



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:34 AM UTC

PDB ID : 5WB7 / pdb_00005wb7
Title : Crystal structure of the epidermal growth factor receptor extracellular region
in complex with epiregulin
Authors : Freed, D.M.; Bessman, N.J.; Ferguson, K.M.; Lemmon, M.A.
Deposited on : 2017-06-28
Resolution : 2.94 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

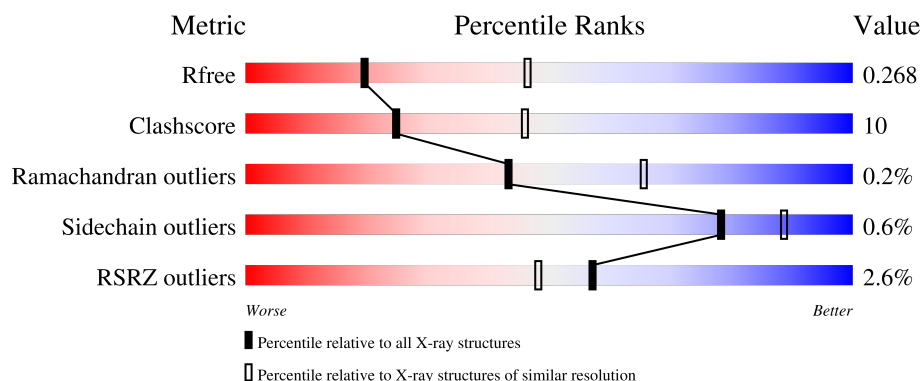
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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.



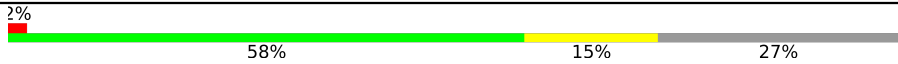
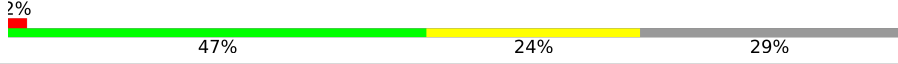
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	507	85% 13%
1	B	507	80% 19%
1	C	507	79% 19%
1	D	507	70% 27%
2	E	62	69% 6% 24%

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Mol	Chain	Length	Quality of chain
2	F	62	
2	G	62	
2	H	62	
3	I	4	
3	M	4	
3	O	4	
4	J	5	
5	K	3	
6	L	2	
6	N	2	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17103 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3816	2364	674	736	42			
1	B	504	Total	C	N	O	S	0	0	0
			3882	2402	694	744	42			
1	C	500	Total	C	N	O	S	0	0	0
			3791	2349	665	735	42			
1	D	499	Total	C	N	O	S	0	0	0
			3757	2331	656	728	42			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	HIS	-	expression tag	UNP P00533
A	503	HIS	-	expression tag	UNP P00533
A	504	HIS	-	expression tag	UNP P00533
A	505	HIS	-	expression tag	UNP P00533
A	506	HIS	-	expression tag	UNP P00533
A	507	HIS	-	expression tag	UNP P00533
B	502	HIS	-	expression tag	UNP P00533
B	503	HIS	-	expression tag	UNP P00533
B	504	HIS	-	expression tag	UNP P00533
B	505	HIS	-	expression tag	UNP P00533
B	506	HIS	-	expression tag	UNP P00533
B	507	HIS	-	expression tag	UNP P00533
C	502	HIS	-	expression tag	UNP P00533
C	503	HIS	-	expression tag	UNP P00533
C	504	HIS	-	expression tag	UNP P00533
C	505	HIS	-	expression tag	UNP P00533
C	506	HIS	-	expression tag	UNP P00533
C	507	HIS	-	expression tag	UNP P00533
D	502	HIS	-	expression tag	UNP P00533
D	503	HIS	-	expression tag	UNP P00533
D	504	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
D	505	HIS	-	expression tag	UNP P00533
D	506	HIS	-	expression tag	UNP P00533
D	507	HIS	-	expression tag	UNP P00533

- Molecule 2 is a protein called Proepiregulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	47	Total	C	N	O	S	0	0	0
			370	230	62	70	8			
2	F	45	Total	C	N	O	S	0	0	0
			347	215	58	66	8			
2	G	47	Total	C	N	O	S	0	0	0
			357	223	57	69	8			
2	H	44	Total	C	N	O	S	0	0	0
			338	209	55	66	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	SER	-	expression tag	UNP O14944
F	-7	SER	-	expression tag	UNP O14944
G	-7	SER	-	expression tag	UNP O14944
H	-7	SER	-	expression tag	UNP O14944

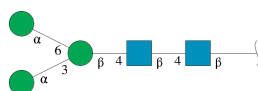
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	O	4	Total	C	N	O	0	0	0
			50	28	2	20			

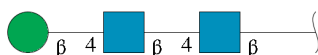
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called 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
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	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	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	O	0	0
			5	5		
8	B	20	Total	O	0	0
			20	20		
8	C	9	Total	O	0	0
			9	9		
8	D	5	Total	O	0	0
			5	5		
8	E	1	Total	O	0	0
			1	1		

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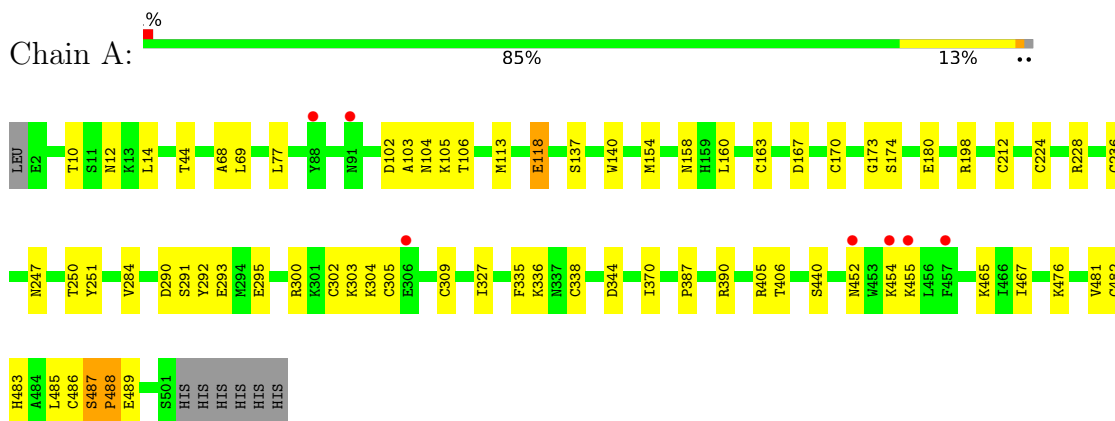
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	1	Total	O	0	0
			1	1		

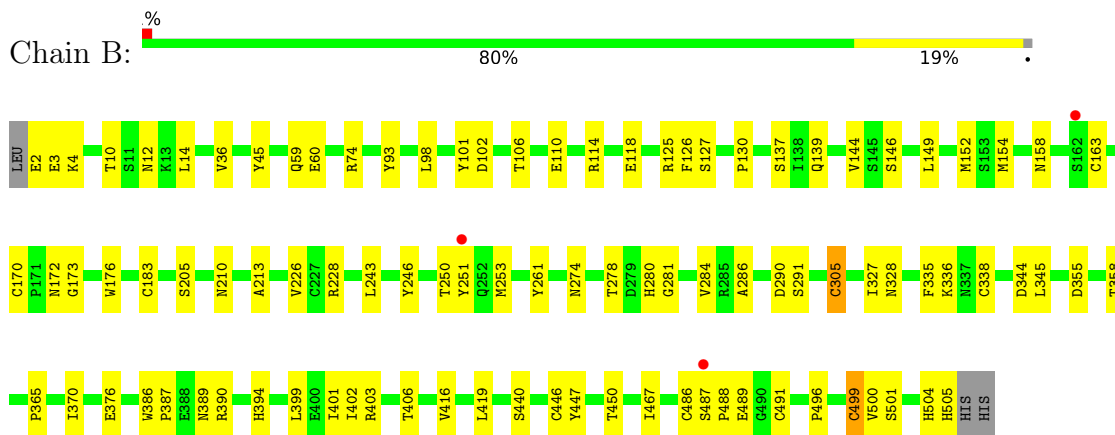
3 Residue-property plots [i](#)

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.

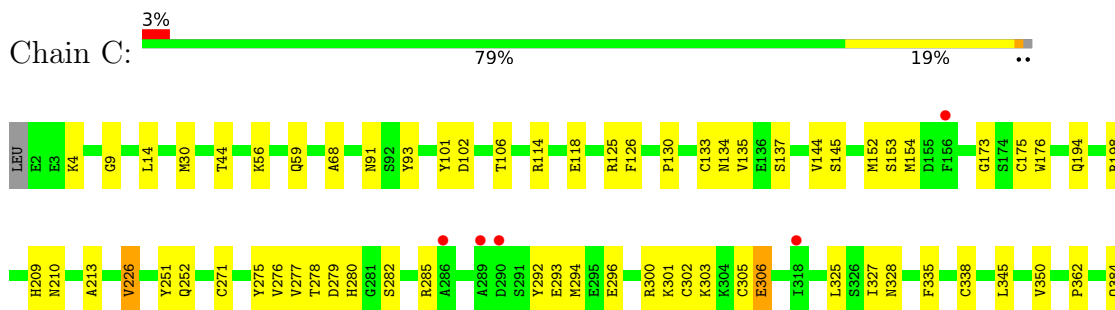
- Molecule 1: Epidermal growth factor receptor

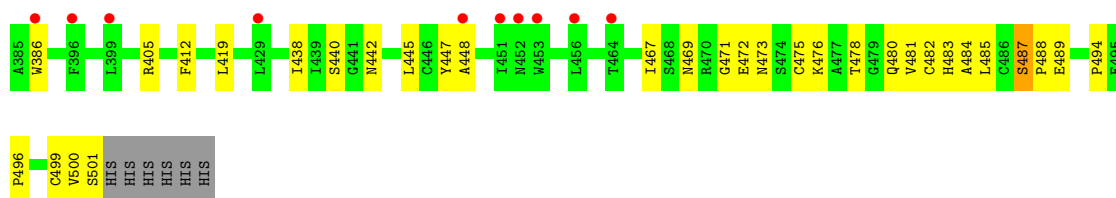


- Molecule 1: Epidermal growth factor receptor

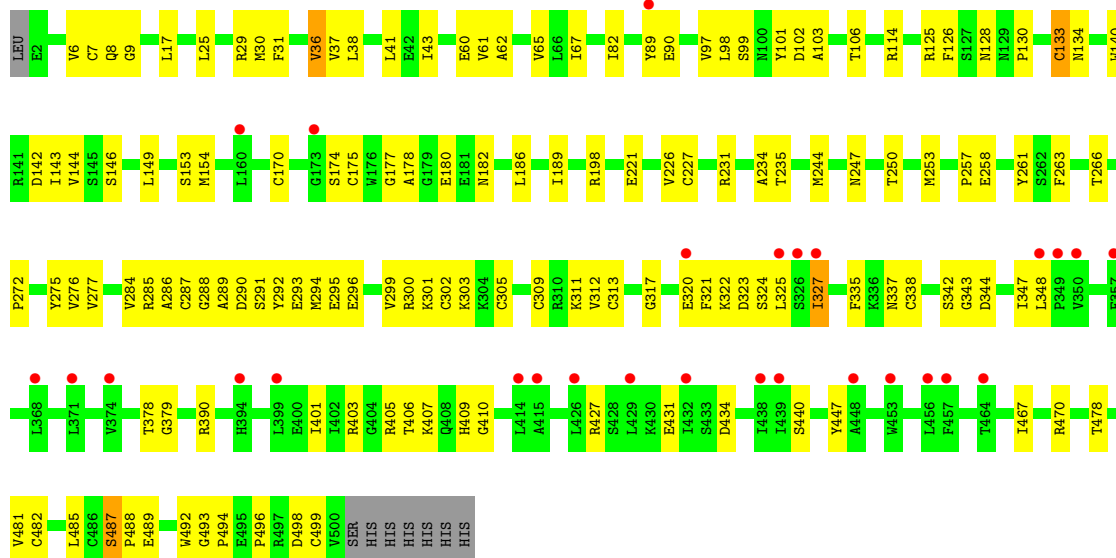


- Molecule 1: Epidermal growth factor receptor





• Molecule 1: Epidermal growth factor receptor



• Molecule 2: Proepiregulin



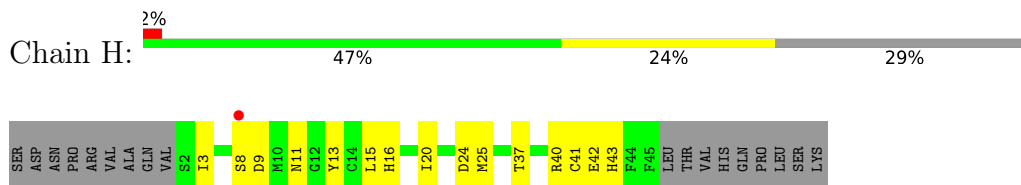
• Molecule 2: Proepiregulin



• Molecule 2: Proepiregulin



- Molecule 2: Proepiregulin



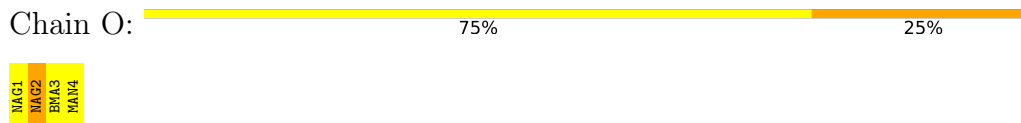
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



