



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:42 PM UTC

PDB ID : 7EKW / pdb_00007ekw
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (D535N) in complex with maltotetraose
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 : 4-5-2 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

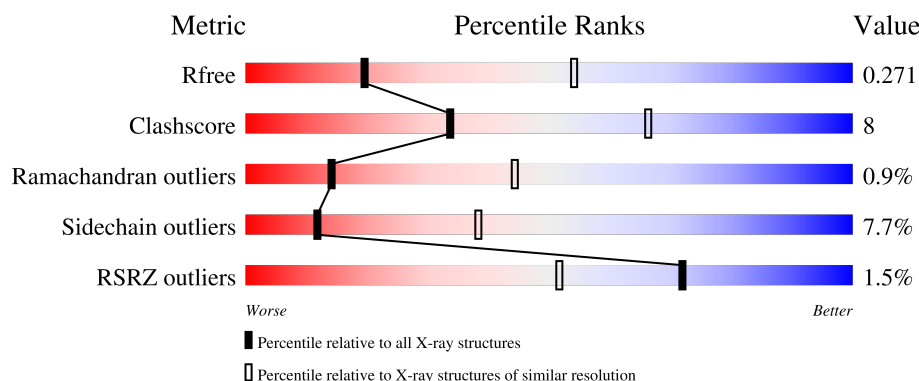
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	1536	 2% 76% 20% ..
1	B	1536	 2% 76% 21% ..
2	C	2	 100%

2 Entry composition

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.

