



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:30 am GMT

PDB ID : 1I8Q  
Title : CRYSTAL STRUCTURE OF STREPTOCOCCUS AGALACTIAE  
HYALURONATE LYASE COMPLEXED WITH ENZYME PRODUCT,  
UNSATURATED DISACCHARIDE HYALURONAN  
Authors : Li, S.; Jedrzejas, M.J.  
Deposited on : 2001-03-15  
Resolution : 2.20 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

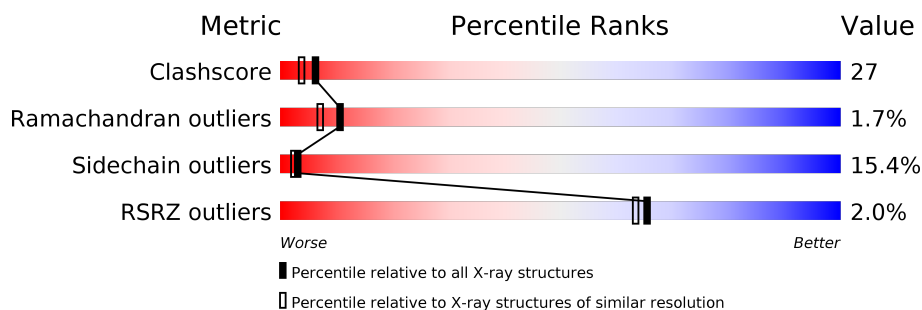
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	814	

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	GC4	A	1001	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6794 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 HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	S	0	0	0
			6513	4101	1108	1286	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	ALA	GLY	SEE REMARK 999	UNP Q53591
A	248	THR	PRO	SEE REMARK 999	UNP Q53591
A	280	ASN	THR	SEE REMARK 999	UNP Q53591
A	288	ALA	GLY	SEE REMARK 999	UNP Q53591
A	583	THR	ALA	SEE REMARK 999	UNP Q53591
A	688	PHE	LEU	SEE REMARK 999	UNP Q53591
A	689	TRP	GLY	SEE REMARK 999	UNP Q53591
A	882	GLN	LEU	SEE REMARK 999	UNP Q53591
A	894	MET	LEU	SEE REMARK 999	UNP Q53591

- Molecule 2 is a polymer of unknown type called SUGAR (DISACCHARIDE HYALURONAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			26	14	1	11		
2	A	2	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	229	Total	O	0	0
			229	229		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.03Å 155.02Å 237.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 47.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.20) 97.6 (47.49-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.182 , 0.252 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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, GC4

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	0.40	0/6640	0.62	0/8988

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	A	6513	0	6405	350	1
2	A	52	0	42	3	0
3	A	229	0	0	15	0
All	All	6794	0	6447	350	1

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 27.

All (350) 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:808:ASN:HD21	1:A:826:LYS:H	1.07	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LYS:HB3	1:A:728:GLN:HB2	1.43	1.00
1:A:504:GLN:HE22	1:A:510:ILE:H	1.07	0.95
1:A:468:GLU:HG2	1:A:478:ASP:HA	1.50	0.94
1:A:742:ASN:HD22	1:A:744:HIS:H	1.16	0.94
1:A:513:GLN:HE21	1:A:513:GLN:H	1.14	0.94
1:A:944:LEU:HD21	1:A:950:LYS:HG3	1.51	0.92
1:A:716:SER:O	1:A:717:LYS:HB3	1.71	0.91
1:A:228:LYS:HG3	1:A:239:GLU:HG3	1.51	0.91
1:A:939:ASP:O	1:A:954:ALA:HB2	1.69	0.91
1:A:859:THR:HG22	1:A:862:SER:H	1.34	0.90
1:A:944:LEU:CD2	1:A:950:LYS:HG3	2.02	0.90
1:A:972:GLN:NE2	1:A:975:THR:H	1.71	0.89
