Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:18 AM JST

PDB ID	:	7EKW
Title	:	Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (D535N) in complex with maltotetrose
Authors	:	Shen, M.; Xiang, S.
Deposited on	:	2021-04-07
Resolution	:	3.10 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:

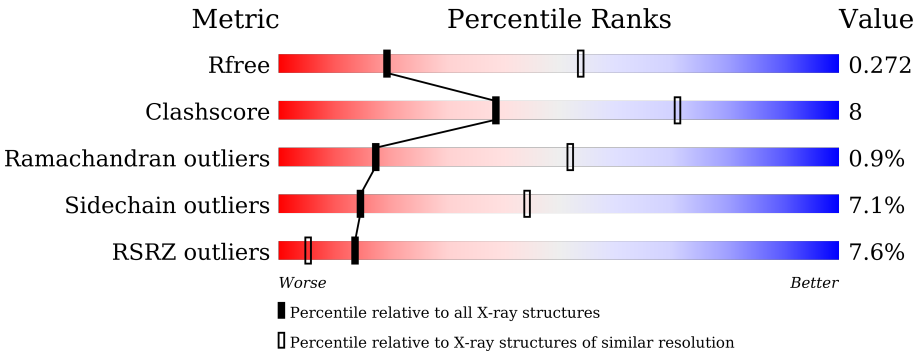
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	1536	7% 77% 20%
1	B	1536	8% 76% 22%
2	C	2	100%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24530 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 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1520	Total	C	N	O	S	0	0	0
			12229	7800	2058	2319	52			
1	B	1526	Total	C	N	O	S	0	0	0
			12278	7830	2066	2330	52			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	ASN	ASP	engineered mutation	UNP Q6FSK0
A	1529	LEU	-	expression tag	UNP Q6FSK0
A	1530	GLU	-	expression tag	UNP Q6FSK0
A	1531	HIS	-	expression tag	UNP Q6FSK0
A	1532	HIS	-	expression tag	UNP Q6FSK0
A	1533	HIS	-	expression tag	UNP Q6FSK0
A	1534	HIS	-	expression tag	UNP Q6FSK0
A	1535	HIS	-	expression tag	UNP Q6FSK0
A	1536	HIS	-	expression tag	UNP Q6FSK0
B	535	ASN	ASP	engineered mutation	UNP Q6FSK0
B	1529	LEU	-	expression tag	UNP Q6FSK0
B	1530	GLU	-	expression tag	UNP Q6FSK0
B	1531	HIS	-	expression tag	UNP Q6FSK0
B	1532	HIS	-	expression tag	UNP Q6FSK0
B	1533	HIS	-	expression tag	UNP Q6FSK0
B	1534	HIS	-	expression tag	UNP Q6FSK0
B	1535	HIS	-	expression tag	UNP Q6FSK0
B	1536	HIS	-	expression tag	UNP Q6FSK0

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

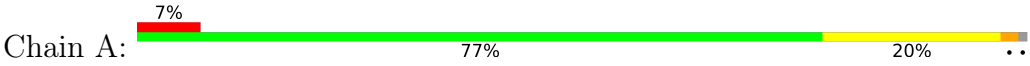
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			

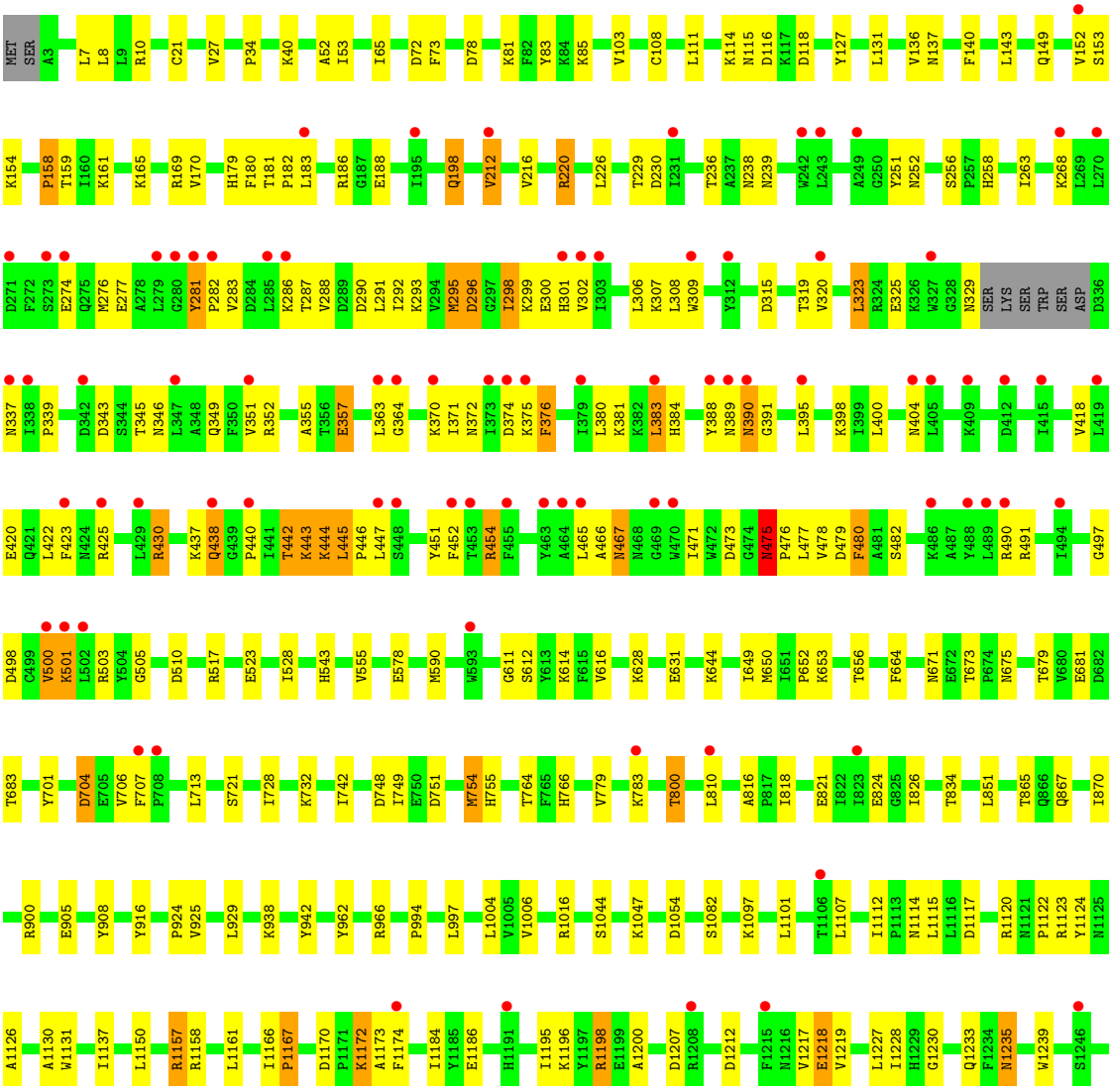
3 Residue-property plots (i)

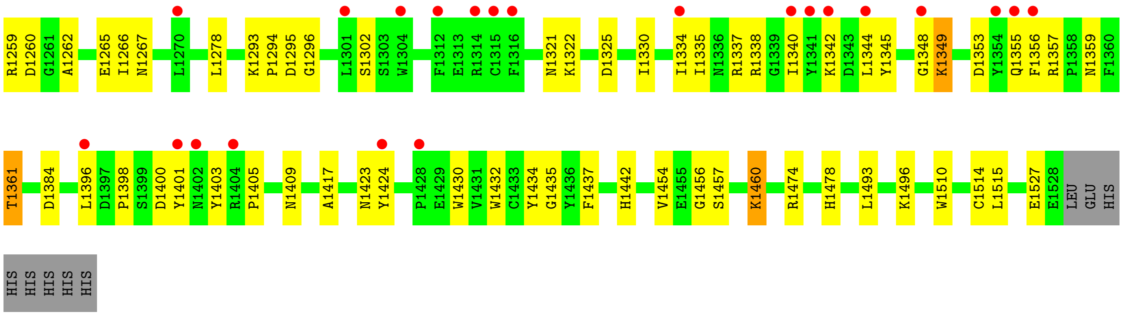
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-alpha-glucanotransferase

Chain A:

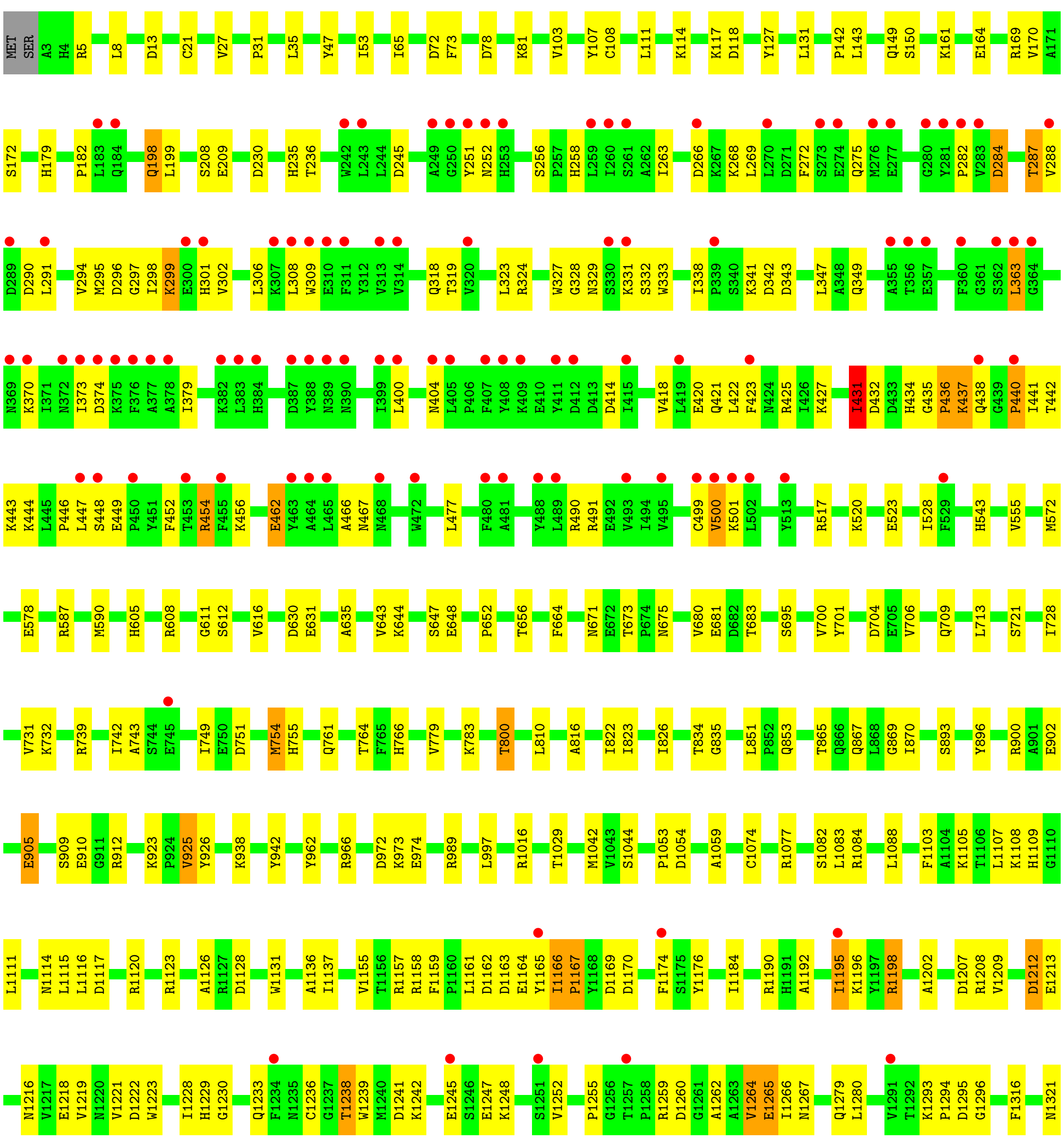


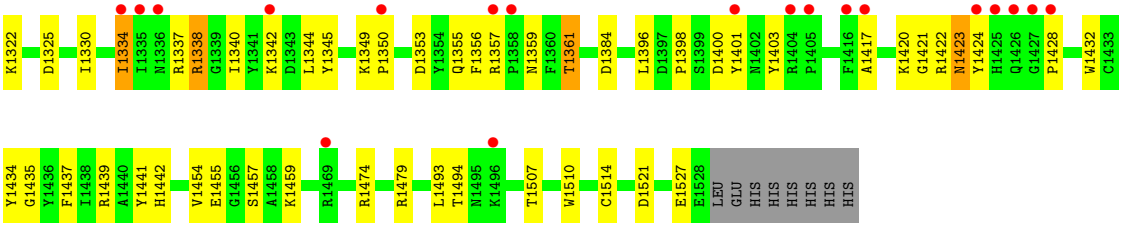




• Molecule 1: 4-alpha-glucanotransferase

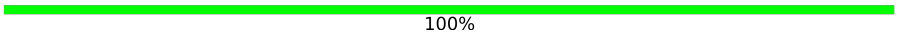
Chain B:





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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	160.25Å 198.94Å 134.59Å 90.00° 104.87° 90.00°	Depositor
Resolution (Å)	25.26 – 3.10 99.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.26-3.10) 99.8 (99.71-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.248 , 0.272 0.248 , 0.272	Depositor DCC
R_{free} test set	3769 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	76.4	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24530	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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

5.1 Standard geometry

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

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	0.25	0/12537	0.42	0/16999
1	B	0.24	0/12589	0.41	0/17071
All	All	0.24	0/25126	0.41	0/34070

There are no bond length outliers.

There are no bond angle outliers.

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	12229	0	11919	173	0
1	B	12278	0	11962	192	0
2	C	23	0	21	0	0
All	All	24530	0	23902	364	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 8.