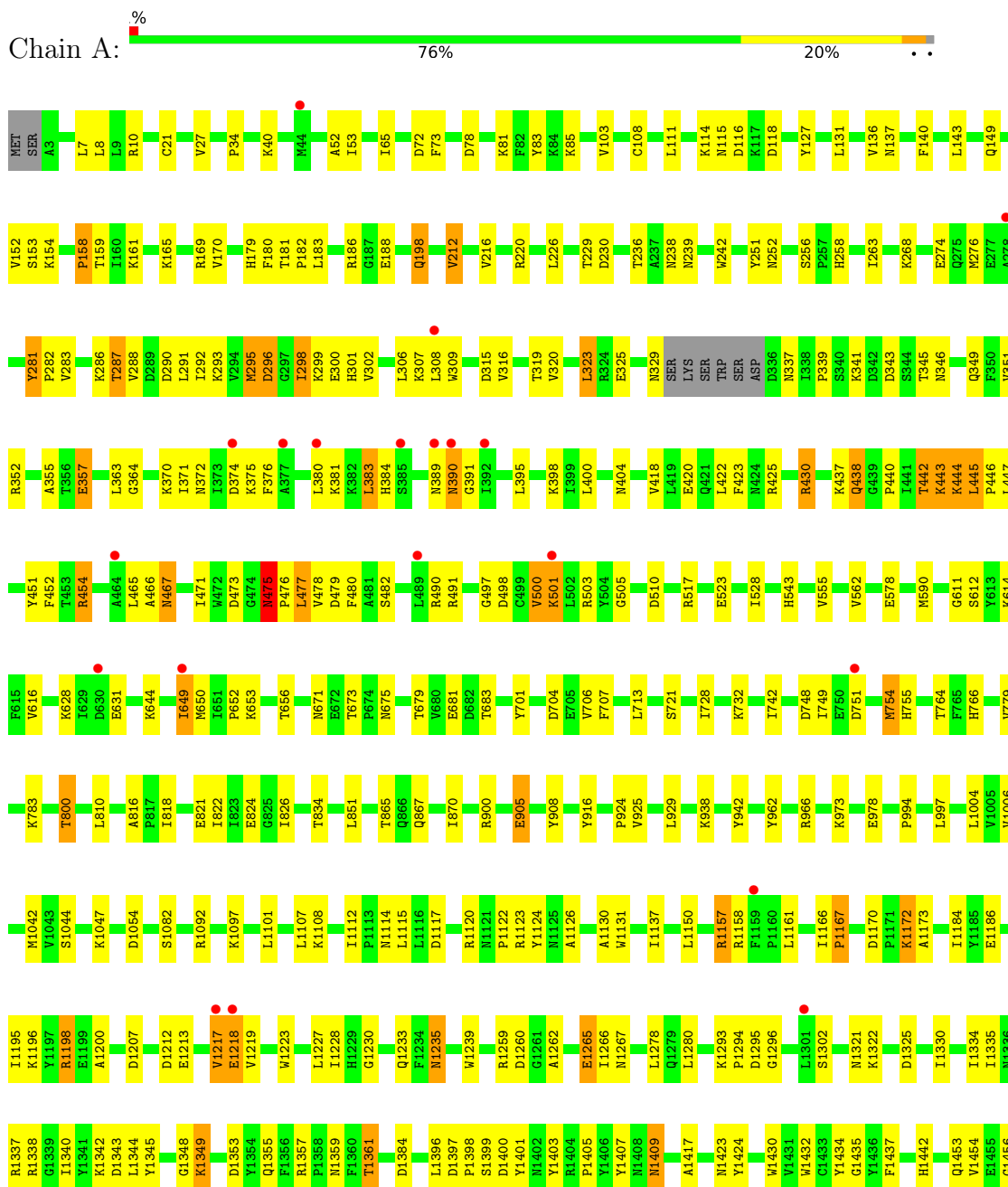


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			

3 Residue-property plots

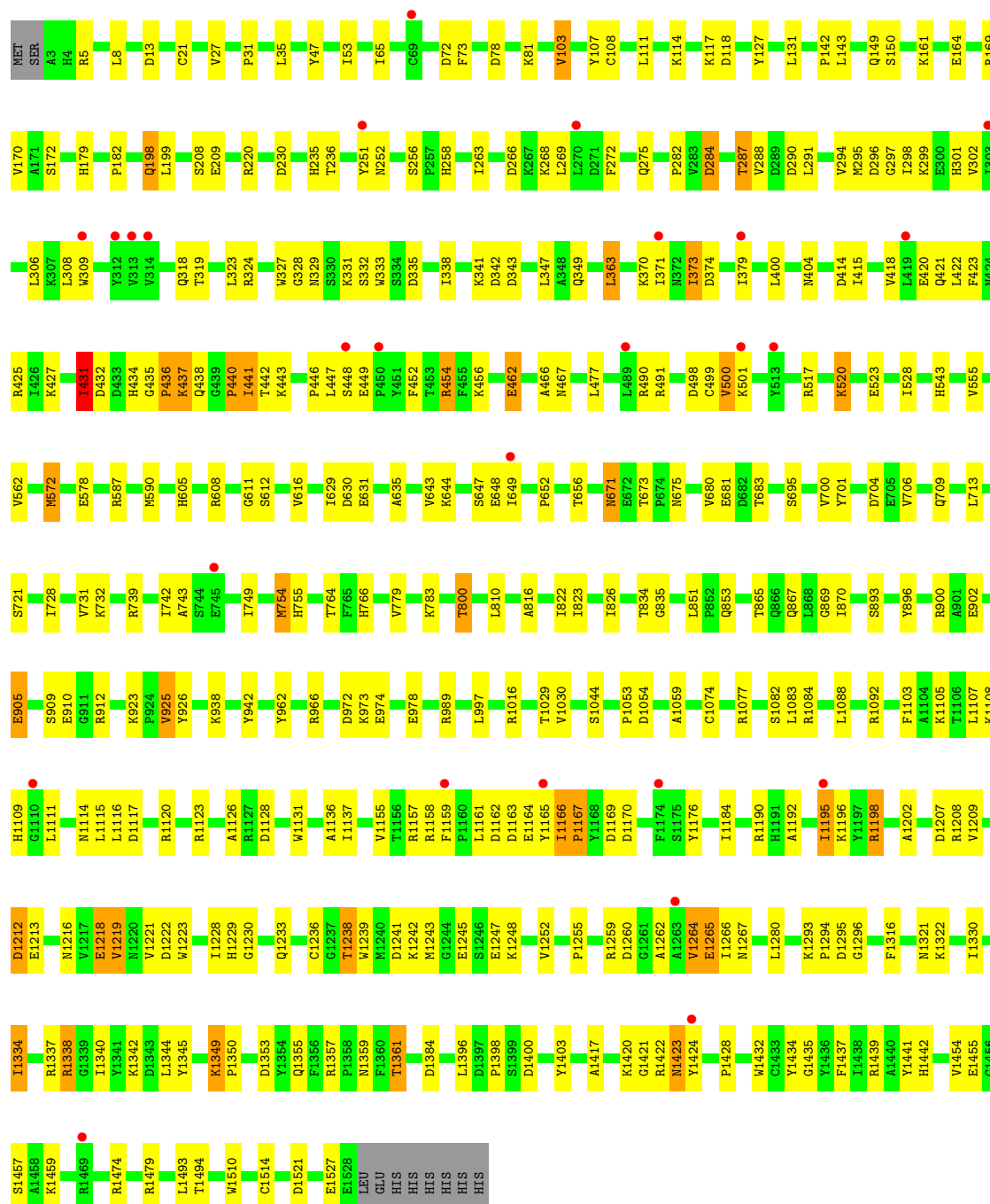
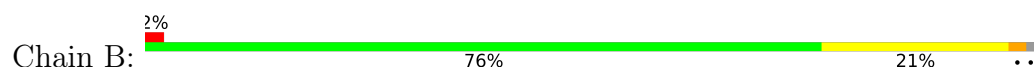
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: 4-alpha-glucanotransferase



