



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:15 PM BST

PDB ID : 1AZX  
Title : ANTITHROMBIN/PENTASACCHARIDE COMPLEX  
Authors : Jin, L.; Abrahams, J.P.; Skinner, R.; Petitou, M.; Pike, R.N.; Carrell, R.W.  
Deposited on : 1997-11-23  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

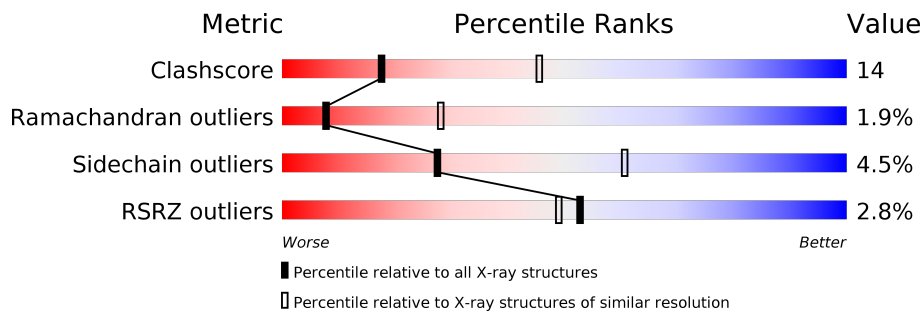
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	432	 4% 65% 29% ..
1	L	432	 2% 64% 30% ..
2	A	5	 80% 20%
2	B	5	 60% 40%

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
3	NAG	L	502	-	-	-	X

## 2 Entry composition i

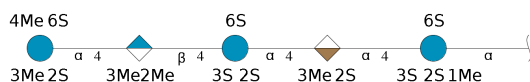
There are 3 unique types of molecules in this entry. The entry contains 6881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANTITHROMBIN.

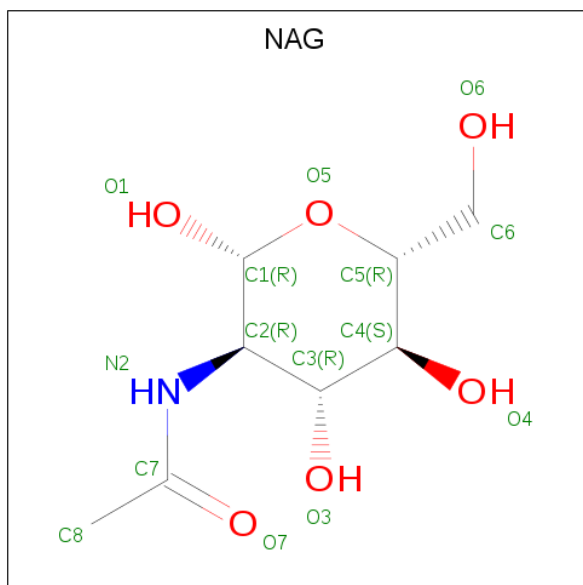
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	417	3328	2121	562	627	18	0	0	0
1	L	414	3311	2111	559	623	18	0	0	0

- Molecule 2 is an oligosaccharide called 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranos e-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucop yranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-su lfo-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	A	5	100	36	55	9	0	0	0
2	B	5	100	36	55	9	0	0	0

- Molecule 3 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>).

