



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:23 AM UTC

PDB ID : 3BT2 / pdb_00003bt2
Title : Structure of urokinase receptor, urokinase and vitronectin complex
Authors : Huang, M.
Deposited on : 2007-12-27
Resolution : 2.50 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

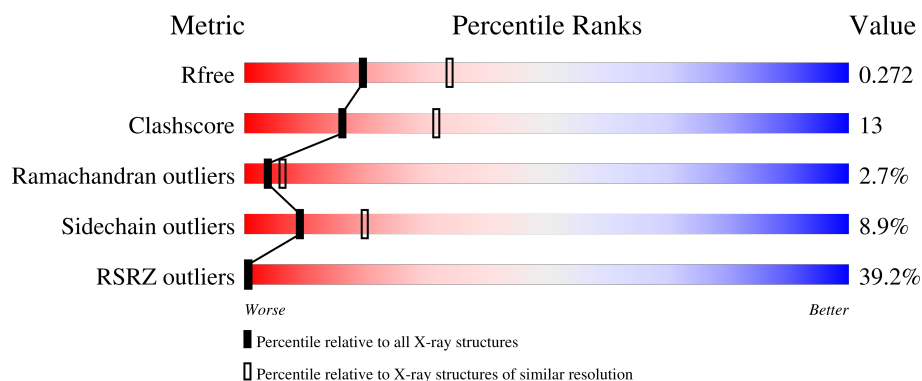
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	135	70% 62% 27% 8%
2	B	40	100% 68% 30%
3	L	212	19% 76% 19%
4	H	214	28% 85% 12%
5	U	283	34% 62% 22% 6% 8%

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Mol	Chain	Length	Quality of chain
6	C	2	 100%
6	D	2	 100%

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
6	NAG	D	1	-	-	X	-
6	NAG	D	2	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6654 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 Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			980	603	186	177	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP P00749
A	0	SER	-	expression tag	UNP P00749

- Molecule 2 is a protein called Vitronectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	S	0	0	0
			312	185	51	68	8			

- Molecule 3 is a protein called anti-uPAR antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1628	1020	268	333	7			

- Molecule 4 is a protein called anti-uPAR antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	212	Total	C	N	O	S	0	0	0
			1617	1035	262	314	6			

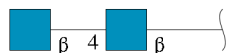
- Molecule 5 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	U	259	Total	C	N	O	S	0	0	0
			1990	1192	366	398	34			

There are 2 discrepancies between the modelled and reference sequences:

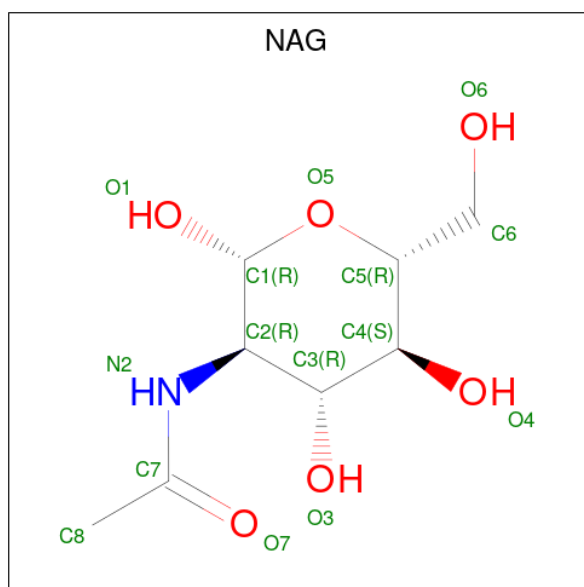
Chain	Residue	Modelled	Actual	Comment	Reference
U	0	ARG	-	expression tag	UNP Q03405
U	1A	SER	-	expression tag	UNP Q03405

- Molecule 6 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
6	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	U	1	Total	C	N	O	0	0
			14	8	1	5		

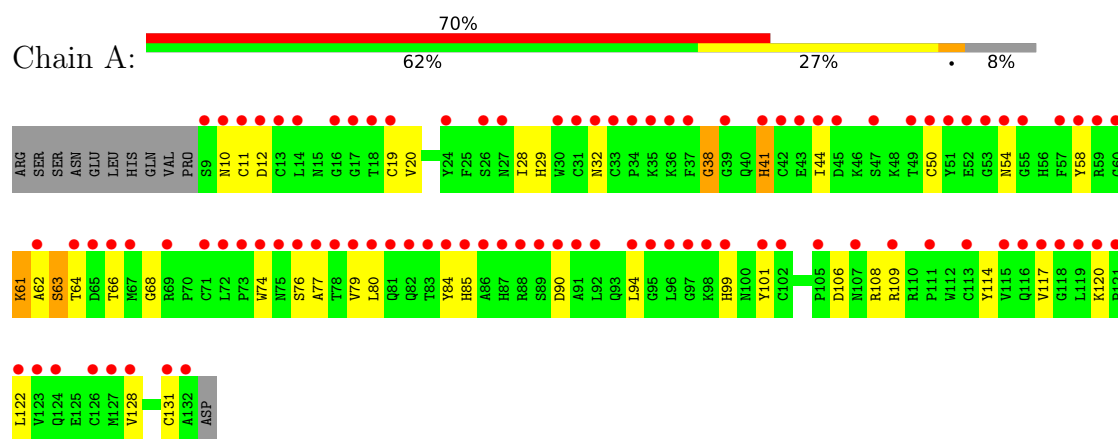
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total 4	O 4	0	0
8	L	20	Total 20	O 20	0	0
8	H	26	Total 26	O 26	0	0
8	U	7	Total 7	O 7	0	0

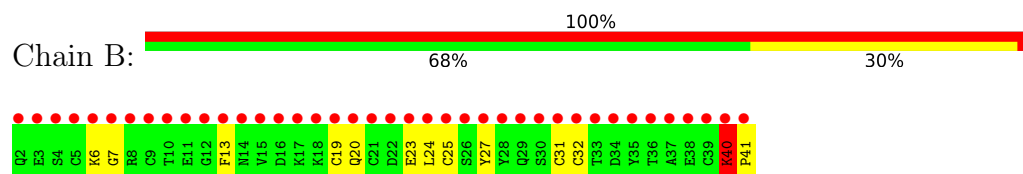
3 Residue-property plots [i](#)

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.

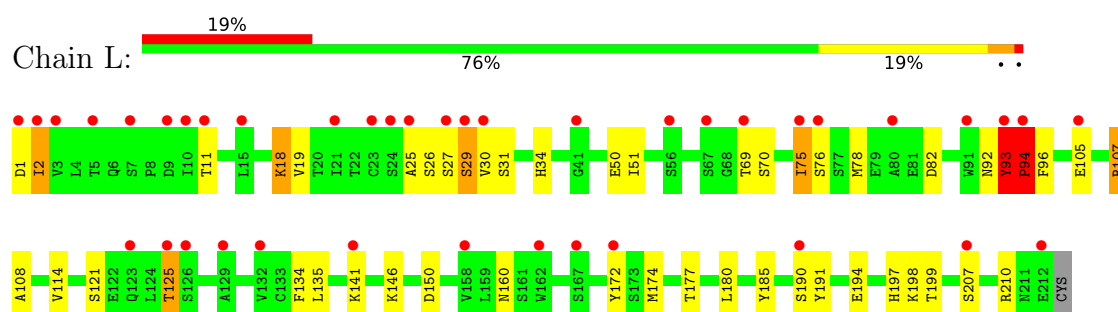
- Molecule 1: Urokinase-type plasminogen activator



