



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 07:22 pm GMT

PDB ID : 6R0X  
Title : The extracellular domain of G6b-B in complex with Fab fragment and DP12 heparin oligosaccharide.  
Authors : Ogg, D.J.; McMiken, H.J.; Howard, T.D.  
Deposited on : 2019-03-13  
Resolution : 3.13 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

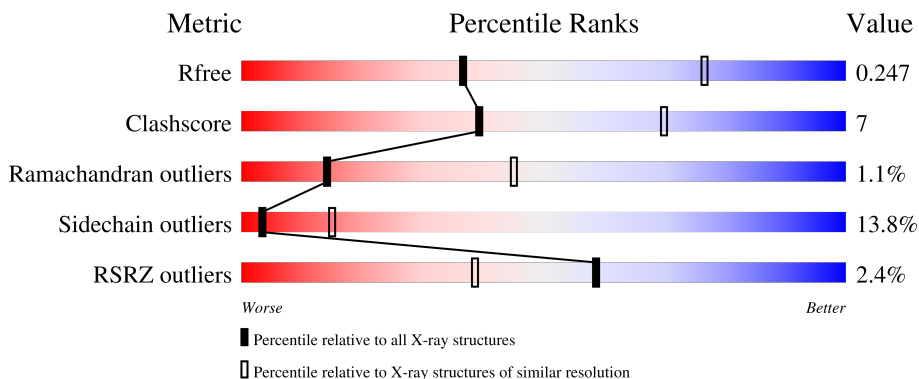
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	240	 2% 69% 18% • 12%
1	C	240	 % 71% 16% • 11%
2	B	234	 % 69% 19% • 9%
2	D	234	 6% 69% 19% • 10%
3	E	116	 2% 53% 28% • 15%

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Mol	Chain	Length	Quality of chain
3	F	116	 % 59% 17% 8% 16%
4	G	3	 33% 33% 33%
4	I	3	 100%
5	H	8	 100%

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	A2G	G	1	X	-	-	-
4	A2G	I	1	X	-	-	-
5	IDS	H	2	X	-	-	-
5	IDS	H	6	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7896 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 antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1575	996	255	319	5	0	0	0
1	C	213	1576	999	252	319	6	0	0	0

- Molecule 2 is a protein called antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1597	995	257	339	6	0	0	0
2	D	211	1537	949	249	332	7	0	0	0

- Molecule 3 is a protein called Megakaryocyte and platelet inhibitory receptor G6b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	99	693	438	127	124	4	0	0	0
3	F	98	688	438	124	123	3	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

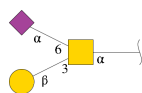
Chain	Residue	Modelled	Actual	Comment	Reference
E	32	ASP	ASN	engineered mutation	UNP O95866
E	67	ALA	SER	engineered mutation	UNP O95866
E	68	ALA	SER	engineered mutation	UNP O95866
E	69	ALA	SER	engineered mutation	UNP O95866
E	71	ALA	THR	engineered mutation	UNP O95866
F	32	ASP	ASN	engineered mutation	UNP O95866
F	67	ALA	SER	engineered mutation	UNP O95866
F	68	ALA	SER	engineered mutation	UNP O95866

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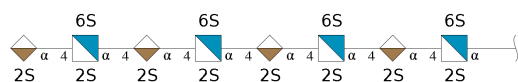
Chain	Residue	Modelled	Actual	Comment	Reference
F	69	ALA	SER	engineered mutation	UNP O95866
F	71	ALA	THR	engineered mutation	UNP O95866

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			45	25	2	18			
4	I	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 5 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.

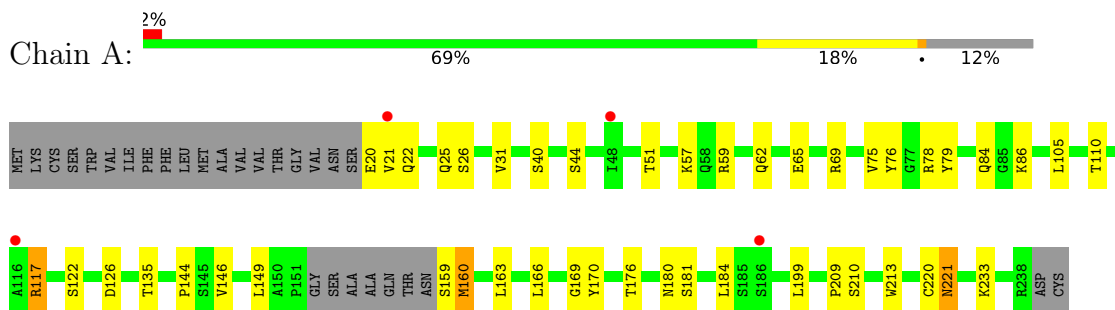


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	8	Total	C	N	O	S	0	0	0
			140	48	4	76	12			

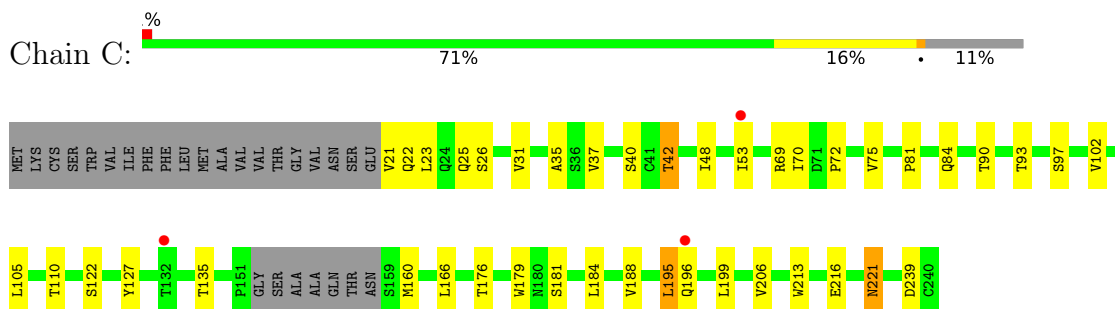
### 3 Residue-property plots [i](#)

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.

