



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:14 pm GMT

PDB ID : 1NQ9  
Title : Crystal Structure of Antithrombin in the Pentasaccharide-Bound Intermediate State  
Authors : Huntington, J.A.; Johnson, D.J.D.  
Deposited on : 2003-01-21  
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

<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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

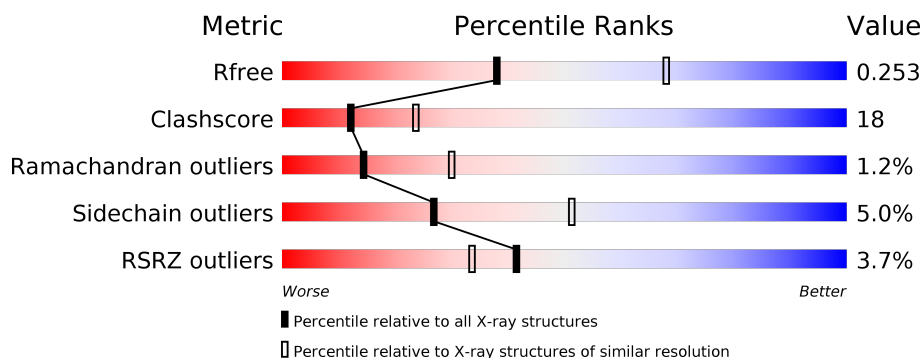
# 1 Overall quality at a glance

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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (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	I	432	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>31%</div> <div>• 6%</div> </div> </div>
1	L	432	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• • •</div> </div> </div>

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	NAG	I	801	-	-	-	X
2	NAG	L	842	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6779 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-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	406	Total	C	N	O	S	0	1	0
			3162	2021	529	595	17			
1	L	413	Total	C	N	O	S	0	0	0
			3216	2055	530	613	18			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



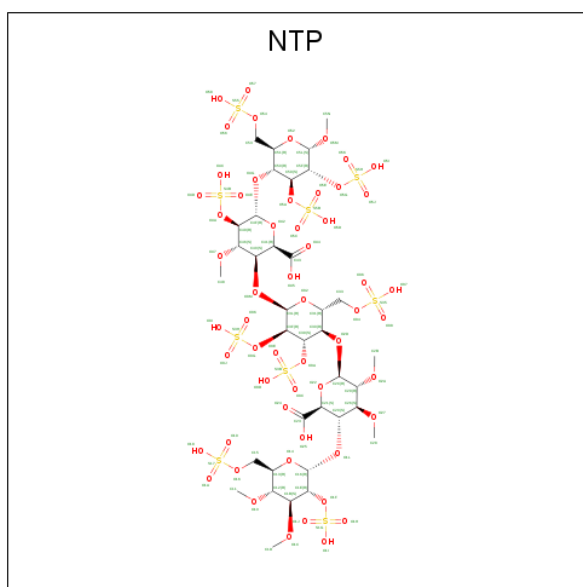
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is HEPARIN PENTASACCHARIDE (three-letter code: NTP) (formula:  $C_{36}H_{60}O_{55}S_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	O	S	0	0
			100	36	55	9		
3	L	1	Total	C	O	S	0	0
			100	36	55	9		

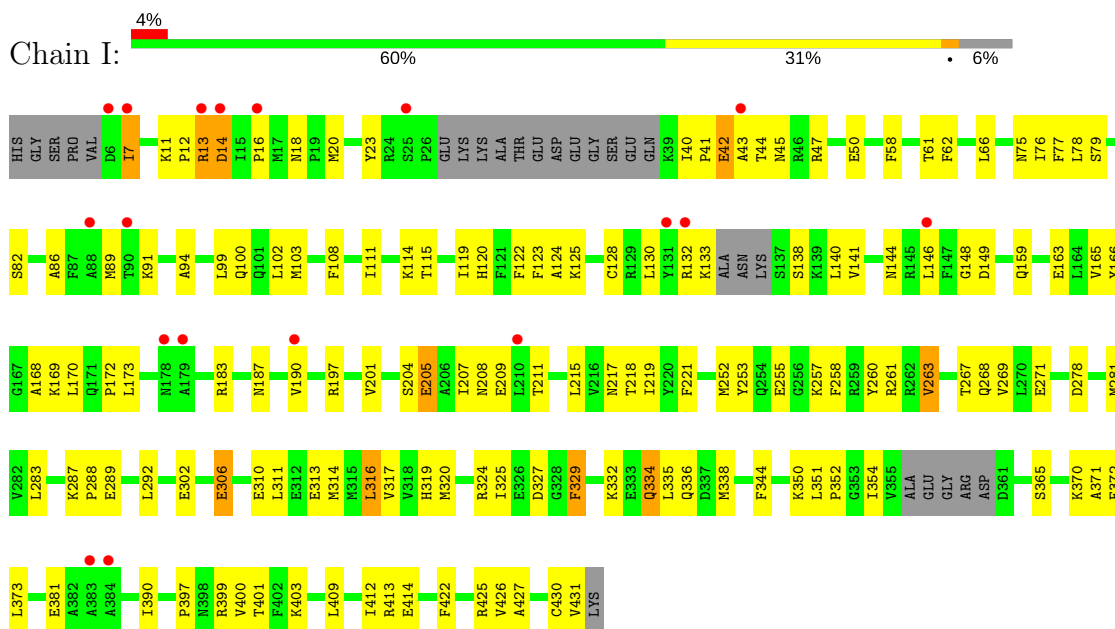
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	36	Total	O	0	0
			36	36		
4	L	53	Total	O	0	0
			53	53		

