Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 07:12 PM EST

PDB ID	:	1ULV
Title	:	Crystal Structure of Glucodextranase Complexed with Acarbose
Authors	:	Mizuno, M.; Tonozuka, T.; Suzuki, S.; Uotsu-Tomita, R.; Kamitori, S.; Nishikawa, A.; Sakano, Y.
Deposited on	:	2003-09-16
Resolution	:	2.42 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 (i)) were used in the production of this report:

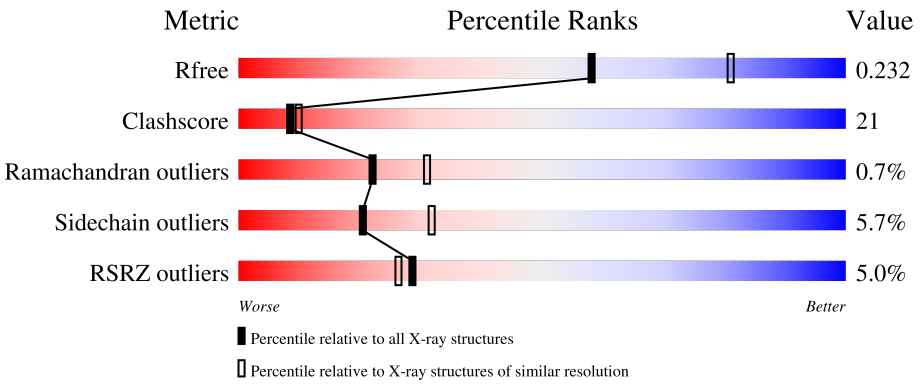
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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-RAY DIFFRACTION

The reported resolution of this entry is 2.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	A	1020	5% 67% 30% .
2	B	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7980 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 glucodextranase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1019	7506	4681	1286	1527	12	0	0	0

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	32	19	1	12	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	6	6	6	0	0

- Molecule 4 is water.

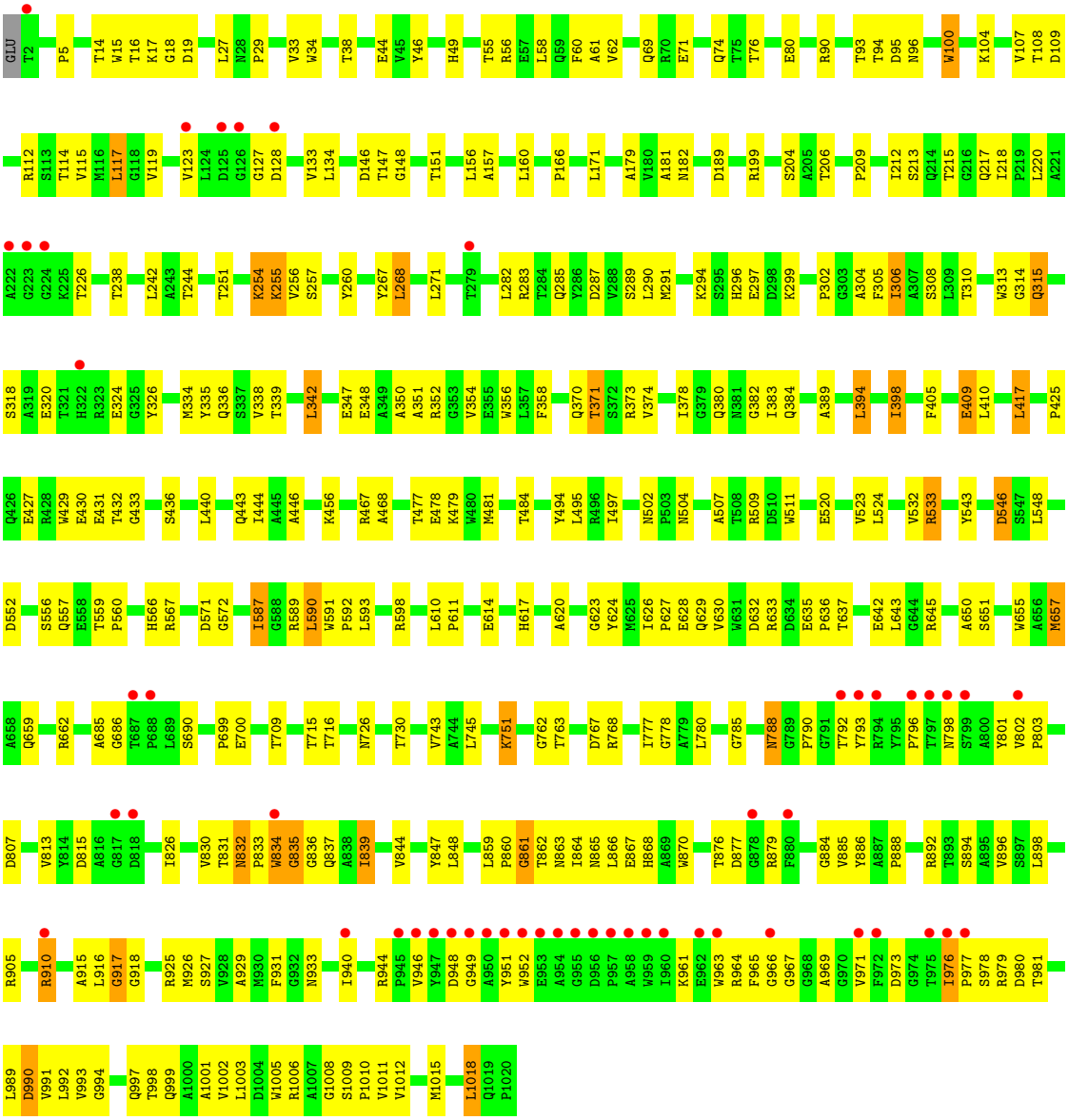
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	436	436	436	0	0

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: glucodextranase

Chain A: 5% 67% 30%



• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	198.79Å 88.25Å 80.99Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	49.59 – 2.42 49.59 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.59-2.42) 98.1 (49.59-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.27 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.238 0.188 , 0.232	Depositor DCC
R_{free} test set	4919 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7980	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA, GLC, AC1

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	0.33	0/7683	0.61	1/10508 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	546	ASP	CB-CG-OD1	7.20	124.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7506	0	7137	306	0
2	B	32	0	19	3	0
3	A	6	0	0	0	0
4	A	436	0	0	14	0
All	All	7980	0	7156	306	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 21.

