



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:13 PM UTC

PDB ID : 4JUN / pdb\_00004jun  
Title : Crystal structure of H5N1 influenza virus hemagglutinin, clade 5  
Authors : DuBois, R.M.; Zaraket, H.; Reddivari, M.; Coop, T.; Heath, R.J.; White, S.W.; Russell, C.J.  
Deposited on : 2013-03-25  
Resolution : 2.34 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](mailto: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>.

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

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

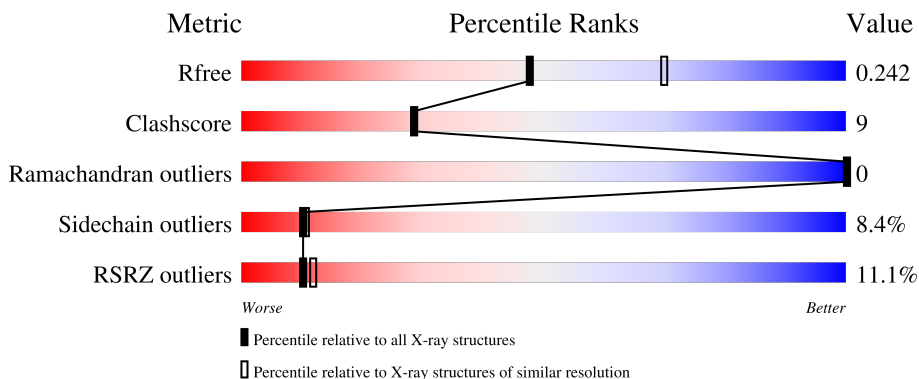
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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.




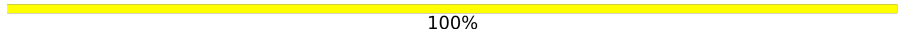

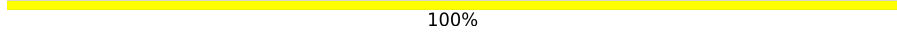
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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  $\geq 3$ , 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	 2% 83% 12% ..
1	C	329	 4% 78% 17% ..
1	E	329	 4% 78% 17% ..
2	B	182	 6% 74% 16% . 7%
2	D	182	 34% 65% 20% . . 10%

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Mol	Chain	Length	Quality of chain
2	F	182	
3	G	2	
3	H	2	
3	I	2	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 12083 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2543	1605	442	482	14	0	1	0
1	C	321	2543	1605	442	482	14	0	1	0
1	E	321	2543	1605	442	482	14	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	expression tag	UNP Q2F4V6
A	6	SER	-	expression tag	UNP Q2F4V6
A	7	ALA	-	expression tag	UNP Q2F4V6
A	8	ASP	-	expression tag	UNP Q2F4V6
A	9	PRO	-	expression tag	UNP Q2F4V6
A	10	GLY	-	expression tag	UNP Q2F4V6
C	5	GLY	-	expression tag	UNP Q2F4V6
C	6	SER	-	expression tag	UNP Q2F4V6
C	7	ALA	-	expression tag	UNP Q2F4V6
C	8	ASP	-	expression tag	UNP Q2F4V6
C	9	PRO	-	expression tag	UNP Q2F4V6
C	10	GLY	-	expression tag	UNP Q2F4V6
E	5	GLY	-	expression tag	UNP Q2F4V6
E	6	SER	-	expression tag	UNP Q2F4V6
E	7	ALA	-	expression tag	UNP Q2F4V6
E	8	ASP	-	expression tag	UNP Q2F4V6
E	9	PRO	-	expression tag	UNP Q2F4V6
E	10	GLY	-	expression tag	UNP Q2F4V6

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1382	859	243	272	8			
2	D	164	Total	C	N	O	S	0	0	0
			1329	827	230	264	8			
2	F	166	Total	C	N	O	S	0	0	0
			1343	835	232	268	8			

There are 18 discrepancies between the modelled and reference sequences:

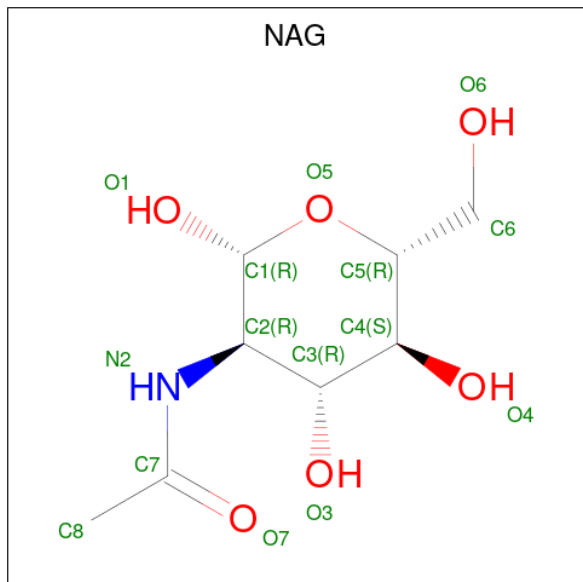
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP Q2F4V6
B	178	SER	-	expression tag	UNP Q2F4V6
B	179	LEU	-	expression tag	UNP Q2F4V6
B	180	VAL	-	expression tag	UNP Q2F4V6
B	181	PRO	-	expression tag	UNP Q2F4V6
B	182	ARG	-	expression tag	UNP Q2F4V6
D	177	ARG	-	expression tag	UNP Q2F4V6
D	178	SER	-	expression tag	UNP Q2F4V6
D	179	LEU	-	expression tag	UNP Q2F4V6
D	180	VAL	-	expression tag	UNP Q2F4V6
D	181	PRO	-	expression tag	UNP Q2F4V6
D	182	ARG	-	expression tag	UNP Q2F4V6
F	177	ARG	-	expression tag	UNP Q2F4V6
F	178	SER	-	expression tag	UNP Q2F4V6
F	179	LEU	-	expression tag	UNP Q2F4V6
F	180	VAL	-	expression tag	UNP Q2F4V6
F	181	PRO	-	expression tag	UNP Q2F4V6
F	182	ARG	-	expression tag	UNP Q2F4V6

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



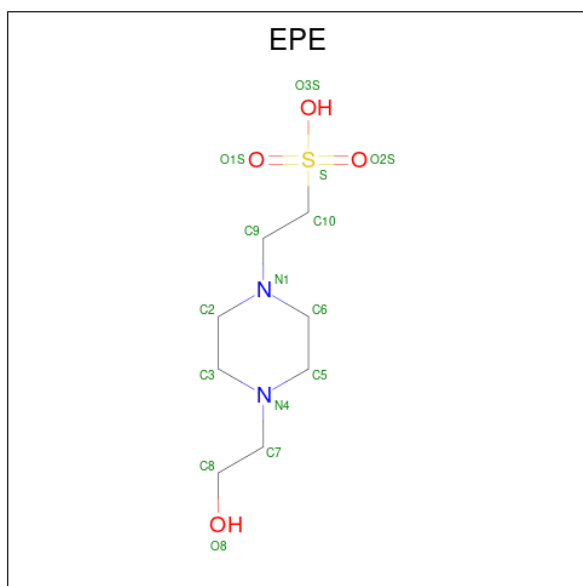
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	E	1	15	8	2	4	1	0	0

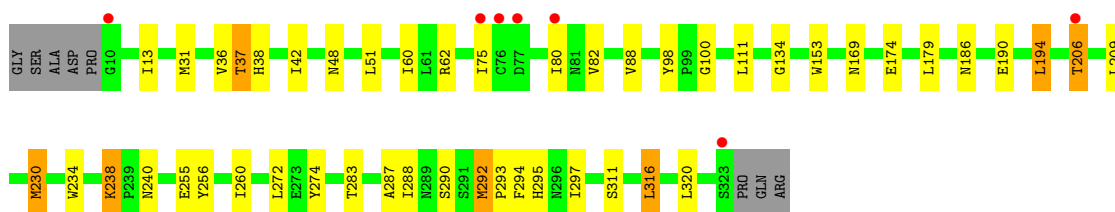
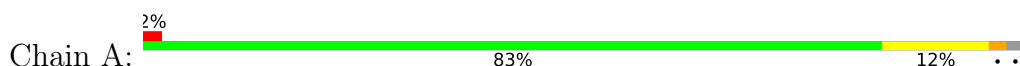
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total 77	O 77	0	0
6	B	14	Total 14	O 14	0	0
6	C	68	Total 68	O 68	0	0
6	D	14	Total 14	O 14	0	0
6	E	66	Total 66	O 66	0	0
6	F	20	Total 20	O 20	0	0

