



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 09:47 AM BST

PDB ID : 5C6T  
Title : Crystal structure of HCMV glycoprotein B in complex with 1G2 Fab  
Authors : Chandramouli, S.; Ciferri, C.; Settembre, E.C.; Carfi, A.  
Deposited on : 2015-06-23  
Resolution : 3.60 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

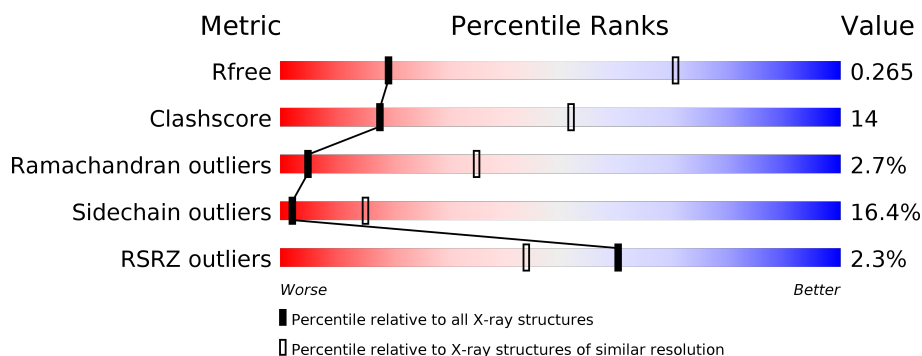
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	A	636	
2	H	233	
3	L	214	
4	B	2	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	2	-	-	-	X
5	NAG	A	1003	-	-	-	X
5	NAG	A	1004	-	-	-	X
5	NAG	A	1005	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6411 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	1	0
			4578	2900	781	873	24			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	expression tag	UNP P13201
A	64	GLU	-	expression tag	UNP P13201
A	65	SER	-	expression tag	UNP P13201
A	66	ARG	-	expression tag	UNP P13201
A	67	ILE	-	expression tag	UNP P13201
A	68	TRP	-	expression tag	UNP P13201
A	69	CYS	-	expression tag	UNP P13201
A	70	LEU	-	expression tag	UNP P13201
A	71	VAL	-	expression tag	UNP P13201
A	72	VAL	-	expression tag	UNP P13201
A	73	CYS	-	expression tag	UNP P13201
A	74	VAL	-	expression tag	UNP P13201
A	75	ASN	-	expression tag	UNP P13201
A	76	LEU	-	expression tag	UNP P13201
A	77	CYS	-	expression tag	UNP P13201
A	78	ILE	-	expression tag	UNP P13201
A	79	VAL	-	expression tag	UNP P13201
A	80	CYS	-	expression tag	UNP P13201
A	81	LEU	-	expression tag	UNP P13201
A	82	GLY	-	expression tag	UNP P13201
A	83	ALA	-	expression tag	UNP P13201
A	84	ALA	-	expression tag	UNP P13201
A	85	VAL	-	expression tag	UNP P13201
A	86	SER	-	expression tag	UNP P13201
A	156	HIS	ILE	engineered mutation	UNP P13201
A	157	ARG	HIS	engineered mutation	UNP P13201
A	240	ASN	TRP	engineered mutation	UNP P13201

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Chain	Residue	Modelled	Actual	Comment	Reference
A	242	THR	TYR	engineered mutation	UNP P13201
A	246	SER	CYS	engineered mutation	UNP P13201
A	457	SER	ARG	engineered mutation	UNP P13201
A	460	SER	ARG	engineered mutation	UNP P13201

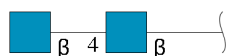
- Molecule 2 is a protein called 1G2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	113	Total	C	N	O	S	0	0	0
			908	586	152	168	2			

- Molecule 3 is a protein called 1G2 Fab light chain.

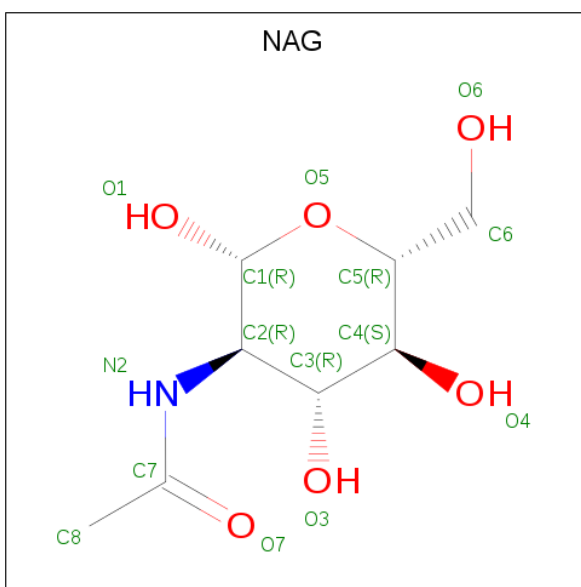
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	104	Total	C	N	O	S	0	0	0
			784	486	135	161	2			