All (306) 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:133:VAL:HG23	1:A:218:ILE:HD11	1.28	1.14
1:A:371:THR:HG22	1:A:380:GLN:H	1.12	1.14
1:A:29:PRO:HA	1:A:299:LYS:HD2	1.37	1.06
1:A:313:TRP:HA	1:A:315:GLN:HE22	1.23	1.02
1:A:831:THR:HG22	1:A:833:PRO:HD3	1.44	1.00
1:A:104:LYS:HB3	1:A:117:LEU:HD21	1.41	0.99
1:A:123:VAL:HG11	1:A:127:GLY:HA2	1.43	0.96
1:A:285:GLN:HE21	1:A:617:HIS:HD2	1.03	0.96
1:A:339:THR:HG21	1:A:662:ARG:HH21	1.35	0.91
1:A:358:PHE:HB3	1:A:409:GLU:HG3	1.53	0.90
1:A:285:GLN:HE21	1:A:617:HIS:CD2	1.94	0.84
1:A:342:LEU:HD11	1:A:398:ILE:HD11	1.59	0.84
1:A:133:VAL:CG2	1:A:218:ILE:HD11	2.08	0.83
1:A:370:GLN:HE21	1:A:382:GLY:H	1.24	0.83
1:A:342:LEU:HD21	1:A:398:ILE:HD13	1.62	0.82
1:A:925:ARG:HB3	1:A:1015:MET:HG3	1.61	0.80
1:A:17:LYS:HD3	1:A:19:ASP:HB3	1.63	0.80
1:A:339:THR:HG23	1:A:662:ARG:HD3	1.64	0.79
1:A:862:THR:CG2	1:A:864:ILE:HG12	2.12	0.79
1:A:371:THR:HG22	1:A:380:GLN:N	1.96	0.79
1:A:865:ASN:ND2	1:A:1010:PRO:HG2	1.96	0.78
1:A:587:ILE:HG23	1:A:589:ARG:NH2	2.00	0.76
1:A:302:PRO:HB2	1:A:352:ARG:HD2	1.69	0.74
1:A:107:VAL:HG23	1:A:260:TYR:CD2	2.23	0.73
1:A:620:ALA:HB2	1:A:626:ILE:HD13	1.71	0.73
1:A:862:THR:HG21	1:A:864:ILE:HG12	1.69	0.73
1:A:726:ASN:HD21	1:A:751:LYS:H	1.36	0.72
1:A:885:VAL:HG11	1:A:915:ALA:HB1	1.71	0.72
1:A:117:LEU:HD22	1:A:119:VAL:HG22	1.70	0.72
1:A:17:LYS:HA	1:A:315:GLN:HE21	1.53	0.71
1:A:839:ILE:HD13	1:A:839:ILE:H	1.55	0.71
1:A:71:GLU:HB2	1:A:93:THR:HG21	1.71	0.71
1:A:831:THR:CG2	1:A:833:PRO:HD3	2.18	0.71
1:A:289:SER:HA	1:A:657:MET:HG3	1.73	0.70
1:A:14:THR:HG23	1:A:15:TRP:O	1.91	0.70
1:A:33:VAL:HG21	1:A:115:VAL:HG23	1.72	0.70
1:A:285:GLN:NE2	1:A:617:HIS:HD2	1.85	0.70
1:A:884:GLY:HA2	1:A:896:VAL:HG13	1.74	0.70
1:A:49:HIS:CD2	1:A:373:ARG:HH12	2.09	0.69
1:A:342:LEU:HD21	1:A:398:ILE:CD1	2.22	0.69
1:A:590:LEU:HD22	1:A:632:ASP:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD13	1:A:238:THR:CG2	2.23	0.68
1:A:976:ILE:HD13	1:A:976:ILE:H	1.56	0.68
1:A:313:TRP:HA	1:A:315:GLN:NE2	2.02	0.67
1:A:348:GLU:HG2	1:A:352:ARG:NH1	2.10	0.67
1:A:384:GLN:NE2	1:A:430:GLU:HG2	2.10	0.67
1:A:49:HIS:HD2	1:A:373:ARG:HH12	1.39	0.66
1:A:339:THR:HG21	1:A:662:ARG:NH2	2.11	0.66
1:A:993:VAL:HB	1:A:997:GLN:HG3	1.78	0.66
1:A:348:GLU:HG2	1:A:352:ARG:HH11	1.60	0.65
1:A:948:ASP:HB3	1:A:951:TYR:HB3	1.79	0.65
1:A:560:PRO:HG2	4:A:3349:HOH:O	1.96	0.65
1:A:844:VAL:CG1	1:A:876:THR:HB	2.27	0.64
1:A:999:GLN:HA	1:A:1002:VAL:CG1	2.28	0.64
1:A:254:LYS:HE3	1:A:254:LYS:HA	1.79	0.64
1:A:429:TRP:O	1:A:431:GLU:HG3	1.98	0.64
1:A:220:LEU:HD22	1:A:226:THR:HG21	1.81	0.63
1:A:726:ASN:ND2	1:A:751:LYS:H	1.96	0.63
1:A:999:GLN:HA	1:A:1002:VAL:HG12	1.80	0.63
1:A:282:LEU:HD11	1:A:614:GLU:OE2	1.99	0.63
1:A:117:LEU:HD22	1:A:119:VAL:CG2	2.29	0.63
1:A:189:ASP:HB2	1:A:213:SER:OG	1.99	0.63
1:A:156:LEU:HD13	1:A:238:THR:HG23	1.80	0.62
1:A:324:GLU:OE2	1:A:371:THR:HG21	2.00	0.62
1:A:844:VAL:HG13	1:A:876:THR:HB	1.82	0.62
1:A:60:PHE:CE1	1:A:133:VAL:HG22	2.35	0.61
1:A:477:THR:HG22	1:A:494:TYR:OH	2.01	0.61
1:A:306:ILE:HD13	1:A:306:ILE:H	1.65	0.60
1:A:885:VAL:CG1	1:A:894:SER:HB3	2.30	0.60
1:A:587:ILE:CG2	1:A:589:ARG:NH2	2.65	0.60
1:A:49:HIS:CD2	1:A:373:ARG:HH22	2.19	0.60
1:A:220:LEU:CD2	1:A:226:THR:HG21	2.30	0.60
1:A:933:ASN:O	1:A:944:ARG:NH1	2.34	0.60
1:A:859:LEU:O	1:A:862:THR:HB	2.01	0.60
1:A:940:ILE:HG23	1:A:977:PRO:HB2	1.83	0.60
1:A:296:HIS:O	1:A:306:ILE:HD13	2.01	0.60