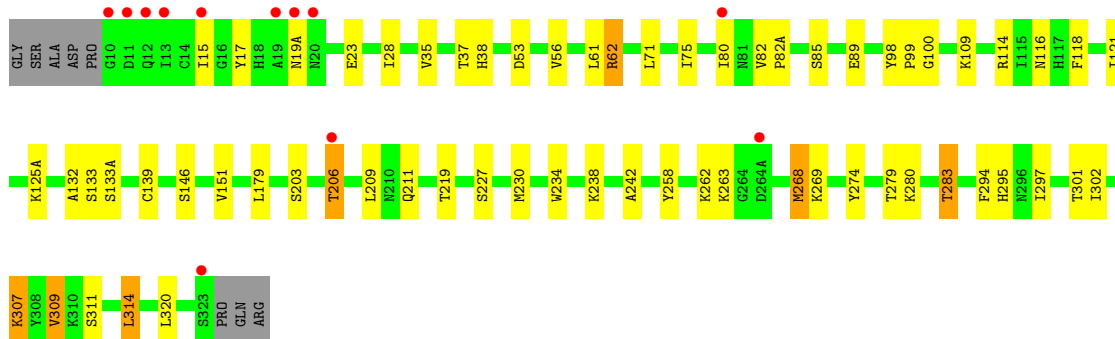
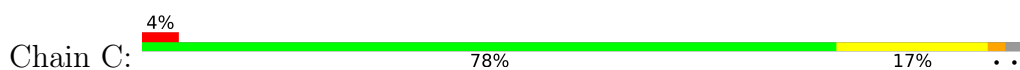
### 3 Residue-property plots [i](#)

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

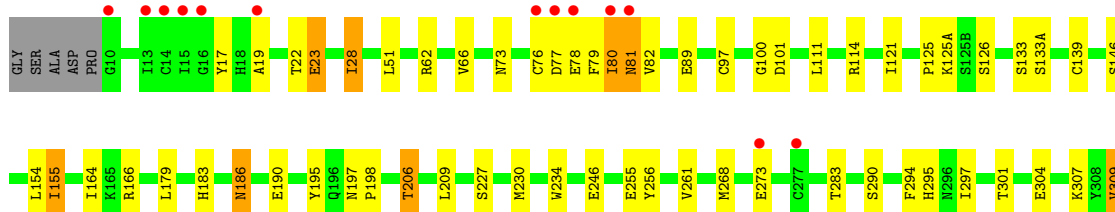
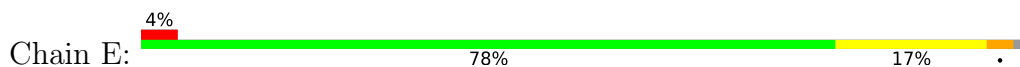
- Molecule 1: Hemagglutinin HA1

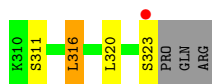


- Molecule 1: Hemagglutinin HA1

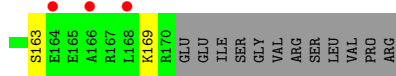
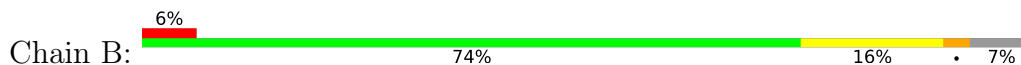


- Molecule 1: Hemagglutinin HA1

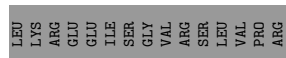
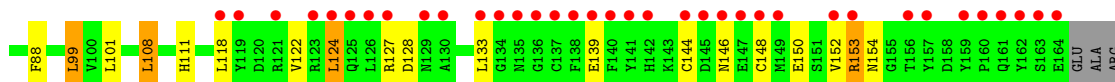
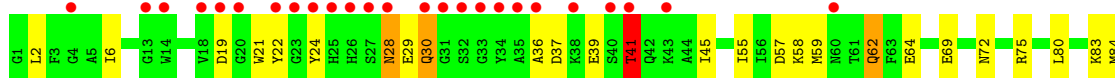




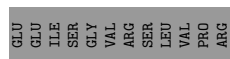
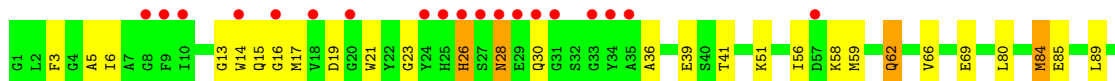
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



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

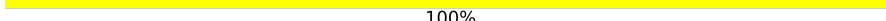


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

MAG1  
MAG2

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

Chain I:  100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.04Å 237.06Å 72.86Å 90.00° 119.18° 90.00°	Depositor
Resolution (Å)	49.62 – 2.34 49.62 – 2.34	Depositor EDS
% Data completeness (in resolution range)	81.7 (49.62-2.34) 86.3 (49.62-2.34)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.201 , 0.245 0.197 , 0.242	Depositor DCC
$R_{free}$ test set	3946 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,k,-h-l 0.008 for -h-l,k,h 0.027 for -h-l,-k,l 0.023 for h,-k,-h-l 0.028 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 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	0.60	2/2608 (0.1%)	0.86	2/3542 (0.1%)
1	C	0.57	0/2608	0.91	2/3542 (0.1%)
1	E	0.56	0/2608	0.89	3/3542 (0.1%)
2	B	0.49	0/1409	0.79	0/1894
2	D	0.47	0/1356	0.89	2/1825 (0.1%)
2	F	0.49	0/1370	0.86	3/1844 (0.2%)
All	All	0.55	2/11959 (0.0%)	0.87	12/16189 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ARG	C-O	-6.95	1.18	1.24
1	A	230	MET	C-O	-5.05	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	82	VAL	N-CA-C	10.24	119.80	107.61
2	F	146	ASN	N-CA-C	8.79	121.66	111.11
1	E	82	VAL	N-CA-CB	-7.66	104.25	112.37
2	F	5	ALA	N-CA-C	7.56	121.00	111.24
1	A	206	THR	N-CA-C	-6.58	99.33	109.14
1	C	62	ARG	CB-CA-C	-5.90	109.21	117.23
1	E	206	THR	N-CA-C	-5.79	100.70	108.86
2	D	41	THR	N-CA-C	-5.54	106.01	112.89
1	A	82	VAL	N-CA-C	5.46	113.84	107.89
2	F	125	GLN	N-CA-C	-5.39	106.30	112.92
2	D	127	ARG	CB-CA-C	-5.25	110.55	116.63
1	C	206	THR	N-CA-C	-5.09	101.56	109.14

