



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:46 PM GMT

PDB ID : 1YKB  
Title : Crystal Structure of Insect Cell Expressed IL-22  
Authors : Xu, T.; Logsdon, N.J.; Walter, M.R.  
Deposited on : 2005-01-17  
Resolution : 2.60 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

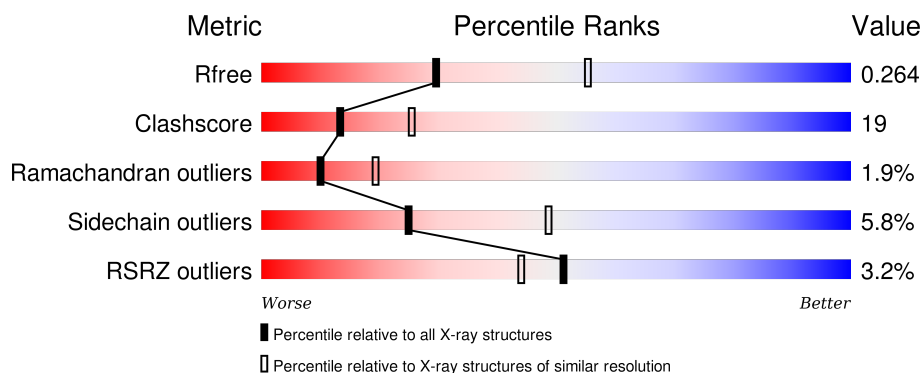
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	142	<div> <div>4%</div> <div>68%</div> <div>28%</div> <div>• •</div> </div>
1	B	142	<div> <div>2%</div> <div>57%</div> <div>35%</div> <div>8%</div> <div>•</div> </div>
1	C	142	<div> <div>3%</div> <div>67%</div> <div>28%</div> <div>• •</div> </div>
1	D	142	<div> <div>%</div> <div>72%</div> <div>25%</div> <div>•</div> </div>
1	E	142	<div> <div>%</div> <div>62%</div> <div>31%</div> <div>7%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	142	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	A	1112	-	-	X	-
3	NAG	E	1531	-	-	-	X
4	NAG	C	1332	X	-	-	-
5	MAN	D	1413	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7197 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 PROTEIN (Interleukin-22).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	1	0
			1144	721	201	212	10			
1	B	142	Total	C	N	O	S	0	1	0
			1150	724	202	214	10			
1	C	142	Total	C	N	O	S	0	1	0
			1150	725	202	214	9			
1	D	142	Total	C	N	O	S	0	2	0
			1153	725	204	214	10			
1	E	142	Total	C	N	O	S	0	0	0
			1147	722	202	214	9			
1	F	142	Total	C	N	O	S	0	1	0
			1150	723	204	214	9			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	5	Total	C	N	O	0	0
			60	34	2	24		

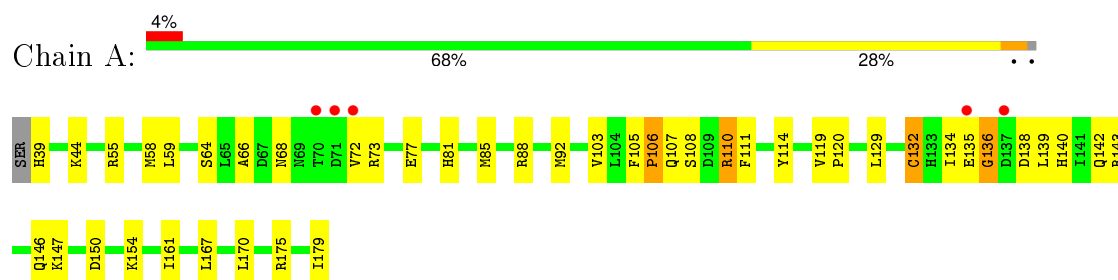
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	O 8	0	0
6	B	8	Total 8	O 8	0	0
6	C	11	Total 11	O 11	0	0
6	D	15	Total 15	O 15	0	0
6	E	5	Total 5	O 5	0	0
6	F	4	Total 4	O 4	0	0

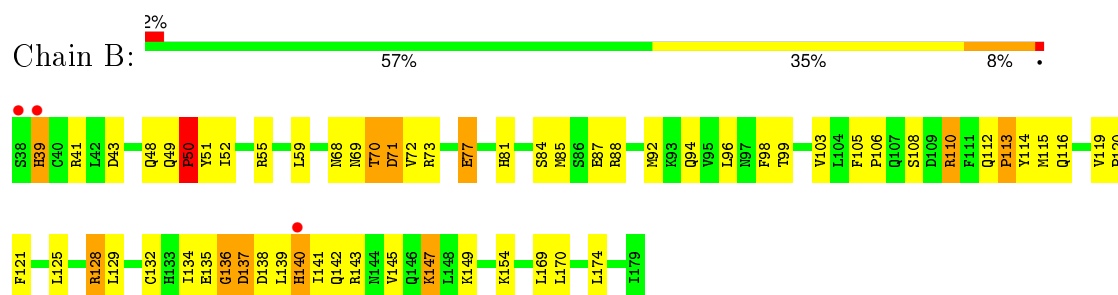
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