1:A:371:THR:CG2	1:A:380:GLN:H	2.01	0.60
1:A:965:PHE:CE1	1:A:989:LEU:HD21	2.37	0.59
1:A:107:VAL:HG21	1:A:257:SER:HA	1.84	0.59
1:A:336:GLN:O	1:A:339:THR:HG22	2.03	0.59
1:A:339:THR:CG2	1:A:662:ARG:HH21	2.13	0.59
1:A:886:TYR:CE1	1:A:892:ARG:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ILE:HB	1:A:425:PRO:HG2	1.84	0.59
1:A:484:THR:H	1:A:504:ASN:HD21	1.49	0.59
1:A:383:ILE:HB	1:A:425:PRO:CG	2.33	0.59
1:A:17:LYS:HA	1:A:315:GLN:NE2	2.16	0.58
1:A:218:ILE:N	1:A:218:ILE:HD12	2.17	0.58
1:A:14:THR:HG21	4:A:3268:HOH:O	2.04	0.58
1:A:767:ASP:O	1:A:768:ARG:HD2	2.03	0.58
1:A:867:GLU:HG2	1:A:868:HIS:CE1	2.38	0.58
1:A:49:HIS:HD2	1:A:373:ARG:HH22	1.51	0.58
1:A:251:THR:HG22	1:A:255:LYS:HB3	1.86	0.57
1:A:566:HIS:HE1	1:A:632:ASP:OD1	1.86	0.57
1:A:862:THR:HG22	1:A:864:ILE:HG12	1.87	0.57
1:A:870:TRP:CH2	1:A:888:PRO:HA	2.40	0.57
1:A:839:ILE:HD13	1:A:839:ILE:N	2.20	0.57
1:A:76:THR:HG23	1:A:94:THR:O	2.05	0.56
1:A:929:ALA:HA	1:A:991:VAL:HG12	1.86	0.56
1:A:315:GLN:NE2	1:A:315:GLN:H	2.02	0.56
1:A:813:VAL:HG21	1:A:1018:LEU:HD21	1.86	0.56
1:A:313:TRP:CA	1:A:315:GLN:HE22	2.08	0.56
1:A:633:ARG:HD2	4:A:3105:HOH:O	2.06	0.56
1:A:777:ILE:HD11	1:A:815:ASP:HB2	1.86	0.56
1:A:335:TYR:CD1	1:A:394:LEU:HD13	2.41	0.56
1:A:507:ALA:O	1:A:520:GLU:HG3	2.05	0.56
1:A:994:GLY:O	1:A:997:GLN:HG2	2.05	0.56
1:A:112:ARG:HB2	1:A:244:THR:HG23	1.88	0.55
1:A:160:LEU:HD12	1:A:166:PRO:HB2	1.88	0.55
1:A:832:ASN:HD21	1:A:836:GLY:H	1.54	0.55
1:A:831:THR:HG22	1:A:832:ASN:N	2.22	0.55
1:A:876:THR:HG23	1:A:898:LEU:HD22	1.87	0.55
1:A:623:GLY:O	1:A:624:TYR:HB2	2.07	0.55
1:A:373:ARG:HG2	1:A:373:ARG:HH11	1.72	0.55
1:A:95:ASP:HB2	1:A:100:TRP:CD2	2.42	0.54
1:A:342:LEU:HD13	1:A:350:ALA:HB2	1.89	0.54
1:A:383:ILE:O	1:A:425:PRO:HG2	2.07	0.54
1:A:370:GLN:NE2	1:A:382:GLY:H	2.01	0.54
1:A:636:PRO:O	1:A:636:PRO:HG2	2.07	0.54
1:A:831:THR:HG22	1:A:832:ASN:H	1.72	0.54
1:A:790:PRO:HG2	1:A:792:THR:HG22	1.90	0.54
1:A:989:LEU:O	1:A:990:ASP:HB3	2.06	0.54
1:A:370:GLN:HE21	1:A:382:GLY:N	2.01	0.54
1:A:511:TRP:CE2	1:A:523:VAL:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG21	1:A:115:VAL:CG2	2.37	0.54
1:A:567:ARG:NH1	2:B:2:AC1:O3	2.38	0.54
1:A:839:ILE:HD11	1:A:898:LEU:HD13	1.89	0.54
1:A:916:LEU:O	1:A:918:GLY:N	2.40	0.54
1:A:567:ARG:HD3	1:A:571:ASP:OD2	2.06	0.54
1:A:977:PRO:HA	1:A:979:ARG:HH12	1.73	0.54
1:A:5:PRO:HD3	1:A:204:SER:OG	2.07	0.53
1:A:690:SER:HA	4:A:3161:HOH:O	2.06	0.53
1:A:802:VAL:CG1	1:A:803:PRO:HD2	2.39	0.53
1:A:114:THR:OG1	1:A:244:THR:HG22	2.09	0.53
1:A:268:LEU:HD21	1:A:291:MET:SD	2.48	0.53
1:A:335:TYR:HD1	1:A:394:LEU:HD13	1.73	0.53
1:A:74:GLN:HE21	1:A:95:ASP:HA	1.74	0.53
1:A:432:THR:HB	1:A:509:ARG:HH11	1.73	0.53
1:A:318:SER:HB2	1:A:320:GLU:OE2	2.07	0.53
1:A:440:LEU:HD23	1:A:481:MET:CE	2.38	0.53
1:A:963:TRP:O	1:A:964:ARG:HD3	2.09	0.53
1:A:49:HIS:HD2	1:A:373:ARG:NH1	2.05	0.53
1:A:226:THR:HG22	4:A:3244:HOH:O	2.08	0.52
1:A:1002:VAL:O	1:A:1011:VAL:HB	2.10	0.52
1:A:74:GLN:NE2	1:A:96:ASN:H	2.08	0.52
1:A:1012:VAL:O	1:A:1012:VAL:HG13	2.10	0.52
1:A:910:ARG:HD3	1:A:910:ARG:N	2.24	0.52
1:A:289:SER:CA	1:A:657:MET:HG3	2.39	0.52
1:A:347:GLU:OE1	1:A:398:ILE:HG13	2.10	0.52
1:A:862:THR:HG22	1:A:864:ILE:HG23	1.91	0.51
1:A:305:PHE:HB2	1:A:334:MET:HG3	1.91	0.51
1:A:885:VAL:HG12	1:A:894:SER:HB3	1.90	0.51
1:A:432:THR:HB	1:A:509:ARG:NH1	2.25	0.51
1:A:378:ILE:HG22	4:A:3124:HOH:O	2.10	0.51