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2543	0	2486	29	0
1	C	2543	0	2486	37	0
1	E	2543	0	2484	42	0
2	B	1382	0	1291	24	0
2	D	1329	0	1230	42	0
2	F	1343	0	1241	48	0
3	G	28	0	25	2	0
3	H	28	0	25	2	0
3	I	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	0	0
5	E	15	0	17	1	0
6	A	77	0	0	0	0
6	B	14	0	0	0	0
6	C	68	0	0	1	0
6	D	14	0	0	0	0
6	E	66	0	0	1	0
6	F	20	0	0	0	0
All	All	12083	0	11349	201	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 9.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:GLN:NE2	2:F:145:ASP:HB2	1.56	1.16
2:F:30:GLN:HE21	2:F:145:ASP:HB2	0.96	1.08
2:D:29:GLU:HB3	2:D:30:GLN:NE2	1.73	1.02
2:D:30:GLN:NE2	2:D:30:GLN:H	1.60	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LEU:HD12	2:B:80:LEU:O	1.63	0.98
2:B:80:LEU:HD12	2:B:80:LEU:C	1.94	0.92
2:D:29:GLU:HB3	2:D:30:GLN:HE21	1.27	0.92
2:D:30:GLN:HE21	2:D:30:GLN:N	1.69	0.91
1:A:295:HIS:HD2	1:A:297:ILE:H	1.18	0.91
2:F:146:ASN:HD22	2:F:146:ASN:N	1.72	0.87
2:F:30:GLN:HE21	2:F:145:ASP:CB	1.86	0.86
2:B:28:ASN:HD22	2:B:28:ASN:C	1.82	0.85
1:E:295:HIS:HD2	1:E:297:ILE:H	1.25	0.82
2:F:26:HIS:HD2	2:F:149:MET:HG3	1.48	0.78
2:D:150:GLU:O	2:D:154:ASN:HB2	1.85	0.77
1:A:240:ASN:HD22	3:G:1:NAG:H5	1.50	0.77
2:D:30:GLN:H	2:D:30:GLN:HE21	1.23	0.77
2:D:150:GLU:HA	2:D:150:GLU:OE1	1.85	0.76
2:F:158:ASP:HB3	2:F:161:GLN:HB2	1.69	0.74
2:D:30:GLN:NE2	2:D:30:GLN:N	2.30	0.74
2:D:24:TYR:CE2	2:D:153:ARG:HG3	2.22	0.74
2:F:146:ASN:N	2:F:146:ASN:ND2	2.36	0.73
1:E:126:SER:OG	1:E:166:ARG:NH2	2.23	0.72
2:D:19:ASP:HB2	2:D:36:ALA:HB2	1.72	0.70
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.73	0.70
2:D:124:LEU:HD12	2:F:134:GLY:HA2	1.74	0.69
1:E:97:CYS:CB	1:E:139:CYS:SG	2.81	0.69
1:E:62:ARG:NH2	1:E:78:GLU:OE1	2.26	0.68
2:D:28:ASN:C	2:D:28:ASN:HD22	2.02	0.68
2:B:28:ASN:C	2:B:28:ASN:ND2	2.50	0.66
1:E:81:ASN:OD1	1:E:81:ASN:N	2.26	0.66
2:D:28:ASN:C	2:D:28:ASN:ND2	2.53	0.65
2:F:26:HIS:HB2	2:F:149:MET:HE3	1.79	0.65
1:E:295:HIS:CD2	1:E:297:ILE:H	2.12	0.64
2:F:165:GLU:O	2:F:166:ALA:C	2.40	0.64
2:F:142:HIS:HB3	2:F:165:GLU:HG2	1.81	0.61
1:E:206:THR:OG1	1:E:209:LEU:N	2.29	0.61
2:D:146:ASN:HD22	2:D:146:ASN:N	1.98	0.61
1:E:97:CYS:HB2	1:E:139:CYS:SG	2.40	0.61
1:A:295:HIS:CD2	1:A:297:ILE:H	2.09	0.60
1:C:294:PHE:HZ	2:D:59:MET:HG3	1.66	0.60
1:C:295:HIS:HD2	1:C:297:ILE:H	1.50	0.60
1:C:242:ALA:H	3:H:1:NAG:H82	1.66	0.60
1:E:307:LYS:HD2	2:F:62:GLN:HG2	1.84	0.59
2:D:29:GLU:CB	2:D:30:GLN:HE21	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:ASP:HB2	2:D:36:ALA:CB	2.32	0.59
1:C:19(A):ASN:ND2	1:C:37:THR:HB	2.17	0.59
1:E:77:ASP:O	1:E:79:PHE:N	2.36	0.58
2:F:30:GLN:NE2	2:F:145:ASP:CB	2.50	0.58
2:F:21:TRP:HB2	2:F:41:THR:HG23	1.86	0.58
2:F:165:GLU:OE2	2:F:165:GLU:CA	2.52	0.57
1:C:242:ALA:N	3:H:1:NAG:H82	2.20	0.57
2:F:28:ASN:ND2	2:F:28:ASN:C	2.62	0.57
2:F:146:ASN:ND2	2:F:146:ASN:H	2.03	0.56
2:B:80:LEU:C	2:B:80:LEU:CD1	2.69	0.56
2:B:30:GLN:HE21	2:B:30:GLN:H	1.54	0.56
1:C:19(A):ASN:HD21	1:C:37:THR:HB	1.70	0.56
2:F:165:GLU:OE2	2:F:165:GLU:N	2.37	0.56
2:B:68:ARG:NH1	2:B:81:ASN:OD1	2.38	0.55
1:E:154:LEU:O	1:E:155:ILE:HD13	2.05	0.55
1:E:294:PHE:HZ	2:F:59:MET:HG3	1.71	0.55
2:F:145:ASP:O	2:F:148:CYS:HB3	2.07	0.55
2:D:84:MET:HE3	2:D:88:PHE:CD2	2.42	0.55
2:B:30:GLN:HE21	2:B:30:GLN:N	2.05	0.54
2:D:72:ASN:HB2	2:D:75:ARG:HH21	1.73	0.54
1:E:206:THR:OG1	1:E:209:LEU:CB	2.57	0.53
1:E:166:ARG:NH1	6:E:556:HOH:O	2.42	0.53
2:F:17:MET:SD	2:F:23:GLY:HA3	2.49	0.52
2:D:29:GLU:CB	2:D:30:GLN:NE2	2.61	0.52
1:C:309:VAL:HG13	1:C:311:SER:H	1.73	0.52
1:A:288:ILE:HD11	1:A:297:ILE:HG13	1.91	0.52
2:F:125:GLN:O	2:F:126:LEU:HD23	2.10	0.52
1:A:75:ILE:O	1:A:75:ILE:HG22	2.09	0.51
1:A:100:GLY:HA3	1:A:230:MET:O	2.10	0.51
1:C:116:ASN:HB2	1:C:262:LYS:HG3	1.90	0.51
2:F:28:ASN:OD1	2:F:145:ASP:HA	2.11	0.51
2:F:142:HIS:ND1	2:F:143:LYS:O	2.38	0.51
1:E:77:ASP:C	1:E:79:PHE:H	2.18	0.51
1:C:219:THR:HG23	6:C:530:HOH:O	2.10	0.51
1:E:139:CYS:HB2	1:E:146:SER:O	2.11	0.50
2:D:150:GLU:OE1	2:D:150:GLU:CA	2.57	0.50
1:A:60:ILE:HD12	1:A:274:TYR:HB2	1.93	0.50
2:D:28:ASN:OD1	2:D:146:ASN:ND2	2.45	0.50
1:E:100:GLY:HA3	1:E:230:MET:O	2.11	0.50
2:D:84:MET:HE3	2:D:88:PHE:HD2	1.76	0.49
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:HIS:CD2	2:F:149:MET:HG3	2.39	0.49
1:E:186:ASN:HB3	1:E:190:GLU:OE1	2.13	0.48
1:C:125(A):LYS:HE3	1:C:132:ALA:O	2.13	0.48
1:A:174:GLU:HG2	1:A:260:ILE:O	2.13	0.48
1:E:206:THR:OG1	1:E:209:LEU:HB3	2.14	0.48
2:F:84:MET:HG3	2:F:85:GLU:N	2.26	0.48
1:C:114:ARG:O	1:C:263:LYS:HG2	2.14	0.48
1:C:35:VAL:HG11	2:D:108:LEU:HD21	1.96	0.48
1:A:290:SER:OG	1:A:292:MET:HB2	2.14	0.48
1:C:206:THR:OG1	1:C:209:LEU:N	2.47	0.47
1:C:75:ILE:HD12	1:C:75:ILE:H	1.78	0.47
1:C:100:GLY:HA3	1:C:230:MET:O	2.15	0.47
1:A:206:THR:HG23	1:A:209:LEU:HB3	1.96	0.47
1:C:109:LYS:NZ	2:D:69:GLU:OE2	2.42	0.47
1:A:51:LEU:HD13	1:A:88:VAL:HG21	1.97	0.47
1:C:89:GLU:O	1:C:269:LYS:HA	2.14	0.47
1:E:183:HIS:ND1	1:E:195:TYR:OH	2.43	0.47
1:C:206:THR:OG1	1:C:209:LEU:HB3	2.14	0.47
2:F:28:ASN:C	2:F:28:ASN:HD22	2.23	0.46
2:F:165:GLU:OE2	2:F:165:GLU:HA	2.15	0.46
1:E:77:ASP:C	1:E:79:PHE:N	2.70	0.46
2:F:142:HIS:CB	2:F:165:GLU:HG2	2.45	0.46
1:A:37:THR:HG22	1:A:38:HIS:ND1	2.29	0.46
1:A:190:GLU:HG2	1:A:194:LEU:HD22	1.98	0.46
1:E:77:ASP:O	1:E:78:GLU:C	2.59	0.46
2:F:150:GLU:HA	2:F:150:GLU:OE2	2.15	0.46
2:F:19:ASP:HB3	2:F:36:ALA:CB	2.45	0.46
1:A:255:GLU:HG2	1:A:256:TYR:CD2	2.51	0.46
2:B:30:GLN:H	2:B:30:GLN:NE2	2.14	0.46
1:C:283:THR:HG22	1:C:301:THR:HG22	1.98	0.45
2:F:26:HIS:O	2:F:26:HIS:ND1	2.49	0.45
1:E:164:ILE:O	1:E:246:GLU:HA	2.15	0.45
1:E:309:VAL:HG13	1:E:311:SER:H	1.82	0.45
2:F:160:PRO:HA	2:F:163:SER:HB2	1.98	0.45
2:B:150:GLU:HG2	2:B:153:ARG:HH21	1.81	0.45
2:B:2:LEU:HG	2:F:3:PHE:HZ	1.82	0.45
2:B:73:LEU:CD2	5:E:404:EPE:H31	2.46	0.45
1:E:19:ALA:HB2	2:F:13:GLY:HA3	1.99	0.45
1:E:125(A):LYS:HB2	1:E:125(A):LYS:HE2	1.70	0.45
1:E:28:ILE:HD11	2:F:102:MET:HG2	1.99	0.44
2:F:132:GLU:HG2	2:F:138:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:LEU:HG	2:F:3:PHE:CZ	2.52	0.44
1:C:53:ASP:OD2	1:C:274:TYR:OH	2.28	0.44
2:B:133:LEU:HD21	2:B:139:GLU:HB2	1.99	0.44
1:A:169:ASN:C	1:A:169:ASN:OD1	2.61	0.44
2:F:51:LYS:HD2	2:F:103:GLU:HB3	2.00	0.44
1:A:295:HIS:HD2	1:A:297:ILE:N	2.00	0.43
2:F:58:LYS:HA	2:F:58:LYS:HD2	1.75	0.43
1:C:61:LEU:O	1:C:62:ARG:HB2	2.18	0.43
1:A:134:GLY:HA3	1:A:153:TRP:HB3	2.01	0.43
1:A:294:PHE:HZ	2:B:59:MET:HG3	1.83	0.43
1:E:283:THR:HG22	1:E:301:THR:HG22	2.00	0.43
1:C:139:CYS:HB2	1:C:146:SER:O	2.18	0.43
1:C:268:MET:HB3	1:C:268:MET:HE3	1.70	0.43
2:F:15:GLN:O	2:F:15:GLN:HG3	2.18	0.43
2:F:132:GLU:HG2	2:F:138:PHE:CE1	2.54	0.43
1:A:48:ASN:HD21	1:A:287:ALA:HB3	1.84	0.43
1:C:80:ILE:HD13	1:C:80:ILE:HA	1.79	0.43
2:D:2:LEU:HD12	2:D:2:LEU:HA	1.89	0.43
1:E:23:GLU:H	1:E:23:GLU:HG2	1.52	0.43
2:D:72:ASN:HB2	2:D:75:ARG:NH2	2.33	0.43
2:D:118:LEU:HD12	2:D:118:LEU:HA	1.88	0.43
1:C:56:VAL:HB	1:C:85:SER:HB3	2.00	0.43
1:A:13:ILE:HB	2:B:149:MET:HE1	2.00	0.42
2:D:58:LYS:HE3	2:F:97:GLU:HB3	2.00	0.42
2:B:150:GLU:HG2	2:B:153:ARG:NH2	2.35	0.42
1:E:51:LEU:HD22	1:E:268:MET:HE1	2.01	0.42
2:B:160:PRO:HA	2:B:163:SER:OG	2.20	0.42
1:C:17:TYR:CZ	2:D:6:ILE:HG23	2.54	0.42
1:C:206:THR:OG1	1:C:209:LEU:CB	2.67	0.42
1:E:28:ILE:H	1:E:28:ILE:HG12	1.54	0.42
2:B:144:CYS:SG	2:B:149:MET:HE3	2.60	0.42
1:C:203:SER:HA	1:C:211:GLN:O	2.20	0.42
1:E:66:VAL:HG23	1:E:89:GLU:OE1	2.20	0.42
2:D:30:GLN:H	2:D:30:GLN:CD	2.23	0.42
1:E:255:GLU:HG2	1:E:256:TYR:CD1	2.54	0.42
2:D:37:ASP:O	2:D:41:THR:HB	2.19	0.42
2:D:153:ARG:HG2	2:D:153:ARG:NH1	2.34	0.42
1:E:80:ILE:HD13	1:E:80:ILE:HA	1.93	0.42
2:F:14:TRP:C	2:F:16:GLY:H	2.27	0.42
1:C:98:TYR:CD2	1:C:99:PRO:HD2	2.55	0.42
1:C:307:LYS:HG3	2:D:62:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:LEU:HD23	1:E:234:TRP:HB3	2.02	0.42
1:E:73:ASN:O	1:E:76:CYS:N	2.44	0.42
1:C:15:ILE:HD11	2:D:122:VAL:HG21	2.02	0.41
1:A:31:MET:HE1	2:F:110:PHE:CE1	2.55	0.41
2:F:19:ASP:HB3	2:F:36:ALA:HB2	2.00	0.41
1:C:320:LEU:HB3	2:D:111:HIS:CD2	2.55	0.41
1:A:240:ASN:ND2	3:G:1:NAG:H5	2.28	0.41
1:C:38:HIS:CE1	2:D:21:TRP:HE1	2.37	0.41
1:E:166:ARG:HA	1:E:166:ARG:HD2	1.80	0.41
2:B:131:LYS:O	2:B:138:PHE:HA	2.21	0.41
2:D:133:LEU:HD13	2:D:139:GLU:HB2	2.02	0.41
1:A:42:ILE:HD13	1:A:316:LEU:HD22	2.02	0.41
2:B:17:MET:HE3	2:B:17:MET:HB2	1.93	0.41
2:D:28:ASN:ND2	2:D:30:GLN:O	2.45	0.41
2:D:55:ILE:HG12	2:D:99:LEU:HD13	2.03	0.41
2:F:159:TYR:HB3	2:F:160:PRO:HD3	2.01	0.41
2:B:145:ASP:OD2	2:B:145:ASP:C	2.64	0.41
1:C:279:THR:OG1	1:C:280:LYS:N	2.54	0.41
2:D:41:THR:O	2:D:45:ILE:HG13	2.21	0.41
1:E:316:LEU:HD12	1:E:316:LEU:HA	1.93	0.41
1:A:42:ILE:HB	1:A:293:PRO:HG2	2.03	0.41
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.94	0.40
2:D:148:CYS:O	2:D:152:VAL:HG23	2.21	0.40
1:E:17:TYR:CZ	2:F:6:ILE:HG23	2.56	0.40
1:A:238:LYS:HD2	1:A:238:LYS:HA	1.80	0.40
1:E:62:ARG:CZ	1:E:78:GLU:OE1	2.68	0.40
1:A:98:TYR:CD2	1:A:230:MET:HG2	2.57	0.40
1:C:118:PHE:CD1	1:C:258:TYR:HB3	2.57	0.40
1:A:294:PHE:CZ	2:B:59:MET:HG3	2.56	0.40
1:A:42:ILE:C	1:A:292:MET:HG3	2.47	0.40
2:B:123:ARG:HD2	2:B:132:GLU:OE1	2.22	0.40
1:E:125:PRO:O	1:E:126:SER:HB3	2.21	0.40
1:E:197:ASN:HA	1:E:198:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/329 (97%)	314 (98%)	6 (2%)	0	100	100
1	C	320/329 (97%)	314 (98%)	6 (2%)	0	100	100
1	E	320/329 (97%)	314 (98%)	6 (2%)	0	100	100
2	B	168/182 (92%)	166 (99%)	2 (1%)	0	100	100
2	D	162/182 (89%)	157 (97%)	5 (3%)	0	100	100
2	F	164/182 (90%)	156 (95%)	8 (5%)	0	100	100
All	All	1454/1533 (95%)	1421 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/291 (98%)	273 (96%)	13 (4%)	24	32
1	C	286/291 (98%)	269 (94%)	17 (6%)	18	21
1	E	286/291 (98%)	264 (92%)	22 (8%)	12	12
2	B	145/156 (93%)	127 (88%)	18 (12%)	4	3
2	D	140/156 (90%)	123 (88%)	17 (12%)	5	4
2	F	141/156 (90%)	121 (86%)	20 (14%)	3	2
All	All	1284/1341 (96%)	1177 (92%)	107 (8%)	10	11