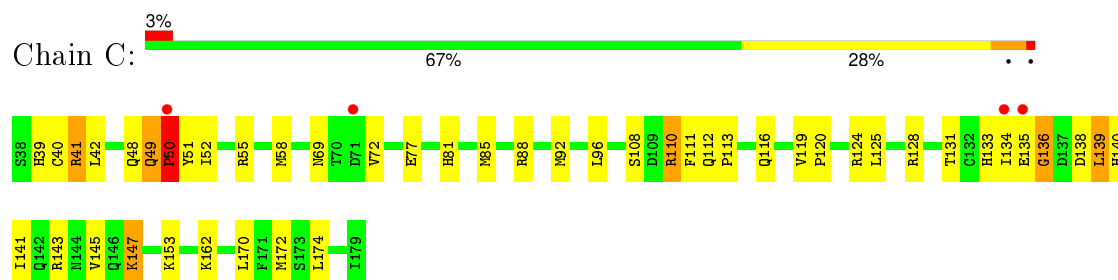
- Molecule 1: PROTEIN (Interleukin-22)



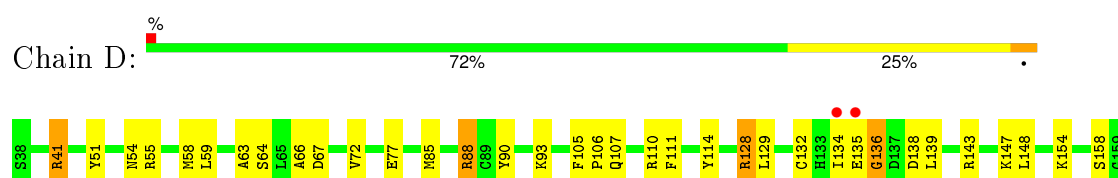
- Molecule 1: PROTEIN (Interleukin-22)



- Molecule 1: PROTEIN (Interleukin-22)

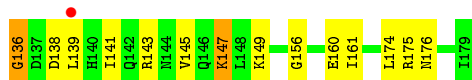


- Molecule 1: PROTEIN (Interleukin-22)





• Molecule 1: PROTEIN (Interleukin-22)



• Molecule 1: PROTEIN (Interleukin-22)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.88Å 62.23Å 139.52Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	19.93 – 2.60 42.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.93-2.60) 91.3 (42.95-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.265 0.239 , 0.264	Depositor DCC
$R_{free}$ test set	1651 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.5	EDS
Estimated twinning fraction	0.006 for k,h,-l 0.012 for -k,-h,-l 0.025 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 35584 reflections (0.011%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7197	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FUC, 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	A	0.49	0/1167	0.65	0/1566
1	B	0.49	0/1173	0.65	0/1574
1	C	0.50	0/1173	0.66	0/1575
1	D	0.49	0/1184	0.63	0/1588
1	E	0.45	0/1165	0.63	0/1564
1	F	0.41	0/1176	0.65	0/1578
All	All	0.47	0/7038	0.65	0/9445

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
4	C	1	0
5	D	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1332	NAG	C1
5	D	1413	MAN	C1

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	A	1144	0	1149	40	0
1	B	1150	0	1155	64	0
1	C	1150	0	1157	53	0
1	D	1153	0	1151	34	0
1	E	1147	0	1150	50	0
1	F	1150	0	1146	36	0
2	A	38	0	34	9	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	E	14	0	13	0	0
4	C	28	0	25	0	0
4	D	28	0	25	2	0
4	F	56	0	50	4	0
5	D	60	0	52	6	0
6	A	8	0	0	2	0
6	B	8	0	0	0	0
6	C	11	0	0	0	0
6	D	15	0	0	4	0
6	E	5	0	0	2	0
6	F	4	0	0	2	0
All	All	7197	0	7133	269	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 19.