1:A:566:HIS:CE1	1:A:590:LEU:HD13	2.46	0.51
1:A:160:LEU:N	1:A:160:LEU:HD22	2.26	0.51
1:A:826:ILE:HD11	1:A:830:VAL:HG22	1.92	0.50
1:A:833:PRO:C	1:A:835:GLY:H	2.14	0.50
1:A:147:THR:O	1:A:157:ALA:HA	2.11	0.50
1:A:479:LYS:HE2	4:A:3269:HOH:O	2.09	0.50
1:A:848:LEU:HD23	1:A:926:MET:HB3	1.93	0.50
1:A:969:ALA:HB2	1:A:1005:TRP:CH2	2.46	0.50
1:A:690:SER:O	1:A:762:GLY:HA3	2.11	0.50
1:A:95:ASP:HB2	1:A:100:TRP:CE3	2.47	0.50
1:A:338:VAL:O	1:A:342:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:THR:O	1:A:1002:VAL:HG12	2.11	0.50
1:A:511:TRP:CZ2	1:A:523:VAL:HG21	2.47	0.49
1:A:552:ASP:OD1	1:A:598:ARG:NH1	2.45	0.49
1:A:58:LEU:HA	1:A:134:LEU:O	2.12	0.49
1:A:156:LEU:HD13	1:A:238:THR:HG21	1.95	0.49
1:A:484:THR:O	1:A:484:THR:CG2	2.61	0.49
1:A:1006:ARG:HH21	1:A:1006:ARG:HG2	1.77	0.49
1:A:940:ILE:HG12	1:A:978:SER:HA	1.95	0.49
1:A:100:TRP:CD1	1:A:100:TRP:C	2.86	0.49
1:A:71:GLU:CB	1:A:93:THR:HG21	2.41	0.49
1:A:884:GLY:HA2	1:A:896:VAL:CG1	2.42	0.48
1:A:572:GLY:HA2	1:A:587:ILE:HA	1.95	0.48
1:A:946:VAL:HG22	1:A:965:PHE:HB2	1.94	0.48
1:A:998:THR:HG23	1:A:1001:ALA:H	1.79	0.48
1:A:358:PHE:CB	1:A:409:GLU:HG3	2.35	0.48
1:A:866:LEU:N	1:A:866:LEU:HD22	2.28	0.48
1:A:16:THR:CG2	1:A:38:THR:HG21	2.43	0.48
1:A:62:VAL:HG11	1:A:100:TRP:CE2	2.48	0.48
1:A:107:VAL:HG23	1:A:260:TYR:CG	2.48	0.48
1:A:283:ARG:NH1	1:A:287:ASP:OD2	2.46	0.48
1:A:952:TRP:NE1	1:A:961:LYS:HA	2.28	0.48
1:A:294:LYS:HD3	1:A:294:LYS:O	2.13	0.47
1:A:477:THR:CG2	1:A:494:TYR:OH	2.62	0.47
1:A:559:THR:HB	1:A:560:PRO:HD2	1.96	0.47
1:A:199:ARG:HH21	1:A:199:ARG:HG3	1.78	0.47
1:A:700:GLU:O	1:A:768:ARG:HG3	2.13	0.47
1:A:976:ILE:H	1:A:976:ILE:CD1	2.25	0.47
1:A:977:PRO:HA	1:A:979:ARG:NH1	2.28	0.47
1:A:610:LEU:N	1:A:611:PRO:HD2	2.30	0.47
1:A:587:ILE:HG23	1:A:589:ARG:HH21	1.79	0.47
1:A:151:THR:HB	1:A:156:LEU:HD11	1.97	0.47
1:A:107:VAL:HG22	1:A:108:THR:N	2.30	0.47
1:A:659:GLN:HE22	1:A:662:ARG:HH11	1.62	0.47
1:A:16:THR:O	1:A:314:GLY:HA3	2.15	0.46
1:A:146:ASP:O	1:A:209:PRO:HA	2.15	0.46
1:A:384:GLN:HE22	1:A:430:GLU:HG2	1.78	0.46
1:A:546:ASP:OD1	1:A:546:ASP:O	2.33	0.46
1:A:715:THR:CG2	1:A:716:THR:N	2.77	0.46
1:A:802:VAL:HG13	1:A:803:PRO:HD2	1.98	0.46
1:A:61:ALA:HA	1:A:69:GLN:O	2.15	0.46
1:A:796:PRO:HG2	1:A:801:TYR:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:HB2	1:A:305:PHE:CE2	2.51	0.46
1:A:34:TRP:HB2	1:A:46:TYR:HB2	1.98	0.46
1:A:16:THR:CG2	1:A:17:LYS:N	2.79	0.46
1:A:633:ARG:HG3	1:A:633:ARG:HH11	1.81	0.46
1:A:313:TRP:CA	1:A:315:GLN:NE2	2.75	0.46
1:A:961:LYS:HG2	1:A:961:LYS:O	2.16	0.46
1:A:940:ILE:CG2	1:A:977:PRO:HB2	2.46	0.46
1:A:655:TRP:HD1	1:A:655:TRP:O	1.99	0.46
1:A:780:LEU:HB3	1:A:992:LEU:HD23	1.98	0.45
1:A:335:TYR:OH	1:A:533:ARG:NH1	2.49	0.45
1:A:49:HIS:HD2	1:A:373:ARG:NH2	2.13	0.45
1:A:55:THR:HG23	4:A:3279:HOH:O	2.17	0.45
1:A:837:GLN:O	1:A:839:ILE:HD13	2.17	0.45
1:A:179:ALA:H	1:A:217:GLN:HB3	1.82	0.45
1:A:326:TYR:CZ	2:B:2:AC1:HC7	2.52	0.45
1:A:335:TYR:O	1:A:339:THR:HB	2.17	0.45
1:A:440:LEU:HA	1:A:443:GLN:OE1	2.17	0.45
1:A:627:PRO:HB3	1:A:651:SER:OG	2.17	0.45
1:A:148:GLY:HA3	1:A:182:ASN:ND2	2.31	0.45
1:A:861:GLY:HA3	1:A:940:ILE:O	2.17	0.45
1:A:813:VAL:CG2	1:A:1018:LEU:HD21	2.47	0.44
1:A:951:TYR:CE2	1:A:971:VAL:HA	2.52	0.44
1:A:792:THR:O	1:A:967:GLY:HA3	2.18	0.44
1:A:405:PHE:O	1:A:409:GLU:HB2	2.17	0.44
1:A:436:SER:O	1:A:440:LEU:HB2	2.17	0.44
1:A:590:LEU:O	1:A:629:GLN:HA	2.18	0.44
1:A:948:ASP:OD2	1:A:949:GLY:N	2.50	0.44
