



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 10:39 PM EDT

PDB ID : 7B01
Title : ADAMTS13-CUB12
Authors : Kim, H.J.; Emsley, J.
Deposited on : 2020-11-18
Resolution : 2.80 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	:	2.37.1
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)	:	2.37.1

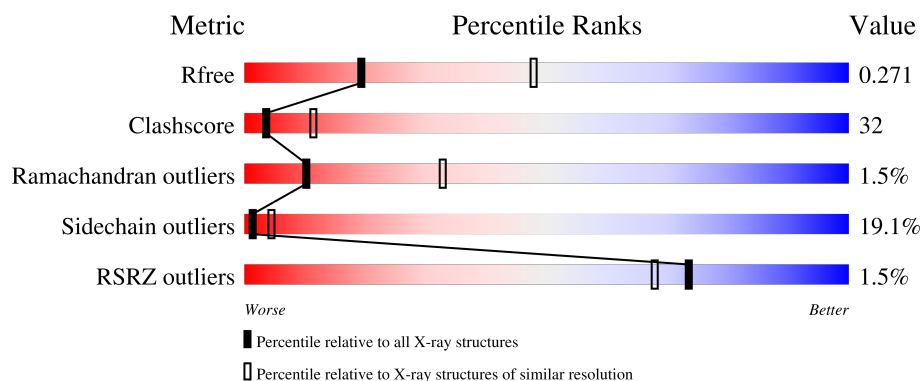
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	608	<div> <div></div> <div>53%</div> <div>34%</div> <div>10%</div> <div>.</div> </div>
2	B	2	<div>100%</div>
3	C	2	<div>50%</div> <div>50%</div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4578 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 Maltodextrin-binding protein, Maltodextrin-binding protein, Maltodextrin-binding protein, ADAMTS13 CUB12, A disintegrin and metalloproteinase with thrombospondin motifs 13, A disintegrin and metalloproteinase with thrombospondin motifs 13, A disintegrin and metalloproteinase with thrombospondin motifs 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4501	2868	766	848	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1275	SER	CYS	conflict	UNP Q76LX8

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

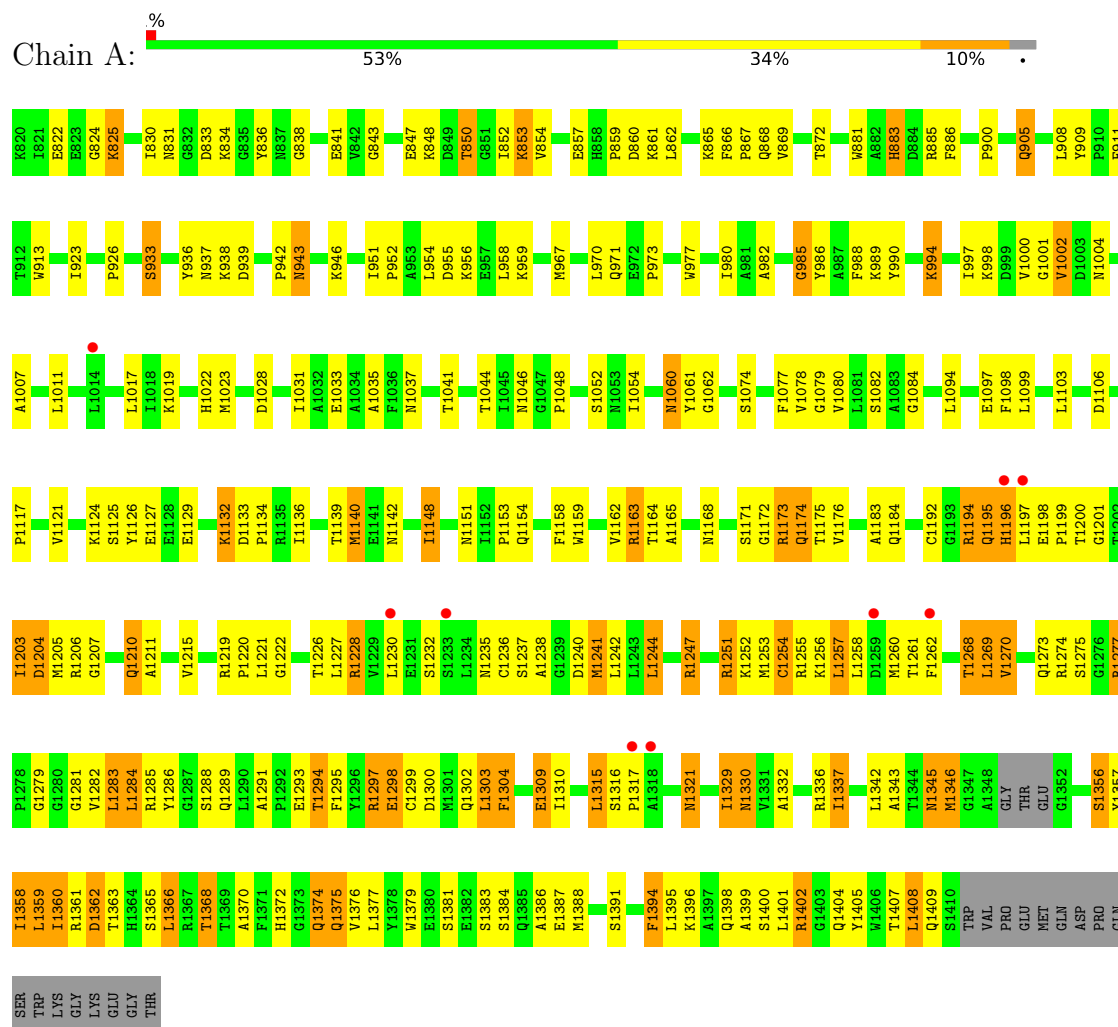
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total 26	O 26	0	0

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: Maltodextrin-binding protein, Maltodextrin-binding protein, Maltodextrin-binding protein, ADAMTS13 CUB12, A disintegrin and metalloproteinase with thrombospondin motifs 13, A disintegrin and metalloproteinase with thrombospondin motifs 13, A disintegrin and metalloproteinase with thrombospondin motifs 13



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 

MAG1
MAG2

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

Chain C:

50%

50%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.58Å 105.58Å 125.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.00 – 2.80 91.43 – 2.75	Depositor EDS
% Data completeness (in resolution range)	58.7 (70.00-2.80) 55.7 (91.43-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.201 , 0.292 0.203 , 0.271	Depositor DCC
R_{free} test set	570 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4578	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NAG, 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	0.66	0/4605	0.83	0/6252

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	4501	0	4425	283	0
2	B	28	0	25	4	0
3	C	23	0	21	1	0
4	A	26	0	0	3	0
All	All	4578	0	4471	285	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 32.

