



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:42 PM EDT

PDB ID : 1M4U / pdb_00001m4u
Title : Crystal structure of Bone Morphogenetic Protein-7 (BMP-7) in complex with the secreted antagonist Noggin
Authors : Groppe, J.; Greenwald, J.; Wiater, E.; Rodriguez-Leon, J.; Economides, A.N.; Kwiatkowski, W.; Affolter, M.; Vale, W.W.; Izpisua-Belmonte, J.C.; Choe, S.
Deposited on : 2002-07-03
Resolution : 2.42 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

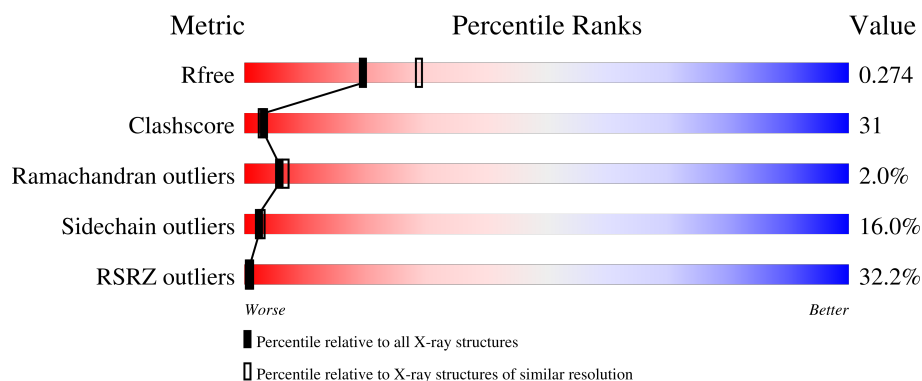
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	L	139	
2	A	206	
3	B	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2559 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 Bone Morphogenetic Protein-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	112	Total	C	N	O	S	0	0	0
			890	563	152	166	9			

- Molecule 2 is a protein called Noggin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	199	Total	C	N	O	S	0	0	0
			1595	1012	289	280	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP Q13253

- Molecule 3 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
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

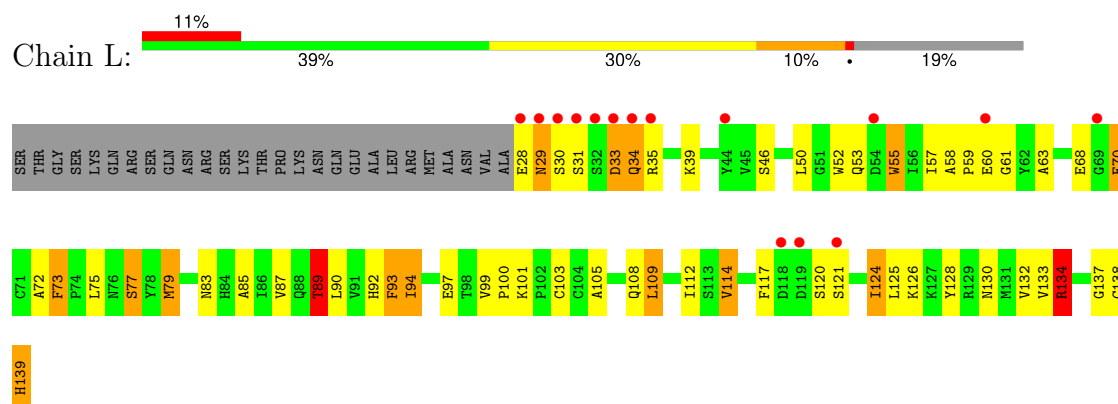
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	22	Total	O	0	0
			22	22		
4	A	24	Total	O	0	0
			24	24		

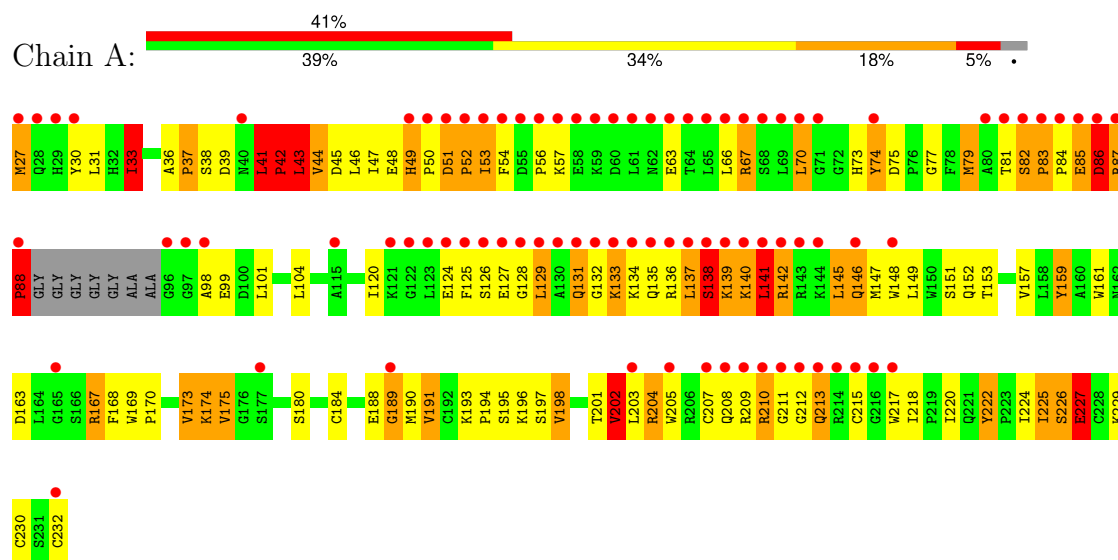
3 Residue-property plots [i](#)

