



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:32 PM BST

PDB ID : 3VE0  
Title : Crystal structure of Sudan Ebolavirus Glycoprotein (strain Boniface) bound to 16F6  
Authors : Sapphire, E.O.; Bale, S.; Dias, J.M.  
Deposited on : 2012-01-06  
Resolution : 3.35 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

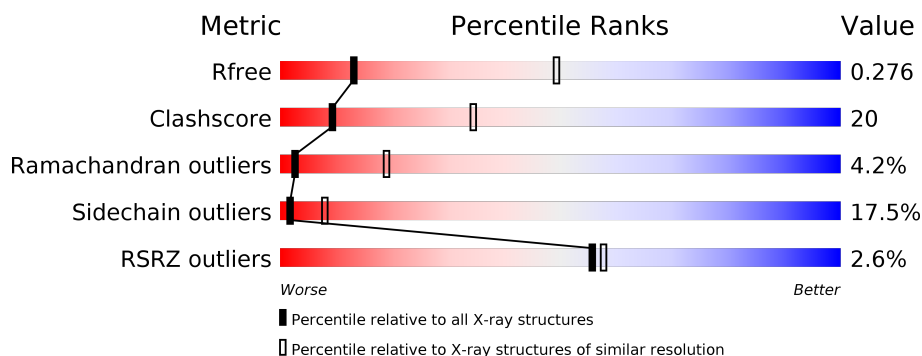
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	I	298	<div> <div>5%</div> <div> <div>44%</div> <div>33%</div> <div>6%</div> <div>18%</div> </div> </div>
2	J	167	<div> <div>2%</div> <div> <div>35%</div> <div>25%</div> <div>•</div> <div>37%</div> </div> </div>
3	A	220	<div> <div>57%</div> <div>34%</div> <div>8%</div> </div>
4	B	212	<div> <div>%</div> <div> <div>52%</div> <div>39%</div> <div>8%</div> </div> </div>
5	C	3	<div> <div>100%</div> </div>
5	D	3	<div> <div>33%</div> <div>67%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6002 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	245	Total	C	N	O	S	0	0	0
			1806	1150	304	346	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	16	TYR	-	expression tag	UNP Q66814
I	17	PRO	-	expression tag	UNP Q66814
I	18	TYR	-	expression tag	UNP Q66814
I	19	ASP	-	expression tag	UNP Q66814
I	20	VAL	-	expression tag	UNP Q66814
I	21	PRO	-	expression tag	UNP Q66814
I	22	ASP	-	expression tag	UNP Q66814
I	23	TYR	-	expression tag	UNP Q66814
I	24	ALA	-	expression tag	UNP Q66814
I	25	ILE	-	expression tag	UNP Q66814
I	26	GLU	-	expression tag	UNP Q66814
I	27	GLY	-	expression tag	UNP Q66814
I	28	ARG	-	expression tag	UNP Q66814
I	29	GLY	-	expression tag	UNP Q66814
I	30	ALA	-	expression tag	UNP Q66814
I	31	ARG	-	expression tag	UNP Q66814
I	32	SER	-	expression tag	UNP Q66814
I	95	LYS	GLN	conflict	UNP Q66814
I	203	VAL	ALA	conflict	UNP Q66814
I	261	HIS	GLN	conflict	UNP Q66814

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	105	Total	C	N	O	S	0	0	0
			804	507	146	145	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	638	VAL	GLN	conflict	UNP Q66814

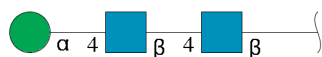
- Molecule 3 is a protein called 16F6 Antibody chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	220	Total	C	N	O	S	0	0	0
			1666	1058	276	324	8			

- Molecule 4 is a protein called 16F6 Antibody chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	212	Total	C	N	O	S	0	0	0
			1648	1030	281	330	7			

