



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:43 AM UTC

PDB ID : 4QWW / pdb_00004qww
Title : Crystal structure of the Fab410-BfAChE complex
Authors : Bourne, Y.; Renault, L.; Marchot, P.
Deposited on : 2014-07-17
Resolution : 2.70 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

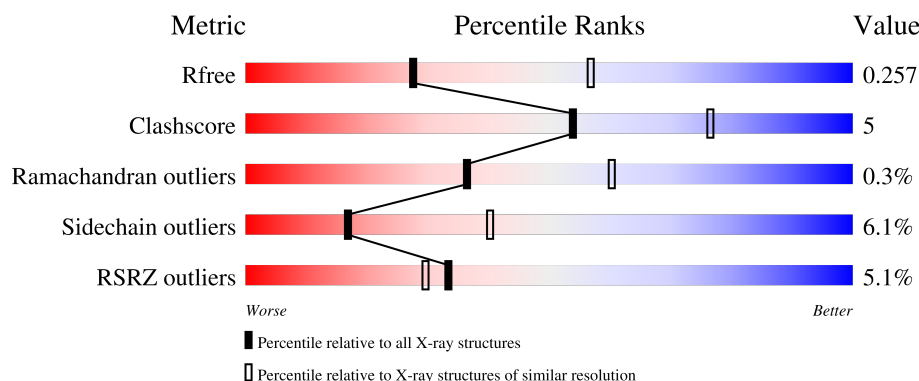
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



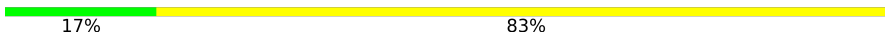
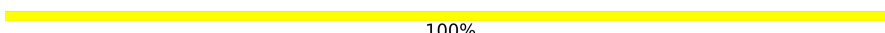
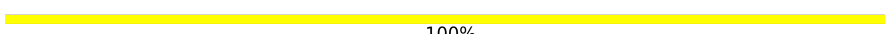
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	542	11% 77% 19% ..
1	B	542	6% 78% 18% ..
2	C	213	81% 17% .
2	E	213	84% 15%
3	D	234	3% 78% 17% ..

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Mol	Chain	Length	Quality of chain
3	F	234	 76% 15% 6%
4	G	6	 17% 83%
4	I	6	 17% 83%
5	H	5	 100%
5	J	5	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15524 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	1	0
			4173	2678	711	767	17			
1	B	529	Total	C	N	O	S	0	1	0
			4173	2678	711	767	17			

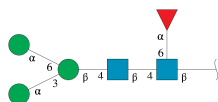
- Molecule 2 is a protein called Fab410 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	212	Total	C	N	O	S	0	0	0
			1626	1011	272	334	9			
2	E	212	Total	C	N	O	S	0	1	0
			1632	1015	272	336	9			

- Molecule 3 is a protein called Fab410 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	225	Total	C	N	O	S	0	1	0
			1723	1089	285	339	10			
3	F	219	Total	C	N	O	S	0	1	0
			1683	1067	277	329	10			

- 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



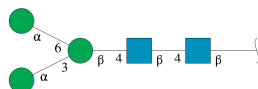
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			71	40	2	29			

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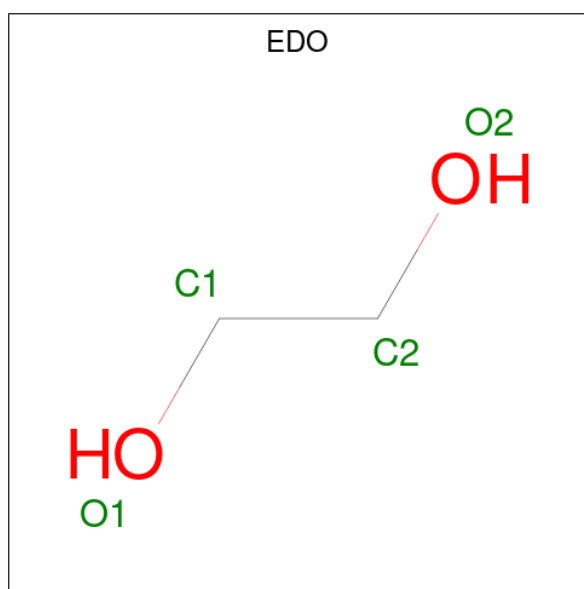
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 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-acetamido-2-deoxy-beta-D-glucopyranose.



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

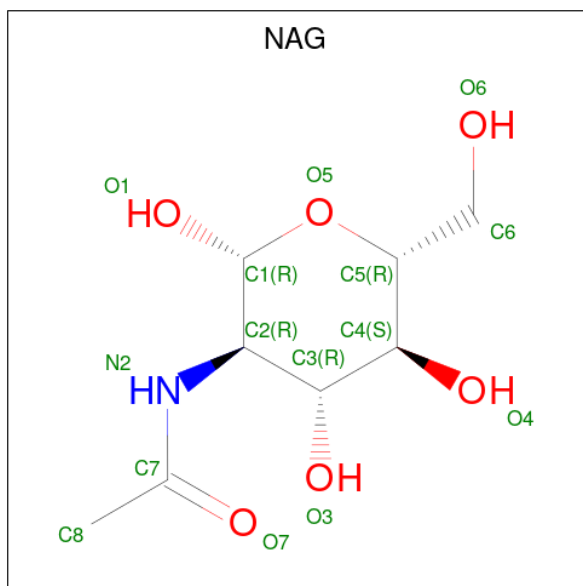
- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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

C₈H₁₅NO₆).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	48	Total	O	0	0
			48	48		
8	B	40	Total	O	0	0
			40	40		
8	C	44	Total	O	0	0
			44	44		
8	D	26	Total	O	0	0
			26	26		
8	E	54	Total	O	0	0
			54	54		
8	F	16	Total	O	0	0
			16	16		

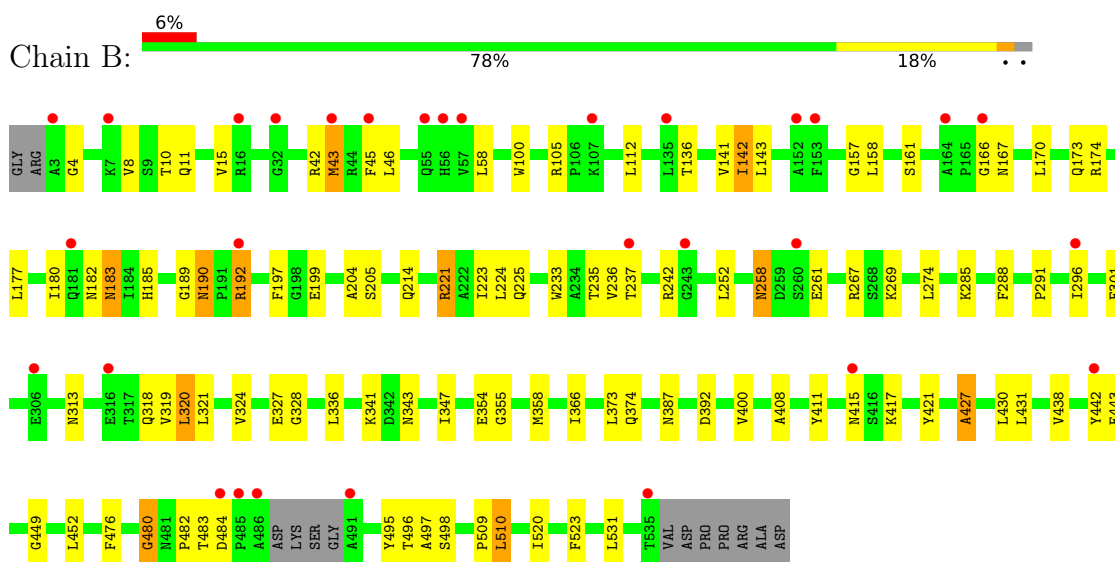
3 Residue-property plots [i](#)

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: Acetylcholinesterase

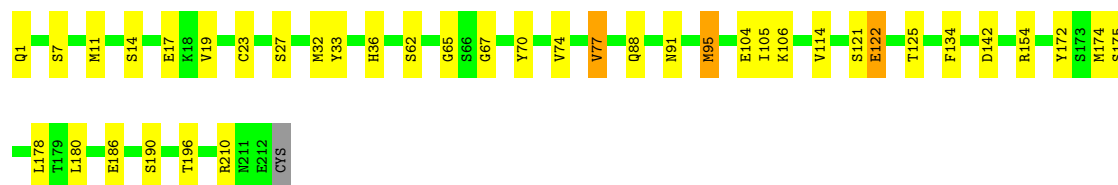


• Molecule 1: Acetylcholinesterase



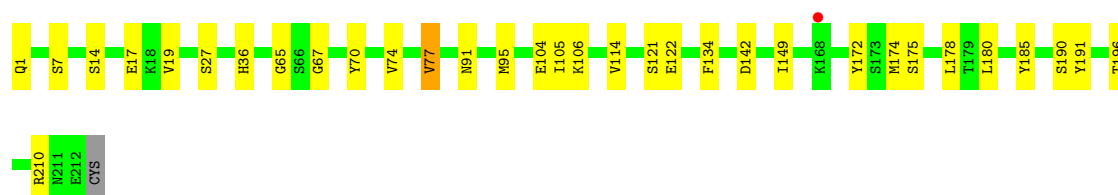
- Molecule 2: Fab410 antibody light chain

