



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:11 PM UTC

PDB ID : 4FGU / pdb_00004fgu
Title : Crystal structure of prolegumain
Authors : Dall, E.; Brandstetter, H.
Deposited on : 2012-06-05
Resolution : 3.90 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

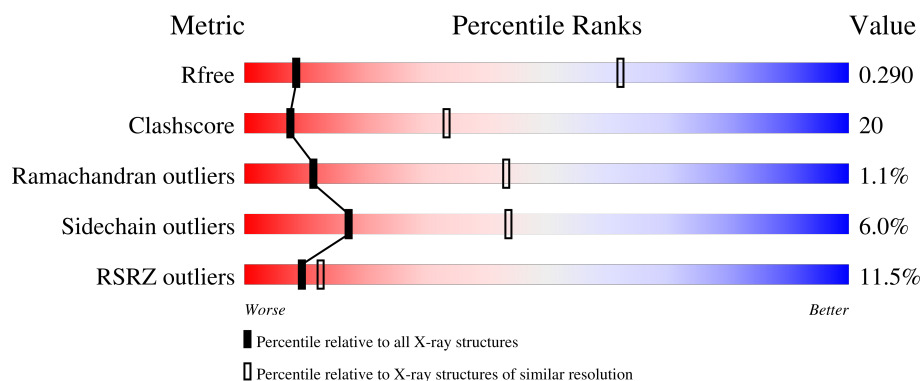
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	429	9% 63% 27% 5% 5%
1	B	429	13% 66% 24% 5% 6%
2	C	2	50% 50%
2	D	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	503	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6688 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 Legumain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3287	2082	569	614	22			
1	B	404	Total	C	N	O	S	0	0	0
			3261	2065	564	610	22			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP Q99538
A	14	ALA	-	expression tag	UNP Q99538
A	15	SER	-	expression tag	UNP Q99538
A	16	LEU	-	expression tag	UNP Q99538
A	17	GLU	-	expression tag	UNP Q99538
A	18	ILE	VAL	variant	UNP Q99538
A	272	GLN	ASN	engineered mutation	UNP Q99538
A	434	GLY	-	expression tag	UNP Q99538
A	435	THR	-	expression tag	UNP Q99538
A	436	HIS	-	expression tag	UNP Q99538
A	437	HIS	-	expression tag	UNP Q99538
A	438	HIS	-	expression tag	UNP Q99538
A	439	HIS	-	expression tag	UNP Q99538
A	440	HIS	-	expression tag	UNP Q99538
A	441	HIS	-	expression tag	UNP Q99538
B	13	GLY	-	expression tag	UNP Q99538
B	14	ALA	-	expression tag	UNP Q99538
B	15	SER	-	expression tag	UNP Q99538
B	16	LEU	-	expression tag	UNP Q99538
B	17	GLU	-	expression tag	UNP Q99538
B	18	ILE	VAL	variant	UNP Q99538
B	272	GLN	ASN	engineered mutation	UNP Q99538
B	434	GLY	-	expression tag	UNP Q99538
B	435	THR	-	expression tag	UNP Q99538
B	436	HIS	-	expression tag	UNP Q99538

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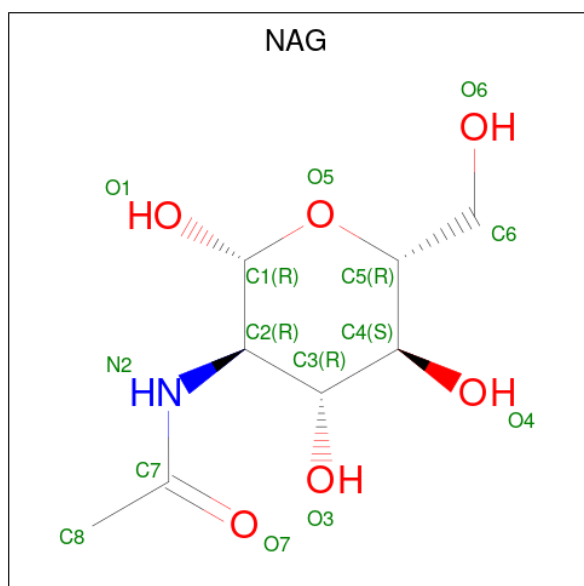
Chain	Residue	Modelled	Actual	Comment	Reference
B	437	HIS	-	expression tag	UNP Q99538
B	438	HIS	-	expression tag	UNP Q99538
B	439	HIS	-	expression tag	UNP Q99538
B	440	HIS	-	expression tag	UNP Q99538
B	441	HIS	-	expression tag	UNP Q99538

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

- 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		

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

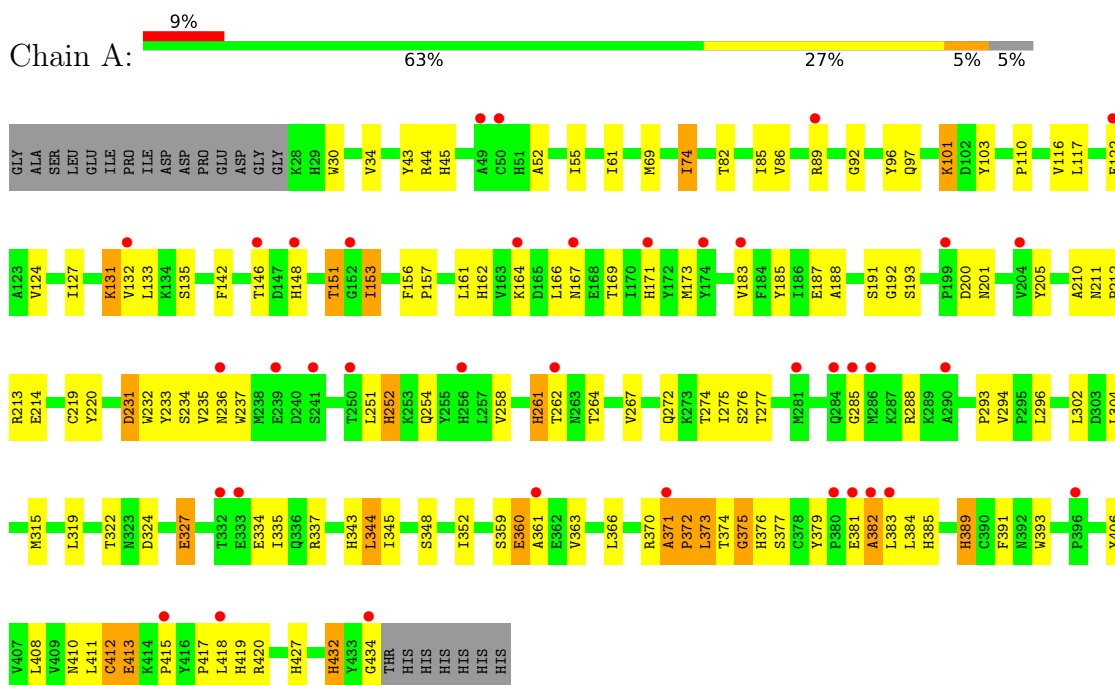
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	24	Total	O	0	0
			24	24		

