



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 09:22 AM BST

PDB ID : 1XWD  
Title : Crystal Structure of Human Follicle Stimulating Hormone Complexed with its Receptor  
Authors : Fan, Q.R.; Hendrickson, W.A.  
Deposited on : 2004-10-30  
Resolution : 2.92 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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

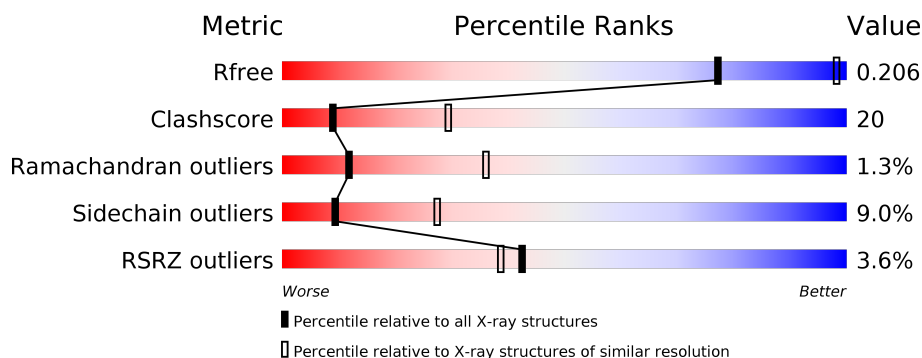
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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.



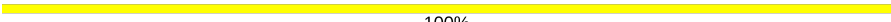
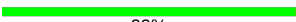

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	92	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>33%</div> <div>• •</div> </div> </div>
1	D	92	<div> <div>5%</div> <div> <div></div> <div>58%</div> <div>33%</div> <div>• 5%</div> </div> </div>
2	B	111	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>• 5%</div> </div> </div>
2	E	111	<div> <div>10%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>• 5%</div> </div> </div>
3	C	252	<div> <div>3%</div> <div> <div></div> <div>45%</div> <div>44%</div> <div>7%</div> <div>•</div> </div> </div>
3	F	252	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>30%</div> <div>5%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
5	H	3	 33%  67%

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
6	NAG	B	112	-	-	-	X
6	NAG	B	113	X	-	-	-
6	NAG	E	112	X	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7031 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 Glycoprotein hormones alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			694	429	120	132	13			
1	D	87	Total	C	N	O	S	0	0	0
			670	415	116	126	13			

- Molecule 2 is a protein called Follitropin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	105	Total	C	N	O	S	0	0	0
			817	510	137	158	12			
2	E	105	Total	C	N	O	S	0	0	0
			817	510	137	158	12			

- Molecule 3 is a protein called Follicle stimulating hormone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	242	Total	C	N	O	S	0	0	0
			1945	1233	345	362	5			
3	F	233	Total	C	N	O	S	0	0	0
			1872	1185	333	349	5			

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



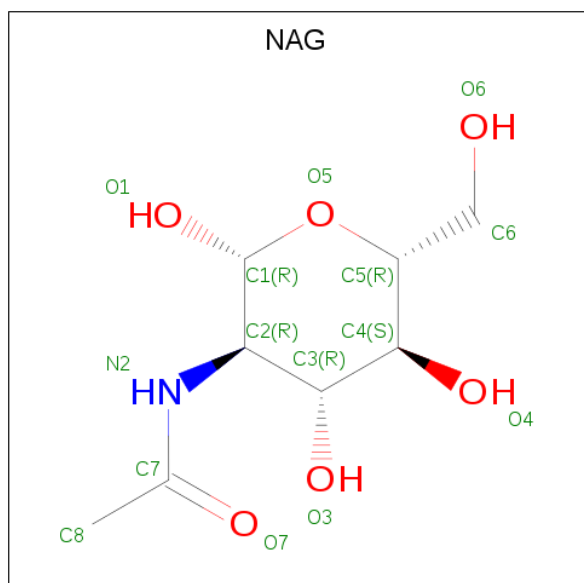
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

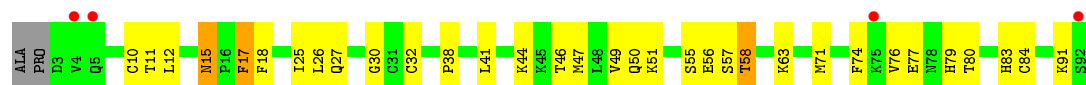
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	O	0	0
			4	4		
8	B	6	Total	O	0	0
			6	6		
8	C	13	Total	O	0	0
			13	13		
8	D	2	Total	O	0	0
			2	2		
8	E	4	Total	O	0	0
			4	4		
8	F	21	Total	O	0	0
			21	21		

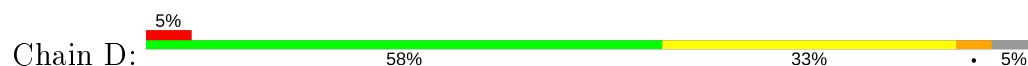
### 3 Residue-property plots [i](#)

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.

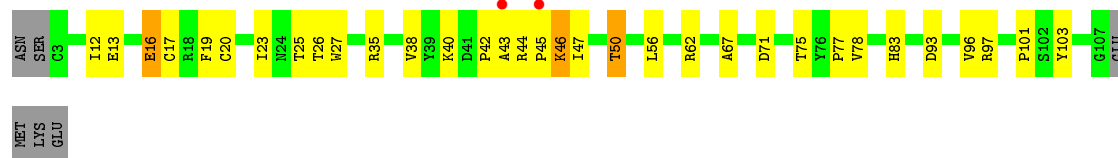
- Molecule 1: Glycoprotein hormones alpha chain



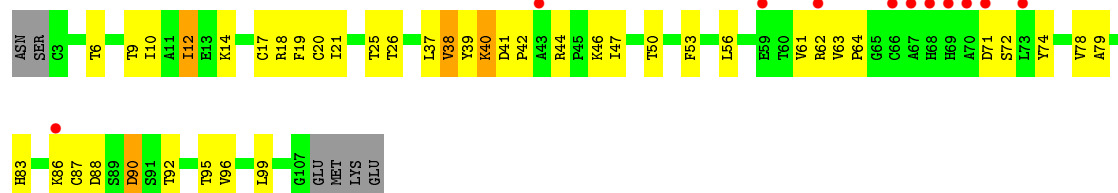
- Molecule 1: Glycoprotein hormones alpha chain