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

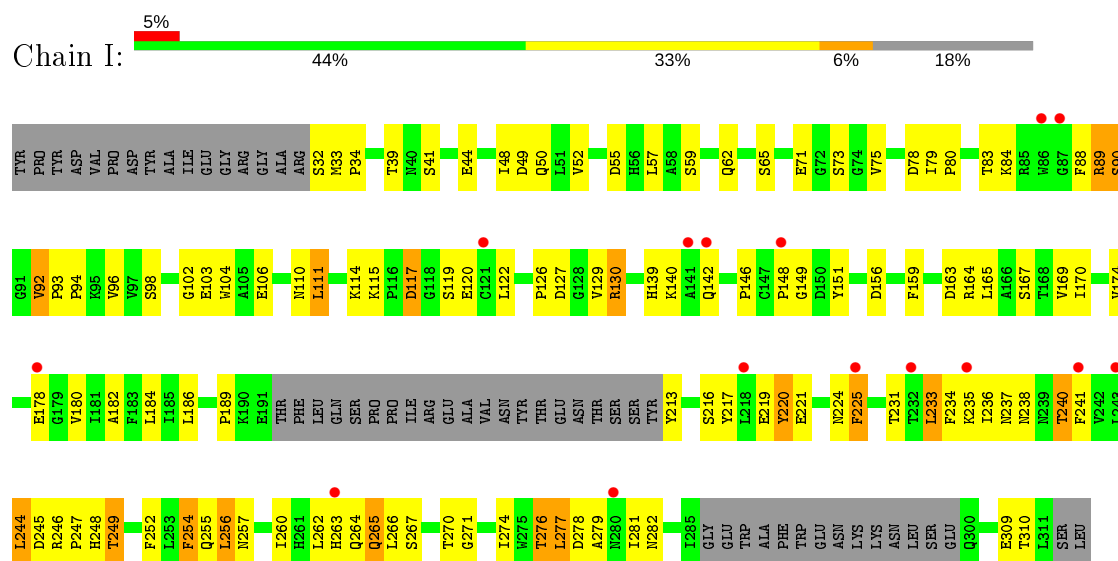


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

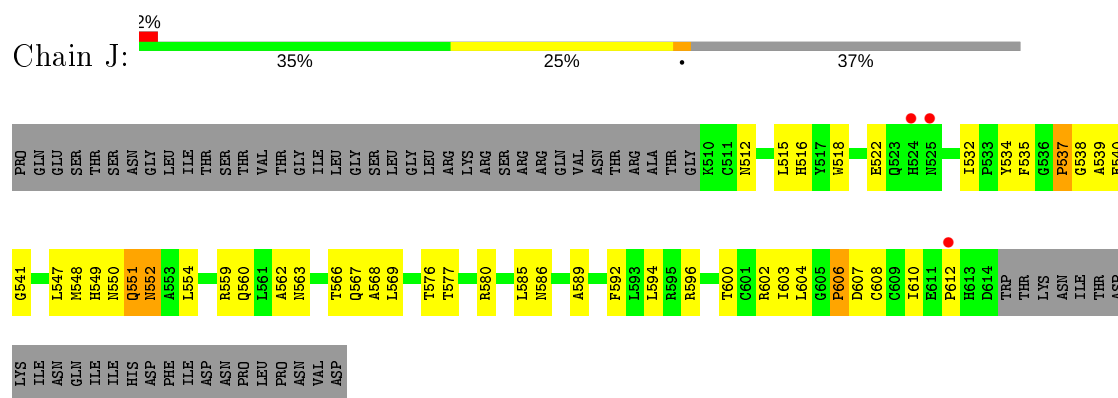
### 3 Residue-property plots

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.

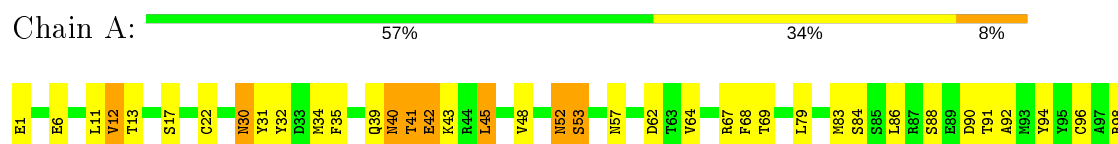
#### • Molecule 1: Envelope glycoprotein

