



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:35 PM BST

PDB ID : 3RJQ  
Title : Crystal structure of anti-HIV llama VHH antibody A12 in complex with C186 gp120  
Authors : Chen, L.; McLellan, J.S.; Kwon, Y.D.; Schmidt, S.; Wu, X.; Zhou, T.; Yang, Y.; Zhang, B.; Forsman, A.; Weiss, R.A.; Verrips, T.; Mascola, J.; Kwong, P.D.  
Deposited on : 2011-04-15  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

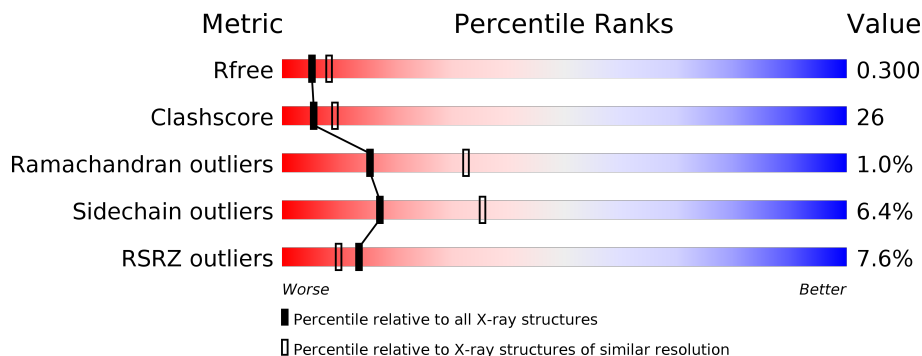
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	382	
2	B	143	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	734	X	-	-	-
3	NAG	A	741	-	-	-	X
3	NAG	A	897	X	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3390 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.

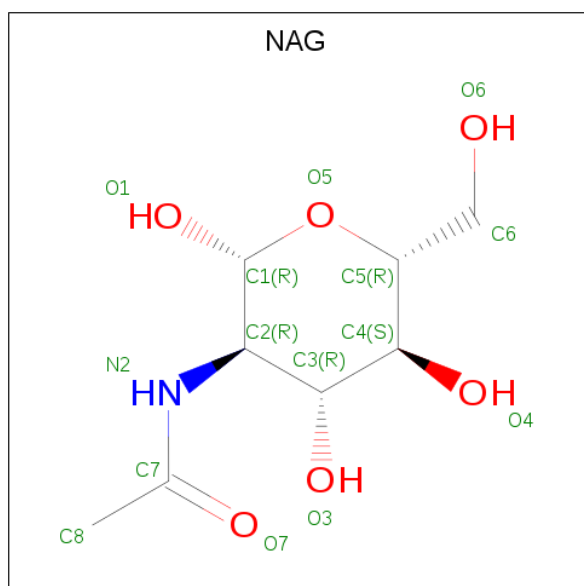
- Molecule 1 is a protein called C186 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2302	1443	396	446	17	0	0	0

