



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:33 PM UTC

PDB ID : 2BOA / pdb_00002boa
Title : Human procarboxypeptidase A4.
Authors : Garcia-Castellanos, R.; Bonet-Figueredo, R.; Pallares, I.; Ventura, S.; Aviles, F.X.; Vendrell, J.; Gomis-Ruth, F.X.
Deposited on : 2005-04-08
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

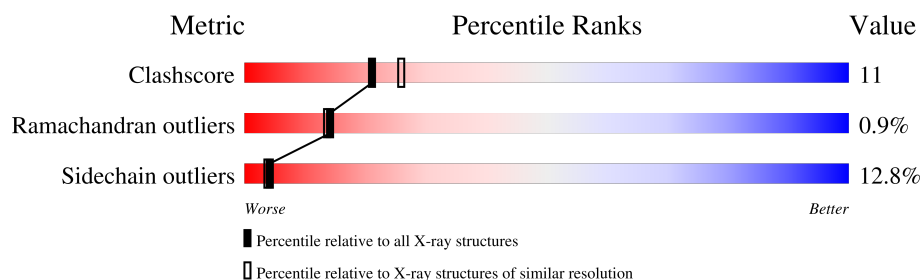
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	404	
1	B	404	
2	C	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6882 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 A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3220	2038	561	612	9			
1	B	404	Total	C	N	O	S	0	0	0
			3220	2038	561	612	9			

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

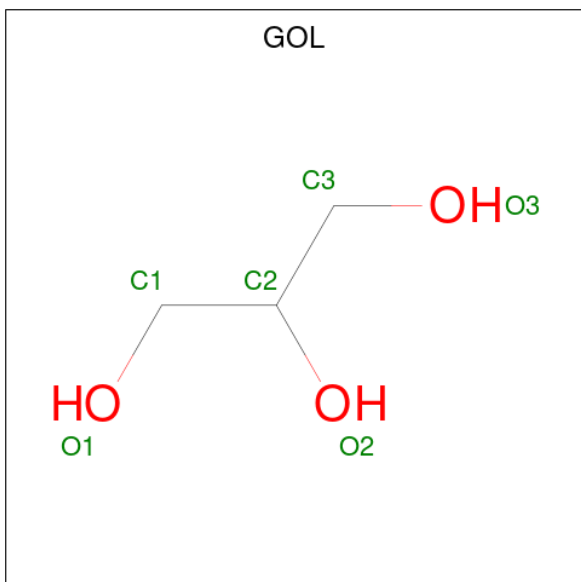


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	202	Total	O	0	0
			202	202		
6	B	172	Total	O	0	0
			172	172		

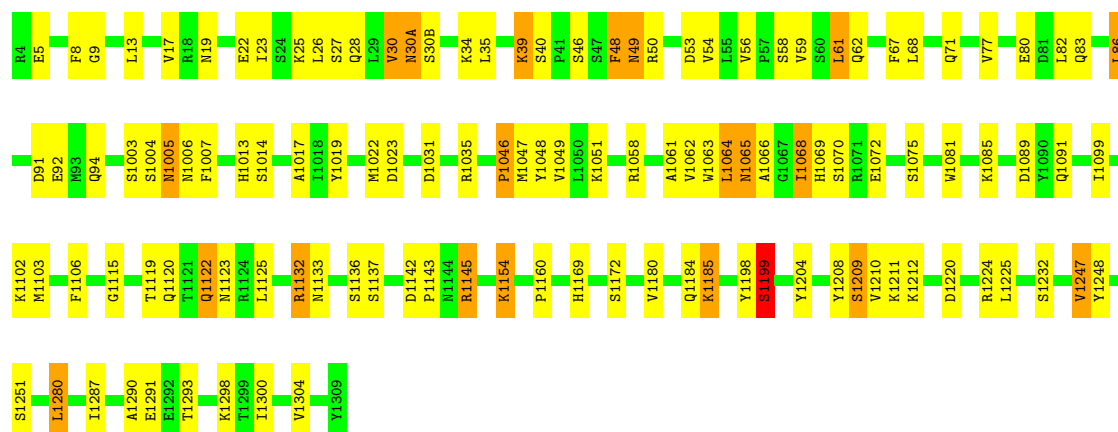
3 Residue-property plots

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.

