



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:24 PM BST

PDB ID : 3ALW  
Title : Crystal structure of the measles virus hemagglutinin bound to its cellular receptor SLAM (Form I, MV-H-SLAM(N102H/R108Y) fusion)  
Authors : Hashiguchi, T.; Ose, T.; Kubota, M.; Maita, N.; Kamishikiryo, J.; Maenaka, K.; Yanagi, Y.  
Deposited on : 2010-08-09  
Resolution : 3.55 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

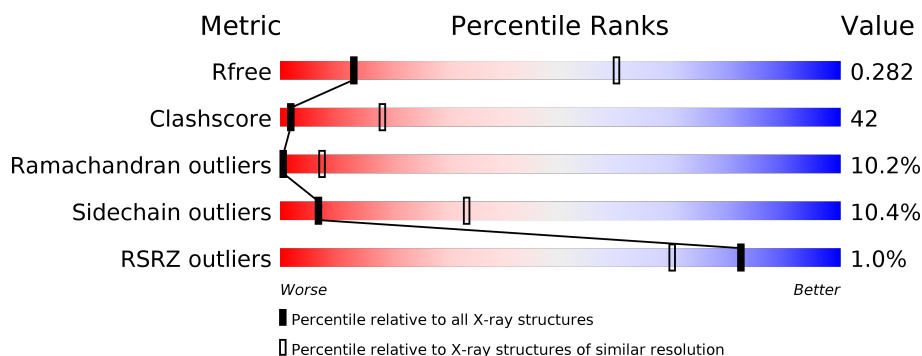
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	559	<div> <div></div> <div>35%</div> <div>45%</div> <div>10%</div> <div>9%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4033 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 Hemagglutinin, CDw150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4005	2570	668	739	28			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	-	expression tag	UNP E2RZS2
A	182	THR	-	expression tag	UNP E2RZS2
A	183	GLY	-	expression tag	UNP E2RZS2
A	102	HIS	ASN	engineered mutation	UNP Q9GJT3
A	108	TYR	ARG	engineered mutation	UNP Q9GJT3
A	141	GLY	-	expression tag	UNP Q9GJT3
A	142	THR	-	expression tag	UNP Q9GJT3
A	143	LYS	-	expression tag	UNP Q9GJT3
A	144	HIS	-	expression tag	UNP Q9GJT3
A	145	HIS	-	expression tag	UNP Q9GJT3
A	146	HIS	-	expression tag	UNP Q9GJT3
A	147	HIS	-	expression tag	UNP Q9GJT3
A	148	HIS	-	expression tag	UNP Q9GJT3
A	149	HIS	-	expression tag	UNP Q9GJT3

- Molecule 2 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>).