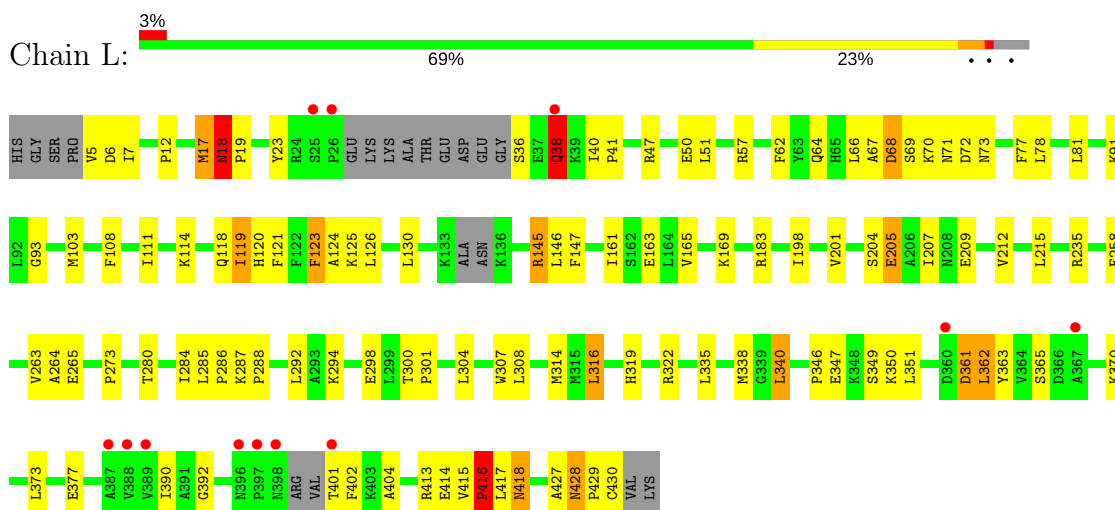
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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-III



#### • Molecule 1: Antithrombin-III



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.68Å 86.76Å 96.92Å 90.00° 109.54° 90.00°	Depositor
Resolution (Å)	24.43 – 2.60 24.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.43-2.60) 99.6 (24.43-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.209 , 0.250 0.212 , 0.253	Depositor DCC
$R_{free}$ test set	1666 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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: NTP, NAG

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	0.38	0/3226	0.60	0/4374
1	L	0.40	0/3279	0.65	0/4440
All	All	0.39	0/6505	0.63	0/8814

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

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	3162	0	3061	128	0
1	L	3216	0	3136	108	0
2	I	42	0	38	5	0
2	L	70	0	63	5	0
3	I	100	0	49	5	0
3	L	100	0	49	0	0
4	I	36	0	0	0	0
4	L	53	0	0	2	0
All	All	6779	0	6396	240	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 18.