1:A:582:LYS:O	1:A:586:THR:HG23	1.74	0.88
1:A:861:ASN:HA	1:A:867:SER:HB3	1.57	0.85
1:A:916:LEU:HB2	1:A:924:VAL:HG22	1.58	0.82
1:A:732:THR:OG1	1:A:753:THR:HG21	1.80	0.82
1:A:281:GLN:O	1:A:285:GLU:HG3	1.79	0.82
1:A:783:ASN:OD1	1:A:785:ILE:HG22	1.80	0.82
1:A:785:ILE:HD12	1:A:786:GLY:H	1.46	0.81
1:A:808:ASN:HD21	1:A:826:LYS:N	1.79	0.81
1:A:864:ASN:ND2	1:A:866:THR:HB	1.98	0.79
1:A:340:ASN:HD22	1:A:343:ALA:H	1.29	0.77
1:A:808:ASN:ND2	1:A:827:SER:H	1.83	0.76
1:A:219:PRO:HB3	1:A:244:VAL:HG11	1.68	0.76
1:A:227:VAL:HG22	1:A:242:LEU:HB2	1.67	0.75
1:A:800:LYS:O	1:A:802:PRO:HD3	1.85	0.74
1:A:678:ASN:ND2	1:A:680:ASP:H	1.84	0.74
1:A:683:HIS:HE1	1:A:796:LYS:H	1.33	0.73
1:A:808:ASN:ND2	1:A:826:LYS:H	1.85	0.73
1:A:972:GLN:HG3	3:A:1248:HOH:O	1.88	0.73
1:A:258:LYS:O	1:A:262:VAL:HG23	1.88	0.73
1:A:919:SER:OG	1:A:921:LYS:HG2	1.89	0.73
1:A:201:GLN:HA	1:A:201:GLN:NE2	2.02	0.73
1:A:814:LEU:C	1:A:816:GLN:H	1.90	0.73
1:A:683:HIS:CE1	1:A:796:LYS:H	2.07	0.72
1:A:742:ASN:ND2	1:A:744:HIS:H	1.89	0.71
1:A:513:GLN:HE21	1:A:513:GLN:N	1.87	0.70
1:A:742:ASN:HA	3:A:1231:HOH:O	1.92	0.69
1:A:820:GLN:HE22	1:A:852:GLU:HG3	1.55	0.69
1:A:785:ILE:HD12	1:A:786:GLY:N	2.06	0.69
1:A:227:VAL:CG2	1:A:242:LEU:HB2	2.23	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ASN:C	1:A:693:ASN:HD22	1.96	0.68
1:A:864:ASN:HD21	1:A:866:THR:HB	1.56	0.68
1:A:513:GLN:NE2	1:A:513:GLN:H	1.89	0.67
1:A:340:ASN:ND2	1:A:343:ALA:H	1.92	0.67
1:A:972:GLN:HE22	1:A:974:GLN:N	1.92	0.67
1:A:678:ASN:C	1:A:678:ASN:HD22	1.99	0.65
1:A:360:ASN:HA	1:A:404:PRO:HG3	1.78	0.65
1:A:944:LEU:HD22	1:A:949:PHE:O	1.96	0.65
1:A:719:SER:C	1:A:720:LYS:HG2	2.17	0.65
1:A:972:GLN:HE21	1:A:975:THR:H	1.45	0.64
1:A:774:PHE:O	1:A:775:LEU:HD23	1.98	0.64
1:A:359:TYR:CE2	1:A:404:PRO:HB2	2.33	0.64
1:A:202:TYR:CE2	1:A:229:ILE:HG12	2.33	0.64
1:A:579:SER:OG	1:A:618:LYS:HD2	1.98	0.64
1:A:736:VAL:HG13	1:A:750:MET:HB2	1.80	0.63
1:A:814:LEU:C	1:A:816:GLN:N	2.51	0.62
1:A:758:THR:HA	1:A:782:THR:HG21	1.81	0.62
1:A:504:GLN:NE2	1:A:510:ILE:H	1.89	0.62
1:A:496:LEU:HG	1:A:500:LEU:CD2	2.30	0.62
1:A:434:GLY:O	1:A:438:ILE:HG12	2.00	0.61
1:A:604:ALA:O	1:A:608:LYS:HG3	2.00	0.61
1:A:859:THR:HG22	1:A:862:SER:HB3	1.82	0.61
1:A:367:GLY:O	1:A:368:SER:HB3	2.00	0.61
1:A:859:THR:HG22	1:A:862:SER:N	2.11	0.61
1:A:371:TRP:O	1:A:375:GLU:HG3	2.01	0.61
1:A:448:THR:O	1:A:452:LYS:HD2	2.02	0.60
1:A:741:LEU:HD13	1:A:969:VAL:HG22	1.84	0.60
1:A:916:LEU:HD12	1:A:916:LEU:H	1.66	0.60
1:A:255:LEU:HD21	1:A:505:GLU:HB3	1.83	0.59
1:A:940:ASN:O	1:A:941:GLN:HB2	2.02	0.59
1:A:723:LYS:HA	1:A:726:THR:OG1	2.02	0.59
1:A:416:ARG:HH22	2:A:1004:NAG:H5	1.68	0.59
1:A:722:ALA:O	1:A:724:GLU:N	2.29	0.59
1:A:648:LEU:HD23	1:A:672:GLY:HA2	1.84	0.59
1:A:179:THR:HA	3:A:1192:HOH:O	2.02	0.59