Chain C:  81% 17%



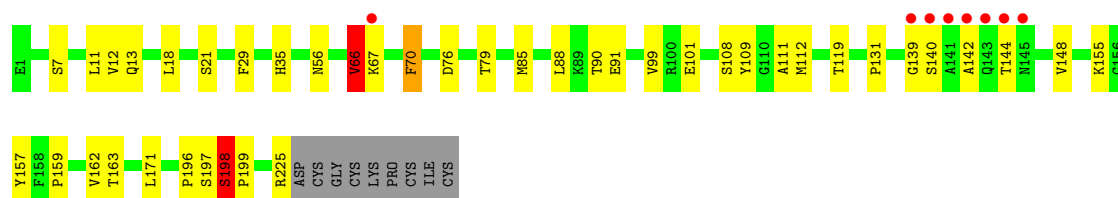
- Molecule 2: Fab410 antibody light chain

Chain E:  84% 15%



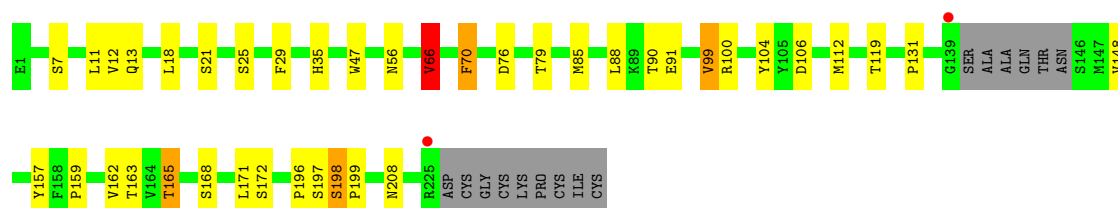
- Molecule 3: Fab410 antibody heavy chain

Chain D:  3% 78% 17%



- Molecule 3: Fab410 antibody heavy chain

Chain F:  76% 15% 6%



- 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  17% 83%



- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain I:  17% 83%

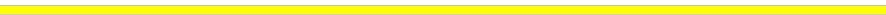
MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain H:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.59Å 251.34Å 73.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.70 39.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.53-2.70) 99.9 (39.53-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.69Å)	Xtrriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.199 , 0.239 0.218 , 0.257	Depositor DCC
R_{free} test set	4060 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15524	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7941e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, NAG, FUC, BMA, EDO

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	0.92	1/4303 (0.0%)	1.39	26/5873 (0.4%)
1	B	0.93	0/4303	1.38	26/5873 (0.4%)
2	C	0.84	1/1667 (0.1%)	1.22	4/2266 (0.2%)
2	E	0.83	1/1676 (0.1%)	1.22	4/2278 (0.2%)
3	D	0.84	1/1772 (0.1%)	1.29	17/2418 (0.7%)
3	F	0.78	0/1731	1.26	11/2360 (0.5%)
All	All	0.88	4/15452 (0.0%)	1.33	88/21068 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	MET	SD-CE	-5.98	1.64	1.79
2	C	95	MET	SD-CE	-5.56	1.65	1.79
2	E	95	MET	SD-CE	-5.24	1.66	1.79
3	D	198	SER	CA-C	5.08	1.58	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	THR	N-CA-C	14.16	128.30	111.02
1	A	343	ASN	CA-CB-CG	9.70	122.30	112.60
1	B	343	ASN	CA-CB-CG	9.53	122.13	112.60
1	A	510	LEU	CB-CA-C	9.42	121.39	109.80
1	B	510	LEU	CB-CA-C	8.69	120.49	109.80
1	B	190	ASN	CA-CB-CG	8.23	120.83	112.60
1	A	212	SER	CA-C-N	7.78	131.60	120.79
1	A	212	SER	C-N-CA	7.78	131.60	120.79
3	D	67	LYS	N-CA-C	7.72	124.11	111.37
1	B	415	ASN	CA-CB-CG	7.65	120.25	112.60
1	B	328	GLY	N-CA-C	7.27	123.11	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	GLY	N-CA-C	-6.72	105.83	115.64
1	A	314	PHE	CA-CB-CG	6.62	120.42	113.80
1	B	313	ASN	CA-CB-CG	6.56	119.16	112.60
2	E	91	ASN	CA-CB-CG	6.51	119.11	112.60
2	E	121	SER	CA-C-N	6.47	130.53	120.82
2	E	121	SER	C-N-CA	6.47	130.53	120.82
2	C	62	SER	CA-C-N	6.45	126.63	122.18
2	C	62	SER	C-N-CA	6.45	126.63	122.18
3	D	144	THR	CA-C-N	6.30	133.04	121.70
3	D	144	THR	C-N-CA	6.30	133.04	121.70
3	D	66	VAL	N-CA-CB	-6.17	102.06	111.57
1	A	341	LYS	N-CA-C	-6.04	105.88	113.18
1	A	213	THR	CB-CA-C	-6.03	101.33	110.92
1	A	45	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	474	ALA	CA-C-N	6.02	128.35	120.28
1	A	474	ALA	C-N-CA	6.02	128.35	120.28
3	F	66	VAL	N-CA-CB	-6.02	102.30	111.57
1	A	510	LEU	N-CA-C	-5.94	101.85	110.64
3	D	76	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	197	PHE	CA-CB-CG	5.86	119.66	113.80
1	B	341	LYS	N-CA-C	-5.85	106.10	113.18
1	B	45	PHE	CA-CB-CG	5.83	119.64	113.80
3	D	197	SER	CA-C-N	5.75	126.21	119.83
3	D	197	SER	C-N-CA	5.75	126.21	119.83
1	B	197	PHE	CA-CB-CG	5.62	119.42	113.80
3	F	70	PHE	CA-CB-CG	5.62	119.42	113.80
3	F	197	SER	CA-C-N	5.60	126.05	119.83
3	F	197	SER	C-N-CA	5.60	126.05	119.83
1	A	443	GLU	CA-C-N	5.56	127.77	120.60
1	A	443	GLU	C-N-CA	5.56	127.77	120.60
1	B	258	ASN	CA-CB-CG	5.53	118.13	112.60
2	C	91	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	183	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	413	LYS	CA-C-N	5.40	128.49	120.17
1	A	413	LYS	C-N-CA	5.40	128.49	120.17
1	B	443	GLU	CA-C-N	5.36	127.52	120.60
1	B	443	GLU	C-N-CA	5.36	127.52	120.60
1	A	285	LYS	N-CA-C	-5.35	100.38	108.67
1	A	480	GLY	N-CA-C	-5.30	107.80	115.27
3	F	106	ASP	CA-CB-CG	5.29	117.89	112.60
3	D	142	ALA	N-CA-C	-5.27	101.82	109.31
1	A	497	ALA	CA-C-N	5.26	129.50	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	ALA	C-N-CA	5.26	129.50	120.71
1	B	510	LEU	N-CA-C	-5.26	102.85	110.64
2	C	180	LEU	N-CA-CB	-5.26	103.10	111.62
3	D	67	LYS	CA-C-N	-5.25	114.41	122.60
3	D	67	LYS	C-N-CA	-5.25	114.41	122.60
3	D	56	ASN	CA-C-N	5.24	129.79	122.08
3	D	56	ASN	C-N-CA	5.24	129.79	122.08
1	B	285	LYS	N-CA-C	-5.17	100.65	108.67
1	B	4	GLY	CA-C-N	5.17	127.21	120.28
1	B	4	GLY	C-N-CA	5.17	127.21	120.28
3	F	76	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	387	ASN	CA-CB-CG	5.16	117.76	112.60
1	B	392	ASP	CA-CB-CG	5.15	117.75	112.60
3	F	56	ASN	CA-C-N	5.15	129.65	122.08
3	F	56	ASN	C-N-CA	5.15	129.65	122.08
1	A	380	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	204	ALA	CA-C-N	5.13	127.16	120.28
1	B	204	ALA	C-N-CA	5.13	127.16	120.28
1	A	240	GLU	CB-CG-CD	5.12	121.30	112.60
2	E	122	GLU	CB-CG-CD	5.11	121.29	112.60
1	B	387	ASN	CA-CB-CG	5.11	117.71	112.60
3	D	70	PHE	CA-CB-CG	5.10	118.90	113.80
3	F	119	THR	CB-CA-C	5.10	118.00	110.14
3	D	90	THR	CA-C-N	5.09	127.61	120.28
3	D	90	THR	C-N-CA	5.09	127.61	120.28
3	F	90	THR	CA-C-N	5.07	127.59	120.28
3	F	90	THR	C-N-CA	5.07	127.59	120.28
1	A	392	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	182	ASN	CA-CB-CG	5.07	117.67	112.60
1	B	497	ALA	N-CA-C	-5.06	105.85	111.36
1	B	183	ASN	CA-CB-CG	5.05	117.65	112.60
3	D	142	ALA	CB-CA-C	-5.05	102.50	114.16
1	B	427	ALA	CA-C-N	5.03	128.65	120.60
1	B	427	ALA	C-N-CA	5.03	128.65	120.60
3	D	119	THR	CB-CA-C	5.01	118.16	110.14

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	4173	0	4027	46	0
1	B	4173	0	4026	48	0
2	C	1626	0	1544	12	0
2	E	1632	0	1550	8	0
3	D	1723	0	1674	17	0
3	F	1683	0	1637	19	0
4	G	71	0	61	0	0
4	I	71	0	61	0	0
5	H	61	0	52	0	0
5	J	61	0	52	0	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
7	B	14	0	13	0	0
8	A	48	0	0	0	0
8	B	40	0	0	1	0
8	C	44	0	0	0	0
8	D	26	0	0	0	0
8	E	54	0	0	0	0
8	F	16	0	0	0	0
All	All	15524	0	14709	146	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 5.