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	37	THR
1	A	80	ILE
1	A	111	LEU
1	A	186	ASN
1	A	194	LEU
1	A	238	LYS
1	A	272	LEU
1	A	283	THR
1	A	292	MET
1	A	311	SER
1	A	316	LEU
1	A	320	LEU
2	B	18	VAL
2	B	28	ASN
2	B	30	GLN
2	B	45	ILE
2	B	60	ASN
2	B	77	ILE
2	B	80	LEU
2	B	89	LEU
2	B	101	LEU
2	B	106	ARG
2	B	108	LEU
2	B	113	SER
2	B	124	LEU
2	B	149	MET
2	B	150	GLU
2	B	151	SER
2	B	152	VAL
2	B	169	LYS
1	C	23	GLU
1	C	28	ILE
1	C	71	LEU
1	C	82	VAL
1	C	82(A)	PRO
1	C	121	ILE
1	C	133	SER
1	C	133(A)	SER
1	C	151	VAL
1	C	227	SER
1	C	238	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	268	MET
1	C	283	THR
1	C	302	ILE
1	C	307	LYS
1	C	309	VAL
1	C	314	LEU
2	D	22	TYR
2	D	28	ASN
2	D	30	GLN
2	D	39	GLU
2	D	41	THR
2	D	57	ASP
2	D	62	GLN
2	D	64	GLU
2	D	80	LEU
2	D	83	LYS
2	D	99	LEU
2	D	101	LEU
2	D	108	LEU
2	D	124	LEU
2	D	128	ASP
2	D	144	CYS
2	D	153	ARG
1	E	22	THR
1	E	23	GLU
1	E	28	ILE
1	E	80	ILE
1	E	81	ASN
1	E	101	ASP
1	E	111	LEU
1	E	114	ARG
1	E	121	ILE
1	E	133	SER
1	E	133(A)	SER
1	E	155	ILE
1	E	186	ASN
1	E	227	SER
1	E	261	VAL
1	E	273	GLU
1	E	290	SER
1	E	304	GLU
1	E	309	VAL

