Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 04:05 AM BST

PDB ID	:	1HGF
Title	:	BINDING OF INFLUENZA VIRUS HEMAGGLUTININ TO ANALOGS OF ITS CELL-SURFACE RECEPTOR, SIALIC ACID: ANALYSIS BY PROTON NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY AND X-RAY CRYSTALLOGRAPHY
Authors	:	Sauter, N.K.; Hanson, J.E.; Glick, G.D.; Brown, J.H.; Crowther, R.L.; Park, S.-J.; Skehel, J.J.; Wiley, D.C.
Deposited on	:	1991-11-01
Resolution	:	3.00 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.00 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.
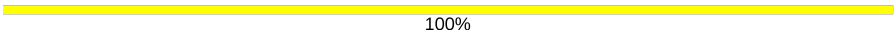
■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
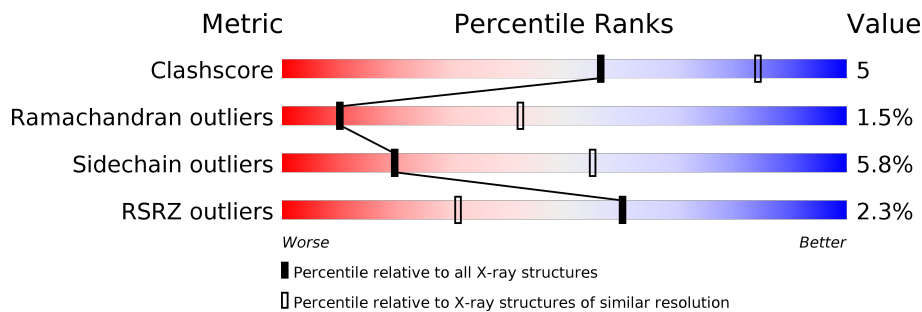
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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 <=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	328	3% 76% 20% ••
1	C	328	3% 75% 22% •
1	E	328	3% 75% 22% ••
2	B	175	% 78% 19% •
2	D	175	% 79% 17% 5%
2	F	175	% 81% 16% ••
3	G	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	3	33%　　　　67%
3	I	3	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15192 atoms, of which 3048 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, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	328	3122	1581	590	445	493	13	0	0	0
1	C	328	Total 3122	C 1581	H 590	N 445	O 493	S 13	0	0	0
1	E	328	Total 3122	C 1581	H 590	N 445	O 493	S 13	0	0	0

- Molecule 2 is a protein called HEMAGGLUTININ, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	175	1754	882	333	250	283	6	0	0	0
2	D	175	Total 1754	C 882	H 333	N 250	O 283	S 6	0	0	0
2	F	175	Total 1754	C 882	H 333	N 250	O 283	S 6	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
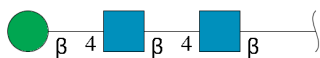
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	G	3	76	22	37	2	15	0	0	0
3	H	3	Total 76	C 22	H 37	N 2	O 15	0	0	0
3	I	3	Total 76	C 22	H 37	N 2	O 15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	F	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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: HEMAGGLUTININ, CHAIN HA1
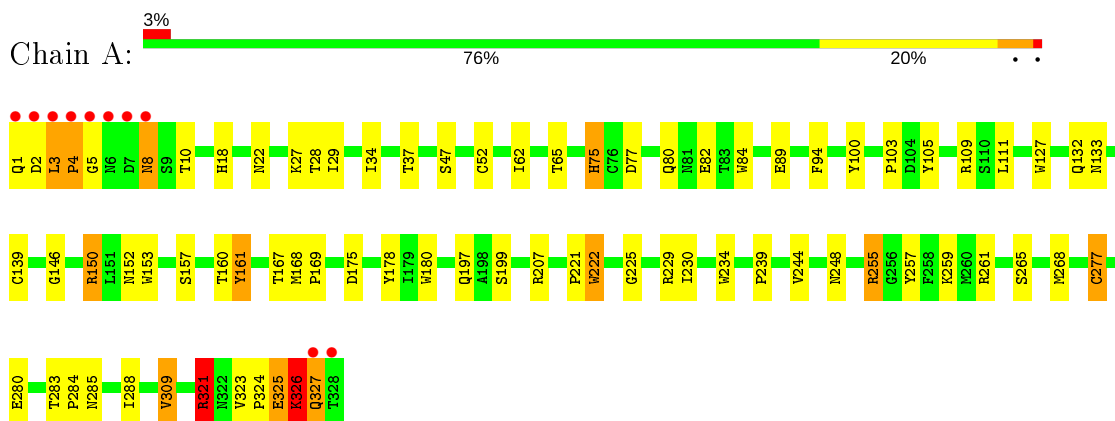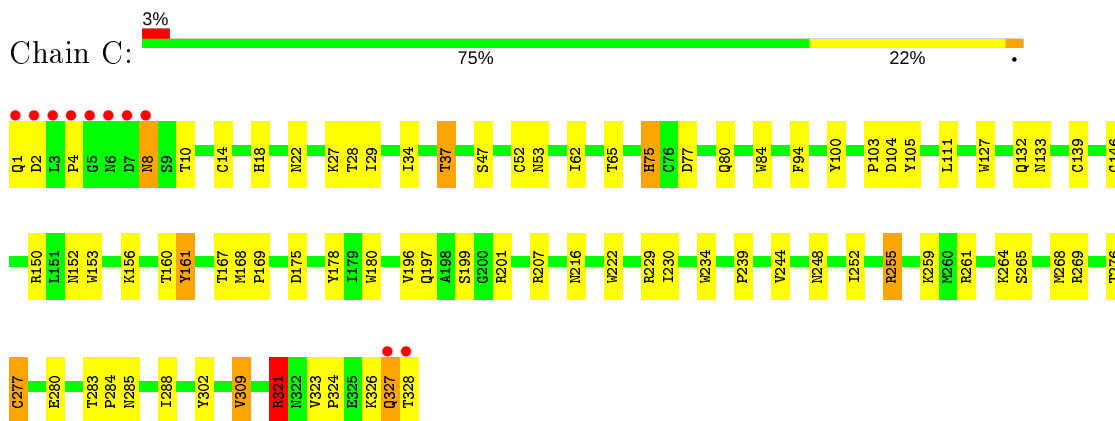
- Molecule 1: HEMAGGLUTININ, CHAIN HA1

- Molecule 1: HEMAGGLUTININ, CHAIN HA1

R269 C277 E280 T283 P284 N285 I288 N298 Y302 V309 K310 Q311 R321 N322 V323 P324 E325 K326 Q327 T328

● Molecule 2: HEMAGGLUTININ, CHAIN HA1

Chain B:

G1 A7 G13 W14 W21 E30 L52 N53 R54 V55 K58 T59 Y83 V84 E85 D86 T87 D90 L91 W92 S93 Y94 L102 Q105 R124 R127 E131 E132 M133 G134 K139 I140 Y141 N146 E150 R153 D160 R163 A166

N169 R170 F171 Q172 I173 K174 G175

● Molecule 2: HEMAGGLUTININ, CHAIN HA1

Chain D:

G1 A7 W14 W21 Q27 N28 T32 R54 V55 K58 T59 L80 Y83 D86 T87 D90 L91 W92 S93 Y94 L102 Q105 R127 E132 M133 G134 C137 F138 K139 I140 Y141 C144 E150 R153 D160 A166 N169 R170

F171 Q172 I173 K174 G175

● Molecule 2: HEMAGGLUTININ, CHAIN HA1

Chain F:

G1 A7 W14 W21 R54 V55 K58 T59 Y83 D86 T87 D90 L91 W92 S93 Y94 E97 L102 Q105 R124 R127 E131 E132 M133 G134 C137 F138 K139 I140 Y141 E150 D160 A166 N169 R170 F171 Q172 I173 K174 G175

● Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain G:

NAG1 NAG2 BMA3

● Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain H:

NAG1 NAG2 BMA3
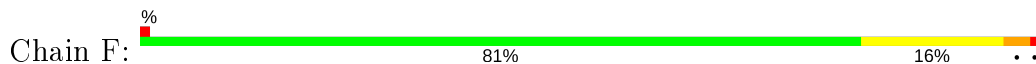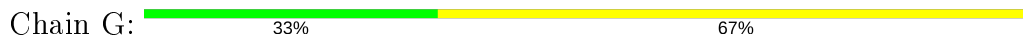
● Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain I:

100%

NAG1 NAG2 BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	163.20Å 163.20Å 177.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-3.00) 76.9 (10.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.45 (at 2.99Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available) 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.6	EDS
L-test for twinning [2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	15192	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.94	1/2589 (0.0%)	1.55	41/3527 (1.2%)
1	C	0.91	0/2589	1.53	42/3527 (1.2%)
1	E	0.96	1/2589 (0.0%)	1.53	42/3527 (1.2%)
2	B	0.97	1/1445 (0.1%)	1.48	19/1939 (1.0%)
2	D	0.99	0/1445	1.49	19/1939 (1.0%)
2	F	0.99	1/1445 (0.1%)	1.49	20/1939 (1.0%)
All	All	0.96	4/12102 (0.0%)	1.52	183/16398 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	150	GLU	CA-CB	-6.01	1.40	1.53
1	E	234	TRP	CG-CD2	-5.58	1.34	1.43
1	A	234	TRP	CG-CD2	-5.32	1.34	1.43
2	B	85	GLU	CD-OE1	-5.25	1.19	1.25

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	ARG	NE-CZ-NH2	-15.10	112.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	ARG	NE-CZ-NH2	-14.08	113.26	120.30
1	C	321	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	E	321	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	E	180	TRP	CD1-CG-CD2	10.14	114.41	106.30
1	A	321	ARG	NE-CZ-NH1	10.13	125.37	120.30
1	C	321	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	C	255	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	222	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	A	255	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	C	180	TRP	CD1-CG-CD2	9.11	113.59	106.30
1	C	222	TRP	CD1-CG-CD2	9.08	113.56	106.30
2	B	92	TRP	CD1-CG-CD2	8.99	113.49	106.30
1	A	180	TRP	CD1-CG-CD2	8.91	113.43	106.30
1	E	222	TRP	CD1-CG-CD2	8.91	113.43	106.30
2	B	14	TRP	CD1-CG-CD2	8.86	113.38	106.30
1	C	127	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	A	127	TRP	CD1-CG-CD2	8.75	113.30	106.30
2	B	170	ARG	NE-CZ-NH2	-8.75	115.93	120.30
2	F	14	TRP	CD1-CG-CD2	8.74	113.30	106.30
2	D	92	TRP	CD1-CG-CD2	8.58	113.17	106.30
2	D	170	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	E	127	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	E	180	TRP	CE2-CD2-CG	-8.31	100.65	107.30
1	C	229	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	E	207	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	C	153	TRP	CD1-CG-CD2	8.14	112.82	106.30
2	F	92	TRP	CD1-CG-CD2	8.14	112.81	106.30
2	D	14	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	C	207	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	C	180	TRP	CE2-CD2-CG	-7.97	100.92	107.30
1	A	207	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	C	161	TYR	CB-CG-CD2	-7.90	116.26	121.00
1	E	180	TRP	CG-CD2-CE3	7.81	140.93	133.90
1	A	180	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	E	229	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	D	21	TRP	CD1-CG-CD2	7.61	112.39	106.30
2	F	21	TRP	CD1-CG-CD2	7.58	112.36	106.30
2	B	14	TRP	CE2-CD2-CG	-7.50	101.30	107.30
2	B	92	TRP	CE2-CD2-CG	-7.49	101.31	107.30
2	D	94	TYR	CB-CG-CD2	-7.46	116.52	121.00
1	E	222	TRP	CE2-CD2-CG	-7.46	101.33	107.30
2	B	21	TRP	CD1-CG-CD2	7.44	112.25	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	TYR	CB-CG-CD2	-7.43	116.54	121.00
1	C	222	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	C	127	TRP	CE2-CD2-CG	-7.34	101.42	107.30
2	F	14	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	127	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	C	153	TRP	CE2-CD2-CG	-7.27	101.49	107.30
1	E	153	TRP	CD1-CG-CD2	7.26	112.11	106.30
2	F	92	TRP	CE2-CD2-CG	-7.26	101.49	107.30
2	D	92	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	E	255	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	E	127	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	E	84	TRP	CD1-CG-CD2	7.14	112.02	106.30
1	A	222	TRP	CE2-CD2-CG	-7.13	101.59	107.30
2	F	150	GLU	CA-CB-CG	-7.07	97.86	113.40
2	F	21	TRP	CE2-CD2-CG	-7.06	101.65	107.30
2	F	170	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	E	326	LYS	CA-CB-CG	7.00	128.81	113.40
2	D	14	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	A	234	TRP	CD1-CG-CD2	6.89	111.81	106.30
2	B	90	ASP	CB-CG-OD1	6.88	124.50	118.30
1	E	153	TRP	CE2-CD2-CG	-6.86	101.82	107.30
1	A	84	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	C	180	TRP	CG-CD2-CE3	6.83	140.05	133.90
1	A	84	TRP	CD1-CG-CD2	6.82	111.76	106.30
1	A	153	TRP	CD1-CG-CD2	6.82	111.75	106.30
1	A	326	LYS	CA-CB-CG	6.81	128.38	113.40
1	A	180	TRP	CG-CD2-CE3	6.79	140.01	133.90
1	A	161	TYR	CB-CG-CD2	-6.78	116.93	121.00
1	C	84	TRP	CD1-CG-CD2	6.77	111.71	106.30
1	C	84	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	A	324	PRO	O-C-N	6.76	133.52	122.70
1	C	28	THR	CA-CB-CG2	6.74	121.84	112.40