All (269) 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)
4:F:1631:NAG:H62	4:F:1632:NAG:H82	1.41	1.03
1:A:55:ARG:NH2	2:A:1112:FUC:H5	1.77	0.99
2:A:1113:NAG:H83	1:B:48:GLN:HE22	1.31	0.95
1:B:134:ILE:HD11	1:B:138:ASP:HB3	1.50	0.94
1:D:134:ILE:HD11	1:D:138:ASP:HB3	1.52	0.92
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.39	0.87
1:F:110:ARG:HH22	1:F:161:ILE:HD11	1.43	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ILE:HD11	1:F:138:ASP:HB3	1.61	0.81
1:C:40:CYS:O	1:C:41:ARG:HG2	1.81	0.81
1:A:110:ARG:HG3	1:A:111:PHE:H	1.43	0.81
1:D:110:ARG:NH1	1:D:161:ILE:HD11	1.98	0.79
1:E:69:ASN:N	1:E:69:ASN:HD22	1.78	0.79
1:D:158:SER:HB2	6:D:1437:HOH:O	1.82	0.79
4:F:1631:NAG:C6	4:F:1632:NAG:H82	2.14	0.78
1:A:134:ILE:HD11	1:A:138:ASP:HB3	1.69	0.74
1:D:59:LEU:HD13	1:D:114:TYR:HB2	1.69	0.74
1:C:147:LYS:HA	1:C:147:LYS:HE2	1.71	0.72
1:A:150:ASP:OD1	6:A:325:HOH:O	2.08	0.71
4:F:1631:NAG:H62	4:F:1632:NAG:C8	2.17	0.71
1:C:110:ARG:HG3	1:C:111:PHE:N	2.06	0.70
1:A:55:ARG:HH22	2:A:1112:FUC:H5	1.57	0.70
1:E:112:GLN:HE22	1:E:116:GLN:H	1.40	0.69
1:F:67:ASP:HA	6:F:1634:HOH:O	1.91	0.69
1:C:49:GLN:O	1:C:52:ILE:HG22	1.93	0.69
1:E:51:TYR:H	1:E:51:TYR:HD2	1.41	0.69
1:A:179:ILE:HD11	1:B:73:ARG:CZ	2.23	0.69
1:C:72:VAL:HG23	1:C:162:LYS:HE3	1.75	0.68
1:F:59:LEU:HD13	1:F:114:TYR:HB2	1.75	0.68
1:C:42:LEU:HD13	1:C:125[B]:LEU:HD11	1.73	0.68
1:B:96:LEU:HD22	1:B:174:LEU:HD11	1.74	0.68
1:E:134:ILE:HD11	1:E:138:ASP:HB3	1.75	0.68
1:A:55:ARG:NH2	2:A:1112:FUC:C5	2.55	0.68
1:E:73:ARG:HD2	1:F:176:ASN:OD1	1.93	0.67
1:A:110:ARG:HG3	1:A:111:PHE:N	2.10	0.67
1:C:39:HIS:HB2	1:C:131:THR:O	1.94	0.67
1:C:55:ARG:HA	1:C:58:MET:HE3	1.77	0.66
1:E:147:LYS:HE2	1:E:147:LYS:HA	1.78	0.66
1:C:135:GLU:HG2	1:C:136:GLY:H	1.60	0.66
1:B:128:ARG:O	1:B:128:ARG:HD2	1.95	0.66
2:A:1113:NAG:H2	1:B:48:GLN:NE2	2.12	0.65
1:C:134:ILE:HD11	1:C:138:ASP:HB3	1.79	0.65
1:B:128:ARG:CD	1:B:128:ARG:O	2.45	0.65
1:F:71:ASP:O	1:F:72:VAL:HG23	1.97	0.65
1:F:105:PHE:HB2	1:F:106:PRO:HD3	1.79	0.64
1:B:105:PHE:HB2	1:B:106:PRO:HD3	1.78	0.64
1:C:49:GLN:O	1:C:51:TYR:N	2.30	0.64
1:B:135:GLU:HG2	1:B:136:GLY:H	1.62	0.64
1:A:103:VAL:C	1:A:106:PRO:HD2	2.20	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:GLN:HG2	1:E:160:GLU:OE1	1.98	0.63
1:C:48:GLN:C	1:C:50:PRO:HD3	2.20	0.62
5:D:1412:NAG:O3	5:D:1414:MAN:H5	2.00	0.62
1:C:96:LEU:HD22	1:C:174:LEU:HD11	1.82	0.62
1:C:124:ARG:CZ	1:E:156:GLY:HA2	2.30	0.61
1:F:150:ASP:HA	1:F:153:LYS:HE2	1.82	0.61
1:C:125[B]:LEU:HD23	1:C:174:LEU:HD13	1.82	0.61
1:E:112:GLN:NE2	1:E:116:GLN:H	1.98	0.61
1:F:129:LEU:O	1:F:132:CYS:HB3	2.00	0.61
1:C:172:MET:HE1	1:D:54:ASN:HA	1.83	0.61
1:C:110:ARG:NH1	1:C:110:ARG:HG2	2.06	0.61
1:E:69:ASN:N	1:E:69:ASN:ND2	2.48	0.61
1:B:112:GLN:OE1	1:B:116:GLN:HG3	2.01	0.60
1:A:85:MET:HE2	1:A:88:ARG:NE	2.15	0.60
1:F:110:ARG:NH2	1:F:161:ILE:HD11	2.13	0.60
1:C:69:ASN:OD1	1:C:72:VAL:HG22	2.01	0.60
1:B:147:LYS:HA	1:B:147:LYS:HE2	1.83	0.59
1:A:129:LEU:O	1:A:132:CYS:HB3	2.02	0.59
1:F:58:MET:HE1	4:F:1611:NAG:C1	2.32	0.59
1:E:73:ARG:HG3	1:F:176:ASN:HB3	1.83	0.59
1:C:135:GLU:HG2	1:C:136:GLY:N	2.17	0.59
1:E:110:ARG:NH2	1:E:161:ILE:HD11	2.18	0.59
1:B:154:LYS:HZ2	1:B:154:LYS:HB2	1.68	0.59
1:E:119:VAL:HB	1:E:120:PRO:HD3	1.85	0.58
1:B:70:THR:HG23	1:B:73:ARG:NH2	2.19	0.58
1:B:112:GLN:NE2	1:B:115:MET:HB3	2.18	0.58
1:D:135:GLU:HG2	1:D:136:GLY:N	2.18	0.58
1:F:54:ASN:OD1	1:F:58:MET:HE2	2.03	0.58
1:E:135:GLU:HG2	1:E:136:GLY:H	1.68	0.57
1:C:125[B]:LEU:CD2	1:C:174:LEU:HD13	2.34	0.57
1:D:107:GLN:OE1	1:D:110:ARG:HD2	2.03	0.57
1:C:42:LEU:CD1	1:C:125[B]:LEU:HD11	2.35	0.57
1:B:154:LYS:NZ	1:B:154:LYS:CB	2.68	0.57
1:E:45:SER:O	1:E:49:GLN:NE2	2.38	0.56
1:C:50:PRO:HB3	6:D:1439:HOH:O	2.05	0.56
1:B:112:GLN:HE22	1:B:115:MET:HB3	1.70	0.56
1:B:112:GLN:OE1	1:B:113:PRO:HA	2.05	0.56
1:F:85:MET:HE2	1:F:85:MET:HA	1.88	0.56
1:E:39:HIS:HB2	1:E:131:THR:O	2.06	0.56
1:B:135:GLU:HG2	1:B:136:GLY:N	2.21	0.56
1:D:85:MET:HE2	1:D:85:MET:HA	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:GLU:HG2	1:D:136:GLY:H	1.72	0.55
1:A:135:GLU:HG2	1:A:136:GLY:N	2.22	0.55
1:C:81:HIS:CE1	1:D:77:GLU:HB2	2.41	0.55
1:C:41:ARG:HH11	1:C:41:ARG:HG3	1.72	0.55
1:B:69:ASN:OD1	1:B:72:VAL:HG23	2.07	0.55
1:E:112:GLN:HE22	1:E:116:GLN:N	2.05	0.55
1:C:55:ARG:HD3	1:C:58:MET:HE1	1.89	0.55
1:D:129:LEU:O	1:D:132:CYS:HB3	2.06	0.54
1:E:73:ARG:HG3	1:F:176:ASN:CB	2.38	0.54
1:A:55:ARG:HH22	2:A:1112:FUC:C6	2.21	0.54
1:B:39:HIS:HE1	1:B:128:ARG:HH22	1.55	0.54
1:F:150:ASP:HA	1:F:153:LYS:CE	2.38	0.54
1:B:85:MET:CE	1:B:88:ARG:CZ	2.86	0.54
1:E:69:ASN:C	1:E:71:ASP:H	2.11	0.53
1:C:55:ARG:HD3	1:C:58:MET:CE	2.39	0.53
4:D:1431:NAG:C6	4:D:1432:NAG:H82	2.39	0.53
1:F:90:TYR:O	1:F:93:LYS:HB3	2.08	0.53
1:D:105:PHE:HB2	1:D:106:PRO:HD3	1.92	0.52
1:C:41:ARG:NH1	1:C:41:ARG:HG3	2.25	0.52
1:F:135:GLU:HG2	1:F:136:GLY:N	2.24	0.52
1:D:55:ARG:HH21	5:D:1415:FUC:H5	1.74	0.52
1:C:85:MET:HE2	1:C:88:ARG:NE	2.25	0.52
1:C:110:ARG:HG3	1:C:111:PHE:CG	2.44	0.52
1:B:139:LEU:HD21	1:B:143:ARG:HH22	1.74	0.52
1:D:107:GLN:NE2	1:D:160:GLU:OE1	2.39	0.52
1:E:135:GLU:HG2	1:E:136:GLY:N	2.24	0.52
1:C:85:MET:HE1	1:C:88:ARG:NH2	2.25	0.52
1:E:103:VAL:C	1:E:106:PRO:HD2	2.31	0.51
1:C:119:VAL:HB	1:C:120:PRO:HD3	1.92	0.51
1:E:106:PRO:C	1:E:108:SER:H	2.13	0.51
1:A:81:HIS:O	1:A:140:HIS:HE1	1.93	0.51
1:B:49:GLN:CG	1:B:50:PRO:HD2	2.42	0.51
4:D:1431:NAG:H61	4:D:1432:NAG:H82	1.92	0.50
1:C:77:GLU:OE2	1:C:81:HIS:NE2	2.44	0.50
1:C:141:ILE:O	1:C:145:VAL:HG23	2.11	0.50
1:A:135:GLU:HG2	1:A:136:GLY:H	1.76	0.50
1:B:128:ARG:O	1:B:128:ARG:HD3	2.11	0.50
1:A:179:ILE:HD11	1:B:73:ARG:NH2	2.27	0.50
1:E:70:THR:O	1:E:73:ARG:NH2	2.45	0.50
1:E:73:ARG:NH2	1:F:179:ILE:HD11	2.27	0.50
1:B:110:ARG:CG	1:B:110:ARG:HH11	2.25	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH2	1:A:161:ILE:HD11	2.27	0.49
1:D:55:ARG:NH2	5:D:1415:FUC:H5	2.27	0.49
1:B:92:MET:CE	1:B:170:LEU:HD12	2.42	0.49
1:B:98:PHE:CE1	1:B:149:LYS:HG2	2.46	0.49
1:A:55:ARG:HH22	2:A:1112:FUC:C5	2.20	0.49
1:F:107:GLN:O	1:F:109:ASP:N	2.46	0.49
1:B:98:PHE:CD1	1:B:149:LYS:HG2	2.47	0.49
