



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 03:50 PM BST

PDB ID : 1UWY
Title : Crystal structure of human carboxypeptidase M
Authors : Maskos, K.; Reverter, D.; Bode, W.
Deposited on : 2004-02-17
Resolution : 3.00 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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

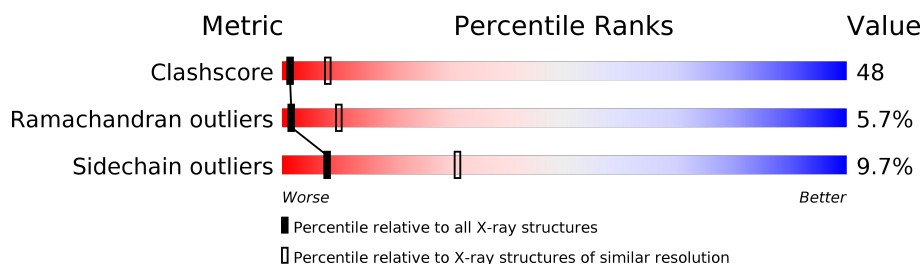
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	426	
2	B	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3230 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 CARBOXYPEPTIDASE M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	90	0	1
			3176	2033	542	585	16			

- 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	3	0	0
			28	16	2	10			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

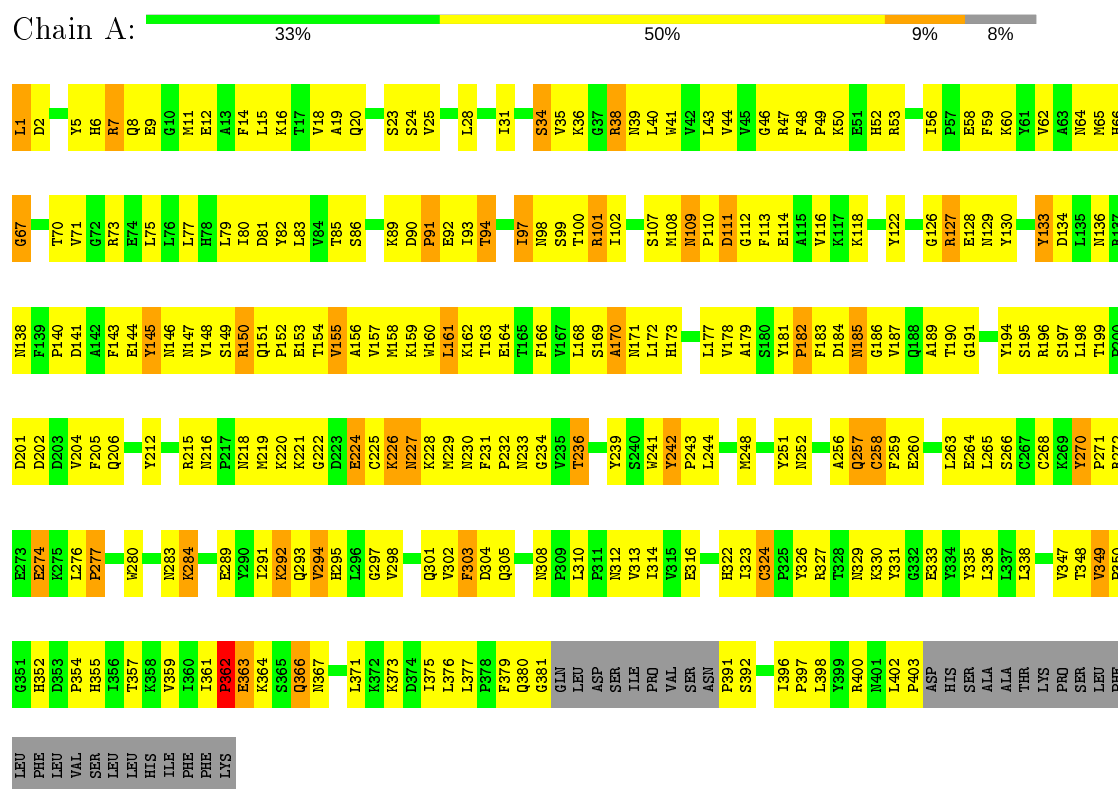
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		

3 Residue-property plots

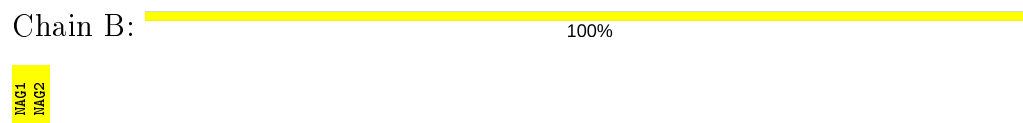
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: CARBOXYPEPTIDASE M



