Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 10:18 PM EDT

PDB ID	:	6XPZ
Title	:	Human antibody S1V2-83 in complex with the influenza hemagglutinin head domain of A/Moscow/10/1999(H3N2)
Authors	:	McCarthy, K.R.; Harrison, S.C.
Deposited on	:	2020-07-09
Resolution	:	3.45 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:

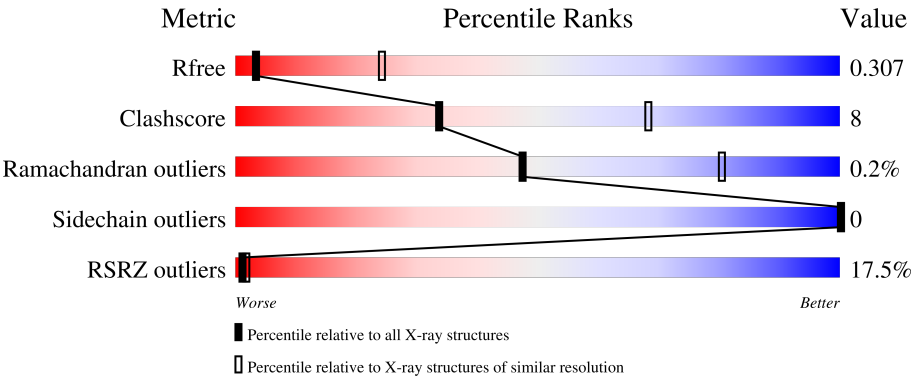
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.45 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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 <=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	290	19% 73% 19% 8%
1	D	290	9% 72% 20% 7%
2	B	243	23% 74% 22% .
2	E	243	16% 73% 23% .
3	C	214	16% 81% 17% .

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Mol	Chain	Length	Quality of chain
3	F	214	18% 84% 15%
4	G	2	100%
5	H	3	33% 33% 33%
5	J	3	33% 33% 33%
6	I	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	G	2	-	-	-	X
5	NAG	J	1	-	-	-	X
5	BMA	J	3	-	-	-	X
6	BMA	I	3	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11182 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2107	1319	377	401	10			
1	D	269	Total	C	N	O	S	0	0	0
			2116	1323	381	402	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	ALA	-	expression tag	UNP Q1NZ37
A	321	LEU	-	expression tag	UNP Q1NZ37
A	322	GLU	-	expression tag	UNP Q1NZ37
A	323	VAL	-	expression tag	UNP Q1NZ37
A	324	LEU	-	expression tag	UNP Q1NZ37
A	325	PHE	-	expression tag	UNP Q1NZ37
A	326	GLN	-	expression tag	UNP Q1NZ37
D	320	ALA	-	expression tag	UNP Q1NZ37
D	321	LEU	-	expression tag	UNP Q1NZ37
D	322	GLU	-	expression tag	UNP Q1NZ37
D	323	VAL	-	expression tag	UNP Q1NZ37
D	324	LEU	-	expression tag	UNP Q1NZ37
D	325	PHE	-	expression tag	UNP Q1NZ37
D	326	GLN	-	expression tag	UNP Q1NZ37

- Molecule 2 is a protein called antibody S1V2-83 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1761	1114	298	342	7			
2	E	233	Total	C	N	O	S	0	0	0
			1761	1114	298	342	7			

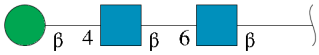
- Molecule 3 is a protein called antibody S1V2-83 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1632	1021	271	335	5			
3	F	211	Total	C	N	O	S	0	0	0
			1632	1021	271	335	5			

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

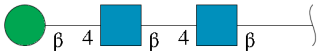
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



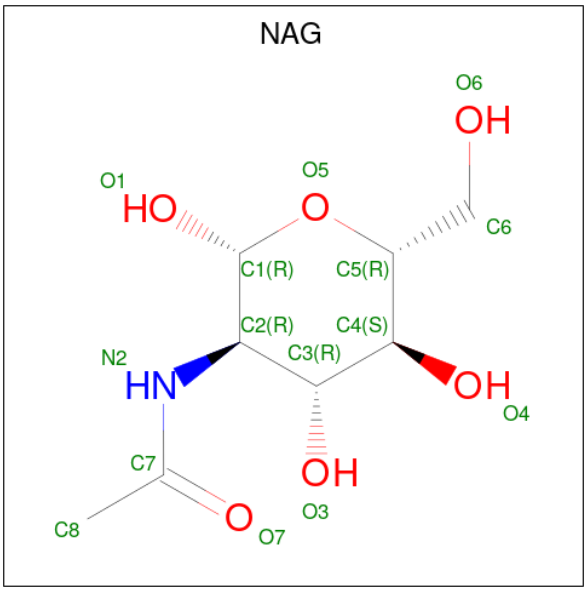
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



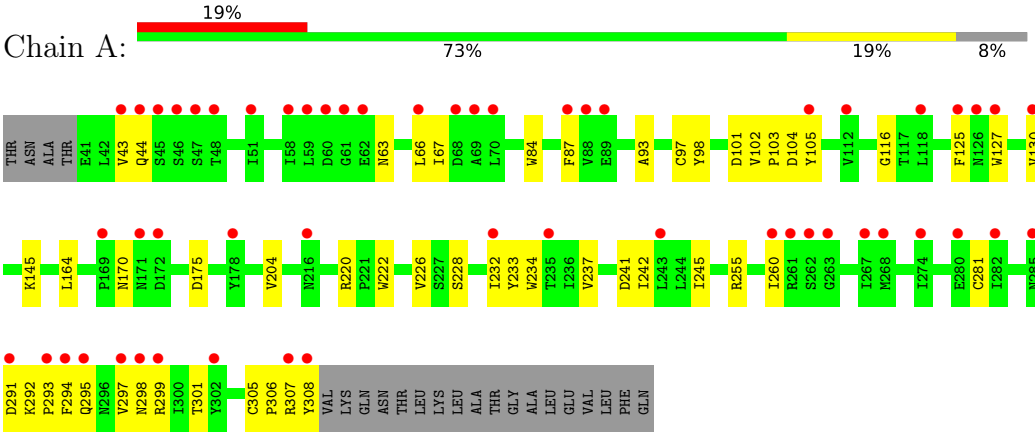
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0

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.

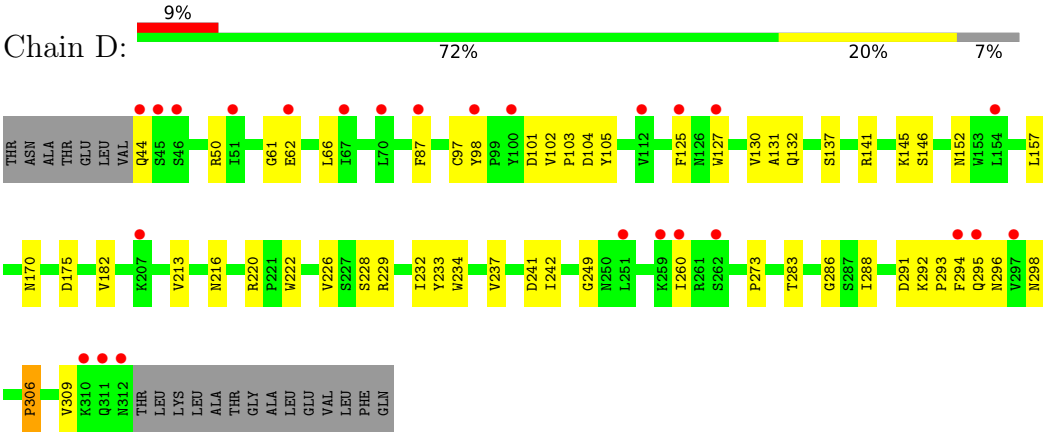
• Molecule 1: Hemagglutinin

Chain A:



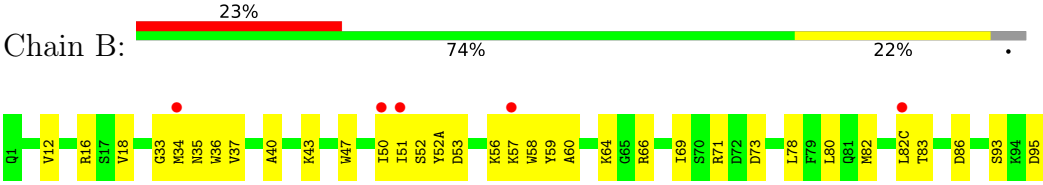
• Molecule 1: Hemagglutinin

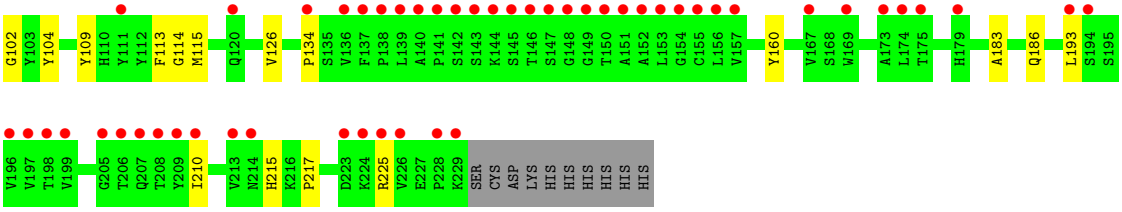
Chain D:



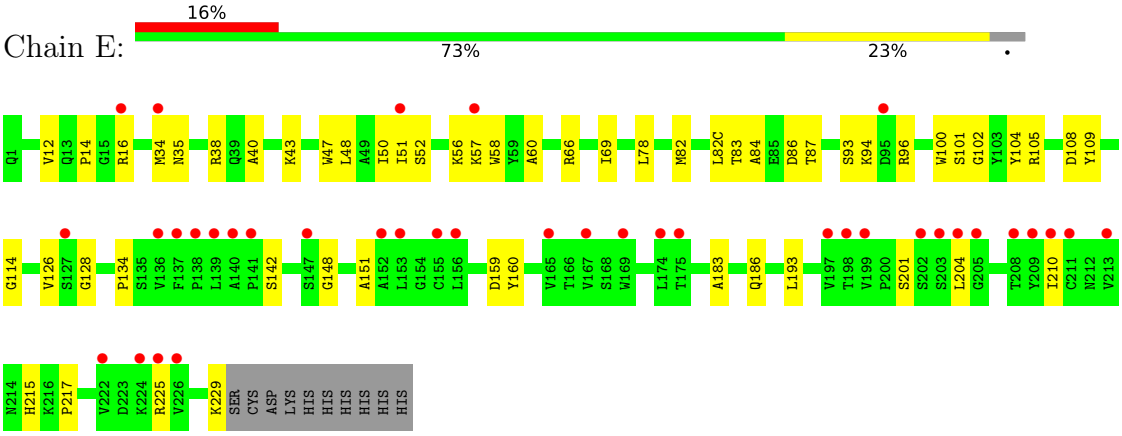
• Molecule 2: antibody S1V2-83 heavy chain

Chain B:

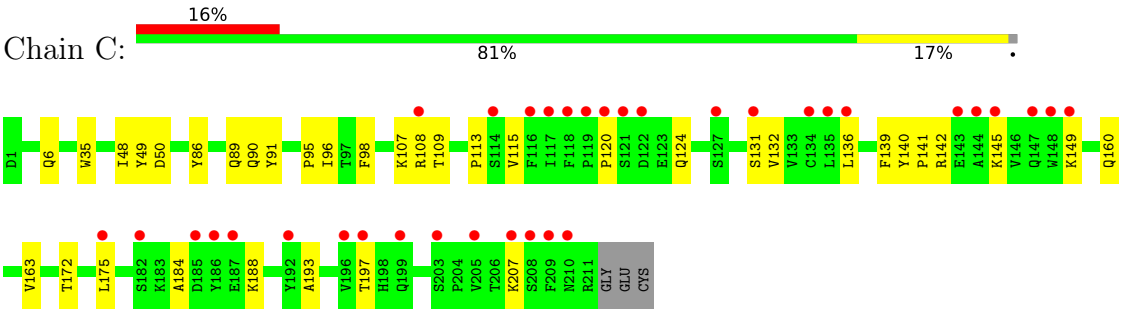




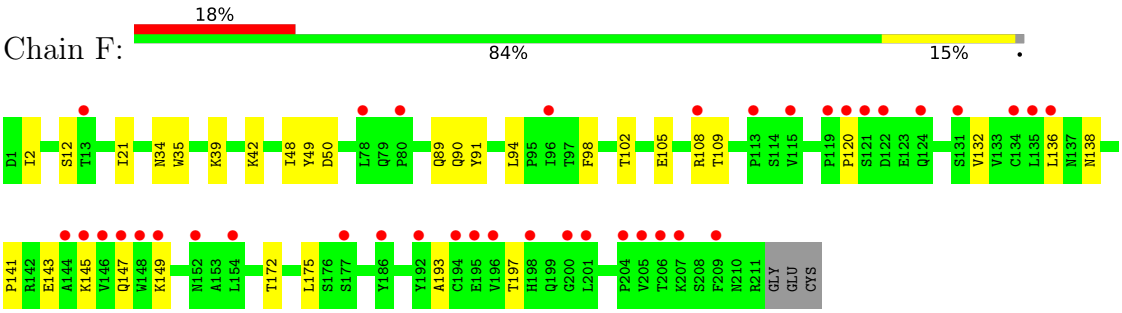
• Molecule 2: antibody S1V2-83 heavy chain



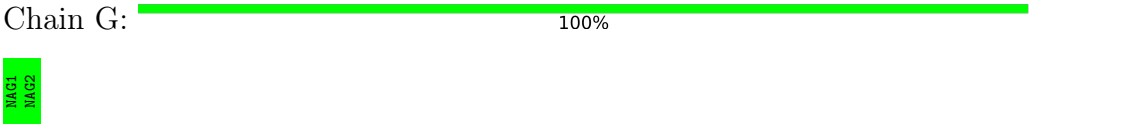
• Molecule 3: antibody S1V2-83 light chain



• Molecule 3: antibody S1V2-83 light chain

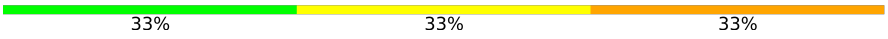


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



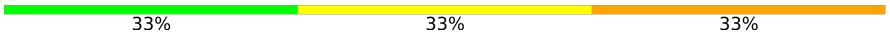
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	85.79Å 103.71Å 220.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 3.45 49.10 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.10-3.45) 85.4 (49.10-3.45)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.251 , 0.307 0.251 , 0.307	Depositor DCC
R_{free} test set	1327 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	83.6	Xtriage
Anisotropy	1.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 81.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11182	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.24	0/2159	0.43	0/2935
1	D	0.24	0/2168	0.44	0/2946
2	B	0.25	0/1807	0.46	0/2457
2	E	0.26	0/1807	0.46	0/2457
3	C	0.25	0/1667	0.46	0/2265
3	F	0.25	0/1667	0.45	0/2265
All	All	0.25	0/11275	0.45	0/15325

There are no bond length outliers.

There are no bond angle outliers.

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	2107	0	2042	37	0
1	D	2116	0	2052	42	0
2	B	1761	0	1703	43	0
2	E	1761	0	1703	41	0
3	C	1632	0	1574	23	0
3	F	1632	0	1574	20	0
4	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	39	0	34	1	0
5	J	39	0	34	1	0
6	I	39	0	34	0	0
7	A	14	0	13	0	0
7	D	14	0	13	0	0
All	All	11182	0	10801	186	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 8.

