



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:07 PM EDT

PDB ID : 7KBT  
Title : Factor VIII in complex with the anti-C2 domain antibody, G99  
Authors : Ronayne, E.K.; Gish, J.; Wilson, C.; Peters, S.; Spencer, H.T.; Spiegel, P.C.; Childers, K.C.  
Deposited on : 2020-10-02  
Resolution : 4.15 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

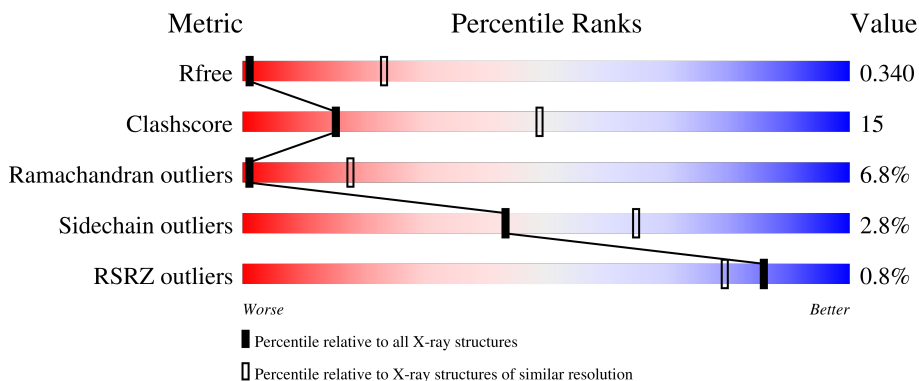
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.15 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	1020 (4.54-3.76)
Clashscore	141614	1028 (4.52-3.80)
Ramachandran outliers	138981	1005 (4.54-3.78)
Sidechain outliers	138945	1024 (4.54-3.76)
RSRZ outliers	127900	1055 (4.62-3.70)

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	1467	
2	E	224	
3	F	214	
4	B	2	
4	G	2	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	NAG	B	2	X	-	-	-

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 11366 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 Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1233	9809	6272	1700	1785	52	0	0	0

- Molecule 2 is a protein called G99 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	115	818	503	139	173	3	0	0	0

- Molecule 3 is a protein called G99 light chain.

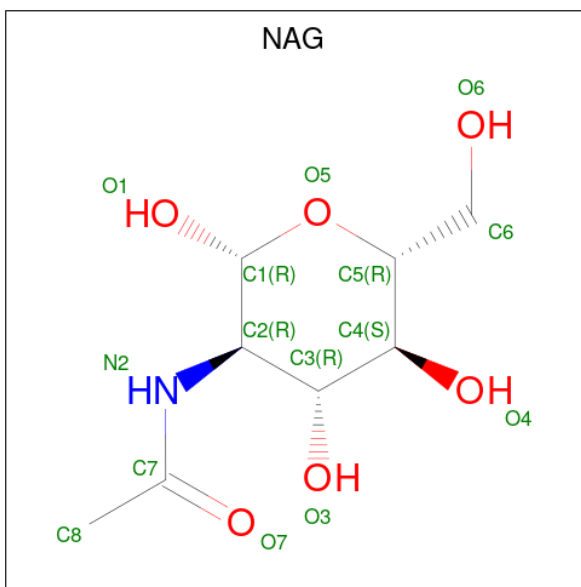
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	96	666	403	120	140	3	0	0	0

- 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
			Total	C	N	O			
4	G	2	28	16	2	10	0	0	0
4	B	2	28	16	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		





SER THR TYR SER MET SER SER THR LEU THR LEU THR LYS ASP GLU TYR GLU ARG HIS ASN SER TYR THR CYS GLU ALA THR HIS LYS THR SER THR SER PRO ILE VAL LYS SER PHE ASN ARG ASN GLU CYS

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

Chain G:  50%

MAG1  
MAG2

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

Chain B:  100%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.24Å 132.24Å 380.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.48 – 4.15 25.72 – 4.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (25.48-4.15) 99.7 (25.72-4.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 4.10Å)	Xtrriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, $R_{free}$	0.300 , 0.338 0.300 , 0.340	Depositor DCC
$R_{free}$ test set	1987 reflections (7.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	195.9	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 139.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	253.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: CU, NAG, ZN, CA

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	0.29	0/10070	0.63	3/13647 (0.0%)
2	E	0.26	0/833	0.48	0/1129
3	F	0.25	0/673	0.48	0/906
All	All	0.29	0/11576	0.61	3/15682 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	C-N-CA	6.71	138.46	121.70
1	A	491	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	449	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2057	GLY	Peptide
1	A	2141	ASN	Peptide
1	A	2178	LEU	Mainchain
1	A	2278	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	404	ASP	Peptide
1	A	570	LYS	Peptide
1	A	691	GLY	Peptide
1	A	696	ASP	Peptide

## 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	9809	0	9455	310	0
2	E	818	0	700	16	0
3	F	666	0	587	10	0
4	B	28	0	25	0	0
4	G	28	0	25	1	0
5	A	14	0	13	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
All	All	11366	0	10805	331	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 15.