All (240) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:263:VAL:HG12	1:L:264:ALA:H	1.07	1.12
1:L:428:ASN:HD21	1:L:430:CYS:HB2	1.27	0.97
1:L:263:VAL:HG12	1:L:264:ALA:N	1.82	0.93
1:L:263:VAL:CG1	1:L:264:ALA:H	1.83	0.91
1:L:428:ASN:ND2	1:L:430:CYS:H	1.70	0.90
1:I:351:LEU:HB3	1:I:354:ILE:HD13	1.59	0.84
1:L:5:VAL:HG23	1:L:6:ASP:H	1.44	0.81
1:L:91:LYS:HE2	1:L:103:MET:HE3	1.64	0.79
1:I:66:LEU:HA	1:I:334:GLN:OE1	1.83	0.78
1:I:18:ASN:H	2:I:842:NAG:C8	1.95	0.78
1:L:258:PHE:HB2	1:L:316:LEU:HD21	1.67	0.76
2:L:841:NAG:H62	2:L:842:NAG:O5	1.85	0.76
1:I:14:ASP:O	1:I:16:PRO:HD3	1.87	0.75
1:I:23:TYR:CE2	1:I:100:GLN:HG3	2.22	0.75
1:L:428:ASN:HD22	1:L:430:CYS:H	1.32	0.74
2:L:861:NAG:H61	2:L:862:NAG:N2	2.02	0.74
2:L:861:NAG:H61	2:L:862:NAG:HN2	1.51	0.74
2:I:841:NAG:H62	2:I:842:NAG:HN2	1.53	0.73
1:L:183:ARG:HB2	1:L:207:ILE:HD12	1.70	0.72
1:L:235:ARG:HH11	1:L:235:ARG:HG3	1.55	0.71
1:I:18:ASN:H	2:I:842:NAG:H82	1.55	0.71
1:I:124:ALA:HB2	1:I:165:VAL:HG13	1.74	0.70
1:I:335:LEU:HD23	1:I:338:MET:HE3	1.74	0.70
1:I:425:ARG:HD3	1:I:427:ALA:HB2	1.75	0.69
1:I:133:LYS:HB3	1:I:278:ASP:OD2	1.93	0.69
1:I:207:ILE:HG23	1:I:211:THR:HG21	1.75	0.68
1:I:13:ARG:NH2	3:I:901:NTP:H482	2.09	0.68
1:I:62:PHE:HD2	1:I:338:MET:HE1	1.59	0.67
1:L:286:PRO:HD3	1:L:292:LEU:HD13	1.77	0.67
1:L:103:MET:HE1	1:L:108:PHE:CD2	2.30	0.67
1:I:258:PHE:HB2	1:I:316:LEU:HD21	1.77	0.66
1:L:62:PHE:HD1	1:L:338:MET:CE	2.10	0.65
1:I:325:ILE:HD11	1:I:426:VAL:HG22	1.78	0.65
1:L:62:PHE:HD1	1:L:338:MET:HE1	1.61	0.64
1:L:428:ASN:HD22	1:L:428:ASN:C	1.99	0.64
1:L:204:SER:O	1:L:205:GLU:HB2	1.96	0.63
1:L:362:LEU:HB3	1:L:390:ILE:CG2	2.29	0.63
1:I:62:PHE:HD2	1:I:338:MET:CE	2.11	0.63
1:I:11:LYS:O	1:I:14:ASP:HB2	1.99	0.63
1:L:17:MET:HB2	1:L:161:ILE:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:108:PHE:O	1:I:111:ILE:HG12	1.99	0.62
1:L:130:LEU:CD2	1:L:414:GLU:HG3	2.29	0.62
1:I:204:SER:O	1:I:205:GLU:HG3	2.00	0.62
1:I:190:VAL:HG11	1:I:201:VAL:HG21	1.80	0.62
1:I:75:ASN:HB3	1:I:325:ILE:HG23	1.82	0.61
1:I:77:PHE:CZ	1:I:373:LEU:HB2	2.35	0.61
1:L:235:ARG:NH1	1:L:235:ARG:HG3	2.14	0.61
1:L:414:GLU:OE1	1:L:417:LEU:HD23	2.00	0.61
1:I:288:PRO:HB2	1:I:289:GLU:OE2	2.01	0.61
1:L:57:ARG:HG2	1:L:301:PRO:HG2	1.83	0.61
1:L:404:ALA:HB2	1:L:428:ASN:HB2	1.83	0.60
1:L:12:PRO:HB3	1:L:118:GLN:OE1	2.01	0.60
1:L:322:ARG:HD2	1:L:377:GLU:OE1	2.01	0.60
1:L:103:MET:HE1	1:L:108:PHE:CB	2.32	0.59
1:I:163:GLU:OE1	1:I:168:ALA:HA	2.03	0.58
1:I:91:LYS:HD2	1:I:119:ILE:HG21	1.86	0.58
1:I:332:LYS:O	1:I:336:GLN:HG3	2.04	0.58
1:L:428:ASN:HD21	1:L:430:CYS:CB	2.08	0.58
1:L:415:VAL:O	1:L:416:PRO:C	2.43	0.57
1:L:126:LEU:CD1	1:L:417:LEU:HD11	2.34	0.57