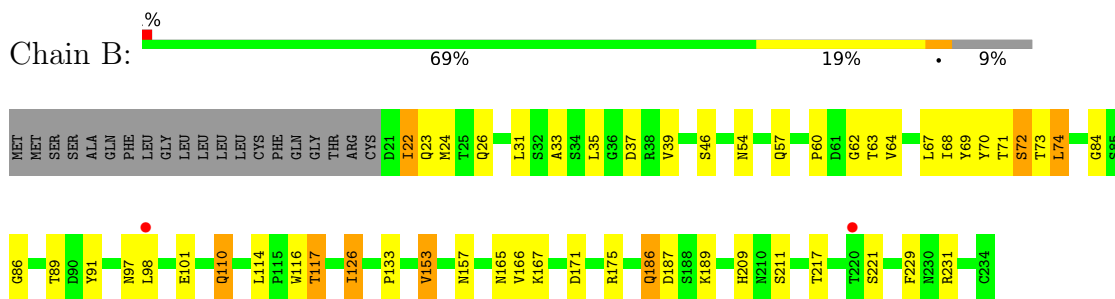
- Molecule 1: antibody fab fragment heavy chain



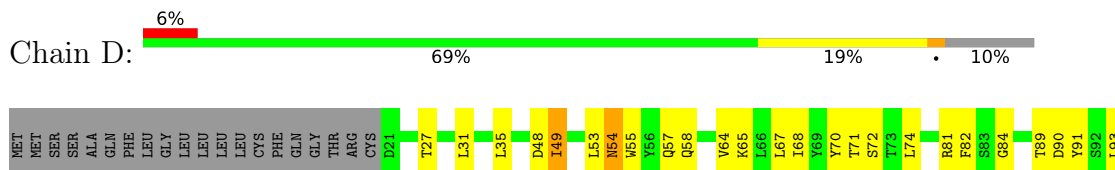
- Molecule 1: antibody fab fragment heavy chain

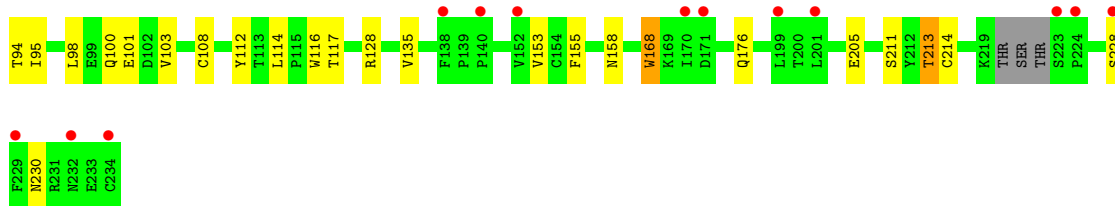


- Molecule 2: antibody fab fragment light chain

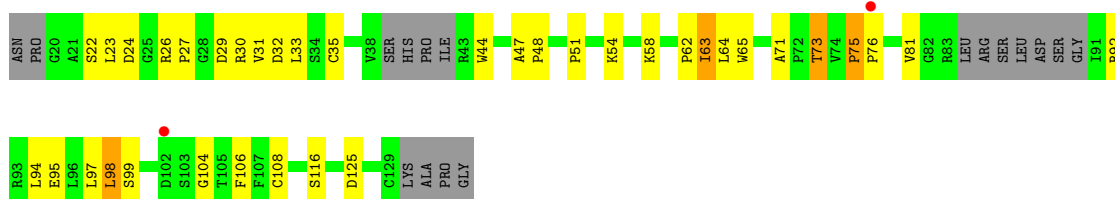


- Molecule 2: antibody fab fragment light chain

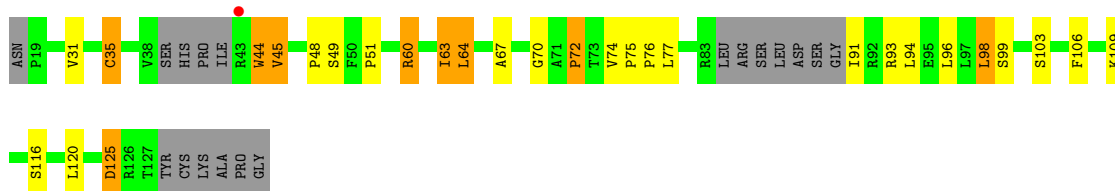




- Molecule 3: Megakaryocyte and platelet inhibitory receptor G6b



- Molecule 3: Megakaryocyte and platelet inhibitory receptor G6b




- Molecule 4: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose



- Molecule 4: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose



- Molecule 5: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain H:  100%

5G11  
1D82  
5G13  
1D84  
5G15  
1D86  
5G17  
1D88



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.80Å 72.34Å 131.04Å 90.00° 124.52° 90.00°	Depositor
Resolution (Å)	63.10 – 3.13 63.10 – 3.13	Depositor EDS
% Data completeness (in resolution range)	97.1 (63.10-3.13) 97.2 (63.10-3.13)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 3.13Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.230 , 0.266 0.256 , 0.247	Depositor DCC
$R_{free}$ test set	1253 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.3	Xtrriage
Anisotropy	0.415	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 103.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: A2G, IDS, SGN, SIA, GAL

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	0.42	0/1617	0.68	0/2219
1	C	0.44	0/1618	0.69	0/2222
2	B	0.47	0/1632	0.74	0/2229
2	D	0.42	0/1569	0.68	0/2146
3	E	0.64	0/710	0.88	0/966
3	F	0.64	0/705	0.89	1/960 (0.1%)
All	All	0.48	0/7851	0.73	1/10742 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	93	ARG	N-CA-C	-5.18	97.01	111.00

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	1575	0	1482	14	0
1	C	1576	0	1490	15	0
2	B	1597	0	1441	26	0
2	D	1537	0	1348	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	693	0	643	21	0
3	F	688	0	644	18	0
4	G	45	0	37	4	0
4	I	45	0	37	1	0
5	H	140	0	48	0	0
All	All	7896	0	7170	111	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 7.