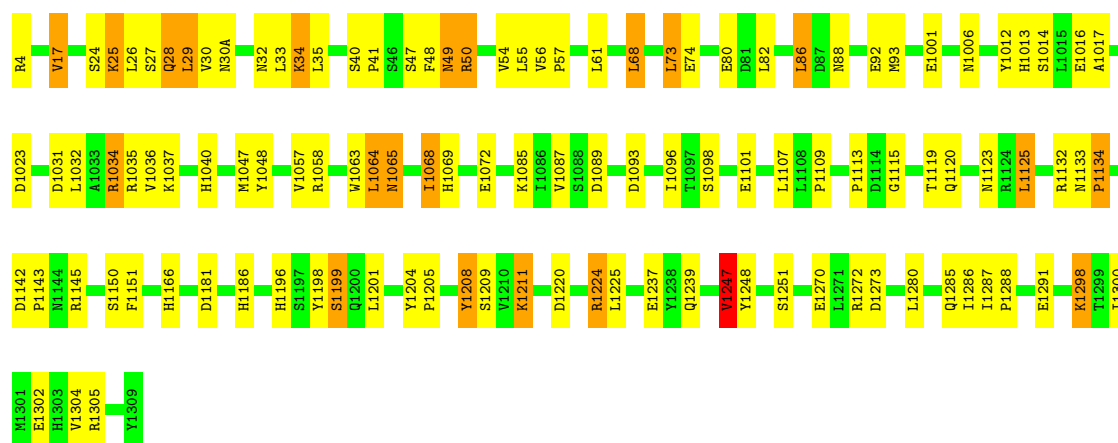
• Molecule 1: CARBOXYPEPTIDASE A4

Chain A: 



• Molecule 1: CARBOXYPEPTIDASE A4

Chain B: 



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

Chain C:

100%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.80Å 87.20Å 89.70Å 90.00° 117.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	96.4 (50.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.220 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6882	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.67	2/3301 (0.1%)	0.98	2/4479 (0.0%)
1	B	0.64	0/3301	1.00	1/4479 (0.0%)
All	All	0.65	2/6602 (0.0%)	0.99	3/8958 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1046	PRO	CA-CB	6.29	1.62	1.53
1	A	1047	MET	SD-CE	5.56	1.93	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30(A)	ASN	N-CA-C	-6.35	104.48	112.93
1	A	1070	SER	N-CA-C	5.94	117.76	111.28
1	A	1061	ALA	N-CA-C	5.33	117.49	109.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1034	ARG	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	3220	0	3109	67	0
1	B	3220	0	3109	75	0
2	C	28	0	25	0	0
3	A	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	16	0	0
5	B	12	0	16	2	0
6	A	202	0	0	1	0
6	B	172	0	0	3	0
All	All	6882	0	6288	141	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 11.