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



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.83Å 85.83Å 124.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	97.8 (30.00-3.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3230	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.61	2/3263 (0.1%)	0.83	1/4430 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	391	PRO	CG-CD	-6.84	1.28	1.50
1	A	391	PRO	N-CD	6.10	1.56	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	CYS	N-CA-C	-5.31	96.66	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	TYR	Sidechain

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	3176	0	3094	289	3
2	B	28	0	25	3	0
3	A	1	0	0	0	0
4	A	25	0	0	2	0
All	All	3230	0	3119	290	3

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 48.

All (290) 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:402:LEU:O	1:A:403:PRO:N	1.82	1.13
1:A:86:SER:HB2	1:A:93:ILE:HD13	1.29	1.13
1:A:47:ARG:HD2	2:B:1:NAG:H61	1.29	1.11
1:A:56:ILE:HD12	1:A:56:ILE:O	1.47	1.10
1:A:31:ILE:HG12	1:A:160:TRP:HB2	1.17	1.10
1:A:224:GLU:H	1:A:230:ASN:ND2	1.60	0.99
1:A:225:CYS:H	1:A:230:ASN:HD21	1.09	0.98
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.29	0.94
1:A:35:VAL:HG12	1:A:152:PRO:HG2	1.51	0.92
1:A:126:GLY:O	1:A:127:ARG:HB3	1.67	0.92
1:A:31:ILE:CG1	1:A:160:TRP:HB2	2.02	0.89
1:A:110:PRO:O	1:A:114:GLU:HG2	1.73	0.89
1:A:16:LYS:O	1:A:19:ALA:HB3	1.73	0.89
1:A:298:VAL:HG12	1:A:371:LEU:HB3	1.54	0.87
1:A:222:GLY:O	1:A:230:ASN:HB3	1.75	0.86
1:A:1:LEU:CD2	1:A:2:ASP:H	1.91	0.84
1:A:1:LEU:HD22	1:A:2:ASP:H	1.44	0.83
1:A:86:SER:CB	1:A:93:ILE:HD13	2.08	0.83
1:A:362:PRO:HD3	1:A:371:LEU:HD12	1.61	0.81
1:A:8:GLN:OE1	1:A:38:ARG:HD3	1.79	0.80
1:A:138:ASN:HD21	1:A:151:GLN:H	1.29	0.80
1:A:46:GLY:O	1:A:49:PRO:HD3	1.81	0.80
1:A:402:LEU:C	1:A:403:PRO:N	2.34	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:HB3	1:A:219:MET:HB3	1.65	0.79
1:A:301:GLN:HA	1:A:333:GLU:HA	1.65	0.78
1:A:65:MET:HE3	1:A:173:HIS:HE2	1.48	0.78
1:A:35:VAL:CG1	1:A:152:PRO:HG2	2.14	0.78
1:A:35:VAL:CG2	1:A:130:TYR:HB3	2.14	0.77
1:A:297:GLY:HA2	1:A:361:ILE:HD13	1.67	0.77
1:A:11:MET:HG3	1:A:77:LEU:HD11	1.64	0.77
1:A:184:ASP:HB3	1:A:244:LEU:HB3	1.66	0.76
1:A:185:ASN:HD22	1:A:186:GLY:H	1.32	0.75
1:A:304:ASP:HB3	1:A:310:LEU:HD21	1.68	0.74
1:A:47:ARG:CD	2:B:1:NAG:H61	2.15	0.74
1:A:190:THR:HG22	1:A:197:SER:HA	1.69	0.74
1:A:298:VAL:HG11	1:A:359:VAL:HG11	1.70	0.74
1:A:136:ASN:ND2	1:A:244:LEU:HD21	2.04	0.72
1:A:168:LEU:HB3	1:A:294:VAL:HG23	1.72	0.72
1:A:71:VAL:HG21	1:A:266:SER:HB3	1.70	0.72
1:A:329:ASN:OD1	1:A:333:GLU:HG2	1.89	0.72
1:A:35:VAL:HG21	1:A:130:TYR:HB3	1.71	0.72
1:A:225:CYS:N	1:A:230:ASN:HD21	1.86	0.71