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Mol	Chain	Res	Type
1	E	316	LEU
1	E	320	LEU
1	E	323	SER
2	F	26	HIS
2	F	28	ASN
2	F	39	GLU
2	F	56	ILE
2	F	62	GLN
2	F	66	VAL
2	F	69	GLU
2	F	80	LEU
2	F	84	MET
2	F	89	LEU
2	F	108	LEU
2	F	113	SER
2	F	121	ARG
2	F	127	ARG
2	F	137	CYS
2	F	146	ASN
2	F	147	GLU
2	F	158	ASP
2	F	164	GLU
2	F	165	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	20	ASN
1	A	150	ASN
1	A	186	ASN
1	A	240	ASN
1	A	295	HIS
2	B	28	ASN
2	B	60	ASN
2	B	62	GLN
2	B	95	ASN
2	B	114	ASN
2	B	146	ASN
2	B	161	GLN
1	C	117	HIS
1	C	186	ASN

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Mol	Chain	Res	Type
1	C	196	GLN
1	C	240	ASN
1	C	295	HIS
2	D	25	HIS
2	D	28	ASN
2	D	30	GLN
2	D	62	GLN
2	D	95	ASN
2	D	114	ASN
2	D	129	ASN
2	D	146	ASN
2	D	154	ASN
1	E	18	HIS
1	E	20	ASN
1	E	158	ASN
1	E	276	ASN
1	E	295	HIS
2	F	30	GLN
2	F	95	ASN
2	F	114	ASN
2	F	129	ASN
2	F	146	ASN
2	F	161	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	G	1	3,1	14,14,15	0.71	0	17,19,21	0.79	0
3	NAG	G	2	3	14,14,15	0.60	0	17,19,21	1.30	2 (11%)
3	NAG	H	1	3,1	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
3	NAG	H	2	3	14,14,15	0.67	0	17,19,21	1.10	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.68	0	17,19,21	1.58	4 (23%)
3	NAG	I	2	3	14,14,15	0.68	0	17,19,21	1.10	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	O5-C1-C2	-4.00	105.09	111.29
3	I	1	NAG	C2-N2-C7	2.82	126.67	122.90
3	I	2	NAG	C1-O5-C5	2.61	115.68	112.19
3	H	2	NAG	C1-O5-C5	2.60	115.67	112.19
3	I	1	NAG	C1-O5-C5	-2.41	108.95	112.19
3	I	1	NAG	O5-C5-C6	2.35	112.25	107.66
3	I	1	NAG	O5-C1-C2	-2.32	107.70	111.29
3	G	2	NAG	C3-C4-C5	2.16	114.15	110.23
3	H	1	NAG	O5-C1-C2	-2.04	108.14	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

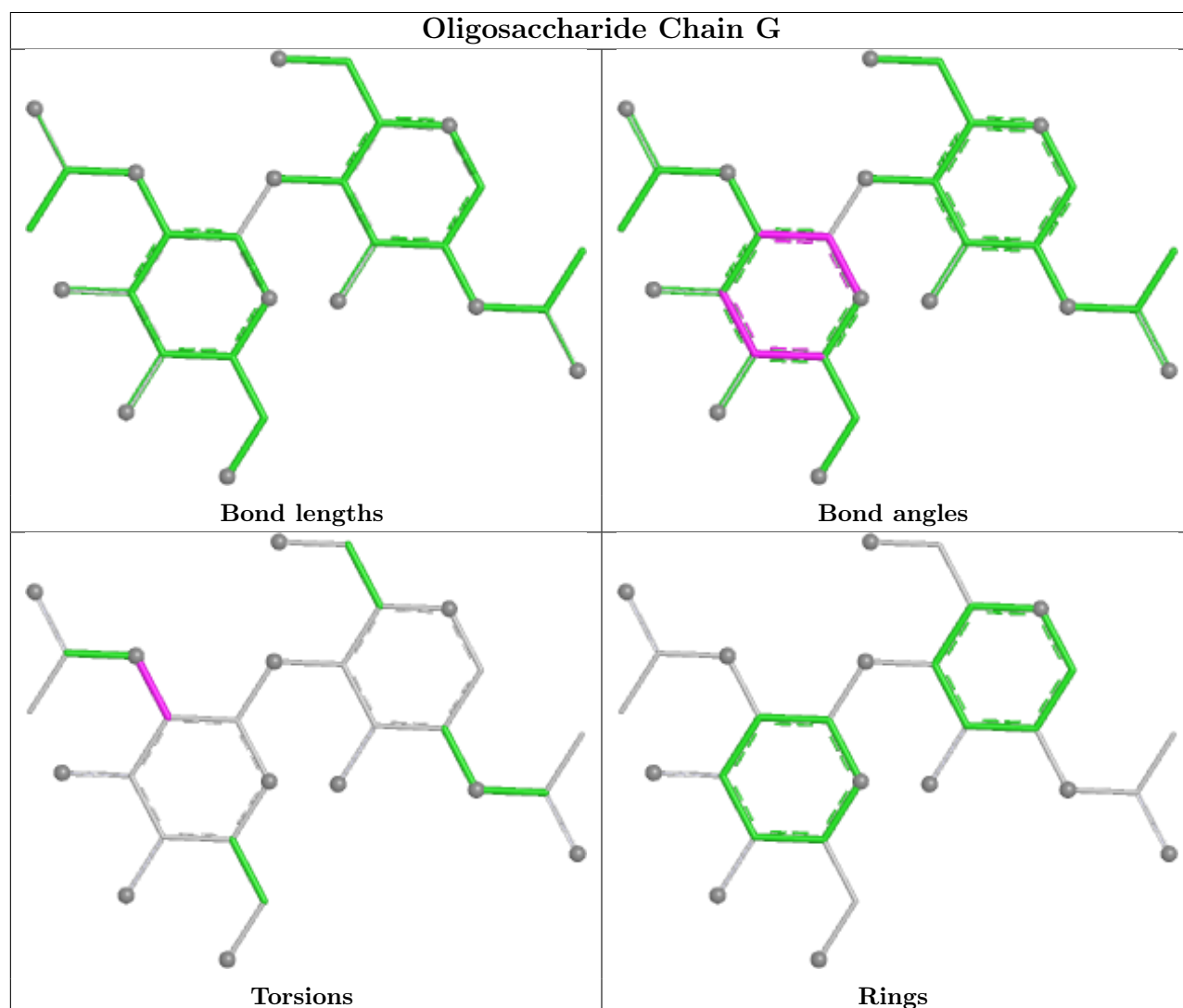
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7