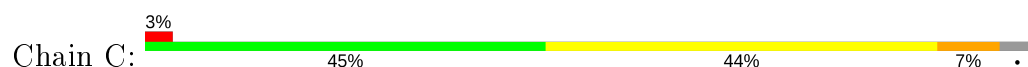
- Molecule 2: Follitropin beta chain

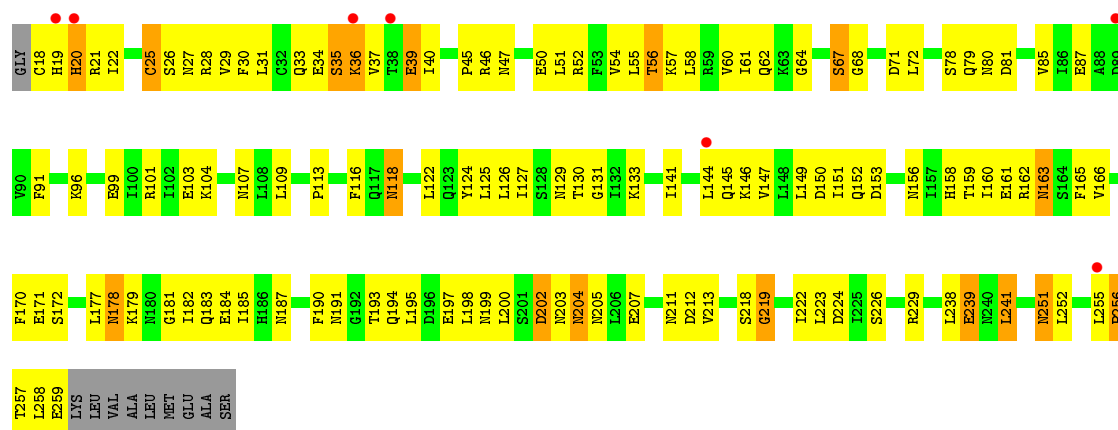


- Molecule 2: Follitropin beta chain

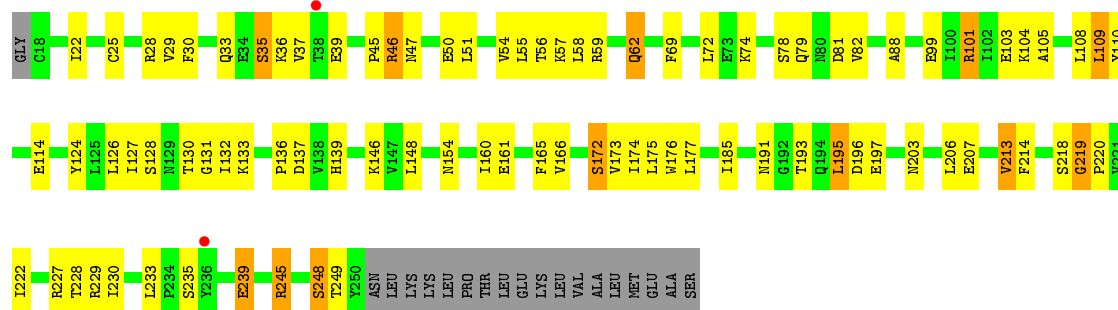


- Molecule 3: Follicle stimulating hormone receptor

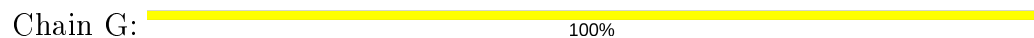




- Molecule 3: Follicle stimulating hormone receptor



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.33Å 66.94Å 148.63Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	25.00 – 2.92 24.84 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.0 (25.00-2.92) 98.0 (24.84-2.92)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.94Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.219 , 0.259 0.220 , 0.206	Depositor DCC
$R_{free}$ test set	1287 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: BMA, NAG, SO4

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	0.51	0/710	0.75	0/959
1	D	0.44	0/686	0.66	0/926
2	B	0.50	0/836	0.80	1/1136 (0.1%)
2	E	0.43	0/836	0.72	0/1136
3	C	0.44	0/1981	0.77	3/2684 (0.1%)
3	F	0.47	0/1907	0.73	0/2584
All	All	0.46	0/6956	0.74	4/9425 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	ASP	CB-CG-OD2	6.13	123.81	118.30
3	C	20	HIS	N-CA-C	-5.39	96.45	111.00
3	C	153	ASP	CB-CG-OD2	5.05	122.85	118.30
3	C	202	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	694	0	658	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	670	0	638	27	0
2	B	817	0	769	28	0
2	E	817	0	770	30	0
3	C	1945	0	1961	118	0
3	F	1872	0	1876	82	0
4	G	28	0	25	0	0
5	H	39	0	34	1	0
6	A	28	0	26	2	0
6	B	28	0	26	0	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
7	B	10	0	0	2	0
7	C	5	0	0	0	0
8	A	4	0	0	1	0
8	B	6	0	0	0	0
8	C	13	0	0	3	0
8	D	2	0	0	0	0
8	E	4	0	0	0	0
8	F	21	0	0	0	0
All	All	7031	0	6809	278	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 20.