1:A:93:ILE:O	1:A:97:ILE:HG13	1.89	0.71
1:A:1:LEU:HD22	1:A:2:ASP:N	2.06	0.71
1:A:159:LYS:O	1:A:162:LYS:HB2	1.92	0.70
1:A:204:VAL:HG11	1:A:259:PHE:HE2	1.55	0.69
1:A:182:PRO:HB3	1:A:183:PHE:HA	1.73	0.69
1:A:93:ILE:HG12	1:A:97:ILE:HD11	1.73	0.69
1:A:31:ILE:HG12	1:A:160:TRP:CB	2.10	0.68
1:A:67:GLY:HA3	1:A:127:ARG:H	1.59	0.68
1:A:8:GLN:O	1:A:12:GLU:HB2	1.94	0.67
1:A:138:ASN:ND2	1:A:154:THR:OG1	2.27	0.66
1:A:28:LEU:HD11	1:A:41:TRP:HE3	1.61	0.65
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.02	0.65
1:A:56:ILE:CD1	1:A:56:ILE:O	2.37	0.65
1:A:185:ASN:ND2	1:A:186:GLY:H	1.92	0.65
1:A:60:LYS:HZ3	1:A:252:ASN:HD21	1.44	0.65
1:A:71:VAL:O	1:A:75:LEU:HG	1.97	0.65
1:A:380:GLN:HG2	1:A:381:GLY:N	2.11	0.64
1:A:178:VAL:HG21	1:A:236:THR:HG22	1.78	0.64
1:A:316:GLU:OE2	1:A:322:HIS:HD2	1.80	0.64
1:A:198:LEU:HD22	1:A:202:ASP:OD2	1.98	0.64
1:A:160:TRP:HA	1:A:163:THR:HG23	1.79	0.63
1:A:304:ASP:HB2	1:A:380:GLN:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD11	1:A:41:TRP:CE3	2.33	0.63
1:A:362:PRO:CD	1:A:371:LEU:HD12	2.26	0.63
1:A:59:PHE:CE2	1:A:291:ILE:HA	2.34	0.62
1:A:136:ASN:HD22	1:A:244:LEU:HD21	1.63	0.62
1:A:169:SER:CB	1:A:260:GLU:HG3	2.29	0.62
1:A:6:HIS:O	1:A:73:ARG:NH2	2.32	0.62
1:A:242:TYR:HD2	1:A:242:TYR:C	2.03	0.62
1:A:362:PRO:HD3	1:A:371:LEU:CD1	2.30	0.62
1:A:43:LEU:HD13	1:A:80:ILE:HD13	1.81	0.62
1:A:183:PHE:CZ	1:A:199:THR:HG22	2.35	0.62
1:A:185:ASN:HD22	1:A:186:GLY:N	1.97	0.62
1:A:168:LEU:HD12	1:A:169:SER:H	1.64	0.62
1:A:90:ASP:OD2	1:A:93:ILE:HG22	2.00	0.62
1:A:349:VAL:O	1:A:352:HIS:HB2	2.00	0.61
1:A:90:ASP:HB3	1:A:93:ILE:CG2	2.30	0.61
1:A:1:LEU:CD2	1:A:2:ASP:N	2.62	0.61
1:A:242:TYR:C	1:A:242:TYR:CD2	2.74	0.61
1:A:169:SER:HB3	1:A:260:GLU:HG3	1.82	0.61
1:A:109:ASN:ND2	1:A:112:GLY:H	1.99	0.61
1:A:183:PHE:CE1	1:A:199:THR:HG22	2.36	0.61
1:A:62:VAL:O	1:A:171:ASN:HA	2.01	0.60
1:A:49:PRO:O	1:A:50:LYS:HB3	2.02	0.59
1:A:64:ASN:HB3	1:A:107:SER:HA	1.84	0.59
1:A:126:GLY:O	1:A:127:ARG:CB	2.45	0.59
1:A:232:PRO:O	1:A:233:ASN:HB2	2.03	0.59
1:A:150:ARG:HG2	1:A:150:ARG:HH11	1.68	0.58
1:A:161:LEU:HD21	1:A:252:ASN:ND2	2.19	0.58
1:A:168:LEU:HD12	1:A:169:SER:N	2.18	0.58
1:A:298:VAL:HG12	1:A:371:LEU:HD22	1.86	0.58
1:A:152:PRO:O	1:A:155:VAL:HG12	2.03	0.58
1:A:172:LEU:CD2	1:A:263:LEU:HD12	2.34	0.58
1:A:31:ILE:HG13	1:A:31:ILE:O	2.03	0.58
1:A:302:VAL:HG22	1:A:375:ILE:HB	1.86	0.58
1:A:201:ASP:HB3	1:A:204:VAL:HG12	1.86	0.57
1:A:224:GLU:H	1:A:230:ASN:HD22	1.48	0.57
1:A:38:ARG:NH1	1:A:111:ASP:HA	2.19	0.57
1:A:25:VAL:HG11	1:A:47:ARG:NH1	2.19	0.57
1:A:1:LEU:HD23	1:A:2:ASP:H	1.69	0.57
1:A:257:GLN:HG3	1:A:326:TYR:CD2	2.40	0.57
1:A:225:CYS:H	1:A:230:ASN:ND2	1.92	0.56