1:A:800:LYS:HE2	3:A:1276:HOH:O	2.01	0.59
1:A:217:LEU:HD22	1:A:242:LEU:HD11	1.84	0.58
1:A:499:LEU:HB3	1:A:503:ILE:CD1	2.33	0.58
1:A:712:LYS:HA	1:A:715:MET:HB2	1.85	0.58
1:A:758:THR:O	1:A:781:ASN:O	2.21	0.58
1:A:687:HIS:C	1:A:690:PRO:HD2	2.24	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:VAL:HG22	1:A:730:THR:N	2.19	0.58
1:A:581:ILE:O	1:A:585:ILE:HG12	2.03	0.58
1:A:864:ASN:HD22	1:A:866:THR:H	1.50	0.58
1:A:484:TYR:CE1	1:A:541:GLY:HA3	2.39	0.57
1:A:781:ASN:O	1:A:782:THR:HB	2.01	0.57
1:A:430:LEU:HD23	1:A:460:LEU:HG	1.84	0.57
1:A:678:ASN:HD21	1:A:680:ASP:HB3	1.69	0.57
1:A:944:LEU:HD12	1:A:947:ASN:HA	1.87	0.57
1:A:227:VAL:O	1:A:239:GLU:HA	2.05	0.57
1:A:950:LYS:O	1:A:984:ILE:HG22	2.05	0.57
1:A:781:ASN:C	1:A:781:ASN:HD22	2.08	0.57
1:A:273:ASP:OD1	1:A:275:ASN:HB2	2.05	0.56
1:A:473:ASP:OD2	1:A:629:SER:HB2	2.06	0.56
1:A:814:LEU:HD13	1:A:853:ARG:HB3	1.87	0.56
1:A:808:ASN:HD22	1:A:827:SER:H	1.54	0.56
1:A:475:SER:HB2	1:A:629:SER:HB2	1.87	0.55
1:A:719:SER:C	1:A:721:ASP:H	2.08	0.55
1:A:820:GLN:HE22	1:A:852:GLU:CG	2.19	0.55
1:A:721:ASP:OD2	1:A:725:LYS:HB2	2.06	0.55
1:A:205:THR:O	1:A:207:PRO:HD3	2.07	0.55
1:A:919:SER:HG	1:A:921:LYS:HG2	1.71	0.55
1:A:918:ASN:HA	1:A:923:GLN:HG3	1.88	0.55
1:A:711:THR:O	1:A:715:MET:HG3	2.07	0.55
1:A:771:LYS:HD3	1:A:907:LEU:HD11	1.89	0.55
1:A:824:ASP:HA	1:A:846:ASN:HB3	1.89	0.55
1:A:230:SER:HA	1:A:237:ILE:HD12	1.89	0.54
1:A:690:PRO:HG3	1:A:860:TRP:CE2	2.42	0.54
1:A:250:ASP:O	1:A:254:LYS:HG2	2.07	0.54
1:A:435:ARG:O	1:A:439:ILE:HG12	2.07	0.54
1:A:763:LYS:HG2	1:A:891:TYR:OH	2.07	0.54
1:A:402:THR:HA	1:A:405:ILE:HD12	1.90	0.54
1:A:523:ASN:O	1:A:528:PRO:HD3	2.07	0.54
1:A:582:LYS:HD3	1:A:615:VAL:HG12	1.88	0.54
1:A:693:ASN:HD22	1:A:694:PRO:N	2.06	0.54
1:A:538:MET:HG3	3:A:1267:HOH:O	2.08	0.53
1:A:654:LEU:HD13	1:A:656:TYR:O	2.08	0.53
1:A:872:ILE:O	1:A:872:ILE:HG13	2.08	0.53
1:A:410:PRO:HD2	3:A:1151:HOH:O	2.08	0.53
1:A:718:HIS:O	1:A:721:ASP:HB3	2.09	0.53
1:A:826:LYS:HG3	1:A:846:ASN:ND2	2.24	0.53
1:A:703:LYS:NZ	1:A:781:ASN:ND2	2.57	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:LYS:HG3	1:A:788:VAL:HG22	1.91	0.53
1:A:806:TYR:HA	1:A:810:LYS:O	2.07	0.53
1:A:781:ASN:ND2	1:A:781:ASN:O	2.41	0.53
1:A:782:THR:HG22	1:A:783:ASN:N	2.24	0.52
1:A:468:GLU:CG	1:A:478:ASP:HA	2.33	0.52
1:A:651:LYS:HA	1:A:731:GLY:O	2.09	0.52
1:A:496:LEU:HG	1:A:500:LEU:HD22	1.91	0.52
1:A:468:GLU:OE1	1:A:480:THR:N	2.39	0.52
1:A:820:GLN:HA	1:A:851:ILE:O	2.10	0.52
1:A:479:HIS:O	1:A:480:THR:HB	2.10	0.52
1:A:806:TYR:HB2	1:A:829:PHE:HB3	1.92	0.51
1:A:313:SER:HB2	1:A:373:ASP:HB2	1.92	0.51
1:A:258:LYS:HE2	1:A:501:PRO:O	2.10	0.51
1:A:703:LYS:NZ	1:A:781:ASN:HD21	2.09	0.51
1:A:766:VAL:HB	1:A:773:VAL:HB	1.93	0.51
1:A:499:LEU:O	1:A:503:ILE:HD12	2.11	0.51
1:A:594:PHE:CD1	1:A:597:LEU:HD12	2.45	0.51
