



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:07 PM UTC

PDB ID : 3LZG / pdb_00003lzg
Title : Crystal structure of a 2009 H1N1 influenza virus hemagglutinin
Authors : Xu, R.; Wilson, I.A.
Deposited on : 2010-03-01
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:

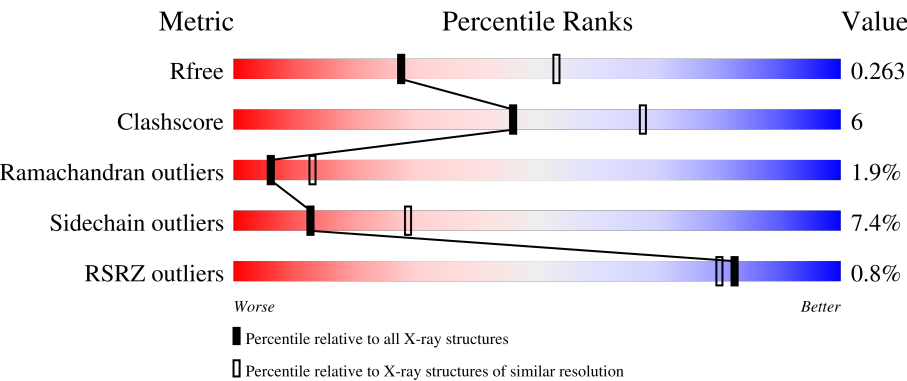
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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



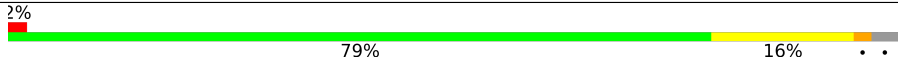
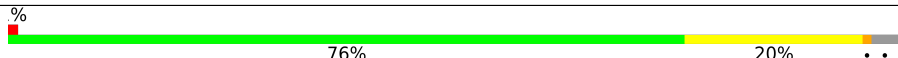
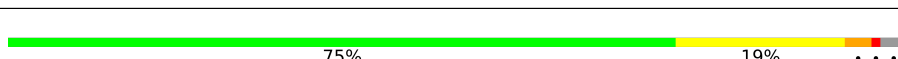
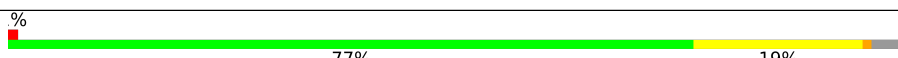
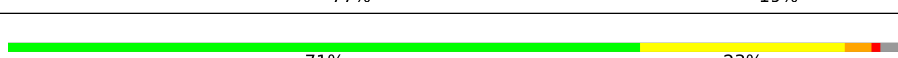
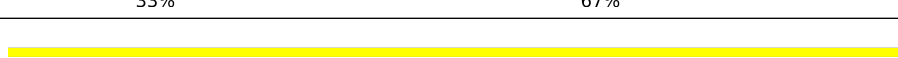
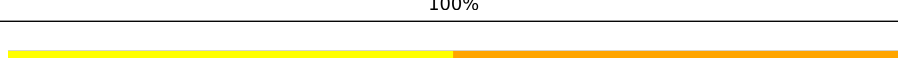
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	329	71%23%..
1	C	329	% 74%21%..
1	E	329	% 67%27%..
1	G	329	% 68%27%..
1	I	329	2% 72%22%..

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Mol	Chain	Length	Quality of chain
1	K	329	
2	B	177	
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	
3	M	3	
4	N	2	
4	O	2	
5	P	5	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24137 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, HA1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2525	1597	435	482	11			
1	C	323	Total	C	N	O	S	0	0	0
			2525	1597	435	482	11			
1	E	323	Total	C	N	O	S	0	0	0
			2525	1597	435	482	11			
1	G	323	Total	C	N	O	S	0	0	0
			2525	1597	435	482	11			
1	I	323	Total	C	N	O	S	0	0	0
			2525	1597	435	482	11			
1	K	325	Total	C	N	O	S	0	0	0
			2536	1604	437	484	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP C3W5S1
A	10	GLY	-	expression tag	UNP C3W5S1
C	9	PRO	-	expression tag	UNP C3W5S1
C	10	GLY	-	expression tag	UNP C3W5S1
E	9	PRO	-	expression tag	UNP C3W5S1
E	10	GLY	-	expression tag	UNP C3W5S1
G	9	PRO	-	expression tag	UNP C3W5S1
G	10	GLY	-	expression tag	UNP C3W5S1
I	9	PRO	-	expression tag	UNP C3W5S1
I	10	GLY	-	expression tag	UNP C3W5S1
K	9	PRO	-	expression tag	UNP C3W5S1
K	10	GLY	-	expression tag	UNP C3W5S1

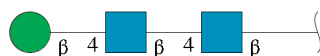
- Molecule 2 is a protein called Hemagglutinin, HA2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1411	884	238	283	6			
2	D	171	Total	C	N	O	S	0	0	0
			1380	866	234	274	6			
2	F	171	Total	C	N	O	S	0	0	0
			1380	866	234	274	6			
2	H	171	Total	C	N	O	S	0	0	0
			1380	866	234	274	6			
2	J	172	Total	C	N	O	S	0	0	0
			1389	871	235	277	6			
2	L	172	Total	C	N	O	S	0	0	0
			1389	871	235	277	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP C3W5S1
B	176	GLY	-	expression tag	UNP C3W5S1
B	177	ARG	-	expression tag	UNP C3W5S1
D	175	SER	-	expression tag	UNP C3W5S1
D	176	GLY	-	expression tag	UNP C3W5S1
D	177	ARG	-	expression tag	UNP C3W5S1
F	175	SER	-	expression tag	UNP C3W5S1
F	176	GLY	-	expression tag	UNP C3W5S1
F	177	ARG	-	expression tag	UNP C3W5S1
H	175	SER	-	expression tag	UNP C3W5S1
H	176	GLY	-	expression tag	UNP C3W5S1
H	177	ARG	-	expression tag	UNP C3W5S1
J	175	SER	-	expression tag	UNP C3W5S1
J	176	GLY	-	expression tag	UNP C3W5S1
J	177	ARG	-	expression tag	UNP C3W5S1
L	175	SER	-	expression tag	UNP C3W5S1
L	176	GLY	-	expression tag	UNP C3W5S1
L	177	ARG	-	expression tag	UNP C3W5S1

- 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.



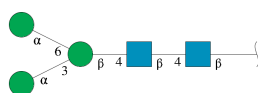
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	69	Total	O	0	0
			69	69		
7	B	32	Total	O	0	0
			32	32		
7	C	54	Total	O	0	0
			54	54		
7	D	23	Total	O	0	0
			23	23		
7	E	60	Total	O	0	0
			60	60		
7	F	23	Total	O	0	0
			23	23		
7	G	59	Total	O	0	0
			59	59		
7	H	24	Total	O	0	0
			24	24		
7	I	39	Total	O	0	0
			39	39		
7	J	20	Total	O	0	0
			20	20		

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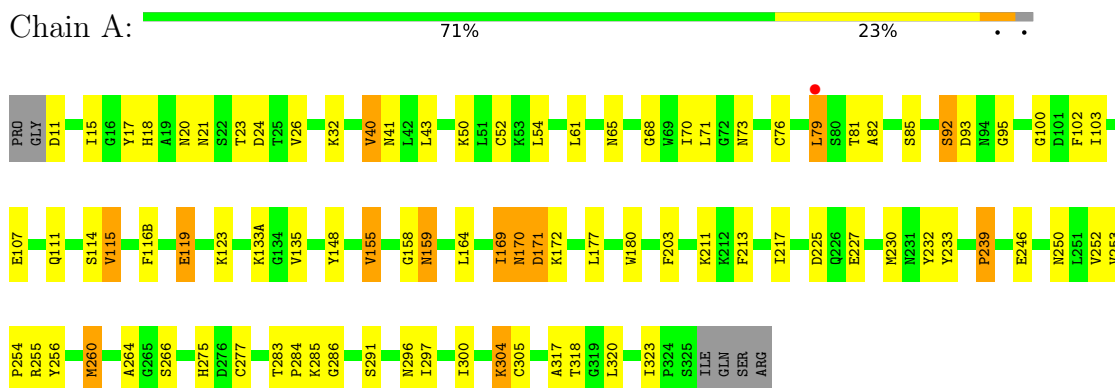
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	34	Total 34	O 34	0	0
7	L	26	Total 26	O 26	0	0

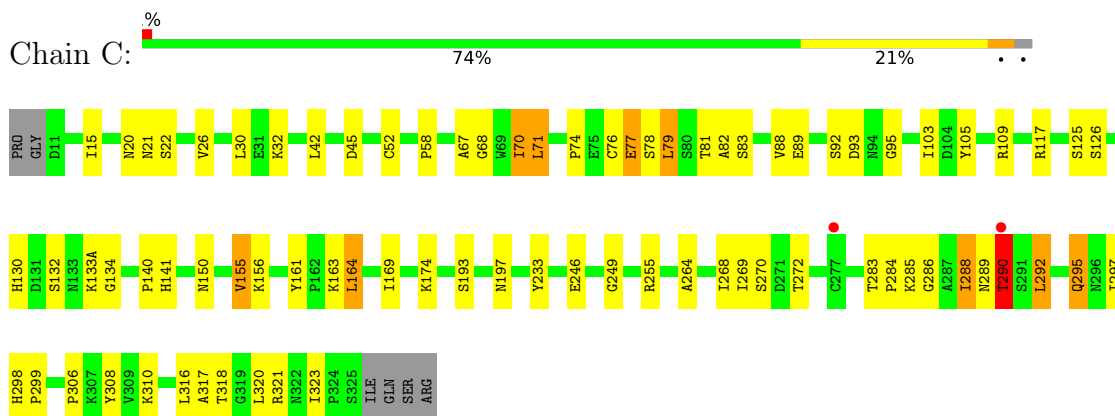
3 Residue-property plots

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.

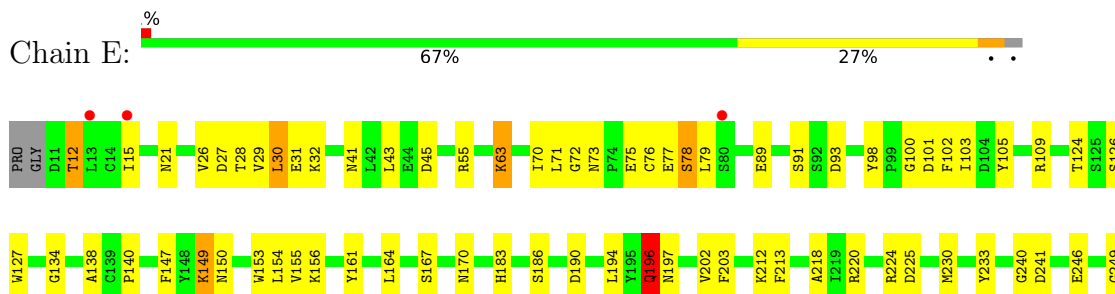
• Molecule 1: Hemagglutinin, HA1 SUBUNIT

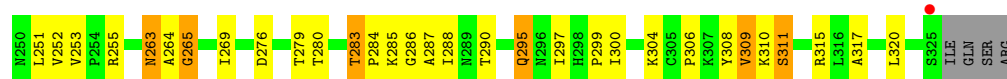


• Molecule 1: Hemagglutinin, HA1 SUBUNIT

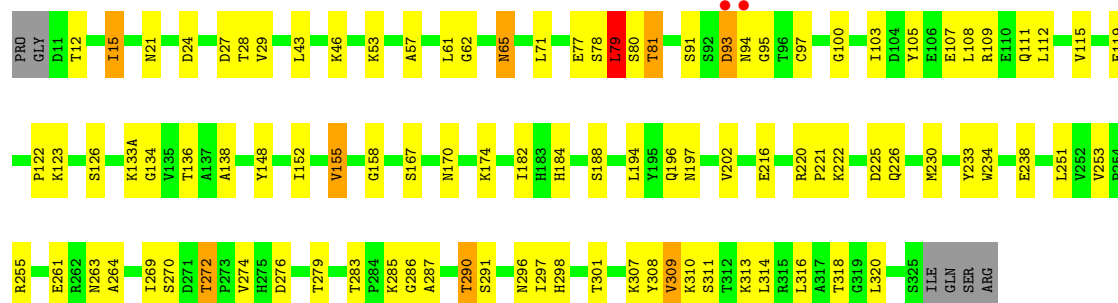


• Molecule 1: Hemagglutinin, HA1 SUBUNIT

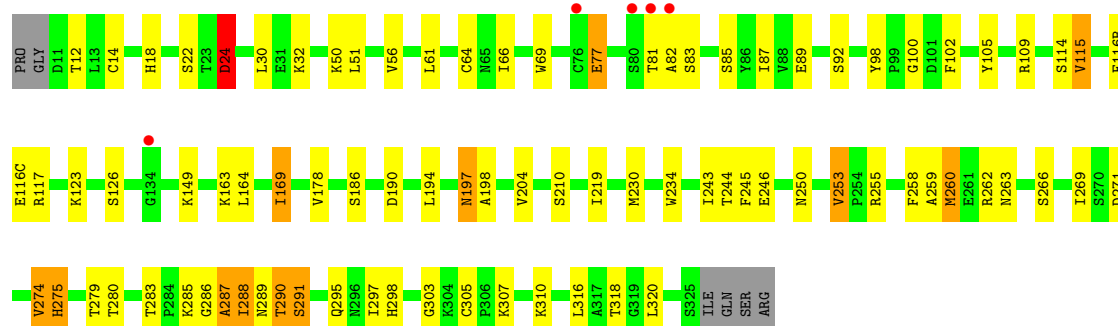




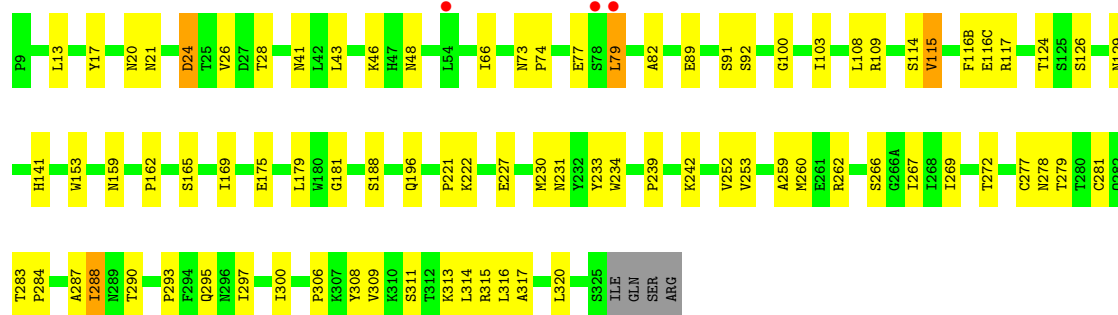
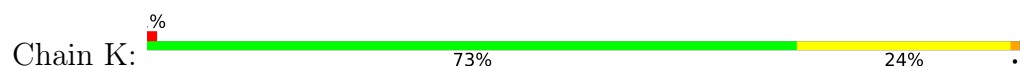
• Molecule 1: Hemagglutinin, HA1 SUBUNIT