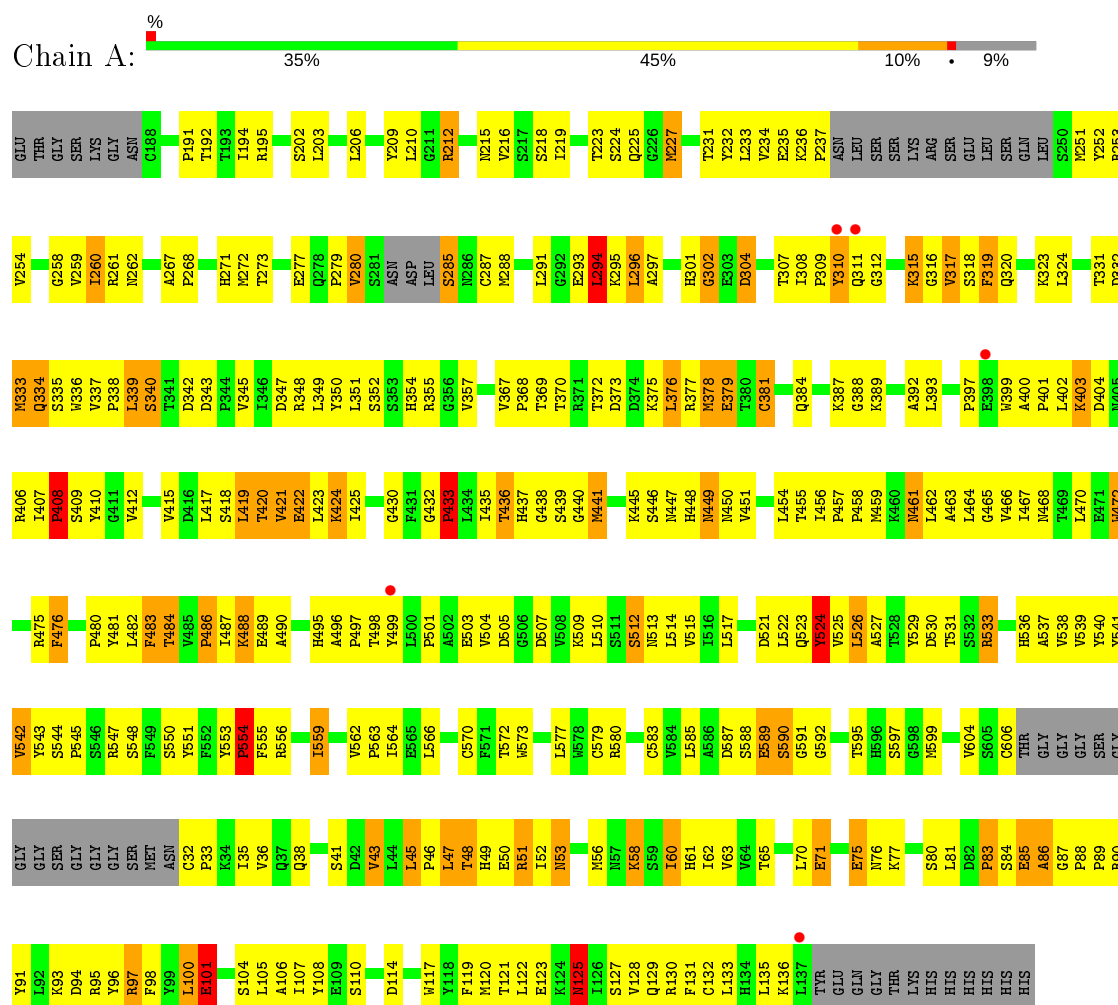


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

### 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: Hemagglutinin, CDw150



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.91Å 209.91Å 180.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.89 – 3.55 29.89 – 3.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.89-3.55) 98.8 (29.89-3.55)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.67 (at 3.56Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.250 , 0.283 0.251 , 0.282	Depositor DCC
$R_{free}$ test set	1449 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.3	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 89.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4033	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 3.72% 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

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	0.43	0/4105	0.70	0/5577

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	232	TYR	Sidechain

### 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	4005	0	3984	336	0
2	A	28	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4033	0	4010	337	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 42.