All (141) 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:1132:ARG:HH22	1:A:1137:SER:HA	1.28	0.98
1:A:30:VAL:HG11	1:A:35:LEU:HB2	1.47	0.96
1:B:40:SER:HB2	1:B:41:PRO:HD2	1.48	0.95
1:B:1247:VAL:HG12	1:B:1248:TYR:H	1.33	0.90
1:A:1023:ASP:HB2	1:A:1035:ARG:NH1	1.89	0.88
1:B:1034:ARG:HE	1:B:1036:VAL:HG22	1.42	0.82
1:B:1247:VAL:CG1	1:B:1248:TYR:H	1.95	0.80
1:B:1065:ASN:H	1:B:1065:ASN:HD22	1.30	0.80
1:A:1132:ARG:NH2	1:A:1137:SER:HA	1.98	0.78
1:A:30:VAL:HG21	1:A:35:LEU:H	1.47	0.78
1:A:1132:ARG:HD3	1:B:1132:ARG:HG2	1.68	0.76
1:B:88:ASN:O	1:B:92:GLU:HG3	1.96	0.67
1:A:1247:VAL:HG12	1:A:1248:TYR:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:ARG:NH2	1:B:1048:TYR:CZ	2.63	0.66
1:B:30:VAL:HG12	1:B:30:VAL:O	1.94	0.66
1:B:1014:SER:HA	1:B:1120:GLN:HE22	1.60	0.65
1:B:1247:VAL:CG1	1:B:1248:TYR:N	2.56	0.64
1:B:30:VAL:HG22	1:B:32:ASN:H	1.64	0.63
1:A:1063:TRP:HE1	1:A:1065:ASN:HB3	1.64	0.63
1:A:1065:ASN:HD22	1:A:1065:ASN:H	1.47	0.62
1:B:1023:ASP:OD1	5:B:1404:GOL:H11	2.00	0.61
1:B:30:VAL:HG11	1:B:35:LEU:H	1.66	0.60
1:A:1133:ASN:HD22	1:A:1160:PRO:HB3	1.66	0.60
1:B:40:SER:HB2	1:B:41:PRO:CD	2.28	0.59
1:B:1068:ILE:HG12	1:B:1143:PRO:HB2	1.83	0.59
1:B:40:SER:CB	1:B:41:PRO:HD2	2.28	0.59
1:A:1115:GLY:O	1:A:1119:THR:HG23	2.02	0.59
1:B:48:PHE:HB2	1:B:50:ARG:HG2	1.86	0.57
1:B:1063:TRP:HE1	1:B:1065:ASN:HB3	1.69	0.57
1:A:1004:SER:HB3	1:A:1006:ASN:HB2	1.86	0.57
1:B:1285:GLN:C	1:B:1288:PRO:HD2	2.29	0.57
1:B:1150:SER:O	1:B:1251:SER:HB2	2.05	0.57
1:B:25:LYS:HD3	1:B:28:GLN:HE22	1.70	0.56
1:A:86:LEU:HD22	1:A:1280:LEU:HD11	1.87	0.56
1:B:1085:LYS:O	1:B:1089:ASP:HB2	2.05	0.55
1:B:17:VAL:O	1:B:49:ASN:HA	2.07	0.54
1:A:1085:LYS:O	1:A:1089:ASP:HB2	2.07	0.54
1:B:1142:ASP:OD2	1:B:1145:ARG:HD3	2.07	0.54
1:B:1065:ASN:HD22	1:B:1065:ASN:N	1.94	0.54
1:B:1037:LYS:NZ	1:B:1040:HIS:NE2	2.53	0.54
1:B:1035:ARG:CZ	1:B:1048:TYR:CE1	2.91	0.54
1:A:1062:VAL:HG12	1:A:1064:LEU:HD13	1.90	0.54
1:B:1014:SER:HA	1:B:1120:GLN:NE2	2.22	0.54
1:B:1201:LEU:HB2	1:B:1270:GLU:HB2	1.89	0.54
1:B:1287:ILE:O	1:B:1291:GLU:HG3	2.09	0.53
1:A:1287:ILE:O	1:A:1291:GLU:HG3	2.09	0.53
1:A:67:PHE:CE2	1:A:71:GLN:HG3	2.43	0.53
1:B:1198:TYR:O	1:B:1199:SER:CB	2.56	0.52
1:A:1004:SER:O	1:A:1005:ASN:HB2	2.09	0.52
1:B:1107:LEU:O	1:B:1109:PRO:HD3	2.10	0.52
1:A:30:VAL:HG13	1:A:30:VAL:O	2.10	0.52
1:A:1099:ILE:HG23	1:A:1103:MET:HE3	1.92	0.52
1:B:1089:ASP:HB3	1:B:1096:ILE:HG21	1.92	0.52
1:B:1142:ASP:CG	1:B:1145:ARG:HD3	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:GLY:O	1:B:1119:THR:HG23	2.09	0.52
1:A:1068:ILE:HG12	1:A:1143:PRO:HB2	1.92	0.51
1:B:1300:ILE:O	1:B:1304:VAL:HG23	2.11	0.51
1:B:1285:GLN:O	1:B:1288:PRO:HD2	2.10	0.51
1:B:1220:ASP:O	1:B:1224:ARG:HB2	2.11	0.51
1:A:1198:TYR:O	1:A:1199:SER:CB	2.59	0.50
1:A:1198:TYR:O	1:A:1199:SER:HB2	2.11	0.50
1:B:1119:THR:HA	1:B:1123:ASN:O	2.11	0.50
1:B:1298:LYS:O	1:B:1302:GLU:HG3	2.12	0.50
1:B:1064:LEU:O	1:B:1107:LEU:HA	2.12	0.49
1:B:1034:ARG:HE	1:B:1036:VAL:CG2	2.18	0.49
1:A:1180:VAL:O	1:A:1184:GLN:HG3	2.12	0.49
1:A:1065:ASN:HD22	1:A:1065:ASN:N	2.11	0.49
1:A:1132:ARG:NH2	1:A:1137:SER:CA	2.72	0.49
1:B:1208:TYR:HB3	1:B:1251:SER:HA	1.94	0.49
1:B:68:LEU:HD12	1:B:73:LEU:HD12	1.96	0.48
1:A:39:LYS:HD3	1:A:1199:SER:OG	2.13	0.48
1:B:1098:SER:OG	1:B:1305:ARG:NH1	2.45	0.48
1:A:1014:SER:HA	1:A:1120:GLN:OE1	2.13	0.48
1:A:30:VAL:HG21	1:A:35:LEU:N	2.24	0.48
1:B:1198:TYR:O	1:B:1199:SER:HB2	2.14	0.48
1:A:1247:VAL:HG12	1:A:1248:TYR:CD2	2.45	0.48
