



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:49 AM UTC

PDB ID : 1LX5 / pdb_00001lx5
Title : Crystal Structure of the BMP7/ActRII Extracellular Domain Complex
Authors : Greenwald, J.; Groppe, J.; Kwiatkowski, W.; Choe, S.
Deposited on : 2002-06-04
Resolution : 3.30 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

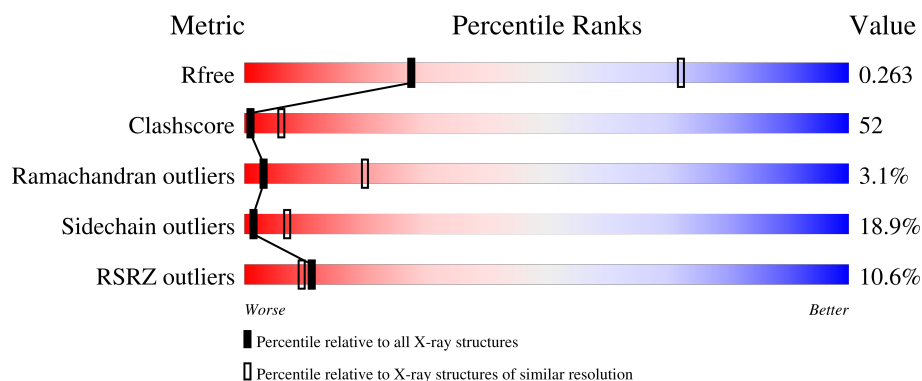
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	139	
2	B	102	
3	C	6	

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
4	NAG	B	124	X	-	-	-
4	NAG	B	147	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1695 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.

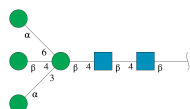
- Molecule 1 is a protein called bone morphogenetic protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	30	0	0
			827	530	139	149	9			

- Molecule 2 is a protein called Activin Type II Receptor.

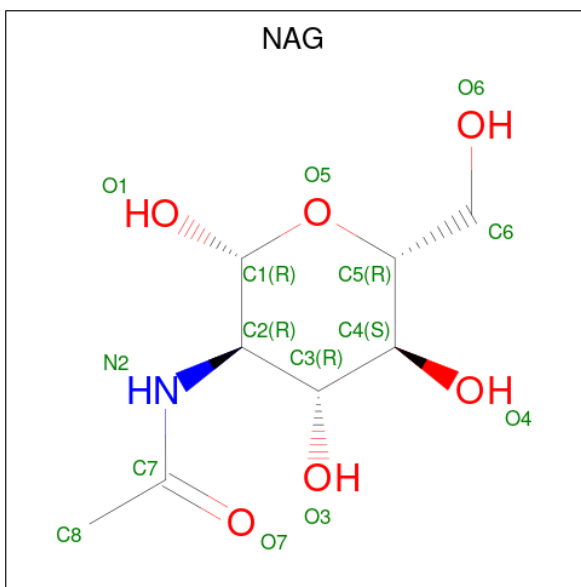
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	S	27	0	0
			768	477	131	149	11			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