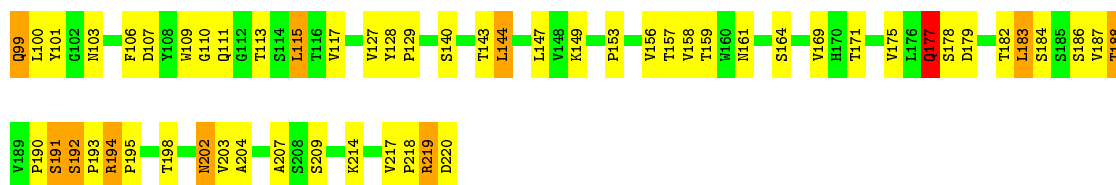


#### • Molecule 2: Envelope glycoprotein

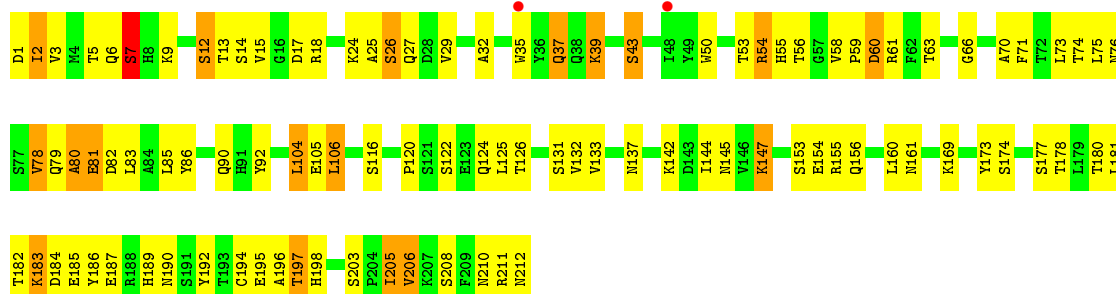


#### • Molecule 3: 16F6 Antibody chain A

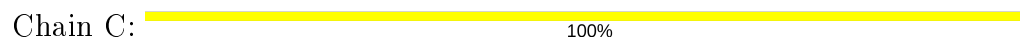




• Molecule 4: 16F6 Antibody chain B



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.86Å 194.86Å 194.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.93 – 3.35 45.93 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.93-3.35) 99.8 (45.93-3.35)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.222 , 0.289 0.213 , 0.276	Depositor DCC
$R_{free}$ test set	907 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 90.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.015 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	I	0.53	0/1849	0.72	2/2522 (0.1%)
2	J	0.55	0/824	0.72	0/1125
3	A	0.69	1/1710 (0.1%)	0.75	1/2333 (0.0%)
4	B	0.59	0/1687	0.74	0/2295
All	All	0.60	1/6070 (0.0%)	0.74	3/8275 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	42	GLU	CG-CD	6.00	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	233	LEU	CA-CB-CG	5.71	128.44	115.30
1	I	111	LEU	CA-CB-CG	5.60	128.17	115.30
3	A	115	LEU	CA-CB-CG	5.43	127.78	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1806	0	1645	69	0
2	J	804	0	747	38	0
3	A	1666	0	1623	82	0
4	B	1648	0	1588	61	0
5	C	39	0	34	0	0
5	D	39	0	34	2	0
All	All	6002	0	5671	231	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:THR:HG22	3:A:117:VAL:H	1.11	1.14
4:B:3:VAL:H	4:B:26:SER:HB3	1.09	1.09
3:A:52:ASN:HD21	3:A:57:ASN:H	1.13	0.92
3:A:17:SER:HB3	3:A:84:SER:HA	1.51	0.89
1:I:234:PHE:HB2	1:I:244:LEU:HD21	1.56	0.85
1:I:156:ASP:OD1	5:D:2:NAG:H61	1.75	0.85
3:A:194:ARG:CG	3:A:194:ARG:HH11	1.91	0.83
3:A:194:ARG:HG3	3:A:194:ARG:HH11	1.42	0.82
4:B:3:VAL:H	4:B:26:SER:CB	1.90	0.82
3:A:88:SER:HA	3:A:117:VAL:HB	1.62	0.82
3:A:6:GLU:OE1	3:A:96:CYS:HB3	1.80	0.82
4:B:24:LYS:NZ	4:B:70:ALA:HB2	1.95	0.81
4:B:3:VAL:N	4:B:26:SER:HB3	1.94	0.81
3:A:64:VAL:HG12	3:A:67:ARG:NH2	1.95	0.81
3:A:52:ASN:H	3:A:52:ASN:HD22	1.27	0.79
3:A:91:THR:HG22	3:A:117:VAL:N	1.95	0.79
3:A:52:ASN:HD21	3:A:57:ASN:N	1.81	0.78
1:I:180:VAL:CG1	2:J:566:THR:HB	2.14	0.78
3:A:194:ARG:NH1	3:A:194:ARG:HG3	2.00	0.76
3:A:40:ASN:C	3:A:40:ASN:HD22	1.88	0.75
4:B:24:LYS:HZ2	4:B:70:ALA:HB2	1.53	0.74
4:B:2:ILE:H	4:B:2:ILE:HD12	1.52	0.74
3:A:177:GLN:HA	3:A:177:GLN:HE21	1.53	0.72
4:B:196:ALA:HB3	4:B:205:ILE:HG23	1.72	0.72
3:A:52:ASN:H	3:A:52:ASN:ND2	1.89	0.70
2:J:537:PRO:HB3	2:J:541:GLY:HA3	1.73	0.70
3:A:52:ASN:ND2	3:A:57:ASN:H	1.91	0.68
2:J:560:GLN:HB3	3:A:101:TYR:CE1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:VAL:O	3:A:117:VAL:HA	1.94	0.68
3:A:149:LYS:HA	3:A:182:THR:HG23	1.76	0.67
3:A:177:GLN:HA	3:A:177:GLN:NE2	2.09	0.67
1:I:89:ARG:HD3	1:I:90:SER:H	1.57	0.67
2:J:566:THR:HG21	5:D:1:NAG:H82	1.77	0.67
4:B:147:LYS:HD3	4:B:154:GLU:HG3	1.76	0.67