All (186) 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:44:GLN:HE22	1:A:289:PRO:HD2	1.43	0.84
1:A:295:GLN:HE21	1:A:297:VAL:HB	1.45	0.82
1:D:137:SER:HB3	1:D:145:LYS:HE2	1.66	0.75
1:A:104:ASP:HB3	1:A:234:TRP:HH2	1.52	0.75
2:E:66:ARG:NH2	2:E:86:ASP:OD2	2.21	0.74
1:D:104:ASP:HB3	1:D:234:TRP:HH2	1.53	0.73
1:A:301:THR:OG1	1:A:305:CYS:SG	2.47	0.72
1:A:137:SER:HB3	1:A:145:LYS:HE2	1.72	0.71
1:D:50:ARG:NH2	2:B:52(A):TYR:O	2.20	0.71
5:J:1:NAG:H3	5:J:1:NAG:H83	1.75	0.69
1:D:102:VAL:H	2:E:104:TYR:HE2	1.39	0.69
1:A:226:VAL:HG12	1:A:228:SER:H	1.60	0.67
2:B:58:TRP:HE1	3:C:95:PRO:HB3	1.61	0.65
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.78	0.65
1:A:220:ARG:HG3	2:B:101:SER:HB3	1.79	0.65
3:C:50:ASP:OD1	3:C:91:TYR:OH	2.17	0.63
1:D:226:VAL:HG12	1:D:228:SER:H	1.66	0.61
3:F:145:LYS:HB3	3:F:197:THR:HB	1.83	0.60
1:D:102:VAL:HG22	1:D:232:ILE:HB	1.82	0.60
2:B:82:MET:HB3	2:B:82(C):LEU:HD21	1.83	0.60
2:E:82:MET:HB3	2:E:82(C):LEU:HD21	1.82	0.60
2:E:114:GLY:HA2	3:F:89:GLN:HE22	1.67	0.60
1:D:295:GLN:NE2	1:D:306:PRO:HD2	2.16	0.60
3:F:149:LYS:HB2	3:F:193:ALA:HB3	1.83	0.60
2:B:52:SER:HB3	2:B:56:LYS:HB2	1.83	0.60
2:B:96:ARG:HH21	2:B:114:GLY:H	1.48	0.60
3:F:12:SER:OG	3:F:105:GLU:OE1	2.20	0.60
2:E:34:MET:HB3	2:E:78:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:GLY:HA2	2:B:71:ARG:HH22	1.66	0.59
2:B:35:ASN:HD22	2:B:115:MET:HG2	1.68	0.59
2:B:134:PRO:HB3	2:B:160:TYR:HB3	1.86	0.58
1:A:43:VAL:HG11	1:A:294:PHE:HB2	1.87	0.57
2:B:47:TRP:HH2	2:B:58:TRP:HD1	1.52	0.57
2:E:51:ILE:HG22	2:E:52:SER:O	2.05	0.56
1:D:273:PRO:HG2	2:B:73:ASP:HB3	1.86	0.56
2:E:51:ILE:HG13	2:E:69:ILE:HD13	1.88	0.56
3:F:50:ASP:OD1	3:F:91:TYR:OH	2.24	0.56
3:C:145:LYS:HB3	3:C:197:THR:HB	1.88	0.55
1:A:220:ARG:HH21	2:B:100:TRP:HB2	1.72	0.55
1:D:130:VAL:HG11	1:D:164:LEU:HD11	1.89	0.55
3:C:149:LYS:HB2	3:C:193:ALA:HB3	1.89	0.55
1:D:161:TYR:CE2	1:D:249:GLY:HA2	2.41	0.55
1:D:220:ARG:HG2	1:D:229:ARG:HG2	1.87	0.55
2:B:47:TRP:HZ2	2:B:50:ILE:HG13	1.72	0.55
2:B:183:ALA:HB2	2:B:193:LEU:HD23	1.88	0.55
3:F:35:TRP:HB2	3:F:48:ILE:HB	1.89	0.55
5:H:2:NAG:H83	5:H:2:NAG:H3	1.89	0.54
1:D:97:CYS:SG	1:D:98:TYR:N	2.77	0.54
2:B:51:ILE:HG13	2:B:69:ILE:HD13	1.88	0.54
2:B:33:GLY:C	2:B:95:ASP:HB2	2.29	0.54
2:E:183:ALA:HB2	2:E:193:LEU:HD23	1.88	0.54
3:C:89:GLN:HG3	3:C:98:PHE:CE1	2.43	0.53
2:B:33:GLY:HA2	2:B:71:ARG:NH2	2.23	0.53
1:A:295:GLN:O	1:A:308:TYR:HA	2.08	0.53
1:D:104:ASP:HB3	1:D:234:TRP:CH2	2.39	0.53
1:A:288:ILE:HG13	1:A:295:GLN:HE22	1.74	0.53
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.91	0.53
2:E:87:THR:OG1	2:E:126:VAL:HG22	2.09	0.52
2:E:14:PRO:HD3	2:E:128:GLY:HA3	1.91	0.52
1:A:204:VAL:HG22	1:A:245:ILE:HG12	1.90	0.52
2:B:51:ILE:HG12	2:B:57:LYS:HG2	1.91	0.52
1:A:97:CYS:SG	1:A:98:TYR:N	2.82	0.52
1:A:170:ASN:HD22	1:A:237:VAL:HG12	1.74	0.52
3:C:35:TRP:HB2	3:C:48:ILE:HB	1.91	0.52
2:E:105:ARG:HB2	2:E:108:ASP:HB3	1.92	0.52
1:A:44:GLN:HB2	1:A:292:LYS:HD2	1.90	0.52
2:B:183:ALA:HA	2:B:193:LEU:HB3	1.90	0.52
1:D:241:ASP:OD1	1:D:242:ILE:N	2.43	0.51
1:D:50:ARG:CZ	2:B:53:ASP:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:SER:HA	2:E:204:LEU:HG	1.93	0.51
1:A:241:ASP:OD1	1:A:242:ILE:N	2.44	0.51
1:D:170:ASN:HD22	1:D:237:VAL:HG12	1.76	0.51
1:D:170:ASN:ND2	1:D:237:VAL:O	2.43	0.51
1:A:104:ASP:HB3	1:A:234:TRP:CH2	2.38	0.51
1:D:216:ASN:OD1	2:E:100:TRP:NE1	2.44	0.51
1:A:295:GLN:HG2	1:A:297:VAL:H	1.75	0.50
3:F:136:LEU:HB2	3:F:175:LEU:HB3	1.94	0.50
1:D:220:ARG:HH21	2:E:100:TRP:HB2	1.77	0.50
2:E:183:ALA:HA	2:E:193:LEU:HB3	1.94	0.50
1:A:294:PHE:HE2	1:A:307:ARG:HE	1.57	0.50
2:E:210:ILE:HG12	2:E:225:ARG:HG2	1.94	0.49
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.94	0.49
3:C:107:LYS:HG2	3:C:108:ARG:H	1.77	0.49
3:F:89:GLN:HG3	3:F:98:PHE:CE1	2.48	0.49
2:E:47:TRP:HZ3	2:E:60:ALA:HA	1.78	0.49
1:D:141:ARG:NH1	1:D:146:SER:OG	2.46	0.49
1:A:298:ASN:OD1	1:A:299:ARG:N	2.45	0.49
2:B:37:VAL:HG22	2:B:47:TRP:HA	1.94	0.49
1:D:283:THR:HG22	1:D:301:THR:HG22	1.95	0.48
1:D:291:ASP:OD1	1:D:292:LYS:N	2.45	0.48
2:B:60:ALA:O	2:B:64:LYS:N	2.40	0.48
1:D:44:GLN:HG2	1:D:288:ILE:HG23	1.95	0.48
1:D:137:SER:HA	1:D:145:LYS:HG2	1.95	0.48
3:C:115:VAL:O	3:C:207:LYS:NZ	2.46	0.48
1:D:175:ASP:HB2	1:D:260:ILE:HG22	1.95	0.48
2:E:134:PRO:HB3	2:E:160:TYR:HB3	1.95	0.48
3:C:140:TYR:CD1	3:C:141:PRO:HA	2.49	0.48
3:F:138:ASN:ND2	3:F:172:THR:OG1	2.36	0.48
1:D:101:ASP:HB3	2:E:102:GLY:O	2.13	0.48
1:D:298:ASN:OD1	1:D:299:ARG:N	2.46	0.48
3:F:120:PRO:HD3	3:F:132:VAL:HG22	1.96	0.47
1:D:161:TYR:HE2	1:D:249:GLY:HA2	1.77	0.47
3:C:89:GLN:NE2	3:C:90:GLN:O	2.45	0.47