1:I:23:TYR:HE2	1:I:100:GLN:HG3	1.66	0.57
1:I:283:LEU:HD11	1:I:320:MET:HE3	1.87	0.57
1:L:316:LEU:N	1:L:316:LEU:HD23	2.20	0.57
1:I:413:ARG:HH11	1:I:413:ARG:HG2	1.71	0.56
1:I:42:GLU:HG2	1:I:43:ALA:N	2.20	0.56
1:I:335:LEU:HD23	1:I:338:MET:CE	2.35	0.56
1:I:269:VAL:HG12	1:I:311:LEU:HD21	1.88	0.56
1:I:99:LEU:O	1:I:103:MET:HG2	2.06	0.56
1:I:400:VAL:HG12	1:I:401:THR:N	2.21	0.56
1:I:7:ILE:N	1:I:7:ILE:HD12	2.22	0.55
1:L:77:PHE:CZ	1:L:373:LEU:HB2	2.40	0.55
1:I:120:HIS:H	1:I:120:HIS:CD2	2.22	0.55
1:I:13:ARG:HH11	1:I:13:ARG:CG	2.20	0.55
1:L:62:PHE:CD1	1:L:338:MET:CE	2.90	0.55
1:I:281:MET:HE3	1:I:320:MET:HE3	1.89	0.55
1:I:289:GLU:CD	1:I:289:GLU:H	2.09	0.54
1:I:144:ASN:HB3	1:I:166:TYR:OH	2.08	0.54
1:I:190:VAL:HG21	1:I:201:VAL:HG21	1.89	0.54
1:I:219:ILE:O	1:I:371:ALA:HA	2.06	0.54
1:I:281:MET:HE3	1:I:283:LEU:HD21	1.89	0.54
1:L:18:ASN:HD22	2:L:842:NAG:H62	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:308:LEU:HD13	1:L:413:ARG:CZ	2.37	0.54
1:L:130:LEU:HD23	1:L:414:GLU:HG3	1.90	0.54
1:L:415:VAL:HB	1:L:416:PRO:HD3	1.89	0.54
1:L:417:LEU:HD23	1:L:417:LEU:H	1.73	0.53
1:I:13:ARG:NH1	1:I:13:ARG:HG3	2.22	0.53
1:I:316:LEU:HD23	1:I:316:LEU:H	1.72	0.53
1:L:91:LYS:NZ	1:L:120:HIS:NE2	2.37	0.53
1:L:347:GLU:OE2	1:L:347:GLU:N	2.41	0.53
1:L:77:PHE:CE1	1:L:373:LEU:HD22	2.42	0.53
1:L:285:LEU:HD12	1:L:285:LEU:N	2.24	0.53
1:I:91:LYS:O	1:I:91:LYS:HD3	2.09	0.52
1:L:145:ARG:HG2	1:L:147:PHE:CZ	2.43	0.52
1:L:263:VAL:HG11	1:L:307:TRP:HE1	1.74	0.52
1:I:283:LEU:HD11	1:I:320:MET:CE	2.40	0.52
1:L:298:GLU:O	1:L:300:THR:HG23	2.10	0.52
1:L:5:VAL:HG23	1:L:6:ASP:N	2.19	0.52
1:I:91:LYS:C	1:I:91:LYS:HD3	2.29	0.52
1:L:91:LYS:CE	1:L:103:MET:HE3	2.38	0.52
1:I:47:ARG:O	1:I:50:GLU:HG2	2.10	0.51
1:I:79:SER:HB3	1:I:82:SER:HB3	1.92	0.51
1:L:64:GLN:O	1:L:68:ASP:HB2	2.10	0.51
1:I:45:ASN:HA	3:I:901:NTP:H282	1.91	0.51
1:L:119:ILE:HD12	1:L:119:ILE:N	2.25	0.51
1:I:260:TYR:CG	1:I:261:ARG:N	2.79	0.51
1:L:91:LYS:HZ1	1:L:120:HIS:CE1	2.24	0.51
1:I:138:SER:HB3	1:I:221:PHE:CZ	2.45	0.50
1:I:257:LYS:HA	1:I:314:MET:O	2.12	0.50
1:I:350:LYS:C	1:I:352:PRO:HD3	2.31	0.50
1:L:365:SER:HB3	1:L:392:GLY:H	1.75	0.50
1:I:183:ARG:NH1	1:I:187:ASN:ND2	2.60	0.50
1:L:163:GLU:OE2	1:L:169:LYS:HE2	2.11	0.50
1:L:413:ARG:HH21	1:L:418:ASN:ND2	2.09	0.50
1:I:148:GLY:O	1:I:172:PRO:HA	2.11	0.50
1:L:287:LYS:HG3	1:L:288:PRO:HD2	1.94	0.50
1:L:322:ARG:HD2	1:L:377:GLU:OE2	2.12	0.50
1:L:12:PRO:HG3	1:L:121:PHE:CD2	2.47	0.50
1:L:51:LEU:CD2	1:L:123:PHE:HA	2.42	0.50
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.94	0.49
1:I:40:ILE:HD11	1:I:44:THR:O	2.13	0.49
1:L:322:ARG:HD2	1:L:377:GLU:CD	2.31	0.49
1:I:197:ARG:HB3	1:I:372:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:335:LEU:HD23	1:L:338:MET:HE1	1.93	0.49