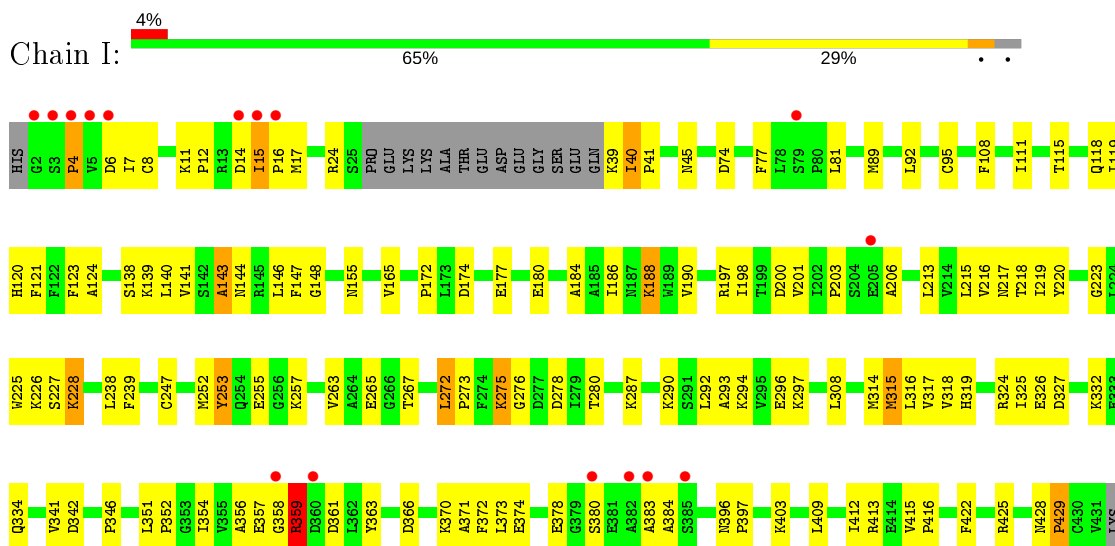


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	I	1	Total 14	8	1	5	0	0
3	L	1	Total 14	8	1	5	0	0
3	L	1	Total 14	8	1	5	0	0

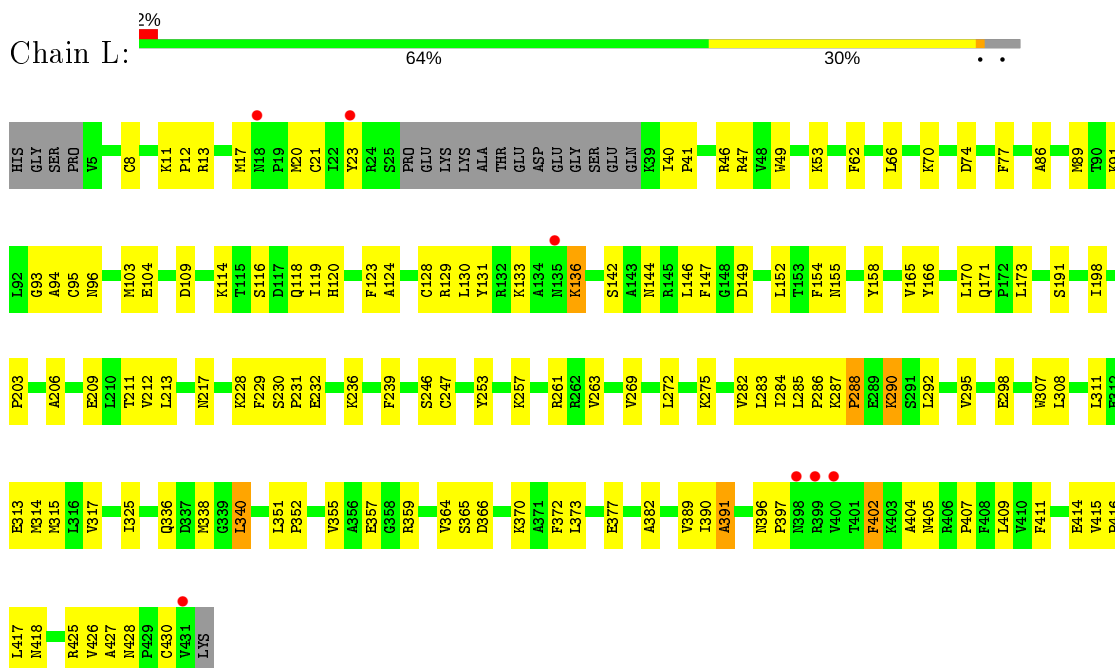
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


#### • Molecule 1: ANTITHROMBIN



#### • Molecule 1: ANTITHROMBIN



- Molecule 2: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain A:  80% 20%

Z9L1  
Z9K2  
G063  
G114  
Z9H5

- Molecule 2: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain B:  60% 40%

Z9L1  
Z9K2  
G063  
G114  
Z9H5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.44Å 86.97Å 97.22Å 90.00° 108.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 27.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-2.90) 94.5 (27.65-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 2.90Å)	Xtrriage
Refinement program	TNT 5D	Depositor
R, $R_{free}$	0.195 , 0.280 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 94.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: NAG, Z9L, Z9K, Z9H, GU1, GU6

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	0.34	0/3394	0.59	0/4582
1	L	0.35	0/3376	0.58	0/4557
All	All	0.35	0/6770	0.59	0/9139

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3328	0	3333	90	0
1	L	3311	0	3323	89	0
2	A	100	0	16	4	0
2	B	100	0	16	5	0
3	I	14	0	13	5	0
3	L	28	0	26	3	0
All	All	6881	0	6727	183	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 14.