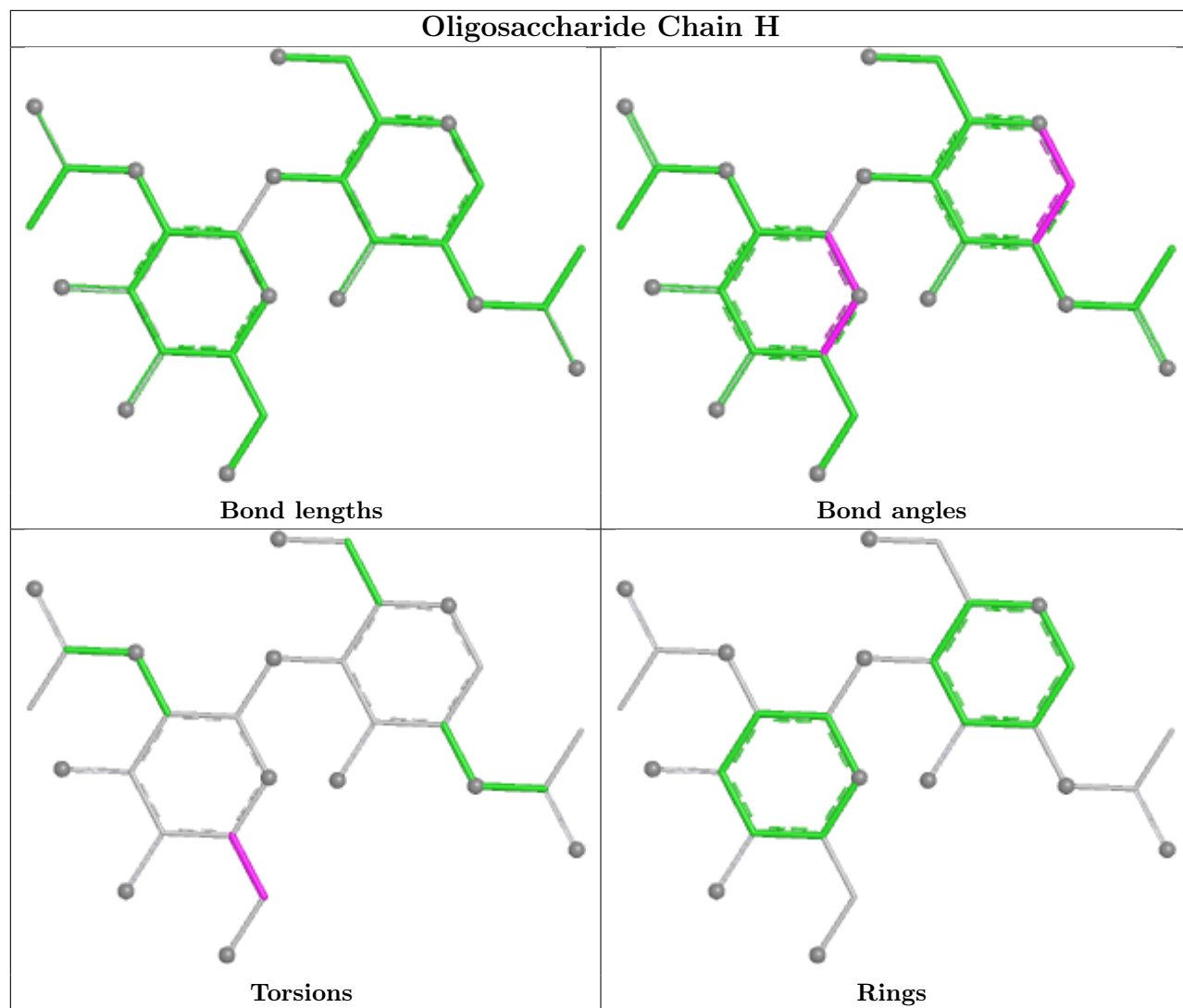
There are no ring outliers.

