



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:54 AM UTC

PDB ID : 1ULV / pdb_00001ulv
Title : Crystal Structure of Glucodextranase Complexed with Acarbose
Authors : Mizuno, M.; Tonozuka, T.; Suzuki, S.; Uotsu-Tomita, R.; Kamitori, S.;
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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 ⓘ 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

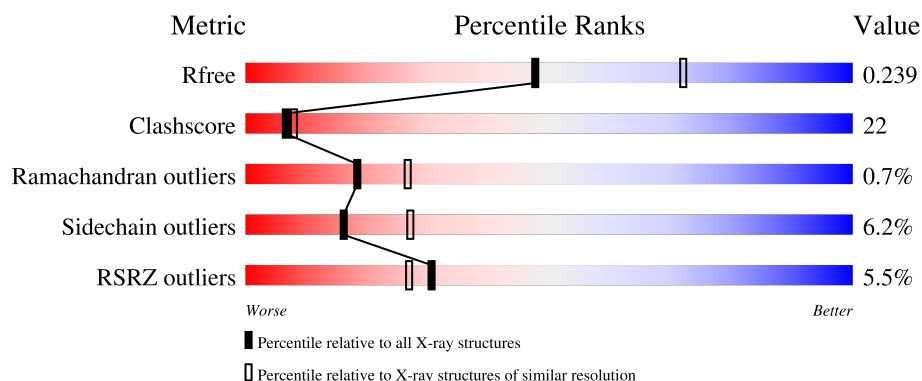
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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 $\leq 5\%$. 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	1020	5% 65% 30% .
2	B	2	50% 50%

2 Entry composition

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
1	A	1019	Total	C	N	O	S	0	0	0
			7506	4681	1286	1527	12			

- 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
2	B	2	Total	C	N	O	0	0	0
			32	19	1	12			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

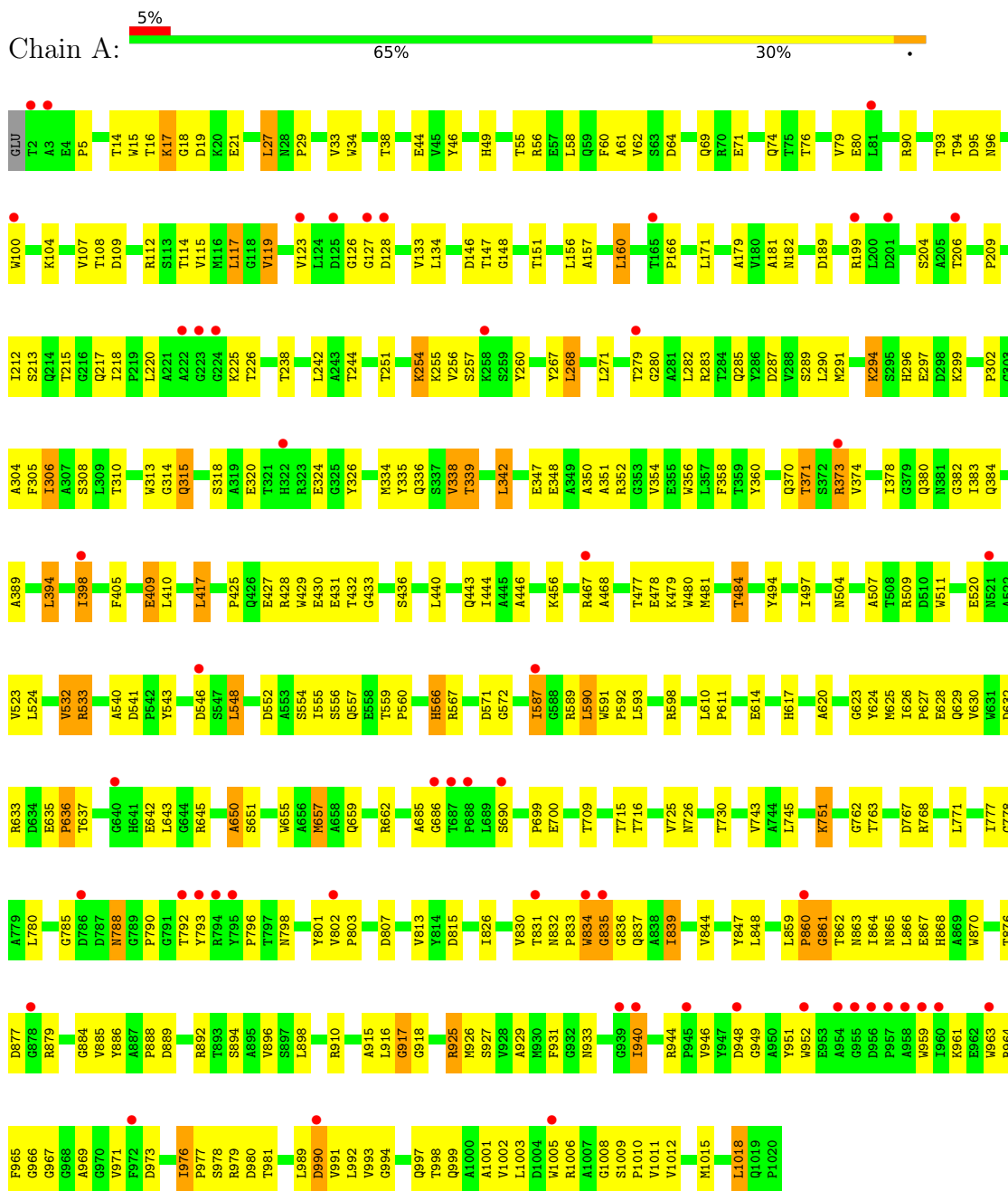
- Molecule 4 is water.

