



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:08 PM UTC

PDB ID : 6V47 / pdb_00006v47
Title : The crystal structure of hemagglutinin from A/duck/Memphis/546/1974 (H11N9)
Authors : Yang, H.; Stevens, J.
Deposited on : 2019-11-27
Resolution : 2.80 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:

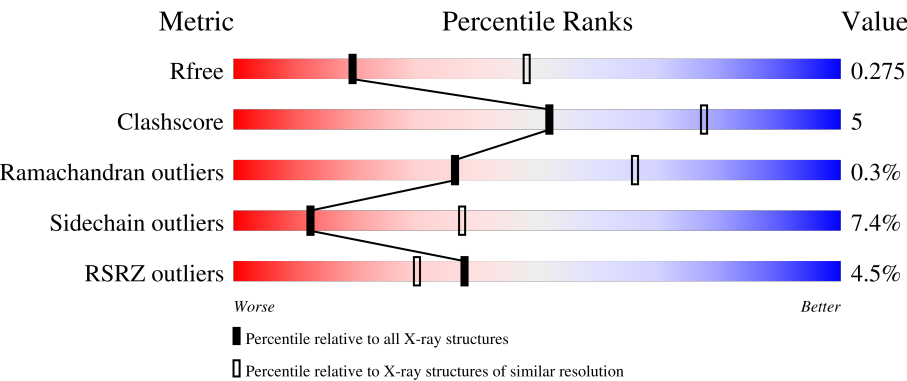
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	326	
1	C	326	
1	E	326	
2	B	181	
2	D	181	

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Mol	Chain	Length	Quality of chain
2	F	181	6% 71% 18% 8%
3	G	2	50% 50%
3	H	2	50% 50%
3	I	2	50% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11712 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2513	1588	430	482	13			
1	C	321	Total	C	N	O	S	0	0	0
			2513	1588	430	482	13			
1	E	321	Total	C	N	O	S	0	0	0
			2513	1588	430	482	13			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1363	839	244	275	5			
2	D	167	Total	C	N	O	S	0	0	0
			1363	839	244	275	5			
2	F	167	Total	C	N	O	S	0	0	0
			1363	839	244	275	5			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A2V851
B	176	GLY	-	expression tag	UNP A2V851
B	177	ARG	-	expression tag	UNP A2V851
B	178	LEU	-	expression tag	UNP A2V851
B	179	VAL	-	expression tag	UNP A2V851
B	180	PRO	-	expression tag	UNP A2V851
B	181	ARG	-	expression tag	UNP A2V851
D	175	SER	-	expression tag	UNP A2V851
D	176	GLY	-	expression tag	UNP A2V851
D	177	ARG	-	expression tag	UNP A2V851
D	178	LEU	-	expression tag	UNP A2V851
D	179	VAL	-	expression tag	UNP A2V851

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Chain	Residue	Modelled	Actual	Comment	Reference
D	180	PRO	-	expression tag	UNP A2V851
D	181	ARG	-	expression tag	UNP A2V851
F	175	SER	-	expression tag	UNP A2V851
F	176	GLY	-	expression tag	UNP A2V851
F	177	ARG	-	expression tag	UNP A2V851
F	178	LEU	-	expression tag	UNP A2V851
F	179	VAL	-	expression tag	UNP A2V851
F	180	PRO	-	expression tag	UNP A2V851
F	181	ARG	-	expression tag	UNP A2V851

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

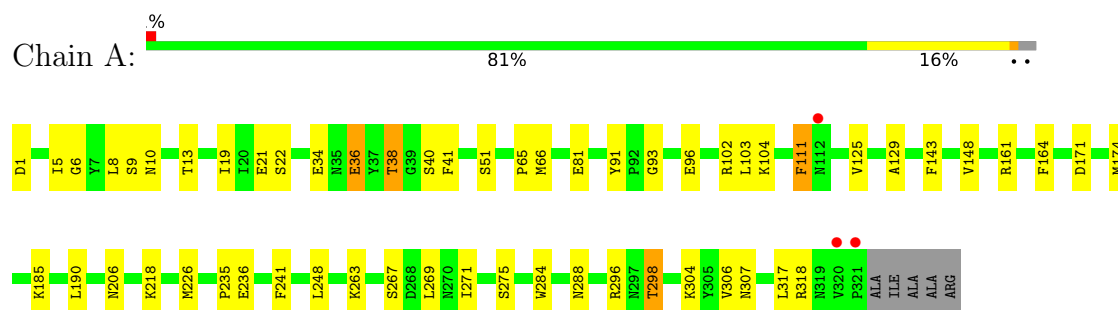


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

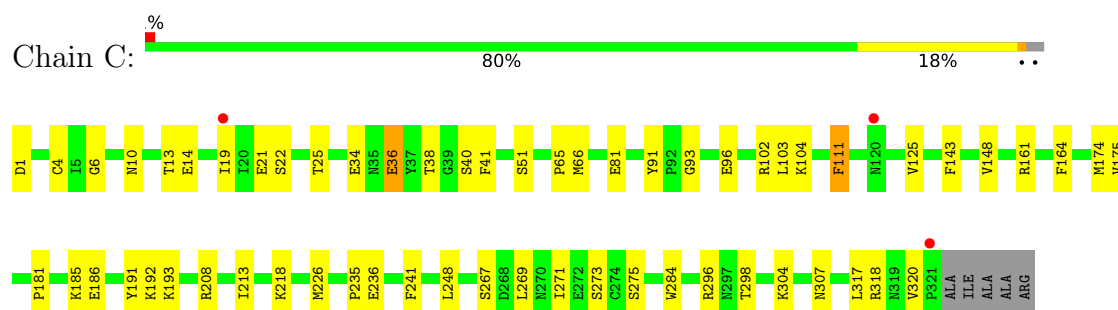
3 Residue-property plots

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.

