



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:30 AM BST

PDB ID : 4GMT  
Title : Crystal structure of heterosubtypic Fab S139/1  
Authors : Lee, P.S.; Ekiert, D.C.; Wilson, I.A.  
Deposited on : 2012-08-16  
Resolution : 2.05 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

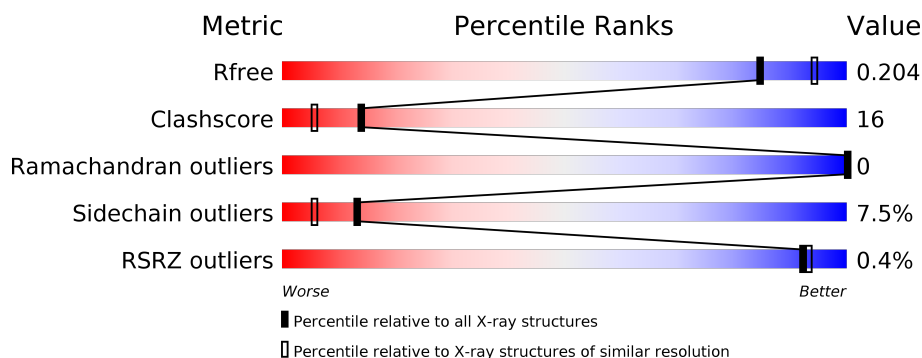
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	L	214	<div> <div></div> <div>68%29%•</div> </div>
1	M	214	<div> <div></div> <div>75%21%•</div> </div>
2	H	225	<div> <div></div> <div>63%29%• 5%</div> </div>
2	I	225	<div> <div></div> <div>62%31%• 5%</div> </div>
3	A	2	<div> <div></div> <div>50%50%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6690 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 Fab S139/1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1662	1031	278	346	7			
1	M	213	Total	C	N	O	S	0	0	0
			1662	1031	278	346	7			

- Molecule 2 is a protein called Fab S139/1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1635	1046	262	320	7			
2	I	213	Total	C	N	O	S	0	0	0
			1635	1046	262	320	7			

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



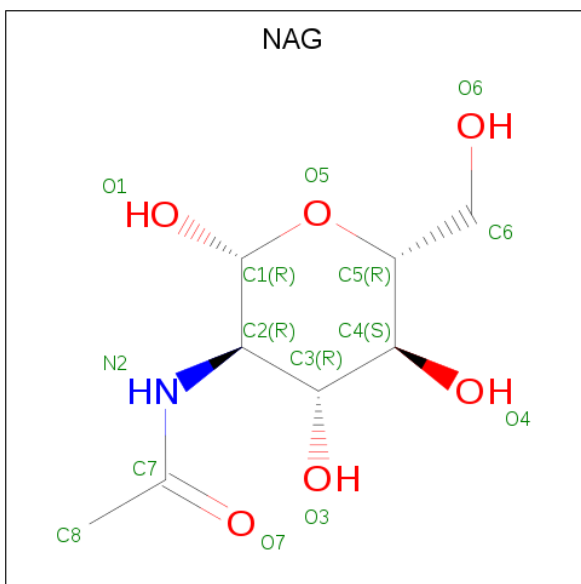
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total	C	N	O	0	0
			14	8	1	5		

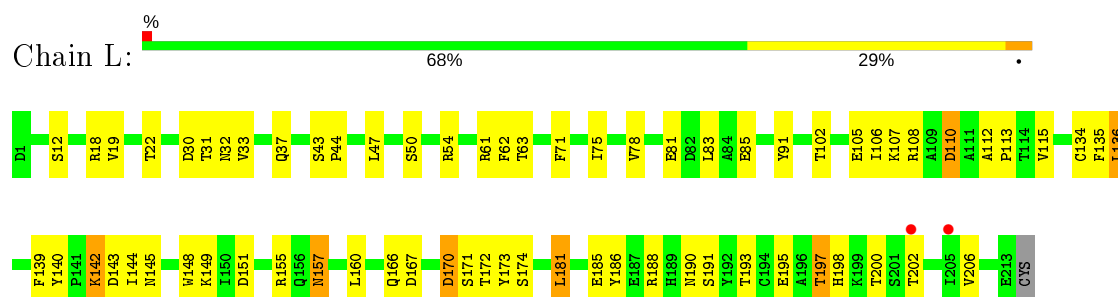
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	11	Total 11	O 11	0	0
6	H	8	Total 8	O 8	0	0
6	M	15	Total 15	O 15	0	0
6	I	10	Total 10	O 10	0	0