1:A:30:VAL:HB	1:A:35:LEU:HD12	1.96	0.47
1:A:9:GLY:C	1:A:58:SER:HB2	2.39	0.47
1:B:1209:SER:HB3	1:B:1211:LYS:HG2	1.95	0.47
1:A:1023:ASP:OD2	1:A:1035:ARG:NH2	2.48	0.47
1:B:1032:LEU:HD23	1:B:1087:VAL:HG12	1.97	0.46
1:B:1012:TYR:CZ	1:B:1286:ILE:HD11	2.50	0.46
1:A:1063:TRP:NE1	1:A:1065:ASN:HB3	2.29	0.46
1:A:1185:LYS:HB3	1:A:1185:LYS:HE2	1.53	0.46
1:B:1001:GLU:HG2	1:B:1006:ASN:O	2.16	0.46
1:A:1209:SER:C	1:A:1211:LYS:H	2.24	0.45
1:B:1093:ASP:OD2	1:B:1298:LYS:HE3	2.16	0.45
1:A:1081:TRP:CE3	1:A:1290:ALA:HB1	2.51	0.45
1:B:1181:ASP:OD2	5:B:1405:GOL:O2	2.35	0.45
1:A:35:LEU:HD22	1:A:56:VAL:HG22	1.99	0.45
1:A:58:SER:HA	1:A:61:LEU:HD22	1.99	0.45
1:B:1047:MET:HE3	1:B:1047:MET:HB3	1.94	0.45
1:A:1013:HIS:HB3	1:A:1017:ALA:HB3	1.99	0.44
1:B:4:ARG:N	6:B:1512:HOH:O	2.50	0.44
1:B:34:LYS:HB2	1:B:34:LYS:HE2	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:HIS:CE1	1:B:1196:HIS:HE1	2.36	0.44
1:A:39:LYS:HB2	1:A:53:ASP:HB2	1.99	0.44
1:A:1051:LYS:HE3	1:A:1106:PHE:CZ	2.52	0.44
1:A:1132:ARG:NH2	1:A:1137:SER:C	2.75	0.44
1:B:50:ARG:NH2	1:B:1239:GLN:HE22	2.16	0.44
1:B:1151:PHE:CE1	1:B:1166:HIS:HB2	2.52	0.44
1:A:8:PHE:CE2	1:A:83:GLN:HG2	2.52	0.44
1:A:1023:ASP:HB2	1:A:1035:ARG:CZ	2.47	0.44
1:B:1113:PRO:HD2	6:B:1552:HOH:O	2.17	0.44
1:A:1154:LYS:H	1:A:1154:LYS:HG2	1.59	0.44
1:B:1016:GLU:HB2	6:B:1580:HOH:O	2.17	0.44
1:A:27:SER:O	1:A:30(A):ASN:ND2	2.50	0.44
1:B:30:VAL:O	1:B:30:VAL:CG1	2.64	0.44
1:B:29:LEU:HD13	1:B:30:VAL:HG23	2.00	0.43
1:B:1204:TYR:HB2	1:B:1205:PRO:HD2	2.00	0.43
1:A:1132:ARG:HH21	1:A:1137:SER:C	2.26	0.43
1:A:1068:ILE:O	1:A:1143:PRO:HG2	2.18	0.43
1:A:1069:HIS:HB2	1:A:1072:GLU:CD	2.44	0.43
1:B:86:LEU:HD13	1:B:86:LEU:HA	1.90	0.43
1:A:1122:GLN:HG3	6:A:1561:HOH:O	2.18	0.43
1:B:56:VAL:HA	1:B:57:PRO:HD3	1.90	0.42
1:A:1019:TYR:O	1:A:1035:ARG:NH1	2.50	0.42
1:B:55:LEU:HD13	1:B:1125:LEU:HD21	2.01	0.42
1:B:1013:HIS:HB3	1:B:1017:ALA:HB3	2.01	0.42
1:A:1007:PHE:CZ	1:A:1013:HIS:CE1	3.07	0.42
1:A:1142:ASP:HB3	1:A:1145:ARG:HB2	2.00	0.42
1:B:1272:ARG:HA	1:B:1273:ASP:HA	1.73	0.42
1:B:1069:HIS:HB2	1:B:1072:GLU:CD	2.44	0.42
1:A:1300:ILE:O	1:A:1304:VAL:HG23	2.20	0.42
1:A:1081:TRP:CD2	1:A:1290:ALA:HB1	2.55	0.42
1:A:9:GLY:HA3	1:A:58:SER:HB2	2.02	0.41
1:A:17:VAL:HG23	1:A:22:GLU:HB3	2.02	0.41
1:A:1169:HIS:O	1:A:1172:SER:HB3	2.20	0.41
1:A:1046:PRO:CB	1:A:1048:TYR:CZ	3.04	0.41
1:A:1119:THR:HA	1:A:1123:ASN:O	2.20	0.41
1:B:1133:ASN:HA	1:B:1134:PRO:HD2	1.79	0.41
1:B:1035:ARG:CZ	1:B:1048:TYR:CZ	3.04	0.41
1:A:1066:ALA:HB1	1:A:1075:SER:HB2	2.01	0.41
1:B:30:VAL:CG2	1:B:33:LEU:H	2.34	0.41
1:A:1022:MET:HE1	1:A:1048:TYR:O	2.21	0.41
1:A:1204:TYR:OH	1:A:1220:ASP:OD2	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:TYR:HB3	1:A:1251:SER:HA	2.02	0.40
1:A:13:LEU:CD2	1:A:77:VAL:HG22	2.50	0.40
1:A:13:LEU:HD22	1:A:77:VAL:HG22	2.03	0.40
1:B:1058:ARG:HD2	1:B:1186:HIS:O	2.21	0.40
1:B:1208:TYR:HE2	1:B:1211:LYS:HE3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/404 (100%)	377 (94%)	21 (5%)	4 (1%)	12	11
1	B	402/404 (100%)	374 (93%)	25 (6%)	3 (1%)	18	19
All	All	804/808 (100%)	751 (93%)	46 (6%)	7 (1%)	14	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1199	SER
1	B	1199	SER
1	A	49	ASN
1	B	1247	VAL
1	A	48	PHE
1	B	1134	PRO
1	A	1247	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	347/347 (100%)	293 (84%)	54 (16%)	2	2
1	B	347/347 (100%)	312 (90%)	35 (10%)	7	7
All	All	694/694 (100%)	605 (87%)	89 (13%)	4	4