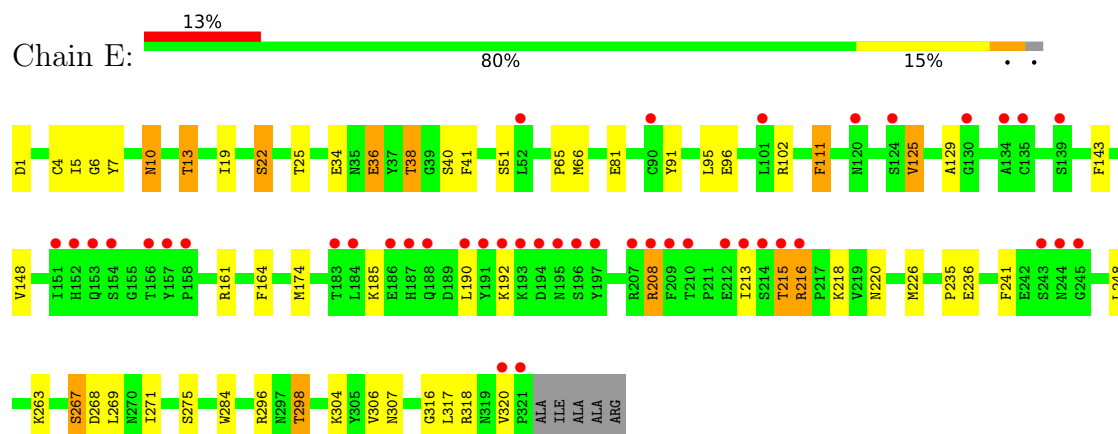
- Molecule 1: Hemagglutinin HA1 chain



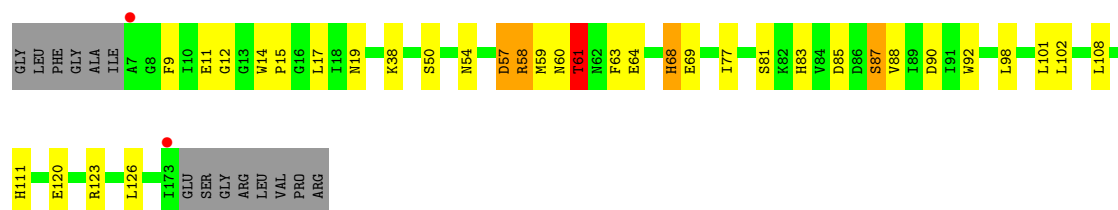
- Molecule 1: Hemagglutinin HA1 chain



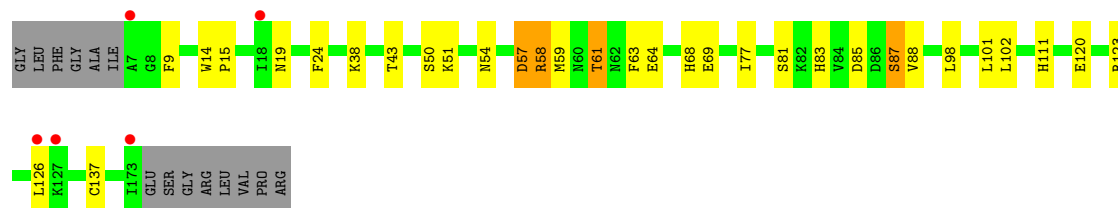
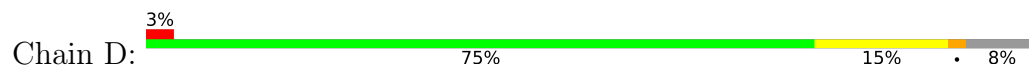
- Molecule 1: Hemagglutinin HA1 chain



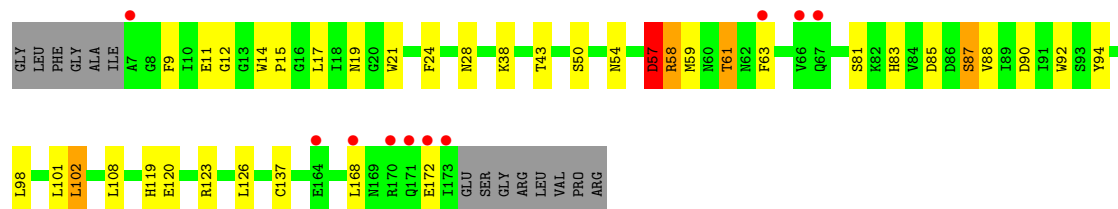
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



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



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



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

Chain I:

50%

50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.12Å 121.15Å 217.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.80 49.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.3 (49.21-2.80) 89.3 (49.21-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.234 , 0.278 0.235 , 0.275	Depositor DCC
R_{free} test set	2370 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 16.3	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	0.91	EDS
Total number of atoms	11712	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: 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	1.06	1/2573 (0.0%)	1.43	8/3489 (0.2%)
1	C	1.07	1/2573 (0.0%)	1.43	10/3489 (0.3%)
1	E	1.09	2/2573 (0.1%)	1.51	17/3489 (0.5%)
2	B	1.10	2/1387 (0.1%)	1.54	5/1868 (0.3%)
2	D	1.08	0/1387	1.53	4/1868 (0.2%)
2	F	1.09	1/1387 (0.1%)	1.56	4/1868 (0.2%)
All	All	1.08	7/11880 (0.1%)	1.49	48/16071 (0.3%)

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	E	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	12	GLY	C-O	6.66	1.29	1.23
2	B	68	HIS	CE1-NE2	6.27	1.38	1.32
2	B	12	GLY	C-O	6.09	1.28	1.23
1	E	220	ASN	C-O	5.27	1.31	1.23
1	A	129	ALA	C-O	5.05	1.30	1.23
1	E	129	ALA	C-O	5.03	1.30	1.23
1	C	181	PRO	C-O	-5.01	1.17	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	15	PRO	N-CA-C	-8.25	98.34	110.80
2	B	15	PRO	N-CA-C	-7.71	99.16	110.80
1	E	267	SER	CA-C-N	7.46	131.02	120.28
1	E	267	SER	C-N-CA	7.46	131.02	120.28
1	A	307	ASN	CB-CA-C	-7.36	98.57	110.79
1	A	1	ASP	CA-CB-CG	7.03	119.63	112.60
2	D	15	PRO	N-CA-C	-6.86	100.47	111.03
2	D	61	THR	CB-CA-C	6.71	120.36	109.90
1	E	307	ASN	CB-CA-C	-6.66	99.36	110.68
2	F	61	THR	CB-CA-C	6.61	120.22	109.90
2	B	61	THR	CB-CA-C	6.49	120.74	109.65
1	E	268	ASP	CB-CA-C	-6.28	99.01	110.63
1	E	208	ARG	CB-CA-C	6.17	119.85	109.48
1	E	306	VAL	CA-C-N	6.13	128.78	120.38
1	E	306	VAL	C-N-CA	6.13	128.78	120.38
1	E	215	THR	N-CA-CB	6.08	119.66	109.94
2	B	90	ASP	CA-CB-CG	6.06	118.66	112.60
1	C	307	ASN	CB-CA-C	-6.01	100.46	110.68
2	F	57	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	1	ASP	CA-CB-CG	5.78	118.38	112.60
1	E	213	ILE	CB-CA-C	5.78	119.54	111.34
1	E	38	THR	CA-CB-OG1	-5.61	101.19	109.60
1	A	306	VAL	CA-C-N	5.56	127.73	120.28
1	A	306	VAL	C-N-CA	5.56	127.73	120.28
1	E	125	VAL	CA-C-O	-5.53	116.31	120.96
1	E	95	LEU	CA-C-O	-5.52	114.80	120.54
1	E	10	ASN	CA-C-N	5.51	128.42	120.38
1	E	10	ASN	C-N-CA	5.51	128.42	120.38
2	D	64	GLU	CA-C-N	5.50	128.58	120.82
2	D	64	GLU	C-N-CA	5.50	128.58	120.82
1	E	13	THR	CB-CA-C	5.49	119.54	109.99
2	F	90	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	36	GLU	CB-CA-C	5.39	118.53	109.48
1	E	316	GLY	CA-C-O	-5.31	116.34	121.92
1	A	36	GLU	CB-CA-C	5.29	118.37	109.48
1	E	36	GLU	CB-CA-C	5.28	118.35	109.48
1	C	13	THR	CB-CA-C	5.18	119.00	109.99
1	C	175	VAL	O-C-N	5.18	128.54	123.00
1	C	193	LYS	CA-C-O	-5.15	115.50	121.26
2	B	64	GLU	CA-C-N	5.14	128.07	120.82
2	B	64	GLU	C-N-CA	5.14	128.07	120.82
1	A	288	ASN	N-CA-C	-5.11	107.05	113.28
1	C	273	SER	CA-C-N	5.06	130.18	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	SER	C-N-CA	5.06	130.18	121.87
1	A	171	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	186	GLU	N-CA-C	-5.06	105.89	111.71
1	C	208	ARG	CB-CA-C	5.05	117.96	109.48
1	A	38	THR	CA-CB-OG1	-5.03	102.06	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	216	ARG	Peptide