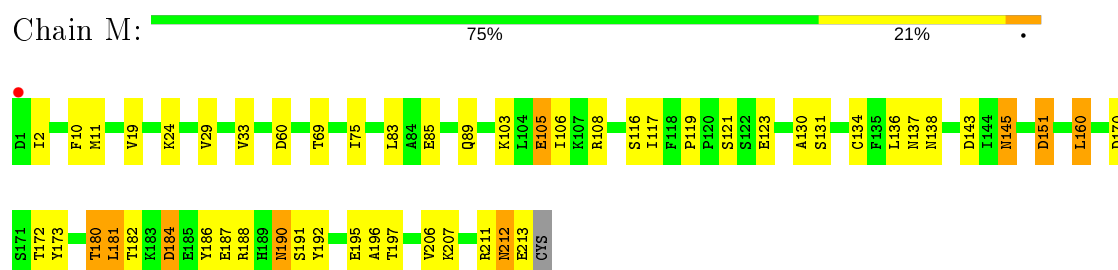
### 3 Residue-property plots [i](#)

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.

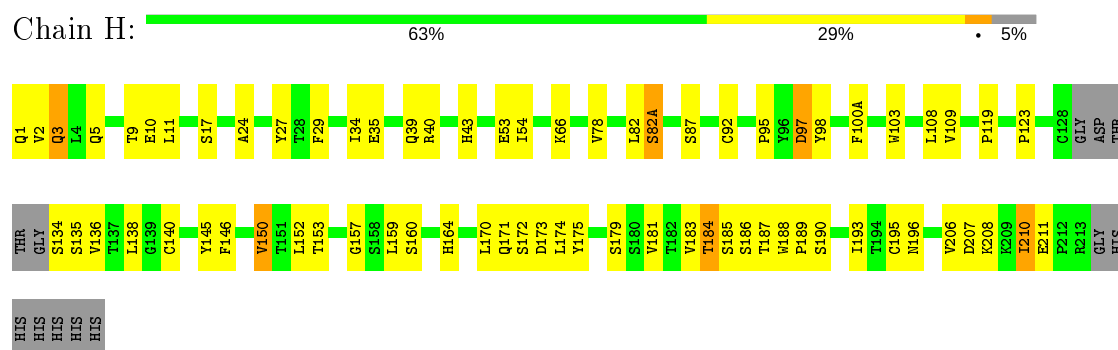
- Molecule 1: Fab S139/1 light chain



- Molecule 1: Fab S139/1 light chain

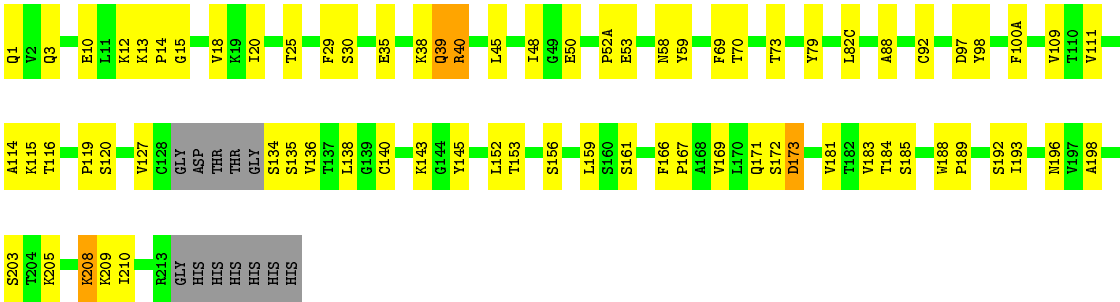


- Molecule 2: Fab S139/1 heavy chain



- Molecule 2: Fab S139/1 heavy chain





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

Chain A: 