All (285) 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:1235:ASN:HD21	2:B:1:NAG:C1	1.35	1.40
1:A:1192:CYS:SG	1:A:1210:GLN:NE2	2.26	1.07
1:A:1277:ARG:HE	1:A:1277:ARG:HA	1.18	1.07
1:A:1211:ALA:HB1	1:A:1275:SER:O	1.60	1.00
1:A:1235:ASN:HD22	1:A:1238:ALA:HB2	1.24	1.00
1:A:1304:PHE:HB2	1:A:1330:ASN:O	1.60	1.00
1:A:1173:ARG:HG3	1:A:1173:ARG:HH11	1.22	0.99
1:A:1366:LEU:HD12	1:A:1366:LEU:H	1.27	0.98
1:A:1235:ASN:HD22	1:A:1238:ALA:CB	1.81	0.93
1:A:1011:LEU:HD23	1:A:1176:VAL:HG13	1.51	0.91
1:A:1303:LEU:HD23	1:A:1405:TYR:CE2	2.05	0.91
1:A:1235:ASN:ND2	1:A:1238:ALA:HB2	1.86	0.90
1:A:1316:SER:OG	1:A:1317:PRO:HD2	1.73	0.89
1:A:1257:LEU:HD12	1:A:1257:LEU:H	1.35	0.88
1:A:1195:GLN:HA	1:A:1195:GLN:NE2	1.89	0.88
1:A:1000:VAL:HG23	1:A:1002:VAL:HG22	1.54	0.87
1:A:1154:GLN:OE1	1:A:1154:GLN:N	2.06	0.87
1:A:977:TRP:HA	1:A:980:ILE:HD12	1.56	0.86
1:A:1346:MET:CE	1:A:1399:ALA:HB1	2.05	0.86
1:A:1277:ARG:HA	1:A:1277:ARG:NE	1.85	0.85
1:A:1204:ASP:OD1	1:A:1204:ASP:N	2.11	0.83
1:A:1302:GLN:HE22	1:A:1330:ASN:ND2	1.78	0.82
1:A:1240:ASP:HA	1:A:1274:ARG:O	1.78	0.81
1:A:1205:MET:HE1	1:A:1273:GLN:HB2	1.63	0.80
1:A:985:GLY:CA	1:A:1004:ASN:HD21	1.96	0.79
1:A:1124:LYS:HB2	4:A:1506:HOH:O	1.83	0.78
1:A:1204:ASP:HA	1:A:1283:LEU:HD23	1.64	0.78
1:A:985:GLY:HA2	1:A:1004:ASN:HD21	1.49	0.77
1:A:1303:LEU:O	1:A:1329:ILE:HA	1.84	0.77
1:A:1356:SER:HB3	1:A:1394:PHE:HA	1.65	0.77
1:A:985:GLY:H	1:A:1004:ASN:HD21	1.33	0.77
1:A:857:GLU:HB3	1:A:859:PRO:HD3	1.68	0.76
1:A:985:GLY:N	1:A:1004:ASN:HD21	1.83	0.75
1:A:1257:LEU:HD12	1:A:1257:LEU:N	2.01	0.75
1:A:1303:LEU:HD13	1:A:1303:LEU:H	1.49	0.75
1:A:943:ASN:N	1:A:943:ASN:HD22	1.85	0.75
1:A:1232:SER:HA	1:A:1282:VAL:HG12	1.69	0.74
1:A:1356:SER:HB3	1:A:1394:PHE:CA	2.17	0.74
1:A:1337:ILE:CD1	1:A:1386:ALA:CB	2.66	0.73
1:A:1316:SER:OG	1:A:1317:PRO:CD	2.36	0.73
1:A:1205:MET:CE	1:A:1273:GLN:HB2	2.19	0.73
1:A:1366:LEU:HD12	1:A:1366:LEU:N	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:LYS:O	1:A:1256:LYS:HG3	1.89	0.72
1:A:994:LYS:NZ	1:A:994:LYS:HB3	2.06	0.71
1:A:909:TYR:HE1	1:A:1124:LYS:HA	1.56	0.70
1:A:1377:LEU:HD12	1:A:1377:LEU:O	1.90	0.70
1:A:1054:ILE:HG22	1:A:1061:TYR:CD1	2.26	0.69
1:A:1219:ARG:HD3	1:A:1220:PRO:HD3	1.74	0.69
1:A:883:HIS:CE1	1:A:1080:VAL:H	2.10	0.69
1:A:1242:LEU:HD21	1:A:1282:VAL:HG21	1.75	0.69
1:A:1337:ILE:CD1	1:A:1386:ALA:HB3	2.23	0.69
1:A:1140:MET:HE3	1:A:1140:MET:HA	1.74	0.69
1:A:1356:SER:HB3	1:A:1394:PHE:N	2.08	0.69
1:A:1201:GLY:HA3	1:A:1286:TYR:CE2	2.28	0.68
1:A:1377:LEU:HD12	1:A:1377:LEU:C	2.12	0.68
1:A:900:PRO:HG2	1:A:905:GLN:HG3	1.76	0.68
1:A:1302:GLN:HE22	1:A:1330:ASN:HD22	1.42	0.68
1:A:886:PHE:HE2	1:A:1084:GLY:HA3	1.59	0.68
1:A:1346:MET:HE3	1:A:1399:ALA:HB1	1.76	0.68
1:A:1253:MET:HE3	1:A:1262:PHE:CE2	2.29	0.67
1:A:1302:GLN:NE2	1:A:1330:ASN:ND2	2.42	0.67
1:A:994:LYS:HB3	1:A:994:LYS:HZ2	1.60	0.66
1:A:1329:ILE:HG12	1:A:1329:ILE:O	1.94	0.66
1:A:1206:ARG:HD3	1:A:1283:LEU:HB2	1.76	0.66
1:A:1002:VAL:HG21	1:A:1184:GLN:HA	1.77	0.66
1:A:1222:GLY:O	1:A:1291:ALA:HB2	1.94	0.66
1:A:831:ASN:ND2	1:A:833:ASP:OD1	2.28	0.65
1:A:1219:ARG:HD2	1:A:1220:PRO:HD2	1.78	0.65
1:A:985:GLY:H	1:A:1004:ASN:ND2	1.93	0.65
1:A:1342:LEU:HG	1:A:1376:VAL:HG13	1.76	0.65