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	2513	0	2431	34	0
1	C	2513	0	2431	28	0
1	E	2513	0	2431	29	0
2	B	1363	0	1272	19	0
2	D	1363	0	1272	16	0
2	F	1363	0	1272	20	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	1	0
All	All	11712	0	11184	117	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 (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HD3	2:B:69:GLU:HG3	1.62	0.81
2:B:54:ASN:O	2:B:59:MET:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:OE2	1:C:102:ARG:NH2	2.23	0.72
1:A:81:GLU:OE2	1:A:102:ARG:NH2	2.23	0.71
1:A:206:ASN:OD1	1:E:216:ARG:NH2	2.20	0.70
1:E:81:GLU:OE2	1:E:102:ARG:NH2	2.25	0.69
1:A:271:ILE:HD12	1:A:271:ILE:H	1.60	0.66
1:C:102:ARG:HD3	2:D:69:GLU:HG3	1.75	0.66
2:D:57:ASP:O	2:D:58:ARG:HB3	1.97	0.65
2:F:57:ASP:O	2:F:58:ARG:HB3	1.97	0.64
1:A:206:ASN:CG	1:E:216:ARG:HH21	2.06	0.63
2:B:57:ASP:O	2:B:58:ARG:HB3	1.98	0.62
1:E:164:PHE:CD2	1:E:174:MET:HE1	2.34	0.62
2:D:98:LEU:HG	2:D:102:LEU:HD13	1.82	0.60
2:F:168:LEU:O	2:F:172:GLU:HG2	2.02	0.59
1:A:22:SER:HB3	3:G:1:NAG:H82	1.85	0.59
2:D:120:GLU:HG2	2:D:123:ARG:NH1	2.18	0.58
1:E:235:PRO:O	1:E:236:GLU:HB2	2.01	0.58
2:F:120:GLU:HG2	2:F:123:ARG:NH1	2.20	0.56
1:E:22:SER:HB3	3:I:1:NAG:H82	1.87	0.56
1:E:1:ASP:OD2	2:F:28:ASN:HA	2.04	0.56
1:A:304:LYS:HD3	2:B:60:ASN:HD21	1.70	0.56
2:F:63:PHE:CE1	2:F:88:VAL:HG11	2.42	0.54
2:B:120:GLU:HG2	2:B:123:ARG:NH1	2.21	0.54
1:A:304:LYS:HD3	2:B:60:ASN:ND2	2.22	0.53
2:D:54:ASN:O	2:D:59:MET:HB2	2.09	0.53
1:E:5:ILE:O	2:F:9:PHE:HB3	2.09	0.53
2:F:9:PHE:C	2:F:9:PHE:CD1	2.87	0.53
1:A:304:LYS:HE2	2:B:92:TRP:HB3	1.90	0.53
1:C:317:LEU:HG	2:D:111:HIS:CG	2.45	0.52
2:F:54:ASN:O	2:F:59:MET:HB2	2.09	0.52
2:B:9:PHE:C	2:B:9:PHE:CD1	2.87	0.52
2:D:83:HIS:O	2:D:87:SER:OG	2.27	0.52
1:E:65:PRO:HG3	1:E:143:PHE:O	2.10	0.52
1:A:65:PRO:HG3	1:A:143:PHE:O	2.11	0.51
1:C:19:ILE:H	1:C:19:ILE:HD12	1.76	0.51
1:C:213:ILE:O	1:E:208:ARG:NH2	2.39	0.51
2:D:9:PHE:CD1	2:D:9:PHE:C	2.88	0.51
2:F:83:HIS:O	2:F:87:SER:OG	2.28	0.51
1:E:304:LYS:HE3	2:F:92:TRP:HB3	1.92	0.51
1:C:91:TYR:CD2	1:C:226:MET:HG3	2.46	0.51
2:B:63:PHE:CE1	2:B:88:VAL:HG11	2.46	0.50
2:B:98:LEU:HG	2:B:102:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLY:HA3	1:C:226:MET:O	2.11	0.50
1:C:65:PRO:HG3	1:C:143:PHE:O	2.12	0.50
2:B:83:HIS:O	2:B:87:SER:OG	2.29	0.50
1:A:317:LEU:HD12	1:A:317:LEU:N	2.27	0.50
2:D:63:PHE:CE1	2:D:88:VAL:HG11	2.46	0.50
1:A:51:SER:HB2	1:A:271:ILE:CD1	2.43	0.48
1:A:103:LEU:HD13	2:B:68:HIS:CE1	2.49	0.48
1:A:51:SER:HB2	1:A:271:ILE:HD11	1.95	0.48
1:E:51:SER:HB2	1:E:271:ILE:HD13	1.95	0.48
1:A:6:GLY:HA3	2:B:14:TRP:CH2	2.48	0.48
1:C:317:LEU:HD12	1:C:317:LEU:N	2.28	0.48
1:A:19:ILE:HD12	1:A:19:ILE:H	1.79	0.47
1:E:304:LYS:CE	2:F:92:TRP:HB3	2.44	0.47
1:E:111:PHE:HD2	1:E:111:PHE:C	2.22	0.47
1:E:317:LEU:HD12	1:E:317:LEU:N	2.29	0.47
1:A:317:LEU:HG	2:B:111:HIS:CG	2.48	0.47
1:C:51:SER:HB2	1:C:271:ILE:HD13	1.96	0.46
1:A:8:LEU:HD12	2:B:17:LEU:HB3	1.96	0.46
1:A:161:ARG:HA	1:A:241:PHE:O	2.15	0.46
1:C:161:ARG:HA	1:C:241:PHE:O	2.15	0.46
1:C:235:PRO:O	1:C:236:GLU:HB2	2.15	0.46
1:A:5:ILE:O	2:B:9:PHE:HB3	2.15	0.46