1:E:96:LEU:HD22	1:E:174:LEU:HD11	1.93	0.49
1:E:77:GLU:OE2	1:E:81:HIS:CE1	2.66	0.48
1:A:44:LYS:HE3	1:A:179:ILE:CD1	2.43	0.48
1:B:85:MET:HE1	1:B:88:ARG:CZ	2.43	0.48
1:D:55:ARG:NH1	1:D:114:TYR:CE1	2.82	0.48
1:B:154:LYS:NZ	1:B:154:LYS:HB2	2.28	0.48
1:D:139:LEU:HD23	1:D:143:ARG:NH2	2.28	0.48
1:A:146:GLN:NE2	6:A:325:HOH:O	2.47	0.48
1:C:124:ARG:NH2	1:E:156:GLY:HA2	2.29	0.48
1:C:110:ARG:CG	1:C:111:PHE:N	2.77	0.47
1:F:109:ASP:OD1	1:F:110:ARG:N	2.45	0.47
1:E:110:ARG:HH21	1:E:161:ILE:HD11	1.78	0.47
1:A:175:ARG:CZ	1:B:169:LEU:HD11	2.44	0.47
1:B:110:ARG:HG3	1:B:110:ARG:HH11	1.79	0.47
1:B:119:VAL:HB	1:B:120:PRO:HD3	1.96	0.47
1:D:128:ARG:HD3	6:D:1433:HOH:O	2.13	0.47
1:A:110:ARG:CG	1:A:111:PHE:N	2.77	0.47
1:B:51:TYR:HE1	1:B:55:ARG:HE	1.59	0.47
1:A:105:PHE:HD2	1:F:128:ARG:HH12	1.63	0.47
1:D:64:SER:C	1:D:66:ALA:H	2.18	0.47
1:A:59:LEU:HD23	1:A:167:LEU:CD1	2.45	0.47
1:B:70:THR:O	1:B:70:THR:HG23	2.15	0.47
1:C:42:LEU:HD22	1:C:128:ARG:HG3	1.97	0.47
1:F:143:ARG:HH11	1:F:143:ARG:CB	2.28	0.47
1:B:128:ARG:HD2	1:B:128:ARG:C	2.34	0.46
1:E:175:ARG:C	1:E:175:ARG:HD2	2.36	0.46
1:B:121:PHE:CE2	1:B:125:LEU:HD11	2.50	0.46
1:F:135:GLU:HG2	1:F:136:GLY:H	1.79	0.46
1:A:139:LEU:HD23	1:A:143:ARG:HH22	1.81	0.46
1:C:128:ARG:O	1:C:128:ARG:NH1	2.47	0.46
1:B:85:MET:HE2	1:B:88:ARG:NE	2.29	0.46
1:B:99:THR:O	1:B:103:VAL:HB	2.16	0.46
1:A:59:LEU:HD13	1:A:114:TYR:HB2	1.97	0.46
1:A:106:PRO:O	1:A:108:SER:N	2.43	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:MET:CE	1:C:170:LEU:HD12	2.46	0.46
1:C:139:LEU:HD21	1:C:143:ARG:HH22	1.79	0.46
1:A:55:ARG:NH1	1:A:114:TYR:CE1	2.83	0.46
1:B:105:PHE:N	1:B:106:PRO:CD	2.79	0.46
1:F:131:THR:HA	6:F:1635:HOH:O	2.15	0.46
1:B:141:ILE:O	1:B:145:VAL:HG23	2.15	0.46
1:B:112:GLN:CD	1:B:116:GLN:HG3	2.36	0.46
1:D:67:ASP:OD1	6:D:1437:HOH:O	2.21	0.46
1:E:42:LEU:HD13	1:E:125:LEU:HD22	1.98	0.46
1:F:73:ARG:HD3	1:F:166:GLU:OE2	2.17	0.45
1:D:58[A]:MET:HE1	5:D:1411:NAG:C1	2.47	0.45
1:C:110:ARG:O	1:C:112:GLN:NE2	2.49	0.45
1:F:59:LEU:HD23	1:F:167:LEU:CD1	2.46	0.45
1:E:134:ILE:HD11	1:E:138:ASP:CB	2.46	0.45
1:D:85:MET:HE2	1:D:88:ARG:NE	2.31	0.45
1:D:41:ARG:NH1	1:D:41:ARG:HG3	2.30	0.45
1:C:49:GLN:N	1:C:50:PRO:HD3	2.32	0.45
1:F:143:ARG:NH1	1:F:143:ARG:HB2	2.32	0.44
1:B:128:ARG:CD	1:B:128:ARG:C	2.85	0.44
1:B:129:LEU:O	1:B:132:CYS:HB3	2.17	0.44
1:B:112:GLN:HA	1:B:112:GLN:OE1	2.17	0.44
1:C:134:ILE:HD11	1:C:138:ASP:CB	2.46	0.44
1:E:46:ASN:C	1:E:49:GLN:HE21	2.21	0.44
1:D:85:MET:HE1	1:D:88:ARG:CZ	2.47	0.44
1:E:105:PHE:N	1:E:106:PRO:CD	2.81	0.44
1:F:96:LEU:HD22	1:F:174:LEU:HD11	2.00	0.44
1:D:72:VAL:HB	1:D:162:LYS:HE3	1.99	0.44
1:B:108:SER:HA	1:B:115:MET:HG2	1.98	0.44
1:A:55:ARG:HD3	1:A:58[A]:MET:CE	2.48	0.44
1:E:69:ASN:C	1:E:71:ASP:N	2.71	0.44
1:E:51:TYR:O	1:E:55:ARG:HG2	2.18	0.44
1:E:98:PHE:CE1	1:E:149:LYS:HG2	2.53	0.44
1:E:54:ASN:HB3	1:E:58:MET:HE2	2.00	0.44
1:C:85:MET:CE	1:C:88:ARG:CZ	2.96	0.44
1:B:49:GLN:HG3	1:B:50:PRO:HD2	2.00	0.44
1:E:141:ILE:O	1:E:145:VAL:HG23	2.18	0.44
1:E:78:LYS:HA	1:E:81:HIS:CD2	2.53	0.43
1:B:41:ARG:NH2	1:B:43:ASP:HA	2.32	0.43
1:B:85:MET:HE1	1:B:88:ARG:NH2	2.33	0.43
1:E:54:ASN:O	1:E:58:MET:HG3	2.17	0.43
1:B:71:ASP:OD1	1:B:71:ASP:N	2.51	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:LEU:HD21	1:E:143:ARG:HH22	1.83	0.43
1:E:38:SER:HB3	6:E:403:HOH:O	2.17	0.43
1:A:59:LEU:HD23	1:A:167:LEU:HD12	2.01	0.43
1:F:55:ARG:NH1	1:F:114:TYR:CE1	2.87	0.43
1:A:44:LYS:HE3	1:A:179:ILE:HD12	1.99	0.43
1:B:77:GLU:OE2	1:B:81:HIS:NE2	2.48	0.43
1:F:64:SER:C	1:F:66:ALA:H	2.20	0.43
1:F:148:LEU:HD23	1:F:148:LEU:C	2.39	0.43
1:A:39:HIS:N	1:A:39:HIS:HD1	2.17	0.43
1:D:154:LYS:HG2	1:D:154:LYS:O	2.18	0.43
1:F:52:ILE:HD12	1:F:52:ILE:HA	1.91	0.43
1:E:98:PHE:CD1	1:E:149:LYS:HG2	2.54	0.42
1:C:42:LEU:HD22	1:C:128:ARG:CG	2.48	0.42
1:E:54:ASN:HB3	1:E:58:MET:CE	2.48	0.42
1:B:59:LEU:HD13	1:B:114:TYR:HB2	2.00	0.42
1:E:175:ARG:NH2	1:E:176:ASN:OD1	2.41	0.42
1:F:92:MET:CE	1:F:170:LEU:HD12	2.49	0.42
1:D:63:ALA:HA	1:D:111:PHE:CE1	2.53	0.42
2:A:1113:NAG:H83	1:B:48:GLN:NE2	2.14	0.42
1:A:77:GLU:HG3	1:B:81:HIS:CE1	2.55	0.42
1:E:112:GLN:NE2	1:E:116:GLN:HB2	2.34	0.42
1:A:55:ARG:NH2	2:A:1112:FUC:C6	2.83	0.42
1:B:94:GLN:HE21	1:B:142:GLN:HE22	1.66	0.42
1:C:85:MET:HE1	1:C:88:ARG:CZ	2.49	0.42
1:D:175[B]:ARG:NH1	1:D:176:ASN:OD1	2.53	0.42
1:C:42:LEU:CD2	1:C:128:ARG:HG3	2.49	0.42
1:F:140:HIS:HA	1:F:143:ARG:HH11	1.85	0.42
1:D:51:TYR:HE1	5:D:1415:FUC:H3	1.85	0.41
1:B:51:TYR:O	1:B:55:ARG:HG2	2.20	0.41
1:F:160:GLU:O	1:F:164:ILE:HG13	2.19	0.41
1:E:92:MET:HB3	1:E:174:LEU:HD23	2.03	0.41
1:A:64:SER:C	1:A:66:ALA:H	2.24	0.41
1:D:55:ARG:NH2	5:D:1415:FUC:C6	2.84	0.41
1:A:39:HIS:ND1	1:A:39:HIS:N	2.68	0.41
1:C:153:LYS:HA	1:C:153:LYS:HD3	1.91	0.41
1:B:85:MET:HE2	1:B:88:ARG:CZ	2.50	0.41
1:D:90:TYR:O	1:D:93:LYS:HB3	2.21	0.41
1:B:39:HIS:CE1	1:B:128:ARG:HH22	2.36	0.41
1:C:172:MET:CE	1:D:54:ASN:HA	2.48	0.41
1:E:40:CYS:O	1:E:41:ARG:HG2	2.20	0.41
1:A:85:MET:HE2	1:A:88:ARG:CD	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:LYS:HE3	1:E:129:LEU:O	2.21	0.41
1:D:148:LEU:C	1:D:148:LEU:HD23	2.40	0.41
1:C:139:LEU:HD21	1:C:143:ARG:NH2	2.36	0.41
1:B:84:SER:OG	1:B:87:GLU:HG3	2.21	0.41
1:B:137:ASP:O	1:B:140:HIS:CE1	2.74	0.41
1:B:73:ARG:HD3	1:B:73:ARG:HA	1.94	0.40
1:C:125[B]:LEU:HD23	1:C:174:LEU:CD1	2.50	0.40
1:A:119:VAL:HB	1:A:120:PRO:HD3	2.03	0.40
1:A:138:ASP:O	1:A:142:GLN:HG2	2.21	0.40
1:B:70:THR:O	1:B:73:ARG:NH2	2.54	0.40
1:C:124:ARG:HG2	6:E:388:HOH:O	2.20	0.40
1:D:41:ARG:HG3	1:D:41:ARG:HH11	1.86	0.40
1:E:110:ARG:HG2	1:E:111:PHE:CD2	2.57	0.40
1:A:92:MET:CE	1:A:170:LEU:HD12	2.51	0.40
1:B:110:ARG:CG	1:B:110:ARG:NH1	2.84	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	140/142 (99%)	134 (96%)	3 (2%)	3 (2%)	9	16
1	B	141/142 (99%)	134 (95%)	5 (4%)	2 (1%)	14	28
1	C	141/142 (99%)	133 (94%)	5 (4%)	3 (2%)	9	16
1	D	142/142 (100%)	136 (96%)	5 (4%)	1 (1%)	26	51
1	E	140/142 (99%)	126 (90%)	10 (7%)	4 (3%)	6	9
1	F	141/142 (99%)	133 (94%)	5 (4%)	3 (2%)	9	16
All	All	845/852 (99%)	796 (94%)	33 (4%)	16 (2%)	10	19