1:I:249:THR:HG23	1:I:252:PHE:HB3	1.77	0.66
3:A:32:TYR:HB3	3:A:34:MET:CE	2.26	0.66
2:J:552:ASN:H	2:J:552:ASN:HD22	1.44	0.65
4:B:12:SER:HA	4:B:105:GLU:O	1.97	0.65
2:J:560:GLN:HB3	3:A:101:TYR:HE1	1.61	0.65
2:J:551:GLN:HG3	2:J:554:LEU:HD12	1.80	0.64
4:B:120:PRO:HD3	4:B:132:VAL:HG22	1.79	0.64
3:A:22:CYS:HB3	3:A:79:LEU:HB3	1.80	0.64
4:B:37:GLN:HG3	4:B:86:TYR:CE1	2.33	0.63
1:I:169:VAL:HG12	1:I:170:ILE:N	2.12	0.63
4:B:2:ILE:N	4:B:2:ILE:HD12	2.13	0.62
3:A:183:LEU:HD12	3:A:184:SER:N	2.14	0.62
3:A:129:PRO:HG3	3:A:214:LYS:HG2	1.82	0.61
3:A:157:THR:HB	3:A:204:ALA:HB3	1.81	0.61
4:B:137:ASN:HB3	4:B:174:SER:HB3	1.81	0.61
2:J:532:ILE:HG22	2:J:534:TYR:H	1.64	0.61
1:I:180:VAL:HG11	2:J:566:THR:HB	1.81	0.61
4:B:195:GLU:HG3	4:B:206:VAL:HB	1.83	0.60
4:B:190:ASN:HD21	4:B:212:ASN:HD21	1.47	0.60
2:J:550:ASN:OD1	2:J:551:GLN:N	2.35	0.59
3:A:17:SER:HB2	3:A:83:MET:O	2.02	0.59
1:I:71:GLU:OE2	1:I:106:GLU:HB3	2.02	0.59
4:B:55:HIS:HB3	4:B:58:VAL:HG21	1.83	0.59
1:I:88:PHE:HB3	1:I:149:GLY:H	1.68	0.59
4:B:161:ASN:HD22	4:B:177:SER:HA	1.68	0.59
1:I:110:ASN:O	1:I:140:LYS:HA	2.03	0.59
3:A:159:THR:OG1	3:A:202:ASN:ND2	2.36	0.58
1:I:236:ILE:HG21	1:I:260:ILE:HG21	1.85	0.58
1:I:96:VAL:HG22	1:I:167:SER:HB2	1.86	0.58
3:A:41:THR:HG23	3:A:42:GLU:OE1	2.03	0.57
1:I:89:ARG:HD2	1:I:92:VAL:HG22	1.86	0.57
3:A:88:SER:O	3:A:91:THR:HG23	2.04	0.57
3:A:143:THR:HG23	3:A:188:THR:HG22	1.87	0.57
3:A:187:VAL:O	3:A:187:VAL:HG13	2.05	0.56
3:A:64:VAL:HG12	3:A:67:ARG:HH21	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:183:LYS:O	4:B:187:GLU:HG2	2.05	0.56
2:J:563:ASN:O	2:J:566:THR:HG22	2.05	0.56
2:J:552:ASN:H	2:J:552:ASN:ND2	2.03	0.56
1:I:265:GLN:O	1:I:267:SER:N	2.39	0.56
1:I:234:PHE:CG	1:I:235:LYS:N	2.73	0.56
1:I:246:ARG:O	1:I:248:HIS:CE1	2.59	0.55
4:B:155:ARG:NH1	4:B:185:GLU:OE1	2.32	0.55
4:B:17:ASP:O	4:B:78:VAL:HG23	2.07	0.55
3:A:140:SER:O	3:A:191:SER:HB2	2.06	0.55
1:I:221:GLU:HB2	1:I:233:LEU:HD12	1.89	0.55
3:A:194:ARG:HD2	3:A:195:PRO:HA	1.88	0.55
4:B:29:VAL:O	4:B:29:VAL:HG12	2.07	0.55
4:B:122:SER:HA	4:B:125:LEU:HD12	1.89	0.54
1:I:264:GLN:O	1:I:265:GLN:CB	2.54	0.54
4:B:24:LYS:HZ3	4:B:70:ALA:HB2	1.71	0.54
1:I:32:SER:O	3:A:31:TYR:OH	2.25	0.54
1:I:57:LEU:HA	1:I:62:GLN:NE2	2.23	0.54
1:I:276:THR:O	1:I:277:LEU:CB	2.57	0.53
4:B:122:SER:O	4:B:126:THR:HG23	2.08	0.53
1:I:163:ASP:OD1	1:I:164:ARG:HG3	2.08	0.53
2:J:552:ASN:ND2	2:J:552:ASN:N	2.56	0.53
4:B:32:ALA:HB3	4:B:92:TYR:HB2	1.90	0.53
4:B:55:HIS:HB3	4:B:58:VAL:CG2	2.39	0.53
3:A:107:ASP:OD2	3:A:107:ASP:N	2.38	0.52
3:A:99:GLN:HG3	3:A:103:ASN:O	2.10	0.52
3:A:171:THR:CG2	3:A:183:LEU:HD11	2.40	0.52
4:B:66:GLY:HA3	4:B:71:PHE:HA	1.91	0.51
1:I:151:TYR:HD2	1:I:169:VAL:HG11	1.73	0.51
1:I:236:ILE:O	1:I:240:THR:O	2.28	0.51
2:J:551:GLN:CG	2:J:554:LEU:HD12	2.39	0.51
1:I:49:ASP:OD1	1:I:50:GLN:N	2.44	0.51
4:B:189:HIS:O	4:B:211:ARG:HD3	2.11	0.51
4:B:131:SER:HA	4:B:180:THR:HA	1.93	0.51