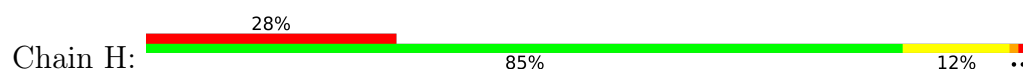
- Molecule 2: Vitronectin

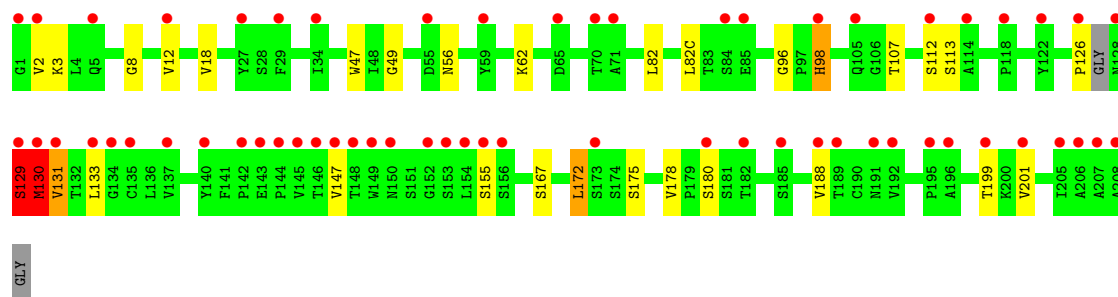


- Molecule 3: anti-uPAR antibody, light chain

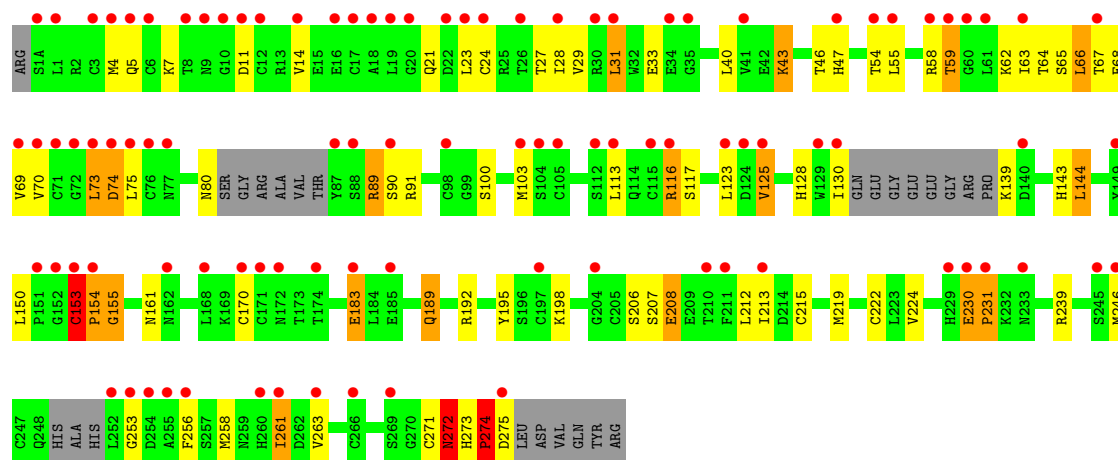


- Molecule 4: anti-uPAR antibody, heavy chain





- Molecule 5: Urokinase plasminogen activator surface receptor



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.10Å 87.20Å 124.27Å 90.00° 94.31° 90.00°	Depositor
Resolution (Å)	42.88 – 2.50 42.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.88-2.50) 99.2 (42.88-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.229 , 0.272 0.232 , 0.272	Depositor DCC
R_{free} test set	1191 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	1.01	5/1007 (0.5%)	0.98	3/1361 (0.2%)
2	B	0.53	0/316	0.87	1/421 (0.2%)
3	L	1.17	3/1668 (0.2%)	1.16	7/2267 (0.3%)
4	H	1.14	0/1667	1.02	4/2282 (0.2%)
5	U	1.07	8/2019 (0.4%)	0.99	6/2715 (0.2%)
All	All	1.09	16/6677 (0.2%)	1.04	21/9046 (0.2%)

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
4	H	0	1
5	U	0	1
All	All	1	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	7	LYS	C-O	14.15	1.42	1.23
1	A	41	HIS	CE1-NE2	11.73	1.44	1.32
5	U	7	LYS	C-N	9.77	1.47	1.33
1	A	38	GLY	C-O	9.63	1.36	1.23
5	U	183	GLU	CB-CG	8.68	1.78	1.52
5	U	43	LYS	C-O	8.23	1.33	1.23
1	A	41	HIS	CG-CD2	6.67	1.43	1.35
1	A	41	HIS	CG-ND1	6.45	1.45	1.38
5	U	183	GLU	CA-C	6.19	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	274	PRO	C-O	-6.09	1.16	1.24
5	U	11	ASP	C-O	5.78	1.31	1.24
3	L	27	SER	CA-C	5.52	1.59	1.52
3	L	114	VAL	C-O	-5.44	1.18	1.24
5	U	43	LYS	C-N	5.25	1.39	1.33
1	A	38	GLY	C-N	5.11	1.40	1.33
3	L	94	PRO	CA-C	5.04	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	93	TYR	CA-C-N	-9.14	108.41	119.84
3	L	93	TYR	C-N-CA	-9.14	108.41	119.84
1	A	38	GLY	O-C-N	8.50	131.16	123.42
2	B	40	LYS	N-CA-C	8.37	128.30	109.81
5	U	272	ASN	N-CA-C	6.45	124.54	110.80
4	H	129	SER	N-CA-C	6.29	124.19	110.80
3	L	27	SER	CA-C-N	6.21	130.18	121.24
3	L	27	SER	C-N-CA	6.21	130.18	121.24
3	L	29	SER	N-CA-C	6.03	118.45	109.59
5	U	153	CYS	CA-C-N	-6.00	112.34	119.84
5	U	153	CYS	C-N-CA	-6.00	112.34	119.84
5	U	7	LYS	CA-C-O	5.96	128.85	121.81
4	H	96	GLY	CA-C-N	5.95	126.10	119.32
4	H	96	GLY	C-N-CA	5.95	126.10	119.32
4	H	147	VAL	N-CA-C	5.37	115.59	107.80
1	A	120	LYS	CA-C-N	5.24	125.00	119.76
1	A	120	LYS	C-N-CA	5.24	125.00	119.76
3	L	92	ASN	N-CA-C	5.17	118.12	110.46
5	U	73	LEU	N-CA-C	5.10	119.58	112.90
3	L	31	SER	N-CA-C	5.09	117.57	111.71
5	U	155	GLY	N-CA-C	5.08	116.69	111.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	40	LYS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	LYS	Peptide

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Mol	Chain	Res	Type	Group
4	H	130	MET	Peptide
5	U	271	CYS	Peptide

5.2 Too-close contacts [i](#)

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	980	0	911	29	0
2	B	312	0	272	6	0
3	L	1628	0	1554	33	0
4	H	1617	0	1558	20	0
5	U	1990	0	1856	77	0
6	C	28	0	25	0	0
6	D	28	0	25	12	0
7	U	14	0	13	0	0
8	A	4	0	0	0	0
8	H	26	0	0	0	0
8	L	20	0	0	1	0
8	U	7	0	0	0	0
All	All	6654	0	6214	168	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 13.