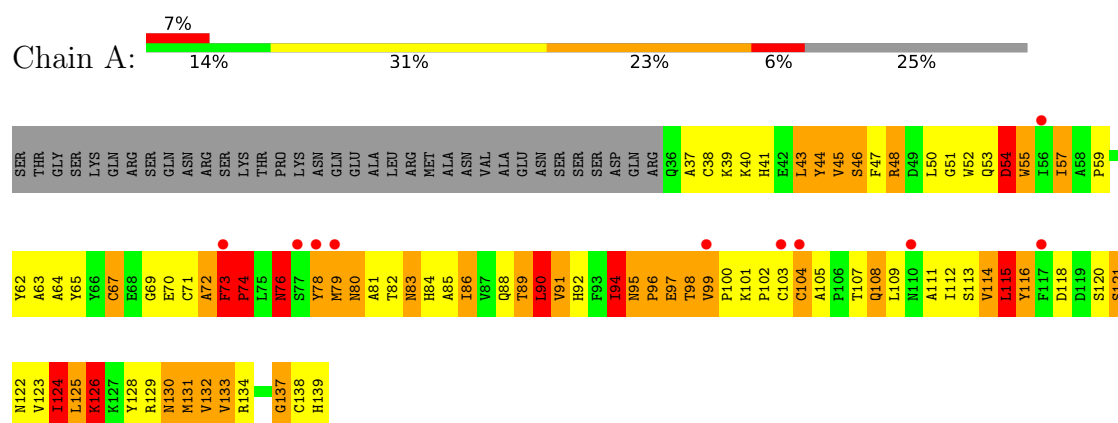


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

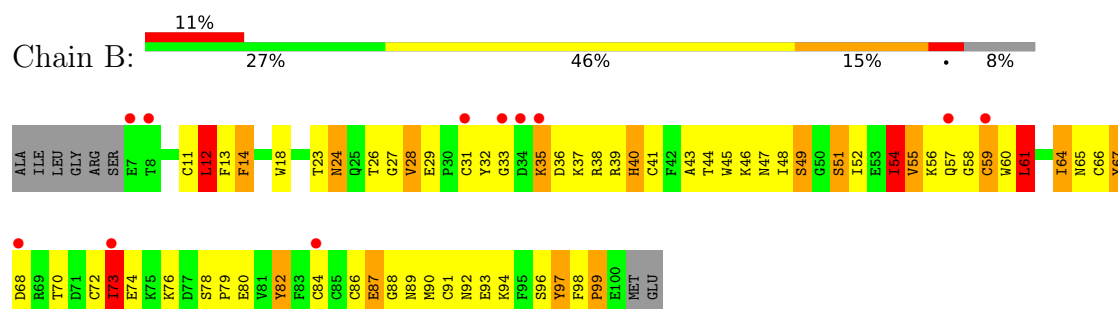
3 Residue-property plots

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

- Molecule 1: bone morphogenetic protein 7



- Molecule 2: Activin Type II Receptor



- Molecule 3: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	140.92Å 140.92Å 90.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.12 – 3.30 27.12 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (27.12-3.30) 96.7 (27.12-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.238 , 0.279 0.267 , 0.263	Depositor DCC
R_{free} test set	381 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	123.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	1695	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	2.95	33/851 (3.9%)	2.23	41/1160 (3.5%)
2	B	1.68	12/787 (1.5%)	1.67	18/1061 (1.7%)
All	All	2.42	45/1638 (2.7%)	1.98	59/2221 (2.7%)

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
2	B	1	0
All	All	1	1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	ASP	CB-CG	49.65	2.76	1.52
1	A	78	TYR	CB-CG	22.97	2.02	1.51
2	B	94	LYS	CB-CG	13.71	1.93	1.52
1	A	63	ALA	CA-CB	-13.27	1.36	1.53
1	A	39	LYS	CB-CG	12.79	1.90	1.52
1	A	129	ARG	CB-CG	-10.46	1.21	1.52
2	B	35	LYS	CB-CG	-10.15	1.22	1.52
2	B	55	VAL	CA-CB	-9.87	1.44	1.55
1	A	112	ILE	CA-CB	-9.56	1.40	1.54
2	B	43	ALA	CA-CB	-8.03	1.40	1.53
2	B	14	PHE	CA-C	-7.99	1.42	1.52
1	A	104	CYS	C-O	-7.96	1.14	1.24
1	A	115	LEU	CA-C	-7.42	1.43	1.52
1	A	86	ILE	CA-CB	-7.31	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ALA	CA-CB	-7.27	1.41	1.53
1	A	45	VAL	CA-CB	-6.97	1.45	1.54
1	A	73	PHE	CB-CG	6.88	1.66	1.50
2	B	54	ILE	CA-CB	-6.68	1.46	1.54
1	A	133	VAL	CA-CB	-6.54	1.46	1.54
1	A	67	CYS	CA-C	-6.38	1.44	1.52
1	A	57	ILE	CA-CB	-6.37	1.46	1.54
1	A	125	LEU	CA-C	-6.21	1.45	1.52
1	A	133	VAL	CA-C	-6.13	1.45	1.52
1	A	81	ALA	CA-CB	-6.05	1.43	1.53
1	A	99	VAL	CA-CB	-5.94	1.46	1.54
1	A	102	PRO	C-O	-5.67	1.16	1.23
1	A	91	VAL	C-O	-5.59	1.17	1.24
2	B	28	VAL	CA-CB	-5.54	1.47	1.54
2	B	65	ASN	CA-C	-5.54	1.45	1.52
1	A	123	VAL	CA-CB	-5.47	1.47	1.54
1	A	131	MET	SD-CE	-5.38	1.66	1.79
1	A	70	GLU	C-O	-5.35	1.16	1.23
1	A	116	TYR	CA-CB	-5.32	1.44	1.53
2	B	23	THR	CA-C	-5.32	1.45	1.53
2	B	24	ASN	CA-C	-5.30	1.46	1.53
1	A	130	ASN	CA-C	-5.27	1.46	1.53
1	A	101	LYS	C-N	-5.25	1.27	1.33
1	A	41	HIS	CA-C	-5.22	1.46	1.52
2	B	37	LYS	CB-CG	-5.20	1.36	1.52
1	A	94	ILE	C-O	-5.18	1.18	1.24
1	A	57	ILE	CA-C	-5.17	1.46	1.53
1	A	101	LYS	C-O	-5.06	1.17	1.23
1	A	37	ALA	C-O	-5.06	1.16	1.23
2	B	73	ILE	CB-CG1	-5.04	1.43	1.53
1	A	105	ALA	CA-CB	-5.03	1.47	1.54

