1:A:506:ALA:N	2.57	0.62
1:A:533:MET:HE3	1:A:545:LYS:HB3	1.83	0.61
1:A:339:ASN:ND2	1:A:340:HIS:HD2	1.99	0.61
1:B:505:LYS:O	1:B:506:ALA:CB	2.50	0.60
1:A:111:THR:HG22	1:A:114:HIS:N	1.98	0.60
1:B:120:TRP:CZ2	1:B:382:MET:HG3	2.35	0.60
1:B:111:THR:HG23	1:B:113:ASP:H	1.66	0.60
1:B:39:GLU:HG3	1:B:40:ILE:HG13	1.84	0.59
1:B:133:HIS:HB3	1:B:136:LYS:HB2	1.83	0.59
1:B:631:LEU:C	1:B:631:LEU:HD23	2.27	0.59
1:A:628:GLN:HE21	1:A:628:GLN:HA	1.68	0.59
1:A:211:HIS:CD2	1:A:213:VAL:HG22	2.36	0.59
1:B:120:TRP:CH2	1:B:382:MET:HG3	2.38	0.59
1:A:370:THR:HG23	1:A:375:ASP:OD2	2.03	0.58
1:B:22:ILE:HD12	1:B:59:TYR:HE1	1.67	0.58
1:B:406:ASP:OD1	4:E:1:GLC:H1	2.03	0.58
1:B:435:GLU:OE1	4:E:1:GLC:H1	2.03	0.58
1:B:1:MET:HG2	1:B:2:VAL:HG23	1.84	0.58
1:B:345:GLU:H	1:B:345:GLU:CD	2.10	0.58
1:A:606:ILE:HD11	8:A:911:HOH:O	2.02	0.58
1:A:38:THR:OG1	1:A:41:THR:HB	2.04	0.58
1:A:631:LEU:C	1:A:631:LEU:HD23	2.29	0.58
1:B:370:THR:OG1	1:B:372:VAL:HG22	2.05	0.57
1:A:223:ARG:HD2	7:A:761:GOL:O3	2.03	0.57
1:A:544:ARG:O	1:A:548:ARG:HG3	2.03	0.57
1:B:536:ALA:C	1:B:537:LEU:HD12	2.30	0.56
1:A:26:GLN:NE2	1:A:30:MET:HE3	2.20	0.56
1:A:695:LYS:O	1:A:697:THR:N	2.36	0.56
1:B:251:ASN:HB2	1:B:597:GLU:OE2	2.06	0.56
1:A:607:ARG:HD3	8:A:1151:HOH:O	2.06	0.56
1:B:307:ASN:HD21	1:B:309:HIS:HB2	1.71	0.56
1:A:553:VAL:HG12	1:A:557:LEU:HD12	1.86	0.56
1:A:549:GLN:O	1:A:553:VAL:HG23	2.06	0.56
1:A:118:LYS:HG2	1:A:152:ALA:HB2	1.88	0.55
1:A:135:ASN:N	1:A:135:ASN:ND2	2.54	0.55
1:B:41:THR:HG22	1:B:42:ASP:N	2.21	0.55
1:A:73:HIS:HB2	1:A:85:LEU:HB2	1.88	0.55
1:B:41:THR:HG21	1:B:43:PHE:CE1	2.42	0.55
1:B:496:HIS:HD2	8:B:1221:HOH:O	1.89	0.55
1:B:73:HIS:HE1	8:B:943:HOH:O	1.89	0.54
1:A:631:LEU:HD23	1:A:632:GLU:N	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:HG13	1:A:171:ASN:ND2	2.23	0.54
1:A:640:LEU:HD13	1:A:641:ILE:N	2.23	0.54
1:A:445:HIS:HD2	1:B:632:GLU:OE2	1.91	0.54
1:A:469:ASP:OD2	1:A:475:THR:HG23	2.09	0.53
1:B:536:ALA:O	1:B:537:LEU:HD12	2.08	0.53
1:A:17:ILE:HG13	1:A:17:ILE:O	2.09	0.53
1:A:39:GLU:O	1:A:40:ILE:CG1	2.56	0.53
1:A:570:GLU:CB	1:A:606:ILE:HD13	2.34	0.53
1:A:571:PHE:CE2	1:A:596:ARG:HB2	2.43	0.53
1:B:341:VAL:H	1:B:374:ASN:HD21	1.56	0.53
1:B:505:LYS:HD2	1:B:505:LYS:N	2.23	0.53
1:A:628:GLN:HA	1:A:628:GLN:NE2	2.24	0.53
1:A:571:PHE:HZ	1:A:591:LEU:HD22	1.74	0.52
1:B:207:LYS:HB2	1:B:208:PRO:HD2	1.91	0.52
1:B:679:ARG:NH2	1:B:693:GLU:HG3	2.25	0.52
1:A:364:GLY:C	1:A:365:LYS:HD2	2.34	0.52
1:A:427:LYS:O	1:A:430:ILE:HG23	2.09	0.52