All (183) 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:I:356:ALA:O	3:I:501:NAG:H81	1.60	1.01
1:L:129:ARG:HD3	1:L:417:LEU:HD21	1.56	0.87
1:L:20:MET:HA	3:L:501:NAG:H61	1.55	0.87
1:I:17:MET:HB2	1:I:120:HIS:HE1	1.39	0.86
1:I:144:ASN:HB3	1:I:217:ASN:HA	1.67	0.77
1:I:324:ARG:HG2	1:I:374:GLU:HG3	1.67	0.75
2:B:2:Z9K:O10	2:B:3:GU6:H5	1.91	0.71
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.73	0.69
1:I:155:ASN:HD22	3:I:501:NAG:H83	1.55	0.69
2:B:4:GU1:H72	2:B:4:GU1:H83	1.75	0.69
1:I:356:ALA:O	3:I:501:NAG:C8	2.41	0.68
1:I:108:PHE:O	1:I:111:ILE:HG12	1.94	0.67
1:I:358:GLY:O	1:I:359:ARG:HD3	1.94	0.66
1:L:20:MET:CA	3:L:501:NAG:H61	2.26	0.66
1:L:355:VAL:HG21	1:L:359:ARG:HB2	1.78	0.65
1:I:17:MET:HB2	1:I:120:HIS:CE1	2.28	0.65
1:I:257:LYS:HA	1:I:314:MET:O	1.96	0.65
1:I:77:PHE:CZ	1:I:373:LEU:HB2	2.33	0.64
1:L:47:ARG:NH1	1:L:114:LYS:HB3	2.11	0.64
1:I:308:LEU:HD13	1:I:413:ARG:NH1	2.14	0.63
1:I:255:GLU:HG2	1:I:317:VAL:HG22	1.80	0.62
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.81	0.62
1:L:415:VAL:HB	1:L:416:PRO:HD3	1.80	0.62
1:L:229:PHE:O	1:L:377:GLU:HB3	2.00	0.62
1:I:17:MET:SD	1:I:121:PHE:HB2	2.40	0.61
1:L:286:PRO:HD3	1:L:292:LEU:HD13	1.81	0.61
1:L:257:LYS:HG2	1:L:315:MET:HG2	1.82	0.61
1:L:247:CYS:HG	1:L:430:CYS:CB	2.13	0.60
1:I:239:PHE:HB3	1:I:247:CYS:HB3	1.83	0.60
1:I:412:ILE:HB	1:I:422:PHE:HB2	1.84	0.59
1:L:152:LEU:HD13	1:L:212:VAL:HG13	1.83	0.59
1:I:139:LYS:HZ3	1:I:197:ARG:HH22	1.48	0.59
1:L:211:THR:HA	1:L:391:ALA:O	2.01	0.59
1:L:407:PRO:HB3	1:L:427:ALA:HA	1.85	0.59
1:I:265:GLU:O	1:I:287:LYS:HD2	2.03	0.58
1:I:140:LEU:HD11	1:I:219:ILE:HD11	1.85	0.58
1:I:228:LYS:HB3	1:I:228:LYS:HZ2	1.69	0.58
1:I:198:ILE:HG23	1:I:370:LYS:HD3	1.87	0.57
1:I:228:LYS:HZ2	1:I:378:GLU:HB2	1.69	0.57
1:L:272:LEU:HD11	1:L:283:LEU:HD11	1.87	0.57
1:L:313:GLU:CD	1:L:313:GLU:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:364:VAL:HG22	1:L:390:ILE:HD13	1.88	0.56
1:L:21:CYS:SG	1:L:95:CYS:CB	2.94	0.56
1:I:4:PRO:HB2	1:I:8:CYS:SG	2.46	0.55
1:L:308:LEU:HA	1:L:311:LEU:HG	1.88	0.55
1:I:138:SER:HB3	1:I:223:GLY:HA2	1.88	0.55
1:L:355:VAL:CG2	1:L:359:ARG:HB2	2.36	0.55
1:L:116:SER:O	1:L:119:ILE:HG12	2.07	0.55
1:I:143:ALA:HB3	1:I:218:THR:OG1	2.07	0.55
1:L:95:CYS:SG	1:L:96:ASN:ND2	2.80	0.55
1:L:21:CYS:SG	1:L:95:CYS:HB2	2.47	0.54
1:L:236:LYS:NZ	1:L:236:LYS:HB2	2.22	0.54
1:I:356:ALA:O	3:I:501:NAG:O7	2.26	0.53
1:L:12:PRO:HB3	1:L:118:GLN:NE2	2.24	0.53
1:I:238:LEU:HA	1:I:247:CYS:O	2.10	0.52
1:L:253:TYR:CE1	1:L:317:VAL:HG13	2.45	0.52
1:L:40:ILE:HB	1:L:41:PRO:HD2	1.92	0.52
1:I:146:LEU:HG	1:I:215:LEU:HG	1.91	0.52
2:A:4:GU1:H83	2:A:4:GU1:H72	1.92	0.51
1:L:365:SER:HB3	1:L:389:VAL:HG23	1.91	0.51
1:L:130:LEU:HD23	1:L:414:GLU:OE1	2.11	0.51