All (146) 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:A:374:GLN:HE22	1:B:374:GLN:HE22	1.25	0.84
3:F:99:VAL:HG11	3:F:112:MET:HB3	1.65	0.76
3:F:35:HIS:HD2	3:F:47:TRP:HE1	1.33	0.75
3:F:168:SER:H	3:F:208:ASN:HD21	1.33	0.74
1:A:427:ALA:HB3	1:A:430:LEU:HB2	1.70	0.73
1:B:366:ILE:HG23	1:B:531:LEU:HD21	1.71	0.73
1:A:366:ILE:HG23	1:A:531:LEU:HD21	1.72	0.72
1:B:112:LEU:HD12	1:B:141:VAL:HG11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:165:THR:HG23	3:F:208:ASN:HB2	1.73	0.70
1:A:224:LEU:HB2	1:A:321:LEU:HD23	1.74	0.69
1:A:12:THR:HG21	1:A:179:TRP:HE1	1.59	0.68
1:B:427:ALA:HB2	1:B:442[B]:TYR:OH	1.95	0.66
1:B:100:TRP:HB3	1:B:136:THR:HG21	1.78	0.66
1:A:149:ARG:HD3	1:A:172:ASP:OD2	1.95	0.65
1:B:224:LEU:HB2	1:B:321:LEU:HD23	1.79	0.65
1:B:354:GLU:HG3	1:B:358:MET:HE3	1.78	0.65
2:C:95:MET:HE1	3:D:112:MET:HE2	1.78	0.64
3:F:66:VAL:HG13	3:F:70:PHE:HB2	1.80	0.64
1:A:419:TYR:HD1	1:A:492:TRP:CD1	2.15	0.63
1:A:427:ALA:HB2	1:A:442[B]:TYR:OH	1.98	0.63
3:F:99:VAL:CG1	3:F:112:MET:HB3	2.29	0.62
1:B:417:LYS:HD3	8:B:704:HOH:O	1.98	0.62
1:A:258:ASN:HB2	1:A:261:GLU:HB2	1.82	0.61
3:F:11:LEU:HB2	3:F:159:PRO:HG3	1.82	0.61
3:D:99:VAL:HG11	3:D:112:MET:HB3	1.83	0.61
1:B:258:ASN:HB2	1:B:261:GLU:HB2	1.83	0.60
3:D:66:VAL:HG13	3:D:70:PHE:HB2	1.84	0.60
3:D:11:LEU:HB2	3:D:159:PRO:HG3	1.84	0.59
1:B:8:VAL:HG22	1:B:105:ARG:HH21	1.67	0.59
1:B:43:MET:HA	1:B:46:LEU:HD12	1.85	0.59
1:A:43:MET:HA	1:A:46:LEU:HD12	1.85	0.59
1:A:174:ARG:HA	1:A:177:LEU:HD12	1.86	0.57
1:A:412:ALA:C	1:A:414:ARG:H	2.14	0.56
2:C:154:ARG:HG2	2:C:178:LEU:HD11	1.86	0.56
3:F:35:HIS:HD2	3:F:47:TRP:NE1	2.03	0.56
1:A:8:VAL:HG22	1:A:105:ARG:HH21	1.70	0.56
1:B:174:ARG:HA	1:B:177:LEU:HD12	1.86	0.56
2:C:88:GLN:HE21	2:C:95:MET:HE3	1.70	0.55
1:A:427:ALA:HB2	1:A:442[B]:TYR:CZ	2.42	0.55
1:A:426:ARG:HB2	1:A:438:VAL:HG22	1.89	0.54
1:B:167:ASN:HB3	1:B:170:LEU:HD12	1.89	0.54
1:B:427:ALA:HB3	1:B:430:LEU:HB2	1.90	0.54
3:F:168:SER:H	3:F:208:ASN:ND2	2.04	0.54
1:B:496:THR:HG22	1:B:498:SER:H	1.73	0.53
1:B:173:GLN:OE1	1:B:205:SER:HB3	2.08	0.53
1:A:252:LEU:HD22	1:A:269:LYS:HG2	1.90	0.53
3:D:99:VAL:CG1	3:D:112:MET:HB3	2.38	0.52
1:A:132:GLY:HA3	1:A:143:LEU:HD22	1.91	0.52
1:A:199:GLU:HA	1:A:225:GLN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:35:HIS:CD2	3:F:47:TRP:HE1	2.21	0.52
1:B:252:LEU:HD22	1:B:269:LYS:HG2	1.90	0.52
1:B:296:ILE:HA	1:B:301:PHE:HB2	1.90	0.52
1:A:296:ILE:HA	1:A:301:PHE:HB2	1.90	0.52
1:A:17:GLY:O	1:A:61:THR:HG22	2.10	0.52
1:B:199:GLU:HA	1:B:225:GLN:O	2.10	0.51
2:C:104:GLU:HG3	2:C:172:TYR:OH	2.11	0.51
2:E:14:SER:HA	2:E:106:LYS:HB2	1.93	0.50
2:E:104:GLU:HG3	2:E:172:TYR:OH	2.12	0.50
3:D:85:MET:HE2	3:D:88:LEU:HD21	1.94	0.49
2:C:14:SER:HA	2:C:106:LYS:HB2	1.93	0.49
1:B:324:VAL:HG22	1:B:327:GLU:OE2	2.13	0.49
1:A:12:THR:HG21	1:A:179:TRP:NE1	2.26	0.49
1:A:233:TRP:HB3	1:A:288:PHE:O	2.12	0.49
1:B:221:ARG:HD3	1:B:480:GLY:HA2	1.94	0.49
1:A:509:PRO:O	1:A:510:LEU:C	2.55	0.49
3:D:29:PHE:HB2	3:D:79:THR:HG23	1.95	0.49
1:B:233:TRP:HB3	1:B:288:PHE:O	2.13	0.48
1:A:207:GLY:O	1:A:211:LEU:HG	2.13	0.48
2:E:77:VAL:HG13	2:E:105:ILE:HD12	1.94	0.48
3:F:85:MET:HE2	3:F:88:LEU:HD21	1.95	0.47
1:B:427:ALA:HB2	1:B:442[B]:TYR:CZ	2.49	0.47
2:C:77:VAL:HG13	2:C:105:ILE:HD12	1.95	0.47
2:C:122:GLU:HA	2:C:125:THR:HG22	1.97	0.47
3:F:131:PRO:HB3	3:F:157:TYR:HB3	1.96	0.46
1:A:191:PRO:HA	1:A:194:VAL:HG23	1.97	0.46
2:E:185:TYR:HA	2:E:191:TYR:OH	2.15	0.46
3:F:12:VAL:HG21	3:F:18:LEU:HB2	1.96	0.46
3:D:131:PRO:HB3	3:D:157:TYR:HB3	1.96	0.46
3:D:35:HIS:CG	3:D:112:MET:HE1	2.51	0.46
3:D:12:VAL:HG21	3:D:18:LEU:HB2	1.97	0.46
3:D:29:PHE:CB	3:D:79:THR:HG23	2.46	0.46
1:A:18:LEU:HD13	1:A:61:THR:HB	1.96	0.45
1:B:509:PRO:O	1:B:510:LEU:C	2.59	0.45
3:F:29:PHE:HB2	3:F:79:THR:HG23	1.98	0.45
1:A:479:THR:HB	1:A:481:ASN:H	1.82	0.45
2:E:149:ILE:HD11	2:E:178:LEU:HD21	1.99	0.45
1:A:10:THR:HB	1:A:183:ASN:OD1	2.17	0.45
1:A:132:GLY:CA	1:A:143:LEU:HD22	2.47	0.45
1:B:141:VAL:HG12	1:B:142:ILE:N	2.32	0.45
1:B:190:ASN:HD22	1:B:192:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HA	1:A:267:ARG:HD3	1.99	0.44
1:B:10:THR:HB	1:B:183:ASN:OD1	2.17	0.44
1:B:42:ARG:HA	1:B:267:ARG:HD3	2.00	0.44
2:C:114:VAL:HA	2:C:134:PHE:O	2.17	0.44
2:C:33:TYR:HB2	2:C:88:GLN:OE1	2.18	0.44
3:D:101:GLU:HA	3:D:111:ALA:O	2.17	0.44
1:A:230:ASN:HD22	1:A:406:GLN:HE21	1.64	0.43
1:A:110:PRO:HG2	1:A:141:VAL:HG22	1.99	0.43
1:A:336:LEU:HD22	1:A:355:GLY:HA2	2.00	0.43
3:F:29:PHE:CB	3:F:79:THR:HG23	2.49	0.43
2:E:114:VAL:HA	2:E:134:PHE:O	2.18	0.43
1:A:452:LEU:HD11	1:A:467:ARG:HG3	2.00	0.43
1:B:438:VAL:HG13	1:B:442[B]:TYR:HD2	1.84	0.43
3:D:198:SER:HB2	3:D:199:PRO:HD3	2.00	0.43
1:A:223:ILE:HG12	1:A:320:LEU:HB3	2.01	0.42
1:A:177:LEU:HA	1:A:180:ILE:HD12	2.01	0.42
1:B:157:GLY:HA2	1:B:166:GLY:HA2	2.01	0.42
1:B:476:PHE:HD1	1:B:482:PRO:HD3	1.84	0.42
1:A:213:THR:HA	1:A:216:ARG:HE	1.85	0.42
1:B:336:LEU:HD22	1:B:355:GLY:HA2	2.01	0.42
2:C:174:MET:HG2	2:C:175:SER:N	2.34	0.42
3:F:198:SER:HB2	3:F:199:PRO:HD3	2.01	0.42
1:B:177:LEU:HA	1:B:180:ILE:HD12	2.01	0.42
3:D:139:GLY:HA2	3:D:225:ARG:HG3	2.01	0.42
1:A:71:VAL:HG11	3:F:104[A]:TYR:CG	2.55	0.42
1:B:520:ILE:O	1:B:523:PHE:HB3	2.20	0.42
3:F:196:PRO:O	3:F:199:PRO:HD2	2.20	0.42
1:B:158:LEU:HD23	1:B:242:ARG:HG2	2.02	0.41
1:B:318:GLN:H	1:B:318:GLN:CD	2.28	0.41
1:A:388:ARG:HD3	1:A:435:TRP:CE3	2.56	0.41
1:B:438:VAL:HG13	1:B:442[B]:TYR:CD2	2.56	0.41
1:B:8:VAL:CG2	1:B:105:ARG:HH21	2.33	0.41
3:D:196:PRO:O	3:D:199:PRO:HD2	2.20	0.41
3:D:108:SER:O	3:D:109:TYR:C	2.63	0.41
1:A:520:ILE:O	1:A:523:PHE:HB3	2.21	0.41
2:C:23:CYS:SG	2:C:32:MET:HE3	2.60	0.41
1:A:527:PHE:HB2	1:B:373:LEU:HD13	2.03	0.41
2:E:174:MET:HG2	2:E:175:SER:N	2.35	0.41
1:A:528:LEU:HD12	1:A:528:LEU:HA	1.94	0.41
1:B:223:ILE:HG12	1:B:320:LEU:HB3	2.03	0.41
1:B:327:GLU:OE1	1:B:400:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:CG	1:B:318:GLN:HE21	2.34	0.41
1:B:225:GLN:HG2	1:B:421:TYR:OH	2.20	0.41
1:B:449:GLY:O	1:B:452:LEU:HB2	2.20	0.41
2:C:65:GLY:HA3	2:C:70:TYR:HA	2.03	0.41
3:D:196:PRO:HD2	3:D:199:PRO:HG2	2.03	0.41
3:F:196:PRO:HD2	3:F:199:PRO:HG2	2.02	0.41
1:A:8:VAL:CG2	1:A:105:ARG:HH21	2.34	0.40
1:A:3:ALA:HB2	1:A:6:LEU:HD12	2.03	0.40
1:B:408:ALA:HB1	1:B:495:TYR:CD1	2.57	0.40
2:E:65:GLY:HA3	2:E:70:TYR:HA	2.04	0.40
1:A:55:GLN:HA	1:A:56:HIS:HA	1.70	0.40
1:B:185:HIS:HA	1:B:189:GLY:O	2.22	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	526/542 (97%)	488 (93%)	36 (7%)	2 (0%)	30	54
1	B	526/542 (97%)	496 (94%)	28 (5%)	2 (0%)	30	54
2	C	210/213 (99%)	205 (98%)	4 (2%)	1 (0%)	24	48
2	E	211/213 (99%)	205 (97%)	5 (2%)	1 (0%)	24	48
3	D	224/234 (96%)	211 (94%)	13 (6%)	0	100	100
3	F	216/234 (92%)	205 (95%)	11 (5%)	0	100	100
All	All	1913/1978 (97%)	1810 (95%)	97 (5%)	6 (0%)	36	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	484	ASP