All (278) 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)
3:C:56:THR:HG22	3:C:58:LEU:H	1.11	1.09
2:B:12:ILE:HD12	2:B:23:ILE:HD12	1.38	1.04
3:F:35:SER:HB3	3:F:37:VAL:HG22	1.48	0.96
3:F:101:ARG:HG2	3:F:126:LEU:HD23	1.46	0.95
3:C:204:ASN:HD22	3:C:204:ASN:H	1.10	0.93
3:C:56:THR:HB	3:C:80:ASN:OD1	1.70	0.91
3:C:56:THR:CG2	3:C:58:LEU:H	1.85	0.88
3:F:35:SER:CB	3:F:37:VAL:HG22	2.02	0.88
2:B:12:ILE:CD1	2:B:23:ILE:HD12	2.02	0.88
3:C:60:VAL:HG23	3:F:109:LEU:CD1	2.03	0.88
3:C:239:GLU:HA	3:C:258:LEU:HD13	1.56	0.87
2:B:16:GLU:CD	2:B:16:GLU:H	1.76	0.86
3:C:204:ASN:H	3:C:204:ASN:ND2	1.74	0.86
3:C:60:VAL:CG2	3:F:109:LEU:CD1	2.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:GLU:HG3	3:C:124:TYR:HD2	1.38	0.86
1:A:57:SER:HB3	2:B:50:THR:OG1	1.75	0.85
3:C:190:PHE:O	3:C:193:THR:HG22	1.77	0.85
1:D:20:GLN:HE22	1:D:71:MET:HB2	1.43	0.82
1:A:77:GLU:O	2:B:38:VAL:HG13	1.79	0.82
2:B:12:ILE:HD12	2:B:23:ILE:CD1	2.10	0.81
1:D:33:PHE:O	1:D:58:THR:HG22	1.80	0.81
3:C:60:VAL:CG2	3:F:109:LEU:HD12	2.11	0.80
3:C:204:ASN:HD22	3:C:204:ASN:N	1.77	0.80
1:D:44:LYS:HE2	1:D:50:GLN:OE1	1.82	0.80
3:F:207:GLU:HB3	3:F:229:ARG:HB2	1.63	0.79
3:C:194:GLN:HA	3:C:218:SER:HB2	1.65	0.78
3:C:18:CYS:HB3	3:C:25:CYS:O	1.83	0.77
3:C:71:ASP:HA	3:C:96:LYS:HD2	1.67	0.77
3:C:22:ILE:HD12	3:C:37:VAL:HG13	1.69	0.75
3:F:25:CYS:HB3	3:F:30:PHE:CD2	2.22	0.75
3:C:56:THR:HG22	3:C:58:LEU:N	1.97	0.75
3:F:62:GLN:H	3:F:62:GLN:HE21	1.33	0.74
2:E:14:LYS:HD3	2:E:63:VAL:HG12	1.69	0.74
1:D:32:CYS:HB3	1:D:58:THR:HG23	1.69	0.74
3:C:60:VAL:HG21	3:F:109:LEU:HD12	1.71	0.73
3:F:56:THR:HG21	3:F:58:LEU:HG	1.71	0.73
3:C:36:LYS:HG3	3:C:36:LYS:O	1.89	0.72
3:C:25:CYS:SG	3:C:25:CYS:O	2.47	0.72
2:B:101:PRO:HD2	7:B:402:SO4:O4	1.90	0.72
3:F:29:VAL:HG22	3:F:50:GLU:HB3	1.72	0.71
3:F:207:GLU:OE1	3:F:229:ARG:NH1	2.23	0.71
1:A:58:THR:HG23	1:A:84:CYS:HB3	1.71	0.70
3:C:166:VAL:HG22	3:C:191:ASN:O	1.90	0.70
1:D:47:MET:CE	1:D:51:LYS:H	2.03	0.70
3:C:256:PRO:C	3:C:258:LEU:H	1.95	0.70
2:B:27:TRP:HZ2	2:B:77:PRO:HB2	1.55	0.70
3:C:60:VAL:HG23	3:F:109:LEU:HD11	1.73	0.70
3:C:60:VAL:CG2	3:F:109:LEU:HD11	2.21	0.69
3:C:56:THR:HG21	3:C:58:LEU:HG	1.75	0.69
3:C:239:GLU:HA	3:C:258:LEU:CD1	2.23	0.69
1:A:44:LYS:HB3	1:A:50:GLN:HE22	1.58	0.68
3:F:62:GLN:H	3:F:62:GLN:NE2	1.91	0.68
3:C:22:ILE:HD12	3:C:37:VAL:CG1	2.23	0.68
3:C:255:LEU:N	8:C:413:HOH:O	2.27	0.68
2:B:13:GLU:HB3	2:B:20:CYS:SG	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:THR:HG22	3:C:131:GLY:H	1.59	0.67
3:F:227:ARG:NH2	3:F:245:ARG:HH22	1.90	0.67
3:C:101:ARG:HG2	3:C:126:LEU:HD23	1.77	0.66
3:C:56:THR:HG21	3:C:58:LEU:CG	2.25	0.66
3:F:101:ARG:CG	3:F:126:LEU:HD23	2.23	0.66
3:C:179:LYS:HG2	3:C:202:ASP:HB2	1.79	0.65
3:F:108:LEU:HB3	3:F:130:THR:HG23	1.77	0.65
3:C:99:GLU:HG3	3:C:124:TYR:CD2	2.28	0.64
3:C:251:ASN:CG	3:C:252:LEU:H	2.01	0.64
2:B:13:GLU:CB	2:B:20:CYS:SG	2.86	0.64
1:A:32:CYS:HB3	1:A:58:THR:HG22	1.79	0.64
3:C:152:GLN:HG2	3:C:178:ASN:HB3	1.80	0.63
3:F:35:SER:HB3	3:F:37:VAL:H	1.62	0.63
3:C:165:PHE:CZ	3:C:177:LEU:HD11	2.34	0.62
3:C:99:GLU:OE2	3:C:101:ARG:HD3	1.98	0.62
1:A:32:CYS:HB3	1:A:58:THR:CG2	2.29	0.62
3:C:22:ILE:CG2	3:C:36:LYS:HB3	2.29	0.62
3:F:30:PHE:CZ	3:F:45:PRO:HG2	2.35	0.62
1:A:15:ASN:HD21	1:A:17:PHE:HD1	1.49	0.61
1:A:58:THR:CG2	1:A:84:CYS:HB3	2.30	0.61
3:F:166:VAL:HG22	3:F:191:ASN:O	2.00	0.61
1:D:27:GLN:HG3	2:E:38:VAL:HG23	1.83	0.60
3:C:35:SER:OG	3:C:37:VAL:HG22	2.02	0.60
3:C:99:GLU:OE2	3:C:101:ARG:CD	2.50	0.60
3:F:130:THR:HG22	3:F:132:ILE:H	1.67	0.60
2:B:40:LYS:HZ3	2:B:42:PRO:HG3	1.67	0.60
1:A:25:ILE:HG22	6:A:94:NAG:H82	1.84	0.59
3:F:126:LEU:HD11	3:F:128:SER:OG	2.01	0.59
3:C:130:THR:HG22	3:C:131:GLY:N	2.16	0.59
1:D:63:LYS:HB2	1:D:63:LYS:NZ	2.18	0.59
3:F:30:PHE:HZ	3:F:45:PRO:HG2	1.68	0.59
1:D:10:CYS:HA	1:D:30:GLY:HA3	1.84	0.58
3:F:51:LEU:HG	3:F:72:LEU:HD11	1.85	0.58
3:C:40:ILE:HD12	3:C:61:ILE:HG23	1.85	0.58
2:B:103:TYR:OH	3:C:34:GLU:OE2	2.21	0.58
3:C:56:THR:CG2	3:C:57:LYS:N	2.66	0.58
3:F:130:THR:HB	3:F:154:ASN:OD1	2.04	0.58
3:C:198:LEU:HD23	3:C:223:LEU:CD1	2.34	0.57
1:D:28:CYS:SG	1:D:62:ALA:HA	2.45	0.57
3:F:56:THR:CG2	3:F:58:LEU:HG	2.34	0.57