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: Bone Morphogenetic Protein-7



• Molecule 2: Noggin



• Molecule 3: 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	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.83Å 99.83Å 150.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.05 – 2.42 60.05 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.7 (60.05-2.42) 95.7 (60.05-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.241 , 0.273 0.247 , 0.274	Depositor DCC
R_{free} test set	1441 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2559	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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	L	2.19	29/914 (3.2%)	1.64	15/1244 (1.2%)
2	A	1.88	36/1639 (2.2%)	1.84	52/2214 (2.3%)
All	All	2.00	65/2553 (2.5%)	1.77	67/3458 (1.9%)

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
2	A	0	1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	36	ALA	CA-C	9.96	1.66	1.52
1	L	79	MET	SD-CE	-9.28	1.56	1.79
2	A	190	MET	SD-CE	-9.11	1.56	1.79
1	L	133	VAL	C-O	-9.01	1.14	1.24
1	L	103	CYS	C-O	-8.84	1.12	1.23
2	A	79	MET	SD-CE	-8.56	1.58	1.79
1	L	55	TRP	CA-C	8.52	1.60	1.52
1	L	117	PHE	C-O	-8.25	1.13	1.23
2	A	147	MET	C-O	-8.14	1.14	1.24
1	L	63	ALA	CA-C	8.06	1.63	1.52
1	L	77	SER	CA-C	-7.83	1.41	1.52
2	A	147	MET	SD-CE	-7.44	1.60	1.79
1	L	83	ASN	N-CA	-7.42	1.37	1.46
1	L	87	VAL	C-O	-7.31	1.16	1.24
1	L	94	ILE	CA-CB	-7.29	1.43	1.54
2	A	159	TYR	CA-C	-7.18	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	73	PHE	C-O	-7.11	1.14	1.23
2	A	193	LYS	C-O	-6.97	1.17	1.24
2	A	194	PRO	C-O	-6.80	1.15	1.23
2	A	146	GLN	N-CA	-6.71	1.38	1.46
1	L	50	LEU	CA-C	-6.68	1.43	1.52
2	A	43	LEU	C-O	-6.61	1.16	1.24
2	A	44	VAL	CA-CB	-6.56	1.47	1.54
1	L	130	ASN	C-O	-6.47	1.15	1.23
2	A	191	VAL	CB-CG2	-6.47	1.31	1.52
2	A	47	ILE	CA-CB	-6.38	1.46	1.53
1	L	72	ALA	CA-C	-6.29	1.45	1.52
1	L	85	ALA	C-O	-6.28	1.16	1.24
2	A	201	THR	CA-C	-6.21	1.45	1.52
1	L	101	LYS	CB-CG	-6.13	1.34	1.52
2	A	46	LEU	CA-C	-6.05	1.45	1.52
2	A	38	SER	CA-C	5.96	1.59	1.52
2	A	230	CYS	CA-C	5.94	1.60	1.52
2	A	229	LYS	CA-CB	-5.88	1.43	1.53
2	A	152	GLN	C-O	-5.87	1.16	1.24
1	L	73	PHE	CA-C	-5.86	1.46	1.53
1	L	125	LEU	C-O	5.76	1.30	1.24
2	A	33	ILE	CA-CB	5.63	1.60	1.54
2	A	159	TYR	C-O	-5.62	1.16	1.23
1	L	124	ILE	CA-CB	-5.61	1.47	1.55
1	L	68	GLU	CA-C	-5.58	1.45	1.52
2	A	41	LEU	CG-CD2	-5.53	1.34	1.52
2	A	163	ASP	C-O	-5.53	1.17	1.24
2	A	204	ARG	N-CA	5.50	1.52	1.46
1	L	57	ILE	C-O	-5.48	1.18	1.24
2	A	168	PHE	C-O	-5.43	1.17	1.23
2	A	230	CYS	C-O	-5.42	1.17	1.23
2	A	224	ILE	C-O	-5.41	1.18	1.24
2	A	41	LEU	N-CA	-5.39	1.41	1.45
1	L	117	PHE	CA-C	-5.34	1.45	1.52
1	L	77	SER	C-O	-5.29	1.17	1.24
1	L	79	MET	CA-C	5.29	1.59	1.52
1	L	109	LEU	C-O	-5.28	1.17	1.23
1	L	112	ILE	N-CA	5.27	1.51	1.46
2	A	145	LEU	C-O	-5.26	1.17	1.24
2	A	180	SER	N-CA	-5.23	1.40	1.46
2	A	222	TYR	CA-CB	-5.22	1.44	1.53
2	A	42	PRO	CG-CD	5.18	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	134	ARG	NE-CZ	5.13	1.38	1.33
2	A	74	TYR	CD1-CE1	-5.09	1.23	1.38
1	L	108	GLN	CA-C	-5.08	1.46	1.52