All (168) 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)
5:U:183:GLU:CB	5:U:183:GLU:CG	1.78	1.57
6:D:1:NAG:C3	6:D:2:NAG:H82	1.85	1.07
5:U:4:MET:HE3	5:U:75:LEU:HD22	1.38	1.05
5:U:128:HIS:NE2	5:U:183:GLU:OE2	1.92	1.02
5:U:116:ARG:CZ	5:U:116:ARG:HB2	1.86	1.02
4:H:131:VAL:CG1	4:H:178:VAL:O	2.12	0.98
5:U:143:HIS:NE2	5:U:183:GLU:OE2	1.96	0.98
3:L:93:TYR:O	3:L:96:PHE:CD2	2.19	0.96
3:L:105:GLU:OE1	3:L:172:TYR:OH	1.83	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:128:HIS:HE2	5:U:183:GLU:CD	1.73	0.95
6:D:1:NAG:H3	6:D:2:NAG:H82	1.42	0.94
5:U:273:HIS:O	5:U:275:ASP:N	1.99	0.94
3:L:93:TYR:O	3:L:96:PHE:N	2.01	0.93
6:D:1:NAG:H3	6:D:2:NAG:C8	2.00	0.92
1:A:12:ASP:OD2	1:A:41:HIS:NE2	2.03	0.91
5:U:23:LEU:HD13	5:U:70:VAL:HG11	1.51	0.91
5:U:4:MET:HE1	5:U:14:VAL:HG22	1.50	0.90
5:U:4:MET:CE	5:U:75:LEU:HD22	2.04	0.88
3:L:93:TYR:O	3:L:94:PRO:C	2.17	0.83
3:L:93:TYR:HA	3:L:96:PHE:CZ	2.15	0.81
6:D:1:NAG:O3	6:D:2:NAG:C7	2.28	0.81
4:H:130:MET:SD	4:H:130:MET:O	2.40	0.79
3:L:25:ALA:O	3:L:69:THR:OG1	2.00	0.79
5:U:128:HIS:NE2	5:U:183:GLU:CD	2.38	0.79
5:U:59:THR:O	5:U:59:THR:CG2	2.31	0.79
1:A:58:TYR:OH	1:A:61:LYS:O	2.01	0.79
4:H:131:VAL:HG13	4:H:178:VAL:O	1.84	0.77
5:U:273:HIS:C	5:U:275:ASP:H	1.93	0.77
3:L:50:GLU:OE2	4:H:98:HIS:ND1	2.19	0.76
4:H:130:MET:O	4:H:131:VAL:HG12	1.86	0.75
1:A:12:ASP:OD2	1:A:29:HIS:NE2	2.13	0.73
3:L:75:ILE:HD11	3:L:78:MET:HA	1.70	0.73
1:A:117:VAL:O	1:A:117:VAL:HG23	1.87	0.73
5:U:23:LEU:HD22	5:U:70:VAL:CG1	2.18	0.73
1:A:12:ASP:CG	1:A:41:HIS:HE2	1.96	0.73
6:D:1:NAG:C3	6:D:2:NAG:C8	2.62	0.73
1:A:12:ASP:CG	1:A:29:HIS:HE2	1.95	0.72
5:U:23:LEU:HD22	5:U:70:VAL:HG12	1.71	0.72
4:H:130:MET:C	4:H:131:VAL:HG12	2.15	0.72
6:D:1:NAG:H3	6:D:2:NAG:N2	2.04	0.72
5:U:153:CYS:O	5:U:155:GLY:N	2.21	0.72
3:L:105:GLU:CD	3:L:172:TYR:OH	2.33	0.72
5:U:73:LEU:O	5:U:74:ASP:HB2	1.89	0.71
1:A:12:ASP:CG	1:A:41:HIS:NE2	2.49	0.71
6:D:1:NAG:O3	6:D:2:NAG:H82	1.91	0.70
5:U:128:HIS:NE2	5:U:183:GLU:OE1	2.25	0.70
5:U:189:GLN:HE21	5:U:189:GLN:H	1.40	0.69
5:U:153:CYS:O	5:U:154:PRO:C	2.35	0.68
6:D:1:NAG:O3	6:D:2:NAG:C8	2.42	0.68
1:A:80:LEU:HD23	1:A:85:HIS:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:93:TYR:O	3:L:96:PHE:CG	2.49	0.66
5:U:4:MET:HE2	5:U:4:MET:HA	1.79	0.65
5:U:222:CYS:HB3	5:U:272:ASN:HB2	1.78	0.64
6:D:1:NAG:H3	6:D:2:NAG:C7	2.26	0.64
4:H:131:VAL:HG13	4:H:131:VAL:O	1.97	0.64
5:U:59:THR:HG22	5:U:62:LYS:HB3	1.79	0.64
5:U:230:GLU:HB3	5:U:231:PRO:HD2	1.79	0.63
5:U:59:THR:O	5:U:59:THR:HG23	1.99	0.62
6:D:1:NAG:C3	6:D:2:NAG:N2	2.63	0.62
5:U:256:PHE:CB	5:U:258:MET:HE2	2.31	0.61
1:A:74:TRP:HA	1:A:79:VAL:HG11	1.83	0.60
1:A:61:LYS:HG2	1:A:62:ALA:N	2.16	0.60
4:H:56:ASN:OD1	5:U:192:ARG:NH2	2.31	0.60
6:D:1:NAG:C3	6:D:2:NAG:C7	2.79	0.60
5:U:4:MET:HE2	5:U:4:MET:CA	2.32	0.59
5:U:23:LEU:HD13	5:U:70:VAL:CG1	2.30	0.59
3:L:75:ILE:CD1	3:L:82:ASP:OD2	2.51	0.58
3:L:107:ARG:HG2	3:L:108:ALA:N	2.18	0.58
3:L:18:LYS:HD3	3:L:76:SER:HA	1.84	0.58
5:U:116:ARG:HB2	5:U:116:ARG:NH1	2.19	0.58
5:U:116:ARG:CZ	5:U:116:ARG:CB	2.72	0.58
5:U:73:LEU:O	5:U:74:ASP:CB	2.52	0.57
1:A:54:ASN:ND2	1:A:108:ARG:O	2.38	0.57
5:U:4:MET:HE2	5:U:4:MET:N	2.19	0.57
1:A:28:ILE:HD13	5:U:29:VAL:HG23	1.86	0.57
5:U:153:CYS:O	5:U:170:CYS:HB3	2.04	0.57
2:B:24:LEU:HD11	5:U:58:ARG:HH21	1.70	0.56
3:L:93:TYR:O	3:L:96:PHE:CE2	2.59	0.56
5:U:59:THR:O	5:U:59:THR:HG22	2.05	0.56
5:U:103:MET:HE2	5:U:103:MET:HA	1.88	0.56
1:A:61:LYS:CG	1:A:62:ALA:N	2.69	0.55
5:U:273:HIS:C	5:U:275:ASP:N	2.59	0.55
2:B:27:TYR:CZ	5:U:63:ILE:HG21	2.42	0.55
1:A:61:LYS:HG2	1:A:62:ALA:H	1.73	0.54
5:U:89:ARG:HD2	5:U:90:SER:H	1.72	0.54
2:B:24:LEU:HD11	5:U:58:ARG:NH2	2.23	0.53
4:H:126:PRO:HD3	4:H:133:LEU:HD23	1.90	0.53
4:H:131:VAL:HG12	4:H:178:VAL:O	2.05	0.53
