



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:51 AM UTC

PDB ID : 3VI4 / pdb_00003vi4
Title : Crystal structure of alpha5beta1 integrin headpiece in complex with RGD peptide
Authors : Nagae, M.; Nogi, T.; Takagi, J.
Deposited on : 2011-09-21
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

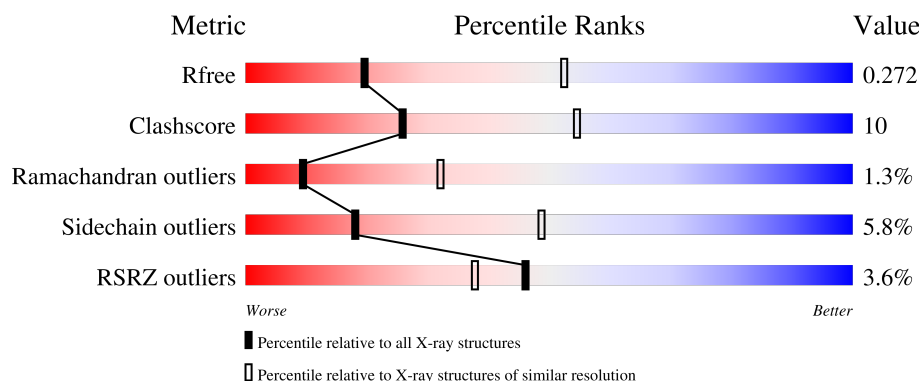
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	632	2% 76% 17% • 5%
1	C	632	5% 63% 27% • 7%
2	B	454	5% 70% 23% • 5%
2	D	454	5% 68% 25% • 5%
3	E	219	0% 72% 25% •

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Mol	Chain	Length	Quality of chain
3	L	219	
4	F	218	
4	H	218	
5	G	5	
5	I	5	
6	J	2	
6	M	2	
7	K	6	
7	N	6	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22882 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4567	2892	768	893	14			
1	C	589	Total	C	N	O	S	0	0	0
			4466	2828	747	877	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	GLY	-	expression tag	UNP P08648
A	625	GLY	-	expression tag	UNP P08648
A	626	LEU	-	expression tag	UNP P08648
A	627	GLU	-	expression tag	UNP P08648
A	628	ASN	-	expression tag	UNP P08648
A	629	LEU	-	expression tag	UNP P08648
A	630	TYR	-	expression tag	UNP P08648
A	631	PHE	-	expression tag	UNP P08648
A	632	GLN	-	expression tag	UNP P08648
C	624	GLY	-	expression tag	UNP P08648
C	625	GLY	-	expression tag	UNP P08648
C	626	LEU	-	expression tag	UNP P08648
C	627	GLU	-	expression tag	UNP P08648
C	628	ASN	-	expression tag	UNP P08648
C	629	LEU	-	expression tag	UNP P08648
C	630	TYR	-	expression tag	UNP P08648
C	631	PHE	-	expression tag	UNP P08648
C	632	GLN	-	expression tag	UNP P08648

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	0	0
			3353	2096	572	661	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	433	Total	C	N	O	S	0	0	0
			3372	2109	575	664	24			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	SEE REMARK 999	UNP P05556
B	195	THR	SER	SEE REMARK 999	UNP P05556
B	446	GLY	-	expression tag	UNP P05556
B	447	GLY	-	expression tag	UNP P05556
B	448	LEU	-	expression tag	UNP P05556
B	449	GLU	-	expression tag	UNP P05556
B	450	ASN	-	expression tag	UNP P05556
B	451	LEU	-	expression tag	UNP P05556
B	452	TYR	-	expression tag	UNP P05556
B	453	PHE	-	expression tag	UNP P05556
B	454	GLN	-	expression tag	UNP P05556
D	92	HIS	THR	SEE REMARK 999	UNP P05556
D	195	THR	SER	SEE REMARK 999	UNP P05556
D	446	GLY	-	expression tag	UNP P05556
D	447	GLY	-	expression tag	UNP P05556
D	448	LEU	-	expression tag	UNP P05556
D	449	GLU	-	expression tag	UNP P05556
D	450	ASN	-	expression tag	UNP P05556
D	451	LEU	-	expression tag	UNP P05556
D	452	TYR	-	expression tag	UNP P05556
D	453	PHE	-	expression tag	UNP P05556
D	454	GLN	-	expression tag	UNP P05556

- Molecule 3 is a protein called SG/19 Fab fragment (Light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1701	1066	292	335	8			
3	E	219	Total	C	N	O	S	0	0	0
			1701	1066	292	335	8			

- Molecule 4 is a protein called SG/19 Fab fragment (Heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	218	Total	C	N	O	S	0	0	0
			1651	1051	268	324	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	218	Total	C	N	O	S	0	0	0
			1651	1051	268	324	8			

- Molecule 5 is a protein called RGD peptide.

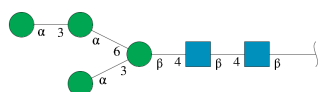
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	4	Total	C	N	O		0	0	0
			31	16	8	7				
5	I	3	Total	C	N	O		0	0	0
			23	12	6	5				

- 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	J	2	Total	C	N	O		0	0	0
			28	16	2	10				
6	M	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.

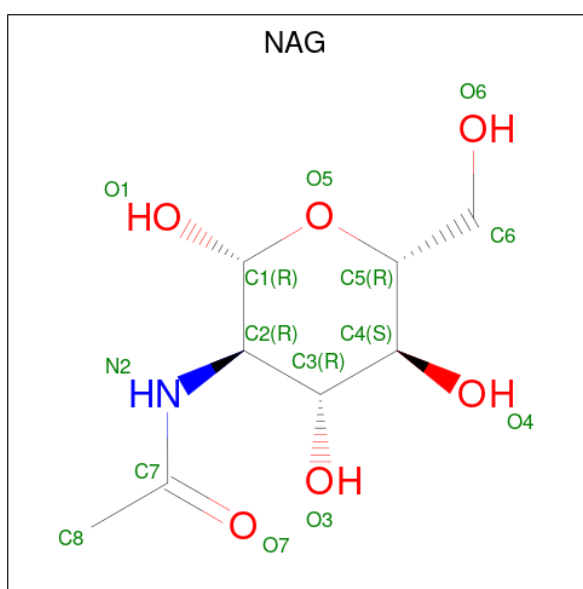


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	K	6	Total	C	N	O		0	0	0
			72	40	2	30				
7	N	6	Total	C	N	O		0	0	0
			72	40	2	30				

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total 4	Ca 4	0	0
8	B	1	Total 1	Ca 1	0	0
8	C	4	Total 4	Ca 4	0	0
8	D	1	Total 1	Ca 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		

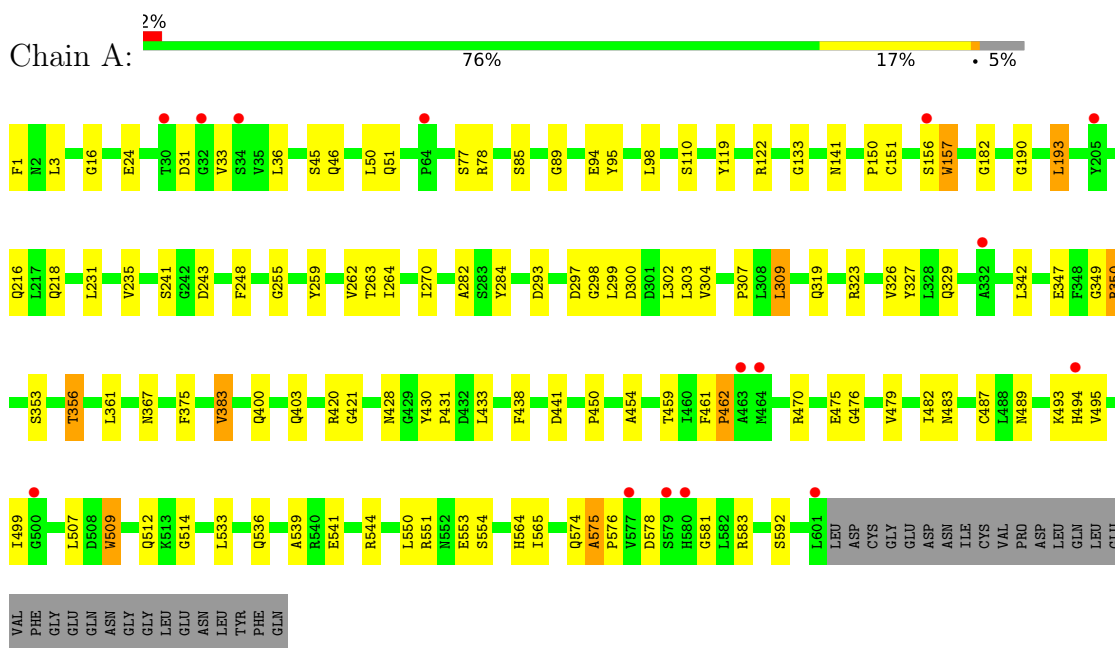
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		

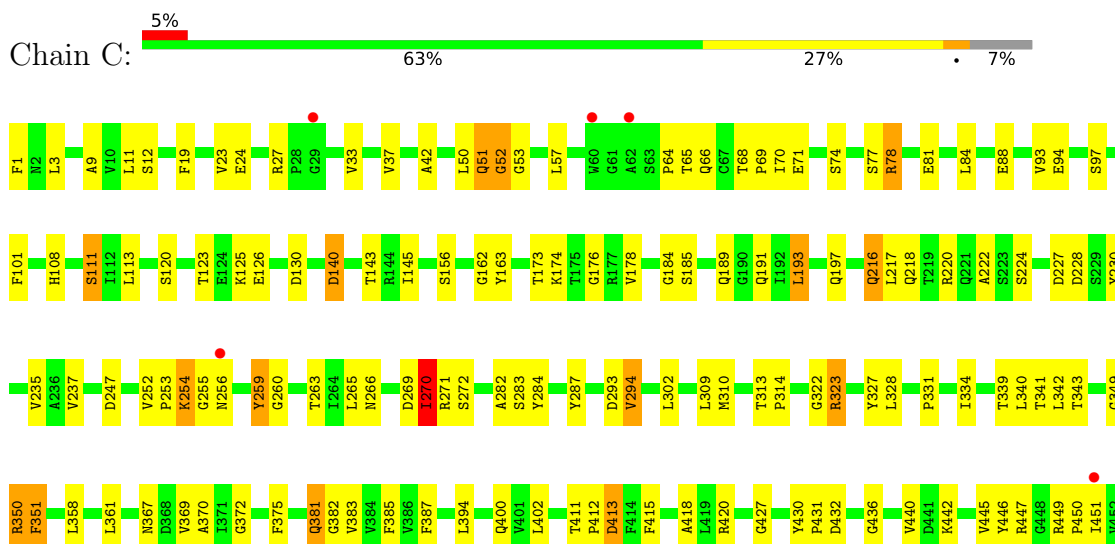
3 Residue-property plots

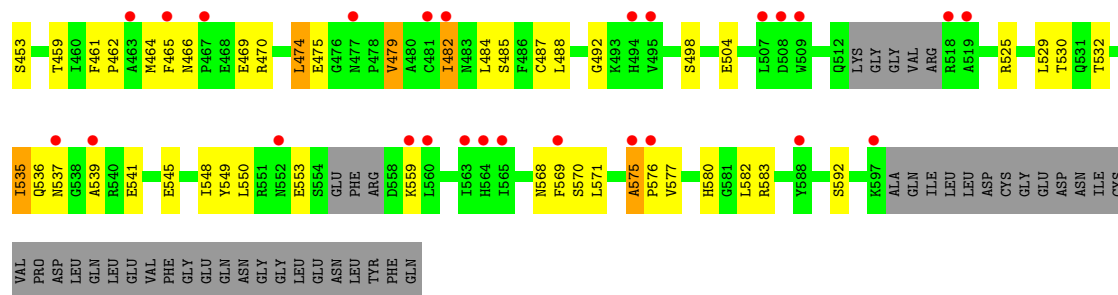
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Integrin alpha-5