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	B	50	PRO
1	C	50	PRO
1	E	50	PRO
1	E	106	PRO
1	A	106	PRO
1	A	136	GLY
1	B	136	GLY
1	C	136	GLY
1	D	136	GLY
1	E	107	GLN
1	E	136	GLY
1	F	108	SER
1	F	136	GLY
1	C	108	SER
1	F	72	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	130/130 (100%)	123 (95%)	7 (5%)	27	52	
1	B	131/130 (101%)	118 (90%)	13 (10%)	10	18	
1	C	131/130 (101%)	121 (92%)	10 (8%)	16	32	
1	D	132/130 (102%)	128 (97%)	4 (3%)	48	76	
1	E	130/130 (100%)	123 (95%)	7 (5%)	27	52	
1	F	131/130 (101%)	127 (97%)	4 (3%)	47	76	
All	All	785/780 (101%)	740 (94%)	45 (6%)	25	49	

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	72	VAL
1	A	73	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	110	ARG
1	A	132	CYS
1	A	147	LYS
1	A	154	LYS
1	B	39	HIS
1	B	50	PRO
1	B	52	ILE
1	B	68	ASN
1	B	70	THR
1	B	71	ASP
1	B	77	GLU
1	B	110	ARG
1	B	113	PRO
1	B	128	ARG
1	B	137	ASP
1	B	140	HIS
1	B	147	LYS
1	C	41	ARG
1	C	49	GLN
1	C	50	PRO
1	C	110	ARG
1	C	113	PRO
1	C	116	GLN
1	C	133	HIS
1	C	139	LEU
1	C	140	HIS
1	C	147	LYS
1	D	41	ARG
1	D	88	ARG
1	D	128	ARG
1	D	147	LYS
1	E	51	TYR
1	E	69	ASN
1	E	71	ASP
1	E	77	GLU
1	E	112	GLN
1	E	116	GLN
1	E	147	LYS
1	F	68	ASN
1	F	71	ASP
1	F	110	ARG
1	F	147	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	B	48	GLN
1	B	94	GLN
1	C	48	GLN
1	C	94	GLN
1	C	112	GLN
1	C	116	GLN
1	C	140	HIS
1	D	69	ASN
1	D	133	HIS
1	E	49	GLN
1	E	69	ASN
1	E	112	GLN
1	E	140	HIS
1	E	142	GLN
1	F	140	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