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASP	CA-CB-CG	-18.61	93.99	112.60
1	A	129	ARG	CA-CB-CG	17.12	148.35	114.10
1	A	105	ALA	N-CA-C	-10.47	98.70	108.13
1	A	72	ALA	N-CA-C	10.00	125.11	109.81
1	A	79	MET	N-CA-C	-9.16	98.71	113.19
2	B	55	VAL	CB-CA-C	-9.10	101.06	111.80
2	B	73	ILE	CA-CB-CG1	8.55	124.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	LYS	CA-CB-CG	8.20	130.49	114.10
1	A	71	CYS	CB-CA-C	-8.10	99.94	111.85
1	A	39	LYS	CA-CB-CG	-7.38	99.34	114.10
2	B	23	THR	N-CA-C	-7.33	99.13	109.69
1	A	78	TYR	CA-CB-CG	7.28	126.99	113.90
1	A	102	PRO	CA-C-O	-7.20	112.94	121.95
1	A	130	ASN	N-CA-C	7.10	121.03	111.24
1	A	91	VAL	N-CA-C	-6.99	102.97	110.23
1	A	90	LEU	CA-CB-CG	6.82	140.16	116.30
2	B	52	ILE	N-CA-C	6.80	117.67	107.75
1	A	86	ILE	N-CA-C	-6.77	103.62	111.00
2	B	36	ASP	N-CA-C	-6.54	96.87	110.80
1	A	103	CYS	CA-C-N	6.53	130.84	121.50
1	A	103	CYS	C-N-CA	6.53	130.84	121.50
1	A	96	PRO	N-CD-CG	-6.46	93.50	103.20
1	A	102	PRO	CB-CA-C	-6.42	102.83	111.12
1	A	131	MET	CA-C-N	-6.36	114.29	123.06
1	A	131	MET	C-N-CA	-6.36	114.29	123.06
1	A	132	VAL	CA-C-N	-6.27	114.54	122.37
1	A	132	VAL	C-N-CA	-6.27	114.54	122.37
2	B	80	GLU	N-CA-C	-6.24	104.39	111.07
1	A	97	GLU	CB-CG-CD	6.21	123.15	112.60
2	B	12	LEU	N-CA-C	-6.17	99.95	109.76
1	A	40	LYS	N-CA-C	-6.17	101.36	110.48
1	A	74	PRO	N-CA-C	-6.12	96.19	112.10
1	A	51	GLY	CA-C-O	6.11	125.80	119.27
2	B	78	SER	CB-CA-C	-6.09	106.88	111.20
1	A	137	GLY	N-CA-C	6.09	119.49	110.42
2	B	24	ASN	N-CA-C	-5.98	102.81	110.53
1	A	130	ASN	CB-CA-C	-5.85	103.08	112.09
1	A	94	ILE	N-CA-C	-5.83	97.20	109.34
1	A	76	ASN	N-CA-C	5.74	117.47	109.31
1	A	83	ASN	N-CA-C	-5.71	104.42	111.33
2	B	18	TRP	N-CA-C	5.68	118.21	111.33
2	B	27	GLY	CA-C-N	-5.67	114.80	122.91
2	B	27	GLY	C-N-CA	-5.67	114.80	122.91
1	A	90	LEU	N-CA-CB	5.60	118.44	110.16
1	A	44	TYR	CA-C-N	-5.59	112.32	122.43
1	A	44	TYR	C-N-CA	-5.59	112.32	122.43
2	B	54	ILE	CB-CA-C	-5.53	103.49	111.34
1	A	124	ILE	N-CA-C	5.43	116.48	108.45
2	B	67	TYR	N-CA-C	-5.43	100.86	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	SER	N-CA-C	-5.37	101.22	109.76
1	A	95	ASN	N-CA-C	5.36	121.65	109.81
1	A	126	LYS	CA-C-N	-5.18	114.92	122.65
1	A	126	LYS	C-N-CA	-5.18	114.92	122.65
2	B	59	CYS	N-CA-C	-5.16	102.88	110.52
1	A	89	THR	OG1-CB-CG2	-5.11	99.09	109.30
1	A	133	VAL	CB-CA-C	-5.09	104.80	110.96
2	B	26	THR	CB-CA-C	-5.08	99.45	111.65
1	A	107	THR	N-CA-C	-5.01	105.98	113.89
1	A	41	HIS	CB-CA-C	-5.00	99.53	109.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	73	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	78	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	827	0	788	82	0
2	B	768	0	684	70	2
3	C	72	0	61	9	0
4	B	28	0	26	9	0
All	All	1695	0	1559	163	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 52.