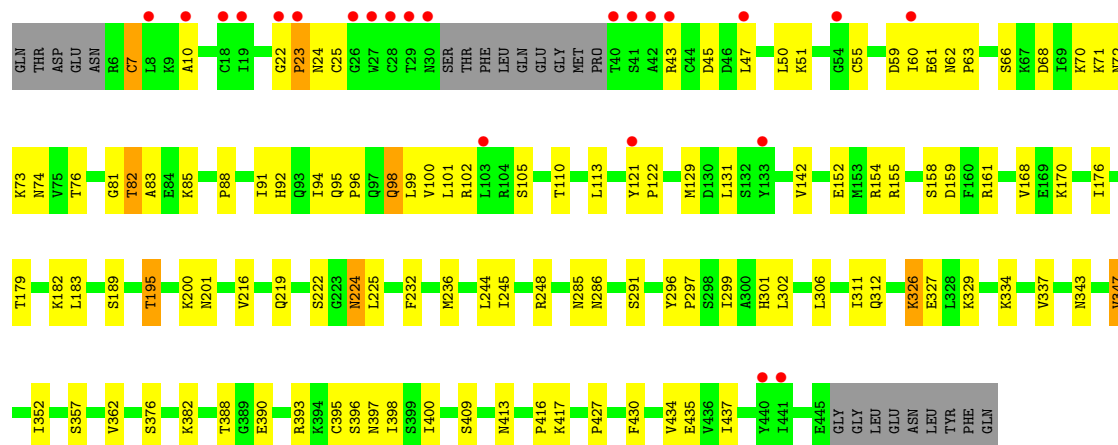


• Molecule 1: Integrin alpha-5

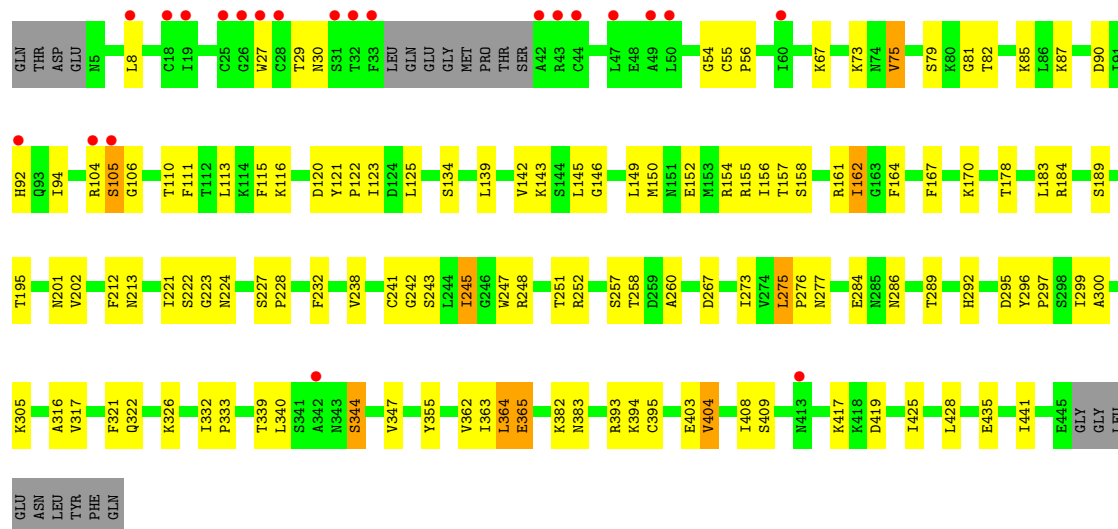




• Molecule 2: Integrin beta-1

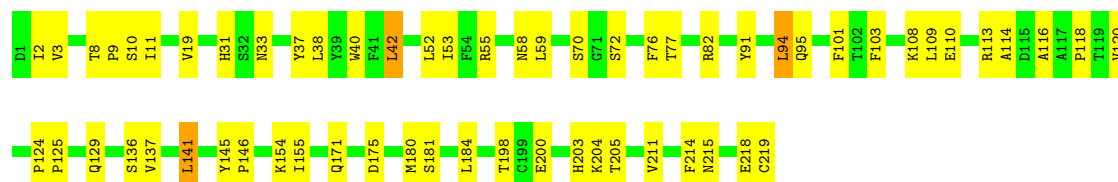


• Molecule 2: Integrin beta-1

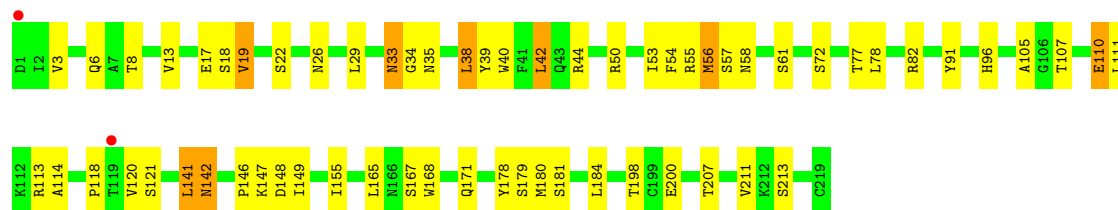


• Molecule 3: SG/19 Fab fragment (Light chain)

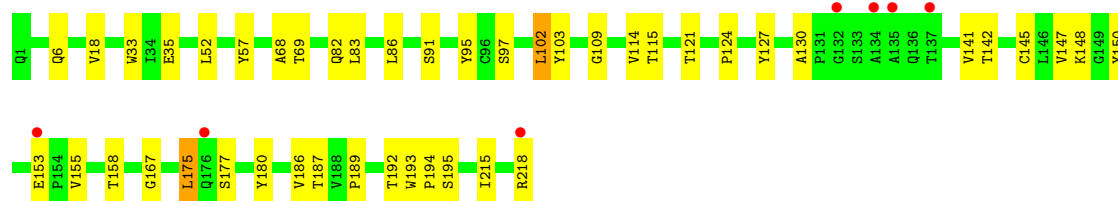
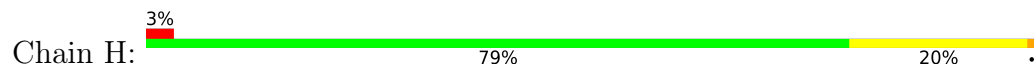




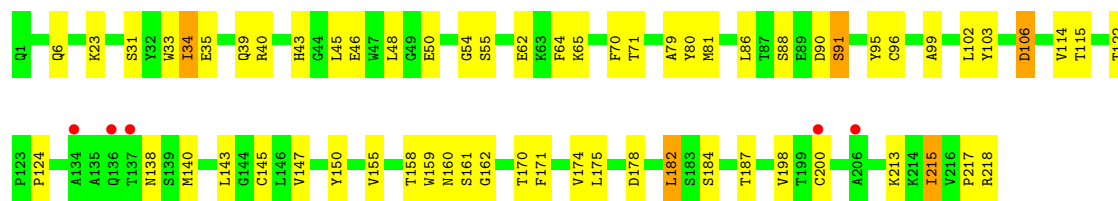
• Molecule 3: SG/19 Fab fragment (Light chain)



• Molecule 4: SG/19 Fab fragment (Heavy chain)



• Molecule 4: SG/19 Fab fragment (Heavy chain)



• Molecule 5: RGD peptide



• Molecule 5: RGD peptide





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

Chain J: 50% 50%



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

Chain M: 100%



- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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

Chain K: 33% 67%



- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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

Chain N: 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.81Å 103.87Å 125.26Å 75.72° 70.16° 70.90°	Depositor
Resolution (Å)	100.00 – 2.90 100.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (100.00-2.90) 98.4 (100.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.215 , 0.275 0.213 , 0.272	Depositor DCC
R_{free} test set	4464 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.5	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	0.93	EDS
Total number of atoms	22882	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: MAN, BMA, MG, NAG, CA

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	0.59	0/4684	0.88	9/6374 (0.1%)
1	C	0.61	0/4580	0.90	7/6234 (0.1%)
2	B	0.56	0/3410	0.86	5/4601 (0.1%)
2	D	0.57	0/3430	0.92	1/4628 (0.0%)
3	E	0.63	0/1741	0.90	3/2364 (0.1%)
3	L	0.66	0/1741	0.85	0/2364
4	F	0.68	0/1698	0.89	1/2323 (0.0%)
4	H	0.69	0/1698	0.91	6/2323 (0.3%)
5	G	0.54	0/30	0.60	0/38
5	I	0.55	0/22	0.49	0/27
All	All	0.61	0/23034	0.89	32/31276 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	142	ASN	N-CA-C	9.62	125.53	111.96
1	A	554	SER	N-CA-C	-7.75	102.17	112.72
1	A	259	TYR	N-CA-C	-7.49	99.95	110.50
4	H	153	GLU	CA-C-N	-7.43	112.33	119.76
4	H	153	GLU	C-N-CA	-7.43	112.33	119.76
1	A	353	SER	N-CA-C	6.84	118.73	111.28
1	C	156	SER	N-CA-C	6.80	119.70	111.40
1	C	259	TYR	N-CA-C	-6.67	100.16	110.10
1	A	31	ASP	N-CA-C	6.61	118.64	110.91
2	D	30	ASN	N-CA-C	6.59	120.47	111.17
2	B	55	CYS	CA-C-N	6.54	124.37	119.66
2	B	55	CYS	C-N-CA	6.54	124.37	119.66
1	A	255	GLY	N-CA-C	6.19	119.98	112.49
4	H	153	GLU	N-CA-C	5.94	121.59	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	GLY	N-CA-C	-5.86	103.71	113.02
1	C	283	SER	N-CA-C	-5.53	101.67	109.96
2	B	347	VAL	CB-CA-C	-5.42	104.94	112.04
4	H	148	LYS	N-CA-C	5.40	117.61	109.23
1	C	474	LEU	N-CA-C	-5.39	102.03	110.17
1	C	568	ASN	N-CA-C	5.39	118.24	109.24
1	A	578	ASP	N-CA-C	5.33	113.86	108.75
3	E	105	ALA	N-CA-C	-5.33	102.39	110.28
1	C	216	GLN	N-CA-C	5.32	117.40	110.43
1	A	182	GLY	CA-C-N	5.30	125.11	119.28
1	A	182	GLY	C-N-CA	5.30	125.11	119.28
2	B	129	MET	N-CA-C	5.26	117.97	109.40
4	H	52	LEU	CA-C-N	5.24	126.39	119.84
4	H	52	LEU	C-N-CA	5.24	126.39	119.84
1	A	433	LEU	N-CA-C	5.16	116.45	107.93
2	B	326	LYS	N-CA-C	-5.06	105.66	111.07
4	F	99	ALA	N-CA-C	5.05	116.92	108.99
3	E	34	GLY	N-CA-C	-5.05	108.65	115.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4567	0	4363	63	0
1	C	4466	0	4247	104	0
2	B	3353	0	3305	67	0
2	D	3372	0	3321	78	0
3	E	1701	0	1649	46	0
3	L	1701	0	1649	35	0
4	F	1651	0	1610	38	0
4	H	1651	0	1610	21	0
5	G	31	0	25	1	0
5	I	23	0	19	0	0
6	J	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	28	0	25	0	0
7	K	72	0	61	0	0
7	N	72	0	61	1	0
8	A	4	0	0	0	0
8	B	1	0	0	0	0
8	C	4	0	0	0	0
8	D	1	0	0	0	0
9	A	56	0	52	0	0
9	B	28	0	26	0	0
9	C	56	0	52	1	0
9	D	14	0	13	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
All	All	22882	0	22113	428	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 10.