All (364) 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:1196:LYS:HA	1:A:1218:GLU:HG3	1.47	0.94
1:B:1361:THR:HG21	1:B:1437:PHE:HA	1.61	0.82
1:B:8:LEU:HB2	1:B:652:PRO:HG2	1.64	0.78
1:A:1361:THR:HG21	1:A:1437:PHE:HA	1.65	0.76
1:B:1123:ARG:HH22	1:B:1207:ASP:HB2	1.48	0.76
1:A:343:ASP:HB3	1:A:346:ASN:HB3	1.68	0.76
1:A:198:GLN:HG2	1:A:517:ARG:HH21	1.51	0.75
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.71	0.72
1:A:1123:ARG:HH22	1:A:1207:ASP:HB2	1.54	0.72
1:B:182:PRO:HD3	1:B:230:ASP:HB2	1.71	0.72
1:A:169:ARG:NH1	1:A:721:SER:O	2.23	0.71
1:A:8:LEU:HB2	1:A:652:PRO:HG2	1.72	0.70
1:B:1190:ARG:HG3	1:B:1195:ILE:HG12	1.74	0.69
1:A:179:HIS:NE2	1:A:230:ASP:OD1	2.26	0.69
1:A:1342:LYS:HE2	1:A:1353:ASP:HB3	1.75	0.69
1:B:466:ALA:H	1:B:501:LYS:HD2	1.58	0.69
1:A:1157:ARG:NH2	1:A:1186:GLU:OE2	2.26	0.69
1:B:1115:LEU:HB3	1:B:1123:ARG:HB3	1.76	0.68
1:B:1167:PRO:HB2	1:B:1170:ASP:HB2	1.76	0.68
1:A:1115:LEU:HB3	1:A:1123:ARG:HB3	1.75	0.68
1:A:351:VAL:HG13	1:A:355:ALA:HB3	1.75	0.67
1:B:1342:LYS:HE2	1:B:1353:ASP:HB3	1.77	0.67
1:B:198:GLN:HG2	1:B:517:ARG:HH21	1.61	0.66
1:B:673:THR:HG22	1:B:675:ASN:H	1.61	0.66
1:B:1295:ASP:OD1	1:B:1296:GLY:N	2.29	0.66
1:B:590:MET:HB2	1:B:671:ASN:HD22	1.60	0.65
1:B:169:ARG:NH1	1:B:721:SER:O	2.29	0.65
1:B:179:HIS:NE2	1:B:230:ASP:OD1	2.26	0.65
1:A:1166:ILE:HD11	1:A:1200:ALA:HB1	1.79	0.64
1:A:816:ALA:HB2	1:A:826:ILE:HG12	1.78	0.64
1:A:1259:ARG:NH2	1:A:1265:GLU:OE2	2.31	0.64
1:A:293:LYS:HA	1:A:296:ASP:HB2	1.79	0.64
1:A:298:ILE:HA	1:A:301:HIS:HB2	1.81	0.63
1:A:400:LEU:O	1:A:404:ASN:ND2	2.32	0.62
1:B:400:LEU:O	1:B:404:ASN:ND2	2.32	0.62
1:B:169:ARG:NH1	1:B:701:TYR:OH	2.33	0.62
1:B:452:PHE:HA	1:B:466:ALA:HA	1.80	0.62
1:B:1262:ALA:HB1	1:B:1267:ASN:HD21	1.65	0.62
1:B:13:ASP:OD2	1:B:1479:ARG:NH2	2.22	0.62
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.32	0.61
1:A:1217:VAL:HB	1:A:1235:ASN:HD21	1.65	0.61
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:PRO:HB2	1:A:1170:ASP:HB2	1.82	0.61
1:B:1229:HIS:HE1	1:B:1345:TYR:HD2	1.47	0.61
1:A:1295:ASP:OD1	1:A:1296:GLY:N	2.34	0.60
1:A:27:VAL:HG22	1:A:578:GLU:HG3	1.82	0.60
1:A:452:PHE:CD1	1:A:466:ALA:HB2	2.37	0.60
1:B:268:LYS:HG3	1:B:302:VAL:HG12	1.84	0.59
1:B:306:LEU:HD13	1:B:309:TRP:HZ2	1.67	0.59
1:B:319:THR:OG1	1:B:370:LYS:NZ	2.35	0.59
1:B:1384:ASP:OD1	1:B:1474:ARG:NH1	2.35	0.59
1:B:27:VAL:HG22	1:B:578:GLU:HG3	1.84	0.58
1:A:673:THR:HG22	1:A:675:ASN:H	1.68	0.58
1:A:1293:LYS:HD2	1:A:1294:PRO:HD2	1.84	0.58
1:B:456:LYS:HG3	1:B:462:GLU:HG2	1.86	0.58
1:A:1384:ASP:OD1	1:A:1474:ARG:NH1	2.36	0.58
1:B:816:ALA:HB2	1:B:826:ILE:HG13	1.86	0.57
1:A:1219:VAL:HG22	1:A:1230:GLY:HA3	1.84	0.57
1:B:103:VAL:O	1:B:107:TYR:OH	2.13	0.57
1:A:287:THR:HB	1:A:290:ASP:HB3	1.86	0.57
1:A:180:PHE:HB3	1:A:183:LEU:HD13	1.85	0.57
1:B:1428:PRO:HB3	1:B:1493:LEU:HD21	1.87	0.57
1:A:614:LYS:HB2	1:A:1004:LEU:HD13	1.87	0.56
1:A:523:GLU:HB2	1:A:555:VAL:HG21	1.87	0.56
1:A:590:MET:HB2	1:A:671:ASN:HD22	1.69	0.56
1:B:425:ARG:HH22	1:B:491:ARG:HB3	1.69	0.56
1:B:523:GLU:HB2	1:B:555:VAL:HG21	1.87	0.56
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.87	0.56
1:A:131:LEU:HD13	1:A:143:LEU:HD13	1.88	0.56
1:B:721:SER:HA	1:B:822:ILE:HD11	1.88	0.56
1:B:1322:LYS:H	1:B:1322:LYS:HD2	1.70	0.56
1:B:681:GLU:HB2	1:B:783:LYS:HG2	1.88	0.56
1:B:909:SER:O	1:B:912:ARG:HG2	2.06	0.56
1:B:1293:LYS:HD2	1:B:1294:PRO:HD2	1.88	0.55
1:A:268:LYS:HG3	1:A:302:VAL:HG12	1.89	0.55
1:A:1432:TRP:CG	1:A:1510:TRP:HD1	2.24	0.55
1:A:1218:GLU:HA	1:A:1218:GLU:OE1	2.05	0.55
1:B:721:SER:OG	1:B:823:ILE:O	2.20	0.55
1:A:1322:LYS:H	1:A:1322:LYS:HD2	1.70	0.55
1:B:1114:ASN:HB2	1:B:1126:ALA:HB2	1.89	0.55
1:A:1196:LYS:HD2	1:A:1218:GLU:HG3	1.88	0.55
1:A:1417:ALA:O	1:A:1423:ASN:ND2	2.39	0.55
1:A:870:ILE:HD11	1:A:997:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:THR:O	1:B:500:VAL:N	2.39	0.54
1:B:1355:GLN:OE1	1:B:1357:ARG:NH1	2.40	0.54
1:A:425:ARG:HH22	1:A:491:ARG:HB3	1.73	0.54
1:B:114:LYS:NZ	1:B:118:ASP:OD1	2.41	0.54
1:B:1432:TRP:CG	1:B:1510:TRP:HD1	2.25	0.54
1:A:238:ASN:OD1	1:A:239:ASN:ND2	2.36	0.54
1:B:323:LEU:HD23	1:B:373:ILE:HG23	1.89	0.54
1:A:1355:GLN:OE1	1:A:1357:ARG:NH1	2.40	0.54
1:B:131:LEU:HD13	1:B:143:LEU:HD13	1.90	0.54
1:B:1229:HIS:HE1	1:B:1345:TYR:CD2	2.24	0.54
1:B:275:GLN:OE1	1:B:275:GLN:N	2.40	0.54
1:A:306:LEU:HD13	1:A:309:TRP:HZ2	1.72	0.54
1:B:680:VAL:HG11	1:B:826:ILE:HD13	1.88	0.54
1:A:1137:ILE:HG21	1:A:1184:ILE:HD11	1.89	0.54
1:B:452:PHE:CD1	1:B:466:ALA:HB2	2.42	0.54
1:B:431:ILE:HG22	1:B:432:ASP:H	1.73	0.54
1:A:1195:ILE:HD11	1:A:1219:VAL:HB	1.88	0.53
1:A:188:GLU:H	1:A:239:ASN:HD21	1.57	0.53
1:A:1435:GLY:HA3	1:A:1514:CYS:HB3	1.91	0.53
1:B:611:GLY:HA2	1:B:997:LEU:HD23	1.89	0.53
1:B:1441:TYR:OH	1:B:1474:ARG:NH2	2.42	0.53
1:A:1198:ARG:NH2	1:A:1212:ASP:O	2.41	0.53
1:B:291:LEU:HA	1:B:294:VAL:HG23	1.91	0.53
1:A:475:ASN:O	1:A:477:LEU:N	2.42	0.53
1:B:728:ILE:HD11	1:B:810:LEU:HD22	1.91	0.53
1:B:800:THR:HG23	1:B:867:GLN:HA	1.90	0.52
1:B:295:MET:O	1:B:299:LYS:N	2.41	0.52
1:A:152:VAL:HG22	1:A:181:THR:HG21	1.91	0.52
1:A:430:ARG:HB3	1:A:438:GLN:HA	1.91	0.52
1:A:115:ASN:OD1	1:A:116:ASP:N	2.43	0.52
1:B:1117:ASP:O	1:B:1120:ARG:HG2	2.09	0.52
1:B:1239:TRP:HE1	1:B:1359:ASN:ND2	2.06	0.52
1:A:452:PHE:HA	1:A:466:ALA:HA	1.91	0.52
1:A:779:VAL:HG11	1:A:851:LEU:HD11	1.91	0.52
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.92	0.52
1:A:83:TYR:HD2	1:B:1459:LYS:HE3	1.76	0.51
1:B:695:SER:O	1:B:739:ARG:NH2	2.40	0.51
1:B:1196:LYS:HA	1:B:1218:GLU:HG3	1.92	0.51