2:B:98:LEU:HG	2:B:102:LEU:CD1	2.46	0.46
1:E:6:GLY:HA3	2:F:14:TRP:CH2	2.50	0.46
1:A:235:PRO:O	1:A:236:GLU:HB2	2.16	0.46
1:C:103:LEU:HD13	2:D:68:HIS:CE1	2.51	0.46
1:A:271:ILE:HD12	1:A:271:ILE:N	2.28	0.45
1:C:38:THR:HB	1:C:284:TRP:NE1	2.32	0.45
1:E:34:GLU:OE1	1:E:36:GLU:HG2	2.17	0.45
1:E:6:GLY:HA3	2:F:14:TRP:CZ3	2.52	0.45
1:E:111:PHE:C	1:E:111:PHE:CD2	2.94	0.45
1:A:21:GLU:OE2	1:A:318:ARG:NH1	2.50	0.45
1:E:19:ILE:HD12	1:E:19:ILE:H	1.80	0.45
1:E:161:ARG:HA	1:E:241:PHE:O	2.16	0.45
1:C:164:PHE:CD2	1:C:174:MET:HE1	2.52	0.45
1:E:7:TYR:HA	2:F:21:TRP:O	2.17	0.45
1:A:38:THR:HB	1:A:284:TRP:CE2	2.53	0.44
1:C:111:PHE:HD2	1:C:111:PHE:C	2.26	0.44
1:A:91:TYR:CD2	1:A:226:MET:HG3	2.53	0.44
1:C:4:CYS:HA	2:D:137:CYS:HA	1.98	0.44
1:E:4:CYS:HA	2:F:137:CYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:LEU:HG	2:F:102:LEU:HD13	1.99	0.44
2:B:61:THR:HG21	2:F:94:TYR:HB2	1.98	0.44
1:C:38:THR:HB	1:C:284:TRP:CE2	2.52	0.44
1:C:41:PHE:CE2	1:C:269:LEU:HB2	2.53	0.44
1:A:38:THR:HB	1:A:284:TRP:NE1	2.33	0.43
2:D:98:LEU:HG	2:D:102:LEU:CD1	2.48	0.43
1:C:6:GLY:HA2	2:D:9:PHE:HB3	1.99	0.43
2:B:77:ILE:HD12	2:B:77:ILE:H	1.84	0.43
2:D:77:ILE:H	2:D:77:ILE:HD12	1.84	0.43
1:A:164:PHE:CD2	1:A:174:MET:HE1	2.53	0.43
1:C:25:THR:O	1:C:318:ARG:O	2.36	0.43
1:E:5:ILE:HG13	2:F:119:HIS:HA	2.00	0.43
1:E:263:LYS:HE2	1:E:298:THR:O	2.19	0.43
2:F:17:LEU:HD12	2:F:17:LEU:HA	1.91	0.43
1:A:263:LYS:HE2	1:A:298:THR:O	2.18	0.43
1:C:34:GLU:OE1	1:C:36:GLU:HG2	2.19	0.42
1:C:111:PHE:C	1:C:111:PHE:CD2	2.97	0.42
1:A:111:PHE:CD2	1:A:111:PHE:C	2.98	0.42
1:A:111:PHE:C	1:A:111:PHE:HD2	2.27	0.42
1:C:191:TYR:O	1:C:192:LYS:C	2.63	0.42
1:E:91:TYR:CD2	1:E:226:MET:HG3	2.55	0.41
1:A:41:PHE:CE2	1:A:269:LEU:HB2	2.55	0.41
1:C:271:ILE:H	1:C:271:ILE:HD12	1.84	0.41
2:F:98:LEU:HG	2:F:102:LEU:CD1	2.51	0.41
1:E:41:PHE:CE2	1:E:269:LEU:HB2	2.56	0.41
1:A:19:ILE:HG22	2:D:51:LYS:HA	2.01	0.41
1:C:6:GLY:HA3	2:D:14:TRP:CH2	2.55	0.41
1:E:38:THR:HB	1:E:284:TRP:NE1	2.36	0.41
1:A:34:GLU:OE1	1:A:36:GLU:HG2	2.20	0.41
1:C:21:GLU:OE2	1:C:318:ARG:NH1	2.54	0.41
1:A:93:GLY:HA3	1:A:226:MET:O	2.21	0.40
1:C:271:ILE:HD12	1:C:271:ILE:N	2.36	0.40
1:E:25:THR:O	1:E:318:ARG:O	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/326 (98%)	298 (93%)	21 (7%)	0	100	100
1	C	319/326 (98%)	296 (93%)	23 (7%)	0	100	100
1	E	319/326 (98%)	297 (93%)	21 (7%)	1 (0%)	36	66
2	B	165/181 (91%)	156 (94%)	8 (5%)	1 (1%)	21	51
2	D	165/181 (91%)	156 (94%)	8 (5%)	1 (1%)	21	51
2	F	165/181 (91%)	155 (94%)	9 (6%)	1 (1%)	21	51
All	All	1452/1521 (96%)	1358 (94%)	90 (6%)	4 (0%)	36	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	58	ARG
2	B	58	ARG
2	D	58	ARG
1	E	192	LYS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/282 (99%)	262 (94%)	18 (6%)	16	44
1	C	280/282 (99%)	261 (93%)	19 (7%)	14	42
1	E	280/282 (99%)	261 (93%)	19 (7%)	14	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	149/160 (93%)	137 (92%)	12 (8%)	11	33
2	D	149/160 (93%)	137 (92%)	12 (8%)	11	33
2	F	149/160 (93%)	134 (90%)	15 (10%)	7	23
All	All	1287/1326 (97%)	1192 (93%)	95 (7%)	13	37