All (428) 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)
4:F:48:LEU:CD1	4:F:81:MET:HE1	1.81	1.08
2:B:110:THR:HG22	2:B:409:SER:HB3	1.15	1.07
2:D:110:THR:HG22	2:D:409:SER:HB3	1.36	1.05
2:B:7:CYS:HB3	2:B:45:ASP:HA	1.39	1.01
2:D:284:GLU:HG2	2:D:289:THR:HG21	1.50	0.94
2:D:110:THR:HG22	2:D:409:SER:CB	1.98	0.93
2:B:110:THR:HG22	2:B:409:SER:CB	2.01	0.91
4:F:48:LEU:HD13	4:F:81:MET:HE1	1.53	0.90
2:B:236:MET:HE3	2:B:301:HIS:HD2	1.35	0.89
2:B:152:GLU:HG2	2:B:352:ILE:HD11	1.54	0.88
1:C:189:GLN:HE22	1:C:222:ALA:H	1.19	0.88
2:B:68:ASP:HB3	2:B:70:LYS:HE2	1.55	0.86
3:E:147:LYS:HG3	3:E:147:LYS:O	1.76	0.86
1:A:475:GLU:HG3	1:A:476:GLY:H	1.40	0.85
2:B:71:LYS:HB3	2:B:98:GLN:HB2	1.59	0.84
4:F:48:LEU:HD12	4:F:81:MET:HE1	1.59	0.84
2:B:158:SER:HA	3:E:55:ARG:HH12	1.43	0.83
3:E:54:PHE:HE2	3:E:55:ARG:HH21	1.27	0.82
1:A:241:SER:HB2	6:J:1:NAG:H82	1.61	0.81
2:B:113:LEU:HD11	2:B:434:VAL:HG21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:200:GLU:HG2	3:L:211:VAL:HG22	1.63	0.81
1:A:150:PRO:HB3	1:A:216:GLN:HE22	1.44	0.80
1:C:461:PHE:HB3	1:C:462:PRO:HD3	1.63	0.80
1:A:462:PRO:HD2	1:A:482:ILE:HG23	1.64	0.79
1:A:193:LEU:HD23	1:A:218:GLN:HG2	1.67	0.77
1:A:356:THR:HG21	1:A:421:GLY:H	1.47	0.77
1:C:504:GLU:HG3	1:C:530:THR:HG22	1.67	0.76
2:D:170:LYS:HD2	2:D:296:TYR:CZ	2.20	0.76
1:C:328:LEU:HD12	1:C:339:THR:HG21	1.68	0.75
2:D:161:ARG:NH2	2:D:248:ARG:HD3	2.00	0.75
3:E:33:ASN:HB3	3:E:35:ASN:HD22	1.52	0.75
2:B:45:ASP:H	2:B:50:LEU:HD12	1.52	0.75
1:C:78:ARG:HD3	1:C:94:GLU:OE2	1.87	0.74
2:B:152:GLU:CG	2:B:352:ILE:HD11	2.16	0.74
2:B:236:MET:HE3	2:B:301:HIS:CD2	2.22	0.74
2:D:273:ILE:HD12	2:D:292:HIS:O	1.85	0.74
1:C:349:GLY:HA2	1:C:375:PHE:HB2	1.70	0.73
1:C:293:ASP:O	1:C:367:ASN:HB2	1.88	0.73
4:F:62:GLU:HA	4:F:65:LYS:HG3	1.71	0.73
1:A:509:TRP:O	1:A:512:GLN:HG2	1.89	0.72
1:C:323:ARG:NH1	1:C:343:THR:OG1	2.24	0.71
2:D:247:TRP:HB3	2:D:252:ARG:HE	1.56	0.71
2:B:236:MET:CE	2:B:301:HIS:HD2	2.03	0.71
1:A:293:ASP:O	1:A:367:ASN:HB2	1.90	0.71
2:D:162:ILE:HG21	2:D:212:PHE:CD1	2.26	0.71
1:C:427:GLY:HA3	1:C:580:HIS:CE1	2.25	0.70
2:D:73:LYS:HD3	2:D:92:HIS:CE1	2.26	0.70
2:D:247:TRP:HB3	2:D:252:ARG:NE	2.07	0.70
2:D:75:VAL:CG1	2:D:116:LYS:HD3	2.21	0.69
2:B:72:ASN:HB2	2:B:96:PRO:HA	1.74	0.68
1:C:53:GLY:HA3	1:C:101:PHE:O	1.92	0.68
4:F:48:LEU:CD1	4:F:81:MET:CE	2.67	0.68
1:A:574:GLN:C	1:A:576:PRO:HD3	2.18	0.68
2:B:400:ILE:O	4:F:31:SER:HB3	1.95	0.67
1:A:24:GLU:HB3	1:A:36:LEU:HB2	1.77	0.67
1:A:77:SER:HB2	1:A:94:GLU:HG3	1.77	0.67
3:E:142:ASN:O	3:E:179:SER:OG	2.10	0.67
3:E:3:VAL:H	3:E:26:ASN:HB2	1.60	0.66
2:B:122:PRO:HB3	2:B:159:ASP:HB3	1.78	0.66
1:A:356:THR:HG21	1:A:421:GLY:N	2.09	0.66
1:C:569:PHE:HB2	1:C:592:SER:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:40:TRP:HB2	3:E:53:ILE:HB	1.78	0.65
3:E:13:VAL:HG21	3:E:19:VAL:HG21	1.78	0.64
2:D:201:ASN:HB3	2:D:286:ASN:HB3	1.79	0.64
1:A:575:ALA:N	1:A:576:PRO:HD3	2.12	0.64
1:C:453:SER:H	1:C:492:GLY:HA3	1.62	0.64
2:D:162:ILE:CG2	2:D:212:PHE:CD1	2.81	0.64
1:A:576:PRO:HG2	1:A:583:ARG:HG2	1.81	0.63
1:C:3:LEU:HB2	1:C:400:GLN:HE22	1.63	0.63
2:B:99:LEU:HD21	2:B:101:LEU:HD13	1.81	0.63
1:A:157:TRP:CZ2	2:B:225:LEU:HD11	2.34	0.63
2:B:158:SER:HA	3:E:55:ARG:NH1	2.13	0.63
2:D:104:ARG:HG3	2:D:105:SER:H	1.64	0.62
1:C:27:ARG:HG2	1:C:33:VAL:HG13	1.80	0.62
3:E:17:GLU:HG2	3:E:18:SER:H	1.64	0.62
1:C:256:ASN:HB2	1:C:259:TYR:HB2	1.82	0.62
1:A:1:PHE:H1	1:A:400:GLN:HB2	1.64	0.62
1:C:351:PHE:O	1:C:372:GLY:O	2.17	0.62
2:D:284:GLU:CG	2:D:289:THR:HG21	2.27	0.62
2:D:115:PHE:CE2	2:D:362:VAL:HG21	2.34	0.62
3:E:33:ASN:HB3	3:E:35:ASN:ND2	2.13	0.62
1:C:487:CYS:HB3	1:C:541:GLU:HB3	1.82	0.62
4:F:48:LEU:HD13	4:F:81:MET:CE	2.26	0.62
4:F:46:GLU:OE2	4:F:64:PHE:HE1	1.83	0.61
2:B:236:MET:CE	2:B:301:HIS:CD2	2.81	0.61
2:D:85:LYS:HG2	3:L:37:TYR:CZ	2.35	0.60
2:B:176:ILE:HG22	2:B:224:ASN:HB2	1.83	0.60
2:D:156:ILE:HG21	2:D:355:TYR:CE2	2.36	0.60
3:L:120:VAL:HG13	3:L:141:LEU:HD23	1.83	0.60
3:E:8:THR:O	3:E:107:THR:HG22	2.01	0.60
2:D:178:THR:HA	2:D:183:LEU:HD13	1.82	0.60
3:E:146:PRO:HB2	3:E:148:ASP:HB2	1.84	0.60
4:F:48:LEU:HD12	4:F:81:MET:CE	2.29	0.60
3:E:13:VAL:HG21	3:E:19:VAL:CG2	2.30	0.60
2:D:395:CYS:SG	2:D:404:VAL:HG11	2.42	0.59
3:L:113:ARG:HG2	3:L:114:ALA:N	2.17	0.59
4:F:70:PHE:CE1	4:F:81:MET:HG3	2.36	0.59
2:B:201:ASN:HB3	2:B:286:ASN:HB3	1.83	0.59
4:H:142:THR:OG1	4:H:187:THR:HG22	2.01	0.59
1:C:575:ALA:HB3	1:C:576:PRO:HD3	1.83	0.59
1:C:411:THR:HB	1:C:412:PRO:HD2	1.84	0.59
1:A:110:SER:HB2	1:A:141:ASN:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:PRO:HB2	1:A:350:ARG:HB3	1.86	0.58
1:C:77:SER:HB2	1:C:94:GLU:HG3	1.86	0.58
1:C:113:LEU:HD11	1:C:178:VAL:HG13	1.84	0.58
2:B:142:VAL:HG12	2:B:216:VAL:HG11	1.86	0.58
2:B:121:TYR:CD2	2:B:122:PRO:HD2	2.39	0.57
3:E:6:GLN:NE2	3:E:107:THR:HG23	2.19	0.57
4:F:159:TRP:CZ3	4:F:200:CYS:HB3	2.39	0.57
4:F:143:LEU:HB3	4:F:215:ILE:HD12	1.86	0.57
1:C:111:SER:OG	1:C:197:GLN:NE2	2.37	0.57
1:A:85:SER:HA	1:A:89:GLY:HA3	1.86	0.57
1:A:95:TYR:OH	1:A:122:ARG:HB2	2.05	0.57
2:B:110:THR:CG2	2:B:409:SER:HB3	2.10	0.57
1:C:485:SER:HB3	1:C:545:GLU:HG2	1.86	0.57
4:F:91:SER:HA	4:F:114:VAL:O	2.05	0.57
1:C:361:LEU:HA	1:C:431:PRO:HG2	1.87	0.57
1:A:487:CYS:HB3	1:A:541:GLU:HG2	1.86	0.56
2:B:83:ALA:HA	2:B:85:LYS:HZ3	1.70	0.56
1:C:323:ARG:HG2	1:C:342:LEU:O	2.05	0.56
1:C:382:GLY:HA3	1:C:415:PHE:O	2.05	0.56
2:B:61:GLU:C	2:B:63:PRO:HD3	2.31	0.56
3:L:118:PRO:HD3	3:L:203:HIS:ND1	2.21	0.56
2:B:170:LYS:HE3	2:B:291:SER:O	2.06	0.56
1:C:140:ASP:HB2	1:C:143:THR:OG1	2.06	0.56
2:D:164:PHE:HD2	2:D:202:VAL:HB	1.71	0.56
1:C:449:ARG:HG2	1:C:582:LEU:HB3	1.87	0.56
2:D:284:GLU:HG2	2:D:289:THR:CG2	2.31	0.56
2:D:152:GLU:HA	2:D:155:ARG:HH11	1.69	0.55
1:C:302:LEU:HB3	1:C:327:TYR:HB2	1.88	0.55
2:D:408:ILE:HD13	2:D:425:ILE:HD13	1.87	0.55
2:B:312:GLN:HG2	2:B:334:LYS:HG3	1.88	0.55
3:E:113:ARG:HG2	3:E:114:ALA:H	1.72	0.55
1:A:461:PHE:HB3	1:A:462:PRO:HD3	1.88	0.55
1:C:282:ALA:HB3	2:D:299:ILE:HD12	1.88	0.55
3:E:6:GLN:HE21	3:E:107:THR:HG23	1.73	0.54
3:E:111:LEU:H	3:E:171:GLN:HE22	1.55	0.54
4:F:39:GLN:HG3	4:F:45:LEU:HD23	1.88	0.54
1:C:78:ARG:O	1:C:93:VAL:HG12	2.07	0.54
3:E:17:GLU:HG2	3:E:18:SER:N	2.23	0.54
3:L:42:LEU:HD13	3:L:91:TYR:CZ	2.42	0.54
3:E:113:ARG:HG2	3:E:114:ALA:N	2.22	0.54
3:E:147:LYS:O	3:E:147:LYS:CG	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:SER:HB3	7:N:1:NAG:H83	1.89	0.54
4:F:160:ASN:HD21	4:F:198:VAL:HA	1.71	0.54
2:D:110:THR:HG22	2:D:409:SER:HB2	1.87	0.54
2:B:82:THR:HG23	3:E:96:HIS:NE2	2.23	0.53
1:A:3:LEU:HB2	1:A:400:GLN:HE22	1.72	0.53
2:B:154:ARG:O	3:E:55:ARG:NH2	2.41	0.53
1:C:269:ASP:O	1:C:270:ILE:C	2.51	0.53
3:L:40:TRP:HB2	3:L:53:ILE:HB	1.91	0.53
2:D:238:VAL:HA	2:D:245:ILE:HD13	1.90	0.53
2:B:82:THR:O	2:B:85:LYS:NZ	2.41	0.53
1:C:50:LEU:O	1:C:97:SER:HA	2.09	0.53
1:C:430:TYR:CE1	1:C:450:PRO:HA	2.43	0.53
1:A:193:LEU:CD2	1:A:218:GLN:HG2	2.37	0.53
1:C:313:THR:HB	1:C:314:PRO:HD2	1.89	0.53
2:D:154:ARG:NH1	3:L:58:ASN:OD1	2.41	0.53
3:E:54:PHE:O	3:E:55:ARG:HG3	2.09	0.53
1:A:536:GLN:HB3	1:A:539:ALA:HB2	1.90	0.53
4:F:160:ASN:C	4:F:162:GLY:H	2.17	0.53
4:F:217:PRO:O	4:F:218:ARG:HB2	2.09	0.53
1:C:310:MET:HG3	2:D:300:ALA:HB2	1.89	0.53
2:B:236:MET:HE2	2:B:302:LEU:HD23	1.91	0.52
2:D:67:LYS:NZ	2:D:111:PHE:HA	2.25	0.52
2:D:121:TYR:CD2	2:D:122:PRO:HD2	2.45	0.52
4:F:62:GLU:HG2	4:F:65:LYS:HE3	1.92	0.52
2:B:390:GLU:O	2:B:393:ARG:HG2	2.10	0.52
1:A:356:THR:HG21	1:A:420:ARG:HA	1.91	0.52
2:D:260:ALA:HA	2:D:321:PHE:CE2	2.44	0.52
1:C:12:SER:HB3	1:C:442:LYS:HG2	1.91	0.52
1:A:156:SER:O	1:A:157:TRP:HB2	2.10	0.51
1:A:302:LEU:HB3	1:A:327:TYR:HB2	1.92	0.51
2:D:104:ARG:HA	2:D:441:ILE:HB	1.92	0.51
1:C:81:GLU:O	1:C:84:LEU:HG	2.11	0.51
4:H:91:SER:HA	4:H:114:VAL:O	2.10	0.51
2:B:170:LYS:HD2	2:B:296:TYR:CZ	2.46	0.51
2:D:257:SER:HA	2:D:316:ALA:O	2.11	0.51
3:L:219:CYS:HB2	4:H:218:ARG:HH12	1.75	0.51
4:H:6:GLN:HE22	4:H:95:TYR:HA	1.75	0.51
1:C:331:PRO:O	3:E:82:ARG:NH1	2.44	0.50
2:D:167:PHE:CD1	2:D:167:PHE:C	2.89	0.50
1:C:474:LEU:HD23	1:C:475:GLU:N	2.26	0.50
1:C:349:GLY:O	1:C:351:PHE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:C	1:A:553:GLU:H	2.17	0.50
3:E:120:VAL:HG22	3:E:141:LEU:HD22	1.92	0.50
4:F:40:ARG:HB2	4:F:43:HIS:HB2	1.93	0.50
1:A:509:TRP:CE3	1:A:564:HIS:HB3	2.46	0.50
2:B:74:ASN:HA	2:B:95:GLN:OE1	2.12	0.50
1:A:297:ASP:O	1:A:299:LEU:N	2.34	0.49
2:B:83:ALA:HA	2:B:85:LYS:NZ	2.26	0.49
1:C:71:GLU:OE1	1:C:74:SER:HB3	2.11	0.49
1:C:488:LEU:HD12	1:C:535:ILE:HD11	1.94	0.49
1:A:383:VAL:HG22	1:A:403:GLN:HG2	1.93	0.49
2:D:104:ARG:HG3	2:D:105:SER:N	2.27	0.49
1:A:323:ARG:HG3	1:A:342:LEU:O	2.11	0.49
2:B:105:SER:HB2	2:B:413:ASN:O	2.13	0.49
3:L:55:ARG:NH1	4:H:102:LEU:O	2.45	0.49
4:F:6:GLN:HE22	4:F:95:TYR:HA	1.77	0.49
2:B:98:GLN:HG2	2:B:435:GLU:HB2	1.93	0.49
1:C:465:PHE:CD1	1:C:550:LEU:HB2	2.47	0.49
1:C:254:LYS:HE3	2:D:267:ASP:OD2	2.13	0.49
1:C:570:SER:HB2	9:C:2016:NAG:O7	2.13	0.49
2:B:100:VAL:HG22	2:B:437:ILE:HB	1.95	0.49
2:B:47:LEU:HA	2:B:51:LYS:HD2	1.95	0.48
3:E:147:LYS:HB3	3:E:178:TYR:CZ	2.48	0.48
1:C:382:GLY:HA3	1:C:415:PHE:HB3	1.95	0.48
2:D:222:SER:OG	2:D:223:GLY:N	2.46	0.48
2:B:72:ASN:CB	2:B:96:PRO:HA	2.41	0.48
1:C:163:TYR:O	1:C:184:GLY:HA3	2.13	0.48
2:D:221:ILE:HG22	2:D:222:SER:O	2.13	0.48
1:C:418:ALA:HB3	1:C:436:GLY:HA3	1.95	0.48
2:B:232:PHE:HB3	2:B:297:PRO:HD2	1.96	0.48
1:C:498:SER:HA	1:C:536:GLN:HG2	1.96	0.48
3:E:53:ILE:HA	3:E:58:ASN:O	2.13	0.48
1:A:493:LYS:HE3	1:A:494:HIS:CE1	2.49	0.48
2:B:66:SER:H	2:B:102:ARG:HB2	1.78	0.48
3:E:155:ILE:HD11	3:E:184:LEU:HD21	1.95	0.48
1:A:303:LEU:HD22	1:A:326:VAL:HG22	1.95	0.48
2:D:417:LYS:C	2:D:419:ASP:H	2.22	0.48