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

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: glucodextranase



- 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:



GLC1
GLC2

4 Data and refinement statistics

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) 98.3 (49.59-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.27 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.238 0.196 , 0.239	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 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h-2*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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, AC1, CA

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	0.39	0/7683	0.90	15/10508 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLY	N-CA-C	-7.55	106.36	114.67
1	A	566	HIS	N-CA-C	-7.32	99.98	110.59
1	A	64	ASP	N-CA-C	-6.52	105.24	113.72
1	A	548	LEU	N-CA-C	6.34	117.89	110.97
1	A	119	VAL	N-CA-C	6.21	117.42	108.48
1	A	27	LEU	N-CA-C	-5.76	105.14	111.82
1	A	428	ARG	N-CA-C	5.57	119.18	112.38
1	A	650	ALA	N-CA-C	5.56	118.42	110.24
1	A	373	ARG	N-CA-C	-5.56	103.36	110.53
1	A	555	ILE	N-CA-C	5.29	118.28	113.20
1	A	360	TYR	N-CA-C	5.26	119.69	113.12
1	A	554	SER	N-CA-C	5.16	116.98	111.36
1	A	636	PRO	N-CA-C	-5.13	101.90	112.47
1	A	480	TRP	N-CA-C	5.04	118.58	112.23
1	A	225	LYS	N-CA-C	5.02	117.76	109.72

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	317	0
2	B	32	0	19	3	0
3	A	6	0	0	0	0
4	A	436	0	0	15	0
All	All	7980	0	7156	317	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 22.

All (317) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:833:PRO:C	1:A:835:GLY:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:100:TRP:CD1	1:A:100:TRP:C	2.86	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:998:THR:O	1:A:1002:VAL:HG12	2.11	0.50
1:A:978:SER:C	1:A:980:ASP:H	2.20	0.49
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: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:58:LEU:C	1:A:58:LEU:HD23	2.39	0.48
1:A:212:ILE:C	1:A:212:ILE:HD12	2.39	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:297:GLU:CD	1:A:352:ARG:HH21	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD23	1:A:481:MET:HE1	1.95	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:593:LEU:C	1:A:593:LEU:HD12	2.40	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
1:A:1015:MET:HE3	4:A:3099:HOH:O	2.15	0.46
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:80:GLU:CD	1:A:90:ARG:HH21	2.24	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:959:TRP:H	1:A:959:TRP:CD1	2.34	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:433:GLY:C	1:A:497:ILE:HD11	2.41	0.45
1:A:916:LEU:O	1:A:917:GLY:C	2.60	0.45
1:A:1009:SER:HA	1:A:1010:PRO:C	2.42	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:625:MET:HA	1:A:657:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:788:ASN:C	1:A:788:ASN:HD22	2.24	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:540:ALA:O	1:A:541:ASP:C	2.60	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: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:860:PRO:C	1:A:862:THR:H	2.25	0.43
1:A:978:SER:C	1:A:980:ASP:N	2.76	0.43
1:A:655:TRP:CD1	1:A:655:TRP:C	2.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:889:ASP:OD1	1:A:889:ASP:C	2.63	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:279:THR:O	1:A:280:GLY:C	2.64	0.41
1:A:310:THR:HA	4:A:3137:HOH:O	2.20	0.41
1:A:833:PRO:C	1:A:835:GLY:N	2.78	0.41
1:A:877:ASP:OD1	1:A:879:ARG:HB3	2.21	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:21:GLU:CD	1:A:79:VAL:HG21	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HA	1:A:743:VAL:O	2.21	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%)	18	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	860	PRO
1	A	917	GLY
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%)	705 (94%)	47 (6%)	16	27