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	10	ASN
1	A	13	THR
1	A	40	SER
1	A	66	MET
1	A	96	GLU
1	A	104	LYS
1	A	111	PHE
1	A	125	VAL
1	A	148	VAL
1	A	185	LYS
1	A	190	LEU
1	A	218	LYS
1	A	248	LEU
1	A	267	SER
1	A	275	SER
1	A	296	ARG
1	A	298	THR
2	B	11	GLU
2	B	19	ASN
2	B	38	LYS
2	B	50	SER
2	B	57	ASP
2	B	61	THR
2	B	81	SER
2	B	85	ASP
2	B	87	SER
2	B	101	LEU
2	B	108	LEU
2	B	126	LEU
1	C	10	ASN
1	C	14	GLU
1	C	22	SER

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Mol	Chain	Res	Type
1	C	40	SER
1	C	66	MET
1	C	96	GLU
1	C	104	LYS
1	C	111	PHE
1	C	125	VAL
1	C	148	VAL
1	C	185	LYS
1	C	218	LYS
1	C	248	LEU
1	C	267	SER
1	C	275	SER
1	C	296	ARG
1	C	298	THR
1	C	304	LYS
1	C	320	VAL
2	D	19	ASN
2	D	24	PHE
2	D	38	LYS
2	D	43	THR
2	D	50	SER
2	D	57	ASP
2	D	61	THR
2	D	81	SER
2	D	85	ASP
2	D	87	SER
2	D	101	LEU
2	D	126	LEU
1	E	10	ASN
1	E	13	THR
1	E	22	SER
1	E	40	SER
1	E	66	MET
1	E	96	GLU
1	E	111	PHE
1	E	125	VAL
1	E	148	VAL
1	E	185	LYS
1	E	190	LEU
1	E	215	THR
1	E	218	LYS
1	E	248	LEU

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Mol	Chain	Res	Type
1	E	267	SER
1	E	275	SER
1	E	296	ARG
1	E	298	THR
1	E	320	VAL
2	F	11	GLU
2	F	19	ASN
2	F	24	PHE
2	F	38	LYS
2	F	43	THR
2	F	50	SER
2	F	57	ASP
2	F	61	THR
2	F	81	SER
2	F	85	ASP
2	F	87	SER
2	F	101	LEU
2	F	102	LEU
2	F	108	LEU
2	F	126	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
2	B	19	ASN
2	B	47	GLN
2	B	60	ASN
2	B	67	GLN
1	C	307	ASN
2	D	25	GLN
2	D	60	ASN
2	D	67	GLN
2	D	68	HIS
2	D	83	HIS
2	D	97	GLN
1	E	307	ASN
2	F	47	GLN
2	F	60	ASN
2	F	159	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	G	1	3,1	14,14,15	1.05	1 (7%)	17,19,21	2.47	4 (23%)
3	NAG	G	2	3	14,14,15	1.19	1 (7%)	17,19,21	1.74	7 (41%)
3	NAG	H	1	3,1	14,14,15	0.69	0	17,19,21	1.35	0
3	NAG	H	2	3	14,14,15	1.08	0	17,19,21	2.36	5 (29%)
3	NAG	I	1	3,1	14,14,15	2.33	6 (42%)	17,19,21	2.54	7 (41%)
3	NAG	I	2	3	14,14,15	1.56	3 (21%)	17,19,21	2.11	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
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	C4-C5	5.01	1.63	1.53
3	I	1	NAG	C1-C2	3.59	1.57	1.52
3	I	2	NAG	C3-C2	3.28	1.59	1.52
3	I	1	NAG	O4-C4	2.90	1.50	1.43
3	I	1	NAG	C6-C5	2.68	1.60	1.51
3	G	2	NAG	C1-C2	2.66	1.56	1.52
3	I	1	NAG	O3-C3	2.39	1.48	1.43
3	I	2	NAG	C1-C2	2.36	1.55	1.52
3	I	1	NAG	C4-C3	2.30	1.58	1.52
3	I	2	NAG	O4-C4	2.27	1.48	1.43
3	G	1	NAG	C4-C5	2.20	1.57	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	7.36	122.05	112.19
3	I	1	NAG	C1-O5-C5	5.58	119.66	112.19
3	H	2	NAG	C4-C3-C2	4.57	117.72	111.02
3	H	2	NAG	C2-N2-C7	4.46	128.87	122.90
3	H	2	NAG	O5-C5-C6	4.37	116.16	107.66
3	I	1	NAG	O4-C4-C5	4.29	119.90	109.32
3	I	1	NAG	C6-C5-C4	3.98	122.80	113.02
3	I	2	NAG	C2-N2-C7	3.98	128.24	122.90
3	I	2	NAG	O3-C3-C2	3.57	116.82	109.40
3	H	2	NAG	C3-C4-C5	3.44	116.47	110.23
3	I	2	NAG	O5-C5-C6	3.43	114.34	107.66
3	I	2	NAG	O4-C4-C5	3.39	117.66	109.32
3	I	2	NAG	C3-C4-C5	-3.35	104.16	110.23
3	G	1	NAG	O5-C1-C2	3.21	116.26	111.29
3	G	2	NAG	O4-C4-C5	3.12	117.01	109.32
3	G	2	NAG	O3-C3-C2	3.07	115.78	109.40
3	G	1	NAG	C1-C2-N2	-3.01	105.69	110.43
3	I	1	NAG	O6-C6-C5	2.94	121.35	111.33
3	I	1	NAG	C1-C2-N2	2.92	115.03	110.43
3	G	1	NAG	C6-C5-C4	2.76	119.80	113.02
3	H	2	NAG	C6-C5-C4	-2.64	106.55	113.02
3	I	1	NAG	O3-C3-C4	2.51	116.28	110.38
3	G	2	NAG	C2-N2-C7	2.50	126.26	122.90
3	G	2	NAG	O5-C5-C4	-2.47	104.81	110.83
3	I	1	NAG	C4-C3-C2	-2.47	107.40	111.02
3	G	2	NAG	C3-C4-C5	-2.14	106.35	110.23
3	G	2	NAG	O5-C1-C2	2.10	114.54	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	O5-C5-C6	2.08	111.70	107.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