3:C:124:TYR:CZ	3:C:126:LEU:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:203:ASN:O	3:F:228:THR:HG22	2.03	0.57
1:A:76:VAL:HB	2:B:38:VAL:HG12	1.86	0.57
1:A:47:MET:CE	1:A:51:LYS:H	2.18	0.57
3:F:227:ARG:NH2	3:F:245:ARG:NH2	2.53	0.55
3:F:137:ASP:OD1	3:F:139:HIS:ND1	2.38	0.55
1:A:15:ASN:ND2	1:A:17:PHE:HD1	2.04	0.55
1:D:47:MET:HE3	1:D:51:LYS:H	1.72	0.55
3:F:124:TYR:CZ	3:F:126:LEU:HB2	2.42	0.55
3:C:160:ILE:HD12	3:C:185:ILE:HG12	1.89	0.55
3:C:241:LEU:HB3	3:C:257:THR:HG22	1.88	0.55
2:E:37:LEU:HB2	2:E:40:LYS:HD2	1.88	0.55
1:A:46:THR:HG21	3:C:79:GLN:HB3	1.87	0.55
3:C:197:GLU:HG3	3:C:222:ILE:HB	1.88	0.54
1:D:46:THR:HG22	3:F:81:ASP:OD1	2.07	0.54
3:F:79:GLN:HG2	3:F:104:LYS:HD2	1.90	0.54
3:F:105:ALA:HB1	3:F:108:LEU:HB2	1.90	0.54
2:B:16:GLU:CD	2:B:16:GLU:N	2.56	0.53
3:F:197:GLU:HG3	3:F:222:ILE:HB	1.91	0.53
3:C:28:ARG:HD2	3:C:47:ASN:O	2.07	0.53
3:C:251:ASN:CG	3:C:252:LEU:N	2.61	0.53
2:E:25:THR:HG23	2:E:78:VAL:HG13	1.90	0.53
3:C:109:LEU:HD12	3:F:59:ARG:HD2	1.89	0.53
3:C:118:ASN:HA	3:C:141:ILE:O	2.09	0.53
3:C:29:VAL:HG22	3:C:50:GLU:HB3	1.89	0.53
3:C:56:THR:HG21	3:C:58:LEU:CD1	2.39	0.53
3:C:31:LEU:HD11	3:C:33:GLN:HB2	1.90	0.53
1:D:20:GLN:HE22	1:D:71:MET:CB	2.19	0.53
3:F:33:GLN:HA	3:F:54:VAL:O	2.09	0.53
2:E:42:PRO:O	3:F:222:ILE:HD11	2.09	0.53
2:B:44:ARG:O	2:B:44:ARG:HG2	2.09	0.52
2:B:35:ARG:HD3	7:B:403:SO4:O1	2.09	0.52
2:B:44:ARG:N	2:B:45:PRO:HD3	2.25	0.52
3:C:159:THR:HG22	3:C:161:GLU:HG2	1.92	0.52
3:C:18:CYS:CB	3:C:25:CYS:O	2.56	0.52
3:C:35:SER:CB	3:C:37:VAL:HG22	2.39	0.52
2:E:14:LYS:HE2	2:E:64:PRO:O	2.09	0.52
3:F:175:LEU:HD12	3:F:195:LEU:HD11	1.91	0.52
1:A:47:MET:HE1	1:A:51:LYS:H	1.75	0.52
3:C:56:THR:HG21	3:C:58:LEU:HD12	1.91	0.52
2:B:13:GLU:HB2	2:B:20:CYS:SG	2.50	0.52
3:F:130:THR:HG22	3:F:131:GLY:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:ASN:OD1	3:C:212:ASP:HB2	2.09	0.52
2:E:99:LEU:HD21	3:F:55:LEU:HD12	1.92	0.52
1:D:63:LYS:HB2	1:D:63:LYS:HZ2	1.75	0.52
3:F:206:LEU:HG	3:F:230:ILE:HD11	1.92	0.52
3:C:146:LYS:HG2	3:C:172:SER:HB3	1.92	0.51
2:B:43:ALA:C	2:B:45:PRO:HD3	2.30	0.51
1:D:77:GLU:O	2:E:38:VAL:HG22	2.10	0.51
5:H:1:NAG:H62	5:H:2:NAG:C1	2.41	0.51
2:E:17:CYS:HB3	2:E:19:PHE:CE2	2.46	0.51
3:F:54:VAL:HA	3:F:78:SER:O	2.11	0.51
3:C:60:VAL:HG22	3:C:85:VAL:HB	1.93	0.51
3:C:198:LEU:HD21	3:C:200:LEU:HD11	1.93	0.50
3:C:204:ASN:N	3:C:204:ASN:ND2	2.44	0.50
3:C:207:GLU:HB3	3:C:229:ARG:HB2	1.93	0.50
3:C:255:LEU:HG	8:C:413:HOH:O	2.10	0.50
2:E:14:LYS:HE3	2:E:17:CYS:SG	2.51	0.50
3:C:87:GLU:CG	3:F:110:TYR:CE1	2.94	0.50
1:A:56:GLU:HB3	2:B:96:VAL:O	2.11	0.50
3:F:46:ARG:HH11	3:F:46:ARG:HB2	1.76	0.50
3:F:35:SER:HB2	3:F:56:THR:HG23	1.94	0.50
3:F:39:GLU:HG3	3:F:62:GLN:NE2	2.27	0.50
3:C:146:LYS:HE2	3:C:172:SER:HB3	1.94	0.49
1:D:38:PRO:HG2	2:E:10:ILE:HG21	1.93	0.49
2:E:87:CYS:HB2	2:E:92:THR:HG21	1.94	0.49
3:C:22:ILE:HG21	3:C:36:LYS:HB3	1.93	0.49
3:C:51:LEU:HD12	3:C:72:LEU:HD21	1.93	0.49
1:D:11:THR:HG22	1:D:12:LEU:H	1.77	0.49
1:D:43:SER:OG	2:E:99:LEU:HD12	2.13	0.49
3:F:218:SER:O	3:F:219:GLY:O	2.30	0.49
2:E:96:VAL:HG23	3:F:101:ARG:NH2	2.27	0.49
3:F:39:GLU:HG3	3:F:62:GLN:CD	2.33	0.49
1:A:57:SER:HB3	2:B:50:THR:HG1	1.75	0.49
3:C:161:GLU:O	3:C:162:ARG:C	2.51	0.49
3:C:26:SER:OG	3:C:27:ASN:N	2.45	0.49
1:D:20:GLN:NE2	1:D:71:MET:HB2	2.20	0.49
1:A:77:GLU:O	2:B:38:VAL:CG1	2.58	0.48
3:F:148:LEU:HD11	3:F:176:TRP:CE3	2.48	0.48
3:F:139:HIS:HA	3:F:166:VAL:O	2.13	0.48
3:F:165:PHE:CZ	3:F:177:LEU:HD11	2.48	0.48
3:C:163:ASN:N	3:C:163:ASN:HD22	2.12	0.48
3:C:126:LEU:HD12	3:C:150:ASP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:SER:HB3	2:E:50:THR:HG23	1.96	0.48
3:C:22:ILE:HG22	3:C:36:LYS:HB3	1.94	0.48
1:D:63:LYS:HE2	1:D:81:ALA:HB1	1.96	0.48
3:F:39:GLU:HG3	3:F:62:GLN:OE1	2.12	0.48
3:C:55:LEU:HA	3:C:55:LEU:HD23	1.69	0.47
3:C:81:ASP:O	3:C:107:ASN:ND2	2.47	0.47
3:F:174:ILE:HG23	3:F:197:GLU:HB3	1.96	0.47
3:F:227:ARG:HH22	3:F:245:ARG:HH22	1.58	0.47
3:C:256:PRO:C	3:C:258:LEU:N	2.66	0.47
1:D:47:MET:HE3	1:D:51:LYS:N	2.30	0.47
3:C:29:VAL:HG12	3:C:29:VAL:O	2.15	0.46
3:C:56:THR:CG2	3:C:58:LEU:HG	2.42	0.46
2:B:40:LYS:HE3	3:C:146:LYS:HZ3	1.80	0.46
3:C:218:SER:O	3:C:219:GLY:O	2.33	0.46
3:C:39:GLU:OE2	3:F:133:LYS:HD2	2.16	0.46
3:F:230:ILE:O	3:F:249:THR:HG21	2.16	0.46