50%

50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.84Å 106.84Å 185.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.29 – 2.05 46.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.29-2.05) 93.5 (46.29-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.93 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.158 , 0.209 0.160 , 0.204	Depositor DCC
$R_{free}$ test set	3999 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l	Xtriage
Reported twinning fraction	0.497 for -h,-k,l	Depositor
Outliers	0 of 75884 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: PCA, 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	L	0.42	0/1698	0.58	0/2306
1	M	0.46	0/1698	0.59	0/2306
2	H	0.41	0/1674	0.59	0/2291
2	I	0.42	0/1674	0.59	0/2291
All	All	0.43	0/6744	0.58	0/9194

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 [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	L	1662	0	1575	62	0
1	M	1662	0	1575	42	0
2	H	1635	0	1587	47	2
2	I	1635	0	1587	58	2
3	A	28	0	25	2	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
5	I	14	0	13	0	0
6	H	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	10	0	0	1	0
6	L	11	0	0	0	0
6	M	15	0	0	0	0
All	All	6690	0	6362	204	2

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 16.

All (204) 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:L:83:LEU:HD11	1:L:106:ILE:HD11	1.60	0.81
1:M:151:ASP:HA	1:M:191:SER:HB3	1.70	0.72
2:H:196:ASN:ND2	2:H:207:ASP:OD1	2.26	0.68
2:H:11:LEU:HD21	2:H:146:PHE:CE2	2.30	0.67
1:L:83:LEU:HD11	1:L:106:ILE:CD1	2.26	0.66
2:H:3:GLN:NE2	2:H:5:GLN:OE1	2.29	0.66
1:L:145:ASN:HB3	1:L:197:THR:HG22	1.77	0.65
1:L:136:LEU:N	1:L:136:LEU:HD12	2.12	0.64
2:H:170:LEU:HD13	2:H:175:TYR:CE1	2.33	0.62
1:L:83:LEU:HD21	1:L:106:ILE:CD1	2.29	0.62
1:M:136:LEU:HD12	1:M:136:LEU:N	2.13	0.62
2:I:152:LEU:HD23	2:I:153:THR:N	2.15	0.62
1:M:83:LEU:HD21	1:M:106:ILE:HB	1.82	0.62
2:H:95:PRO:HA	2:H:100(A):PHE:HA	1.82	0.61
1:L:83:LEU:HD21	1:L:106:ILE:HD11	1.82	0.60
1:M:160:LEU:HD21	2:I:169:VAL:HB	1.82	0.60
1:L:61:ARG:O	1:L:75:ILE:HA	2.02	0.60
2:I:18:VAL:CG1	2:I:82(C):LEU:HD11	2.31	0.60
1:M:184:ASP:O	1:M:188:ARG:HG3	2.02	0.59
1:L:83:LEU:CD1	1:L:106:ILE:HD11	2.33	0.59
2:H:123:PRO:HD3	2:H:208:LYS:HG2	1.83	0.59
2:H:170:LEU:CD1	2:H:175:TYR:CE1	2.87	0.58
2:I:38:LYS:HB2	2:I:48:ILE:HD11	1.84	0.58
2:H:40:ARG:HB2	2:H:43:HIS:HB2	1.85	0.58
1:M:187:GLU:HA	1:M:211:ARG:CD	2.34	0.58
1:L:181:LEU:CD1	1:L:186:TYR:HB2	2.34	0.57
2:I:161:SER:HB2	6:I:407:HOH:O	2.05	0.56
1:M:121:SER:HB2	1:M:123:GLU:OE1	2.05	0.56
2:H:97:ASP:N	2:H:97:ASP:OD2	2.37	0.56