3:A:157:THR:O	3:A:203:VAL:HA	2.11	0.50
3:A:6:GLU:OE1	3:A:110:GLY:HA3	2.11	0.50
1:I:247:PRO:HG2	1:I:279:ALA:O	2.10	0.50
1:I:78:ASP:OD1	1:I:80:PRO:HD2	2.11	0.50
3:A:40:ASN:ND2	3:A:40:ASN:C	2.59	0.50
4:B:145:ASN:HB2	4:B:197:THR:HG22	1.94	0.50
4:B:37:GLN:NE2	4:B:39:LYS:HD3	2.27	0.50
2:J:538:GLY:O	2:J:540:GLU:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:ARG:CG	3:A:194:ARG:NH1	2.57	0.49
1:I:103:GLU:OE1	2:J:559:ARG:NH2	2.44	0.49
3:A:109:TRP:HB2	4:B:43:SER:OG	2.12	0.49
3:A:178:SER:O	3:A:179:ASP:HB2	2.13	0.49
4:B:144:ILE:HG13	4:B:198:HIS:HB2	1.94	0.49
4:B:29:VAL:O	4:B:29:VAL:CG1	2.61	0.49
1:I:104:TRP:HB2	2:J:516:HIS:HB3	1.94	0.49
3:A:149:LYS:HG3	3:A:182:THR:CG2	2.43	0.49
4:B:6:GLN:O	4:B:7:SER:C	2.51	0.49
1:I:139:HIS:HD2	1:I:220:TYR:OH	1.95	0.49
3:A:41:THR:HG23	3:A:42:GLU:CD	2.33	0.48
4:B:2:ILE:HG13	4:B:27:GLN:HE21	1.78	0.48
1:I:83:THR:HB	1:I:84:LYS:HD2	1.95	0.48
3:A:92:ALA:HB3	3:A:94:TYR:CE2	2.49	0.48
1:I:236:ILE:HG23	1:I:257:ASN:OD1	2.13	0.48
1:I:139:HIS:HB3	1:I:220:TYR:HE2	1.77	0.48
1:I:140:LYS:HB2	1:I:219:GLU:HB3	1.96	0.47
2:J:547:LEU:HD11	2:J:549:HIS:HD2	1.79	0.47
1:I:127:ASP:O	2:J:580:ARG:NH2	2.47	0.47
3:A:144:LEU:HD21	3:A:194:ARG:HD3	1.95	0.47
4:B:186:TYR:HA	4:B:192:TYR:OH	2.15	0.47
1:I:94:PRO:HG3	1:I:151:TYR:CE2	2.50	0.47
4:B:25:ALA:O	4:B:27:GLN:N	2.47	0.47
4:B:161:ASN:ND2	4:B:177:SER:HA	2.30	0.47
1:I:117:ASP:N	1:I:117:ASP:OD1	2.48	0.47
1:I:114:LYS:HA	1:I:120:GLU:HA	1.96	0.47
1:I:62:GLN:NE2	1:I:186:LEU:O	2.47	0.46
1:I:180:VAL:HG11	2:J:562:ALA:O	2.15	0.46
3:A:128:TYR:HA	3:A:129:PRO:HD3	1.70	0.46
4:B:35:TRP:CE2	4:B:73:LEU:HB2	2.51	0.46
1:I:169:VAL:CG1	1:I:170:ILE:N	2.76	0.46
2:J:515:LEU:HD23	2:J:548:MET:HG3	1.97	0.46
3:A:158:VAL:HG13	3:A:203:VAL:HG12	1.97	0.46
3:A:149:LYS:HG3	3:A:182:THR:HG23	1.96	0.46
3:A:194:ARG:HG2	3:A:194:ARG:HH11	1.78	0.46
4:B:75:LEU:HG	4:B:78:VAL:HG22	1.97	0.46
1:I:219:GLU:OE1	1:I:219:GLU:N	2.49	0.46
1:I:236:ILE:HG13	1:I:256:LEU:HD12	1.98	0.46
4:B:61:ARG:HB2	4:B:76:ASN:H	1.80	0.45
1:I:139:HIS:CD2	1:I:220:TYR:OH	2.69	0.45
1:I:88:PHE:HB2	1:I:148:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:43:LYS:HA	3:A:43:LYS:HD3	1.81	0.45
3:A:171:THR:HG22	3:A:183:LEU:HD11	1.98	0.45
3:A:156:VAL:HG12	3:A:157:THR:N	2.31	0.45
4:B:17:ASP:O	4:B:78:VAL:CG2	2.65	0.45
1:I:93:PRO:HA	1:I:94:PRO:HD2	1.63	0.45
4:B:142:LYS:HG3	4:B:173:TYR:CE1	2.52	0.45
1:I:254:PHE:O	1:I:256:LEU:N	2.50	0.45
2:J:537:PRO:HB3	2:J:541:GLY:CA	2.45	0.45
3:A:109:TRP:CD1	3:A:109:TRP:N	2.84	0.44
3:A:17:SER:CB	3:A:83:MET:O	2.64	0.44
2:J:552:ASN:HB2	4:B:50:TRP:CE2	2.52	0.44
1:I:78:ASP:HB3	1:I:248:HIS:O	2.18	0.44
3:A:190:PRO:HB2	3:A:193:PRO:CG	2.47	0.44
3:A:153:PRO:HD2	3:A:207:ALA:CB	2.48	0.44
1:I:224:ASN:O	1:I:225:PHE:HB2	2.16	0.44
1:I:234:PHE:HB2	1:I:244:LEU:CD2	2.39	0.44
4:B:18:ARG:HA	4:B:75:LEU:O	2.17	0.44
1:I:104:TRP:CD1	2:J:516:HIS:ND1	2.86	0.44