1:B:661:HIS:HE1	8:B:1043:HOH:O	1.93	0.52
1:B:504:TRP:O	1:B:505:LYS:C	2.52	0.52
1:B:692:THR:HG22	8:B:1243:HOH:O	2.08	0.51
1:A:307:ASN:C	1:A:307:ASN:HD22	2.18	0.51
1:A:380:ARG:HE	1:A:380:ARG:HA	1.76	0.51
1:B:571:PHE:CE2	1:B:596:ARG:HB2	2.46	0.51
1:A:39:GLU:C	1:A:40:ILE:HG23	2.35	0.50
1:A:6:ARG:HD3	1:A:84:ASP:OD2	2.11	0.50
1:A:637:LYS:HE3	8:A:922:HOH:O	2.10	0.50
1:A:178:VAL:HG21	1:A:296:HIS:CE1	2.46	0.50
1:A:32:PRO:HG3	1:A:34:PHE:CE1	2.46	0.50
1:B:211:HIS:HD2	1:B:213:VAL:HG22	1.77	0.50
1:B:549:GLN:O	1:B:553:VAL:HG23	2.12	0.49
1:A:87:ILE:HG13	1:A:171:ASN:HD21	1.75	0.49
1:A:230:ASN:HD21	1:A:250:ALA:N	2.09	0.49
1:B:496:HIS:CE1	1:B:503:GLY:H	2.25	0.49
1:B:250:ALA:HB3	8:B:1276:HOH:O	2.12	0.49
1:B:596:ARG:HD2	1:B:596:ARG:C	2.37	0.49
1:B:682:CYS:O	1:B:706:VAL:HA	2.12	0.49
1:B:22:ILE:HD12	1:B:59:TYR:CE1	2.48	0.49
1:B:33:PRO:HD2	1:B:78:SER:HB3	1.94	0.49
1:B:32:PRO:HG3	1:B:34:PHE:CE1	2.47	0.48
1:A:41:THR:HG23	1:A:43:PHE:CE1	2.47	0.48
1:A:307:ASN:ND2	1:A:307:ASN:C	2.70	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:N	1:A:53:LEU:HD12	2.29	0.48
1:A:133:HIS:CD2	1:A:134:PRO:HD2	2.49	0.48
1:A:427:LYS:HB3	1:A:430:ILE:CG2	2.44	0.48
1:A:680:LEU:C	1:A:680:LEU:HD13	2.39	0.48
1:A:682:CYS:O	1:A:706:VAL:HA	2.13	0.48
1:A:362:GLU:HG2	1:B:636:LEU:HD13	1.96	0.48
1:A:492:GLN:HE22	1:A:505:LYS:HD2	1.77	0.47
1:B:463:PHE:HA	1:B:518:ILE:HB	1.96	0.47
1:A:477:HIS:HB3	1:A:479:LYS:HZ2	1.79	0.47
1:A:406:ASP:OD1	2:C:1:GLC:C1	2.55	0.47
1:A:307:ASN:HD21	1:A:309:HIS:HB2	1.80	0.47
1:A:592:ASP:OD1	1:A:594:ASP:HB2	2.14	0.47
1:A:694:ILE:C	1:A:694:ILE:HD12	2.39	0.47
1:B:660:ILE:CG2	1:B:706:VAL:HG13	2.31	0.47
1:A:243:THR:HG22	1:A:321:MET:HA	1.97	0.47
1:B:288:TYR:CD1	1:B:289:ASN:N	2.83	0.46
1:B:427:LYS:HE2	8:B:988:HOH:O	2.15	0.46
1:B:111:THR:CG2	1:B:114:HIS:H	2.05	0.46
1:A:38:THR:HG22	1:A:72:ILE:O	2.15	0.46
1:A:41:THR:HG23	1:A:43:PHE:HE1	1.81	0.46
1:B:582:TYR:CD2	4:E:2:GLC:H4	2.51	0.46
1:B:406:ASP:OD1	4:E:1:GLC:C1	2.63	0.46
1:A:221:HIS:CD2	1:A:223:ARG:H	2.34	0.46
1:B:221:HIS:CD2	1:B:223:ARG:H	2.34	0.46
1:A:628:GLN:HE21	1:A:628:GLN:CA	2.25	0.46
1:B:542:ASP:O	1:B:546:ARG:HG3	2.16	0.46
1:A:472:LYS:CE	1:A:475:THR:HG22	2.44	0.45
1:A:41:THR:HG22	1:A:42:ASP:N	2.31	0.45
1:A:136:LYS:NZ	8:A:837:HOH:O	2.49	0.45
1:A:553:VAL:CG2	8:A:904:HOH:O	2.64	0.45
1:B:616:HIS:HB3	1:B:652:ASP:OD2	2.15	0.45
1:B:683:ASP:HB2	1:B:684:PRO:CD	2.47	0.45
1:B:6:ARG:HD3	1:B:84:ASP:OD2	2.16	0.45