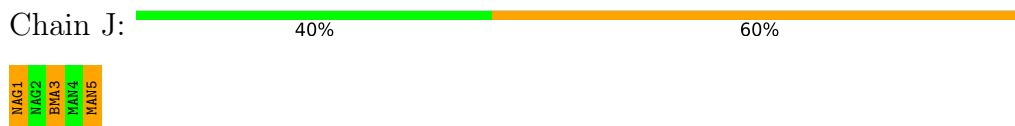
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



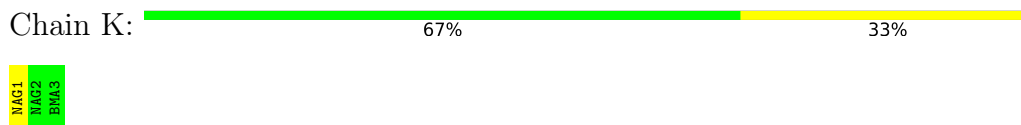
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-[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



- Molecule 5: beta-D-mannopyranose-(1-4)-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

Chain L:  50% 50%

MAG1
MAG2

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

Chain N:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.65Å 199.29Å 87.92Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	47.68 – 2.94 47.68 – 2.94	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.68-2.94) 96.5 (47.68-2.94)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.225 , 0.268 0.226 , 0.268	Depositor DCC
R_{free} test set	2597 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17103	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.16	0/3885	0.43	2/5256 (0.0%)
1	B	0.20	1/3957 (0.0%)	0.42	0/5350
1	C	0.16	0/3861	0.41	0/5235
1	D	0.18	0/3827	0.42	1/5193 (0.0%)
2	E	0.15	0/377	0.37	0/507
2	F	0.50	0/354	0.44	0/476
2	G	0.17	0/364	0.39	0/492
2	H	0.25	0/345	0.49	0/465
All	All	0.19	1/16970 (0.0%)	0.42	3/22974 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	ASN	C-O	-6.50	1.15	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ILE	N-CA-C	-12.75	93.14	109.58
1	D	327	ILE	N-CA-C	-6.89	99.62	108.93
1	A	327	ILE	CB-CA-C	5.24	119.22	111.26

There are no chirality outliers.

There are no planarity outliers.

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	3816	0	3670	42	2
1	B	3882	0	3731	61	0
1	C	3791	0	3597	78	1
1	D	3757	0	3539	117	1
2	E	370	0	340	5	0
2	F	347	0	302	8	1
2	G	357	0	314	15	0
2	H	338	0	291	17	1
3	I	50	0	43	1	0
3	M	50	0	43	1	0
3	O	50	0	43	6	0
4	J	61	0	52	2	1
5	K	39	0	34	0	0
6	L	28	0	25	5	0
6	N	28	0	25	1	0
7	A	42	0	39	0	0
7	B	28	0	26	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	5	0	0	0	0
8	B	20	0	0	1	0
8	C	9	0	0	2	0
8	D	5	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
All	All	17103	0	16140	324	4

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 10.