1:I:130:ARG:H	1:I:130:ARG:HD2	1.82	0.44
3:A:35:PHE:HE2	3:A:99:GLN:HB2	1.82	0.44
4:B:147:LYS:O	4:B:147:LYS:HG3	2.18	0.44
4:B:79:GLN:O	4:B:80:ALA:C	2.56	0.44
3:A:128:TYR:CE1	4:B:124:GLN:HA	2.53	0.43
4:B:13:THR:O	4:B:106:LEU:HA	2.18	0.43
2:J:534:TYR:HD1	2:J:535:PHE:CE1	2.35	0.43
3:A:127:VAL:HG21	3:A:203:VAL:HG21	2.00	0.43
3:A:192:SER:O	3:A:194:ARG:N	2.46	0.43
3:A:35:PHE:HE2	3:A:99:GLN:CB	2.31	0.43
3:A:83:MET:HB3	3:A:86:LEU:HD21	2.00	0.43
1:I:233:LEU:HD13	1:I:234:PHE:O	2.19	0.43
2:J:594:LEU:C	2:J:596:ARG:H	2.22	0.43
3:A:187:VAL:CG1	3:A:187:VAL:O	2.67	0.43
4:B:124:GLN:NE2	4:B:131:SER:H	2.16	0.43
4:B:190:ASN:O	4:B:210:ASN:HA	2.19	0.43
1:I:245:ASP:H	1:I:248:HIS:CE1	2.36	0.43
2:J:549:HIS:O	2:J:550:ASN:ND2	2.51	0.43
2:J:567:GLN:O	2:J:568:ALA:C	2.56	0.43
1:I:220:TYR:CD2	1:I:220:TYR:N	2.86	0.43
2:J:606:PRO:HB2	2:J:607:ASP:H	1.64	0.43
3:A:175:VAL:HG21	4:B:160:LEU:HD13	2.00	0.43
2:J:594:LEU:HA	2:J:594:LEU:HD12	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:88:PHE:HB3	1:I:149:GLY:N	2.32	0.42
4:B:79:GLN:O	4:B:81:GLU:N	2.52	0.42
1:I:309:GLU:HB3	1:I:310:THR:H	1.61	0.42
2:J:569:LEU:HD12	2:J:569:LEU:HA	1.81	0.42
3:A:31:TYR:C	3:A:53:SER:OG	2.57	0.42
4:B:54:ARG:HH22	4:B:60:ASP:HA	1.84	0.42
1:I:115:LYS:HB2	1:I:119:SER:O	2.19	0.42
2:J:576:THR:OG1	2:J:577:THR:N	2.53	0.42
3:A:42:GLU:N	3:A:42:GLU:OE1	2.53	0.42
4:B:181:LEU:HD22	4:B:185:GLU:CD	2.40	0.42
4:B:29:VAL:HG12	4:B:32:ALA:H	1.84	0.42
1:I:34:PRO:HG3	3:A:31:TYR:CE1	2.54	0.42
2:J:602:ARG:C	2:J:604:LEU:H	2.23	0.42
3:A:217:VAL:CG2	3:A:218:PRO:HD2	2.50	0.42
3:A:128:TYR:HB2	3:A:147:LEU:HB3	2.02	0.41
1:I:126:PRO:O	1:I:129:VAL:HG12	2.20	0.41
4:B:86:TYR:CE2	4:B:104:LEU:HD23	2.55	0.41
3:A:39:GLN:HB2	3:A:45:LEU:HD12	2.01	0.41
1:I:182:ALA:HB2	2:J:562:ALA:HB2	2.01	0.41
3:A:219:ARG:O	3:A:220:ASP:HB2	2.20	0.41
3:A:35:PHE:CE2	3:A:99:GLN:HB2	2.55	0.41
4:B:79:GLN:O	4:B:82:ASP:N	2.53	0.41
1:I:221:GLU:O	1:I:233:LEU:HB3	2.20	0.41
1:I:221:GLU:N	1:I:233:LEU:O	2.39	0.41
1:I:98:SER:HA	1:I:165:LEU:HD23	2.03	0.41
1:I:159:PHE:O	1:I:178:GLU:HA	2.21	0.41
2:J:586:ASN:H	2:J:586:ASN:HD22	1.67	0.41
3:A:190:PRO:HB2	3:A:193:PRO:CD	2.51	0.41
1:I:103:GLU:CD	2:J:559:ARG:HH22	2.24	0.41
1:I:33:MET:HA	1:I:34:PRO:HD3	1.84	0.41
3:A:175:VAL:CG2	4:B:160:LEU:HD13	2.51	0.41
1:I:102:GLY:HA3	2:J:518:TRP:CZ2	2.55	0.41
2:J:589:ALA:O	2:J:592:PHE:HB3	2.21	0.41
4:B:37:GLN:HG3	4:B:86:TYR:CZ	2.55	0.40
3:A:194:ARG:CD	3:A:195:PRO:HA	2.51	0.40
3:A:67:ARG:C	3:A:68:PHE:HD1	2.25	0.40
3:A:161:ASN:O	3:A:164:SER:HB2	2.22	0.40
3:A:88:SER:C	3:A:90:ASP:H	2.24	0.40
1:I:94:PRO:HB3	1:I:169:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	I	239/298 (80%)	191 (80%)	31 (13%)	17 (7%)	1	8
2	J	103/167 (62%)	78 (76%)	18 (18%)	7 (7%)	1	9
3	A	218/220 (99%)	191 (88%)	25 (12%)	2 (1%)	17	51
4	B	210/212 (99%)	183 (87%)	21 (10%)	6 (3%)	4	26
All	All	770/897 (86%)	643 (84%)	95 (12%)	32 (4%)	3	19