1:I:147:PHE:CE2	1:I:186:ILE:HG23	2.45	0.51
1:L:20:MET:HA	3:L:501:NAG:C6	2.36	0.51
1:L:257:LYS:HA	1:L:314:MET:O	2.10	0.51
1:L:287:LYS:HB3	1:L:290:LYS:HG3	1.91	0.51
1:L:370:LYS:NZ	1:L:370:LYS:HB2	2.25	0.51
1:I:15:ILE:HD13	1:I:15:ILE:N	2.26	0.51
1:I:174:ASP:OD2	1:I:177:GLU:HB2	2.11	0.51
1:I:40:ILE:HG13	1:I:41:PRO:HD2	1.94	0.50
1:I:148:GLY:O	1:I:172:PRO:HA	2.12	0.50
1:L:23:TYR:CD1	1:L:103:MET:HG3	2.47	0.50
1:I:184:ALA:O	1:I:188:LYS:HD2	2.12	0.50
1:I:253:TYR:HA	1:I:318:VAL:O	2.12	0.50
1:L:402:PHE:HD1	1:L:402:PHE:O	1.95	0.50
1:L:77:PHE:CE2	1:L:373:LEU:HB2	2.46	0.50
1:I:220:TYR:HD1	1:I:372:PHE:HB3	1.77	0.49
1:L:86:ALA:O	1:L:89:MET:HB2	2.12	0.49
1:I:380:SER:HB2	1:I:384:ALA:HB2	1.94	0.49
1:I:314:MET:HG2	1:I:315:MET:N	2.26	0.49
1:I:290:LYS:HD2	1:I:294:LYS:HD3	1.93	0.49
1:L:120:HIS:HD2	1:L:166:TYR:OH	1.96	0.49
1:I:17:MET:HG3	1:I:118:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:93:GLY:O	1:L:351:LEU:HA	2.13	0.49
1:L:91:LYS:NZ	1:L:120:HIS:NE2	2.61	0.49
1:I:326:GLU:HA	1:I:371:ALA:O	2.13	0.49
1:I:396:ASN:OD1	1:I:397:PRO:HD2	2.13	0.48
1:L:149:ASP:HA	1:L:173:LEU:O	2.13	0.48
1:L:203:PRO:HG2	1:L:206:ALA:HB2	1.94	0.48
1:L:21:CYS:HG	1:L:95:CYS:HG	0.48	0.48
1:I:12:PRO:HD2	2:A:3:GU6:O14	2.14	0.48
1:L:155:ASN:HB3	1:L:158:TYR:HB3	1.96	0.48
1:L:290:LYS:NZ	1:L:290:LYS:HB3	2.28	0.48
1:L:77:PHE:CE1	1:L:373:LEU:HD22	2.48	0.48
1:L:370:LYS:HZ2	1:L:370:LYS:HB2	1.79	0.48
1:I:272:LEU:N	1:I:272:LEU:HD12	2.29	0.47
1:I:141:VAL:HG23	1:I:220:TYR:HB3	1.94	0.47
1:L:131:TYR:CE1	1:L:142:SER:HB2	2.49	0.47
1:L:144:ASN:OD1	1:L:217:ASN:ND2	2.47	0.47
1:L:239:PHE:O	1:L:246:SER:HA	2.13	0.47
1:L:62:PHE:HA	1:L:338:MET:HE1	1.96	0.47
1:L:407:PRO:HB2	1:L:425:ARG:HG2	1.97	0.47
1:L:154:PHE:HA	1:L:355:VAL:HA	1.96	0.47
1:L:247:CYS:SG	1:L:430:CYS:CB	3.03	0.47
1:L:47:ARG:HH12	1:L:114:LYS:HB3	1.78	0.47
1:I:188:LYS:N	1:I:188:LYS:HE3	2.30	0.46
1:L:8:CYS:HG	1:L:128:CYS:CB	2.26	0.46
1:I:119:ILE:O	1:I:123:PHE:HD2	1.98	0.46
1:L:13:ARG:NH1	2:B:3:GU6:O13	2.48	0.46
1:I:293:ALA:O	1:I:297:LYS:HG3	2.16	0.46
1:L:229:PHE:HB2	1:L:377:GLU:HA	1.96	0.46
1:I:273:PRO:HA	1:I:280:THR:HG22	1.97	0.46
1:L:47:ARG:CZ	1:L:114:LYS:HD3	2.46	0.46
1:L:282:VAL:HB	1:L:411:PHE:HB2	1.97	0.46
1:I:292:LEU:O	1:I:296:GLU:HG3	2.16	0.45
1:L:191:SER:HA	1:L:198:ILE:O	2.16	0.45
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.97	0.45
1:I:141:VAL:CG2	1:I:220:TYR:HB3	2.47	0.45
1:I:147:PHE:O	1:I:213:LEU:HD12	2.18	0.44
1:I:324:ARG:HA	1:I:373:LEU:O	2.17	0.44
1:L:275:LYS:HD2	1:L:275:LYS:HA	1.79	0.44
1:L:133:LYS:O	1:L:136:LYS:HE2	2.17	0.44
1:I:95:CYS:SG	1:I:352:PRO:CG	3.05	0.44
1:L:261:ARG:HB2	1:L:311:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:ALA:HB2	1:L:165:VAL:HG13	2.00	0.44