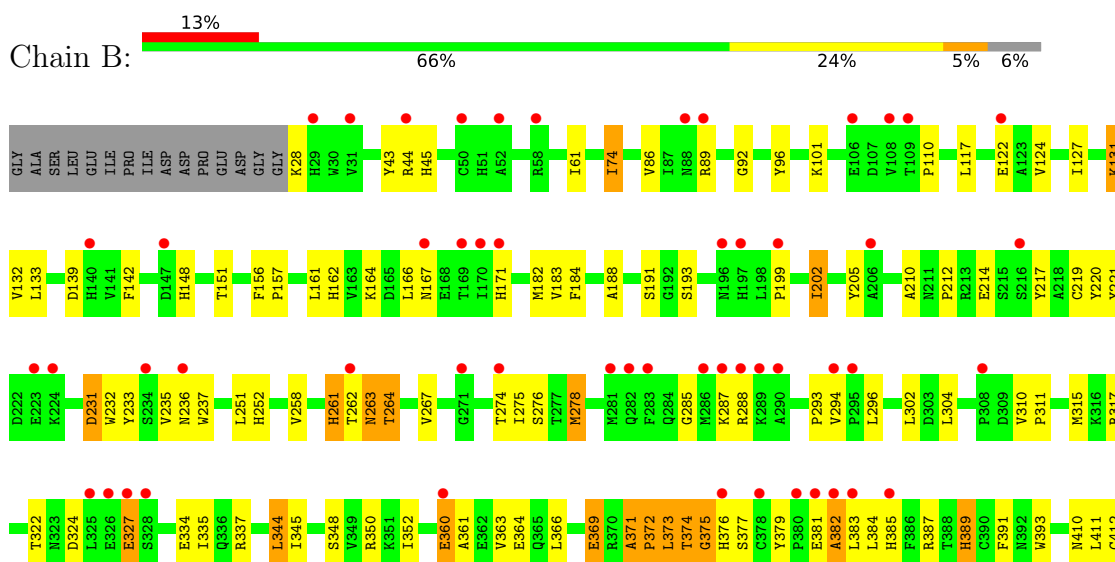
3 Residue-property plots [i](#)

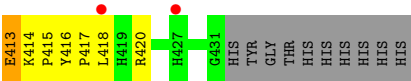
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Legumain



• Molecule 1: Legumain





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	185.10Å 185.10Å 173.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.63 – 3.90 49.63 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.63-3.90) 99.2 (49.63-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.286 , 0.300 0.287 , 0.290	Depositor DCC
R_{free} test set	505 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	6688	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

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	0/3377	0.93	12/4589 (0.3%)
1	B	0.68	2/3349 (0.1%)	0.92	12/4551 (0.3%)
All	All	0.68	2/6726 (0.0%)	0.92	24/9140 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	GLU	C-N	6.61	1.42	1.33
1	B	261	HIS	ND1-CE1	5.42	1.38	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	GLY	N-CA-C	12.59	127.10	112.50
1	B	375	GLY	N-CA-C	12.48	126.97	112.50
1	B	371	ALA	CA-C-N	11.55	131.43	119.19
1	B	371	ALA	C-N-CA	11.55	131.43	119.19
1	A	371	ALA	CA-C-N	11.39	131.26	119.19
1	A	371	ALA	C-N-CA	11.39	131.26	119.19
1	A	374	THR	N-CA-C	9.03	120.73	111.07
1	B	374	THR	N-CA-C	8.58	120.25	111.07
1	B	372	PRO	N-CA-C	8.41	124.59	113.57
1	A	372	PRO	N-CA-C	8.13	124.22	113.57
1	A	361	ALA	N-CA-C	-7.57	104.55	114.31
1	B	377	SER	N-CA-C	-7.28	106.32	114.62
1	A	377	SER	N-CA-C	-7.21	106.40	114.62
1	B	361	ALA	N-CA-C	-6.96	104.45	114.12
1	A	374	THR	CB-CA-C	-6.69	100.38	110.88
1	B	374	THR	CB-CA-C	-6.50	100.67	110.88
1	A	432	HIS	N-CA-C	6.40	118.05	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	GLU	N-CA-C	6.04	122.70	113.51
1	A	359	SER	N-CA-C	5.91	117.92	110.24
1	A	45	HIS	CB-CG-CD2	-5.52	124.03	131.20
1	B	360	GLU	CB-CA-C	-5.43	104.46	109.83
1	A	360	GLU	N-CA-C	5.22	121.48	113.28
1	B	45	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	B	264	THR	N-CA-C	5.16	116.71	111.14

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	3287	0	3179	142	0
1	B	3261	0	3159	121	0
2	C	28	0	25	2	0
2	D	28	0	25	1	0
3	A	14	0	13	8	0
3	B	14	0	13	5	0
4	A	32	0	0	0	0
4	B	24	0	0	0	0
All	All	6688	0	6414	263	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 20.