2	A	43	LEU	CA-C	-5.08	1.46	1.52
1	L	124	ILE	N-CA	-5.06	1.40	1.46
2	A	226	SER	C-O	-5.03	1.17	1.23
2	A	151	SER	CA-C	-5.03	1.46	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	43	LEU	N-CA-C	10.57	127.01	109.46
2	A	232	CYS	CA-C-O	-10.23	103.41	120.80
1	L	94	ILE	N-CA-C	10.13	125.16	111.17
1	L	139	HIS	CA-C-O	-8.86	105.74	120.80
2	A	87	ARG	CA-C-O	-8.79	112.13	121.27
2	A	133	LYS	N-CA-C	-8.41	97.85	108.45
2	A	82	SER	CA-C-N	7.99	128.61	120.38
2	A	82	SER	C-N-CA	7.99	128.61	120.38
2	A	88	PRO	N-CA-C	7.75	131.46	112.10
2	A	43	LEU	CB-CA-C	-7.73	97.13	109.80
2	A	52	PRO	N-CA-C	7.70	123.44	114.20
1	L	93	PHE	CA-C-N	7.61	133.09	120.62
1	L	93	PHE	C-N-CA	7.61	133.09	120.62
1	L	55	TRP	N-CA-C	-7.38	103.28	112.72
2	A	39	ASP	N-CA-C	7.15	121.60	113.02
2	A	30	TYR	N-CA-C	7.07	118.77	111.14
2	A	86	ASP	CB-CG-OD1	-7.02	102.24	118.40
2	A	86	ASP	CB-CA-C	-6.92	97.18	113.02
1	L	94	ILE	CB-CA-C	-6.80	102.11	112.05
2	A	87	ARG	N-CA-C	-6.59	102.40	110.31
2	A	99	GLU	N-CA-C	-6.49	104.30	111.82
2	A	86	ASP	CA-CB-CG	6.47	119.07	112.60
2	A	225	ILE	N-CA-CB	-6.42	103.69	110.82
2	A	198	VAL	N-CA-C	-6.32	99.49	108.65
2	A	198	VAL	N-CA-CB	-6.31	102.95	112.35
2	A	83	PRO	CB-CA-C	-6.15	103.42	110.92
2	A	126	SER	N-CA-C	6.14	120.88	112.04
2	A	86	ASP	CB-CG-OD2	6.07	132.36	118.40
2	A	87	ARG	O-C-N	-6.06	115.23	120.99
2	A	227	GLU	N-CA-C	6.00	118.53	109.23
2	A	120	ILE	N-CA-C	-5.96	106.01	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	49	HIS	N-CA-C	5.63	116.76	109.72
2	A	189	GLY	CA-C-N	5.60	129.73	120.94
2	A	189	GLY	C-N-CA	5.60	129.73	120.94
2	A	36	ALA	CA-C-N	5.60	126.07	120.14
2	A	36	ALA	C-N-CA	5.60	126.07	120.14
2	A	175	VAL	N-CA-CB	-5.59	101.67	111.39
2	A	218	ILE	N-CA-CB	-5.59	105.66	111.64
2	A	98	ALA	N-CA-C	-5.57	107.03	113.88
2	A	147	MET	N-CA-C	-5.56	105.30	111.36
2	A	83	PRO	N-CA-C	5.56	117.48	110.70
2	A	145	LEU	N-CA-C	-5.56	105.38	111.82
1	L	53	GLN	CA-C-N	-5.54	113.83	122.37
1	L	53	GLN	C-N-CA	-5.54	113.83	122.37
2	A	37	PRO	CB-CA-C	-5.53	102.72	110.63
2	A	173	VAL	N-CA-CB	-5.50	101.64	111.92
2	A	202	VAL	N-CA-CB	-5.46	106.04	112.32
2	A	134	LYS	N-CA-C	-5.42	105.93	112.54
1	L	61	GLY	CA-C-O	-5.37	116.53	121.63
2	A	42	PRO	N-CD-CG	-5.36	97.37	103.80
2	A	74	TYR	CA-C-N	-5.31	116.36	122.52
2	A	74	TYR	C-N-CA	-5.31	116.36	122.52
2	A	137	LEU	N-CA-C	5.29	117.21	108.48
1	L	70	GLU	CA-C-N	5.28	130.10	123.03
1	L	70	GLU	C-N-CA	5.28	130.10	123.03
2	A	157	VAL	CB-CA-C	-5.26	104.60	110.96
1	L	60	GLU	N-CA-C	-5.21	107.09	113.50
2	A	190	MET	N-CA-C	5.20	117.83	110.50
2	A	87	ARG	C-N-CD	-5.19	103.74	125.00
2	A	77	GLY	N-CA-C	-5.18	108.24	114.66
2	A	188	GLU	CA-CB-CG	5.16	124.43	114.10
2	A	167	ARG	CA-C-N	-5.11	114.22	122.81
2	A	167	ARG	C-N-CA	-5.11	114.22	122.81
1	L	126	LYS	N-CA-C	5.06	116.50	108.96
1	L	73	PHE	CB-CA-C	5.05	116.68	109.26
1	L	89	THR	OG1-CB-CG2	-5.03	99.23	109.30
2	A	104	LEU	CB-CG-CD1	5.02	125.75	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	86	ASP	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	L	890	0	840	25	1
2	A	1595	0	1587	127	2
3	B	28	0	25	1	0
4	A	24	0	0	0	0
4	L	22	0	0	1	0
All	All	2559	0	2452	153	2