2:B:34:MET:HB3	2:B:78:LEU:HD22	1.96	0.47
2:B:47:TRP:CZ2	2:B:50:ILE:HG13	2.49	0.47
3:F:141:PRO:HG2	3:F:143:GLU:HG2	1.97	0.47
3:C:136:LEU:HB2	3:C:175:LEU:HB3	1.97	0.47
2:E:84:ALA:HA	2:E:126:VAL:HG23	1.95	0.47
2:E:159:ASP:OD1	2:E:186:GLN:NE2	2.48	0.47
3:F:2:ILE:HB	3:F:90:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ASN:HB2	2:B:93:SER:OG	2.15	0.47
2:E:151:ALA:HB2	2:E:201:SER:HB3	1.96	0.46
1:D:132:GLN:HB3	1:D:152:ASN:HD21	1.80	0.46
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.96	0.46
2:B:50:ILE:HD11	3:C:96:ILE:HD12	1.97	0.46
3:F:145:LYS:HE2	3:F:147:GLN:HE21	1.80	0.46
3:F:39:LYS:HB2	3:F:42:LYS:HD2	1.96	0.46
1:D:220:ARG:HG3	2:E:101:SER:CB	2.46	0.46
2:B:12:VAL:HG21	2:B:18:VAL:HG21	1.98	0.46
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.48	0.46
2:E:47:TRP:CZ3	2:E:60:ALA:HA	2.51	0.45
3:C:89:GLN:HG3	3:C:98:PHE:HE1	1.81	0.45
1:D:131:ALA:HB2	1:D:157:LEU:HD13	1.99	0.45
2:B:102:GLY:HA3	2:B:109:TYR:CZ	2.51	0.45
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.37	0.45
2:B:96:ARG:NH2	2:B:113:PHE:HB3	2.32	0.45
3:C:6:GLN:NE2	3:C:86:TYR:O	2.50	0.45
1:A:63:ASN:HA	1:A:93:ALA:HA	1.99	0.44
2:B:16:ARG:HD2	2:B:16:ARG:HA	1.79	0.44
2:E:114:GLY:HA3	3:F:34:ASN:ND2	2.32	0.44
1:D:296:ASN:HA	1:D:309:VAL:HA	1.98	0.44
3:C:113:PRO:HB3	3:C:139:PHE:HB3	2.00	0.44
2:B:35:ASN:OD1	2:B:50:ILE:HG12	2.18	0.44
2:B:210:ILE:HG12	2:B:225:ARG:HG2	2.00	0.44
1:A:222:TRP:HZ3	3:C:49:TYR:HE2	1.65	0.43
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.52	0.43
1:A:175:ASP:HB2	1:A:260:ILE:HG22	1.99	0.43
1:D:125:PHE:HB2	1:D:127:TRP:NE1	2.33	0.43
1:D:105:TYR:HB2	2:E:104:TYR:OH	2.19	0.43
2:E:38:ARG:HB3	2:E:48:LEU:HD11	1.99	0.43
1:A:130:VAL:HG11	1:A:164:LEU:HD11	2.01	0.43
1:A:291:ASP:OD1	1:A:292:LYS:N	2.51	0.43
3:C:107:LYS:O	3:C:108:ARG:HG2	2.19	0.43
2:B:47:TRP:CH2	2:B:58:TRP:HD1	2.35	0.42
2:B:82(C):LEU:HB3	2:B:126:VAL:HG11	2.01	0.42
3:C:142:ARG:CZ	3:C:163:VAL:HG21	2.49	0.42
2:B:59:TYR:CZ	2:B:69:ILE:HG22	2.54	0.42
2:E:51:ILE:HG12	2:E:57:LYS:HG2	2.01	0.42
1:A:125:PHE:HB2	1:A:127:TRP:NE1	2.33	0.42
1:D:102:VAL:N	2:E:104:TYR:HE2	2.13	0.42
2:E:12:VAL:HG13	2:E:126:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:HA	1:A:145:LYS:HG2	2.01	0.42
2:E:58:TRP:NE1	3:F:94:LEU:HB3	2.34	0.42
2:E:58:TRP:CD1	3:F:94:LEU:HB3	2.55	0.42
2:B:215:HIS:CE1	2:B:217:PRO:HB2	2.54	0.42
2:E:215:HIS:CE1	2:E:217:PRO:HB2	2.55	0.42
1:A:66:LEU:HA	1:A:87:PHE:HE2	1.85	0.41
1:D:61:GLY:C	1:D:62:GLU:HG2	2.41	0.41
1:D:182:VAL:HG21	1:D:213:VAL:HB	2.01	0.41
1:D:283:THR:OG1	1:D:286:GLY:O	2.30	0.41
1:A:101:ASP:HA	2:B:104:TYR:CD2	2.54	0.41
1:D:293:PRO:HG2	1:D:294:PHE:HD1	1.85	0.41
1:D:222:TRP:HZ3	3:F:49:TYR:HE2	1.67	0.41
1:A:293:PRO:O	1:A:306:PRO:HB3	2.20	0.41
2:B:83:THR:O	2:B:126:VAL:HG21	2.20	0.41
2:E:35:ASN:OD1	2:E:50:ILE:HG12	2.20	0.41
2:E:94:LYS:HG2	2:E:96:ARG:H	1.84	0.41
3:F:21:ILE:HG21	3:F:102:THR:HG21	2.01	0.41
2:E:83:THR:O	2:E:126:VAL:HG21	2.20	0.41
2:E:142:SER:HB3	2:E:229:LYS:HD2	2.01	0.41
3:C:124:GLN:OE1	3:C:131:SER:N	2.53	0.41
3:C:184:ALA:O	3:C:188:LYS:HG3	2.20	0.41
1:A:281:CYS:HB3	1:A:288:ILE:O	2.21	0.41
2:B:36:TRP:CG	2:B:80:LEU:HD22	2.56	0.41
3:C:109:THR:HG21	3:C:172:THR:HG22	2.01	0.41
1:D:103:PRO:HG2	1:D:233:TYR:CE1	2.56	0.41
2:B:52:SER:O	2:B:71:ARG:NH2	2.53	0.41
1:A:103:PRO:HG2	1:A:233:TYR:CE1	2.55	0.41
2:B:186:GLN:HA	3:C:160:GLN:HE22	1.85	0.41
2:E:16:ARG:HA	2:E:16:ARG:HD2	1.85	0.41
3:F:108:ARG:HD2	3:F:109:THR:H	1.86	0.41
1:A:98:TYR:CZ	1:A:226:VAL:HG11	2.56	0.40
2:E:35:ASN:HB2	2:E:93:SER:OG	2.21	0.40
1:A:67:ILE:HG13	1:A:105:TYR:CE1	2.56	0.40
1:D:66:LEU:HA	1:D:87:PHE:HE2	1.86	0.40
2:E:52:SER:HB3	2:E:56:LYS:HB2	2.03	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	266/290 (92%)	254 (96%)	12 (4%)	0	100 100
1	D	267/290 (92%)	254 (95%)	12 (4%)	1 (0%)	34 70
2	B	231/243 (95%)	218 (94%)	13 (6%)	0	100 100
2	E	231/243 (95%)	211 (91%)	18 (8%)	2 (1%)	17 54
3	C	209/214 (98%)	198 (95%)	11 (5%)	0	100 100
3	F	209/214 (98%)	197 (94%)	12 (6%)	0	100 100
All	All	1413/1494 (95%)	1332 (94%)	78 (6%)	3 (0%)	47 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	306	PRO
2	E	109	TYR
2	E	148	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	239/257 (93%)	239 (100%)	0	100 100
1	D	240/257 (93%)	240 (100%)	0	100 100
2	B	193/203 (95%)	193 (100%)	0	100 100
2	E	193/203 (95%)	193 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	188/190 (99%)	188 (100%)	0	100	100
3	F	188/190 (99%)	188 (100%)	0	100	100
All	All	1241/1300 (96%)	1241 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	295	GLN
1	D	170	ASN
2	B	35	ASN