1:A:958:LEU:O	1:A:968:ASN:HA	2.11	0.51
1:A:182:GLU:HG3	1:A:196:ASN:ND2	2.26	0.51
1:A:416:ARG:NH2	2:A:1004:NAG:H5	2.25	0.51
1:A:540:ARG:O	1:A:543:SER:HB2	2.11	0.51
1:A:693:ASN:ND2	1:A:695:TYR:H	2.07	0.51
1:A:411:ASP:HA	3:A:1149:HOH:O	2.10	0.51
1:A:493:ILE:O	1:A:497:THR:HG23	2.11	0.51
1:A:944:LEU:HD23	1:A:950:LYS:HG3	1.87	0.51
1:A:403:ASP:N	1:A:404:PRO:CD	2.74	0.51
1:A:814:LEU:HG	1:A:819:SER:HB3	1.93	0.51
1:A:504:GLN:HE22	1:A:510:ILE:N	1.91	0.50
1:A:708:GLU:HG3	1:A:714:PHE:CE1	2.46	0.50
1:A:762:GLN:HE22	1:A:920:SER:HA	1.76	0.50
1:A:461:PHE:CD2	1:A:514:GLU:HG2	2.46	0.50
1:A:716:SER:O	1:A:717:LYS:CB	2.52	0.50
1:A:324:GLU:HA	1:A:385:THR:OG1	2.12	0.50
1:A:958:LEU:HB2	1:A:969:VAL:HG23	1.92	0.50
1:A:466:LYS:O	1:A:467:ALA:HB3	2.12	0.49
1:A:547:GLU:HG3	1:A:860:TRP:CE2	2.47	0.49
1:A:329:GLN:HA	1:A:329:GLN:OE1	2.11	0.49
1:A:417:LYS:HA	1:A:422:PRO:HB3	1.95	0.49
1:A:859:THR:CG2	1:A:862:SER:H	2.18	0.49
1:A:590:PHE:CE1	1:A:682:SER:HB3	2.47	0.49
1:A:780:LYS:HA	1:A:886:ASN:HD21	1.75	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LYS:HA	1:A:730:THR:HG23	1.94	0.49
1:A:936:ILE:HG12	1:A:956:LEU:HD22	1.95	0.49
1:A:729:VAL:HG11	1:A:757:ARG:NH1	2.27	0.49
1:A:504:GLN:O	1:A:509:LYS:HE3	2.12	0.49
1:A:972:GLN:NE2	1:A:975:THR:N	2.52	0.49
1:A:295:LYS:HB2	1:A:295:LYS:NZ	2.28	0.49
1:A:363:LYS:HE2	3:A:1184:HOH:O	2.13	0.49
1:A:506:THR:O	1:A:509:LYS:HD2	2.13	0.49
1:A:490:ASN:HD21	1:A:535:LEU:CD1	2.25	0.49
1:A:690:PRO:HG3	1:A:860:TRP:NE1	2.28	0.49
1:A:729:VAL:HG11	1:A:757:ARG:HH12	1.77	0.49
1:A:952:ASN:ND2	1:A:953:LYS:HD2	2.28	0.49
1:A:461:PHE:CG	1:A:514:GLU:HG2	2.47	0.49
1:A:210:GLY:HA2	1:A:220:ASN:HB2	1.95	0.48
1:A:256:LEU:O	1:A:259:TRP:HB3	2.12	0.48
1:A:917:GLU:HB3	1:A:924:VAL:HG13	1.95	0.48
1:A:814:LEU:O	1:A:816:GLN:N	2.46	0.48
1:A:708:GLU:HG3	1:A:714:PHE:HE1	1.78	0.48
1:A:406:GLU:OE1	1:A:437:LYS:NZ	2.46	0.48
1:A:591:TYR:OH	1:A:596:ASN:HB2	2.14	0.48
1:A:820:GLN:NE2	1:A:852:GLU:OE1	2.47	0.48
1:A:739:VAL:HG23	1:A:978:LYS:HD2	1.95	0.48
1:A:333:PRO:HA	1:A:338:TYR:CD2	2.49	0.48
1:A:439:ILE:N	1:A:439:ILE:HD13	2.29	0.48
1:A:509:LYS:HD2	1:A:509:LYS:H	1.78	0.48
1:A:921:LYS:HE2	3:A:1301:HOH:O	2.14	0.48
1:A:280:ASN:OD1	1:A:332:ASN:ND2	2.47	0.47
1:A:725:LYS:HD2	1:A:725:LYS:HA	1.64	0.47
1:A:818:SER:HB3	1:A:819:SER:H	1.44	0.47
1:A:771:LYS:HE3	1:A:912:GLU:OE1	2.13	0.47
1:A:379:PRO:HB3	1:A:405:ILE:HG12	1.97	0.47
1:A:504:GLN:HA	1:A:509:LYS:HB3	1.96	0.47
1:A:742:ASN:HD21	1:A:745:PHE:HD1	1.63	0.47
1:A:197:LYS:O	1:A:202:TYR:OH	2.23	0.47
1:A:850:ASP:O	1:A:880:ILE:HA	2.14	0.47
1:A:173:HIS:O	1:A:175:GLN:HG3	2.14	0.47
1:A:225:THR:HG23	1:A:226:THR:N	2.29	0.47
1:A:264:ILE:HB	3:A:1204:HOH:O	2.15	0.47
1:A:868:LYS:HA	1:A:868:LYS:HD3	1.66	0.47