1:A:288:TYR:CD1	1:A:288:TYR:C	2.95	0.45
1:A:22:ILE:HD12	1:A:27:LYS:HA	1.97	0.45
1:A:359:ARG:NH2	1:A:443:LEU:HD11	2.32	0.45
1:B:27:LYS:NZ	8:B:1161:HOH:O	2.49	0.45
1:B:307:ASN:C	1:B:307:ASN:HD22	2.25	0.44
1:B:211:HIS:CE1	1:B:622:ARG:HD2	2.52	0.44
1:B:344:ARG:HG3	1:B:358:PHE:CE2	2.53	0.44
1:A:211:HIS:O	1:A:214:ASP:HB2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LYS:O	1:B:506:ALA:HB3	2.17	0.44
1:A:232:GLY:O	1:A:247:THR:HG23	2.17	0.44
1:A:288:TYR:CD1	1:A:289:ASN:N	2.86	0.44
1:A:445:HIS:CE1	1:A:446:GLU:HG3	2.53	0.44
1:A:235:ASN:O	1:A:241:ALA:HB2	2.18	0.44
1:A:207:LYS:HB3	1:A:208:PRO:HD2	2.00	0.44
1:A:485:LEU:HA	1:A:548:ARG:HE	1.82	0.44
1:B:101:TYR:CE1	1:B:382:MET:HE3	2.52	0.44
1:A:133:HIS:HD2	1:A:134:PRO:N	2.14	0.44
1:A:228:HIS:HD2	1:A:590:GLN:NE2	2.15	0.44
1:A:309:HIS:O	1:A:311:PRO:HD3	2.18	0.44
1:A:14:ASP:HB3	1:A:17:ILE:CG2	2.35	0.43
1:A:680:LEU:HD12	1:A:688:GLN:HG3	2.00	0.43
1:A:683:ASP:OD2	1:A:683:ASP:C	2.62	0.43
1:B:553:VAL:HG12	1:B:557:LEU:HD12	2.00	0.43
1:A:38:THR:OG1	1:A:41:THR:CB	2.66	0.43
1:A:271:LEU:HB3	1:A:272:PRO:HD2	2.01	0.43
1:A:339:ASN:ND2	1:A:340:HIS:CD2	2.84	0.43
1:B:117:PHE:O	1:B:152:ALA:HA	2.18	0.43
1:B:339:ASN:ND2	1:B:340:HIS:CD2	2.77	0.43
1:A:380:ARG:HA	1:A:380:ARG:NE	2.34	0.43
1:A:683:ASP:HB2	1:A:684:PRO:HD2	2.01	0.43
1:B:12:VAL:O	1:B:12:VAL:HG13	2.18	0.43
1:B:171:ASN:O	1:B:172:SER:HB2	2.17	0.43
1:B:621:LEU:HD23	1:B:627:ILE:HA	2.00	0.43
1:A:91:ILE:HD13	1:A:354:PRO:O	2.19	0.43
1:A:640:LEU:HD13	1:A:640:LEU:C	2.44	0.43
1:B:694:ILE:HD11	1:B:708:LEU:CD2	2.48	0.43
1:A:472:LYS:HD2	1:A:532:LYS:HG2	2.01	0.43
1:B:73:HIS:HD2	7:B:762:GOL:H12	1.84	0.43
1:A:435:GLU:HB2	1:A:437:TRP:CE2	2.53	0.42
1:A:621:LEU:HD23	1:A:627:ILE:HA	2.01	0.42
1:A:204:ALA:N	1:A:205:PRO:HD3	2.34	0.42
1:A:492:GLN:NE2	1:A:505:LYS:HD2	2.35	0.42
1:A:661:HIS:HD2	1:A:705:THR:OG1	2.02	0.42
1:B:49:GLU:HG2	1:B:60:VAL:HG22	2.02	0.42
1:B:160:HIS:CD2	1:B:196:ARG:HG2	2.54	0.42
1:A:466:MET:SD	1:A:466:MET:C	3.02	0.42
1:A:160:HIS:CD2	1:A:196:ARG:H	2.28	0.42
1:B:91:ILE:HD13	1:B:354:PRO:O	2.19	0.42
1:B:466:MET:C	1:B:466:MET:SD	3.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LYS:N	1:B:505:LYS:CD	2.82	0.42
1:B:75:VAL:CG2	1:B:83:THR:HG22	2.49	0.42
1:B:496:HIS:HE1	1:B:503:GLY:N	2.10	0.42
1:A:17:ILE:HD13	1:A:60:VAL:HG13	2.02	0.42
1:A:692:THR:HG22	8:A:929:HOH:O	2.20	0.42
1:B:628:GLN:HE21	1:B:628:GLN:HA	1.84	0.41
1:B:694:ILE:HD11	1:B:708:LEU:HD22	2.02	0.41