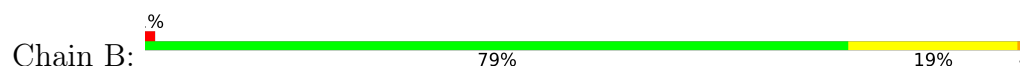
• Molecule 1: Hemagglutinin, HA1 SUBUNIT

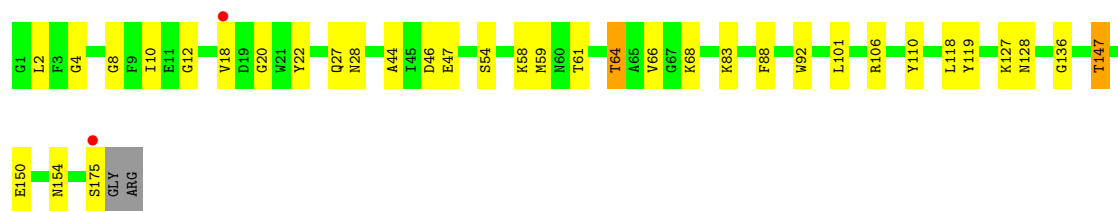


• Molecule 1: Hemagglutinin, HA1 SUBUNIT

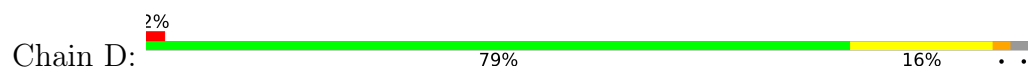


• Molecule 2: Hemagglutinin, HA2 SUBUNIT

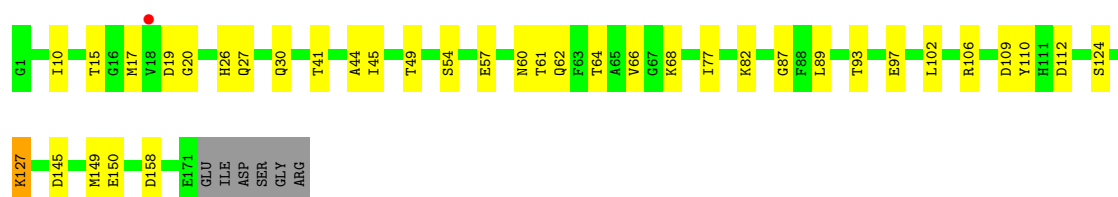
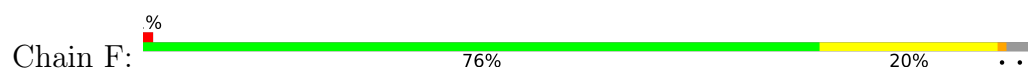




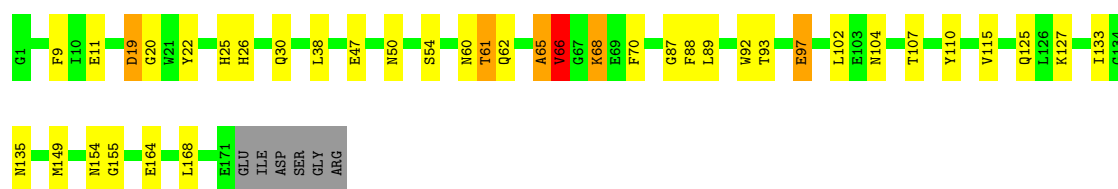
• Molecule 2: Hemagglutinin, HA2 SUBUNIT



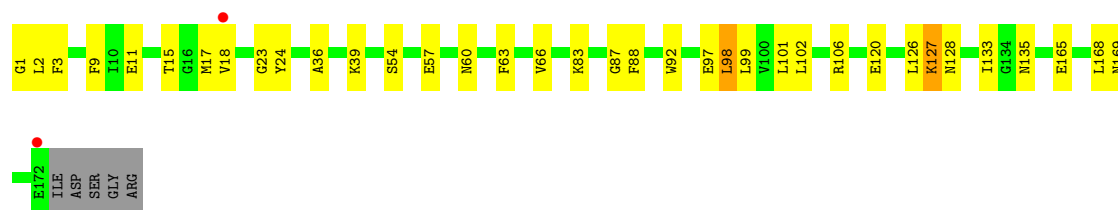
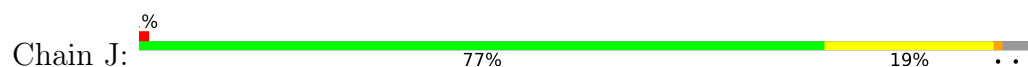
• Molecule 2: Hemagglutinin, HA2 SUBUNIT



• Molecule 2: Hemagglutinin, HA2 SUBUNIT

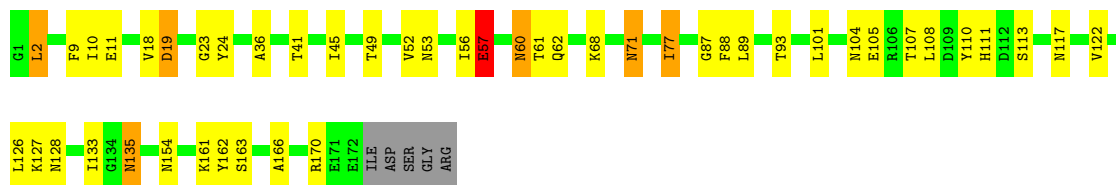


• Molecule 2: Hemagglutinin, HA2 SUBUNIT



• Molecule 2: Hemagglutinin, HA2 SUBUNIT

Chain L:  71% 23% . . .

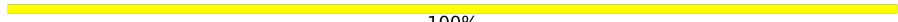


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 67%



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

Chain N:  100%



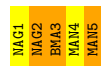
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%



- Molecule 5: 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

Chain P:  40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.68Å 118.31Å 120.07Å 117.37° 92.67° 100.84°	Depositor
Resolution (Å)	45.00 – 2.60 45.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.7 (45.00-2.60) 91.7 (45.00-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.181 , 0.252 0.188 , 0.263	Depositor DCC
R_{free} test set	4548 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.3	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	0.95	EDS
Total number of atoms	24137	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, 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	0.89	0/2589	1.40	24/3519 (0.7%)
1	C	0.87	0/2589	1.42	22/3519 (0.6%)
1	E	0.85	0/2589	1.39	22/3519 (0.6%)
1	G	0.89	0/2589	1.41	27/3519 (0.8%)
1	I	0.83	0/2589	1.40	30/3519 (0.9%)
1	K	0.82	0/2601	1.35	17/3535 (0.5%)
2	B	0.83	0/1439	1.51	11/1939 (0.6%)
2	D	0.85	0/1408	1.49	5/1897 (0.3%)
2	F	0.87	0/1408	1.48	8/1897 (0.4%)
2	H	0.84	0/1408	1.51	8/1897 (0.4%)
2	J	0.82	0/1417	1.49	13/1909 (0.7%)
2	L	0.85	0/1417	1.54	22/1909 (1.2%)
All	All	0.85	0/24043	1.43	209/32578 (0.6%)

There are no bond length outliers.