1:A:389:ASN:O	1:A:391:GLY:N	2.40	0.51
1:A:479:ASP:HB3	1:A:482:SER:HB3	1.92	0.51
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:HB3	1:A:465:LEU:HD23	1.93	0.51
1:B:870:ILE:HD11	1:B:997:LEU:HD13	1.92	0.51
1:A:471:ILE:HD11	1:A:480:PHE:HB3	1.93	0.51
1:B:422:LEU:HD23	1:B:425:ARG:HE	1.76	0.51
1:A:188:GLU:HB2	1:A:239:ASN:ND2	2.26	0.51
1:A:319:THR:O	1:A:323:LEU:N	2.41	0.51
1:A:1239:TRP:HE1	1:A:1359:ASN:HD21	1.59	0.51
1:B:263:ILE:HG23	1:B:454:ARG:HH21	1.75	0.51
1:B:608:ARG:HD2	1:B:749:ILE:HG12	1.93	0.51
1:A:611:GLY:HA2	1:A:997:LEU:HD23	1.93	0.50
1:A:681:GLU:HB2	1:A:783:LYS:HG2	1.92	0.50
1:A:236:THR:O	1:A:500:VAL:N	2.45	0.50
1:A:357:GLU:HG3	1:A:372:ASN:HB2	1.94	0.50
1:B:161:LYS:HD2	1:B:164:GLU:HB2	1.94	0.50
1:B:779:VAL:HG11	1:B:851:LEU:HD11	1.93	0.50
1:B:902:GLU:OE2	1:B:923:LYS:NZ	2.35	0.50
1:B:1107:LEU:O	1:B:1157:ARG:NH1	2.28	0.50
1:B:21:CYS:H	1:B:656:THR:HG21	1.75	0.50
1:B:1417:ALA:O	1:B:1422:ARG:HB2	2.12	0.49
1:A:905:GLU:OE1	1:A:966:ARG:NH1	2.45	0.49
1:A:1158:ARG:HD3	1:A:1173:ALA:HB1	1.94	0.49
1:B:266:ASP:OD2	1:B:452:PHE:N	2.45	0.49
1:B:1131:TRP:CD1	1:B:1266:ILE:HG23	2.47	0.49
1:A:263:ILE:HG23	1:A:454:ARG:HH21	1.78	0.49
1:A:916:TYR:O	1:A:924:PRO:HD2	2.13	0.49
1:B:1245:GLU:HG3	1:B:1420:LYS:HB3	1.93	0.49
1:B:284:ASP:OD1	1:B:440:PRO:HA	2.13	0.49
1:B:466:ALA:HB3	1:B:501:LYS:HE3	1.95	0.49
1:A:65:ILE:HG12	1:A:111:LEU:HD22	1.95	0.49
1:B:1137:ILE:HG21	1:B:1184:ILE:HD11	1.95	0.49
1:A:1322:LYS:HG3	1:A:1338:ARG:NH1	2.28	0.49
1:A:1337:ARG:HB2	1:A:1340:ILE:HD12	1.95	0.49
1:B:328:GLY:H	1:B:331:LYS:HG3	1.78	0.49
1:B:306:LEU:HD13	1:B:309:TRP:CZ2	2.45	0.48
1:B:251:TYR:HB2	1:B:501:LYS:HZ3	1.77	0.48
1:B:477:LEU:HD11	1:B:572:MET:HG3	1.94	0.48
1:B:149:GLN:HG2	1:B:170:VAL:HG11	1.96	0.48
1:B:1219:VAL:HG12	1:B:1230:GLY:HA3	1.95	0.48
1:A:420:GLU:HA	1:A:423:PHE:CE2	2.48	0.48
1:A:425:ARG:NH2	1:A:491:ARG:HB3	2.27	0.48
1:A:475:ASN:OD1	1:A:478:VAL:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HD23	1:A:425:ARG:HE	1.78	0.48
1:B:65:ILE:HG12	1:B:111:LEU:HD22	1.96	0.48
1:B:520:LYS:HA	1:B:523:GLU:HG2	1.95	0.48
1:B:671:ASN:OD1	1:B:671:ASN:N	2.39	0.48
1:A:1117:ASP:HB3	1:A:1120:ARG:O	2.14	0.48
1:B:1157:ARG:HG2	1:B:1176:TYR:CZ	2.49	0.48
1:B:1159:PHE:CZ	1:B:1166:ILE:HG22	2.49	0.48
1:A:503:ARG:NH2	1:A:510:ASP:O	2.46	0.48
1:A:108:CYS:HB3	1:A:127:TYR:CD2	2.49	0.47
1:A:1260:ASP:OD1	1:A:1260:ASP:N	2.47	0.47
1:A:1117:ASP:O	1:A:1120:ARG:HG2	2.13	0.47
1:A:1239:TRP:HE1	1:A:1359:ASN:ND2	2.11	0.47
1:B:295:MET:HA	1:B:298:ILE:HB	1.95	0.47
1:B:323:LEU:O	1:B:327:TRP:N	2.46	0.47
1:B:72:ASP:OD1	1:B:73:PHE:N	2.41	0.47
1:B:427:LYS:O	1:B:431:ILE:N	2.47	0.47
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.96	0.47
1:A:1278:LEU:HD11	1:A:1302:SER:HA	1.95	0.47
1:A:179:HIS:HE2	1:A:230:ASP:CG	2.17	0.47
1:B:296:ASP:HA	1:B:299:LYS:HB3	1.97	0.47
1:A:1172:LYS:HB3	1:A:1172:LYS:HE2	1.74	0.47
1:B:728:ILE:O	1:B:731:VAL:N	2.48	0.47
1:B:972:ASP:OD1	1:B:972:ASP:N	2.47	0.47
1:B:1042:MET:HE1	1:B:1507:THR:HG22	1.95	0.47
1:B:1459:LYS:HA	1:B:1459:LYS:HD3	1.69	0.47
1:A:72:ASP:OD1	1:A:73:PHE:N	2.40	0.47
1:B:251:TYR:HB2	1:B:501:LYS:NZ	2.30	0.47
1:A:704:ASP:OD2	1:A:732:LYS:HG3	2.14	0.47
1:A:800:THR:HG23	1:A:867:GLN:HA	1.97	0.47
1:B:1164:GLU:HG2	1:B:1165:TYR:CD2	2.50	0.47
1:A:306:LEU:HD13	1:A:309:TRP:CZ2	2.50	0.46
1:A:1259:ARG:HB3	1:A:1344:LEU:HD21	1.97	0.46
1:A:1400:ASP:OD1	1:A:1401:TYR:N	2.48	0.46
1:B:420:GLU:HA	1:B:423:PHE:CE2	2.49	0.46
1:A:114:LYS:NZ	1:A:118:ASP:OD1	2.49	0.46
1:B:938:LYS:HE2	1:B:942:TYR:HE2	1.78	0.46
1:B:1242:LYS:HE2	1:B:1421:GLY:HA3	1.97	0.46
1:B:1322:LYS:HG3	1:B:1338:ARG:NH1	2.30	0.46
1:A:766:HIS:NE2	1:A:865:THR:HG21	2.30	0.46
1:A:962:TYR:CZ	1:A:966:ARG:HD3	2.51	0.46
1:A:1054:ASP:OD1	1:A:1054:ASP:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1077:ARG:HH21	1:B:1128:ASP:HB2	1.81	0.46
1:A:161:LYS:HD2	1:A:161:LYS:HA	1.79	0.46
1:B:1236:CYS:HB3	1:B:1241:ASP:HA	1.98	0.46
1:A:34:PRO:HG3	1:A:140:PHE:CD2	2.50	0.46
1:A:315:ASP:O	1:A:319:THR:OG1	2.25	0.46
1:A:136:VAL:HG13	1:A:137:ASN:H	1.81	0.46
1:A:389:ASN:OD1	1:A:390:ASN:N	2.49	0.46
1:B:1222:ASP:HB2	1:B:1229:HIS:CD2	2.51	0.46
1:A:154:LYS:HG2	1:A:186:ARG:NH1	2.31	0.46
1:A:1398:PRO:HA	1:A:1403:TYR:CG	2.51	0.46
1:B:53:ILE:HD11	1:B:65:ILE:HD11	1.98	0.45
1:B:78:ASP:HB3	1:B:81:LYS:HB3	1.99	0.45
1:A:728:ILE:HD11	1:A:810:LEU:HD22	1.98	0.45
1:A:1112:ILE:H	1:A:1130:ALA:HB2	1.80	0.45
1:B:466:ALA:N	1:B:501:LYS:HD2	2.30	0.45
1:B:1053:PRO:O	1:B:1120:ARG:NH2	2.48	0.45
1:A:418:VAL:HG22	1:A:490:ARG:HA	1.99	0.45
1:A:466:ALA:HB3	1:A:501:LYS:CE	2.47	0.45
1:A:158:PRO:HG2	1:A:159:THR:HG23	1.99	0.45
1:A:683:THR:HG22	1:A:728:ILE:HG13	1.98	0.45
1:A:1233:GLN:OE1	1:A:1348:GLY:HA3	2.16	0.45
1:B:282:PRO:HG2	1:B:294:VAL:HG22	1.98	0.45
1:B:1223:TRP:HD1	1:B:1293:LYS:HZ2	1.65	0.45
1:A:1357:ARG:NH2	1:A:1396:LEU:HD12	2.31	0.45
1:B:1434:TYR:OH	1:B:1474:ARG:HB3	2.17	0.45
1:A:256:SER:HB2	1:A:258:HIS:CE1	2.51	0.45
1:B:31:PRO:O	1:B:47:TYR:OH	2.24	0.45
1:A:10:ARG:HA	1:A:52:ALA:HB3	1.97	0.45
1:A:754:MET:HG2	1:A:755:HIS:N	2.31	0.45
1:B:256:SER:HB2	1:B:258:HIS:CE1	2.52	0.45
1:B:1229:HIS:CE1	1:B:1345:TYR:HD2	2.32	0.45
1:B:683:THR:HG22	1:B:728:ILE:HG13	1.98	0.44
1:A:1349:LYS:H	1:A:1349:LYS:HG2	1.54	0.44
1:B:1165:TYR:O	1:B:1167:PRO:HD3	2.17	0.44
1:B:869:GLY:O	1:B:989:ARG:NH1	2.36	0.44
1:A:251:TYR:CE2	1:A:503:ARG:HG3	2.52	0.44
1:A:1262:ALA:HB1	1:A:1267:ASN:HD21	1.82	0.44
1:B:338:ILE:HD13	1:B:379:ILE:HG23	1.99	0.44
1:B:754:MET:HG2	1:B:755:HIS:N	2.32	0.44
1:B:1105:LYS:HG2	1:B:1155:VAL:HB	2.00	0.44