All (331) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1781:ARG:HG2	1:A:1782:PRO:HD2	1.49	0.93
1:A:540:GLU:HG2	1:A:583:ARG:HH21	1.39	0.85
1:A:64:ARG:HH21	1:A:65:PRO:HD2	1.41	0.85
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.58	0.84
1:A:54:GLU:HG2	1:A:75:PRO:HG3	1.58	0.83
1:A:1846:ASP:HB3	1:A:1889:TRP:HE1	1.46	0.81
1:A:708:VAL:HG23	1:A:709:SER:H	1.45	0.81
1:A:12:LEU:N	1:A:49:LYS:O	2.17	0.77
1:A:2246:GLN:HB3	1:A:2320:ARG:HB2	1.66	0.76
1:A:401:ALA:O	1:A:403:ASP:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:OE1	1:A:318:HIS:NE2	2.19	0.75
1:A:1874:GLN:HE22	1:A:1934:MET:HA	1.51	0.75
1:A:406:SER:O	1:A:408:LYS:N	2.15	0.75
1:A:2261:LEU:HD11	1:A:2282:VAL:HG12	1.69	0.75
1:A:2179:GLY:HA3	1:A:2184:ALA:HB3	1.69	0.73
1:A:2100:GLN:HB2	1:A:2155:HIS:HB2	1.70	0.73
1:A:243:LEU:HD12	1:A:246:LEU:HD23	1.70	0.73
1:A:435:THR:HG23	1:A:437:LYS:H	1.53	0.73
1:A:256:TRP:HE1	1:A:299:THR:HG22	1.54	0.72
1:A:293:THR:HA	1:A:1977:ASN:HD21	1.54	0.72
1:A:2274:PHE:HB3	1:A:2281:LYS:HE2	1.71	0.72
1:A:2265:SER:O	1:A:2303:THR:OG1	2.09	0.71
1:A:80:GLU:HG2	1:A:182:GLU:HA	1.73	0.71
1:A:120:SER:OG	1:A:123:GLU:OE1	2.08	0.70
1:A:2187:ASP:OD1	1:A:2209:ARG:NH2	2.25	0.69
1:A:1709:TYR:O	1:A:1925:VAL:HG12	1.93	0.68
1:A:467:ASN:OD1	1:A:468:GLN:N	2.27	0.68
1:A:130:LEU:HG	1:A:131:PRO:HD2	1.75	0.67
2:E:34:ILE:HD11	2:E:51:ILE:HD12	1.77	0.67
1:A:620:TYR:HB3	1:A:624:SER:HB2	1.77	0.66
1:A:2236:LYS:NZ	1:A:2237:THR:OG1	2.29	0.66
1:A:238:TYR:HD2	1:A:243:LEU:HA	1.60	0.66
1:A:2142:PRO:HG3	4:G:1:NAG:H81	1.78	0.65
1:A:1993:VAL:HA	1:A:2016:VAL:HG23	1.78	0.65
1:A:280:ARG:O	1:A:281:HIS:ND1	2.30	0.65
1:A:1782:PRO:HB3	1:A:1809:PRO:HD3	1.78	0.65
3:F:56:SER:OG	3:F:57:SER:N	2.30	0.64
1:A:1776:LYS:HD2	1:A:1812:THR:HB	1.78	0.64
1:A:1756:LEU:HD21	1:A:1762:TYR:CE2	2.32	0.64
1:A:121:GLN:OE1	1:A:121:GLN:N	2.31	0.64
1:A:114:GLU:HB2	1:A:127:ASP:HB3	1.80	0.64
1:A:1946:SER:HB3	1:A:1978:LEU:HD22	1.80	0.64
1:A:160:LEU:HD22	1:A:169:LEU:HD21	1.79	0.63
1:A:1805:ASN:O	1:A:1813:ARG:NH1	2.32	0.63
1:A:80:GLU:CG	1:A:182:GLU:HA	2.28	0.63
1:A:2198:ASN:OD1	1:A:2199:MET:N	2.32	0.63
1:A:504:LEU:O	1:A:506:GLY:N	2.32	0.63
1:A:666:ASP:HB2	1:A:1835:TRP:HZ3	1.64	0.62
1:A:2169:CYS:SG	1:A:2173:SER:HA	2.39	0.62
1:A:2260:PHE:HE1	1:A:2262:ILE:HD11	1.63	0.62
1:A:235:VAL:HG23	1:A:321:MET:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:NH1	1:A:328:GLU:OE2	2.33	0.62
1:A:73:LEU:HD21	1:A:199:LEU:HB2	1.81	0.62
1:A:427:ARG:HE	1:A:448:ILE:HA	1.65	0.61
2:E:47:TRP:HE3	2:E:61:ASN:HD22	1.49	0.61
1:A:522:THR:O	1:A:524:SER:N	2.31	0.61
1:A:110:SER:OG	1:A:137:TYR:O	2.09	0.60
1:A:2274:PHE:HD2	1:A:2281:LYS:HD3	1.66	0.60
1:A:73:LEU:HD12	1:A:236:ASN:ND2	2.16	0.60
1:A:239:VAL:O	1:A:242:SER:OG	2.18	0.60
1:A:649:LEU:HA	1:A:694:ASN:ND2	2.18	0.58
1:A:2021:CYS:SG	1:A:2175:SER:OG	2.61	0.58
1:A:696:ASP:HA	1:A:699:ASN:OD1	2.03	0.58
1:A:2106:SER:N	1:A:2148:TYR:O	2.36	0.58
1:A:54:GLU:HG2	1:A:75:PRO:CG	2.33	0.58
1:A:444:HIS:O	1:A:445:GLU:HB2	2.04	0.58
1:A:2194:SER:OG	1:A:2228:GLU:OE2	2.21	0.58
1:A:654:SER:O	1:A:656:TYR:N	2.36	0.57
1:A:293:THR:HA	1:A:1977:ASN:ND2	2.18	0.57
1:A:496:LYS:H	1:A:496:LYS:HD3	1.68	0.57
1:A:2246:GLN:HE22	1:A:2292:PRO:HD3	1.70	0.57
1:A:189:ARG:HB3	1:A:192:ASN:OD1	2.05	0.57
1:A:591:ILE:HG23	1:A:595:LEU:HD22	1.87	0.57
1:A:2254:SER:O	1:A:2315:HIS:ND1	2.37	0.57
2:E:108:ASP:O	3:F:46:ARG:NH1	2.34	0.57
1:A:2044:GLY:C	1:A:2046:TRP:H	2.08	0.57
1:A:2235:GLN:O	1:A:2304:ARG:NH1	2.37	0.57
1:A:601:VAL:HG23	1:A:602:GLN:H	1.70	0.56
1:A:73:LEU:HD12	1:A:236:ASN:HD22	1.69	0.56
1:A:525:ASP:HB2	1:A:526:PRO:HD2	1.87	0.56
1:A:1870:GLN:O	1:A:1871:VAL:HG22	2.05	0.56
1:A:1706:LEU:HD21	1:A:1729:ARG:HD3	1.87	0.56
1:A:2262:ILE:HD13	1:A:2281:LYS:HZ1	1.70	0.56
1:A:686:GLY:O	1:A:708:VAL:HG22	2.06	0.56
1:A:649:LEU:HA	1:A:694:ASN:HD21	1.70	0.56
1:A:107:TRP:O	1:A:108:LYS:HB2	2.04	0.55
1:A:1786:TYR:CD1	1:A:1790:ILE:HD11	2.42	0.55
1:A:311:CYS:SG	1:A:313:ILE:HG22	2.48	0.54
1:A:541:ARG:HG2	1:A:583:ARG:HB3	1.89	0.54
1:A:629:VAL:HG23	1:A:708:VAL:HG12	1.88	0.54
1:A:104:VAL:HG12	1:A:105:SER:H	1.73	0.54
1:A:694:ASN:O	1:A:696:ASP:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:TYR:CE2	1:A:77:ILE:HG23	2.43	0.54
1:A:491:LEU:HD23	1:A:495:VAL:HB	1.89	0.54
1:A:601:VAL:O	1:A:603:LEU:N	2.37	0.54
1:A:1951:GLU:OE2	1:A:1952:ASN:ND2	2.40	0.54
1:A:2115:TYR:OH	1:A:2142:PRO:HD2	2.08	0.54
1:A:2104:MET:O	1:A:2150:ARG:N	2.36	0.54
1:A:2119:SER:O	1:A:2121:GLY:N	2.40	0.54
1:A:1826:THR:HG22	1:A:1828:ASP:H	1.73	0.54
1:A:162:HIS:NE2	1:A:1999:GLU:OE2	2.33	0.53
1:A:2201:ALA:HB1	1:A:2203:TRP:NE1	2.23	0.53
1:A:246:LEU:HD12	1:A:325:VAL:HG13	1.89	0.53
1:A:692:CYS:HB3	1:A:698:ARG:HB2	1.90	0.53
1:A:631:LEU:HD11	1:A:685:PRO:HB3	1.91	0.53
1:A:176:ALA:HB2	1:A:197:VAL:HG11	1.92	0.52
1:A:2100:GLN:O	1:A:2154:THR:HG22	2.09	0.52
1:A:2091:GLN:O	1:A:2093:PHE:N	2.42	0.52
1:A:1764:ARG:HG2	1:A:1856:LEU:HB2	1.91	0.52
1:A:2174:CYS:HG	1:A:2326:CYS:HG	1.58	0.52
1:A:2193:SER:HB3	2:E:103:PHE:CD2	2.44	0.52
