



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:14 PM UTC

PDB ID : 4KTH / pdb_00004kth
Title : Structure of A/Hubei/1/2010 H5 HA
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Deposited on : 2013-05-20
Resolution : 2.60 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:

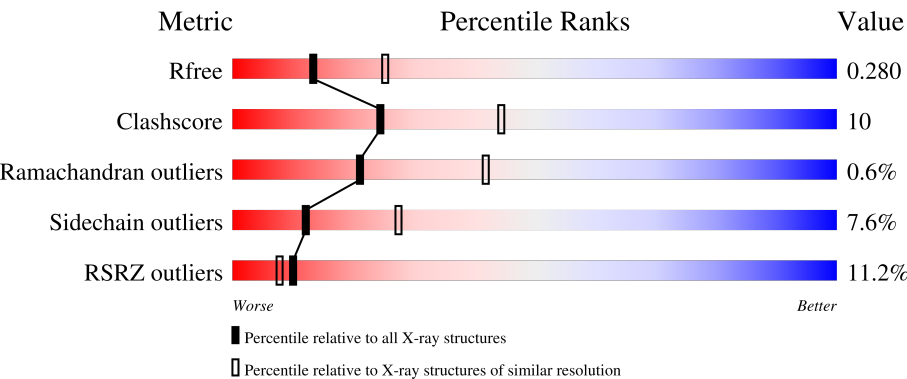
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	330	5% 75% 19% • •
1	C	330	9% 75% 18% • •
1	E	330	16% 76% 18% • •
2	B	181	2% 77% 13% • 9%
2	D	181	13% 69% 22% • • 6%

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Mol	Chain	Length	Quality of chain
2	F	181	
3	G	2	
3	H	2	
3	I	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	I	1	X	-	-	-
4	NAG	A	406	X	-	-	-
4	NAG	E	402	X	-	-	-
4	NAG	F	201	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11987 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2553	1617	441	482	13			
1	E	321	Total	C	N	O	S	0	0	0
			2546	1612	440	481	13			
1	C	321	Total	C	N	O	S	0	0	0
			2546	1612	440	481	13			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP G2U0T8
A	-2	ASP	-	expression tag	UNP G2U0T8
A	-1	PRO	-	expression tag	UNP G2U0T8
A	0	GLY	-	expression tag	UNP G2U0T8
A	325	THR	ARG	conflict	UNP G2U0T8
E	-3	ALA	-	expression tag	UNP G2U0T8
E	-2	ASP	-	expression tag	UNP G2U0T8
E	-1	PRO	-	expression tag	UNP G2U0T8
E	0	GLY	-	expression tag	UNP G2U0T8
E	325	THR	ARG	conflict	UNP G2U0T8
C	-3	ALA	-	expression tag	UNP G2U0T8
C	-2	ASP	-	expression tag	UNP G2U0T8
C	-1	PRO	-	expression tag	UNP G2U0T8
C	0	GLY	-	expression tag	UNP G2U0T8
C	325	THR	ARG	conflict	UNP G2U0T8

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1352	836	236	272	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	163	Total	C	N	O	S	0	0	0
			1338	827	234	269	8			
2	D	170	Total	C	N	O	S	0	0	0
			1384	858	241	277	8			

There are 18 discrepancies between the modelled and reference sequences:

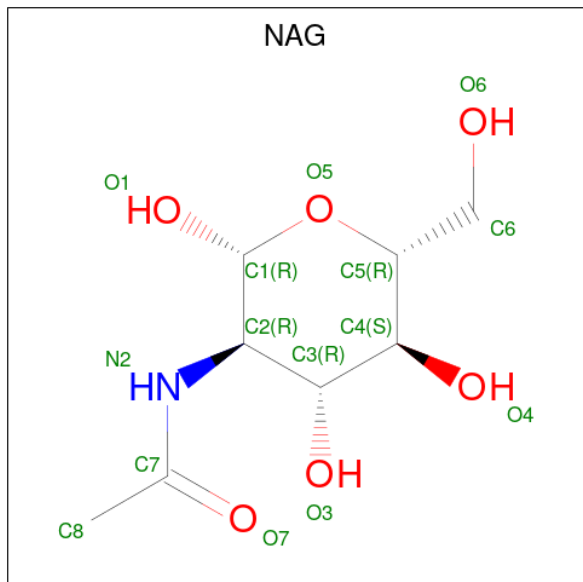
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	GLY	conflict	UNP G2U0T8
B	176	GLY	VAL	conflict	UNP G2U0T8
B	177	ARG	LYS	conflict	UNP G2U0T8
B	179	VAL	-	expression tag	UNP G2U0T8
B	180	PRO	-	expression tag	UNP G2U0T8
B	181	ARG	-	expression tag	UNP G2U0T8
F	175	SER	GLY	conflict	UNP G2U0T8
F	176	GLY	VAL	conflict	UNP G2U0T8
F	177	ARG	LYS	conflict	UNP G2U0T8
F	179	VAL	-	expression tag	UNP G2U0T8
F	180	PRO	-	expression tag	UNP G2U0T8
F	181	ARG	-	expression tag	UNP G2U0T8
D	175	SER	GLY	conflict	UNP G2U0T8
D	176	GLY	VAL	conflict	UNP G2U0T8
D	177	ARG	LYS	conflict	UNP G2U0T8
D	179	VAL	-	expression tag	UNP G2U0T8
D	180	PRO	-	expression tag	UNP G2U0T8
D	181	ARG	-	expression tag	UNP G2U0T8

- Molecule 3 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
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	E	13	Total	O	0	0
			13	13		

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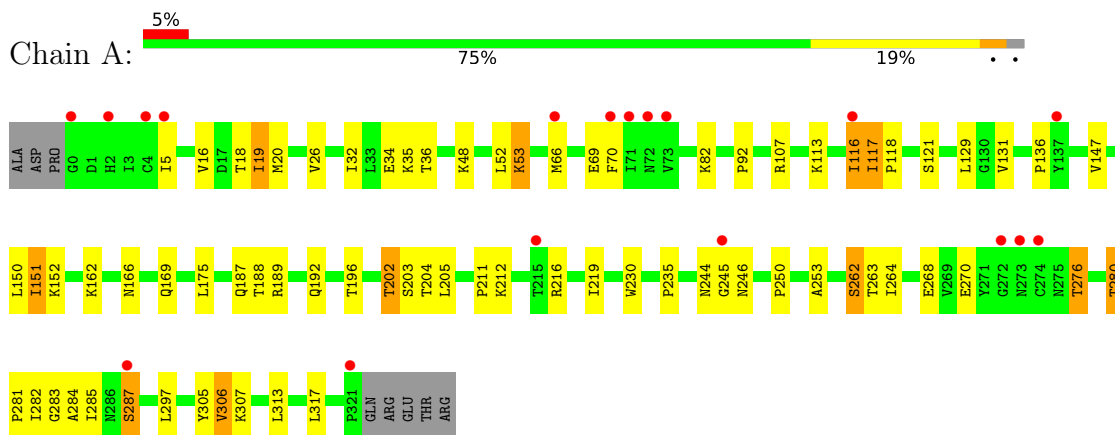
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	7	Total 7	O 7	0	0
5	C	17	Total 17	O 17	0	0
5	F	6	Total 6	O 6	0	0
5	D	6	Total 6	O 6	0	0

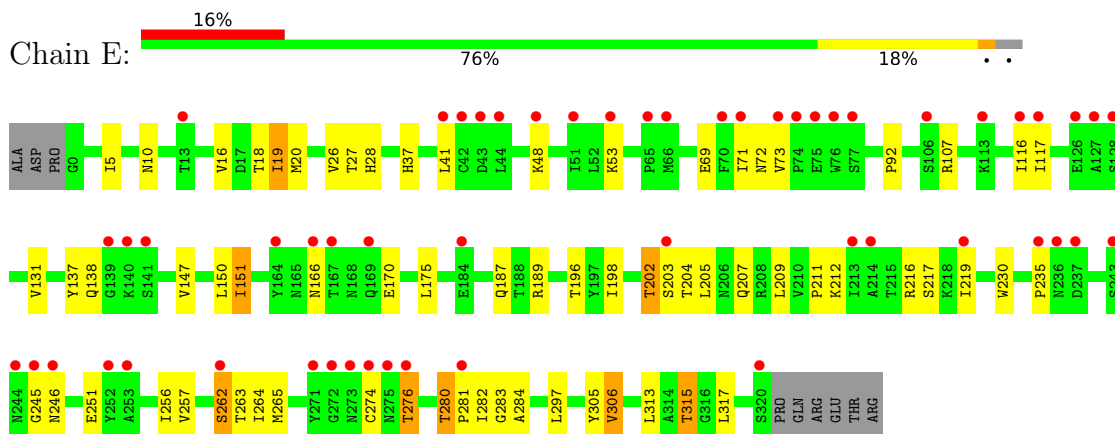
3 Residue-property plots [i](#)