1:A:272:ARG:NH2	1:A:274:GLU:OE2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLN:OE1	1:A:326:TYR:HA	2.05	0.56
1:A:77:LEU:O	1:A:80:ILE:HB	2.06	0.56
1:A:178:VAL:HG21	1:A:236:THR:CG2	2.34	0.56
1:A:143:PHE:CD1	1:A:185:ASN:HB3	2.41	0.56
1:A:39:ASN:HB3	1:A:41:TRP:CE2	2.40	0.56
1:A:80:ILE:HG22	1:A:81:ASP:N	2.20	0.56
1:A:60:LYS:NZ	1:A:252:ASN:ND2	2.54	0.56
1:A:161:LEU:HD23	1:A:256:ALA:HB2	1.88	0.56
1:A:218:ASN:HA	1:A:221:LYS:HE2	1.89	0.55
1:A:268:CYS:O	1:A:271:PRO:HD3	2.06	0.55
1:A:144:GLU:O	1:A:145:TYR:C	2.44	0.55
1:A:60:LYS:NZ	1:A:252:ASN:HD21	2.04	0.55
1:A:60:LYS:HE2	1:A:161:LEU:HD11	1.88	0.55
1:A:239:TYR:CE2	1:A:243:PRO:HG3	2.41	0.55
1:A:323:ILE:HG23	1:A:324:CYS:N	2.22	0.55
1:A:177:LEU:HA	1:A:264:GLU:O	2.07	0.55
1:A:38:ARG:CG	1:A:38:ARG:HH11	2.09	0.55
1:A:71:VAL:HG21	1:A:266:SER:CB	2.36	0.54
1:A:178:VAL:CG2	1:A:236:THR:HG22	2.38	0.54
1:A:138:ASN:ND2	1:A:151:GLN:HG2	2.22	0.54
1:A:349:VAL:HG11	1:A:379:PHE:CE1	2.43	0.54
1:A:100:THR:HG22	1:A:101:ARG:N	2.23	0.54
1:A:101:ARG:NH2	1:A:101:ARG:HG2	2.23	0.54
1:A:161:LEU:HD23	1:A:256:ALA:CB	2.38	0.53
1:A:178:VAL:HG22	1:A:179:ALA:N	2.22	0.53
1:A:144:GLU:O	1:A:144:GLU:HG3	2.08	0.53
1:A:102:ILE:HD13	1:A:291:ILE:HD13	1.91	0.53
1:A:335:TYR:O	1:A:336:LEU:HD23	2.09	0.53
1:A:169:SER:OG	1:A:260:GLU:HG3	2.09	0.53
1:A:313:VAL:O	1:A:327:ARG:HA	2.09	0.53
1:A:252:ASN:HA	1:A:256:ALA:HB3	1.89	0.53
1:A:83:LEU:HA	1:A:93:ILE:HD11	1.90	0.52
1:A:90:ASP:HB3	1:A:93:ILE:HG22	1.91	0.52
1:A:178:VAL:HG23	1:A:234:GLY:O	2.09	0.52
1:A:314:ILE:HG13	1:A:327:ARG:NH1	2.24	0.52
1:A:138:ASN:HD21	1:A:151:GLN:N	2.05	0.52
1:A:101:ARG:HH21	1:A:101:ARG:HG2	1.75	0.52
1:A:366:GLN:HE21	1:A:366:GLN:HA	1.75	0.52
1:A:65:MET:HE3	1:A:173:HIS:NE2	2.19	0.52
1:A:133:TYR:OH	1:A:149:SER:HB3	2.10	0.52
1:A:100:THR:HG22	1:A:101:ARG:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:SER:O	1:A:170:ALA:HB2	2.09	0.52
1:A:70:THR:HG21	1:A:270:TYR:CE2	2.45	0.52
1:A:349:VAL:HG13	1:A:352:HIS:HB2	1.92	0.52
1:A:149:SER:O	1:A:151:GLN:NE2	2.28	0.51
1:A:111:ASP:OD1	1:A:111:ASP:N	2.42	0.51
1:A:212:TYR:CE2	1:A:263:LEU:HD13	2.45	0.51
1:A:310:LEU:HD11	1:A:377:LEU:HD12	1.93	0.51
4:A:2024:HOH:O	2:B:2:NAG:H5	2.11	0.51
1:A:257:GLN:OE1	1:A:327:ARG:N	2.42	0.51
1:A:31:ILE:O	1:A:31:ILE:CG1	2.58	0.51
1:A:338:LEU:HD12	1:A:361:ILE:HD11	1.93	0.51
1:A:127:ARG:NH1	1:A:134:ASP:OD2	2.44	0.50
1:A:185:ASN:ND2	1:A:186:GLY:N	2.56	0.50
1:A:204:VAL:CG1	1:A:259:PHE:HE2	2.23	0.50
1:A:190:THR:HG22	1:A:198:LEU:H	1.77	0.50
1:A:53:ARG:O	1:A:56:ILE:HG13	2.11	0.50
1:A:66:HIS:O	1:A:67:GLY:C	2.50	0.50
1:A:166:PHE:O	1:A:258:CYS:HB3	2.11	0.50
1:A:305:GLN:HB2	4:A:2023:HOH:O	2.11	0.50
1:A:396:ILE:O	1:A:396:ILE:HG13	2.12	0.50
1:A:276:LEU:O	1:A:277:PRO:C	2.49	0.50