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)

11 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	$\#\|Z\| > 2$
4	NAG	G	1	4,1	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	G	2	4	14,14,15	0.34	0	17,19,21	0.54	0
5	NAG	H	1	5,1	14,14,15	0.19	0	17,19,21	0.41	0
5	NAG	H	2	5	14,14,15	0.42	0	17,19,21	1.40	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	H	3	5	11,11,12	0.57	0	15,15,17	0.82	1 (6%)
6	NAG	I	1	6,1	14,14,15	0.31	0	17,19,21	0.59	0
6	NAG	I	2	6	14,14,15	0.29	0	17,19,21	0.49	0
6	BMA	I	3	6	11,11,12	1.00	1 (9%)	15,15,17	0.94	1 (6%)
5	NAG	J	1	5,1	14,14,15	1.14	1 (7%)	17,19,21	1.21	1 (5%)
5	NAG	J	2	5	14,14,15	0.88	1 (7%)	17,19,21	0.92	1 (5%)
5	BMA	J	3	5	11,11,12	0.69	0	15,15,17	0.70	0

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	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	NAG	C1-C2	3.90	1.58	1.52
5	J	2	NAG	O5-C1	-3.09	1.38	1.43
6	I	3	BMA	C1-C2	2.70	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	2	NAG	C2-N2-C7	4.42	129.20	122.90
5	J	1	NAG	C2-N2-C7	3.71	128.19	122.90
5	H	2	NAG	C1-C2-N2	2.21	114.27	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	3	BMA	O2-C2-C3	-2.15	105.82	110.14
5	H	3	BMA	C1-O5-C5	2.06	114.99	112.19
5	J	2	NAG	C3-C4-C5	2.04	113.87	110.24

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
6	I	2	NAG	O5-C5-C6-O6
5	J	3	BMA	O5-C5-C6-O6
5	J	3	BMA	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7
5	J	1	NAG	C3-C2-N2-C7
6	I	1	NAG	C3-C2-N2-C7
6	I	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C1-C2-N2-C7
5	H	2	NAG	C3-C2-N2-C7

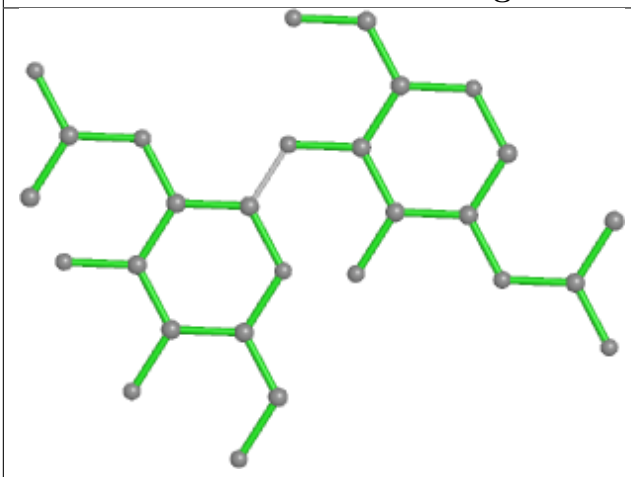
There are no ring outliers.