1:A:620:ALA:O	1:A:645:ARG:NH1	2.51	0.44
1:A:628:GLU:HG2	1:A:629:GLN:HG3	2.00	0.44
1:A:44:GLU:HG3	1:A:55:THR:O	2.17	0.44
1:A:383:ILE:HB	1:A:425:PRO:HG3	2.00	0.44
1:A:620:ALA:HB2	1:A:626:ILE:CD1	2.46	0.44
1:A:978:SER:C	1:A:980:ASP:H	2.20	0.44
1:A:109:ASP:HA	1:A:256:VAL:HG13	1.99	0.43
1:A:778:GLY:HA3	1:A:1018:LEU:HB3	1.99	0.43
1:A:862:THR:HG23	1:A:931:PHE:CE2	2.53	0.43
1:A:212:ILE:C	1:A:212:ILE:HD12	2.39	0.43
1:A:58:LEU:C	1:A:58:LEU:HD23	2.39	0.43
1:A:793:TYR:HA	1:A:966:GLY:O	2.19	0.43
1:A:862:THR:O	1:A:863:ASN:HB2	2.18	0.43
1:A:867:GLU:HG2	1:A:868:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:HG22	1:A:56:ARG:N	2.34	0.43
1:A:308:SER:OG	1:A:310:THR:HG22	2.19	0.43
1:A:1005:TRP:HA	1:A:1008:GLY:O	2.18	0.43
1:A:467:ARG:NH1	4:A:3057:HOH:O	2.52	0.43
1:A:699:PRO:HG2	1:A:768:ARG:HG2	2.00	0.43
1:A:973:ASP:O	1:A:979:ARG:HA	2.18	0.43
1:A:532:VAL:HG22	4:A:3046:HOH:O	2.19	0.43
1:A:976:ILE:HB	1:A:977:PRO:HD2	2.01	0.43
1:A:304:ALA:HB2	1:A:356:TRP:CE2	2.54	0.43
1:A:127:GLY:O	1:A:128:ASP:HB2	2.18	0.42
1:A:630:VAL:HA	1:A:645:ARG:O	2.18	0.42
1:A:973:ASP:HB2	1:A:981:THR:HG22	2.00	0.42
1:A:351:ALA:O	1:A:354:VAL:HG12	2.20	0.42
1:A:389:ALA:HB1	1:A:446:ALA:HB2	2.01	0.42
1:A:587:ILE:HG23	1:A:589:ARG:CZ	2.48	0.42
1:A:798:ASN:ND2	1:A:963:TRP:CZ2	2.87	0.42
1:A:685:ALA:HB3	4:A:3111:HOH:O	2.20	0.42
1:A:74:GLN:HE21	1:A:96:ASN:H	1.68	0.42
1:A:297:GLU:CD	1:A:352:ARG:HH21	2.22	0.42
1:A:593:LEU:C	1:A:593:LEU:HD12	2.40	0.42
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.93	0.42
1:A:148:GLY:O	1:A:206:THR:HA	2.20	0.41
1:A:484:THR:O	1:A:484:THR:HG22	2.20	0.41
1:A:636:PRO:O	1:A:636:PRO:CG	2.68	0.41
1:A:862:THR:HG23	1:A:931:PHE:CZ	2.54	0.41
1:A:80:GLU:CD	1:A:90:ARG:HH21	2.24	0.41
1:A:504:ASN:N	1:A:504:ASN:HD22	2.17	0.41
1:A:49:HIS:HB3	1:A:374:VAL:HG21	2.02	0.41
1:A:90:ARG:HD3	4:A:3186:HOH:O	2.19	0.41
1:A:430:GLU:OE1	2:B:2:AC1:N4A	2.54	0.41
1:A:788:ASN:HD22	1:A:788:ASN:H	1.68	0.41
1:A:552:ASP:HA	1:A:556:SER:HB3	2.02	0.41
1:A:785:GLY:N	1:A:807:ASP:OD1	2.48	0.41
1:A:14:THR:HG21	1:A:315:GLN:O	2.21	0.41
1:A:847:TYR:O	1:A:926:MET:HA	2.20	0.41
1:A:112:ARG:HD3	1:A:244:THR:HG23	2.02	0.41
1:A:478:GLU:HG2	1:A:543:TYR:CD2	2.54	0.41
1:A:18:GLY:HA2	1:A:310:THR:OG1	2.20	0.41
1:A:199:ARG:HG3	1:A:199:ARG:NH2	2.35	0.41
1:A:310:THR:HA	4:A:3137:HOH:O	2.20	0.41
1:A:433:GLY:C	1:A:497:ILE:HD11	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD23	1:A:481:MET:HE2	2.02	0.41
1:A:877:ASP:OD1	1:A:879:ARG:HB3	2.21	0.41
1:A:916:LEU:O	1:A:917:GLY:C	2.60	0.41
1:A:1009:SER:HA	1:A:1010:PRO:C	2.42	0.41
1:A:1002:VAL:HG13	1:A:1003:LEU:HD13	2.03	0.41
1:A:591:TRP:HA	1:A:592:PRO:HD2	1.97	0.40
1:A:440:LEU:O	1:A:444:ILE:HG13	2.22	0.40
1:A:468:ALA:HA	1:A:763:THR:OG1	2.22	0.40
1:A:310:THR:HG21	1:A:650:ALA:HA	2.03	0.40
1:A:315:GLN:HE21	1:A:315:GLN:H	1.67	0.40
1:A:866:LEU:HD12	1:A:927:SER:CB	2.52	0.40
1:A:27:LEU:HD13	1:A:27:LEU:O	2.22	0.40
1:A:181:ALA:HB3	1:A:215:THR:CG2	2.51	0.40
1:A:206:THR:HG22	4:A:3215:HOH:O	2.21	0.40
1:A:267:TYR:CZ	1:A:271:LEU:HD11	2.56	0.40
1:A:709:THR:HA	1:A:743:VAL:O	2.21	0.40
1:A:788:ASN:HD22	1:A:788:ASN:C	2.24	0.40
1:A:69:GLN:OE1	1:A:100:TRP:CH2	2.75	0.40
1:A:946:VAL:HG22	1:A:965:PHE:CB	2.52	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	1017/1020 (100%)	963 (95%)	47 (5%)	7 (1%)	22 31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	860	PRO
1	A	917	GLY