3:E:42:LEU:HD13	3:E:91:TYR:CZ	2.49	0.48
1:C:475:GLU:OE2	1:C:525:ARG:NH2	2.46	0.48
2:B:326:LYS:O	2:B:329:LYS:HB3	2.14	0.48
1:C:173:THR:HG22	1:C:237:VAL:HG11	1.96	0.48
2:D:125:LEU:C	2:D:125:LEU:HD23	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:ARG:HA	2:D:195:THR:HG22	1.95	0.47
4:H:35:GLU:HB2	4:H:97:SER:HB3	1.96	0.47
4:H:175:LEU:HD13	4:H:180:TYR:CE1	2.48	0.47
1:C:19:PHE:CE1	1:C:37:VAL:HG11	2.49	0.47
1:C:224:SER:HB3	5:G:5001:ARG:HE	1.80	0.47
2:D:143:LYS:O	2:D:213:ASN:ND2	2.47	0.47
2:B:168:VAL:HG21	2:B:222:SER:HB3	1.97	0.47
2:B:200:LYS:NZ	2:B:219:GLN:HE22	2.12	0.47
2:D:241:CYS:HB2	2:D:245:ILE:HD12	1.97	0.47
4:F:124:PRO:HB2	4:F:147:VAL:HG13	1.97	0.47
1:C:255:GLY:O	1:C:256:ASN:C	2.58	0.47
1:C:385:PHE:HB3	1:C:387:PHE:CE1	2.49	0.47
2:D:75:VAL:HG11	2:D:116:LYS:HD3	1.95	0.47
1:A:507:LEU:HD23	1:A:565:ILE:HG23	1.96	0.47
1:C:265:LEU:HA	1:C:271:ARG:O	2.15	0.47
2:D:322:GLN:O	2:D:326:LYS:HG2	2.15	0.47
2:B:161:ARG:HH11	2:B:248:ARG:HE	1.62	0.47
2:D:149:LEU:HD23	2:D:162:ILE:HD11	1.96	0.47
1:C:57:LEU:HB2	1:C:70:ILE:HD11	1.97	0.46
1:C:255:GLY:H	1:C:260:GLY:HA2	1.79	0.46
3:L:95:GLN:NE2	3:L:101:PHE:HA	2.30	0.46
3:L:129:GLN:HE22	3:L:136:SER:HB2	1.80	0.46
4:H:193:TRP:CD1	4:H:194:PRO:HA	2.49	0.46
1:A:190:GLY:HA3	1:A:231:LEU:HB3	1.96	0.46
2:B:179:THR:HB	2:B:182:LYS:HB2	1.97	0.46
2:D:238:VAL:HA	2:D:245:ILE:CD1	2.45	0.46
1:C:474:LEU:HD23	1:C:475:GLU:H	1.79	0.46
4:F:170:THR:HG23	4:F:184:SER:HB2	1.96	0.46
1:C:19:PHE:CZ	1:C:37:VAL:HG11	2.50	0.46
2:D:116:LYS:HB2	2:D:403:GLU:HG2	1.98	0.46
3:L:52:LEU:C	3:L:53:ILE:HD12	2.40	0.46
3:E:44:ARG:NH1	3:E:50:ARG:HH11	2.13	0.46
1:A:50:LEU:O	1:A:51:GLN:C	2.59	0.46
1:A:282:ALA:HB3	2:B:299:ILE:HD12	1.96	0.46
1:C:465:PHE:CE1	1:C:550:LEU:HB2	2.51	0.46
3:L:113:ARG:HG2	3:L:114:ALA:O	2.16	0.46
1:C:525:ARG:HG2	1:C:549:TYR:OH	2.16	0.46
4:H:18:VAL:HG12	4:H:86:LEU:HD11	1.98	0.46
4:F:124:PRO:HB3	4:F:150:TYR:HB3	1.98	0.46
2:B:50:LEU:HD22	2:B:51:LYS:HG3	1.98	0.46
2:B:73:LYS:HD3	2:B:92:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:TYR:CE1	1:A:450:PRO:HA	2.51	0.45
2:D:152:GLU:HA	2:D:155:ARG:NH1	2.31	0.45
2:D:156:ILE:HG21	2:D:355:TYR:HE2	1.81	0.45
3:L:31:HIS:HD2	3:L:33:ASN:H	1.63	0.45
2:B:427:PRO:HG2	2:B:430:PHE:HB2	1.97	0.45
1:C:294:VAL:HG11	1:C:394:LEU:HB2	1.97	0.45
1:C:349:GLY:O	1:C:350:ARG:C	2.59	0.45
1:C:577:VAL:HG22	1:C:583:ARG:HE	1.80	0.45
1:C:24:GLU:HA	1:C:420:ARG:HG2	1.98	0.45
1:C:130:ASP:HB3	1:C:162:GLY:O	2.17	0.45
1:A:454:ALA:HA	1:A:489:ASN:O	2.16	0.45
3:L:125:PRO:HD3	3:L:137:VAL:HG22	1.98	0.45
3:E:198:THR:HG22	3:E:213:SER:OG	2.16	0.45
1:C:340:LEU:HG	1:C:341:THR:N	2.30	0.45
2:B:62:ASN:N	2:B:63:PRO:HD3	2.32	0.45
1:C:474:LEU:O	1:C:475:GLU:C	2.60	0.45
3:L:154:LYS:HB2	3:L:198:THR:HB	1.98	0.45
3:E:110:GLU:OE2	3:E:147:LYS:HD2	2.16	0.45
2:D:162:ILE:CG2	2:D:212:PHE:HD1	2.29	0.45
2:B:88:PRO:HA	2:B:91:ILE:HD12	1.99	0.44
2:D:340:LEU:HD11	2:D:344:SER:HA	1.99	0.44
3:L:110:GLU:HB3	3:L:171:GLN:HE22	1.82	0.44
3:E:22:SER:HB3	3:E:77:THR:HG22	1.99	0.44
4:F:35:GLU:OE2	4:F:50:GLU:OE1	2.35	0.44
4:F:86:LEU:HA	4:F:90:ASP:OD2	2.17	0.44
1:A:438:PHE:CD1	1:A:438:PHE:C	2.95	0.44
1:C:3:LEU:HD22	1:C:446:TYR:HB3	1.99	0.44
1:C:470:ARG:HD2	1:C:479:VAL:HA	1.99	0.44
1:C:216:GLN:HG2	1:C:217:LEU:N	2.32	0.44
2:D:364:LEU:O	2:D:393:ARG:HD3	2.16	0.44
2:D:395:CYS:SG	2:D:404:VAL:CG1	3.06	0.44
3:L:155:ILE:HD11	3:L:184:LEU:HD21	1.98	0.44
1:A:428:ASN:HB2	1:A:430:TYR:HD1	1.82	0.44
4:H:130:ALA:HB2	4:H:215:ILE:HG23	2.00	0.44
4:F:91:SER:OG	4:F:115:THR:HA	2.18	0.44
4:F:71:THR:OG1	4:F:80:TYR:HB2	2.16	0.44
1:A:361:LEU:HA	1:A:431:PRO:HG2	2.00	0.44
1:A:509:TRP:HE3	1:A:564:HIS:HB3	1.83	0.44
3:L:124:PRO:HB3	3:L:214:PHE:CZ	2.53	0.44
1:C:3:LEU:HD22	1:C:446:TYR:CB	2.48	0.44
2:D:305:LYS:HD3	2:D:305:LYS:HA	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:LEU:HD22	1:C:323:ARG:HB2	2.00	0.43
1:C:413:ASP:HB3	1:C:440:VAL:HG22	2.00	0.43
2:D:82:THR:O	2:D:85:LYS:NZ	2.48	0.43
1:A:309:LEU:HD22	1:A:323:ARG:HB2	2.00	0.43
1:A:349:GLY:HA2	1:A:375:PHE:HB2	2.00	0.43
2:B:22:GLY:HA3	2:B:23:PRO:HD3	1.77	0.43
2:D:75:VAL:HG11	2:D:116:LYS:HB3	2.00	0.43
4:H:124:PRO:HB3	4:H:150:TYR:HB3	2.00	0.43
4:H:167:GLY:O	4:H:186:VAL:HA	2.17	0.43
4:F:174:VAL:HG12	4:F:175:LEU:N	2.33	0.43
1:C:466:ASN:HB3	1:C:469:GLU:HB2	1.99	0.43
2:D:154:ARG:HB3	3:L:55:ARG:NH2	2.33	0.43
3:L:31:HIS:CD2	3:L:33:ASN:H	2.36	0.43
1:C:185:SER:HB2	1:C:191:GLN:HB2	2.01	0.43
3:E:38:LEU:HG	3:E:39:TYR:N	2.32	0.43
2:B:131:LEU:HD23	2:B:131:LEU:HA	1.70	0.43
4:H:68:ALA:HA	4:H:82:GLN:O	2.19	0.43
1:A:248:PHE:O	1:A:264:ILE:HA	2.18	0.43
1:C:50:LEU:O	1:C:51:GLN:C	2.62	0.43
1:C:322:GLY:HA3	1:C:351:PHE:HB3	2.00	0.43
2:D:363:ILE:HG12	2:D:394:LYS:HG2	2.00	0.43
1:A:475:GLU:HG3	1:A:476:GLY:N	2.19	0.43
3:L:94:LEU:HB2	3:L:103:PHE:CD1	2.54	0.43
3:E:3:VAL:H	3:E:26:ASN:CB	2.28	0.43
4:F:35:GLU:O	4:F:96:CYS:HA	2.19	0.43
1:C:432:ASP:OD1	1:C:447:ARG:HA	2.18	0.43
1:C:465:PHE:CE1	1:C:482:ILE:HD13	2.54	0.43
2:D:85:LYS:HB2	3:L:31:HIS:CE1	2.53	0.43
2:D:120:ASP:OD2	2:D:158:SER:OG	2.31	0.43
4:H:189:PRO:O	4:H:192:THR:OG1	2.35	0.43
1:C:23:VAL:HG23	1:C:420:ARG:HB2	2.01	0.42
1:C:358:LEU:HD11	1:C:370:ALA:HB2	2.00	0.42
1:C:284:TYR:CD2	1:C:287:TYR:HD1	2.37	0.42
4:H:102:LEU:HG	4:H:103:TYR:HB2	2.02	0.42
3:E:200:GLU:HG2	3:E:211:VAL:HG22	2.01	0.42
4:F:106:ASP:OD1	4:F:106:ASP:N	2.44	0.42
4:F:103:TYR:CE2	4:F:106:ASP:HB3	2.55	0.42
1:A:461:PHE:HB3	1:A:483:ASN:HB2	2.00	0.42
1:C:120:SER:HA	1:C:130:ASP:O	2.19	0.42
1:C:569:PHE:HD2	1:C:592:SER:HA	1.85	0.42
2:D:123:ILE:HD12	2:D:157:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:LYS:HD2	2:D:296:TYR:CE2	2.53	0.42
1:A:50:LEU:HD23	1:A:98:LEU:HD21	2.01	0.42
2:D:227:SER:HB3	2:D:228:PRO:HD3	2.01	0.42
3:E:168:TRP:CE2	3:E:180:MET:HE3	2.55	0.42
1:C:68:THR:HA	1:C:69:PRO:HD3	1.95	0.42
2:D:67:LYS:HZ2	2:D:111:PHE:HA	1.84	0.42
2:D:79:SER:HA	4:H:57:TYR:CD2	2.54	0.42
3:E:167:SER:OG	4:F:171:PHE:HB3	2.20	0.42
1:A:119:TYR:HB3	1:A:133:GLY:HA2	2.02	0.42
2:B:183:LEU:O	2:B:195:THR:HB	2.19	0.42
2:D:55:CYS:HA	2:D:56:PRO:HD3	1.83	0.42
2:B:155:ARG:NH1	3:E:61:SER:HB3	2.35	0.41
3:L:8:THR:HG21	3:L:11:ILE:HG12	2.02	0.41
2:D:365:GLU:HG2	2:D:428:LEU:HG	2.01	0.41
1:A:151:CYS:SG	1:A:193:LEU:HD11	2.60	0.41
1:A:300:ASP:O	1:A:329:GLN:NE2	2.49	0.41
1:A:319:GLN:HB2	1:A:347:GLU:HG2	2.01	0.41
3:L:180:MET:HG2	3:L:181:SER:N	2.36	0.41
1:A:262:VAL:HG21	1:A:304:VAL:CG2	2.50	0.41
1:A:470:ARG:HB3	1:A:479:VAL:C	2.46	0.41
4:H:124:PRO:HB2	4:H:147:VAL:HG13	2.01	0.41
1:A:24:GLU:OE2	1:A:24:GLU:HA	2.21	0.41
1:C:382:GLY:CA	1:C:415:PHE:HB3	2.50	0.41
2:D:81:GLY:HA2	4:H:33:TRP:CZ2	2.55	0.41
2:D:382:LYS:HG2	2:D:383:ASN:HD22	1.86	0.41
3:L:10:SER:HB2	3:L:108:LYS:HB3	2.02	0.41
3:E:113:ARG:NH1	3:E:114:ALA:O	2.51	0.41
2:B:142:VAL:O	2:B:142:VAL:CG1	2.67	0.41
2:B:395:CYS:HB3	2:B:398:ILE:HD11	2.03	0.41
1:C:53:GLY:H	1:C:101:PHE:H	1.68	0.41
1:C:230:TYR:HB2	1:C:253:PRO:HD2	2.02	0.41
1:C:484:LEU:HD12	1:C:548:ILE:HD13	2.03	0.41
2:D:232:PHE:HB3	2:D:297:PRO:HG2	2.02	0.41
2:D:275:LEU:HD12	2:D:276:PRO:HD2	2.01	0.41
2:D:277:ASN:HB2	2:D:295:ASP:O	2.21	0.41
3:L:215:ASN:HB2	3:L:218:GLU:HG3	2.03	0.41
1:A:45:SER:O	1:A:46:GLN:C	2.64	0.41
1:C:42:ALA:O	1:C:52:GLY:O	2.39	0.41
2:D:87:LYS:HB2	2:D:90:ASP:OD1	2.21	0.41
1:C:427:GLY:HA3	1:C:580:HIS:HE1	1.81	0.41
3:L:116:ALA:O	3:L:205:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:CG2	1:A:421:GLY:H	2.26	0.41
1:A:533:LEU:CD2	1:A:544:ARG:HE	2.33	0.41
1:A:551:ARG:C	1:A:553:GLU:N	2.79	0.41
2:B:81:GLY:HA2	4:F:33:TRP:CZ2	2.56	0.41
2:B:236:MET:HE1	2:B:301:HIS:CD2	2.56	0.41
1:C:1:PHE:H1	1:C:400:GLN:HB2	1.86	0.41
1:C:125:LYS:HB2	1:C:126:GLU:H	1.53	0.41
2:D:332:ILE:HA	2:D:333:PRO:HD3	1.92	0.41
3:L:175:ASP:OD1	3:L:175:ASP:C	2.64	0.41
4:H:6:GLN:HE21	4:H:109:GLY:HA3	1.86	0.41
4:F:138:ASN:C	4:F:140:MET:H	2.28	0.41
4:F:150:TYR:OH	4:F:182:LEU:HD23	2.20	0.41
4:F:213:LYS:HD3	4:F:213:LYS:HA	1.90	0.41
3:L:145:TYR:CG	3:L:146:PRO:HA	2.56	0.41
3:E:33:ASN:CB	3:E:35:ASN:HD22	2.28	0.41
3:E:168:TRP:NE1	3:E:180:MET:HE3	2.36	0.41
1:A:16:GLY:N	1:A:441:ASP:OD1	2.50	0.40
2:B:7:CYS:HB3	2:B:45:ASP:CA	2.29	0.40
1:C:247:ASP:OD1	1:C:266:ASN:HA	2.20	0.40
2:D:85:LYS:HG2	3:L:37:TYR:OH	2.21	0.40
2:D:145:LEU:HG	2:D:146:GLY:N	2.35	0.40
2:B:306:LEU:HD22	2:B:311:ILE:HB	2.03	0.40
1:C:381:GLN:HB3	1:C:413:ASP:OD2	2.21	0.40
1:C:537:ASN:C	1:C:539:ALA:H	2.28	0.40
3:L:8:THR:HA	3:L:9:PRO:HD3	1.97	0.40
4:H:175:LEU:HD12	4:H:175:LEU:HA	1.88	0.40
1:C:9:ALA:HB3	1:C:445:VAL:HB	2.03	0.40
1:C:108:HIS:CD2	1:C:176:GLY:CA	3.04	0.40
3:E:118:PRO:HG3	3:E:149:ILE:HD11	2.03	0.40
1:C:193:LEU:HD23	1:C:218:GLN:HG2	2.04	0.40
3:L:38:LEU:HD22	3:L:76:PHE:CG	2.55	0.40
3:L:129:GLN:HG3	4:H:127:TYR:CE2	2.57	0.40
3:E:29:LEU:HD12	3:E:38:LEU:HB2	2.03	0.40
4:F:34:ILE:HD13	4:F:79:ALA:HB2	2.04	0.40
4:F:215:ILE:H	4:F:215:ILE:HG12	1.78	0.40
2:B:179:THR:HG22	2:B:182:LYS:H	1.87	0.40
2:B:417:LYS:H	2:B:417:LYS:HG2	1.72	0.40
1:C:224:SER:HA	1:C:227:ASP:OD2	2.22	0.40
3:E:55:ARG:C	3:E:57:SER:H	2.30	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	599/632 (95%)	533 (89%)	56 (9%)	10 (2%)	7	26
1	C	583/632 (92%)	504 (86%)	69 (12%)	10 (2%)	7	26
2	B	427/454 (94%)	376 (88%)	46 (11%)	5 (1%)	10	34
2	D	429/454 (94%)	386 (90%)	38 (9%)	5 (1%)	10	34
3	E	217/219 (99%)	193 (89%)	22 (10%)	2 (1%)	14	41
3	L	217/219 (99%)	201 (93%)	13 (6%)	3 (1%)	9	30
4	F	216/218 (99%)	192 (89%)	22 (10%)	2 (1%)	14	41
4	H	216/218 (99%)	199 (92%)	16 (7%)	1 (0%)	24	54
5	G	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
5	I	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2907/3056 (95%)	2586 (89%)	283 (10%)	38 (1%)	9	32