1:A:2273:LEU:HD21	2:E:101:TYR:CE1	2.45	0.52
1:A:1894:ASN:HA	1:A:1896:GLU:HG3	1.92	0.52
1:A:497:HIS:C	1:A:499:LYS:H	2.13	0.52
2:E:14:PRO:HG3	2:E:120:VAL:HG12	1.92	0.51
1:A:687:LEU:HD21	1:A:705:LEU:HD23	1.92	0.51
1:A:248:GLY:O	1:A:327:VAL:HA	2.10	0.51
1:A:148:THR:O	1:A:181:ARG:NH2	2.35	0.51
1:A:200:PHE:HE2	1:A:270:ILE:HG21	1.76	0.51
1:A:447:GLY:O	1:A:448:ILE:HG22	2.09	0.51
1:A:1832:CYS:HA	1:A:1858:CYS:HA	1.93	0.51
1:A:1834:ALA:HB2	1:A:1943:TYR:CD1	2.46	0.51
1:A:2103:ILE:HD13	1:A:2140:PHE:CE1	2.46	0.51
3:F:39:LYS:HB2	3:F:43:THR:HB	1.92	0.51
1:A:4:ARG:O	1:A:5:TYR:HD1	1.93	0.51
1:A:2080:ILE:HG12	1:A:2145:ILE:HD12	1.91	0.51
1:A:2246:GLN:HE22	1:A:2292:PRO:CD	2.23	0.51
1:A:1829:GLU:O	1:A:1859:ARG:NH2	2.44	0.50
1:A:708:VAL:HG23	1:A:709:SER:N	2.22	0.50
2:E:88:SER:HA	2:E:120:VAL:HB	1.93	0.50
1:A:1732:LYS:NZ	1:A:1885:GLU:OE2	2.28	0.50
1:A:409:SER:HB2	1:A:413:ASN:HD22	1.77	0.50
1:A:2250:SER:O	1:A:2252:LEU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:ASP:HA	3:F:46:ARG:HD3	1.93	0.50
1:A:70:MET:O	1:A:236:ASN:ND2	2.42	0.50
1:A:1808:GLN:HB2	1:A:1811:GLU:HG2	1.92	0.50
1:A:2101:PHE:HE2	1:A:2103:ILE:HD11	1.76	0.50
1:A:50:THR:HG21	1:A:95:HIS:NE2	2.27	0.50
3:F:12:SER:HA	3:F:104:VAL:HG12	1.92	0.50
1:A:1742:SER:O	1:A:1744:THR:N	2.44	0.50
1:A:2009:GLY:O	1:A:2011:SER:N	2.45	0.50
1:A:2281:LYS:HZ2	1:A:2283:PHE:HE2	1.60	0.49
1:A:1756:LEU:HD21	1:A:1762:TYR:HE2	1.76	0.49
1:A:2036:GLN:NE2	1:A:2074:ASP:O	2.44	0.49
1:A:2058:SER:OG	1:A:2059:ILE:N	2.45	0.49
1:A:2207:LYS:HE2	1:A:2216:SER:O	2.12	0.49
1:A:684:ASN:O	1:A:708:VAL:HG21	2.12	0.49
1:A:1712:SER:OG	1:A:1713:GLU:OE1	2.21	0.49
1:A:2049:LYS:HG3	1:A:2050:LEU:HD22	1.93	0.49
1:A:119:THR:HG23	1:A:123:GLU:HB2	1.95	0.49
1:A:1764:ARG:HB3	1:A:1863:LEU:HD11	1.94	0.49
1:A:91:ASN:ND2	1:A:97:VAL:HG22	2.27	0.49
1:A:2027:MET:HA	1:A:2032:ILE:CG2	2.43	0.49
1:A:2313:TRP:HB3	1:A:2317:ILE:HD13	1.94	0.49
1:A:1737:GLU:HB2	1:A:1761:PRO:HG3	1.94	0.48
1:A:2098:ILE:HD13	1:A:2162:LEU:HD13	1.95	0.48
1:A:2112:TRP:CZ3	1:A:2150:ARG:HB2	2.48	0.48
1:A:1808:GLN:O	1:A:1810:ASN:N	2.46	0.48
1:A:2042:GLN:O	1:A:2044:GLY:N	2.47	0.48
1:A:495:VAL:HG12	1:A:498:LEU:H	1.78	0.48
1:A:1934:MET:SD	1:A:1940:ILE:HD13	2.54	0.48
1:A:1781:ARG:C	1:A:1809:PRO:HG3	2.33	0.48
1:A:2228:GLU:HG3	1:A:2229:TRP:N	2.29	0.48
1:A:77:ILE:HD12	1:A:177:LEU:HD13	1.95	0.48
1:A:666:ASP:HB2	1:A:1835:TRP:CZ3	2.48	0.48
1:A:1707:TRP:HB3	1:A:1732:LYS:HG3	1.95	0.48
1:A:1756:LEU:O	1:A:1759:LEU:HB2	2.14	0.48
1:A:2241:THR:HA	1:A:2300:PRO:HB3	1.95	0.48
1:A:486:LEU:HG	1:A:487:TYR:CD2	2.49	0.47
1:A:2241:THR:HG22	1:A:2325:GLY:HA2	1.96	0.47
1:A:616:SER:HA	1:A:621:VAL:HG12	1.96	0.47
1:A:489:ARG:HE	1:A:489:ARG:HB2	1.48	0.47
1:A:404:ASP:N	1:A:404:ASP:OD1	2.47	0.47
1:A:658:PHE:HA	1:A:680:MET:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:PHE:O	1:A:700:ARG:N	2.43	0.47
2:E:110:ASP:OD1	2:E:110:ASP:N	2.47	0.47
1:A:2053:LEU:HG	1:A:2087:GLN:OE1	2.15	0.47
1:A:631:LEU:HD12	1:A:710:SER:HB3	1.97	0.47
1:A:2103:ILE:HD13	1:A:2140:PHE:HE1	1.79	0.47
1:A:2116:ARG:HG3	1:A:2123:LEU:HA	1.97	0.47
1:A:1936:GLN:O	1:A:1990:PRO:HG2	2.15	0.47
1:A:540:GLU:HG2	1:A:583:ARG:NH2	2.18	0.47
3:F:41:ASP:OD1	3:F:41:ASP:N	2.44	0.47
1:A:602:GLN:O	1:A:604:GLU:N	2.46	0.47
1:A:648:PHE:CZ	1:A:1953:ILE:HD11	2.50	0.47
1:A:2046:TRP:CZ2	1:A:2059:ILE:HG22	2.50	0.47
1:A:155:LEU:HD11	1:A:1972:LYS:O	2.15	0.46
1:A:1751:GLU:H	1:A:1754:LYS:HG3	1.80	0.46
1:A:2038:THR:O	1:A:2072:LYS:N	2.48	0.46
1:A:703:THR:O	1:A:704:ALA:HB3	2.15	0.46
1:A:1846:ASP:HB3	1:A:1889:TRP:NE1	2.24	0.46
3:F:67:SER:O	3:F:70:ASP:N	2.40	0.46
1:A:1759:LEU:HD22	1:A:1922:ASN:ND2	2.29	0.46
1:A:2080:ILE:HG13	1:A:2171:LEU:HD23	1.97	0.46
1:A:164:ASP:HB3	1:A:167:LYS:HB2	1.96	0.46
1:A:525:ASP:HB2	1:A:526:PRO:CD	2.44	0.46
1:A:1735:PHE:O	1:A:1760:GLY:HA2	2.16	0.46
1:A:102:VAL:HG13	1:A:1957:HIS:CE1	2.50	0.46
1:A:472:PRO:HB2	1:A:502:PRO:HB2	1.98	0.46
1:A:2093:PHE:HD1	1:A:2093:PHE:H	1.64	0.46
1:A:497:HIS:O	1:A:499:LYS:N	2.48	0.46
1:A:2096:LEU:HD23	1:A:2159:ARG:HB2	1.97	0.46
2:E:96:CYS:O	2:E:113:GLY:N	2.48	0.46
1:A:279:VAL:O	1:A:281:HIS:N	2.49	0.46
1:A:1870:GLN:C	1:A:1872:THR:H	2.19	0.46
1:A:599:ALA:O	1:A:601:VAL:HG13	2.16	0.46
1:A:703:THR:OG1	1:A:704:ALA:N	2.48	0.45
1:A:2228:GLU:HG3	1:A:2229:TRP:H	1.81	0.45
1:A:1762:TYR:OH	1:A:1877:ALA:N	2.49	0.45
1:A:1731:LYS:HD3	1:A:1890:TYR:HB3	1.98	0.45
1:A:2274:PHE:HD1	1:A:2301:LEU:HD12	1.81	0.45
1:A:290:SER:O	1:A:291:PRO:C	2.55	0.45
1:A:1753:ASN:HB3	1:A:1756:LEU:HD23	1.98	0.45
1:A:591:ILE:O	1:A:595:LEU:HB2	2.17	0.45
1:A:651:VAL:HG12	1:A:668:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2230:LEU:HB3	1:A:2308:ILE:HG22	1.99	0.45
1:A:279:VAL:HG12	1:A:297:ALA:HB2	1.99	0.45
1:A:542:ASP:O	1:A:545:SER:OG	2.31	0.45
1:A:1781:ARG:HH21	1:A:1783:TYR:HE1	1.64	0.45
1:A:1996:TRP:HB2	1:A:2014:PHE:CZ	2.52	0.45
1:A:445:GLU:O	1:A:618:ASN:ND2	2.50	0.45
1:A:1714:SER:HA	1:A:1715:PRO:HD2	1.88	0.45
1:A:1732:LYS:HD3	1:A:1758:LEU:HD21	1.99	0.45
1:A:1783:TYR:O	1:A:1807:VAL:HB	2.17	0.45