16 carbohydrates 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	NAG	A	1111	1,2	14,14,15	0.78	0	15,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FUC	A	1112	2	10,10,11	0.73	0	14,14,16	0.66	0
2	NAG	A	1113	2	14,14,15	0.66	0	15,19,21	0.73	0
4	NAG	C	1331	1,4	14,14,15	0.68	0	15,19,21	1.37	2 (13%)
4	NAG	C	1332	4	14,14,15	0.73	0	15,19,21	0.96	1 (6%)
5	NAG	D	1411	1,5	14,14,15	0.55	0	15,19,21	0.81	0
5	NAG	D	1412	5	14,14,15	0.54	0	15,19,21	0.79	1 (6%)
5	MAN	D	1413	5	11,11,12	0.72	0	14,15,17	0.30	0
5	MAN	D	1414	5	11,11,12	0.58	0	14,15,17	0.95	2 (14%)
5	FUC	D	1415	5	10,10,11	0.76	0	14,14,16	0.86	1 (7%)
4	NAG	D	1431	1,4	14,14,15	0.58	0	15,19,21	0.87	1 (6%)
4	NAG	D	1432	4	14,14,15	0.71	0	15,19,21	0.80	1 (6%)
4	NAG	F	1611	1,4	14,14,15	0.60	0	15,19,21	0.88	0
4	NAG	F	1612	4	14,14,15	0.68	0	15,19,21	0.73	0
4	NAG	F	1631	1,4	14,14,15	0.65	0	15,19,21	0.77	1 (6%)
4	NAG	F	1632	4	14,14,15	0.72	0	15,19,21	0.89	1 (6%)