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	ALA
2	B	416	PRO
1	C	350	ARG
1	C	575	ALA
1	A	514	GLY
1	A	581	GLY
2	B	10	ALA
2	B	43	ARG
2	B	189	SER
1	C	51	GLN
2	D	105	SER
4	F	54	GLY
1	A	78	ARG
1	A	350	ARG

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Mol	Chain	Res	Type
2	B	23	PRO
1	C	553	GLU
1	C	559	LYS
2	D	54	GLY
2	D	189	SER
2	D	242	GLY
3	L	72	SER
3	E	56	MET
4	F	178	ASP
1	A	298	GLY
1	C	174	LYS
1	C	351	PHE
1	A	157	TRP
1	C	64	PRO
4	H	177	SER
3	E	33	ASN
1	A	243	ASP
1	A	462	PRO
1	C	140	ASP
2	D	106	GLY
3	L	82	ARG
1	A	270	ILE
1	C	270	ILE
3	L	2	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	486/513 (95%)	472 (97%)	14 (3%)	37	71
1	C	476/513 (93%)	443 (93%)	33 (7%)	14	41
2	B	382/402 (95%)	357 (94%)	25 (6%)	15	44
2	D	384/402 (96%)	359 (94%)	25 (6%)	15	44
3	E	194/194 (100%)	182 (94%)	12 (6%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	194/194 (100%)	184 (95%)	10 (5%)	21	52
4	F	186/186 (100%)	171 (92%)	15 (8%)	11	33
4	H	186/186 (100%)	175 (94%)	11 (6%)	18	48
5	G	3/4 (75%)	3 (100%)	0	100	100
5	I	2/4 (50%)	2 (100%)	0	100	100
All	All	2493/2598 (96%)	2348 (94%)	145 (6%)	18	49

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	193	LEU
1	A	235	VAL
1	A	263	THR
1	A	284	TYR
1	A	309	LEU
1	A	356	THR
1	A	383	VAL
1	A	459	THR
1	A	495	VAL
1	A	499	ILE
1	A	509	TRP
1	A	550	LEU
1	A	592	SER
2	B	7	CYS
2	B	24	ASN
2	B	25	CYS
2	B	59	ASP
2	B	60	ILE
2	B	76	THR
2	B	82	THR
2	B	94	ILE
2	B	98	GLN
2	B	195	THR
2	B	224	ASN
2	B	244	LEU
2	B	245	ILE
2	B	285	ASN
2	B	327	GLU
2	B	337	VAL

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Mol	Chain	Res	Type
2	B	343	ASN
2	B	347	VAL
2	B	357	SER
2	B	362	VAL
2	B	376	SER
2	B	382	LYS
2	B	388	THR
2	B	396	SER
2	B	397	ASN
1	C	11	LEU
1	C	65	THR
1	C	66	GLN
1	C	78	ARG
1	C	88	GLU
1	C	111	SER
1	C	123	THR
1	C	145	ILE
1	C	193	LEU
1	C	220	ARG
1	C	228	ASP
1	C	235	VAL
1	C	252	VAL
1	C	254	LYS
1	C	263	THR
1	C	270	ILE
1	C	294	VAL
1	C	323	ARG
1	C	334	ILE
1	C	369	VAL
1	C	381	GLN
1	C	383	VAL
1	C	402	LEU
1	C	413	ASP
1	C	451	ILE
1	C	459	THR
1	C	464	MET
1	C	479	VAL
1	C	482	ILE
1	C	529	LEU
1	C	532	THR
1	C	535	ILE
1	C	571	LEU

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Mol	Chain	Res	Type
2	D	8	LEU
2	D	27	TRP
2	D	29	THR
2	D	75	VAL
2	D	94	ILE
2	D	113	LEU
2	D	134	SER
2	D	139	LEU
2	D	142	VAL
2	D	150	MET
2	D	162	ILE
2	D	224	ASN
2	D	243	SER
2	D	245	ILE
2	D	251	THR
2	D	258	THR
2	D	275	LEU
2	D	317	VAL
2	D	339	THR
2	D	344	SER
2	D	347	VAL
2	D	364	LEU
2	D	365	GLU
2	D	404	VAL
2	D	435	GLU
3	L	3	VAL
3	L	19	VAL
3	L	42	LEU
3	L	59	LEU
3	L	70	SER
3	L	77	THR
3	L	94	LEU
3	L	109	LEU
3	L	141	LEU
3	L	204	LYS
4	H	69	THR
4	H	83	LEU
4	H	102	LEU
4	H	115	THR
4	H	121	THR
4	H	141	VAL
4	H	145	CYS

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Mol	Chain	Res	Type
4	H	155	VAL
4	H	158	THR
4	H	175	LEU
4	H	195	SER
3	E	19	VAL
3	E	38	LEU
3	E	42	LEU
3	E	56	MET
3	E	72	SER
3	E	78	LEU
3	E	110	GLU
3	E	121	SER
3	E	141	LEU
3	E	165	LEU
3	E	181	SER
3	E	207	THR
4	F	23	LYS
4	F	34	ILE
4	F	55	SER
4	F	88	SER
4	F	91	SER
4	F	102	LEU
4	F	106	ASP
4	F	122	THR
4	F	145	CYS
4	F	155	VAL
4	F	158	THR
4	F	161	SER
4	F	182	LEU
4	F	187	THR
4	F	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	165	GLN
1	A	211	ASN
1	A	214	GLN
1	A	216	GLN
1	A	329	GLN
1	A	380	GLN

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Mol	Chain	Res	Type
1	A	381	GLN
1	A	400	GLN
1	A	477	ASN
2	B	72	ASN
2	B	92	HIS
2	B	151	ASN
2	B	219	GLN
2	B	277	ASN
2	B	292	HIS
2	B	301	HIS
2	B	310	ASN
2	B	405	GLN
1	C	108	HIS
1	C	165	GLN
1	C	189	GLN
1	C	197	GLN
1	C	211	ASN
1	C	400	GLN
1	C	552	ASN
1	C	574	GLN
1	C	580	HIS
2	D	5	ASN
2	D	20	GLN
2	D	92	HIS
2	D	201	ASN
2	D	213	ASN
2	D	310	ASN
2	D	383	ASN
2	D	397	ASN
3	L	31	HIS
3	L	129	GLN
3	L	171	GLN
3	L	217	ASN
4	H	6	GLN
4	H	77	ASN
3	E	6	GLN
3	E	26	ASN
3	E	35	ASN
3	E	194	HIS
4	F	6	GLN
4	F	77	ASN
4	F	160	ASN

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Mol	Chain	Res	Type
4	F	176	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 ⓘ