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



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

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



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

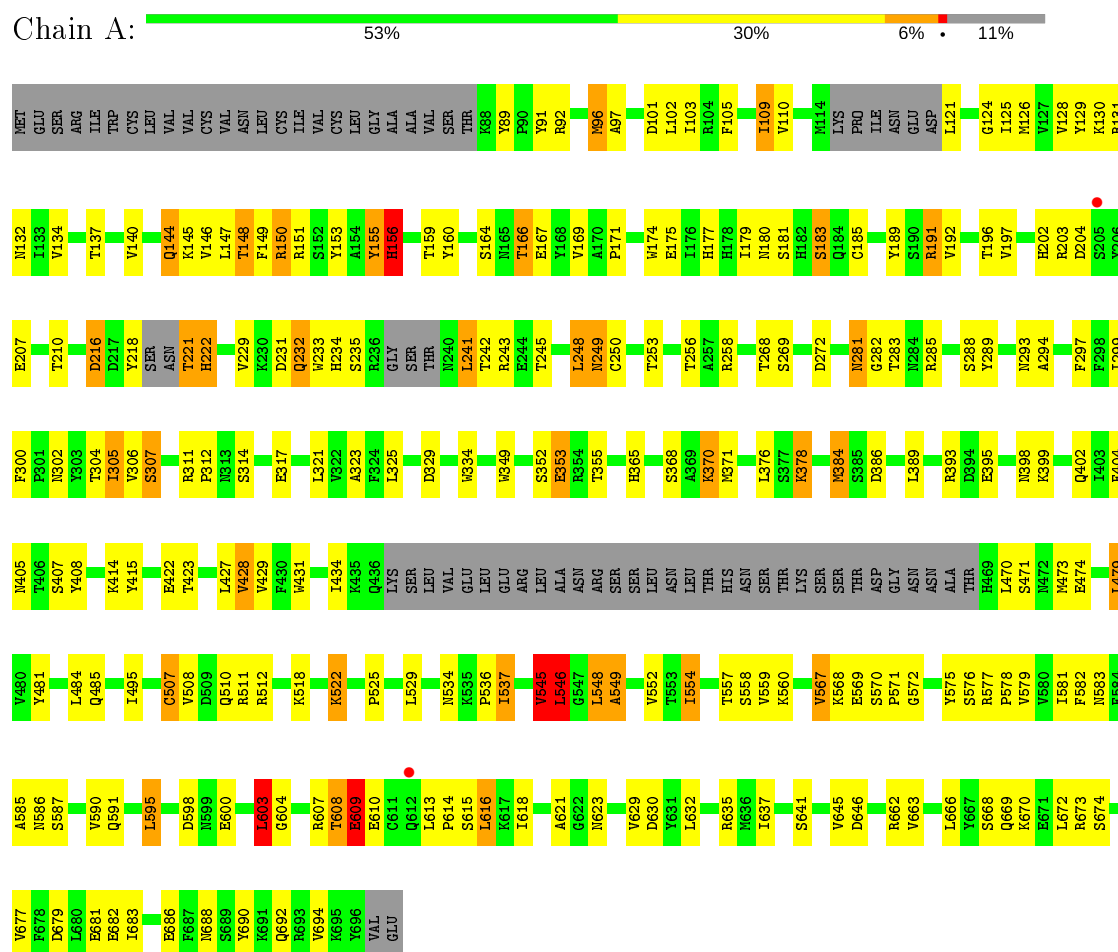
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