3:C:64:GLY:O	3:C:67:SER:HB2	2.15	0.46
2:E:12:ILE:HD11	2:E:74:TYR:HD2	1.81	0.45
1:D:63:LYS:NZ	1:D:63:LYS:CB	2.79	0.45
2:E:17:CYS:O	2:E:18:ARG:HB2	2.16	0.45
3:F:88:ALA:HB1	3:F:114:GLU:HB2	1.99	0.45
3:F:239:GLU:HG2	3:F:239:GLU:H	1.56	0.45
3:C:195:LEU:HD23	3:C:195:LEU:HA	1.81	0.45
3:C:256:PRO:O	3:C:259:GLU:HG3	2.17	0.45
1:A:12:LEU:HB3	1:A:26:LEU:HD23	1.98	0.44
3:C:183:GLN:HG2	3:C:205:ASN:HB2	1.98	0.44
2:E:37:LEU:H	2:E:46:LYS:HE2	1.82	0.44
3:F:74:LYS:HG2	3:F:99:GLU:HB3	1.99	0.44
1:D:25:ILE:HD13	1:D:76:VAL:CG2	2.47	0.44
2:B:17:CYS:HB3	2:B:19:PHE:CE2	2.52	0.44
3:F:146:LYS:HA	3:F:172:SER:O	2.18	0.44
1:A:27:GLN:HA	1:A:79:HIS:ND1	2.32	0.44
3:C:46:ARG:HD2	3:C:68:GLY:O	2.17	0.44
1:D:76:VAL:HB	2:E:38:VAL:HG13	2.00	0.44
3:F:219:GLY:HA2	3:F:220:PRO:HD3	1.88	0.44
3:F:56:THR:HG22	3:F:57:LYS:N	2.33	0.44
3:F:59:ARG:HA	3:F:82:VAL:O	2.18	0.44
1:D:42:ARG:NH1	1:D:45:LYS:HD3	2.32	0.44
3:F:59:ARG:HB2	3:F:59:ARG:HE	1.68	0.44
3:C:127:ILE:O	3:C:151:ILE:HA	2.18	0.43
2:E:88:ASP:OD1	2:E:90:ASP:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:SER:HB3	3:C:37:VAL:HG22	2.01	0.43
2:E:12:ILE:HG22	2:E:21:ILE:HG12	2.00	0.43
2:E:61:VAL:HG22	2:E:62:ARG:H	1.83	0.43
3:C:30:PHE:CZ	3:C:45:PRO:HB2	2.53	0.43
3:F:213:VAL:HG23	3:F:214:PHE:CD2	2.54	0.43
3:C:199:ASN:HA	3:C:224:ASP:HB3	1.99	0.43
3:C:238:LEU:HD22	3:C:241:LEU:HG	1.99	0.43
2:B:46:LYS:HG2	2:B:46:LYS:H	1.23	0.43
1:A:18:PHE:HB2	1:A:25:ILE:HD11	2.01	0.43
2:E:53:PHE:CD1	2:E:56:LEU:HG	2.54	0.43
2:E:63:VAL:HB	2:E:72:SER:O	2.18	0.43
1:A:10:CYS:HA	1:A:30:GLY:HA3	2.01	0.43
3:C:18:CYS:SG	3:C:25:CYS:O	2.77	0.43
3:C:193:THR:HG23	3:C:195:LEU:HG	2.01	0.42
3:C:99:GLU:OE2	3:C:101:ARG:HD2	2.19	0.42
1:D:35:ARG:HE	1:D:37:TYR:HE2	1.68	0.42
3:F:227:ARG:HA	3:F:248:SER:O	2.19	0.42
2:E:99:LEU:HD21	3:F:55:LEU:CD1	2.50	0.42
3:C:54:VAL:HA	3:C:78:SER:O	2.19	0.42
2:E:25:THR:CG2	2:E:78:VAL:HG13	2.49	0.42
3:F:227:ARG:HG3	3:F:248:SER:HB2	2.01	0.42
3:C:133:LYS:HG2	3:C:156:ASN:HB3	2.00	0.42
3:F:101:ARG:HG3	3:F:126:LEU:HB3	2.02	0.42
3:C:122:LEU:O	3:C:147:VAL:HG22	2.19	0.42
3:C:30:PHE:HZ	3:C:45:PRO:HB2	1.84	0.42
3:F:103:GLU:HB3	3:F:104:LYS:HE3	2.02	0.42
3:C:182:ILE:HB	3:C:203:ASN:OD1	2.19	0.42
3:C:20:HIS:ND1	3:C:21:ARG:N	2.67	0.42
1:A:38:PRO:HD3	2:B:27:TRP:CD1	2.55	0.42
1:A:49:VAL:HG23	3:C:129:ASN:OD1	2.20	0.42
3:C:255:LEU:N	3:C:256:PRO:CD	2.82	0.42
3:F:69:PHE:HB3	3:F:72:LEU:HB2	2.00	0.42
1:A:91:LYS:HE3	3:C:152:GLN:HE22	1.84	0.42
3:C:56:THR:CG2	3:C:58:LEU:N	2.68	0.42
3:F:22:ILE:HD11	3:F:36:LYS:HB3	2.02	0.42
3:F:99:GLU:HG3	3:F:124:TYR:HD2	1.85	0.41
2:B:25:THR:OG1	2:B:78:VAL:HG22	2.20	0.41
3:F:206:LEU:O	3:F:228:THR:HB	2.20	0.41
3:F:28:ARG:HD3	3:F:47:ASN:ND2	2.35	0.41
1:A:25:ILE:CG2	6:A:94:NAG:H82	2.51	0.41
3:C:103:GLU:HB3	3:C:104:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:LEU:HD23	3:C:170:PHE:HD2	1.86	0.41
3:C:158:HIS:HA	3:C:181:GLY:O	2.20	0.41
3:C:40:ILE:CD1	3:C:61:ILE:HG23	2.49	0.41
3:C:91:PHE:CD2	3:C:116:PHE:CE1	3.09	0.41
3:F:130:THR:CG2	3:F:131:GLY:N	2.84	0.41
3:F:127:ILE:HD12	3:F:136:PRO:HG3	2.03	0.41
1:A:63:LYS:NZ	8:A:95:HOH:O	2.54	0.40
2:E:39:TYR:CE2	2:E:41:ASP:HB2	2.56	0.40
3:C:241:LEU:HD13	3:C:257:THR:CG2	2.51	0.40
2:E:56:LEU:HD23	2:E:79:ALA:HA	2.02	0.40
3:F:160:ILE:HD12	3:F:185:ILE:HG12	2.04	0.40
3:F:51:LEU:HG	3:F:72:LEU:CD1	2.50	0.40
2:B:97:ARG:CZ	3:C:52:ARG:NH1	2.85	0.40
3:C:56:THR:HG23	3:C:57:LYS:N	2.36	0.40
3:C:62:GLN:HB3	8:C:414:HOH:O	2.20	0.40
2:E:47:ILE:HG23	2:E:86:LYS:HE2	2.03	0.40
1:D:92:SER:OXT	2:E:86:LYS:HD3	2.22	0.40
3:C:125:LEU:HD23	3:C:149:LEU:CD1	2.52	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	88/92 (96%)	83 (94%)	4 (4%)	1 (1%)	14	41
1	D	85/92 (92%)	81 (95%)	2 (2%)	2 (2%)	6	21
2	B	103/111 (93%)	94 (91%)	7 (7%)	2 (2%)	8	27
2	E	103/111 (93%)	96 (93%)	7 (7%)	0	100	100
3	C	240/252 (95%)	208 (87%)	27 (11%)	5 (2%)	7	24
3	F	231/252 (92%)	199 (86%)	31 (13%)	1 (0%)	34	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	850/910 (93%)	761 (90%)	78 (9%)	11 (1%)	12	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	MET
2	B	67	ALA
3	C	219	GLY
3	C	118	ASN
1	D	8	PRO
3	F	219	GLY
3	C	251	ASN
2	B	71	ASP
1	D	10	CYS
3	C	113	PRO
3	C	256	PRO