All (337) 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:459:MET:HB3	1:A:463:ALA:HB3	1.31	1.08
1:A:93:LYS:HD2	1:A:96:TYR:H	1.29	0.97
1:A:85:GLU:HG2	1:A:86:ALA:H	1.31	0.96
1:A:97:ARG:HB3	1:A:106:ALA:HB3	1.46	0.96
1:A:419:LEU:HD22	1:A:423:LEU:HD11	1.48	0.94
1:A:589:GLU:HG3	1:A:590:SER:H	1.29	0.94
1:A:448:HIS:HB2	1:A:451:VAL:HG12	1.51	0.93
1:A:191:PRO:HB3	1:A:131:PHE:CE2	2.11	0.85
1:A:253:ARG:HH21	1:A:285:SER:HB3	1.41	0.84
1:A:378:MET:HG2	1:A:407:ILE:HG21	1.61	0.83
1:A:384:GLN:HG3	1:A:490:ALA:HB2	1.59	0.82
1:A:368:PRO:HD3	1:A:441:MET:HE3	1.59	0.81
1:A:589:GLU:CG	1:A:590:SER:H	1.92	0.81
1:A:194:ILE:HG12	1:A:604:VAL:HG12	1.64	0.79
1:A:375:LYS:HA	1:A:379:GLU:HG2	1.65	0.79
1:A:218:SER:HB3	1:A:233:LEU:HD12	1.65	0.79
1:A:35:ILE:HD11	1:A:45:LEU:HD23	1.65	0.78
1:A:354:HIS:ND1	1:A:367:VAL:HG12	1.96	0.78
1:A:318:SER:HB3	1:A:337:VAL:O	1.82	0.78
1:A:123:GLU:HB3	1:A:128:VAL:HG22	1.66	0.77
1:A:81:LEU:HD23	1:A:83:PRO:HD3	1.65	0.77
1:A:58:LYS:HA	1:A:58:LYS:HE3	1.65	0.76
1:A:38:GLN:HB2	1:A:41:SER:HB3	1.66	0.76
1:A:91:TYR:HB3	1:A:93:LYS:HG2	1.68	0.75
1:A:548:SER:HB3	1:A:70:LEU:HB3	1.69	0.75
1:A:343:ASP:OD1	1:A:345:VAL:HG12	1.87	0.74
1:A:589:GLU:C	1:A:591:GLY:H	1.91	0.74
1:A:194:ILE:HD13	1:A:551:TYR:CD2	2.21	0.74
1:A:52:ILE:HD11	1:A:101:GLU:O	1.87	0.74
1:A:354:HIS:CE1	1:A:367:VAL:HG12	2.23	0.73
1:A:461:ASN:ND2	1:A:462:LEU:HD23	2.03	0.73
1:A:227:MET:HE1	1:A:291:LEU:HD22	1.71	0.73
1:A:563:PRO:HA	1:A:585:LEU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HG3	1:A:370:THR:OG1	1.90	0.72
1:A:236:LYS:HB3	1:A:237:PRO:HD2	1.71	0.72
1:A:280:VAL:CG1	1:A:285:SER:HB2	2.20	0.71
1:A:437:HIS:CB	1:A:459:MET:HE3	2.21	0.71
1:A:418:SER:O	1:A:420:THR:HG23	1.91	0.71
1:A:339:LEU:H	1:A:339:LEU:HD23	1.55	0.71
1:A:323:LYS:HE2	1:A:333:MET:HE2	1.73	0.70
1:A:480:PRO:HB2	1:A:484:THR:HG21	1.72	0.70
1:A:316:GLY:O	1:A:339:LEU:HD21	1.93	0.69
1:A:60:ILE:HG22	1:A:60:ILE:O	1.94	0.68
1:A:448:HIS:HB2	1:A:451:VAL:CG1	2.24	0.68
1:A:526:LEU:HD13	1:A:527:ALA:H	1.59	0.68
1:A:531:THR:HG22	1:A:536:HIS:CD2	2.28	0.68
1:A:318:SER:HB2	1:A:336:TRP:NE1	2.09	0.68
1:A:81:LEU:HD13	1:A:98:PHE:CD2	2.29	0.68
1:A:315:LYS:HD2	1:A:315:LYS:O	1.94	0.67
1:A:580:ARG:HE	1:A:599:MET:CE	2.09	0.66
1:A:505:ASP:OD2	1:A:77:LYS:HD3	1.95	0.66
1:A:570:CYS:HB3	1:A:577:LEU:HD11	1.76	0.66
1:A:514:LEU:HD21	1:A:524:TYR:HD1	1.61	0.66
1:A:526:LEU:CD1	1:A:527:ALA:H	2.08	0.66
1:A:318:SER:OG	1:A:338:PRO:HA	1.95	0.66
1:A:397:PRO:HG2	1:A:403:LYS:HG2	1.78	0.66
1:A:437:HIS:HB2	1:A:459:MET:HE3	1.78	0.66
1:A:483:PHE:CD1	1:A:483:PHE:N	2.60	0.65
1:A:514:LEU:HD23	1:A:515:VAL:N	2.11	0.65
1:A:81:LEU:HD13	1:A:98:PHE:HD2	1.61	0.65
1:A:438:GLY:O	1:A:440:GLY:N	2.30	0.64
1:A:450:ASN:HA	1:A:472:TRP:CH2	2.32	0.64
1:A:43:VAL:HG22	1:A:110:SER:HB3	1.78	0.64
1:A:236:LYS:HD2	1:A:277:GLU:OE2	1.98	0.64
1:A:85:GLU:HG2	1:A:86:ALA:N	2.10	0.63
1:A:580:ARG:HE	1:A:599:MET:HE3	1.63	0.63
1:A:93:LYS:HD2	1:A:96:TYR:N	2.06	0.63
1:A:378:MET:HB3	1:A:407:ILE:HD12	1.81	0.62
1:A:433:PRO:CG	1:A:480:PRO:HB3	2.30	0.62
1:A:419:LEU:HA	1:A:423:LEU:HD21	1.82	0.62
1:A:446:SER:HB3	1:A:451:VAL:O	1.99	0.62
1:A:33:PRO:HB2	1:A:133:LEU:HD23	1.82	0.62
1:A:531:THR:HG22	1:A:536:HIS:NE2	2.15	0.62
1:A:481:TYR:O	1:A:482:LEU:HD23	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ARG:NH1	1:A:123:GLU:OE2	2.32	0.61
1:A:589:GLU:CG	1:A:590:SER:N	2.62	0.61
1:A:533:ARG:HB3	1:A:61:HIS:CD2	2.36	0.61
1:A:218:SER:CB	1:A:233:LEU:HD12	2.30	0.60
1:A:384:GLN:HB3	1:A:487:ILE:HG21	1.83	0.60
1:A:77:LYS:CE	1:A:80:SER:HB2	2.31	0.60
1:A:467:ILE:C	1:A:468:ASN:HD22	2.05	0.60
1:A:592:GLY:HA3	2:A:901:NAG:H61	1.84	0.60
1:A:339:LEU:CD2	1:A:339:LEU:H	2.15	0.60