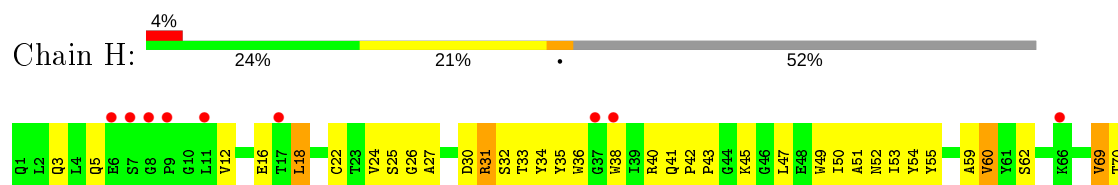
### 3 Residue-property plots

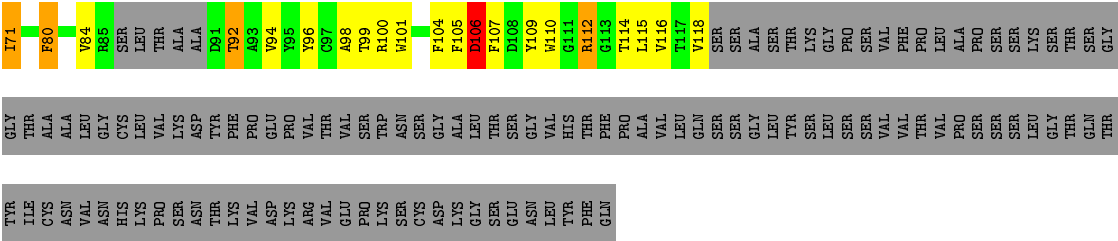
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Envelope glycoprotein B

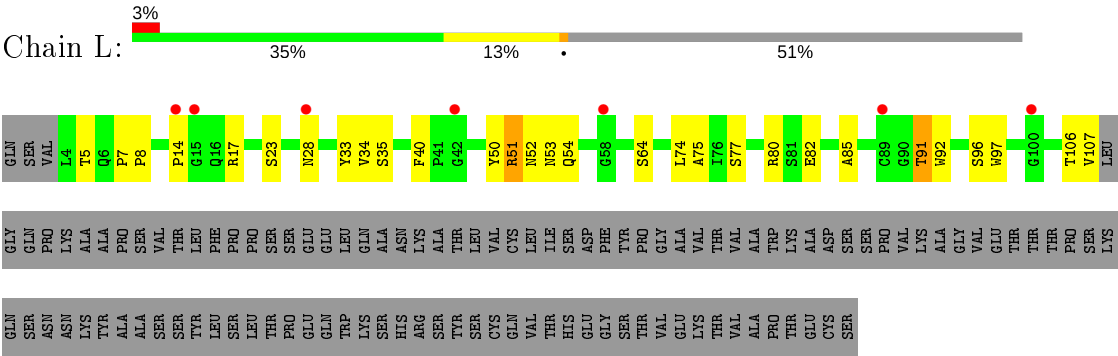


#### • Molecule 2: 1G2 Fab heavy chain

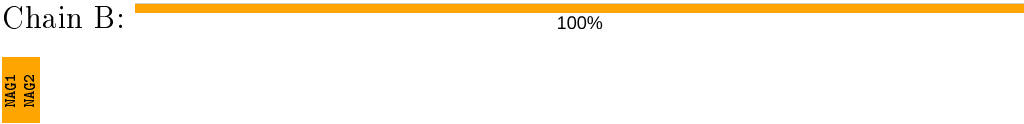




● Molecule 3: 1G2 Fab light chain



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.49 Å   176.49 Å   176.49 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.98 – 3.60 19.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-3.60) 100.0 (19.98-3.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.44 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.212 , 0.260 0.216 , 0.265	Depositor DCC
$R_{free}$ test set	1290 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	117.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: MG, 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	A	0.32	0/4680	0.56	0/6342
2	H	0.25	0/934	0.50	0/1274
3	L	0.24	0/804	0.48	0/1095
All	All	0.30	0/6418	0.54	0/8711