1:I:413:ARG:HH11	1:I:413:ARG:CG	2.25	0.49
1:I:263:VAL:HG22	1:I:267:THR:O	2.13	0.49
1:L:428:ASN:HD22	1:L:429:PRO:N	2.11	0.49
1:I:62:PHE:CD2	1:I:338:MET:CE	2.95	0.49
1:I:260:TYR:OH	1:I:268:GLN:HG2	2.14	0.48
1:I:130:LEU:C	1:I:132:ARG:H	2.16	0.48
1:I:12:PRO:HG2	3:I:901:NTP:O3C	2.14	0.48
1:I:253:TYR:CE1	1:I:317:VAL:HG13	2.49	0.48
1:L:145:ARG:HG3	1:L:146:LEU:N	2.29	0.48
1:I:281:MET:HE3	1:I:320:MET:CE	2.43	0.48
1:L:401:THR:HG22	1:L:402:PHE:N	2.29	0.48
1:I:390:ILE:HG12	1:L:319:HIS:HB2	1.95	0.48
1:I:329:PHE:CD2	1:I:329:PHE:N	2.82	0.47
1:I:45:ASN:OD1	1:I:47:ARG:HB2	2.14	0.47
1:I:271:GLU:OE2	1:I:413:ARG:NH1	2.38	0.47
1:L:103:MET:HE1	1:L:108:PHE:HD2	1.77	0.47
1:L:40:ILE:HB	1:L:41:PRO:HD2	1.95	0.47
1:I:351:LEU:N	1:I:352:PRO:HD3	2.29	0.47
1:I:390:ILE:HA	1:L:319:HIS:HB2	1.96	0.47
1:I:306:GLU:O	1:I:310:GLU:HG3	2.14	0.47
1:L:428:ASN:C	1:L:428:ASN:ND2	2.68	0.47
1:I:324:ARG:HA	1:I:373:LEU:O	2.15	0.47
1:L:212:VAL:HG21	1:L:362:LEU:HD22	1.95	0.47
1:I:255:GLU:HG2	1:I:317:VAL:HG22	1.95	0.47
1:I:316:LEU:HD23	1:I:316:LEU:N	2.30	0.47
1:L:67:ALA:C	1:L:69:SER:H	2.18	0.47
1:L:91:LYS:HE3	1:L:120:HIS:CE1	2.50	0.47
1:I:204:SER:O	1:I:205:GLU:CG	2.63	0.46
1:I:119:ILE:HG23	1:I:120:HIS:N	2.31	0.46
1:I:18:ASN:H	2:I:842:NAG:H83	1.80	0.46
1:L:103:MET:CE	1:L:108:PHE:HD2	2.28	0.46
1:I:218:THR:HA	1:I:370:LYS:O	2.15	0.46
1:L:12:PRO:HG3	1:L:121:PHE:CE2	2.50	0.46
1:L:47:ARG:HG2	1:L:47:ARG:HH11	1.80	0.46
1:L:428:ASN:ND2	1:L:430:CYS:N	2.52	0.46
1:L:62:PHE:CD1	1:L:338:MET:HE2	2.51	0.46
1:I:253:TYR:HE1	1:I:317:VAL:CG1	2.29	0.46
1:L:284:ILE:HD13	1:L:307:TRP:CZ3	2.51	0.46
1:I:13:ARG:NH1	1:I:13:ARG:CG	2.77	0.46
1:I:208:ASN:OD1	1:I:209:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.99	0.45
1:L:125:LYS:HD2	4:L:915:HOH:O	2.16	0.45
1:I:159:GLN:OE1	1:I:169:LYS:HB2	2.16	0.45
1:I:332:LYS:HG3	1:I:344:PHE:CD1	2.51	0.45
1:I:58:PHE:HA	1:I:61:THR:HG22	1.99	0.45
1:L:62:PHE:CD1	1:L:338:MET:HE1	2.46	0.45
1:L:346:PRO:HG3	1:L:363:TYR:CE2	2.52	0.45
1:L:38:GLN:H	1:L:38:GLN:HG2	1.55	0.45
1:L:50:GLU:OE2	1:L:111:ILE:HB	2.17	0.45
1:I:306:GLU:OE1	1:I:310:GLU:OE2	2.35	0.45
1:I:183:ARG:HG2	1:I:183:ARG:HH11	1.82	0.44
1:L:414:GLU:OE2	1:L:416:PRO:HD2	2.16	0.44
1:I:62:PHE:CD2	1:I:338:MET:HE2	2.51	0.44
1:I:76:ILE:HA	1:I:327:ASP:OD2	2.17	0.44
1:L:263:VAL:HG11	1:L:307:TRP:NE1	2.31	0.44
1:I:13:ARG:HH11	1:I:13:ARG:HG3	1.81	0.44
1:I:149:ASP:HA	1:I:173:LEU:O	2.17	0.44
1:L:316:LEU:N	1:L:316:LEU:CD2	2.81	0.44
1:I:430:CYS:O	1:I:431:VAL:HB	2.17	0.44
1:I:316:LEU:CD2	1:I:316:LEU:N	2.81	0.44
1:I:351:LEU:HB3	1:I:354:ILE:CD1	2.39	0.43
1:I:400:VAL:CG1	1:I:401:THR:N	2.80	0.43