All (111) 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:D:54:ASN:HD22	2:D:70:TYR:H	1.32	0.76
2:B:86:GLY:HA3	2:B:91:TYR:HA	1.68	0.74
1:A:22:GLN:HB3	1:A:44:SER:HB2	1.69	0.73
2:D:213:THR:OG1	2:D:228:SER:HA	1.92	0.69
2:D:168:TRP:HB3	2:D:214:CYS:HA	1.76	0.65
3:E:48:PRO:CD	3:E:63:ILE:HD12	2.27	0.65
1:A:159:SER:HB3	1:A:210:SER:HB2	1.79	0.65
2:B:57:GLN:HB2	2:B:67:LEU:HD11	1.79	0.64
3:F:44:TRP:HB3	3:F:109:LYS:O	1.97	0.64
3:E:81:VAL:CG2	3:E:92:ARG:HH11	2.10	0.64
2:B:22:ILE:HD11	2:B:110:GLN:HG2	1.80	0.63
3:E:73:THR:HA	4:G:1:A2G:N2	2.15	0.62
3:E:75:PRO:HB2	3:E:76:PRO:HD3	1.83	0.61
1:C:35:ALA:O	1:C:105:LEU:HD23	2.02	0.59
3:E:48:PRO:HD3	3:E:63:ILE:HD12	1.84	0.59
2:B:24:MET:HG2	2:B:117:THR:HG22	1.85	0.58
3:F:63:ILE:HG12	3:F:64:LEU:HD22	1.85	0.58
3:E:47:ALA:HA	3:E:62:PRO:HA	1.86	0.57
3:F:51:PRO:HD2	3:F:103:SER:O	2.04	0.57
2:D:57:GLN:HB2	2:D:67:LEU:HD11	1.85	0.56
2:D:72:SER:HA	2:D:84:GLY:O	2.04	0.56
1:A:110:THR:HG23	1:A:135:THR:HA	1.87	0.56
2:D:54:ASN:ND2	2:D:70:TYR:H	2.01	0.55
2:B:68:ILE:CD1	2:B:84:GLY:HA3	2.38	0.54
1:C:110:THR:HG23	1:C:135:THR:HA	1.90	0.53
2:B:165:ASN:HB3	2:B:217:THR:HB	1.89	0.53
2:B:68:ILE:HB	2:B:73:THR:O	2.09	0.53
2:D:58:GLN:HG3	2:D:64:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:HE2	1:A:59:ARG:HD3	1.90	0.52
3:F:48:PRO:HD3	3:F:63:ILE:HD12	1.91	0.52
3:F:67:ALA:HB1	3:F:72:PRO:HG2	1.92	0.52
3:E:73:THR:HA	4:G:1:A2G:C7	2.40	0.52
3:E:81:VAL:HG21	3:E:92:ARG:HH11	1.75	0.51
3:F:91:ILE:N	4:I:2:GAL:HO3	2.08	0.51
1:A:22:GLN:HB3	1:A:44:SER:CB	2.38	0.51
2:D:211:SER:HA	2:D:230:ASN:HA	1.92	0.50
3:E:51:PRO:HD3	3:E:104:GLY:HA2	1.91	0.50
2:D:53:LEU:HD11	2:D:108:CYS:HB2	1.92	0.50
3:E:108:CYS:HB3	3:E:116:SER:HB3	1.93	0.50
2:D:168:TRP:N	2:D:168:TRP:CD1	2.80	0.50
1:C:181:SER:H	1:C:221:ASN:HD21	1.59	0.50
2:B:114:LEU:H	3:E:22:SER:HB3	1.78	0.49
1:C:42:THR:HG23	1:C:97:SER:HB3	1.95	0.49
2:D:49:ILE:HD11	2:D:91:TYR:CE1	2.48	0.49
2:B:24:MET:HG2	2:B:117:THR:CG2	2.44	0.48
3:F:31:VAL:HG22	3:F:98:LEU:HD11	1.95	0.48
3:E:29:ASP:HB2	3:E:98:LEU:HD23	1.95	0.48
1:A:31:VAL:HG21	1:A:105:LEU:HD13	1.94	0.48
1:A:149:LEU:HD13	2:B:153:VAL:HG21	1.95	0.48
2:D:114:LEU:O	2:D:116:TRP:HD1	1.97	0.47
3:E:32:ASP:HA	3:E:94:LEU:O	2.15	0.47
1:A:26:SER:HB3	1:A:40:SER:HB3	1.96	0.47
2:B:69:TYR:O	2:B:73:THR:HB	2.15	0.47
1:A:51:THR:HG21	1:A:117:ARG:HG3	1.96	0.47
2:B:114:LEU:N	3:E:22:SER:HB3	2.29	0.47
2:B:24:MET:CG	2:B:117:THR:HG22	2.45	0.47
2:D:49:ILE:HG22	2:D:112:TYR:HB3	1.96	0.47
3:E:73:THR:HA	4:G:1:A2G:C2	2.45	0.47
2:B:126:ILE:H	2:B:186:GLN:HE21	1.63	0.47
2:B:24:MET:HE2	2:B:110:GLN:HB3	1.96	0.46
3:F:48:PRO:HB3	3:F:106:PHE:HA	1.98	0.46
1:C:70:ILE:HD11	1:C:75:VAL:HA	1.97	0.45
1:C:81:PRO:HA	1:C:84:GLN:HB2	1.98	0.45
3:F:63:ILE:O	3:F:76:PRO:HD2	2.17	0.45
3:E:81:VAL:CG2	3:E:92:ARG:NH1	2.78	0.45
3:F:63:ILE:HA	3:F:76:PRO:HD2	1.98	0.45
1:C:26:SER:HB3	1:C:40:SER:HB3	1.97	0.45
3:E:27:PRO:HB3	3:E:99:SER:O	2.17	0.45
1:C:48:ILE:HD11	1:C:93:THR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:LEU:HD12	2:D:114:LEU:HA	1.77	0.45
1:C:21:VAL:HG12	1:C:21:VAL:O	2.17	0.44
3:E:71:ALA:CB	4:G:1:A2G:O4	2.65	0.44
3:E:48:PRO:HD2	3:E:63:ILE:HG23	1.98	0.44
1:A:169:GLY:HA2	1:A:199:LEU:HB3	2.00	0.44
2:B:133:PRO:HA	2:B:157:ASN:O	2.18	0.44
2:B:68:ILE:HD12	2:B:71:THR:O	2.17	0.43
2:D:135:VAL:HA	2:D:155:PHE:O	2.18	0.43
2:D:57:GLN:OE1	2:D:65:LYS:HD3	2.18	0.43
3:E:30:ARG:HH11	3:E:95:GLU:HG3	1.83	0.43
2:B:33:ALA:HB2	2:B:39:VAL:HG11	2.00	0.43
1:C:179:TRP:CD1	1:C:188:VAL:HG23	2.54	0.43
1:A:160:MET:HA	1:A:209:PRO:HA	2.01	0.43
3:F:45:VAL:HG13	3:F:109:LYS:HB2	2.01	0.43
1:A:181:SER:H	1:A:221:ASN:HD21	1.67	0.42
2:B:54:ASN:ND2	2:B:70:TYR:H	2.18	0.42
1:C:102:VAL:HG13	1:C:105:LEU:HD21	2.01	0.42
2:B:71:THR:HG23	2:B:72:SER:H	1.83	0.42
3:F:64:LEU:HD22	3:F:75:PRO:HB3	2.00	0.42
3:F:64:LEU:CD2	3:F:75:PRO:HB3	2.50	0.42
2:B:68:ILE:HG22	2:B:74:LEU:HA	2.02	0.42
1:C:48:ILE:HD12	1:C:72:PRO:HB3	2.01	0.42
1:C:195:LEU:HA	1:C:199:LEU:O	2.20	0.42
2:D:100:GLN:O	2:D:103:VAL:HG12	2.20	0.42
2:B:60:PRO:C	2:B:62:GLY:H	2.23	0.41
2:B:114:LEU:O	2:B:116:TRP:HD1	2.03	0.41
2:B:171:ASP:HA	2:B:211:SER:HB3	2.02	0.41
3:F:35:CYS:HB3	3:F:116:SER:HB3	2.03	0.41
2:D:55:TRP:CD2	2:D:93:LEU:HB2	2.55	0.41
1:A:146:VAL:HB	1:A:233:LYS:HE3	2.02	0.41
2:B:114:LEU:HD12	2:B:114:LEU:HA	1.90	0.41
3:E:48:PRO:HB3	3:E:106:PHE:HA	2.02	0.41
2:D:168:TRP:H	2:D:168:TRP:HD1	1.68	0.41
3:F:49:SER:HB2	3:F:60:ARG:HA	2.03	0.41
1:C:31:VAL:HG21	1:C:37:VAL:HB	2.02	0.40
1:A:144:PRO:HB3	1:A:170:TYR:HB3	2.03	0.40
3:F:103:SER:HB3	3:F:125:ASP:OD2	2.21	0.40
2:B:33:ALA:O	2:B:126:ILE:HA	2.21	0.40
1:C:23:LEU:HD12	1:C:127:TYR:HD2	1.87	0.40
2:D:82:PHE:CE1	2:D:95:ILE:HG12	2.57	0.40
3:F:70:GLY:C	3:F:72:PRO:HD3	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:98:LEU:CD2	3:F:120:LEU:HD21	2.51	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	208/240 (87%)	198 (95%)	8 (4%)	2 (1%)	15	47
1	C	209/240 (87%)	193 (92%)	16 (8%)	0	100	100
2	B	212/234 (91%)	190 (90%)	20 (9%)	2 (1%)	17	50
2	D	207/234 (88%)	190 (92%)	15 (7%)	2 (1%)	15	47
3	E	93/116 (80%)	74 (80%)	17 (18%)	2 (2%)	6	27
3	F	92/116 (79%)	71 (77%)	18 (20%)	3 (3%)	4	19
All	All	1021/1180 (86%)	916 (90%)	94 (9%)	11 (1%)	14	45