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

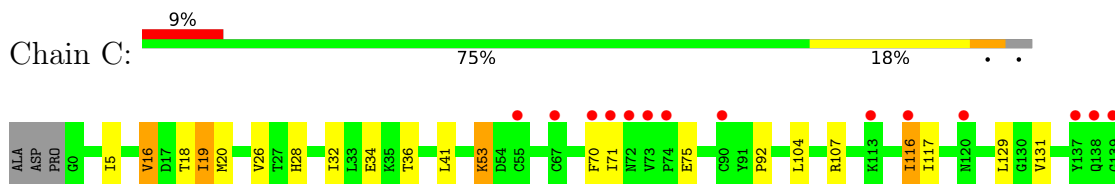
• Molecule 1: Hemagglutinin

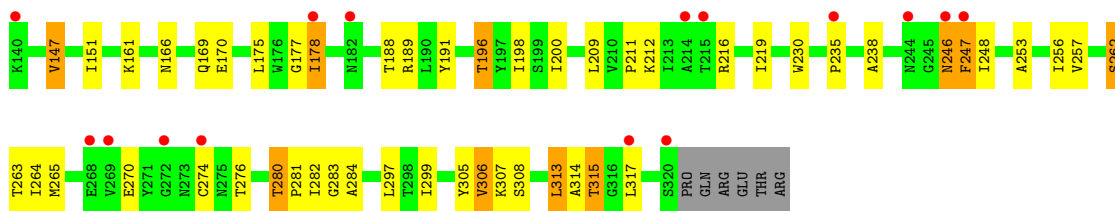


• Molecule 1: Hemagglutinin

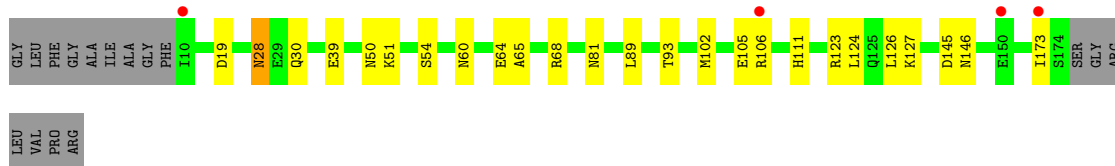
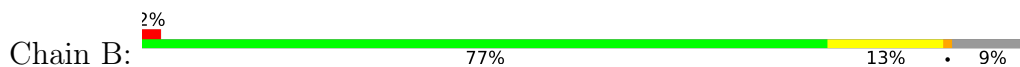


• Molecule 1: Hemagglutinin

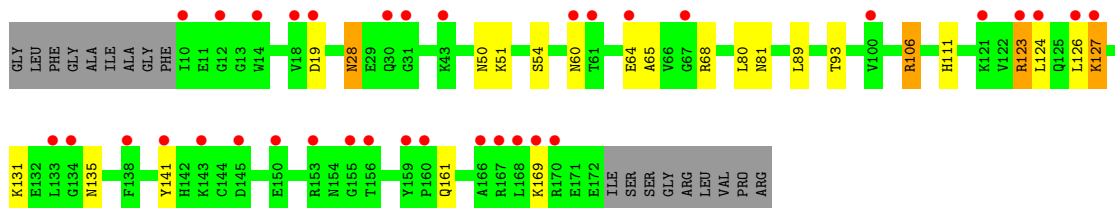




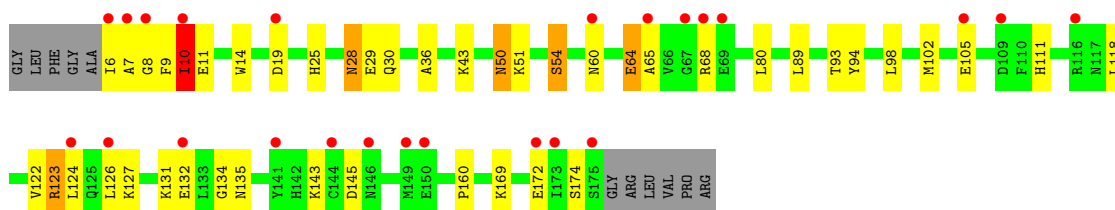
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