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



2019
12/11

4 Data and refinement statistics

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 25.26 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.26-3.10) 99.6 (25.26-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.248 , 0.272 0.248 , 0.271	Depositor DCC
R_{free} test set	3769 reflections (5.11%)	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)	0.29 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.11	0/12537	0.32	0/16999
1	B	0.11	0/12589	0.31	0/17071
All	All	0.11	0/25126	0.32	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	183	0
1	B	12278	0	11962	192	0
2	C	23	0	21	0	0
All	All	24530	0	23902	374	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 (374) 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:242:TRP:CG	1:A:517:ARG:HH12	2.16	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.34	0.61
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:319:THR:OG1	1:B:370:LYS:NZ	2.35	0.60
1:B:721:SER:OG	1:B:823:ILE:O	2.20	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ILE:HD11	1:A:997:LEU:HD13	1.90	0.54
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:A:179:HIS:HE2	1:A:230:ASP:CG	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1223:TRP:CD1	1:A:1293:LYS:HZ3	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:242:TRP:NE1	1:A:517:ARG:HH22	2.12	0.48
1:A:422:LEU:HD23	1:A:425:ARG:HE	1.78	0.48
1:A:389:ASN:C	1:A:391:GLY:H	2.21	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:B:169:ARG:O	1:B:172:SER:OG	2.28	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: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: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:307:LYS:C	1:A:309:TRP:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1198:ARG:HH22	1:B:1212:ASP:CG	2.24	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:B:1243:MET:HE1	1:B:1255:PRO:HG3	1.97	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: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:A:1259:ARG:HH12	1:A:1343:ASP:CG	2.25	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:A:1042:MET:HE2	1:A:1507:THR:HG22	1.99	0.44
1:B:869:GLY:O	1:B:989:ARG:NH1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:295:MET:HE2	1:A:295:MET:HB2	1.95	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:A:307:LYS:C	1:A:309:TRP:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLY:O	1:B:301:HIS:HB2	2.19	0.43
1:B:31:PRO:O	1:B:47:TYR:OH	2.24	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
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:A:315:ASP:O	1:A:319:THR:OG1	2.25	0.42
1:B:905:GLU:OE2	1:B:966:ARG:HD2	2.20	0.42
1:B:1218:GLU:CD	1:B:1219:VAL:H	2.27	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:B:1107:LEU:HD12	1:B:1111:LEU:O	2.19	0.42
1:A:242:TRP:CD1	1:A:517:ARG:HH12	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:TYR:OH	1:A:1409:ASN:OD1	2.38	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
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:A:1397:ASP:CG	1:A:1399:SER:HG	2.28	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:1265:GLU:CD	1:A:1265:GLU:H	2.29	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: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: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