1:A:91:ILE:HD12	1:A:355:GLY:C	2.44	0.41
1:A:110:TYR:CG	1:A:111:THR:N	2.87	0.41
1:A:280:ASP:OD2	1:A:283:LYS:HE3	2.20	0.41
1:A:362:GLU:OE1	1:A:362:GLU:N	2.48	0.41
1:B:240:LEU:HG	8:B:1190:HOH:O	2.19	0.41
1:B:496:HIS:CE1	1:B:501:SER:HA	2.55	0.41
1:A:129:VAL:O	1:A:129:VAL:HG13	2.20	0.41
1:A:463:PHE:HA	1:A:518:ILE:HB	2.01	0.41
1:B:204:ALA:HA	1:B:205:PRO:HD3	1.82	0.41
1:B:427:LYS:O	1:B:430:ILE:HG23	2.21	0.41
4:E:2:GLC:H62	4:E:3:BGC:C1	2.51	0.41
1:A:616:HIS:HB3	1:A:652:ASP:OD2	2.21	0.41
1:A:333:ILE:HD11	1:A:431:LEU:HD12	2.03	0.41
1:A:496:HIS:HE1	1:A:503:GLY:N	2.12	0.41
1:A:646:TYR:CD1	1:A:647:ASP:HB2	2.56	0.41
1:A:661:HIS:HE1	8:A:913:HOH:O	2.04	0.41
1:B:288:TYR:CD1	1:B:288:TYR:C	2.98	0.41
1:B:391:VAL:HG13	1:B:403:PHE:CE1	2.56	0.41
1:B:533:MET:HE3	1:B:545:LYS:HB3	2.03	0.41
1:A:139:ARG:NH1	8:A:838:HOH:O	2.51	0.41
1:B:690:ASP:OD2	1:B:690:ASP:N	2.51	0.41
1:A:111:THR:HG21	1:A:114:HIS:CE1	2.57	0.40
1:A:117:PHE:O	1:A:152:ALA:HA	2.21	0.40
1:B:681:LEU:O	1:B:681:LEU:HD22	2.21	0.40
1:A:454:ALA:N	1:A:455:PRO:CD	2.84	0.40
1:A:667:SER:OG	1:A:701:ASN:OD1	2.40	0.40
1:B:211:HIS:CD2	1:B:213:VAL:H	2.34	0.40
1:B:231:SER:HB2	1:B:233:MET:HE3	2.02	0.40
1:A:290:TRP:CD2	1:A:582:TYR:HA	2.57	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	Percentiles	
1	A	710/718 (99%)	670 (94%)	28 (4%)	12 (2%)	7	7
1	B	710/718 (99%)	675 (95%)	31 (4%)	4 (1%)	21	27
All	All	1420/1436 (99%)	1345 (95%)	59 (4%)	16 (1%)	11	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	651	VAL
1	B	506	ALA
1	A	42	ASP
1	A	136	LYS
1	A	696	LYS
1	B	505	LYS
1	A	40	ILE
1	A	137	SER
1	A	15	MET
1	A	24	ALA
1	A	343	LYS
1	A	684	PRO
1	B	2	VAL
1	B	272	PRO
1	A	272	PRO
1	A	690	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/615 (99%)	579 (95%)	30 (5%)	22	34
1	B	609/615 (99%)	588 (97%)	21 (3%)	32	49
All	All	1218/1230 (99%)	1167 (96%)	51 (4%)	26	40

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

Mol	Chain	Res	Type
1	A	17	ILE
1	A	25	GLU
1	A	28	GLU
1	A	40	ILE
1	A	85	LEU
1	A	97	ASP
1	A	111	THR
1	A	135	ASN
1	A	165	LEU
1	A	178	VAL
1	A	242	LEU
1	A	247	THR
1	A	251	ASN
1	A	257	LEU
1	A	337	VAL
1	A	345	GLU
1	A	362	GLU
1	A	408	LEU
1	A	427	LYS
1	A	446	GLU
1	A	451	LEU
1	A	479	LYS
1	A	537	LEU
1	A	591	LEU
1	A	621	LEU
1	A	622	ARG
1	A	634	LEU
1	A	640	LEU
1	A	645	LEU
1	A	706	VAL
1	B	28	GLU
1	B	60	VAL
1	B	85	LEU
1	B	111	THR
1	B	207	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	242	LEU
1	B	316	THR
1	B	332	VAL
1	B	408	LEU