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Mol	Chain	Res	Type
1	A	482	PRO
2	C	67	GLY
2	E	67	GLY
1	A	291	PRO
1	B	291	PRO

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	448/457 (98%)	424 (95%)	24 (5%)	20	45
1	B	448/457 (98%)	428 (96%)	20 (4%)	24	52
2	C	186/187 (100%)	170 (91%)	16 (9%)	10	25
2	E	187/187 (100%)	174 (93%)	13 (7%)	14	34
3	D	194/201 (96%)	182 (94%)	12 (6%)	16	39
3	F	190/201 (94%)	175 (92%)	15 (8%)	11	28
All	All	1653/1690 (98%)	1553 (94%)	100 (6%)	17	41

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	31	LEU
1	A	43	MET
1	A	58	LEU
1	A	97	LEU
1	A	141	VAL
1	A	142	ILE
1	A	143	LEU
1	A	161	SER
1	A	214	GLN
1	A	215	SER
1	A	217	THR
1	A	235	THR

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Mol	Chain	Res	Type
1	A	236	VAL
1	A	237	THR
1	A	274	LEU
1	A	318	GLN
1	A	320	LEU
1	A	347	ILE
1	A	411	TYR
1	A	413	LYS
1	A	431	LEU
1	A	479	THR
1	A	498	SER
1	B	11	GLN
1	B	15	VAL
1	B	43	MET
1	B	58	LEU
1	B	142	ILE
1	B	143	LEU
1	B	161	SER
1	B	192	ARG
1	B	214	GLN
1	B	221	ARG
1	B	235	THR
1	B	236	VAL
1	B	237	THR
1	B	274	LEU
1	B	319	VAL
1	B	320	LEU
1	B	347	ILE
1	B	411	TYR
1	B	431	LEU
1	B	483	THR
2	C	1	GLN
2	C	7	SER
2	C	11	MET
2	C	17	GLU
2	C	19	VAL
2	C	27	SER
2	C	36	HIS
2	C	74	VAL
2	C	77	VAL
2	C	121	SER
2	C	122	GLU

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Mol	Chain	Res	Type
2	C	142	ASP
2	C	186	GLU
2	C	190	SER
2	C	196	THR
2	C	210	ARG
3	D	7	SER
3	D	13	GLN
3	D	21	SER
3	D	66	VAL
3	D	91	GLU
3	D	140	SER
3	D	148	VAL
3	D	155	LYS
3	D	162	VAL
3	D	163	THR
3	D	171	LEU
3	D	198	SER
2	E	1	GLN
2	E	7	SER
2	E	17	GLU
2	E	19	VAL
2	E	27	SER
2	E	36	HIS
2	E	74	VAL
2	E	77	VAL
2	E	142	ASP
2	E	180	LEU
2	E	190	SER
2	E	196	THR
2	E	210	ARG
3	F	7	SER
3	F	13	GLN
3	F	21	SER
3	F	25	SER
3	F	66	VAL
3	F	91	GLU
3	F	99	VAL
3	F	100	ARG
3	F	148	VAL
3	F	162	VAL
3	F	163	THR
3	F	165	THR

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Mol	Chain	Res	Type
3	F	171	LEU
3	F	172	SER
3	F	198	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	139	GLN
1	A	178	GLN
1	A	251	GLN
1	A	364	ASN
1	A	374	GLN
1	A	406	GLN
1	A	415	ASN
1	A	508	GLN
1	A	525	ASN
1	B	11	GLN
1	B	139	GLN
1	B	140	ASN
1	B	178	GLN
1	B	190	ASN
1	B	209	HIS
1	B	225	GLN
1	B	251	GLN
1	B	313	ASN
1	B	364	ASN
1	B	374	GLN
1	B	415	ASN
1	B	475	ASN
1	B	504	GLN
1	B	508	GLN
1	B	525	ASN
2	C	137	ASN
2	C	156	ASN
2	E	137	ASN
2	E	156	ASN
2	E	209	ASN
2	E	211	ASN
3	F	35	HIS
3	F	176	HIS
3	F	208	ASN