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	SER	N-CA-C	10.40	122.62	111.28
1	I	77	GLU	N-CA-C	10.12	122.07	111.14
1	G	272	THR	CB-CA-C	9.88	123.78	109.26
1	C	197	ASN	N-CA-C	9.46	122.59	111.71
1	G	197	ASN	N-CA-C	9.43	122.74	111.33
2	J	2	LEU	N-CA-C	8.74	120.42	111.07
1	E	241	ASP	N-CA-C	8.51	121.58	110.43
1	I	126	SER	N-CA-C	8.46	120.50	111.28
1	A	159	ASN	CA-CB-CG	8.42	121.02	112.60
1	C	71	LEU	N-CA-C	-8.22	98.32	110.48
2	F	10	ILE	CA-C-N	7.95	132.75	120.82
2	F	10	ILE	C-N-CA	7.95	132.75	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	ASN	N-CA-C	7.87	118.64	108.34
1	K	126	SER	N-CA-C	7.82	119.89	111.36
2	L	71	ASN	CA-CB-CG	7.80	120.40	112.60
1	C	255	ARG	N-CA-C	-7.74	102.81	112.72
1	E	71	LEU	N-CA-C	-7.62	100.70	110.53
2	F	77	ILE	N-CA-CB	7.52	120.77	110.54
1	E	197	ASN	N-CA-C	7.22	120.99	111.75
2	J	18	VAL	CA-C-N	7.17	130.20	120.38
2	J	18	VAL	C-N-CA	7.17	130.20	120.38
2	L	19	ASP	CA-CB-CG	7.16	119.75	112.60
1	K	20	ASN	CA-C-N	7.06	130.45	120.28
1	K	20	ASN	C-N-CA	7.06	130.45	120.28
1	K	24	ASP	CA-CB-CG	7.02	119.62	112.60
1	G	170	ASN	CA-C-N	6.99	133.36	121.14
1	G	170	ASN	C-N-CA	6.99	133.36	121.14
1	G	126	SER	N-CA-C	6.92	119.67	111.71
1	A	172	LYS	N-CA-C	-6.87	99.35	110.20
1	E	196	GLN	CA-C-N	6.82	130.34	120.38
1	E	196	GLN	C-N-CA	6.82	130.34	120.38
2	J	1	GLY	CA-C-N	6.80	129.28	120.44
2	J	1	GLY	C-N-CA	6.80	129.28	120.44
1	C	289	ASN	CA-C-N	6.75	134.43	121.54
1	C	289	ASN	C-N-CA	6.75	134.43	121.54
1	I	280	THR	N-CA-C	-6.69	104.82	114.12
1	G	93	ASP	CA-CB-CG	6.69	119.29	112.60
1	G	24	ASP	CA-CB-CG	6.68	119.28	112.60
1	C	52	CYS	N-CA-C	6.62	120.25	110.46
1	E	255	ARG	N-CA-C	-6.60	104.27	112.72
2	D	128	ASN	CA-C-N	6.54	129.93	120.38
2	D	128	ASN	C-N-CA	6.54	129.93	120.38
1	A	24	ASP	CA-CB-CG	6.49	119.09	112.60
1	I	24	ASP	CA-CB-CG	6.43	119.03	112.60
1	I	253	VAL	N-CA-C	6.41	116.02	108.96
2	J	99	LEU	N-CA-C	-6.41	104.21	111.14
2	F	109	ASP	CA-CB-CG	6.41	119.01	112.60
1	G	225	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	125	SER	N-CA-C	6.30	119.44	111.69
2	H	127	LYS	CA-C-N	6.29	130.67	120.60
2	H	127	LYS	C-N-CA	6.29	130.67	120.60
2	L	57	GLU	N-CA-C	6.27	120.54	113.01
1	K	278	ASN	CA-CB-CG	6.18	118.78	112.60
2	F	57	GLU	N-CA-C	6.18	120.08	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	19	ASP	CA-CB-CG	6.17	118.77	112.60
1	G	155	VAL	N-CA-CB	-6.16	102.09	112.44
2	L	10	ILE	CA-C-N	6.15	128.84	120.54
2	L	10	ILE	C-N-CA	6.15	128.84	120.54
1	I	123	LYS	CA-C-N	6.11	128.78	120.54
1	I	123	LYS	C-N-CA	6.11	128.78	120.54
2	D	2	LEU	N-CA-C	6.09	117.59	111.07
1	A	171	ASP	N-CA-C	-6.07	105.52	113.17
1	G	291	SER	CA-C-N	6.05	130.54	120.86
1	G	291	SER	C-N-CA	6.05	130.54	120.86
1	I	258	PHE	N-CA-C	6.03	118.23	108.34
1	A	17	TYR	CA-C-N	5.98	129.21	120.71
1	A	17	TYR	C-N-CA	5.98	129.21	120.71
1	I	289	ASN	CA-C-N	5.96	132.92	121.54
1	I	289	ASN	C-N-CA	5.96	132.92	121.54
1	A	239	PRO	N-CA-C	5.93	124.68	112.47
1	E	21	ASN	CA-CB-CG	5.92	118.52	112.60
1	C	78	SER	N-CA-C	5.92	118.96	109.02
1	A	32	LYS	CA-C-N	-5.89	114.05	122.77
1	A	32	LYS	C-N-CA	-5.89	114.05	122.77
1	E	280	THR	N-CA-C	-5.86	106.47	113.97
2	L	163	SER	N-CA-C	5.86	118.17	111.02
1	C	155	VAL	N-CA-CB	-5.86	101.53	112.36
1	K	288	ILE	N-CA-C	5.84	117.85	108.85
1	A	20	ASN	N-CA-C	5.84	115.94	108.24
1	E	263	ASN	CA-C-N	5.82	132.66	121.54
1	E	263	ASN	C-N-CA	5.82	132.66	121.54
2	B	127	LYS	CA-C-N	5.81	129.90	120.60
2	B	127	LYS	C-N-CA	5.81	129.90	120.60
1	K	314	LEU	CA-C-N	-5.80	115.05	122.77
1	K	314	LEU	C-N-CA	-5.80	115.05	122.77
2	F	19	ASP	N-CA-C	5.80	119.46	112.38
1	K	159	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	155	VAL	N-CA-CB	-5.79	103.72	112.35
1	I	318	THR	N-CA-C	-5.79	106.14	113.43
2	H	66	VAL	N-CA-CB	5.76	120.73	111.23
1	K	196	GLN	CA-C-N	5.75	129.27	121.05
1	K	196	GLN	C-N-CA	5.75	129.27	121.05
1	C	21	ASN	CA-CB-CG	5.75	118.35	112.60
1	G	12	THR	N-CA-C	5.74	118.13	109.23
2	L	133	ILE	N-CA-C	5.73	117.73	111.77
1	K	48	ASN	CA-CB-CG	5.72	118.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	LYS	N-CA-C	5.68	117.92	111.11
1	I	197	ASN	N-CA-C	5.67	122.88	110.80
1	G	196	GLN	CA-C-N	5.66	128.14	120.38
1	G	196	GLN	C-N-CA	5.66	128.14	120.38
1	I	253	VAL	CB-CA-C	5.66	116.42	110.88
1	A	135	VAL	N-CA-C	-5.65	100.31	108.89
2	B	147	THR	CA-C-N	5.63	127.76	120.44
2	B	147	THR	C-N-CA	5.63	127.76	120.44
1	E	203	PHE	CA-CB-CG	-5.63	108.17	113.80
2	L	11	GLU	N-CA-C	5.63	117.86	111.11
1	K	73	ASN	CA-CB-CG	5.63	118.23	112.60
2	L	154	ASN	CA-CB-CG	5.63	118.23	112.60
1	C	32	LYS	CA-C-N	-5.61	114.46	122.77
1	C	32	LYS	C-N-CA	-5.61	114.46	122.77
2	L	122	VAL	CA-C-N	5.61	127.73	120.44
2	L	122	VAL	C-N-CA	5.61	127.73	120.44
1	G	133(A)	LYS	N-CA-C	-5.60	103.10	110.33
2	J	128	ASN	CA-CB-CG	5.59	118.19	112.60
1	I	305	CYS	N-CA-C	5.58	118.37	110.40
1	C	272	THR	CB-CA-C	5.57	118.37	109.62
1	E	124	THR	N-CA-C	5.56	118.27	111.82
1	A	255	ARG	N-CA-C	-5.55	106.56	113.55
2	F	112	ASP	CA-CB-CG	5.55	118.15	112.60
2	J	165	GLU	CA-C-N	5.55	128.27	120.28
2	J	165	GLU	C-N-CA	5.55	128.27	120.28
1	E	220	ARG	N-CA-C	-5.54	102.94	110.36
1	A	92	SER	CA-C-N	5.53	130.03	120.58
1	A	92	SER	C-N-CA	5.53	130.03	120.58
2	J	120	GLU	CA-C-N	5.53	127.95	120.38
2	J	120	GLU	C-N-CA	5.53	127.95	120.38
1	I	190	ASP	CA-C-N	5.53	127.94	120.65
1	I	190	ASP	C-N-CA	5.53	127.94	120.65
1	I	260	MET	N-CA-C	5.52	117.24	108.79
1	E	276	ASP	CA-CB-CG	5.51	118.11	112.60
1	I	64	CYS	N-CA-C	5.50	118.66	110.52
1	A	305	CYS	N-CA-C	5.48	118.49	110.10
1	G	270	SER	N-CA-C	5.48	117.43	108.55
1	K	315	ARG	N-CA-C	5.46	117.63	108.73
2	H	38	LEU	N-CA-C	5.44	117.91	111.33
1	A	296	ASN	CA-C-N	5.43	127.49	120.70
1	A	296	ASN	C-N-CA	5.43	127.49	120.70
2	H	20	GLY	CA-C-N	5.43	127.83	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	20	GLY	C-N-CA	5.43	127.83	120.44
1	I	291	SER	CA-C-N	5.43	129.56	120.86
1	I	291	SER	C-N-CA	5.43	129.56	120.86
1	C	76	CYS	N-CA-C	5.43	120.78	113.72
2	B	10	ILE	CA-C-N	5.41	128.93	120.82
2	B	10	ILE	C-N-CA	5.41	128.93	120.82
1	E	284	PRO	CA-C-N	5.37	129.69	120.72
1	E	284	PRO	C-N-CA	5.37	129.69	120.72
2	B	64	THR	CB-CA-C	5.34	120.55	109.38
1	I	290	THR	CA-C-N	5.33	131.72	121.54
1	I	290	THR	C-N-CA	5.33	131.72	121.54
1	E	240	GLY	CA-C-N	5.32	129.86	120.87
1	E	240	GLY	C-N-CA	5.32	129.86	120.87
1	I	288	ILE	N-CA-C	5.31	115.51	107.75
1	E	31	GLU	N-CA-C	5.31	116.47	108.46
1	G	226	GLN	N-CA-C	5.31	117.39	107.99
2	J	168	LEU	N-CA-C	5.31	117.75	111.33
1	K	272	THR	CB-CA-C	5.30	117.06	109.26
1	G	79	LEU	CA-C-N	5.30	131.66	121.54
1	G	79	LEU	C-N-CA	5.30	131.66	121.54
1	C	133(A)	LYS	N-CA-C	-5.28	100.64	109.24
1	A	227	GLU	N-CA-C	-5.27	106.90	113.38
2	L	10	ILE	N-CA-CB	5.25	117.34	111.89
2	L	111	HIS	CA-C-N	5.24	127.30	120.28
2	L	111	HIS	C-N-CA	5.24	127.30	120.28
1	G	182	ILE	N-CA-C	-5.22	100.13	107.75
1	C	284	PRO	CA-C-N	5.20	130.24	121.14
1	C	284	PRO	C-N-CA	5.20	130.24	121.14
2	J	57	GLU	N-CA-C	5.18	119.32	112.89
1	A	250	ASN	N-CA-C	5.18	119.17	112.86
1	G	221	PRO	CA-C-N	5.18	131.43	121.54
1	G	221	PRO	C-N-CA	5.18	131.43	121.54
1	G	318	THR	N-CA-C	-5.17	107.63	114.04
2	L	77	ILE	N-CA-CB	5.17	119.48	110.65
1	G	255	ARG	N-CA-C	-5.16	106.11	112.72
1	I	12	THR	N-CA-C	5.16	117.66	109.50
1	E	225	ASP	CA-CB-CG	5.16	117.75	112.60
1	I	169	ILE	N-CA-C	5.15	118.73	112.80
1	C	318	THR	N-CA-C	-5.15	106.13	112.72
2	B	128	ASN	CA-CB-CG	5.14	117.74	112.60
1	I	287	ALA	N-CA-C	5.13	118.38	110.42
2	F	15	THR	CB-CA-C	5.13	120.71	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	VAL	N-CA-CB	5.13	119.69	111.23
1	C	83	SER	N-CA-C	-5.12	106.96	114.39
1	C	292	LEU	N-CA-C	5.12	117.14	110.08
1	I	255	ARG	N-CA-C	-5.11	106.18	112.72
2	H	92	TRP	N-CA-C	5.11	116.85	111.28
2	L	126	LEU	N-CA-C	5.11	116.65	111.14
1	E	126	SER	N-CA-C	5.10	117.74	111.82
1	I	98	TYR	N-CA-C	-5.10	102.16	109.24
2	L	24	TYR	N-CA-C	5.08	117.40	109.52
1	A	61	LEU	N-CA-C	-5.08	101.03	109.46
2	L	105	GLU	CA-C-N	5.08	127.08	120.28
2	L	105	GLU	C-N-CA	5.08	127.08	120.28
1	A	304	LYS	N-CA-C	-5.05	99.11	107.99
1	K	46	LYS	N-CA-C	5.04	117.62	109.40
1	G	134	GLY	CA-C-N	5.04	129.85	122.69
1	G	134	GLY	C-N-CA	5.04	129.85	122.69
2	B	2	LEU	N-CA-C	5.04	117.43	111.33
2	L	49	THR	CB-CA-C	5.04	119.15	110.79
2	B	12	GLY	N-CA-C	5.04	118.62	111.12
1	E	12	THR	N-CA-C	5.03	117.60	109.40
1	I	250	ASN	N-CA-C	5.03	119.27	113.38
1	K	260	MET	N-CA-C	5.03	116.72	109.07
1	A	65	ASN	CA-CB-CG	5.03	117.63	112.60
2	L	117	ASN	CA-C-N	5.02	126.97	120.44
2	L	117	ASN	C-N-CA	5.02	126.97	120.44
2	D	109	ASP	CA-C-N	5.01	126.99	120.28
2	D	109	ASP	C-N-CA	5.01	126.99	120.28
1	G	27	ASP	CA-CB-CG	5.01	117.61	112.60
1	I	290	THR	N-CA-C	5.01	121.47	110.80

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	2525	0	2474	30	0
1	C	2525	0	2475	34	0
1	E	2525	0	2475	47	0
1	G	2525	0	2476	31	0
1	I	2525	0	2475	36	0
1	K	2536	0	2486	34	0
2	B	1411	0	1329	15	0
2	D	1380	0	1303	16	0
2	F	1380	0	1303	13	0
2	H	1380	0	1303	22	0
2	J	1389	0	1309	13	0
2	L	1389	0	1309	19	0
3	M	39	0	34	1	0
4	N	28	0	25	0	0
4	O	28	0	25	2	0
5	P	61	0	52	2	0
6	E	14	0	13	1	0
6	K	14	0	13	0	0
7	A	69	0	0	0	0
7	B	32	0	0	0	0
7	C	54	0	0	0	0
7	D	23	0	0	0	0
7	E	60	0	0	0	0
7	F	23	0	0	0	0
7	G	59	0	0	0	0
7	H	24	0	0	2	0
7	I	39	0	0	1	0
7	J	20	0	0	0	0
7	K	34	0	0	1	0
7	L	26	0	0	0	0
All	All	24137	0	22879	271	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 6.