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 31.

All (153) 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)
2:A:125:PHE:CB	2:A:137:LEU:HD12	1.69	1.21
2:A:125:PHE:HB2	2:A:137:LEU:HD12	1.26	1.09
2:A:140:LYS:HG2	2:A:141:LEU:N	1.48	1.08
2:A:127:GLU:HA	2:A:132:GLY:HA2	1.26	1.07
2:A:128:GLY:HA3	2:A:136:ARG:HD3	1.34	1.04
2:A:140:LYS:CG	2:A:141:LEU:N	2.18	1.04
2:A:140:LYS:HG2	2:A:141:LEU:H	0.86	1.03
2:A:145:LEU:C	2:A:145:LEU:HD23	1.85	1.02
2:A:125:PHE:CZ	2:A:145:LEU:HD22	1.96	1.01
2:A:125:PHE:HB3	2:A:137:LEU:HD12	1.46	0.95
2:A:140:LYS:CG	2:A:141:LEU:H	1.78	0.94
2:A:145:LEU:HD23	2:A:145:LEU:O	1.70	0.92
2:A:125:PHE:CB	2:A:137:LEU:CD1	2.50	0.89
2:A:127:GLU:CA	2:A:132:GLY:HA2	2.03	0.89
1:L:34:GLN:O	1:L:70:GLU:HG3	1.77	0.84
1:L:105:ALA:HB3	1:L:139:HIS:CD2	2.12	0.84
1:L:134:ARG:HG2	1:L:134:ARG:HH11	1.40	0.84
2:A:125:PHE:HB3	2:A:137:LEU:CD1	2.05	0.83
2:A:139:LYS:HD2	2:A:139:LYS:C	2.01	0.83
2:A:145:LEU:HD21	2:A:149:LEU:CD1	2.09	0.83
2:A:129:LEU:HB2	2:A:133:LYS:HD2	1.58	0.83
2:A:145:LEU:HD21	2:A:149:LEU:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:48:GLU:OE2	2:A:204:ARG:NH2	2.16	0.78
1:L:114:VAL:HG13	1:L:128:TYR:CD2	2.18	0.78
2:A:128:GLY:HA3	2:A:136:ARG:CD	2.14	0.77
2:A:125:PHE:CE2	2:A:145:LEU:HD22	2.21	0.75
2:A:125:PHE:HB2	2:A:137:LEU:CD1	2.12	0.75
2:A:220:ILE:HD12	2:A:220:ILE:C	2.13	0.74
2:A:54:PHE:O	2:A:205:TRP:HD1	1.70	0.74
2:A:139:LYS:HD2	2:A:139:LYS:O	1.88	0.73
2:A:67:ARG:CG	2:A:67:ARG:HH11	2.02	0.73
2:A:54:PHE:O	2:A:205:TRP:CD1	2.41	0.72
2:A:139:LYS:C	2:A:139:LYS:CD	2.63	0.72
2:A:139:LYS:HE3	2:A:140:LYS:HA	1.70	0.71
2:A:207:CYS:HB3	2:A:212:GLY:HA2	1.72	0.71
2:A:142:ARG:HH11	2:A:146:GLN:NE2	1.90	0.69
2:A:125:PHE:CD1	2:A:125:PHE:N	2.61	0.69
2:A:128:GLY:CA	2:A:136:ARG:HD3	2.19	0.68
2:A:70:LEU:HD22	2:A:73:HIS:HB2	1.76	0.68
2:A:27:MET:O	2:A:27:MET:HG3	1.94	0.66
1:L:114:VAL:CG1	1:L:128:TYR:CD2	2.78	0.66
3:B:1:NAG:O7	3:B:1:NAG:O3	2.11	0.66
2:A:139:LYS:HE3	2:A:140:LYS:CA	2.27	0.65
1:L:109:LEU:HA	1:L:132:VAL:O	1.99	0.63
2:A:145:LEU:C	2:A:145:LEU:CD2	2.60	0.63
1:L:97:GLU:OE2	1:L:97:GLU:HA	1.98	0.62
2:A:148:TRP:CZ3	2:A:149:LEU:HD23	2.34	0.61
2:A:56:PRO:HG3	2:A:205:TRP:CG	2.36	0.61
2:A:43:LEU:HD23	2:A:43:LEU:N	2.15	0.61
2:A:84:PRO:O	2:A:85:GLU:C	2.42	0.61
2:A:207:CYS:CB	2:A:212:GLY:HA2	2.31	0.61
1:L:90:LEU:O	1:L:90:LEU:HD12	2.01	0.60
2:A:139:LYS:O	2:A:140:LYS:C	2.45	0.60
2:A:139:LYS:HE3	2:A:140:LYS:N	2.16	0.60
2:A:48:GLU:HG3	2:A:167:ARG:NH1	2.17	0.60
2:A:84:PRO:O	2:A:86:ASP:N	2.35	0.60
2:A:145:LEU:CD2	2:A:149:LEU:CD1	2.81	0.59
1:L:79:MET:HE3	1:L:138:CYS:SG	2.43	0.59
2:A:169:TRP:HA	2:A:170:PRO:C	2.27	0.58
2:A:148:TRP:CZ3	2:A:149:LEU:CD2	2.86	0.58
2:A:48:GLU:CG	2:A:167:ARG:NH1	2.67	0.58
1:L:92:HIS:O	1:L:93:PHE:C	2.47	0.57
2:A:37:PRO:O	2:A:37:PRO:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:148:TRP:CE3	2:A:149:LEU:HD23	2.40	0.56
2:A:129:LEU:HG	2:A:133:LYS:NZ	2.20	0.56
2:A:125:PHE:HD1	2:A:125:PHE:H	1.50	0.56
2:A:124:GLU:HG2	2:A:142:ARG:NH2	2.20	0.56
2:A:140:LYS:O	2:A:142:ARG:N	2.39	0.56
2:A:159:TYR:HB3	2:A:174:LYS:HD3	1.87	0.55
2:A:142:ARG:HH11	2:A:146:GLN:HE22	1.53	0.55
2:A:67:ARG:HH11	2:A:67:ARG:HG2	1.70	0.55
1:L:31:SER:OG	1:L:33:ASP:OD2	2.23	0.54
2:A:211:GLY:C	2:A:213:GLN:NE2	2.66	0.54
2:A:66:LEU:HD13	2:A:169:TRP:CD1	2.43	0.54
1:L:97:GLU:OE2	1:L:97:GLU:CA	2.57	0.53