3:L:177:THR:HG22	8:L:230:HOH:O	2.08	0.53
5:U:143:HIS:HE2	5:U:183:GLU:CD	2.09	0.52
5:U:195:TYR:O	5:U:272:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:ASP:HA	3:L:190:SER:HB3	1.91	0.52
4:H:82:LEU:HB3	4:H:82(C):LEU:HD21	1.92	0.51
1:A:90:ASP:OD2	1:A:94:LEU:HD22	2.10	0.51
5:U:161:ASN:HA	5:U:213:ILE:CD1	2.40	0.51
1:A:117:VAL:O	1:A:117:VAL:CG2	2.57	0.51
5:U:256:PHE:HB2	5:U:258:MET:HE2	1.92	0.51
5:U:55:LEU:HD13	5:U:123:LEU:HD13	1.93	0.51
1:A:12:ASP:CG	1:A:41:HIS:CD2	2.89	0.51
2:B:13:PHE:CE1	5:U:91:ARG:HD2	2.45	0.51
3:L:107:ARG:HG2	3:L:108:ALA:H	1.76	0.51
1:A:79:VAL:HG22	1:A:114:TYR:CD2	2.46	0.50
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.46	0.50
1:A:12:ASP:N	1:A:12:ASP:OD1	2.41	0.50
4:H:172:LEU:C	4:H:172:LEU:HD23	2.37	0.50
5:U:29:VAL:HG12	5:U:31:LEU:HD13	1.94	0.50
1:A:28:ILE:HD13	5:U:29:VAL:CG2	2.42	0.49
3:L:135:LEU:N	3:L:135:LEU:HD12	2.27	0.49
3:L:93:TYR:C	3:L:96:PHE:N	2.70	0.49
4:H:18:VAL:HG12	4:H:82(C):LEU:HD11	1.94	0.49
5:U:31:LEU:CD1	5:U:64:THR:HG23	2.43	0.49
3:L:134:PHE:CE2	4:H:175:SER:HB3	2.48	0.49
5:U:128:HIS:CD2	5:U:183:GLU:OE1	2.66	0.49
5:U:5:GLN:HA	5:U:43:LYS:O	2.13	0.48
5:U:23:LEU:HB3	5:U:70:VAL:HG13	1.95	0.48
1:A:61:LYS:O	1:A:62:ALA:HB3	2.14	0.48
3:L:93:TYR:HA	3:L:96:PHE:CE2	2.48	0.48
3:L:93:TYR:CG	3:L:94:PRO:N	2.81	0.48
1:A:12:ASP:CG	1:A:29:HIS:NE2	2.69	0.47
1:A:61:LYS:HD2	1:A:63:SER:OG	2.14	0.47
2:B:25:CYS:C	2:B:31:CYS:SG	2.97	0.47
1:A:38:GLY:O	1:A:44:ILE:HB	2.15	0.47
5:U:4:MET:CE	5:U:4:MET:HA	2.39	0.47
6:D:1:NAG:C2	6:D:2:NAG:H82	2.45	0.47
5:U:66:LEU:N	5:U:66:LEU:CD2	2.78	0.47
5:U:55:LEU:HD12	5:U:123:LEU:HD12	1.97	0.46
3:L:185:TYR:CZ	3:L:210:ARG:HG3	2.50	0.46
4:H:133:LEU:CD1	4:H:188:VAL:HG11	2.46	0.46
5:U:206:SER:OG	5:U:208:GLU:OE1	2.33	0.46
5:U:274:PRO:O	5:U:275:ASP:O	2.34	0.46
3:L:197:HIS:HD2	3:L:199:THR:OG1	1.99	0.45
3:L:141:LYS:HD2	3:L:172:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:8:GLY:O	4:H:107:THR:HG23	2.16	0.45
5:U:150:LEU:O	5:U:153:CYS:HB2	2.16	0.45
5:U:274:PRO:C	5:U:275:ASP:O	2.57	0.45
1:A:99:HIS:HD2	1:A:101:TYR:H	1.65	0.45
4:H:130:MET:O	4:H:131:VAL:CG1	2.62	0.44
5:U:261:ILE:HG23	5:U:261:ILE:O	2.18	0.44
5:U:54:THR:HG23	5:U:66:LEU:O	2.18	0.44
5:U:222:CYS:HB3	5:U:272:ASN:CB	2.47	0.44
4:H:130:MET:HA	4:H:180:SER:HB3	2.00	0.44
3:L:19:VAL:HB	3:L:75:ILE:HG23	2.00	0.44
1:A:61:LYS:CD	1:A:63:SER:OG	2.65	0.44
2:B:40:LYS:O	2:B:41:PRO:C	2.61	0.44
5:U:125:VAL:HG13	5:U:144:LEU:HB2	2.00	0.43
5:U:31:LEU:HD12	5:U:64:THR:HG23	2.01	0.43
5:U:215:CYS:HB3	5:U:219:MET:O	2.18	0.43
1:A:61:LYS:O	1:A:62:ALA:CB	2.66	0.43
5:U:55:LEU:HD21	5:U:144:LEU:HD23	2.00	0.43
5:U:116:ARG:NH1	5:U:116:ARG:CB	2.82	0.43
5:U:224:VAL:HG22	5:U:239:ARG:HG2	2.00	0.43
5:U:230:GLU:O	5:U:231:PRO:C	2.62	0.43
5:U:263:VAL:HG23	5:U:263:VAL:O	2.19	0.43
3:L:146:LYS:HB3	3:L:194:GLU:HB2	2.02	0.42
5:U:24:CYS:O	5:U:70:VAL:HA	2.20	0.42
3:L:75:ILE:CD1	3:L:78:MET:HA	2.44	0.42
5:U:27:THR:OG1	5:U:68:GLU:OE1	2.36	0.42
5:U:89:ARG:NH1	5:U:116:ARG:O	2.52	0.42
3:L:191:TYR:O	3:L:207:SER:HA	2.19	0.42
5:U:256:PHE:HB2	5:U:258:MET:CE	2.50	0.41
3:L:160:ASN:HB3	3:L:174:MET:HE3	2.03	0.41
1:A:76:SER:O	1:A:77:ALA:C	2.61	0.41
3:L:34:HIS:HD2	3:L:50:GLU:H	1.67	0.41
4:H:133:LEU:HD12	4:H:188:VAL:HG11	2.03	0.41
3:L:121:SER:O	3:L:125:THR:HG23	2.20	0.41
5:U:23:LEU:HD12	5:U:47:HIS:O	2.20	0.40
3:L:1:ASP:O	3:L:2:ILE:C	2.65	0.40
1:A:84:TYR:OH	1:A:106:ASP:HB3	2.21	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	122/135 (90%)	104 (85%)	15 (12%)	3 (2%)	4	7
2	B	38/40 (95%)	28 (74%)	6 (16%)	4 (10%)	0	0
3	L	209/212 (99%)	195 (93%)	9 (4%)	5 (2%)	4	8
4	H	208/214 (97%)	200 (96%)	5 (2%)	3 (1%)	9	17
5	U	251/283 (89%)	229 (91%)	15 (6%)	7 (3%)	4	6
All	All	828/884 (94%)	756 (91%)	50 (6%)	22 (3%)	4	6