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	NAG	A	1111	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1112	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1113	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1331	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1332	4	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	D	1411	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1412	5	-	0/6/23/26	0/1/1/1
5	MAN	D	1413	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	D	1414	5	-	0/2/19/22	0/1/1/1
5	FUC	D	1415	5	-	0/0/17/20	0/1/1/1
4	NAG	D	1431	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	1432	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1611	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	1612	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1631	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	1632	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1331	NAG	C2-N2-C7	-3.21	118.92	123.04
4	C	1331	NAG	C4-C3-C2	-3.04	106.51	111.23
4	C	1332	NAG	C2-N2-C7	-2.91	119.30	123.04
4	D	1431	NAG	C2-N2-C7	-2.63	119.66	123.04
4	F	1631	NAG	C2-N2-C7	-2.55	119.76	123.04
4	F	1632	NAG	C2-N2-C7	-2.41	119.94	123.04
5	D	1412	NAG	C2-N2-C7	-2.40	119.95	123.04
4	D	1432	NAG	C2-N2-C7	-2.27	120.12	123.04
5	D	1414	MAN	C1-O5-C5	2.23	115.08	112.25
5	D	1415	FUC	C1-C2-C3	2.26	112.21	109.54
5	D	1414	MAN	C1-C2-C3	2.32	112.28	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1332	NAG	C1
5	D	1413	MAN	C1