1	C	255	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	234	TRP	CD1-CG-CD2	6.71	111.67	106.30
2	D	86	ASP	CB-CG-OD1	6.70	124.33	118.30
1	E	255	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	E	180	TRP	CG-CD1-NE1	-6.69	103.41	110.10
2	B	21	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	C	178	TYR	CB-CG-CD2	-6.60	117.04	121.00
1	A	28	THR	CA-CB-CG2	6.56	121.59	112.40
1	E	84	TRP	CE2-CD2-CG	-6.51	102.09	107.30
2	B	86	ASP	CB-CG-OD1	6.39	124.05	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	28	THR	CA-CB-CG2	6.38	121.34	112.40
2	B	94	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	A	180	TRP	CG-CD1-NE1	-6.30	103.80	110.10
1	E	180	TRP	CB-CG-CD1	-6.29	118.83	127.00
2	D	21	TRP	CE2-CD2-CG	-6.24	102.31	107.30
1	E	1	GLN	N-CA-C	-6.24	94.16	111.00
1	E	234	TRP	CD1-CG-CD2	6.21	111.27	106.30
1	C	180	TRP	CG-CD1-NE1	-6.21	103.89	110.10
1	A	111	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	153	TRP	CE2-CD2-CG	-6.16	102.37	107.30
1	C	180	TRP	CB-CG-CD1	-6.16	119.00	127.00
2	F	94	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	325	GLU	CA-CB-CG	6.08	126.78	113.40
1	A	105	TYR	CB-CG-CD2	-6.05	117.37	121.00
2	F	14	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	A	234	TRP	CE2-CD2-CG	-6.02	102.48	107.30
2	F	124	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	E	111	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	180	TRP	CB-CG-CD1	-5.92	119.31	127.00
2	F	55	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	A	321	ARG	CB-CG-CD	-5.91	96.23	111.60
1	C	153	TRP	CG-CD1-NE1	-5.90	104.20	110.10
2	D	153	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	D	27	GLN	CA-CB-CG	-5.89	100.45	113.40
1	A	127	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	C	234	TRP	CE2-CD2-CG	-5.88	102.59	107.30
1	A	75	HIS	CA-CB-CG	5.87	123.57	113.60
1	E	234	TRP	CE2-CD2-CG	-5.86	102.61	107.30
2	B	92	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	E	37	THR	CA-CB-CG2	5.85	120.59	112.40
1	C	127	TRP	CG-CD1-NE1	-5.84	104.26	110.10
2	D	55	VAL	CG1-CB-CG2	-5.83	101.58	110.90
2	F	132	GLU	CA-CB-CG	-5.82	100.59	113.40
2	F	86	ASP	CB-CG-OD1	5.82	123.54	118.30
2	D	132	GLU	CA-CB-CG	-5.81	100.61	113.40
1	C	37	THR	CA-CB-CG2	5.81	120.53	112.40
2	B	14	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	E	75	HIS	CA-CB-CG	5.80	123.45	113.60
1	A	229	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	C	248	ASN	N-CA-CB	-5.79	100.18	110.60
1	A	150	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	B	132	GLU	CA-CB-CG	-5.77	100.72	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	ARG	CB-CG-CD	-5.75	96.66	111.60
1	E	82	GLU	N-CA-CB	-5.72	100.31	110.60
2	B	55	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	C	222	TRP	CG-CD1-NE1	-5.69	104.41	110.10
2	D	90	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	321	ARG	CB-CG-CD	-5.67	96.87	111.60
2	D	92	TRP	CG-CD1-NE1	-5.65	104.45	110.10
2	D	14	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	C	111	LEU	N-CA-CB	-5.56	99.28	110.40
2	B	21	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	E	326	LYS	N-CA-CB	-5.54	100.63	110.60
1	E	73	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	248	ASN	N-CA-CB	-5.49	100.72	110.60
1	E	248	ASN	N-CA-CB	-5.48	100.73	110.60
2	F	54	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	222	TRP	CG-CD1-NE1	-5.47	104.63	110.10
2	B	169	ASN	CA-CB-CG	5.46	125.42	113.40
1	E	104	ASP	CB-CG-OD1	5.46	123.22	118.30
2	D	21	TRP	CG-CD1-NE1	-5.46	104.64	110.10
2	B	124	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	1	GLN	N-CA-C	-5.42	96.36	111.00
1	E	178	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	C	111	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	75	HIS	CA-CB-CG	5.39	122.76	113.60
1	E	37	THR	CA-CB-OG1	-5.35	97.77	109.00
1	C	37	THR	CA-CB-OG1	-5.35	97.77	109.00
1	A	153	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	C	104	ASP	CB-CG-OD1	5.33	123.10	118.30
2	F	92	TRP	CG-CD1-NE1	-5.33	104.77	110.10
2	D	169	ASN	CA-CB-CG	5.28	125.01	113.40
1	C	321	ARG	CG-CD-NE	5.25	122.83	111.80
2	B	14	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	E	321	ARG	CG-CD-NE	5.21	122.74	111.80
1	C	229	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	E	127	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	C	153	TRP	CG-CD2-CE3	5.20	138.58	133.90
2	F	21	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	A	8	ASN	N-CA-CB	-5.19	101.26	110.60
1	E	153	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	C	105	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	C	201	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	F	169	ASN	CA-CB-CG	5.16	124.76	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	14	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	E	111	LEU	N-CA-CB	-5.14	100.12	110.40
1	A	324	PRO	CA-C-N	-5.12	105.93	117.20
1	A	111	LEU	N-CA-CB	-5.11	100.18	110.40
1	E	156	LYS	CD-CE-NZ	-5.10	99.96	111.70
1	E	309	VAL	N-CA-CB	-5.09	100.30	111.50
1	A	257	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	C	252	ILE	N-CA-C	-5.07	97.33	111.00
1	A	321	ARG	CG-CD-NE	5.05	122.40	111.80
2	D	80	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	E	269	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	B	52	LEU	CB-CG-CD2	-5.01	102.49	111.00
2	F	90	ASP	CB-CG-OD1	5.00	122.80	118.30
1	C	269	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain
1	C	161	TYR	Sidechain