1:A:1934:MET:HE2	1:A:2016:VAL:HG12	1.99	0.45
1:A:2026:GLY:O	1:A:2032:ILE:HG22	2.16	0.45
1:A:2107:LEU:HD13	1:A:2146:ALA:HA	1.98	0.45
1:A:130:LEU:H	1:A:133:LYS:NZ	2.15	0.44
1:A:2070:TRP:HB3	1:A:2152:HIS:CE1	2.52	0.44
1:A:2112:TRP:CH2	1:A:2148:TYR:HB3	2.51	0.44
1:A:1826:THR:HB	1:A:1829:GLU:HG3	2.00	0.44
1:A:1732:LYS:HD3	1:A:1758:LEU:HD11	1.99	0.44
1:A:2178:LEU:HD13	1:A:2323:VAL:HB	1.99	0.44
1:A:64:ARG:HD2	1:A:65:PRO:HD2	1.99	0.44
2:E:98:ARG:NH2	2:E:107:TYR:HB3	2.33	0.44
1:A:2187:ASP:HB3	1:A:2206:SER:HB2	1.99	0.44
1:A:91:ASN:HD21	1:A:96:PRO:HA	1.82	0.44
1:A:165:LEU:HD23	1:A:2003:GLY:HA2	2.00	0.44
1:A:250:HIS:O	1:A:252:LYS:N	2.44	0.44
1:A:259:ILE:HG23	1:A:294:PHE:CE1	2.52	0.44
1:A:430:ALA:HB2	1:A:451:PRO:HG3	1.99	0.43
2:E:41:PRO:HD3	2:E:92:ALA:HA	2.00	0.43
1:A:69:TRP:CE2	1:A:196:PHE:HD1	2.35	0.43
1:A:467:ASN:O	1:A:468:GLN:HG3	2.17	0.43
1:A:1924:TYR:CD1	1:A:1928:THR:HG22	2.54	0.43
1:A:1781:ARG:O	1:A:1809:PRO:HG3	2.18	0.43
1:A:103:GLY:HA2	1:A:1962:VAL:HG12	2.00	0.43
1:A:516:THR:OG1	1:A:517:VAL:N	2.51	0.43
1:A:692:CYS:SG	1:A:694:ASN:HB2	2.59	0.43
1:A:1758:LEU:HD23	1:A:1883:PHE:CZ	2.53	0.43
1:A:1769:ASP:O	1:A:1819:VAL:HG12	2.19	0.43
1:A:101:ALA:HB2	1:A:139:TRP:CZ2	2.53	0.43
1:A:486:LEU:HD12	1:A:487:TYR:H	1.83	0.43
1:A:1768:GLU:H	1:A:1819:VAL:HG13	1.82	0.43
1:A:306:GLN:HA	1:A:325:VAL:O	2.19	0.43
1:A:422:LYS:HB2	1:A:422:LYS:HE3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:HB2	1:A:135:GLN:HE22	1.83	0.43
1:A:1778:GLN:HB3	1:A:1779:ALA:H	1.59	0.43
1:A:1784:SER:OG	1:A:1805:ASN:OD1	2.37	0.43
1:A:2098:ILE:HG21	1:A:2101:PHE:HB3	2.01	0.43
1:A:2192:ALA:HB2	1:A:2230:LEU:HD12	2.01	0.43
1:A:431:TYR:CE2	1:A:439:ARG:HG2	2.53	0.43
1:A:15:ASP:O	1:A:16:TYR:HB2	2.19	0.42
1:A:2258:LYS:HB2	1:A:2258:LYS:HE3	1.84	0.42
1:A:397:PRO:HD2	1:A:624:SER:HB3	2.01	0.42
1:A:2027:MET:O	1:A:2052:ARG:NH1	2.52	0.42
1:A:2044:GLY:O	1:A:2046:TRP:N	2.50	0.42
1:A:2207:LYS:HB3	1:A:2207:LYS:HE3	1.78	0.42
1:A:2236:LYS:HG3	1:A:2237:THR:N	2.34	0.42
1:A:115:TYR:CE2	1:A:117:ASP:HB3	2.54	0.42
1:A:626:GLN:HB3	1:A:707:LYS:HE2	2.01	0.42
1:A:101:ALA:HB2	1:A:139:TRP:CH2	2.54	0.42
1:A:265:PRO:HB2	1:A:266:GLU:H	1.55	0.42
1:A:398:LEU:HD22	1:A:398:LEU:HA	1.86	0.42
1:A:1929:LEU:HD23	1:A:2012:THR:HG21	2.02	0.42
1:A:418:ARG:CZ	1:A:607:GLU:HG2	2.50	0.42
1:A:1704:GLU:OE2	1:A:1780:SER:N	2.49	0.42
1:A:2080:ILE:HG22	1:A:2082:HIS:CE1	2.55	0.42
1:A:182:GLU:OE1	1:A:182:GLU:N	2.25	0.42
1:A:381:THR:HG22	1:A:460:THR:OG1	2.19	0.42
1:A:2194:SER:HB2	1:A:2222:GLN:HB2	2.02	0.42
1:A:2313:TRP:CE3	1:A:2317:ILE:HD11	2.55	0.42
1:A:119:THR:CG2	1:A:123:GLU:HB2	2.50	0.42
1:A:192:ASN:HB2	1:A:193:LEU:H	1.64	0.42
1:A:246:LEU:HD11	1:A:325:VAL:HG22	2.01	0.42
1:A:315:SER:O	1:A:318:HIS:HB2	2.20	0.42
1:A:446:SER:O	1:A:449:LEU:HG	2.19	0.42
1:A:453:LEU:HD22	1:A:533:TYR:CE2	2.55	0.42
1:A:1874:GLN:NE2	1:A:1934:MET:HA	2.25	0.42
1:A:2116:ARG:CG	1:A:2123:LEU:HA	2.50	0.42
1:A:167:LYS:HB3	1:A:209:TRP:CD1	2.55	0.41
1:A:417:GLN:O	1:A:418:ARG:NE	2.52	0.41
1:A:1700:ILE:O	1:A:1775:PHE:HA	2.20	0.41
1:A:2105:TYR:HA	1:A:2149:ILE:HA	2.02	0.41
3:F:68:GLY:HA2	3:F:69:SER:HA	1.51	0.41
1:A:211:SER:HB2	1:A:212:ALA:H	1.62	0.41
1:A:2128:GLY:O	1:A:2136:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:55:ASP:OD1	3:F:56:SER:N	2.37	0.41
1:A:2204:SER:O	1:A:2207:LYS:HG2	2.20	0.41
1:A:2230:LEU:O	1:A:2307:ARG:HA	2.20	0.41
1:A:2258:LYS:HE2	1:A:2314:VAL:HG23	2.02	0.41
2:E:5:GLN:O	2:E:22:CYS:HA	2.20	0.41
3:F:59:PRO:HG2	3:F:61:ARG:NH2	2.35	0.41
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.79	0.41
1:A:69:TRP:CE2	1:A:196:PHE:CD1	3.09	0.41
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.81	0.41
1:A:2260:PHE:CE1	1:A:2262:ILE:HD11	2.49	0.41
1:A:2280:VAL:HB	2:E:55:SER:HB3	2.01	0.41
1:A:208:SER:OG	1:A:209:TRP:N	2.53	0.41
1:A:433:ASP:OD1	1:A:435:THR:HG22	2.20	0.41
1:A:474:ASN:O	1:A:535:SER:HB2	2.21	0.41
1:A:684:ASN:HD21	1:A:1791:SER:HA	1.86	0.41
1:A:1998:ILE:HG13	1:A:2014:PHE:CE1	2.56	0.41
1:A:157:TYR:HB2	1:A:177:LEU:HB3	2.03	0.41
1:A:627:LEU:HD23	1:A:705:LEU:O	2.20	0.41
1:A:654:SER:HB2	1:A:688:TRP:HB3	2.02	0.41
1:A:689:ILE:O	1:A:689:ILE:HG13	2.21	0.41
1:A:708:VAL:O	1:A:709:SER:HB3	2.20	0.41
1:A:1760:GLY:N	1:A:1852:ILE:O	2.47	0.41
1:A:112:GLY:HA2	1:A:126:ASP:O	2.21	0.41
1:A:2248:VAL:O	1:A:2289:SER:HB2	2.21	0.41
1:A:620:TYR:CD1	1:A:625:LEU:HB2	2.56	0.40
1:A:2033:ARG:HB2	1:A:2035:PHE:CE1	2.56	0.40
1:A:266:GLU:CD	1:A:318:HIS:HE2	2.23	0.40
1:A:128:LYS:HB3	1:A:128:LYS:HE3	1.78	0.40
1:A:521:PRO:HG3	1:A:529:LEU:HD23	2.03	0.40
2:E:61:ASN:O	2:E:65:LYS:HG2	2.20	0.40
1:A:189:ARG:O	1:A:191:GLN:N	2.54	0.40
1:A:2027:MET:HA	1:A:2032:ILE:HG22	2.04	0.40
1:A:2281:LYS:NZ	1:A:2297:LEU:HD21	2.37	0.40
2:E:17:SER:HA	2:E:84:SER:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1211/1467 (82%)	952 (79%)	170 (14%)	89 (7%)	1	16
2	E	105/224 (47%)	82 (78%)	19 (18%)	4 (4%)	3	27
3	F	90/214 (42%)	63 (70%)	24 (27%)	3 (3%)	4	30
All	All	1406/1905 (74%)	1097 (78%)	213 (15%)	96 (7%)	1	18