All (324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:VAL:HG21	1:C:152:MET:HE1	1.35	1.04
2:H:13:TYR:O	2:H:40:ARG:NE	2.07	0.87
1:B:158:ASN:ND2	1:B:163:CYS:SG	2.49	0.85
1:B:327:ILE:HD11	1:B:345:LEU:HD22	1.61	0.82
1:D:344:ASP:OD1	1:D:406:THR:OG1	2.02	0.77
1:D:31:PHE:CE2	1:D:41:LEU:HG	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:TYR:OH	2:G:24:ASP:OD2	2.03	0.76
6:L:1:NAG:O7	6:L:1:NAG:H5	1.86	0.76
8:B:701:HOH:O	4:J:5:MAN:O2	2.04	0.75
1:C:102:ASP:N	1:C:106:THR:O	2.17	0.74
1:D:327:ILE:HD12	1:D:347:ILE:HG12	1.72	0.72
1:C:327:ILE:HD11	1:C:345:LEU:HD22	1.73	0.71
1:C:144:VAL:HG21	1:C:152:MET:CE	2.18	0.70
1:D:294:MET:O	1:D:301:LYS:N	2.24	0.70
2:F:37:THR:HG21	2:F:45:PHE:HD2	1.56	0.70
1:D:327:ILE:HD12	1:D:347:ILE:CG1	2.23	0.69
1:D:427:ARG:NH2	1:D:498:ASP:OD1	2.26	0.68
2:H:37:THR:N	2:H:43:HIS:O	2.28	0.66
1:A:102:ASP:OD1	1:A:103:ALA:N	2.28	0.66
1:A:291:SER:HB3	1:A:302:CYS:SG	2.36	0.66
1:B:290:ASP:OD1	1:B:291:SER:N	2.29	0.65
1:D:292:TYR:N	1:D:303:LYS:O	2.26	0.65
1:B:358:THR:HG21	4:J:1:NAG:HN2	1.62	0.64
6:N:2:NAG:O7	6:N:2:NAG:O3	2.12	0.64
1:C:4:LYS:NZ	1:C:59:GLN:OE1	2.18	0.63
1:C:294:MET:O	1:C:301:LYS:N	2.31	0.63
1:D:311:LYS:NZ	1:D:313:CYS:SG	2.71	0.62
2:H:37:THR:O	2:H:43:HIS:N	2.20	0.62
1:D:487:SER:HB3	1:D:488:PRO:HD3	1.82	0.62
1:B:278:THR:HG22	1:B:280:HIS:H	1.65	0.62
1:C:91:ASN:O	6:L:1:NAG:H62	2.00	0.61
1:D:140:TRP:O	1:D:144:VAL:N	2.28	0.61
1:D:293:GLU:HA	1:D:302:CYS:HA	1.83	0.61
1:B:274:ASN:ND2	1:B:403:ARG:O	2.31	0.61
1:C:327:ILE:O	1:C:327:ILE:HG22	2.00	0.61
1:B:101:TYR:HB3	1:B:130:PRO:HD2	1.82	0.60
1:D:257:PRO:O	1:D:258:GLU:HB2	2.01	0.60
1:A:158:ASN:ND2	1:A:163:CYS:SG	2.75	0.60
1:C:294:MET:HE2	1:C:296:GLU:HB2	1.84	0.59
1:D:407:LYS:O	1:D:410:GLY:N	2.33	0.59
1:D:31:PHE:HE2	1:D:41:LEU:HG	1.67	0.59
1:D:102:ASP:N	1:D:106:THR:O	2.22	0.59
1:C:473:ASN:HA	1:C:476:LYS:HD2	1.83	0.59
1:C:292:TYR:N	1:C:303:LYS:O	2.24	0.59
1:C:445:LEU:HD21	1:C:448:ALA:HB2	1.85	0.58
2:F:37:THR:HG21	2:F:45:PHE:CD2	2.39	0.58
1:D:296:GLU:N	1:D:299:VAL:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:1:NAG:H5	6:L:1:NAG:C7	2.33	0.58
1:B:210:ASN:O	1:B:228:ARG:NH1	2.36	0.58
1:A:452:ASN:O	1:A:455:LYS:HG2	2.03	0.57
1:C:471:GLY:O	1:C:475:CYS:N	2.37	0.57
1:A:487:SER:N	1:A:488:PRO:HD3	2.19	0.57
1:C:276:VAL:HG23	1:C:300:ARG:C	2.30	0.57
1:C:362:PRO:HG2	1:D:234:ALA:HB2	1.87	0.56
1:C:475:CYS:SG	1:C:480:GLN:HB2	2.45	0.56
1:D:146:SER:HA	1:D:149:LEU:HD13	1.87	0.56
1:B:290:ASP:O	1:B:305:CYS:SG	2.64	0.56
1:B:344:ASP:OD1	1:B:406:THR:OG1	2.24	0.56
1:C:292:TYR:O	1:C:303:LYS:N	2.39	0.55
2:H:8:SER:O	2:H:11:ASN:HB2	2.06	0.55
2:G:6:CYS:SG	2:G:20:ILE:N	2.78	0.55
1:C:14:LEU:HD11	2:G:25:MET:HE1	1.88	0.55
1:D:325:LEU:HD11	2:H:40:ARG:HD3	1.89	0.55
1:D:134:ASN:O	1:D:175:CYS:O	2.24	0.55
1:D:487:SER:O	1:D:489:GLU:N	2.40	0.55
1:D:311:LYS:NZ	1:D:312:VAL:O	2.32	0.55
1:D:293:GLU:OE2	1:D:300:ARG:NH1	2.40	0.55
1:D:291:SER:HB2	1:D:303:LYS:C	2.30	0.54
1:D:142:ASP:O	1:D:198:ARG:NH2	2.40	0.54
1:D:263:PHE:CE1	1:D:272:PRO:HG3	2.42	0.54
1:A:14:LEU:CD1	2:E:25:MET:HG2	2.38	0.54
1:D:323:ASP:HB2	3:O:2:NAG:H5	1.90	0.54
1:B:98:LEU:HD21	1:B:125:ARG:HG2	1.89	0.54
1:D:142:ASP:O	1:D:198:ARG:NH1	2.39	0.54
1:B:170:CYS:N	1:B:183:CYS:SG	2.80	0.53
1:B:389:ASN:OD1	1:B:390:ARG:HG2	2.09	0.53
1:D:496:PRO:O	1:D:499:CYS:HB2	2.08	0.53
2:G:16:HIS:HB3	2:G:36:TYR:CD2	2.43	0.53
1:D:41:LEU:HD22	1:D:65:VAL:HG23	1.90	0.53
1:B:213:ALA:HB3	1:B:226:VAL:HG23	1.91	0.53
3:O:2:NAG:O7	3:O:2:NAG:H3	2.08	0.53
1:A:440:SER:HA	1:A:467:ILE:O	2.09	0.52
1:B:440:SER:HA	1:B:467:ILE:O	2.10	0.52
1:C:442:ASN:HB2	1:C:469:ASN:OD1	2.10	0.52
1:C:125:ARG:HA	1:C:153:SER:O	2.09	0.52
1:C:485:LEU:HD12	1:C:499:CYS:SG	2.49	0.52
1:D:101:TYR:HB3	1:D:130:PRO:HD2	1.91	0.51
1:C:485:LEU:CD1	1:C:499:CYS:SG	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ALA:HB3	1:C:226:VAL:HG13	1.92	0.51
1:C:293:GLU:OE2	1:C:405:ARG:NH2	2.43	0.51
1:B:496:PRO:O	1:B:499:CYS:HB2	2.11	0.51
1:D:8:GLN:OE1	1:D:285:ARG:NH2	2.43	0.51
1:C:114:ARG:HA	1:C:176:TRP:CD1	2.46	0.51
1:A:290:ASP:O	1:A:309:CYS:SG	2.70	0.50
1:B:489:GLU:O	1:B:500:VAL:HG21	2.12	0.50
1:D:324:SER:HA	3:O:1:NAG:H2	1.93	0.50
1:D:485:LEU:HD21	1:D:496:PRO:HB3	1.92	0.50
1:A:290:ASP:OD1	1:A:291:SER:N	2.45	0.50
1:D:261:TYR:CE1	1:D:277:VAL:HG21	2.47	0.50
1:D:25:LEU:HB3	1:D:29:ARG:HH12	1.76	0.49
1:C:118:GLU:OE1	1:C:198:ARG:NH2	2.45	0.49
1:D:82:ILE:HG21	1:D:226:VAL:HG11	1.94	0.49
1:D:134:ASN:ND2	1:D:177:GLY:O	2.45	0.49
1:B:98:LEU:HD22	1:B:127:SER:HB3	1.94	0.49
1:D:301:LYS:CB	1:D:303:LYS:HG3	2.42	0.49
1:D:6:VAL:HG21	1:D:38:LEU:HD21	1.95	0.49
1:A:344:ASP:OD1	1:A:406:THR:OG1	2.31	0.49
1:B:4:LYS:NZ	1:B:59:GLN:OE1	2.46	0.49
1:D:285:ARG:HG2	1:D:405:ARG:HD2	1.95	0.49
1:D:487:SER:HB3	1:D:488:PRO:CD	2.43	0.48
2:G:22:LEU:O	2:G:26:SER:N	2.36	0.48
3:I:1:NAG:H61	3:I:2:NAG:N2	2.28	0.48
1:A:137:SER:HB2	1:A:173:GLY:O	2.12	0.48
1:B:487:SER:N	1:B:488:PRO:HD2	2.28	0.48
1:C:91:ASN:HB3	6:L:1:NAG:H62	1.95	0.48
1:C:386:TRP:HB2	1:C:419:LEU:HD22	1.95	0.48
1:D:288:GLY:HA2	1:D:342:SER:OG	2.14	0.48
1:B:447:TYR:O	1:B:450:THR:HG22	2.14	0.48
1:D:261:TYR:CZ	1:D:277:VAL:HG21	2.49	0.48
1:A:387:PRO:HB2	1:A:390:ARG:HG2	1.95	0.48
1:B:144:VAL:HG11	1:B:152:MET:HE2	1.95	0.48
1:D:487:SER:CB	1:D:488:PRO:CD	2.91	0.48
1:B:101:TYR:OH	2:F:24:ASP:OD2	2.15	0.48
1:C:483:HIS:ND1	1:C:484:ALA:N	2.62	0.48
1:C:276:VAL:HG22	1:C:302:CYS:HB2	1.96	0.48
1:D:320:GLU:HG3	1:D:321:PHE:CE1	2.49	0.48
2:H:40:ARG:N	2:H:42:GLU:OE1	2.39	0.48
3:O:3:BMA:H3	3:O:4:MAN:H2	1.38	0.48
1:B:416:VAL:CG1	1:B:419:LEU:HD12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:CYS:HB3	1:D:174:SER:O	2.14	0.47
1:B:144:VAL:HG21	1:B:152:MET:HE1	1.96	0.47
3:O:1:NAG:O7	3:O:1:NAG:H3	2.13	0.47
1:A:476:LYS:HD2	1:A:481:VAL:HG21	1.96	0.47
1:C:485:LEU:HD11	1:C:496:PRO:HB3	1.96	0.47
1:D:99:SER:HA	1:D:128:ASN:O	2.14	0.47
1:A:14:LEU:HD13	2:E:25:MET:HG2	1.96	0.47
1:D:7:CYS:SG	1:D:37:VAL:HB	2.55	0.47
1:D:41:LEU:HD21	1:D:43:ILE:HD11	1.95	0.47
1:D:67:ILE:HB	1:D:97:VAL:HG12	1.96	0.47
1:D:17:LEU:HD21	1:D:409:HIS:HB3	1.96	0.47
1:D:97:VAL:HG23	1:D:97:VAL:O	2.15	0.47
1:D:98:LEU:HB3	2:H:25:MET:HE1	1.96	0.47
1:C:91:ASN:HB3	6:L:1:NAG:C6	2.44	0.47
1:D:126:PHE:CD1	1:D:154:MET:HE3	2.50	0.47
1:B:146:SER:HA	1:B:149:LEU:HD13	1.96	0.46
1:D:296:GLU:OE1	1:D:303:LYS:NZ	2.44	0.46
1:D:335:PHE:HA	1:D:338:CYS:SG	2.55	0.46
1:C:93:TYR:CE1	1:C:125:ARG:HB2	2.50	0.46
1:D:272:PRO:HG2	1:D:275:TYR:CD1	2.50	0.46
1:A:295:GLU:OE1	1:A:295:GLU:N	2.36	0.46
1:D:292:TYR:O	1:D:303:LYS:N	2.49	0.46
1:B:336:LYS:O	1:B:370:ILE:HG23	2.15	0.46
1:C:412:PHE:CE2	2:G:46:LEU:HB2	2.49	0.46
2:G:8:SER:HA	2:G:11:ASN:HB2	1.96	0.46
1:C:362:PRO:CG	1:D:234:ALA:HB2	2.45	0.46
1:A:167:ASP:OD2	1:A:180:GLU:HB3	2.16	0.46
1:A:212:CYS:O	1:A:228:ARG:NH2	2.49	0.46
1:B:355:ASP:HB3	1:B:358:THR:HG22	1.98	0.46
1:D:221:GLU:CG	1:D:235:THR:HG23	2.46	0.46
1:D:287:CYS:SG	1:D:293:GLU:HB2	2.56	0.46
1:D:289:ALA:C	1:D:291:SER:N	2.73	0.46
2:H:3:ILE:HG23	2:H:20:ILE:HB	1.97	0.46
2:E:47:THR:O	2:E:48:VAL:C	2.58	0.46
1:C:472:GLU:O	1:C:476:LYS:HG3	2.16	0.46
1:D:125:ARG:HA	1:D:153:SER:O	2.16	0.46
2:H:40:ARG:O	2:H:41:CYS:HB2	2.15	0.46
1:C:350:VAL:CG1	2:G:15:LEU:HD13	2.46	0.46
1:C:483:HIS:ND1	1:C:485:LEU:HG	2.30	0.46
1:B:450:THR:HG23	1:B:491:CYS:H	1.82	0.45
1:A:293:GLU:OE2	1:A:405:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLU:OE1	1:B:213:ALA:O	2.35	0.45
1:C:489:GLU:HB3	1:C:500:VAL:CG1	2.47	0.45
1:A:336:LYS:HA	1:A:370:ILE:HG23	1.97	0.45
1:D:407:LYS:NZ	1:D:434:ASP:OD2	2.36	0.45
1:A:10:THR:OG1	1:A:12:ASN:ND2	2.49	0.45
1:C:481:VAL:HG12	1:C:482:CYS:N	2.31	0.45
1:C:496:PRO:O	1:C:499:CYS:HB2	2.17	0.45
1:D:324:SER:CB	3:O:1:NAG:H2	2.47	0.45
1:D:343:GLY:O	1:D:379:GLY:N	2.49	0.45
1:A:295:GLU:HB3	1:A:300:ARG:HD2	1.99	0.45
1:D:289:ALA:C	1:D:291:SER:H	2.24	0.45
1:D:487:SER:O	1:D:488:PRO:C	2.60	0.45
1:A:335:PHE:HA	1:A:338:CYS:SG	2.57	0.45
1:B:74:ARG:NH1	1:B:110:GLU:OE1	2.46	0.45
1:B:390:ARG:HD3	1:B:394:HIS:CE1	2.52	0.45
1:C:126:PHE:CE2	1:C:135:VAL:HG11	2.52	0.45
1:A:224:CYS:HB2	1:A:236:CYS:SG	2.56	0.45
1:D:379:GLY:HA3	1:D:406:THR:OG1	2.17	0.45
1:A:483:HIS:CE1	1:A:485:LEU:HG	2.52	0.44
1:C:335:PHE:HA	1:C:338:CYS:SG	2.57	0.44
1:A:140:TRP:CD1	1:A:154:MET:HE1	2.53	0.44
1:C:500:VAL:O	1:C:501:SER:C	2.60	0.44
2:H:42:GLU:HG2	2:H:43:HIS:ND1	2.32	0.44
1:D:275:TYR:CE2	1:D:285:ARG:HB2	2.52	0.44
1:A:44:THR:HA	1:A:68:ALA:O	2.17	0.44
1:A:465:LYS:HG3	2:E:48:VAL:C	2.43	0.44
1:B:284:VAL:HA	1:C:251:TYR:O	2.18	0.44
1:D:89:TYR:O	1:D:90:GLU:HB2	2.17	0.44
1:D:290:ASP:O	1:D:305:CYS:HB2	2.18	0.44
1:A:69:LEU:HD11	2:E:22:LEU:HD23	2.00	0.44
1:A:291:SER:HA	1:A:304:LYS:HA	1.99	0.44
1:D:9:GLY:H	1:D:30:MET:HE2	1.83	0.44
1:B:114:ARG:HA	1:B:176:TRP:CD1	2.53	0.44
1:C:305:CYS:O	1:C:306:GLU:HB3	2.18	0.44
1:D:378:THR:HA	1:D:403:ARG:HG3	2.00	0.44
1:A:106:THR:HA	1:A:160:LEU:HD11	1.98	0.44
1:A:481:VAL:HG12	1:A:482:CYS:N	2.33	0.44
1:D:493:GLY:N	1:D:498:ASP:HB3	2.33	0.44
2:F:3:ILE:HG23	2:F:20:ILE:HB	2.00	0.44
1:D:133:CYS:O	1:D:134:ASN:HB2	2.18	0.43
1:D:470:ARG:NH2	1:D:478:THR:HG21	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ILE:O	1:D:97:VAL:HA	2.17	0.43
1:B:14:LEU:CD1	2:F:25:MET:HG2	2.48	0.43
1:B:139:GLN:OE1	1:B:172:ASN:ND2	2.51	0.43
1:C:278:THR:HG22	1:C:279:ASP:N	2.33	0.43
2:H:15:LEU:HG	2:H:16:HIS:ND1	2.33	0.43
1:A:118:GLU:OE1	1:A:198:ARG:NE	2.51	0.43
1:D:481:VAL:HG12	1:D:482:CYS:N	2.33	0.43
1:A:118:GLU:OE1	1:A:198:ARG:NH2	2.52	0.43
1:B:14:LEU:HD13	2:F:25:MET:HE3	2.00	0.43
1:B:335:PHE:HA	1:B:338:CYS:SG	2.59	0.43
1:C:101:TYR:HB3	1:C:130:PRO:HD2	2.01	0.43
1:C:152:MET:HG2	1:C:154:MET:HG2	2.01	0.43
1:C:275:TYR:HA	1:C:285:ARG:HA	2.00	0.43
1:D:221:GLU:HG2	1:D:235:THR:HG23	2.00	0.43
1:D:401:ILE:HG12	1:D:431:GLU:HB3	2.00	0.43
1:A:105:LYS:O	1:A:160:LEU:HD11	2.19	0.43
1:B:261:TYR:HA	1:B:281:GLY:O	2.19	0.43
1:C:384:GLN:CD	2:G:44:PHE:H	2.27	0.43
1:C:478:THR:HB	1:C:480:GLN:OE1	2.19	0.43
1:D:99:SER:OG	2:H:24:ASP:HB3	2.19	0.43
1:D:309:CYS:SG	1:D:312:VAL:HG23	2.58	0.43
1:C:209:HIS:CE1	8:C:708:HOH:O	2.72	0.43
1:C:447:TYR:OH	1:C:480:GLN:HB3	2.19	0.43
1:D:244:MET:HB3	1:D:253:MET:HE3	2.01	0.43
2:H:15:LEU:HD23	2:H:42:GLU:HA	2.00	0.43
1:B:205:SER:HB3	1:C:194:GLN:O	2.19	0.42
1:C:438:ILE:HG21	2:G:46:LEU:HD13	2.01	0.42
1:D:36:VAL:HG23	1:D:60:GLU:HG3	2.00	0.42
2:G:6:CYS:SG	2:G:19:CYS:C	3.02	0.42
1:D:317:GLY:N	1:D:321:PHE:O	2.52	0.42
1:B:93:TYR:CE1	1:B:125:ARG:HB2	2.53	0.42
1:B:250:THR:O	1:B:251:TYR:HB2	2.20	0.42
1:C:328:ASN:HD22	3:M:1:NAG:H82	1.84	0.42
1:C:440:SER:HA	1:C:467:ILE:O	2.19	0.42
1:D:295:GLU:HA	1:D:300:ARG:HA	2.01	0.42
2:G:10:MET:SD	2:G:28:ASN:CG	3.02	0.42
1:C:280:HIS:CD2	1:C:282:SER:HB2	2.55	0.42
1:C:487:SER:HB2	1:C:488:PRO:CD	2.49	0.42
1:D:99:SER:OG	2:H:25:MET:HE3	2.18	0.42
1:D:294:MET:O	1:D:300:ARG:HA	2.19	0.42
1:D:407:LYS:HB2	1:D:410:GLY:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ASP:OD1	1:D:103:ALA:N	2.52	0.42
1:A:487:SER:N	1:A:488:PRO:CD	2.82	0.42
1:B:286:ALA:HB3	1:C:252:GLN:HE22	1.85	0.42
1:C:9:GLY:H	1:C:30:MET:HE3	1.85	0.42
1:D:485:LEU:HD11	1:D:499:CYS:SG	2.59	0.42
1:B:36:VAL:HG13	1:B:60:GLU:HG3	2.02	0.42
1:C:276:VAL:CG2	1:C:302:CYS:HB2	2.50	0.42
1:D:178:ALA:N	1:D:182:ASN:HD22	2.17	0.42
1:D:427:ARG:HA	1:D:492:TRP:CE3	2.55	0.42
1:A:251:TYR:O	1:D:288:GLY:C	2.63	0.42
1:D:227:CYS:SG	1:D:231:ARG:HB2	2.60	0.42
2:G:19:CYS:O	2:G:20:ILE:HD13	2.20	0.42
1:B:243:LEU:HD11	1:B:261:TYR:CE2	2.55	0.42
1:C:210:ASN:HB3	8:C:708:HOH:O	2.20	0.42
1:A:292:TYR:CD2	1:A:303:LYS:O	2.73	0.42
1:B:2:GLU:OE1	1:B:3:GLU:N	2.53	0.42
1:B:416:VAL:HG12	1:B:419:LEU:HD12	2.01	0.42
1:C:487:SER:CB	1:C:488:PRO:CD	2.98	0.42
1:B:246:TYR:HD1	1:B:253:MET:SD	2.43	0.41
1:C:500:VAL:HG12	1:C:501:SER:N	2.35	0.41
1:D:284:VAL:HG22	1:D:286:ALA:H	1.85	0.41
1:B:14:LEU:HD11	2:F:25:MET:HG2	2.02	0.41
1:C:483:HIS:CE1	1:C:485:LEU:HG	2.55	0.41
1:D:348:LEU:HD23	2:H:42:GLU:O	2.20	0.41
1:C:144:VAL:HG12	1:C:145:SER:N	2.35	0.41
1:C:277:VAL:HG12	1:C:278:THR:N	2.35	0.41
1:D:140:TRP:O	1:D:143:ILE:N	2.53	0.41
1:D:285:ARG:CG	1:D:405:ARG:HD2	2.50	0.41
1:D:447:TYR:OH	1:D:494:PRO:HB3	2.20	0.41
1:A:77:LEU:HD12	1:A:113:MET:HE2	2.02	0.41
1:B:10:THR:OG1	1:B:12:ASN:ND2	2.53	0.41
1:B:14:LEU:O	1:B:45:TYR:OH	2.33	0.41
1:B:386:TRP:CG	1:B:387:PRO:HD2	2.55	0.41
1:C:278:THR:HG21	1:C:280:HIS:CE1	2.56	0.41
1:D:276:VAL:HG23	1:D:300:ARG:O	2.21	0.41
1:C:478:THR:O	1:C:478:THR:HG22	2.21	0.41
1:D:38:LEU:O	1:D:62:ALA:HB3	2.20	0.41
1:D:101:TYR:CE1	2:H:24:ASP:OD2	2.74	0.41
1:A:292:TYR:HB3	1:A:305:CYS:SG	2.61	0.41
1:C:44:THR:HA	1:C:68:ALA:O	2.20	0.41
1:C:137:SER:HB2	1:C:173:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LEU:HD11	2:G:40:ARG:HD3	2.03	0.41
1:B:504:HIS:O	1:B:505:HIS:HB2	2.21	0.41
1:D:140:TRP:CZ2	1:D:154:MET:HE1	2.56	0.41
1:A:247:ASN:HB3	1:A:250:THR:HB	2.02	0.41
1:B:137:SER:HB2	1:B:173:GLY:O	2.20	0.41
1:B:376:GLU:HB2	1:B:401:ILE:HG23	2.02	0.41
1:B:488:PRO:HB2	1:B:501:SER:HB3	2.03	0.41
1:C:447:TYR:OH	1:C:494:PRO:HB3	2.20	0.41
1:D:290:ASP:O	1:D:312:VAL:HG21	2.21	0.41
1:D:440:SER:HA	1:D:467:ILE:O	2.21	0.41
2:F:7:SER:C	2:F:9:ASP:H	2.29	0.41
1:B:365:PRO:HB3	1:B:387:PRO:HG3	2.02	0.41
1:C:275:TYR:CE2	1:C:285:ARG:HB2	2.56	0.41
1:D:37:VAL:HG13	1:D:61:VAL:HG13	2.02	0.41
1:D:114:ARG:HD3	1:D:182:ASN:OD1	2.21	0.40
1:D:263:PHE:O	1:D:266:THR:OG1	2.31	0.40
1:D:317:GLY:C	1:D:322:LYS:HA	2.46	0.40
1:A:452:ASN:OD1	1:A:454:LYS:HE2	2.21	0.40
1:B:102:ASP:HB2	1:B:106:THR:O	2.22	0.40
1:B:399:LEU:HD21	1:B:402:ILE:HD11	2.02	0.40
1:C:134:ASN:O	1:C:175:CYS:O	2.39	0.40
1:D:186:LEU:HD22	1:D:189:ILE:HD11	2.01	0.40
2:G:3:ILE:CG2	2:G:20:ILE:CG2	2.99	0.40
1:A:170:CYS:HB3	1:A:174:SER:O	2.22	0.40
1:D:97:VAL:HG21	1:D:126:PHE:CE2	2.56	0.40
1:D:247:ASN:HB3	1:D:250:THR:HB	2.04	0.40
1:D:311:LYS:HB3	1:D:337:ASN:O	2.21	0.40
1:B:486:CYS:C	1:B:488:PRO:HD2	2.47	0.40
2:H:15:LEU:HG	2:H:16:HIS:CE1	2.57	0.40
1:B:126:PHE:HB2	1:B:154:MET:HB2	2.02	0.40
1:D:293:GLU:OE2	1:D:300:ARG:HD3	2.21	0.40