All (271) 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:E:279:THR:HG21	1:E:287:ALA:HB1	1.28	1.11
1:E:290:THR:HG21	1:E:304:LYS:O	1.75	0.87
1:A:283:THR:HB	1:A:286:GLY:O	1.75	0.87
1:C:283:THR:HB	1:C:286:GLY:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:SER:HB2	1:I:266:SER:HB2	1.68	0.76
1:A:283:THR:HG22	1:A:285:LYS:H	1.52	0.74
1:I:283:THR:HB	1:I:286:GLY:O	1.90	0.70
1:I:61:LEU:HD11	1:I:66:ILE:HD13	1.74	0.69
1:K:222:LYS:HG3	1:K:227:GLU:HG2	1.74	0.69
1:I:24:ASP:HB3	7:I:357:HOH:O	1.93	0.68
1:I:260:MET:HE2	1:I:262:ARG:HG2	1.74	0.68
1:G:103:ILE:HG13	1:G:233:TYR:CE2	2.29	0.67
1:K:103:ILE:HG13	1:K:233:TYR:CE2	2.30	0.67
1:E:279:THR:HG21	1:E:287:ALA:CB	2.17	0.66
1:E:288:ILE:HG21	1:E:297:ILE:HG13	1.78	0.66
1:G:283:THR:HB	1:G:286:GLY:O	1.96	0.66
1:C:70:ILE:CG2	1:C:71:LEU:N	2.59	0.65
1:E:138:ALA:O	1:E:224:ARG:NH1	2.29	0.65
1:G:107:GLU:O	1:G:111:GLN:HG2	1.96	0.65
1:K:100:GLY:HA3	1:K:230:MET:O	1.96	0.64
1:G:283:THR:HG22	1:G:285:LYS:H	1.63	0.64
1:C:42:LEU:HD11	1:C:316:LEU:HG	1.79	0.63
2:D:47:GLU:HB3	1:E:30:LEU:HG	1.79	0.63
1:K:290:THR:HG22	1:K:306:PRO:HD3	1.79	0.63
1:I:100:GLY:HA3	1:I:230:MET:O	1.99	0.63
1:A:177:LEU:HB2	1:A:260:MET:HE3	1.81	0.62
1:G:309:VAL:HG22	2:H:93:THR:HA	1.81	0.62
1:K:309:VAL:HG12	1:K:311:SER:H	1.63	0.62
1:A:107:GLU:O	1:A:111:GLN:HG2	2.00	0.62
2:B:18:VAL:HG12	2:B:18:VAL:O	1.98	0.62
1:E:26:VAL:HG21	1:E:317:ALA:HB2	1.82	0.62
1:E:288:ILE:HD13	1:E:295:GLN:HG3	1.80	0.61
2:B:58:LYS:HD2	2:D:97:GLU:HG2	1.80	0.61
2:H:9:PHE:O	2:H:135:ASN:HA	2.00	0.61
1:E:140:PRO:HD2	6:E:330:NAG:H83	1.84	0.60
1:G:279:THR:HG21	1:G:287:ALA:HB1	1.82	0.60
1:K:26:VAL:HG21	1:K:317:ALA:HB2	1.84	0.60
1:E:89:GLU:O	1:E:269:ILE:HA	2.03	0.59
1:I:51:LEU:HB2	1:I:274:VAL:HA	1.84	0.59
1:A:169:ILE:O	1:A:170:ASN:HB2	2.03	0.59
2:H:68:LYS:HB3	2:H:70:PHE:CE2	2.38	0.58
1:I:102:PHE:HB3	1:I:105:TYR:HB2	1.85	0.58
1:K:316:LEU:HD23	2:L:52:VAL:HG22	1.86	0.58
1:G:97:CYS:HB2	1:G:138:ALA:O	2.04	0.57
2:D:30:GLN:HE22	2:D:145:ASP:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:65:ALA:O	2:H:66:VAL:HG23	2.04	0.57
1:E:100:GLY:HA3	1:E:230:MET:O	2.03	0.57
1:G:123:LYS:HG3	1:G:152:ILE:HD11	1.87	0.56
1:A:114:SER:HB2	1:A:266:SER:HB2	1.87	0.56
2:H:66:VAL:O	2:J:83:LYS:NZ	2.38	0.56
1:E:263:ASN:O	1:E:265:GLY:N	2.38	0.56
2:B:83:LYS:NZ	2:F:66:VAL:O	2.39	0.55
1:K:169:ILE:HG12	1:K:242:LYS:HG3	1.87	0.55
1:E:98:TYR:CD1	1:E:230:MET:HB2	2.41	0.55
1:E:73:ASN:HB3	1:E:76:CYS:SG	2.47	0.55
1:C:89:GLU:O	1:C:269:ILE:HA	2.04	0.55
1:C:105:TYR:CE2	1:C:109:ARG:HD2	2.42	0.55
1:C:283:THR:HG22	1:C:285:LYS:H	1.70	0.55
1:K:66:ILE:HG13	1:K:109:ARG:HG2	1.87	0.55
1:I:61:LEU:HD12	1:I:89:GLU:HG2	1.89	0.55
1:A:26:VAL:HG21	1:A:317:ALA:HB2	1.89	0.54
1:K:116(C):GLU:HB3	1:K:259:ALA:HB3	1.90	0.54
1:E:72:GLY:HA3	1:E:149:LYS:H	1.71	0.54
2:L:53:ASN:O	2:L:57:GLU:HG2	2.08	0.54
1:E:103:ILE:HG13	1:E:233:TYR:CE2	2.42	0.54
2:D:88:PHE:CZ	2:F:87:GLY:HA3	2.43	0.54
1:K:293:PRO:HD3	2:L:56:ILE:HG12	1.90	0.54
1:I:116(C):GLU:HB3	1:I:259:ALA:HB3	1.90	0.54
1:I:260:MET:CE	1:I:262:ARG:HG2	2.38	0.54
1:I:115:VAL:HG11	1:I:116(B):PHE:HB2	1.90	0.53
1:A:50:LYS:HD2	1:A:275:HIS:HB2	1.89	0.53
1:C:156:LYS:HE2	1:C:193:SER:O	2.08	0.53
1:I:186:SER:HB2	1:I:219:ILE:HG12	1.90	0.53
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.91	0.53
1:K:115:VAL:HG11	1:K:116(B):PHE:HB2	1.91	0.53
1:C:70:ILE:O	1:C:150:ASN:ND2	2.38	0.53
1:C:288:ILE:HD12	1:C:295:GLN:HG3	1.91	0.53
1:K:77:GLU:HG3	1:K:79:LEU:HB2	1.91	0.53
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.24	0.52
1:G:79:LEU:C	1:G:81:THR:H	2.17	0.52
1:C:45:ASP:C	1:C:297:ILE:HD11	2.34	0.52
1:E:156:LYS:HD2	1:E:196:GLN:HB2	1.92	0.52
1:K:309:VAL:HG13	2:L:93:THR:HA	1.90	0.52
2:F:45:ILE:O	2:F:49:THR:HG23	2.10	0.52
2:L:9:PHE:O	2:L:135:ASN:HA	2.10	0.52
1:A:100:GLY:HA3	1:A:230:MET:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:PHE:HB2	2:D:78:GLU:HG3	1.92	0.51
1:K:114:SER:HB2	1:K:266:SER:HB3	1.92	0.51
1:E:290:THR:HG22	1:E:306:PRO:HD3	1.93	0.51
1:E:202:VAL:HG11	1:E:251:LEU:HD13	1.91	0.51
2:F:44:ALA:HA	2:F:110:TYR:OH	2.10	0.51
1:I:69:TRP:HE1	1:I:81:THR:HG22	1.76	0.51
2:D:9:PHE:O	2:D:135:ASN:HA	2.10	0.51
1:K:41:ASN:ND2	1:K:43:LEU:O	2.43	0.51
1:A:133(A):LYS:HG2	5:P:2:NAG:H83	1.92	0.51
1:E:288:ILE:CD1	1:E:295:GLN:HG3	2.40	0.51
1:I:164:LEU:O	1:I:246:GLU:HA	2.10	0.51
2:B:4:GLY:O	2:B:8:GLY:HA3	2.10	0.51
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.92	0.51
1:G:53:LYS:HE3	1:G:57:ALA:HB2	1.93	0.50
1:G:301:THR:O	2:H:65:ALA:O	2.30	0.50
1:C:283:THR:HG21	1:C:297:ILE:HG22	1.94	0.50
2:F:93:THR:O	2:F:97:GLU:HB2	2.12	0.50
1:G:28:THR:HG22	2:H:104:ASN:HB3	1.93	0.50
1:A:18:HIS:HB2	2:B:20:GLY:O	2.12	0.50
2:B:88:PHE:CZ	2:D:87:GLY:HA3	2.47	0.50
1:A:11:ASP:OD1	2:B:28:ASN:HA	2.12	0.49
1:C:70:ILE:HG22	1:C:71:LEU:H	1.77	0.49
2:J:9:PHE:O	2:J:135:ASN:HA	2.12	0.49
1:E:283:THR:HB	1:E:286:GLY:O	2.12	0.49
1:G:71:LEU:O	1:G:148:TYR:HB3	2.12	0.49
1:C:70:ILE:HG23	1:C:71:LEU:N	2.27	0.49
2:J:88:PHE:CZ	2:L:87:GLY:HA3	2.47	0.49
1:K:28:THR:HG22	2:L:104:ASN:HB3	1.94	0.49
1:I:178:VAL:O	1:I:234:TRP:HA	2.12	0.49
1:E:309:VAL:HG13	1:E:311:SER:OG	2.12	0.49
1:K:24:ASP:HB2	7:K:352:HOH:O	2.12	0.49
1:K:74:PRO:HB3	1:K:141:HIS:HB2	1.95	0.49
1:E:186:SER:HA	1:E:218:ALA:O	2.12	0.49
1:I:66:ILE:HG13	1:I:109:ARG:HG2	1.95	0.49
2:H:107:THR:O	2:H:110:TYR:HB3	2.12	0.49
1:G:100:GLY:HA3	1:G:230:MET:O	2.13	0.48
1:I:283:THR:HG22	1:I:285:LYS:H	1.78	0.48
1:A:41:ASN:ND2	1:A:43:LEU:O	2.46	0.48
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.53	0.48
1:E:72:GLY:HA3	1:E:149:LYS:N	2.29	0.48
2:H:50:ASN:HD21	1:I:32:LYS:HE3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:LEU:HB2	2:D:109:ASP:OD1	2.13	0.48
1:G:307:LYS:HE2	2:H:61:THR:HG21	1.96	0.48
1:K:175:GLU:CD	1:K:262:ARG:HH12	2.22	0.47
2:L:18:VAL:O	2:L:18:VAL:HG12	2.13	0.47
1:E:26:VAL:HG12	1:E:315:ARG:HG3	1.95	0.47
2:B:18:VAL:O	2:B:18:VAL:CG1	2.61	0.47
1:E:105:TYR:CZ	1:E:109:ARG:HD2	2.49	0.47
2:F:30:GLN:HE22	2:F:145:ASP:HB2	1.80	0.47
2:H:97:GLU:HG3	7:H:450:HOH:O	2.14	0.47
1:C:70:ILE:HD12	1:C:70:ILE:HA	1.73	0.47
1:A:68:GLY:CA	1:A:95:GLY:HA2	2.45	0.47
2:D:58:LYS:HD2	2:F:97:GLU:HG2	1.97	0.47
1:E:147:PHE:HZ	1:E:252:VAL:HG11	1.79	0.46
1:E:295:GLN:OE1	1:E:308:TYR:HD1	1.99	0.46
1:G:15:ILE:HD11	2:H:115:VAL:HG13	1.97	0.46
2:H:62:GLN:H	2:H:62:GLN:CD	2.23	0.46
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.50	0.46
1:G:283:THR:HG23	1:G:298:HIS:CB	2.46	0.46
2:L:107:THR:O	2:L:110:TYR:HB3	2.15	0.46
1:A:211:LYS:HE3	1:A:213:PHE:CE1	2.51	0.46
1:E:154:LEU:HD12	1:E:253:VAL:HG11	1.96	0.46
1:K:279:THR:HG21	1:K:287:ALA:HB1	1.97	0.46
1:C:74:PRO:HB3	1:C:141:HIS:HB2	1.97	0.46
1:G:108:LEU:HB2	1:G:234:TRP:CE2	2.51	0.46
1:I:279:THR:HG21	1:I:287:ALA:HB1	1.97	0.46
1:G:308:TYR:CD2	2:H:89:LEU:HD13	2.50	0.46
2:H:30:GLN:O	2:H:30:GLN:HG2	2.16	0.46
1:A:114:SER:HB2	1:A:266:SER:CB	2.45	0.45
2:F:41:THR:O	2:F:45:ILE:HG12	2.17	0.45
1:I:89:GLU:O	1:I:269:ILE:HA	2.16	0.45
1:K:308:TYR:CD2	2:L:89:LEU:HD13	2.51	0.45
2:D:88:PHE:CE2	2:F:87:GLY:HA3	2.51	0.45
1:A:71:LEU:O	1:A:148:TYR:HB3	2.16	0.45
1:A:115:VAL:HG11	1:A:116(B):PHE:HB2	1.98	0.45
2:B:59:MET:HE1	2:B:92:TRP:CZ3	2.51	0.45
1:E:41:ASN:ND2	1:E:43:LEU:O	2.45	0.45
1:E:70:ILE:O	1:E:150:ASN:ND2	2.50	0.45
2:H:47:GLU:HB3	1:I:30:LEU:HD22	1.97	0.45
1:K:17:TYR:HB2	1:K:320:LEU:HD11	1.98	0.45
1:E:63:LYS:HD2	1:E:75:GLU:HB3	1.98	0.45
1:E:102:PHE:HB3	1:E:105:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:GLN:HB3	1:E:306:PRO:HB2	1.99	0.45
2:L:128:ASN:HB3	2:L:170:ARG:NH2	2.32	0.45
1:A:230:MET:SD	1:A:252:VAL:HG21	2.57	0.45
1:C:70:ILE:HG22	1:C:71:LEU:N	2.30	0.45
2:F:17:MET:HE3	2:F:20:GLY:O	2.17	0.45
1:I:307:LYS:HG3	2:J:92:TRP:CE2	2.52	0.44
1:C:164:LEU:O	1:C:246:GLU:HA	2.17	0.44
2:D:160:PRO:HA	2:D:163:SER:HB2	1.98	0.44
1:A:203:PHE:HB3	1:A:246:GLU:HB3	2.00	0.44
2:B:101:LEU:HD13	2:F:54:SER:HB3	1.99	0.44
1:G:184:HIS:HB3	1:G:220:ARG:HH22	1.82	0.44
1:E:127:TRP:CD2	1:E:154:LEU:HD11	2.52	0.44
1:I:66:ILE:CD1	1:I:87:ILE:HG21	2.48	0.44
1:K:153:TRP:HA	1:K:252:VAL:HG22	2.00	0.44
2:B:44:ALA:HA	2:B:110:TYR:OH	2.17	0.44
2:B:88:PHE:CE2	2:D:87:GLY:HA3	2.52	0.44
1:G:65:ASN:OD1	1:G:95:GLY:HA2	2.18	0.44
1:C:290:THR:HG23	1:C:306:PRO:HG3	1.99	0.44
1:G:61:LEU:HA	1:G:79:LEU:CD1	2.47	0.44
1:K:281:CYS:HB3	1:K:288:ILE:HG13	1.98	0.44
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.53	0.44
1:A:54:LEU:HB3	1:A:85:SER:HB2	1.99	0.44
1:G:43:LEU:HD11	1:G:296:ASN:HB3	1.99	0.44
2:H:54:SER:HB3	2:J:101:LEU:HD13	2.00	0.44
1:K:308:TYR:CE2	2:L:89:LEU:HD13	2.53	0.44
5:P:3:BMA:H62	5:P:5:MAN:H5	2.00	0.44
1:E:29:VAL:HG13	1:E:30:LEU:HD13	1.99	0.43
1:A:103:ILE:HG13	1:A:233:TYR:CE2	2.53	0.43
1:E:27:ASP:HB3	1:E:32:LYS:HD2	2.00	0.43
1:E:164:LEU:O	1:E:246:GLU:HA	2.17	0.43
1:G:61:LEU:HA	1:G:79:LEU:HD12	1.99	0.43
2:D:93:THR:O	2:D:97:GLU:HB2	2.18	0.43
1:I:66:ILE:HD11	1:I:87:ILE:HG21	2.01	0.43
1:A:79:LEU:HD22	1:I:271:ASP:HB2	2.00	0.43
1:E:45:ASP:C	1:E:297:ILE:HD11	2.43	0.43
1:I:18:HIS:ND1	2:J:17:MET:O	2.45	0.43
2:H:87:GLY:HA3	2:L:88:PHE:CZ	2.54	0.43
2:J:54:SER:HB3	2:L:101:LEU:HD13	2.00	0.43
2:L:41:THR:O	2:L:45:ILE:HG12	2.18	0.43
2:L:166:ALA:O	2:L:170:ARG:HB2	2.18	0.43
1:A:119:GLU:HG3	1:A:256:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:CYS:O	2:J:24:TYR:HA	2.19	0.43
1:I:283:THR:HG23	1:I:298:HIS:CB	2.48	0.43
1:K:281:CYS:SG	1:K:288:ILE:HD11	2.58	0.43
2:H:125:GLN:NE2	2:H:155:GLY:HA2	2.34	0.43
1:C:295:GLN:OE1	1:C:308:TYR:HD1	2.02	0.42
1:E:77:GLU:O	1:E:78:SER:HB3	2.19	0.42
2:H:25:HIS:HD2	7:H:181:HOH:O	2.03	0.42
1:I:56:VAL:HB	1:I:85:SER:HB3	2.02	0.42
1:E:70:ILE:HD12	1:E:70:ILE:HA	1.96	0.42
1:E:299:PRO:HG2	1:E:300:ILE:HD12	2.01	0.42
1:G:43:LEU:HB2	1:G:314:LEU:HB2	2.02	0.42
1:G:103:ILE:HG13	1:G:233:TYR:CZ	2.54	0.42
2:J:3:PHE:CZ	2:L:2:LEU:HG	2.54	0.42
1:C:79:LEU:C	1:C:81:THR:H	2.27	0.42
1:C:130:HIS:CE1	1:C:164:LEU:HB3	2.55	0.42
1:E:310:LYS:HG3	2:F:89:LEU:HD11	2.01	0.42
1:I:244:THR:HG22	1:K:221:PRO:HD3	2.00	0.42
2:L:161:LYS:HD3	2:L:162:TYR:CZ	2.55	0.42
1:C:93:ASP:OD2	4:O:1:NAG:H62	2.19	0.42
1:K:169:ILE:HG22	1:K:169:ILE:O	2.20	0.42
1:K:284:PRO:HD3	1:K:300:ILE:O	2.20	0.42
1:A:40:VAL:HG13	1:A:318:THR:HG21	2.00	0.42
1:G:202:VAL:HG11	1:G:251:LEU:HD13	2.02	0.42
1:I:288:ILE:HD11	1:I:297:ILE:HG13	2.01	0.42
1:C:103:ILE:HG12	1:C:233:TYR:CE2	2.55	0.42
2:D:23:GLY:HA3	2:D:36:ALA:HA	2.01	0.42
2:J:23:GLY:HA3	2:J:36:ALA:HA	2.02	0.42
1:A:180:TRP:HB3	1:A:254:PRO:HG3	2.02	0.41
2:H:88:PHE:CZ	2:J:87:GLY:HA3	2.55	0.41
1:K:89:GLU:O	1:K:269:ILE:HA	2.20	0.41
1:A:52:CYS:HB3	1:A:277:CYS:O	2.20	0.41
2:F:64:THR:HG22	2:F:66:VAL:H	1.85	0.41
1:C:283:THR:HG23	1:C:298:HIS:HB2	2.01	0.41
1:E:134:GLY:HA3	1:E:153:TRP:HB3	2.03	0.41
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.55	0.41
1:G:283:THR:HG21	1:G:297:ILE:HG22	2.03	0.41
1:I:204:VAL:HG22	1:I:245:PHE:CD2	2.56	0.41
1:K:108:LEU:HD13	1:K:234:TRP:CD2	2.56	0.41
1:K:129:ASN:HB3	1:K:162:PRO:HG3	2.01	0.41
1:C:68:GLY:CA	1:C:95:GLY:HA2	2.50	0.41
1:G:53:LYS:HG2	1:G:57:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:SER:HB3	2:D:101:LEU:HD13	2.03	0.41
1:C:321:ARG:HD2	1:C:323:ILE:HD11	2.02	0.41
1:A:284:PRO:HD3	1:A:300:ILE:O	2.20	0.41
1:C:58:PRO:HB2	1:C:88:VAL:HG23	2.03	0.41
1:C:67:ALA:HB2	1:C:105:TYR:CE1	2.56	0.41
3:M:1:NAG:H61	3:M:2:NAG:C7	2.51	0.41
1:C:140:PRO:HD2	4:O:1:NAG:H83	2.03	0.41
2:H:26:HIS:HB2	2:H:149:MET:HE3	2.01	0.41
1:C:42:LEU:HA	1:C:292:LEU:HD22	2.03	0.40
1:E:202:VAL:HB	1:E:213:PHE:HB2	2.03	0.40
1:G:119:GLU:CD	1:G:122:PRO:HA	2.45	0.40
1:E:183:HIS:HB2	1:E:230:MET:HE2	2.03	0.40
1:I:303:GLY:HA2	2:J:63:PHE:CD1	2.56	0.40
2:B:47:GLU:HB3	1:C:30:LEU:HB3	2.03	0.40
2:D:133:ILE:HD11	2:D:137:CYS:HB2	2.02	0.40
2:J:97:GLU:O	2:J:98:LEU:HB2	2.21	0.40
1:A:102:PHE:HA	1:A:232:TYR:HB2	2.03	0.40
1:I:83:SER:O	1:I:116(B):PHE:N	2.54	0.40
1:G:105:TYR:CE2	1:G:109:ARG:HD2	2.56	0.40
1:I:50:LYS:HG2	1:I:275:HIS:ND1	2.36	0.40
1:K:181:GLY:HA2	1:K:231:ASN:O	2.22	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	321/329 (98%)	295 (92%)	18 (6%)	8 (2%)	4	8
1	C	321/329 (98%)	294 (92%)	20 (6%)	7 (2%)	5	10
1	E	321/329 (98%)	292 (91%)	24 (8%)	5 (2%)	7	16
1	G	321/329 (98%)	294 (92%)	18 (6%)	9 (3%)	4	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	321/329 (98%)	293 (91%)	21 (6%)	7 (2%)	5	10
1	K	323/329 (98%)	293 (91%)	26 (8%)	4 (1%)	10	23
2	B	173/177 (98%)	160 (92%)	12 (7%)	1 (1%)	21	42
2	D	169/177 (96%)	149 (88%)	17 (10%)	3 (2%)	6	14
2	F	169/177 (96%)	151 (89%)	15 (9%)	3 (2%)	6	14
2	H	169/177 (96%)	153 (90%)	11 (6%)	5 (3%)	3	6
2	J	170/177 (96%)	161 (95%)	5 (3%)	4 (2%)	4	9
2	L	170/177 (96%)	158 (93%)	11 (6%)	1 (1%)	21	42
All	All	2948/3036 (97%)	2693 (91%)	198 (7%)	57 (2%)	6	13