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	229	GLN
1	A	250	HIS
1	A	265	PRO
1	A	291	PRO
1	A	318	HIS
1	A	321	MET
1	A	402	PRO
1	A	407	TYR
1	A	416	PRO
1	A	505	PRO
1	A	572	ASN
1	A	603	LEU
1	A	655	GLY
1	A	1713	GLU
1	A	1796	GLN
1	A	1804	HIS
1	A	1871	VAL
1	A	1889	TRP
1	A	1936	GLN
1	A	2010	MET
1	A	2120	THR
1	A	2183	LYS
1	A	2206	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	24	GLU
1	A	189	ARG
1	A	280	ARG
1	A	400	LEU
1	A	403	ASP
1	A	419	ILE
1	A	445	GLU
1	A	468	GLN
1	A	523	LYS
1	A	600	GLY
1	A	707	LYS
1	A	1743	PHE
1	A	1809	PRO
1	A	2092	LYS
1	A	2119	SER
1	A	2184	ALA
1	A	2199	MET
1	A	2251	LEU
2	E	43	HIS
3	F	19	VAL
1	A	193	LEU
1	A	211	SER
1	A	230	PRO
1	A	251	LYS
1	A	266	GLU
1	A	319	GLY
1	A	1742	SER
1	A	1751	GLU
1	A	1778	GLN
1	A	1897	ARG
1	A	1938	GLN
1	A	2040	SER
1	A	2043	TYR
1	A	2045	GLN
1	A	2067	PRO
1	A	2218	ALA
1	A	2252	LEU
2	E	85	SER
3	F	98	PHE
1	A	138	VAL
1	A	273	GLU
1	A	331	ALA