1:A:206:LEU:HD11	1:A:216:VAL:HG11	1.85	0.59
1:A:412:VAL:HG21	1:A:470:LEU:HD21	1.85	0.59
1:A:482:LEU:O	1:A:484:THR:HG22	2.03	0.58
1:A:537:ALA:HB2	1:A:556:ARG:HA	1.85	0.58
1:A:459:MET:HB3	1:A:463:ALA:CB	2.21	0.58
1:A:47:LEU:HD12	1:A:133:LEU:HD12	1.85	0.58
1:A:288:MET:CE	1:A:351:LEU:HD22	2.34	0.57
1:A:60:ILE:O	1:A:61:HIS:HB2	2.04	0.57
1:A:378:MET:CG	1:A:407:ILE:HG21	2.33	0.57
1:A:319:PHE:HD1	1:A:425:ILE:HD12	1.69	0.57
1:A:192:THR:HG22	1:A:606:CYS:SG	2.45	0.57
1:A:219:ILE:HD12	1:A:219:ILE:N	2.19	0.57
1:A:349:LEU:HD22	1:A:369:THR:CG2	2.35	0.57
1:A:409:SER:HB2	1:A:430:GLY:O	2.05	0.57
1:A:378:MET:HB3	1:A:407:ILE:CD1	2.35	0.57
1:A:524:TYR:CE2	1:A:543:TYR:HB2	2.39	0.57
1:A:127:SER:O	1:A:128:VAL:HG23	2.05	0.57
1:A:350:TYR:HE2	1:A:370:THR:HG23	1.70	0.57
1:A:585:LEU:HD12	1:A:585:LEU:O	2.05	0.56
1:A:91:TYR:CD1	1:A:93:LYS:HD3	2.40	0.56
1:A:564:ILE:HG13	1:A:585:LEU:HA	1.87	0.56
1:A:467:ILE:HD11	1:A:524:TYR:CD1	2.41	0.56
1:A:304:ASP:O	1:A:350:TYR:HA	2.06	0.56
1:A:448:HIS:O	1:A:450:ASN:N	2.38	0.55
1:A:475:ARG:HG2	1:A:476:PHE:H	1.70	0.55
1:A:486:PRO:HG3	1:A:495:HIS:ND1	2.21	0.55
1:A:33:PRO:HD2	1:A:132:CYS:O	2.07	0.55
1:A:349:LEU:HD22	1:A:369:THR:HG22	1.88	0.55
1:A:97:ARG:NH1	1:A:97:ARG:HG2	2.21	0.55
1:A:323:LYS:O	1:A:324:LEU:HD12	2.07	0.55
1:A:97:ARG:O	1:A:105:LEU:HA	2.07	0.55
1:A:421:VAL:O	1:A:422:GLU:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLU:C	1:A:591:GLY:N	2.59	0.55
1:A:317:VAL:O	1:A:339:LEU:HD22	2.06	0.55
1:A:524:TYR:HD2	1:A:524:TYR:N	2.05	0.55
1:A:590:SER:C	1:A:592:GLY:H	2.10	0.55
1:A:219:ILE:H	1:A:219:ILE:HD12	1.71	0.55
1:A:433:PRO:HG2	1:A:480:PRO:HB3	1.89	0.54
1:A:592:GLY:HA3	2:A:901:NAG:C6	2.37	0.54
1:A:515:VAL:HG13	1:A:515:VAL:O	2.07	0.54
1:A:43:VAL:HG23	1:A:107:ILE:HB	1.89	0.54
1:A:280:VAL:HG11	1:A:285:SER:HB2	1.88	0.54
1:A:317:VAL:HG12	1:A:318:SER:N	2.23	0.54
1:A:433:PRO:HG3	1:A:480:PRO:HB3	1.89	0.54
1:A:122:LEU:HB2	1:A:129:GLN:HB3	1.89	0.54
1:A:589:GLU:O	1:A:591:GLY:N	2.41	0.54
1:A:43:VAL:CG2	1:A:107:ILE:HD12	2.38	0.53
1:A:46:PRO:O	1:A:48:THR:N	2.41	0.53
1:A:481:TYR:HD2	1:A:482:LEU:HG	1.73	0.53
1:A:440:GLY:O	1:A:441:MET:HB2	2.09	0.53
1:A:559:ILE:HD13	1:A:559:ILE:H	1.72	0.53
1:A:71:GLU:CD	1:A:71:GLU:H	2.09	0.53
1:A:496:ALA:HB1	1:A:497:PRO:CD	2.38	0.53
1:A:91:TYR:C	1:A:93:LYS:H	2.11	0.53
1:A:323:LYS:HD3	1:A:417:LEU:HD22	1.89	0.53
1:A:121:THR:HG23	1:A:128:VAL:HG13	1.89	0.53
1:A:89:PRO:HG2	1:A:91:TYR:CE2	2.44	0.53
1:A:529:TYR:CE1	1:A:563:PRO:HD3	2.43	0.53
1:A:318:SER:HB3	1:A:337:VAL:C	2.30	0.52
1:A:378:MET:HE2	1:A:381:CYS:HB3	1.92	0.52
1:A:524:TYR:CD2	1:A:524:TYR:N	2.75	0.52
1:A:43:VAL:HG23	1:A:107:ILE:HD12	1.90	0.52
1:A:120:MET:CE	1:A:122:LEU:HD21	2.39	0.52
1:A:421:VAL:HG23	1:A:422:GLU:H	1.74	0.52
1:A:438:GLY:C	1:A:440:GLY:H	2.11	0.52
1:A:522:LEU:HD12	1:A:523:GLN:N	2.24	0.52
1:A:526:LEU:CD1	1:A:527:ALA:N	2.72	0.52
1:A:119:PHE:HA	1:A:131:PHE:O	2.09	0.52
1:A:527:ALA:HA	1:A:539:VAL:O	2.10	0.52
1:A:507:ASP:HA	1:A:531:THR:OG1	2.10	0.51
1:A:323:LYS:HB3	1:A:333:MET:HE2	1.92	0.51
1:A:542:VAL:O	1:A:542:VAL:HG12	2.09	0.51
1:A:89:PRO:HG2	1:A:91:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:CG1	1:A:425:ILE:HG12	2.41	0.51
1:A:556:ARG:HH12	1:A:125:ASN:HA	1.75	0.51
1:A:377:ARG:O	1:A:377:ARG:HD2	2.11	0.51
1:A:437:HIS:N	1:A:437:HIS:ND1	2.59	0.51
1:A:514:LEU:HD21	1:A:524:TYR:CD1	2.46	0.51
1:A:531:THR:HA	1:A:536:HIS:CD2	2.46	0.51
1:A:296:LEU:HD12	1:A:297:ALA:N	2.26	0.50
1:A:50:GLU:HB3	1:A:51:ARG:NH2	2.26	0.50
1:A:456:ILE:HB	1:A:466:VAL:HB	1.93	0.50
1:A:415:VAL:HG12	1:A:425:ILE:HG12	1.93	0.50
1:A:45:LEU:HD12	1:A:105:LEU:O	2.11	0.50
1:A:587:ASP:CG	1:A:588:SER:N	2.65	0.50
1:A:458:PRO:HG3	1:A:465:GLY:CA	2.42	0.50