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Mol	Chain	Res	Type
1	A	637	THR
1	A	834	TRP
1	A	835	GLY
1	A	861	GLY
1	A	686	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	752/753 (100%)	709 (94%)	43 (6%)	20 32

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	TRP
1	A	117	LEU
1	A	171	LEU
1	A	242	LEU
1	A	254	LYS
1	A	255	LYS
1	A	268	LEU
1	A	290	LEU
1	A	306	ILE
1	A	315	GLN
1	A	342	LEU
1	A	371	THR
1	A	394	LEU
1	A	398	ILE
1	A	409	GLU
1	A	410	LEU
1	A	417	LEU
1	A	427	GLU
1	A	456	LYS
1	A	495	LEU
1	A	502	ASN

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Mol	Chain	Res	Type
1	A	524	LEU
1	A	533	ARG
1	A	548	LEU
1	A	557	GLN
1	A	587	ILE
1	A	590	LEU
1	A	635	GLU
1	A	642	GLU
1	A	643	LEU
1	A	657	MET
1	A	730	THR
1	A	745	LEU
1	A	751	LYS
1	A	788	ASN
1	A	832	ASN
1	A	834	TRP
1	A	839	ILE
1	A	905	ARG
1	A	910	ARG
1	A	976	ILE
1	A	990	ASP
1	A	1018	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	74	GLN
1	A	182	ASN
1	A	214	GLN
1	A	285	GLN
1	A	315	GLN
1	A	370	GLN
1	A	408	ASN
1	A	502	ASN
1	A	504	ASN
1	A	557	GLN
1	A	566	HIS
1	A	607	GLN
1	A	617	HIS
1	A	641	HIS
1	A	659	GLN