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	608	THR	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4578	0	4384	113	0
2	H	908	0	872	42	0
3	L	784	0	736	20	0
4	B	28	0	25	1	0
5	A	112	0	104	4	0
6	A	1	0	0	0	0
All	All	6411	0	6121	170	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 (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:HG23	1:A:166:THR:HB	1.57	0.86
1:A:150:ARG:HB2	1:A:150:ARG:HH11	1.47	0.78
1:A:167:GLU:OE1	1:A:191:ARG:NH2	2.17	0.77
1:A:352:SER:HA	1:A:370:LYS:HD3	1.68	0.75
1:A:169:VAL:HG11	1:A:189:TYR:CZ	2.23	0.74
1:A:192:VAL:HB	1:A:197:VAL:HG12	1.70	0.73
1:A:180:ASN:HB2	1:A:305:ILE:HD13	1.70	0.73
1:A:307:SER:HB2	1:A:317:GLU:HG3	1.71	0.72
3:L:52:ASN:O	3:L:54:GLN:N	2.22	0.72
3:L:96:SER:OG	3:L:97:TRP:N	2.22	0.72
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.72	0.71
1:A:144:GLN:HA	1:A:171:PRO:HD3	1.72	0.71
1:A:204:ASP:OD2	1:A:243:ARG:NH2	2.24	0.70
1:A:221:THR:OG1	1:A:222:HIS:N	2.26	0.68
2:H:52:ASN:HB3	2:H:60:VAL:HG13	1.78	0.66
2:H:49:TRP:HZ2	2:H:52:ASN:HB2	1.61	0.65
2:H:35:TYR:HB3	2:H:54:TYR:HE1	1.62	0.63
2:H:12:VAL:HG13	2:H:16:GLU:HG2	1.79	0.63
2:H:24:VAL:HG12	2:H:26:GLY:H	1.63	0.62
1:A:603:LEU:HD12	1:A:604:GLY:H	1.63	0.62
2:H:92:THR:HB	2:H:118:VAL:H	1.64	0.61
2:H:94:VAL:HG22	2:H:115:LEU:HD13	1.82	0.61
1:A:131:ARG:HG2	1:A:474:GLU:HA	1.81	0.61
1:A:235:SER:OG	1:A:243:ARG:NH1	2.33	0.60
1:A:525:PRO:HB3	1:A:546:LEU:HD11	1.81	0.60
3:L:5:THR:HB	3:L:23:SER:HB3	1.82	0.60
1:A:153:TYR:HB3	1:A:160:TYR:HB2	1.84	0.59
1:A:376:LEU:HD21	1:A:485:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ALA:HA	1:A:587:SER:N	2.16	0.59
2:H:49:TRP:CZ2	2:H:52:ASN:HB2	2.38	0.59
1:A:183:SER:OG	1:A:183:SER:O	2.20	0.58
2:H:40:ARG:HB3	2:H:50:ILE:HD11	1.84	0.58
1:A:630:ASP:C	1:A:632:LEU:H	2.07	0.58
1:A:130:LYS:HG3	1:A:349:TRP:HB2	1.86	0.58
2:H:51:ALA:HB1	2:H:71:ILE:HD13	1.86	0.58
1:A:241:LEU:HD12	1:A:241:LEU:H	1.70	0.57
2:H:18:LEU:HD11	2:H:116:VAL:HG11	1.87	0.57
2:H:26:GLY:N	2:H:27:ALA:HA	2.20	0.57
2:H:42:PRO:HB2	2:H:45:LYS:HD3	1.87	0.56
1:A:384:MET:O	1:A:393:ARG:NH1	2.27	0.56
2:H:53:ILE:HB	2:H:71:ILE:HD12	1.87	0.56
2:H:3:GLN:HB3	2:H:25:SER:HB3	1.88	0.55
1:A:175:GLU:O	1:A:179:ILE:HG12	2.07	0.55
4:B:1:NAG:H62	4:B:2:NAG:C7	2.36	0.55
1:A:89:TYR:HE1	1:A:536:PRO:HB3	1.72	0.54
1:A:583:ASN:ND2	5:A:1009:NAG:H82	2.23	0.54
2:H:59:ALA:HB1	2:H:71:ILE:HD11	1.90	0.54
1:A:89:TYR:CE1	1:A:536:PRO:HB3	2.42	0.53
1:A:281:ASN:O	1:A:283:THR:N	2.41	0.53
1:A:368:SER:OG	1:A:371:MET:HG2	2.07	0.53
1:A:479:LEU:HD12	1:A:481:TYR:HE1	1.73	0.53
1:A:92:ARG:HH21	1:A:600:GLU:HB2	1.74	0.53
1:A:613:LEU:HD13	1:A:614:PRO:HA	1.90	0.53
1:A:554:ILE:HD12	1:A:582:PHE:HB2	1.89	0.52
2:H:22:CYS:HB3	2:H:80:PHE:CE1	2.44	0.52
1:A:234:HIS:ND1	1:A:245:THR:OG1	2.35	0.52
1:A:145:LYS:HD3	1:A:248:LEU:HD11	1.92	0.51
1:A:126:MET:HG3	1:A:429:VAL:HG13	1.92	0.51
1:A:294:ALA:HB2	2:H:32:SER:HA	1.92	0.51
1:A:249:ASN:HD22	1:A:249:ASN:C	2.13	0.51
1:A:288:SER:OG	1:A:289:TYR:N	2.40	0.51
1:A:595:LEU:HD11	1:A:621:ALA:HB2	1.91	0.51
1:A:635:ARG:CZ	1:A:637:ILE:HD11	2.41	0.51
1:A:92:ARG:NH2	1:A:598:ASP:O	2.36	0.51
1:A:329:ASP:OD1	1:A:329:ASP:N	2.44	0.51
2:H:41:GLN:HB2	2:H:47:LEU:HD23	1.92	0.51
5:A:1010:NAG:H61	3:L:54:GLN:NE2	2.26	0.50
1:A:299:ILE:HG22	1:A:321:LEU:HD22	1.94	0.50
1:A:570:SER:OG	1:A:571:PRO:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:THR:HB	1:A:431:TRP:HZ3	1.77	0.50
1:A:608:THR:HA	1:A:609:GLU:CB	2.42	0.49
3:L:82:GLU:CD	3:L:82:GLU:H	2.15	0.49
2:H:38:TRP:HB2	2:H:50:ILE:HB	1.94	0.49
3:L:33:TYR:HB3	3:L:51:ARG:HA	1.93	0.49
1:A:150:ARG:HB2	1:A:150:ARG:NH1	2.24	0.49
1:A:560:LYS:HB2	1:A:581:ILE:CG1	2.43	0.49
2:H:30:ASP:HB3	2:H:32:SER:H	1.78	0.49
2:H:35:TYR:CE1	2:H:100:ARG:HB2	2.48	0.48
1:A:179:ILE:HD12	1:A:185:CYS:SG	2.53	0.48
2:H:98:ALA:HB2	2:H:110:TRP:CE3	2.49	0.48
1:A:679:ASP:O	1:A:683:ILE:HG13	2.14	0.48
2:H:35:TYR:HB3	2:H:54:TYR:CE1	2.47	0.48
5:A:1010:NAG:H61	3:L:54:GLN:HE22	1.78	0.48
1:A:150:ARG:HD3	1:A:164:SER:HB2	1.95	0.48
1:A:285:ARG:HD3	2:H:101:TRP:O	2.14	0.48
2:H:32:SER:O	2:H:32:SER:OG	2.29	0.48
2:H:105:PHE:HA	3:L:50:TYR:HB2	1.94	0.47