All (4) 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:A:180:GLU:OE2	4:J:3:BMA:O4[1_556]	1.69	0.51
1:A:489:GLU:OE2	2:F:26:SER:OG[1_656]	1.99	0.21
1:C:56:LYS:NZ	2:H:9:ASP:OD2[1_454]	2.13	0.07
1:D:180:GLU:OE2	1:D:390:ARG:NH1[1_455]	2.19	0.01

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	498/507 (98%)	471 (95%)	25 (5%)	2 (0%)	30	54
1	B	502/507 (99%)	475 (95%)	27 (5%)	0	100	100
1	C	498/507 (98%)	464 (93%)	32 (6%)	2 (0%)	30	54
1	D	497/507 (98%)	463 (93%)	33 (7%)	1 (0%)	43	65
2	E	45/62 (73%)	43 (96%)	2 (4%)	0	100	100
2	F	43/62 (69%)	40 (93%)	3 (7%)	0	100	100
2	G	45/62 (73%)	44 (98%)	1 (2%)	0	100	100
2	H	42/62 (68%)	39 (93%)	3 (7%)	0	100	100
All	All	2170/2276 (95%)	2039 (94%)	126 (6%)	5 (0%)	43	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	PRO
1	C	306	GLU
1	D	487	SER
1	C	487	SER
1	A	487	SER

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	426/446 (96%)	422 (99%)	4 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	435/446 (98%)	432 (99%)	3 (1%)	76	86
1	C	419/446 (94%)	416 (99%)	3 (1%)	76	86
1	D	410/446 (92%)	408 (100%)	2 (0%)	81	90
2	E	43/57 (75%)	43 (100%)	0	100	100
2	F	38/57 (67%)	38 (100%)	0	100	100
2	G	40/57 (70%)	40 (100%)	0	100	100
2	H	38/57 (67%)	38 (100%)	0	100	100
All	All	1849/2012 (92%)	1837 (99%)	12 (1%)	78	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	118	GLU
1	A	284	VAL
1	A	486	CYS
1	B	305	CYS
1	B	446	CYS
1	B	499	CYS
1	C	133	CYS
1	C	226	VAL
1	C	271	CYS
1	D	36	VAL
1	D	133	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	193	GLN
1	A	359	HIS
1	B	28	GLN
1	B	33	ASN
1	B	121	HIS
1	B	274	ASN
1	B	409	HIS
1	B	452	ASN
1	B	502	HIS

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Mol	Chain	Res	Type
1	C	139	GLN
1	C	359	HIS
1	D	33	ASN
1	D	79	ASN
1	D	100	ASN
1	D	134	ASN
1	D	359	HIS
1	D	409	HIS

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](#)

24 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	I	1	1,3	14,14,15	0.56	0	17,19,21	1.13	2 (11%)
3	NAG	I	2	3	14,14,15	0.37	0	17,19,21	0.86	1 (5%)
3	BMA	I	3	3	11,11,12	0.22	0	15,15,17	0.51	0
3	MAN	I	4	3	11,11,12	0.30	0	15,15,17	0.89	0
4	NAG	J	1	1,4	14,14,15	0.50	0	17,19,21	1.20	2 (11%)
4	NAG	J	2	4	14,14,15	0.39	0	17,19,21	0.85	0
4	BMA	J	3	4	11,11,12	0.43	0	15,15,17	1.20	2 (13%)
4	MAN	J	4	4	11,11,12	0.24	0	15,15,17	0.74	0
4	MAN	J	5	4	11,11,12	0.42	0	15,15,17	1.58	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	1	1,5	14,14,15	0.28	0	17,19,21	1.02	2 (11%)
5	NAG	K	2	5	14,14,15	0.32	0	17,19,21	0.61	0
5	BMA	K	3	5	11,11,12	0.27	0	15,15,17	0.66	0
6	NAG	L	1	1,6	14,14,15	0.33	0	17,19,21	0.95	1 (5%)
6	NAG	L	2	6	14,14,15	0.35	0	17,19,21	0.68	0
3	NAG	M	1	1,3	14,14,15	0.44	0	17,19,21	0.88	1 (5%)
3	NAG	M	2	3	14,14,15	0.32	0	17,19,21	0.72	1 (5%)
3	BMA	M	3	3	11,11,12	0.24	0	15,15,17	0.52	0
3	MAN	M	4	3	11,11,12	0.25	0	15,15,17	0.51	0
6	NAG	N	1	1,6	14,14,15	0.35	0	17,19,21	0.87	1 (5%)
6	NAG	N	2	6	14,14,15	0.37	0	17,19,21	1.10	2 (11%)
3	NAG	O	1	1,3	14,14,15	0.41	0	17,19,21	0.70	0
3	NAG	O	2	3	14,14,15	0.35	0	17,19,21	0.90	1 (5%)
3	BMA	O	3	3	11,11,12	0.25	0	15,15,17	0.62	0
3	MAN	O	4	3	11,11,12	0.23	0	15,15,17	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	3/6/23/26	0/1/1/1
5	BMA	K	3	5	-	1/2/19/22	0/1/1/1
6	NAG	L	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	4/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	M	3	3	-	1/2/19/22	0/1/1/1
3	MAN	M	4	3	-	2/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	0/2/19/22	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(°)
4	J	5	MAN	C1-C2-C3	4.25	115.83	109.64
3	O	2	NAG	O5-C1-C2	-3.05	106.57	111.29
4	J	1	NAG	C4-C3-C2	2.88	115.24	111.02
4	J	5	MAN	O5-C1-C2	2.87	117.64	110.79
5	K	1	NAG	O5-C1-C2	-2.67	107.16	111.29
3	I	1	NAG	C1-O5-C5	-2.65	108.64	112.19
5	K	1	NAG	C1-O5-C5	2.47	115.50	112.19
4	J	3	BMA	C1-C2-C3	2.43	113.19	109.64
6	L	1	NAG	C1-O5-C5	-2.41	108.95	112.19
6	N	2	NAG	O5-C1-C2	-2.37	107.62	111.29
3	I	1	NAG	C2-N2-C7	-2.37	119.72	122.90
3	I	2	NAG	O5-C1-C2	-2.36	107.64	111.29
6	N	2	NAG	C3-C4-C5	2.34	114.48	110.23
6	N	1	NAG	C1-O5-C5	-2.27	109.14	112.19
3	M	1	NAG	C2-N2-C7	-2.23	119.91	122.90
4	J	1	NAG	C3-C4-C5	2.12	114.08	110.23
4	J	3	BMA	C3-C4-C5	2.10	114.05	110.23
3	M	2	NAG	O5-C1-C2	-2.05	108.12	111.29
4	J	5	MAN	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	M	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C1-C2-N2-C7
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	4	MAN	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
6	N	1	NAG	C8-C7-N2-C2
3	I	4	MAN	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	L	2	NAG	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	M	4	MAN	C4-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O7-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
5	K	2	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C3-C2-N2-C7
3	O	2	NAG	C3-C2-N2-C7
6	N	1	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
4	J	5	MAN	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6