2:A:50:PRO:O	2:A:52:PRO:HD3	2.08	0.53
2:A:142:ARG:NH1	2:A:146:GLN:HE22	2.07	0.53
2:A:202:VAL:CG1	2:A:203:LEU:N	2.70	0.53
2:A:142:ARG:NH1	2:A:146:GLN:NE2	2.57	0.52
2:A:141:LEU:HD12	2:A:141:LEU:O	2.10	0.52
1:L:120:SER:O	1:L:121:SER:C	2.51	0.51
2:A:48:GLU:CG	2:A:167:ARG:HH11	2.23	0.51
2:A:145:LEU:CD2	2:A:149:LEU:HD12	2.40	0.51
2:A:124:GLU:CD	2:A:142:ARG:NH2	2.70	0.50
1:L:120:SER:O	1:L:121:SER:OG	2.25	0.50
1:L:137:GLY:O	1:L:139:HIS:CD2	2.65	0.50
2:A:41:LEU:CB	2:A:42:PRO:HA	2.32	0.50
2:A:49:HIS:CD2	2:A:51:ASP:H	2.30	0.49
2:A:129:LEU:HG	2:A:133:LYS:HZ2	1.77	0.49
2:A:127:GLU:HB2	2:A:131:GLN:C	2.37	0.49
2:A:148:TRP:HZ3	2:A:149:LEU:CD2	2.25	0.49
1:L:52:TRP:CD2	1:L:55:TRP:HZ3	2.30	0.49
2:A:124:GLU:HG2	2:A:142:ARG:HH22	1.78	0.48
1:L:134:ARG:HG2	1:L:134:ARG:NH1	2.17	0.48
2:A:140:LYS:C	2:A:142:ARG:N	2.71	0.48
2:A:148:TRP:HZ3	2:A:149:LEU:HD21	1.78	0.48
2:A:67:ARG:HH11	2:A:67:ARG:HG3	1.79	0.48
2:A:48:GLU:HG3	2:A:167:ARG:HH11	1.79	0.48
1:L:58:ALA:HA	1:L:59:PRO:C	2.39	0.48
2:A:149:LEU:HD23	2:A:149:LEU:HA	1.73	0.47
2:A:67:ARG:CZ	2:A:74:TYR:CE2	2.97	0.47
1:L:29:ASN:O	1:L:30:SER:OG	2.25	0.47
1:L:120:SER:C	1:L:121:SER:OG	2.57	0.47
2:A:202:VAL:HG13	2:A:203:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:67:ARG:HG3	2:A:67:ARG:NH1	2.29	0.46
2:A:140:LYS:C	2:A:142:ARG:H	2.24	0.46
2:A:205:TRP:CZ2	2:A:215:CYS:HB2	2.51	0.46
2:A:49:HIS:HD2	2:A:51:ASP:HB2	1.80	0.46
2:A:127:GLU:HB2	2:A:131:GLN:HA	1.97	0.45
2:A:75:ASP:OD1	2:A:75:ASP:C	2.59	0.45
2:A:142:ARG:O	2:A:146:GLN:HG3	2.17	0.45
2:A:204:ARG:O	2:A:217:TRP:HA	2.16	0.45
2:A:31:LEU:HB3	2:A:33:ILE:HG23	1.98	0.45
2:A:128:GLY:N	2:A:132:GLY:HA2	2.32	0.45
2:A:139:LYS:C	2:A:139:LYS:HE3	2.41	0.45
2:A:137:LEU:HB3	2:A:141:LEU:HG	1.98	0.45
2:A:148:TRP:CE3	2:A:149:LEU:CD2	2.99	0.45
2:A:195:SER:O	2:A:196:LYS:HG2	2.18	0.44
2:A:48:GLU:HG2	2:A:167:ARG:NH1	2.32	0.44
2:A:124:GLU:CG	2:A:142:ARG:NH2	2.80	0.44
1:L:99:VAL:HG22	1:L:100:PRO:HD2	1.99	0.44
2:A:138:SER:OG	2:A:140:LYS:NZ	2.49	0.43
2:A:226:SER:O	2:A:227:GLU:HG2	2.18	0.43
2:A:82:SER:HA	2:A:83:PRO:HD2	1.77	0.43
2:A:139:LYS:O	2:A:142:ARG:CB	2.67	0.43
2:A:128:GLY:H	2:A:132:GLY:CA	2.31	0.43
1:L:73:PHE:HB2	1:L:89:THR:HG23	2.00	0.43
1:L:94:ILE:HD13	1:L:94:ILE:HG21	1.61	0.43
2:A:66:LEU:HD23	2:A:66:LEU:HA	1.66	0.43
2:A:148:TRP:CZ3	2:A:149:LEU:HD21	2.54	0.43
2:A:211:GLY:O	2:A:213:GLN:NE2	2.52	0.43
2:A:41:LEU:HA	2:A:42:PRO:HA	1.58	0.42
2:A:209:ARG:HB2	2:A:213:GLN:HB2	2.01	0.42
1:L:114:VAL:HG13	1:L:128:TYR:HD2	1.78	0.42
2:A:66:LEU:HD13	2:A:169:TRP:CG	2.55	0.42
2:A:153:THR:HG22	2:A:184:CYS:O	2.20	0.42
2:A:51:ASP:HB3	2:A:53:ILE:HD11	2.02	0.42
2:A:42:PRO:HB3	2:A:225:ILE:HD11	2.01	0.42
1:L:33:ASP:HB3	4:L:197:HOH:O	2.19	0.42
2:A:128:GLY:HA3	2:A:136:ARG:CG	2.49	0.41
2:A:70:LEU:HD23	2:A:70:LEU:HA	1.91	0.41
2:A:125:PHE:CE2	2:A:145:LEU:CD2	3.00	0.41
2:A:44:VAL:HG12	2:A:45:ASP:N	2.35	0.41
2:A:128:GLY:C	2:A:136:ARG:HH11	2.28	0.41
2:A:139:LYS:C	2:A:139:LYS:CE	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:222:TYR:CD2	2:A:222:TYR:C	2.98	0.40
2:A:125:PHE:CE2	2:A:145:LEU:HD13	2.57	0.40
2:A:127:GLU:HA	2:A:132:GLY:CA	2.20	0.40
2:A:138:SER:CB	2:A:140:LYS:HZ3	2.33	0.40
2:A:127:GLU:HB3	2:A:131:GLN:NE2	2.37	0.40
2:A:129:LEU:N	2:A:132:GLY:O	2.54	0.40
2:A:169:TRP:CA	2:A:170:PRO:C	2.94	0.40
2:A:85:GLU:HB2	2:A:161:TRP:HD1	1.87	0.40