1:A:45:LEU:H	1:A:45:LEU:HD12	1.77	0.50
1:A:307:THR:O	1:A:309:PRO:HD3	2.12	0.49
1:A:294:LEU:H	1:A:294:LEU:HD23	1.77	0.49
1:A:503:GLU:OE1	1:A:76:ASN:HB3	2.11	0.49
1:A:526:LEU:HB3	1:A:541:TYR:HB2	1.94	0.49
2:A:901:NAG:H83	2:A:901:NAG:O3	2.13	0.49
1:A:482:LEU:HB3	1:A:483:PHE:CE1	2.47	0.49
1:A:487:ILE:HG23	1:A:488:LYS:HE2	1.94	0.49
1:A:525:VAL:HG12	1:A:526:LEU:N	2.26	0.49
1:A:101:GLU:N	1:A:101:GLU:CD	2.66	0.49
1:A:512:SER:HB3	1:A:566:LEU:HD23	1.93	0.49
1:A:572:THR:HG22	1:A:573:TRP:N	2.26	0.49
1:A:85:GLU:O	1:A:87:GLY:N	2.44	0.49
1:A:402:LEU:C	1:A:404:ASP:H	2.16	0.49
1:A:475:ARG:HG2	1:A:476:PHE:N	2.28	0.49
1:A:522:LEU:HD12	1:A:523:GLN:H	1.77	0.49
1:A:81:LEU:CD2	1:A:83:PRO:HD3	2.41	0.49
1:A:399:TRP:CZ2	1:A:438:GLY:HA3	2.48	0.49
1:A:537:ALA:CB	1:A:556:ARG:HA	2.43	0.48
1:A:258:GLY:HA2	1:A:273:THR:OG1	2.13	0.48
1:A:583:CYS:O	1:A:595:THR:HA	2.13	0.48
1:A:77:LYS:HE3	1:A:80:SER:HB2	1.94	0.48
1:A:318:SER:HB2	1:A:336:TRP:CE2	2.48	0.48
1:A:547:ARG:O	1:A:548:SER:HB2	2.13	0.48
1:A:70:LEU:N	1:A:70:LEU:HD22	2.28	0.48
1:A:376:LEU:H	1:A:376:LEU:HD23	1.78	0.48
1:A:517:LEU:HD11	1:A:525:VAL:HG23	1.94	0.48
1:A:36:VAL:HG12	1:A:136:LYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:THR:HA	1:A:536:HIS:HD2	1.79	0.48
1:A:65:THR:OG1	1:A:119:PHE:HB2	2.14	0.48
1:A:317:VAL:O	1:A:339:LEU:CD2	2.62	0.48
1:A:368:PRO:HD3	1:A:441:MET:CE	2.38	0.48
1:A:378:MET:CE	1:A:378:MET:HA	2.44	0.48
1:A:304:ASP:N	1:A:304:ASP:OD2	2.44	0.48
1:A:384:GLN:HB3	1:A:487:ILE:CG2	2.44	0.48
1:A:315:LYS:HD2	1:A:315:LYS:C	2.34	0.47
1:A:348:ARG:HD3	1:A:350:TYR:CZ	2.49	0.47
1:A:262:ASN:HB2	1:A:573:TRP:HZ2	1.79	0.47
1:A:101:GLU:CD	1:A:101:GLU:H	2.18	0.47
1:A:285:SER:HA	1:A:302:GLY:HA2	1.95	0.47
1:A:49:HIS:HD2	1:A:51:ARG:HH21	1.62	0.47
1:A:60:ILE:CG2	1:A:60:ILE:O	2.60	0.47
1:A:65:THR:HA	1:A:76:ASN:O	2.14	0.47
1:A:45:LEU:HD21	1:A:135:LEU:HD22	1.96	0.47
1:A:97:ARG:HH11	1:A:97:ARG:HG2	1.76	0.47
1:A:488:LYS:O	1:A:489:GLU:HB2	2.14	0.47
1:A:432:GLY:O	1:A:433:PRO:C	2.53	0.46
1:A:96:TYR:HA	1:A:106:ALA:O	2.15	0.46
1:A:407:ILE:O	1:A:408:PRO:C	2.54	0.46
1:A:548:SER:CB	1:A:70:LEU:HB3	2.42	0.46
1:A:253:ARG:NH2	1:A:285:SER:O	2.48	0.46
1:A:294:LEU:N	1:A:294:LEU:HD23	2.29	0.46
1:A:293:GLU:O	1:A:295:LYS:HG2	2.16	0.46
1:A:316:GLY:O	1:A:317:VAL:O	2.33	0.46
1:A:486:PRO:HA	1:A:495:HIS:HA	1.98	0.46
1:A:538:VAL:O	1:A:555:PHE:N	2.44	0.46
1:A:45:LEU:O	1:A:104:SER:HA	2.16	0.46
1:A:32:CYS:HA	1:A:33:PRO:HD3	1.82	0.45
1:A:50:GLU:O	1:A:50:GLU:HG3	2.17	0.45
1:A:507:ASP:OD2	1:A:90:ARG:NH1	2.50	0.45
1:A:71:GLU:N	1:A:71:GLU:CD	2.70	0.45
1:A:393:LEU:HD23	1:A:436:THR:OG1	2.17	0.45
1:A:70:LEU:HD21	1:A:117:TRP:CZ2	2.52	0.45
1:A:259:VAL:O	1:A:261:ARG:N	2.50	0.45
1:A:47:LEU:O	1:A:48:THR:HB	2.16	0.45
1:A:445:LYS:HB3	1:A:445:LYS:HE2	1.77	0.45
1:A:122:LEU:HD12	1:A:131:PHE:HE1	1.81	0.44
1:A:347:ASP:OD1	1:A:348:ARG:HG2	2.17	0.44
1:A:457:PRO:HB3	1:A:513:ASN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:CD2	1:A:252:TYR:N	2.86	0.44
1:A:407:ILE:HG22	1:A:407:ILE:O	2.17	0.44
1:A:484:THR:HA	1:A:496:ALA:O	2.17	0.44
1:A:526:LEU:HD13	1:A:527:ALA:N	2.30	0.44
1:A:318:SER:CB	1:A:338:PRO:HA	2.47	0.44
1:A:459:MET:CB	1:A:463:ALA:HB3	2.23	0.44
1:A:488:LYS:HD2	1:A:488:LYS:O	2.17	0.44
1:A:35:ILE:HD13	1:A:45:LEU:HB3	1.98	0.44
1:A:311:GLN:HG2	1:A:312:GLY:N	2.33	0.44
1:A:339:LEU:CD2	1:A:339:LEU:N	2.79	0.44
1:A:577:LEU:HG	1:A:577:LEU:O	2.18	0.44
1:A:62:ILE:HG23	1:A:122:LEU:HD23	1.99	0.44
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.83	0.44
1:A:209:TYR:CE1	1:A:234:VAL:HG11	2.53	0.44
1:A:231:THR:HG21	1:A:287:CYS:HB2	1.99	0.44
1:A:481:TYR:CD2	1:A:482:LEU:HG	2.52	0.44
1:A:392:ALA:HB3	1:A:499:TYR:CE2	2.53	0.44