1:L:295:VAL:HG13	1:L:307:TRP:HH2	1.83	0.44
1:I:124:ALA:HB2	1:I:165:VAL:HG13	2.00	0.44
1:I:358:GLY:C	1:I:359:ARG:HD3	2.37	0.44
1:L:66:LEU:O	1:L:70:LYS:HG3	2.17	0.44
1:I:325:ILE:O	1:I:372:PHE:HA	2.17	0.44
1:I:201:VAL:HG11	1:I:216:VAL:HG13	1.99	0.44
1:I:252:MET:O	1:I:319:HIS:HA	2.18	0.43
1:I:357:GLU:HB2	1:I:359:ARG:NH1	2.34	0.43
1:I:74:ASP:O	1:I:425:ARG:NH1	2.50	0.43
1:L:239:PHE:HB3	1:L:430:CYS:SG	2.58	0.43
1:I:341:VAL:HG23	1:I:342:ASP:H	1.83	0.43
1:L:287:LYS:HB3	1:L:290:LYS:HB2	2.00	0.43
1:L:336:GLN:HA	1:L:340:LEU:O	2.18	0.43
1:I:155:ASN:ND2	3:I:501:NAG:H83	2.28	0.43
1:L:407:PRO:HB3	1:L:427:ALA:CA	2.48	0.43
1:L:325:ILE:HD13	1:L:426:VAL:HG22	2.01	0.43
1:I:198:ILE:HG21	1:I:218:THR:HB	2.01	0.42
1:I:11:LYS:HB3	2:A:3:GU6:O14	2.19	0.42
1:I:319:HIS:CB	1:I:403:LYS:HG3	2.49	0.42
1:L:147:PHE:HA	1:L:171:GLN:O	2.20	0.42
1:I:17:MET:HG3	1:I:118:GLN:OE1	2.20	0.42
1:I:203:PRO:HG2	1:I:206:ALA:HB2	2.00	0.42
1:I:139:LYS:HA	1:I:139:LYS:HD2	1.92	0.42
1:I:294:LYS:HZ2	1:I:294:LYS:HB3	1.84	0.42
1:L:124:ALA:O	1:L:128:CYS:SG	2.78	0.42
1:I:14:ASP:HB2	1:I:15:ILE:HD13	2.02	0.42
1:L:285:LEU:HD12	1:L:285:LEU:N	2.35	0.42
1:I:190:VAL:HG21	1:I:201:VAL:HG21	2.02	0.42
1:L:230:SER:HA	1:L:231:PRO:HD3	1.90	0.42
1:L:292:LEU:HD21	1:L:409:LEU:HG	2.01	0.41
1:I:39:LYS:O	1:I:40:ILE:HB	2.20	0.41
1:L:239:PHE:HZ	1:L:405:ASN:O	2.02	0.41
1:I:308:LEU:HD13	1:I:413:ARG:HH11	1.85	0.41
1:I:351:LEU:HD13	1:I:354:ILE:HD12	2.01	0.41
1:I:327:ASP:O	1:I:370:LYS:HA	2.20	0.41
1:I:45:ASN:HA	2:A:4:GU1:H82	2.02	0.41
1:L:20:MET:HG2	1:L:352:PRO:HG2	2.01	0.41
1:L:366:ASP:O	1:L:389:VAL:HG22	2.21	0.41
1:I:228:LYS:NZ	1:I:378:GLU:HB2	2.34	0.41
1:L:372:PHE:O	1:L:382:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:LYS:HD3	2:B:3:GU6:H2	2.02	0.41
1:I:276:GLY:C	1:I:278:ASP:H	2.24	0.41
1:L:74:ASP:O	1:L:425:ARG:HD2	2.21	0.41
1:I:314:MET:HG2	1:I:315:MET:H	1.85	0.41
1:L:147:PHE:O	1:L:213:LEU:HD12	2.21	0.41
2:B:3:GU6:O15	2:B:3:GU6:C1	2.67	0.41
1:I:263:VAL:CG2	1:I:267:THR:HB	2.51	0.41
1:I:15:ILE:HA	1:I:16:PRO:HD2	1.87	0.40
1:I:346:PRO:HG3	1:I:363:TYR:CE2	2.56	0.40
1:L:146:LEU:HB2	1:L:170:LEU:HA	2.04	0.40
1:L:230:SER:HB3	1:L:232:GLU:CD	2.41	0.40
1:L:94:ALA:HA	1:L:351:LEU:HD23	2.03	0.40
1:I:17:MET:HG3	1:I:118:GLN:NE2	2.35	0.40
1:I:226:LYS:HA	1:I:275:LYS:HD2	2.02	0.40
1:I:89:MET:O	1:I:92:LEU:HB3	2.21	0.40
1:L:269:VAL:HG13	1:L:284:ILE:HD13	2.04	0.40
1:L:49:TRP:CZ2	1:L:53:LYS:HD3	2.56	0.40
1:I:115:THR:O	1:I:119:ILE:N	2.54	0.40
1:L:104:GLU:HA	1:L:109:ASP:OD1	2.22	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	I	413/432 (96%)	367 (89%)	36 (9%)	10 (2%)	6	22
1	L	410/432 (95%)	377 (92%)	27 (7%)	6 (2%)	10	34
All	All	823/864 (95%)	744 (90%)	63 (8%)	16 (2%)	8	28