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Mol	Chain	Res	Type
1	A	498	LEU
1	A	654	SER
1	A	694	ASN
1	A	695	SER
1	A	704	ALA
1	A	1714	SER
1	A	1798	GLN
1	A	2132	SER
1	A	2315	HIS
2	E	76	SER
3	F	51	ALA
1	A	187	ARG
1	A	540	GLU
1	A	569	ASP
1	A	622	PHE
1	A	1810	ASN
1	A	1843	LEU
1	A	1860	ALA
1	A	1890	TYR
1	A	2142	PRO
1	A	474	ASN
1	A	708	VAL
1	A	1779	ALA
1	A	2058	SER
1	A	2116	ARG
1	A	141	VAL
1	A	174	ILE
1	A	448	ILE
1	A	494	GLY
2	E	48	ILE

### 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	1052/1301 (81%)	1026 (98%)	26 (2%)	47 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	80/191 (42%)	77 (96%)	3 (4%)	33 58
3	F	64/191 (34%)	60 (94%)	4 (6%)	18 45
All	All	1196/1683 (71%)	1163 (97%)	33 (3%)	43 65

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	26	HIS
1	A	66	ARG
1	A	72	LEU
1	A	107	TRP
1	A	153	PRO
1	A	185	LEU
1	A	193	LEU
1	A	210	HIS
1	A	312	HIS
1	A	440	GLU
1	A	647	ASP
1	A	699	ASN
1	A	1697	HIS
1	A	1753	ASN
1	A	1983	PHE
1	A	1997	ARG
1	A	2000	CYS
1	A	2018	SER
1	A	2034	ASP
1	A	2093	PHE
1	A	2110	LYS
1	A	2157	SER
1	A	2206	SER
1	A	2250	SER
1	A	2304	ARG
2	E	27	TYR
2	E	80	TYR
2	E	107	TYR
3	F	4	MET
3	F	56	SER
3	F	83	PHE
3	F	88	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	645	GLN
1	A	694	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

4 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	B	1	1,4	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	B	2	4	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	G	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.65	1 (5%)
4	NAG	G	2	4	14,14,15	0.91	1 (7%)	17,19,21	1.24	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	NAG	O5-C1	-2.52	1.39	1.43
4	G	1	NAG	O5-C1	2.28	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C4-C3-C2	2.72	115.00	111.02
4	G	2	NAG	C2-N2-C7	2.46	126.41	122.90
4	G	1	NAG	C1-O5-C5	2.05	114.97	112.19
4	G	2	NAG	C3-C4-C5	2.01	113.83	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2	NAG	C1

All (9) torsion outliers are listed below:

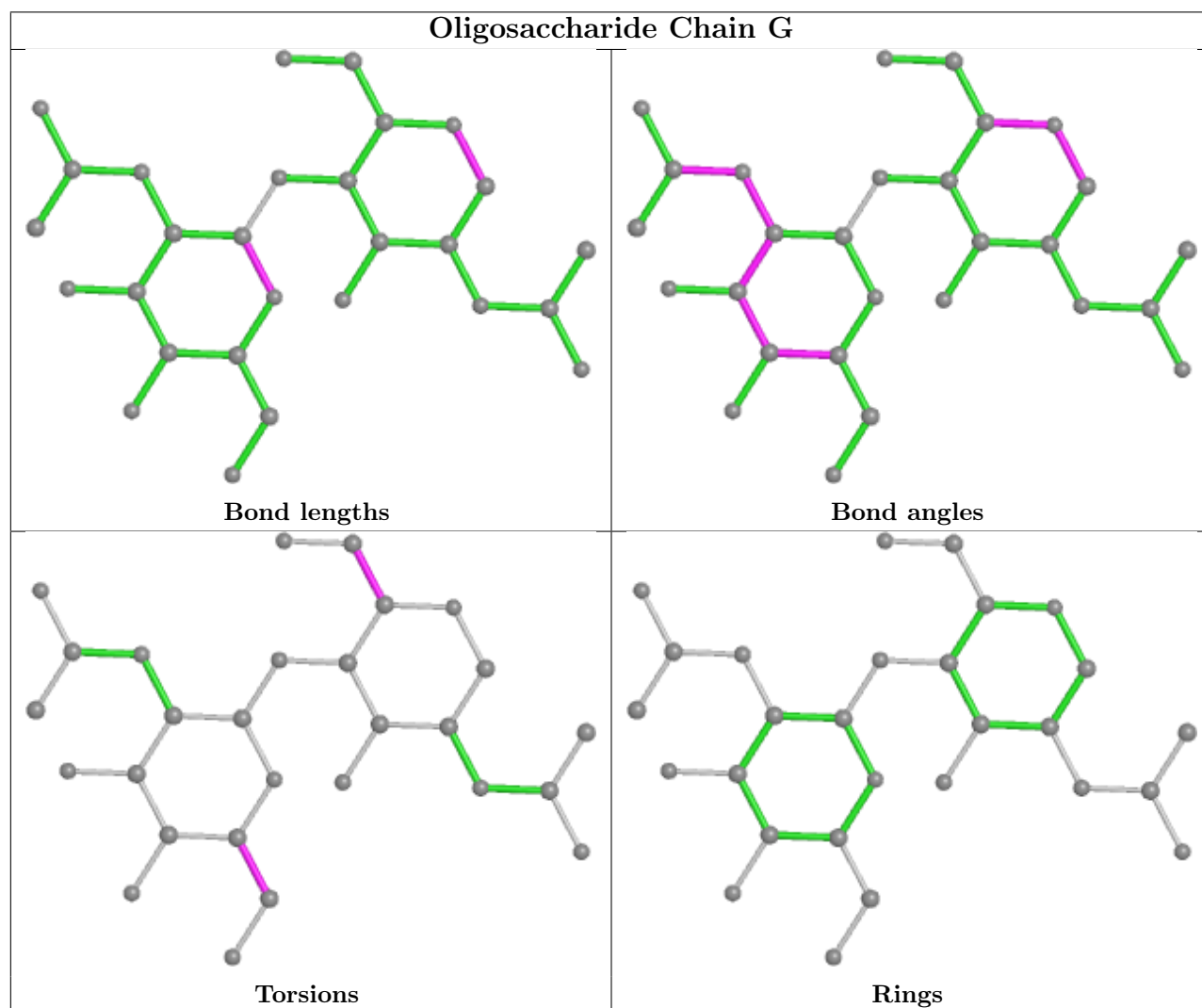
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	G	1	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