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 ⓘ

22 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	$\# Z > 2$
4	NAG	G	1	1,4	14,14,15	0.44	0	17,19,21	2.05	3 (17%)
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	BMA	G	3	4	11,11,12	0.36	0	15,15,17	0.91	2 (13%)
4	MAN	G	4	4	11,11,12	0.32	0	15,15,17	0.74	1 (6%)
4	MAN	G	5	4	11,11,12	0.41	0	15,15,17	1.01	1 (6%)
4	FUC	G	6	4	10,10,11	0.53	0	14,14,16	0.89	1 (7%)
5	NAG	H	1	1,5	14,14,15	0.20	0	17,19,21	1.10	2 (11%)
5	NAG	H	2	5	14,14,15	0.26	0	17,19,21	0.81	1 (5%)
5	BMA	H	3	5	11,11,12	0.30	0	15,15,17	1.06	1 (6%)
5	MAN	H	4	5	11,11,12	0.26	0	15,15,17	0.93	1 (6%)
5	MAN	H	5	5	11,11,12	0.46	0	15,15,17	0.98	1 (6%)
4	NAG	I	1	1,4	14,14,15	0.40	0	17,19,21	2.20	3 (17%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.41	0
4	BMA	I	3	4	11,11,12	0.35	0	15,15,17	1.03	2 (13%)
4	MAN	I	4	4	11,11,12	0.34	0	15,15,17	0.72	1 (6%)
4	MAN	I	5	4	11,11,12	0.41	0	15,15,17	1.03	1 (6%)
4	FUC	I	6	4	10,10,11	0.54	0	14,14,16	0.94	1 (7%)
5	NAG	J	1	1,5	14,14,15	0.26	0	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	2	5	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
5	BMA	J	3	5	11,11,12	0.25	0	15,15,17	1.06	1 (6%)
5	MAN	J	4	5	11,11,12	0.26	0	15,15,17	0.86	1 (6%)
5	MAN	J	5	5	11,11,12	0.49	0	15,15,17	0.99	1 (6%)

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

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

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-C2-N2	5.93	119.78	110.43
4	I	1	NAG	C1-C2-N2	5.80	119.58	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C2-N2-C7	4.86	129.42	122.90
4	I	1	NAG	O5-C1-C2	-4.47	104.37	111.29
4	G	1	NAG	O5-C1-C2	-4.16	104.85	111.29
4	I	5	MAN	C1-O5-C5	3.69	117.13	112.19
4	G	1	NAG	C2-N2-C7	3.61	127.74	122.90
4	G	5	MAN	C1-O5-C5	3.60	117.01	112.19
5	J	5	MAN	C1-O5-C5	3.53	116.92	112.19
5	H	5	MAN	C1-O5-C5	3.53	116.92	112.19
5	H	1	NAG	C1-O5-C5	3.52	116.91	112.19
5	J	3	BMA	C1-O5-C5	3.29	116.59	112.19
5	J	1	NAG	C1-O5-C5	3.27	116.57	112.19
5	H	3	BMA	C1-O5-C5	3.25	116.55	112.19
5	H	4	MAN	C1-O5-C5	3.17	116.43	112.19
5	J	4	MAN	C1-O5-C5	2.96	116.16	112.19
4	I	3	BMA	C1-O5-C5	2.88	116.05	112.19
4	I	6	FUC	C1-O5-C5	2.79	119.54	112.97
5	H	2	NAG	C1-O5-C5	2.60	115.68	112.19
4	G	3	BMA	O3-C3-C2	2.47	115.10	110.05
4	G	6	FUC	C1-O5-C5	2.47	118.78	112.97
4	I	3	BMA	O3-C3-C2	2.44	115.03	110.05
5	H	1	NAG	O5-C1-C2	-2.38	107.62	111.29
5	J	1	NAG	O5-C1-C2	-2.23	107.84	111.29
5	J	2	NAG	C1-O5-C5	2.21	115.14	112.19
4	G	4	MAN	C1-O5-C5	2.15	115.07	112.19
4	G	3	BMA	C1-O5-C5	2.09	114.99	112.19
4	I	4	MAN	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C1-C2-N2-C7
5	H	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
5	J	5	MAN	O5-C5-C6-O6

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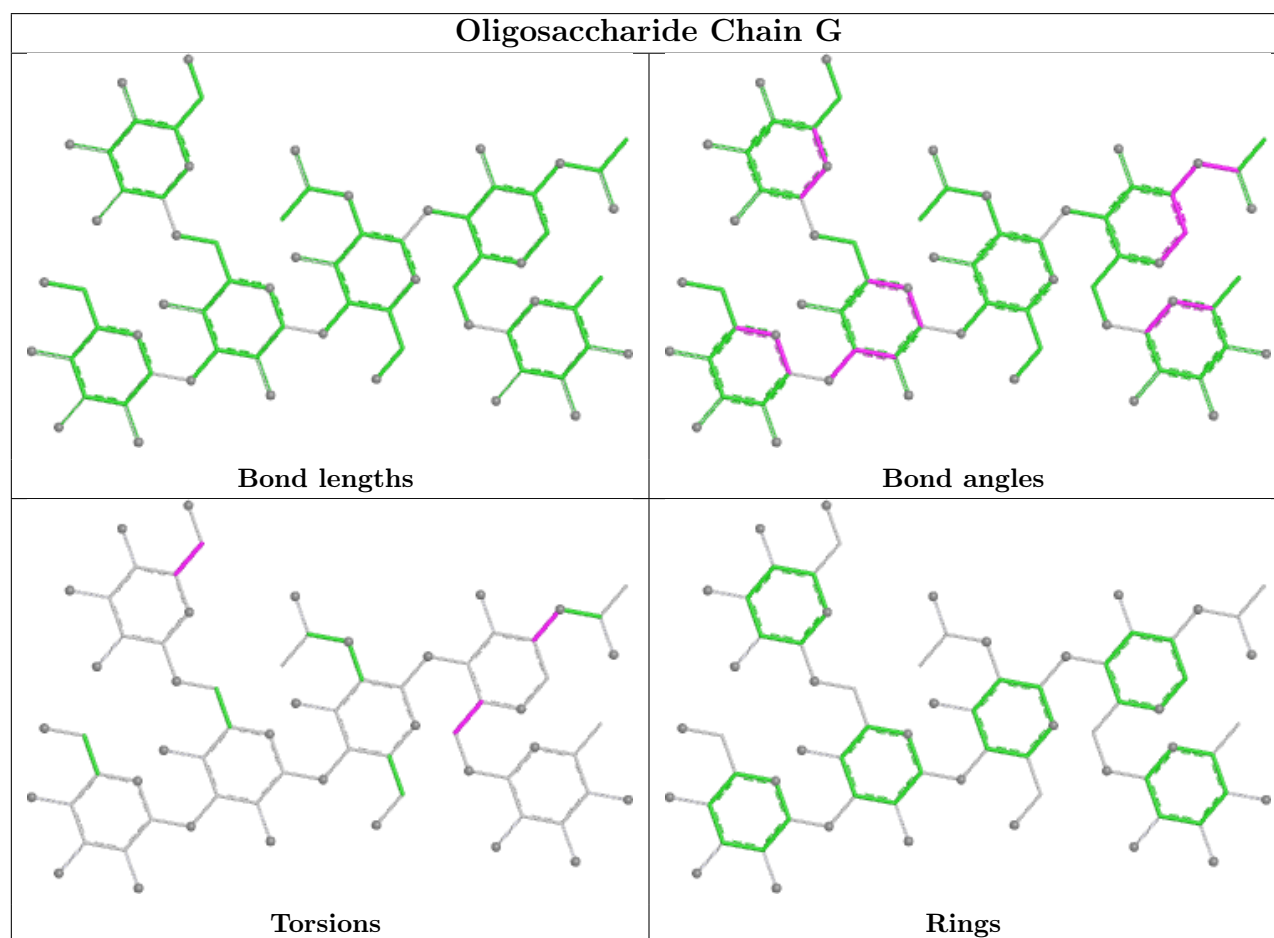
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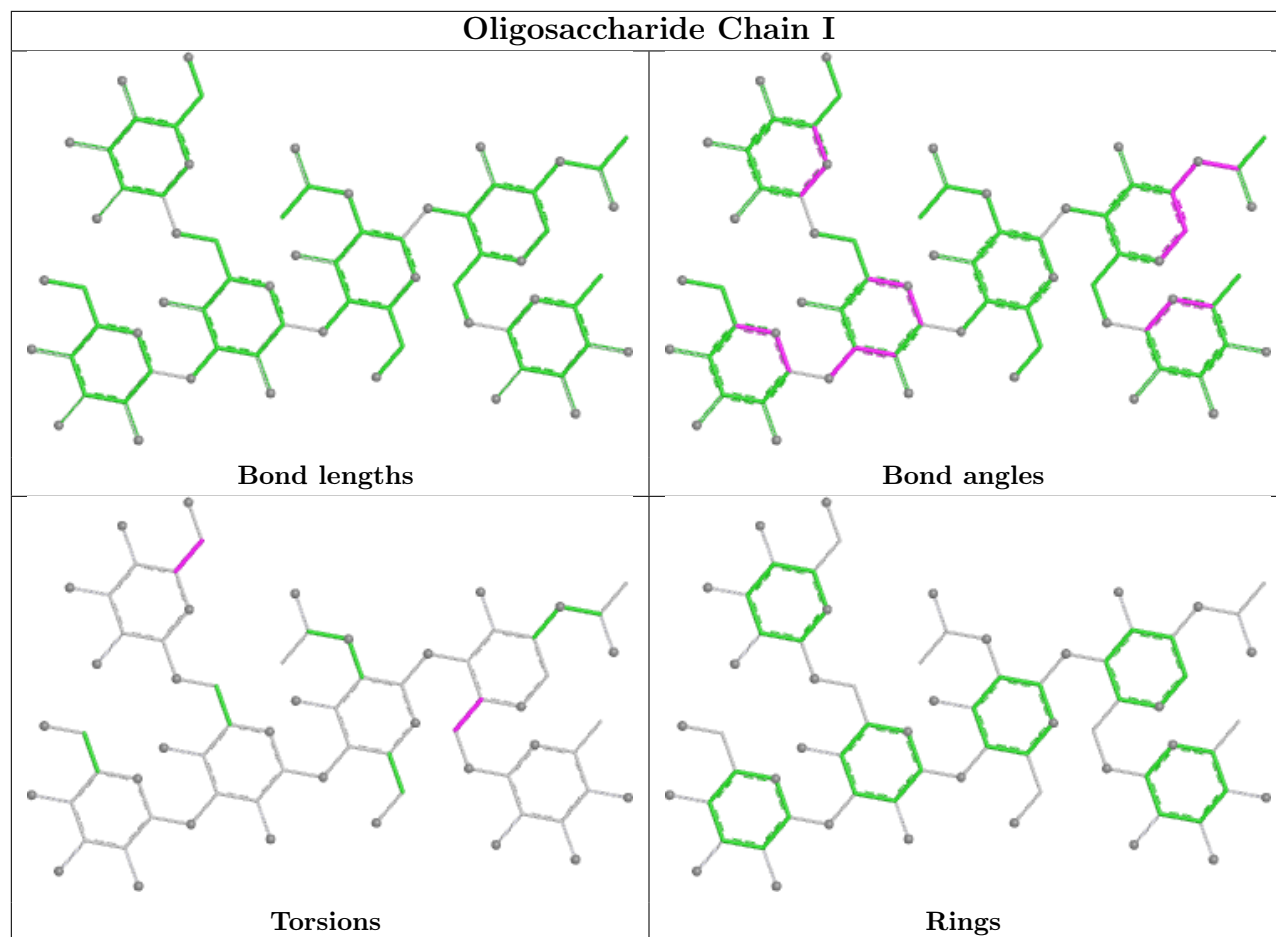
Mol	Chain	Res	Type	Atoms
5	H	5	MAN	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6