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	40	LYS
3	L	2	ILE
3	L	93	TYR
4	H	129	SER
5	U	74	ASP
5	U	272	ASN
5	U	274	PRO
1	A	68	GLY
2	B	6	LYS
2	B	7	GLY
2	B	19	CYS
3	L	26	SER
3	L	94	PRO
4	H	130	MET
5	U	231	PRO
5	U	253	GLY
4	H	131	VAL
1	A	128	VAL
3	L	51	ILE
5	U	154	PRO

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Mol	Chain	Res	Type
5	U	230	GLU

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	108/119 (91%)	97 (90%)	11 (10%)	7	15
2	B	37/37 (100%)	34 (92%)	3 (8%)	11	23
3	L	185/186 (100%)	175 (95%)	10 (5%)	20	41
4	H	182/182 (100%)	169 (93%)	13 (7%)	13	29
5	U	232/251 (92%)	203 (88%)	29 (12%)	4	9
All	All	744/775 (96%)	678 (91%)	66 (9%)	9	20

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	CYS
1	A	19	CYS
1	A	20	VAL
1	A	32	ASN
1	A	50	CYS
1	A	63	SER
1	A	64	THR
1	A	66	THR
1	A	109	ARG
1	A	122	LEU
1	A	131	CYS
2	B	20	GLN
2	B	23	GLU
2	B	32	CYS
3	L	11	THR
3	L	18	LYS
3	L	29	SER
3	L	30	VAL

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Mol	Chain	Res	Type
3	L	70	SER
3	L	75	ILE
3	L	107	ARG
3	L	125	THR
3	L	180	LEU
3	L	198	LYS
4	H	2	VAL
4	H	3	LYS
4	H	12	VAL
4	H	62	LYS
4	H	98	HIS
4	H	112	SER
4	H	113	SER
4	H	129	SER
4	H	155	SER
4	H	167	SER
4	H	172	LEU
4	H	199	THR
4	H	201	VAL
5	U	21	GLN
5	U	28	ILE
5	U	31	LEU
5	U	33	GLU
5	U	40	LEU
5	U	46	THR
5	U	59	THR
5	U	65	SER
5	U	66	LEU
5	U	67	THR
5	U	69	VAL
5	U	80	ASN
5	U	89	ARG
5	U	100	SER
5	U	113	LEU
5	U	116	ARG
5	U	117	SER
5	U	125	VAL
5	U	130	ILE
5	U	139	LYS
5	U	144	LEU
5	U	153	CYS
5	U	189	GLN

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Mol	Chain	Res	Type
5	U	198	LYS
5	U	207	SER
5	U	208	GLU
5	U	212	LEU
5	U	246	MET
5	U	261	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	54	ASN
2	B	20	GLN
3	L	34	HIS
3	L	90	GLN
3	L	137	ASN
3	L	197	HIS
4	H	52(A)	HIS
4	H	81	GLN
4	H	159	HIS
5	U	47	HIS
5	U	114	GLN
5	U	166	HIS
5	U	189	GLN
5	U	193	GLN
5	U	229	HIS
5	U	272	ASN

5.3.3 RNA [i](#)

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](#)

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	$\# Z > 2$
6	NAG	C	1	5,6	14,14,15	0.65	0	17,19,21	0.94	1 (5%)
6	NAG	C	2	6	14,14,15	0.45	0	17,19,21	1.71	4 (23%)
6	NAG	D	1	5,6	14,14,15	0.58	0	17,19,21	3.02	7 (41%)
6	NAG	D	2	6	14,14,15	0.57	0	17,19,21	3.02	7 (41%)

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
6	NAG	C	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	4/6/23/26	0/1/1/1
6	NAG	D	1	5,6	-	4/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1	NAG	C1-O5-C5	6.62	121.05	112.19
6	D	2	NAG	C1-O5-C5	6.61	121.05	112.19
6	D	1	NAG	C4-C3-C2	-6.59	101.36	111.02
6	D	2	NAG	C4-C3-C2	-6.58	101.38	111.02
6	D	2	NAG	O4-C4-C5	4.61	120.69	109.32
6	D	1	NAG	O4-C4-C5	4.60	120.65	109.32
6	C	2	NAG	C4-C3-C2	-3.92	105.27	111.02
6	C	2	NAG	C1-O5-C5	3.33	116.65	112.19
6	D	1	NAG	C3-C4-C5	-3.26	104.31	110.23
6	D	2	NAG	C3-C4-C5	-3.26	104.33	110.23
6	D	2	NAG	O5-C5-C6	2.96	113.43	107.66
6	D	1	NAG	O5-C5-C6	2.96	113.42	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1	NAG	O4-C4-C3	2.92	117.26	110.38
6	D	2	NAG	O4-C4-C3	2.90	117.22	110.38
6	D	2	NAG	O3-C3-C4	2.61	116.53	110.38
6	D	1	NAG	O3-C3-C4	2.61	116.52	110.38
6	C	2	NAG	C8-C7-N2	2.48	120.23	116.12
6	C	2	NAG	O7-C7-C8	-2.27	118.01	122.05
6	C	1	NAG	O3-C3-C4	2.15	115.45	110.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

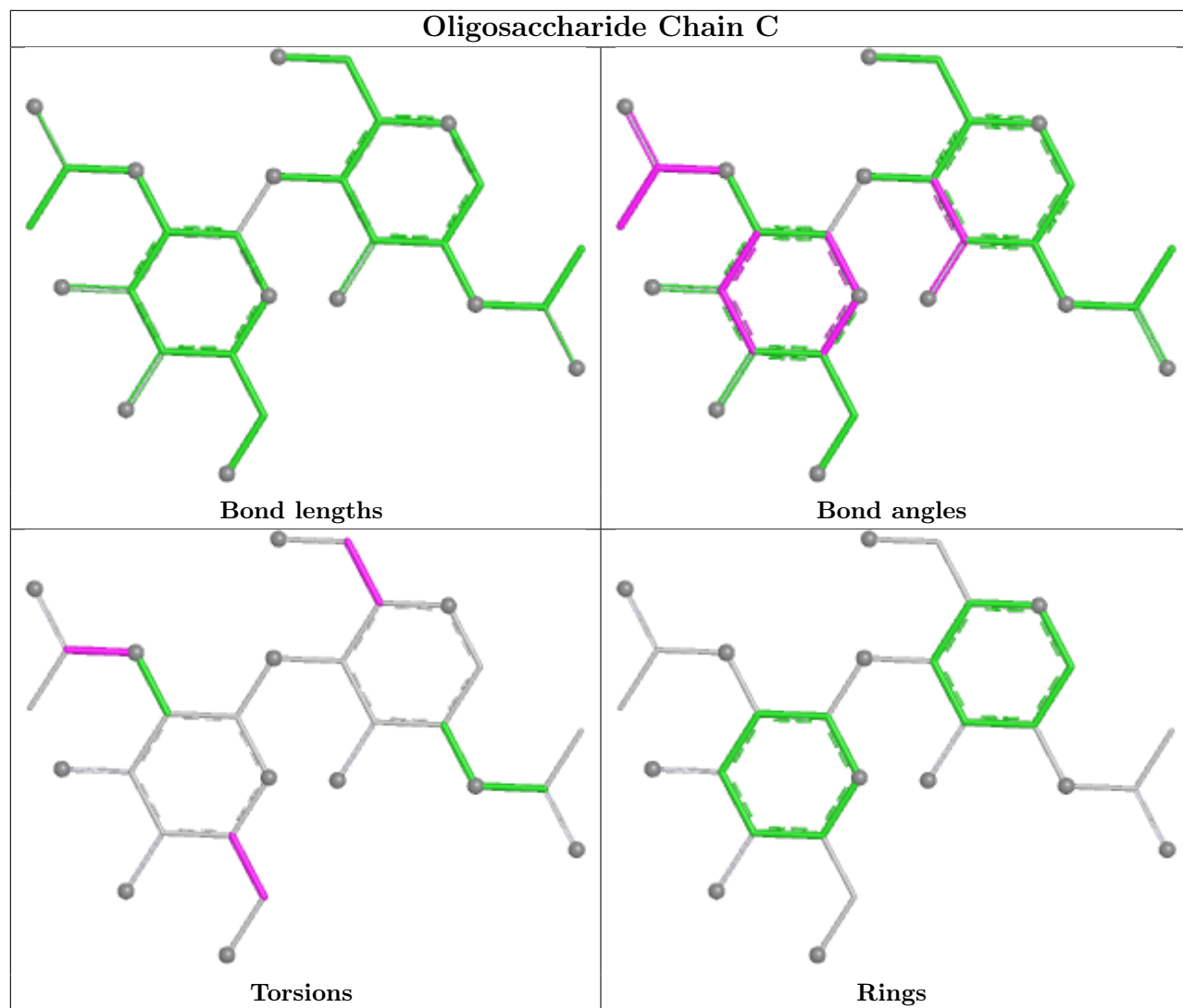
Mol	Chain	Res	Type	Atoms
6	C	1	NAG	C4-C5-C6-O6
6	C	1	NAG	O5-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
6	C	2	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
6	C	2	NAG	C8-C7-N2-C2
6	C	2	NAG	O7-C7-N2-C2
6	D	1	NAG	C8-C7-N2-C2
6	D	2	NAG	C8-C7-N2-C2
6	D	1	NAG	O7-C7-N2-C2
6	D	2	NAG	O7-C7-N2-C2
6	C	2	NAG	C4-C5-C6-O6