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	4	PRO
1	I	200	ASP
1	I	359	ARG
1	L	404	ALA
1	L	288	PRO
1	I	6	ASP
1	I	383	ALA
1	I	429	PRO
1	L	357	GLU
1	I	143	ALA
1	I	361	ASP
1	L	391	ALA
1	I	332	LYS
1	I	40	ILE
1	L	397	PRO
1	L	263	VAL

### 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	370/383 (97%)	351 (95%)	19 (5%)	24	56
1	L	368/383 (96%)	354 (96%)	14 (4%)	33	67
All	All	738/766 (96%)	705 (96%)	33 (4%)	27	61

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

Mol	Chain	Res	Type
1	I	7	ILE
1	I	15	ILE
1	I	24	ARG
1	I	81	LEU
1	I	180	GLU
1	I	188	LYS
1	I	225	TRP
1	I	227	SER

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Mol	Chain	Res	Type
1	I	228	LYS
1	I	253	TYR
1	I	272	LEU
1	I	275	LYS
1	I	315	MET
1	I	316	LEU
1	I	334	GLN
1	I	359	ARG
1	I	366	ASP
1	I	428	ASN
1	I	429	PRO
1	L	17	MET
1	L	46	ARG
1	L	123	PHE
1	L	136	LYS
1	L	209	GLU
1	L	228	LYS
1	L	288	PRO
1	L	290	LYS
1	L	298	GLU
1	L	340	LEU
1	L	396	ASN
1	L	402	PHE
1	L	418	ASN
1	L	428	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	120	HIS
1	I	127	ASN
1	I	233	ASN
1	I	428	ASN
1	L	96	ASN
1	L	118	GLN
1	L	120	HIS
1	L	396	ASN

### 5.3.3 RNA

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](#)

10 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
2	Z9L	A	1	2	25,25,25	1.08	0	30,39,39	0.96	1 (3%)
2	Z9K	A	2	2	14,17,18	1.27	3 (21%)	15,25,27	1.05	1 (6%)
2	GU6	A	3	2	23,23,24	1.29	4 (17%)	25,36,38	1.16	1 (4%)
2	GU1	A	4	2	11,14,15	0.69	0	13,19,21	0.66	0
2	Z9H	A	5	2	21,21,22	1.03	1 (4%)	25,31,33	1.16	1 (4%)
2	Z9L	B	1	2	25,25,25	1.03	1 (4%)	30,39,39	1.00	1 (3%)
2	Z9K	B	2	2	14,17,18	1.19	1 (7%)	15,25,27	1.16	2 (13%)
2	GU6	B	3	2	23,23,24	1.19	3 (13%)	25,36,38	1.22	2 (8%)
2	GU1	B	4	2	11,14,15	0.63	0	13,19,21	0.69	0
2	Z9H	B	5	2	21,21,22	1.09	1 (4%)	25,31,33	1.05	1 (4%)