All (163) 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:B:97:TYR:CE2	2:B:99:PRO:HD3	1.65	1.30
3:C:3:BMA:H3	3:C:5:BMA:H2	1.13	1.10
1:A:126:LYS:HG2	1:A:128:TYR:HE2	1.20	1.07
2:B:97:TYR:CD2	2:B:99:PRO:HD3	1.95	1.00
1:A:126:LYS:HG2	1:A:128:TYR:CE2	2.00	0.95
2:B:97:TYR:CE2	2:B:99:PRO:CD	2.48	0.95
2:B:97:TYR:HE2	2:B:99:PRO:HD3	1.29	0.94
3:C:3:BMA:C3	3:C:5:BMA:H2	1.98	0.92
1:A:95:ASN:OD1	1:A:97:GLU:HB2	1.69	0.91
1:A:118:ASP:OD1	1:A:122:ASN:N	2.06	0.88
2:B:47:ASN:HD22	4:B:147:NAG:H82	1.42	0.85
1:A:116:TYR:CZ	1:A:124:ILE:HG21	2.12	0.85
1:A:74:PRO:HG2	1:A:74:PRO:O	1.76	0.83
2:B:29:GLU:OE1	2:B:59:CYS:HB2	1.80	0.81
1:A:64:ALA:O	1:A:65:TYR:HB2	1.81	0.80
2:B:97:TYR:HE2	2:B:99:PRO:CD	1.89	0.80
2:B:44:THR:HG23	2:B:55:VAL:HB	1.65	0.78
1:A:74:PRO:O	1:A:74:PRO:CG	2.31	0.78
1:A:43:LEU:C	1:A:43:LEU:HD23	2.12	0.74
2:B:40:HIS:HB3	2:B:86:CYS:O	1.88	0.74
1:A:95:ASN:C	1:A:97:GLU:H	1.95	0.73
2:B:31:CYS:O	2:B:39:ARG:NE	2.20	0.73
2:B:45:TRP:CE2	2:B:82:TYR:HB2	2.24	0.73
1:A:95:ASN:O	1:A:97:GLU:N	2.22	0.73
1:A:114:VAL:HG23	1:A:115:LEU:N	2.02	0.73
2:B:45:TRP:HE1	4:B:147:NAG:C8	2.02	0.72
3:C:3:BMA:H3	3:C:5:BMA:C2	2.06	0.71
1:A:38:CYS:HA	1:A:69:GLY:HA3	1.73	0.70
1:A:95:ASN:C	1:A:97:GLU:N	2.48	0.69
2:B:14:PHE:CE2	2:B:54:ILE:HD12	2.28	0.68
1:A:53:GLN:H	1:A:53:GLN:CD	2.01	0.68
2:B:97:TYR:HE2	2:B:99:PRO:CG	2.06	0.68
1:A:48:ARG:HA	1:A:53:GLN:HB3	1.75	0.67
2:B:97:TYR:CD2	2:B:97:TYR:C	2.73	0.65
2:B:38:ARG:NH1	2:B:87:GLU:OE1	2.29	0.65
2:B:73:ILE:HA	2:B:96:SER:O	1.97	0.65
2:B:97:TYR:HE2	2:B:99:PRO:HG3	1.62	0.65
4:B:124:NAG:O6	4:B:124:NAG:O4	2.10	0.65
3:C:1:NAG:H62	3:C:2:NAG:HN2	1.61	0.64
2:B:47:ASN:ND2	4:B:147:NAG:H82	2.11	0.64
1:A:79:MET:O	1:A:80:ASN:C	2.40	0.63
2:B:55:VAL:HG12	2:B:56:LYS:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:CE2	1:A:124:ILE:HG21	2.34	0.63
2:B:97:TYR:HD2	2:B:98:PHE:N	1.98	0.62
1:A:62:TYR:CZ	1:A:131:MET:HE3	2.34	0.61
1:A:116:TYR:CZ	1:A:124:ILE:CG2	2.81	0.61
1:A:45:VAL:HG12	1:A:46:SER:N	2.15	0.61
1:A:90:LEU:O	1:A:91:VAL:C	2.39	0.61
1:A:94:ILE:HG22	1:A:95:ASN:N	2.16	0.61
1:A:116:TYR:CD2	1:A:116:TYR:C	2.79	0.60
1:A:43:LEU:C	1:A:43:LEU:CD2	2.74	0.60
2:B:29:GLU:OE1	2:B:59:CYS:CB	2.48	0.60
1:A:82:THR:O	1:A:85:ALA:HB3	2.02	0.60
2:B:28:VAL:CG1	2:B:90:MET:HE1	2.31	0.60
2:B:13:PHE:HA	2:B:57:GLN:O	2.02	0.60
1:A:109:LEU:HA	1:A:132:VAL:O	2.02	0.59
2:B:47:ASN:O	2:B:49:SER:N	2.35	0.59
2:B:64:ILE:HG12	2:B:64:ILE:O	2.01	0.59
2:B:97:TYR:CE2	2:B:99:PRO:CG	2.85	0.58
2:B:38:ARG:HD2	2:B:67:TYR:CE1	2.38	0.58
1:A:62:TYR:OH	1:A:131:MET:HE3	2.03	0.58
3:C:1:NAG:H62	3:C:2:NAG:N2	2.19	0.57
2:B:97:TYR:C	2:B:97:TYR:HD2	2.12	0.57
2:B:44:THR:HA	2:B:82:TYR:O	2.04	0.57
2:B:44:THR:HG22	2:B:56:LYS:H	1.68	0.57
2:B:60:TRP:O	2:B:61:LEU:C	2.48	0.56
2:B:45:TRP:NE1	4:B:147:NAG:C8	2.67	0.56
2:B:28:VAL:HG13	2:B:90:MET:HE1	1.88	0.56
1:A:88:GLN:HG3	1:A:99:VAL:HG21	1.88	0.56
3:C:3:BMA:H4	3:C:6:MAN:H2	1.87	0.56
1:A:53:GLN:CD	1:A:53:GLN:N	2.64	0.55
1:A:82:THR:O	1:A:83:ASN:C	2.47	0.54
1:A:94:ILE:O	1:A:96:PRO:CD	2.55	0.54
2:B:45:TRP:NE1	4:B:147:NAG:H81	2.22	0.54
2:B:12:LEU:O	2:B:92:ASN:ND2	2.34	0.53
1:A:115:LEU:HD12	1:A:124:ILE:O	2.08	0.53
1:A:99:VAL:HG23	1:A:100:PRO:HD2	1.90	0.53
1:A:54:ASP:O	1:A:55:TRP:HE3	1.92	0.53
2:B:48:ILE:O	2:B:51:SER:HB2	2.08	0.53
1:A:74:PRO:O	1:A:74:PRO:CD	2.56	0.53
3:C:1:NAG:O7	3:C:1:NAG:O3	2.23	0.53
1:A:43:LEU:HD23	1:A:44:TYR:N	2.24	0.52