1:A:509:LYS:HE2	1:A:531:THR:OG1	2.18	0.44
1:A:553:TYR:CE2	1:A:554:PRO:O	2.71	0.44
1:A:350:TYR:O	1:A:368:PRO:HG2	2.18	0.44
1:A:553:TYR:CD2	1:A:554:PRO:N	2.85	0.44
1:A:310:TYR:CE1	1:A:372:THR:HG21	2.53	0.43
1:A:458:PRO:HA	1:A:464:LEU:O	2.18	0.43
1:A:529:TYR:CD1	1:A:563:PRO:HG3	2.53	0.43
1:A:446:SER:OG	1:A:447:ASN:N	2.51	0.43
1:A:539:VAL:HG22	1:A:554:PRO:HA	2.00	0.43
1:A:521:ASP:N	1:A:521:ASP:OD2	2.52	0.43
1:A:231:THR:OG1	1:A:253:ARG:HD2	2.18	0.43
1:A:86:ALA:O	1:A:88:PRO:HD2	2.18	0.43
1:A:376:LEU:N	1:A:376:LEU:HD23	2.33	0.43
1:A:62:ILE:HA	1:A:121:THR:O	2.18	0.43
1:A:98:PHE:HA	1:A:104:SER:O	2.18	0.43
1:A:464:LEU:HD23	1:A:483:PHE:HB3	2.01	0.43
1:A:482:LEU:HB3	1:A:483:PHE:CD1	2.54	0.43
1:A:122:LEU:CD1	1:A:131:PHE:HE1	2.32	0.43
1:A:35:ILE:CD1	1:A:45:LEU:HB3	2.48	0.43
1:A:526:LEU:O	1:A:540:TYR:HA	2.19	0.43
1:A:212:ARG:HE	1:A:212:ARG:HB3	1.35	0.42
1:A:267:ALA:HB1	1:A:268:PRO:HD2	2.01	0.42
1:A:293:GLU:O	1:A:295:LYS:N	2.52	0.42
1:A:402:LEU:HD23	1:A:406:ARG:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:HB3	1:A:227:MET:HE3	2.01	0.42
1:A:332:ASP:O	1:A:333:MET:HB3	2.18	0.42
1:A:419:LEU:CD2	1:A:423:LEU:HD11	2.34	0.42
1:A:547:ARG:HD3	1:A:547:ARG:HA	1.70	0.42
1:A:210:LEU:HD13	1:A:597:SER:HB3	2.01	0.42
1:A:436:THR:CG2	1:A:497:PRO:HG2	2.50	0.42
1:A:271:HIS:CD2	1:A:272:MET:O	2.73	0.42
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.76	0.42
1:A:480:PRO:HG3	1:A:495:HIS:CD2	2.55	0.42
1:A:579:CYS:O	1:A:599:MET:HA	2.20	0.42
1:A:308:ILE:N	1:A:308:ILE:HD12	2.34	0.42
1:A:377:ARG:HH11	1:A:377:ARG:HG3	1.85	0.42
1:A:307:THR:HA	1:A:348:ARG:HB3	2.02	0.42
1:A:459:MET:HE2	1:A:459:MET:HA	2.01	0.42
1:A:441:MET:HG3	1:A:454:LEU:HD21	2.02	0.42
1:A:430:GLY:HA3	1:A:476:PHE:CE2	2.55	0.42
1:A:464:LEU:HD22	1:A:498:THR:HG21	2.01	0.42
1:A:223:THR:HG22	1:A:260:ILE:HD11	2.02	0.42
1:A:348:ARG:HG3	1:A:370:THR:HG1	1.81	0.42
1:A:539:VAL:HG13	1:A:553:TYR:O	2.20	0.42
1:A:235:GLU:HG2	1:A:251:MET:HG3	2.02	0.42
1:A:400:ALA:N	1:A:401:PRO:HD2	2.34	0.42
1:A:85:GLU:CG	1:A:86:ALA:H	2.08	0.42
1:A:451:VAL:HG23	1:A:470:LEU:O	2.20	0.41
1:A:501:PRO:O	1:A:504:VAL:HG23	2.20	0.41
1:A:53:ASN:O	1:A:56:MET:HG2	2.20	0.41
1:A:523:GLN:C	1:A:524:TYR:HD2	2.23	0.41
1:A:572:THR:CG2	1:A:573:TRP:N	2.83	0.41
1:A:215:ASN:HB2	1:A:235:GLU:CG	2.50	0.41
1:A:100:LEU:HB3	1:A:101:GLU:H	1.75	0.41
1:A:514:LEU:HD23	1:A:515:VAL:H	1.82	0.41
1:A:210:LEU:C	1:A:212:ARG:H	2.24	0.41
1:A:268:PRO:HD3	1:A:573:TRP:CE3	2.56	0.41
1:A:231:THR:HA	1:A:254:VAL:O	2.19	0.41
1:A:424:LYS:HZ2	1:A:424:LYS:HB2	1.86	0.41
1:A:410:TYR:HD2	1:A:454:LEU:HD11	1.85	0.41
1:A:523:GLN:O	1:A:524:TYR:HB3	2.21	0.41
1:A:94:ASP:OD1	1:A:95:ARG:HG3	2.19	0.41
1:A:203:LEU:HB2	1:A:271:HIS:HA	2.02	0.41
1:A:354:HIS:CG	1:A:367:VAL:HG12	2.56	0.41
1:A:421:VAL:O	1:A:422:GLU:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ASN:HD21	1:A:462:LEU:HD23	1.82	0.41
1:A:88:PRO:HA	1:A:89:PRO:HD2	1.91	0.41
1:A:271:HIS:CD2	1:A:272:MET:N	2.89	0.41
1:A:215:ASN:HB2	1:A:235:GLU:HG3	2.02	0.41
1:A:467:ILE:C	1:A:468:ASN:ND2	2.74	0.41
1:A:410:TYR:CE1	1:A:435:ILE:HD11	2.56	0.41
1:A:580:ARG:HE	1:A:599:MET:HE2	1.84	0.41
1:A:271:HIS:HD2	1:A:272:MET:N	2.19	0.40
1:A:340:SER:C	1:A:342:ASP:H	2.23	0.40
1:A:461:ASN:ND2	1:A:504:VAL:HG13	2.36	0.40
1:A:415:VAL:HG12	1:A:425:ILE:HA	2.03	0.40
1:A:62:ILE:HG22	1:A:63:VAL:N	2.36	0.40
1:A:195:ARG:HH11	1:A:195:ARG:HG3	1.85	0.40
1:A:61:HIS:C	1:A:62:ILE:HG13	2.41	0.40
1:A:65:THR:HB	1:A:75:GLU:HG3	2.03	0.40
1:A:334:GLN:HE21	1:A:334:GLN:HB2	1.55	0.40
1:A:526:LEU:HD12	1:A:527:ALA:N	2.36	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	A	502/559 (90%)	372 (74%)	79 (16%)	51 (10%)	<b>0</b> <b>7</b>