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
2	D	27	THR
3	F	45	VAL
2	B	189	LYS
3	E	73	THR
3	F	74	VAL
2	B	97	ASN
2	D	71	THR
1	A	21	VAL
3	E	75	PRO
3	F	72	PRO

### 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	174/206 (84%)	152 (87%)	22 (13%)	4 17
1	C	176/206 (85%)	158 (90%)	18 (10%)	7 25
2	B	177/209 (85%)	150 (85%)	27 (15%)	2 11
2	D	168/209 (80%)	147 (88%)	21 (12%)	4 18
3	E	65/91 (71%)	50 (77%)	15 (23%)	1 3
3	F	64/91 (70%)	53 (83%)	11 (17%)	2 8
All	All	824/1012 (81%)	710 (86%)	114 (14%)	3 15

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	25	GLN
1	A	62	GLN
1	A	65	GLU
1	A	69	ARG
1	A	75	VAL
1	A	76	TYR
1	A	78	ARG
1	A	79	TYR
1	A	86	LYS
1	A	117	ARG
1	A	122	SER
1	A	126	ASP
1	A	160	MET
1	A	163	LEU
1	A	166	LEU
1	A	176	THR
1	A	180	ASN
1	A	184	LEU
1	A	213	TRP
1	A	220	CYS
1	A	221	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	22	ILE
2	B	23	GLN
2	B	26	GLN
2	B	31	LEU
2	B	35	LEU
2	B	37	ASP
2	B	46	SER
2	B	63	THR
2	B	64	VAL
2	B	72	SER
2	B	74	LEU
2	B	89	THR
2	B	98	LEU
2	B	101	GLU
2	B	110	GLN
2	B	117	THR
2	B	126	ILE
2	B	153	VAL
2	B	166	VAL
2	B	167	LYS
2	B	175	ARG
2	B	186	GLN
2	B	187	ASP
2	B	209	HIS
2	B	221	SER
2	B	229	PHE
2	B	231	ARG
1	C	22	GLN
1	C	25	GLN
1	C	42	THR
1	C	53	ILE
1	C	69	ARG
1	C	90	THR
1	C	122	SER
1	C	160	MET
1	C	166	LEU
1	C	176	THR
1	C	184	LEU
1	C	195	LEU
1	C	196	GLN
1	C	206	VAL
1	C	213	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	216	GLU
1	C	221	ASN
1	C	239	ASP
2	D	31	LEU
2	D	35	LEU
2	D	48	ASP
2	D	49	ILE
2	D	54	ASN
2	D	68	ILE
2	D	74	LEU
2	D	81	ARG
2	D	89	THR
2	D	90	ASP
2	D	94	THR
2	D	98	LEU
2	D	101	GLU
2	D	117	THR
2	D	128	ARG
2	D	153	VAL
2	D	158	ASN
2	D	168	TRP
2	D	176	GLN
2	D	205	GLU
2	D	213	THR
3	E	23	LEU
3	E	24	ASP
3	E	26	ARG
3	E	31	VAL
3	E	33	LEU
3	E	35	CYS
3	E	44	TRP
3	E	54	LYS
3	E	58	LYS
3	E	63	ILE
3	E	64	LEU
3	E	65	TRP
3	E	97	LEU
3	E	98	LEU
3	E	125	ASP
3	F	35	CYS
3	F	44	TRP
3	F	60	ARG

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Mol	Chain	Res	Type
3	F	63	ILE
3	F	64	LEU
3	F	77	LEU
3	F	94	LEU
3	F	96	LEU
3	F	98	LEU
3	F	99	SER
3	F	125	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	180	ASN
1	A	221	ASN
2	B	23	GLN
2	B	54	ASN
2	B	58	GLN
2	B	157	ASN
2	B	186	GLN
1	C	180	ASN
1	C	221	ASN
2	D	54	ASN
3	E	121	HIS
3	F	78	GLN
3	F	121	HIS

### 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](#)

14 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	A2G	G	1	3,4	14,14,15	0.57	0	17,19,21	1.39	3 (17%)
4	GAL	G	2	4	11,11,12	0.56	0	15,15,17	0.87	0
4	SIA	G	3	4	20,20,21	0.67	1 (5%)	24,28,31	1.42	4 (16%)
5	SGN	H	1	5	19,20,20	0.66	1 (5%)	24,31,31	2.07	4 (16%)
5	IDS	H	2	5	16,16,17	0.65	0	17,24,26	2.98	4 (23%)
5	SGN	H	3	5	18,19,20	0.39	0	22,29,31	2.17	4 (18%)
5	IDS	H	4	5	16,16,17	0.95	1 (6%)	17,24,26	2.76	6 (35%)
5	SGN	H	5	5	18,19,20	0.52	0	22,29,31	2.72	4 (18%)
5	IDS	H	6	5	16,16,17	0.56	0	17,24,26	2.67	5 (29%)
5	SGN	H	7	5	18,19,20	3.17	2 (11%)	22,29,31	2.26	5 (22%)
5	IDS	H	8	5	15,15,17	0.81	1 (6%)	15,22,26	2.33	3 (20%)
4	A2G	I	1	3,4	14,14,15	0.33	0	17,19,21	1.33	2 (11%)
4	GAL	I	2	4	11,11,12	0.37	0	15,15,17	0.71	0
4	SIA	I	3	4	20,20,21	1.07	3 (15%)	24,28,31	1.54	5 (20%)