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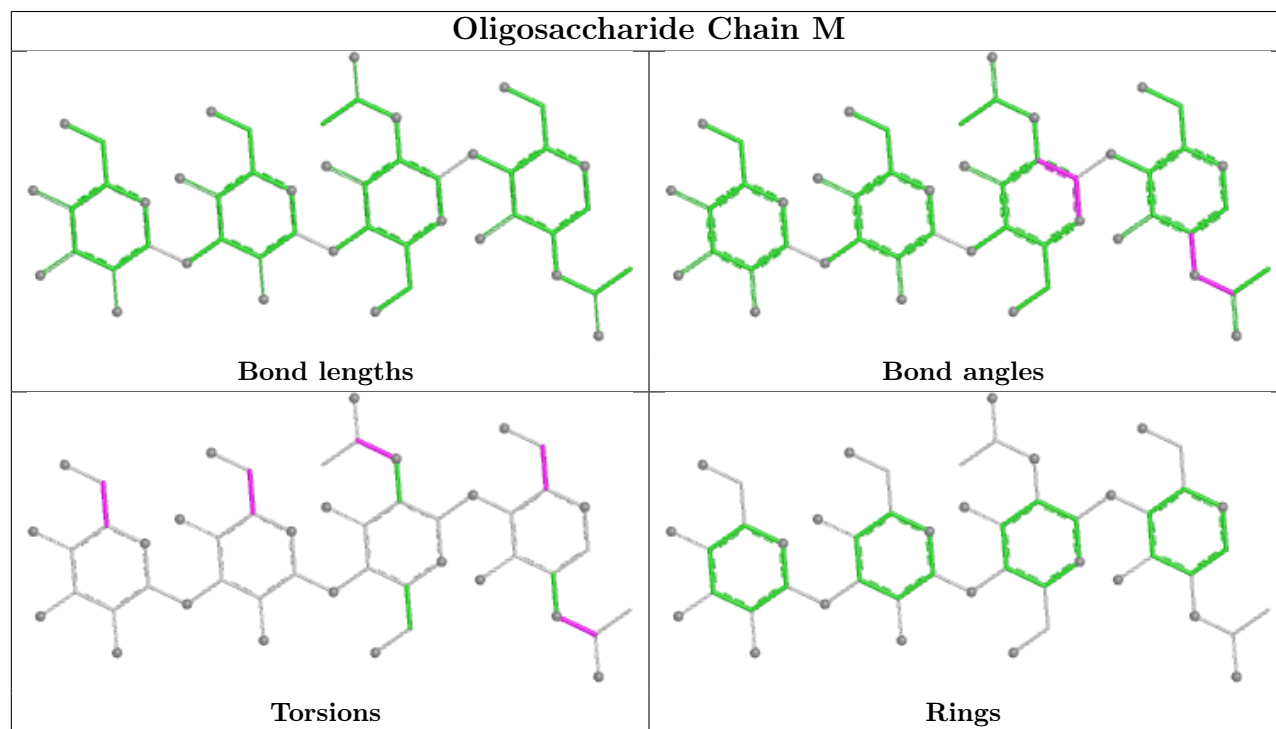
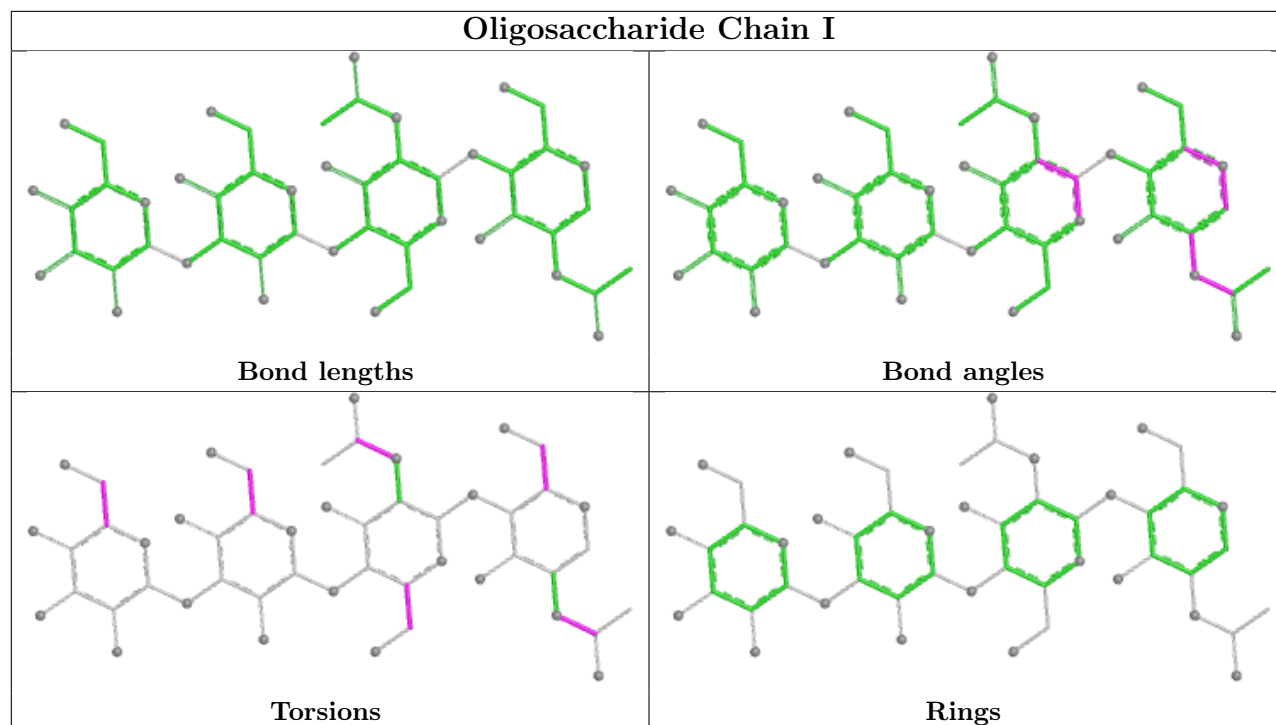
Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	N	2	NAG	C8-C7-N2-C2
3	I	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C1-C2-N2-C7
6	N	2	NAG	C3-C2-N2-C7
4	J	5	MAN	C4-C5-C6-O6
6	N	2	NAG	O7-C7-N2-C2
3	I	2	NAG	O5-C5-C6-O6

There are no ring outliers.

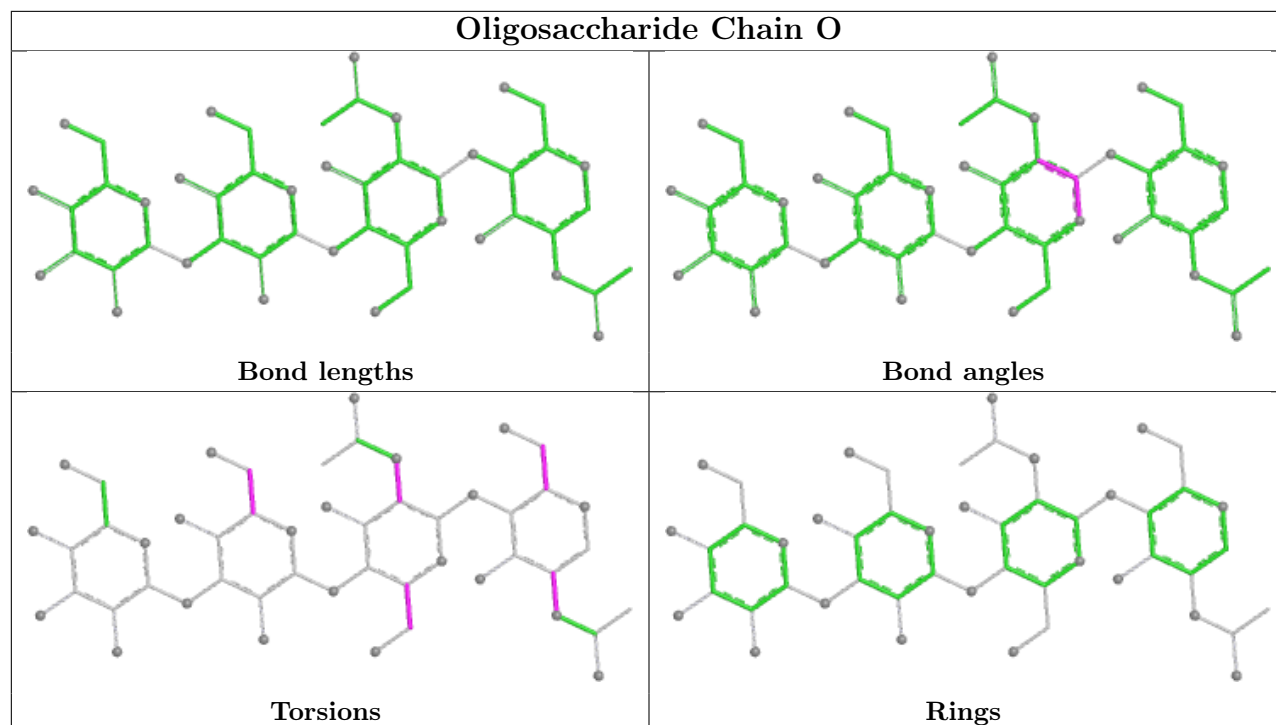
12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	1	0
4	J	3	BMA	0	1
3	I	1	NAG	1	0
3	O	1	NAG	3	0
6	L	1	NAG	5	0
6	N	2	NAG	1	0
3	M	1	NAG	1	0
4	J	5	MAN	1	0
3	I	2	NAG	1	0
3	O	3	BMA	1	0
3	O	4	MAN	1	0
3	O	2	NAG	2	0