1:L:198:ILE:HG23	1:L:370:LYS:HG2	1.99	0.43
1:L:340:LEU:HA	1:L:340:LEU:HD23	1.80	0.43
1:L:47:ARG:HG2	1:L:47:ARG:NH1	2.34	0.43
1:L:81:LEU:HD21	1:L:130:LEU:HD13	1.99	0.43
1:L:47:ARG:CZ	1:L:114:LYS:HD3	2.48	0.43
1:L:66:LEU:O	1:L:70:LYS:HG3	2.18	0.43
1:I:269:VAL:CG1	1:I:311:LEU:HD21	2.48	0.43
1:L:124:ALA:HB2	1:L:165:VAL:HG13	2.00	0.43
1:L:71:ASN:O	1:L:73:ASN:N	2.52	0.43
1:I:13:ARG:NH1	3:I:901:NTP:O56	2.52	0.42
1:L:314:MET:O	1:L:316:LEU:HD22	2.18	0.42
1:I:125:LYS:O	1:I:128:CYS:HB2	2.18	0.42
1:I:183:ARG:HG2	1:I:183:ARG:NH1	2.35	0.42
1:I:62:PHE:HE1	1:I:78:LEU:HD13	1.84	0.42
1:I:86:ALA:O	1:I:89:MET:HB2	2.19	0.42
3:I:901:NTP:O44	3:I:901:NTP:H31	2.19	0.42
1:L:7:ILE:HG22	4:L:924:HOH:O	2.18	0.42
1:I:170:LEU:C	1:I:170:LEU:HD23	2.40	0.42
1:I:313:GLU:O	1:I:314:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:ASN:C	1:L:73:ASN:H	2.23	0.42
2:L:842:NAG:H3	2:L:842:NAG:O7	2.20	0.42
1:I:190:VAL:HG11	1:I:201:VAL:CG2	2.47	0.42
1:I:287:LYS:HD2	1:I:289:GLU:OE1	2.19	0.42
1:L:103:MET:HE1	1:L:108:PHE:HB2	2.00	0.42
1:I:258:PHE:CD2	1:I:316:LEU:HD21	2.55	0.42
1:I:47:ARG:NH1	1:I:114:LYS:HB3	2.34	0.42
1:I:94:ALA:HB3	1:I:99:LEU:HD13	2.02	0.42
1:L:273:PRO:HA	1:L:280:THR:HG22	2.02	0.42
1:I:197:ARG:NE	1:I:381:GLU:OE1	2.53	0.42
1:I:140:LEU:HD12	1:I:140:LEU:HA	1.90	0.41
1:I:332:LYS:HE2	1:I:365:SER:O	2.20	0.41
1:L:335:LEU:HA	1:L:338:MET:HE3	2.02	0.41
1:L:404:ALA:HB3	1:L:427:ALA:HB1	2.01	0.41
1:I:146:LEU:HG	1:I:215:LEU:HD13	2.03	0.41
1:I:183:ARG:HH12	1:I:187:ASN:ND2	2.17	0.41
1:L:126:LEU:HD12	1:L:417:LEU:HD11	2.02	0.41
1:I:115:THR:HA	1:I:122:PHE:CE2	2.56	0.41
1:I:20:MET:CE	2:I:841:NAG:H2	2.51	0.41
1:L:93:GLY:O	1:L:351:LEU:HA	2.21	0.41
1:I:42:GLU:HG2	1:I:43:ALA:H	1.84	0.41
1:L:18:ASN:HA	1:L:19:PRO:HD2	1.98	0.41
1:I:207:ILE:HG23	1:I:211:THR:CG2	2.47	0.41
1:L:119:ILE:N	1:L:119:ILE:CD1	2.84	0.41
1:I:397:PRO:HA	1:I:399:ARG:HH21	1.85	0.41
1:L:215:LEU:N	1:L:215:LEU:HD12	2.36	0.41
1:L:349:SER:O	1:L:350:LYS:HD2	2.21	0.41
1:I:412:ILE:HB	1:I:422:PHE:HB2	2.02	0.40
1:L:71:ASN:C	1:L:73:ASN:N	2.74	0.40
1:I:329:PHE:H	1:I:329:PHE:HD2	1.69	0.40
1:I:61:THR:HG23	1:I:62:PHE:N	2.36	0.40
1:I:40:ILE:HA	1:I:41:PRO:HD3	1.78	0.40
1:I:76:ILE:HG22	1:I:77:PHE:N	2.36	0.40
1:I:252:MET:N	1:I:320:MET:O	2.47	0.40
1:L:103:MET:CE	1:L:108:PHE:CD2	3.00	0.40
1:L:17:MET:O	1:L:18:ASN:O	2.40	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	399/432 (92%)	365 (92%)	31 (8%)	3 (1%)	21	42
1	L	405/432 (94%)	368 (91%)	30 (7%)	7 (2%)	10	20
All	All	804/864 (93%)	733 (91%)	61 (8%)	10 (1%)	14	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	361	ASP
1	I	141	VAL
1	L	418	ASN
1	I	14	ASP
1	L	72	ASP
1	L	68	ASP
1	I	263	VAL
1	L	18	ASN
1	L	416	PRO