1:A:1238:ALA:HB2	2:B:1:NAG:HN2	1.60	0.64
1:A:1106:ASP:OD1	1:A:1126:TYR:HB2	1.97	0.64
1:A:1219:ARG:HD3	1:A:1220:PRO:CD	2.27	0.64
1:A:1173:ARG:HG3	1:A:1173:ARG:NH1	2.02	0.64
1:A:973:PRO:HD3	1:A:1163:ARG:HG3	1.81	0.63
1:A:1303:LEU:HD13	1:A:1303:LEU:N	2.14	0.63
1:A:1299:CYS:HB3	1:A:1315:LEU:HD22	1.81	0.63
1:A:1297:ARG:CG	1:A:1297:ARG:HH21	2.13	0.62
1:A:1199:PRO:HG3	1:A:1219:ARG:NH1	2.14	0.62
1:A:988:PHE:CD1	1:A:1000:VAL:HG12	2.35	0.62
1:A:1173:ARG:NH2	1:A:1288:SER:OG	2.33	0.61
1:A:1240:ASP:OD1	1:A:1275:SER:HA	2.00	0.61
1:A:825:LYS:HB2	1:A:853:LYS:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:ILE:CG2	1:A:1061:TYR:CD1	2.82	0.61
1:A:1133:ASP:OD1	1:A:1134:PRO:HD2	2.01	0.61
1:A:1337:ILE:HD12	1:A:1386:ALA:HB3	1.81	0.61
1:A:1035:ALA:HB2	4:A:1507:HOH:O	2.01	0.60
1:A:881:TRP:NE1	1:A:885:ARG:HG3	2.15	0.60
1:A:1346:MET:CE	1:A:1399:ALA:CB	2.78	0.60
1:A:1219:ARG:CD	1:A:1220:PRO:HD2	2.31	0.60
1:A:1230:LEU:HD11	1:A:1285:ARG:HB2	1.83	0.60
1:A:1379:TRP:CH2	1:A:1381:SER:HA	2.37	0.60
1:A:1002:VAL:HG23	1:A:1184:GLN:HB2	1.84	0.59
1:A:1159:TRP:CE2	3:C:2:GLC:H4	2.38	0.59
1:A:1257:LEU:H	1:A:1257:LEU:CD1	2.08	0.59
1:A:1136:ILE:O	1:A:1139:THR:N	2.36	0.58
1:A:1359:LEU:HD12	1:A:1370:ALA:CB	2.32	0.58
1:A:1342:LEU:HD12	1:A:1342:LEU:N	2.20	0.57
1:A:951:ILE:N	1:A:952:PRO:HD2	2.20	0.57
1:A:1304:PHE:N	1:A:1304:PHE:CD1	2.71	0.57
1:A:1004:ASN:OD1	1:A:1007:ALA:N	2.34	0.56
1:A:943:ASN:HD22	1:A:943:ASN:H	1.51	0.56
1:A:1251:ARG:NH1	1:A:1262:PHE:CE1	2.73	0.56
1:A:1206:ARG:HA	1:A:1281:GLY:HA3	1.88	0.56
1:A:1129:GLU:O	1:A:1132:LYS:HB2	2.06	0.56
1:A:1240:ASP:CG	1:A:1275:SER:HA	2.26	0.56
1:A:1000:VAL:HG22	1:A:1184:GLN:NE2	2.21	0.56
1:A:1173:ARG:HH11	1:A:1173:ARG:CG	2.04	0.56
1:A:1273:GLN:HE21	1:A:1282:VAL:HG22	1.71	0.56
1:A:1346:MET:HE2	1:A:1399:ALA:CB	2.36	0.56
1:A:1297:ARG:NH2	1:A:1297:ARG:HG3	2.20	0.55
1:A:1253:MET:CE	1:A:1262:PHE:CE2	2.89	0.55
1:A:1297:ARG:HH21	1:A:1297:ARG:HB2	1.71	0.55
1:A:1345:ASN:HB3	1:A:1399:ALA:HA	1.87	0.55
1:A:1309:GLU:OE1	1:A:1404:GLN:HG2	2.06	0.55
1:A:1000:VAL:CG2	1:A:1002:VAL:HG22	2.31	0.55
1:A:1195:GLN:HG2	1:A:1203:ILE:CD1	2.37	0.55
1:A:1227:LEU:HD23	1:A:1228:ARG:N	2.22	0.55
1:A:1165:ALA:HB2	1:A:1183:ALA:HB2	1.89	0.54
1:A:1207:GLY:HA2	1:A:1279:GLY:HA2	1.89	0.54
1:A:1310:ILE:HD11	1:A:1405:TYR:HB3	1.89	0.54
1:A:1401:LEU:C	1:A:1401:LEU:HD23	2.27	0.54
1:A:1303:LEU:HD23	1:A:1405:TYR:HE2	1.70	0.54
1:A:985:GLY:HA2	1:A:1004:ASN:ND2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:LEU:O	1:A:1097:GLU:HB3	2.08	0.54
1:A:1219:ARG:CD	1:A:1220:PRO:CD	2.86	0.54
1:A:1362:ASP:HB3	1:A:1383:SER:OG	2.08	0.53
1:A:1121:VAL:HG23	1:A:1127:GLU:HB2	1.89	0.53
1:A:1136:ILE:O	1:A:1139:THR:HB	2.08	0.53
1:A:1284:LEU:O	1:A:1284:LEU:HD22	2.09	0.53
1:A:1360:ILE:HD11	1:A:1379:TRP:CZ3	2.43	0.53
1:A:943:ASN:N	1:A:943:ASN:ND2	2.51	0.53
1:A:1241:MET:HB2	1:A:1253:MET:O	2.09	0.53
1:A:1275:SER:O	1:A:1275:SER:OG	2.23	0.53
1:A:1023:MET:CE	4:A:1505:HOH:O	2.56	0.52
1:A:1033:GLU:O	1:A:1037:ASN:ND2	2.41	0.52
1:A:1165:ALA:O	1:A:1168:ASN:OD1	2.27	0.52
1:A:1357:TYR:O	1:A:1391:SER:HB3	2.10	0.52
1:A:1103:LEU:O	1:A:1103:LEU:HD12	2.09	0.52
1:A:1235:ASN:ND2	1:A:1238:ALA:CB	2.57	0.52
1:A:1303:LEU:N	1:A:1303:LEU:CD1	2.72	0.52
1:A:1151:ASN:CG	1:A:1151:ASN:O	2.46	0.52