1	B	446	GLU
1	B	451	LEU
1	B	591	LEU
1	B	596	ARG
1	B	621	LEU
1	B	629	ARG
1	B	634	LEU
1	B	645	LEU
1	B	660	ILE
1	B	671	ARG
1	B	706	VAL
1	B	710	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	133	HIS
1	A	135	ASN
1	A	160	HIS
1	A	171	ASN
1	A	180	GLN
1	A	199	GLN
1	A	211	HIS
1	A	221	HIS
1	A	230	ASN
1	A	248	GLN
1	A	274	ASN
1	A	307	ASN
1	A	312	GLN
1	A	320	GLN
1	A	327	GLN
1	A	339	ASN
1	A	340	HIS
1	A	374	ASN
1	A	445	HIS
1	A	492	GLN
1	A	496	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	526	ASN
1	A	549	GLN
1	A	580	ASN
1	A	583	GLN
1	A	590	GLN
1	A	628	GLN
1	A	639	HIS
1	A	661	HIS
1	B	26	GLN
1	B	73	HIS
1	B	86	GLN
1	B	133	HIS
1	B	142	GLN
1	B	160	HIS
1	B	170	ASN
1	B	171	ASN
1	B	180	GLN
1	B	211	HIS
1	B	221	HIS
1	B	230	ASN
1	B	248	GLN
1	B	274	ASN
1	B	307	ASN
1	B	312	GLN
1	B	320	GLN
1	B	327	GLN
1	B	328	HIS
1	B	339	ASN
1	B	340	HIS
1	B	346	ASN
1	B	447	GLN
1	B	496	HIS
1	B	526	ASN
1	B	527	HIS
1	B	539	GLN
1	B	549	GLN
1	B	580	ASN
1	B	583	GLN
1	B	590	GLN
1	B	628	GLN
1	B	630	HIS
1	B	661	HIS

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 ⓘ

8 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	C	1	2	12,12,12	0.55	0	17,17,17	0.38	0
2	GLC	C	2	2	11,11,12	0.60	0	15,15,17	0.75	1 (6%)
2	GLC	C	3	2	11,11,12	0.56	0	15,15,17	0.56	1 (6%)
3	GLC	D	1	3	12,12,12	0.54	0	17,17,17	0.42	0
3	GLC	D	2	3	11,11,12	0.56	0	15,15,17	0.64	1 (6%)
4	GLC	E	1	4	12,12,12	0.56	0	17,17,17	0.41	0
4	GLC	E	2	4	11,11,12	0.62	0	15,15,17	1.18	2 (13%)
4	BGC	E	3	4	11,11,12	0.52	0	15,15,17	0.52	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	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
3	GLC	D	1	3	-	2/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	E	1	4	-	2/2/22/22	0/1/1/1
4	GLC	E	2	4	-	0/2/19/22	0/1/1/1
4	BGC	E	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	GLC	C1-O5-C5	2.98	116.18	112.19
4	E	2	GLC	C2-C3-C4	-2.22	106.95	110.86
2	C	2	GLC	C1-O5-C5	2.21	115.15	112.19
3	D	2	GLC	C1-O5-C5	2.04	114.92	112.19
2	C	3	GLC	C1-O5-C5	2.04	114.91	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

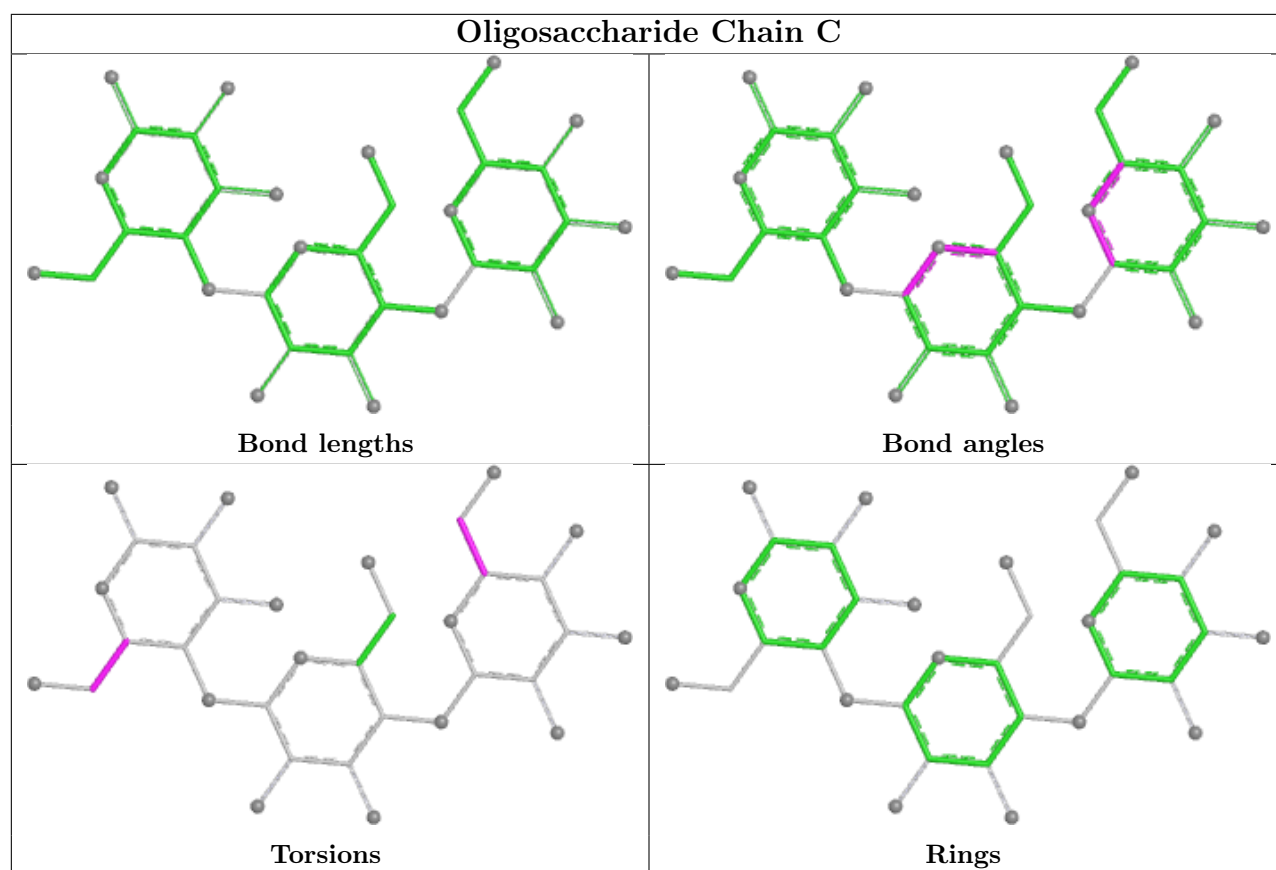
Mol	Chain	Res	Type	Atoms
4	E	3	BGC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
4	E	3	BGC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6
4	E	1	GLC	C4-C5-C6-O6
4	E	1	GLC	O5-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6
3	D	1	GLC	O5-C5-C6-O6

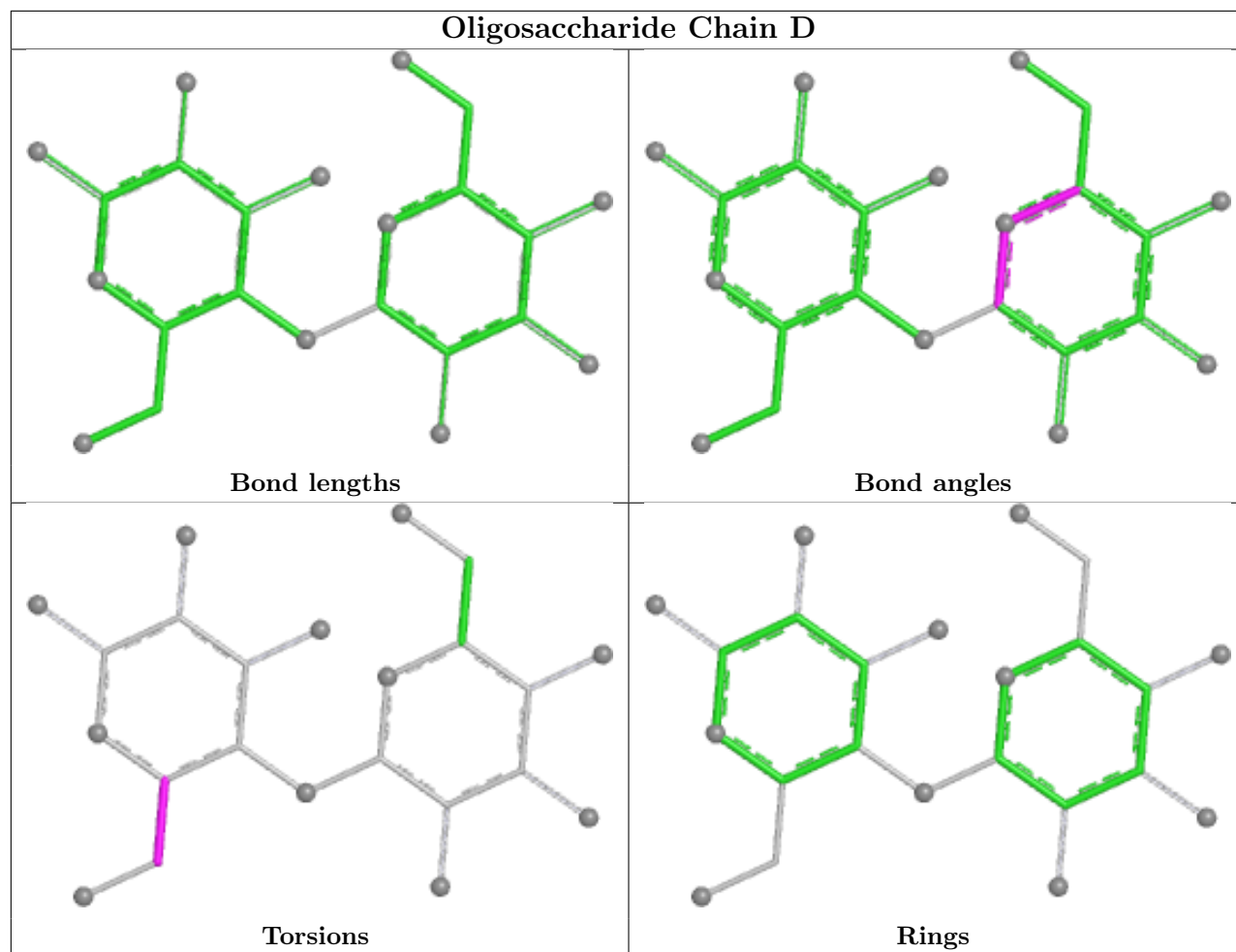
There are no ring outliers.