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	LEU
1	A	317	VAL
1	A	422	GLU
1	A	439	SER

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Mol	Chain	Res	Type
1	A	441	MET
1	A	449	ASN
1	A	533	ARG
1	A	542	VAL
1	A	550	SER
1	A	48	THR
1	A	53	ASN
1	A	75	GLU
1	A	100	LEU
1	A	378	MET
1	A	389	LYS
1	A	421	VAL
1	A	433	PRO
1	A	589	GLU
1	A	47	LEU
1	A	60	ILE
1	A	86	ALA
1	A	114	ASP
1	A	225	GLN
1	A	301	HIS
1	A	319	PHE
1	A	408	PRO
1	A	419	LEU
1	A	420	THR
1	A	486	PRO
1	A	512	SER
1	A	590	SER
1	A	84	SER
1	A	101	GLU
1	A	340	SER
1	A	352	SER
1	A	373	ASP
1	A	403	LYS
1	A	476	PHE
1	A	524	TYR
1	A	125	ASN
1	A	260	ILE
1	A	43	VAL
1	A	108	TYR
1	A	302	GLY
1	A	545	PRO
1	A	85	GLU

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Mol	Chain	Res	Type
1	A	279	PRO
1	A	554	PRO
1	A	388	GLY
1	A	544	SER
1	A	83	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	A	452/489 (92%)	405 (90%)	47 (10%)	7 33