1:A:1052:SER:HB2	1:A:1117:PRO:HD3	1.91	0.52
1:A:1273:GLN:HE22	1:A:1281:GLY:CA	2.22	0.52
1:A:825:LYS:CB	1:A:853:LYS:HD3	2.40	0.51
1:A:868:GLN:O	1:A:872:THR:HG23	2.10	0.51
1:A:1094:LEU:O	1:A:1098:PHE:N	2.39	0.51
1:A:1273:GLN:NE2	1:A:1281:GLY:HA2	2.25	0.51
1:A:1273:GLN:NE2	1:A:1282:VAL:H	2.07	0.51
1:A:1336:ARG:O	1:A:1409:GLN:OE1	2.28	0.51
1:A:1277:ARG:HE	1:A:1277:ARG:CA	2.07	0.51
1:A:954:LEU:O	1:A:958:LEU:HD12	2.11	0.50
1:A:1236:CYS:SG	1:A:1255:ARG:N	2.69	0.50
1:A:847:GLU:CD	1:A:853:LYS:HA	2.31	0.50
1:A:1247:ARG:HH21	1:A:1247:ARG:HB2	1.77	0.50
1:A:1297:ARG:HH21	1:A:1297:ARG:HG3	1.75	0.50
1:A:1054:ILE:HG22	1:A:1061:TYR:CE1	2.47	0.50
1:A:1297:ARG:CG	1:A:1297:ARG:NH2	2.73	0.50
1:A:1304:PHE:CB	1:A:1330:ASN:O	2.48	0.50
1:A:982:ALA:HB2	1:A:1074:SER:HA	1.94	0.49
1:A:1078:VAL:HB	1:A:1148:ILE:HA	1.94	0.49
1:A:847:GLU:OE1	1:A:853:LYS:HA	2.11	0.49
1:A:1346:MET:HE2	1:A:1399:ALA:HB1	1.88	0.49
1:A:1337:ILE:HD11	1:A:1386:ALA:CB	2.42	0.49
1:A:971:GLN:HG3	1:A:1028:ASP:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:PHE:C	1:A:1394:PHE:CD1	2.84	0.49
1:A:1158:PHE:O	1:A:1162:VAL:HG23	2.13	0.49
1:A:1304:PHE:HB3	1:A:1330:ASN:H	1.77	0.49
1:A:883:HIS:HE1	1:A:1079:GLY:HA2	1.78	0.49
1:A:1028:ASP:HB2	1:A:1031:ILE:HG13	1.94	0.48
1:A:1297:ARG:HH21	1:A:1297:ARG:CB	2.26	0.48
1:A:1211:ALA:CB	1:A:1275:SER:O	2.47	0.48
1:A:866:PHE:CD1	1:A:866:PHE:C	2.87	0.48
1:A:997:ILE:C	1:A:997:ILE:HD12	2.33	0.48
1:A:1302:GLN:NE2	1:A:1330:ASN:HD21	2.12	0.48
1:A:1052:SER:HB2	1:A:1117:PRO:CD	2.43	0.48
1:A:1357:TYR:H	1:A:1391:SER:CB	2.27	0.48
1:A:1337:ILE:HG12	1:A:1337:ILE:O	2.11	0.47
1:A:909:TYR:CE1	1:A:1124:LYS:HA	2.43	0.47
1:A:1197:LEU:HA	1:A:1219:ARG:NH2	2.29	0.47
1:A:1037:ASN:OD1	1:A:1054:ILE:HA	2.14	0.47
1:A:1198:GLU:HB2	1:A:1286:TYR:OH	2.14	0.47
1:A:1299:CYS:HB3	1:A:1315:LEU:CD2	2.45	0.47
1:A:1168:ASN:HB2	1:A:1174:GLN:HG3	1.94	0.47
1:A:1361:ARG:HD3	1:A:1368:THR:HG22	1.95	0.47
1:A:913:TRP:CZ3	1:A:926:PRO:HD3	2.50	0.47
1:A:1164:THR:O	1:A:1168:ASN:CG	2.53	0.47
1:A:1253:MET:CE	1:A:1262:PHE:CD2	2.98	0.47
1:A:994:LYS:NZ	1:A:994:LYS:CB	2.73	0.47
1:A:1230:LEU:HB2	1:A:1283:LEU:HD13	1.97	0.47
1:A:1304:PHE:HD1	1:A:1304:PHE:H	1.63	0.46
1:A:865:LYS:O	1:A:869:VAL:HG13	2.16	0.46
1:A:1140:MET:HE2	1:A:1140:MET:HB3	1.79	0.46
1:A:1241:MET:HG2	1:A:1242:LEU:O	2.15	0.46
1:A:1297:ARG:HG3	1:A:1297:ARG:O	2.15	0.46
1:A:881:TRP:CD1	1:A:885:ARG:HG3	2.51	0.46
1:A:1304:PHE:CD1	1:A:1304:PHE:O	2.69	0.46
1:A:1195:GLN:HG2	1:A:1203:ILE:HD12	1.96	0.46
1:A:1195:GLN:HB3	1:A:1196:HIS:H	1.52	0.46
1:A:1196:HIS:CD2	1:A:1197:LEU:HB2	2.51	0.46
1:A:1140:MET:HE3	1:A:1140:MET:CA	2.43	0.46
1:A:1235:ASN:HD22	1:A:1238:ALA:HB3	1.73	0.46
1:A:1247:ARG:HH22	1:A:1268:THR:HB	1.81	0.46
1:A:1284:LEU:N	1:A:1284:LEU:HD13	2.30	0.46
1:A:881:TRP:HE1	1:A:885:ARG:HG3	1.79	0.45
1:A:1048:PRO:O	1:A:1117:PRO:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:ARG:HD3	1:A:1196:HIS:HB3	1.97	0.45
1:A:1154:GLN:H	1:A:1154:GLN:CD	2.13	0.45
1:A:967:MET:HB2	1:A:1041:THR:HG21	1.97	0.45
1:A:1221:LEU:HG	1:A:1302:GLN:HB2	1.98	0.45
1:A:955:ASP:HB3	1:A:1022:HIS:ND1	2.32	0.45
1:A:1256:LYS:O	1:A:1256:LYS:CG	2.57	0.45
1:A:1295:PHE:CD2	1:A:1295:PHE:O	2.70	0.45
1:A:843:GLY:HA3	1:A:854:VAL:HG11	1.97	0.45