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



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

Chain H:  50% 50%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.12Å 101.58Å 124.93Å 90.00° 121.66° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.60) 99.2 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.234 , 0.266 0.254 , 0.280	Depositor DCC
R_{free} test set	2876 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.7	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	0.91	EDS
Total number of atoms	11987	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	0/2617	0.72	1/3557 (0.0%)
1	C	0.67	0/2609	0.73	3/3545 (0.1%)
1	E	0.66	0/2609	0.69	0/3545
2	B	0.62	0/1377	0.70	0/1851
2	D	0.63	0/1410	0.70	0/1895
2	F	0.63	0/1363	0.71	0/1832
All	All	0.65	0/11985	0.71	4/16225 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	ASN	N-CA-C	7.41	121.61	111.54
1	C	71	ILE	N-CA-C	-6.29	106.32	111.91
1	A	287	SER	N-CA-C	5.63	117.96	107.99
1	C	247	PHE	N-CA-C	5.18	117.89	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2553	0	2491	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2546	0	2485	65	0
1	E	2546	0	2486	44	0
2	B	1352	0	1256	21	0
2	D	1384	0	1286	65	0
2	F	1338	0	1239	49	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
4	A	28	0	26	0	0
4	C	42	0	39	1	0
4	E	28	0	26	0	0
4	F	14	0	13	0	0
5	A	23	0	0	1	0
5	B	7	0	0	2	0
5	C	17	0	0	1	0
5	D	6	0	0	2	0
5	E	13	0	0	1	0
5	F	6	0	0	0	0
All	All	11987	0	11422	231	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 (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:123:ARG:NH1	2:F:124:LEU:CD1	1.72	1.51
2:F:123:ARG:NH1	2:F:124:LEU:HD11	1.20	1.46
2:F:127:LYS:HZ3	2:D:132:GLU:N	1.33	1.25
2:F:123:ARG:NH2	2:D:132:GLU:OE1	1.74	1.20
2:F:127:LYS:NZ	2:D:132:GLU:N	1.94	1.14
2:F:127:LYS:HZ2	2:D:131:LYS:HG3	1.15	1.08
1:E:297:LEU:HD21	2:F:68:ARG:NH2	1.71	1.04
2:F:123:ARG:NH1	2:F:124:LEU:HD12	1.70	1.02
2:F:127:LYS:HZ2	2:D:131:LYS:CG	1.75	1.00
1:A:116:ILE:HG22	1:A:117:ILE:HG22	1.43	0.99
1:C:178:ILE:HD11	1:C:209:LEU:HD13	1.46	0.97
2:F:123:ARG:CZ	2:F:124:LEU:CD1	2.43	0.96
2:D:9:PHE:CE2	2:D:10:ILE:HG23	2.02	0.95
2:F:123:ARG:CZ	2:F:124:LEU:HD12	1.98	0.92
1:C:178:ILE:HD11	1:C:209:LEU:CD1	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:HD12	1:C:198:ILE:HD12	1.51	0.90
2:F:127:LYS:HZ3	2:D:131:LYS:C	1.81	0.89
1:C:276:THR:HG21	1:C:284:ALA:HB1	1.54	0.89
2:F:127:LYS:HE2	2:D:132:GLU:HB2	1.51	0.89
2:F:127:LYS:HZ3	2:D:132:GLU:H	1.15	0.87
2:F:127:LYS:NZ	2:D:131:LYS:C	2.32	0.86
1:C:20:MET:HE3	5:D:206:HOH:O	1.75	0.86
2:F:127:LYS:NZ	2:D:131:LYS:CG	2.40	0.83
1:E:27:THR:HG22	1:E:28:HIS:CD2	2.14	0.83
1:C:178:ILE:CD1	1:C:209:LEU:HD13	2.09	0.83
2:F:123:ARG:CZ	2:F:124:LEU:HD11	2.08	0.82
1:A:69:GLU:HB3	1:A:70:PHE:HA	1.66	0.77
2:F:123:ARG:HH11	2:F:124:LEU:CD1	1.97	0.77
1:A:196:THR:HA	1:A:244:ASN:HD21	1.51	0.76
1:E:297:LEU:HD21	2:F:68:ARG:HH22	1.49	0.73
1:C:177:GLY:C	1:C:178:ILE:HD13	2.14	0.72
2:F:123:ARG:NH2	2:D:132:GLU:CD	2.47	0.72
1:C:317:LEU:HD23	2:D:111:HIS:CG	2.25	0.72
1:C:18:THR:HG22	1:C:20:MET:H	1.54	0.72
1:A:202:THR:HG22	1:A:204:THR:H	1.54	0.71
1:E:202:THR:HG21	5:E:510:HOH:O	1.89	0.71
2:B:102:MET:HE1	2:D:102:MET:CE	2.21	0.71
2:B:173:ILE:HD12	2:D:160:PRO:HB3	1.72	0.70
1:C:20:MET:HE2	2:F:51:LYS:HE3	1.73	0.70
1:C:198:ILE:CD1	1:C:247:PHE:HB2	2.22	0.70
1:E:18:THR:HG22	1:E:20:MET:H	1.57	0.69
1:A:18:THR:HG22	1:A:20:MET:H	1.57	0.69
1:A:66:MET:HE3	1:A:136:PRO:HD2	1.75	0.69
1:A:34:GLU:OE2	1:A:36:THR:HG22	1.94	0.67
1:C:34:GLU:OE2	1:C:36:THR:HG22	1.93	0.67
2:D:9:PHE:CD2	2:D:10:ILE:HG23	2.29	0.66
1:E:196:THR:HG21	1:E:246:ASN:OD1	1.96	0.66
2:D:10:ILE:HD11	2:D:135:ASN:HA	1.77	0.66
1:E:107:ARG:HB2	1:E:262:SER:HB3	1.79	0.65
1:E:198:ILE:HD11	1:E:246:ASN:O	1.97	0.64
2:F:127:LYS:HZ1	2:D:132:GLU:N	1.93	0.64
1:C:263:THR:HG22	2:D:65:ALA:HB1	1.80	0.64
2:F:123:ARG:HH21	2:D:132:GLU:CD	2.06	0.64
1:A:285:ILE:HG22	1:A:287:SER:HB3	1.78	0.63
1:E:280:THR:HG22	1:E:282:ILE:H	1.63	0.63
2:F:127:LYS:NZ	2:D:131:LYS:HG2	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:CD1	1:C:209:LEU:CD1	2.74	0.63
2:F:127:LYS:HZ3	2:D:131:LYS:CA	2.12	0.63
1:E:10:ASN:ND2	1:E:27:THR:HG23	2.15	0.62
1:C:116:ILE:HD13	1:C:253:ALA:HB3	1.81	0.62
1:C:280:THR:HG22	1:C:282:ILE:H	1.65	0.62
1:A:196:THR:HA	1:A:244:ASN:ND2	2.17	0.59
1:C:178:ILE:HG23	1:C:198:ILE:HD12	1.84	0.59
2:F:127:LYS:NZ	2:D:131:LYS:CA	2.65	0.59
2:F:127:LYS:CE	2:D:132:GLU:O	2.51	0.59
1:A:169:GLN:HE21	1:A:169:GLN:HA	1.66	0.59
1:A:69:GLU:HB3	1:A:70:PHE:CA	2.31	0.59
2:F:81:ASN:HD22	2:D:80:LEU:CD1	2.16	0.59
1:A:196:THR:HG21	1:A:246:ASN:OD1	2.03	0.58
1:C:196:THR:HG22	1:C:211:PRO:HG2	1.85	0.58
1:C:306:VAL:HG22	2:D:93:THR:HA	1.85	0.58
1:A:262:SER:OG	1:A:263:THR:N	2.37	0.58
1:A:280:THR:HG22	1:A:282:ILE:H	1.69	0.58
1:E:262:SER:OG	1:E:263:THR:N	2.36	0.58
1:C:178:ILE:HG23	1:C:198:ILE:CD1	2.32	0.58
1:A:69:GLU:CB	1:A:70:PHE:HA	2.29	0.58
1:A:117:ILE:HD13	1:A:162:LYS:HE3	1.86	0.58
2:F:127:LYS:HZ1	2:D:132:GLU:C	2.12	0.58
1:A:306:VAL:HG22	2:B:93:THR:HA	1.86	0.57
1:A:196:THR:CG2	1:A:211:PRO:HG2	2.35	0.57
1:C:198:ILE:HD11	1:C:247:PHE:HB2	1.87	0.57
1:C:262:SER:OG	1:C:263:THR:N	2.36	0.57
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.88	0.56
1:A:305:TYR:CD2	2:B:89:LEU:HD12	2.40	0.56
2:B:106:ARG:HD3	5:B:304:HOH:O	2.04	0.56
2:D:123:ARG:HG2	2:D:124:LEU:CD1	2.36	0.56
1:A:196:THR:HG23	1:A:211:PRO:HG2	1.88	0.55
1:C:280:THR:HB	1:C:283:GLY:O	2.06	0.55
1:C:280:THR:HG23	1:C:281:PRO:HD2	1.88	0.55
1:A:280:THR:HB	1:A:283:GLY:O	2.07	0.55
2:D:8:GLY:HA3	2:D:135:ASN:O	2.06	0.55
1:A:19:ILE:HD12	2:D:51:LYS:HG3	1.89	0.54
1:A:118:PRO:HG2	1:A:121:SER:HB2	1.89	0.54
1:C:276:THR:HG21	1:C:284:ALA:CB	2.33	0.54
1:A:175:LEU:HD23	1:A:230:TRP:HB3	1.88	0.54
1:A:297:LEU:HD21	2:B:68:ARG:NH1	2.23	0.54
1:A:70:PHE:HB2	1:A:113:LYS:NZ	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:GLN:NE2	2:D:145:ASP:HB2	2.23	0.54
1:C:166:ASN:O	1:C:235:PRO:O	2.26	0.54
1:A:166:ASN:O	1:A:235:PRO:O	2.25	0.54
1:E:175:LEU:HD23	1:E:230:TRP:HB3	1.90	0.54