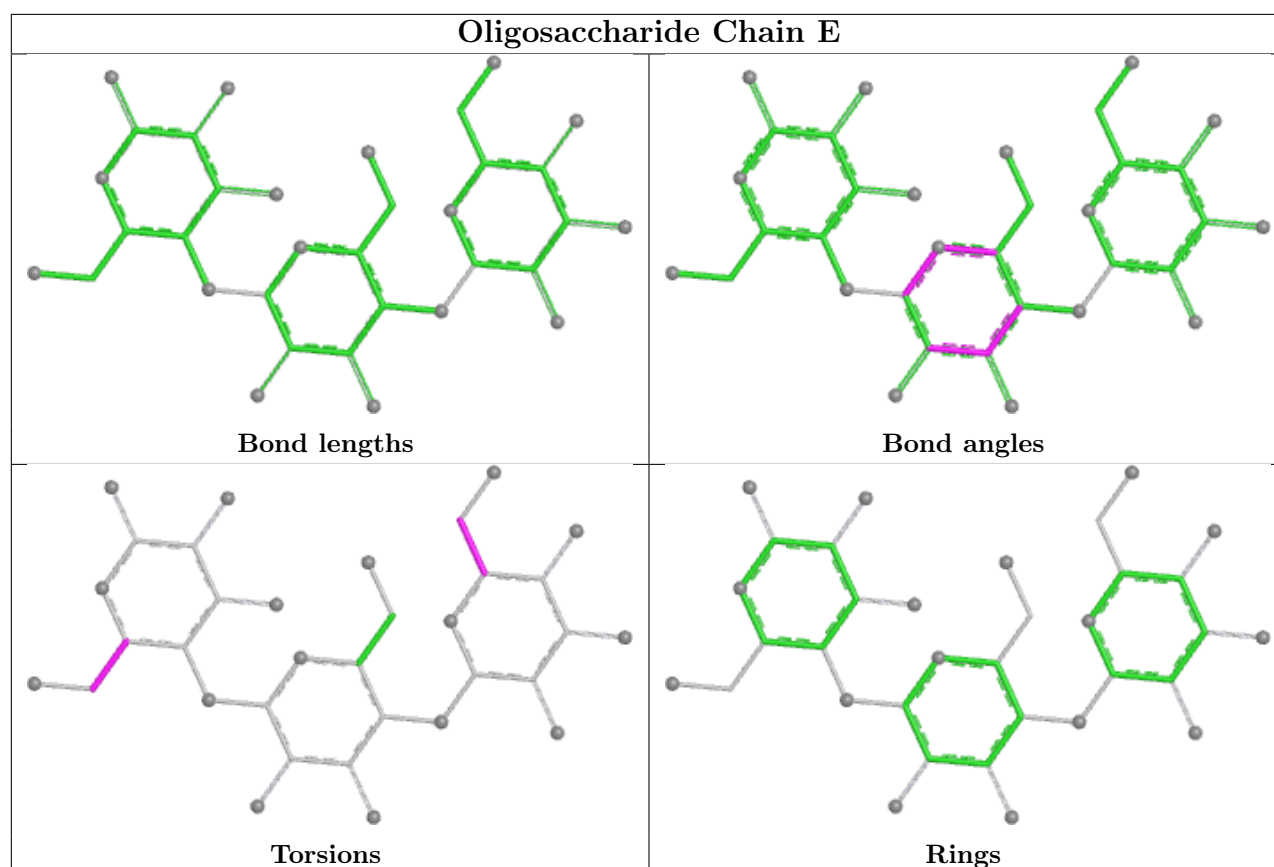
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	3	BGC	2	0
4	E	2	GLC	3	0
2	C	1	GLC	2	0
4	E	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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ACT	A	753	-	3,3,3	1.28	1 (33%)	3,3,3	0.75	0
7	GOL	A	761	-	5,5,5	4.44	5 (100%)	5,5,5	6.16	3 (60%)
6	ACT	A	751	-	3,3,3	1.30	1 (33%)	3,3,3	0.81	0
6	ACT	B	752	-	3,3,3	1.27	1 (33%)	3,3,3	0.68	0
7	GOL	B	762	-	5,5,5	4.39	5 (100%)	5,5,5	6.20	3 (60%)

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
7	GOL	B	762	-	-	2/4/4/4	-
7	GOL	A	761	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	761	GOL	C3-C2	-8.09	1.20	1.51
7	B	762	GOL	C3-C2	-7.93	1.21	1.51
7	B	762	GOL	O3-C3	3.35	1.56	1.42
7	A	761	GOL	O3-C3	3.20	1.55	1.42
7	A	761	GOL	O2-C2	-2.99	1.34	1.43
7	B	762	GOL	O2-C2	-2.93	1.34	1.43
7	B	762	GOL	C1-C2	-2.91	1.40	1.51
7	A	761	GOL	C1-C2	-2.89	1.40	1.51
7	A	761	GOL	O1-C1	-2.38	1.32	1.42
7	B	762	GOL	O1-C1	-2.32	1.32	1.42
6	A	751	ACT	O-C	2.18	1.31	1.22
6	A	753	ACT	O-C	2.14	1.31	1.22
6	B	752	ACT	O-C	2.09	1.31	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	762	GOL	O3-C3-C2	11.48	162.07	110.38