1:A:850:THR:HG22	1:A:852:ILE:HD13	1.98	0.45
1:A:986:TYR:CE1	1:A:1001:GLY:HA2	2.51	0.45
1:A:1374:GLN:HG3	1:A:1375:GLN:NE2	2.31	0.45
1:A:1171:SER:O	1:A:1173:ARG:N	2.50	0.45
1:A:1159:TRP:HA	1:A:1159:TRP:CE3	2.52	0.44
1:A:1235:ASN:C	1:A:1237:SER:H	2.20	0.44
1:A:1356:SER:CB	1:A:1394:PHE:N	2.79	0.44
1:A:1273:GLN:NE2	1:A:1281:GLY:CA	2.80	0.44
2:B:1:NAG:O7	2:B:1:NAG:O3	2.29	0.44
1:A:933:SER:HA	1:A:1142:ASN:ND2	2.33	0.44
1:A:937:ASN:OD1	1:A:939:ASP:HB2	2.18	0.44
1:A:1153:PRO:HD2	1:A:1154:GLN:OE1	2.17	0.44
1:A:1204:ASP:CA	1:A:1283:LEU:HD23	2.41	0.44
1:A:911:PHE:CD1	1:A:911:PHE:C	2.90	0.44
1:A:938:LYS:HB2	1:A:1060:ASN:O	2.18	0.44
1:A:1315:LEU:HD12	1:A:1315:LEU:HA	1.66	0.44
1:A:1357:TYR:H	1:A:1391:SER:HB3	1.83	0.44
1:A:1221:LEU:CD1	1:A:1300:ASP:O	2.66	0.43
2:B:2:NAG:O7	2:B:2:NAG:H3	2.17	0.43
1:A:866:PHE:HA	1:A:869:VAL:HG22	1.98	0.43
1:A:830:ILE:CG2	1:A:836:TYR:HB3	2.49	0.43
1:A:1357:TYR:O	1:A:1391:SER:CB	2.67	0.43
1:A:1303:LEU:HD22	1:A:1329:ILE:HB	2.00	0.43
1:A:1359:LEU:HD12	1:A:1370:ALA:HA	2.00	0.43
1:A:1195:GLN:HG2	1:A:1203:ILE:HD11	2.00	0.43
1:A:1254:CYS:SG	1:A:1255:ARG:N	2.90	0.43
1:A:1198:GLU:N	1:A:1219:ARG:HH22	2.16	0.43
1:A:1321:ASN:CG	1:A:1396:LYS:HE3	2.39	0.43
1:A:1203:ILE:HD13	1:A:1203:ILE:N	2.33	0.43
1:A:1099:LEU:HA	1:A:1103:LEU:HB3	2.01	0.43
1:A:1375:GLN:N	1:A:1375:GLN:CD	2.71	0.43
1:A:824:GLY:O	1:A:852:ILE:HG23	2.19	0.43
1:A:866:PHE:N	1:A:867:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:ASN:O	1:A:1151:ASN:OD1	2.36	0.43
1:A:1194:ARG:HH12	1:A:1304:PHE:HB2	1.83	0.43
1:A:1206:ARG:H	1:A:1206:ARG:HG3	1.66	0.43
1:A:1358:ILE:CD1	1:A:1388:MET:HE2	2.49	0.43
1:A:838:GLY:O	1:A:841:GLU:HB2	2.19	0.42
1:A:908:LEU:HD23	1:A:926:PRO:HG2	2.01	0.42
1:A:1310:ILE:O	1:A:1402:ARG:HA	2.18	0.42
1:A:951:ILE:H	1:A:952:PRO:HD2	1.84	0.42
1:A:1407:THR:HB	1:A:1408:LEU:H	1.61	0.42
1:A:1253:MET:HE1	1:A:1262:PHE:CD2	2.55	0.42
1:A:1244:LEU:N	1:A:1244:LEU:HD23	2.35	0.42
1:A:1199:PRO:HG3	1:A:1219:ARG:HH11	1.85	0.42
1:A:1133:ASP:OD1	1:A:1134:PRO:CD	2.66	0.41
1:A:977:TRP:CD1	1:A:1077:PHE:CD2	3.08	0.41
1:A:1269:LEU:HD23	1:A:1270:VAL:H	1.85	0.41
1:A:1284:LEU:HD22	1:A:1284:LEU:C	2.41	0.41
1:A:1359:LEU:HD13	1:A:1359:LEU:N	2.35	0.41
1:A:1173:ARG:NH1	1:A:1173:ARG:CG	2.71	0.41
1:A:1221:LEU:HD12	1:A:1300:ASP:O	2.19	0.41
1:A:1194:ARG:HB2	1:A:1332:ALA:CB	2.50	0.41
1:A:970:LEU:HD21	1:A:1023:MET:HE1	2.02	0.41
1:A:988:PHE:CD1	1:A:1000:VAL:CG1	3.04	0.41
1:A:1207:GLY:CA	1:A:1279:GLY:HA2	2.50	0.41
1:A:883:HIS:CE1	1:A:1080:VAL:N	2.84	0.40
1:A:971:GLN:CG	1:A:1028:ASP:OD1	2.69	0.40
1:A:1017:LEU:HD23	1:A:1017:LEU:N	2.36	0.40
1:A:1194:ARG:NH1	1:A:1330:ASN:O	2.54	0.40
1:A:1361:ARG:NH1	1:A:1363:THR:O	2.53	0.40
1:A:936:TYR:CE1	1:A:1062:GLY:HA3	2.57	0.40
1:A:946:LYS:HA	1:A:946:LYS:HE2	2.03	0.40
1:A:986:TYR:O	1:A:1001:GLY:N	2.54	0.40
1:A:1165:ALA:C	1:A:1168:ASN:OD1	2.59	0.40
1:A:955:ASP:O	1:A:959:LYS:N	2.51	0.40
1:A:1197:LEU:HA	1:A:1197:LEU:HD12	1.85	0.40
1:A:886:PHE:HE2	1:A:1084:GLY:CA	2.31	0.40
1:A:1174:GLN:HE21	1:A:1174:GLN:HA	1.86	0.40
1:A:1343:ALA:HA	1:A:1401:LEU:HA	2.03	0.40
1:A:1387:GLU:O	1:A:1387:GLU:HG2	2.21	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	584/608 (96%)	514 (88%)	61 (10%)	9 (2%)	10	33