1:B:1108:LYS:HG2	1:B:1109:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD22	1:A:653:LYS:HB3	2.00	0.44
1:A:370:LYS:HD2	1:A:370:LYS:HA	1.63	0.44
1:A:628:LYS:O	1:A:650:MET:HB2	2.18	0.44
1:B:269:LEU:HA	1:B:272:PHE:HB3	2.00	0.44
1:B:425:ARG:NH2	1:B:491:ARG:HB3	2.32	0.44
1:B:713:LEU:HD12	1:B:713:LEU:H	1.81	0.44
1:B:1349:LYS:H	1:B:1349:LYS:HG2	1.55	0.44
1:A:748:ASP:OD1	1:A:749:ILE:N	2.41	0.44
1:A:908:TYR:CE2	1:A:1047:LYS:HE2	2.52	0.44
1:B:1259:ARG:HB3	1:B:1344:LEU:HD21	2.00	0.44
1:B:1109:HIS:O	1:B:1195:ILE:HD13	2.18	0.44
1:A:1432:TRP:CG	1:A:1510:TRP:CD1	3.05	0.44
1:B:295:MET:SD	1:B:423:PHE:HB3	2.58	0.44
1:A:65:ILE:HB	1:A:85:LYS:HB2	2.00	0.43
1:B:893:SER:HA	1:B:896:TYR:CD2	2.52	0.43
1:B:1265:GLU:H	1:B:1265:GLU:HG3	1.30	0.43
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.53	0.43
1:A:1430:TRP:CE2	1:A:1493:LEU:HD12	2.53	0.43
1:B:414:ASP:O	1:B:418:VAL:HG23	2.18	0.43
1:B:466:ALA:HB3	1:B:501:LYS:CE	2.47	0.43
1:B:587:ARG:HG3	1:B:605:HIS:CE1	2.53	0.43
1:B:630:ASP:OD1	1:B:635:ALA:HB3	2.18	0.43
1:B:1192:ALA:HB1	1:B:1223:TRP:HZ2	1.83	0.43
1:B:1334:ILE:HD13	1:B:1350:PRO:HB2	2.00	0.43
1:A:938:LYS:HE2	1:A:942:TYR:HE2	1.83	0.43
1:B:169:ARG:O	1:B:172:SER:OG	2.28	0.43
1:A:389:ASN:C	1:A:391:GLY:H	2.21	0.43
1:A:1131:TRP:CD1	1:A:1266:ILE:HG23	2.54	0.43
1:B:235:HIS:HB2	1:B:499:CYS:HB3	2.00	0.43
1:B:962:TYR:CZ	1:B:966:ARG:HD3	2.53	0.43
1:B:1054:ASP:OD1	1:B:1054:ASP:N	2.41	0.43
1:B:1083:LEU:HD22	1:B:1136:ALA:HB1	2.01	0.43
1:A:649:ILE:H	1:A:649:ILE:HG13	1.46	0.43
1:A:1228:ILE:O	1:A:1262:ALA:HA	2.19	0.43
1:B:209:GLU:HG2	1:B:528:ILE:HD11	2.00	0.43
1:B:297:GLY:O	1:B:301:HIS:HB2	2.19	0.43
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.53	0.43
1:B:363:LEU:H	1:B:363:LEU:HG	1.50	0.43
1:A:212:VAL:HG22	1:A:528:ILE:HD13	2.01	0.43
1:A:1217:VAL:HB	1:A:1235:ASN:ND2	2.32	0.43
1:B:608:ARG:O	1:B:754:MET:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LYS:H	1:A:443:LYS:HG2	1.68	0.42
1:A:320:VAL:HA	1:A:323:LEU:HB2	2.02	0.42
1:A:383:LEU:HB3	1:A:384:HIS:H	1.55	0.42
1:B:5:ARG:HA	1:B:643:VAL:HG12	2.00	0.42
1:B:418:VAL:HG22	1:B:490:ARG:HA	2.00	0.42
1:B:1432:TRP:CG	1:B:1510:TRP:CD1	3.06	0.42
1:B:1435:GLY:HA3	1:B:1514:CYS:HB3	2.01	0.42
1:A:149:GLN:HG2	1:A:170:VAL:HG11	2.01	0.42
1:B:905:GLU:OE2	1:B:966:ARG:HD2	2.20	0.42
1:A:53:ILE:HD11	1:A:65:ILE:HD11	2.02	0.42
1:B:287:THR:HG22	1:B:288:VAL:H	1.85	0.42
1:B:290:ASP:OD1	1:B:290:ASP:N	2.52	0.42
1:B:1264:VAL:HG13	1:B:1316:PHE:CD1	2.54	0.42
1:A:1097:LYS:O	1:A:1101:LEU:HG	2.19	0.42
1:B:142:PRO:HG2	1:B:743:ALA:HB1	2.02	0.42
1:B:150:SER:OG	1:B:700:VAL:HA	2.19	0.42
1:B:647:SER:OG	1:B:648:GLU:N	2.50	0.42
1:B:1157:ARG:HG2	1:B:1176:TYR:OH	2.20	0.42
1:B:1357:ARG:NH2	1:B:1396:LEU:HD12	2.35	0.42
1:A:1122:PRO:HG2	1:A:1124:TYR:CE1	2.55	0.42
1:B:1117:ASP:HB3	1:B:1120:ARG:O	2.20	0.42
1:A:238:ASN:ND2	1:A:497:GLY:O	2.51	0.42
1:A:307:LYS:C	1:A:309:TRP:H	2.22	0.42
1:B:1107:LEU:HD12	1:B:1111:LEU:O	2.19	0.42
1:A:372:ASN:O	1:A:376:PHE:HB2	2.19	0.42
1:A:505:GLY:HA3	1:A:510:ASP:HB2	2.01	0.42
1:A:1456:GLY:HA3	1:A:1460:LYS:O	2.20	0.42
1:B:1084:ARG:HG3	1:B:1088:LEU:HD12	2.02	0.42
1:B:1107:LEU:HB3	1:B:1157:ARG:NH1	2.35	0.42
1:B:435:GLY:HA2	1:B:436:PRO:HD3	1.81	0.42
1:B:1236:CYS:SG	1:B:1255:PRO:HB3	2.60	0.42
1:A:281:TYR:CD2	1:A:282:PRO:HD3	2.55	0.41
1:B:766:HIS:NE2	1:B:865:THR:HG21	2.35	0.41
1:B:834:THR:HG22	1:B:835:GLY:H	1.85	0.41
1:B:1493:LEU:HD23	1:B:1494:THR:N	2.35	0.41
1:B:284:ASP:OD2	1:B:438:GLN:HG3	2.20	0.41
1:B:1103:PHE:CZ	1:B:1116:LEU:HD22	2.55	0.41
1:B:1423:ASN:HD22	1:B:1423:ASN:HA	1.64	0.41
1:A:442:THR:N	1:A:445:LEU:O	2.53	0.41
1:A:673:THR:HG21	1:A:707:PHE:O	2.20	0.41
1:A:994:PRO:HD2	1:A:997:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1337:ARG:HB2	1:B:1340:ILE:HD12	2.03	0.41
1:A:136:VAL:HA	1:A:226:LEU:HD21	2.01	0.41
1:A:380:LEU:HD23	1:A:383:LEU:HD23	2.03	0.41
1:A:444:LYS:H	1:A:444:LYS:HD2	1.85	0.41
1:B:1262:ALA:HB1	1:B:1267:ASN:ND2	2.32	0.41
1:A:713:LEU:H	1:A:713:LEU:HD12	1.85	0.41
1:B:370:LYS:HD2	1:B:370:LYS:HA	1.86	0.41
1:B:893:SER:HA	1:B:896:TYR:HD2	1.86	0.41
1:A:295:MET:HA	1:A:298:ILE:HB	2.02	0.41
1:A:1434:TYR:OH	1:A:1474:ARG:HB3	2.21	0.41
1:A:1478:HIS:ND1	1:A:1515:LEU:HD11	2.35	0.41
1:B:1198:ARG:HH22	1:B:1212:ASP:CG	2.24	0.41
1:A:216:VAL:O	1:A:220:ARG:HD3	2.20	0.41
1:A:1097:LYS:HG3	1:A:1150:LEU:HD13	2.01	0.41
1:A:1405:PRO:HB2	1:A:1496:LYS:HB2	2.01	0.41
1:B:1166:ILE:H	1:B:1166:ILE:HG13	1.67	0.41
1:B:1242:LYS:HA	1:B:1242:LYS:HD2	1.91	0.41
1:B:1439:ARG:HD2	1:B:1521:ASP:OD2	2.20	0.41
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.87	0.41
1:A:78:ASP:HB3	1:A:81:LYS:HB3	2.03	0.40
1:A:251:TYR:OH	1:A:479:ASP:OD2	2.37	0.40
1:A:451:TYR:HE2	1:A:491:ARG:HA	1.86	0.40
1:B:1221:VAL:HG22	1:B:1228:ILE:HG12	2.02	0.40
1:A:40:LYS:HE2	1:A:40:LYS:HB3	1.81	0.40
1:A:467:ASN:HA	1:A:500:VAL:HA	2.02	0.40
1:A:929:LEU:HD22	1:A:1006:VAL:HG13	2.02	0.40
1:B:925:VAL:HG12	1:B:926:TYR:CD2	2.56	0.40
1:A:1107:LEU:HB3	1:A:1157:ARG:NH1	2.36	0.40
1:B:421:GLN:O	1:B:425:ARG:HG2	2.21	0.40
1:B:1238:THR:OG1	1:B:1259:ARG:HD3	2.20	0.40
1:B:1265:GLU:HG2	1:B:1359:ASN:HB3	2.04	0.40
1:B:35:LEU:HD12	1:B:35:LEU:H	1.86	0.40
1:B:1059:ALA:HB1	1:B:1074:CYS:SG	2.61	0.40
1:B:1396:LEU:HD21	1:B:1400:ASP:HB3	2.02	0.40
1:A:21:CYS:H	1:A:656:THR:HG21	1.87	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	1516/1536 (99%)	1391 (92%)	111 (7%)	14 (1%)	17	52
1	B	1524/1536 (99%)	1408 (92%)	102 (7%)	14 (1%)	17	52
All	All	3040/3072 (99%)	2799 (92%)	213 (7%)	28 (1%)	17	52