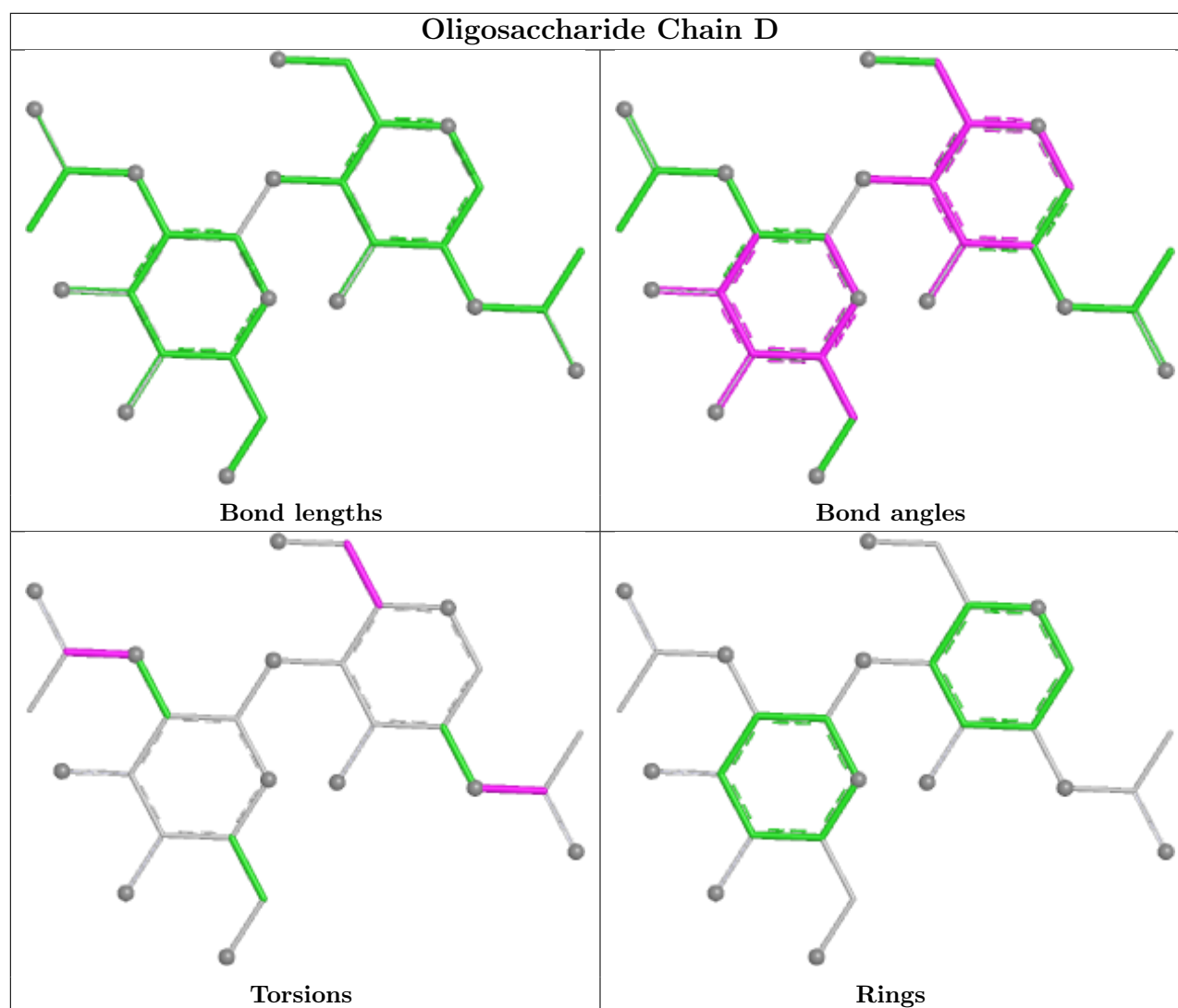
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2	NAG	12	0
6	D	1	NAG	12	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](#)

1 ligand is 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	$\# Z > 2$
7	NAG	U	1052	5	14,14,15	0.53	0	17,19,21	1.23	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
7	NAG	U	1052	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	1052	NAG	C1-O5-C5	3.93	117.45	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	U	1052	NAG	C8-C7-N2-C2
7	U	1052	NAG	O7-C7-N2-C2
7	U	1052	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	124/135 (91%)	2.91	95 (76%) 0 0	63, 74, 81, 83	0
2	B	40/40 (100%)	5.81	40 (100%) 0 0	51, 54, 54, 54	40 (100%)
3	L	211/212 (99%)	1.44	40 (18%) 3 2	51, 68, 80, 86	0
4	H	212/214 (99%)	1.74	60 (28%) 1 1	59, 70, 83, 88	0
5	U	259/283 (91%)	1.89	97 (37%) 1 1	57, 74, 91, 102	0
All	All	846/884 (95%)	2.07	332 (39%) 1 0	51, 71, 84, 102	40 (4%)