7	A	761	GOL	O3-C3-C2	11.32	161.36	110.38
7	A	761	GOL	O2-C2-C3	6.99	138.12	109.18
7	B	762	GOL	O2-C2-C3	6.95	137.97	109.18
7	A	761	GOL	O1-C1-C2	3.48	126.05	110.38
7	B	762	GOL	O1-C1-C2	3.37	125.54	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	761	GOL	O1-C1-C2-C3
7	A	761	GOL	C1-C2-C3-O3
7	B	762	GOL	C1-C2-C3-O3
7	B	762	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	761	GOL	1	0
7	B	762	GOL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	712/718 (99%)	-0.27	6 (0%) 82 83	21, 34, 58, 80	0
1	B	712/718 (99%)	-0.32	5 (0%) 84 85	22, 33, 54, 70	0
All	All	1424/1436 (99%)	-0.30	11 (0%) 82 83	21, 34, 56, 80	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ASN	2.9
1	B	1	MET	2.7
1	A	53	LEU	2.7
1	B	366	PRO	2.6
1	A	692	THR	2.2
1	B	476	PHE	2.1
1	A	712	SER	2.1
1	B	649	ASP	2.1
1	B	692	THR	2.1
1	A	476	PHE	2.0
1	A	22	ILE	2.0

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

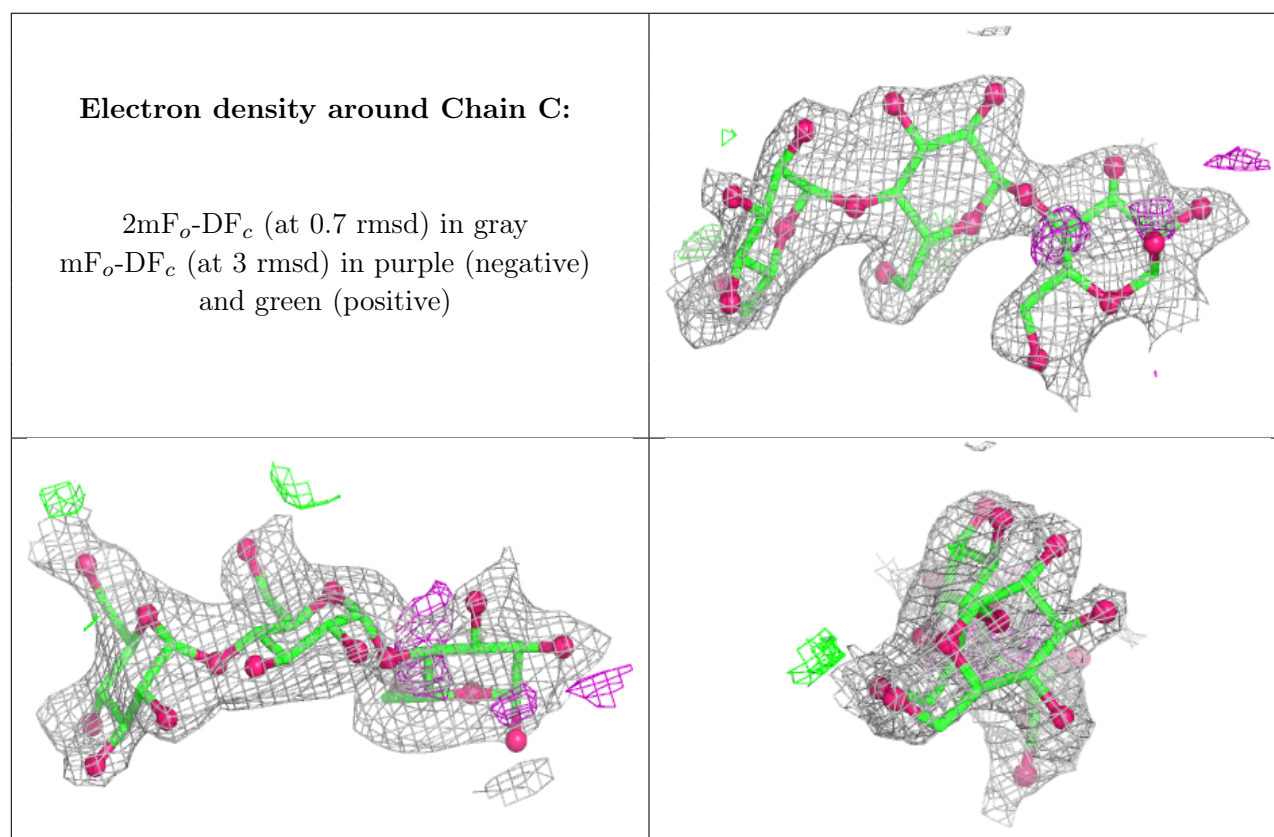
There are no non-standard protein/DNA/RNA residues in this entry.

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.