2 monomers are involved in 2 short contacts:

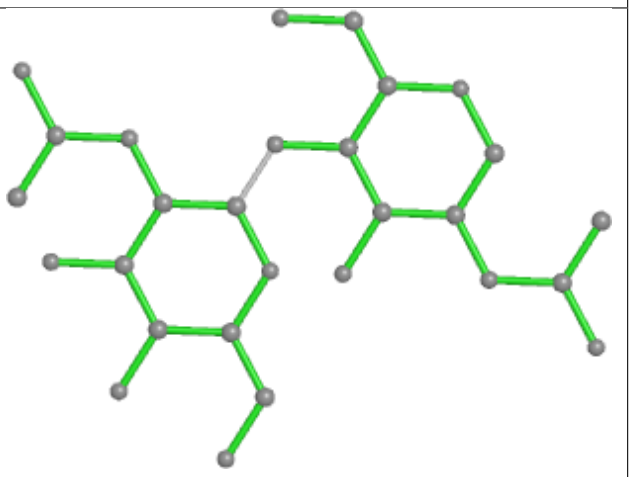
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
5	J	1	NAG	1	0

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

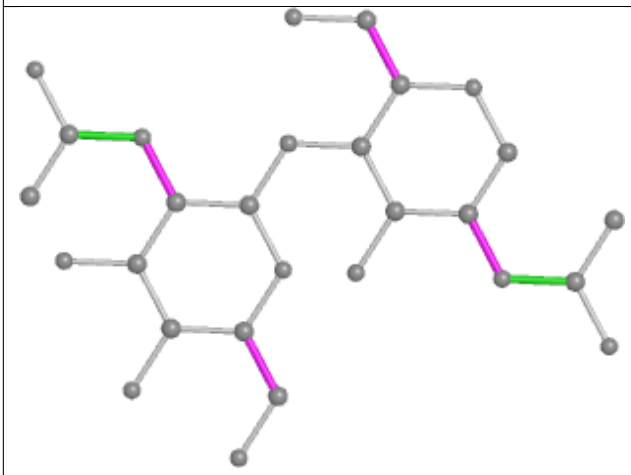
Oligosaccharide Chain G



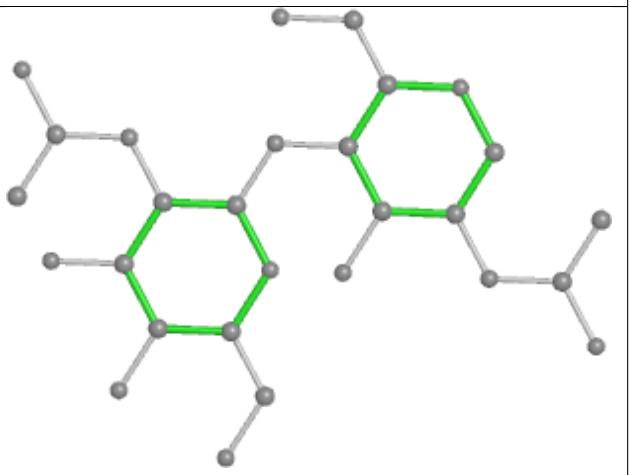
Bond lengths



Bond angles

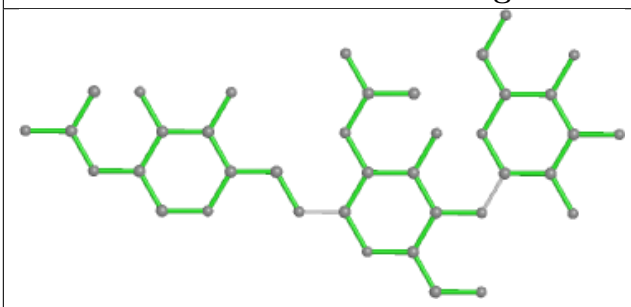


Torsions

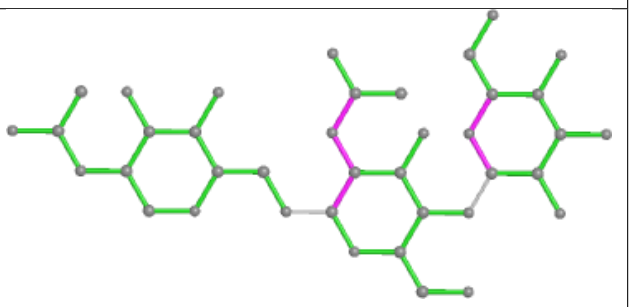


Rings

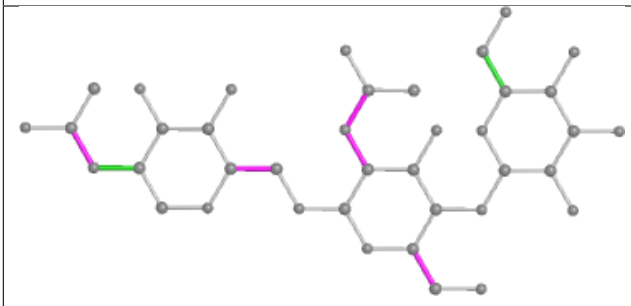
Oligosaccharide Chain H



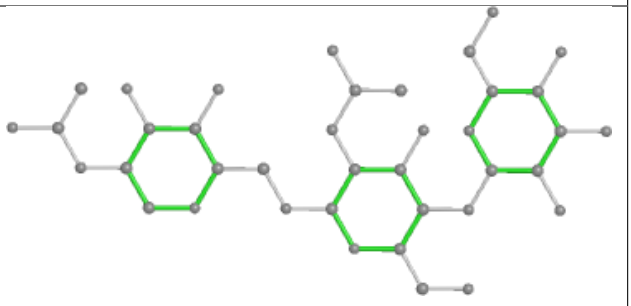
Bond lengths



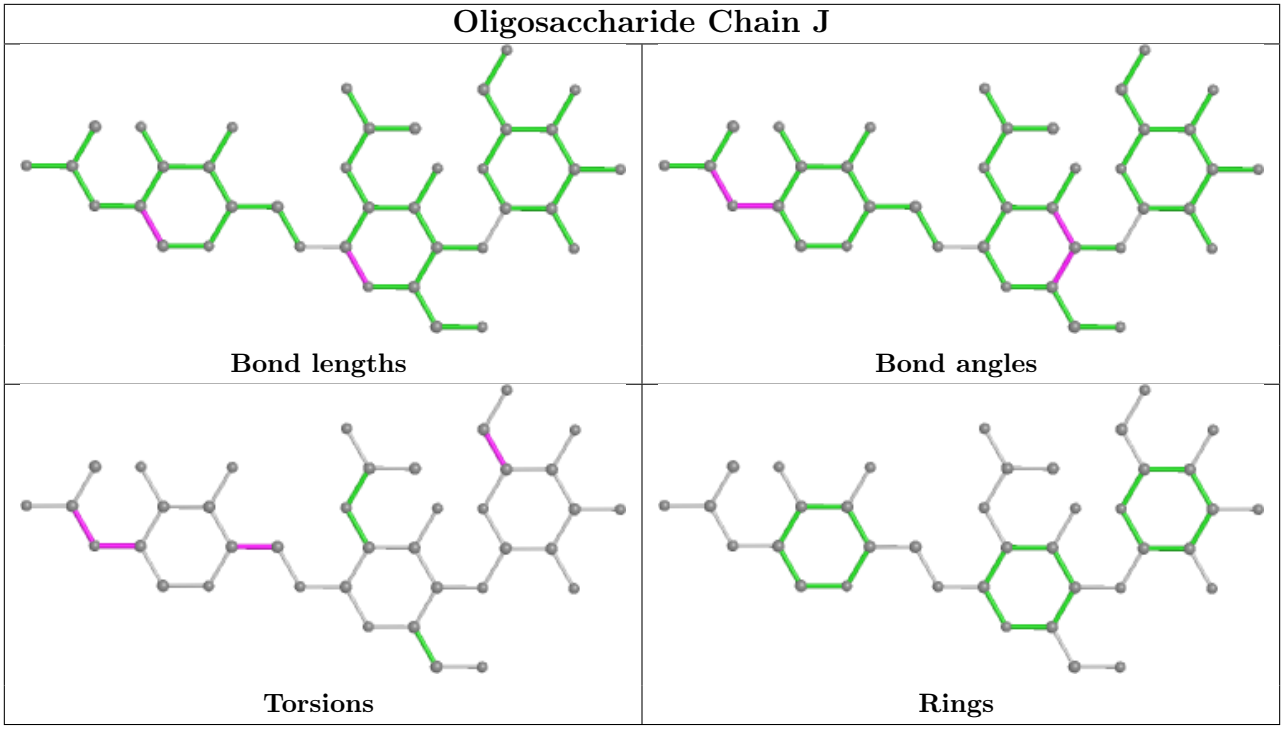
Bond angles

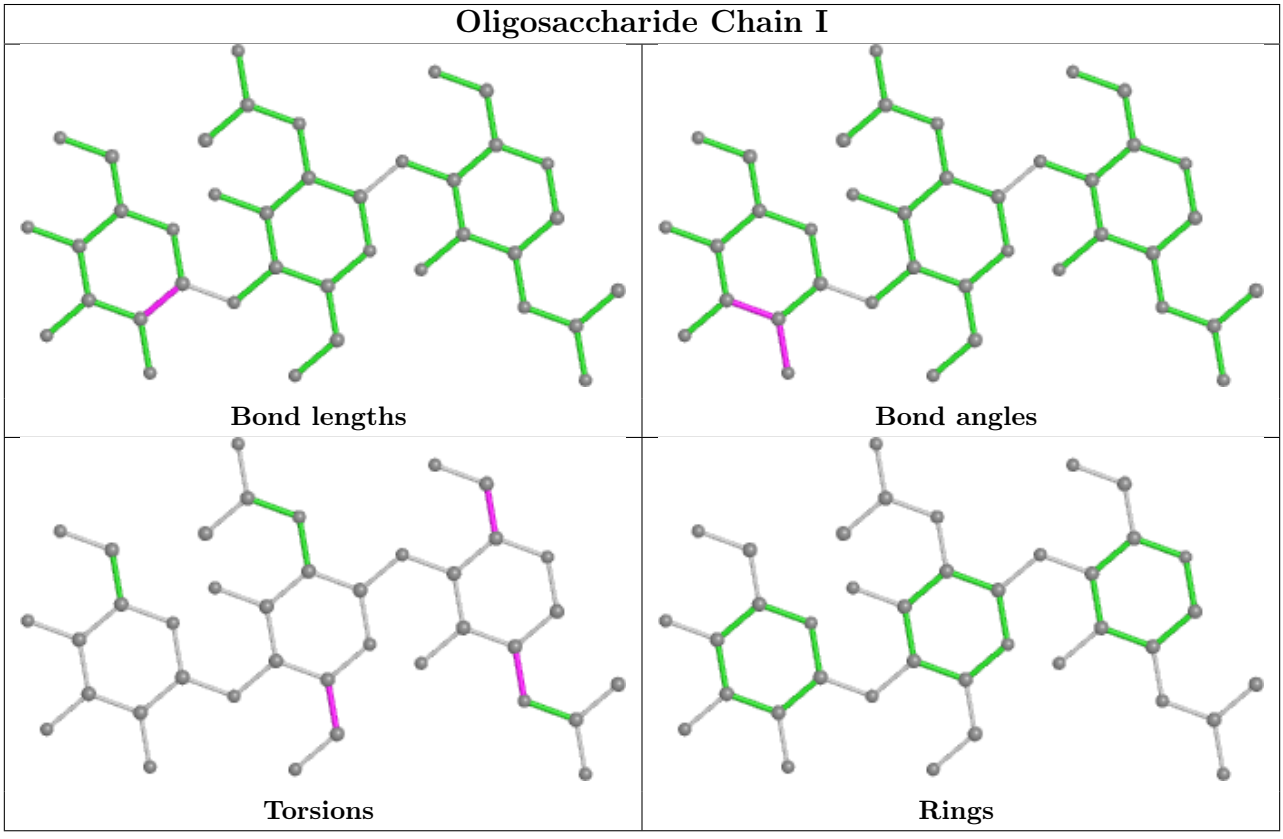


Torsions



Rings





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	$\#\|Z\| > 2$
7	NAG	A	401	1	14,14,15	0.24	0	17,19,21	0.54	0
7	NAG	D	401	1	14,14,15	0.17	0	17,19,21	0.43	0

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
7	NAG	A	401	1	-	3/6/23/26	0/1/1/1
7	NAG	D	401	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	NAG	O5-C5-C6-O6
7	A	401	NAG	C4-C5-C6-O6
7	D	401	NAG	C8-C7-N2-C2
7	D	401	NAG	O7-C7-N2-C2
7	D	401	NAG	O5-C5-C6-O6
7	A	401	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	268/290 (92%)	1.12	56 (20%) 1 1	95, 139, 186, 226	0
1	D	269/290 (92%)	0.82	26 (9%) 7 10	75, 113, 171, 240	0
2	B	233/243 (95%)	1.49	56 (24%) 0 0	89, 128, 253, 442	0
2	E	233/243 (95%)	1.07	38 (16%) 1 2	79, 124, 271, 333	0
3	C	211/214 (98%)	1.11	35 (16%) 1 2	81, 135, 229, 282	0
3	F	211/214 (98%)	1.04	38 (18%) 1 2	70, 146, 214, 261	0
All	All	1425/1494 (95%)	1.10	249 (17%) 1 2	70, 129, 232, 442	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	145	SER	13.5
2	B	152	ALA	13.5
2	B	153	LEU	12.6
2	B	136	VAL	8.6
2	B	141	PRO	8.2
2	B	209	TYR	8.0
2	B	174	LEU	8.0
2	E	153	LEU	7.8
2	B	225	ARG	7.8
2	E	209	TYR	7.6
3	C	186	TYR	7.3
2	B	154	GLY	7.2
2	B	138	PRO	7.0
3	C	208	SER	6.6
2	E	204	LEU	6.5
3	C	196	VAL	6.4
3	F	194	CYS	6.1
1	A	88	VAL	5.9
2	E	208	THR	5.8