1:E:280:THR:HB	1:E:283:GLY:O	2.07	0.54
1:E:196:THR:OG1	1:E:245:GLY:N	2.42	0.53
2:D:6:ILE:HD13	2:D:25:HIS:NE2	2.23	0.53
1:C:178:ILE:HD13	1:C:178:ILE:N	2.24	0.53
1:E:263:THR:HB	2:F:65:ALA:HB1	1.90	0.53
2:D:7:ALA:HB1	2:D:11:GLU:HG3	1.91	0.53
1:E:276:THR:HG21	1:E:284:ALA:HB1	1.89	0.53
1:E:280:THR:HG23	1:E:281:PRO:HD2	1.91	0.53
2:F:81:ASN:HD22	2:D:80:LEU:HD13	1.72	0.53
1:A:196:THR:HG23	1:A:211:PRO:CG	2.39	0.53
1:A:263:THR:HG22	2:B:65:ALA:HB1	1.90	0.52
1:C:117:ILE:HD12	1:C:117:ILE:O	2.08	0.52
1:C:263:THR:CG2	2:D:65:ALA:HB1	2.39	0.52
2:B:81:ASN:HD22	2:F:80:LEU:CD1	2.21	0.52
1:E:116:ILE:HG22	1:E:251:GLU:O	2.09	0.52
1:E:202:THR:CG2	1:E:203:SER:N	2.73	0.52
1:E:306:VAL:HG22	2:F:93:THR:HA	1.92	0.52
2:D:14:TRP:NE1	5:D:204:HOH:O	2.10	0.52
1:A:52:LEU:O	1:A:53:LYS:C	2.53	0.52
1:C:116:ILE:HG23	1:C:117:ILE:HG23	1.92	0.52
1:A:117:ILE:HD13	1:A:162:LYS:CE	2.40	0.51
1:A:307:LYS:HB2	2:B:89:LEU:HD21	1.91	0.51
1:E:19:ILE:HD12	2:B:51:LYS:HG3	1.92	0.51
2:D:123:ARG:HG2	2:D:124:LEU:HD12	1.92	0.51
1:A:202:THR:HB	1:A:205:LEU:HB3	1.91	0.51
1:E:166:ASN:O	1:E:235:PRO:O	2.27	0.51
1:E:37:HIS:CE1	1:E:282:ILE:HG22	2.45	0.51
2:F:127:LYS:HE2	2:D:132:GLU:CB	2.31	0.51
1:C:107:ARG:HB2	1:C:262:SER:HB3	1.92	0.51
1:A:280:THR:HG23	1:A:281:PRO:HD2	1.92	0.51
1:A:276:THR:HG21	1:A:284:ALA:HB1	1.92	0.51
1:E:305:TYR:CD2	2:F:89:LEU:HD13	2.46	0.51
1:E:28:HIS:C	1:E:315:THR:HG22	2.37	0.50
1:C:41:LEU:HD22	1:C:265:MET:HE1	1.93	0.50
1:C:175:LEU:HD23	1:C:230:TRP:HB3	1.92	0.50
1:A:18:THR:HG23	2:B:105:GLU:HB2	1.92	0.50
2:B:106:ARG:CD	5:B:304:HOH:O	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:LYS:HE3	2:D:132:GLU:O	2.12	0.49
2:D:29:GLU:OE1	2:D:143:LYS:NZ	2.44	0.49
1:A:116:ILE:HD13	1:A:253:ALA:HB3	1.94	0.49
1:C:92:PRO:HG3	1:C:219:ILE:HG23	1.94	0.49
1:A:116:ILE:HG22	1:A:117:ILE:N	2.27	0.49
2:F:127:LYS:HZ1	2:D:131:LYS:C	2.17	0.49
1:E:92:PRO:HG3	1:E:219:ILE:HG23	1.94	0.49
1:E:202:THR:HB	1:E:205:LEU:HB3	1.95	0.49
2:D:28:ASN:C	2:D:28:ASN:HD22	2.20	0.49
1:A:107:ARG:HB2	1:A:262:SER:HB3	1.95	0.48
1:C:19:ILE:HD12	2:F:51:LYS:HG3	1.94	0.48
1:A:92:PRO:HG3	1:A:219:ILE:HG23	1.95	0.48
1:C:305:TYR:CD2	2:D:89:LEU:HD12	2.49	0.48
1:E:71:ILE:O	1:E:73:VAL:HG23	2.13	0.48
2:D:7:ALA:O	2:D:14:TRP:HH2	1.97	0.48
1:E:10:ASN:HD21	1:E:27:THR:HG23	1.78	0.48
1:C:41:LEU:HD22	1:C:265:MET:CE	2.44	0.48
2:F:127:LYS:HZ1	2:D:131:LYS:HG2	1.77	0.48
2:B:28:ASN:C	2:B:28:ASN:HD22	2.22	0.47
2:F:127:LYS:HZ3	2:D:131:LYS:HA	1.80	0.47
2:B:102:MET:HE1	2:D:102:MET:HE3	1.96	0.47
2:F:106:ARG:HH22	2:D:102:MET:HB3	1.80	0.47
1:A:263:THR:CG2	2:B:65:ALA:HB1	2.45	0.47
2:D:7:ALA:C	2:D:14:TRP:HH2	2.23	0.47
1:A:317:LEU:HD23	2:B:111:HIS:CG	2.49	0.46
1:C:299:ILE:HA	2:D:64:GLU:O	2.15	0.46
2:B:126:LEU:O	2:B:127:LYS:C	2.55	0.46
1:C:5:ILE:HD12	1:C:5:ILE:N	2.30	0.46
1:A:264:ILE:N	1:A:264:ILE:HD12	2.30	0.46
1:C:20:MET:CE	2:F:51:LYS:HE3	2.45	0.46
2:B:123:ARG:NH2	2:B:124:LEU:CD1	2.79	0.46
1:C:307:LYS:HB2	2:D:89:LEU:HD21	1.98	0.46
1:C:178:ILE:CG1	1:C:209:LEU:HD13	2.46	0.46
1:E:202:THR:HG22	1:E:203:SER:N	2.31	0.45
1:C:147:VAL:HG22	1:C:248:ILE:HG22	1.98	0.45
1:E:137:TYR:CD2	1:E:138:GLN:HG2	2.52	0.45
2:F:124:LEU:HD23	2:D:134:GLY:HA2	1.99	0.45
1:E:116:ILE:HG23	1:E:117:ILE:HG12	1.99	0.45
2:D:30:GLN:HE22	2:D:145:ASP:HB2	1.81	0.45
1:E:207:GLN:NE2	1:E:209:LEU:HD21	2.32	0.45
1:A:107:ARG:HD2	5:A:510:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ARG:HD2	5:C:513:HOH:O	2.17	0.45
1:C:238:ALA:N	4:C:401:NAG:H82	2.32	0.45
2:D:10:ILE:HD11	2:D:134:GLY:O	2.17	0.45
1:C:200:ILE:N	1:C:200:ILE:HD12	2.32	0.44
2:F:28:ASN:HD22	2:F:28:ASN:C	2.25	0.44
1:A:152:LYS:HD2	1:A:192:GLN:HG2	1.99	0.44
1:C:5:ILE:HD11	2:D:122:VAL:HG21	2.00	0.44
2:F:127:LYS:CE	2:D:132:GLU:N	2.78	0.44
1:C:264:ILE:N	1:C:264:ILE:HD12	2.32	0.44
1:C:297:LEU:HD21	2:D:68:ARG:NH1	2.32	0.44
1:E:264:ILE:HD12	1:E:264:ILE:N	2.33	0.44
2:D:7:ALA:HB1	2:D:11:GLU:CG	2.48	0.44
1:C:16:VAL:HG11	1:C:314:ALA:HB2	1.98	0.43
1:C:178:ILE:HD12	1:C:198:ILE:CD1	2.37	0.43
2:D:94:TYR:CZ	2:D:98:LEU:HD11	2.53	0.43
1:A:202:THR:CG2	1:A:203:SER:N	2.80	0.43
1:A:82:LYS:CD	1:A:268:GLU:HG2	2.49	0.43
1:E:150:LEU:O	1:E:151:ILE:HD12	2.18	0.43
1:C:28:HIS:C	1:C:315:THR:HG22	2.43	0.43
1:E:41:LEU:HD22	1:E:265:MET:CE	2.49	0.43
1:E:170:GLU:HG2	1:E:257:VAL:CG2	2.48	0.43
2:F:127:LYS:NZ	2:D:132:GLU:CA	2.77	0.43
1:C:178:ILE:HD11	1:C:209:LEU:HD12	1.96	0.43
1:A:5:ILE:HD12	1:A:5:ILE:N	2.34	0.43
1:A:117:ILE:HG23	1:A:250:PRO:O	2.18	0.42
1:E:5:ILE:N	1:E:5:ILE:HD12	2.33	0.42
1:C:196:THR:HG22	1:C:211:PRO:CG	2.48	0.42
1:C:18:THR:HG23	2:D:105:GLU:HB2	2.02	0.42
1:C:70:PHE:O	1:C:70:PHE:CG	2.72	0.42
1:C:306:VAL:HG13	1:C:308:SER:HB3	2.01	0.42
1:C:196:THR:CG2	1:C:211:PRO:CG	2.98	0.42
1:E:317:LEU:HD23	2:F:111:HIS:CG	2.54	0.42
1:C:212:LYS:O	1:C:216:ARG:NH2	2.52	0.42
2:F:131:LYS:HB2	2:F:141:TYR:CZ	2.55	0.42
1:A:150:LEU:O	1:A:151:ILE:HD12	2.20	0.42
1:C:191:TYR:CZ	1:C:246:ASN:HA	2.54	0.42
1:A:212:LYS:O	1:A:216:ARG:NH2	2.53	0.41
2:B:123:ARG:NH2	2:B:124:LEU:HD12	2.36	0.41
1:C:170:GLU:HG2	1:C:257:VAL:CG2	2.50	0.41
1:C:248:ILE:N	1:C:248:ILE:HD12	2.34	0.41
1:E:217:SER:HB3	3:G:1:NAG:H81	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HG23	2:D:118:LEU:HD23	2.02	0.41
1:E:280:THR:CG2	1:E:282:ILE:H	2.30	0.41
1:C:280:THR:CG2	1:C:282:ILE:H	2.32	0.41
1:E:212:LYS:O	1:E:216:ARG:NH2	2.54	0.41
1:E:41:LEU:HD22	1:E:265:MET:HE1	2.03	0.41
1:E:196:THR:CG2	1:E:211:PRO:HG2	2.50	0.41
1:C:313:LEU:HD12	1:C:313:LEU:HA	1.95	0.41
2:D:50:ASN:O	2:D:54:SER:OG	2.39	0.41
2:F:127:LYS:NZ	2:D:132:GLU:H	1.89	0.41
2:B:30:GLN:HE22	2:B:146:ASN:H	1.69	0.40
2:B:30:GLN:HE22	2:B:145:ASP:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/330 (97%)	300 (94%)	18 (6%)	2 (1%)	21	42
1	C	319/330 (97%)	301 (94%)	17 (5%)	1 (0%)	36	58
1	E	319/330 (97%)	294 (92%)	23 (7%)	2 (1%)	21	42
2	B	163/181 (90%)	160 (98%)	3 (2%)	0	100	100
2	D	168/181 (93%)	162 (96%)	4 (2%)	2 (1%)	10	23
2	F	161/181 (89%)	158 (98%)	2 (1%)	1 (1%)	21	42
All	All	1450/1533 (95%)	1375 (95%)	67 (5%)	8 (1%)	21	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	LYS