1:A:348:THR:OG1	1:A:354:PRO:HB3	2.12	0.49
1:A:280:TRP:CZ2	1:A:284:LYS:HG3	2.47	0.49
1:A:347:VAL:HB	1:A:355:HIS:HB3	1.93	0.49
1:A:86:SER:HB3	1:A:93:ILE:HG21	1.94	0.49
1:A:396:ILE:O	1:A:398:LEU:HD23	2.12	0.49
1:A:265:LEU:HD22	1:A:283:ASN:HD21	1.77	0.49
1:A:190:THR:CG2	1:A:198:LEU:N	2.76	0.49
1:A:190:THR:HG22	1:A:190:THR:O	2.13	0.49
1:A:86:SER:HB2	1:A:93:ILE:CD1	2.21	0.48
1:A:108:MET:CE	1:A:157:VAL:HG21	2.43	0.48
1:A:109:ASN:HD21	1:A:112:GLY:H	1.60	0.48
1:A:160:TRP:HA	1:A:163:THR:CG2	2.42	0.48
1:A:90:ASP:CG	1:A:93:ILE:HG22	2.34	0.48
1:A:224:GLU:N	1:A:230:ASN:ND2	2.45	0.48
1:A:5:TYR:CE1	1:A:270:TYR:HE2	2.32	0.47
1:A:141:ASP:OD2	1:A:143:PHE:HB2	2.14	0.47
1:A:366:GLN:NE2	1:A:366:GLN:CA	2.78	0.47
1:A:59:PHE:C	1:A:59:PHE:CD1	2.87	0.47
1:A:178:VAL:H	1:A:264:GLU:HB2	1.80	0.47
1:A:12:GLU:HA	1:A:15:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HA	1:A:102:ILE:O	2.15	0.47
1:A:60:LYS:HE2	1:A:161:LEU:CD1	2.44	0.47
1:A:38:ARG:CG	1:A:38:ARG:NH1	2.69	0.47
1:A:116:VAL:HG21	1:A:270:TYR:HE1	1.79	0.47
1:A:215:ARG:NE	1:A:289:GLU:HG3	2.29	0.47
1:A:146:ASN:O	1:A:148:VAL:HG22	2.15	0.47
1:A:222:GLY:HA2	1:A:231:PHE:O	2.15	0.47
1:A:85:THR:O	1:A:89:LYS:HD2	2.14	0.47
1:A:349:VAL:HG11	1:A:379:PHE:CZ	2.50	0.47
1:A:70:THR:HG21	1:A:270:TYR:CZ	2.50	0.47
1:A:181:TYR:CZ	1:A:206:GLN:HG2	2.50	0.46
1:A:289:GLU:OE1	1:A:292:LYS:HE3	2.15	0.46
1:A:14:PHE:O	1:A:18:VAL:HG23	2.16	0.46
1:A:187:VAL:HG12	1:A:189:ALA:H	1.79	0.46
1:A:263:LEU:HB3	1:A:265:LEU:HD21	1.98	0.46
1:A:380:GLN:CG	1:A:381:GLY:N	2.78	0.46
1:A:81:ASP:O	1:A:82:TYR:C	2.54	0.46
1:A:313:VAL:CG1	1:A:314:ILE:N	2.78	0.46
1:A:190:THR:HG22	1:A:197:SER:CA	2.44	0.46
1:A:330:LYS:HD2	1:A:331:TYR:CZ	2.51	0.46
1:A:7:ARG:HA	1:A:113:PHE:HE2	1.80	0.46
1:A:44:VAL:CG1	1:A:101:ARG:HG3	2.46	0.45
1:A:64:ASN:ND2	1:A:107:SER:OG	2.37	0.45
1:A:150:ARG:HG2	1:A:150:ARG:NH1	2.31	0.45
1:A:239:TYR:C	1:A:241:TRP:N	2.67	0.45
1:A:133:TYR:CE2	1:A:151:GLN:NE2	2.84	0.45
1:A:190:THR:HG22	1:A:198:LEU:N	2.31	0.45
1:A:293:GLN:C	1:A:295:HIS:H	2.20	0.45
1:A:14:PHE:HE1	1:A:80:ILE:HG21	1.81	0.45
1:A:155:VAL:CG1	1:A:156:ALA:N	2.80	0.45
1:A:204:VAL:HG13	1:A:205:PHE:N	2.32	0.45
1:A:396:ILE:O	1:A:398:LEU:N	2.49	0.45
1:A:90:ASP:CB	1:A:93:ILE:HG22	2.46	0.45
1:A:93:ILE:O	1:A:97:ILE:CG1	2.63	0.44
1:A:108:MET:SD	1:A:248:MET:CE	3.05	0.44
1:A:140:PRO:HG3	1:A:150:ARG:NH2	2.32	0.44
1:A:226:LYS:C	1:A:228:LYS:H	2.20	0.44
1:A:239:TYR:C	1:A:241:TRP:H	2.21	0.44
1:A:283:ASN:O	1:A:284:LYS:C	2.56	0.44
1:A:229:MET:CG	1:A:230:ASN:N	2.80	0.44
1:A:366:GLN:NE2	1:A:366:GLN:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:HG23	1:A:116:VAL:O	2.17	0.44
1:A:191:GLY:O	1:A:196:ARG:O	2.36	0.44
1:A:169:SER:OG	1:A:170:ALA:N	2.50	0.44