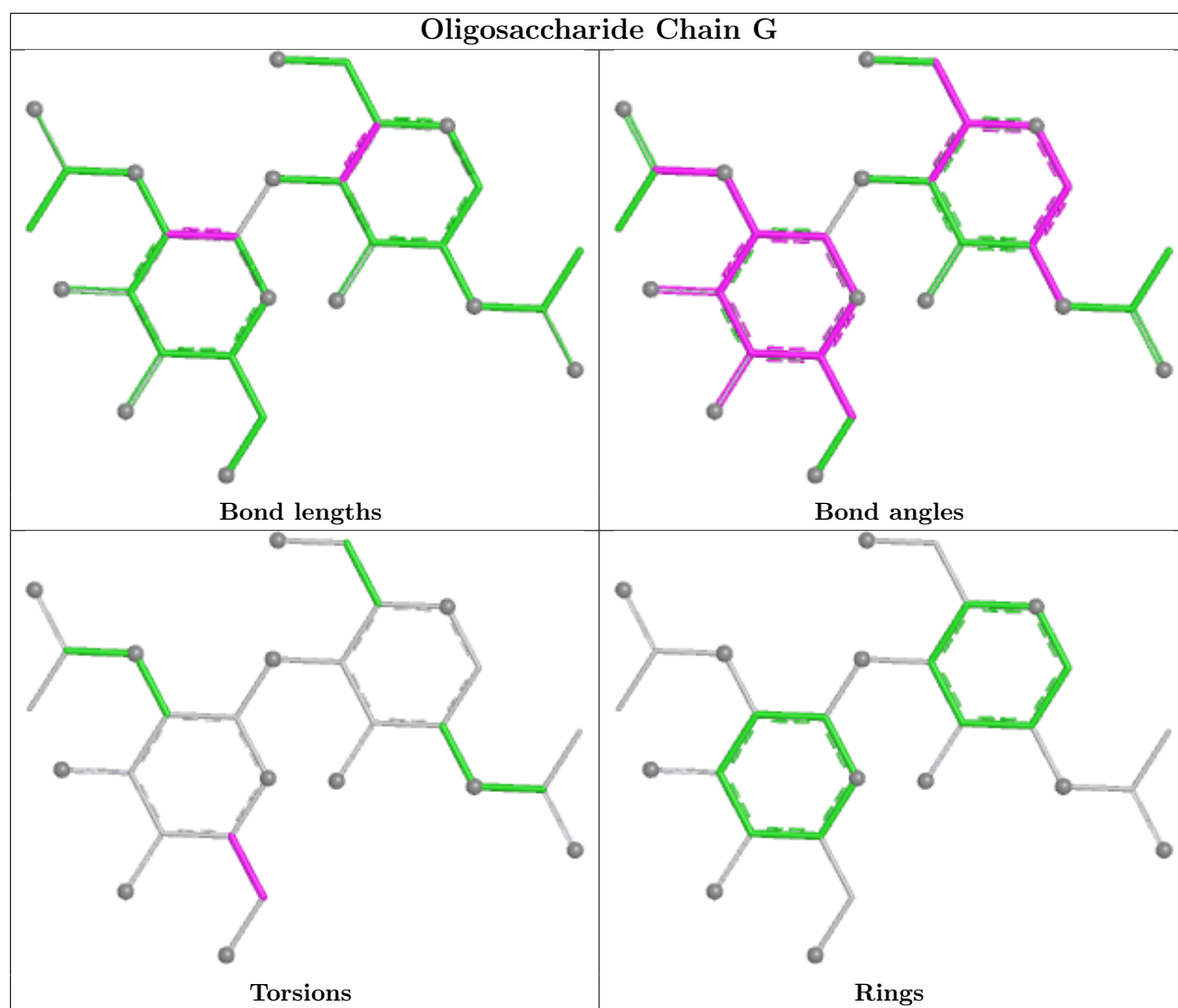
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

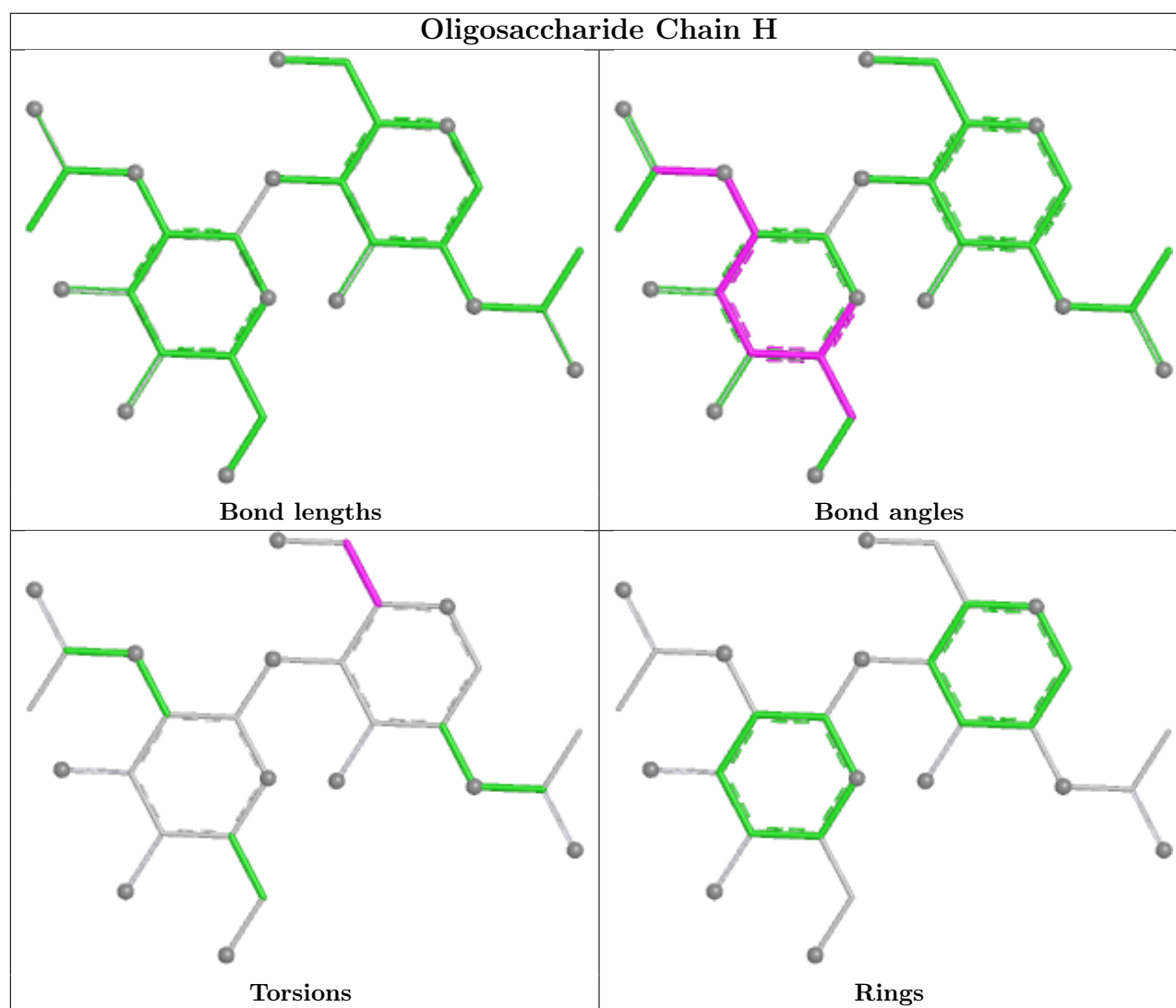
There are no ring outliers.