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	24	LEU	10.9
2	B	27	TYR	10.8
2	B	23	GLU	10.4
2	B	15	VAL	9.6
2	B	28	TYR	9.5
2	B	41	PRO	7.7
2	B	8	ARG	7.7
2	B	16	ASP	7.2
2	B	7	GLY	7.0
5	U	253	GLY	7.0
2	B	20	GLN	6.8
2	B	35	TYR	6.7
2	B	2	GLN	6.4
1	A	86	ALA	6.4
4	H	129	SER	6.3
4	H	130	MET	6.3
2	B	9	CYS	6.1
2	B	13	PHE	6.0
2	B	40	LYS	6.0
2	B	18	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	26	SER	5.9
2	B	10	THR	5.7
4	H	1	GLY	5.6
2	B	11	GLU	5.5
1	A	79	VAL	5.5
5	U	153	CYS	5.5
5	U	129	TRP	5.4
2	B	6	LYS	5.4
1	A	132	ALA	5.3
4	H	128	ASN	5.2
1	A	81	GLN	5.2
1	A	19	CYS	5.1
2	B	39	CYS	5.0
1	A	126	CYS	5.0
2	B	14	ASN	5.0
2	B	29	GLN	4.9
2	B	19	CYS	4.9
2	B	21	CYS	4.8
1	A	12	ASP	4.8
1	A	80	LEU	4.8
1	A	119	LEU	4.8
1	A	77	ALA	4.7
2	B	25	CYS	4.7
1	A	87	HIS	4.7
1	A	75	ASN	4.6
1	A	97	GLY	4.5
4	H	208	ALA	4.5
1	A	115	VAL	4.4
2	B	22	ASP	4.4
1	A	109	ARG	4.4
3	L	1	ASP	4.4
2	B	3	GLU	4.4
2	B	12	GLY	4.3
1	A	36	LYS	4.3
2	B	37	ALA	4.3
2	B	33	THR	4.2
2	B	30	SER	4.2
2	B	36	THR	4.2
4	H	131	VAL	4.2
2	B	4	SER	4.2
1	A	47	SER	4.1
1	A	44	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
5	U	261	ILE	4.1
1	A	78	THR	4.1
1	A	92	LEU	4.1
2	B	32	CYS	4.1
1	A	73	PRO	4.0
1	A	120	LYS	4.0
5	U	87	TYR	4.0
1	A	85	HIS	4.0
1	A	123	VAL	4.0
1	A	66	THR	3.9
1	A	41	HIS	3.9
1	A	65	ASP	3.9
5	U	130	ILE	3.9
1	A	122	LEU	3.9
2	B	17	LYS	3.9
2	B	31	CYS	3.8
4	H	189	THR	3.8
5	U	76	CYS	3.8
5	U	149	TYR	3.8
1	A	121	PRO	3.8
5	U	230	GLU	3.8
1	A	82	GLN	3.8
1	A	74	TRP	3.7
5	U	1(A)	SER	3.7
1	A	43	GLU	3.7
1	A	117	VAL	3.6
5	U	54	THR	3.6
2	B	5	CYS	3.6
1	A	76	SER	3.6
3	L	24	SER	3.6
5	U	12	CYS	3.6
1	A	131	CYS	3.6
3	L	5	THR	3.6
1	A	98	LYS	3.6
5	U	252	LEU	3.6
5	U	30	ARG	3.5
4	H	149	TRP	3.5
3	L	25	ALA	3.5
5	U	154	PRO	3.5
5	U	254	ASP	3.4
1	A	64	THR	3.4
1	A	11	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
5	U	229	HIS	3.4
2	B	38	GLU	3.4
1	A	72	LEU	3.4
1	A	62	ALA	3.4
4	H	206	ALA	3.4
3	L	69	THR	3.3
1	A	127	MET	3.3
5	U	183	GLU	3.3
3	L	29	SER	3.3
3	L	94	PRO	3.3
5	U	34	GLU	3.3
4	H	5	GLN	3.3
1	A	96	LEU	3.3
5	U	116	ARG	3.2
4	H	207	ALA	3.2
5	U	73	LEU	3.2
1	A	53	GLY	3.2
1	A	32	ASN	3.2
4	H	98	HIS	3.2
1	A	49	THR	3.2
4	H	2	VAL	3.2
5	U	246	MET	3.1
1	A	18	THR	3.1
5	U	18	ALA	3.1
4	H	153	SER	3.1
4	H	137	VAL	3.1
4	H	196	ALA	3.1
5	U	6	CYS	3.1
5	U	115	CYS	3.1
4	H	154	LEU	3.1
4	H	146	THR	3.0
5	U	47	HIS	3.0
3	L	27	SER	3.0
1	A	10	ASN	3.0
3	L	21	ILE	3.0
3	L	125	THR	3.0
5	U	19	LEU	3.0
1	A	42	CYS	3.0
1	A	50	CYS	3.0
1	A	55	GLY	3.0
3	L	93	TYR	3.0
1	A	35	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
4	H	12	VAL	2.9
5	U	70	VAL	2.9
1	A	69	ARG	2.9
1	A	17	GLY	2.9
5	U	170	CYS	2.9
1	A	128	VAL	2.9
5	U	1	LEU	2.9
1	A	116	GLN	2.9
1	A	107	ASN	2.9
1	A	118	GLY	2.9
1	A	99	HIS	2.9
4	H	29	PHE	2.9
3	L	76	SER	2.8
3	L	167	SER	2.8
5	U	168	LEU	2.8
4	H	143	GLU	2.8
5	U	20	GLY	2.8
1	A	27	ASN	2.8
5	U	245	SER	2.8
3	L	3	VAL	2.8
1	A	67	MET	2.8
5	U	256	PHE	2.8
5	U	112	SER	2.8
5	U	61	LEU	2.8
1	A	33	CYS	2.8
3	L	75	ILE	2.8
5	U	231	PRO	2.8
1	A	16	GLY	2.7
3	L	10	ILE	2.7
1	A	83	THR	2.7
5	U	113	LEU	2.7
1	A	91	ALA	2.7
1	A	31	CYS	2.7
5	U	71	CYS	2.7
5	U	22	ASP	2.7
4	H	195	PRO	2.7
3	L	56	SER	2.7
5	U	263	VAL	2.7
3	L	15	LEU	2.7
4	H	133	LEU	2.7
4	H	105	GLN	2.7
5	U	72	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
4	H	147	VAL	2.7
1	A	94	LEU	2.7
3	L	172	TYR	2.7
5	U	103	MET	2.7
5	U	58	ARG	2.7
3	L	105	GLU	2.7
4	H	192	VAL	2.7
5	U	88	SER	2.7
5	U	104	SER	2.7
1	A	124	GLN	2.7
1	A	13	CYS	2.6
3	L	158	VAL	2.6
5	U	23	LEU	2.6
5	U	75	LEU	2.6
1	A	58	TYR	2.6
3	L	41	GLY	2.6
5	U	4	MET	2.6
5	U	31	LEU	2.6
1	A	101	TYR	2.6
2	B	34	ASP	2.6
5	U	275	ASP	2.6
5	U	105	CYS	2.6
5	U	69	VAL	2.6
5	U	90	SER	2.6
5	U	8	THR	2.6
5	U	60	GLY	2.6
5	U	213	ILE	2.6
1	A	52	GLU	2.6
5	U	171	CYS	2.6
1	A	39	GLY	2.5
5	U	74	ASP	2.5
3	L	126	SER	2.5
1	A	45	ASP	2.5
4	H	85	GLU	2.5
5	U	255	ALA	2.5
1	A	71	CYS	2.5
4	H	148	THR	2.5
5	U	174	THR	2.5
4	H	145	VAL	2.5
1	A	9	SER	2.5
1	A	111	PRO	2.5
4	H	126	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
5	U	11	ASP	2.5
4	H	188	VAL	2.5
3	L	67	SER	2.5
1	A	102	CYS	2.4
5	U	204	GLY	2.4
4	H	112	SER	2.4
5	U	140	ASP	2.4
5	U	59	THR	2.4
5	U	67	THR	2.4
4	H	156	SER	2.4
4	H	65	ASP	2.4
5	U	55	LEU	2.4
1	A	88	ARG	2.4
1	A	30	TRP	2.4
3	L	2	ILE	2.4
5	U	28	ILE	2.4
3	L	9	ASP	2.4
1	A	113	CYS	2.4
4	H	135	CYS	2.4
1	A	54	ASN	2.4
3	L	212	GLU	2.3
4	H	118	PRO	2.3
4	H	144	PRO	2.3
5	U	26	THR	2.3
3	L	162	TRP	2.3
4	H	180	SER	2.3
5	U	5	GLN	2.3
4	H	55	ASP	2.3
5	U	211	PHE	2.3
5	U	14	VAL	2.3
4	H	70	THR	2.3
5	U	210	THR	2.3
1	A	59	ARG	2.3
5	U	152	GLY	2.3
5	U	260	HIS	2.3
4	H	205	ILE	2.3
1	A	37	PHE	2.3
1	A	57	PHE	2.3
3	L	80	ALA	2.3
5	U	151	PRO	2.3
5	U	233	ASN	2.3
3	L	11	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	H	152	GLY	2.3
4	H	155	SER	2.3
4	H	173	SER	2.3
5	U	269	SER	2.3
4	H	34	ILE	2.2
1	A	34	PRO	2.2
5	U	77	ASN	2.2
4	H	59	TYR	2.2
5	U	17	CYS	2.2
4	H	199	THR	2.2
5	U	16	GLU	2.2
5	U	9	ASN	2.2
1	A	84	TYR	2.2
4	H	140	TYR	2.2
5	U	24	CYS	2.2
4	H	185	SER	2.2
4	H	122	TYR	2.2
4	H	134	GLY	2.2
5	U	98	CYS	2.2
3	L	141	LYS	2.2
5	U	3	CYS	2.1
5	U	197	CYS	2.1
1	A	90	ASP	2.1
3	L	91	TRP	2.1
3	L	132	VAL	2.1
5	U	41	VAL	2.1
5	U	63	ILE	2.1
1	A	24	TYR	2.1
5	U	266	CYS	2.1
1	A	89	SER	2.1
3	L	7	SER	2.1
5	U	124	ASP	2.1
4	H	142	PRO	2.1
4	H	201	VAL	2.1
5	U	162	ASN	2.1
1	A	60	GLY	2.1
1	A	51	TYR	2.1
1	A	26	SER	2.1
3	L	207	SER	2.1
4	H	84	SER	2.1
3	L	123	GLN	2.1
5	U	125	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	H	71	ALA	2.1
4	H	191	ASN	2.1
3	L	190	SER	2.1
3	L	23	CYS	2.1
3	L	129	ALA	2.0
4	H	114	ALA	2.0
4	H	150	ASN	2.0
5	U	123	LEU	2.0
5	U	172	ASN	2.0
1	A	95	GLY	2.0
5	U	185	GLU	2.0
4	H	182	THR	2.0
1	A	105	PRO	2.0
4	H	27	TYR	2.0
3	L	30	VAL	2.0
1	A	14	LEU	2.0
5	U	10	GLY	2.0
5	U	35	GLY	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](#)