### 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	82/83 (99%)	73 (89%)	9 (11%)	6	18
1	D	79/83 (95%)	73 (92%)	6 (8%)	13	35
2	B	93/99 (94%)	84 (90%)	9 (10%)	8	24
2	E	93/99 (94%)	81 (87%)	12 (13%)	4	12
3	C	224/231 (97%)	206 (92%)	18 (8%)	12	32
3	F	215/231 (93%)	198 (92%)	17 (8%)	12	33
All	All	786/826 (95%)	715 (91%)	71 (9%)	9	27

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR

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Mol	Chain	Res	Type
1	A	15	ASN
1	A	17	PHE
1	A	41	LEU
1	A	55	SER
1	A	58	THR
1	A	74	PHE
1	A	80	THR
1	A	83	HIS
2	B	16	GLU
2	B	26	THR
2	B	46	LYS
2	B	47	ILE
2	B	50	THR
2	B	56	LEU
2	B	62	ARG
2	B	75	THR
2	B	83	HIS
3	C	19	HIS
3	C	25	CYS
3	C	35	SER
3	C	36	LYS
3	C	39	GLU
3	C	56	THR
3	C	67	SER
3	C	145	GLN
3	C	163	ASN
3	C	171	GLU
3	C	178	ASN
3	C	184	GLU
3	C	204	ASN
3	C	211	ASN
3	C	213	VAL
3	C	226	SER
3	C	239	GLU
3	C	241	LEU
1	D	7	CYS
1	D	41	LEU
1	D	47	MET
1	D	63	LYS
1	D	83	HIS
1	D	92	SER
2	E	6	THR

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Mol	Chain	Res	Type
2	E	9	THR
2	E	12	ILE
2	E	20	CYS
2	E	26	THR
2	E	38	VAL
2	E	40	LYS
2	E	44	ARG
2	E	71	ASP
2	E	83	HIS
2	E	90	ASP
2	E	95	THR
3	F	35	SER
3	F	46	ARG
3	F	62	GLN
3	F	101	ARG
3	F	109	LEU
3	F	161	GLU
3	F	172	SER
3	F	173	VAL
3	F	193	THR
3	F	195	LEU
3	F	196	ASP
3	F	213	VAL
3	F	233	LEU
3	F	235	SER
3	F	239	GLU
3	F	245	ARG
3	F	248	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	50	GLN
3	C	178	ASN
3	C	204	ASN
1	D	15	ASN
1	D	20	GLN
1	D	83	HIS
2	E	83	HIS
3	F	62	GLN
3	F	93	ASN

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Mol	Chain	Res	Type
3	F	118	ASN
3	F	240	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

5 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	3,4	14,14,15	0.54	0	17,19,21	1.58	2 (11%)
4	NAG	G	2	4	14,14,15	0.69	0	17,19,21	1.69	4 (23%)
5	NAG	H	1	3,5	14,14,15	0.66	0	17,19,21	1.64	2 (11%)
5	NAG	H	2	5	14,14,15	0.53	0	17,19,21	1.80	4 (23%)
5	BMA	H	3	5	11,11,12	0.78	0	15,15,17	0.72	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	3,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	H	1	3,5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C1-O5-C5	5.04	119.02	112.19
5	H	2	NAG	C4-C3-C2	4.57	117.72	111.02
4	G	1	NAG	C1-O5-C5	4.22	117.91	112.19
4	G	2	NAG	C1-O5-C5	4.17	117.85	112.19
5	H	2	NAG	C1-O5-C5	3.61	117.08	112.19
4	G	1	NAG	O5-C1-C2	3.22	116.37	111.29
4	G	2	NAG	O5-C1-C2	2.42	115.12	111.29
4	G	2	NAG	C3-C4-C5	2.40	114.52	110.24
4	G	2	NAG	O5-C5-C6	2.19	110.64	107.20
5	H	2	NAG	O4-C4-C3	-2.17	105.33	110.35
5	H	1	NAG	O3-C3-C2	2.13	113.88	109.47
5	H	2	NAG	C2-N2-C7	2.07	125.85	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

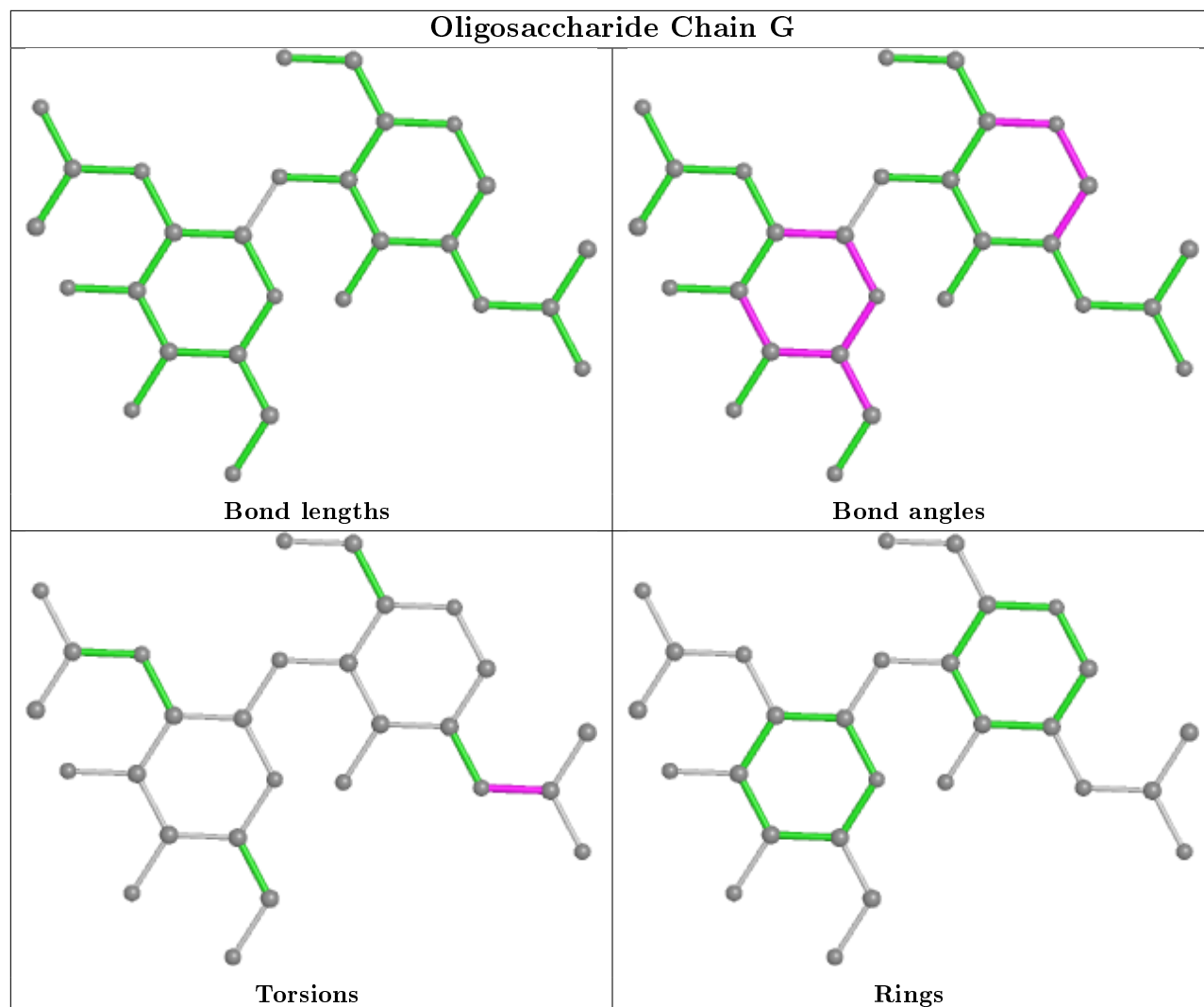
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
5	H	3	BMA	O5-C5-C6-O6
4	G	1	NAG	O7-C7-N2-C2
5	H	3	BMA	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6