1:M:19:VAL:HG13	1:M:75:ILE:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:114:ALA:HB2	2:I:173:ASP:OD1	2.06	0.56
1:M:131:SER:OG	1:M:180:THR:HG23	2.05	0.56
2:I:136:VAL:HG13	2:I:183:VAL:HG23	1.88	0.55
1:L:30:ASP:CG	1:L:31:THR:H	2.09	0.55
1:M:186:TYR:O	1:M:192:TYR:OH	2.21	0.55
2:I:136:VAL:HG13	2:I:183:VAL:CG2	2.37	0.55
1:M:11:MET:CE	1:M:19:VAL:HG23	2.36	0.55
2:I:13:LYS:HG2	2:I:14:PRO:HD2	1.89	0.55
2:H:136:VAL:HG13	2:H:183:VAL:HG22	1.89	0.55
2:I:172:SER:O	2:I:173:ASP:HB3	2.07	0.54
1:L:149:LYS:HB2	1:L:193:THR:HG23	1.89	0.54
1:M:117:ILE:HG22	1:M:207:LYS:HZ2	1.72	0.54
1:L:85:GLU:HA	1:L:102:THR:O	2.07	0.54
1:M:117:ILE:HG22	1:M:207:LYS:NZ	2.23	0.53
2:H:66:LYS:O	2:H:82:LEU:HA	2.09	0.53
2:H:11:LEU:HD21	2:H:146:PHE:HE2	1.72	0.53
1:L:142:LYS:HB3	1:L:173:TYR:CD1	2.44	0.53
1:M:190:ASN:OD1	1:M:212:ASN:OD1	2.27	0.53
2:I:192:SER:HB2	2:I:209:LYS:HE2	1.91	0.53
2:H:35:GLU:HG3	2:H:100(A):PHE:CE1	2.44	0.52
3:A:1:NAG:H61	3:A:2:NAG:C7	2.38	0.52
2:I:18:VAL:HG12	2:I:82(C):LEU:HD11	1.91	0.52
1:L:31:THR:O	1:L:50:SER:HA	2.09	0.52
1:M:180:THR:HG21	2:I:171:GLN:HE22	1.75	0.52
1:L:83:LEU:CD1	1:L:106:ILE:CD1	2.88	0.51
2:H:134:SER:N	2:H:185:SER:HB3	2.26	0.51
2:H:34:ILE:HG13	2:H:78:VAL:HG21	1.91	0.51
1:M:2:ILE:HD13	1:M:29:VAL:HG12	1.91	0.51
2:I:152:LEU:HD23	2:I:152:LEU:C	2.31	0.51
2:H:152:LEU:HD13	2:H:179:SER:HB2	1.93	0.51
2:I:10:GLU:HG3	2:I:20:ILE:HD11	1.91	0.51
1:L:195:GLU:HG2	1:L:206:VAL:HG13	1.93	0.51
1:L:19:VAL:HG12	1:L:75:ILE:HB	1.93	0.51
2:H:53:GLU:HG2	2:H:54:ILE:HG23	1.93	0.51
2:I:35:GLU:HG3	2:I:100(A):PHE:CE1	2.46	0.51
1:L:142:LYS:HB3	1:L:173:TYR:CE1	2.45	0.51
1:L:185:GLU:HA	1:L:188:ARG:HE	1.76	0.50
1:L:83:LEU:CD2	1:L:106:ILE:CD1	2.90	0.50
1:M:136:LEU:CD1	1:M:136:LEU:N	2.75	0.50
2:I:39:GLN:HG3	2:I:45:LEU:HD23	1.92	0.50
2:I:15:GLY:N	2:I:82(C):LEU:O	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:GLN:HB2	1:L:173:TYR:CZ	2.46	0.50
1:L:136:LEU:HD23	1:L:144:ILE:HD11	1.93	0.50
2:I:188:TRP:CD1	2:I:193:ILE:HD12	2.46	0.49
2:I:39:GLN:HB2	2:I:45:LEU:HD23	1.94	0.49
3:A:1:NAG:H61	3:A:2:NAG:H82	1.94	0.49
1:M:119:PRO:CG	2:I:127:VAL:HG12	2.43	0.49
1:L:110:ASP:N	1:L:110:ASP:OD1	2.46	0.49
2:I:135:SER:HA	2:I:185:SER:N	2.28	0.48
1:L:32:ASN:HB3	1:L:91:TYR:CD1	2.48	0.48
2:I:208:LYS:CE	2:I:208:LYS:HA	2.43	0.48
1:M:19:VAL:CG1	1:M:75:ILE:HB	2.43	0.48
1:M:85:GLU:HG3	1:M:103:LYS:HG3	1.95	0.48
2:H:183:VAL:HG11	2:H:193:ILE:HD11	1.96	0.48
2:H:172:SER:O	2:H:173:ASP:HB2	2.14	0.48
1:L:167:ASP:O	1:L:171:SER:HA	2.13	0.48
1:L:139:PHE:O	1:L:172:THR:HB	2.14	0.48
2:H:153:THR:HB	2:H:157:GLY:HA2	1.95	0.48