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

5.3.1 Protein backbone

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%)	14	44
1	B	1524/1536 (99%)	1408 (92%)	102 (7%)	14 (1%)	14	44
All	All	3040/3072 (99%)	2799 (92%)	213 (7%)	28 (1%)	14	44

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

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Mol	Chain	Res	Type
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
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%)	1233 (92%)	105 (8%)	11	38
1	B	1344/1354 (99%)	1242 (92%)	102 (8%)	12	39
All	All	2682/2708 (99%)	2475 (92%)	207 (8%)	12	38

All (207) 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	229	THR
1	A	274	GLU
1	A	276	MET
1	A	281	TYR

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Mol	Chain	Res	Type
1	A	286	LYS
1	A	287	THR
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
1	A	308	LEU
1	A	316	VAL
1	A	323	LEU
1	A	325	GLU
1	A	329	ASN
1	A	337	ASN
1	A	341	LYS
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	381	LYS
1	A	383	LEU
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	477	LEU

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Mol	Chain	Res	Type
1	A	498	ASP
1	A	500	VAL
1	A	543	HIS
1	A	562	VAL
1	A	612	SER
1	A	616	VAL
1	A	631	GLU
1	A	644	LYS
1	A	649	ILE
1	A	679	THR
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	822	ILE
1	A	824	GLU
1	A	834	THR
1	A	905	GLU
1	A	925	VAL
1	A	973	LYS
1	A	978	GLU
1	A	1044	SER
1	A	1082	SER
1	A	1092	ARG
1	A	1108	LYS
1	A	1157	ARG
1	A	1161	LEU
1	A	1172	LYS
1	A	1198	ARG
1	A	1213	GLU
1	A	1217	VAL
1	A	1218	GLU
1	A	1227	LEU
1	A	1235	ASN
1	A	1265	GLU
1	A	1280	LEU
1	A	1321	ASN
1	A	1325	ASP
1	A	1330	ILE

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Mol	Chain	Res	Type
1	A	1334	ILE
1	A	1335	ILE
1	A	1349	LYS
1	A	1361	THR
1	A	1409	ASN
1	A	1424	TYR
1	A	1442	HIS
1	A	1453	GLN
1	A	1454	VAL
1	A	1457	SER
1	A	1460	LYS
1	A	1527	GLU
1	B	103	VAL
1	B	117	LYS
1	B	198	GLN
1	B	199	LEU
1	B	208	SER
1	B	220	ARG
1	B	252	ASN
1	B	284	ASP
1	B	287	THR
1	B	308	LEU
1	B	318	GLN
1	B	324	ARG
1	B	329	ASN
1	B	335	ASP
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	371	ILE
1	B	373	ILE
1	B	374	ASP
1	B	415	ILE
1	B	431	ILE
1	B	437	LYS
1	B	441	ILE
1	B	442	THR
1	B	443	LYS
1	B	447	LEU