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	A2G	G	1	3,4	1/1/5/7	2/6/23/26	0/1/1/1
4	GAL	G	2	4	-	1/2/19/22	0/1/1/1
4	SIA	G	3	4	-	10/18/34/38	0/1/1/1
5	SGN	H	1	5	-	6/11/31/31	0/1/1/1
5	IDS	H	2	5	1/1/6/7	1/9/26/29	1/1/1/1
5	SGN	H	3	5	-	1/11/28/31	0/1/1/1
5	IDS	H	4	5	-	0/9/26/29	0/1/1/1
5	SGN	H	5	5	-	5/11/28/31	0/1/1/1
5	IDS	H	6	5	1/1/6/7	1/9/26/29	1/1/1/1
5	SGN	H	7	5	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IDS	H	8	5	-	1/9/22/29	1/1/1/1
4	A2G	I	1	3,4	1/1/5/7	0/6/23/26	0/1/1/1
4	GAL	I	2	4	-	1/2/19/22	0/1/1/1
4	SIA	I	3	4	-	7/18/34/38	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	7	SGN	O1S-S1	12.99	1.56	1.42
5	H	4	IDS	O4-C4	3.14	1.50	1.43
4	I	3	SIA	O1A-C1	3.04	1.31	1.22
5	H	7	SGN	O4-C4	2.66	1.49	1.43
4	I	3	SIA	O1B-C1	-2.57	1.22	1.30
4	G	3	SIA	C2-C1	2.46	1.54	1.52
4	I	3	SIA	C2-C1	2.41	1.54	1.52
5	H	1	SGN	O4-C4	2.39	1.48	1.43
5	H	8	IDS	C4-C5	2.23	1.56	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5	SGN	O4-C4-C5	11.54	137.94	109.30
5	H	1	SGN	O4-C4-C5	8.19	129.64	109.30
5	H	3	SGN	O4-C4-C3	8.11	129.10	110.35
5	H	2	IDS	O4-C4-C5	8.08	127.85	109.74
5	H	7	SGN	O1S-S1-O2S	-7.52	102.39	120.16
5	H	8	IDS	C2-O2-S	7.43	127.59	117.91
5	H	6	IDS	C2-O2-S	7.00	127.04	117.91
5	H	2	IDS	C2-O2-S	6.46	126.33	117.91
5	H	4	IDS	C2-O2-S	6.22	126.02	117.91
5	H	4	IDS	O3S-S-O1S	5.40	127.26	108.49
5	H	2	IDS	O3S-S-O1S	4.97	125.76	108.49
5	H	7	SGN	C1-O5-C5	4.88	118.80	112.19
5	H	6	IDS	O3S-S-O1S	4.86	125.37	108.49
5	H	4	IDS	O4-C4-C5	4.61	120.09	109.74
5	H	6	IDS	O4-C4-C3	4.44	120.62	110.35
5	H	6	IDS	O4-C4-C5	4.22	119.21	109.74
5	H	4	IDS	O4-C4-C3	-3.96	101.20	110.35
4	G	3	SIA	C8-C7-C6	3.88	120.39	113.03
4	I	1	A2G	C1-C2-N2	-3.88	103.87	110.49
5	H	3	SGN	O4-C4-C5	3.80	118.73	109.30
4	I	3	SIA	O1B-C1-C2	3.58	123.25	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3	SIA	C3-C4-C5	-3.51	107.22	111.46
4	I	3	SIA	O1A-C1-C2	-3.47	114.38	122.57
5	H	8	IDS	O2S-S-O1S	3.44	126.03	112.22
4	G	1	A2G	C1-C2-N2	-3.35	104.76	110.49
5	H	5	SGN	O5S-S2-O4S	3.32	125.56	112.22
5	H	2	IDS	O4-C4-C3	3.29	117.94	110.35
5	H	7	SGN	O5S-S2-O4S	3.23	125.17	112.22
4	G	3	SIA	C4-C3-C2	3.20	115.55	109.81
5	H	4	IDS	O5-C1-C2	3.20	115.89	109.41
5	H	3	SGN	O5S-S2-O4S	3.19	125.03	112.22
4	G	1	A2G	C1-O5-C5	-3.16	107.91	112.19
5	H	1	SGN	O5S-S2-O4S	3.15	124.87	112.22
4	I	1	A2G	O5-C1-C2	3.15	116.26	111.29
5	H	7	SGN	O5-C1-C2	3.08	116.15	111.29
5	H	8	IDS	O5-C1-C2	2.91	115.30	109.41
5	H	4	IDS	C1-C2-C3	2.70	113.44	109.40
4	G	3	SIA	C6-O6-C2	2.64	117.00	111.34
5	H	7	SGN	C1-C2-N2	2.57	114.70	110.27
4	I	3	SIA	C6-O6-C2	2.55	116.80	111.34
5	H	1	SGN	O5-C1-C2	2.54	112.07	109.52
5	H	1	SGN	C1-C2-N2	2.41	113.55	110.67
5	H	5	SGN	C1-O5-C5	2.24	115.23	112.19
4	G	3	SIA	C6-C5-N5	2.22	114.59	110.91
5	H	3	SGN	O5-C1-C2	2.18	114.72	111.29
4	G	1	A2G	O3-C3-C2	2.15	113.92	109.47
4	I	3	SIA	C4-C3-C2	2.15	113.65	109.81
5	H	6	IDS	O2-C2-C3	2.11	109.90	106.95
5	H	5	SGN	O4-C4-C3	-2.03	105.66	110.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	1	A2G	C1
4	I	1	A2G	C1
5	H	2	IDS	C4
5	H	6	IDS	C4