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1002	VAL
1	A	985	GLY
1	A	1172	GLY
1	A	1298	GLU
1	A	1294	THR
1	A	1356	SER
1	A	883	HIS
1	A	942	PRO
1	A	1254	CYS

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	461/485 (95%)	373 (81%)	88 (19%)	1	4

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	822	GLU
1	A	825	LYS

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Mol	Chain	Res	Type
1	A	834	LYS
1	A	848	LYS
1	A	850	THR
1	A	853	LYS
1	A	860	ASP
1	A	861	LYS
1	A	862	LEU
1	A	905	GLN
1	A	923	ILE
1	A	933	SER
1	A	943	ASN
1	A	956	LYS
1	A	989	LYS
1	A	990	TYR
1	A	994	LYS
1	A	998	LYS
1	A	1019	LYS
1	A	1044	THR
1	A	1046	ASN
1	A	1060	ASN
1	A	1082	SER
1	A	1125	SER
1	A	1132	LYS
1	A	1140	MET
1	A	1148	ILE
1	A	1163	ARG
1	A	1173	ARG
1	A	1174	GLN
1	A	1175	THR
1	A	1194	ARG
1	A	1195	GLN
1	A	1196	HIS
1	A	1200	THR
1	A	1203	ILE
1	A	1204	ASP
1	A	1210	GLN
1	A	1215	VAL
1	A	1226	THR
1	A	1228	ARG
1	A	1241	MET
1	A	1244	LEU
1	A	1247	ARG

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Mol	Chain	Res	Type
1	A	1251	ARG
1	A	1252	LYS
1	A	1257	LEU
1	A	1258	LEU
1	A	1260	MET
1	A	1261	THR
1	A	1268	THR
1	A	1269	LEU
1	A	1270	VAL
1	A	1277	ARG
1	A	1283	LEU
1	A	1284	LEU
1	A	1289	GLN
1	A	1293	GLU
1	A	1294	THR
1	A	1297	ARG
1	A	1298	GLU
1	A	1303	LEU
1	A	1304	PHE
1	A	1309	GLU
1	A	1315	LEU
1	A	1321	ASN
1	A	1329	ILE
1	A	1330	ASN
1	A	1337	ILE
1	A	1345	ASN
1	A	1346	MET
1	A	1358	ILE
1	A	1359	LEU
1	A	1360	ILE
1	A	1362	ASP
1	A	1365	SER
1	A	1366	LEU
1	A	1368	THR
1	A	1372	HIS
1	A	1374	GLN
1	A	1375	GLN
1	A	1384	SER
1	A	1394	PHE
1	A	1395	LEU
1	A	1398	GLN
1	A	1400	SER

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Mol	Chain	Res	Type
1	A	1402	ARG
1	A	1408	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	943	ASN
1	A	1024	ASN
1	A	1060	ASN
1	A	1072	GLN
1	A	1174	GLN
1	A	1184	GLN
1	A	1195	GLN
1	A	1196	HIS
1	A	1235	ASN
1	A	1273	GLN
1	A	1321	ASN
1	A	1330	ASN
1	A	1364	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 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	NAG	B	1	2,1	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	B	2	2	14,14,15	0.28	0	17,19,21	0.65	0
3	GLC	C	1	3	12,12,12	0.60	0	17,17,17	1.40	3 (17%)
3	GLC	C	2	3	11,11,12	0.48	0	15,15,17	1.27	2 (13%)

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	NAG	B	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
3	GLC	C	1	3	-	1/2/22/22	0/1/1/1
3	GLC	C	2	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	GLC	O4-C4-C3	-2.69	104.14	110.35
3	C	1	GLC	C3-C4-C5	2.43	114.58	110.24
3	C	2	GLC	O4-C4-C3	-2.40	104.79	110.35
3	C	2	GLC	O5-C5-C6	-2.34	103.54	107.20
3	C	1	GLC	O2-C2-C3	-2.21	105.25	110.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	2	GLC	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C3-C2-N2-C7
3	C	2	GLC	C4-C5-C6-O6

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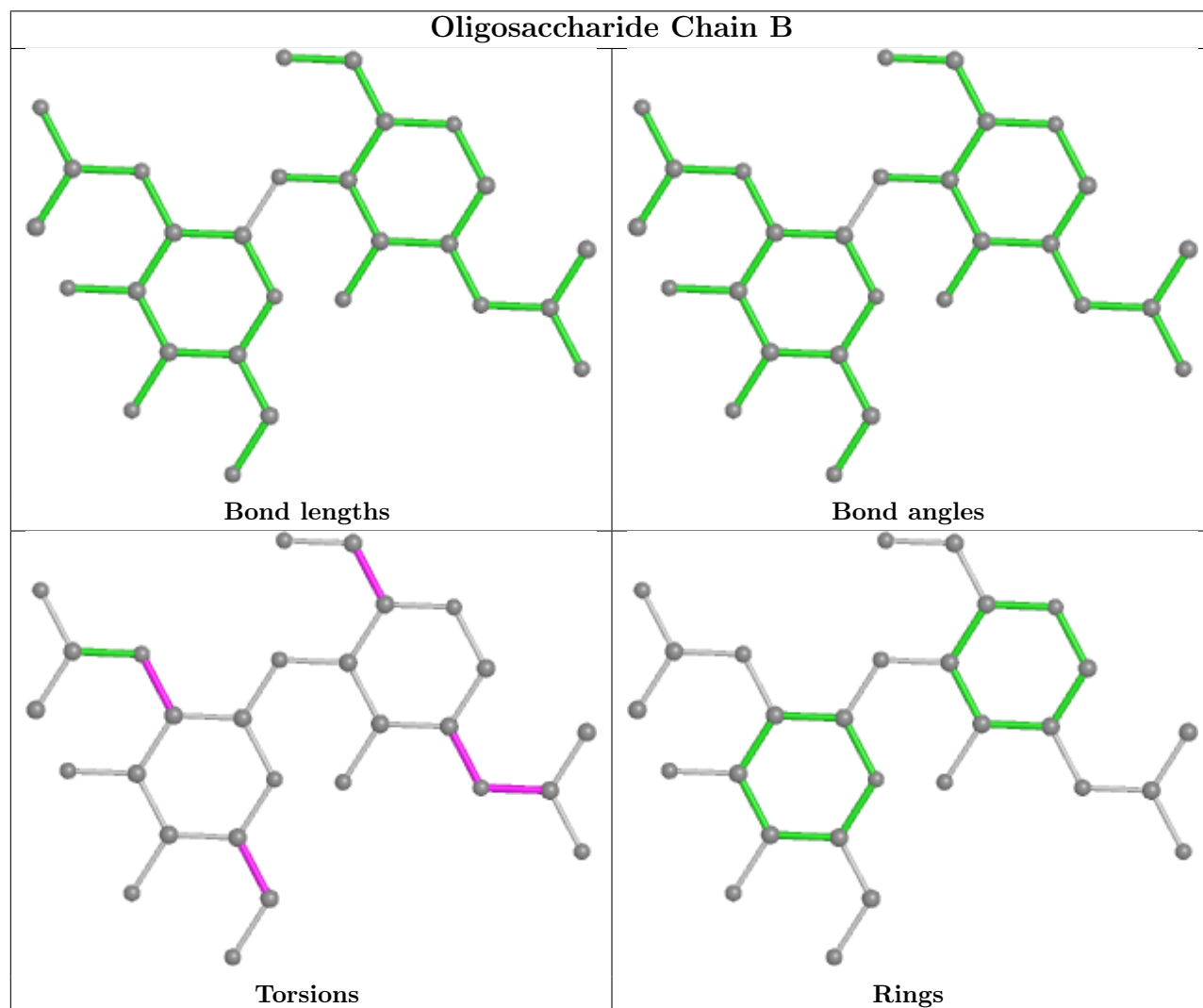
Mol	Chain	Res	Type	Atoms
3	C	1	GLC	C4-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7