1:L:108:ARG:HD3	1:L:171:SER:O	2.13	0.48
1:L:170:ASP:OD1	1:L:172:THR:HG23	2.13	0.47
2:H:135:SER:HA	2:H:185:SER:H	1.79	0.47
2:H:134:SER:C	2:H:185:SER:HB3	2.35	0.47
2:I:115:LYS:CG	2:I:116:THR:H	2.28	0.47
1:L:160:LEU:HD23	1:L:160:LEU:C	2.35	0.47
1:L:12:SER:OG	1:L:107:LYS:HB2	2.14	0.47
1:M:136:LEU:C	1:M:137:ASN:HD22	2.19	0.47
1:M:11:MET:HE1	1:M:19:VAL:HG23	1.96	0.47
1:M:119:PRO:HD3	2:I:127:VAL:CG1	2.44	0.47
2:H:9:THR:HG23	2:H:108:LEU:HB3	1.96	0.46
2:I:20:ILE:O	2:I:79:TYR:HA	2.14	0.46
2:H:184:THR:O	2:H:187:THR:N	2.46	0.46
2:I:29:PHE:CE2	2:I:52(A):PRO:HB3	2.50	0.46
2:I:59:TYR:CE1	2:I:69:PHE:CD2	3.04	0.46
1:L:107:LYS:HA	1:L:140:TYR:OH	2.16	0.46
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.49	0.46
2:I:115:LYS:CG	2:I:116:THR:N	2.79	0.46
2:I:114:ALA:HB2	2:I:173:ASP:OD2	2.15	0.46
1:L:136:LEU:CD1	1:L:136:LEU:N	2.79	0.46
2:I:156:SER:N	2:I:196:ASN:OD1	2.42	0.46
1:L:143:ASP:O	1:L:198:HIS:HD2	1.99	0.45
2:H:87:SER:HA	2:H:109:VAL:O	2.16	0.45
1:L:83:LEU:CD2	1:L:106:ILE:HD12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:166:PHE:HA	2:I:167:PRO:HD3	1.88	0.45
1:M:181:LEU:HD11	1:M:186:TYR:HB2	1.99	0.45
1:M:187:GLU:HA	1:M:211:ARG:HD3	1.99	0.45
1:L:44:PRO:HG2	2:H:103:TRP:CZ3	2.52	0.45
2:H:35:GLU:O	2:H:92:CYS:HA	2.17	0.45
2:I:114:ALA:HB2	2:I:173:ASP:CG	2.37	0.45
2:I:208:LYS:HE3	2:I:208:LYS:CA	2.46	0.45
1:M:130:ALA:HB3	1:M:181:LEU:HD12	1.99	0.45
2:I:12:LYS:O	2:I:111:VAL:HA	2.17	0.45
1:M:85:GLU:OE1	1:M:103:LYS:HE3	2.17	0.45
2:I:188:TRP:CG	2:I:189:PRO:HA	2.52	0.45
1:L:83:LEU:CD2	1:L:106:ILE:HD11	2.47	0.45
2:H:138:LEU:HD11	2:H:193:ILE:HD12	1.98	0.44
1:L:18:ARG:HA	1:L:75:ILE:O	2.16	0.44
1:M:24:LYS:HE3	1:M:69:THR:OG1	2.17	0.44
2:H:188:TRP:CG	2:H:189:PRO:HA	2.52	0.44
2:I:159:LEU:HD21	2:I:181:VAL:HG21	2.00	0.44
1:L:195:GLU:HG2	1:L:206:VAL:HG22	2.00	0.44
1:M:11:MET:HE2	1:M:19:VAL:HG23	1.98	0.44
2:I:30:SER:O	2:I:53:GLU:HB2	2.17	0.44
1:L:115:VAL:HA	1:L:135:PHE:O	2.17	0.44
1:L:166:GLN:HB2	1:L:173:TYR:CE2	2.53	0.44
2:H:134:SER:C	2:H:185:SER:CB	2.86	0.44
2:H:136:VAL:HG13	2:H:183:VAL:CG2	2.48	0.44
2:I:138:LEU:HD22	2:I:210:ILE:HG21	1.98	0.44
2:I:50:GLU:HG3	2:I:58:ASN:HB3	1.99	0.44
1:L:113:PRO:HA	1:L:139:PHE:HB3	2.00	0.44
1:L:139:PHE:CE2	1:L:174:SER:HA	2.53	0.44
2:H:135:SER:N	2:H:185:SER:HB2	2.32	0.44
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.00	0.43
1:L:149:LYS:HB2	1:L:193:THR:CG2	2.48	0.43
2:I:39:GLN:HB2	2:I:45:LEU:CD2	2.48	0.43
2:H:2:VAL:HG13	2:H:27:TYR:CD1	2.53	0.43
2:I:10:GLU:HB2	2:I:109:VAL:HG22	2.01	0.43
2:I:135:SER:HB2	2:I:184:THR:HA	2.01	0.43
1:L:33:VAL:HG21	1:L:71:PHE:CZ	2.54	0.43