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	SER
1	A	212	ARG
1	A	227	MET
1	A	280	VAL
1	A	285	SER
1	A	294	LEU
1	A	296	LEU
1	A	304	ASP
1	A	310	TYR
1	A	315	LYS
1	A	320	GLN
1	A	331	THR
1	A	333	MET
1	A	334	GLN
1	A	335	SER
1	A	339	LEU
1	A	355	ARG
1	A	357	VAL
1	A	376	LEU
1	A	379	GLU
1	A	381	CYS

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Mol	Chain	Res	Type
1	A	387	LYS
1	A	408	PRO
1	A	424	LYS
1	A	433	PRO
1	A	436	THR
1	A	449	ASN
1	A	455	THR
1	A	461	ASN
1	A	472	TRP
1	A	483	PHE
1	A	484	THR
1	A	488	LYS
1	A	510	LEU
1	A	524	TYR
1	A	526	LEU
1	A	530	ASP
1	A	554	PRO
1	A	559	ILE
1	A	562	VAL
1	A	45	LEU
1	A	51	ARG
1	A	58	LYS
1	A	71	GLU
1	A	97	ARG
1	A	101	GLU
1	A	125	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	A	197	GLN
1	A	271	HIS
1	A	278	GLN
1	A	320	GLN
1	A	449	ASN
1	A	461	ASN
1	A	468	ASN
1	A	581	HIS
1	A	49	HIS
1	A	129	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	A	801	1	14,14,15	0.98	1 (7%)	17,19,21	0.56	0
2	NAG	A	901	1	14,14,15	0.87	1 (7%)	17,19,21	0.74	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
2	NAG	A	801	1	-	6/6/23/26	0/1/1/1
2	NAG	A	901	1	-	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)
2	A	801	NAG	C1-C2	2.97	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAG	C1-C2	2.35	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
2	A	901	NAG	C8-C7-N2-C2
2	A	901	NAG	O7-C7-N2-C2
2	A	801	NAG	O5-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6
2	A	801	NAG	C1-C2-N2-C7
2	A	801	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	510/559 (91%)	-0.16	5 (0%) 82 70	68, 136, 201, 220	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	TYR	2.9
1	A	398	GLU	2.6
1	A	310	TYR	2.4
1	A	137	LEU	2.4
1	A	311	GLN	2.1

### 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 monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	NAG	A	801	14/15	0.81	0.32	160,166,168,168	0
2	NAG	A	901	14/15	0.81	0.28	153,156,159,160	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.