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Mol	Chain	Res	Type
1	E	53	LYS
1	C	53	LYS
1	A	245	GLY
2	F	127	LYS
2	D	127	LYS
1	E	72	ASN
2	D	10	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	286/293 (98%)	264 (92%)	22 (8%)	12	27
1	C	285/293 (97%)	260 (91%)	25 (9%)	9	21
1	E	285/293 (97%)	265 (93%)	20 (7%)	14	31
2	B	145/155 (94%)	138 (95%)	7 (5%)	23	47
2	D	147/155 (95%)	135 (92%)	12 (8%)	10	24
2	F	143/155 (92%)	131 (92%)	12 (8%)	10	23
All	All	1291/1344 (96%)	1193 (92%)	98 (8%)	12	27

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	19	ILE
1	A	26	VAL
1	A	32	ILE
1	A	35	LYS
1	A	48	LYS
1	A	116	ILE
1	A	117	ILE
1	A	129	LEU
1	A	131	VAL
1	A	147	VAL

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Mol	Chain	Res	Type
1	A	151	ILE
1	A	187	GLN
1	A	188	THR
1	A	189	ARG
1	A	202	THR
1	A	262	SER
1	A	270	GLU
1	A	276	THR
1	A	280	THR
1	A	306	VAL
1	A	313	LEU
1	E	16	VAL
1	E	19	ILE
1	E	26	VAL
1	E	48	LYS
1	E	69	GLU
1	E	131	VAL
1	E	147	VAL
1	E	151	ILE
1	E	187	GLN
1	E	189	ARG
1	E	202	THR
1	E	204	THR
1	E	256	ILE
1	E	262	SER
1	E	274	CYS
1	E	276	THR
1	E	280	THR
1	E	306	VAL
1	E	313	LEU
1	E	315	THR
2	B	19	ASP
2	B	28	ASN
2	B	39	GLU
2	B	50	ASN
2	B	54	SER
2	B	60	ASN
2	B	64	GLU
1	C	16	VAL
1	C	19	ILE
1	C	26	VAL
1	C	32	ILE

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Mol	Chain	Res	Type
1	C	53	LYS
1	C	75	GLU
1	C	104	LEU
1	C	116	ILE
1	C	129	LEU
1	C	131	VAL
1	C	147	VAL
1	C	151	ILE
1	C	161	LYS
1	C	169	GLN
1	C	178	ILE
1	C	188	THR
1	C	196	THR
1	C	256	ILE
1	C	262	SER
1	C	270	GLU
1	C	274	CYS
1	C	280	THR
1	C	306	VAL
1	C	313	LEU
1	C	315	THR
2	F	19	ASP
2	F	28	ASN
2	F	50	ASN
2	F	54	SER
2	F	60	ASN
2	F	64	GLU
2	F	106	ARG
2	F	123	ARG
2	F	126	LEU
2	F	135	ASN
2	F	161	GLN
2	F	169	LYS
2	D	10	ILE
2	D	28	ASN
2	D	43	LYS
2	D	50	ASN
2	D	54	SER
2	D	60	ASN
2	D	64	GLU
2	D	123	ARG
2	D	126	LEU

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Mol	Chain	Res	Type
2	D	169	LYS
2	D	172	GLU
2	D	174	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	169	GLN
1	A	192	GLN
1	A	193	ASN
1	A	319	ASN
1	E	28	HIS
1	E	109	ASN
1	E	115	GLN
1	E	155	ASN
1	E	192	GLN
1	E	193	ASN
1	E	207	GLN
1	E	319	ASN
2	B	28	ASN
2	B	30	GLN
2	B	81	ASN
2	B	95	ASN
2	B	142	HIS
1	C	155	ASN
1	C	319	ASN
2	F	28	ASN
2	F	81	ASN
2	F	117	ASN
2	F	142	HIS
2	F	161	GLN
2	D	28	ASN
2	D	30	GLN
2	D	95	ASN
2	D	117	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 ⓘ

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	G	1	3,1	14,14,15	0.59	0	17,19,21	0.92	1 (5%)
3	NAG	G	2	3	14,14,15	0.56	0	17,19,21	0.63	0
3	NAG	H	1	3,1	14,14,15	0.69	0	17,19,21	1.41	3 (17%)
3	NAG	H	2	3	14,14,15	0.52	0	17,19,21	0.63	0
3	NAG	I	1	3,2	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
3	NAG	I	2	3	14,14,15	0.69	0	17,19,21	1.19	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
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	O5-C1-C2	-3.76	105.47	111.29
3	I	2	NAG	C4-C3-C2	3.43	116.04	111.02
3	H	1	NAG	C3-C4-C5	2.51	114.78	110.23
3	I	1	NAG	O5-C1-C2	-2.47	107.47	111.29
3	H	1	NAG	C4-C3-C2	2.33	114.43	111.02
3	G	1	NAG	C1-O5-C5	2.02	114.90	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	1	NAG	C1

All (10) torsion outliers are listed below:

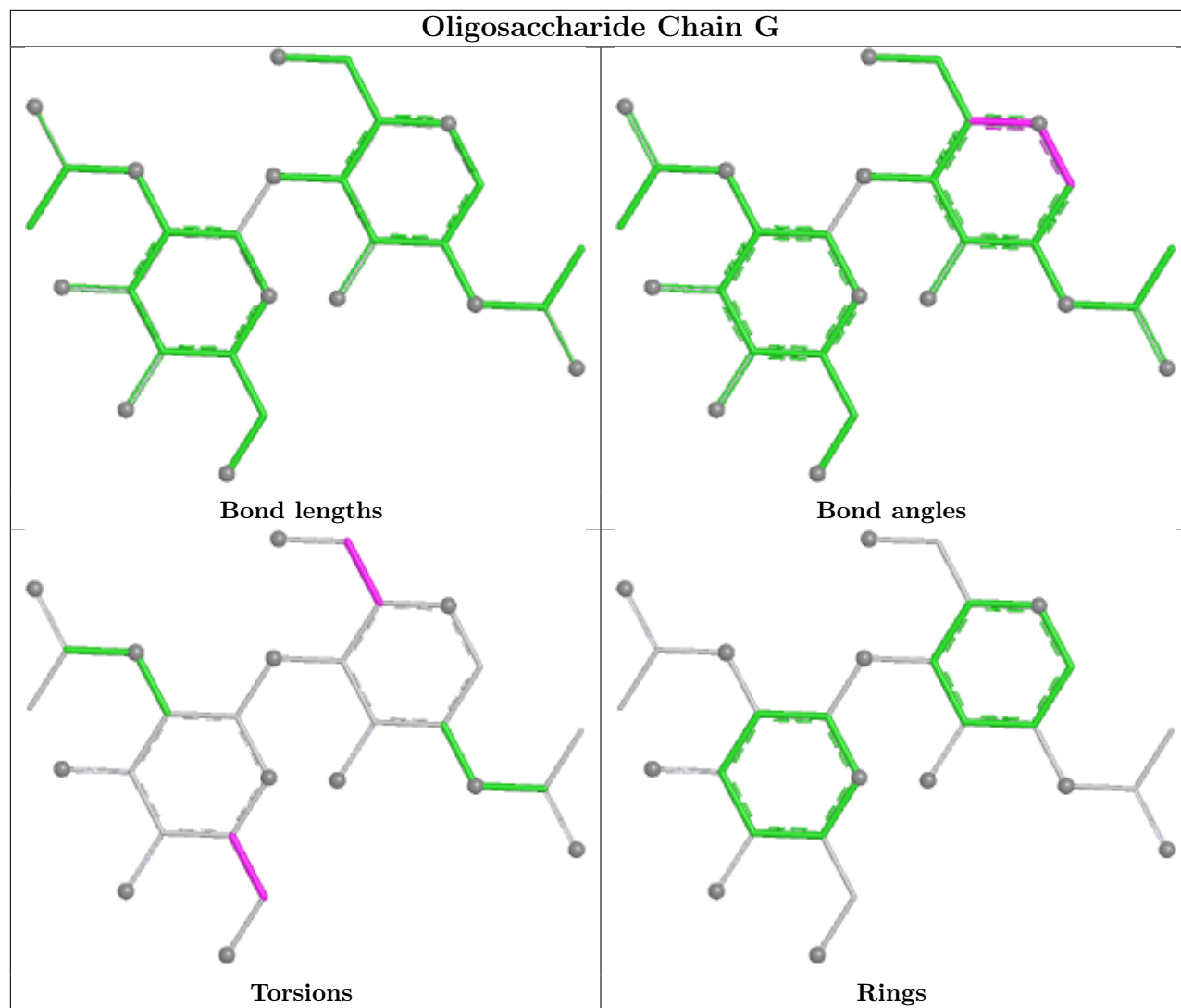
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