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	117	LEU
1	A	160	LEU
1	A	171	LEU
1	A	242	LEU
1	A	254	LYS
1	A	268	LEU
1	A	290	LEU
1	A	294	LYS
1	A	306	ILE
1	A	315	GLN
1	A	338	VAL
1	A	339	THR
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	484	THR
1	A	524	LEU
1	A	532	VAL
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	725	VAL
1	A	730	THR
1	A	745	LEU
1	A	751	LYS

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Mol	Chain	Res	Type
1	A	771	LEU
1	A	788	ASN
1	A	834	TRP
1	A	839	ILE
1	A	925	ARG
1	A	940	ILE
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	361	GLN
1	A	363	GLN
1	A	370	GLN
1	A	397	GLN
1	A	408	ASN
1	A	502	ASN
1	A	504	ASN
1	A	557	GLN
1	A	566	HIS
1	A	617	HIS
1	A	641	HIS
1	A	659	GLN
1	A	677	GLN
1	A	726	ASN
1	A	788	ASN
1	A	832	ASN
1	A	845	ASN
1	A	863	ASN
1	A	868	HIS
1	A	906	GLN
1	A	987	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	B	1	2	11,11,12	1.73	4 (36%)	15,15,17	1.19	1 (6%)
2	AC1	B	2	2	21,22,23	2.96	10 (47%)	22,32,34	1.00	1 (4%)

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	7.67	1.57	1.51
2	B	2	AC1	C7B-C5B	5.89	1.41	1.32
2	B	2	AC1	C3B-C4A	4.38	1.59	1.53
2	B	2	AC1	C2B-C1B	3.88	1.58	1.53
2	B	2	AC1	O5-C5	3.83	1.51	1.43
2	B	2	AC1	C2-C3	3.00	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	AC1	C1B-C7B	2.93	1.54	1.50
2	B	1	GLC	C2-C3	2.88	1.56	1.52
2	B	1	GLC	O5-C5	2.77	1.48	1.43
2	B	2	AC1	C1B-N4A	2.71	1.52	1.47
2	B	1	GLC	C4-C3	2.50	1.58	1.52
2	B	2	AC1	C5-C4	2.29	1.60	1.53
2	B	2	AC1	O5-C1	2.19	1.47	1.43
2	B	1	GLC	O4-C4	2.09	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	C1-O5-C5	2.60	115.68	112.19
2	B	2	AC1	O4-C4A-C3B	-2.49	105.36	110.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