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	A	92	SER
1	A	170	ASN
1	A	264	ALA
1	C	77	GLU
1	C	264	ALA
1	C	290	THR
1	E	264	ALA
2	F	127	LYS
1	G	264	ALA
2	H	66	VAL
1	I	82	ALA
1	I	92	SER
1	I	198	ALA
1	I	290	THR
2	J	98	LEU
2	J	127	LYS
1	K	82	ALA
1	K	277	CYS
1	A	158	GLY
1	A	169	ILE
1	A	239	PRO
1	C	79	LEU
1	C	92	SER
1	E	170	ASN
1	E	265	GLY

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Mol	Chain	Res	Type
1	G	62	GLY
1	G	78	SER
1	G	81	THR
1	G	93	ASP
1	G	94	ASN
1	G	290	THR
2	H	19	ASP
2	H	61	THR
1	I	197	ASN
1	K	92	SER
2	L	60	ASN
1	A	81	THR
1	C	134	GLY
2	D	60	ASN
2	F	61	THR
1	G	222	LYS
1	I	210	SER
2	B	61	THR
2	D	40	SER
1	E	78	SER
2	F	60	ASN
2	H	60	ASN
2	H	65	ALA
2	J	60	ASN
1	C	82	ALA
2	D	11	GLU
1	I	291	SER
1	E	196	GLN
1	G	158	GLY
1	K	239	PRO
2	J	66	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/289 (98%)	262 (92%)	22 (8%)	12	27
1	C	284/289 (98%)	266 (94%)	18 (6%)	16	36
1	E	284/289 (98%)	262 (92%)	22 (8%)	12	27
1	G	284/289 (98%)	251 (88%)	33 (12%)	5	11
1	I	284/289 (98%)	266 (94%)	18 (6%)	16	36
1	K	285/289 (99%)	269 (94%)	16 (6%)	19	40
2	B	151/152 (99%)	140 (93%)	11 (7%)	13	29
2	D	147/152 (97%)	138 (94%)	9 (6%)	17	37
2	F	147/152 (97%)	135 (92%)	12 (8%)	10	24
2	H	147/152 (97%)	138 (94%)	9 (6%)	17	37
2	J	148/152 (97%)	139 (94%)	9 (6%)	17	37
2	L	148/152 (97%)	135 (91%)	13 (9%)	9	21
All	All	2593/2646 (98%)	2401 (93%)	192 (7%)	13	29

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	21	ASN
1	A	23	THR
1	A	40	VAL
1	A	70	ILE
1	A	79	LEU
1	A	93	ASP
1	A	115	VAL
1	A	119	GLU
1	A	155	VAL
1	A	159	ASN
1	A	164	LEU
1	A	171	ASP
1	A	217	ILE
1	A	225	ASP
1	A	253	VAL
1	A	260	MET
1	A	291	SER
1	A	297	ILE

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Mol	Chain	Res	Type
1	A	304	LYS
1	A	320	LEU
1	A	323	ILE
2	B	22	TYR
2	B	27	GLN
2	B	46	ASP
2	B	64	THR
2	B	68	LYS
2	B	106	ARG
2	B	118	LEU
2	B	147	THR
2	B	150	GLU
2	B	154	ASN
2	B	175	SER
1	C	15	ILE
1	C	22	SER
1	C	70	ILE
1	C	77	GLU
1	C	117	ARG
1	C	132	SER
1	C	155	VAL
1	C	163	LYS
1	C	164	LEU
1	C	169	ILE
1	C	174	LYS
1	C	268	ILE
1	C	270	SER
1	C	288	ILE
1	C	290	THR
1	C	295	GLN
1	C	310	LYS
1	C	320	LEU
2	D	11	GLU
2	D	22	TYR
2	D	34	TYR
2	D	62	GLN
2	D	100	VAL
2	D	102	LEU
2	D	106	ARG
2	D	123	ARG
2	D	135	ASN
1	E	12	THR

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Mol	Chain	Res	Type
1	E	15	ILE
1	E	28	THR
1	E	30	LEU
1	E	55	ARG
1	E	63	LYS
1	E	79	LEU
1	E	91	SER
1	E	93	ASP
1	E	101	ASP
1	E	149	LYS
1	E	155	VAL
1	E	167	SER
1	E	190	ASP
1	E	194	LEU
1	E	212	LYS
1	E	283	THR
1	E	285	LYS
1	E	295	GLN
1	E	309	VAL
1	E	311	SER
1	E	320	LEU
2	F	26	HIS
2	F	27	GLN
2	F	62	GLN
2	F	68	LYS
2	F	82	LYS
2	F	102	LEU
2	F	106	ARG
2	F	124	SER
2	F	127	LYS
2	F	149	MET
2	F	150	GLU
2	F	158	ASP
1	G	15	ILE
1	G	21	ASN
1	G	29	VAL
1	G	46	LYS
1	G	65	ASN
1	G	77	GLU
1	G	79	LEU
1	G	80	SER
1	G	91	SER

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Mol	Chain	Res	Type
1	G	112	LEU
1	G	115	VAL
1	G	136	THR
1	G	155	VAL
1	G	167	SER
1	G	174	LYS
1	G	188	SER
1	G	194	LEU
1	G	216	GLU
1	G	238	GLU
1	G	253	VAL
1	G	261	GLU
1	G	263	ASN
1	G	269	ILE
1	G	272	THR
1	G	274	VAL
1	G	276	ASP
1	G	290	THR
1	G	309	VAL
1	G	310	LYS
1	G	311	SER
1	G	313	LYS
1	G	316	LEU
1	G	320	LEU
2	H	11	GLU
2	H	22	TYR
2	H	68	LYS
2	H	97	GLU
2	H	102	LEU
2	H	133	ILE
2	H	154	ASN
2	H	164	GLU
2	H	168	LEU
1	I	22	SER
1	I	24	ASP
1	I	77	GLU
1	I	115	VAL
1	I	117	ARG
1	I	149	LYS
1	I	163	LYS
1	I	169	ILE
1	I	194	LEU