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Mol	Chain	Res	Type
1	B	448	SER
1	B	449	GLU
1	B	454	ARG
1	B	462	GLU
1	B	467	ASN
1	B	498	ASP
1	B	500	VAL
1	B	520	LYS
1	B	543	HIS
1	B	562	VAL
1	B	572	MET
1	B	612	SER
1	B	616	VAL
1	B	629	ILE
1	B	631	GLU
1	B	644	LYS
1	B	649	ILE
1	B	671	ASN
1	B	709	GLN
1	B	742	ILE
1	B	754	MET
1	B	764	THR
1	B	800	THR
1	B	853	GLN
1	B	905	GLU
1	B	910	GLU
1	B	925	VAL
1	B	973	LYS
1	B	974	GLU
1	B	978	GLU
1	B	1016	ARG
1	B	1029	THR
1	B	1030	VAL
1	B	1044	SER
1	B	1082	SER
1	B	1092	ARG
1	B	1158	ARG
1	B	1161	LEU
1	B	1162	ASP
1	B	1166	ILE
1	B	1169	ASP
1	B	1195	ILE

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Mol	Chain	Res	Type
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	1218	GLU
1	B	1219	VAL
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	1280	LEU
1	B	1321	ASN
1	B	1330	ILE
1	B	1334	ILE
1	B	1338	ARG
1	B	1349	LYS
1	B	1361	THR
1	B	1423	ASN
1	B	1424	TYR
1	B	1442	HIS
1	B	1454	VAL
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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	239	ASN
1	A	301	HIS
1	A	329	ASN
1	A	349	GLN
1	A	354	ASN
1	A	424	ASN
1	A	438	GLN

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Mol	Chain	Res	Type
1	A	790	GLN
1	A	866	GLN
1	A	943	ASN
1	A	1359	ASN
1	A	1423	ASN
1	B	137	ASN
1	B	149	GLN
1	B	184	GLN
1	B	190	ASN
1	B	198	GLN
1	B	223	HIS
1	B	384	HIS
1	B	467	ASN
1	B	468	ASN
1	B	525	ASN
1	B	538	HIS
1	B	866	GLN
1	B	1109	HIS
1	B	1229	HIS
1	B	1279	GLN
1	B	1425	HIS
1	B	1426	GLN

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	C	1	2	12,12,12	0.55	0	17,17,17	0.72	0
2	GLC	C	2	2	11,11,12	0.40	0	15,15,17	0.74	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.