2:B:24:ASN:N	2:B:24:ASN:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:CE2	1:A:124:ILE:CG2	2.94	0.51
1:A:82:THR:O	1:A:85:ALA:N	2.42	0.51
2:B:41:CYS:HA	2:B:58:GLY:O	2.11	0.51
4:B:124:NAG:HO4	4:B:124:NAG:HO6	1.55	0.50
2:B:97:TYR:CE2	2:B:99:PRO:HG3	2.42	0.50
2:B:39:ARG:C	2:B:40:HIS:CD2	2.90	0.50
1:A:84:HIS:O	1:A:84:HIS:CG	2.62	0.49
1:A:53:GLN:N	1:A:53:GLN:OE1	2.41	0.49
2:B:12:LEU:HD12	2:B:93:GLU:HA	1.93	0.49
2:B:41:CYS:HB3	2:B:92:ASN:HB3	1.93	0.49
2:B:45:TRP:HE1	4:B:147:NAG:H81	1.72	0.49
1:A:94:ILE:HG22	1:A:95:ASN:H	1.77	0.49
1:A:128:TYR:HD2	1:A:128:TYR:N	2.10	0.48
1:A:128:TYR:N	1:A:128:TYR:CD2	2.80	0.48
1:A:104:CYS:HA	1:A:137:GLY:O	2.12	0.48
2:B:47:ASN:ND2	4:B:147:NAG:C8	2.75	0.48
1:A:94:ILE:O	1:A:96:PRO:HD2	2.13	0.48
2:B:39:ARG:O	2:B:40:HIS:HD2	1.97	0.47
2:B:76:LYS:O	2:B:79:PRO:HD3	2.13	0.47
2:B:45:TRP:CD1	2:B:45:TRP:C	2.89	0.47
1:A:108:GLN:O	1:A:134:ARG:N	2.36	0.47
1:A:67:CYS:HB3	1:A:104:CYS:SG	2.55	0.47
2:B:33:GLY:CA	2:B:39:ARG:HG3	2.45	0.47
2:B:44:THR:CG2	2:B:55:VAL:HB	2.40	0.47
2:B:90:MET:O	2:B:93:GLU:HB2	2.15	0.47
1:A:72:ALA:HB1	1:A:73:PHE:CG	2.50	0.46
1:A:47:PHE:HA	1:A:50:LEU:HB2	1.98	0.46
1:A:62:TYR:CZ	1:A:131:MET:CE	2.98	0.46
2:B:49:SER:C	2:B:51:SER:H	2.23	0.46
1:A:118:ASP:OD2	1:A:122:ASN:ND2	2.49	0.46
1:A:45:VAL:CG1	1:A:46:SER:N	2.78	0.46
2:B:84:CYS:O	2:B:84:CYS:SG	2.74	0.45
1:A:88:GLN:CG	1:A:99:VAL:HG21	2.47	0.45
2:B:54:ILE:H	2:B:54:ILE:HG13	1.08	0.45
3:C:2:NAG:H62	3:C:3:BMA:C1	2.46	0.45
2:B:32:TYR:O	2:B:39:ARG:NH2	2.48	0.45
1:A:126:LYS:CG	1:A:128:TYR:HE2	2.09	0.45
1:A:115:LEU:HD13	1:A:125:LEU:CD1	2.47	0.45
2:B:68:ASP:N	2:B:87:GLU:OE2	2.50	0.45
1:A:92:HIS:O	1:A:96:PRO:N	2.51	0.44
2:B:38:ARG:C	2:B:39:ARG:HG2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:THR:CG2	2:B:56:LYS:H	2.31	0.44
2:B:33:GLY:HA2	2:B:39:ARG:HG3	1.99	0.44
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.34	0.44
1:A:109:LEU:HD23	1:A:133:VAL:HA	1.99	0.44
2:B:44:THR:CG2	2:B:44:THR:O	2.64	0.43
3:C:1:NAG:O3	3:C:1:NAG:C7	2.66	0.43
1:A:138:CYS:O	1:A:139:HIS:HD2	2.00	0.43
1:A:91:VAL:O	1:A:92:HIS:C	2.60	0.43
1:A:62:TYR:OH	1:A:131:MET:CE	2.66	0.42
2:B:88:GLY:O	2:B:89:ASN:C	2.61	0.42
1:A:72:ALA:HB1	1:A:73:PHE:CD2	2.55	0.42
1:A:86:ILE:HG21	1:A:86:ILE:HD13	1.78	0.42
1:A:95:ASN:OD1	1:A:97:GLU:CB	2.54	0.42
1:A:83:ASN:C	1:A:85:ALA:N	2.74	0.42
1:A:115:LEU:HD13	1:A:125:LEU:HD12	2.02	0.42
1:A:76:ASN:H	1:A:76:ASN:HD22	1.66	0.41
1:A:138:CYS:C	1:A:139:HIS:HD2	2.28	0.41
2:B:82:TYR:CD1	2:B:82:TYR:N	2.88	0.41
1:A:57:ILE:HB	1:A:115:LEU:HB3	2.02	0.41
1:A:88:GLN:O	1:A:88:GLN:HG2	2.21	0.41
1:A:131:MET:HE3	1:A:131:MET:HB3	1.24	0.41
2:B:88:GLY:O	2:B:91:CYS:HB3	2.20	0.41
2:B:41:CYS:HB2	2:B:91:CYS:SG	2.60	0.41
2:B:14:PHE:CD2	2:B:54:ILE:HD12	2.53	0.41
2:B:89:ASN:C	2:B:91:CYS:N	2.78	0.41
2:B:11:CYS:SG	2:B:59:CYS:HA	2.60	0.41
1:A:109:LEU:CD1	1:A:130:ASN:HB3	2.51	0.41
1:A:118:ASP:OD1	1:A:121:SER:N	2.54	0.41
2:B:47:ASN:O	2:B:48:ILE:C	2.62	0.41
1:A:83:ASN:O	1:A:84:HIS:C	2.63	0.41
1:A:138:CYS:C	1:A:139:HIS:CD2	2.99	0.41
2:B:82:TYR:HE2	2:B:97:TYR:CE1	2.38	0.41
2:B:90:MET:O	2:B:91:CYS:C	2.62	0.41
1:A:52:TRP:N	1:A:52:TRP:CD1	2.87	0.40
1:A:57:ILE:O	1:A:57:ILE:HG22	2.17	0.40
1:A:98:THR:HB	1:A:99:VAL:H	1.77	0.40
1:A:76:ASN:HD22	1:A:76:ASN:N	2.19	0.40
1:A:89:THR:O	1:A:92:HIS:HB3	2.21	0.40
1:A:111:ALA:HA	1:A:128:TYR:O	2.22	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)
2:B:93:GLU:OE2	2:B:93:GLU:OE2[4_765]	1.86	0.34
2:B:93:GLU:CD	2:B:93:GLU:OE2[4_765]	2.02	0.18