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Mol	Chain	Res	Type
1	I	243	ILE
1	I	253	VAL
1	I	263	ASN
1	I	274	VAL
1	I	275	HIS
1	I	295	GLN
1	I	310	LYS
1	I	316	LEU
1	I	320	LEU
2	J	11	GLU
2	J	15	THR
2	J	39	LYS
2	J	102	LEU
2	J	106	ARG
2	J	126	LEU
2	J	127	LYS
2	J	133	ILE
2	J	169	ASN
1	K	13	LEU
1	K	21	ASN
1	K	79	LEU
1	K	91	SER
1	K	115	VAL
1	K	117	ARG
1	K	124	THR
1	K	165	SER
1	K	179	LEU
1	K	188	SER
1	K	253	VAL
1	K	267	ILE
1	K	283	THR
1	K	295	GLN
1	K	297	ILE
1	K	313	LYS
2	L	2	LEU
2	L	19	ASP
2	L	57	GLU
2	L	60	ASN
2	L	61	THR
2	L	62	GLN
2	L	68	LYS
2	L	71	ASN

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Mol	Chain	Res	Type
2	L	77	ILE
2	L	108	LEU
2	L	113	SER
2	L	127	LYS
2	L	135	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	129	ASN
1	A	226	GLN
2	B	53	ASN
1	C	41	ASN
1	C	278	ASN
2	D	28	ASN
2	D	128	ASN
2	D	146	ASN
1	E	21	ASN
1	E	141	HIS
2	F	28	ASN
2	F	125	GLN
1	G	41	ASN
1	G	60	HIS
1	G	159	ASN
1	G	196	GLN
2	H	25	HIS
2	H	62	GLN
2	H	79	ASN
2	H	95	ASN
2	H	114	ASN
2	H	169	ASN
1	I	33	ASN
1	I	41	ASN
1	I	111	GLN
1	I	150	ASN
1	I	192	GLN
2	J	25	HIS
2	J	60	ASN
2	J	62	GLN
2	J	95	ASN
2	J	154	ASN

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Mol	Chain	Res	Type
1	K	41	ASN
1	K	278	ASN
2	L	25	HIS
2	L	27	GLN
2	L	43	ASN
2	L	169	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 ⓘ

12 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	M	1	1,3	14,14,15	1.78	2 (14%)	17,19,21	2.35	5 (29%)
3	NAG	M	2	3	14,14,15	1.60	2 (14%)	17,19,21	2.44	5 (29%)
3	BMA	M	3	3	11,11,12	1.79	3 (27%)	15,15,17	1.86	5 (33%)
4	NAG	N	1	4,1	14,14,15	1.91	6 (42%)	17,19,21	2.01	5 (29%)
4	NAG	N	2	4	14,14,15	2.31	3 (21%)	17,19,21	1.51	4 (23%)
4	NAG	O	1	4,1	14,14,15	1.09	1 (7%)	17,19,21	1.24	3 (17%)
4	NAG	O	2	4	14,14,15	1.92	5 (35%)	17,19,21	2.95	6 (35%)
5	NAG	P	1	1,5	14,14,15	1.87	4 (28%)	17,19,21	1.62	3 (17%)
5	NAG	P	2	5	14,14,15	1.24	2 (14%)	17,19,21	2.63	6 (35%)
5	BMA	P	3	5	11,11,12	1.64	4 (36%)	15,15,17	3.15	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	P	4	5	11,11,12	2.56	6 (54%)	15,15,17	2.37	7 (46%)
5	MAN	P	5	5	11,11,12	3.35	5 (45%)	15,15,17	2.27	4 (26%)

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	M	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	3/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
5	MAN	P	4	5	-	1/2/19/22	0/1/1/1
5	MAN	P	5	5	-	0/2/19/22	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	5	MAN	C2-C3	7.70	1.64	1.52
5	P	5	MAN	C1-C2	6.00	1.66	1.52
4	N	2	NAG	C1-C2	5.84	1.60	1.52
3	M	1	NAG	C1-C2	5.08	1.59	1.52
5	P	4	MAN	O2-C2	4.14	1.52	1.43
3	M	2	NAG	C1-C2	4.07	1.57	1.52
4	N	2	NAG	C3-C2	3.73	1.60	1.52
4	O	2	NAG	C4-C5	3.55	1.60	1.53
5	P	4	MAN	C1-C2	3.47	1.60	1.52
5	P	1	NAG	C4-C5	3.43	1.60	1.53
5	P	5	MAN	O2-C2	3.42	1.50	1.43
3	M	3	BMA	C1-C2	3.29	1.60	1.52
4	O	2	NAG	C4-C3	3.25	1.60	1.52
5	P	4	MAN	C2-C3	3.24	1.57	1.52
5	P	1	NAG	C1-C2	3.14	1.56	1.52
5	P	4	MAN	C4-C5	3.13	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	3	BMA	C2-C3	3.13	1.57	1.52
4	N	1	NAG	O5-C1	3.11	1.48	1.43
3	M	1	NAG	O5-C5	3.09	1.49	1.43
5	P	4	MAN	C4-C3	3.02	1.60	1.52
4	O	2	NAG	O5-C1	2.97	1.48	1.43
4	O	2	NAG	O5-C5	2.90	1.49	1.43
4	N	1	NAG	C4-C3	2.80	1.59	1.52
4	N	1	NAG	C4-C5	2.73	1.58	1.53
5	P	3	BMA	C4-C5	2.66	1.58	1.53
4	N	2	NAG	C2-N2	2.63	1.50	1.46
5	P	1	NAG	O5-C5	2.59	1.48	1.43
4	N	1	NAG	O5-C5	2.58	1.48	1.43
4	N	1	NAG	C3-C2	2.50	1.57	1.52
4	O	1	NAG	C1-C2	2.37	1.55	1.52
5	P	2	NAG	C1-C2	2.36	1.55	1.52
5	P	5	MAN	C4-C3	2.33	1.58	1.52
5	P	5	MAN	O3-C3	2.30	1.48	1.43
5	P	3	BMA	O5-C1	2.30	1.47	1.43
5	P	4	MAN	O5-C1	2.28	1.47	1.43
5	P	3	BMA	O4-C4	2.28	1.48	1.43
5	P	1	NAG	C4-C3	2.21	1.58	1.52
3	M	2	NAG	C3-C2	2.15	1.57	1.52
5	P	3	BMA	O2-C2	2.10	1.47	1.43
4	N	1	NAG	C1-C2	2.09	1.55	1.52
4	O	2	NAG	C7-N2	2.08	1.41	1.34
3	M	3	BMA	O2-C2	2.06	1.47	1.43
5	P	2	NAG	O5-C5	2.04	1.47	1.43

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	3	BMA	C1-O5-C5	9.12	124.41	112.19
5	P	2	NAG	C1-O5-C5	8.35	123.37	112.19
3	M	2	NAG	C1-C2-N2	-8.01	97.82	110.43
3	M	1	NAG	C1-O5-C5	7.11	121.72	112.19
4	O	2	NAG	C4-C3-C2	-6.61	101.33	111.02
4	O	2	NAG	C1-O5-C5	6.05	120.29	112.19
4	N	1	NAG	C1-O5-C5	5.91	120.11	112.19
5	P	5	MAN	C1-C2-C3	5.12	117.10	109.64
4	O	2	NAG	O5-C1-C2	4.83	118.77	111.29
5	P	4	MAN	C2-C3-C4	4.42	118.64	110.86
5	P	3	BMA	O2-C2-C3	4.17	118.78	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	3	BMA	O5-C1-C2	3.96	120.24	110.79
4	O	2	NAG	O3-C3-C4	3.93	119.65	110.38
5	P	5	MAN	O3-C3-C2	3.85	117.92	110.05
5	P	1	NAG	C1-C2-N2	3.77	116.38	110.43
5	P	2	NAG	C3-C4-C5	3.47	116.52	110.23
5	P	4	MAN	C1-C2-C3	3.45	114.67	109.64
4	O	2	NAG	C1-C2-N2	3.44	115.86	110.43
3	M	3	BMA	O5-C5-C6	3.42	114.31	107.66
5	P	4	MAN	C3-C4-C5	3.41	116.42	110.23
5	P	5	MAN	O4-C4-C5	3.24	117.30	109.32
4	N	1	NAG	C8-C7-N2	-3.23	110.77	116.12
3	M	3	BMA	O2-C2-C1	3.18	116.49	109.22
4	O	2	NAG	O4-C4-C3	2.94	117.31	110.38
3	M	1	NAG	O4-C4-C3	-2.89	103.57	110.38
5	P	4	MAN	O2-C2-C3	2.85	116.06	110.15
3	M	3	BMA	C3-C4-C5	-2.85	105.06	110.23
5	P	2	NAG	C1-C2-N2	-2.79	106.04	110.43
5	P	4	MAN	O6-C6-C5	-2.71	102.11	111.33
5	P	1	NAG	C4-C3-C2	2.67	114.93	111.02
5	P	2	NAG	C2-N2-C7	2.63	126.42	122.90
5	P	1	NAG	C6-C5-C4	2.61	119.44	113.02
5	P	3	BMA	O2-C2-C1	2.59	115.15	109.22
5	P	5	MAN	O2-C2-C1	2.58	115.12	109.22
4	N	2	NAG	O4-C4-C5	2.56	115.64	109.32
3	M	2	NAG	O5-C1-C2	2.56	115.25	111.29
3	M	2	NAG	O4-C4-C5	2.55	115.61	109.32
4	N	2	NAG	O3-C3-C2	2.53	114.65	109.40
3	M	1	NAG	O3-C3-C4	-2.50	104.47	110.38
3	M	2	NAG	C3-C4-C5	-2.50	105.70	110.23
5	P	3	BMA	C1-C2-C3	-2.49	106.01	109.64
5	P	3	BMA	O6-C6-C5	2.47	119.74	111.33
5	P	4	MAN	O2-C2-C1	2.47	114.87	109.22
3	M	1	NAG	O5-C5-C4	2.47	116.83	110.83
5	P	4	MAN	O5-C1-C2	2.44	116.61	110.79
4	N	1	NAG	O5-C1-C2	2.43	115.06	111.29
5	P	2	NAG	O5-C1-C2	2.43	115.05	111.29
3	M	3	BMA	O4-C4-C5	2.42	115.28	109.32
4	N	1	NAG	O7-C7-N2	2.42	126.25	121.98
3	M	1	NAG	C3-C4-C5	-2.41	105.86	110.23
4	O	1	NAG	C4-C3-C2	2.35	114.47	111.02
3	M	2	NAG	C6-C5-C4	2.30	118.68	113.02
4	N	1	NAG	O5-C5-C4	2.26	116.32	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1	NAG	O3-C3-C4	-2.18	105.23	110.38
4	O	1	NAG	C3-C4-C5	2.18	114.18	110.23
5	P	2	NAG	C4-C3-C2	2.16	114.18	111.02
4	N	2	NAG	C8-C7-N2	-2.12	112.61	116.12
4	N	2	NAG	C3-C4-C5	-2.04	106.53	110.23
5	P	3	BMA	O4-C4-C5	2.01	114.28	109.32
3	M	3	BMA	C6-C5-C4	2.01	117.95	113.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

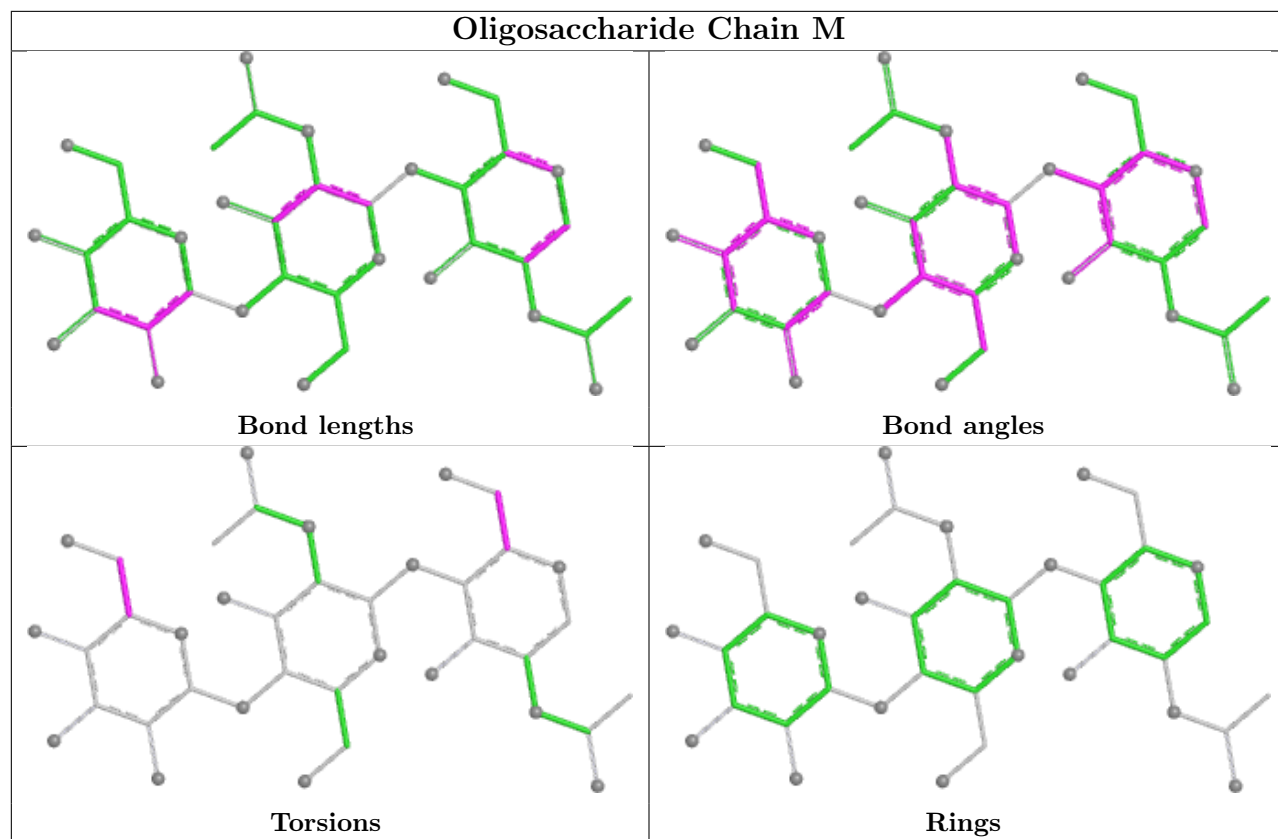
Mol	Chain	Res	Type	Atoms
5	P	3	BMA	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
5	P	4	MAN	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
5	P	3	BMA	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C1-C2-N2-C7