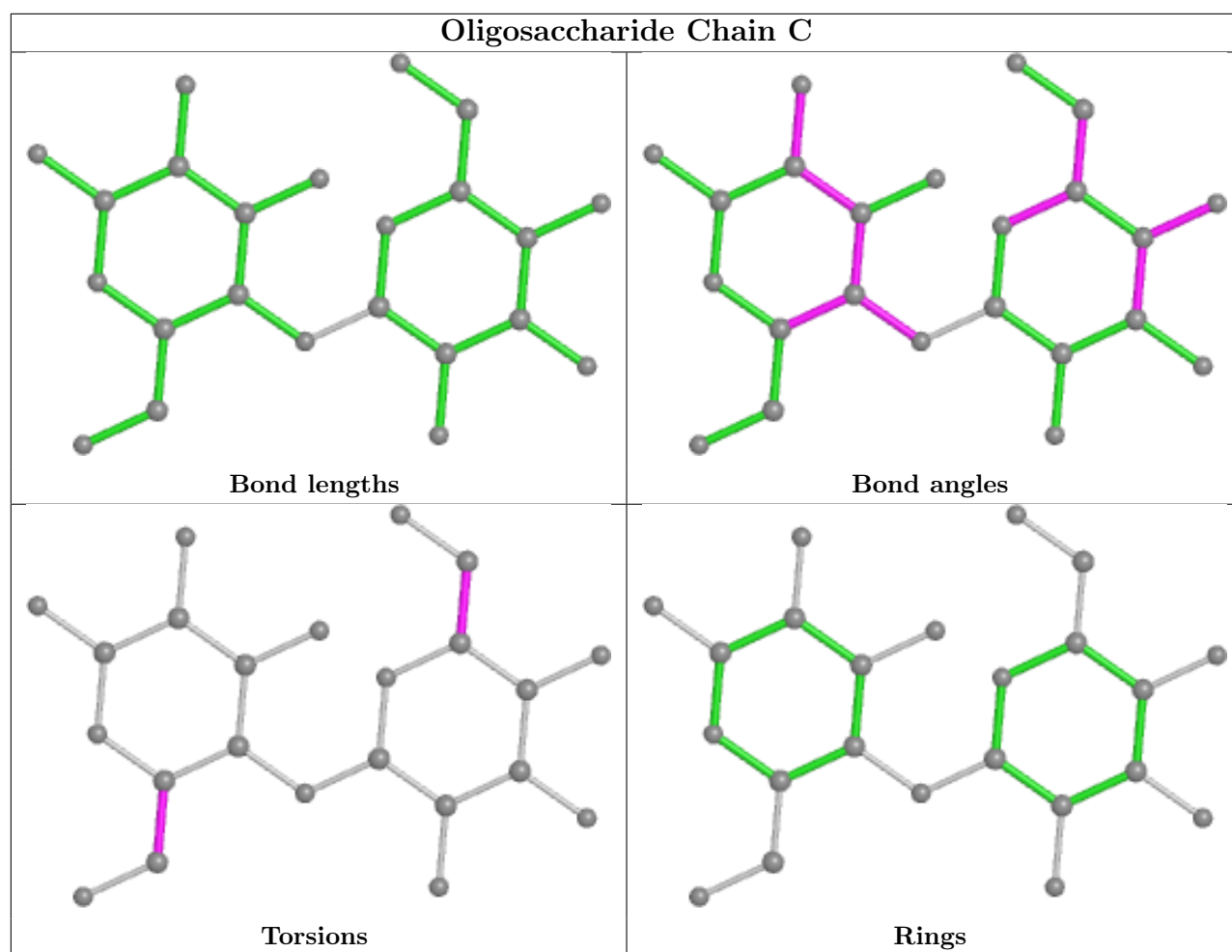
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
3	C	2	GLC	1	0
2	B	1	NAG	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](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	588/608 (96%)	-0.06	9 (1%) 73 68	23, 57, 93, 156	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1196	HIS	3.8
1	A	1318	ALA	3.0
1	A	1259	ASP	2.8
1	A	1262	PHE	2.6
1	A	1317	PRO	2.5
1	A	1014	LEU	2.5
1	A	1197	LEU	2.2
1	A	1233	SER	2.2
1	A	1230	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