All (2) 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:L:77:SER:O	2:A:88:PRO:O[6_455]	1.49	0.71
2:A:135:GLN:OE1	2:A:210:ARG:NH2[4_444]	2.00	0.20

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	L	110/139 (79%)	101 (92%)	8 (7%)	1 (1%)	14	20
2	A	195/206 (95%)	170 (87%)	20 (10%)	5 (3%)	4	4
All	All	305/345 (88%)	271 (89%)	28 (9%)	6 (2%)	6	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	ASN
2	A	85	GLU
2	A	63	GLU
2	A	138	SER

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Mol	Chain	Res	Type
2	A	141	LEU
2	A	189	GLY

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	L	98/121 (81%)	87 (89%)	11 (11%)	6	8
2	A	177/177 (100%)	144 (81%)	33 (19%)	1	2
All	All	275/298 (92%)	231 (84%)	44 (16%)	2	3

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

Mol	Chain	Res	Type
1	L	28	GLU
1	L	33	ASP
1	L	34	GLN
1	L	35	ARG
1	L	39	LYS
1	L	46	SER
1	L	75	LEU
1	L	89	THR
1	L	114	VAL
1	L	124	ILE
1	L	134	ARG
2	A	27	MET
2	A	33	ILE
2	A	41	LEU
2	A	42	PRO
2	A	43	LEU
2	A	51	ASP
2	A	53	ILE
2	A	57	LYS
2	A	67	ARG
2	A	70	LEU

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Mol	Chain	Res	Type
2	A	79	MET
2	A	81	THR
2	A	87	ARG
2	A	88	PRO
2	A	101	LEU
2	A	129	LEU
2	A	131	GLN
2	A	138	SER
2	A	139	LYS
2	A	140	LYS
2	A	141	LEU
2	A	142	ARG
2	A	173	VAL
2	A	174	LYS
2	A	175	VAL
2	A	191	VAL
2	A	197	SER
2	A	198	VAL
2	A	202	VAL
2	A	208	GLN
2	A	210	ARG
2	A	213	GLN
2	A	227	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	32	HIS
2	A	49	HIS
2	A	110	GLN
2	A	131	GLN
2	A	146	GLN
2	A	208	GLN
2	A	213	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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$
3	NAG	B	1	3,1	14,14,15	1.82	3 (21%)	17,19,21	3.53	8 (47%)
3	NAG	B	2	3	14,14,15	1.80	5 (35%)	17,19,21	3.11	10 (58%)

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	B	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	5/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	C2-N2	-5.10	1.37	1.46
3	B	2	NAG	C2-N2	3.28	1.51	1.46
3	B	2	NAG	O5-C1	2.96	1.48	1.43
3	B	1	NAG	C1-C2	2.73	1.56	1.52
3	B	2	NAG	C4-C5	2.51	1.58	1.53
3	B	1	NAG	O5-C1	-2.46	1.39	1.43
3	B	2	NAG	O3-C3	-2.25	1.37	1.43
3	B	2	NAG	C1-C2	2.00	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	O4-C4-C5	-7.48	90.91	109.32
3	B	2	NAG	O5-C1-C2	6.43	121.24	111.29
3	B	1	NAG	O4-C4-C3	6.38	125.42	110.38
3	B	1	NAG	C2-N2-C7	-6.30	114.45	122.90
3	B	2	NAG	C1-C2-N2	5.00	118.31	110.43
3	B	2	NAG	O3-C3-C2	-4.76	99.52	109.40
3	B	1	NAG	O5-C5-C4	4.36	121.44	110.83
3	B	1	NAG	C4-C3-C2	-4.15	104.93	111.02
3	B	2	NAG	C3-C4-C5	-4.09	102.82	110.23
3	B	1	NAG	C1-O5-C5	-4.06	106.74	112.19
3	B	2	NAG	C2-N2-C7	3.75	127.93	122.90
3	B	2	NAG	O4-C4-C5	3.47	117.87	109.32
3	B	2	NAG	C1-O5-C5	2.96	116.15	112.19
3	B	1	NAG	C1-C2-N2	-2.58	106.37	110.43
3	B	2	NAG	O7-C7-C8	-2.50	117.61	122.05
3	B	2	NAG	O3-C3-C4	2.19	115.53	110.38
3	B	2	NAG	O5-C5-C6	2.17	111.89	107.66
3	B	1	NAG	O5-C1-C2	-2.11	108.02	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