All (263) 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:171:HIS:HB2	3:A:503:NAG:C8	1.28	1.60
1:B:171:HIS:HB2	3:B:503:NAG:C8	1.55	1.36
1:B:371:ALA:HB1	1:B:372:PRO:CD	1.60	1.30
1:A:371:ALA:HB1	1:A:372:PRO:CD	1.63	1.29
1:A:201:ASN:HA	1:A:272:GLN:NE2	1.52	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ALA:HB1	1:A:372:PRO:HD2	1.26	1.17
1:A:171:HIS:CB	3:A:503:NAG:H82	1.75	1.16
1:A:171:HIS:CB	3:A:503:NAG:C8	2.23	1.16
1:A:151:THR:HG22	1:A:373:LEU:HD23	1.22	1.15
1:A:201:ASN:CA	1:A:272:GLN:HE21	1.58	1.15
1:A:151:THR:CG2	1:A:373:LEU:HD23	1.81	1.11
1:B:151:THR:CG2	1:B:373:LEU:HD23	1.79	1.10
1:B:151:THR:HG22	1:B:373:LEU:HD23	1.30	1.10
1:B:371:ALA:HB1	1:B:372:PRO:HD2	1.30	1.09
1:A:171:HIS:HB2	3:A:503:NAG:H82	1.07	1.04
1:A:151:THR:CG2	1:A:373:LEU:CD2	2.36	1.03
1:A:151:THR:HG22	1:A:373:LEU:CD2	1.89	1.02
1:B:171:HIS:CB	3:B:503:NAG:H82	1.88	1.02
1:B:151:THR:CG2	1:B:373:LEU:CD2	2.38	1.02
1:B:171:HIS:HB2	3:B:503:NAG:H82	1.01	1.00
1:B:371:ALA:HB1	1:B:372:PRO:HD3	1.36	1.00
1:B:220:TYR:HE2	1:B:235:VAL:HG11	1.27	1.00
1:A:371:ALA:HB1	1:A:372:PRO:HD3	1.45	0.99
1:B:371:ALA:CB	1:B:372:PRO:CD	2.37	0.98
1:A:372:PRO:HG2	1:A:413:GLU:OE1	1.61	0.98
1:A:171:HIS:HB2	3:A:503:NAG:H83	1.40	0.97
1:A:220:TYR:HE2	1:A:235:VAL:HG11	1.26	0.97
1:A:371:ALA:CB	1:A:372:PRO:HD2	1.95	0.96
1:B:89:ARG:HH12	1:B:296:LEU:HD12	1.32	0.95
1:B:371:ALA:CB	1:B:372:PRO:HD2	1.95	0.94
1:A:201:ASN:HA	1:A:272:GLN:HE21	1.09	0.93
1:B:151:THR:HG22	1:B:373:LEU:CD2	1.99	0.91
1:A:171:HIS:HB2	3:A:503:NAG:H81	1.49	0.91
1:B:220:TYR:CE2	1:B:235:VAL:HG11	2.06	0.90
1:A:372:PRO:O	1:A:373:LEU:HD12	1.73	0.87
1:B:89:ARG:NH1	1:B:296:LEU:HD12	1.90	0.86
1:A:103:TYR:CE1	1:A:124:VAL:HG21	2.10	0.85
1:B:372:PRO:O	1:B:373:LEU:HD12	1.76	0.85
1:A:220:TYR:CE2	1:A:235:VAL:HG11	2.13	0.83
1:A:372:PRO:CG	1:A:413:GLU:OE1	2.26	0.82
1:B:372:PRO:HG2	1:B:413:GLU:OE1	1.80	0.81
1:A:344:LEU:C	1:A:344:LEU:HD23	2.06	0.81
1:A:262:THR:HG21	1:A:267:VAL:HG23	1.64	0.79
1:B:262:THR:HG21	1:B:267:VAL:HG23	1.64	0.78
1:A:89:ARG:NH1	1:A:296:LEU:HD12	1.98	0.78
1:A:86:VAL:HG22	1:A:96:TYR:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:HIS:HB2	3:B:503:NAG:H83	1.64	0.78
1:A:201:ASN:CA	1:A:272:GLN:NE2	2.28	0.77
1:B:372:PRO:HG2	1:B:413:GLU:CD	2.11	0.76
1:B:372:PRO:CG	1:B:413:GLU:OE1	2.33	0.75
1:A:201:ASN:C	1:A:272:GLN:HE21	1.94	0.74
1:B:86:VAL:HG22	1:B:96:TYR:HB2	1.68	0.74
1:B:344:LEU:C	1:B:344:LEU:HD23	2.11	0.74
1:B:151:THR:HG23	1:B:373:LEU:CD2	2.16	0.74
1:A:372:PRO:HG3	1:A:413:GLU:HG2	1.69	0.73
1:B:164:LYS:NZ	1:B:376:HIS:O	2.21	0.73
1:B:236:ASN:CG	1:B:261:HIS:HB3	2.14	0.72
1:B:372:PRO:HG3	1:B:413:GLU:HG2	1.73	0.71
1:A:236:ASN:ND2	1:A:261:HIS:HB3	2.06	0.70
1:A:236:ASN:CG	1:A:261:HIS:HB3	2.16	0.70
1:B:236:ASN:ND2	1:B:261:HIS:HB3	2.07	0.70
1:B:28:LYS:O	1:B:139:ASP:HB3	1.91	0.69
1:B:360:GLU:H	1:B:363:VAL:HG12	1.57	0.68
1:B:156:PHE:HB3	1:B:157:PRO:HD2	1.76	0.68
1:A:151:THR:HG23	1:A:373:LEU:CD2	2.22	0.67
1:A:381:GLU:O	1:A:383:LEU:N	2.28	0.67
1:B:232:TRP:HE1	1:B:262:THR:HA	1.59	0.67
1:A:117:LEU:HA	1:A:133:LEU:HD12	1.77	0.67
1:A:264:THR:HG22	2:C:1:NAG:H82	1.76	0.67
1:A:193:SER:HB3	1:A:212:PRO:HB3	1.77	0.67
1:B:217:TYR:CD1	1:B:264:THR:HB	2.30	0.66
1:A:61:ILE:HD11	1:A:285:GLY:HA3	1.76	0.66
1:B:381:GLU:O	1:B:383:LEU:N	2.29	0.66
1:A:372:PRO:C	1:A:373:LEU:HG	2.20	0.66
1:A:372:PRO:O	1:A:373:LEU:CD1	2.42	0.66
1:A:103:TYR:HE1	1:A:124:VAL:HG21	1.59	0.65
1:A:372:PRO:CG	1:A:413:GLU:HG2	2.26	0.65
1:A:201:ASN:C	1:A:272:GLN:NE2	2.54	0.65
1:B:372:PRO:C	1:B:373:LEU:HG	2.21	0.65
1:B:236:ASN:OD1	1:B:261:HIS:HB3	1.96	0.64
1:A:151:THR:CG2	1:A:373:LEU:HD21	2.28	0.64
1:B:334:GLU:HG3	1:B:337:ARG:HH21	1.62	0.64
1:B:264:THR:HG23	1:B:304:LEU:HD23	1.80	0.63
1:A:236:ASN:OD1	1:A:261:HIS:HB3	1.99	0.63
1:B:372:PRO:O	1:B:373:LEU:CD1	2.46	0.62
1:A:372:PRO:O	1:A:373:LEU:CG	2.47	0.62
1:A:151:THR:HG23	1:A:373:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:THR:HG23	1:B:373:LEU:HD21	1.80	0.62