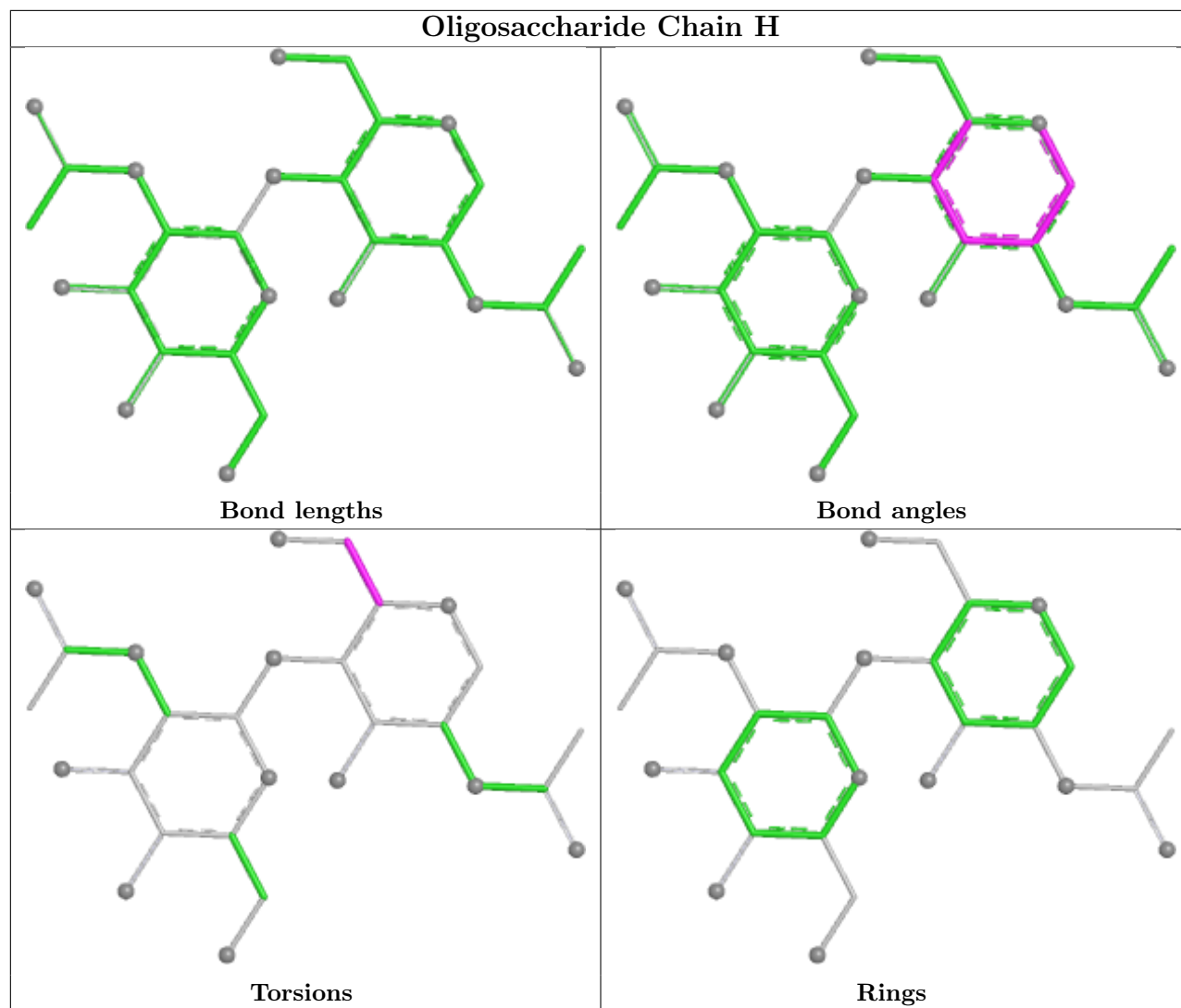
There are no ring outliers.

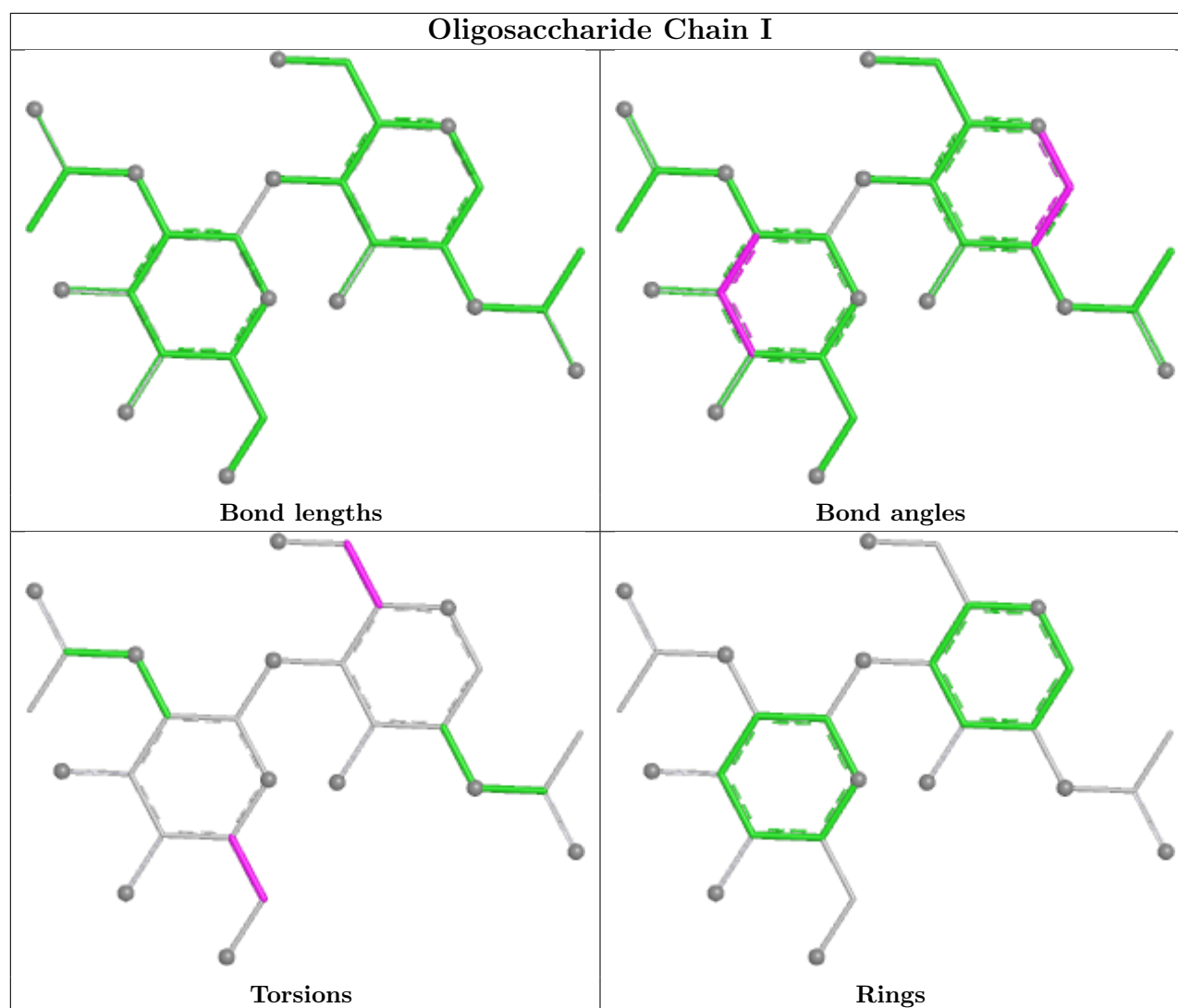
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	406	1	14,14,15	0.77	0	17,19,21	1.23	2 (11%)
4	NAG	E	401	1	14,14,15	0.52	0	17,19,21	1.28	1 (5%)
4	NAG	C	401	1	14,14,15	0.55	0	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	401	1	14,14,15	0.65	0	17,19,21	1.15	2 (11%)
4	NAG	C	403	1	14,14,15	0.73	1 (7%)	17,19,21	2.04	2 (11%)
4	NAG	E	402	1	14,14,15	0.81	0	17,19,21	1.42	2 (11%)
4	NAG	F	201	2	14,14,15	0.65	0	17,19,21	1.02	1 (5%)
4	NAG	C	402	1	14,14,15	0.65	1 (7%)	17,19,21	1.61	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
4	NAG	A	406	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	E	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	403	1	-	2/6/23/26	0/1/1/1
4	NAG	E	402	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	F	201	2	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	NAG	C1-C2	2.40	1.55	1.52
4	C	402	NAG	C1-C2	2.02	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	NAG	C1-O5-C5	6.91	121.44	112.19
4	C	402	NAG	C1-O5-C5	5.38	119.40	112.19
4	E	401	NAG	C1-O5-C5	4.44	118.14	112.19
4	E	402	NAG	C4-C3-C2	4.05	116.96	111.02
4	C	403	NAG	O5-C1-C2	4.05	117.56	111.29
4	C	401	NAG	C1-O5-C5	3.57	116.97	112.19
4	A	406	NAG	C4-C3-C2	3.41	116.01	111.02
4	F	201	NAG	C1-O5-C5	2.67	115.77	112.19
4	A	401	NAG	O5-C1-C2	-2.64	107.21	111.29
4	A	401	NAG	C4-C3-C2	2.53	114.72	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	406	NAG	O5-C5-C4	-2.42	104.94	110.83
4	E	402	NAG	O5-C5-C4	-2.23	105.41	110.83