1:A:900:ASP:OD1	1:A:902:THR:HB	2.15	0.47
1:A:631:ASP:O	1:A:632:ARG:HD3	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ASN:HB2	3:A:1118:HOH:O	2.14	0.47
1:A:656:TYR:CE1	1:A:667:TRP:HA	2.50	0.47
1:A:739:VAL:CG2	1:A:978:LYS:HD2	2.45	0.47
1:A:271:THR:HG22	1:A:277:GLN:HE22	1.80	0.47
1:A:418:THR:HA	3:A:1157:HOH:O	2.14	0.47
1:A:714:PHE:CD2	1:A:714:PHE:C	2.88	0.47
1:A:678:ASN:C	1:A:678:ASN:ND2	2.67	0.47
1:A:887:LYS:HG3	1:A:888:GLY:N	2.29	0.47
1:A:970:TYR:HB3	1:A:979:THR:HB	1.95	0.47
1:A:503:ILE:HG22	1:A:504:GLN:HE21	1.80	0.46
1:A:521:TRP:O	1:A:525:SER:HB2	2.16	0.46
1:A:633:LEU:HD23	1:A:633:LEU:C	2.36	0.46
1:A:264:ILE:HG13	1:A:388:LEU:HD21	1.96	0.46
1:A:230:SER:CA	1:A:237:ILE:HD12	2.45	0.46
1:A:864:ASN:O	1:A:867:SER:HB3	2.16	0.46
1:A:368:SER:O	1:A:369:ALA:O	2.32	0.46
1:A:661:ASP:HB3	1:A:865:ARG:HB2	1.98	0.46
1:A:734:ASP:OD1	1:A:734:ASP:N	2.36	0.46
1:A:826:LYS:CD	1:A:846:ASN:HD21	2.29	0.46
1:A:937:LYS:HE3	1:A:943:SER:HB3	1.98	0.46
1:A:723:LYS:O	1:A:726:THR:N	2.49	0.46
1:A:372:TRP:CD1	1:A:376:ILE:HD12	2.51	0.46
1:A:801:THR:HG21	1:A:834:GLU:H	1.79	0.46
1:A:911:LYS:O	1:A:928:LYS:NZ	2.47	0.46
1:A:648:LEU:CD2	1:A:672:GLY:HA2	2.45	0.45
1:A:941:GLN:N	1:A:952:ASN:O	2.50	0.45
1:A:742:ASN:ND2	1:A:745:PHE:H	2.15	0.45
1:A:754:ASN:HB2	1:A:759:LEU:HB3	1.99	0.45
1:A:949:PHE:HB3	1:A:984:ILE:HB	1.99	0.45
1:A:524:GLN:O	1:A:528:PRO:HG2	2.16	0.45
1:A:552:HIS:O	1:A:556:VAL:HG23	2.16	0.45
1:A:630:MET:HG3	1:A:632:ARG:HG2	1.98	0.45
1:A:570:ASN:HD22	1:A:575:LEU:HD21	1.81	0.45
1:A:250:ASP:OD1	1:A:252:PHE:HB2	2.17	0.45
1:A:475:SER:HB2	1:A:629:SER:CB	2.46	0.45
1:A:693:ASN:C	1:A:693:ASN:ND2	2.66	0.45
1:A:703:LYS:NZ	1:A:758:THR:O	2.49	0.45
1:A:729:VAL:HG22	1:A:730:THR:H	1.81	0.45
1:A:959:VAL:HG22	1:A:968:ASN:HB3	1.99	0.45
1:A:650:SER:C	1:A:652:ARG:H	2.19	0.45
1:A:650:SER:C	1:A:652:ARG:N	2.70	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:GLN:HE22	1:A:975:THR:H	1.61	0.45
1:A:479:HIS:HA	3:A:1123:HOH:O	2.16	0.44
1:A:200:TYR:CE1	1:A:237:ILE:HD13	2.53	0.44
1:A:547:GLU:HB2	1:A:860:TRP:CD2	2.52	0.44
1:A:754:ASN:O	1:A:757:ARG:HD3	2.17	0.44
1:A:939:ASP:CG	1:A:940:ASN:H	2.20	0.44
1:A:576:ASP:OD1	1:A:618:LYS:NZ	2.44	0.44
1:A:421:ASN:N	1:A:422:PRO:CD	2.81	0.44
1:A:703:LYS:HZ3	1:A:781:ASN:HD21	1.63	0.44
1:A:869:ASN:ND2	1:A:871:SER:OG	2.50	0.44
1:A:451:GLU:HB2	1:A:508:TYR:CZ	2.52	0.44
1:A:676:ILE:HD13	1:A:676:ILE:HA	1.68	0.44
1:A:686:ASN:CG	1:A:686:ASN:O	2.56	0.44
1:A:773:VAL:HG11	1:A:925:ILE:HD12	1.99	0.44
1:A:719:SER:C	1:A:721:ASP:N	2.71	0.44
1:A:569:SER:OG	1:A:571:GLU:HG3	2.18	0.44
1:A:696:LYS:O	1:A:794:GLN:NE2	2.48	0.44
1:A:723:LYS:O	1:A:724:GLU:C	2.56	0.44
1:A:446:ASP:OD1	1:A:448:THR:HB	2.17	0.44
1:A:612:ASP:OD1	1:A:614:THR:HB	2.17	0.44
1:A:671:ASP:OD2	1:A:702:GLU:OE2	2.36	0.44