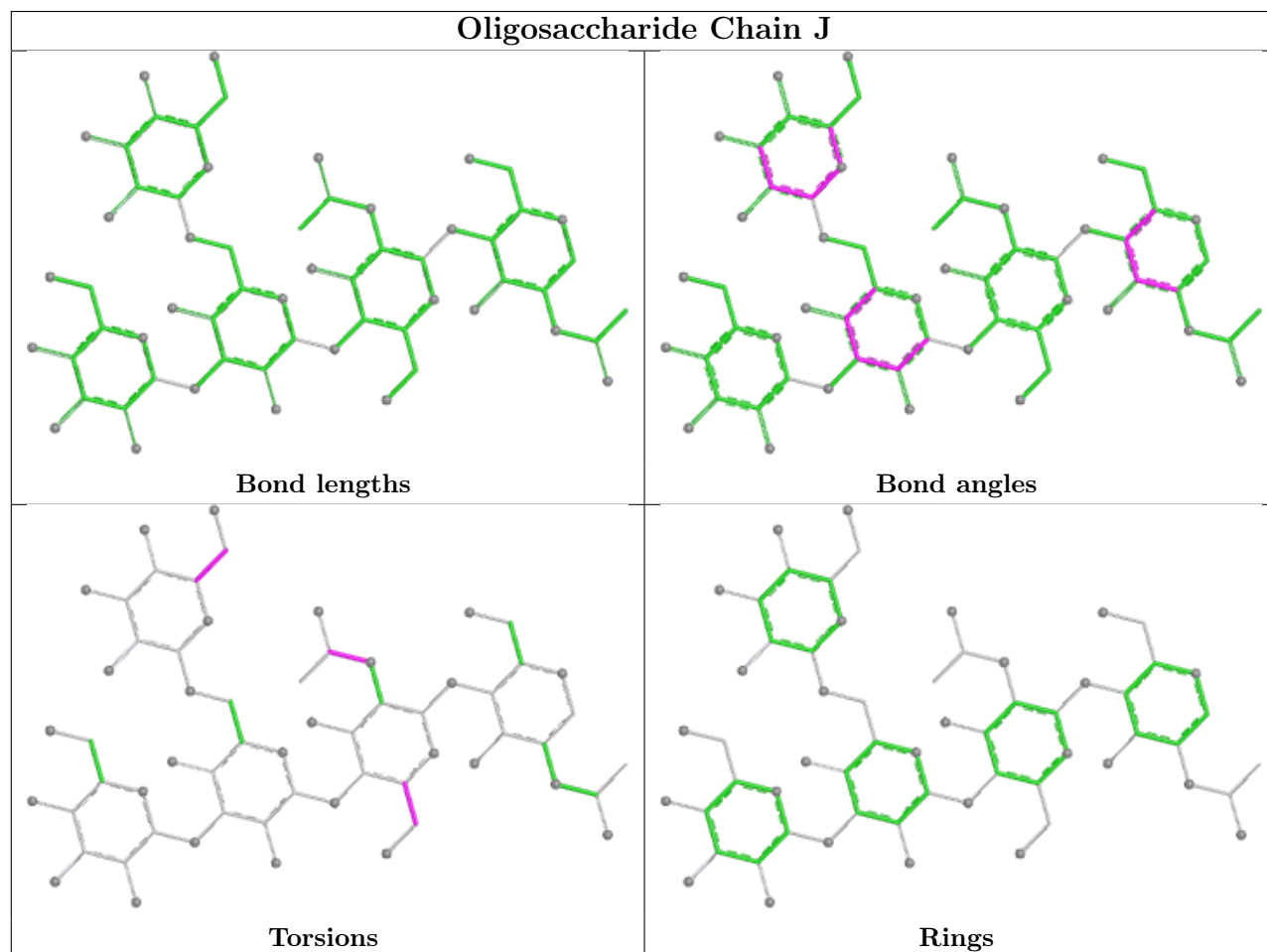
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