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	406	NAG	C1
4	E	402	NAG	C1
4	F	201	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	NAG	O5-C5-C6-O6
4	C	403	NAG	O5-C5-C6-O6
4	F	201	NAG	C4-C5-C6-O6
4	E	402	NAG	O5-C5-C6-O6
4	E	402	NAG	C4-C5-C6-O6
4	C	402	NAG	C4-C5-C6-O6
4	C	401	NAG	O5-C5-C6-O6
4	C	401	NAG	C4-C5-C6-O6
4	C	403	NAG	C4-C5-C6-O6
4	C	402	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	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	322/330 (97%)	0.26	18 (5%) 30 24	19, 32, 59, 126	0
1	C	321/330 (97%)	0.78	29 (9%) 15 11	30, 52, 87, 160	0
1	E	321/330 (97%)	1.08	54 (16%) 4 3	33, 55, 90, 166	0
2	B	165/181 (91%)	0.24	4 (2%) 59 54	13, 32, 59, 86	0
2	D	170/181 (93%)	0.94	24 (14%) 6 5	24, 57, 95, 159	0
2	F	163/181 (90%)	1.17	35 (21%) 2 2	28, 54, 105, 136	0
All	All	1462/1533 (95%)	0.73	164 (11%) 10 8	13, 47, 87, 166	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	127	LYS	6.6
1	C	274	CYS	6.3
2	F	124	LEU	6.3
1	E	203	SER	6.2
1	E	244	ASN	5.2
1	E	74	PRO	5.2
1	C	71	ILE	4.8
1	E	245	GLY	4.8
2	D	150	GLU	4.6
1	A	321	PRO	4.6
2	F	61	THR	4.3
2	D	69	GLU	4.3
2	F	156	THR	4.3
2	B	173	ILE	4.3
1	C	272	GLY	4.2
1	E	66	MET	4.1
2	F	134	GLY	4.0
1	E	273	ASN	4.0
1	C	120	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	126	LEU	3.9
2	F	159	TYR	3.8
2	D	65	ALA	3.7
1	E	274	CYS	3.7
2	D	6	ILE	3.6
2	F	141	TYR	3.6
1	E	73	VAL	3.6
2	D	173	ILE	3.6
1	A	70	PHE	3.6
1	E	276	THR	3.6
2	D	68	ARG	3.6
2	F	168	LEU	3.5
1	E	140	LYS	3.5
2	F	150	GLU	3.5
2	F	133	LEU	3.5
1	A	272	GLY	3.4
2	F	166	ALA	3.4
1	C	90	CYS	3.4
2	F	60	ASN	3.3
1	E	70	PHE	3.3
2	D	7	ALA	3.3
1	E	126	GLU	3.3
1	E	167	THR	3.3
2	F	170	ARG	3.2
1	E	75	GLU	3.2
1	C	138	GLN	3.2
2	F	10	ILE	3.2
2	F	121	LYS	3.2
1	E	139	GLY	3.2
2	D	10	ILE	3.1
1	C	268	GLU	3.1
1	C	116	ILE	3.1
1	C	73	VAL	3.1
2	D	109	ASP	3.0
1	E	213	ILE	3.0
2	F	19	ASP	3.0
1	E	41	LEU	3.0
1	E	106	SER	3.0
1	C	72	ASN	3.0
1	A	71	ILE	3.0
2	F	155	GLY	3.0
2	F	14	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	43	ASP	2.9
1	E	281	PRO	2.9
1	C	235	PRO	2.9
1	E	246	ASN	2.9
1	C	244	ASN	2.9
1	E	71	ILE	2.9
1	E	141	SER	2.9
1	A	0	GLY	2.9
1	E	272	GLY	2.9
2	F	12	GLY	2.9
2	F	169	LYS	2.8
1	E	169	GLN	2.8
1	E	219	ILE	2.8
1	A	245	GLY	2.8
2	F	64	GLU	2.8
1	E	77	SER	2.8
2	F	126	LEU	2.7
1	E	214	ALA	2.7
1	C	70	PHE	2.7
1	E	116	ILE	2.6
2	B	10	ILE	2.6
2	F	31	GLY	2.6
2	D	175	SER	2.6
1	E	184	GLU	2.6
1	A	73	VAL	2.6
1	C	320	SER	2.5
1	E	236	ASN	2.5
2	D	132	GLU	2.5
1	C	214	ALA	2.5
1	C	55	CYS	2.5
2	F	67	GLY	2.5
2	F	18	VAL	2.4
1	C	215	THR	2.4
2	D	8	GLY	2.4
1	E	164	TYR	2.4
1	E	252	TYR	2.4
1	E	271	TYR	2.4
1	A	287	SER	2.4
1	E	127	ALA	2.4
2	B	150	GLU	2.4
2	F	145	ASP	2.4
1	E	53	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	137	TYR	2.3
1	A	72	ASN	2.3
1	E	320	SER	2.3
2	F	30	GLN	2.3
2	D	67	GLY	2.3
1	C	67	CYS	2.3
1	C	137	TYR	2.3
1	E	243	SER	2.3
2	F	100	VAL	2.3
2	D	144	CYS	2.3
2	F	43	LYS	2.3
1	C	182	ASN	2.3
2	D	146	ASN	2.3
1	C	74	PRO	2.3
1	A	116	ILE	2.2
1	E	253	ALA	2.2
1	A	273	ASN	2.2
1	E	51	ILE	2.2
1	C	113	LYS	2.2
1	C	247	PHE	2.2
2	F	143	LYS	2.2
1	A	66	MET	2.2
1	A	4	CYS	2.2
1	E	42	CYS	2.2
2	D	105	GLU	2.2
2	F	153	ARG	2.2
2	D	60	ASN	2.2
1	C	269	VAL	2.2
1	E	13	THR	2.2
1	E	128	SER	2.2
2	D	19	ASP	2.2
1	E	48	LYS	2.2
1	C	139	GLY	2.2
1	E	237	ASP	2.2
2	B	106	ARG	2.1
1	E	65	PRO	2.1
2	F	160	PRO	2.1
1	E	275	ASN	2.1
1	C	140	LYS	2.1
1	C	246	ASN	2.1
1	C	317	LEU	2.1
2	D	124	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	5	ILE	2.1
2	F	138	PHE	2.1
1	E	113	LYS	2.1
1	E	76	TRP	2.1
2	F	123	ARG	2.1
1	C	178	ILE	2.1
2	F	167	ARG	2.1
1	A	2	HIS	2.1
1	E	117	ILE	2.1
2	D	116	ARG	2.0
1	E	262	SER	2.0
2	D	149	MET	2.0
1	E	44	LEU	2.0
1	E	166	ASN	2.0
1	A	274	CYS	2.0
2	D	172	GLU	2.0
1	A	215	THR	2.0
1	E	235	PRO	2.0
2	D	141	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](#)