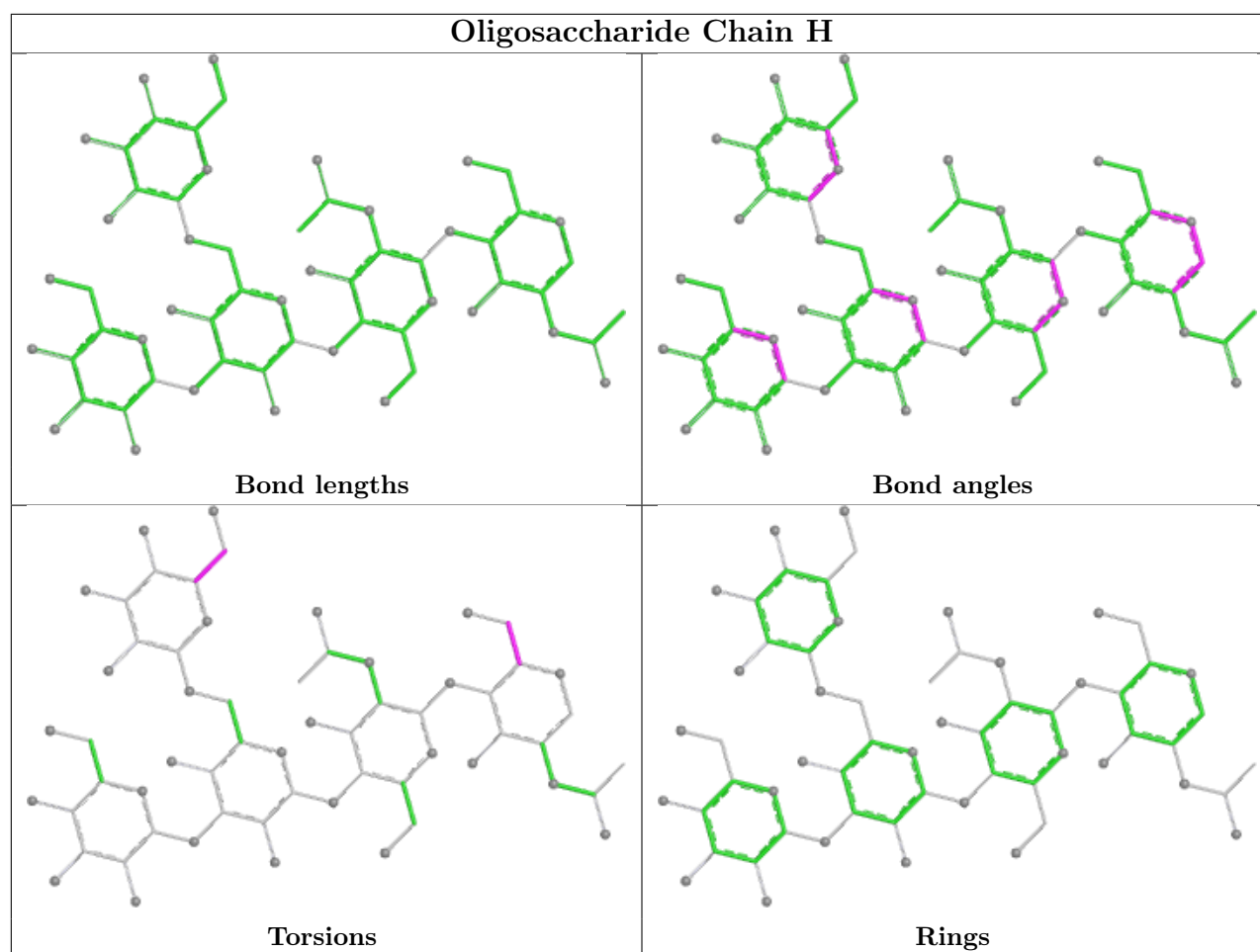
There are no ring outliers.

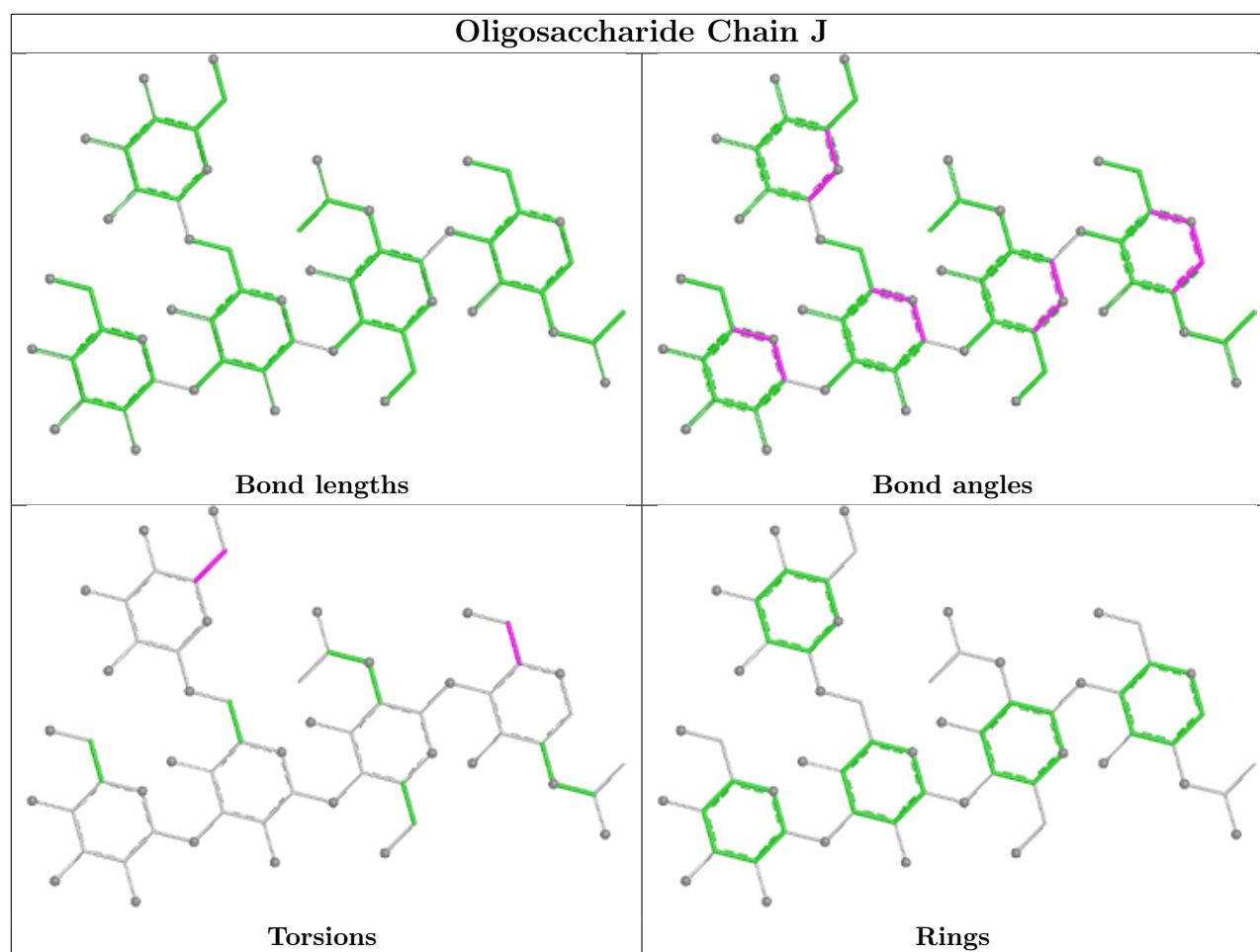
No monomer is involved in short contacts.