1:A:800:LYS:C	1:A:802:PRO:HD3	2.38	0.43
1:A:916:LEU:HB2	1:A:924:VAL:CG2	2.39	0.43
1:A:517:MET:CE	3:A:1240:HOH:O	2.65	0.43
1:A:916:LEU:HD13	1:A:924:VAL:HG23	2.01	0.43
1:A:499:LEU:C	1:A:503:ILE:HD12	2.38	0.43
1:A:509:LYS:CD	1:A:509:LYS:H	2.32	0.43
1:A:937:LYS:HB3	1:A:954:ALA:HA	2.00	0.43
1:A:267:TYR:CE1	1:A:268:VAL:HG13	2.54	0.43
1:A:330:ILE:HG13	1:A:337:ILE:HD12	2.01	0.43
1:A:593:VAL:HG13	1:A:594:PHE:N	2.34	0.43
1:A:865:ARG:HA	1:A:865:ARG:HD3	1.59	0.43
1:A:931:GLN:OE1	1:A:961:LYS:HG2	2.19	0.43
1:A:832:SER:HB3	1:A:837:ARG:HB2	2.00	0.43
1:A:204:LEU:HG	1:A:212:ILE:HD12	1.99	0.42
1:A:780:LYS:HA	1:A:886:ASN:ND2	2.34	0.42
1:A:808:ASN:HD21	1:A:827:SER:H	1.64	0.42
1:A:545:SER:HB2	1:A:863:ILE:HD12	2.01	0.42
1:A:780:LYS:HG2	1:A:780:LYS:H	1.71	0.42
1:A:855:GLU:HA	1:A:876:PRO:HA	2.01	0.42
1:A:826:LYS:CG	1:A:846:ASN:HD21	2.32	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:GLN:HB2	1:A:762:GLN:HE21	1.60	0.42
1:A:773:VAL:HG11	1:A:925:ILE:CD1	2.50	0.42
1:A:814:LEU:HD21	1:A:820:GLN:OE1	2.20	0.42
1:A:247:SER:OG	1:A:249:GLU:HB2	2.19	0.42
1:A:650:SER:HB3	1:A:736:VAL:HB	2.00	0.42
1:A:783:ASN:CG	1:A:785:ILE:HG22	2.40	0.42
1:A:828:VAL:HG23	1:A:843:PHE:HE1	1.83	0.42
1:A:951:MET:HG2	1:A:957:TYR:CE2	2.54	0.42
1:A:620:LEU:HD13	1:A:636:TYR:OH	2.20	0.42
1:A:348:LYS:HE3	1:A:393:PHE:CD2	2.55	0.42
1:A:683:HIS:HE1	1:A:796:LYS:N	2.07	0.42
1:A:475:SER:OG	1:A:627:PHE:HB3	2.19	0.42
1:A:646:LEU:HD23	1:A:646:LEU:HA	1.82	0.42
1:A:711:THR:HG21	1:A:865:ARG:NH1	2.35	0.42
1:A:175:GLN:HB3	1:A:176:PRO:HD2	2.02	0.42
1:A:386:LEU:O	1:A:390:ASN:HB3	2.20	0.42
1:A:715:MET:HG2	1:A:726:THR:HG21	2.02	0.42
1:A:906:LYS:O	1:A:910:SER:HB3	2.20	0.42
1:A:620:LEU:HG	1:A:620:LEU:H	1.65	0.42
1:A:944:LEU:HA	1:A:944:LEU:HD22	1.78	0.42
1:A:860:TRP:O	1:A:863:ILE:HG13	2.20	0.41
1:A:416:ARG:NH1	2:A:1004:NAG:H3	2.35	0.41
1:A:416:ARG:HG3	1:A:419:LEU:HD23	2.02	0.41
1:A:499:LEU:HB3	1:A:503:ILE:HD12	2.01	0.41
1:A:774:PHE:O	1:A:892:GLY:HA2	2.19	0.41
1:A:776:GLY:HA3	1:A:891:TYR:CE2	2.55	0.41
1:A:972:GLN:HE22	1:A:974:GLN:CA	2.33	0.41
1:A:419:LEU:N	1:A:419:LEU:HD13	2.35	0.41
1:A:972:GLN:HA	1:A:973:PRO:HD2	1.82	0.41
1:A:367:GLY:O	1:A:368:SER:CB	2.67	0.41
1:A:504:GLN:NE2	1:A:510:ILE:HG23	2.36	0.41
1:A:781:ASN:ND2	1:A:781:ASN:C	2.73	0.41
1:A:807:VAL:HG21	1:A:812:ILE:HG21	2.01	0.41
1:A:819:SER:C	1:A:820:GLN:HG2	2.41	0.41
1:A:952:ASN:HD21	1:A:953:LYS:HD2	1.84	0.41
1:A:204:LEU:HD22	1:A:225:THR:HG21	2.02	0.41
1:A:538:MET:CE	1:A:632:ARG:HB3	2.50	0.41
1:A:679:SER:OG	1:A:837:ARG:NE	2.48	0.41
1:A:755:TRP:CG	1:A:756:ASP:N	2.89	0.41
1:A:754:ASN:HB2	1:A:759:LEU:N	2.36	0.41
1:A:758:THR:HB	1:A:783:ASN:ND2	2.35	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:LEU:HD13	1:A:788:VAL:HG21	2.03	0.41