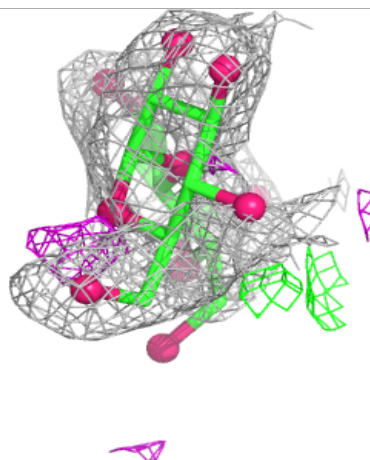
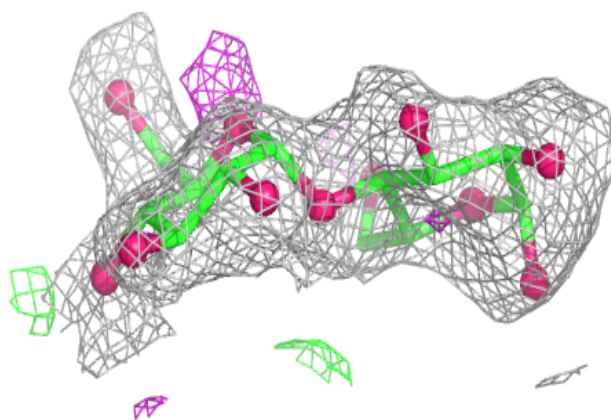
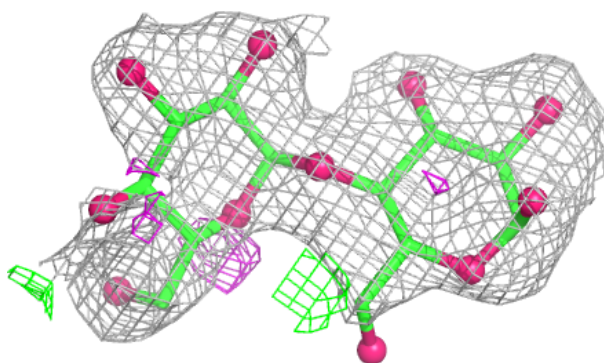
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BGC	E	3	11/12	0.71	0.14	69,71,72,73	0
2	GLC	C	1	12/12	0.75	0.14	57,59,60,62	0
4	GLC	E	1	12/12	0.78	0.18	69,75,77,77	0
3	GLC	D	1	12/12	0.78	0.11	58,61,62,62	0
3	GLC	D	2	11/12	0.80	0.13	50,55,57,58	0
4	GLC	E	2	11/12	0.81	0.13	69,71,72,72	0
2	GLC	C	3	11/12	0.82	0.10	61,61,62,62	0
2	GLC	C	2	11/12	0.90	0.08	51,57,57,58	0

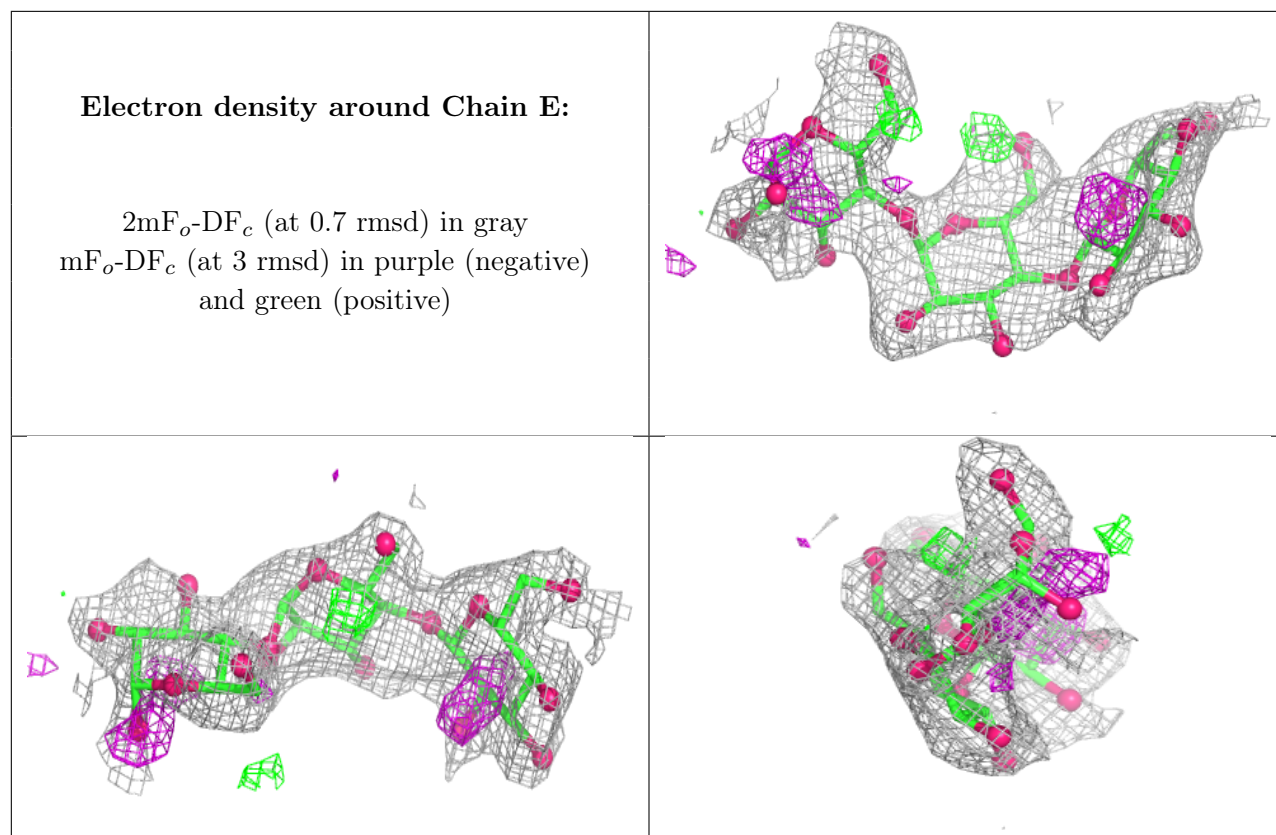
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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
6	ACT	B	752	4/4	0.68	0.17	51,52,52,53	0
7	GOL	B	762	6/6	0.71	0.14	40,44,47,48	0
6	ACT	A	753	4/4	0.81	0.13	58,59,59,59	0
7	GOL	A	761	6/6	0.82	0.12	49,52,53,54	0
6	ACT	A	751	4/4	0.90	0.14	53,53,54,55	0
5	CA	B	742	1/1	0.99	0.02	38,38,38,38	0
5	CA	A	741	1/1	0.99	0.02	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.