1:B:236:ASN:OD1	1:B:261:HIS:CB	2.48	0.61
1:B:275:ILE:HG23	1:B:278:MET:HE2	1.82	0.61
1:B:89:ARG:HG2	1:B:92:GLY:HA3	1.83	0.61
1:A:124:VAL:HG22	1:A:124:VAL:O	2.01	0.60
1:B:171:HIS:CB	3:B:503:NAG:C8	2.52	0.60
1:A:89:ARG:HH12	1:A:296:LEU:HD12	1.64	0.60
1:A:232:TRP:HE1	1:A:262:THR:HA	1.66	0.60
1:B:251:LEU:HB2	1:B:276:SER:HA	1.84	0.60
1:B:262:THR:HG23	1:B:262:THR:O	2.03	0.59
1:B:188:ALA:HB3	1:B:191:SER:HB3	1.84	0.58
1:B:344:LEU:HD23	1:B:345:ILE:N	2.19	0.58
1:A:142:PHE:CE1	1:A:185:TYR:HD2	2.22	0.58
1:B:232:TRP:O	1:B:233:TYR:HB3	2.03	0.58
1:A:372:PRO:HG2	1:A:413:GLU:CD	2.28	0.58
1:A:171:HIS:HB3	3:A:503:NAG:H82	1.77	0.57
1:B:372:PRO:O	1:B:373:LEU:CG	2.52	0.57
1:A:344:LEU:C	1:A:344:LEU:CD2	2.78	0.57
1:B:263:ASN:N	1:B:263:ASN:OD1	2.37	0.57
1:A:142:PHE:HE1	1:A:185:TYR:HD2	1.51	0.57
1:B:117:LEU:HA	1:B:133:LEU:HD12	1.87	0.57
1:A:344:LEU:HD21	1:A:391:PHE:CZ	2.39	0.57
1:A:262:THR:O	1:A:262:THR:HG23	2.06	0.56
1:A:142:PHE:HD1	1:A:183:VAL:HG13	1.71	0.55
1:B:142:PHE:HD1	1:B:183:VAL:HG13	1.70	0.55
1:B:372:PRO:CG	1:B:413:GLU:CD	2.77	0.55
1:B:372:PRO:CG	1:B:413:GLU:HG2	2.36	0.55
1:B:96:TYR:OH	1:B:101:LYS:HE3	2.07	0.55
1:A:427:HIS:NE2	1:A:434:GLY:HA2	2.21	0.55
1:B:61:ILE:HD11	1:B:285:GLY:HA3	1.89	0.55
1:B:142:PHE:CD1	1:B:183:VAL:HG13	2.42	0.54
1:B:417:PRO:HG2	1:B:420:ARG:HE	1.72	0.54
1:B:302:LEU:HG	1:B:304:LEU:HD13	1.89	0.54
1:B:199:PRO:HG2	1:B:202:ILE:HG12	1.89	0.54
1:B:302:LEU:CD2	2:D:1:NAG:H5	2.37	0.54
1:B:182:MET:SD	1:B:184:PHE:HE1	2.30	0.54
1:A:302:LEU:HG	1:A:304:LEU:HD13	1.89	0.54
1:A:219:CYS:SG	1:A:231:ASP:C	2.91	0.53
1:A:156:PHE:HB3	1:A:157:PRO:HD2	1.89	0.53
1:A:344:LEU:HD23	1:A:345:ILE:N	2.23	0.53
1:A:372:PRO:C	1:A:373:LEU:CG	2.80	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ALA:HB3	1:B:410:ASN:HB3	1.90	0.53
1:A:200:ASP:C	1:A:272:GLN:HG2	2.34	0.53
1:B:131:LYS:HD2	1:B:132:VAL:O	2.08	0.53
1:A:96:TYR:OH	1:A:101:LYS:CE	2.57	0.53
1:A:96:TYR:OH	1:A:101:LYS:HE3	2.07	0.53
1:A:131:LYS:HD3	1:A:132:VAL:N	2.23	0.53
1:B:372:PRO:C	1:B:373:LEU:CG	2.82	0.53
1:A:334:GLU:HG3	1:A:337:ARG:HH21	1.74	0.53
1:A:236:ASN:HD21	1:A:261:HIS:HB3	1.74	0.53
1:B:219:CYS:SG	1:B:231:ASP:C	2.92	0.52
1:B:366:LEU:HD11	1:B:414:LYS:HG3	1.90	0.52
1:A:375:GLY:O	1:A:376:HIS:HB2	2.09	0.51
1:A:360:GLU:HA	1:A:363:VAL:HG12	1.92	0.51
1:B:375:GLY:O	1:B:376:HIS:HB2	2.09	0.51
1:B:344:LEU:C	1:B:344:LEU:CD2	2.83	0.51
1:B:315:MET:HB3	1:B:335:ILE:CG2	2.41	0.50
1:A:324:ASP:HB3	1:A:327:GLU:HB2	1.93	0.50
1:B:315:MET:HB3	1:B:335:ILE:HG22	1.92	0.50
1:A:274:THR:O	1:A:277:THR:HG23	2.12	0.50
1:A:131:LYS:HD2	1:A:132:VAL:O	2.10	0.50
1:B:156:PHE:HB3	1:B:157:PRO:CD	2.41	0.50
1:A:379:TYR:HA	1:A:383:LEU:HB2	1.93	0.50
1:B:379:TYR:HA	1:B:383:LEU:HB2	1.93	0.50
1:A:372:PRO:O	1:A:373:LEU:CB	2.60	0.50
1:B:124:VAL:HA	1:B:127:ILE:HD12	1.94	0.50
1:A:52:ALA:O	1:A:55:ILE:HG22	2.12	0.49
1:A:153:ILE:HD13	1:A:384:LEU:HD21	1.95	0.49
1:A:344:LEU:CD2	1:A:391:PHE:CZ	2.96	0.49
1:B:366:LEU:HD23	1:B:411:LEU:HD12	1.95	0.49
1:B:205:TYR:HB2	1:B:275:ILE:HB	1.96	0.48
1:A:348:SER:O	1:A:352:ILE:HG12	2.14	0.48
1:A:232:TRP:O	1:A:233:TYR:HB3	2.12	0.48
1:A:210:ALA:HB1	1:A:214:GLU:HG3	1.94	0.48
1:A:366:LEU:HD23	1:A:411:LEU:HD12	1.95	0.48
1:A:103:TYR:HE1	1:A:124:VAL:CG2	2.24	0.48
1:A:103:TYR:CZ	1:A:124:VAL:HG21	2.47	0.48
1:A:213:ARG:HA	1:A:370:ARG:NH1	2.29	0.48
1:B:96:TYR:OH	1:B:101:LYS:CE	2.62	0.48
1:A:110:PRO:HD3	1:A:156:PHE:CD2	2.49	0.48
1:A:161:LEU:HD21	1:A:166:LEU:HD13	1.96	0.48
1:A:322:THR:HG22	1:A:324:ASP:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:HIS:N	1:B:389:HIS:ND1	2.62	0.47
1:A:103:TYR:OH	1:A:124:VAL:HG11	2.15	0.47
1:B:384:LEU:O	1:B:387:ARG:HB3	2.14	0.47
1:A:142:PHE:CD1	1:A:183:VAL:HG13	2.49	0.47
1:A:254:GLN:O	1:A:258:VAL:HG23	2.15	0.47
1:B:110:PRO:HD3	1:B:156:PHE:CD2	2.50	0.47
1:A:162:HIS:CE1	1:A:384:LEU:HD22	2.50	0.46
1:A:381:GLU:O	1:A:382:ALA:C	2.59	0.46
1:A:406:TYR:O	1:A:410:ASN:ND2	2.49	0.46
1:B:372:PRO:O	1:B:373:LEU:CB	2.62	0.46