16 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	J	1	1,6	14,14,15	0.49	0	17,19,21	2.10	4 (23%)
6	NAG	J	2	6	14,14,15	0.51	0	17,19,21	1.33	2 (11%)
7	NAG	K	1	1,7	14,14,15	0.73	0	17,19,21	0.88	0
7	NAG	K	2	7	14,14,15	0.61	0	17,19,21	2.21	3 (17%)
7	BMA	K	3	7	11,11,12	0.49	0	15,15,17	1.05	1 (6%)
7	MAN	K	4	7	11,11,12	0.57	0	15,15,17	1.28	2 (13%)
7	MAN	K	5	7	11,11,12	0.80	0	15,15,17	1.43	3 (20%)
7	MAN	K	6	7	11,11,12	0.65	0	15,15,17	0.68	0
6	NAG	M	1	1,6	14,14,15	0.50	0	17,19,21	2.39	5 (29%)
6	NAG	M	2	6	14,14,15	0.51	0	17,19,21	0.84	1 (5%)
7	NAG	N	1	1,7	14,14,15	0.68	0	17,19,21	1.28	2 (11%)
7	NAG	N	2	7	14,14,15	0.56	0	17,19,21	2.45	3 (17%)
7	BMA	N	3	7	11,11,12	0.40	0	15,15,17	0.98	1 (6%)
7	MAN	N	4	7	11,11,12	0.60	0	15,15,17	1.49	3 (20%)
7	MAN	N	5	7	11,11,12	0.51	0	15,15,17	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	N	6	7	11,11,12	0.64	0	15,15,17	1.08	2 (13%)

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	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
7	NAG	K	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1
7	MAN	K	5	7	-	2/2/19/22	0/1/1/1
7	MAN	K	6	7	-	2/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
7	NAG	N	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	1/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
7	MAN	N	4	7	-	0/2/19/22	0/1/1/1
7	MAN	N	5	7	-	2/2/19/22	0/1/1/1
7	MAN	N	6	7	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	2	NAG	C2-N2-C7	7.55	133.02	122.90
6	M	1	NAG	C1-O5-C5	6.14	120.41	112.19
7	K	2	NAG	C2-N2-C7	5.87	130.77	122.90
7	K	2	NAG	C4-C3-C2	-5.33	103.21	111.02
6	J	1	NAG	C1-O5-C5	5.22	119.18	112.19
7	N	2	NAG	C4-C3-C2	-4.80	103.98	111.02
6	M	1	NAG	C4-C3-C2	-4.67	104.18	111.02
6	J	1	NAG	C4-C3-C2	3.86	116.67	111.02
7	K	4	MAN	C1-O5-C5	3.66	117.09	112.19
7	N	2	NAG	O5-C1-C2	-3.59	105.73	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	2	NAG	C1-O5-C5	3.53	116.92	112.19
7	K	5	MAN	C2-C3-C4	3.39	116.83	110.86
7	K	5	MAN	C3-C4-C5	3.18	116.00	110.23
6	M	1	NAG	C2-N2-C7	3.14	127.11	122.90
7	K	2	NAG	O5-C1-C2	-3.13	106.44	111.29
6	M	1	NAG	O5-C5-C4	3.07	118.30	110.83
7	N	5	MAN	C1-O5-C5	2.86	116.02	112.19
7	N	4	MAN	C3-C4-C5	2.79	115.29	110.23
7	N	4	MAN	C2-C3-C4	2.75	115.70	110.86
6	J	2	NAG	C2-N2-C7	-2.67	119.32	122.90
7	N	1	NAG	C2-N2-C7	2.61	126.40	122.90
6	M	1	NAG	C1-C2-N2	2.56	114.46	110.43
6	J	1	NAG	C6-C5-C4	-2.49	106.90	113.02
7	K	5	MAN	C1-C2-C3	2.42	113.17	109.64
7	K	4	MAN	O5-C5-C6	2.38	112.29	107.66
7	K	3	BMA	O5-C5-C4	-2.28	105.27	110.83
7	N	6	MAN	C1-C2-C3	2.28	112.97	109.64
7	N	1	NAG	O4-C4-C3	-2.23	105.11	110.38
7	N	3	BMA	C1-O5-C5	-2.21	109.22	112.19
7	N	4	MAN	O5-C5-C6	2.12	111.80	107.66
6	J	1	NAG	C3-C4-C5	2.09	114.03	110.23
6	M	2	NAG	C4-C3-C2	2.09	114.08	111.02
7	N	6	MAN	O5-C5-C6	2.02	111.59	107.66

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	2	NAG	C3-C2-N2-C7
6	J	2	NAG	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
7	K	4	MAN	O5-C5-C6-O6
7	K	6	MAN	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
7	K	6	MAN	C4-C5-C6-O6
7	K	4	MAN	C4-C5-C6-O6
7	K	5	MAN	C4-C5-C6-O6
7	N	5	MAN	C4-C5-C6-O6
7	K	5	MAN	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6

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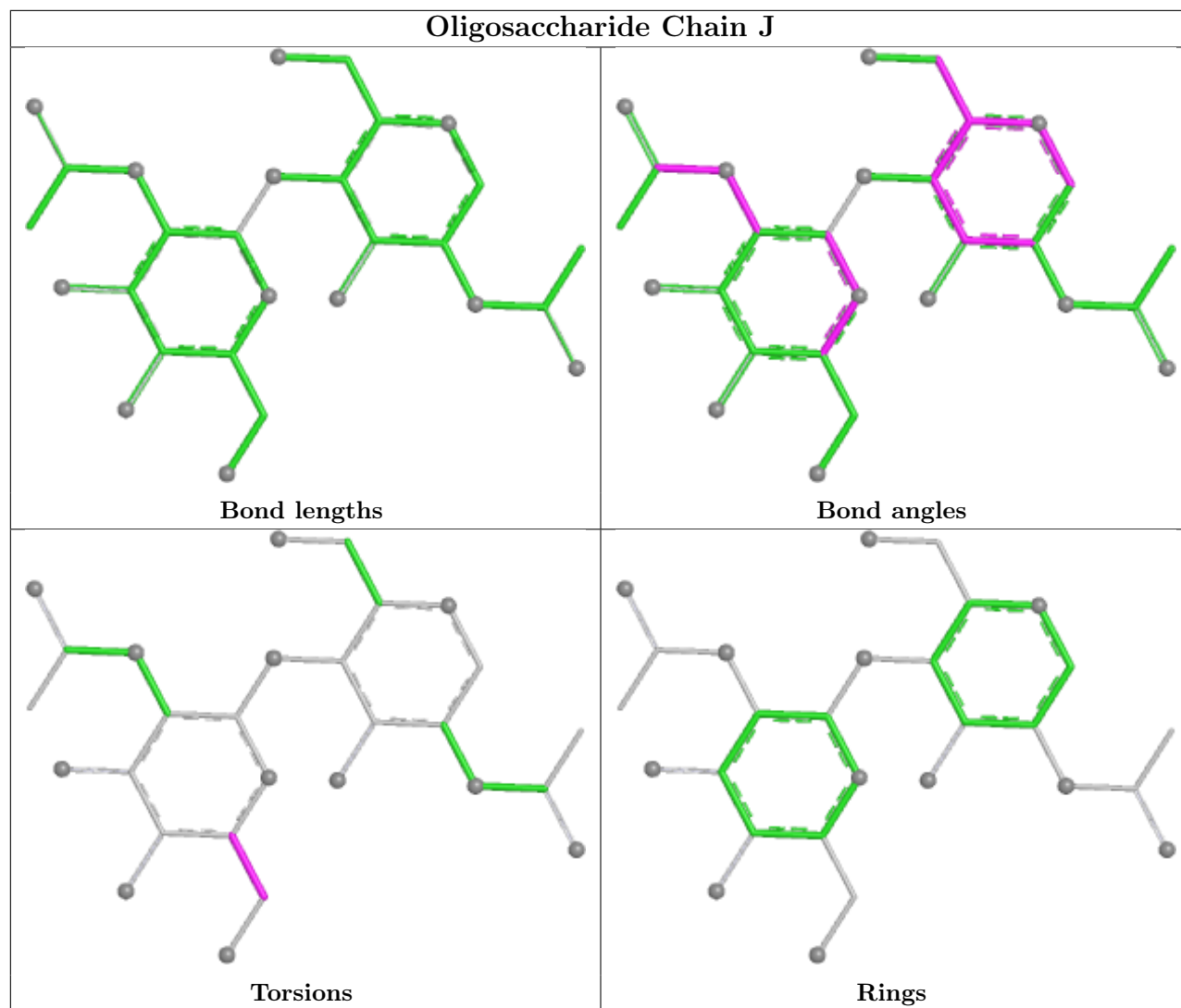
Mol	Chain	Res	Type	Atoms
7	N	5	MAN	O5-C5-C6-O6
7	N	6	MAN	C4-C5-C6-O6
7	N	6	MAN	O5-C5-C6-O6
6	M	1	NAG	C3-C2-N2-C7
7	K	2	NAG	C3-C2-N2-C7
7	N	1	NAG	C4-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
6	M	1	NAG	C1-C2-N2-C7

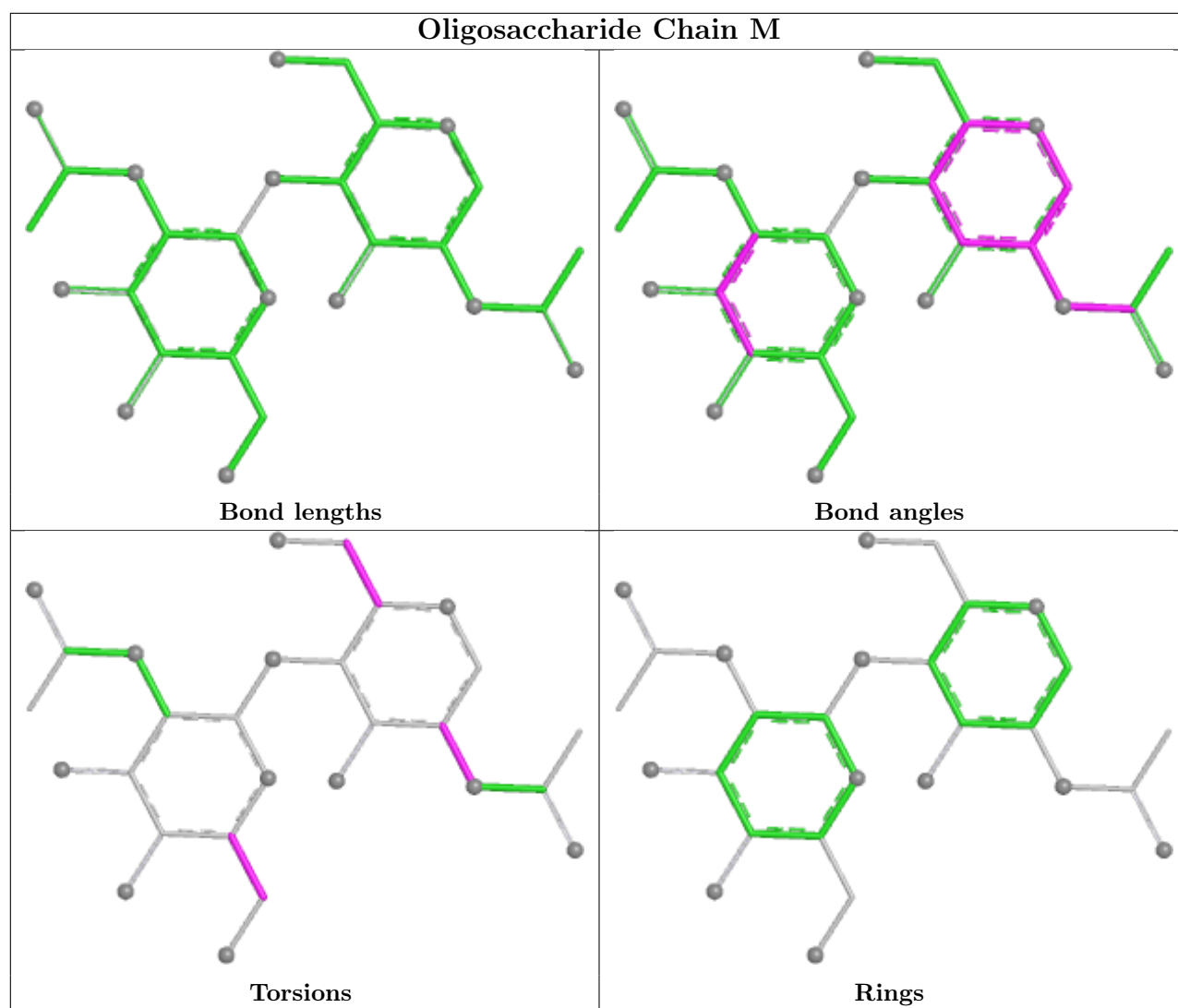
There are no ring outliers.