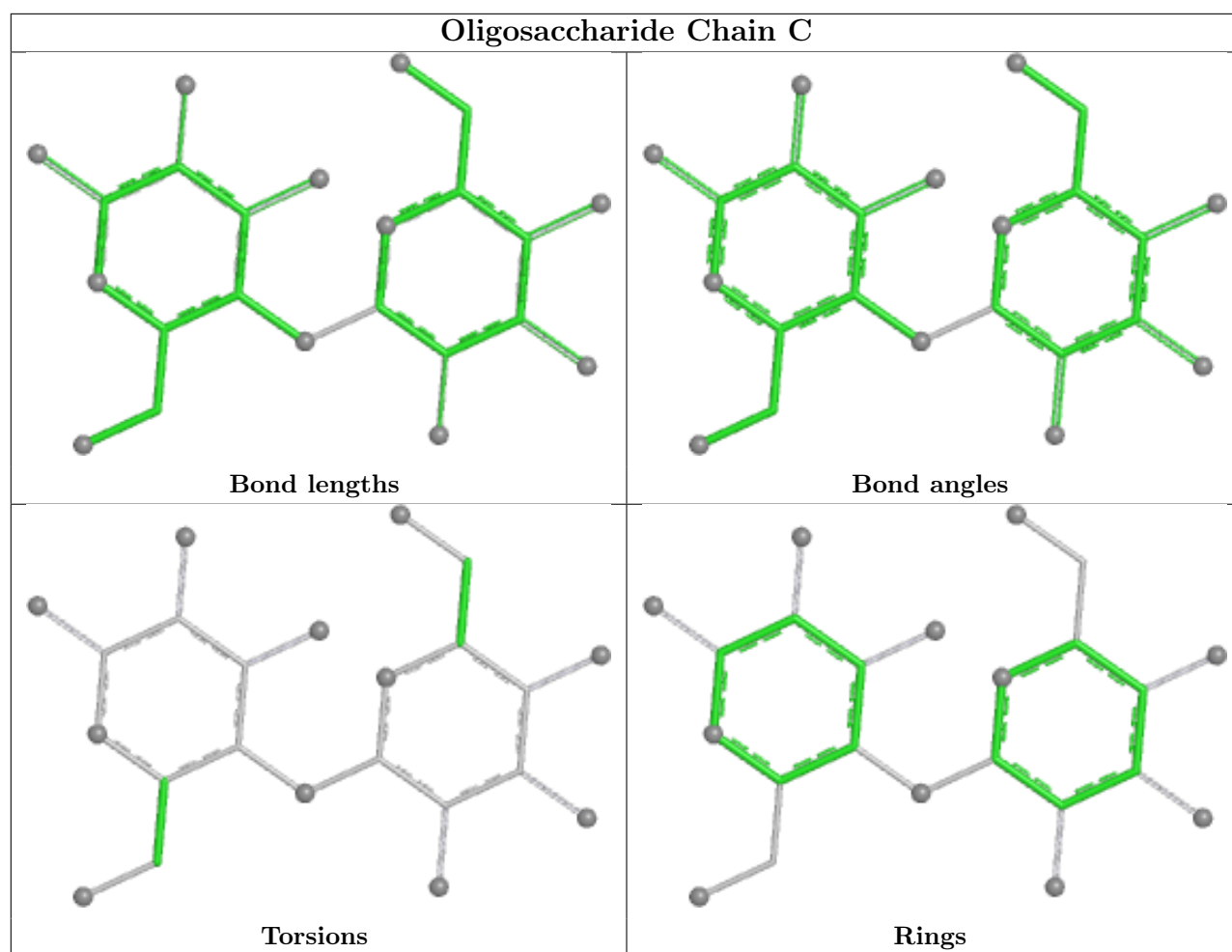
There are no chirality outliers.

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.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1520/1536 (98%)	0.10	20 (1%) 75 56	46, 97, 175, 203	0
1	B	1526/1536 (99%)	0.13	26 (1%) 69 48	48, 88, 153, 194	0
All	All	3046/3072 (99%)	0.11	46 (1%) 72 52	46, 93, 170, 203	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	LYS	4.0
1	A	390	ASN	3.5
1	B	501	LYS	2.9
1	B	1195	ILE	2.9
1	B	251	TYR	2.8
1	B	270	LEU	2.8
1	B	1165	TYR	2.6
1	A	630	ASP	2.6
1	A	1217	VAL	2.6
1	B	309	TRP	2.6
1	B	1469	ARG	2.6
1	B	313	VAL	2.5
1	A	278	ALA	2.5
1	A	649	ILE	2.5
1	A	1159	PHE	2.4
1	B	1174	PHE	2.4
1	B	69	CYS	2.4
1	A	489	LEU	2.4
1	B	379	ILE	2.4
1	B	1110	GLY	2.4
1	B	1424	TYR	2.4
1	B	419	LEU	2.3
1	B	448	SER	2.3
1	A	374	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	2.3
1	B	312	TYR	2.3
1	A	377	ALA	2.2
1	A	389	ASN	2.2
1	B	450	PRO	2.2
1	B	649	ILE	2.2
1	A	385	SER	2.1
1	B	745	GLU	2.1
1	A	392	ILE	2.1
1	A	464	ALA	2.1
1	A	1218	GLU	2.1
1	B	314	VAL	2.1
1	A	44	MET	2.1
1	A	308	LEU	2.1
1	A	380	LEU	2.1
1	B	303	ILE	2.1
1	A	751	ASP	2.0
1	B	1263	ALA	2.0
1	B	513	TYR	2.0
1	B	1159	PHE	2.0
1	A	1301	LEU	2.0
1	B	371	ILE	2.0