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	102/139 (73%)	85 (83%)	14 (14%)	3 (3%)	3	21
2	B	92/102 (90%)	78 (85%)	11 (12%)	3 (3%)	3	19
All	All	194/241 (80%)	163 (84%)	25 (13%)	6 (3%)	3	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	LYS
2	B	61	LEU
2	B	99	PRO
1	A	48	ARG
1	A	94	ILE
1	A	80	ASN

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	90/121 (74%)	72 (80%)	18 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	85/93 (91%)	70 (82%)	15 (18%)	2	9
All	All	175/214 (82%)	142 (81%)	33 (19%)	1	7

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	46	SER
1	A	54	ASP
1	A	55	TRP
1	A	59	PRO
1	A	73	PHE
1	A	74	PRO
1	A	76	ASN
1	A	90	LEU
1	A	98	THR
1	A	108	GLN
1	A	113	SER
1	A	114	VAL
1	A	115	LEU
1	A	120	SER
1	A	121	SER
1	A	124	ILE
1	A	126	LYS
2	B	12	LEU
2	B	40	HIS
2	B	46	LYS
2	B	49	SER
2	B	54	ILE
2	B	61	LEU
2	B	64	ILE
2	B	66	CYS
2	B	70	THR
2	B	72	CYS
2	B	73	ILE
2	B	74	GLU
2	B	82	TYR
2	B	87	GLU
2	B	97	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	130	ASN
1	A	139	HIS
2	B	57	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 ⓘ

6 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	C	1	1,3	14,14,15	1.13	1 (7%)	17,19,21	2.33	5 (29%)
3	NAG	C	2	3	14,14,15	0.72	0	17,19,21	1.79	4 (23%)
3	BMA	C	3	3	11,11,12	0.58	0	15,15,17	0.92	1 (6%)
3	MAN	C	4	3	11,11,12	0.56	0	15,15,17	0.96	0
3	BMA	C	5	3	11,11,12	0.75	0	15,15,17	1.40	2 (13%)
3	MAN	C	6	3	11,11,12	0.76	0	15,15,17	2.53	5 (33%)

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	C	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	BMA	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C1	-2.15	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	MAN	C1-O5-C5	6.61	121.05	112.19
3	C	1	NAG	C2-N2-C7	-6.47	114.23	122.90
3	C	6	MAN	C1-C2-C3	4.39	116.04	109.64
3	C	1	NAG	O4-C4-C3	-4.14	100.61	110.38
3	C	2	NAG	C2-N2-C7	-4.10	117.41	122.90
3	C	5	BMA	C3-C4-C5	3.84	117.19	110.23
3	C	6	MAN	O5-C1-C2	3.42	118.95	110.79
3	C	1	NAG	C1-C2-N2	3.26	115.58	110.43
3	C	2	NAG	C1-C2-N2	2.83	114.89	110.43
3	C	2	NAG	O4-C4-C5	2.62	115.79	109.32
3	C	1	NAG	C3-C4-C5	2.49	114.75	110.23
3	C	6	MAN	C3-C4-C5	2.39	114.56	110.23
3	C	2	NAG	O5-C5-C6	2.38	112.30	107.66
3	C	5	BMA	C1-O5-C5	-2.22	109.20	112.19
3	C	3	BMA	O4-C4-C5	2.12	114.54	109.32
3	C	6	MAN	C2-C3-C4	2.11	114.57	110.86
3	C	1	NAG	O5-C1-C2	-2.07	108.09	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6