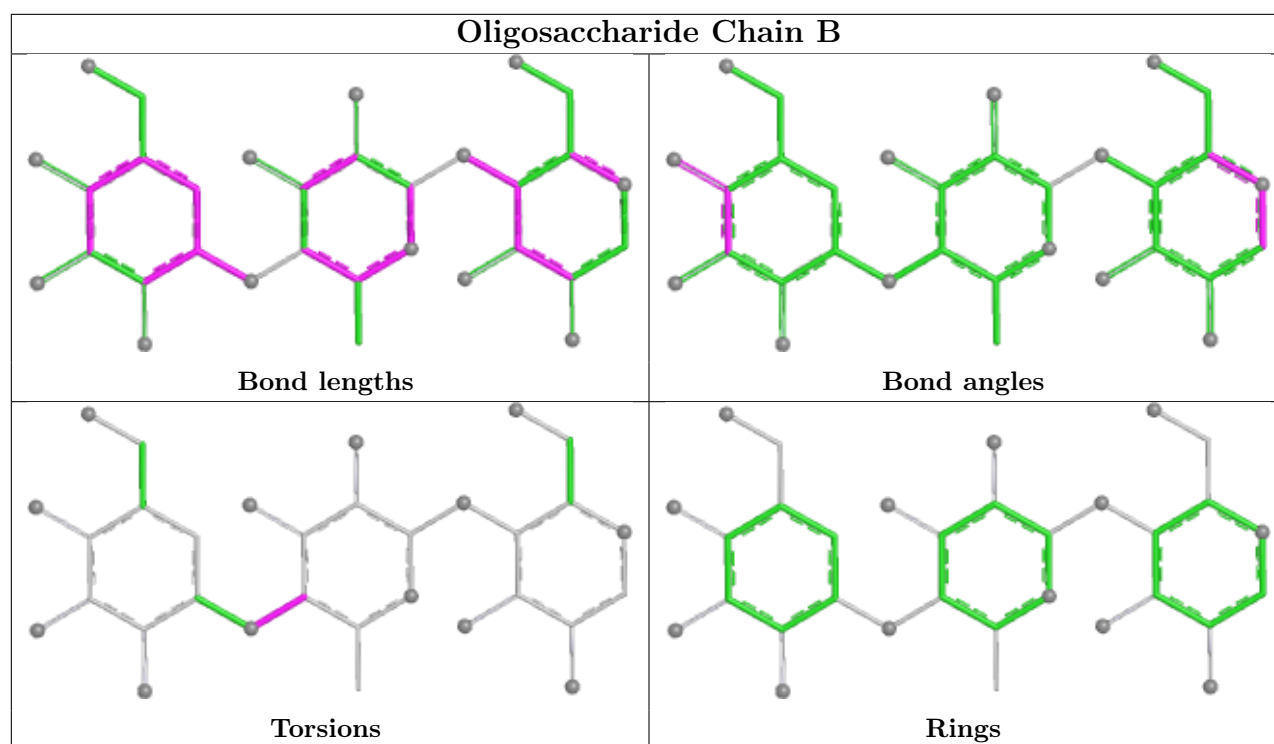
Mol	Chain	Res	Type	Atoms
2	B	2	AC1	C3-C4-N4A-C1B
2	B	2	AC1	C5-C4-N4A-C1B

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1019/1020 (99%)	0.07	56 (5%)	30 27	8, 23, 52, 76	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	GLY	5.4
1	A	2	THR	4.3
1	A	956	ASP	4.1
1	A	687	THR	4.0
1	A	958	ALA	3.8
1	A	125	ASP	3.6
1	A	834	TRP	3.4
1	A	963	TRP	3.3
1	A	688	PRO	3.3
1	A	128	ASP	3.2
1	A	792	THR	3.2
1	A	952	TRP	3.1
1	A	972	PHE	3.1
1	A	990	ASP	3.1
1	A	690	SER	3.0
1	A	794	ARG	3.0
1	A	940	ILE	2.9
1	A	3	ALA	2.9
1	A	959	TRP	2.9
1	A	686	GLY	2.9
1	A	954	ALA	2.8
1	A	1005	TRP	2.8
1	A	878	GLY	2.7
1	A	948	ASP	2.7
1	A	955	GLY	2.6
1	A	945	PRO	2.6
1	A	831	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	279	THR	2.6
1	A	640	GLY	2.5
1	A	860	PRO	2.5
1	A	100	TRP	2.5
1	A	960	ILE	2.5
1	A	786	ASP	2.4
1	A	127	GLY	2.4
1	A	199	ARG	2.4
1	A	81	LEU	2.4
1	A	802	VAL	2.4
1	A	939	GLY	2.3
1	A	835	GLY	2.3
1	A	206	THR	2.3
1	A	398	ILE	2.3
1	A	467	ARG	2.2
1	A	587	ILE	2.2
1	A	201	ASP	2.2
1	A	223	GLY	2.1
1	A	521	ASN	2.1
1	A	258	LYS	2.1
1	A	322	HIS	2.1
1	A	793	TYR	2.0
1	A	123	VAL	2.0
1	A	373	ARG	2.0
1	A	222	ALA	2.0
1	A	165	THR	2.0
1	A	546	ASP	2.0
1	A	957	PRO	2.0
1	A	795	TYR	2.0