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

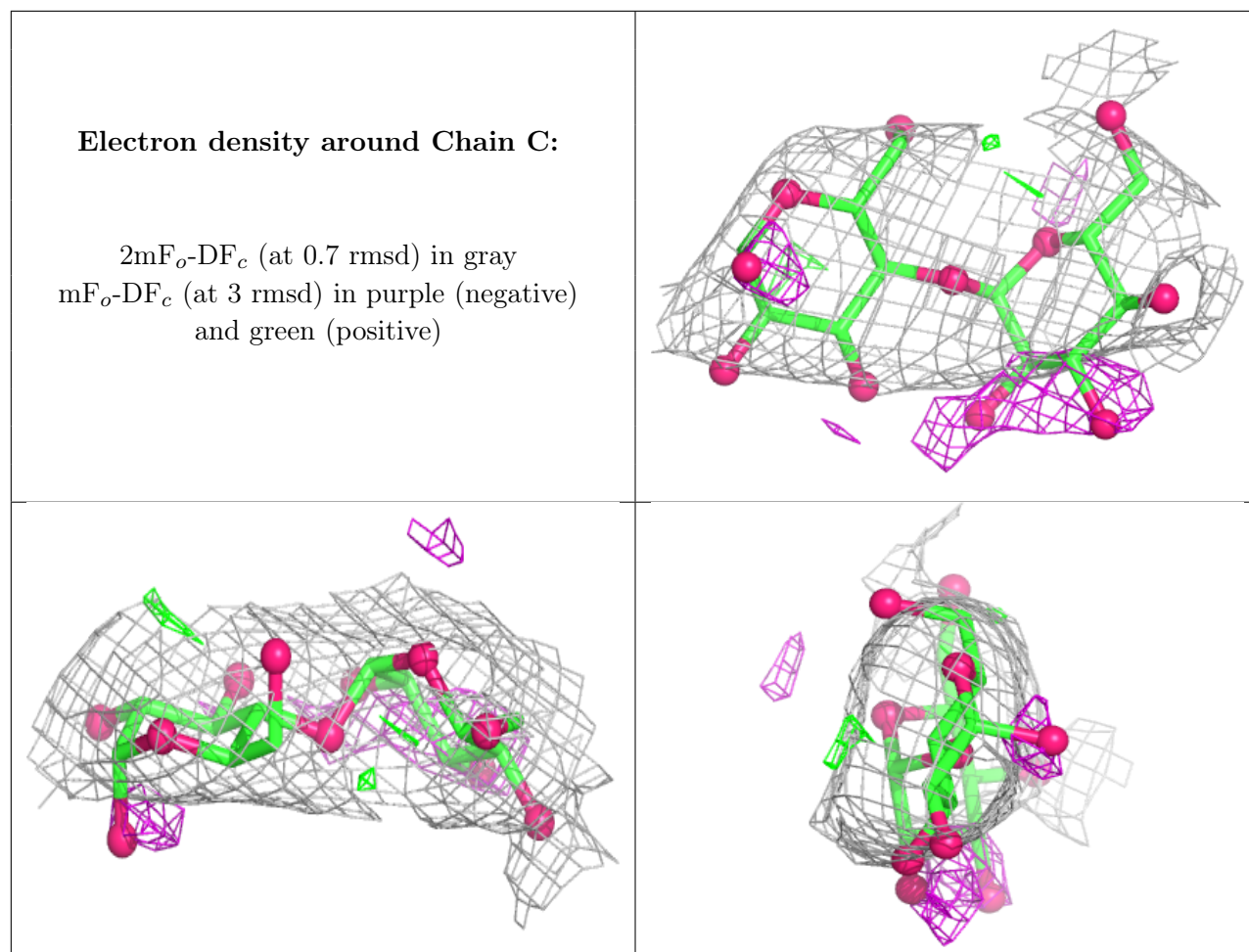
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	2	11/12	0.42	0.16	116,119,128,134	0
2	GLC	C	1	12/12	0.52	0.13	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.