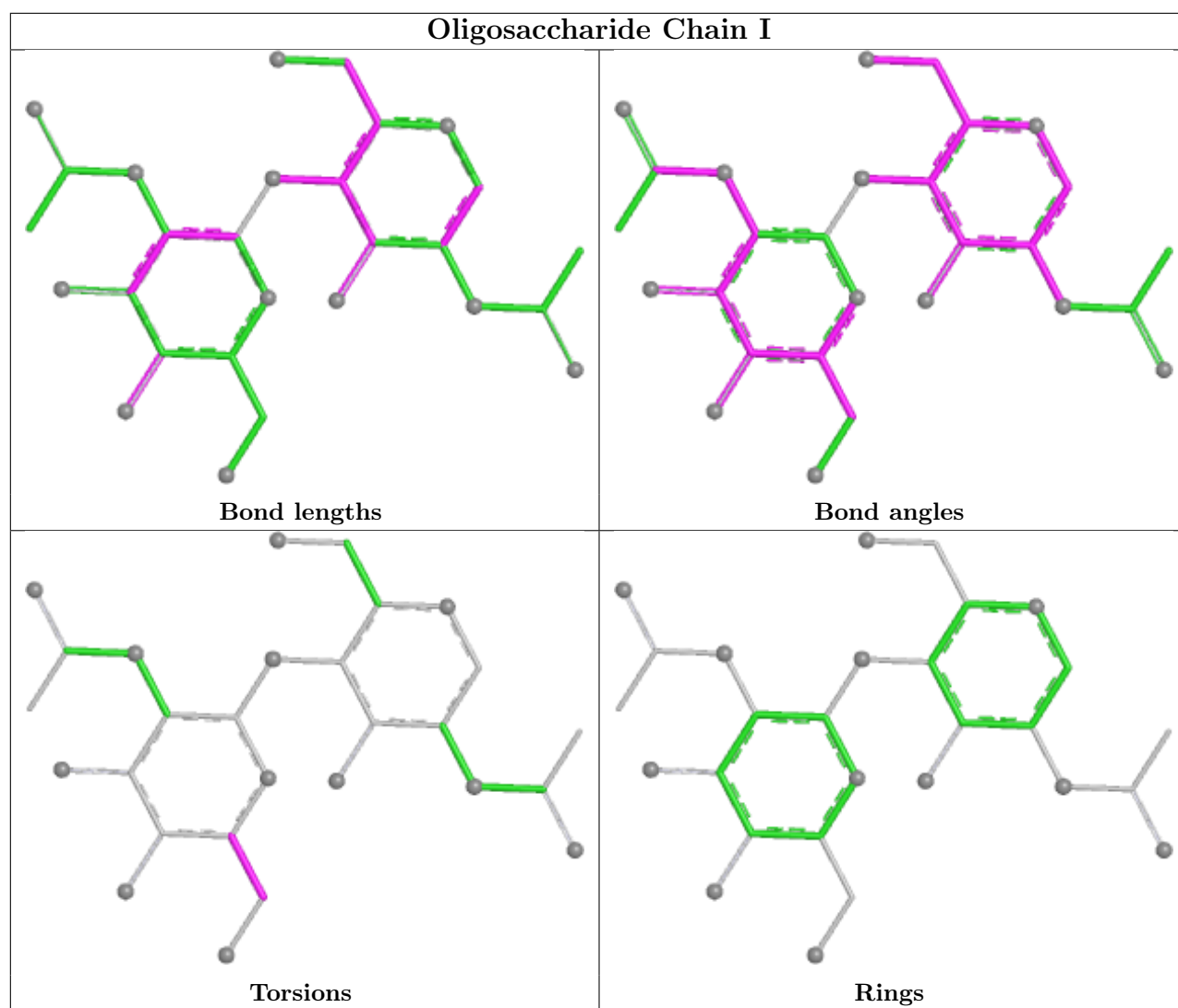
2 monomers are involved in 2 short contacts:

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

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







5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	321/326 (98%)	-0.14	3 (0%) 81 74	39, 50, 72, 108	0
1	C	321/326 (98%)	-0.00	3 (0%) 81 74	39, 54, 77, 111	0
1	E	321/326 (98%)	0.75	43 (13%) 7 5	42, 58, 96, 125	0
2	B	167/181 (92%)	0.09	2 (1%) 76 68	46, 64, 83, 99	0
2	D	167/181 (92%)	0.42	5 (2%) 52 42	44, 78, 117, 150	0
2	F	167/181 (92%)	0.41	10 (5%) 27 21	43, 67, 95, 128	0
All	All	1464/1521 (96%)	0.24	66 (4%) 38 30	39, 58, 93, 150	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	215	THR	7.3
1	E	214	SER	5.6
1	E	213	ILE	5.6
1	A	321	PRO	5.3
2	F	173	ILE	4.7
2	D	7	ALA	4.6
1	E	321	PRO	4.5
2	F	66	VAL	4.4
2	D	173	ILE	4.4
1	E	184	LEU	4.2
1	E	154	SER	4.2
1	E	207	ARG	4.1
1	E	197	TYR	4.1
1	E	244	ASN	4.0
2	B	7	ALA	3.9
2	F	7	ALA	3.7
1	E	212	GLU	3.7
1	E	196	SER	3.7
1	E	208	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	157	TYR	3.5
1	E	192	LYS	3.4
1	E	52	LEU	3.4
1	E	190	LEU	3.4
2	D	126	LEU	3.4
1	E	152	HIS	3.3
1	E	120	ASN	3.3
1	E	135	CYS	3.3
1	A	320	VAL	3.3
1	E	320	VAL	3.3
1	E	194	ASP	3.3
1	E	156	THR	3.3
1	E	186	GLU	3.2
2	F	168	LEU	3.2
1	E	210	THR	3.2
1	C	321	PRO	3.2
1	E	188	GLN	3.0
2	F	164	GLU	3.0
2	F	67	GLN	2.9
1	E	134	ALA	2.9
2	F	170	ARG	2.9
2	B	173	ILE	2.9
1	E	130	GLY	2.9
1	A	112	ASN	2.8
2	F	171	GLN	2.7
2	F	63	PHE	2.7
1	E	124	SER	2.6
1	E	191	TYR	2.5
1	E	187	HIS	2.4
1	E	245	GLY	2.4
1	E	139	SER	2.4
1	E	243	SER	2.3
1	E	216	ARG	2.3
1	E	158	PRO	2.3
1	E	90	CYS	2.3
1	E	193	LYS	2.3
2	D	127	LYS	2.3
1	E	183	THR	2.3
1	E	209	PHE	2.2
1	E	153	GLN	2.2
1	E	101	LEU	2.2
1	E	151	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	195	ASN	2.2
2	D	18	ILE	2.1
1	C	19	ILE	2.1
2	F	172	GLU	2.1
1	C	120	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