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	Z9L	A	1	2	-	8/18/38/38	0/1/1/1
2	Z9K	A	2	2	-	0/7/28/31	0/1/1/1
2	GU6	A	3	2	-	8/16/33/36	0/1/1/1
2	GU1	A	4	2	-	2/4/25/28	0/1/1/1
2	Z9H	A	5	2	-	5/15/32/35	0/1/1/1
2	Z9L	B	1	2	-	6/18/38/38	0/1/1/1
2	Z9K	B	2	2	-	0/7/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GU6	B	3	2	-	8/16/33/36	0/1/1/1
2	GU1	B	4	2	-	2/4/25/28	0/1/1/1
2	Z9H	B	5	2	-	5/15/32/35	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	Z9H	O2-C2	-3.25	1.42	1.47
2	B	2	Z9K	O2-C2	-3.17	1.42	1.47
2	A	5	Z9H	O2-C2	-2.82	1.43	1.47
2	B	3	GU6	O2-C2	-2.77	1.43	1.47
2	A	2	Z9K	C1-C2	2.69	1.56	1.51
2	A	3	GU6	C1-C2	2.51	1.55	1.51
2	A	3	GU6	O2-C2	-2.44	1.43	1.47
2	A	3	GU6	O3-C3	-2.41	1.41	1.46
2	B	3	GU6	C1-C2	2.39	1.55	1.51
2	A	2	Z9K	O2-C2	-2.32	1.43	1.47
2	B	3	GU6	O3-C3	-2.18	1.41	1.46
2	A	3	GU6	O6-S6	2.18	1.62	1.56
2	B	1	Z9L	O3-C3	-2.02	1.42	1.46
2	A	2	Z9K	O2-S1	2.02	1.63	1.57

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	Z9H	O2-C2-C3	3.76	110.81	106.65
2	A	3	GU6	O2-C2-C3	3.49	110.52	106.65
2	B	3	GU6	O2-C2-C3	2.95	109.92	106.65
2	B	5	Z9H	O2-C2-C3	2.75	109.70	106.65
2	A	2	Z9K	O2-C2-C3	2.69	109.63	106.65
2	B	2	Z9K	O2-C2-C3	2.53	109.45	106.65
2	A	1	Z9L	O2-C2-C1	2.20	110.54	107.58
2	B	3	GU6	O6-C6-C5	-2.12	103.67	107.62
2	B	1	Z9L	O2-C2-C1	2.11	110.41	107.58
2	B	2	Z9K	O5-C1-C2	2.09	113.65	109.41

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	Z9L	C6-O6-S1-O7

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Mol	Chain	Res	Type	Atoms
2	A	1	Z9L	C6-O6-S1-O11
2	A	1	Z9L	C6-O6-S1-O15
2	A	5	Z9H	C4-C5-C6-O6
2	A	5	Z9H	O5-C5-C6-O6
2	A	5	Z9H	C6-O6-S1-O7
2	A	5	Z9H	C6-O6-S1-O8
2	A	5	Z9H	C6-O6-S1-O12
2	B	1	Z9L	C6-O6-S1-O7
2	B	1	Z9L	C6-O6-S1-O11
2	B	1	Z9L	C6-O6-S1-O15
2	B	5	Z9H	C4-C5-C6-O6
2	B	5	Z9H	O5-C5-C6-O6
2	B	5	Z9H	C6-O6-S1-O7
2	B	5	Z9H	C6-O6-S1-O8
2	B	5	Z9H	C6-O6-S1-O12
2	A	3	GU6	C1-C2-O2-S2
2	A	3	GU6	C6-O6-S6-O19
2	A	3	GU6	C6-O6-S6-O20
2	A	3	GU6	C6-O6-S6-O21
2	B	3	GU6	C1-C2-O2-S2
2	B	3	GU6	C3-C2-O2-S2
2	B	3	GU6	C6-O6-S6-O19
2	B	3	GU6	C6-O6-S6-O20
2	B	3	GU6	C6-O6-S6-O21
2	A	1	Z9L	O5-C1-O1-C7
2	A	1	Z9L	C2-C1-O1-C7
2	B	4	GU1	C2-C3-O3-C8
2	A	4	GU1	C2-C3-O3-C8
2	A	1	Z9L	C2-O2-S3-O13
2	A	1	Z9L	C2-O2-S3-O14
2	B	1	Z9L	C2-O2-S3-O13
2	B	1	Z9L	C2-O2-S3-O14
2	A	3	GU6	C2-O2-S2-O14
2	A	3	GU6	C2-O2-S2-O15
2	B	3	GU6	C2-O2-S2-O14
2	B	3	GU6	C2-O2-S2-O15
2	A	4	GU1	C4-C3-O3-C8
2	A	3	GU6	C3-C2-O2-S2
2	A	1	Z9L	C2-O2-S3-O12
2	B	1	Z9L	C2-O2-S3-O12
2	A	3	GU6	C2-O2-S2-O13
2	B	3	GU6	C2-O2-S2-O13