1:M:195:GLU:HG2	1:M:206:VAL:HG22	2.00	0.43
1:M:160:LEU:HG	2:I:169:VAL:HG11	2.01	0.43
1:M:105:GLU:OE1	1:M:173:TYR:OH	2.21	0.43
1:M:182:THR:HB	1:M:184:ASP:OD2	2.18	0.43
1:M:145:ASN:O	1:M:196:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:ARG:HE	1:L:157:ASN:HB2	1.84	0.43
1:M:138:ASN:HA	1:M:172:THR:HB	2.01	0.43
1:M:181:LEU:CD1	1:M:186:TYR:HB2	2.49	0.43
2:H:17:SER:HB2	2:H:82(A):SER:HA	2.00	0.42
1:L:174:SER:OG	2:H:164:HIS:CE1	2.72	0.42
1:M:187:GLU:HA	1:M:211:ARG:HD2	2.00	0.42
2:I:29:PHE:O	2:I:52(A):PRO:HG2	2.19	0.42
2:I:40:ARG:HB3	2:I:88:ALA:HB2	2.00	0.42
2:H:210:ILE:N	2:H:210:ILE:CD1	2.82	0.42
1:L:185:GLU:HA	1:L:188:ARG:NE	2.33	0.42
2:I:198:ALA:HB2	2:I:205:LYS:CD	2.50	0.42
2:H:134:SER:N	2:H:185:SER:CB	2.82	0.42
1:L:37:GLN:HB2	1:L:47:LEU:HD11	2.02	0.42
2:I:38:LYS:HE2	2:I:40:ARG:HG2	2.01	0.42
2:I:35:GLU:O	2:I:92:CYS:HA	2.20	0.42
2:I:39:GLN:CG	2:I:45:LEU:HD23	2.50	0.41
1:L:167:ASP:O	1:L:171:SER:N	2.48	0.41
2:H:146:PHE:HB2	2:H:174:LEU:HD23	2.03	0.41
1:L:112:ALA:HA	1:L:200:THR:OG1	2.20	0.41
1:L:151:ASP:HA	1:L:191:SER:HB3	2.02	0.41
1:L:197:THR:O	1:L:197:THR:CG2	2.68	0.41
1:L:195:GLU:CG	1:L:206:VAL:HG22	2.50	0.41
1:L:81:GLU:CD	1:L:81:GLU:H	2.23	0.41
2:I:115:LYS:HG2	2:I:116:THR:N	2.35	0.41
1:L:157:ASN:N	1:L:157:ASN:OD1	2.53	0.41
1:M:85:GLU:CD	1:M:103:LYS:HE3	2.41	0.41
2:I:39:GLN:HG3	2:I:45:LEU:CD2	2.50	0.41
2:H:136:VAL:CG1	2:H:183:VAL:CG2	2.99	0.41
2:I:134:SER:C	2:I:185:SER:OG	2.59	0.41
1:L:185:GLU:HA	1:L:188:ARG:CD	2.50	0.41
2:I:136:VAL:CG1	2:I:183:VAL:HG23	2.49	0.41
1:L:33:VAL:HG21	1:L:71:PHE:CE1	2.56	0.41
1:M:108:ARG:HD2	1:M:170:ASP:O	2.21	0.41
1:M:212:ASN:OD1	1:M:212:ASN:N	2.53	0.41
1:L:170:ASP:OD1	1:L:172:THR:OG1	2.33	0.41
2:I:119:PRO:HB3	2:I:145:TYR:HB3	2.02	0.41
2:I:50:GLU:CG	2:I:58:ASN:HB3	2.51	0.41
1:L:185:GLU:HA	1:L:188:ARG:HD3	2.03	0.41
2:H:10:GLU:HB2	2:H:109:VAL:HG22	2.03	0.40
2:H:27:TYR:CE2	2:H:29:PHE:HA	2.55	0.40
2:I:208:LYS:HE3	2:I:208:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:116:SER:O	1:M:134:CYS:HA	2.22	0.40
2:H:40:ARG:CB	2:H:43:HIS:HB2	2.50	0.40
1:M:33:VAL:HA	1:M:89:GLN:O	2.21	0.40
2:H:136:VAL:CG1	2:H:183:VAL:HG23	2.51	0.40
2:I:38:LYS:HE2	2:I:40:ARG:HD2	2.03	0.40
1:L:142:LYS:HB3	1:L:173:TYR:CG	2.56	0.40
2:H:145:TYR:CZ	2:H:150:VAL:HG22	2.57	0.40
2:H:159:LEU:CD2	2:H:181:VAL:HG21	2.52	0.40
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.57	0.40
1:L:54:ARG:NH1	1:L:62:PHE:O	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:TYR:OH	2:I:53:GLU:OE1[5_555]	2.13	0.07
2:H:53:GLU:OE1	2:I:98:TYR:OH[5_555]	2.15	0.05