1:A:268:THR:OG1	1:A:272:ASP:HB2	2.14	0.47
1:A:567:VAL:HG12	1:A:575:TYR:CE2	2.50	0.47
1:A:578:PRO:HG2	1:A:595:LEU:HD12	1.97	0.47
1:A:175:GLU:HG2	1:A:179:ILE:HD11	1.96	0.46
3:L:34:VAL:HA	3:L:91:THR:HG22	1.96	0.46
1:A:508:VAL:O	1:A:512:ARG:HG2	2.15	0.46
2:H:69:VAL:HG12	2:H:84:VAL:HG22	1.96	0.46
1:A:669:GLN:HA	1:A:672:LEU:HD12	1.97	0.46
3:L:92:TRP:HD1	3:L:97:TRP:HE3	1.63	0.46
1:A:370:LYS:NZ	1:A:370:LYS:HB2	2.31	0.46
1:A:378:LYS:HE2	1:A:422:GLU:O	2.16	0.46
1:A:96:MET:HG3	1:A:549:ALA:HB2	1.96	0.46
1:A:101:ASP:OD1	1:A:101:ASP:N	2.49	0.45
1:A:241:LEU:N	1:A:241:LEU:HD12	2.29	0.45
1:A:529:LEU:HB3	1:A:537:ILE:HD13	1.98	0.45
3:L:64:SER:O	3:L:74:LEU:HD12	2.16	0.45
3:L:91:THR:OG1	3:L:92:TRP:N	2.48	0.45
1:A:203:ARG:NH1	1:A:233:TRP:HB3	2.31	0.45
1:A:529:LEU:HD13	1:A:537:ILE:HD11	1.98	0.45
1:A:353:GLU:CD	1:A:353:GLU:H	2.20	0.45
1:A:668:SER:O	1:A:672:LEU:HG	2.17	0.45
1:A:507:CYS:HA	1:A:510:GLN:HB2	1.98	0.44
1:A:585:ALA:HA	1:A:586:ASN:C	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:THR:HA	1:A:558:SER:HA	1.32	0.44
1:A:149:PHE:O	1:A:164:SER:HA	2.17	0.44
1:A:249:ASN:HD22	1:A:250:CYS:N	2.14	0.44
1:A:129:TYR:HB2	1:A:428:VAL:HG13	2.00	0.44
1:A:109:ILE:HD11	1:A:511:ARG:HA	1.98	0.44
1:A:283:THR:HG23	2:H:105:PHE:CZ	2.53	0.44
2:H:38:TRP:HB3	2:H:50:ILE:HD12	1.99	0.44
1:A:670:LYS:O	1:A:674:SER:HB2	2.18	0.44
2:H:34:TYR:HB3	2:H:100:ARG:HB3	2.00	0.43
1:A:398:ASN:O	1:A:402:GLN:HB2	2.19	0.43
2:H:34:TYR:HB3	2:H:100:ARG:HD3	2.00	0.43
2:H:31:ARG:HA	2:H:55:TYR:CZ	2.53	0.43
1:A:203:ARG:NH2	1:A:231:ASP:OD1	2.44	0.43
1:A:404:PHE:HE2	1:A:414:LYS:HG3	1.84	0.43
1:A:682:GLU:O	1:A:686:GLU:HB2	2.19	0.43
1:A:140:VAL:HG22	1:A:334:TRP:HB3	2.00	0.43
1:A:177:HIS:HE1	1:A:300:PHE:CE2	2.37	0.43
1:A:203:ARG:HD2	1:A:233:TRP:CE3	2.54	0.43
1:A:124:GLY:HA2	1:A:434:ILE:HG12	2.01	0.43
1:A:616:LEU:HD23	1:A:629:VAL:HA	1.99	0.43
2:H:5:GLN:OE1	2:H:112:ARG:NH1	2.51	0.43
1:A:395:GLU:O	1:A:399:LYS:HG2	2.19	0.42
1:A:378:LYS:H	1:A:378:LYS:HD3	1.85	0.42
1:A:568:LYS:HA	1:A:569:GLU:HA	1.64	0.42
2:H:43:PRO:HG3	2:H:94:VAL:HG23	2.01	0.42
1:A:297:PHE:CE1	1:A:323:ALA:HB1	2.54	0.42
1:A:105:PHE:HB2	1:A:518:LYS:HG3	2.00	0.42
1:A:479:LEU:HD12	1:A:481:TYR:CE1	2.54	0.42
1:A:545:VAL:HG13	1:A:545:VAL:O	2.19	0.42
1:A:92:ARG:HA	1:A:552:VAL:O	2.20	0.42
2:H:105:PHE:HB3	2:H:106:ASP:H	1.50	0.42
3:L:80:ARG:O	3:L:107:VAL:HG11	2.20	0.42
1:A:529:LEU:HA	1:A:529:LEU:HD23	1.88	0.42
3:L:33:TYR:O	3:L:91:THR:HB	2.20	0.42
2:H:49:TRP:CD1	3:L:97:TRP:HB3	2.55	0.42
1:A:148:THR:HG21	1:A:232:GLN:OE1	2.20	0.42
1:A:243:ARG:HE	1:A:243:ARG:HB2	1.61	0.42
1:A:495:ILE:HA	1:A:495:ILE:HD13	1.76	0.42
3:L:64:SER:HB3	3:L:75:ALA:HB3	2.01	0.42
1:A:571:PRO:HA	1:A:572:GLY:HA2	1.74	0.42
2:H:96:TYR:CE1	2:H:112:ARG:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:CE3	2:H:99:THR:HG21	2.55	0.42
1:A:548:LEU:HA	1:A:548:LEU:HD13	1.72	0.41
1:A:155:TYR:HB3	1:A:156:HIS:CE1	2.55	0.41
3:L:40:PHE:CD1	3:L:85:ALA:HB2	2.55	0.41
1:A:637:ILE:HA	1:A:637:ILE:HD13	1.81	0.41
1:A:522:LYS:HD2	1:A:522:LYS:N	2.35	0.41
1:A:577:ARG:HD3	1:A:595:LEU:O	2.20	0.41
1:A:153:TYR:CD1	1:A:242:THR:HG22	2.55	0.41
2:H:104:PHE:HA	3:L:51:ARG:HD3	2.03	0.41
3:L:17:ARG:HA	3:L:77:SER:HA	2.01	0.41
1:A:471:SER:C	1:A:473:MET:H	2.23	0.40
1:A:554:ILE:HB	1:A:583:ASN:O	2.21	0.40
3:L:7:PRO:HA	3:L:8:PRO:HD3	1.75	0.40
1:A:204:ASP:H	1:A:233:TRP:HH2	1.70	0.40
2:H:49:TRP:CE3	2:H:62:SER:HB2	2.56	0.40
1:A:174:TRP:CH2	5:A:1002:NAG:H5	2.57	0.40
1:A:311:ARG:HA	1:A:312:PRO:HD3	1.86	0.40
1:A:91:TYR:O	1:A:554:ILE:HG12	2.21	0.40
1:A:603:LEU:HG	1:A:603:LEU:H	1.71	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	557/636 (88%)	479 (86%)	61 (11%)	17 (3%)	4	32
2	H	109/233 (47%)	93 (85%)	14 (13%)	2 (2%)	8	43
3	L	102/214 (48%)	87 (85%)	13 (13%)	2 (2%)	7	41
All	All	768/1083 (71%)	659 (86%)	88 (12%)	21 (3%)	5	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	302	ASN
1	A	405	ASN
1	A	603	LEU
3	L	53	ASN
1	A	97	ALA
1	A	202	HIS
1	A	282	GLY
1	A	314	SER
1	A	549	ALA
1	A	607	ARG
1	A	616	LEU
2	H	106	ASP
1	A	546	LEU
2	H	109	TYR
1	A	216	ASP
1	A	156	HIS
1	A	609	GLU
3	L	14	PRO
1	A	545	VAL
1	A	554	ILE