1:A:959:VAL:HG22	1:A:968:ASN:CB	2.50	0.41
1:A:481:ASN:HB2	1:A:653:THR:HA	2.02	0.41
1:A:707:ARG:HH22	1:A:727:GLY:HA3	1.85	0.41
1:A:341:GLU:O	1:A:345:ARG:HG3	2.21	0.41
1:A:937:LYS:HE3	1:A:943:SER:CB	2.51	0.41
1:A:484:TYR:CZ	1:A:541:GLY:HA3	2.56	0.41
1:A:826:LYS:CG	1:A:846:ASN:ND2	2.84	0.41
1:A:779:ILE:O	1:A:889:ASP:HB2	2.21	0.41
1:A:329:GLN:HB2	1:A:337:ILE:HD11	2.03	0.40
1:A:967:GLN:HA	1:A:981:GLN:OE1	2.21	0.40
1:A:416:ARG:CG	1:A:419:LEU:HD23	2.51	0.40
1:A:537:ASP:O	1:A:539:SER:N	2.55	0.40
1:A:718:HIS:CD2	1:A:725:LYS:HG2	2.56	0.40
1:A:861:ASN:HA	1:A:864:ASN:O	2.22	0.40
1:A:177:VAL:HA	3:A:1191:HOH:O	2.21	0.40
1:A:484:TYR:CD1	1:A:487:ALA:HB3	2.55	0.40
1:A:962:VAL:HG13	1:A:962:VAL:O	2.22	0.40
1:A:173:HIS:O	1:A:174:PRO:C	2.58	0.40
1:A:729:VAL:HG21	1:A:757:ARG:NH2	2.36	0.40
1:A:972:GLN:HE22	1:A:974:GLN:H	1.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:SER:N	1:A:171:SER:N[3_655]	2.07	0.13

## 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	812/814 (100%)	739 (91%)	59 (7%)	14 (2%)	11 7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	SER
1	A	942	GLU
1	A	367	GLY
1	A	369	ALA
1	A	713	GLU
1	A	717	LYS
1	A	939	ASP
1	A	209	LEU
1	A	754	ASN
1	A	769	ASN
1	A	467	ALA
1	A	538	MET
1	A	720	LYS
1	A	368	SER

### 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	729/729 (100%)	617 (85%)	112 (15%)	3 2

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	A	180	GLN
1	A	183	LYS
1	A	191	LYS
1	A	201	GLN
1	A	227	VAL
1	A	232	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	243	SER
1	A	249	GLU
1	A	267	TYR
1	A	271	THR
1	A	274	SER
1	A	277	GLN
1	A	291	ILE
1	A	295	LYS
1	A	298	SER
1	A	305	LYS
1	A	342	LYS
1	A	351	LEU
1	A	363	LYS
1	A	381	SER
1	A	390	ASN
1	A	391	ASN
1	A	399	LYS
1	A	419	LEU
1	A	424	LYS
1	A	447	ASN
1	A	452	LYS
1	A	458	LYS
1	A	484	TYR
1	A	500	LEU
1	A	507	ASP
1	A	509	LYS
1	A	513	GLN
1	A	515	LEU
1	A	535	LEU
1	A	538	MET
1	A	546	ARG
1	A	559	LEU
1	A	569	SER
1	A	587	SER
1	A	601	SER
1	A	614	THR
1	A	618	LYS
1	A	620	LEU
1	A	623	ASN
1	A	629	SER
1	A	639	LYS
1	A	647	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	651	LYS
1	A	654	LEU
1	A	659	MET
1	A	663	ASN
1	A	676	ILE
1	A	678	ASN
1	A	693	ASN
1	A	697	MET
1	A	706	LYS
1	A	713	GLU
1	A	716	SER
1	A	720	LYS
1	A	723	LYS
1	A	725	LYS
1	A	730	THR
1	A	734	ASP
1	A	742	ASN
1	A	771	LYS
1	A	778	ASN
1	A	780	LYS
1	A	781	ASN
1	A	782	THR
1	A	785	ILE
1	A	810	LYS
1	A	813	ASP
1	A	814	LEU
1	A	815	LYS
1	A	818	SER
1	A	819	SER
1	A	820	GLN
1	A	827	SER
1	A	841	TYR
1	A	845	LYS
1	A	849	ILE
1	A	853	ARG
1	A	854	LYS
1	A	859	THR
1	A	862	SER
1	A	863	ILE
1	A	864	ASN
1	A	865	ARG
1	A	868	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	870	THR
1	A	872	ILE
1	A	887	LYS
1	A	906	LYS
1	A	907	LEU
1	A	910	SER
1	A	919	SER
1	A	920	SER