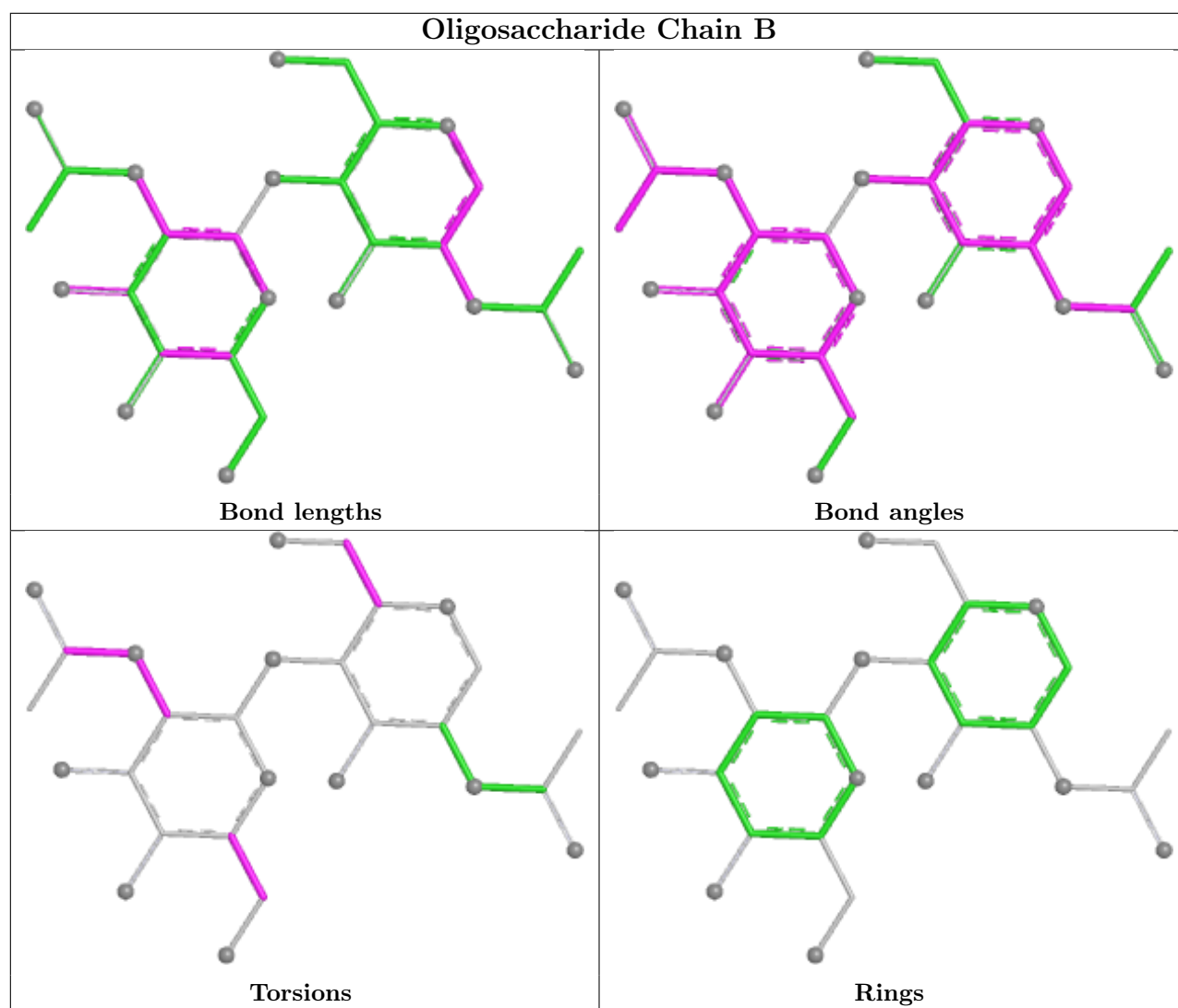
Mol	Chain	Res	Type	Atoms
3	B	2	NAG	C8-C7-N2-C2
3	B	1	NAG	O5-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	B	2	NAG	O7-C7-N2-C2
3	B	1	NAG	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	2	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	112/139 (80%)	0.87	15 (13%) 7 5	33, 46, 105, 141	0
2	A	199/206 (96%)	2.16	85 (42%) 0 0	35, 58, 118, 130	0
All	All	311/345 (90%)	1.70	100 (32%) 1 1	33, 52, 115, 141	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	52	PRO	8.2
2	A	138	SER	8.1
2	A	141	LEU	7.6
2	A	126	SER	7.5
1	L	31	SER	7.2
2	A	62	ASN	6.9
2	A	139	LYS	6.7
2	A	127	GLU	6.6
2	A	129	LEU	6.4
2	A	27	MET	6.2
2	A	50	PRO	6.0
2	A	130	ALA	5.9
2	A	65	LEU	5.8
2	A	88	PRO	5.8
2	A	86	ASP	5.8
2	A	132	GLY	5.7
2	A	133	LYS	5.7
1	L	32	SER	5.7
2	A	60	ASP	5.7
2	A	207	CYS	5.5
2	A	131	GLN	5.4
1	L	33	ASP	5.3
2	A	215	CYS	5.3
2	A	96	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
2	A	134	LYS	5.2
2	A	135	GLN	5.1
2	A	49	HIS	5.0
2	A	53	ILE	4.8
1	L	29	ASN	4.8
1	L	34	GLN	4.7
2	A	214	ARG	4.5
2	A	87	ARG	4.5
2	A	84	PRO	4.4
1	L	119	ASP	4.4
2	A	30	TYR	4.3
2	A	137	LEU	4.2
2	A	51	ASP	4.2
2	A	98	ALA	4.2
2	A	68	SER	4.1
2	A	128	GLY	4.1
2	A	63	GLU	4.0
2	A	125	PHE	4.0
2	A	97	GLY	3.9
2	A	136	ARG	3.9
1	L	35	ARG	3.8
2	A	57	LYS	3.8
2	A	64	THR	3.8
2	A	209	ARG	3.7
2	A	122	GLY	3.7
2	A	29	HIS	3.7
2	A	232	CYS	3.7
2	A	142	ARG	3.7
2	A	54	PHE	3.6
2	A	124	GLU	3.6
2	A	59	LYS	3.6
2	A	82	SER	3.6
2	A	212	GLY	3.5
2	A	28	GLN	3.5
2	A	216	GLY	3.5
2	A	74	TYR	3.4
2	A	58	GLU	3.3
2	A	69	LEU	3.2
1	L	28	GLU	3.2
2	A	144	LYS	3.1
1	L	30	SER	3.1
2	A	123	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	121	LYS	3.1
2	A	67	ARG	3.0
2	A	70	LEU	3.0
2	A	203	LEU	2.9
2	A	208	GLN	2.9
2	A	80	ALA	2.9
2	A	211	GLY	2.8
2	A	83	PRO	2.7
2	A	146	GLN	2.6
2	A	115	ALA	2.6
1	L	121	SER	2.6
2	A	40	ASN	2.5
2	A	61	LEU	2.5
2	A	148	TRP	2.5
2	A	217	TRP	2.5
2	A	85	GLU	2.4
2	A	66	LEU	2.4
2	A	71	GLY	2.4
2	A	56	PRO	2.4
1	L	54	ASP	2.4
2	A	210	ARG	2.4
2	A	213	GLN	2.4
2	A	205	TRP	2.4
2	A	140	LYS	2.3
2	A	55	ASP	2.3
1	L	60	GLU	2.3
2	A	177	SER	2.3
1	L	118	ASP	2.3
2	A	143	ARG	2.3
1	L	44	TYR	2.2
1	L	69	GLY	2.1
2	A	81	THR	2.1
2	A	165	GLY	2.1
2	A	189	GLY	2.1