1:B:193:SER:HB3	1:B:212:PRO:HB3	1.98	0.46
1:B:161:LEU:HD21	1:B:166:LEU:HD13	1.97	0.46
1:B:205:TYR:CZ	1:B:276:SER:HB3	2.51	0.46
1:B:210:ALA:HB1	1:B:214:GLU:HG3	1.97	0.45
1:B:236:ASN:HD21	1:B:261:HIS:HB3	1.78	0.45
1:A:188:ALA:HB3	1:A:191:SER:HB3	1.99	0.45
1:A:389:HIS:ND1	1:A:389:HIS:N	2.64	0.45
1:B:360:GLU:N	1:B:363:VAL:HG12	2.29	0.45
1:B:221:TYR:HE2	1:B:317:ARG:HG2	1.81	0.45
1:B:383:LEU:HD21	1:B:418:LEU:O	2.17	0.45
1:B:89:ARG:CG	1:B:92:GLY:HA3	2.46	0.45
1:B:371:ALA:CB	1:B:410:ASN:HB3	2.47	0.45
1:A:89:ARG:HG2	1:A:92:GLY:HA3	1.98	0.45
1:A:44:ARG:HH22	1:A:148:HIS:CE1	2.35	0.45
1:B:44:ARG:HH22	1:B:148:HIS:CE1	2.35	0.45
1:B:322:THR:HG21	1:B:327:GLU:HB3	1.99	0.45
1:B:372:PRO:HG3	1:B:413:GLU:CG	2.46	0.45
1:A:30:TRP:CD1	1:A:135:SER:HB3	2.52	0.44
1:A:417:PRO:HG2	1:A:420:ARG:HE	1.82	0.44
1:B:381:GLU:O	1:B:382:ALA:C	2.59	0.44
1:A:419:HIS:CE1	1:A:420:ARG:HG3	2.52	0.44
1:B:414:LYS:O	1:B:416:TYR:HD2	2.01	0.44
1:B:156:PHE:HE2	1:B:161:LEU:HB2	1.83	0.44
1:B:236:ASN:OD1	1:B:261:HIS:HB2	2.16	0.44
1:B:372:PRO:HG3	1:B:413:GLU:OE1	2.15	0.44
1:A:82:THR:HB	1:A:85:ILE:HB	1.99	0.44
1:B:360:GLU:HA	1:B:363:VAL:HG12	1.99	0.44
1:B:374:THR:HB	1:B:413:GLU:OE1	2.17	0.44
1:A:89:ARG:CG	1:A:92:GLY:HA3	2.47	0.44
1:A:124:VAL:HA	1:A:127:ILE:HD12	2.00	0.44
1:B:372:PRO:CG	1:B:413:GLU:CG	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:HIS:O	1:A:343:HIS:ND1	2.51	0.43
1:A:418:LEU:HD23	1:A:418:LEU:H	1.82	0.43
1:B:348:SER:O	1:B:352:ILE:HG12	2.17	0.43
1:A:131:LYS:HD3	1:A:132:VAL:H	1.82	0.43
1:A:142:PHE:HE1	1:A:185:TYR:CD2	2.34	0.43
1:A:372:PRO:CG	1:A:413:GLU:CG	2.95	0.43
1:A:252:HIS:ND1	1:A:276:SER:OG	2.47	0.43
1:A:344:LEU:CD2	1:A:345:ILE:N	2.81	0.43
1:A:187:GLU:HG2	1:A:234:SER:HB2	1.99	0.43
1:A:44:ARG:NH2	1:A:148:HIS:CE1	2.87	0.43
1:A:110:PRO:HD3	1:A:156:PHE:HD2	1.83	0.43
1:A:171:HIS:CG	3:A:503:NAG:H83	2.54	0.42
1:A:302:LEU:CD2	2:C:1:NAG:H5	2.49	0.42
1:A:344:LEU:HD21	1:A:391:PHE:CE1	2.54	0.42
1:B:264:THR:CG2	1:B:304:LEU:HD23	2.47	0.42
1:A:251:LEU:HB2	1:A:276:SER:HA	2.01	0.42
1:A:272:GLN:HB2	1:A:275:ILE:HD12	2.00	0.42
1:B:237:TRP:HB3	1:B:258:VAL:HG21	2.02	0.42
1:B:43:TYR:CD1	1:B:74:ILE:HD11	2.55	0.41
1:B:344:LEU:CD2	1:B:345:ILE:N	2.83	0.41
1:B:344:LEU:HD21	1:B:391:PHE:CZ	2.55	0.41
1:A:131:LYS:CD	1:A:132:VAL:N	2.83	0.41
1:B:315:MET:CB	1:B:335:ILE:HG22	2.50	0.41
1:A:43:TYR:CD1	1:A:74:ILE:HD11	2.56	0.41
1:A:371:ALA:CB	1:A:372:PRO:HD3	2.31	0.41
1:B:310:VAL:N	1:B:311:PRO:HD2	2.34	0.41
1:B:350:ARG:NH1	1:B:364:GLU:OE2	2.47	0.41
1:A:262:THR:C	1:A:264:THR:H	2.28	0.41
1:A:360:GLU:H	1:A:363:VAL:HG12	1.85	0.41
1:A:334:GLU:HG3	1:A:337:ARG:NH2	2.34	0.41
1:B:374:THR:CB	1:B:413:GLU:OE1	2.68	0.41
1:A:183:VAL:HG23	1:A:205:TYR:HD2	1.86	0.41
1:A:237:TRP:HB3	1:A:258:VAL:HG21	2.03	0.41
1:A:315:MET:HB3	1:A:335:ILE:CG2	2.51	0.41
1:A:164:LYS:NZ	1:A:376:HIS:O	2.48	0.41
1:A:192:GLY:C	1:A:212:PRO:HG3	2.46	0.41
1:B:324:ASP:HB3	1:B:327:GLU:HB2	2.03	0.41
1:A:34:VAL:HG22	1:A:69:MET:HB2	2.03	0.41
1:A:236:ASN:OD1	1:A:261:HIS:CB	2.68	0.41
1:B:379:TYR:CZ	1:B:384:LEU:HD12	2.56	0.41
1:A:379:TYR:CZ	1:A:384:LEU:HD12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LYS:HD3	1:B:132:VAL:N	2.36	0.40
1:B:162:HIS:CE1	1:B:381:GLU:H	2.38	0.40
1:B:131:LYS:CD	1:B:132:VAL:N	2.83	0.40
1:B:416:TYR:HA	1:B:417:PRO:HD3	1.94	0.40
1:A:61:ILE:HD11	1:A:285:GLY:CA	2.47	0.40
1:A:183:VAL:HA	1:A:205:TYR:O	2.21	0.40
1:A:169:THR:O	1:A:173:MET:HG3	2.22	0.40
1:B:369:GLU:O	1:B:410:ASN:ND2	2.54	0.40
1:A:193:SER:N	1:A:212:PRO:HG3	2.37	0.40
1:A:371:ALA:HB3	1:A:410:ASN:HB3	2.02	0.40
1:A:383:LEU:HD12	1:A:412:CYS:SG	2.62	0.40
1:A:408:LEU:O	1:A:412:CYS:N	2.55	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	405/429 (94%)	363 (90%)	37 (9%)	5 (1%)	10	41
1	B	402/429 (94%)	364 (90%)	34 (8%)	4 (1%)	12	45
All	All	807/858 (94%)	727 (90%)	71 (9%)	9 (1%)	11	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	PRO
1	B	293	PRO
1	A	151	THR
1	A	382	ALA
1	B	382	ALA
1	A	101	LYS