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](#)

3 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	$\# Z > 2$
6	EDO	A	612	-	3,3,3	0.69	0	2,2,2	0.22	0
7	NAG	B	612	1	14,14,15	0.34	0	17,19,21	0.90	1 (5%)
6	EDO	B	613	-	3,3,3	0.71	0	2,2,2	0.15	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
6	EDO	A	612	-	-	0/1/1/1	-
7	NAG	B	612	1	-	0/6/23/26	0/1/1/1
6	EDO	B	613	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	B	612	NAG	C1-C2-N2	3.12	115.35	110.43

There are no chirality outliers.

There are no torsion outliers.

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	529/542 (97%)	0.65	57 (10%) 11 9	21, 66, 105, 135	1 (0%)
1	B	529/542 (97%)	0.56	30 (5%) 29 26	22, 65, 100, 135	1 (0%)
2	C	212/213 (99%)	-0.31	0 100 100	30, 43, 66, 103	0
2	E	212/213 (99%)	-0.25	1 (0%) 87 86	25, 47, 76, 100	1 (0%)
3	D	225/234 (96%)	0.06	8 (3%) 46 42	24, 51, 79, 122	1 (0%)
3	F	219/234 (93%)	0.12	2 (0%) 81 80	24, 59, 91, 124	1 (0%)
All	All	1926/1978 (97%)	0.29	98 (5%) 33 29	21, 57, 96, 135	5 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	ALA	5.4
3	F	139	GLY	4.9
3	D	141	ALA	4.8
1	B	56	HIS	4.7
3	D	142	ALA	4.6
1	A	213	THR	4.1
1	A	486	ALA	3.9
3	D	144	THR	3.7
1	A	56	HIS	3.5
1	A	108	ASP	3.4
1	B	316	GLU	3.4
3	D	143	GLN	3.4
3	D	145	ASN	3.4
1	A	41	GLY	3.4
1	B	3	ALA	3.4
1	A	491	ALA	3.3
1	A	217	THR	3.2
1	B	491	ALA	3.2
1	A	258	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	3.1
1	A	416	SER	3.1
1	A	166	GLY	3.1
1	A	45	PHE	2.9
1	B	57	VAL	2.9
1	B	260	SER	2.9
1	A	256	PHE	2.9
3	D	140	SER	2.8
1	A	109	ALA	2.8
1	B	164	ALA	2.8
1	A	464	GLU	2.8
1	B	107	LYS	2.8
1	A	264	SER	2.7
1	B	243	GLY	2.7
1	A	535	THR	2.7
1	A	50	PRO	2.7
1	B	45	PHE	2.7
1	A	111	VAL	2.6
1	A	91	SER	2.6
1	A	485	PRO	2.6
1	B	485	PRO	2.6
1	A	58	LEU	2.6
1	A	42	ARG	2.6
1	A	47	ARG	2.6
1	A	316	GLU	2.5
1	B	166	GLY	2.5
3	D	139	GLY	2.5
1	A	177	LEU	2.5
1	B	135	LEU	2.5
1	A	315	LYS	2.4
1	A	533	ASN	2.4
1	B	192	ARG	2.4
1	A	412	ALA	2.4
3	F	225	ARG	2.4
1	A	162	PRO	2.4
1	A	192	ARG	2.4
1	A	414	ARG	2.4
1	B	43	MET	2.3
1	A	413	LYS	2.3
3	D	67	LYS	2.3
1	A	35	PHE	2.3
1	A	411	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	237	THR	2.3
1	B	16	ARG	2.3
1	A	174	ARG	2.2
1	B	484	ASP	2.2
1	A	301	PHE	2.2
1	A	237	THR	2.2
1	A	182	ASN	2.2
1	B	181	GLN	2.2
1	B	535	THR	2.2
1	B	153	PHE	2.2
1	A	12	THR	2.2
1	A	158	LEU	2.2
1	A	255	HIS	2.2
1	A	193	ALA	2.1
1	B	152	ALA	2.1
1	B	415	ASN	2.1
1	A	266	LEU	2.1
1	A	496	THR	2.1
1	A	107	LYS	2.1
2	E	168	LYS	2.1
1	A	165	PRO	2.1
1	A	482	PRO	2.1
1	B	55	GLN	2.1
1	B	32	GLY	2.1
1	A	477	ALA	2.1
1	B	306	GLU	2.1
1	B	7	LYS	2.1
1	A	54	TRP	2.0
1	A	38	PRO	2.0
1	A	189	GLY	2.0
1	A	296	ILE	2.0
1	B	296	ILE	2.0
1	B	442[A]	TYR	2.0
1	A	3	ALA	2.0
1	A	493	PRO	2.0
1	A	218	LEU	2.0
1	A	362	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

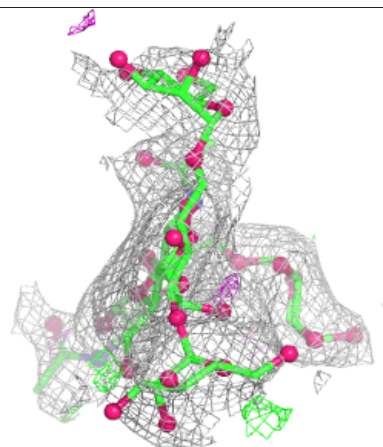
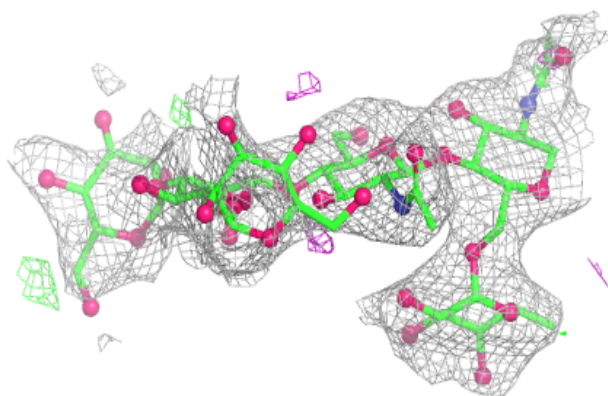
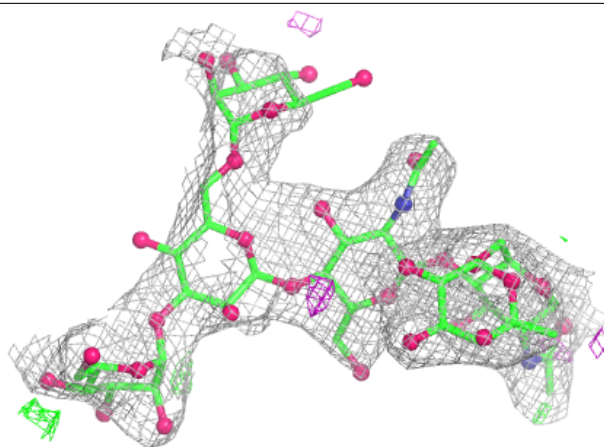
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	G	4	11/12	0.45	0.18	115,117,118,119	0
5	MAN	H	5	11/12	0.53	0.22	93,98,103,105	0
5	MAN	J	5	11/12	0.54	0.21	97,105,110,112	0
4	BMA	G	3	11/12	0.59	0.15	101,114,125,132	0
4	MAN	I	4	11/12	0.62	0.17	107,110,112,113	0
4	MAN	G	5	11/12	0.63	0.22	138,143,145,145	0
4	BMA	I	3	11/12	0.65	0.15	94,102,107,108	0
4	MAN	I	5	11/12	0.71	0.18	111,114,118,119	0
5	BMA	J	3	11/12	0.88	0.09	68,73,89,97	0
5	MAN	J	4	11/12	0.89	0.10	65,69,71,73	0
4	NAG	I	1	14/15	0.89	0.13	38,46,60,64	0
5	MAN	H	4	11/12	0.90	0.10	59,61,67,71	0
4	NAG	G	2	14/15	0.90	0.13	59,63,77,87	0
5	NAG	J	1	14/15	0.90	0.12	55,57,63,63	0
5	NAG	J	2	14/15	0.91	0.10	59,61,63,65	0
4	NAG	I	2	14/15	0.91	0.14	59,70,79,83	0
5	NAG	H	1	14/15	0.92	0.10	42,49,56,62	0
5	BMA	H	3	11/12	0.93	0.09	50,57,74,84	0
4	NAG	G	1	14/15	0.94	0.10	40,42,60,64	0
4	FUC	G	6	10/11	0.95	0.09	31,40,44,46	0
5	NAG	H	2	14/15	0.95	0.08	40,49,56,60	0
4	FUC	I	6	10/11	0.96	0.08	25,39,41,42	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.