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

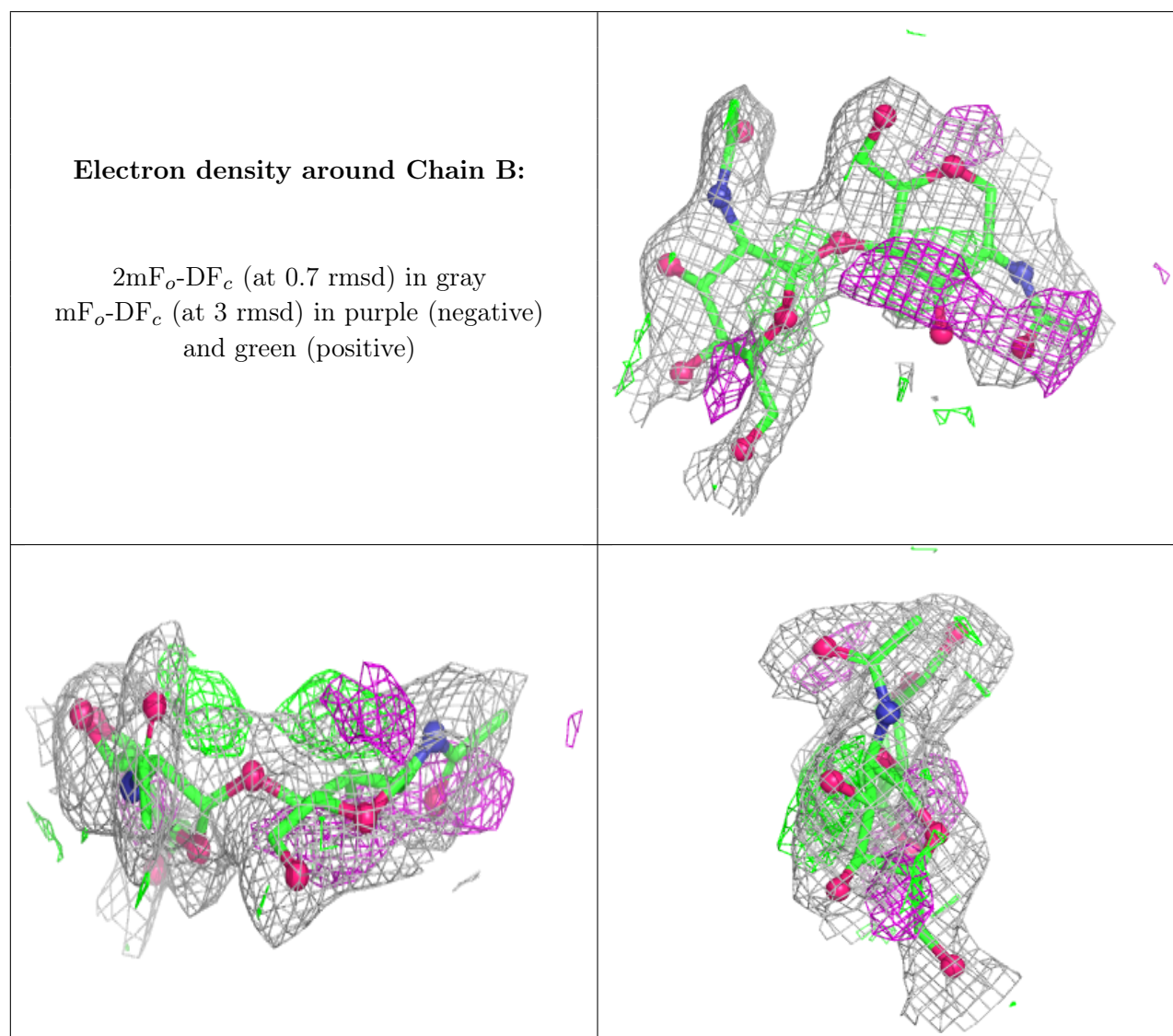
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	1	14/15	-	-	35,54,71,82	0
3	NAG	B	2	14/15	-	-	64,77,84,85	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.