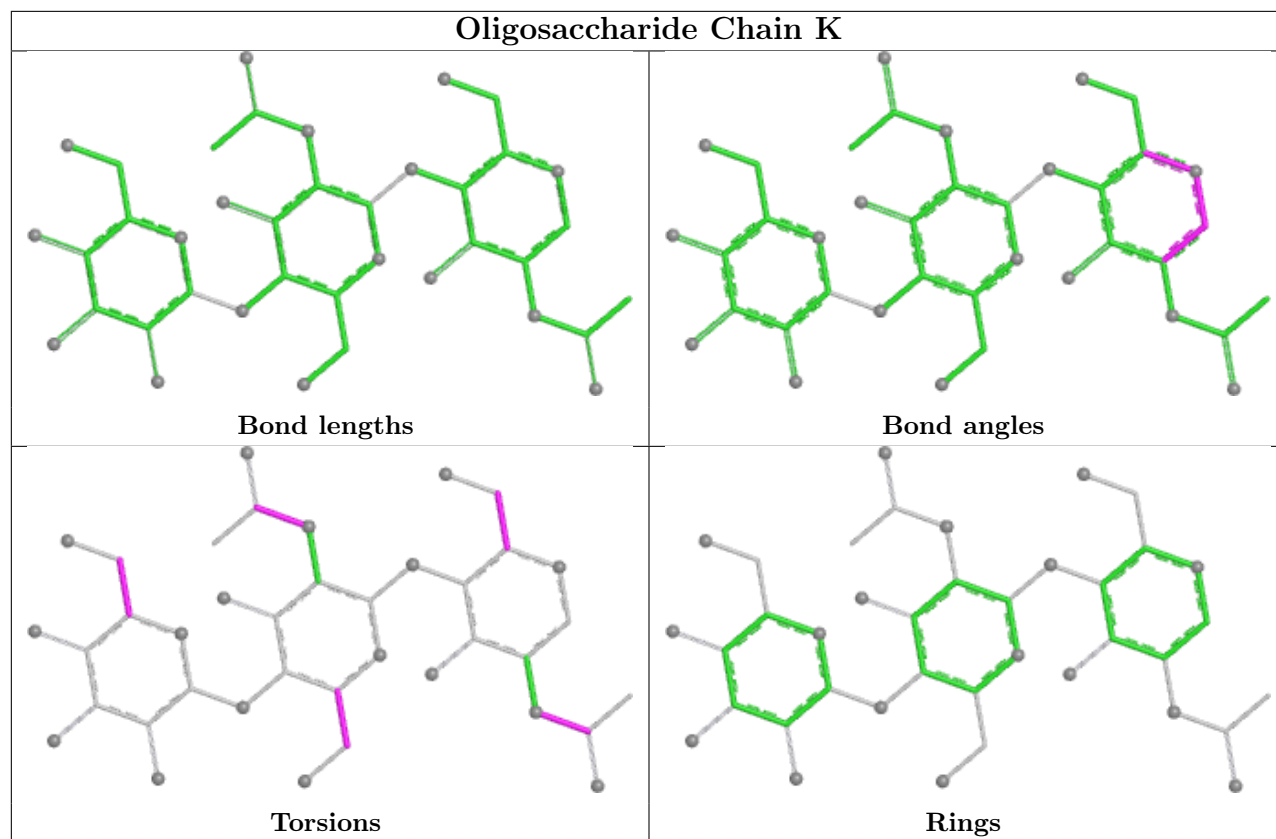


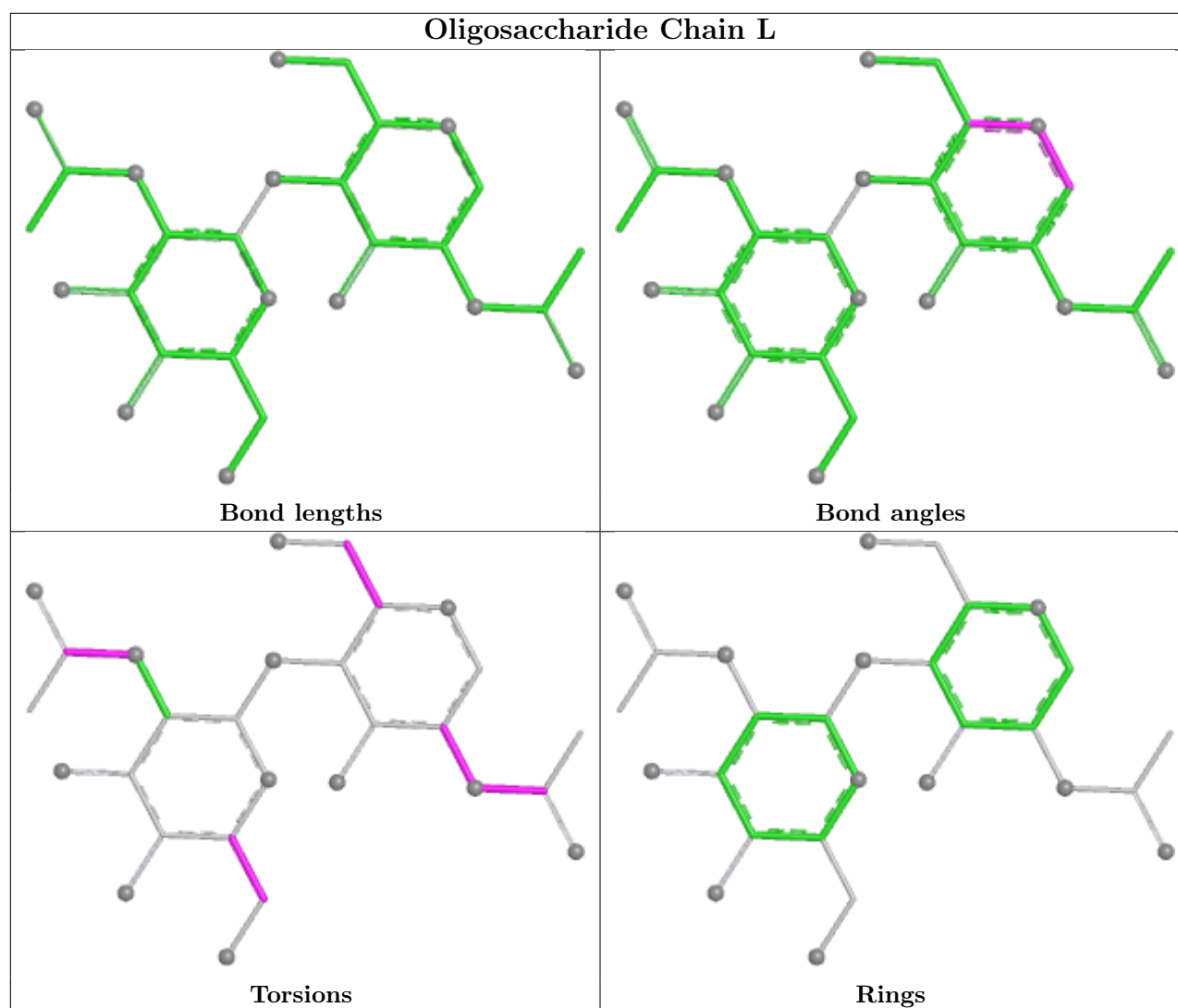
Oligosaccharide Chain O

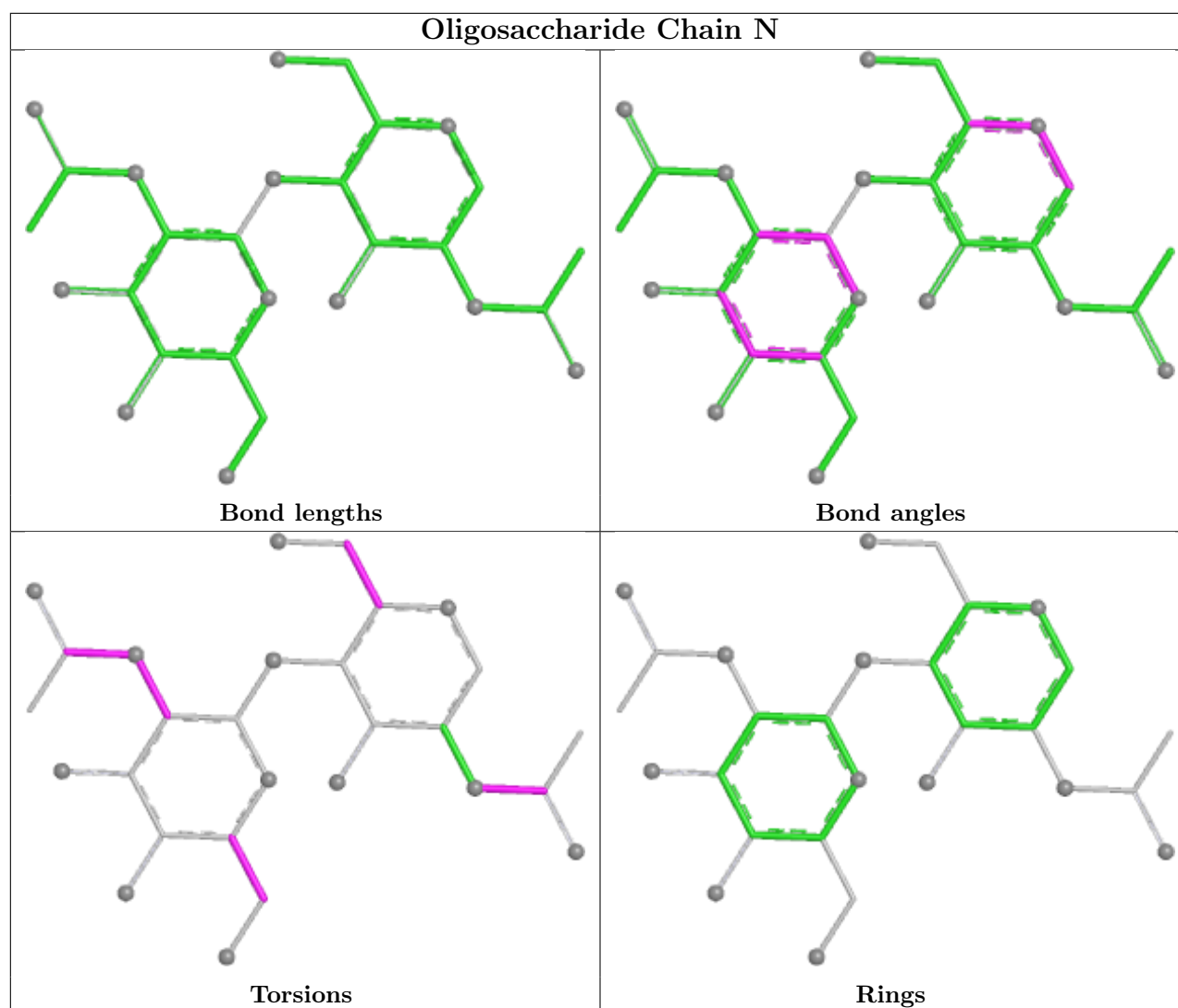


Oligosaccharide Chain J









5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
7	NAG	C	603	1	14,14,15	0.18	0	17,19,21	0.64	0
7	NAG	B	601	1	14,14,15	0.29	0	17,19,21	0.55	0
7	NAG	D	601	1	14,14,15	0.67	1 (7%)	17,19,21	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	602	1	14,14,15	0.30	0	17,19,21	0.46	0
7	NAG	A	3207	1	14,14,15	0.28	0	17,19,21	1.18	2 (11%)
7	NAG	A	3206	1	14,14,15	0.28	0	17,19,21	0.66	0
7	NAG	A	3201	1	14,14,15	0.33	0	17,19,21	1.03	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	C	603	1	-	2/6/23/26	0/1/1/1
7	NAG	B	601	1	-	2/6/23/26	0/1/1/1
7	NAG	D	601	1	-	2/6/23/26	0/1/1/1
7	NAG	B	602	1	-	1/6/23/26	0/1/1/1
7	NAG	A	3207	1	-	2/6/23/26	0/1/1/1
7	NAG	A	3206	1	-	1/6/23/26	0/1/1/1
7	NAG	A	3201	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	601	NAG	C1-C2	2.38	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3207	NAG	C1-O5-C5	3.39	116.73	112.19
7	A	3207	NAG	O5-C1-C2	2.73	115.51	111.29
7	A	3201	NAG	O5-C1-C2	-2.45	107.50	111.29
7	D	601	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	NAG	C8-C7-N2-C2
7	B	601	NAG	O7-C7-N2-C2
7	A	3207	NAG	C4-C5-C6-O6
7	D	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	3207	NAG	O5-C5-C6-O6
7	A	3201	NAG	C8-C7-N2-C2
7	C	603	NAG	C4-C5-C6-O6
7	D	601	NAG	C4-C5-C6-O6
7	A	3201	NAG	O7-C7-N2-C2
7	C	603	NAG	O5-C5-C6-O6
7	A	3206	NAG	O5-C5-C6-O6
7	B	602	NAG	C4-C5-C6-O6
7	A	3201	NAG	O5-C5-C6-O6
7	A	3201	NAG	C4-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	500/507 (98%)	-0.12	7 (1%) 73 66	44, 72, 121, 181	0
1	B	504/507 (99%)	-0.17	3 (0%) 85 81	34, 65, 129, 178	0
1	C	500/507 (98%)	0.18	15 (3%) 52 44	36, 88, 167, 266	0
1	D	499/507 (98%)	0.42	28 (5%) 30 24	60, 120, 188, 253	0
2	E	47/62 (75%)	0.10	2 (4%) 40 31	54, 74, 118, 132	0
2	F	45/62 (72%)	-0.06	1 (2%) 62 53	49, 70, 120, 166	0
2	G	47/62 (75%)	0.21	0 100 100	74, 110, 154, 188	0
2	H	44/62 (70%)	0.58	1 (2%) 61 52	111, 131, 168, 184	0
All	All	2186/2276 (96%)	0.09	57 (2%) 57 48	34, 82, 166, 266	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	374	VAL	5.7
1	C	290	ASP	4.2
1	C	451	ILE	3.9
1	D	448	ALA	3.9
1	D	348	LEU	3.8
1	D	415	ALA	3.7
1	C	456	LEU	3.7
1	D	327	ILE	3.4
2	E	48	VAL	3.4
1	D	371	LEU	3.3
1	A	88	TYR	3.2
1	D	438	ILE	3.2
1	D	453	TRP	3.2
1	B	487	SER	3.1
1	C	429	LEU	3.1
1	D	350	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	325	LEU	3.1
1	C	453	TRP	3.0
1	D	368	LEU	2.9
1	D	349	PRO	2.9
1	C	448	ALA	2.9
1	D	89	TYR	2.8
1	D	399	LEU	2.8
1	D	357	PHE	2.7
1	B	251	TYR	2.7
1	C	452	ASN	2.7
1	D	173	GLY	2.6
2	E	26	SER	2.6
1	D	432	ILE	2.6
2	H	8	SER	2.5
1	D	429	LEU	2.5
1	D	426	LEU	2.4
1	C	318	ILE	2.4
1	C	156	PHE	2.4
1	A	306	GLU	2.4
1	C	399	LEU	2.4
1	D	160	LEU	2.4
1	A	452	ASN	2.3
1	D	414	LEU	2.3
1	D	439	ILE	2.3
1	C	464	THR	2.2
1	A	454	LYS	2.2
1	A	455	LYS	2.2
2	F	46	LEU	2.2
1	B	162	SER	2.2
1	D	320	GLU	2.2
1	C	396	PHE	2.2
1	D	326	SER	2.2
1	D	457	PHE	2.2
1	A	91	ASN	2.1
1	D	394	HIS	2.1
1	C	386	TRP	2.1
1	A	457	PHE	2.1
1	D	456	LEU	2.1
1	C	289	ALA	2.1
1	D	464	THR	2.0
1	C	286	ALA	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](#)

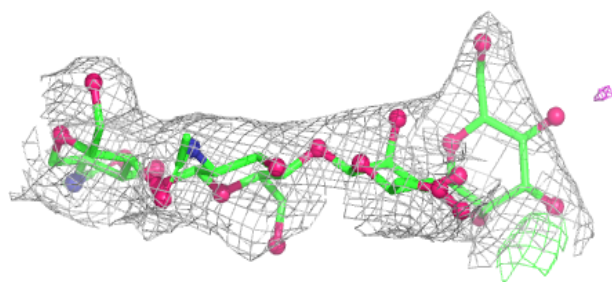
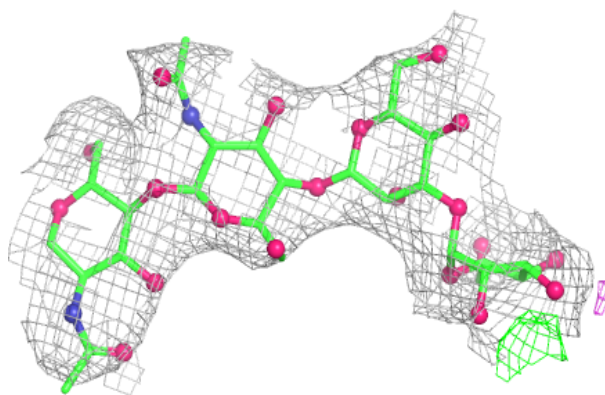
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	K	3	11/12	0.21	0.14	149,174,191,195	0
6	NAG	L	1	14/15	0.44	0.13	122,138,156,159	0
3	BMA	M	3	11/12	0.49	0.10	142,156,167,173	0
3	MAN	M	4	11/12	0.52	0.10	139,142,152,153	0
6	NAG	L	2	14/15	0.57	0.10	106,150,160,161	0
3	NAG	O	2	14/15	0.61	0.17	134,151,170,185	0
3	MAN	I	4	11/12	0.61	0.13	116,148,154,161	0
4	MAN	J	4	11/12	0.64	0.13	146,165,171,173	0
4	BMA	J	3	11/12	0.65	0.12	124,141,152,158	0
5	NAG	K	1	14/15	0.68	0.12	120,145,161,163	0
3	MAN	O	4	11/12	0.68	0.13	114,133,147,148	0
6	NAG	N	2	14/15	0.70	0.10	126,157,164,164	0
5	NAG	K	2	14/15	0.73	0.10	140,161,175,190	0
3	BMA	I	3	11/12	0.75	0.09	123,132,136,141	0
6	NAG	N	1	14/15	0.76	0.12	92,117,137,151	0
4	MAN	J	5	11/12	0.78	0.13	138,153,161,163	0
3	BMA	O	3	11/12	0.79	0.13	135,141,145,149	0
4	NAG	J	2	14/15	0.85	0.13	42,72,112,114	0
3	NAG	O	1	14/15	0.87	0.16	109,145,180,189	0
3	NAG	M	2	14/15	0.89	0.10	114,122,144,156	0
3	NAG	I	2	14/15	0.89	0.12	91,111,124,126	0
4	NAG	J	1	14/15	0.90	0.17	62,85,93,99	0
3	NAG	M	1	14/15	0.92	0.09	81,108,124,128	0
3	NAG	I	1	14/15	0.92	0.12	62,77,92,115	0

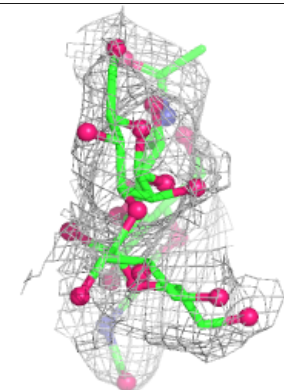
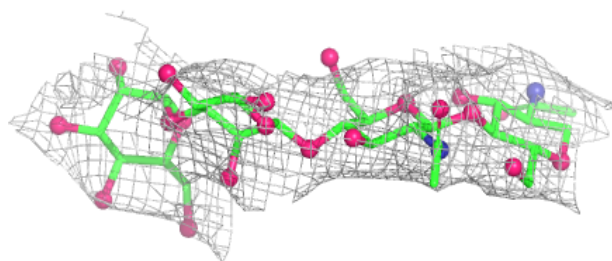
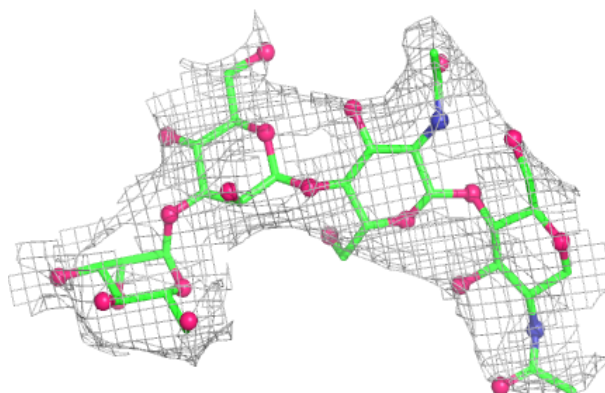
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