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3	SIA	C5-C6-C7-C8
4	G	3	SIA	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
4	G	3	SIA	O6-C6-C7-C8
4	G	3	SIA	O6-C6-C7-O7
4	I	3	SIA	C5-C6-C7-C8
4	I	3	SIA	C5-C6-C7-O7
4	I	3	SIA	O6-C6-C7-C8
4	I	3	SIA	O6-C6-C7-O7
5	H	1	SGN	C4-C5-C6-O6
5	H	1	SGN	O5-C5-C6-O6
5	H	5	SGN	O5-C5-C6-O6
5	H	5	SGN	C2-N2-S1-O1S
5	H	7	SGN	C4-C5-C6-O6
5	H	7	SGN	O5-C5-C6-O6
5	H	7	SGN	C2-N2-S1-O2S
5	H	7	SGN	C2-N2-S1-O3S
5	H	7	SGN	C6-O6-S2-O6S
4	G	3	SIA	C11-C10-N5-C5
4	G	3	SIA	O10-C10-N5-C5
4	G	3	SIA	O7-C7-C8-O8
4	G	1	A2G	C4-C5-C6-O6
5	H	7	SGN	C6-O6-S2-O4S
5	H	1	SGN	C6-O6-S2-O4S
5	H	7	SGN	C6-O6-S2-O5S
4	G	3	SIA	O7-C7-C8-C9
5	H	5	SGN	C6-O6-S2-O6S
4	G	1	A2G	O5-C5-C6-O6
5	H	5	SGN	C6-O6-S2-O5S
4	G	2	GAL	O5-C5-C6-O6
4	I	2	GAL	O5-C5-C6-O6
4	G	3	SIA	O1A-C1-C2-O6
5	H	1	SGN	C2-N2-S1-O1S
5	H	7	SGN	C2-N2-S1-O1S
4	I	3	SIA	C6-C5-N5-C10
5	H	5	SGN	C6-O6-S2-O4S
5	H	2	IDS	C2-O2-S-O1S
5	H	1	SGN	C6-O6-S2-O5S
5	H	3	SGN	C6-O6-S2-O4S
4	G	3	SIA	C6-C7-C8-O8
5	H	1	SGN	C6-O6-S2-O6S
4	I	3	SIA	C4-C5-N5-C10
4	I	3	SIA	O1B-C1-C2-O6
5	H	6	IDS	O5-C5-C6-O6A
5	H	8	IDS	C4-C5-C6-O6A

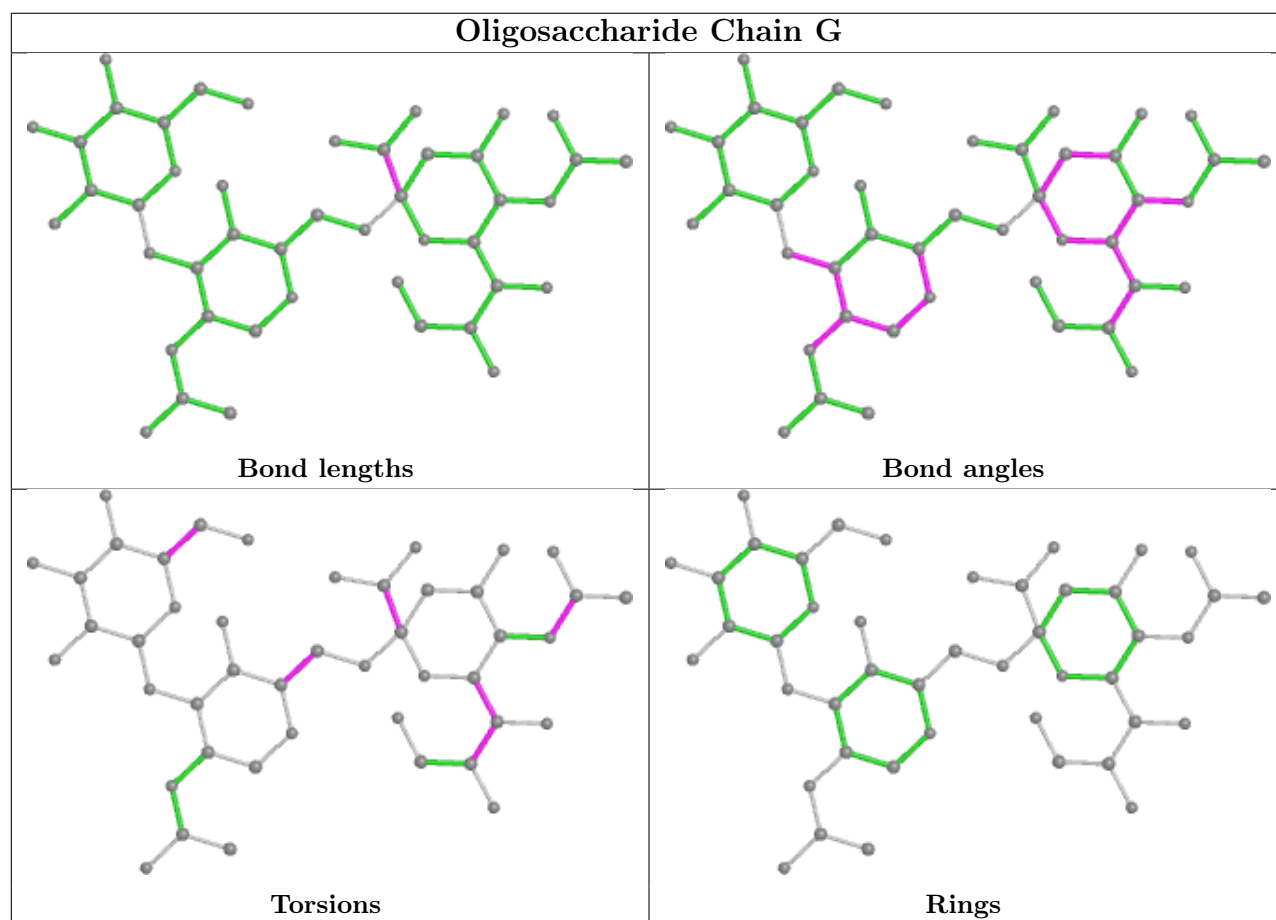
All (3) ring outliers are listed below:

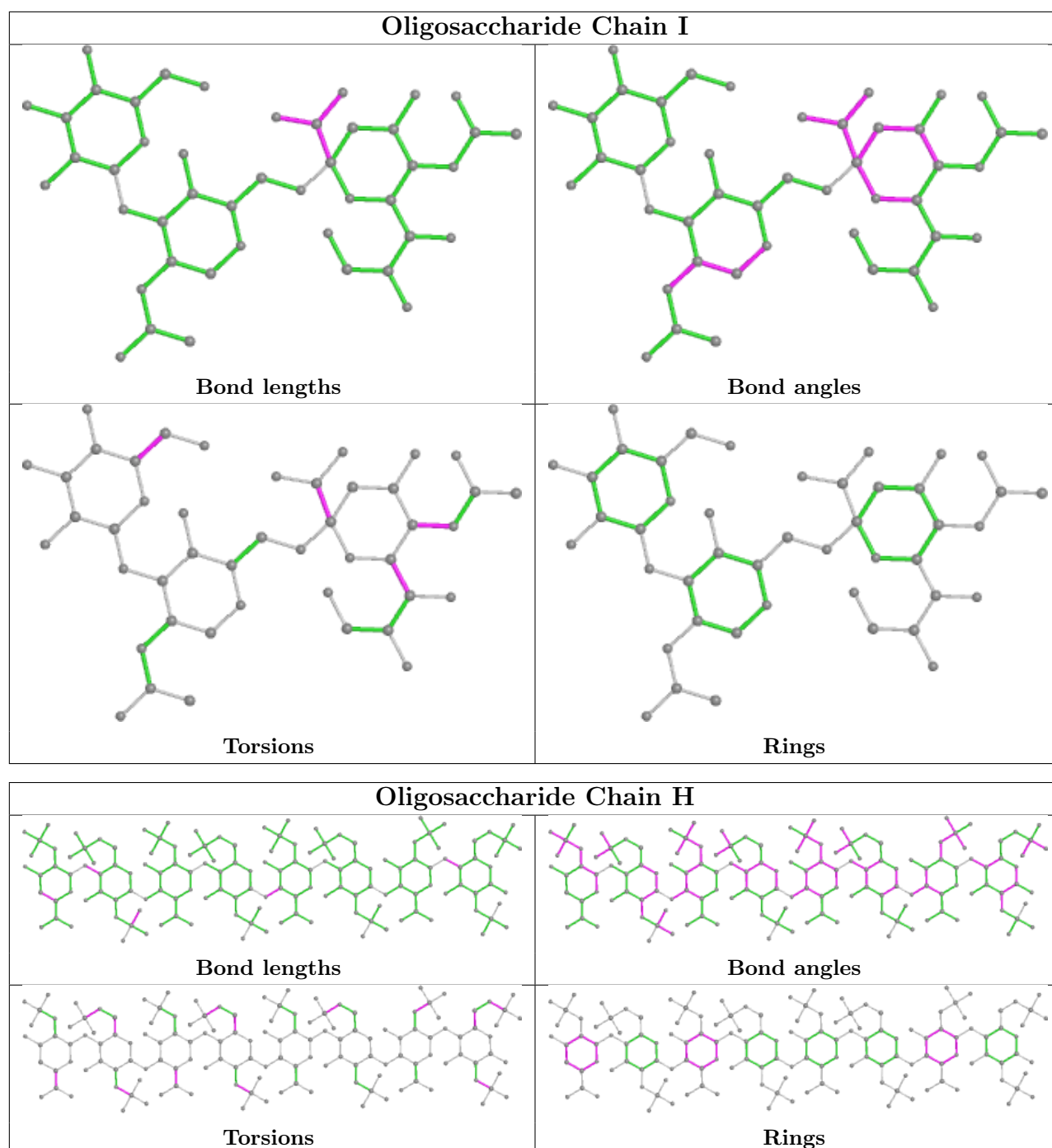
Mol	Chain	Res	Type	Atoms
5	H	2	IDS	C1-C2-C3-C4-C5-O5
5	H	8	IDS	C1-C2-C3-C4-C5-O5
5	H	6	IDS	C1-C2-C3-C4-C5-O5

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	GAL	1	0
4	G	1	A2G	4	0

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





## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

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	212/240 (88%)	0.11	4 (1%) 66 48	63, 101, 132, 167	0
1	C	213/240 (88%)	0.08	3 (1%) 75 59	72, 112, 151, 181	0
2	B	214/234 (91%)	-0.04	2 (0%) 84 72	65, 111, 152, 200	0
2	D	211/234 (90%)	0.35	13 (6%) 20 9	63, 128, 279, 290	0
3	E	99/116 (85%)	0.07	2 (2%) 65 46	70, 100, 142, 252	0
3	F	98/116 (84%)	0.04	1 (1%) 82 70	75, 97, 135, 227	0
All	All	1047/1180 (88%)	0.11	25 (2%) 59 38	63, 107, 177, 290	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	201	LEU	10.0
3	F	43	ARG	4.2
2	D	234	CYS	4.1
2	D	228	SER	3.5
2	D	224	PRO	3.5
2	D	229	PHE	3.4
2	D	152	VAL	3.4
3	E	102	ASP	3.2
1	A	48	ILE	3.0
2	D	199	LEU	2.6
2	D	223	SER	2.5
2	D	170	ILE	2.5
1	C	53	ILE	2.4
1	C	196	GLN	2.4
2	B	220	THR	2.3
1	A	116	ALA	2.3
1	A	21	VAL	2.2
2	B	98	LEU	2.2
1	A	186	SER	2.2

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
2	D	138	PHE	2.2
3	E	76	PRO	2.1
2	D	140	PRO	2.1
2	D	232	ASN	2.1
2	D	171	ASP	2.0
1	C	132	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](#)

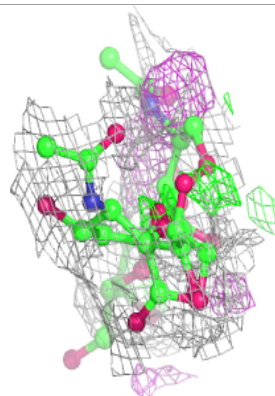
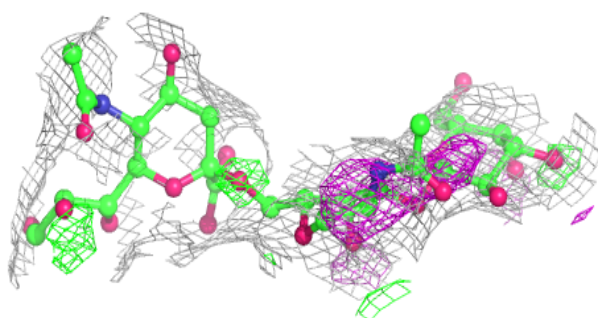
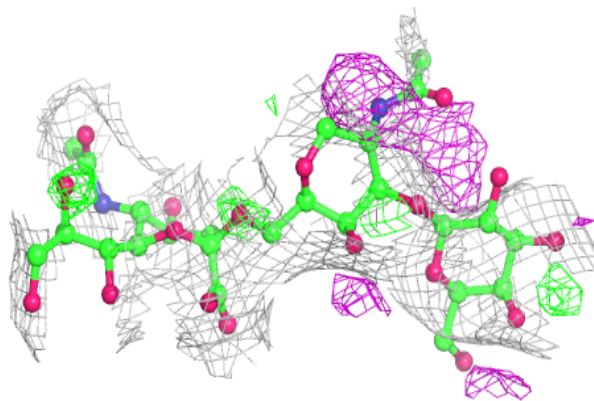
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 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	A2G	G	1	14/15	0.61	0.33	127,136,146,151	0
5	SGN	H	1	20/20	0.71	0.25	187,198,201,201	0
4	GAL	I	2	11/12	0.74	0.23	168,170,171,172	0
4	GAL	G	2	11/12	0.77	0.32	105,111,116,120	0
5	SGN	H	7	19/20	0.77	0.20	143,154,165,165	0
4	SIA	G	3	20/21	0.79	0.19	161,166,174,176	0
5	IDS	H	8	15/17	0.79	0.32	163,164,166,166	0
5	SGN	H	3	19/20	0.84	0.12	136,151,168,169	0
4	A2G	I	1	14/15	0.88	0.20	165,171,191,205	0
4	SIA	I	3	20/21	0.88	0.22	216,228,236,236	0
5	IDS	H	2	16/17	0.89	0.21	166,178,182,182	0
5	IDS	H	6	16/17	0.90	0.17	122,133,136,140	0
5	IDS	H	4	16/17	0.91	0.17	105,117,125,125	0
5	SGN	H	5	19/20	0.93	0.18	97,104,108,112	0