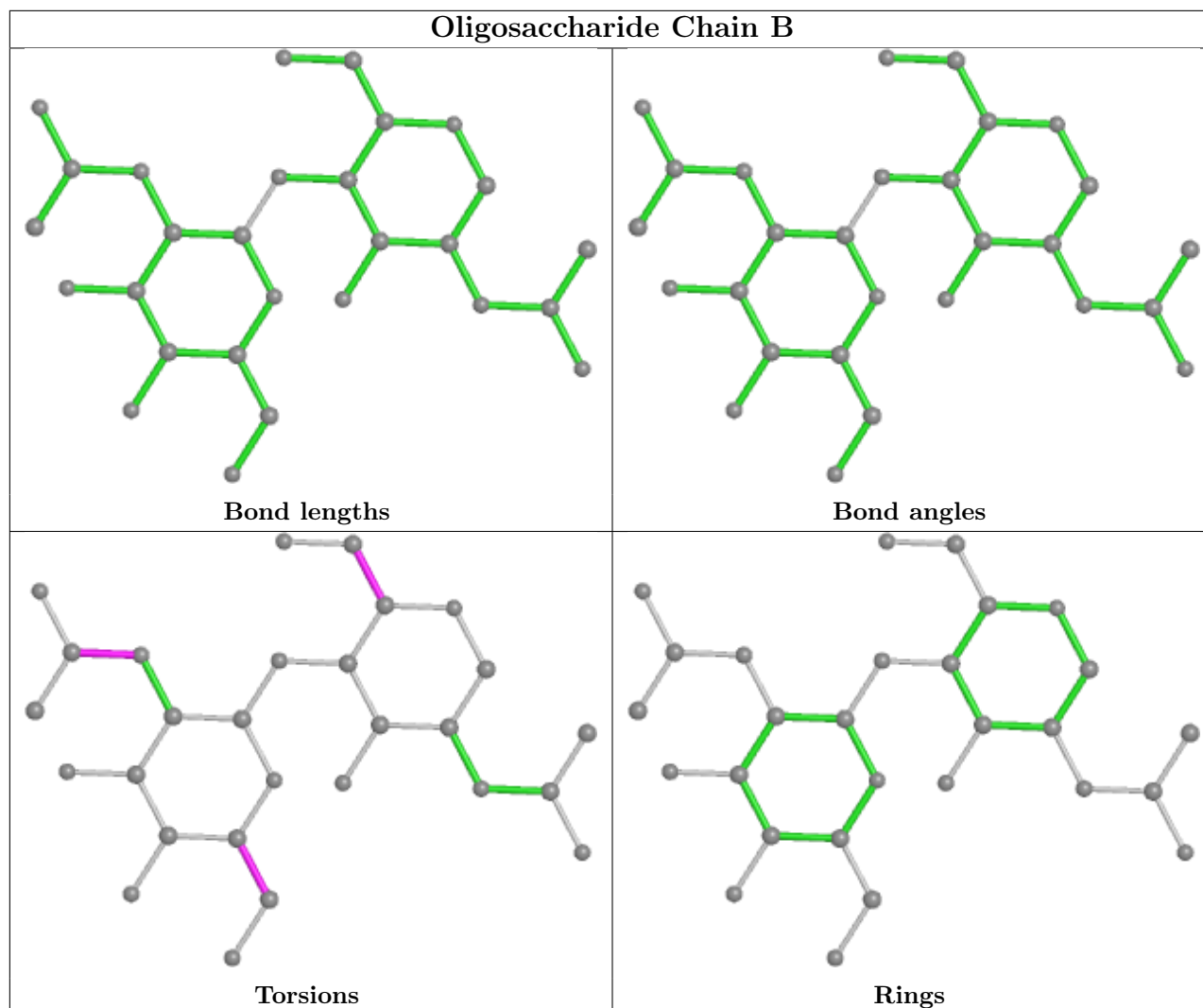
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0

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





## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
5	NAG	A	2401	1	14,14,15	0.30	0	17,19,21	0.50	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
5	NAG	A	2401	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2401	NAG	C4-C5-C6-O6
5	A	2401	NAG	O5-C5-C6-O6
5	A	2401	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1233/1467 (84%)	-0.28	7 (0%) 89 84	194, 241, 289, 329	0
2	E	115/224 (51%)	-0.01	1 (0%) 84 77	265, 306, 326, 335	0
3	F	96/214 (44%)	0.17	3 (3%) 49 38	277, 329, 358, 365	0
All	All	1444/1905 (75%)	-0.23	11 (0%) 86 79	194, 247, 324, 365	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	14	SER	2.8
3	F	82	ASP	2.7
1	A	2201	ALA	2.6
1	A	89	LEU	2.5
1	A	556	LYS	2.4
1	A	88	THR	2.2
1	A	2229	TRP	2.2
2	E	88	SER	2.2
1	A	63	ALA	2.1
3	F	51	ALA	2.0
1	A	2049	LYS	2.0