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	2532	590	2473	31	0
1	C	2532	590	2473	32	0
1	E	2532	590	2473	34	0
2	B	1421	333	1345	20	0
2	D	1421	333	1345	19	0
2	F	1421	333	1345	18	0
3	G	39	37	34	1	0
3	H	39	37	34	2	0
3	I	39	37	34	1	0
4	A	42	42	39	0	0
4	B	14	14	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	42	42	39	0	0
4	D	14	14	13	0	0
4	E	42	42	39	0	0
4	F	14	14	13	0	0
All	All	12144	3048	11712	120	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 (120) 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:B:83:TYR:O	2:B:87:THR:HG23	1.85	0.77
2:F:83:TYR:O	2:F:87:THR:HG23	1.86	0.75
2:D:83:TYR:O	2:D:87:THR:HG23	1.87	0.74
2:D:27:GLN:HG3	2:D:32:THR:HG22	1.69	0.71
2:F:132:GLU:HG2	2:F:134:GLY:H	1.55	0.71
2:B:132:GLU:HG2	2:B:134:GLY:H	1.56	0.70
2:D:132:GLU:HG2	2:D:134:GLY:H	1.56	0.70
1:E:321:ARG:HG2	1:E:321:ARG:HH11	1.61	0.65
1:A:10:THR:HG22	2:B:141:TYR:HA	1.79	0.64
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.62	0.64
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.79	0.63
1:C:283:THR:HG22	1:C:285:ASN:H	1.62	0.63
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.63	0.63
2:D:28:ASN:HB2	2:D:144:CYS:O	1.99	0.63
1:E:10:THR:HG22	2:F:141:TYR:HA	1.80	0.62
1:C:77:ASP:O	1:C:80:GLN:HG3	1.98	0.62
1:E:283:THR:HG22	1:E:285:ASN:H	1.65	0.62
1:C:10:THR:HG22	2:D:141:TYR:HA	1.82	0.62
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.80	0.62
1:A:77:ASP:O	1:A:80:GLN:HG3	2.00	0.62
1:E:77:ASP:O	1:E:80:GLN:HG3	1.99	0.62
1:C:132:GLN:HE21	1:C:152:ASN:HD21	1.47	0.61
1:A:132:GLN:HE21	1:A:152:ASN:HD21	1.46	0.61
2:B:173:ILE:HG22	2:B:174:LYS:HG2	1.83	0.61
2:F:173:ILE:HG22	2:F:174:LYS:HG2	1.83	0.61
2:D:173:ILE:HG22	2:D:174:LYS:HG2	1.84	0.60
1:E:132:GLN:HE21	1:E:152:ASN:HD21	1.47	0.60
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.82	0.60
1:A:325:GLU:HB2	2:B:13:GLY:O	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:THR:HG22	1:A:285:ASN:H	1.65	0.59
1:C:53:ASN:OD1	1:C:276:THR:HA	2.04	0.57
2:F:58:LYS:HE2	2:F:59:THR:O	2.07	0.55
2:B:58:LYS:HE2	2:B:59:THR:O	2.07	0.55
1:E:52:CYS:HB3	1:E:277:CYS:O	2.09	0.53
2:B:141:TYR:O	2:B:166:ALA:HA	2.09	0.52
1:C:27:LYS:HD3	2:F:54:ARG:NH2	2.25	0.52
2:D:58:LYS:HE2	2:D:59:THR:O	2.09	0.52
2:F:141:TYR:O	2:F:166:ALA:HA	2.10	0.52
1:C:52:CYS:HB3	1:C:277:CYS:O	2.10	0.51
2:B:54:ARG:NH2	1:E:27:LYS:HD3	2.25	0.51
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.10	0.51
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.11	0.51
1:A:244:VAL:HG23	1:E:221:PRO:HG3	1.93	0.50
1:A:27:LYS:HD3	2:D:54:ARG:NH2	2.26	0.50
1:A:3:LEU:HB2	1:A:4:PRO:HD2	1.95	0.49
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.13	0.49
1:A:52:CYS:HB3	1:A:277:CYS:O	2.12	0.49
2:D:141:TYR:O	2:D:166:ALA:HA	2.12	0.49
1:E:326:LYS:HD2	1:E:327:GLN:H	1.76	0.49
1:A:167:THR:HB	3:G:1:NAG:H62	1.95	0.48
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.96	0.48
1:A:268:MET:SD	1:A:284:PRO:HD3	2.53	0.48
1:C:132:GLN:HE21	1:C:152:ASN:ND2	2.10	0.48
2:B:127:ARG:NH1	2:F:131:GLU:OE1	2.47	0.48
1:C:167:THR:HB	3:H:1:NAG:H62	1.96	0.48
1:A:283:THR:HG22	1:A:285:ASN:N	2.29	0.47
1:E:132:GLN:HE21	1:E:152:ASN:ND2	2.12	0.47
1:A:326:LYS:HG2	1:A:327:GLN:N	2.29	0.47
1:C:283:THR:HG22	1:C:285:ASN:N	2.28	0.47
1:E:133:ASN:OD1	1:E:255:ARG:NH2	2.47	0.47
1:E:283:THR:HG22	1:E:285:ASN:N	2.30	0.47
1:E:167:THR:HB	3:I:1:NAG:H62	1.96	0.47
1:C:327:GLN:HG2	1:C:328:THR:N	2.30	0.47
1:A:309:VAL:HG22	2:B:93:SER:HA	1.96	0.46
1:C:1:GLN:OE1	1:C:1:GLN:HA	2.15	0.46
1:A:47:SER:HA	1:A:288:ILE:HG22	1.96	0.46
1:A:132:GLN:HE21	1:A:152:ASN:ND2	2.11	0.46
2:D:91:LEU:HD13	2:F:91:LEU:HD13	1.99	0.45
1:E:29:ILE:HB	2:F:105:GLN:OE1	2.17	0.45
1:A:29:ILE:HB	2:B:105:GLN:OE1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:HB	2:D:105:GLN:OE1	2.17	0.45
2:B:30:GLU:HB2	2:B:146:ASN:ND2	2.32	0.45
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.49	0.44
1:E:47:SER:HA	1:E:288:ILE:HG22	1.99	0.44
1:C:47:SER:HA	1:C:288:ILE:HG22	2.00	0.44
1:A:221:PRO:HG3	1:C:244:VAL:HG23	1.98	0.44
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.99	0.44
1:C:139:CYS:HB3	1:C:146:GLY:O	2.18	0.43
1:C:309:VAL:HG22	2:D:93:SER:HA	1.99	0.43
1:A:75:HIS:HE1	1:A:94:PHE:O	2.01	0.43
1:A:221:PRO:HA	3:H:2:NAG:O7	2.18	0.43
1:E:75:HIS:HE1	1:E:94:PHE:O	2.01	0.43
1:E:324:PRO:HG3	1:E:328:THR:HG23	2.01	0.43
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.57	0.43
1:E:53:ASN:HA	1:E:58:ILE:HD13	1.99	0.43
1:C:100:TYR:HA	1:C:230:ILE:O	2.18	0.43
1:E:323:VAL:HG21	2:F:7:ALA:HB2	2.01	0.43
1:E:182:ILE:HD11	1:E:215:PRO:HD3	2.01	0.42
1:C:156:LYS:HD3	1:C:196:VAL:CG2	2.49	0.42
2:D:173:ILE:HD13	2:D:173:ILE:HA	1.93	0.42
1:C:323:VAL:HG21	2:D:7:ALA:HB2	2.02	0.42
1:C:10:THR:HG21	2:D:139:LYS:HE2	2.02	0.42
1:E:109:ARG:HD2	1:E:109:ARG:HH11	1.68	0.42
2:B:150:GLU:OE1	2:B:153:ARG:NH1	2.53	0.42
1:C:133:ASN:OD1	1:C:255:ARG:NH2	2.47	0.42
1:C:264:LYS:HE3	1:C:302:TYR:OH	2.20	0.42
1:C:168:MET:HA	1:C:169:PRO:HD3	1.86	0.42
1:E:284:PRO:HG2	1:E:298:ASN:ND2	2.35	0.42
2:B:131:GLU:OE1	2:D:127:ARG:NH1	2.52	0.42
1:E:309:VAL:HG22	2:F:93:SER:HA	2.01	0.42
1:E:321:ARG:CG	1:E:321:ARG:HH11	2.31	0.42
1:E:89:GLU:OE1	1:E:109:ARG:NH1	2.52	0.41
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.35	0.41
1:E:14:CYS:HA	2:F:137:CYS:HA	2.02	0.41
2:B:163:ARG:NH2	2:F:131:GLU:OE2	2.53	0.41
1:A:323:VAL:HG21	2:B:7:ALA:HB2	2.01	0.41
1:A:168:MET:HA	1:A:169:PRO:HD3	1.87	0.41
1:C:14:CYS:HA	2:D:137:CYS:HA	2.03	0.41
1:A:100:TYR:HA	1:A:230:ILE:O	2.21	0.41
1:C:268:MET:SD	1:C:284:PRO:HD3	2.61	0.41
1:A:139:CYS:HB3	1:A:146:GLY:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.56	0.41
1:C:75:HIS:HE1	1:C:94:PHE:O	2.04	0.41
1:E:71:LEU:O	1:E:148:PHE:HB3	2.20	0.41
1:E:264:LYS:HE3	1:E:302:TYR:OH	2.20	0.41
1:A:10:THR:HG21	2:B:139:LYS:HE2	2.03	0.40
1:E:10:THR:HG21	2:F:139:LYS:HE2	2.02	0.40
1:A:89:GLU:OE1	1:A:109:ARG:NH1	2.54	0.40
2:B:173:ILE:HA	2:B:173:ILE:HD13	1.94	0.40
1:C:8:ASN:HB2	2:D:169:ASN:HD21	1.86	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	326/328 (99%)	303 (93%)	15 (5%)	8 (2%)	5	28
1	C	326/328 (99%)	303 (93%)	19 (6%)	4 (1%)	13	48
1	E	326/328 (99%)	306 (94%)	18 (6%)	2 (1%)	25	64
2	B	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	9	39
2	D	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	9	39
2	F	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	9	39
All	All	1497/1509 (99%)	1393 (93%)	81 (5%)	23 (2%)	10	42