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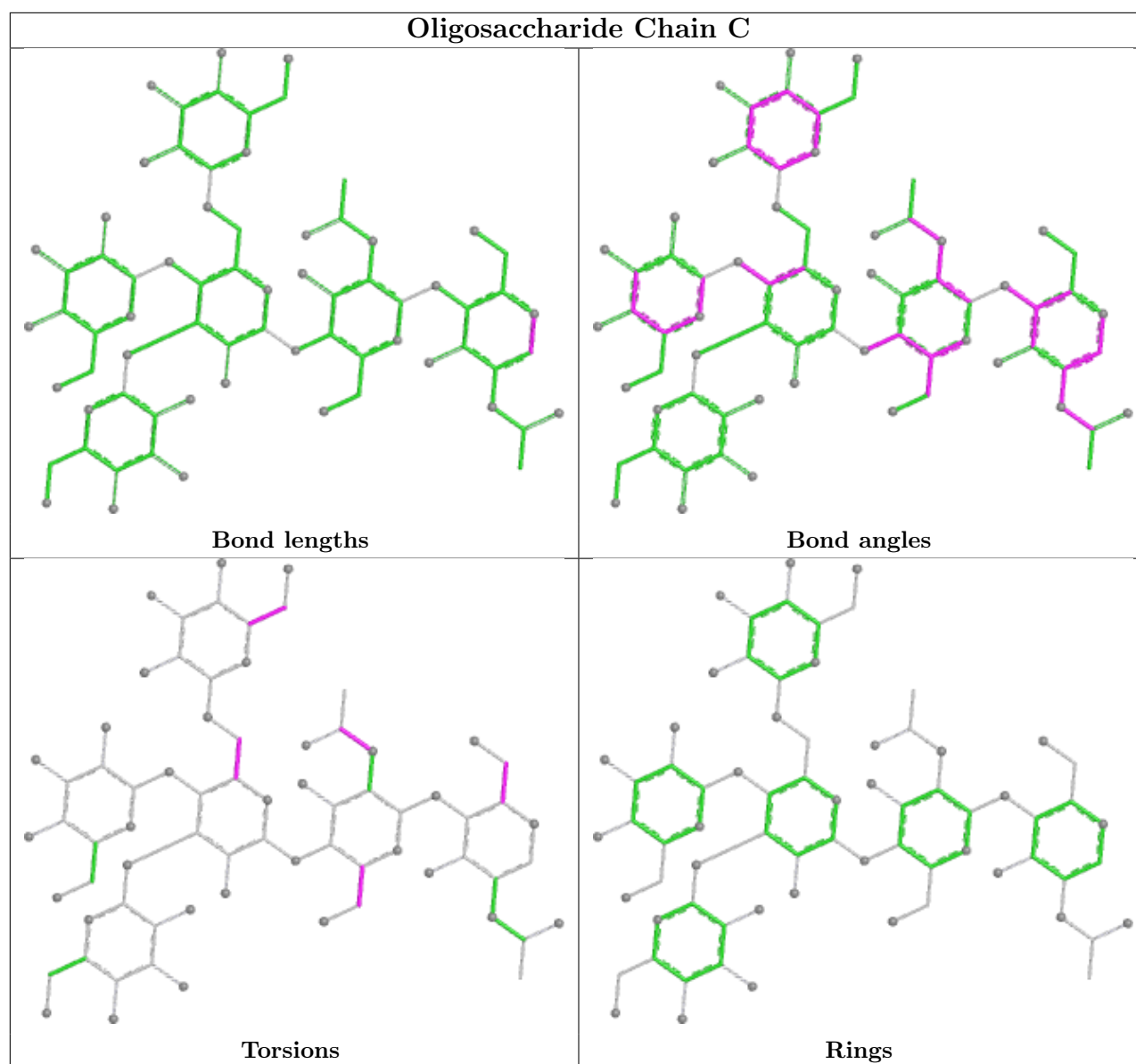
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	3	0
3	C	6	MAN	1	0
3	C	3	BMA	5	0
3	C	1	NAG	4	0
3	C	5	BMA	3	0

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



5.6 Ligand geometry [i](#)

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
4	NAG	B	147	2	14,14,15	1.10	2 (14%)	17,19,21	2.24	9 (52%)
4	NAG	B	124	2	14,14,15	1.50	2 (14%)	17,19,21	3.52	9 (52%)

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
4	NAG	B	147	2	-	3/6/23/26	0/1/1/1
4	NAG	B	124	2	1/1/5/7	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	124	NAG	C2-N2	4.02	1.52	1.46
4	B	124	NAG	C1-C2	3.08	1.56	1.52
4	B	147	NAG	O5-C1	-2.21	1.40	1.43
4	B	147	NAG	C2-N2	-2.04	1.42	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	124	NAG	C2-N2-C7	9.04	135.02	122.90
4	B	124	NAG	O7-C7-C8	-5.71	111.88	122.05
4	B	124	NAG	O5-C1-C2	4.81	118.73	111.29
4	B	124	NAG	C1-O5-C5	-4.01	106.81	112.19
4	B	124	NAG	O7-C7-N2	3.99	129.03	121.98
4	B	147	NAG	C1-C2-N2	-3.92	104.26	110.43
4	B	147	NAG	C3-C4-C5	-3.90	103.15	110.23
4	B	147	NAG	C2-N2-C7	-3.78	117.83	122.90
4	B	124	NAG	C1-C2-N2	3.67	116.21	110.43
4	B	124	NAG	O5-C5-C6	2.94	113.39	107.66
4	B	147	NAG	O4-C4-C5	2.85	116.34	109.32
4	B	147	NAG	C4-C3-C2	-2.71	107.05	111.02
4	B	147	NAG	C1-O5-C5	-2.57	108.73	112.19
4	B	147	NAG	O5-C1-C2	-2.30	107.73	111.29
4	B	124	NAG	C4-C3-C2	-2.17	107.83	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	147	NAG	C6-C5-C4	2.09	118.14	113.02
4	B	147	NAG	O5-C5-C4	-2.07	105.79	110.83
4	B	124	NAG	O3-C3-C2	2.06	113.67	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	124	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	147	NAG	C8-C7-N2-C2
4	B	147	NAG	O7-C7-N2-C2
4	B	124	NAG	C4-C5-C6-O6
4	B	124	NAG	O5-C5-C6-O6
4	B	147	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	147	NAG	7	0
4	B	124	NAG	2	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	104/139 (74%)	0.73	10 (9%) 13 11	25, 63, 79, 88	6 (5%)
2	B	94/102 (92%)	0.83	11 (11%) 9 8	30, 70, 92, 153	6 (6%)
All	All	198/241 (82%)	0.78	21 (10%) 11 9	25, 67, 87, 153	12 (6%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	GLY	5.5
2	B	8	THR	4.4
1	A	79	MET	3.8
1	A	117	PHE	3.3
2	B	31	CYS	3.3
1	A	77	SER	3.1
1	A	78	TYR	3.1
1	A	110	ASN	2.8
2	B	68	ASP	2.6
2	B	34	ASP	2.4
1	A	73	PHE	2.4
2	B	84	CYS	2.3
2	B	7	GLU	2.2
2	B	57	GLN	2.2
2	B	59	CYS	2.2
2	B	73	ILE	2.2
1	A	103	CYS	2.2
2	B	35	LYS	2.1
1	A	99	VAL	2.1
1	A	56	ILE	2.1
1	A	104	CYS	2.0