### 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	I	338/383 (88%)	325 (96%)	13 (4%)	36	63
1	L	348/383 (91%)	327 (94%)	21 (6%)	21	42
All	All	686/766 (90%)	652 (95%)	34 (5%)	27	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	7	ILE
1	I	13	ARG
1	I	42	GLU
1	I	102	LEU
1	I	123	PHE
1	I	205	GLU
1	I	217	ASN
1	I	302	GLU
1	I	306	GLU
1	I	316	LEU
1	I	329	PHE
1	I	334	GLN
1	I	414	GLU
1	L	17	MET
1	L	18	ASN
1	L	23	TYR
1	L	36	SER
1	L	38	GLN
1	L	78	LEU
1	L	119	ILE
1	L	123	PHE
1	L	145	ARG
1	L	201	VAL
1	L	205	GLU
1	L	209	GLU
1	L	265	GLU
1	L	294	LYS
1	L	304	LEU
1	L	316	LEU
1	L	340	LEU
1	L	361	ASP
1	L	362	LEU
1	L	416	PRO
1	L	428	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	120	HIS
1	I	171	GLN
1	I	268	GLN

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Mol	Chain	Res	Type
1	I	319	HIS
1	L	18	ASN
1	L	159	GLN
1	L	233	ASN
1	L	336	GLN
1	L	418	ASN
1	L	428	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	$\# Z  > 2$
2	NAG	I	801	1	14,14,15	0.63	0	17,19,21	0.69	0
2	NAG	I	841	1,2	14,14,15	0.59	0	17,19,21	0.73	0
2	NAG	I	842	2	14,14,15	0.56	0	17,19,21	0.73	1 (5%)
3	NTP	I	901	-	98,104,104	1.34	13 (13%)	126,162,162	1.06	5 (3%)
2	NAG	L	801	1	14,14,15	0.53	0	17,19,21	0.73	0
2	NAG	L	841	1,2	14,14,15	0.66	0	17,19,21	1.20	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	L	842	2	14,14,15	0.60	0	17,19,21	0.52	0
2	NAG	L	861	1,2	14,14,15	0.59	0	17,19,21	0.97	1 (5%)
2	NAG	L	862	2	14,14,15	0.62	0	17,19,21	0.57	0
3	NTP	L	901	-	98,104,104	1.33	12 (12%)	126,162,162	1.07	7 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	801	1	-	0/6/23/26	0/1/1/1
2	NAG	I	841	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	842	2	-	0/6/23/26	0/1/1/1
3	NTP	I	901	-	-	0/76/184/184	0/5/5/5
2	NAG	L	801	1	-	0/6/23/26	0/1/1/1
2	NAG	L	841	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	842	2	-	0/6/23/26	0/1/1/1
2	NAG	L	861	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	862	2	-	0/6/23/26	0/1/1/1
3	NTP	L	901	-	-	0/76/184/184	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	901	NTP	O3A-C39	-2.02	1.42	1.46
3	I	901	NTP	O4A-S4B	2.04	1.62	1.56
3	I	901	NTP	C4F-C49	2.07	1.57	1.52
3	I	901	NTP	O5A-S5B	2.09	1.62	1.56
3	I	901	NTP	C46-C40	2.13	1.56	1.52
3	I	901	NTP	O3A-S3B	2.19	1.62	1.56
3	L	901	NTP	O1F-S1G	2.24	1.63	1.56
3	L	901	NTP	C3L-C3F	2.24	1.58	1.52
3	L	901	NTP	O16-S17	2.25	1.63	1.56
3	L	901	NTP	C1B-C12	2.32	1.57	1.52
3	I	901	NTP	O3G-S3H	2.35	1.63	1.56
3	L	901	NTP	O5G-S5H	2.55	1.63	1.56
3	I	901	NTP	O54-S55	2.56	1.63	1.56
3	I	901	NTP	O5G-S5H	2.56	1.63	1.56
3	L	901	NTP	O32-C3L	2.57	1.48	1.41