1	A	923	GLN
1	A	924	VAL
1	A	925	ILE
1	A	928	LYS
1	A	942	GLU
1	A	944	LEU
1	A	947	ASN
1	A	965	ASP
1	A	969	VAL
1	A	972	GLN
1	A	976	MET
1	A	981	GLN
1	A	982	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	266	ASN
1	A	275	ASN
1	A	277	GLN
1	A	340	ASN
1	A	447	ASN
1	A	504	GLN
1	A	513	GLN
1	A	567	ASN
1	A	570	ASN
1	A	574	ASN
1	A	605	ASN
1	A	660	ASN
1	A	663	ASN
1	A	678	ASN
1	A	683	HIS
1	A	686	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	693	ASN
1	A	742	ASN
1	A	762	GLN
1	A	769	ASN
1	A	778	ASN
1	A	781	ASN
1	A	787	ASN
1	A	808	ASN
1	A	820	GLN
1	A	846	ASN
1	A	864	ASN
1	A	869	ASN
1	A	886	ASN
1	A	923	GLN
1	A	946	ASN
1	A	960	GLN
1	A	972	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 ⓘ

4 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	GC4	A	1001	2	8,11,12	2.48	2 (25%)	9,15,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1002	2	15,15,15	2.33	6 (40%)	21,21,21	1.18	2 (9%)
2	GC4	A	1003	2	8,11,12	1.99	2 (25%)	9,15,17	0.54	0
2	NAG	A	1004	2	15,15,15	1.61	4 (26%)	21,21,21	0.96	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	GC4	A	1001	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1002	2	-	0/6/26/26	0/1/1/1
2	GC4	A	1003	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1004	2	-	0/6/26/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	NAG	O5-C5	2.08	1.49	1.44
2	A	1002	NAG	O5-C5	2.10	1.49	1.44
2	A	1002	NAG	C1-C2	2.14	1.55	1.52
2	A	1004	NAG	O5-C1	2.32	1.47	1.43
2	A	1002	NAG	O3-C3	2.46	1.48	1.43
2	A	1004	NAG	C7-N2	2.55	1.43	1.34
2	A	1002	NAG	O5-C1	2.98	1.48	1.43
2	A	1001	GC4	O5-C1	3.17	1.48	1.43
2	A	1004	NAG	C2-N2	3.30	1.51	1.45
2	A	1003	GC4	O5-C1	3.38	1.49	1.43
2	A	1002	NAG	C7-N2	3.43	1.47	1.34
2	A	1003	GC4	O5-C5	3.65	1.48	1.43
2	A	1001	GC4	O5-C5	5.15	1.50	1.43
2	A	1002	NAG	C2-N2	5.58	1.55	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	NAG	O7-C7-C8	-3.12	116.37	122.06
2	A	1004	NAG	O7-C7-C8	-2.68	117.18	122.06
2	A	1002	NAG	O7-C7-N2	2.18	126.12	121.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1004	NAG	3	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	814/814 (100%)	-0.15	16 (1%) 65 63	17, 35, 63, 94	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	818	SER	9.5
1	A	817	ALA	9.3
1	A	819	SER	5.7
1	A	816	GLN	4.4
1	A	721	ASP	3.6
1	A	367	GLY	3.5
1	A	722	ALA	3.5
1	A	720	LYS	2.8
1	A	947	ASN	2.8
1	A	718	HIS	2.7
1	A	714	PHE	2.7
1	A	716	SER	2.6
1	A	725	LYS	2.5
1	A	867	SER	2.4
1	A	888	GLY	2.2
1	A	941	GLN	2.2

### 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
2	GC4	A	1001	11/12	0.71	0.46	16.50	65,71,74,77	0
2	NAG	A	1002	15/15	0.67	0.43	-	61,68,76,77	0
2	NAG	A	1004	15/15	0.83	0.24	-	59,63,69,69	0
2	GC4	A	1003	11/12	0.78	0.29	-	59,64,70,71	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.