## 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	L	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
1	M	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
2	H	209/225 (93%)	203 (97%)	6 (3%)	0	100	100
2	I	209/225 (93%)	204 (98%)	5 (2%)	0	100	100
All	All	840/878 (96%)	813 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	L	191/192 (100%)	177 (93%)	14 (7%)	14	6
1	M	191/192 (100%)	177 (93%)	14 (7%)	14	6
2	H	184/193 (95%)	169 (92%)	15 (8%)	11	5
2	I	184/193 (95%)	171 (93%)	13 (7%)	14	7
All	All	750/770 (97%)	694 (92%)	56 (8%)	13	6

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	22	THR
1	L	43	SER
1	L	63	THR
1	L	78	VAL
1	L	105	GLU
1	L	110	ASP
1	L	136	LEU
1	L	142	LYS
1	L	157	ASN
1	L	170	ASP
1	L	181	LEU
1	L	190	ASN
1	L	197	THR
1	L	202	THR
2	H	3	GLN
2	H	39	GLN
2	H	82(A)	SER
2	H	97	ASP
2	H	140	CYS
2	H	150	VAL
2	H	160	SER
2	H	171	GLN
2	H	184	THR
2	H	186	SER

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Mol	Chain	Res	Type
2	H	190	SER
2	H	195	CYS
2	H	206	VAL
2	H	210	ILE
2	H	211	GLU
1	M	10	PHE
1	M	60	ASP
1	M	105	GLU
1	M	143	ASP
1	M	145	ASN
1	M	151	ASP
1	M	160	LEU
1	M	180	THR
1	M	181	LEU
1	M	184	ASP
1	M	190	ASN
1	M	197	THR
1	M	212	ASN
1	M	213	GLU
2	I	3	GLN
2	I	25	THR
2	I	39	GLN
2	I	40	ARG
2	I	70	THR
2	I	73	THR
2	I	97	ASP
2	I	120	SER
2	I	140	CYS
2	I	143	LYS
2	I	173	ASP
2	I	203	SER
2	I	208	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	137	ASN
2	H	164	HIS
1	M	28	ASN
1	M	137	ASN
1	M	190	ASN
2	I	81	GLN