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	19	ASN
1	A	23	ILE
1	A	25	LYS
1	A	26	LEU
1	A	28	GLN
1	A	30	VAL
1	A	30(A)	ASN
1	A	30(B)	SER
1	A	34	LYS
1	A	39	LYS
1	A	40	SER
1	A	46	SER
1	A	48	PHE
1	A	49	ASN
1	A	50	ARG
1	A	54	VAL
1	A	59	VAL
1	A	61	LEU
1	A	62	GLN
1	A	68	LEU
1	A	80	GLU
1	A	82	LEU
1	A	86	LEU
1	A	91	ASP
1	A	92	GLU
1	A	94	GLN
1	A	1003	SER
1	A	1005	ASN
1	A	1031	ASP
1	A	1049	VAL
1	A	1058	ARG
1	A	1064	LEU

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Mol	Chain	Res	Type
1	A	1065	ASN
1	A	1068	ILE
1	A	1091	GLN
1	A	1102	LYS
1	A	1122	GLN
1	A	1125	LEU
1	A	1132	ARG
1	A	1136	SER
1	A	1145	ARG
1	A	1154	LYS
1	A	1185	LYS
1	A	1199	SER
1	A	1209	SER
1	A	1210	VAL
1	A	1212	LYS
1	A	1224	ARG
1	A	1225	LEU
1	A	1232	SER
1	A	1280	LEU
1	A	1293	THR
1	A	1298	LYS
1	B	17	VAL
1	B	24	SER
1	B	25	LYS
1	B	26	LEU
1	B	27	SER
1	B	28	GLN
1	B	29	LEU
1	B	34	LYS
1	B	47	SER
1	B	49	ASN
1	B	50	ARG
1	B	54	VAL
1	B	61	LEU
1	B	68	LEU
1	B	73	LEU
1	B	74	GLU
1	B	80	GLU
1	B	82	LEU
1	B	86	LEU
1	B	93	MET
1	B	1031	ASP