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	LEU
2	B	58	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	173	ILE
2	D	58	LYS
2	D	173	ILE
2	F	58	LYS
2	F	173	ILE
1	A	326	LYS
1	C	4	PRO
1	A	327	GLN
1	C	326	LYS
2	F	172	GLN
1	A	62	ILE
2	B	172	GLN
1	C	62	ILE
2	D	172	GLN
1	E	62	ILE
1	A	22	ASN
1	A	4	PRO
1	C	22	ASN
1	E	22	ASN
1	A	5	GLY

5.3.2 Protein sidechains (i)

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	289/289 (100%)	269 (93%)	20 (7%)	15	48
1	C	289/289 (100%)	269 (93%)	20 (7%)	15	48
1	E	289/289 (100%)	267 (92%)	22 (8%)	13	43
2	B	149/149 (100%)	145 (97%)	4 (3%)	44	77
2	D	149/149 (100%)	144 (97%)	5 (3%)	37	72
2	F	149/149 (100%)	144 (97%)	5 (3%)	37	72
All	All	1314/1314 (100%)	1238 (94%)	76 (6%)	20	55

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	18	HIS
1	A	34	ILE
1	A	37	THR
1	A	65	THR
1	A	82	GLU
1	A	103	PRO
1	A	150	ARG
1	A	157	SER
1	A	160	THR
1	A	197	GLN
1	A	199	SER
1	A	259	LYS
1	A	261	ARG
1	A	265	SER
1	A	277	CYS
1	A	280	GLU
1	A	309	VAL
1	A	321	ARG
1	A	326	LYS
2	B	54	ARG
2	B	127	ARG
2	B	160	ASP
2	B	170	ARG
1	C	2	ASP
1	C	8	ASN
1	C	18	HIS
1	C	34	ILE
1	C	37	THR
1	C	65	THR
1	C	103	PRO
1	C	150	ARG
1	C	160	THR
1	C	197	GLN
1	C	199	SER
1	C	259	LYS
1	C	261	ARG
1	C	265	SER
1	C	277	CYS
1	C	280	GLU
1	C	309	VAL
1	C	321	ARG
1	C	324	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	327	GLN
2	D	54	ARG
2	D	127	ARG
2	D	150	GLU
2	D	160	ASP
2	D	170	ARG
1	E	2	ASP
1	E	7	ASP
1	E	8	ASN
1	E	18	HIS
1	E	34	ILE
1	E	37	THR
1	E	65	THR
1	E	103	PRO
1	E	150	ARG
1	E	159	SER
1	E	160	THR
1	E	189	GLN
1	E	199	SER
1	E	259	LYS
1	E	261	ARG
1	E	265	SER
1	E	277	CYS
1	E	280	GLU
1	E	309	VAL
1	E	321	ARG
1	E	326	LYS
1	E	328	THR
2	F	54	ARG
2	F	127	ARG
2	F	150	GLU
2	F	160	ASP
2	F	170	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	132	GLN
1	A	171	ASN
2	B	146	ASN
1	C	132	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	171	ASN
1	C	327	GLN
2	D	12	ASN
2	D	26	HIS
2	D	28	ASN
2	D	169	ASN
1	E	8	ASN
1	E	132	GLN
1	E	171	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 ⓘ

9 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	1,3	14,14,15	0.58	0	17,19,21	0.75	0
3	NAG	G	2	3	14,14,15	0.65	0	17,19,21	1.09	1 (5%)
3	BMA	G	3	3	11,11,12	0.92	0	15,15,17	1.16	0
3	NAG	H	1	1,3	14,14,15	0.74	1 (7%)	17,19,21	0.83	0
3	NAG	H	2	3	14,14,15	0.48	0	17,19,21	1.11	1 (5%)
3	BMA	H	3	3	11,11,12	0.81	0	15,15,17	1.46	3 (20%)
3	NAG	I	1	1,3	14,14,15	0.59	0	17,19,21	0.78	0
3	NAG	I	2	3	14,14,15	0.50	0	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	BMA	I	3	3	11,11,12	0.85	0	15,15,17	1.33	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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-2.08	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	3	BMA	C1-O5-C5	2.83	116.02	112.19
3	H	3	BMA	C1-O5-C5	2.69	115.83	112.19
3	G	2	NAG	C4-C3-C2	-2.62	107.18	111.02
3	H	3	BMA	O5-C1-C2	-2.61	106.74	110.77
3	H	2	NAG	C4-C3-C2	-2.54	107.30	111.02
3	H	3	BMA	C6-C5-C4	-2.43	107.30	113.00
3	I	2	NAG	C4-C3-C2	-2.37	107.54	111.02
3	I	3	BMA	C1-C2-C3	2.31	112.50	109.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	I	1	NAG	1	0
3	G	1	NAG	1	0
3	H	2	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.