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

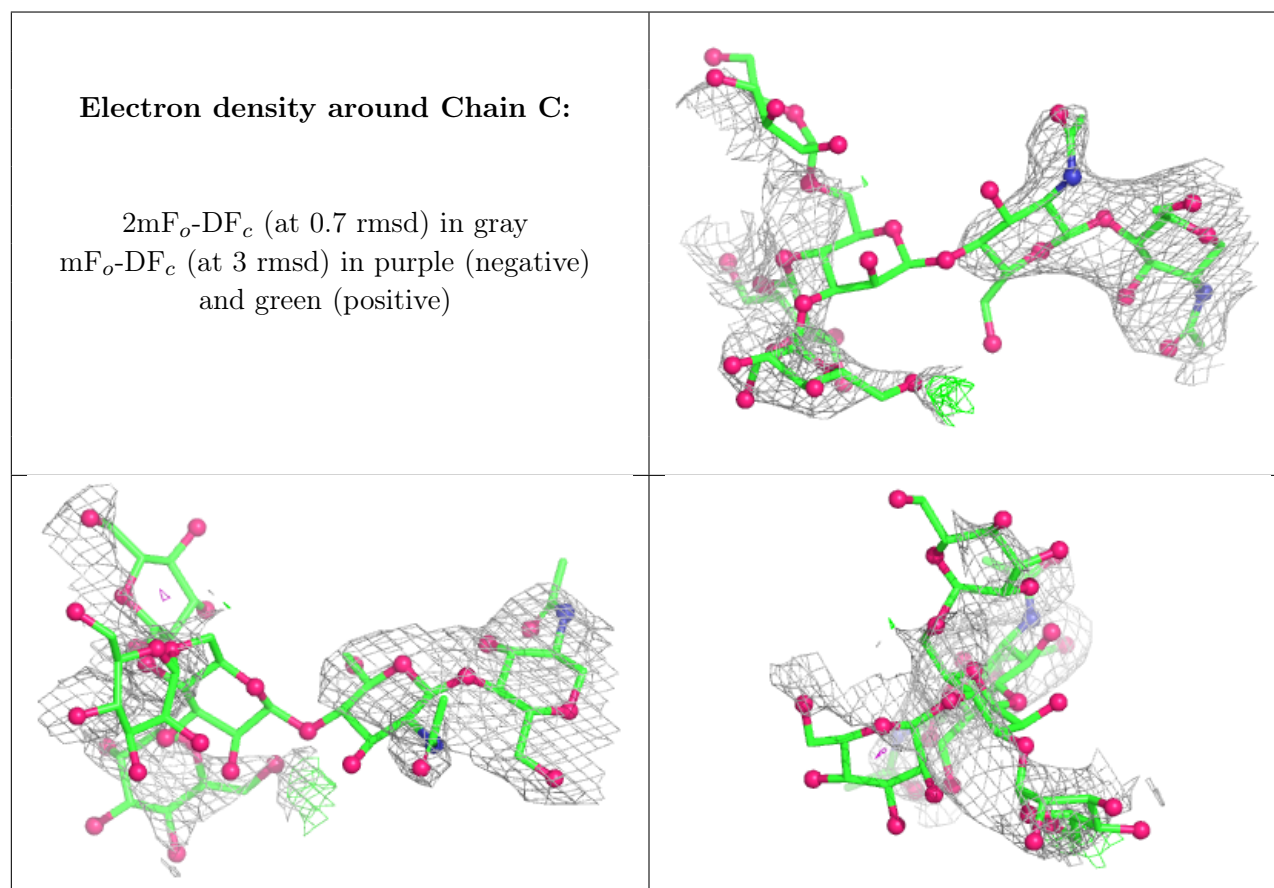
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	MAN	C	4	11/12	0.15	0.20	142,144,145,146	0
3	BMA	C	3	11/12	0.26	0.16	134,136,141,142	0
3	BMA	C	5	11/12	0.26	0.17	142,143,144,145	0
3	NAG	C	2	14/15	0.55	0.17	114,121,131,132	0
3	MAN	C	6	11/12	0.65	0.13	130,131,132,132	0
3	NAG	C	1	14/15	0.95	0.09	71,82,90,102	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](#)

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
4	NAG	B	124	14/15	0.80	0.13	72,75,80,80	0
4	NAG	B	147	14/15	0.87	0.10	64,68,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.