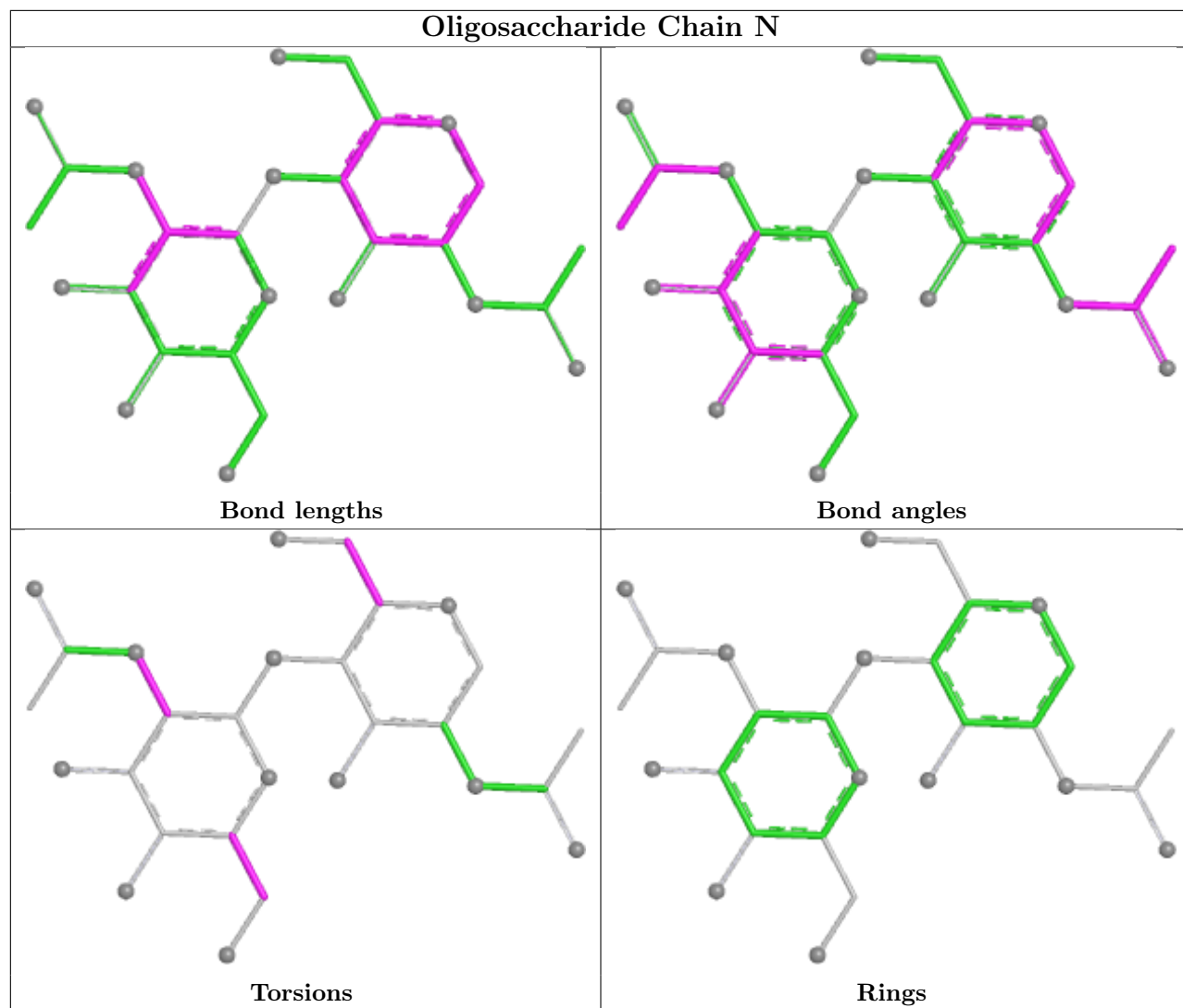
There are no ring outliers.

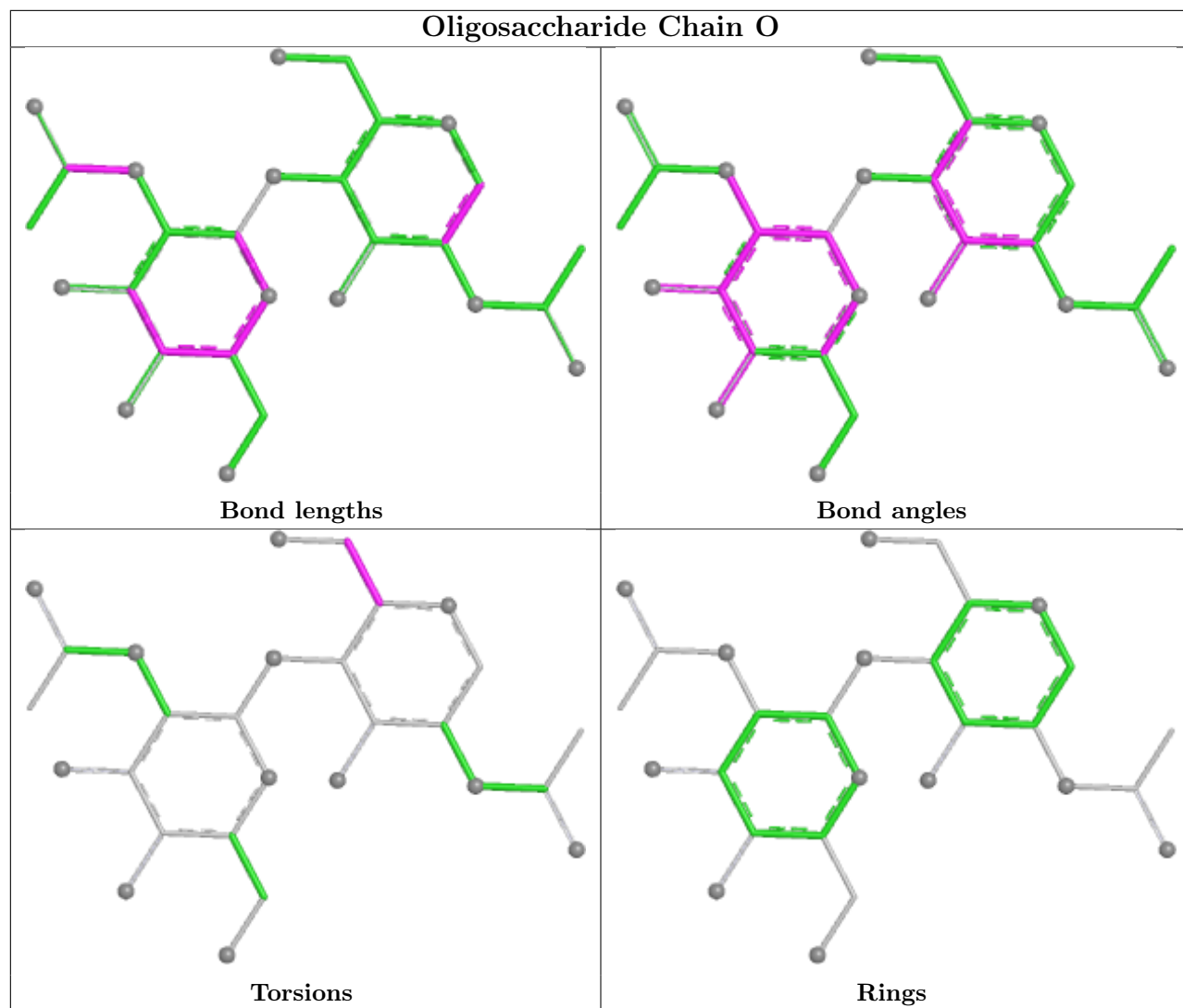
6 monomers are involved in 5 short contacts:

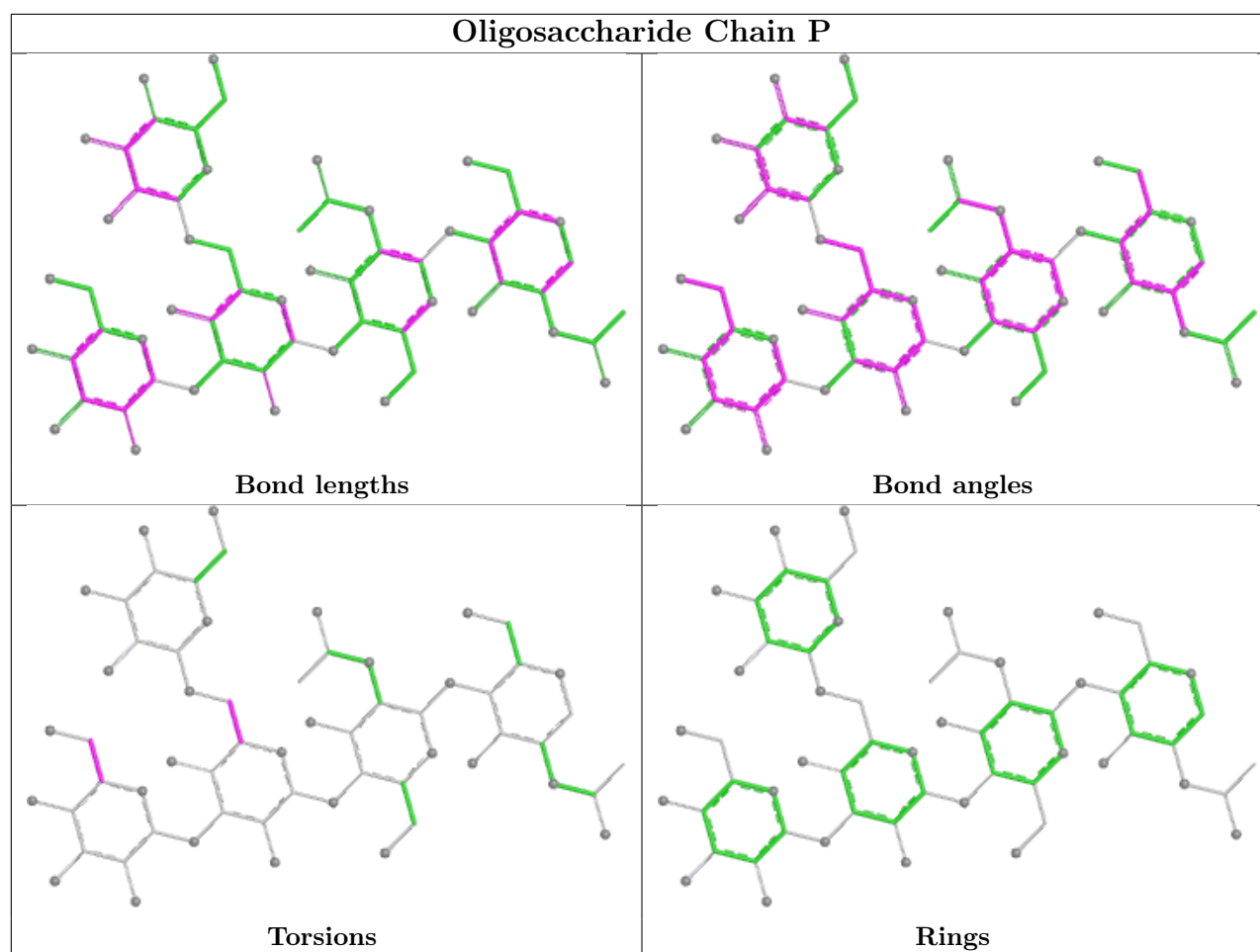
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	2	NAG	1	0
3	M	2	NAG	1	0
5	P	3	BMA	1	0
5	P	5	MAN	1	0
3	M	1	NAG	1	0
4	O	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