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Mol	Chain	Res	Type
1	A	677	GLN
1	A	726	ASN
1	A	788	ASN
1	A	832	ASN
1	A	841	HIS
1	A	845	ASN
1	A	863	ASN
1	A	868	HIS
1	A	906	GLN
1	A	987	ASN
1	A	1019	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	B	1	2	11,11,12	1.75	4 (36%)	15,15,17	1.24	1 (6%)
2	AC1	B	2	2	21,22,23	2.93	10 (47%)	22,32,34	1.13	2 (9%)

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	B	1	2	-	0/2/19/22	0/1/1/1
2	AC1	B	2	2	-	2/6/43/46	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	AC1	C4A-C5B	7.59	1.57	1.51
2	B	2	AC1	C7B-C5B	5.99	1.41	1.32
2	B	2	AC1	C3B-C4A	4.21	1.59	1.53
2	B	2	AC1	C2B-C1B	3.84	1.58	1.52
2	B	2	AC1	O5-C5	3.55	1.51	1.43
2	B	2	AC1	C2-C3	3.10	1.57	1.52
2	B	1	GLC	C2-C3	2.98	1.56	1.52
2	B	2	AC1	C1B-C7B	2.93	1.54	1.50
2	B	1	GLC	O5-C5	2.66	1.48	1.43
2	B	2	AC1	C1B-N4A	2.65	1.52	1.47
2	B	1	GLC	C4-C3	2.55	1.58	1.52
2	B	2	AC1	O5-C1	2.29	1.47	1.43
2	B	1	GLC	O4-C4	2.19	1.48	1.43
2	B	2	AC1	C4-N4A	2.04	1.50	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	GLC	C1-O5-C5	2.57	115.68	112.19
2	B	2	AC1	O4-C4A-C3B	-2.51	105.36	110.53
2	B	2	AC1	C2-C3-C4	-2.49	108.43	110.63

There are no chirality outliers.

All (2) torsion outliers are listed below:

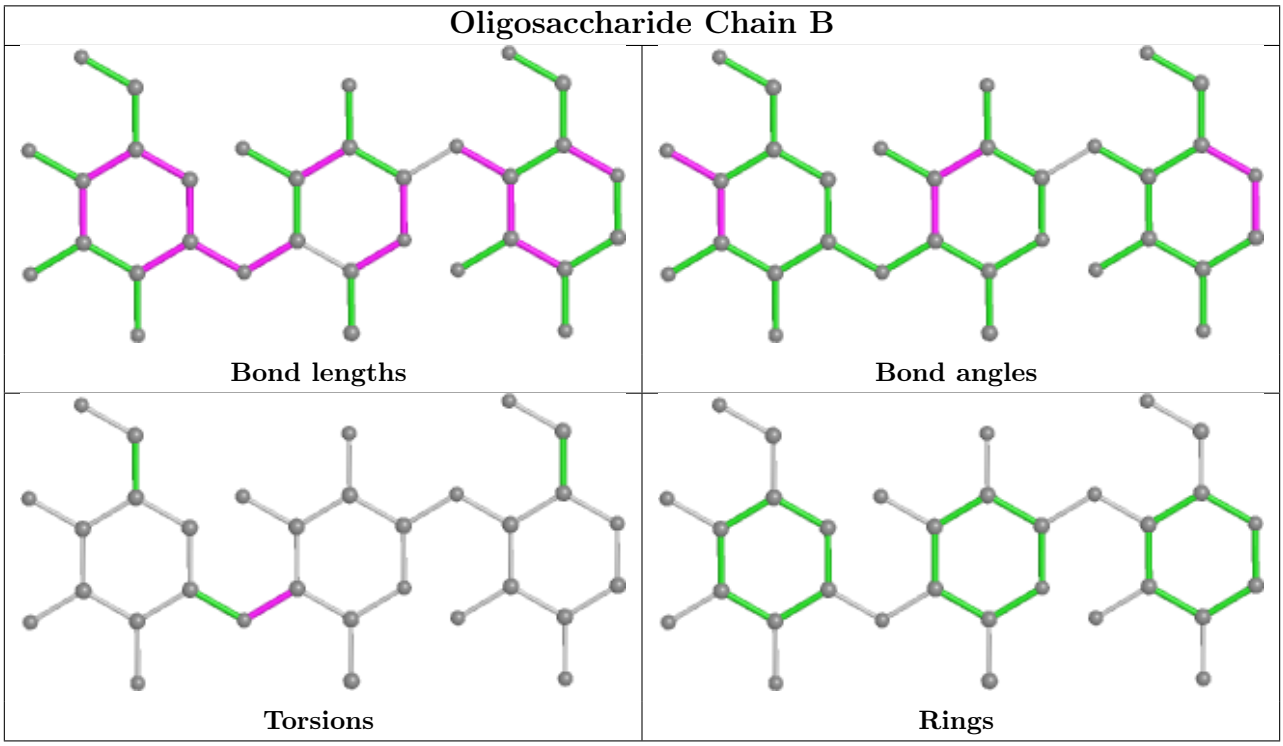
Mol	Chain	Res	Type	Atoms
2	B	2	AC1	C3-C4-N4A-C1B
2	B	2	AC1	C5-C4-N4A-C1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	AC1	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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1019/1020 (99%)	0.01	51 (5%)	28	26	8, 23, 52, 76	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	959	TRP	5.9
1	A	2	THR	5.7
1	A	958	ALA	5.1
1	A	956	ASP	5.0
1	A	954	ALA	4.8
1	A	963	TRP	4.8
1	A	952	TRP	4.6
1	A	972	PHE	4.4
1	A	802	VAL	4.2
1	A	960	ILE	4.2
1	A	794	ARG	4.1
1	A	224	GLY	4.0
1	A	951	TYR	3.9
1	A	797	THR	3.8
1	A	955	GLY	3.7
1	A	128	ASP	3.5
1	A	687	THR	3.5
1	A	953	GLU	3.4
1	A	957	PRO	3.4
1	A	949	GLY	3.3
1	A	940	ILE	3.3
1	A	945	PRO	3.1
1	A	962	GLU	3.1
1	A	948	ASP	3.0
1	A	796	PRO	2.9
1	A	799	SER	2.7
1	A	975	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	947	TYR	2.6
1	A	880	PHE	2.6
1	A	977	PRO	2.6
1	A	950	ALA	2.6
1	A	834	TRP	2.6
1	A	279	THR	2.5
1	A	878	GLY	2.5
1	A	126	GLY	2.4
1	A	125	ASP	2.4
1	A	976	ILE	2.3
1	A	223	GLY	2.3
1	A	793	TYR	2.3
1	A	971	VAL	2.3
1	A	966	GLY	2.3
1	A	222	ALA	2.3
1	A	792	THR	2.2
1	A	688	PRO	2.2
1	A	946	VAL	2.2
1	A	817	GLY	2.2
1	A	910	ARG	2.1
1	A	322	HIS	2.1
1	A	123	VAL	2.1
1	A	798	ASN	2.1
1	A	818	ASP	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.