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	440	PRO
1	A	446	PRO
1	A	475	ASN
1	A	476	PRO
1	A	1167	PRO
1	B	440	PRO
1	B	446	PRO
1	B	1167	PRO
1	B	332	SER
1	B	1163	ASP
1	A	501	LYS
1	B	333	TRP
1	B	434	HIS
1	B	441	ILE
1	A	283	VAL
1	A	339	PRO
1	A	900	ARG
1	B	436	PRO
1	B	437	LYS
1	B	900	ARG
1	B	1202	ALA
1	A	158	PRO
1	A	182	PRO
1	A	364	GLY

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Mol	Chain	Res	Type
1	B	431	ILE
1	A	706	VAL
1	B	706	VAL

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	1338/1354 (99%)	1240 (93%)	98 (7%)	14	43
1	B	1344/1354 (99%)	1251 (93%)	93 (7%)	15	45
All	All	2682/2708 (99%)	2491 (93%)	191 (7%)	14	44

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	A	153	SER
1	A	165	LYS
1	A	198	GLN
1	A	212	VAL
1	A	220	ARG
1	A	229	THR
1	A	274	GLU
1	A	276	MET
1	A	277	GLU
1	A	281	TYR
1	A	286	LYS
1	A	288	VAL
1	A	291	LEU
1	A	292	ILE
1	A	295	MET
1	A	296	ASP
1	A	298	ILE
1	A	299	LYS
1	A	300	GLU

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Mol	Chain	Res	Type
1	A	308	LEU
1	A	323	LEU
1	A	325	GLU
1	A	329	ASN
1	A	337	ASN
1	A	345	THR
1	A	349	GLN
1	A	352	ARG
1	A	357	GLU
1	A	363	LEU
1	A	371	ILE
1	A	374	ASP
1	A	375	LYS
1	A	376	PHE
1	A	381	LYS
1	A	383	LEU
1	A	388	TYR
1	A	395	LEU
1	A	398	LYS
1	A	430	ARG
1	A	437	LYS
1	A	438	GLN
1	A	442	THR
1	A	443	LYS
1	A	444	LYS
1	A	445	LEU
1	A	447	LEU
1	A	454	ARG
1	A	467	ASN
1	A	473	ASP
1	A	475	ASN
1	A	480	PHE
1	A	498	ASP
1	A	500	VAL
1	A	543	HIS
1	A	612	SER
1	A	616	VAL
1	A	631	GLU
1	A	644	LYS
1	A	664	PHE
1	A	679	THR
1	A	704	ASP

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Mol	Chain	Res	Type
1	A	742	ILE
1	A	751	ASP
1	A	754	MET
1	A	764	THR
1	A	800	THR
1	A	818	ILE
1	A	821	GLU
1	A	824	GLU
1	A	834	THR
1	A	925	VAL
1	A	1016	ARG
1	A	1044	SER
1	A	1082	SER
1	A	1157	ARG
1	A	1161	LEU
1	A	1172	LYS
1	A	1174	PHE
1	A	1198	ARG
1	A	1218	GLU
1	A	1227	LEU
1	A	1235	ASN
1	A	1321	ASN
1	A	1325	ASP
1	A	1330	ILE
1	A	1334	ILE
1	A	1335	ILE
1	A	1349	LYS
1	A	1356	PHE
1	A	1361	THR
1	A	1409	ASN
1	A	1424	TYR
1	A	1442	HIS
1	A	1454	VAL
1	A	1457	SER
1	A	1460	LYS
1	A	1527	GLU
1	B	117	LYS
1	B	198	GLN
1	B	199	LEU
1	B	208	SER
1	B	245	ASP
1	B	252	ASN

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Mol	Chain	Res	Type
1	B	284	ASP
1	B	287	THR
1	B	299	LYS
1	B	308	LEU
1	B	318	GLN
1	B	324	ARG
1	B	329	ASN
1	B	341	LYS
1	B	342	ASP
1	B	343	ASP
1	B	347	LEU
1	B	349	GLN
1	B	363	LEU
1	B	374	ASP
1	B	431	ILE
1	B	437	LYS
1	B	442	THR
1	B	443	LYS
1	B	444	LYS
1	B	447	LEU
1	B	448	SER
1	B	449	GLU
1	B	454	ARG
1	B	462	GLU
1	B	467	ASN
1	B	500	VAL
1	B	543	HIS
1	B	612	SER
1	B	616	VAL
1	B	631	GLU
1	B	644	LYS
1	B	664	PHE
1	B	709	GLN
1	B	742	ILE
1	B	751	ASP
1	B	754	MET
1	B	761	GLN
1	B	764	THR
1	B	800	THR
1	B	853	GLN
1	B	905	GLU
1	B	910	GLU

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Mol	Chain	Res	Type
1	B	925	VAL
1	B	973	LYS
1	B	974	GLU
1	B	1016	ARG
1	B	1029	THR
1	B	1044	SER
1	B	1082	SER
1	B	1158	ARG
1	B	1161	LEU
1	B	1162	ASP
1	B	1166	ILE
1	B	1169	ASP
1	B	1174	PHE
1	B	1195	ILE
1	B	1198	ARG
1	B	1208	ARG
1	B	1209	VAL
1	B	1212	ASP
1	B	1213	GLU
1	B	1216	ASN
1	B	1233	GLN
1	B	1238	THR
1	B	1247	GLU
1	B	1248	LYS
1	B	1252	VAL
1	B	1260	ASP
1	B	1264	VAL
1	B	1265	GLU
1	B	1279	GLN
1	B	1280	LEU
1	B	1321	ASN
1	B	1325	ASP
1	B	1330	ILE
1	B	1334	ILE
1	B	1338	ARG
1	B	1356	PHE
1	B	1361	THR
1	B	1401	TYR
1	B	1423	ASN
1	B	1424	TYR
1	B	1442	HIS
1	B	1454	VAL