1:A:116:VAL:CG2	1:A:270:TYR:HE1	2.31	0.44
1:A:159:LYS:O	1:A:162:LYS:N	2.40	0.44
1:A:172:LEU:HD21	1:A:263:LEU:HD12	1.99	0.43
1:A:222:GLY:CA	1:A:231:PHE:O	2.66	0.43
1:A:116:VAL:HG21	1:A:270:TYR:CE1	2.52	0.43
1:A:178:VAL:O	1:A:264:GLU:HB2	2.18	0.43
1:A:323:ILE:HG23	1:A:324:CYS:H	1.82	0.43
1:A:380:GLN:HG2	1:A:381:GLY:OXT	2.17	0.43
1:A:58:GLU:OE2	1:A:101:ARG:NH2	2.51	0.43
1:A:64:ASN:HD22	1:A:107:SER:CB	2.29	0.43
1:A:91:PRO:HG2	1:A:92:GLU:H	1.83	0.43
1:A:93:ILE:HG23	1:A:94:THR:N	2.34	0.43
1:A:313:VAL:HG12	1:A:314:ILE:N	2.34	0.42
1:A:34:SER:HG	1:A:36:LYS:H	1.66	0.42
1:A:146:ASN:O	1:A:147:ASN:C	2.58	0.42
1:A:133:TYR:CZ	1:A:149:SER:HB3	2.54	0.42
1:A:158:MET:HE3	1:A:251:TYR:CE1	2.55	0.42
1:A:265:LEU:HD22	1:A:283:ASN:ND2	2.33	0.42
1:A:155:VAL:O	1:A:156:ALA:C	2.58	0.42
1:A:361:ILE:O	1:A:362:PRO:O	2.38	0.42
1:A:231:PHE:CD2	1:A:231:PHE:N	2.87	0.42
1:A:158:MET:HG2	1:A:251:TYR:CZ	2.55	0.42
1:A:151:GLN:HB3	1:A:152:PRO:HD2	2.01	0.42
1:A:194:TYR:O	1:A:195:SER:HB2	2.20	0.42
1:A:60:LYS:HZ1	1:A:252:ASN:ND2	2.17	0.42
1:A:40:LEU:HD23	1:A:40:LEU:N	2.35	0.42
1:A:190:THR:HG21	1:A:197:SER:OG	2.19	0.42
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.80	0.42
1:A:56:ILE:HD12	1:A:56:ILE:C	2.30	0.42
1:A:91:PRO:O	1:A:94:THR:N	2.53	0.42
1:A:20:GLN:HA	1:A:20:GLN:NE2	2.35	0.42
1:A:242:TYR:CD2	1:A:243:PRO:O	2.73	0.42
1:A:289:GLU:OE1	1:A:292:LYS:CE	2.67	0.42
1:A:79:LEU:O	1:A:82:TYR:HB3	2.20	0.42
1:A:359:VAL:CG2	1:A:373:LYS:HG3	2.50	0.41
1:A:218:ASN:CA	1:A:221:LYS:HE2	2.50	0.41
1:A:329:ASN:CG	1:A:333:GLU:HG2	2.40	0.41
1:A:59:PHE:CD1	1:A:60:LYS:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PRO:CB	1:A:183:PHE:HA	2.41	0.41
1:A:212:TYR:C	1:A:212:TYR:CD1	2.94	0.41
1:A:25:VAL:C	1:A:49:PRO:HG3	2.40	0.41
1:A:91:PRO:O	1:A:92:GLU:C	2.57	0.41
1:A:298:VAL:CG1	1:A:371:LEU:HB3	2.39	0.41
1:A:101:ARG:HH21	1:A:101:ARG:CG	2.32	0.41
1:A:153:GLU:H	1:A:153:GLU:CD	2.24	0.41
1:A:242:TYR:HD2	1:A:243:PRO:N	2.18	0.41
1:A:28:LEU:HD11	1:A:41:TRP:HB3	2.02	0.41
1:A:108:MET:SD	1:A:248:MET:HE1	2.61	0.41
1:A:160:TRP:CA	1:A:163:THR:HG23	2.49	0.41
1:A:172:LEU:HD22	1:A:263:LEU:HB2	2.02	0.41
1:A:122:TYR:HE2	1:A:227:ASN:HB2	1.85	0.40
1:A:178:VAL:CG2	1:A:179:ALA:N	2.84	0.40
1:A:220:LYS:HE2	1:A:220:LYS:HB3	1.87	0.40
1:A:108:MET:SD	1:A:248:MET:HE2	2.61	0.40
1:A:52:HIS:NE2	1:A:333:GLU:OE1	2.51	0.40
1:A:239:TYR:CE2	1:A:243:PRO:HB3	2.57	0.40
1:A:323:ILE:CG2	1:A:324:CYS:N	2.85	0.40
1:A:127:ARG:HG3	1:A:128:GLU:N	2.36	0.40
1:A:303:PHE:HB3	1:A:308:ASN:N	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:NZ	1:A:133:TYR:CE2[5_555]	1.65	0.55
1:A:118:LYS:NZ	1:A:133:TYR:CD2[5_555]	1.94	0.26
1:A:118:LYS:NZ	1:A:133:TYR:CZ[5_555]	2.18	0.02