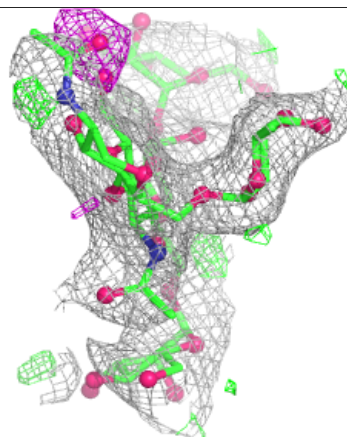
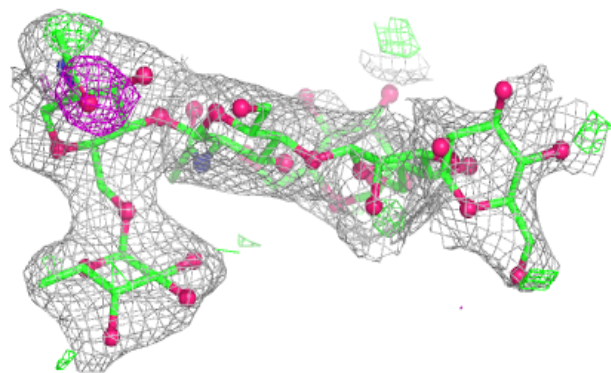
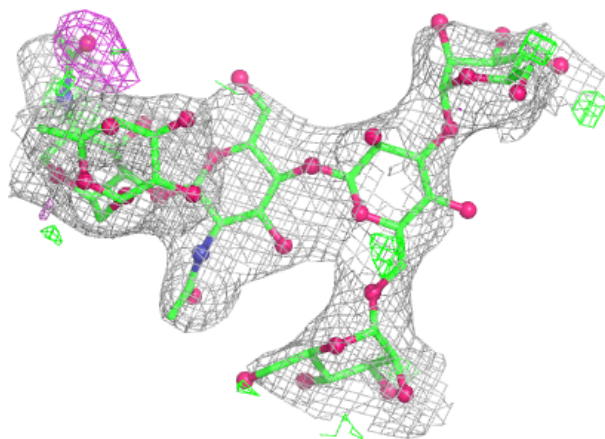
Electron density around Chain G:

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



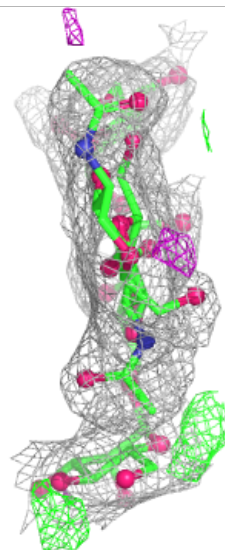
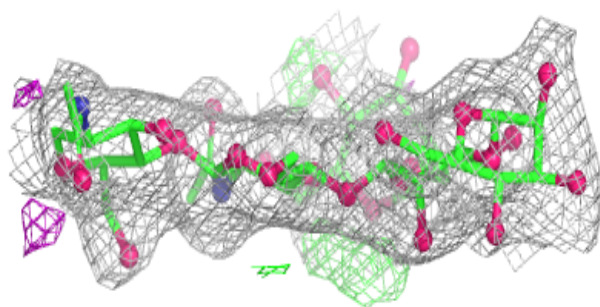
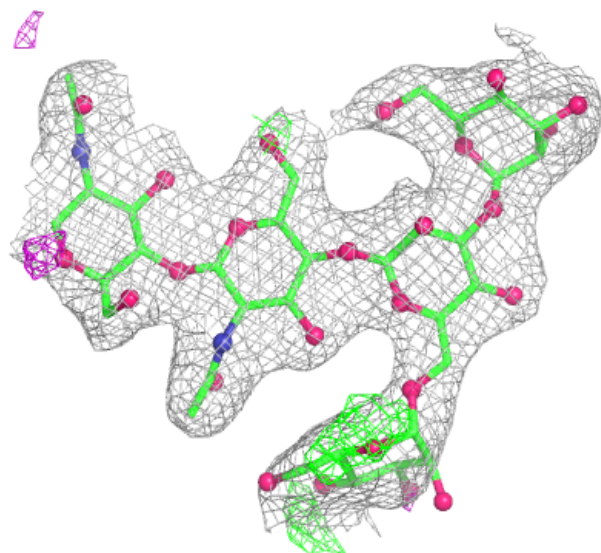
Electron density around Chain I:

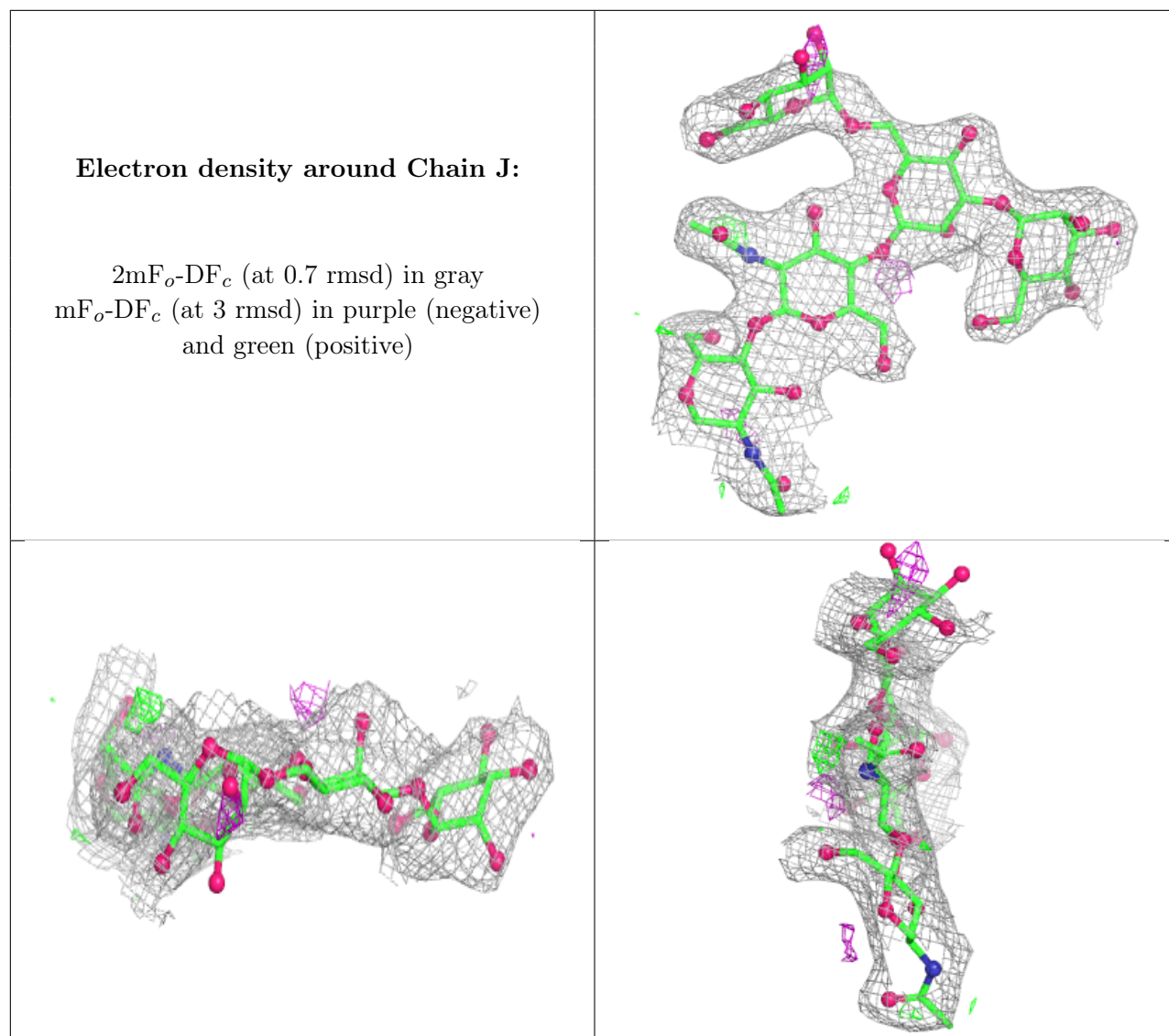
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
7	NAG	B	612	14/15	0.47	0.16	111,117,118,119	0
6	EDO	B	613	4/4	0.73	0.22	52,56,60,63	0
6	EDO	A	612	4/4	0.88	0.15	44,44,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.