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Mol	Chain	Res	Type
1	B	1455	GLU
1	B	1457	SER
1	B	1527	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	1309	GLN
1	A	1423	ASN
1	B	1229	HIS

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	C	1	2	12,12,12	0.54	0	17,17,17	0.73	0
2	GLC	C	2	2	11,11,12	0.40	0	15,15,17	0.83	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	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

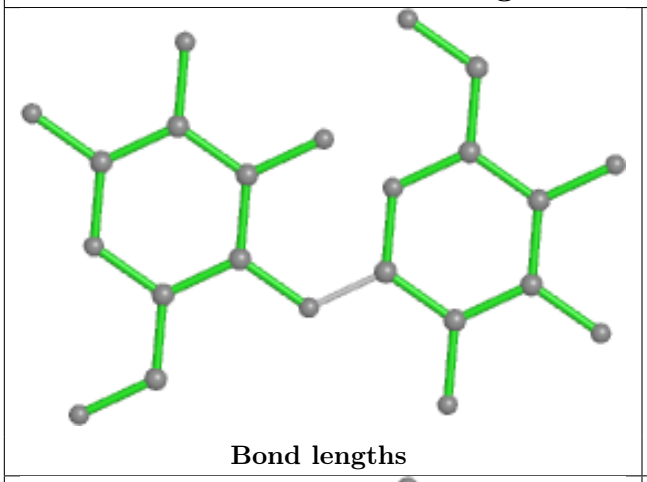
There are no torsion outliers.

There are no ring outliers.

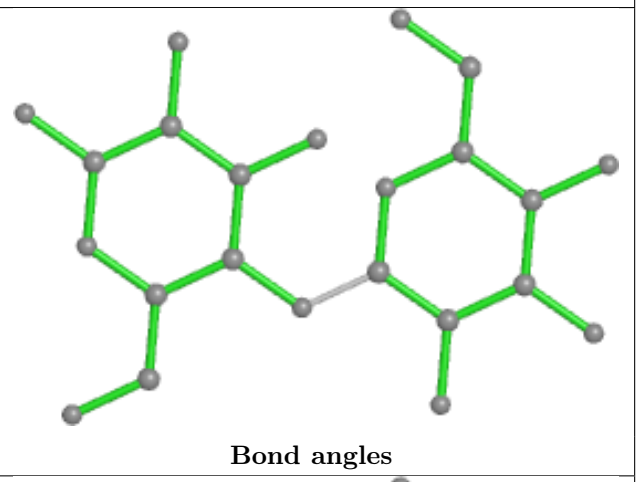
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