### 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	504/576 (88%)	409 (81%)	95 (19%)	1	9
2	H	97/202 (48%)	84 (87%)	13 (13%)	4	23
3	L	87/182 (48%)	82 (94%)	5 (6%)	20	55
All	All	688/960 (72%)	575 (84%)	113 (16%)	2	15

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	MET
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	103	ILE
1	A	109	ILE
1	A	110	VAL
1	A	121	LEU
1	A	125	ILE
1	A	128	VAL
1	A	134	VAL
1	A	137	THR
1	A	144	GLN
1	A	146	VAL
1	A	147	LEU
1	A	148	THR
1	A	150	ARG
1	A	151	ARG
1	A	155	TYR
1	A	156	HIS
1	A	159	THR
1	A	166	THR
1	A	181	SER
1	A	183	SER
1	A	191	ARG
1	A	196	THR
1	A	207	GLU
1	A	210	THR
1	A	216	ASP
1	A	218	TYR
1	A	221	THR
1	A	222	HIS
1	A	229	VAL
1	A	232	GLN
1	A	241	LEU
1	A	248	LEU
1	A	249	ASN
1	A	253	THR
1	A	256	THR
1	A	258	ARG
1	A	269	SER
1	A	281	ASN
1	A	293	ASN
1	A	304	THR
1	A	305	ILE
1	A	306	VAL