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Mol	Chain	Res	Type
1	A	415	PRO
1	B	415	PRO
1	B	202	ILE

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	365/383 (95%)	341 (93%)	24 (7%)	15	41
1	B	363/383 (95%)	343 (94%)	20 (6%)	19	45
All	All	728/766 (95%)	684 (94%)	44 (6%)	17	44

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ILE
1	A	97	GLN
1	A	116	VAL
1	A	122	GLU
1	A	131	LYS
1	A	146	THR
1	A	153	ILE
1	A	167	ASN
1	A	211	ASN
1	A	231	ASP
1	A	252	HIS
1	A	261	HIS
1	A	288	ARG
1	A	294	VAL
1	A	319	LEU
1	A	327	GLU
1	A	344	LEU
1	A	373	LEU
1	A	385	HIS
1	A	389	HIS

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Mol	Chain	Res	Type
1	A	393	TRP
1	A	412	CYS
1	A	413	GLU
1	A	432	HIS
1	B	74	ILE
1	B	122	GLU
1	B	131	LYS
1	B	167	ASN
1	B	231	ASP
1	B	252	HIS
1	B	263	ASN
1	B	274	THR
1	B	278	MET
1	B	287	LYS
1	B	288	ARG
1	B	294	VAL
1	B	327	GLU
1	B	344	LEU
1	B	373	LEU
1	B	385	HIS
1	B	389	HIS
1	B	393	TRP
1	B	412	CYS
1	B	413	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	59	ASN
1	A	148	HIS
1	A	162	HIS
1	A	256	HIS
1	A	272	GLN
1	A	404	HIS
1	A	410	ASN
1	A	419	HIS
1	B	54	GLN
1	B	59	ASN
1	B	65	GLN
1	B	111	GLN
1	B	140	HIS

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Mol	Chain	Res	Type
1	B	148	HIS
1	B	162	HIS
1	B	171	HIS
1	B	301	HIS
1	B	404	HIS
1	B	410	ASN

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	C	1	1,2	14,14,15	0.55	0	17,19,21	1.36	2 (11%)
2	NAG	C	2	2	14,14,15	0.45	0	17,19,21	0.96	0
2	NAG	D	1	1,2	14,14,15	0.67	0	17,19,21	1.68	3 (17%)
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	0.97	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	C	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	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(°)
2	D	1	NAG	C1-O5-C5	5.39	119.41	112.19
2	C	1	NAG	C1-O5-C5	4.30	117.94	112.19
2	D	1	NAG	C4-C3-C2	2.87	115.22	111.02
2	C	1	NAG	C4-C3-C2	2.74	115.03	111.02
2	D	1	NAG	O5-C1-C2	-2.58	107.30	111.29

There are no chirality outliers.

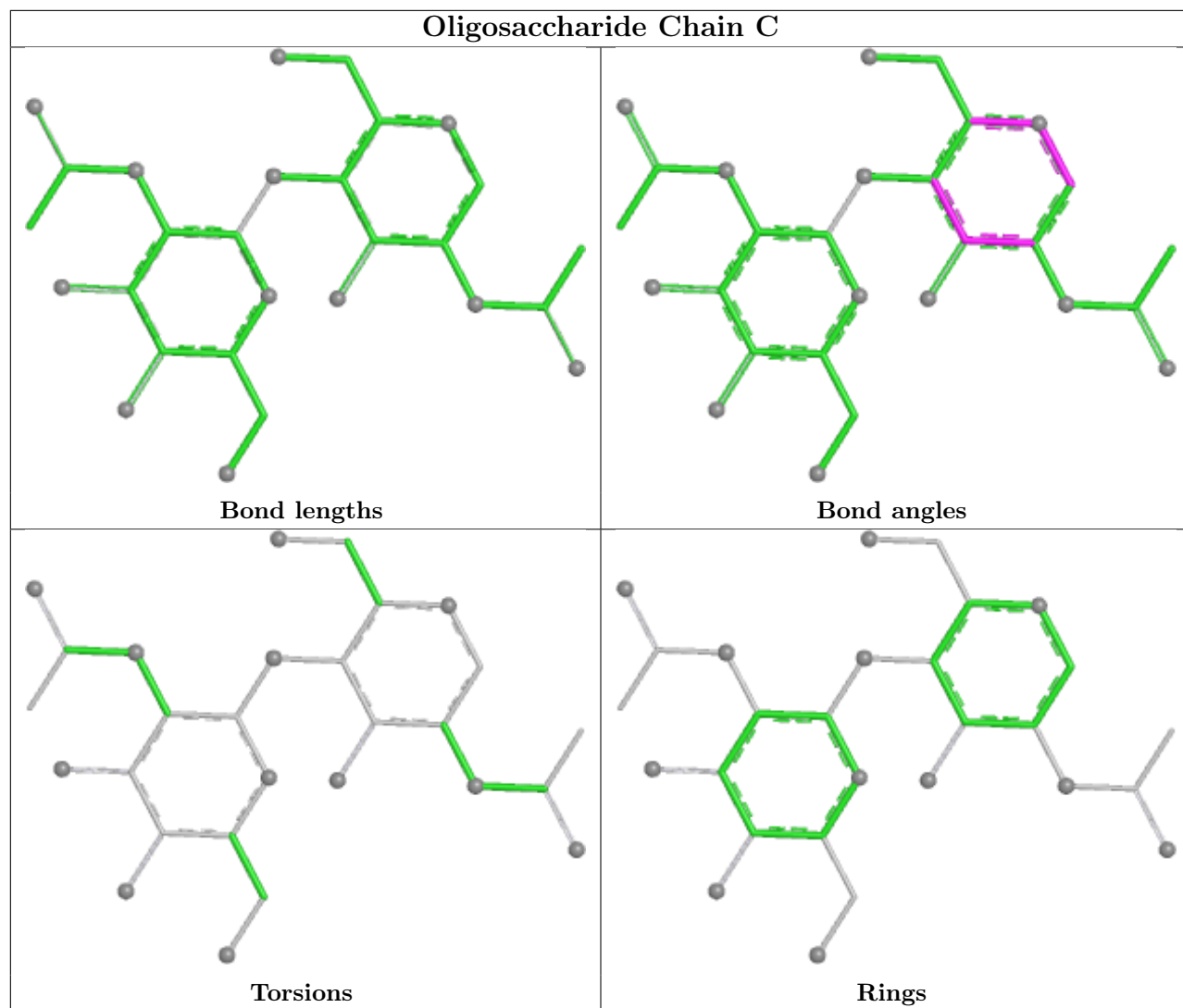
There are no torsion outliers.