There are no ring outliers.

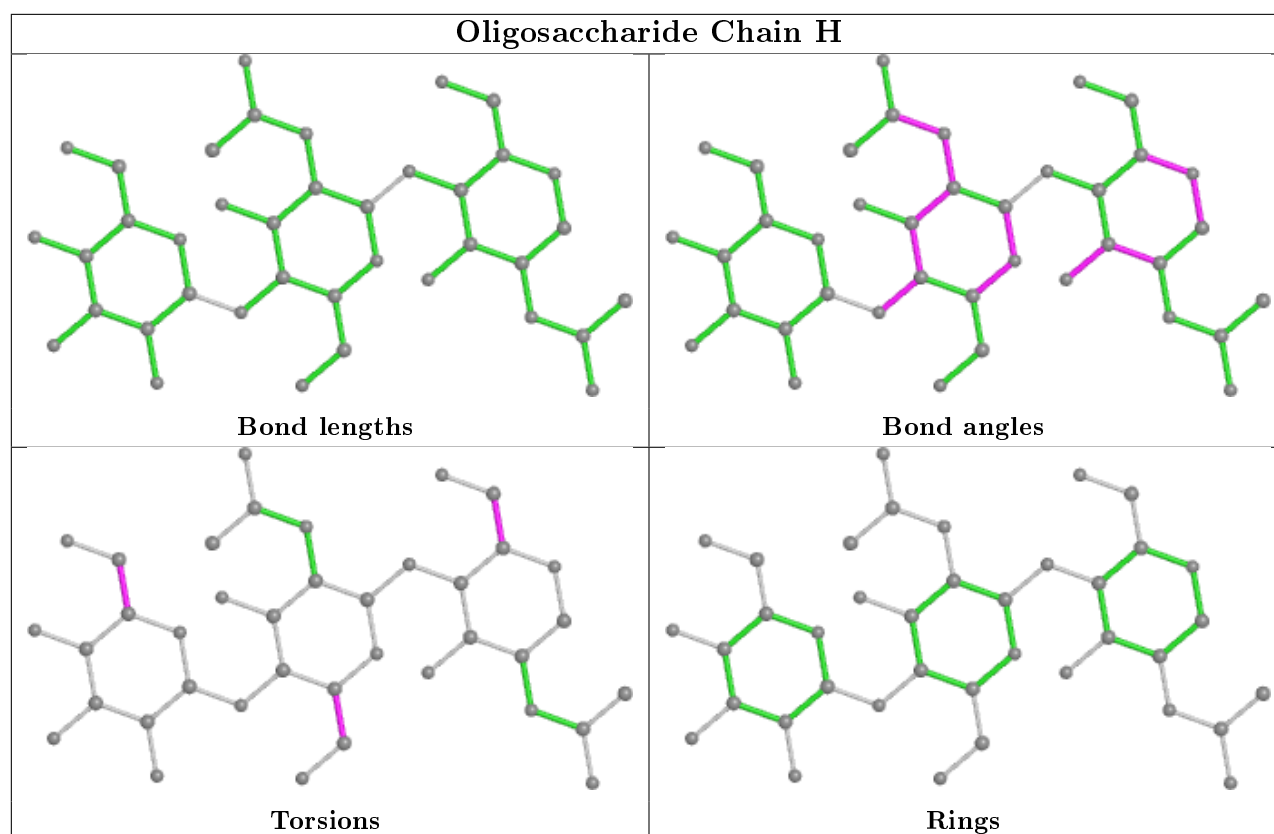
2 monomers are involved in 1 short contact:

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

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







## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	E	112	2	14,14,15	0.59	0	17,19,21	1.26	1 (5%)
7	SO4	C	401	-	4,4,4	0.22	0	6,6,6	0.16	0
7	SO4	B	403	-	4,4,4	0.21	0	6,6,6	0.30	0
6	NAG	B	113	2	14,14,15	0.54	0	17,19,21	1.68	5 (29%)
7	SO4	B	402	-	4,4,4	0.26	0	6,6,6	0.40	0
6	NAG	A	93	1	14,14,15	0.58	0	17,19,21	1.22	1 (5%)
6	NAG	A	94	1	14,14,15	0.51	0	17,19,21	1.59	3 (17%)
6	NAG	B	112	2	14,14,15	0.60	0	17,19,21	1.43	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	D	93	1	14,14,15	0.58	0	17,19,21	1.25	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
6	NAG	E	112	2	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	B	113	2	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	A	93	1	-	0/6/23/26	0/1/1/1
6	NAG	A	94	1	-	0/6/23/26	0/1/1/1
6	NAG	B	112	2	-	2/6/23/26	0/1/1/1
6	NAG	D	93	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	93	NAG	C1-O5-C5	4.11	117.77	112.19
6	B	112	NAG	C1-O5-C5	3.92	117.50	112.19
6	D	93	NAG	C1-O5-C5	3.91	117.49	112.19
6	A	94	NAG	C1-O5-C5	3.84	117.39	112.19
6	B	113	NAG	O5-C1-C2	-3.64	105.54	111.29
6	A	94	NAG	O5-C1-C2	-3.41	105.90	111.29
6	E	112	NAG	O5-C5-C6	3.04	111.97	107.20
6	B	113	NAG	C4-C3-C2	2.72	115.00	111.02
6	B	113	NAG	C3-C4-C5	2.70	115.06	110.24
6	B	113	NAG	O5-C5-C6	2.58	111.24	107.20
6	B	113	NAG	C1-O5-C5	2.35	115.37	112.19
6	A	94	NAG	O7-C7-C8	-2.25	117.87	122.06
6	B	112	NAG	C2-N2-C7	2.02	125.77	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	112	NAG	C1
6	B	113	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	113	NAG	O5-C5-C6-O6
6	B	113	NAG	C4-C5-C6-O6
6	E	112	NAG	C8-C7-N2-C2
6	B	112	NAG	C8-C7-N2-C2
6	E	112	NAG	O7-C7-N2-C2
6	B	112	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	403	SO4	1	0
7	B	402	SO4	1	0
6	A	94	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	90/92 (97%)	0.16	4 (4%) 34 31	28, 52, 91, 115	0
1	D	87/92 (94%)	0.23	5 (5%) 23 20	47, 61, 85, 92	0
2	B	105/111 (94%)	-0.13	2 (1%) 66 65	32, 48, 76, 87	0
2	E	105/111 (94%)	0.67	11 (10%) 6 5	46, 71, 91, 94	0
3	C	242/252 (96%)	-0.02	7 (2%) 51 48	30, 52, 79, 114	0
3	F	233/252 (92%)	-0.22	2 (0%) 84 84	27, 47, 70, 88	0
All	All	862/910 (94%)	0.04	31 (3%) 42 39	27, 53, 87, 115	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	43	ALA	4.5
2	E	70	ALA	4.5
1	D	92	SER	4.3
3	C	19	HIS	4.1
1	D	7	CYS	3.9
2	E	73	LEU	3.9
1	A	5	GLN	3.8
1	D	21	PRO	3.6
2	E	86	LYS	3.2
2	E	62	ARG	3.1
1	A	4	VAL	3.0
3	C	20	HIS	3.0
1	D	72	GLY	2.9
3	F	236	TYR	2.9
2	E	43	ALA	2.9
2	E	71	ASP	2.8
2	E	68	HIS	2.8
2	E	59	GLU	2.8
2	E	67	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	36	LYS	2.7
2	E	69	HIS	2.7
1	D	6	ASP	2.3
1	A	75	LYS	2.3
1	A	92	SER	2.3
3	C	38	THR	2.2
3	C	144	LEU	2.2
2	B	45	PRO	2.2
2	E	66	CYS	2.0
3	C	89	ASP	2.0
3	F	38	THR	2.0
3	C	255	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

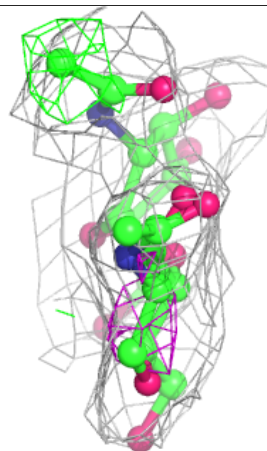
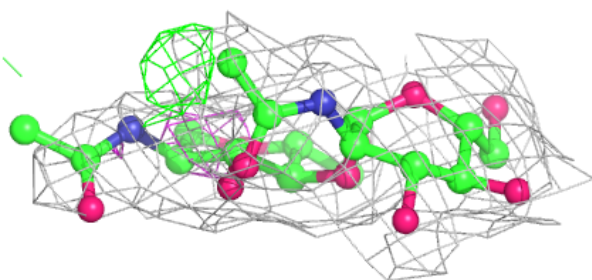
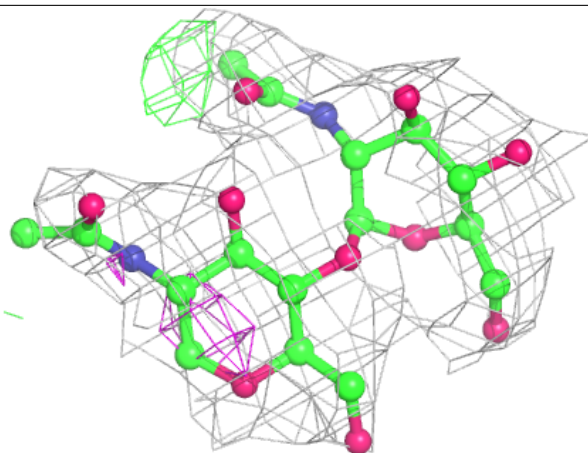
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	BMA	H	3	11/12	0.83	0.33	85,88,90,90	0
4	NAG	G	2	14/15	0.86	0.31	83,88,93,94	0
4	NAG	G	1	14/15	0.88	0.38	76,81,86,86	0
5	NAG	H	1	14/15	0.88	0.29	59,65,69,70	0
5	NAG	H	2	14/15	0.95	0.40	68,71,74,79	0

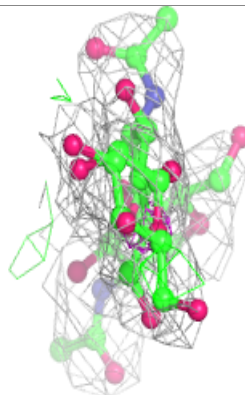
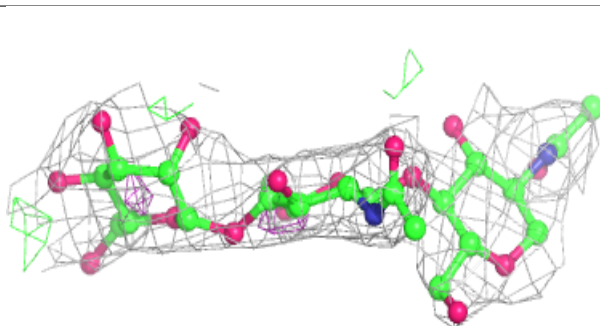
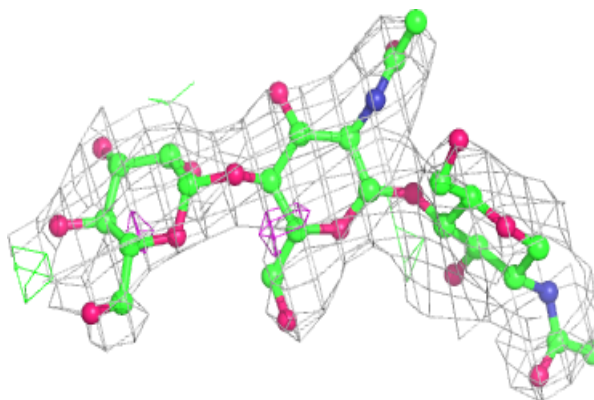
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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
6	NAG	B	112	14/15	0.74	0.42	76,83,84,85	0
6	NAG	E	112	14/15	0.75	0.45	88,90,92,93	0
6	NAG	B	113	14/15	0.85	0.34	73,79,83,85	0
6	NAG	A	94	14/15	0.87	0.28	59,63,67,69	0
6	NAG	A	93	14/15	0.90	0.21	64,68,71,72	0
7	SO4	B	403	5/5	0.91	0.20	82,84,84,85	0
7	SO4	B	402	5/5	0.92	0.33	78,78,82,82	0
6	NAG	D	93	14/15	0.93	0.26	70,72,74,75	0
7	SO4	C	401	5/5	0.96	0.16	82,82,85,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.