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
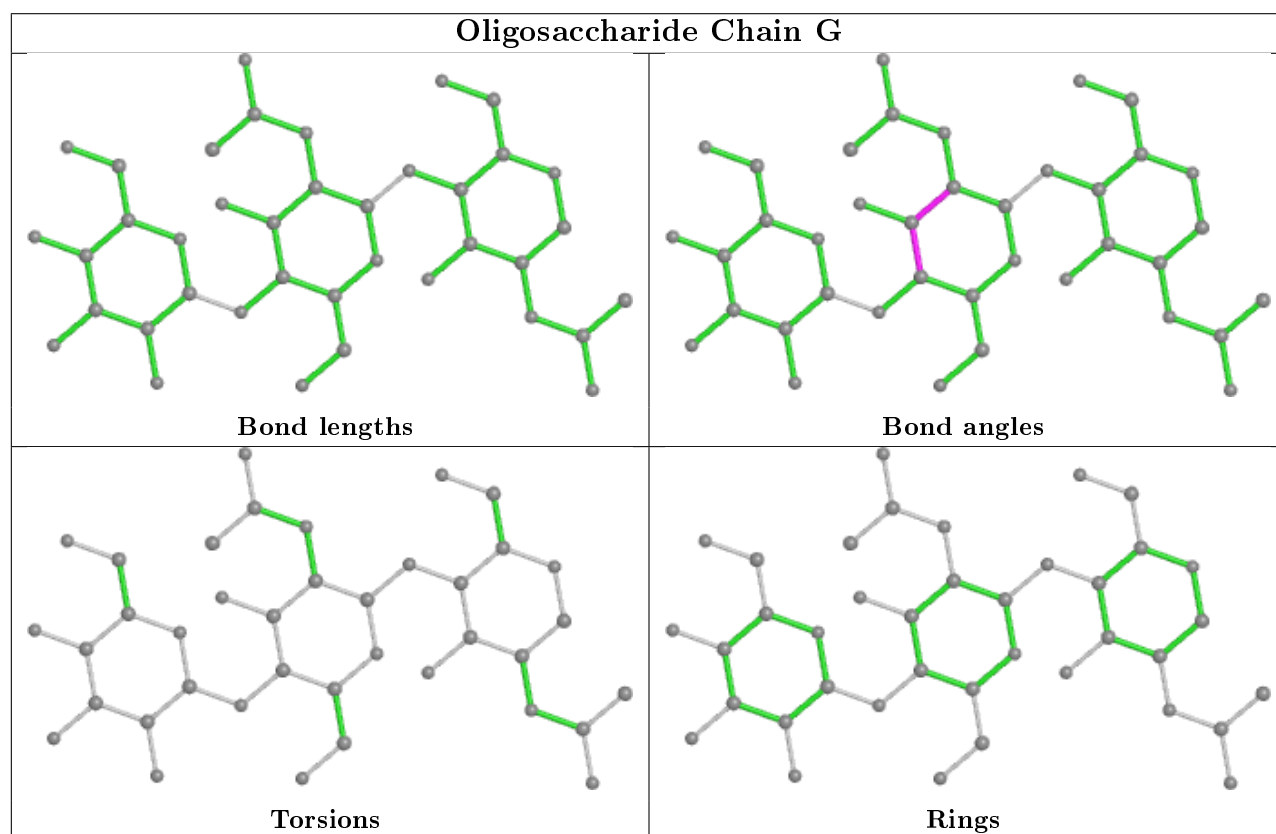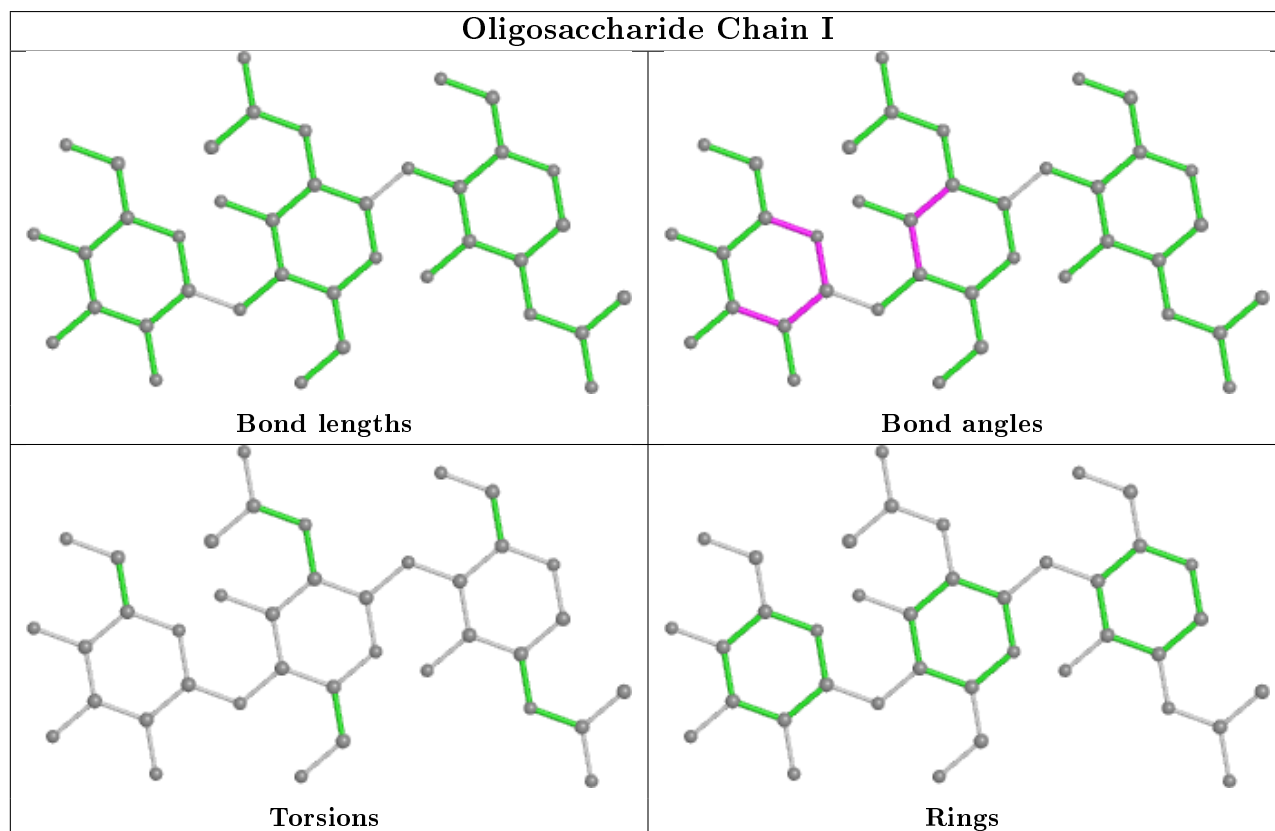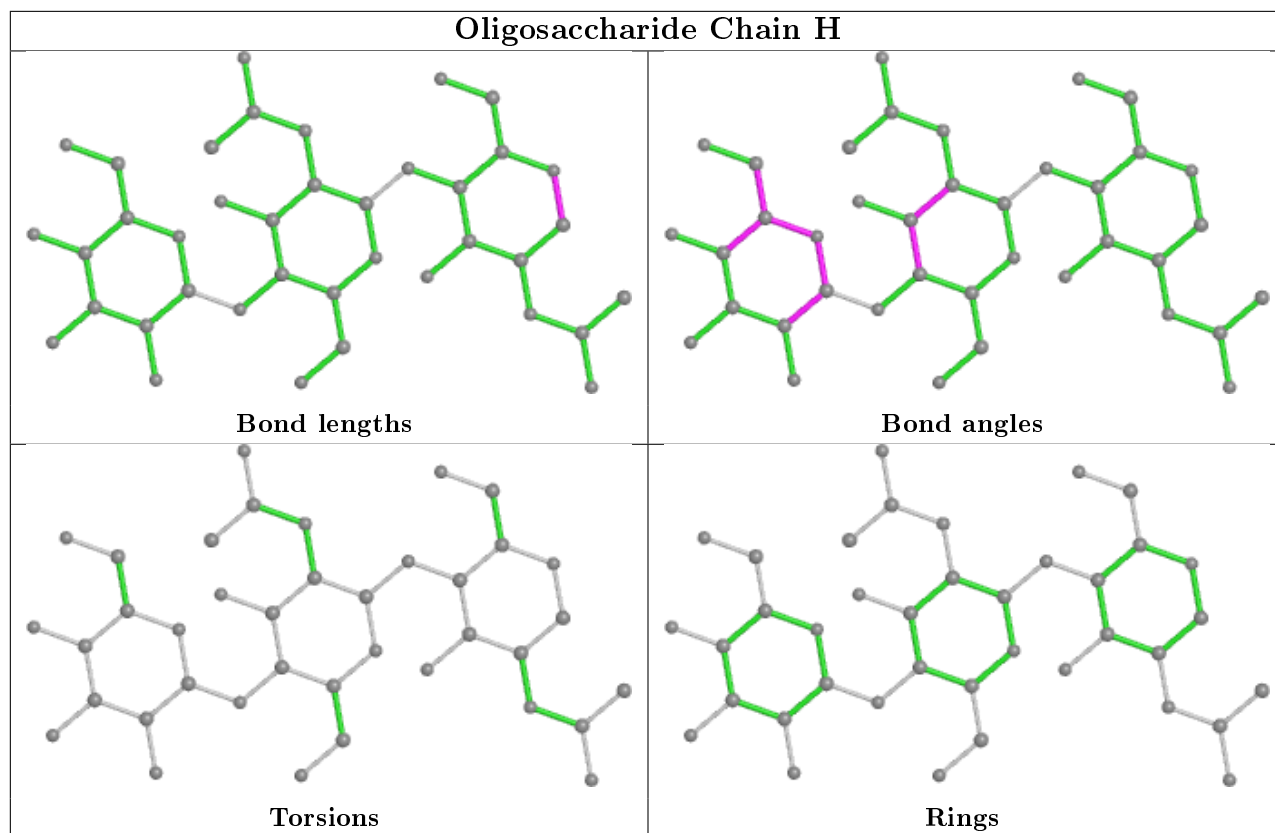
5.6 Ligand geometry (i)