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

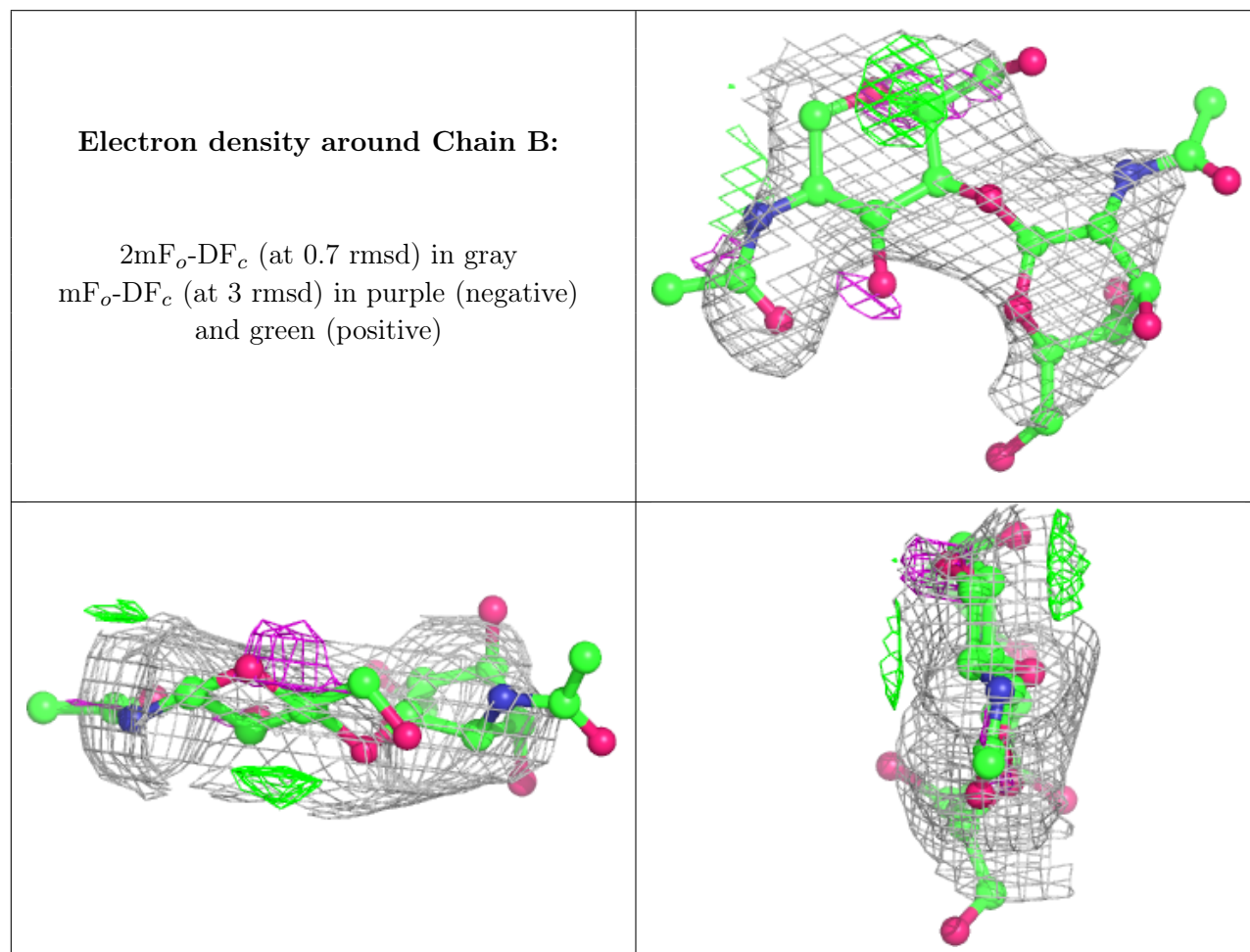
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	1	14/15	0.70	0.33	62,80,91,112	0
2	NAG	B	2	14/15	0.76	0.36	100,125,135,145	0
3	GLC	C	1	12/12	0.95	0.17	37,40,49,57	0

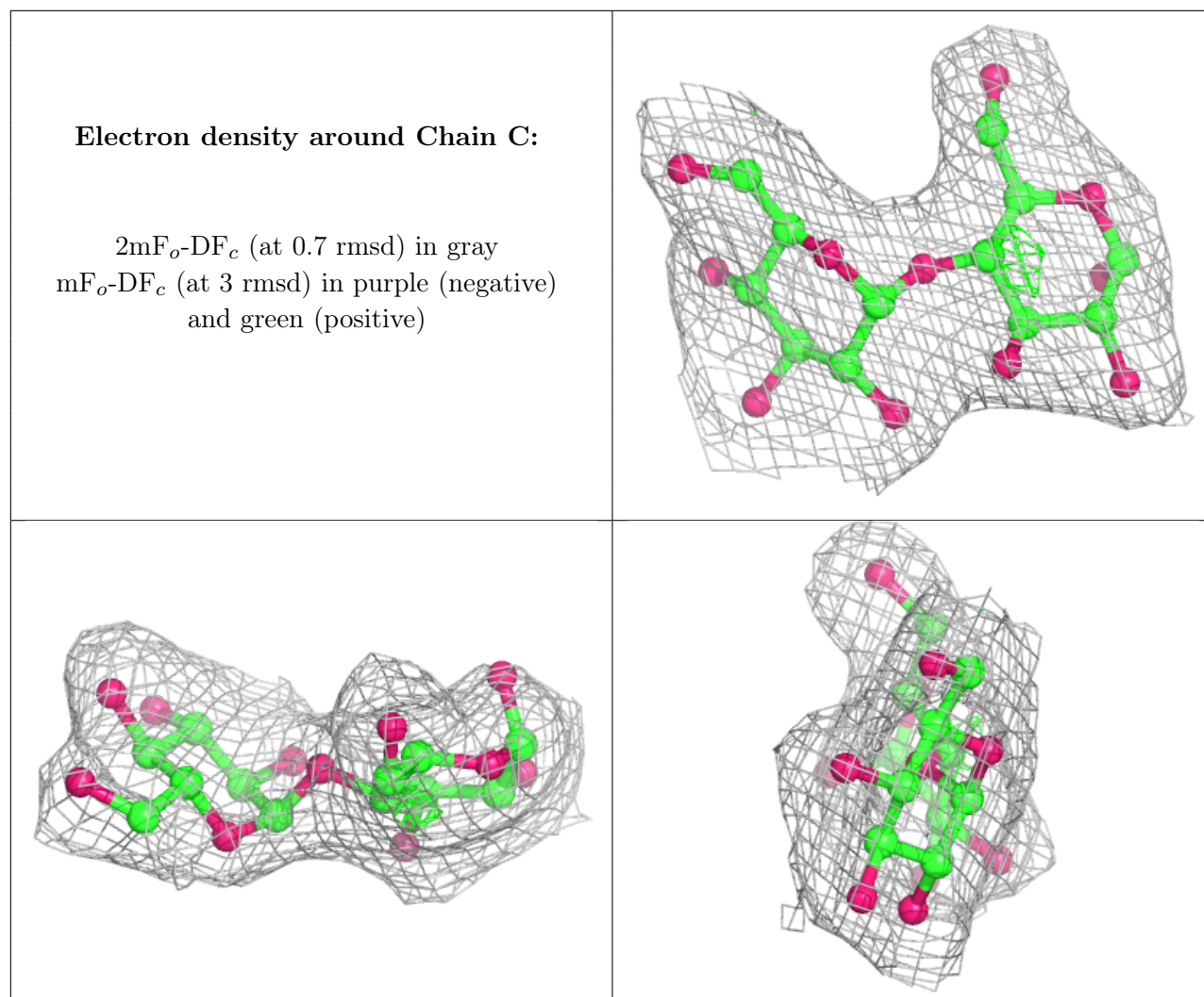
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	C	2	11/12	0.97	0.15	36,39,43,44	0

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.