3	I	901	NTP	O5M-C5L	2.57	1.44	1.40
3	L	901	NTP	C46-C40	2.58	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	901	NTP	O34-S35	2.65	1.64	1.56
3	L	901	NTP	O5M-C5L	2.69	1.44	1.40
3	L	901	NTP	C40-C41	2.78	1.57	1.52
3	L	901	NTP	C26-C20	2.91	1.58	1.52
3	I	901	NTP	C40-C41	3.07	1.57	1.52
3	I	901	NTP	C26-C20	3.16	1.58	1.52
3	L	901	NTP	C20-C21	3.82	1.59	1.52
3	I	901	NTP	C20-C21	4.04	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	861	NAG	C4-C3-C2	-2.68	107.09	111.02
2	I	842	NAG	C2-N2-C7	-2.04	119.96	122.94
3	I	901	NTP	O42-C41-C40	2.01	111.03	108.42
3	L	901	NTP	O16-C15-C13	2.03	111.53	107.64
3	L	901	NTP	O5G-C5F-C5L	2.05	110.42	107.58
3	I	901	NTP	O42-C4F-C49	2.13	113.73	109.50
3	L	901	NTP	O42-C4F-C49	2.15	113.78	109.50
3	I	901	NTP	O3G-C3F-C3L	2.25	110.69	107.58
3	L	901	NTP	O42-C41-C40	2.29	111.39	108.42
3	L	901	NTP	O3G-C3F-C3L	2.46	110.98	107.58
3	L	901	NTP	O4A-C49-C4F	2.55	111.11	107.58
3	I	901	NTP	O4A-C49-C4F	2.72	111.35	107.58
2	L	841	NAG	C4-C3-C2	3.14	115.63	111.02
3	I	901	NTP	C4F-O42-C41	3.45	117.53	112.04
3	L	901	NTP	C4F-O42-C41	4.10	118.57	112.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	841	NAG	2	0
2	I	842	NAG	4	0
3	I	901	NTP	5	0
2	L	841	NAG	1	0
2	L	842	NAG	3	0
2	L	861	NAG	2	0
2	L	862	NAG	2	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	406/432 (93%)	0.10	18 (4%) 34 26	24, 52, 85, 95	0
1	L	413/432 (95%)	-0.04	12 (2%) 51 44	15, 40, 71, 94	0
All	All	819/864 (94%)	0.03	30 (3%) 41 33	15, 46, 82, 95	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	398	ASN	4.7
1	I	384	ALA	4.2
1	I	14	ASP	4.0
1	L	26	PRO	3.5
1	L	38	GLN	3.4
1	L	397	PRO	3.4
1	I	383	ALA	3.3
1	I	43	ALA	3.1
1	L	389	VAL	2.9
1	L	25	SER	2.8
1	I	90	THR	2.8
1	I	7	ILE	2.8
1	I	16	PRO	2.7
1	L	360	ASP	2.6
1	I	131	TYR	2.6
1	I	210	LEU	2.5
1	L	401	THR	2.5
1	I	179	ALA	2.4
1	L	388	VAL	2.3
1	L	396	ASN	2.2
1	I	178	ASN	2.2
1	L	387	ALA	2.2
1	L	367	ALA	2.1
1	I	13	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	88	ALA	2.1
1	I	25	SER	2.1
1	I	146	LEU	2.0
1	I	6	ASP	2.0
1	I	132	ARG	2.0
1	I	190	VAL	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	I	801	14/15	0.74	0.46	77,79,81,81	0
2	NAG	L	842	14/15	0.78	0.44	84,88,90,91	0
2	NAG	I	841	14/15	0.83	0.26	82,86,91,94	0
2	NAG	I	842	14/15	0.84	0.47	98,101,102,103	0
2	NAG	L	801	14/15	0.87	0.27	66,68,70,71	0
2	NAG	L	862	14/15	0.87	0.40	76,78,80,81	0
2	NAG	L	841	14/15	0.91	0.23	60,66,69,77	0
2	NAG	L	861	14/15	0.92	0.23	58,61,66,71	0
3	NTP	I	901	100/100	0.93	0.16	53,67,79,84	0
3	NTP	L	901	100/100	0.95	0.15	45,55,70,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.