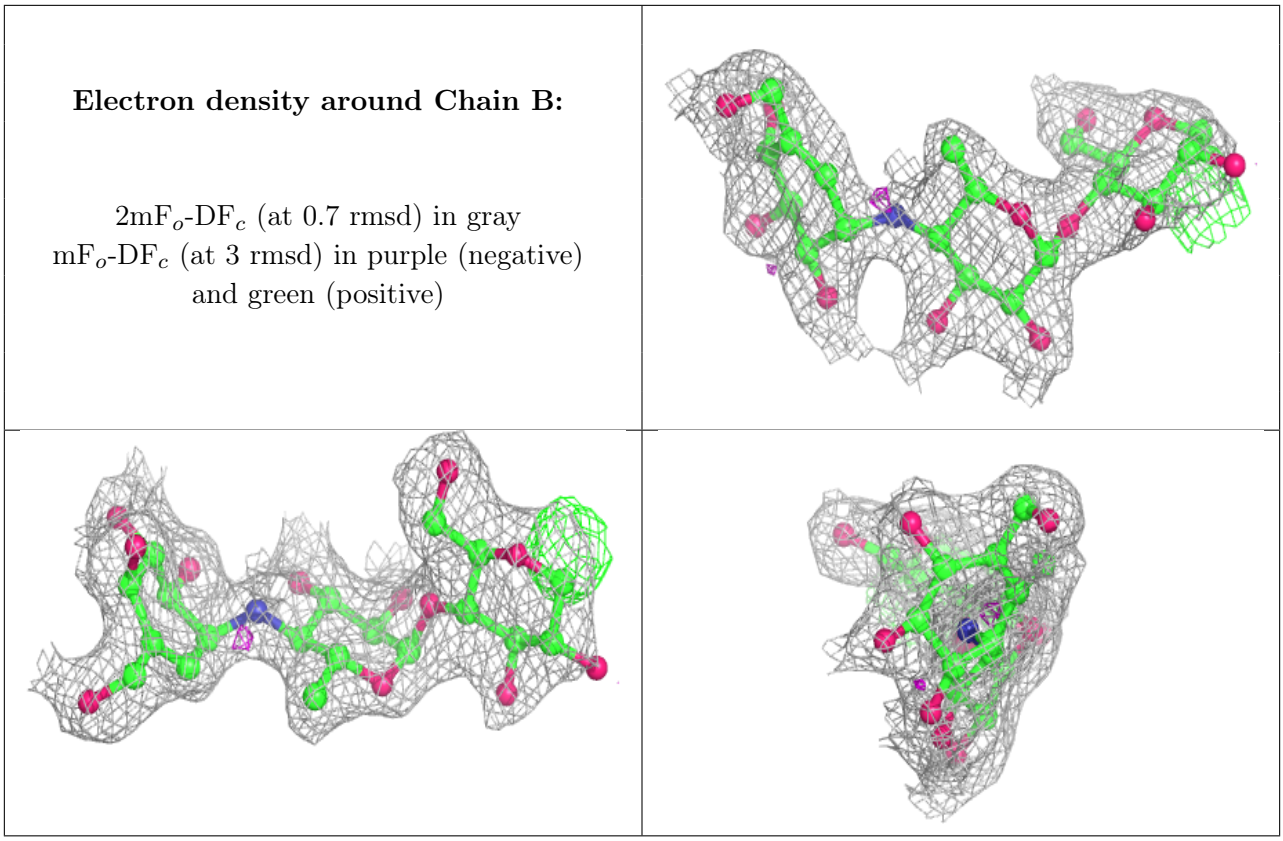
6.3 Carbohydrates (i)

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	B	1	11/12	0.81	0.22	32,39,44,46	0
2	AC1	B	2	21/22	0.95	0.15	15,18,24,26	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. 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(Å^2)	Q<0.9
3	CA	A	2001	1/1	0.95	0.09	36,36,36,36	0
3	CA	A	2006	1/1	0.96	0.07	36,36,36,36	0
3	CA	A	2005	1/1	0.98	0.07	26,26,26,26	0
3	CA	A	2002	1/1	0.98	0.09	34,34,34,34	0
3	CA	A	2003	1/1	0.99	0.04	27,27,27,27	0
3	CA	A	2004	1/1	0.99	0.05	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.