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	389/426 (91%)	320 (82%)	47 (12%)	22 (6%)	1	10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	362	PRO
1	A	363	GLU
1	A	364	LYS
1	A	392	SER
1	A	397	PRO
1	A	67	GLY
1	A	99	SER
1	A	170	ALA
1	A	226	LYS
1	A	284	LYS
1	A	312	ASN
1	A	7	ARG
1	A	9	GLU
1	A	23	SER
1	A	91	PRO
1	A	145	TYR
1	A	400	ARG
1	A	227	ASN
1	A	292	LYS
1	A	34	SER
1	A	98	ASN

5.3.2 Protein sidechains ⓘ

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	351/382 (92%)	317 (90%)	34 (10%)	8	31

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	24	SER
1	A	38	ARG
1	A	48	PHE
1	A	94	THR
1	A	97	ILE
1	A	101	ARG
1	A	109	ASN
1	A	111	ASP
1	A	129	ASN
1	A	150	ARG
1	A	155	VAL
1	A	161	LEU
1	A	164	GLU
1	A	182	PRO
1	A	185	ASN
1	A	224	GLU
1	A	236	THR
1	A	242	TYR
1	A	257	GLN
1	A	258	CYS
1	A	270	TYR
1	A	274	GLU
1	A	277	PRO
1	A	294	VAL
1	A	303	PHE
1	A	349	VAL
1	A	350	PRO
1	A	357	THR
1	A	362	PRO
1	A	363	GLU
1	A	366	GLN
1	A	367	ASN
1	A	376	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	64	ASN
1	A	109	ASN
1	A	138	ASN
1	A	146	ASN