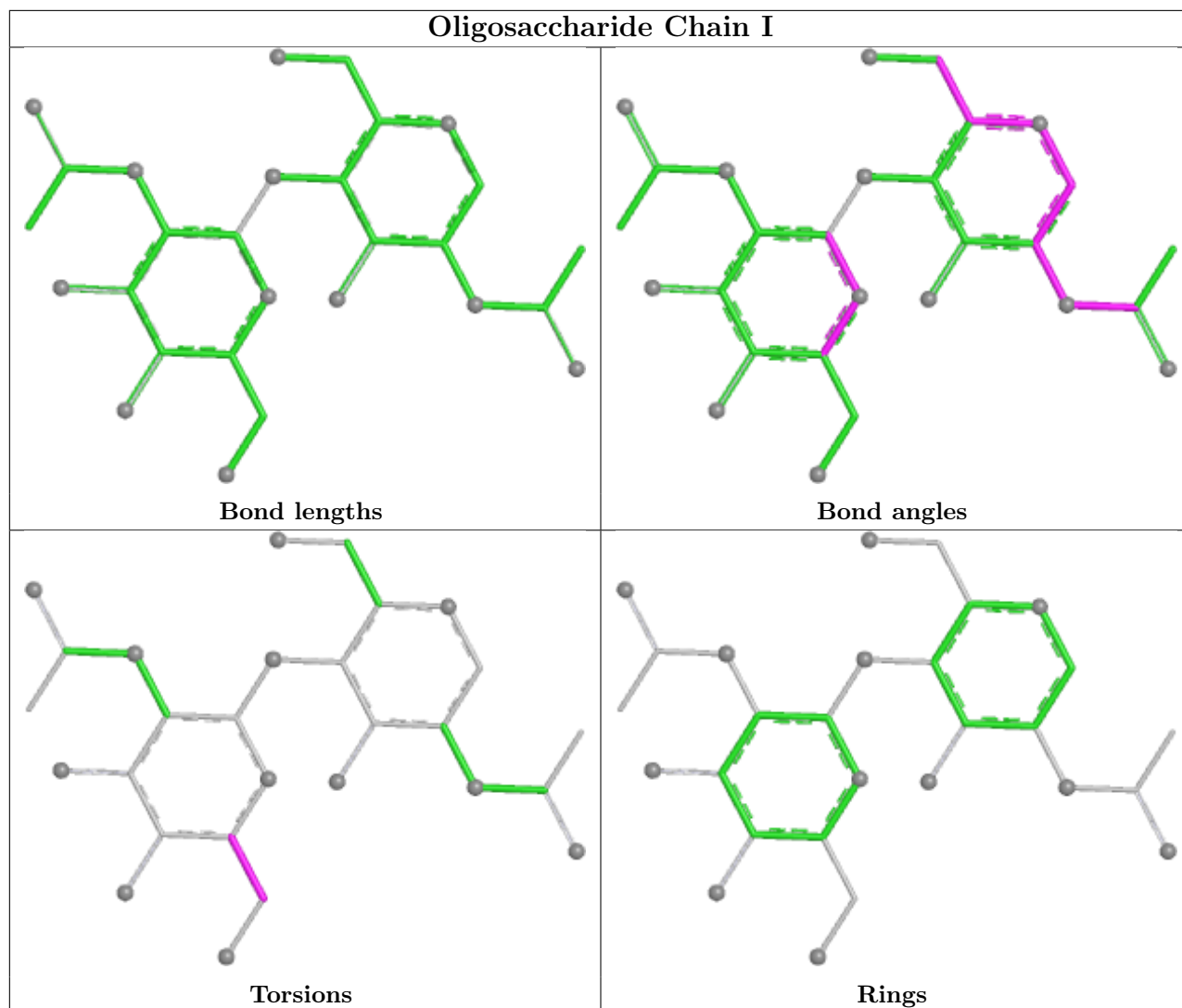
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	2	0
3	G	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	E	403	1	14,14,15	0.58	0	17,19,21	1.37	2 (11%)
4	NAG	C	403	1	14,14,15	0.54	0	17,19,21	1.15	2 (11%)
5	EPE	E	404	-	15,15,15	1.28	1 (6%)	19,20,20	2.12	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	403	1	14,14,15	0.58	0	17,19,21	1.17	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	403	1	-	2/6/23/26	0/1/1/1
5	EPE	E	404	-	-	5/9/19/19	0/1/1/1
4	NAG	A	403	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	404	EPE	C10-S	4.46	1.83	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	404	EPE	C7-N4-C3	4.97	124.49	111.24
5	E	404	EPE	O2S-S-C10	4.61	113.69	106.73
4	E	403	NAG	O5-C1-C2	-3.46	105.93	111.29
4	E	403	NAG	C3-C4-C5	3.17	115.98	110.23
5	E	404	EPE	C5-N4-C3	2.88	115.04	108.84
5	E	404	EPE	C7-N4-C5	2.59	118.14	111.24
5	E	404	EPE	C2-C3-N4	2.59	115.87	110.65
4	C	403	NAG	C3-C4-C5	2.58	114.91	110.23
4	A	403	NAG	O5-C1-C2	-2.49	107.44	111.29
4	A	403	NAG	C2-N2-C7	-2.32	119.80	122.90
4	A	403	NAG	C4-C3-C2	-2.31	107.63	111.02
4	C	403	NAG	O5-C1-C2	-2.24	107.83	111.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	404	EPE	N4-C7-C8-O8
4	E	403	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	403	NAG	O5-C5-C6-O6
5	E	404	EPE	C8-C7-N4-C5
5	E	404	EPE	C9-C10-S-O1S
5	E	404	EPE	C9-C10-S-O2S
4	C	403	NAG	C4-C5-C6-O6
4	E	403	NAG	C4-C5-C6-O6
5	E	404	EPE	C9-C10-S-O3S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	404	EPE	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	321/329 (97%)	-0.10	7 (2%) 62 67	14, 33, 55, 71	1 (0%)
1	C	321/329 (97%)	-0.01	12 (3%) 45 51	12, 33, 61, 112	1 (0%)
1	E	321/329 (97%)	0.11	14 (4%) 39 45	13, 32, 62, 104	1 (0%)
2	B	170/182 (93%)	0.61	11 (6%) 25 29	15, 52, 71, 91	0
2	D	164/182 (90%)	1.39	61 (37%) 1 0	17, 64, 109, 117	0
2	F	166/182 (91%)	1.36	58 (34%) 1 0	18, 65, 117, 125	0
All	All	1463/1533 (95%)	0.38	163 (11%) 10 12	12, 38, 99, 125	3 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	166	ALA	7.8
2	F	141	TYR	5.8
1	E	13	ILE	5.7
2	D	141	TYR	5.4
1	E	80	ILE	5.1
1	E	10	GLY	4.9
2	F	160	PRO	4.9
2	D	133	LEU	4.8
2	D	140	PHE	4.7
2	F	157	TYR	4.6
1	E	77	ASP	4.6
2	D	162	TYR	4.5
2	F	152	VAL	4.5
2	F	162	TYR	4.5
2	D	138	PHE	4.4
2	F	126	LEU	4.3
2	F	156	THR	4.3
1	A	10	GLY	4.3
2	D	157	TYR	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	27	SER	4.2
2	D	159	TYR	4.1
2	B	29	GLU	4.1
1	E	81	ASN	4.0
2	D	164	GLU	4.0
2	F	124	LEU	3.9
1	C	10	GLY	3.9
1	C	13	ILE	3.8
2	D	160	PRO	3.8
1	E	14	CYS	3.8
2	F	138	PHE	3.8
2	F	9	PHE	3.7
2	D	126	LEU	3.7
1	C	323	SER	3.7
1	E	76	CYS	3.6
2	D	152	VAL	3.6
1	C	19(A)	ASN	3.6
2	D	124	LEU	3.5
2	F	159	TYR	3.5
2	D	161	GLN	3.5
2	D	149	MET	3.4
2	F	143	LYS	3.4
2	D	27	SER	3.4
2	F	129	ASN	3.4
2	D	153	ARG	3.3
2	D	35	ALA	3.3
2	D	148	CYS	3.3
1	C	206	THR	3.3
1	A	323	SER	3.3
1	E	16	GLY	3.2
1	E	323	SER	3.2
2	B	168	LEU	3.2
2	F	163	SER	3.2
1	A	76	CYS	3.1
2	D	24	TYR	3.1
2	F	20	GLY	3.1
2	B	166	ALA	3.1
2	D	163	SER	3.1
2	D	144	CYS	3.0
1	A	80	ILE	3.0
1	A	77	ASP	3.0
2	F	149	MET	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	133	LEU	2.9
2	F	29	GLU	2.9
2	D	146	ASN	2.9
2	D	23	GLY	2.8
2	F	130	ALA	2.8
2	F	140	PHE	2.8
2	F	30	GLN	2.8
2	D	60	ASN	2.8
2	F	161	GLN	2.8
2	F	31	GLY	2.8
1	C	19	ALA	2.8
2	D	145	ASP	2.7
2	D	20	GLY	2.7
2	F	139	GLU	2.7
2	F	125	GLN	2.7
2	B	164	GLU	2.7
1	C	15	ILE	2.7
1	C	20	ASN	2.7
2	D	139	GLU	2.7
2	D	41	THR	2.6
1	C	12	GLN	2.6
2	B	31	GLY	2.6
2	F	142	HIS	2.6
2	F	127	ARG	2.6
2	F	154	ASN	2.6
2	F	8	GLY	2.6
2	F	131	LYS	2.6
2	D	31	GLY	2.6
2	D	156	THR	2.6
2	F	26	HIS	2.6
2	D	30	GLN	2.5
1	C	80	ILE	2.5
2	D	26	HIS	2.5
2	F	25	HIS	2.5
2	D	43	LYS	2.5
1	A	206	THR	2.5
2	B	30	GLN	2.5
2	F	10	ILE	2.5
2	D	19	ASP	2.5
2	F	128	ASP	2.5
2	F	146	ASN	2.5
2	D	136	GLY	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	142	HIS	2.5
2	F	35	ALA	2.5
2	D	125	GLN	2.5
1	E	78	GLU	2.4
1	C	264(A)	ASP	2.4
2	D	28	ASN	2.4
1	E	277	CYS	2.4
2	F	164	GLU	2.4
2	F	33	GLY	2.4
2	D	137	CYS	2.4
1	C	11	ASP	2.4
2	F	57	ASP	2.4
2	D	4	GLY	2.4
2	D	36	ALA	2.4
2	F	123	ARG	2.4
2	F	24	TYR	2.3
1	E	19	ALA	2.3
2	D	121	ARG	2.3
2	D	18	VAL	2.3
2	F	165	GLU	2.3
2	D	135	ASN	2.3
2	F	153	ARG	2.3
1	E	15	ILE	2.3
2	F	28	ASN	2.2
2	D	123	ARG	2.2
2	D	130	ALA	2.2
2	F	151	SER	2.2
2	B	124	LEU	2.2
2	D	118	LEU	2.2
2	F	158	ASP	2.2
2	B	134	GLY	2.2
2	D	25	HIS	2.2
2	D	38	LYS	2.2
2	F	18	VAL	2.2
2	D	129	ASN	2.2
2	D	33	GLY	2.2
2	F	155	GLY	2.2
2	F	144	CYS	2.2
2	D	40	SER	2.2
2	D	119	TYR	2.1
2	D	127	ARG	2.1
2	D	14	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	147	GLU	2.1
2	F	148	CYS	2.1
2	D	34	TYR	2.1
2	D	13	GLY	2.1
2	F	16	GLY	2.1
2	F	137	CYS	2.1
1	E	273	GLU	2.1
2	F	34	TYR	2.1
2	D	134	GLY	2.1
2	B	39	GLU	2.1
1	A	75	ILE	2.1
2	D	22	TYR	2.1
2	B	18	VAL	2.1
2	B	33	GLY	2.1
2	D	32	SER	2.0
2	F	14	TRP	2.0
2	D	147	GLU	2.0
2	F	145	ASP	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](#)