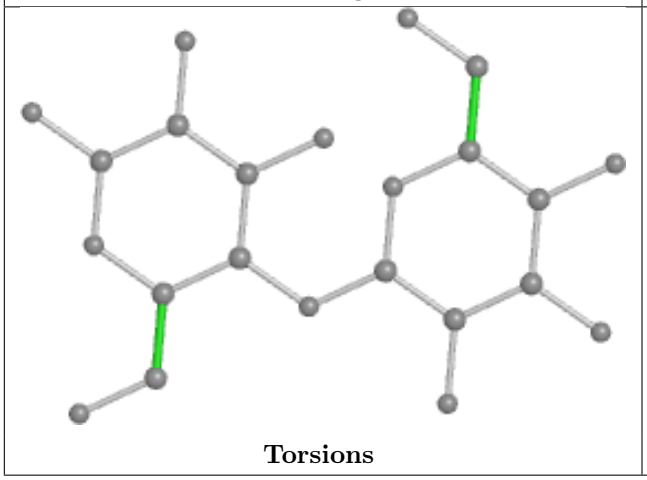
Oligosaccharide Chain C



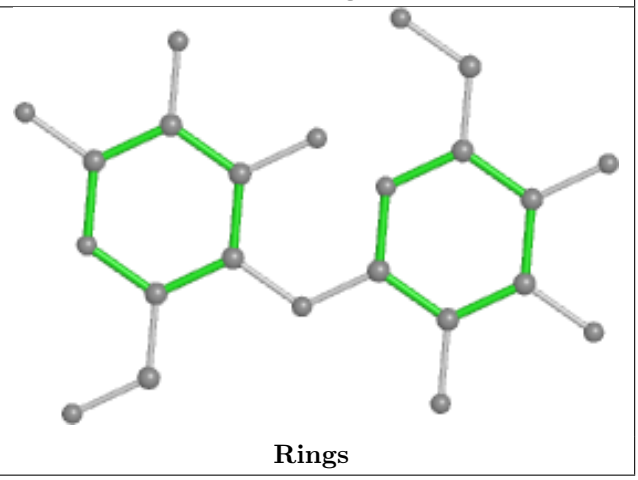
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1520/1536 (98%)	0.47	106 (6%)	16	7	46, 97, 175, 203	0
1	B	1526/1536 (99%)	0.49	125 (8%)	11	4	48, 88, 153, 194	0
All	All	3046/3072 (99%)	0.48	231 (7%)	13	5	46, 93, 170, 203	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	VAL	6.9
1	B	289	ASP	6.9
1	B	273	SER	6.5
1	B	251	TYR	6.2
1	B	270	LEU	5.8
1	A	270	LEU	5.6
1	B	364	GLY	5.5
1	A	374	ASP	5.3
1	A	1316	PHE	5.2
1	B	356	THR	5.1
1	A	389	ASN	5.0
1	A	438	GLN	4.9
1	A	364	GLY	4.8
1	B	389	ASN	4.7
1	B	276	MET	4.6
1	A	390	ASN	4.3
1	B	408	TYR	4.3
1	B	261	SER	4.3
1	B	1245	GLU	4.3
1	B	480	PHE	4.2
1	A	448	SER	4.2
1	B	1424	TYR	4.1
1	B	388	TYR	4.1
1	B	309	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	372	ASN	4.1
1	A	282	PRO	4.1
1	A	447	LEU	4.1
1	A	1340	ILE	4.0
1	B	501	LYS	4.0
1	B	277	GLU	3.9
1	B	281	TYR	3.9
1	B	307	LYS	3.9
1	B	288	VAL	3.9
1	B	242	TRP	3.9
1	B	745	GLU	3.8
1	A	465	LEU	3.8
1	B	314	VAL	3.8
1	B	411	TYR	3.8
1	B	369	ASN	3.8
1	A	363	LEU	3.7
1	A	1401	TYR	3.7
1	B	252	ASN	3.7
1	A	463	TYR	3.7
1	B	374	ASP	3.6
1	B	1165	TYR	3.6
1	B	448	SER	3.6
1	A	281	TYR	3.6
1	A	1356	PHE	3.5
1	A	501	LYS	3.5
1	A	1301	LEU	3.5
1	B	1174	PHE	3.5
1	A	285	LEU	3.5
1	A	1334	ILE	3.5
1	A	375	LYS	3.5
1	B	384	HIS	3.4
1	A	183	LEU	3.4
1	A	312	TYR	3.4
1	B	502	LEU	3.4
1	B	409	LYS	3.4
1	B	438	GLN	3.4
1	A	1342	LYS	3.4
1	B	440	PRO	3.4
1	A	1174	PHE	3.3
1	A	1354	TYR	3.3
1	B	450	PRO	3.3
1	B	320	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	310	GLU	3.3
1	B	243	LEU	3.3
1	B	1426	GLN	3.2
1	A	440	PRO	3.2
1	B	1405	PRO	3.2
1	B	423	PHE	3.2
1	A	1312	PHE	3.2
1	A	464	ALA	3.1
1	A	338	ILE	3.1
1	B	1336	ASN	3.1
1	B	259	LEU	3.1
1	B	412	ASP	3.1
1	B	472	TRP	3.1
1	A	243	LEU	3.1
1	A	489	LEU	3.1
1	A	1396	LEU	3.1
1	B	301	HIS	3.1
1	B	400	LEU	3.1
1	A	379	ILE	3.0
1	B	1401	TYR	3.0
1	A	271	ASP	3.0
1	B	468	ASN	3.0
1	A	273	SER	3.0
1	B	357	GLU	3.0
1	A	490	ARG	3.0
1	B	404	ASN	3.0
1	A	1106	THR	2.9
1	A	1315	CYS	2.9
1	A	425	ARG	2.9
1	A	708	PRO	2.9
1	B	378	ALA	2.9
1	A	1402	ASN	2.9
1	A	1348	GLY	2.9
1	B	447	LEU	2.9
1	A	309	TRP	2.9
1	B	493	VAL	2.9
1	B	481	ALA	2.9
1	B	253	HIS	2.9
1	B	1428	PRO	2.8
1	A	783	LYS	2.8
1	A	302	VAL	2.8
1	A	423	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	282	PRO	2.8
1	B	405	LEU	2.8
1	A	388	TYR	2.8
1	B	1342	LYS	2.8
1	B	363	LEU	2.8
1	A	373	ILE	2.8
1	B	500	VAL	2.8
1	B	1469	ARG	2.8
1	B	453	THR	2.8
1	B	465	LEU	2.8
1	A	419	LEU	2.7
1	A	452	PHE	2.7
1	B	382	LYS	2.7
1	B	399	ILE	2.7
1	A	1404	ARG	2.7
1	B	274	GLU	2.7
1	B	464	ALA	2.7
1	B	331	LYS	2.7
1	A	488	TYR	2.7
1	A	593	TRP	2.7
1	A	810	LEU	2.6
1	B	488	TYR	2.6
1	A	1341	TYR	2.6
1	B	499	CYS	2.6
1	A	494	ILE	2.6
1	A	351	VAL	2.5
1	A	453	THR	2.5
1	A	1304	TRP	2.5
1	A	274	GLU	2.5
1	A	1208	ARG	2.5
1	A	249	ALA	2.5
1	B	362	SER	2.5
1	A	707	PHE	2.5
1	B	183	LEU	2.5
1	A	404	ASN	2.4
1	A	342	ASP	2.4
1	A	470	TRP	2.4
1	A	1344	LEU	2.4
1	B	250	GLY	2.4
1	B	407	PHE	2.4
1	B	1404	ARG	2.4
1	A	455	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1424	TYR	2.4
1	B	280	GLY	2.4
1	B	370	LYS	2.4
1	B	1234	PHE	2.4
1	A	301	HIS	2.4
1	A	412	ASP	2.4
1	B	463	TYR	2.4
1	B	1335	ILE	2.4
1	A	280	GLY	2.4
1	B	513	TYR	2.4
1	B	376	PHE	2.4
1	B	373	ILE	2.4
1	A	383	LEU	2.4
1	A	405	LEU	2.4
1	B	1334	ILE	2.3
1	A	242	TRP	2.3
1	B	1195	ILE	2.3
1	B	1357	ARG	2.3
1	B	419	LEU	2.3
1	A	231	ILE	2.3
1	A	500	VAL	2.3
1	B	495	VAL	2.3
1	A	286	LYS	2.3
1	B	184	GLN	2.3
1	A	370	LYS	2.3
1	B	249	ALA	2.3
1	B	387	ASP	2.2
1	B	330	SER	2.2
1	B	308	LEU	2.2
1	A	195	ILE	2.2
1	A	347	LEU	2.2
1	B	1291	VAL	2.2
1	B	1425	HIS	2.2
1	B	529	PHE	2.2
1	A	486	LYS	2.2
1	A	469	GLY	2.2
1	B	383	LEU	2.2
1	B	260	ILE	2.2
1	A	1314	ARG	2.2
1	B	1350	PRO	2.2
1	A	303	ILE	2.2
1	A	502	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	455	PHE	2.2
1	B	300	GLU	2.2
1	A	152	VAL	2.2
1	A	337	ASN	2.2
1	A	429	LEU	2.1
1	A	1270	LEU	2.1
1	B	339	PRO	2.1
1	B	1358	PRO	2.1
1	B	377	ALA	2.1
1	A	1428	PRO	2.1
1	A	279	LEU	2.1
1	B	489	LEU	2.1
1	B	1257	THR	2.1
1	A	320	VAL	2.1
1	B	283	VAL	2.1
1	A	327	TRP	2.1
1	B	1417	ALA	2.1
1	B	291	LEU	2.1
1	A	1246	SER	2.1
1	B	1416	PHE	2.1
1	B	355	ALA	2.1
1	B	360	PHE	2.1
1	A	1355	GLN	2.1
1	B	375	LYS	2.1
1	B	415	ILE	2.1
1	A	212	VAL	2.1
1	A	409	LYS	2.1
1	A	1191	HIS	2.1
1	A	268	LYS	2.0
1	A	1215	PHE	2.0
1	B	266	ASP	2.0
1	A	415	ILE	2.0
1	B	1427	GLY	2.0
1	B	1251	SER	2.0
1	B	311	PHE	2.0
1	B	390	ASN	2.0
1	A	823	ILE	2.0
1	B	1496	LYS	2.0
1	A	395	LEU	2.0

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

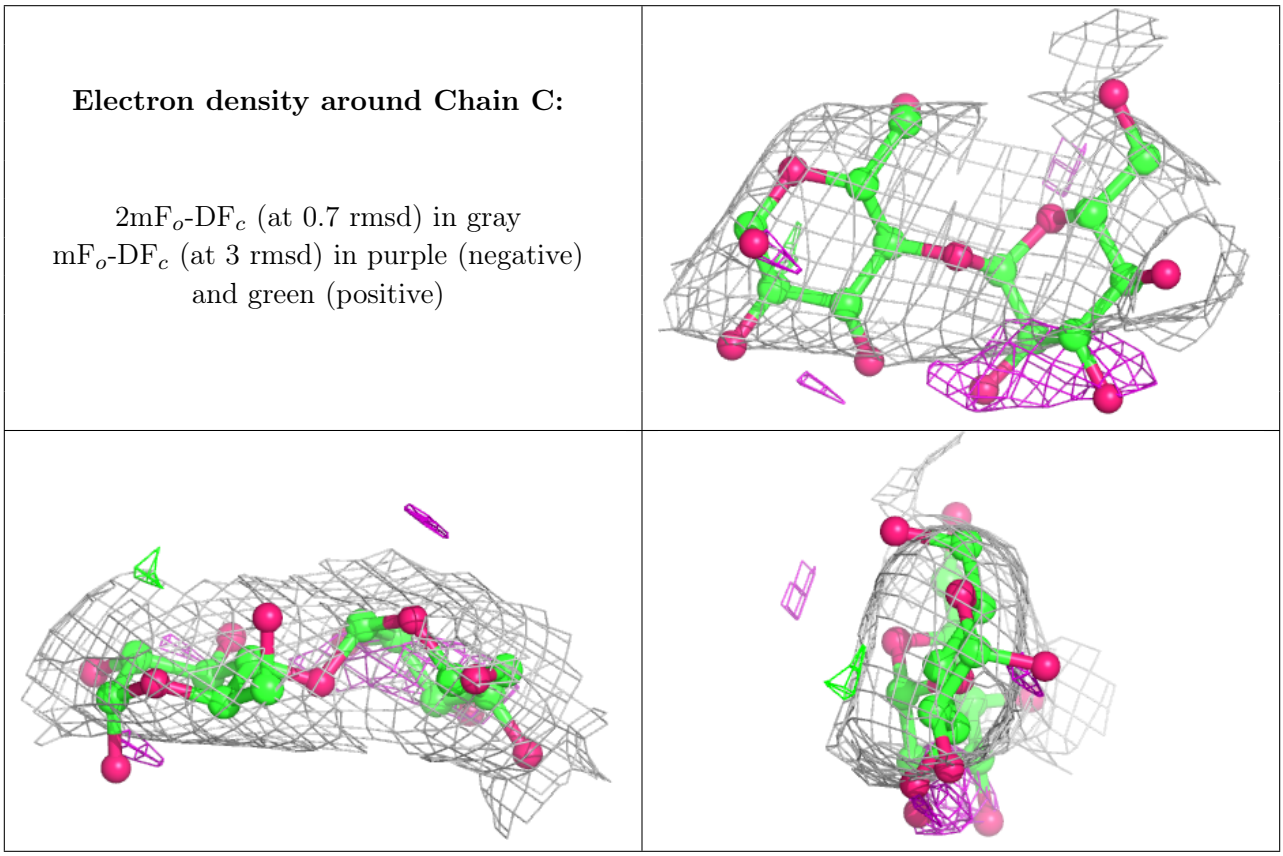
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	2	11/12	0.64	0.36	116,119,128,134	0
2	GLC	C	1	12/12	0.76	0.32	110,110,111,113	0

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



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.