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	262	LEU
1	I	266	LEU
1	I	276	THR
1	I	277	LEU
1	I	278	ASP
1	I	282	ASN
2	J	539	ALA
2	J	612	PRO
3	A	30	ASN
4	B	2	ILE
4	B	26	SER
4	B	59	PRO
4	B	80	ALA
1	I	189	PRO
1	I	225	PHE
1	I	263	HIS
1	I	265	GLN
2	J	603	ILE
2	J	606	PRO
4	B	78	VAL
1	I	270	THR
1	I	274	ILE

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Mol	Chain	Res	Type
1	I	237	ASN
1	I	255	GLN
2	J	537	PRO
2	J	600	THR
4	B	7	SER
2	J	610	ILE
1	I	281	ILE
3	A	177	GLN
1	I	146	PRO
1	I	271	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	178/257 (69%)	145 (82%)	33 (18%)	1	6
2	J	78/142 (55%)	72 (92%)	6 (8%)	13	41
3	A	184/184 (100%)	151 (82%)	33 (18%)	2	7
4	B	187/187 (100%)	149 (80%)	38 (20%)	1	4
All	All	627/770 (81%)	517 (82%)	110 (18%)	2	8

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	39	THR
1	I	41	SER
1	I	44	GLU
1	I	48	ILE
1	I	52	VAL
1	I	55	ASP
1	I	59	SER
1	I	65	SER
1	I	73	SER
1	I	75	VAL
1	I	79	ILE

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Mol	Chain	Res	Type
1	I	89	ARG
1	I	90	SER
1	I	92	VAL
1	I	111	LEU
1	I	117	ASP
1	I	122	LEU
1	I	130	ARG
1	I	142	GLN
1	I	174	VAL
1	I	184	LEU
1	I	213	TYR
1	I	216	SER
1	I	217	TYR
1	I	220	TYR
1	I	231	THR
1	I	238	ASN
1	I	240	THR
1	I	241	PHE
1	I	244	LEU
1	I	249	THR
1	I	254	PHE
1	I	256	LEU
2	J	512	ASN
2	J	522	GLU
2	J	551	GLN
2	J	552	ASN
2	J	585	LEU
2	J	608	CYS
3	A	1	GLU
3	A	11	LEU
3	A	12	VAL
3	A	13	THR
3	A	30	ASN
3	A	40	ASN
3	A	41	THR
3	A	45	LEU
3	A	48	VAL
3	A	52	ASN
3	A	53	SER
3	A	62	ASP
3	A	69	THR
3	A	98	ARG

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Mol	Chain	Res	Type
3	A	99	GLN
3	A	100	LEU
3	A	106	PHE
3	A	111	GLN
3	A	113	THR
3	A	115	LEU
3	A	144	LEU
3	A	169	VAL
3	A	177	GLN
3	A	183	LEU
3	A	186	SER
3	A	188	THR
3	A	191	SER
3	A	192	SER
3	A	194	ARG
3	A	198	THR
3	A	202	ASN
3	A	209	SER
3	A	219	ARG
4	B	1	ASP
4	B	5	THR
4	B	7	SER
4	B	9	LYS
4	B	12	SER
4	B	14	SER
4	B	15	VAL
4	B	37	GLN
4	B	39	LYS
4	B	43	SER
4	B	53	THR
4	B	54	ARG
4	B	56	THR
4	B	60	ASP
4	B	63	THR
4	B	74	THR
4	B	81	GLU
4	B	83	LEU
4	B	85	LEU
4	B	90	GLN
4	B	104	LEU
4	B	106	LEU
4	B	116	SER