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Mol	Chain	Res	Type	RSRZ
3	C	120	PRO	5.8
3	C	209	PHE	5.8
3	C	117	ILE	5.7
1	A	295	GLN	5.6
2	B	146	THR	5.6
3	C	145	LYS	5.6
1	D	311	GLN	5.5
1	A	262	SER	5.5
2	B	143	SER	5.4
2	B	197	VAL	5.4
2	B	205	GLY	5.3
2	E	138	PRO	5.2
2	B	137	PHE	5.2
2	E	225	ARG	5.1
3	C	121	SER	5.1
2	B	213	VAL	5.0
2	B	142	SER	5.0
2	B	198	THR	5.0
2	B	151	ALA	4.9
3	C	122	ASP	4.9
3	F	115	VAL	4.9
2	E	174	LEU	4.8
2	B	155	CYS	4.7
2	B	156	LEU	4.7
3	C	135	LEU	4.7
2	B	224	LYS	4.7
2	B	199	VAL	4.4
2	E	226	VAL	4.4
2	E	199	VAL	4.4
1	A	46	SER	4.4
1	D	260	ILE	4.4
3	C	119	PRO	4.3
3	F	205	VAL	4.3
3	F	147	GLN	4.3
2	B	228	PRO	4.2
1	A	308	TYR	4.2
3	F	152	ASN	4.1
2	E	137	PHE	4.1
3	F	186	TYR	4.1
3	F	131	SER	4.0
2	B	167	VAL	4.0
3	C	175	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	312	ASN	4.0
3	F	122	ASP	4.0
1	A	260	ILE	3.9
2	B	206	THR	3.9
1	D	295	GLN	3.9
2	E	152	ALA	3.8
1	D	297	VAL	3.8
1	D	46	SER	3.8
1	A	302	TYR	3.7
3	F	13	THR	3.7
1	D	262	SER	3.7
2	E	198	THR	3.7
3	F	207	LYS	3.6
1	A	294	PHE	3.6
3	F	201	LEU	3.6
1	A	127	TRP	3.6
1	D	45	SER	3.6
2	B	157	VAL	3.6
2	E	167	VAL	3.5
1	A	59	LEU	3.5
1	A	178	TYR	3.5
1	A	285	ASN	3.5
3	C	116	PHE	3.5
2	E	34	MET	3.5
2	B	210	ILE	3.4
1	A	45	SER	3.4
1	A	268	MET	3.4
2	E	139	LEU	3.4
2	E	202	SER	3.4
3	C	197	THR	3.3
3	F	149	LYS	3.3
3	F	196	VAL	3.3
3	F	192	TYR	3.3
1	A	87	PHE	3.3
2	B	134	PRO	3.3
3	F	113	PRO	3.3
2	E	197	VAL	3.3
1	A	263	GLY	3.3
3	C	207	LYS	3.3
1	A	47	SER	3.2
2	E	141	PRO	3.2
1	A	126	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	3.2
2	B	149	GLY	3.2
2	E	155	CYS	3.2
2	E	169	TRP	3.2
3	C	136	LEU	3.2
2	B	223	ASP	3.1
2	B	139	LEU	3.1
2	E	136	VAL	3.1
2	E	224	LYS	3.1
3	F	108	ARG	3.1
3	C	134	CYS	3.1
2	B	229	LYS	3.0
3	C	144	ALA	3.0
3	F	120	PRO	3.0
3	F	134	CYS	3.0
1	D	98	TYR	3.0
3	F	195	GLU	3.0
1	A	51	ILE	3.0
1	D	112	VAL	3.0
3	F	136	LEU	3.0
2	E	147	SER	3.0
1	A	89	GLU	2.9
2	E	210	ILE	2.9
1	A	261	ARG	2.9
3	F	154	LEU	2.9
2	B	208	THR	2.9
1	D	310	LYS	2.9
3	C	203	SER	2.9
1	A	297	VAL	2.9
2	E	222	VAL	2.8
1	A	172	ASP	2.8
1	A	291	ASP	2.8
3	C	114	SER	2.8
1	A	290	ASN	2.8
2	B	214	ASN	2.8
3	C	192	TYR	2.8
1	A	299	ARG	2.8
2	E	140	ALA	2.8
3	C	205	VAL	2.8
1	A	61	GLY	2.8
1	A	243	LEU	2.8
2	E	205	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	108	ARG	2.8
1	D	207	LYS	2.8
1	D	70	LEU	2.7
2	E	165	VAL	2.7
3	C	127	SER	2.7
1	A	112	VAL	2.7
3	C	143	GLU	2.7
1	D	154	LEU	2.7
2	E	211	CYS	2.7
2	E	156	LEU	2.7
1	D	294	PHE	2.7
2	B	144	LYS	2.7
2	B	173	ALA	2.7
1	A	280	GLU	2.6
1	A	274	ILE	2.6
3	F	119	PRO	2.6
2	B	147	SER	2.6
3	C	199	GLN	2.6
2	B	150	THR	2.6
3	F	209	PHE	2.6
2	B	140	ALA	2.6
1	A	130	VAL	2.6
1	A	58	ILE	2.6
2	E	57	LYS	2.5
1	A	288	ILE	2.5
3	C	131	SER	2.5
2	B	169	TRP	2.5
1	A	60	ASP	2.5
1	D	127	TRP	2.5
1	D	302	TYR	2.5
2	B	57	LYS	2.5
3	C	148	TRP	2.5
2	B	51	ILE	2.5
1	A	125	PHE	2.5
1	D	125	PHE	2.4
3	C	147	GLN	2.4
3	C	149	LYS	2.4
2	E	203	SER	2.4
3	C	185	ASP	2.4
3	F	96	ILE	2.4
1	A	307	ARG	2.4
3	C	118	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	105	TYR	2.4
3	F	145	LYS	2.3
3	F	200	GLY	2.3
2	B	148	GLY	2.3
2	B	196	VAL	2.3
2	B	82(C)	LEU	2.3
3	C	187	GLU	2.3
2	E	16	ARG	2.3
1	A	293	PRO	2.3
3	F	206	THR	2.3
2	B	179	HIS	2.3
1	A	69	ALA	2.3
1	D	51	ILE	2.3
1	D	251	LEU	2.3
1	D	100	TYR	2.3
3	C	210	ASN	2.3
2	B	34	MET	2.3
3	F	198	HIS	2.3
1	A	298	ASN	2.3
1	D	259	LYS	2.3
1	A	282	ILE	2.2
2	B	226	VAL	2.2
2	E	213	VAL	2.2
3	F	146	VAL	2.2
2	B	193	LEU	2.2
1	D	67	ILE	2.2
3	F	124	GLN	2.2
3	F	148	TRP	2.2
1	A	267	ILE	2.2
1	A	68	ASP	2.2
3	C	182	SER	2.2
2	B	111	TYR	2.2
3	F	80	PRO	2.2
2	E	127	SER	2.2
2	E	95	ASP	2.2
3	F	144	ALA	2.2
3	F	204	PRO	2.2
1	D	62	GLU	2.2
2	B	120	GLN	2.2
2	B	50	ILE	2.2
1	A	66	LEU	2.1
3	F	135	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	87	PHE	2.1
3	F	121	SER	2.1
1	A	216	ASN	2.1
1	D	44	GLN	2.1
1	A	62	GLU	2.1
1	A	235	THR	2.1
1	A	169	PRO	2.1
3	F	78	LEU	2.1
2	B	207	GLN	2.1
2	E	175	THR	2.1
1	A	70	LEU	2.1
1	A	232	ILE	2.1
2	E	51	ILE	2.1
1	A	48	THR	2.0
1	A	44	GLN	2.0
1	A	171	ASN	2.0
2	B	194	SER	2.0
3	F	177	SER	2.0
1	A	118	LEU	2.0
2	B	175	THR	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^{th} 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	G	2	14/15	0.53	0.46	162,185,194,196	0
6	BMA	I	3	11/12	0.54	0.41	165,175,180,183	0
5	NAG	J	1	14/15	0.63	0.44	113,137,147,147	0
5	BMA	J	3	11/12	0.66	0.45	160,167,179,182	0
5	NAG	J	2	14/15	0.71	0.40	141,157,174,178	0
5	NAG	H	2	14/15	0.73	0.22	134,153,164,169	0
4	NAG	G	1	14/15	0.74	0.37	153,172,183,186	0
5	NAG	H	1	14/15	0.76	0.39	138,159,167,168	0

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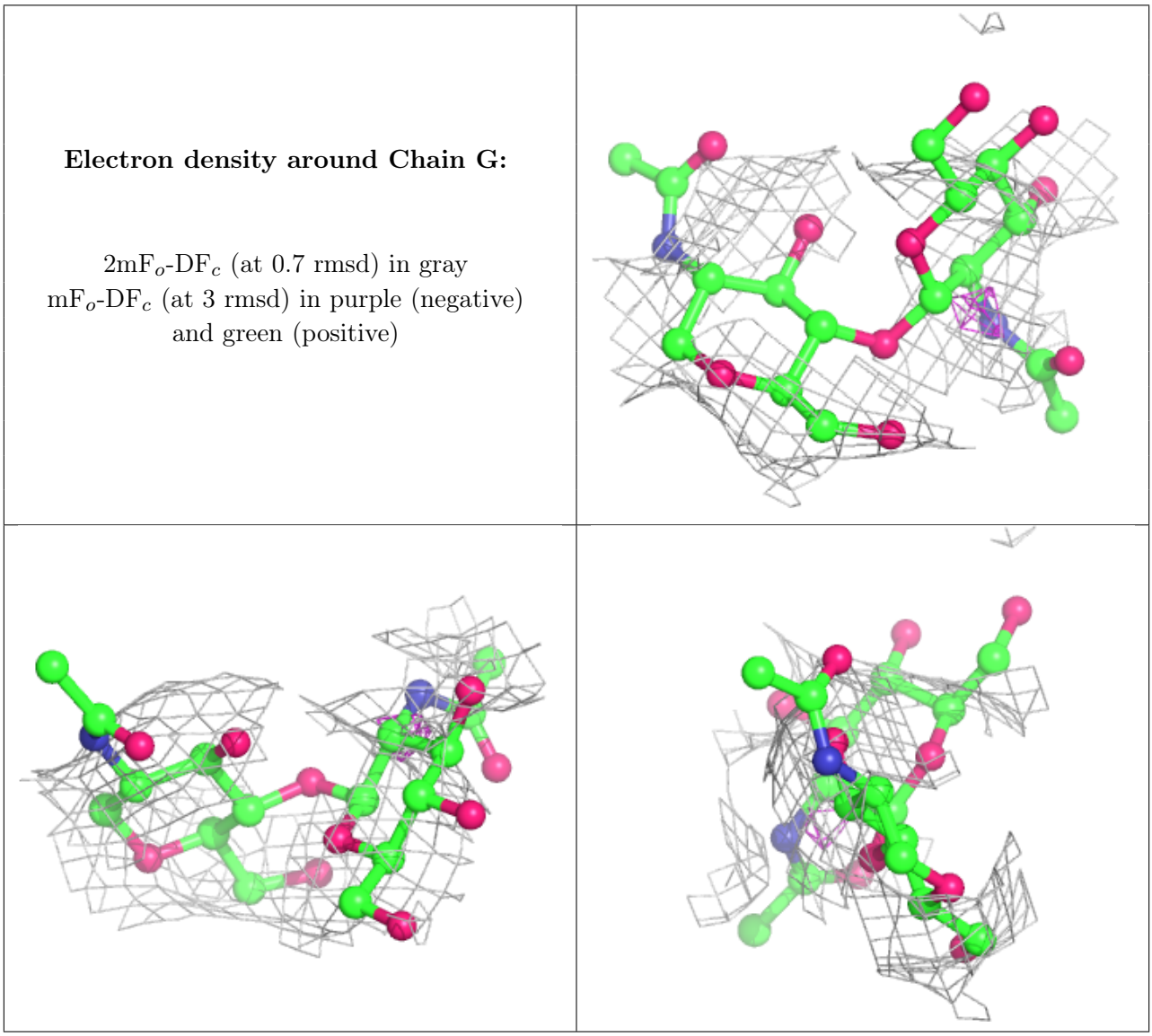
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	I	2	14/15	0.78	0.35	126,157,172,176	0
5	BMA	H	3	11/12	0.78	0.37	155,160,164,164	0
6	NAG	I	1	14/15	0.83	0.26	105,125,143,154	0

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.