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

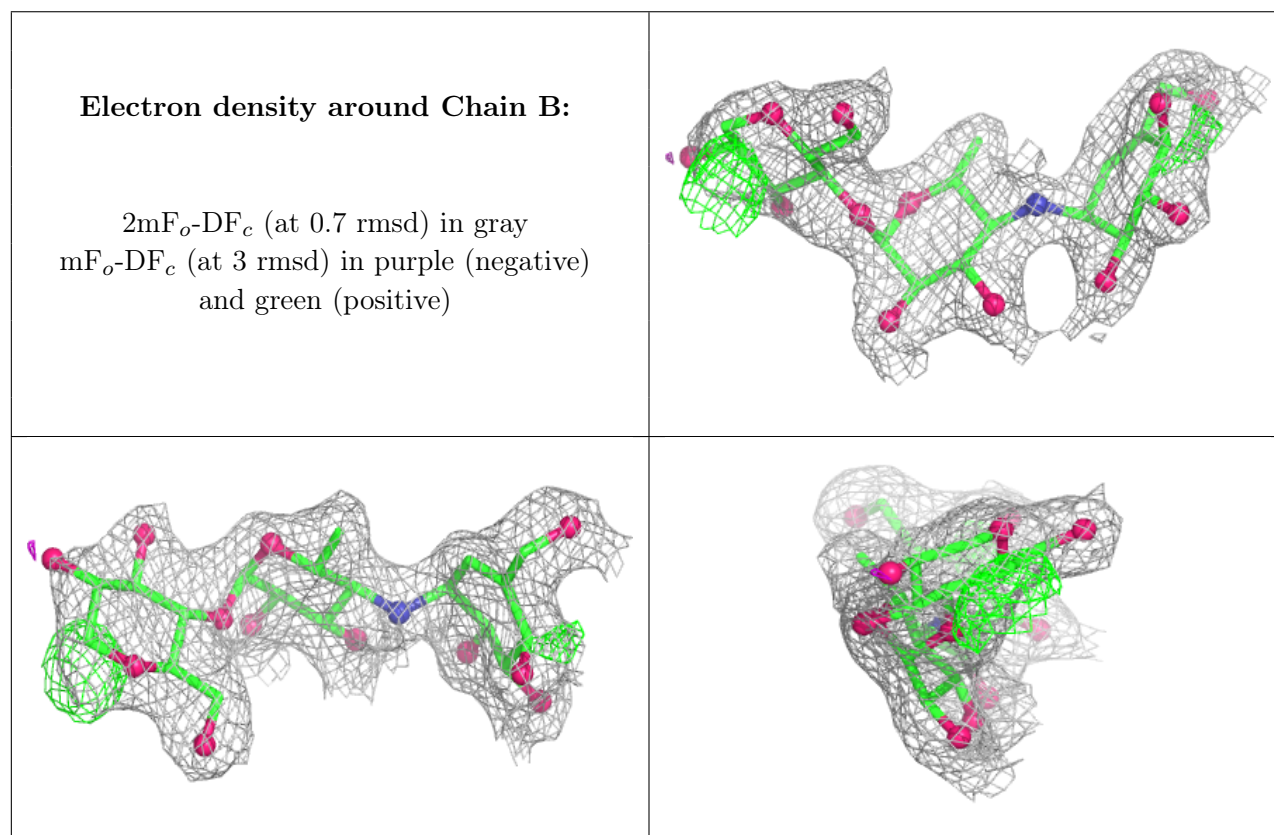
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	GLC	B	1	11/12	0.80	0.14	32,39,44,46	0
2	AC1	B	2	21/22	0.93	0.08	15,18,24,26	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 ⓘ

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
3	CA	A	2006	1/1	0.96	0.04	36,36,36,36	0
3	CA	A	2005	1/1	0.97	0.04	26,26,26,26	0
3	CA	A	2002	1/1	0.97	0.10	34,34,34,34	0
3	CA	A	2001	1/1	0.98	0.08	36,36,36,36	0
3	CA	A	2003	1/1	0.98	0.06	27,27,27,27	0
3	CA	A	2004	1/1	0.99	0.03	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.