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1112	FUC	6	0
2	A	1113	NAG	3	0
5	D	1411	NAG	1	0
5	D	1412	NAG	1	0
5	D	1414	MAN	1	0
5	D	1415	FUC	4	0
4	D	1431	NAG	2	0
4	D	1432	NAG	2	0
4	F	1611	NAG	1	0
4	F	1631	NAG	3	0
4	F	1632	NAG	3	0

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
3	NAG	A	1131	1	14,14,15	0.44	0	15,19,21	1.12	2 (13%)
3	NAG	B	1231	1	14,14,15	0.78	0	15,19,21	1.07	1 (6%)
3	NAG	E	1531	1	14,14,15	0.65	0	15,19,21	0.57	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
3	NAG	A	1131	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1231	1	-	0/6/23/26	0/1/1/1
3	NAG	E	1531	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1231	NAG	C2-N2-C7	-2.96	119.24	123.04
3	A	1131	NAG	C2-N2-C7	-2.44	119.90	123.04
3	A	1131	NAG	C4-C3-C2	-2.02	108.08	111.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1131	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	141/142 (99%)	-0.02	5 (3%)	48	40	25, 53, 82, 97	0
1	B	142/142 (100%)	-0.09	3 (2%)	67	61	34, 52, 86, 103	0
1	C	142/142 (100%)	-0.09	4 (2%)	56	49	29, 47, 79, 100	0
1	D	142/142 (100%)	-0.20	2 (1%)	78	74	24, 54, 88, 100	0
1	E	142/142 (100%)	-0.10	1 (0%)	89	87	39, 60, 89, 103	0
1	F	142/142 (100%)	0.34	12 (8%)	13	9	36, 73, 111, 121	0
All	All	851/852 (99%)	-0.03	27 (3%)	51	44	24, 56, 95, 121	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	134	ILE	4.2
1	F	135	GLU	3.9
1	F	136	GLY	3.8
1	A	70	THR	3.8
1	A	71	ASP	3.4
1	A	72	VAL	3.2
1	B	39	HIS	3.1
1	B	38	SER	3.0
1	F	84	SER	2.8
1	F	82	GLY	2.7
1	C	134	ILE	2.7
1	B	140	HIS	2.6
1	F	38	SER	2.6
1	C	135	GLU	2.6
1	F	113	PRO	2.5
1	F	116	GLN	2.4
1	D	134	ILE	2.4
1	D	135	GLU	2.4
1	C	50	PRO	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	85	MET	2.3
1	A	135	GLU	2.2
1	E	139	LEU	2.2
1	F	83	VAL	2.2
1	F	87	GLU	2.1
1	C	71	ASP	2.0
1	A	137	ASP	2.0
1	F	114	TYR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	D	1431	14/15	0.93	0.18	1.51	59,61,67,71	0
4	NAG	F	1611	14/15	0.87	0.22	0.48	82,86,91,94	0
4	NAG	C	1331	14/15	0.87	0.18	0.42	65,71,78,83	0
2	NAG	A	1111	14/15	0.87	0.20	0.12	69,73,83,86	0
5	NAG	D	1411	14/15	0.89	0.17	-0.20	51,65,75,81	0
4	NAG	F	1631	14/15	0.85	0.17	-0.30	78,81,83,86	0
4	NAG	C	1332	14/15	0.76	0.22	-	86,88,92,93	0
4	NAG	F	1632	14/15	0.64	0.28	-	89,90,92,92	0
5	MAN	D	1413	11/12	0.75	0.40	-	94,96,98,99	0
5	MAN	D	1414	11/12	0.88	0.33	-	98,100,101,101	0
5	FUC	D	1415	10/11	0.73	0.49	-	85,87,88,89	0
4	NAG	F	1612	14/15	0.93	0.26	-	97,98,101,101	0
2	NAG	A	1113	14/15	0.88	0.31	-	87,89,90,90	0
4	NAG	D	1432	14/15	0.86	0.29	-	75,76,81,81	0
2	FUC	A	1112	10/11	0.79	0.43	-	89,91,92,93	0
5	NAG	D	1412	14/15	0.89	0.22	-	79,81,85,91	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	1531	14/15	0.92	0.21	6.29	55,59,61,63	0
3	NAG	B	1231	14/15	0.88	0.18	0.64	67,70,71,73	0
3	NAG	A	1131	14/15	0.94	0.14	-1.08	68,71,74,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.