2 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	NAG	K	601	1	14,14,15	1.60	4 (28%)	17,19,21	2.66	8 (47%)
6	NAG	E	330	1	14,14,15	1.81	4 (28%)	17,19,21	1.73	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	K	601	1	-	1/6/23/26	0/1/1/1
6	NAG	E	330	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	330	NAG	C1-C2	3.89	1.57	1.52
6	K	601	NAG	C1-C2	3.42	1.57	1.52
6	E	330	NAG	C4-C5	2.90	1.59	1.53
6	K	601	NAG	O5-C5	2.64	1.48	1.43
6	E	330	NAG	O4-C4	2.61	1.49	1.43
6	K	601	NAG	C4-C5	2.30	1.57	1.53
6	K	601	NAG	O5-C1	2.16	1.47	1.43
6	E	330	NAG	O5-C5	2.12	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	601	NAG	C1-C2-N2	5.86	119.67	110.43
6	K	601	NAG	C2-N2-C7	4.56	129.00	122.90
6	K	601	NAG	O3-C3-C2	4.12	117.95	109.40
6	E	330	NAG	C1-O5-C5	3.68	117.12	112.19
6	K	601	NAG	C4-C3-C2	-3.63	105.70	111.02
6	K	601	NAG	C1-O5-C5	3.21	116.49	112.19
6	E	330	NAG	C1-C2-N2	2.97	115.12	110.43
6	E	330	NAG	O5-C5-C6	-2.52	102.75	107.66
6	K	601	NAG	C3-C4-C5	-2.39	105.89	110.23
6	E	330	NAG	C4-C3-C2	2.34	114.45	111.02
6	E	330	NAG	C2-N2-C7	2.25	125.91	122.90
6	K	601	NAG	C8-C7-N2	-2.12	112.60	116.12
6	K	601	NAG	O3-C3-C4	2.05	115.20	110.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	601	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
6	E	330	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	323/329 (98%)	-0.22	1 (0%) 90 88	32, 50, 74, 95	0
1	C	323/329 (98%)	-0.07	2 (0%) 85 83	33, 61, 92, 122	0
1	E	323/329 (98%)	-0.07	4 (1%) 76 73	35, 58, 84, 118	0
1	G	323/329 (98%)	-0.16	2 (0%) 85 83	35, 55, 77, 100	0
1	I	323/329 (98%)	0.03	5 (1%) 72 68	44, 64, 91, 108	0
1	K	325/329 (98%)	0.17	3 (0%) 81 78	52, 74, 99, 133	0
2	B	175/177 (98%)	-0.05	2 (1%) 78 74	37, 63, 85, 100	0
2	D	171/177 (96%)	0.18	3 (1%) 67 63	39, 73, 126, 148	0
2	F	171/177 (96%)	0.09	1 (0%) 85 83	38, 74, 119, 144	0
2	H	171/177 (96%)	0.01	0 100 100	46, 65, 88, 98	0
2	J	172/177 (97%)	0.07	2 (1%) 76 73	45, 72, 109, 120	0
2	L	172/177 (97%)	0.07	0 100 100	47, 63, 83, 103	0
All	All	2972/3036 (97%)	-0.01	25 (0%) 82 80	32, 62, 100, 148	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	81	THR	4.4
2	B	18	VAL	3.6
1	G	94	ASN	3.2
2	F	18	VAL	3.0
2	J	172	GLU	2.8
1	A	79	LEU	2.7
1	K	79	LEU	2.7
1	E	13	LEU	2.7
1	K	78	SER	2.7
2	D	18	VAL	2.6
1	C	277	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	15	ILE	2.5
1	I	82	ALA	2.5
2	J	18	VAL	2.5
1	I	80	SER	2.5
2	B	175	SER	2.5
1	G	93	ASP	2.4
1	E	80	SER	2.4
1	I	134	GLY	2.4
1	C	290	THR	2.3
1	E	325	SER	2.2
2	D	38	LEU	2.2
1	I	76	CYS	2.1
2	D	143	LYS	2.0
1	K	54	LEU	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.

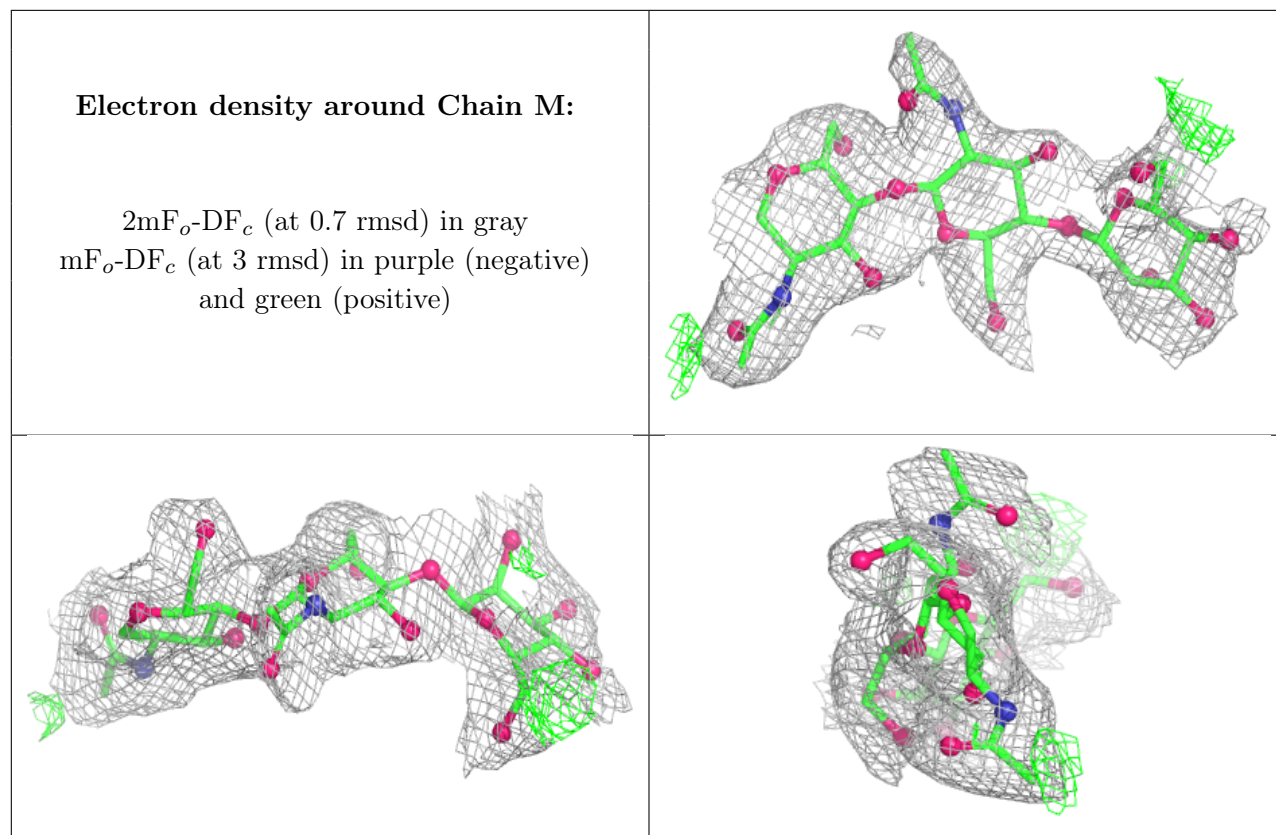
6.3 Carbohydrates [i](#)

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
4	NAG	N	2	14/15	0.52	0.12	94,98,102,103	0
5	MAN	P	5	11/12	0.56	0.17	84,86,88,91	0
3	BMA	M	3	11/12	0.64	0.11	85,88,92,93	0
5	MAN	P	4	11/12	0.66	0.11	81,83,88,89	0
4	NAG	O	2	14/15	0.69	0.13	87,89,96,96	0
5	BMA	P	3	11/12	0.69	0.12	79,82,84,85	0
4	NAG	N	1	14/15	0.77	0.11	84,88,92,93	0
3	NAG	M	2	14/15	0.80	0.11	74,79,82,83	0
5	NAG	P	1	14/15	0.91	0.09	69,72,77,78	0
5	NAG	P	2	14/15	0.92	0.08	71,74,78,81	0
4	NAG	O	1	14/15	0.92	0.09	83,84,87,88	0
3	NAG	M	1	14/15	0.93	0.08	58,62,66,68	0

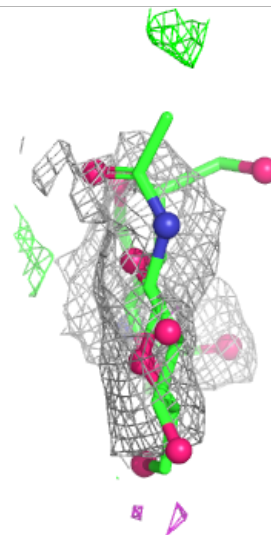
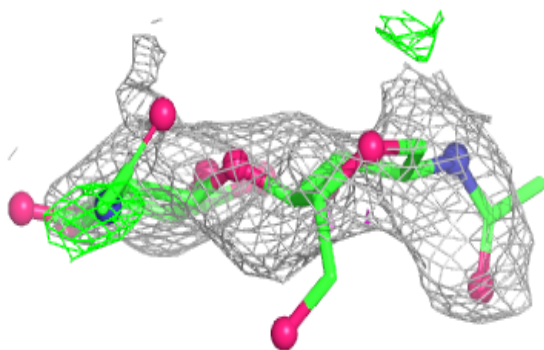
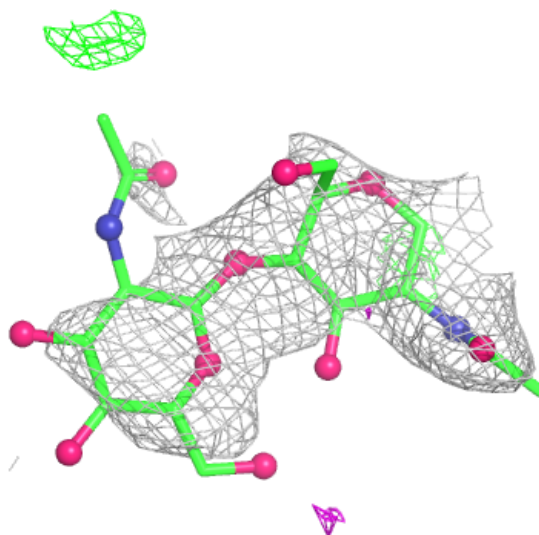
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



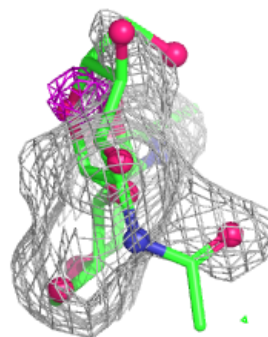
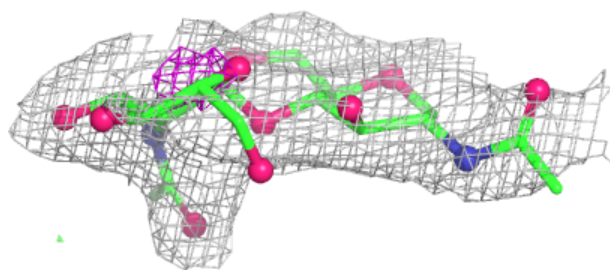
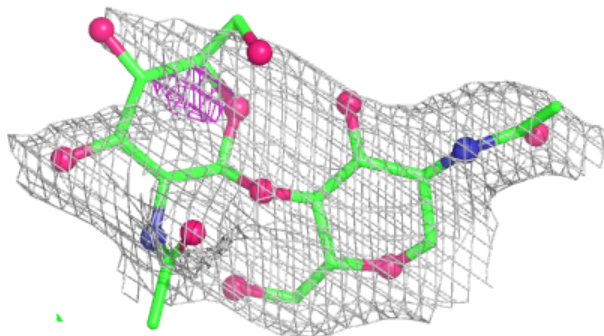
Electron density around Chain N:

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

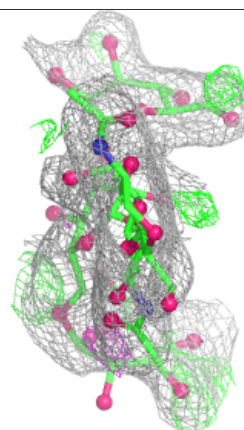
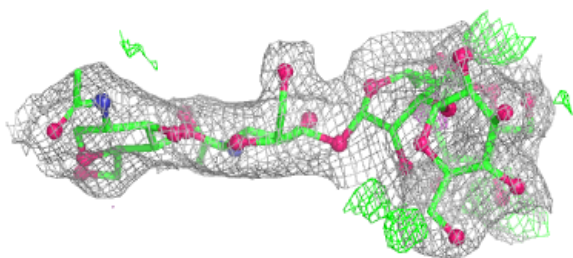
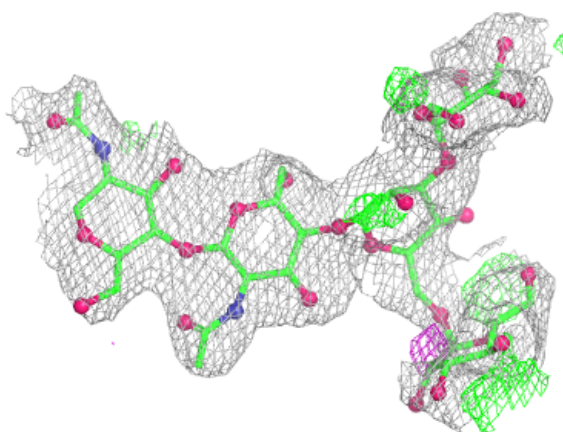


Electron density around Chain O:

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

**Electron density around Chain P:**

$2mF_o-DF_c$ (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
6	NAG	K	601	14/15	0.79	0.14	133,137,144,144	0
6	NAG	E	330	14/15	0.87	0.10	91,95,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.