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Mol	Chain	Res	Type
1	B	1057	VAL
1	B	1064	LEU
1	B	1065	ASN
1	B	1068	ILE
1	B	1101	GLU
1	B	1125	LEU
1	B	1208	TYR
1	B	1211	LYS
1	B	1224	ARG
1	B	1225	LEU
1	B	1237	GLU
1	B	1247	VAL
1	B	1280	LEU
1	B	1298	LYS

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	49	ASN
1	A	1065	ASN
1	A	1091	GLN
1	A	1200	GLN
1	A	1239	GLN
1	A	1261	ASN
1	B	28	GLN
1	B	88	ASN
1	B	1044	ASN
1	B	1065	ASN
1	B	1120	GLN
1	B	1171	ASN
1	B	1239	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	C	1	2,1	14,14,15	0.54	0	17,19,21	1.39	3 (17%)
2	NAG	C	2	2	14,14,15	0.65	0	17,19,21	1.58	3 (17%)

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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C2-N2-C7	4.00	128.27	122.90
2	C	1	NAG	C1-O5-C5	3.04	116.27	112.19
2	C	2	NAG	C1-C2-N2	3.01	115.18	110.43
2	C	2	NAG	C1-O5-C5	2.77	115.90	112.19
2	C	1	NAG	O4-C4-C3	-2.56	104.34	110.38
2	C	1	NAG	O5-C1-C2	-2.47	107.47	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