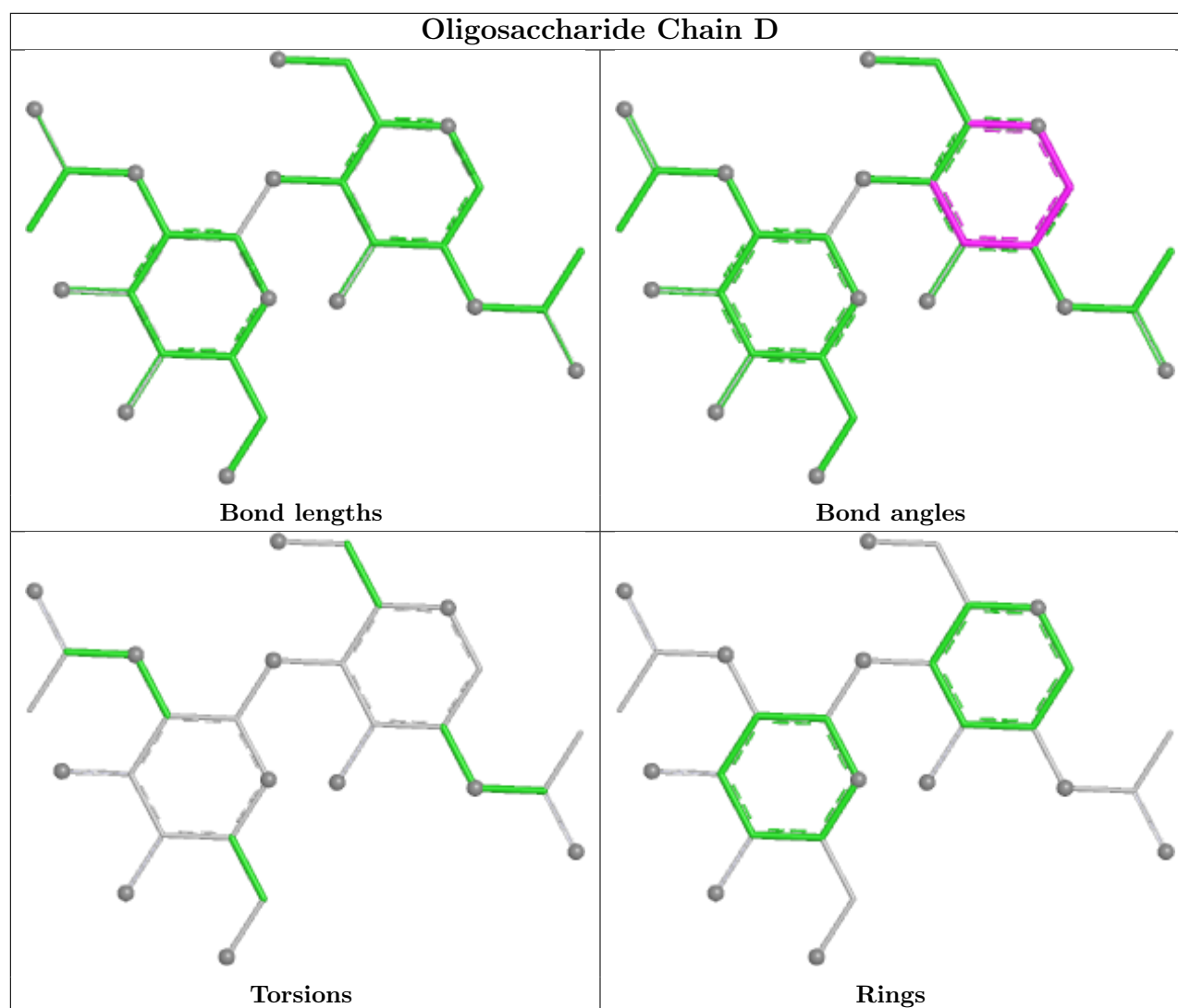
There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

2 ligands 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	$\# Z > 2$
3	NAG	A	503	1	14,14,15	0.44	0	17,19,21	0.98	1 (5%)
3	NAG	B	503	1	14,14,15	0.43	0	17,19,21	0.94	1 (5%)

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
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
3	NAG	B	503	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	NAG	C1-O5-C5	2.80	115.94	112.19
3	B	503	NAG	C1-O5-C5	2.34	115.32	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	NAG	C4-C5-C6-O6
3	B	503	NAG	C4-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	B	503	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	8	0
3	B	503	NAG	5	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

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	407/429 (94%)	1.02	38 (9%) 14 16	22, 53, 93, 125	0
1	B	404/429 (94%)	1.13	55 (13%) 7 10	26, 55, 96, 141	0
All	All	811/858 (94%)	1.07	93 (11%) 9 12	22, 54, 95, 141	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	GLY	4.8
1	B	281	MET	3.6
1	B	380	PRO	3.4
1	B	382	ALA	3.2
1	B	199	PRO	3.2
1	A	418	LEU	3.2
1	B	326	GLU	3.2
1	A	382	ALA	3.1
1	B	89	ARG	3.1
1	A	281	MET	3.1
1	A	286	MET	3.0
1	A	89	ARG	3.0
1	B	171	HIS	2.9
1	B	376	HIS	2.9
1	B	216	SER	2.9
1	B	360	GLU	2.9
1	B	287	LYS	2.9
1	B	381	GLU	2.9
1	A	434	GLY	2.8
1	A	361	ALA	2.8
1	B	271	GLY	2.8
1	B	286	MET	2.7
1	A	380	PRO	2.7
1	B	418	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	289	LYS	2.6
1	A	122	GLU	2.6
1	A	256	HIS	2.6
1	B	108	VAL	2.6
1	B	295	PRO	2.6
1	A	381	GLU	2.6
1	B	308	PRO	2.6
1	A	383	LEU	2.6
1	A	146	THR	2.5
1	A	415	PRO	2.5
1	B	140	HIS	2.5
1	A	148	HIS	2.5
1	A	174	TYR	2.5
1	A	132	VAL	2.5
1	B	122	GLU	2.5
1	B	327	GLU	2.5
1	A	290	ALA	2.5
1	B	147	ASP	2.5
1	B	29	HIS	2.4
1	A	49	ALA	2.4
1	B	196	ASN	2.4
1	B	170	ILE	2.4
1	B	282	GLN	2.3
1	B	274	THR	2.3
1	A	164	LYS	2.3
1	B	31	VAL	2.3
1	A	171	HIS	2.3
1	A	152	GLY	2.3
1	A	284	GLN	2.2
1	A	50	CYS	2.2
1	A	199	PRO	2.2
1	B	325	LEU	2.2
1	B	197	HIS	2.2
1	B	385	HIS	2.2
1	A	239	GLU	2.2
1	B	106	GLU	2.2
1	B	294	VAL	2.2
1	B	44	ARG	2.2
1	A	167	ASN	2.2
1	B	288	ARG	2.2
1	A	333	GLU	2.2
1	B	262	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	241	SER	2.1
1	B	206	ALA	2.1
1	B	236	ASN	2.1
1	B	234	SER	2.1
1	B	427	HIS	2.1
1	A	204	VAL	2.1
1	B	223	GLU	2.1
1	B	383	LEU	2.1
1	B	328	SER	2.1
1	A	183	VAL	2.1
1	B	378	CYS	2.1
1	B	169	THR	2.1
1	B	283	PHE	2.1
1	B	52	ALA	2.1
1	B	224	LYS	2.1
1	B	167	ASN	2.1
1	A	262	THR	2.1
1	B	109	THR	2.1
1	B	50	CYS	2.1
1	A	236	ASN	2.1
1	B	88	ASN	2.1
1	A	396	PRO	2.0
1	A	332	THR	2.0
1	A	371	ALA	2.0
1	B	290	ALA	2.0
1	B	58	ARG	2.0
1	A	250	THR	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	NAG	C	2	14/15	0.65	0.20	5,6,6,7	0