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Mol	Chain	Res	Type
1	A	307	SER
1	A	325	LEU
1	A	353	GLU
1	A	365	HIS
1	A	370	LYS
1	A	378	LYS
1	A	384	MET
1	A	386	ASP
1	A	389	LEU
1	A	407	SER
1	A	408	TYR
1	A	415	TYR
1	A	423	THR
1	A	427	LEU
1	A	428	VAL
1	A	470	LEU
1	A	479	LEU
1	A	484	LEU
1	A	507	CYS
1	A	522	LYS
1	A	534	ASN
1	A	537	ILE
1	A	545	VAL
1	A	546	LEU
1	A	548	LEU
1	A	559	VAL
1	A	567	VAL
1	A	576	SER
1	A	579	VAL
1	A	590	VAL
1	A	591	GLN
1	A	595	LEU
1	A	603	LEU
1	A	609	GLU
1	A	610	GLU
1	A	615	SER
1	A	618	ILE
1	A	623	ASN
1	A	641	SER
1	A	645	VAL
1	A	646	ASP
1	A	662	ARG

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Mol	Chain	Res	Type
1	A	663	VAL
1	A	666	LEU
1	A	673	ARG
1	A	677	VAL
1	A	681	GLU
1	A	688	ASN
1	A	690	TYR
1	A	692	GLN
1	A	694	VAL
2	H	18	LEU
2	H	31	ARG
2	H	33	THR
2	H	60	VAL
2	H	69	VAL
2	H	70	THR
2	H	71	ILE
2	H	80	PHE
2	H	92	THR
2	H	106	ASP
2	H	107	PHE
2	H	112	ARG
2	H	114	THR
3	L	28	ASN
3	L	35	SER
3	L	51	ARG
3	L	91	THR
3	L	106	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	ASN
2	H	79	GLN
3	L	16	GLN