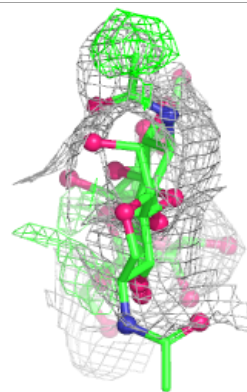
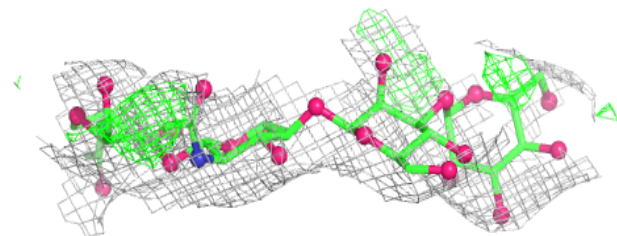
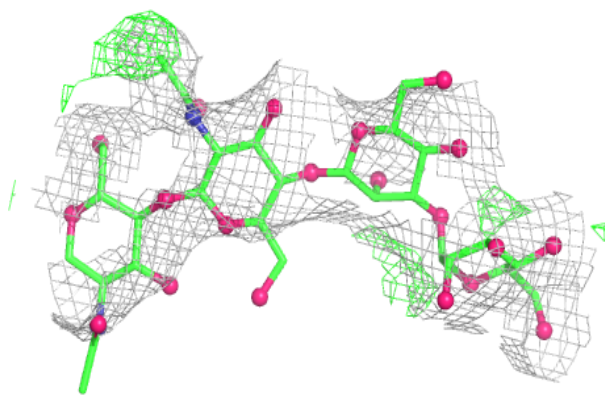
**Electron density around Chain M:**

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



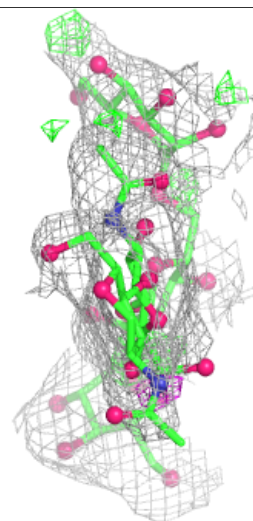
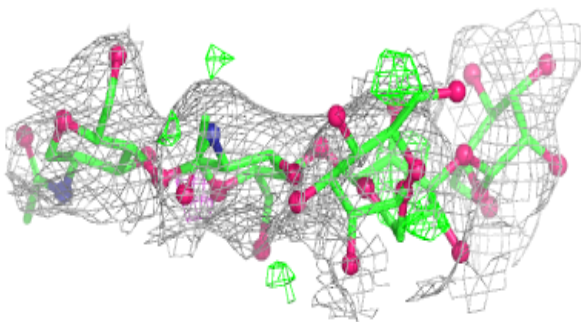
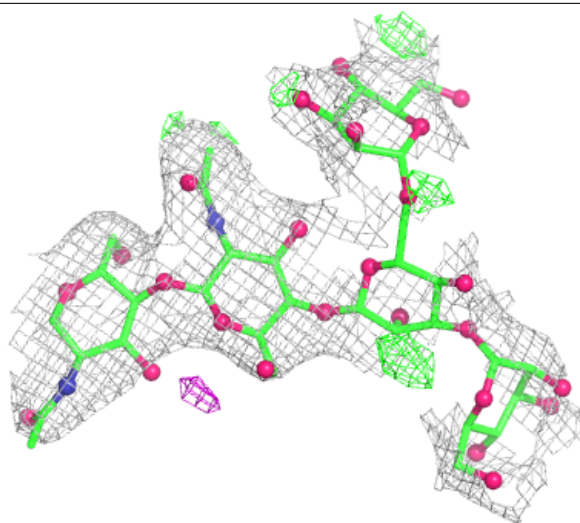
Electron density around Chain O:

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



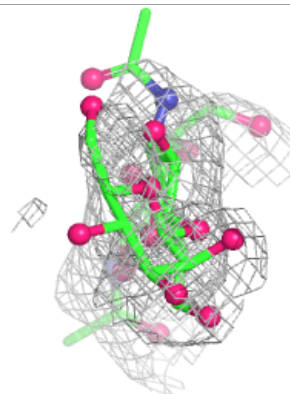
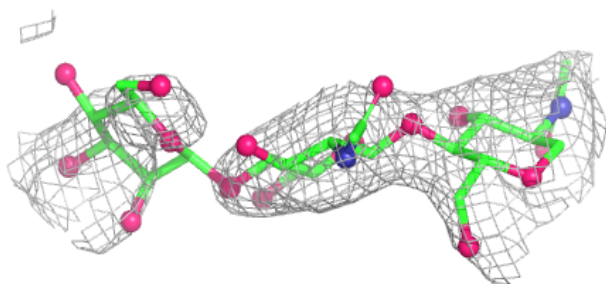
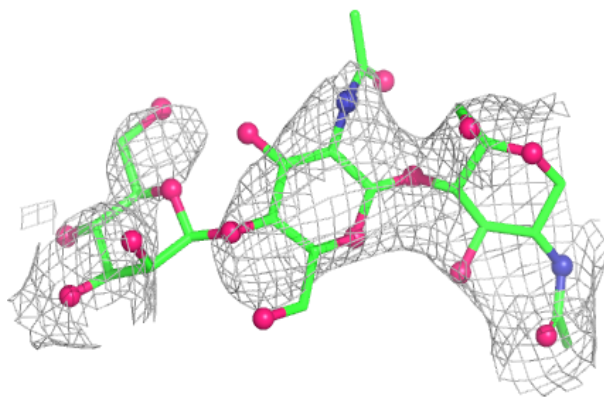
Electron density around Chain J:

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



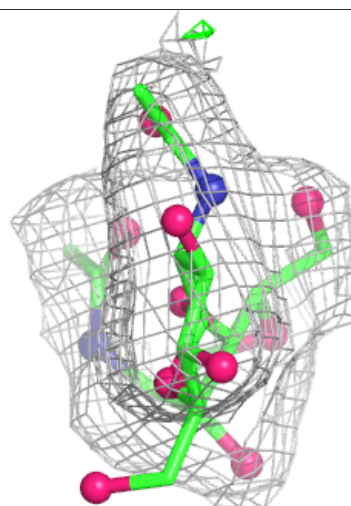
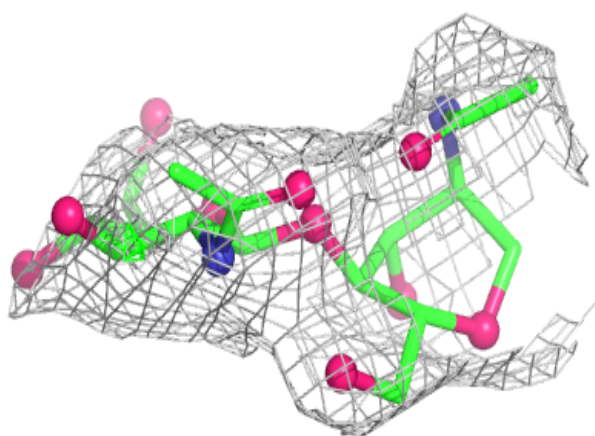
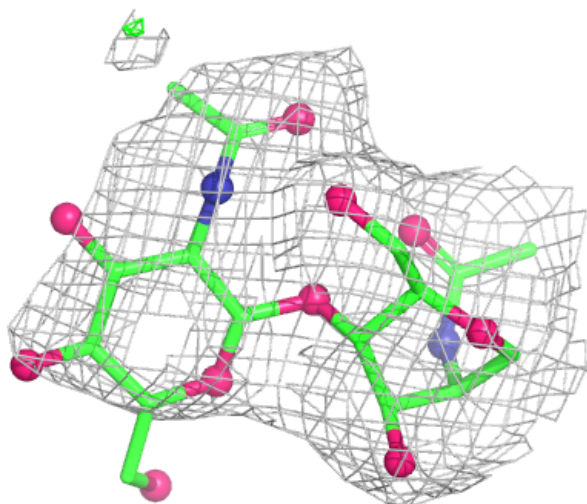
Electron density around Chain K:

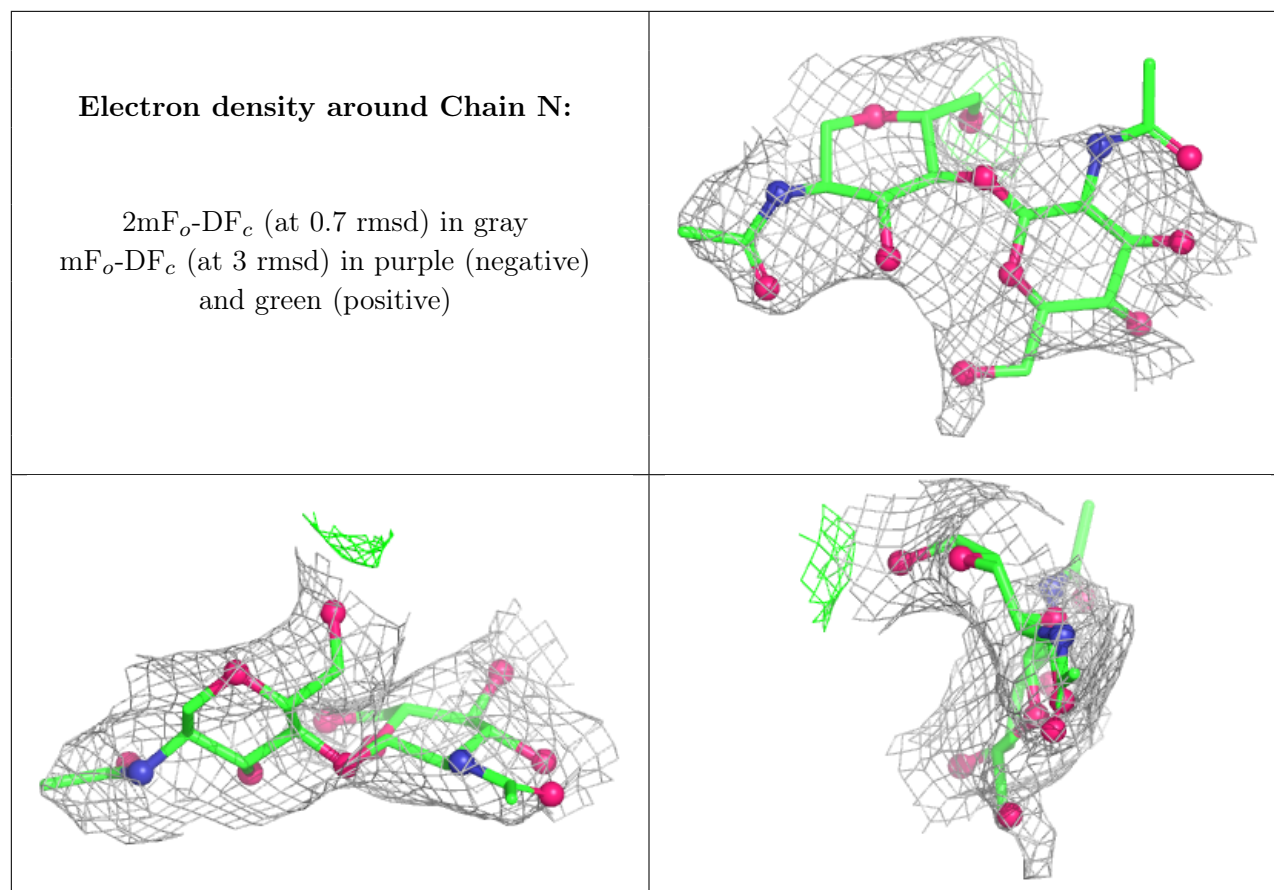
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

$2mF_o-DF_c$ (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	D	601	14/15	0.08	0.16	127,144,158,166	0
7	NAG	A	3207	14/15	0.28	0.17	124,142,162,164	0
7	NAG	A	3206	14/15	0.57	0.12	124,140,169,193	0
7	NAG	A	3201	14/15	0.60	0.12	113,136,143,154	0
7	NAG	B	601	14/15	0.67	0.12	127,150,161,161	0
7	NAG	C	603	14/15	0.72	0.11	74,89,112,123	0
7	NAG	B	602	14/15	0.75	0.10	92,114,128,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.