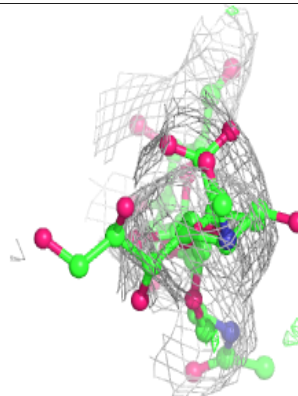
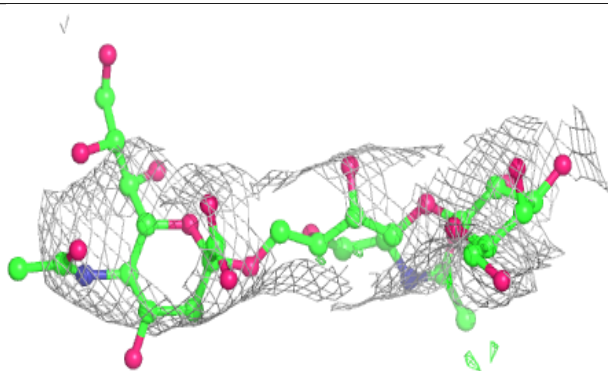
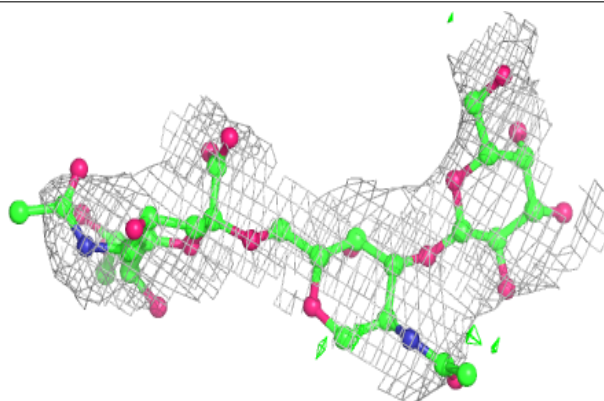
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

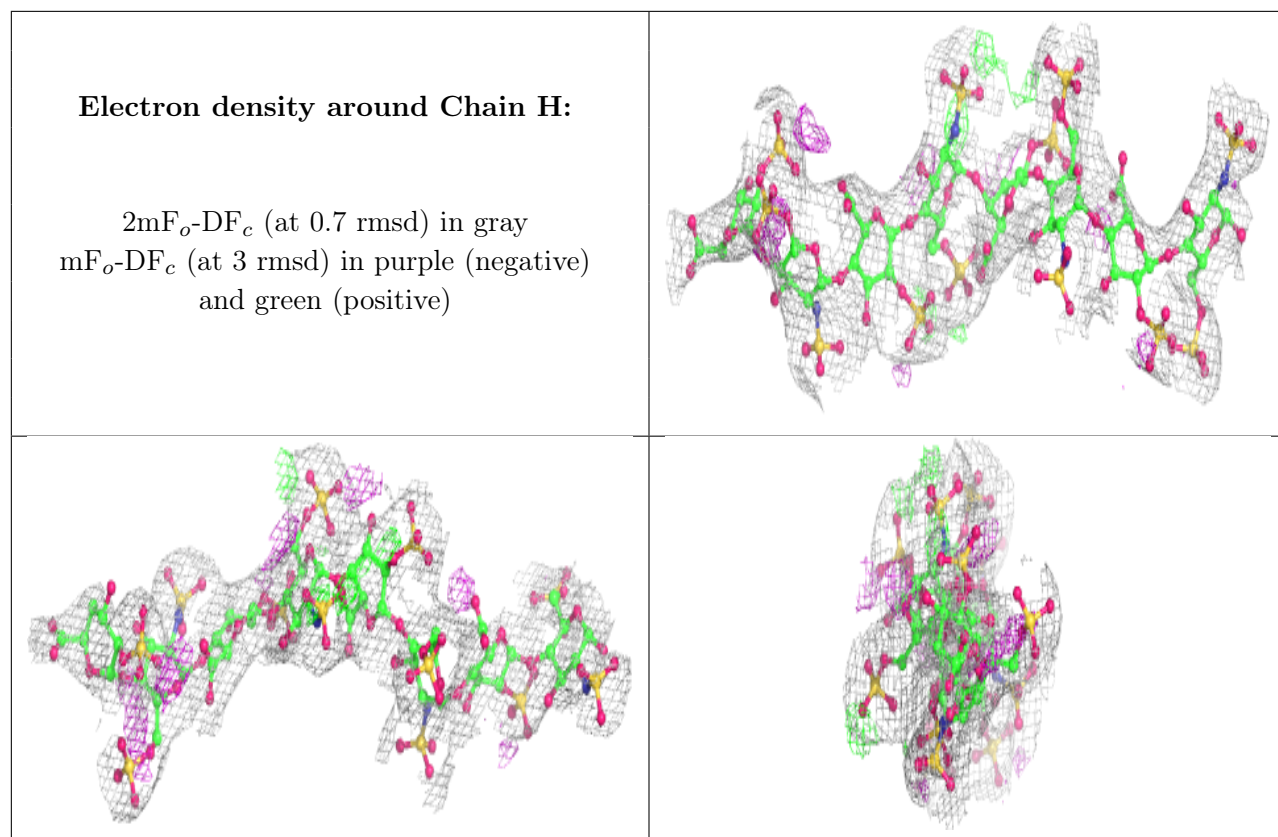
**Electron density around Chain G:**

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

**Electron density around Chain I:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.