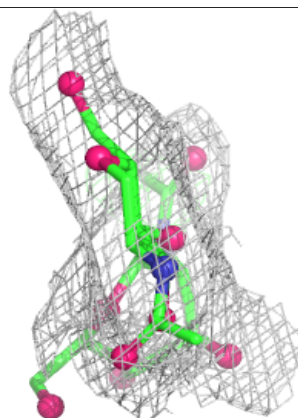
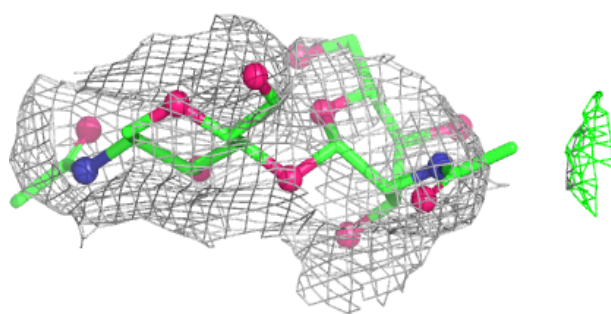
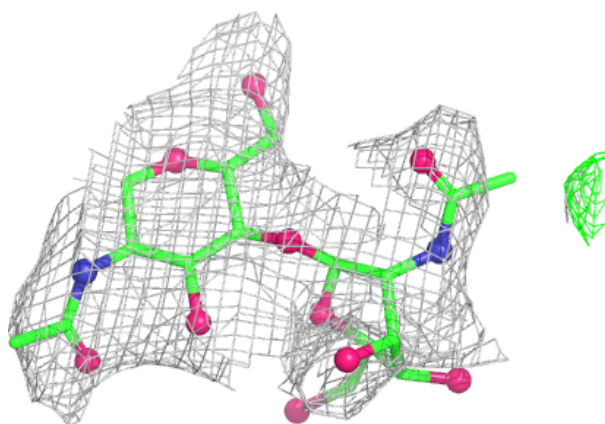
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NAG	H	2	14/15	0.43	0.17	124,141,167,175	0
3	NAG	I	2	14/15	0.47	0.23	88,128,151,160	0
3	NAG	G	2	14/15	0.52	0.17	106,130,149,154	0
3	NAG	H	1	14/15	0.77	0.17	68,101,118,130	0
3	NAG	I	1	14/15	0.79	0.18	99,119,137,160	0
3	NAG	G	1	14/15	0.87	0.10	63,72,81,107	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.

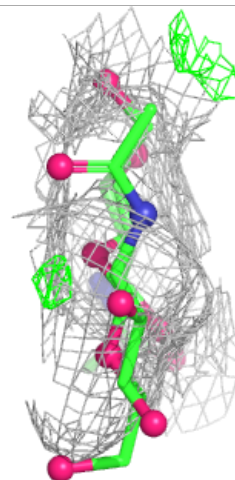
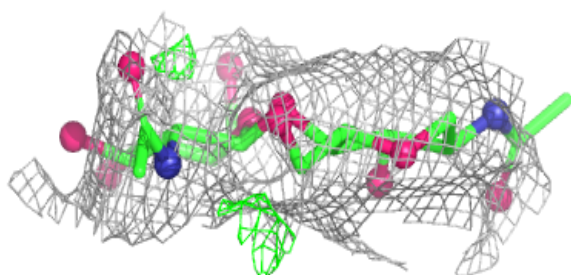
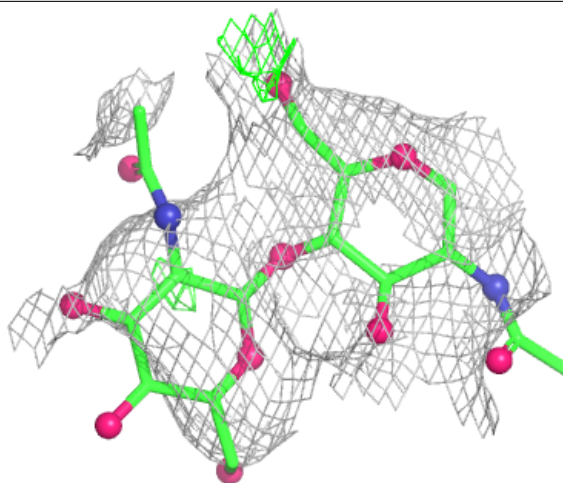
Electron density around Chain G:

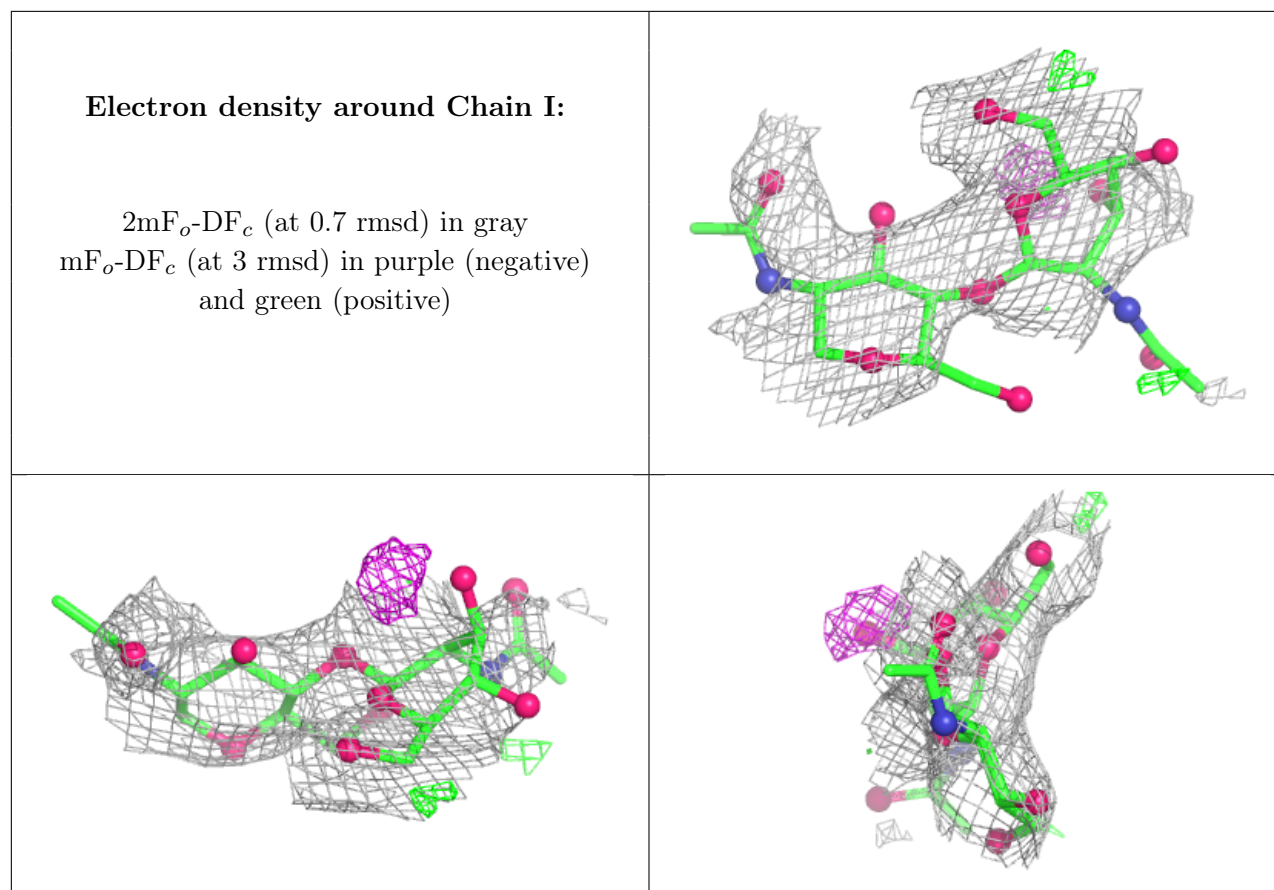
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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 ⓘ

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	NAG	C	403	14/15	0.33	0.18	85,96,115,117	0
4	NAG	A	401	14/15	0.48	0.17	103,118,126,129	0
4	NAG	C	402	14/15	0.51	0.20	86,100,113,115	0
4	NAG	A	406	14/15	0.57	0.18	99,114,125,125	0
4	NAG	E	402	14/15	0.60	0.15	68,80,86,89	0
4	NAG	F	201	14/15	0.60	0.17	97,111,122,123	0
4	NAG	E	401	14/15	0.77	0.12	86,91,97,98	0
4	NAG	C	401	14/15	0.81	0.12	61,66,68,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.