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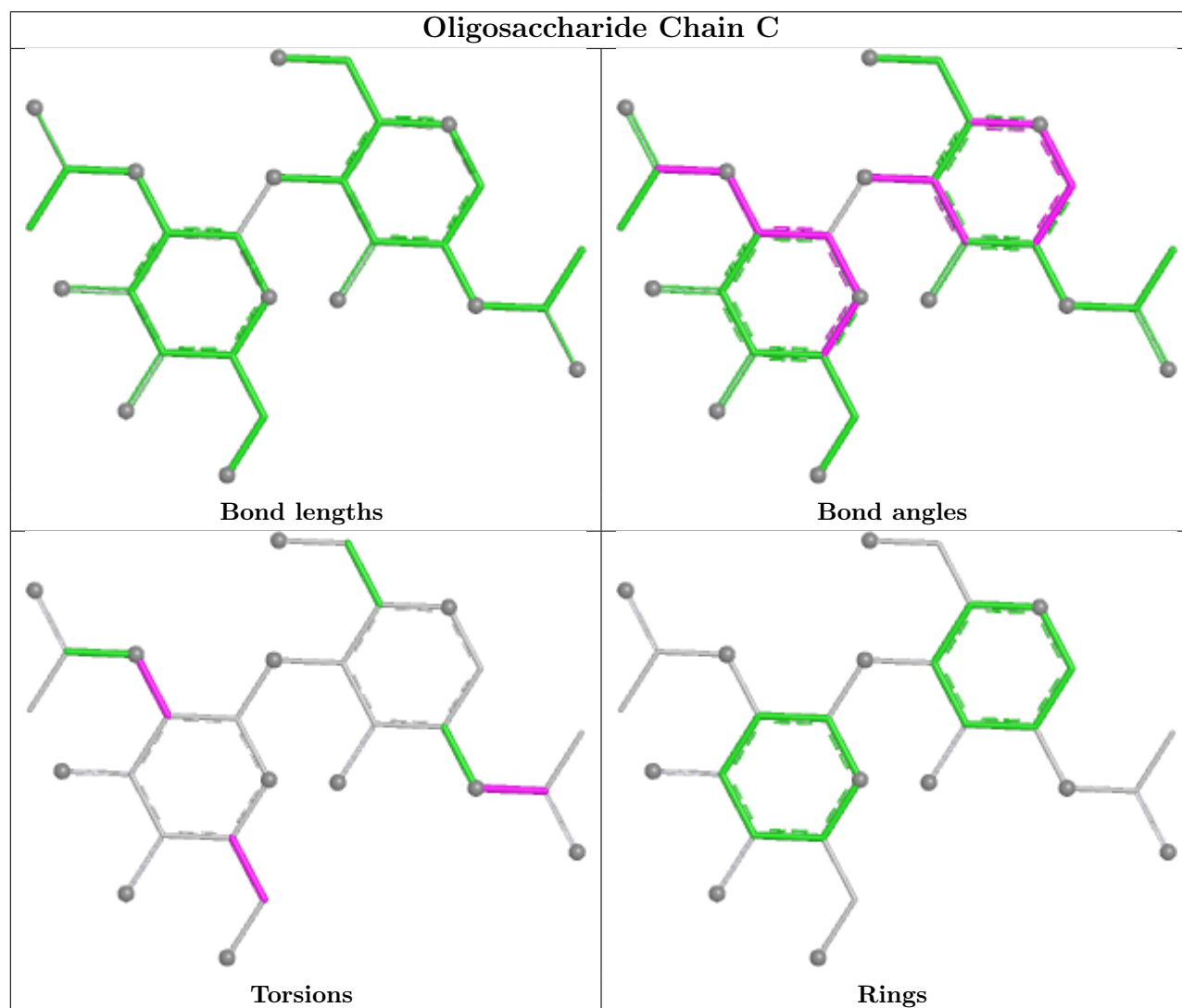
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Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	C	2	NAG	O5-C5-C6-O6

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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
5	GOL	B	1405	-	5,5,5	0.47	0	5,5,5	0.38	0
5	GOL	A	1404	-	5,5,5	0.35	0	5,5,5	0.30	0
3	NAG	A	1401	1	14,14,15	0.48	0	17,19,21	0.65	0
5	GOL	A	1403	-	5,5,5	0.44	0	5,5,5	0.77	0
5	GOL	B	1404	-	5,5,5	0.30	0	5,5,5	0.34	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
5	GOL	B	1405	-	-	2/4/4/4	-
5	GOL	A	1404	-	-	2/4/4/4	-
3	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	GOL	A	1403	-	-	3/4/4/4	-
5	GOL	B	1404	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1403	GOL	O1-C1-C2-C3
5	B	1404	GOL	O1-C1-C2-C3
5	B	1405	GOL	C1-C2-C3-O3
5	A	1403	GOL	C1-C2-C3-O3
5	A	1404	GOL	C1-C2-C3-O3
5	A	1403	GOL	O1-C1-C2-O2
5	B	1404	GOL	O1-C1-C2-O2
5	B	1405	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1401	NAG	C8-C7-N2-C2
5	A	1404	GOL	O2-C2-C3-O3
3	A	1401	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1405	GOL	1	0
5	B	1404	GOL	1	0

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

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.