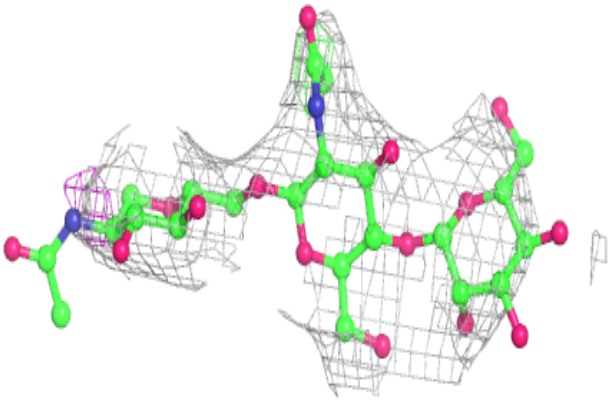
Electron density around Chain G:

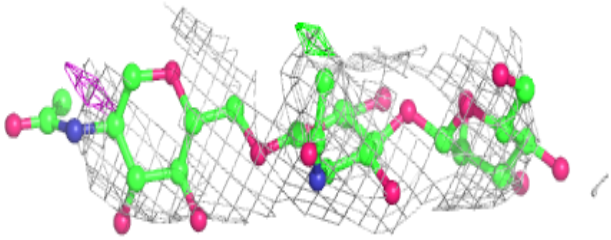
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

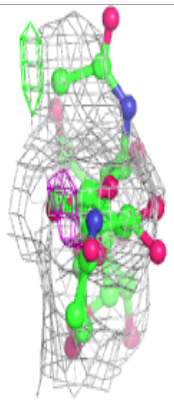


Electron density around Chain H:

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

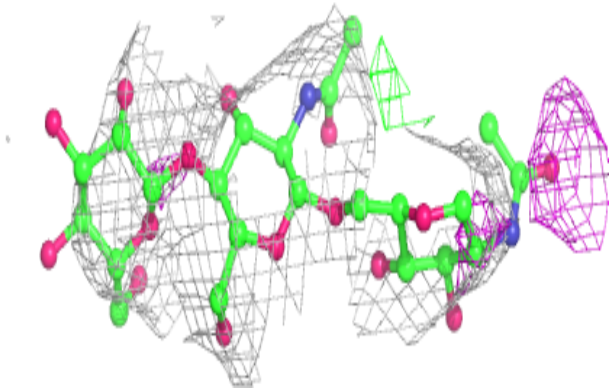


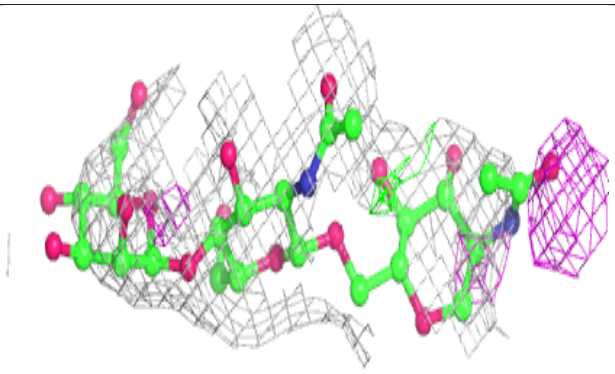


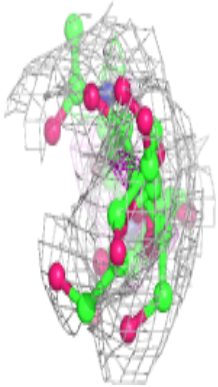


Electron density around Chain J:

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

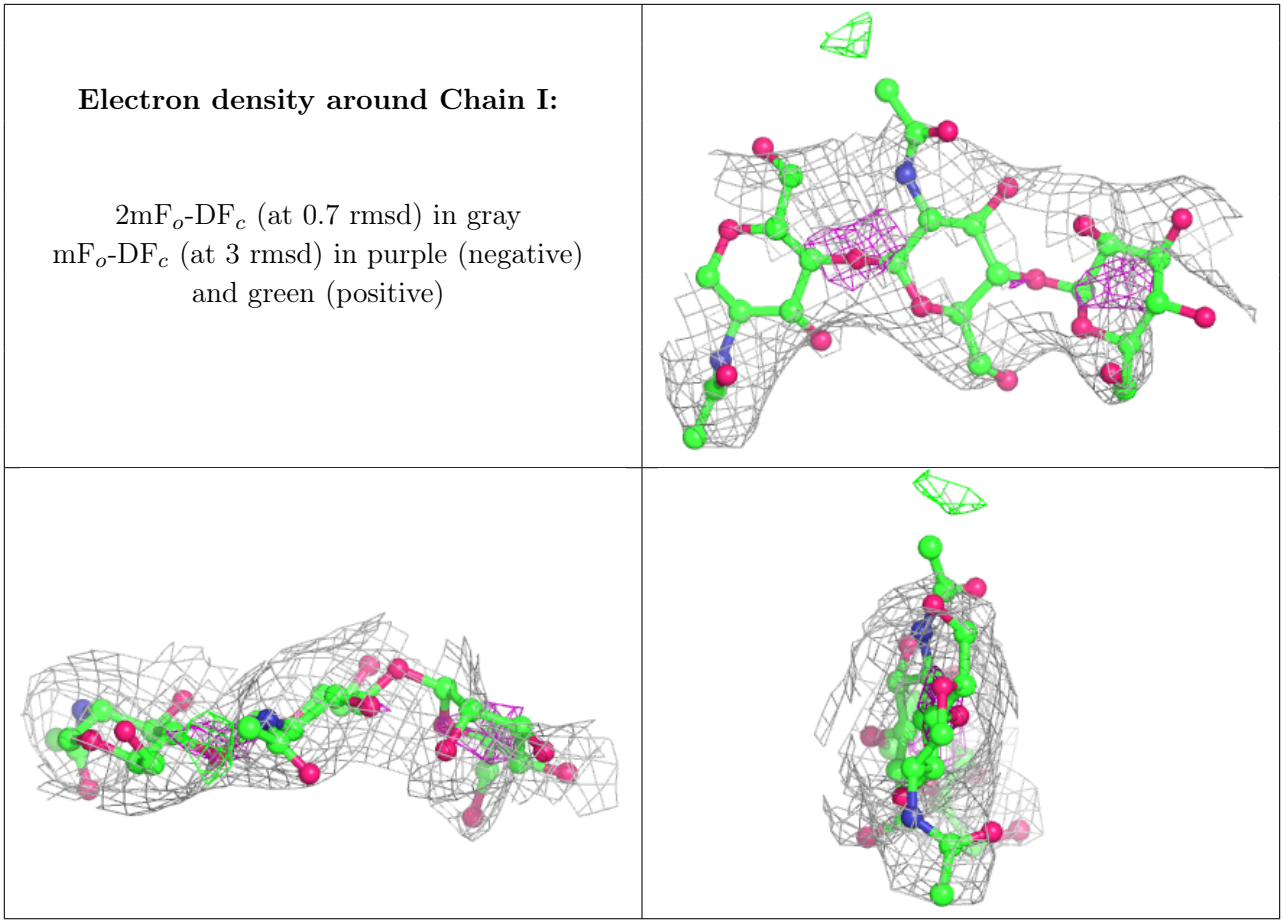






Electron density around Chain I:

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



6.4 Ligands

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^{th} 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
7	NAG	D	401	14/15	0.63	0.34	140,148,158,159	0
7	NAG	A	401	14/15	0.83	0.21	123,135,140,142	0

6.5 Other polymers

There are no such residues in this entry.