### 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 ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1	1,4	14,14,15	0.76	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	B	2	4	14,14,15	1.11	1 (7%)	17,19,21	1.12	1 (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
4	NAG	B	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	NAG	O5-C1	3.82	1.49	1.43
4	B	1	NAG	C1-C2	2.03	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAG	C1-O5-C5	4.22	117.90	112.19
4	B	1	NAG	C1-O5-C5	3.29	116.64	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	NAG	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2	NAG	1	0
4	B	1	NAG	1	0

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	1008	1	14,14,15	0.56	0	17,19,21	0.41	0
5	NAG	A	1004	1	14,14,15	0.32	0	17,19,21	0.35	0
5	NAG	A	1009	1	14,14,15	0.41	0	17,19,21	0.56	0
5	NAG	A	1005	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	A	1001	1	14,14,15	0.30	0	17,19,21	0.33	0
5	NAG	A	1010	1	14,14,15	0.58	0	17,19,21	0.57	0
5	NAG	A	1002	1	14,14,15	0.34	0	17,19,21	0.73	1 (5%)
5	NAG	A	1003	1	14,14,15	0.18	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1004	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1003	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	NAG	C1-O5-C5	2.46	115.53	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1002	NAG	O5-C5-C6-O6
5	A	1004	NAG	O5-C5-C6-O6
5	A	1004	NAG	C4-C5-C6-O6
5	A	1002	NAG	C4-C5-C6-O6
5	A	1003	NAG	O5-C5-C6-O6
5	A	1001	NAG	O5-C5-C6-O6
5	A	1004	NAG	C8-C7-N2-C2
5	A	1004	NAG	O7-C7-N2-C2
5	A	1002	NAG	C8-C7-N2-C2
5	A	1002	NAG	O7-C7-N2-C2
5	A	1003	NAG	C8-C7-N2-C2
5	A	1003	NAG	O7-C7-N2-C2
5	A	1009	NAG	C4-C5-C6-O6
5	A	1001	NAG	C4-C5-C6-O6
5	A	1003	NAG	C4-C5-C6-O6
5	A	1009	NAG	O5-C5-C6-O6
5	A	1010	NAG	O5-C5-C6-O6
5	A	1010	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1009	NAG	1	0
5	A	1010	NAG	2	0
5	A	1002	NAG	1	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	566/636 (88%)	-0.50	2 (0%) 92 86	60, 100, 167, 230	0
2	H	113/233 (48%)	0.39	9 (7%) 12 7	114, 223, 284, 349	0
3	L	104/214 (48%)	0.40	7 (6%) 17 10	151, 228, 266, 310	0
All	All	783/1083 (72%)	-0.25	18 (2%) 60 44	60, 114, 257, 349	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	8	GLY	6.3
2	H	9	PRO	4.8
3	L	89	CYS	4.3
2	H	7	SER	3.6
2	H	11	LEU	3.5
2	H	38	TRP	3.4
2	H	17	THR	2.7
3	L	14	PRO	2.7
1	A	205	SER	2.4
2	H	37	GLY	2.4
3	L	42	GLY	2.3
1	A	612	GLN	2.2
3	L	100	GLY	2.2
2	H	66	LYS	2.1
3	L	15	GLY	2.1
2	H	6	GLU	2.0
3	L	58	GLY	2.0
3	L	28	ASN	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
4	NAG	B	2	14/15	0.79	0.46	158,174,182,189	0
4	NAG	B	1	14/15	0.86	0.20	137,152,161,162	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
5	NAG	A	1003	14/15	0.61	0.53	175,192,205,209	0
5	NAG	A	1005	14/15	0.68	0.52	228,240,254,258	0
5	NAG	A	1004	14/15	0.71	0.50	228,238,246,246	0
5	NAG	A	1001	14/15	0.76	0.37	172,195,199,201	0
5	NAG	A	1008	14/15	0.82	0.45	157,176,183,184	0
5	NAG	A	1009	14/15	0.87	0.44	145,157,161,161	0
5	NAG	A	1010	14/15	0.91	0.20	134,146,164,165	0
6	MG	A	1011	1/1	0.91	0.23	99,99,99,99	1
5	NAG	A	1002	14/15	0.92	0.25	97,109,118,123	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.