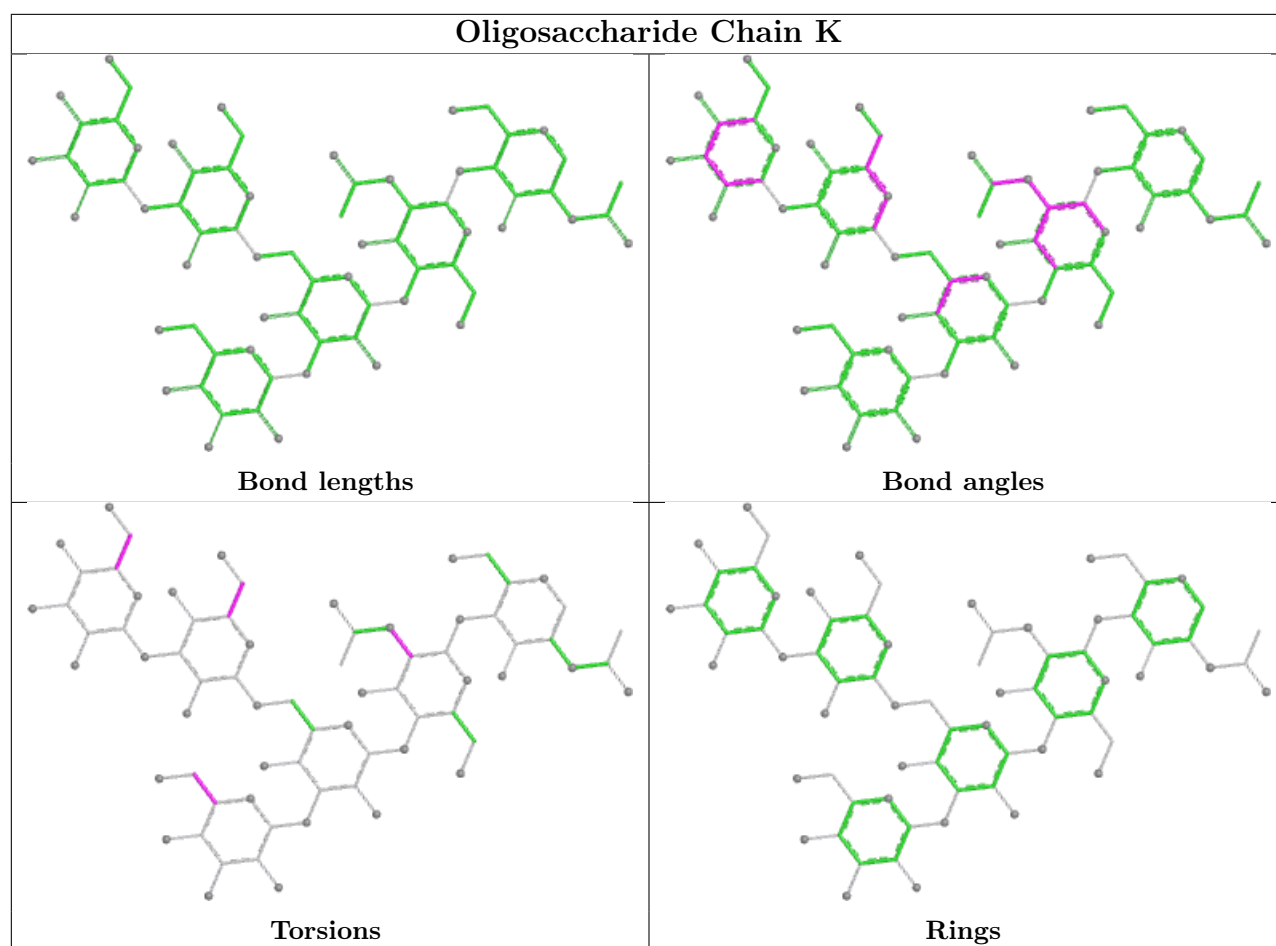
2 monomers are involved in 2 short contacts:

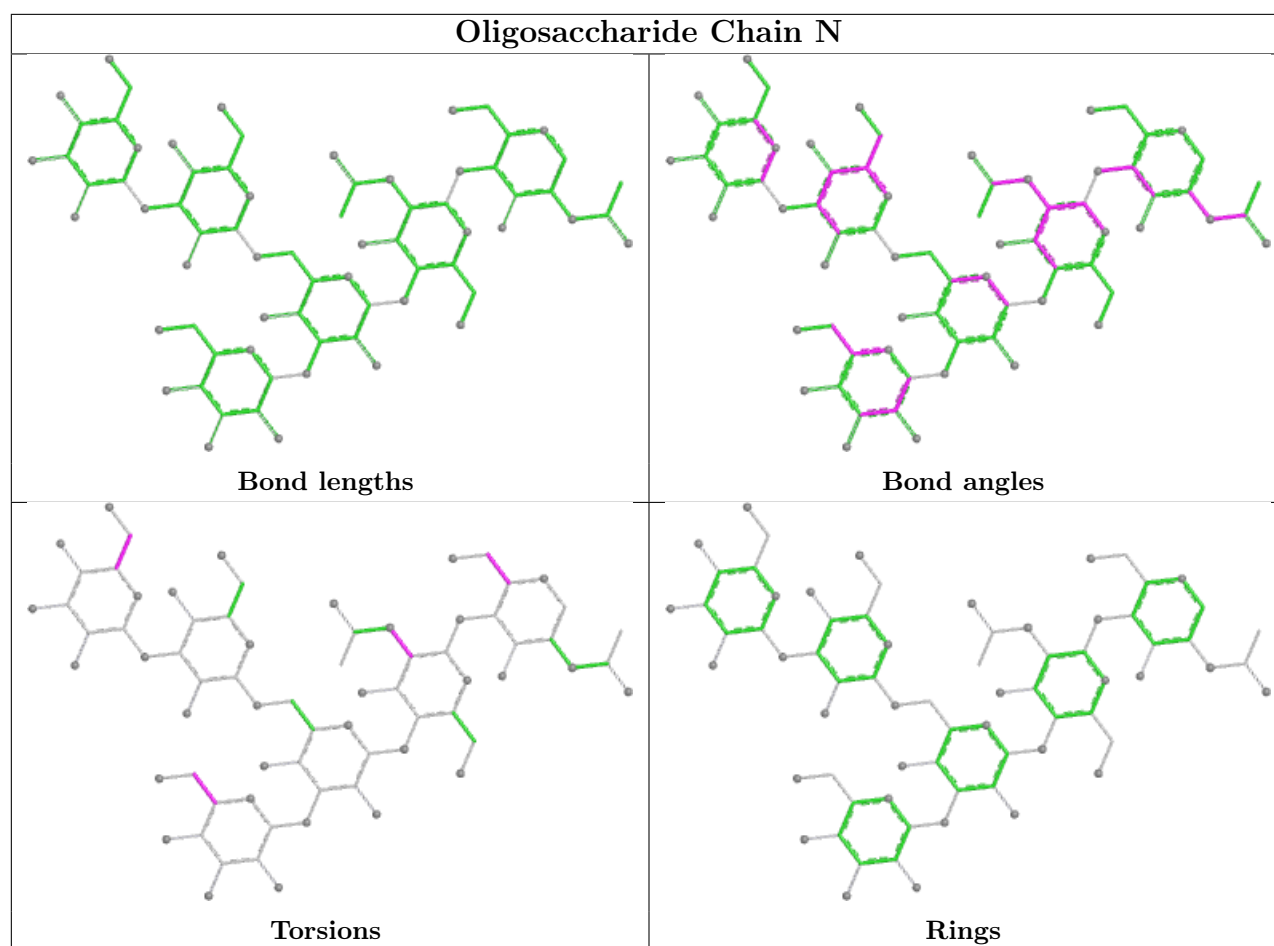
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
7	N	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
9	NAG	A	2005	1	14,14,15	0.48	0	17,19,21	1.10	1 (5%)
9	NAG	C	2009	1	14,14,15	0.54	0	17,19,21	1.28	1 (5%)
9	NAG	C	2016	1	14,14,15	0.45	0	17,19,21	1.39	1 (5%)
9	NAG	C	2007	1	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
9	NAG	C	2008	1	14,14,15	0.54	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	B	503	2	14,14,15	0.58	0	17,19,21	1.00	1 (5%)
9	NAG	D	503	2	14,14,15	0.37	0	17,19,21	1.93	2 (11%)
9	NAG	A	2007	1	14,14,15	0.50	0	17,19,21	0.83	0
9	NAG	A	2006	1	14,14,15	0.58	0	17,19,21	1.07	1 (5%)
9	NAG	A	2016	1	14,14,15	0.51	0	17,19,21	2.09	1 (5%)
9	NAG	B	504	2	14,14,15	0.47	0	17,19,21	1.02	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
9	NAG	A	2005	1	-	0/6/23/26	0/1/1/1
9	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
9	NAG	C	2016	1	-	1/6/23/26	0/1/1/1
9	NAG	C	2007	1	-	0/6/23/26	0/1/1/1
9	NAG	C	2008	1	-	0/6/23/26	0/1/1/1
9	NAG	B	503	2	-	0/6/23/26	0/1/1/1
9	NAG	D	503	2	-	2/6/23/26	0/1/1/1
9	NAG	A	2007	1	-	0/6/23/26	0/1/1/1
9	NAG	A	2006	1	-	1/6/23/26	0/1/1/1
9	NAG	A	2016	1	-	2/6/23/26	0/1/1/1
9	NAG	B	504	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2016	NAG	C1-O5-C5	7.27	121.93	112.19
9	D	503	NAG	C1-O5-C5	6.35	120.69	112.19
9	C	2016	NAG	C1-O5-C5	4.26	117.90	112.19
9	A	2005	NAG	C1-O5-C5	3.58	116.98	112.19
9	C	2009	NAG	C1-O5-C5	3.52	116.90	112.19
9	B	504	NAG	C1-O5-C5	2.99	116.19	112.19
9	C	2008	NAG	C1-O5-C5	2.79	115.92	112.19
9	D	503	NAG	C6-C5-C4	-2.42	107.07	113.02
9	B	503	NAG	C1-O5-C5	2.39	115.38	112.19
9	C	2007	NAG	C1-O5-C5	2.28	115.24	112.19
9	A	2006	NAG	C2-N2-C7	2.26	125.92	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	503	NAG	O5-C5-C6-O6
9	C	2009	NAG	O5-C5-C6-O6
9	D	503	NAG	C4-C5-C6-O6
9	C	2009	NAG	C4-C5-C6-O6
9	A	2016	NAG	C4-C5-C6-O6
9	A	2016	NAG	O5-C5-C6-O6
9	C	2016	NAG	O5-C5-C6-O6
9	A	2006	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2016	NAG	1	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	601/632 (95%)	0.22	15 (2%)	58	48	40, 66, 115, 159	0
1	C	589/632 (93%)	0.38	31 (5%)	32	25	37, 65, 131, 164	0
2	B	431/454 (94%)	0.34	23 (5%)	32	25	41, 64, 161, 217	0
2	D	433/454 (95%)	0.18	22 (5%)	33	26	36, 58, 139, 160	0
3	E	219/219 (100%)	0.02	2 (0%)	81	75	42, 62, 80, 94	0
3	L	219/219 (100%)	-0.06	0	100	100	38, 55, 73, 85	0
4	F	218/218 (100%)	0.28	5 (2%)	61	52	44, 66, 106, 127	0
4	H	218/218 (100%)	0.11	7 (3%)	50	41	35, 58, 97, 111	0
5	G	4/5 (80%)	1.00	0	100	100	85, 87, 88, 99	0
5	I	3/5 (60%)	0.21	0	100	100	77, 77, 82, 86	0
All	All	2935/3056 (96%)	0.22	105 (3%)	46	38	35, 62, 127, 217	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	137	THR	6.1
2	B	19	ILE	6.0
2	B	42	ALA	5.2
1	C	519	ALA	5.2
2	D	27	TRP	4.7
2	B	28	CYS	4.6
2	B	441	ILE	4.3
2	D	26	GLY	4.1
1	C	495	VAL	4.0
2	B	43	ARG	4.0
1	A	577	VAL	3.9
4	H	137	THR	3.8
1	C	588	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	27	TRP	3.6
1	C	576	PRO	3.5
1	C	62	ALA	3.4
1	C	509	TRP	3.4
2	D	50	LEU	3.4
2	D	42	ALA	3.4
1	A	601	LEU	3.3
1	C	564	HIS	3.3
1	C	563	ILE	3.3
1	C	560	LEU	3.2
4	F	134	ALA	3.2
2	D	104	ARG	3.1
1	C	60	TRP	3.0
2	D	47	LEU	3.0
1	C	481	CYS	3.0
1	C	29	GLY	3.0
2	D	60	ILE	2.9
1	A	32	GLY	2.9
1	C	508	ASP	2.9
2	B	8	LEU	2.9
1	C	539	ALA	2.9
1	A	64	PRO	2.8
1	A	30	THR	2.8
1	C	482	ILE	2.8
2	D	105	SER	2.8
2	B	133	TYR	2.8
1	C	256	ASN	2.7
2	D	28	CYS	2.7
1	C	477	ASN	2.7
2	B	23	PRO	2.7
2	D	19	ILE	2.6
2	D	8	LEU	2.6
1	A	579	SER	2.6
1	C	451	ILE	2.6
4	H	176	GLN	2.6
2	B	22	GLY	2.6
1	A	580	HIS	2.6
2	B	18	CYS	2.6
2	B	47	LEU	2.5
2	B	41	SER	2.5
1	C	467	PRO	2.5
1	C	559	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	569	PHE	2.4
4	H	134	ALA	2.4
4	F	200	CYS	2.4
1	C	518	ARG	2.4
1	A	34	SER	2.4
2	D	33	PHE	2.4
2	B	29	THR	2.4
2	D	32	THR	2.4
2	B	60	ILE	2.4
2	B	26	GLY	2.4
2	D	25	CYS	2.4
3	E	1	ASP	2.4
2	B	10	ALA	2.4
1	C	597	LYS	2.3
2	B	440	TYR	2.3
3	E	119	THR	2.3
2	D	413	ASN	2.3
1	C	465	PHE	2.3
2	D	49	ALA	2.3
1	C	537	ASN	2.2
2	D	18	CYS	2.2
4	H	135	ALA	2.2
1	C	552	ASN	2.2
2	B	40	THR	2.2
4	H	218	ARG	2.2
4	F	136	GLN	2.2
2	B	54	GLY	2.2
2	D	342	ALA	2.2
4	H	132	GLY	2.2
2	B	103	LEU	2.2
1	C	575	ALA	2.2
1	A	156	SER	2.1
1	C	463	ALA	2.1
1	C	494	HIS	2.1
1	C	565	ILE	2.1
2	D	92	HIS	2.1
1	C	507	LEU	2.1
2	B	121	TYR	2.1
4	H	153	GLU	2.1
2	D	31	SER	2.1
1	A	464	MET	2.1
1	A	494	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	30	ASN	2.1
4	F	206	ALA	2.1
1	A	332	ALA	2.0
1	A	463	ALA	2.0
2	D	44	CYS	2.0
2	D	43	ARG	2.0
1	A	500	GLY	2.0
1	A	205	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