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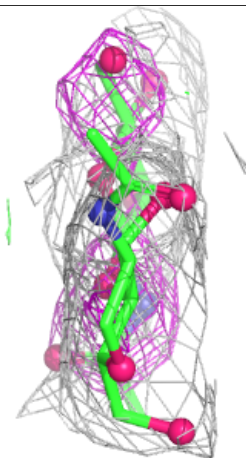
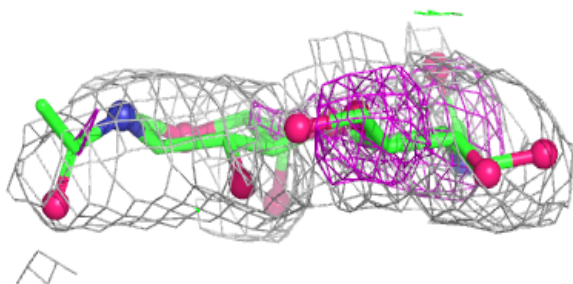
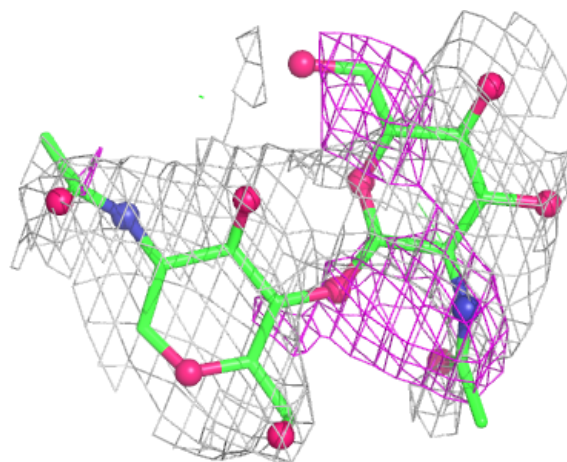
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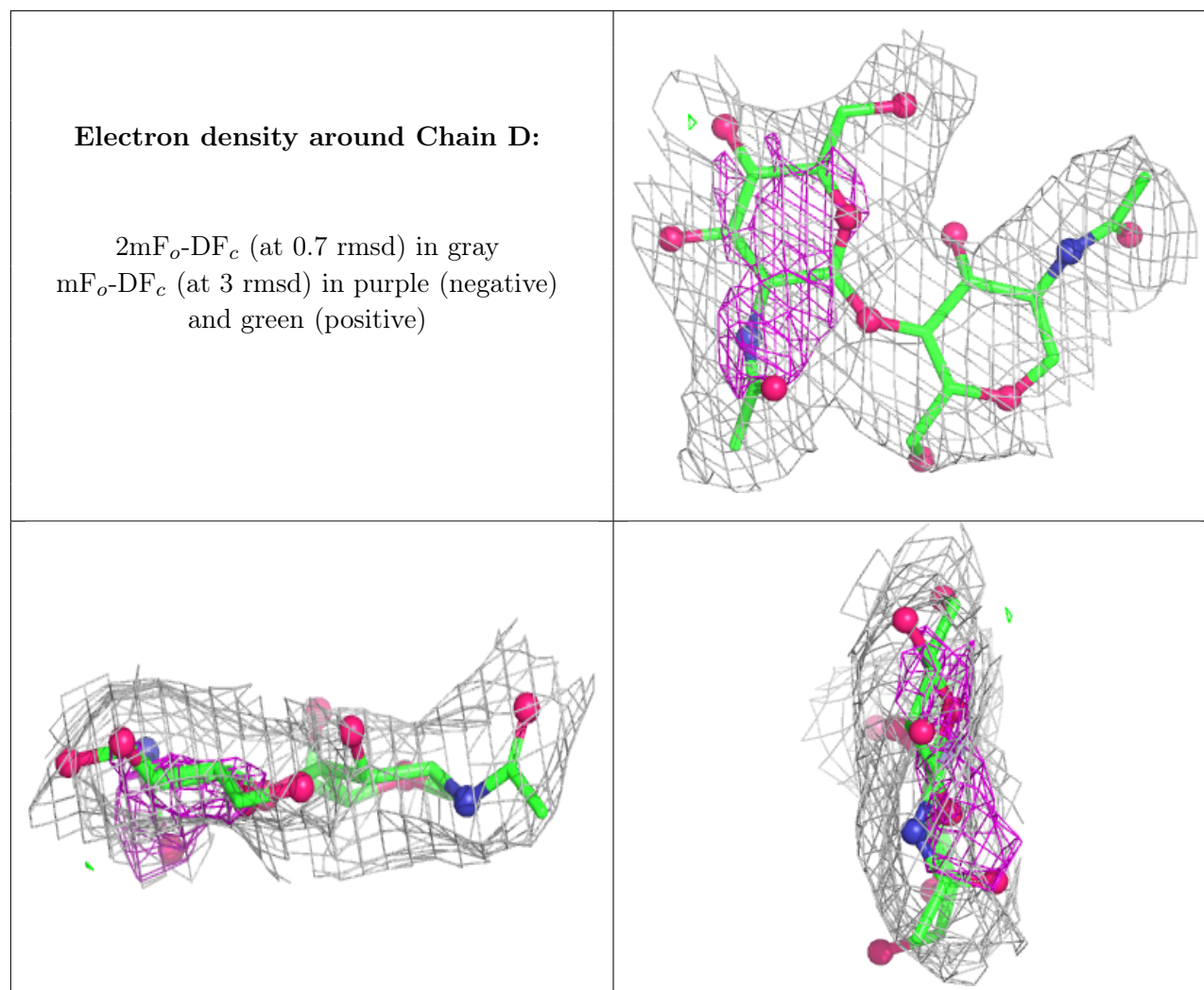
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	1	14/15	0.78	0.15	17,21,22,22	0
2	NAG	D	1	14/15	0.79	0.16	16,20,21,21	0
2	NAG	D	2	14/15	0.79	0.17	5,6,6,6	0

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.

Electron density around Chain C:

2mF_o-DF_c (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)





6.4 Ligands ⓘ

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
3	NAG	B	503	14/15	0.32	0.28	30,30,31,32	0
3	NAG	A	503	14/15	0.51	0.27	29,29,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.