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

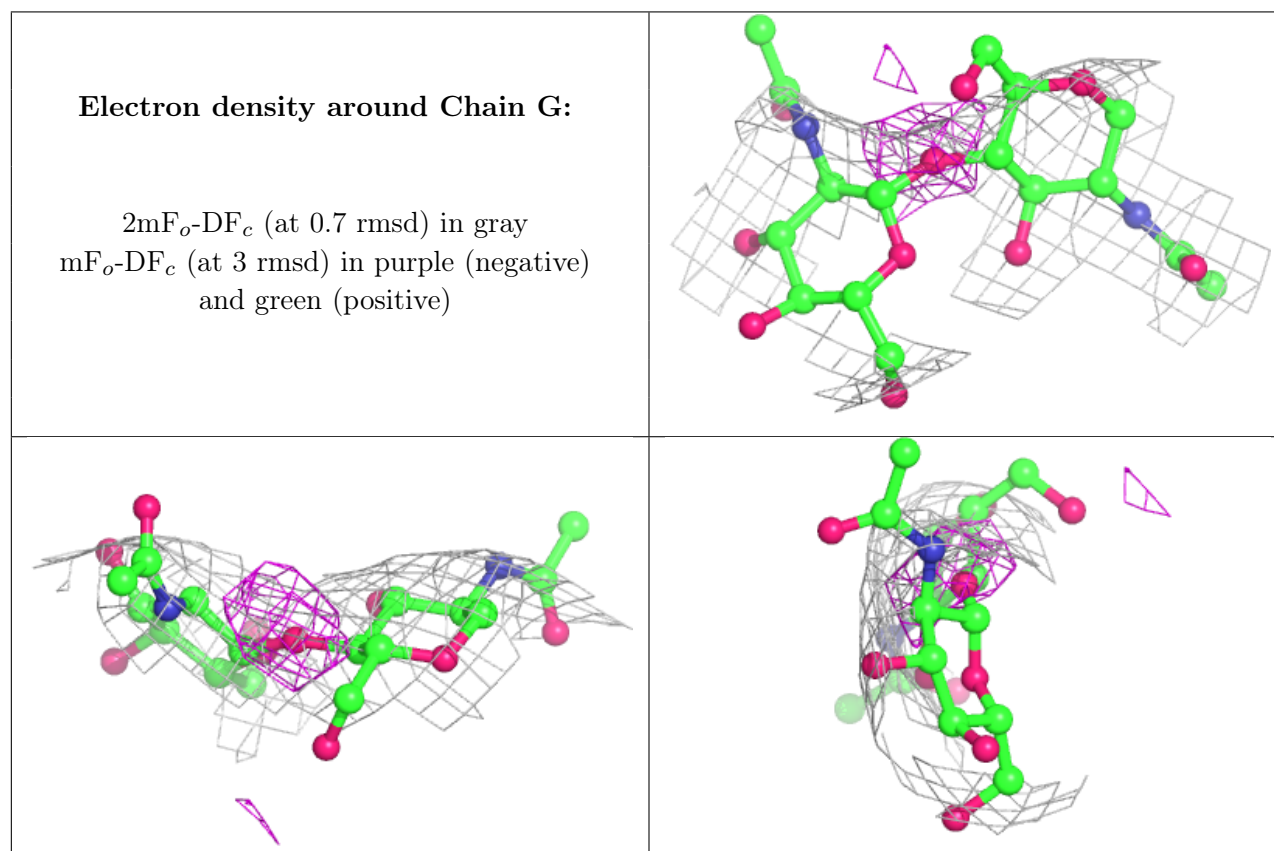
There are no non-standard protein/DNA/RNA residues in this entry.

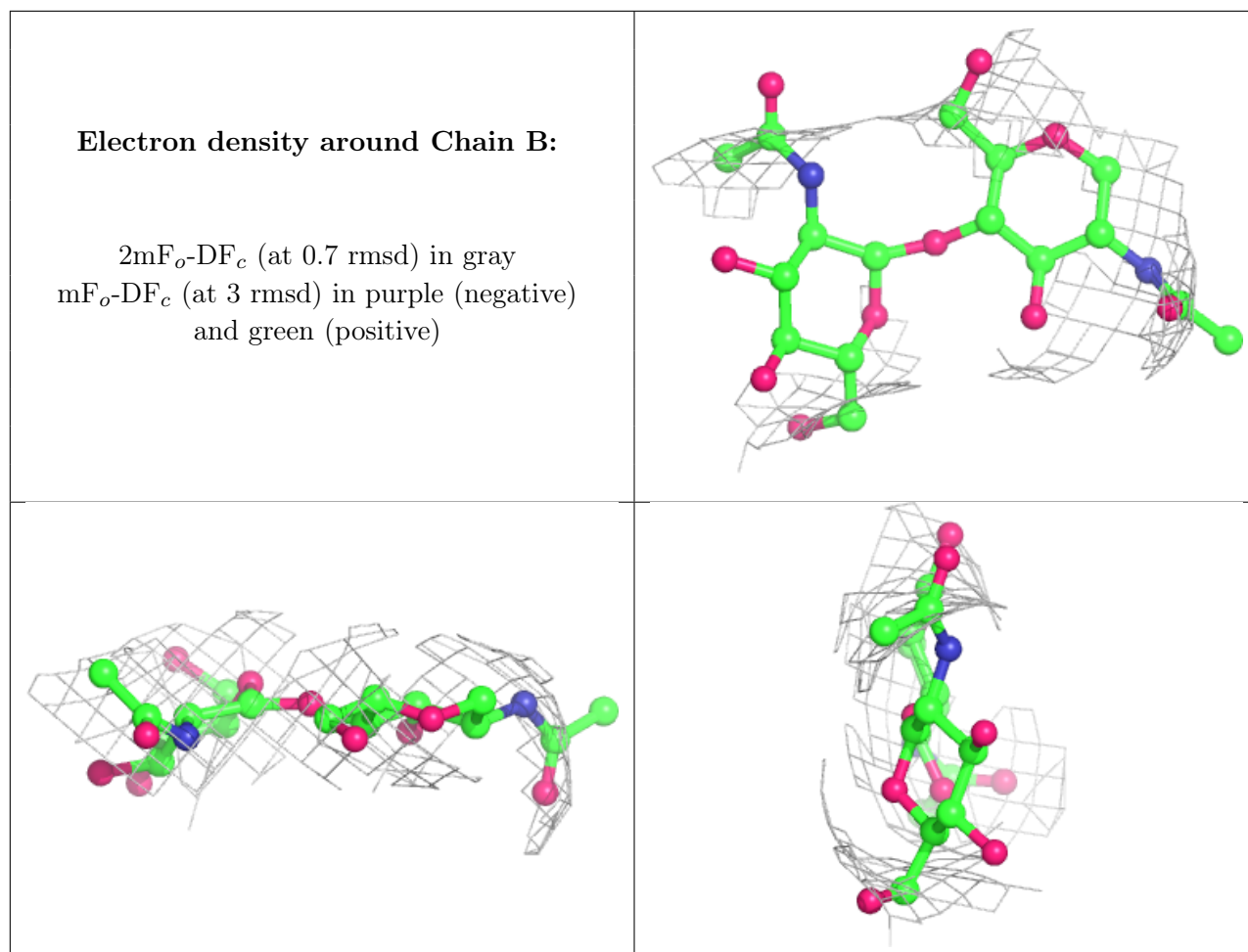
### 6.3 Carbohydrates [i](#)

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( $\text{\AA}^2$ )	Q<0.9
4	NAG	G	2	14/15	0.69	0.38	224,248,256,258	0
4	NAG	G	1	14/15	0.81	0.43	243,253,266,267	0
4	NAG	B	2	14/15	0.81	0.40	301,312,318,318	0
4	NAG	B	1	14/15	0.88	0.35	261,277,285,288	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.





## 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
6	CU	A	2402	1/1	0.83	0.16	229,229,229,229	0
5	NAG	A	2401	14/15	0.87	0.23	273,291,300,302	0
7	ZN	A	2403	1/1	0.90	0.19	213,213,213,213	0
8	CA	A	2404	1/1	0.97	0.22	210,210,210,210	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.