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Mol	Chain	Res	Type
2	I	171	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	PCA	I	1	2	7,8,9	2.01	2 (28%)	9,10,12	2.06	5 (55%)
2	PCA	H	1	2	7,8,9	2.41	2 (28%)	9,10,12	1.96	5 (55%)

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
2	PCA	I	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	4.84	1.47	1.34
2	I	1	PCA	CD-N	4.46	1.46	1.34
2	H	1	PCA	CA-N	4.03	1.51	1.46
2	I	1	PCA	CA-N	2.61	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	OE-CD-CG	-2.95	121.62	126.76
2	I	1	PCA	CA-N-CD	-2.93	103.55	113.58
2	I	1	PCA	OE-CD-CG	-2.80	121.88	126.76
2	H	1	PCA	CA-N-CD	-2.75	104.15	113.58
2	I	1	PCA	CB-CA-C	-2.68	109.01	112.70
2	I	1	PCA	CB-CA-N	2.62	110.83	103.30
2	I	1	PCA	CG-CD-N	2.50	114.85	108.39
2	H	1	PCA	CB-CA-N	2.50	110.46	103.30
2	H	1	PCA	CB-CA-C	-2.35	109.46	112.70
2	H	1	PCA	CG-CD-N	2.09	113.81	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	1	3,2	14,14,15	0.60	0	17,19,21	0.88	0
3	NAG	A	2	3	14,14,15	0.67	0	17,19,21	0.86	1 (5%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	NAG	C2-N2-C7	-2.51	119.33	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	NAG	O5-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	NAG	2	0
3	A	1	NAG	2	0

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	I	302	-	4,4,4	0.13	0	6,6,6	0.15	0
4	SO4	H	303	-	4,4,4	0.15	0	6,6,6	0.24	0
5	NAG	I	301	2	14,14,15	0.54	0	17,19,21	0.74	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
5	NAG	I	301	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	I	301	NAG	C1-O5-C5	2.39	115.42	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	301	NAG	C8-C7-N2-C2
5	I	301	NAG	O7-C7-N2-C2
5	I	301	NAG	C4-C5-C6-O6
5	I	301	NAG	O5-C5-C6-O6

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	L	213/214 (99%)	-0.20	2 (0%) 84 86	34, 55, 96, 130	0
1	M	213/214 (99%)	-0.34	1 (0%) 91 92	31, 46, 84, 107	0
2	H	212/225 (94%)	-0.35	0 100 100	31, 52, 75, 104	0
2	I	212/225 (94%)	-0.37	0 100 100	32, 48, 71, 95	0
All	All	850/878 (96%)	-0.31	3 (0%) 92 93	31, 51, 84, 130	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	205	ILE	3.5
1	L	202	THR	2.4
1	M	1	ASP	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PCA	H	1	8/9	0.96	0.12	68,72,74,77	0
2	PCA	I	1	8/9	0.98	0.11	55,65,70,78	0

### 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	2	14/15	0.89	0.19	93,106,114,119	0
3	NAG	A	1	14/15	0.93	0.11	66,76,87,99	0

## 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( $\text{\AA}^2$ )	Q<0.9
5	NAG	I	301	14/15	0.88	0.19	106,126,131,135	0
4	SO4	H	303	5/5	0.97	0.10	77,85,87,91	0
4	SO4	I	302	5/5	0.99	0.09	72,73,77,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.