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Mol	Chain	Res	Type	Atoms
2	B	4	GU1	C4-C3-O3-C8

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	GU1	1	0
2	B	2	Z9K	1	0
2	A	3	GU6	2	0
2	B	3	GU6	4	0
2	A	4	GU1	2	0

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	501	1	14,14,15	0.85	0	17,19,21	1.68	4 (23%)
3	NAG	L	502	1	14,14,15	0.84	0	17,19,21	1.68	4 (23%)
3	NAG	L	501	1	14,14,15	0.84	0	17,19,21	1.68	4 (23%)

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	I	501	1	-	2/6/23/26	0/1/1/1
3	NAG	L	502	1	-	2/6/23/26	0/1/1/1
3	NAG	L	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	NAG	O5-C1-C2	-3.37	105.96	111.29
3	I	501	NAG	O5-C1-C2	-3.36	105.99	111.29
3	L	502	NAG	O5-C1-C2	-3.34	106.02	111.29
3	L	502	NAG	C1-O5-C5	3.02	116.28	112.19
3	L	501	NAG	O4-C4-C3	-3.02	103.37	110.35
3	I	501	NAG	C1-O5-C5	3.02	116.28	112.19
3	L	502	NAG	O4-C4-C3	-3.02	103.37	110.35
3	I	501	NAG	O4-C4-C3	-3.01	103.38	110.35
3	L	501	NAG	C1-O5-C5	3.01	116.27	112.19
3	L	501	NAG	O7-C7-C8	-2.21	117.95	122.06
3	L	502	NAG	O7-C7-C8	-2.21	117.95	122.06
3	I	501	NAG	O7-C7-C8	-2.18	118.01	122.06

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	501	NAG	C8-C7-N2-C2
3	I	501	NAG	O7-C7-N2-C2
3	L	502	NAG	C8-C7-N2-C2
3	L	502	NAG	O7-C7-N2-C2
3	L	501	NAG	C8-C7-N2-C2
3	L	501	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	501	NAG	5	0
3	L	501	NAG	3	0

## 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	417/432 (96%)	-0.23	16 (3%) 40 36	2, 35, 78, 114	0
1	L	414/432 (95%)	-0.32	7 (1%) 70 69	2, 27, 70, 97	0
All	All	831/864 (96%)	-0.27	23 (2%) 53 49	2, 32, 74, 114	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	3	SER	7.3
1	I	2	GLY	5.8
1	I	5	VAL	4.4
1	I	4	PRO	4.3
1	L	18	ASN	3.9
1	I	385	SER	3.7
1	I	382	ALA	3.7
1	I	15	ILE	3.5
1	L	399	ARG	3.5
1	I	383	ALA	2.9
1	I	6	ASP	2.8
1	L	135	ASN	2.8
1	I	205	GLU	2.7
1	L	23	TYR	2.6
1	I	14	ASP	2.6
1	L	400	VAL	2.4
1	L	398	ASN	2.4
1	L	431	VAL	2.2
1	I	79	SER	2.2
1	I	360	ASP	2.2
1	I	16	PRO	2.1
1	I	358	GLY	2.1
1	I	380	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	Z9K	A	2	17/18	0.87	0.15	35,55,71,71	0
2	GU1	A	4	14/15	0.92	0.13	37,40,53,53	0
2	Z9H	B	5	21/22	0.95	0.14	36,38,45,67	0
2	Z9L	A	1	25/25	0.95	0.12	41,51,52,55	0
2	GU6	A	3	23/24	0.95	0.10	30,50,65,65	0
2	Z9H	A	5	21/22	0.95	0.13	27,41,56,62	0
2	GU1	B	4	14/15	0.96	0.11	28,28,74,74	0
2	Z9K	B	2	17/18	0.96	0.14	26,30,33,33	0
2	GU6	B	3	23/24	0.97	0.11	26,27,56,56	0
2	Z9L	B	1	25/25	0.97	0.14	21,30,44,44	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	L	501	14/15	0.55	0.38	30,60,78,82	0
3	NAG	L	502	14/15	0.65	0.43	30,60,78,82	0
3	NAG	I	501	14/15	0.86	0.31	35,55,55,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.