12 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	F	401	2	14,14,15	0.67	0	17,19,21	1.48	2 (11%)
4	NAG	D	401	2	14,14,15	0.65	0	17,19,21	1.49	1 (5%)
4	NAG	A	348	1	14,14,15	0.69	0	17,19,21	1.42	4 (23%)
4	NAG	E	348	1	14,14,15	0.76	0	17,19,21	1.43	4 (23%)
4	NAG	E	334	1	14,14,15	0.67	0	17,19,21	1.29	1 (5%)
4	NAG	E	329	1	14,14,15	0.67	0	17,19,21	0.90	1 (5%)
4	NAG	A	334	1	14,14,15	0.79	0	17,19,21	1.37	2 (11%)
4	NAG	C	348	1	14,14,15	0.78	0	17,19,21	1.48	4 (23%)
4	NAG	A	329	1	14,14,15	0.65	0	17,19,21	0.93	1 (5%)
4	NAG	C	329	1	14,14,15	0.65	0	17,19,21	0.93	1 (5%)
4	NAG	C	334	1	14,14,15	0.83	1 (7%)	17,19,21	1.35	1 (5%)
4	NAG	B	401	2	14,14,15	0.62	0	17,19,21	1.42	2 (11%)

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	F	401	2	-	0/6/23/26	0/1/1/1
4	NAG	D	401	2	-	0/6/23/26	0/1/1/1
4	NAG	A	348	1	-	2/6/23/26	0/1/1/1
4	NAG	E	348	1	-	2/6/23/26	0/1/1/1
4	NAG	E	334	1	-	0/6/23/26	0/1/1/1
4	NAG	E	329	1	-	0/6/23/26	0/1/1/1
4	NAG	A	334	1	-	0/6/23/26	0/1/1/1
4	NAG	C	348	1	-	2/6/23/26	0/1/1/1
4	NAG	A	329	1	-	0/6/23/26	0/1/1/1

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	329	1	-	0/6/23/26	0/1/1/1
4	NAG	C	334	1	-	0/6/23/26	0/1/1/1
4	NAG	B	401	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	334	NAG	C6-C5	2.15	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	NAG	C1-O5-C5	4.64	118.47	112.19
4	F	401	NAG	C1-O5-C5	4.45	118.22	112.19
4	B	401	NAG	C1-O5-C5	3.96	117.56	112.19
4	A	334	NAG	C1-O5-C5	3.80	117.33	112.19
4	E	334	NAG	C1-O5-C5	3.51	116.95	112.19
4	C	334	NAG	C1-O5-C5	3.30	116.67	112.19
4	A	348	NAG	C1-O5-C5	3.00	116.26	112.19
4	C	348	NAG	C8-C7-N2	2.99	121.17	116.10
4	E	348	NAG	C1-O5-C5	2.87	116.07	112.19
4	C	348	NAG	C1-O5-C5	2.61	115.73	112.19
4	C	329	NAG	C1-O5-C5	2.48	115.55	112.19
4	A	329	NAG	C1-O5-C5	2.42	115.47	112.19
4	A	348	NAG	C8-C7-N2	2.39	120.15	116.10
4	E	329	NAG	C1-O5-C5	2.37	115.41	112.19
4	E	348	NAG	C3-C4-C5	-2.32	106.10	110.24
4	E	348	NAG	C8-C7-N2	2.30	119.99	116.10
4	A	348	NAG	O4-C4-C5	2.29	114.99	109.30
4	E	348	NAG	O4-C4-C5	2.20	114.76	109.30
4	F	401	NAG	C8-C7-N2	2.19	119.81	116.10
4	A	348	NAG	C3-C4-C5	-2.18	106.36	110.24
4	C	348	NAG	O4-C4-C5	2.10	114.52	109.30
4	A	334	NAG	O5-C5-C6	2.03	110.39	107.20
4	B	401	NAG	C8-C7-N2	2.03	119.54	116.10
4	C	348	NAG	C3-C4-C5	-2.02	106.64	110.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	348	NAG	C4-C5-C6-O6
4	A	348	NAG	O5-C5-C6-O6
4	E	348	NAG	C4-C5-C6-O6
4	C	348	NAG	C4-C5-C6-O6
4	C	348	NAG	O5-C5-C6-O6
4	E	348	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	328/328 (100%)	-0.68	10 (3%)	50	22	5, 24, 51, 151	0
1	C	328/328 (100%)	-0.65	10 (3%)	50	22	5, 24, 51, 148	0
1	E	328/328 (100%)	-0.69	9 (2%)	54	26	5, 24, 51, 148	0
2	B	175/175 (100%)	-0.73	2 (1%)	80	56	3, 18, 50, 105	0
2	D	175/175 (100%)	-0.77	1 (0%)	89	72	2, 18, 47, 105	0
2	F	175/175 (100%)	-0.76	2 (1%)	80	56	3, 18, 48, 105	0
All	All	1509/1509 (100%)	-0.70	34 (2%)	60	31	2, 23, 51, 151	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	6	ASN	7.5
1	A	2	ASP	4.7
1	E	1	GLN	4.5
1	C	6	ASN	4.1
1	A	3	LEU	4.1
1	C	328	THR	4.1
1	E	7	ASP	3.9
1	A	328	THR	3.8
1	A	1	GLN	3.7
1	C	4	PRO	3.7
1	A	6	ASN	3.7
1	C	8	ASN	3.5
1	C	2	ASP	3.4
1	A	4	PRO	3.4
1	A	7	ASP	3.4
1	E	327	GLN	3.3
1	C	7	ASP	3.3
1	C	1	GLN	3.3
1	C	5	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	328	THR	3.1
1	C	327	GLN	2.9
1	E	5	GLY	2.9
1	E	2	ASP	2.8
1	A	327	GLN	2.7
1	C	3	LEU	2.7
1	E	3	LEU	2.6
2	F	172	GLN	2.4
1	A	8	ASN	2.3
1	E	4	PRO	2.3
2	B	173	ILE	2.3
2	D	174	LYS	2.3
2	B	174	LYS	2.1
2	F	175	GLY	2.0
1	A	5	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.
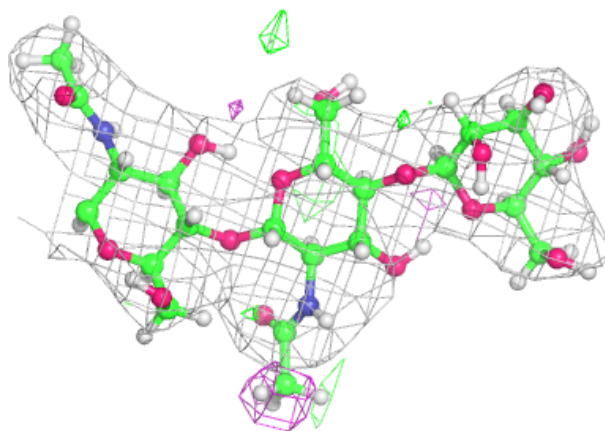
6.3 Carbohydrates (i)