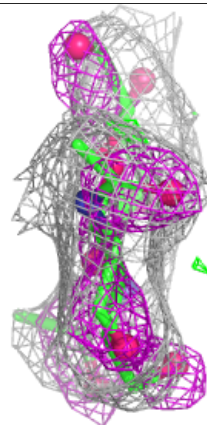
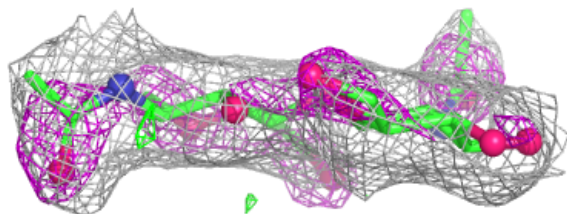
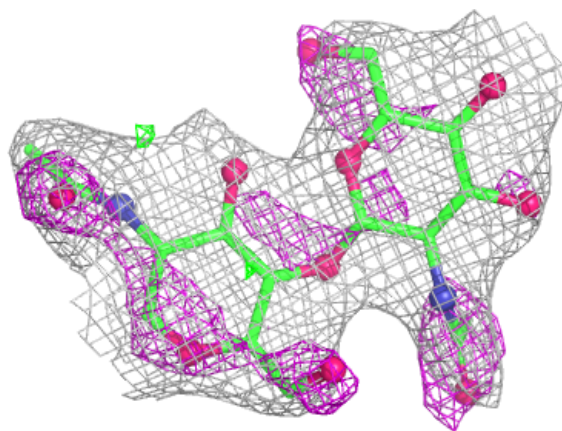
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

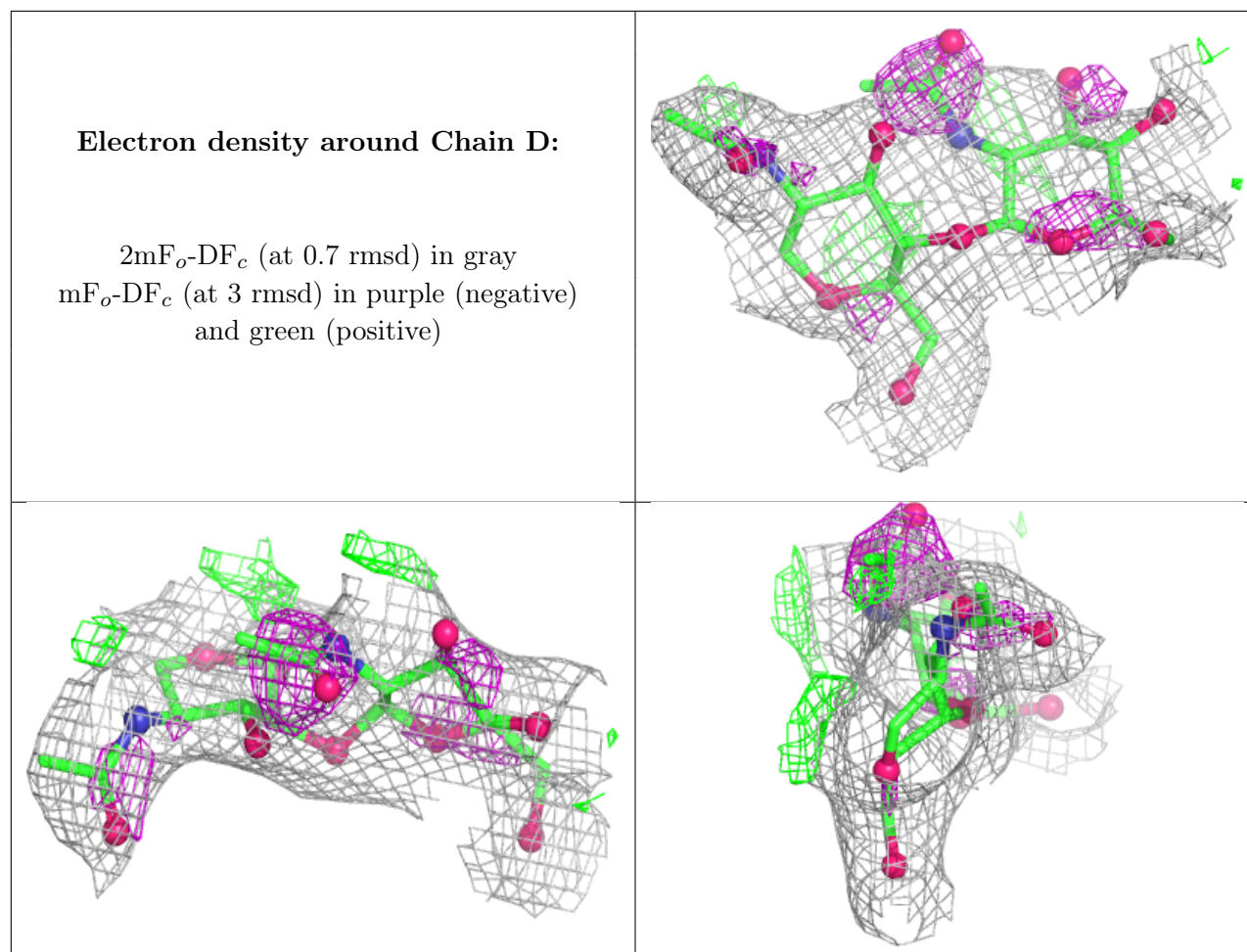
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	C	1	14/15	-	-	65,70,72,74	0
6	NAG	C	2	14/15	-	-	74,77,79,80	0
6	NAG	D	1	14/15	-	-	82,86,88,91	0
6	NAG	D	2	14/15	-	-	92,96,98,101	0

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 [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
7	NAG	U	1052	14/15	0.52	0.22	83,85,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.