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Mol	Chain	Res	Type
1	A	185	ASN
1	A	218	ASN
1	A	230	ASN
1	A	237	ASN
1	A	245	GLN
1	A	252	ASN
1	A	283	ASN
1	A	301	GLN
1	A	306	ASN
1	A	308	ASN
1	A	322	HIS
1	A	352	HIS
1	A	355	HIS
1	A	366	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	NAG	B	1	1,2	14,14,15	0.71	0	17,19,21	0.87	0
2	NAG	B	2	1,2	14,14,15	0.56	0	17,19,21	0.72	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	NAG	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	1,2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

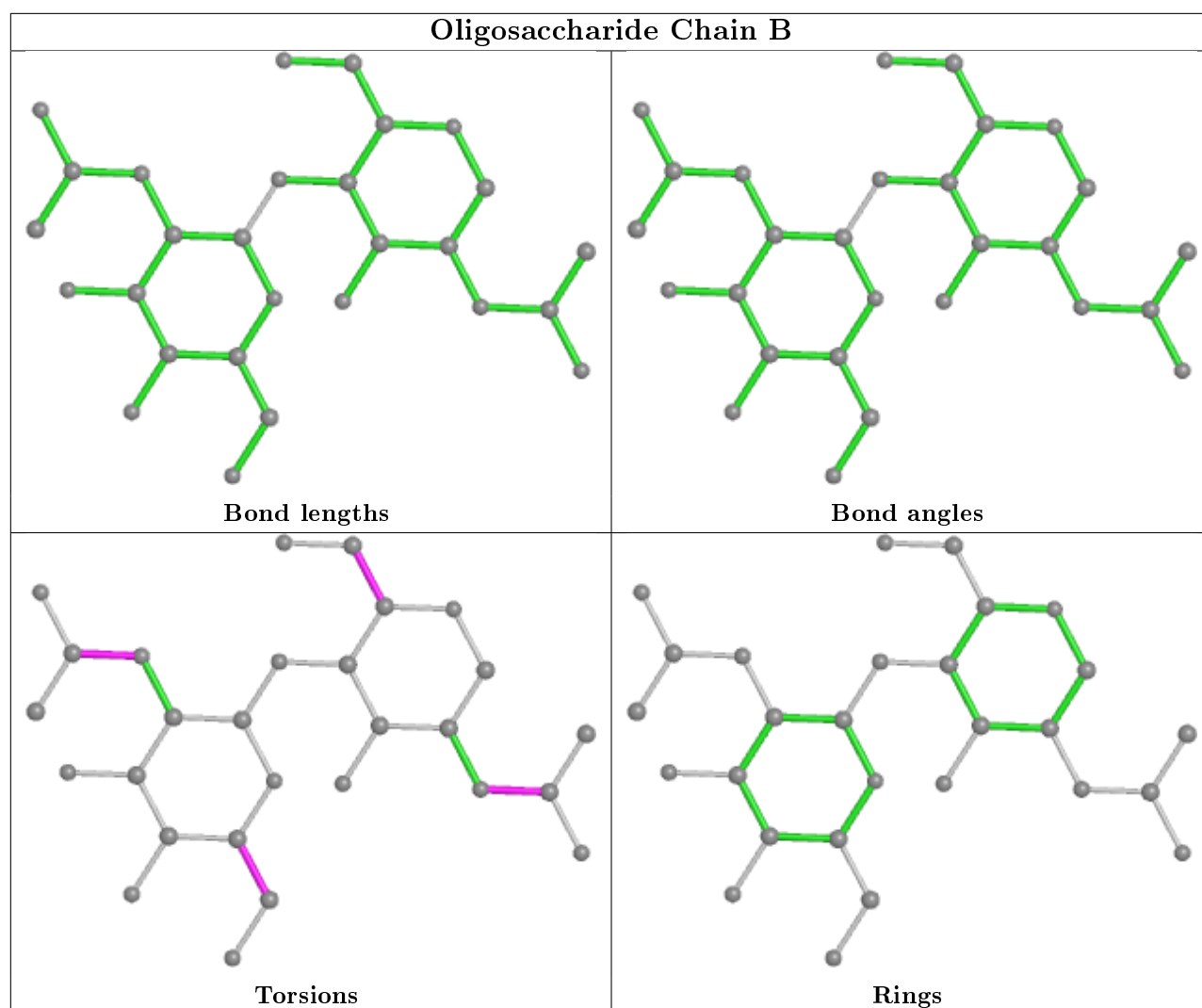
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	2	0
2	B	2	NAG	1	0

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



5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	402:LEU	C	403:PRO	N	2.34

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.