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

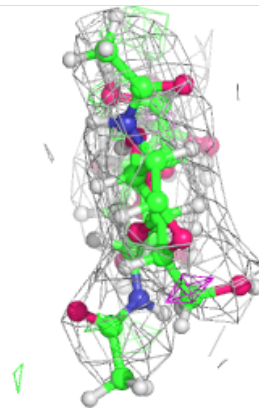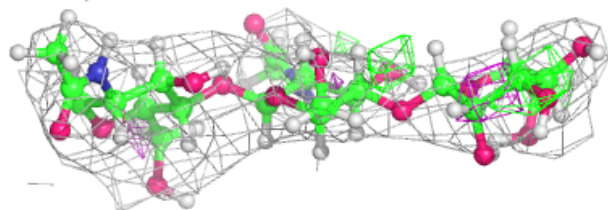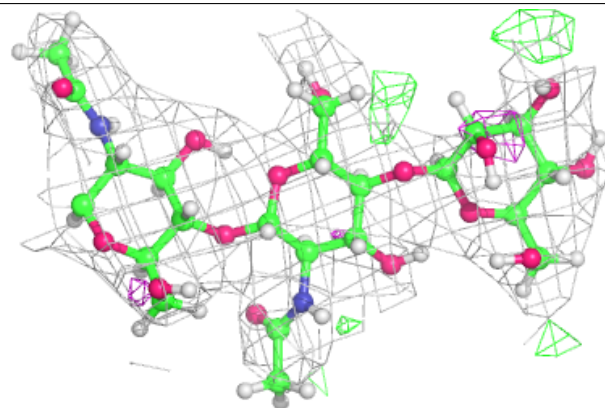| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	H	3	11/12	0.82	0.39	0,0,71,72	0
3	BMA	I	3	11/12	0.86	0.38	0,0,73,75	0
3	NAG	I	2	14/15	0.86	0.23	0,0,60,64	0
3	NAG	G	2	14/15	0.86	0.23	0,0,60,63	0
3	NAG	H	2	14/15	0.88	0.23	0,0,60,64	0
3	NAG	I	1	14/15	0.90	0.17	0,0,47,51	0
3	NAG	H	1	14/15	0.90	0.19	0,0,49,51	0
3	BMA	G	3	11/12	0.90	0.33	0,0,69,70	0
3	NAG	G	1	14/15	0.94	0.15	0,0,48,52	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.
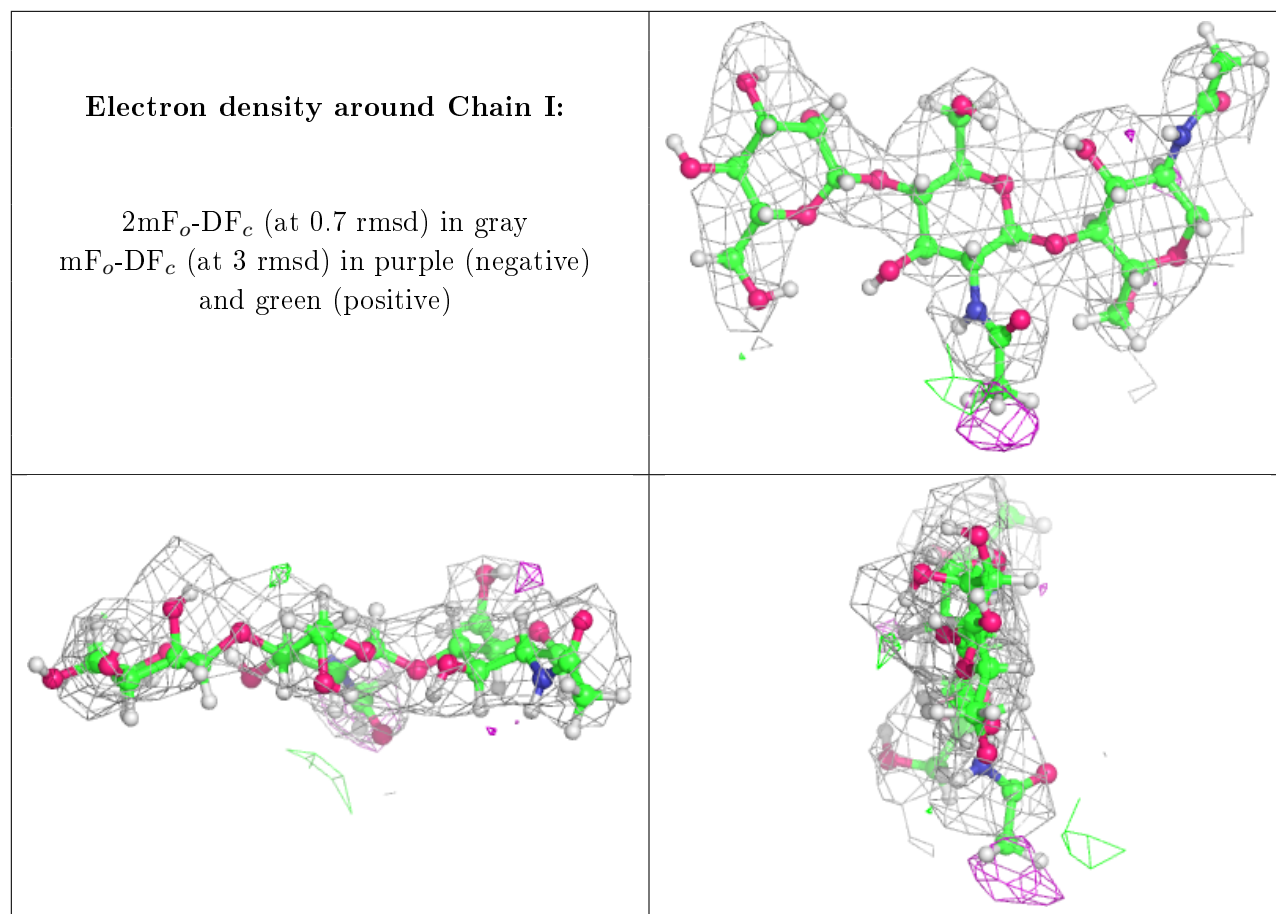
Electron density around Chain G:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
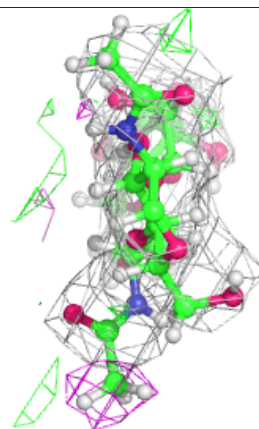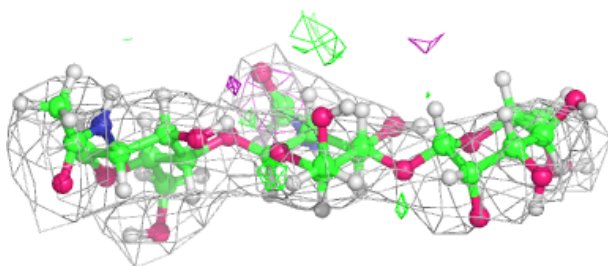
Electron density around Chain H:

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

Electron density around Chain I:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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	B	401	14/15	0.82	0.29	0,0,59,60	0
4	NAG	F	401	14/15	0.86	0.31	0,0,60,60	0
4	NAG	A	334	14/15	0.88	0.22	0,0,44,46	0
4	NAG	C	329	14/15	0.88	0.29	0,0,45,47	0
4	NAG	E	348	14/15	0.89	0.31	0,0,45,47	0
4	NAG	D	401	14/15	0.90	0.29	0,0,59,60	0
4	NAG	A	348	14/15	0.90	0.22	0,0,45,46	0
4	NAG	C	348	14/15	0.91	0.31	0,0,45,48	0
4	NAG	A	329	14/15	0.91	0.28	0,0,45,47	0
4	NAG	C	334	14/15	0.91	0.28	0,0,45,46	0
4	NAG	E	329	14/15	0.91	0.30	0,0,45,47	0
4	NAG	E	334	14/15	0.93	0.19	0,0,44,46	0

6.5 Other polymers (i)

There are no such residues in this entry.