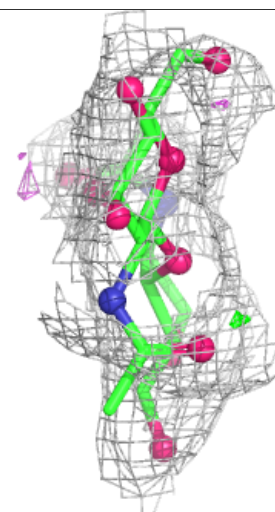
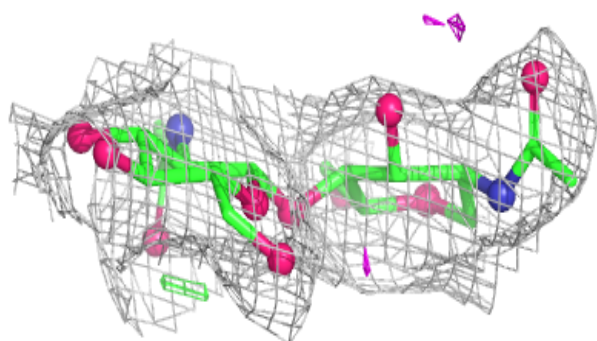
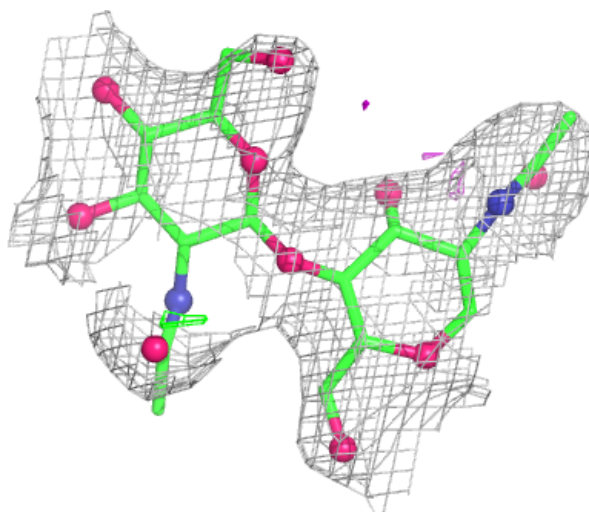
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	J	1	14/15	-	-	74,81,86,92	0
6	NAG	J	2	14/15	-	-	85,99,103,104	0
7	MAN	N	6	11/12	0.66	0.11	81,91,95,96	0
6	NAG	M	2	14/15	0.71	0.12	88,94,98,100	0
7	NAG	K	2	14/15	0.74	0.12	61,64,71,75	0
7	MAN	N	4	11/12	0.75	0.12	83,86,92,97	0
7	BMA	K	3	11/12	-	-	72,80,84,86	0
7	MAN	K	4	11/12	-	-	85,95,103,104	0
7	MAN	K	5	11/12	-	-	84,89,94,97	0
7	MAN	K	6	11/12	-	-	78,84,87,95	0
7	MAN	N	5	11/12	0.80	0.12	79,85,97,103	0
7	NAG	K	1	14/15	0.85	0.09	54,59,62,68	0
6	NAG	M	1	14/15	0.88	0.10	73,78,87,88	0
7	BMA	N	3	11/12	0.90	0.08	71,76,82,85	0
7	NAG	N	1	14/15	0.92	0.10	50,54,60,64	0
7	NAG	N	2	14/15	0.92	0.10	57,61,68,77	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.

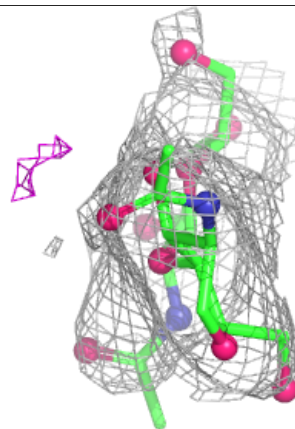
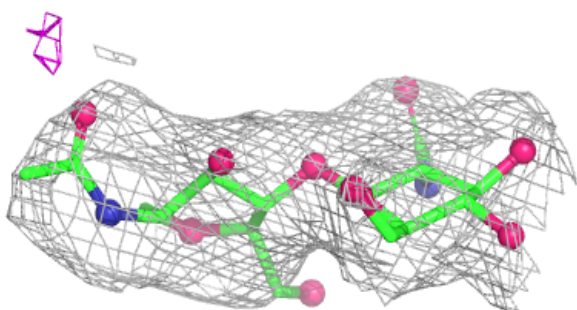
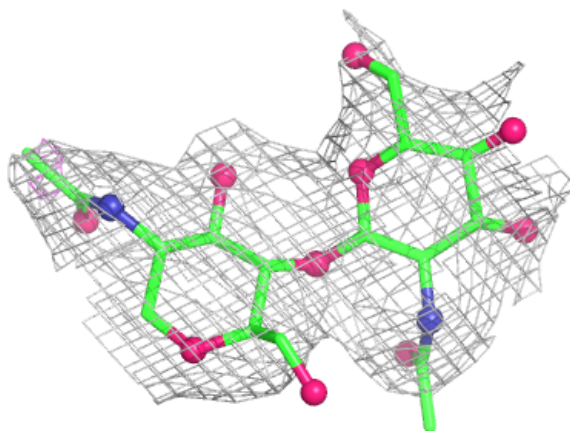
Electron density around Chain J:

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



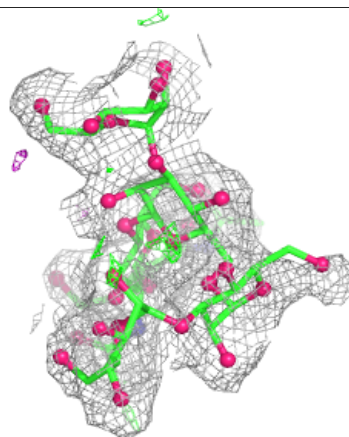
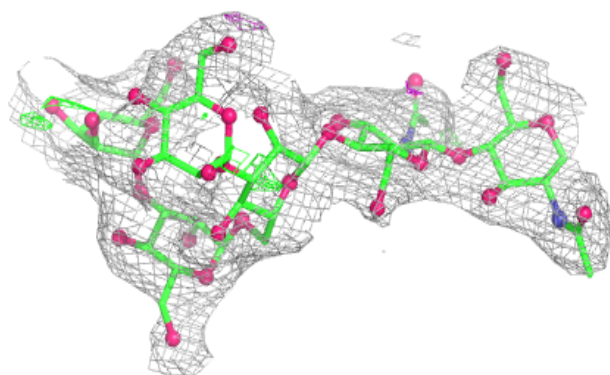
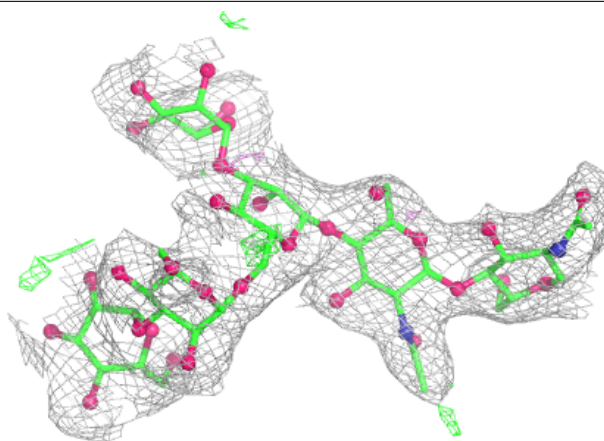
Electron density around Chain M:

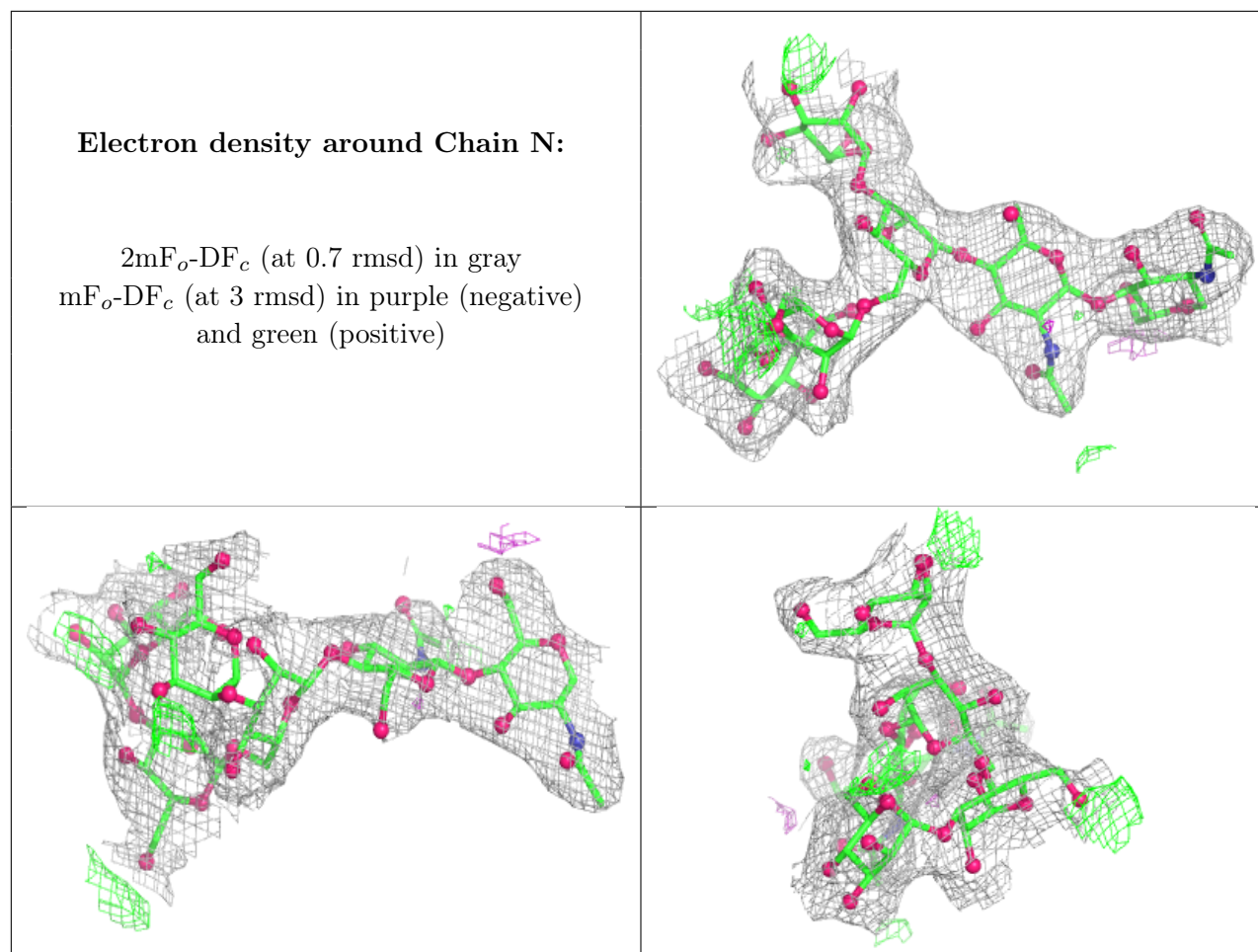
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	A	2006	14/15	0.68	0.13	98,103,109,113	0
9	NAG	D	503	14/15	0.79	0.10	55,62,65,66	0
9	NAG	C	2007	14/15	0.80	0.11	67,78,85,86	0
9	NAG	A	2016	14/15	0.80	0.12	84,89,95,99	0
9	NAG	C	2016	14/15	0.83	0.11	88,94,106,111	0
10	MG	B	502	1/1	0.83	0.11	66,66,66,66	0
9	NAG	C	2008	14/15	0.84	0.13	103,112,114,114	0
9	NAG	C	2009	14/15	0.86	0.09	60,67,71,72	0
9	NAG	A	2007	14/15	0.86	0.10	78,88,93,97	0
10	MG	D	502	1/1	0.87	0.10	66,66,66,66	0
9	NAG	B	504	14/15	0.89	0.10	67,70,76,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	A	2005	14/15	0.90	0.09	64,72,79,79	0
9	NAG	B	503	14/15	0.93	0.07	60,62,67,69	0
8	CA	A	2002	1/1	0.95	0.05	81,81,81,81	0
8	CA	D	501	1/1	0.96	0.07	50,50,50,50	0
8	CA	C	2004	1/1	0.96	0.04	76,76,76,76	0
8	CA	C	2002	1/1	0.97	0.05	80,80,80,80	0
8	CA	A	2004	1/1	0.97	0.04	81,81,81,81	0
8	CA	C	2003	1/1	0.98	0.03	78,78,78,78	0
8	CA	B	501	1/1	0.98	0.06	59,59,59,59	0
8	CA	C	2001	1/1	0.98	0.04	58,58,58,58	0
8	CA	A	2001	1/1	0.98	0.04	69,69,69,69	0
8	CA	A	2003	1/1	0.99	0.04	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.