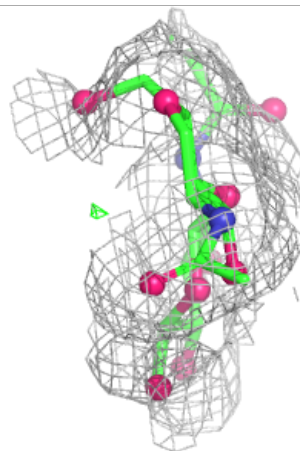
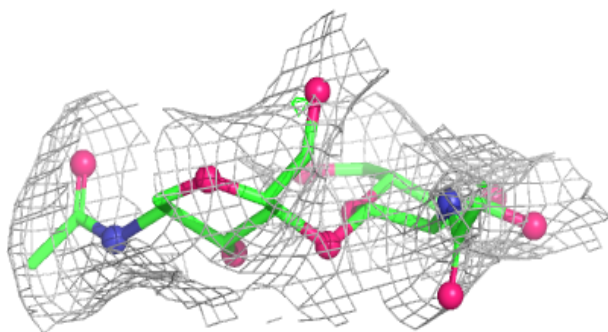
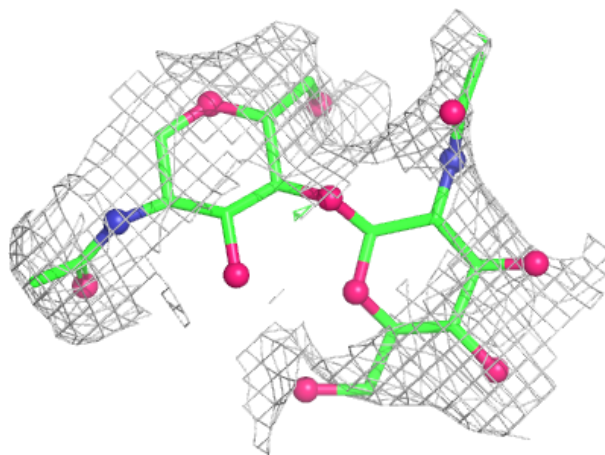
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	H	2	14/15	0.40	0.14	121,149,161,169	0
3	NAG	H	1	14/15	0.49	0.14	110,125,136,150	0
3	NAG	G	2	14/15	0.61	0.15	97,115,119,121	0
3	NAG	G	1	14/15	0.69	0.12	91,96,104,110	0
3	NAG	I	1	14/15	0.70	0.14	81,85,91,93	0
3	NAG	I	2	14/15	0.82	0.12	78,96,102,103	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.

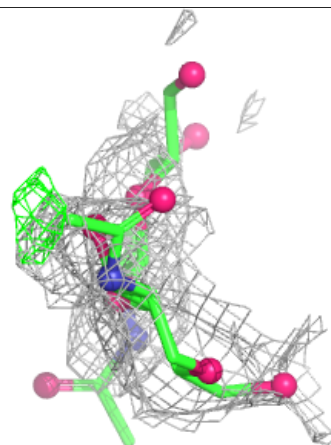
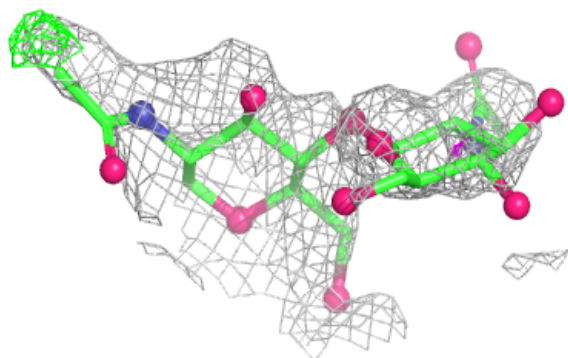
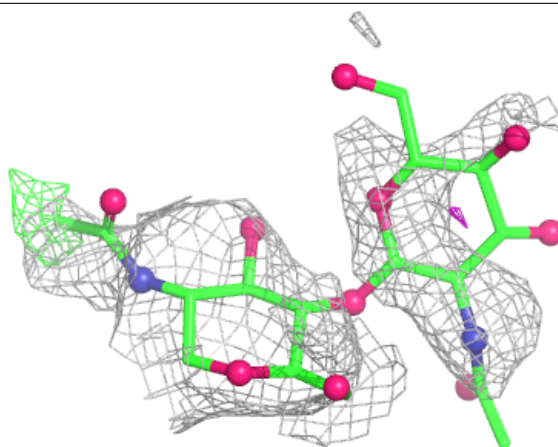
Electron density around Chain G:

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

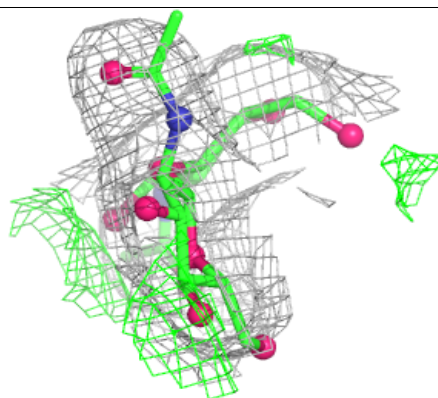
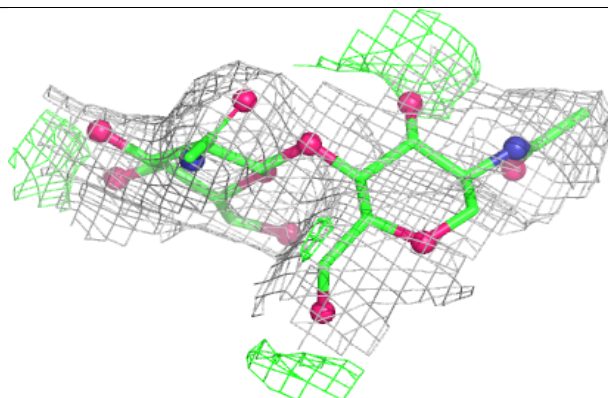
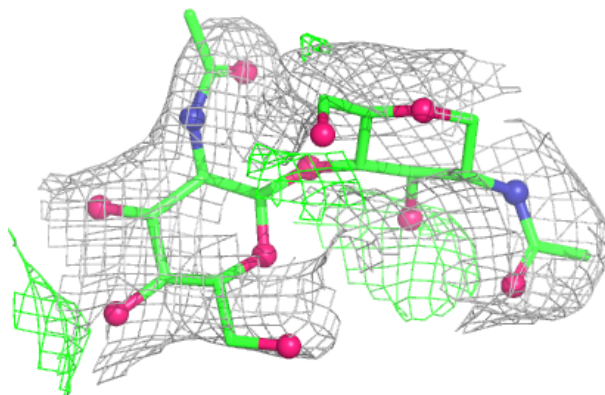


Electron density around Chain H:

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

**Electron density around Chain I:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.