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Mol	Chain	Res	Type
4	B	133	VAL
4	B	147	LYS
4	B	153	SER
4	B	156	GLN
4	B	169	LYS
4	B	178	THR
4	B	182	THR
4	B	183	LYS
4	B	184	ASP
4	B	194	CYS
4	B	197	THR
4	B	203	SER
4	B	205	ILE
4	B	206	VAL
4	B	208	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	62	GLN
1	I	139	HIS
1	I	142	GLN
1	I	224	ASN
1	I	239	ASN
1	I	248	HIS
2	J	549	HIS
2	J	551	GLN
2	J	552	ASN
2	J	586	ASN
3	A	40	ASN
3	A	52	ASN
3	A	177	GLN
3	A	202	ASN
4	B	27	GLN
4	B	37	GLN
4	B	124	GLN
4	B	137	ASN
4	B	138	ASN
4	B	156	GLN
4	B	157	ASN
4	B	161	ASN
4	B	190	ASN

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Mol	Chain	Res	Type
4	B	210	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

6 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
5	NAG	C	1	1,5	14,14,15	0.63	0	17,19,21	1.35	2 (11%)
5	NAG	C	2	5	14,14,15	0.56	0	17,19,21	1.62	2 (11%)
5	MAN	C	3	5	11,11,12	0.62	0	15,15,17	1.25	2 (13%)
5	NAG	D	1	2,5	14,14,15	0.63	0	17,19,21	1.71	1 (5%)
5	NAG	D	2	5	14,14,15	0.44	0	17,19,21	2.07	4 (23%)
5	MAN	D	3	5	11,11,12	0.65	0	15,15,17	1.58	2 (13%)

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	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	C	3	5	-	2/2/19/22	0/1/1/1
5	NAG	D	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	D	2	5	-	4/6/23/26	0/1/1/1
5	MAN	D	3	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2	NAG	C1-O5-C5	6.28	120.69	112.19
5	D	1	NAG	O5-C1-C2	-5.29	102.93	111.29
5	C	2	NAG	C1-O5-C5	4.20	117.88	112.19
5	D	2	NAG	C4-C3-C2	-3.78	105.47	111.02
5	D	3	MAN	C1-O5-C5	3.61	117.08	112.19
5	D	3	MAN	C3-C4-C5	3.31	116.15	110.24
5	C	1	NAG	C1-O5-C5	3.04	116.31	112.19
5	C	2	NAG	C4-C3-C2	-2.99	106.63	111.02
5	C	3	MAN	C1-O5-C5	2.68	115.82	112.19
5	D	2	NAG	C6-C5-C4	-2.17	107.92	113.00
5	D	2	NAG	C8-C7-N2	2.14	119.72	116.10
5	C	3	MAN	C3-C4-C5	2.06	113.92	110.24
5	C	1	NAG	C6-C5-C4	-2.05	108.19	113.00

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2	NAG	O5-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	D	2	NAG	C8-C7-N2-C2
5	D	2	NAG	O7-C7-N2-C2
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
5	D	3	MAN	O5-C5-C6-O6
5	C	3	MAN	C4-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
5	C	3	MAN	O5-C5-C6-O6
5	D	1	NAG	O5-C5-C6-O6
5	D	3	MAN	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	I	245/298 (82%)	0.28	15 (6%) 21 23	102, 178, 299, 339	0
2	J	105/167 (62%)	0.28	3 (2%) 51 54	110, 151, 229, 251	0
3	A	220/220 (100%)	-0.11	0 100 100	87, 111, 152, 205	0
4	B	212/212 (100%)	-0.02	2 (0%) 84 87	86, 120, 166, 187	0
All	All	782/897 (87%)	0.09	20 (2%) 56 58	86, 131, 259, 339	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	142	GLN	5.5
1	I	87	GLY	4.6
1	I	86	TRP	4.0
1	I	218	LEU	3.8
1	I	121	CYS	3.3
1	I	141	ALA	3.0
1	I	148	PRO	2.9
1	I	232	THR	2.9
1	I	225	PHE	2.8
2	J	524	HIS	2.8
1	I	243	LEU	2.6
1	I	241	PHE	2.6
4	B	35	TRP	2.4
2	J	612	PRO	2.3
2	J	525	ASN	2.1
1	I	280	ASN	2.1
4	B	48	ILE	2.0
1	I	263	HIS	2.0
1	I	235	LYS	2.0
1	I	178	GLU	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
5	MAN	C	3	11/12	0.60	0.31	225,232,235,235	0
5	NAG	C	2	14/15	0.73	0.27	192,197,201,210	0
5	MAN	D	3	11/12	0.82	0.19	217,222,223,223	0
5	NAG	C	1	14/15	0.83	0.23	168,182,195,212	0
5	NAG	D	2	14/15	0.95	0.15	183,187,192,201	0
5	NAG	D	1	14/15	0.95	0.22	153,157,165,174	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.