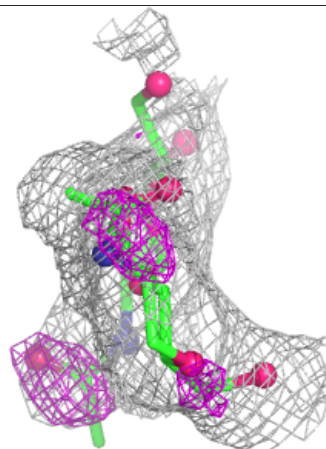
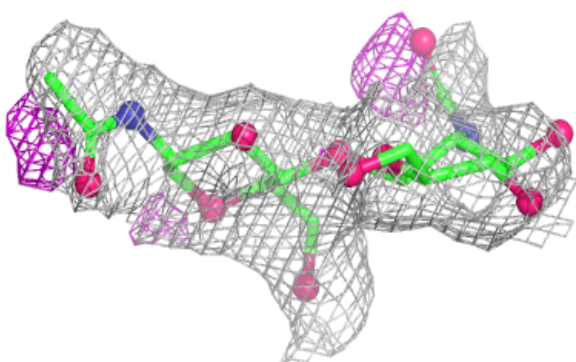
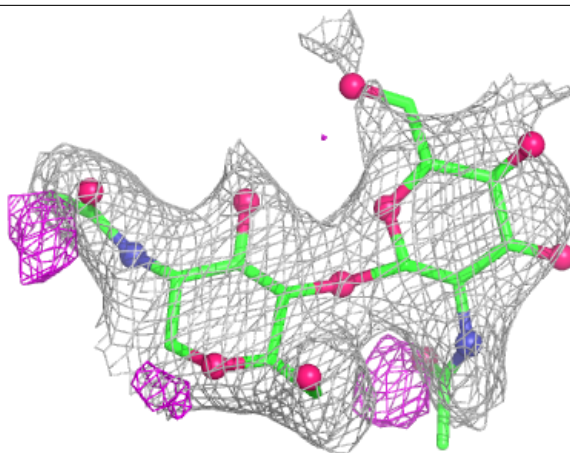
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	H	2	14/15	0.66	0.18	61,74,79,79	0
3	NAG	I	2	14/15	0.67	0.17	61,74,79,79	0
3	NAG	G	2	14/15	0.72	0.18	58,77,84,86	0
3	NAG	H	1	14/15	0.79	0.14	25,44,52,53	0
3	NAG	I	1	14/15	0.81	0.13	31,45,61,69	0
3	NAG	G	1	14/15	0.86	0.12	32,44,52,64	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

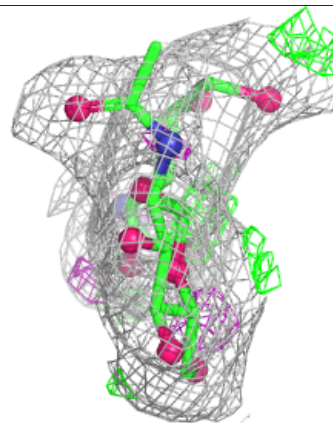
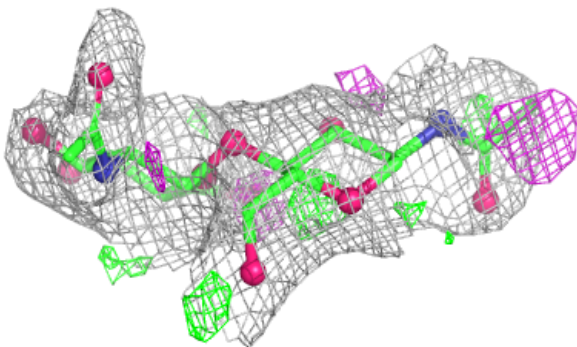
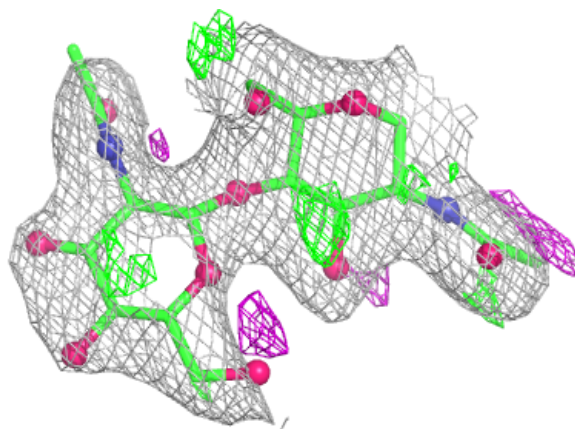
**Electron density around Chain G:**

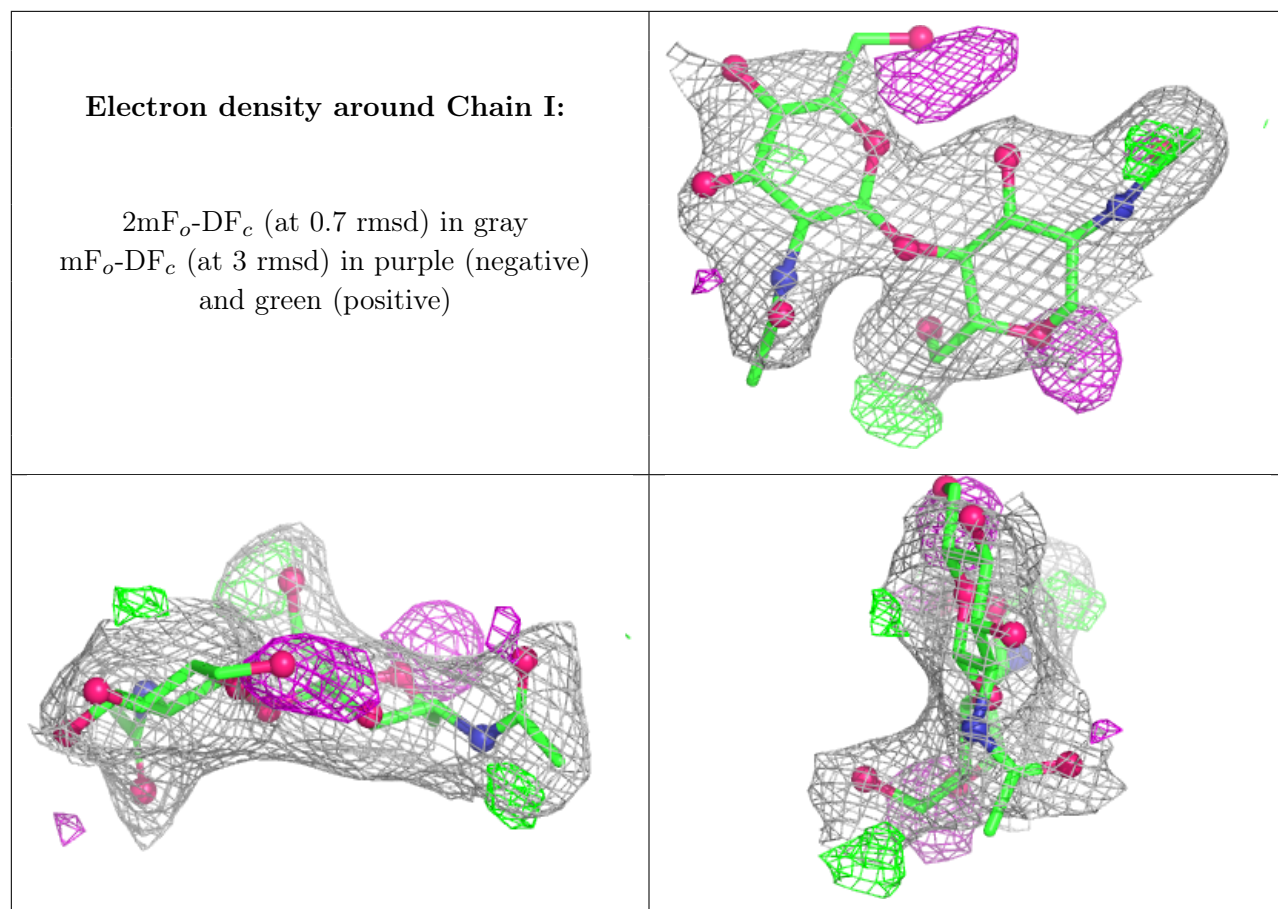
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain H:**

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





## 6.4 Ligands [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	E	403	14/15	0.61	0.19	76,84,89,90	0
4	NAG	C	403	14/15	0.70	0.18	75,78,85,92	0
4	NAG	A	403	14/15	0.71	0.15	77,81,89,89	0
5	EPE	E	404	15/15	0.85	0.13	26,37,62,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.