- Molecule 2 is a protein called Llama VHH A12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	127	976	609	169	194	4	2	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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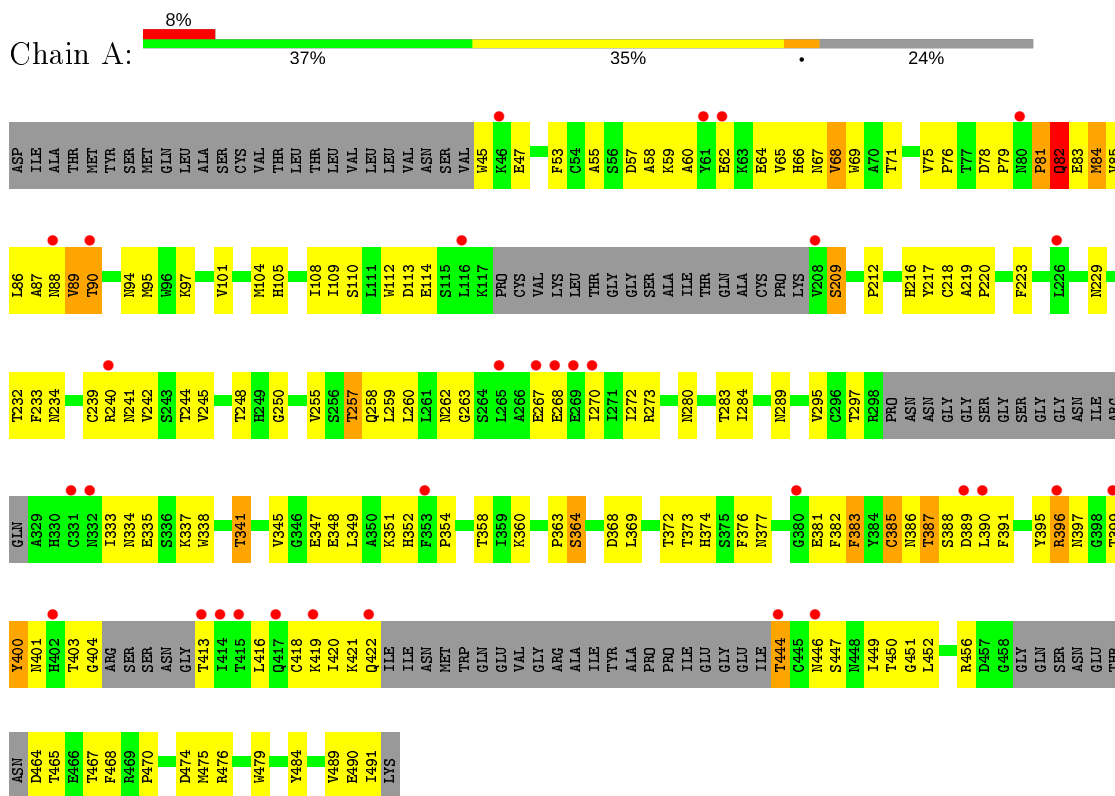
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>ZeroOcc</b>	<b>AltConf</b>
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

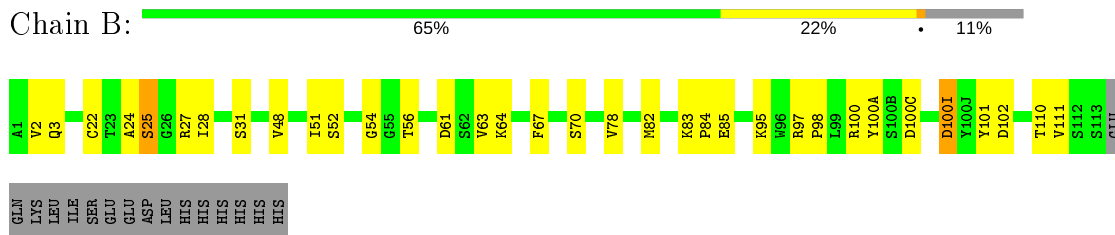
### 3 Residue-property plots i

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

- Molecule 1: C186 gp120



- Molecule 2: Llama VHH A12



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.60Å 66.60Å 266.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.47 – 2.60 23.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	69.0 (23.47-2.60) 69.0 (23.47-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.97 (at 2.60Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.255 , 0.299 0.262 , 0.300	Depositor DCC
$R_{free}$ test set	659 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 68.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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	0.27	0/2348	0.48	1/3181 (0.0%)
2	B	0.27	0/999	0.45	0/1353
All	All	0.27	0/3347	0.47	1/4534 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	PRO	C-N-CA	5.27	134.87	121.70

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	2302	0	2199	150	0
2	B	976	0	922	24	0
3	A	112	0	104	10	0
All	All	3390	0	3225	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 26.



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:389:ASP:OD1	1:A:403:THR:HG22	1.45	1.16
1:A:389:ASP:CA	1:A:403:THR:HG21	1.77	1.15
1:A:395:TYR:CD2	1:A:399:THR:HB	1.81	1.14
1:A:81:PRO:HA	1:A:82:GLN:HB3	1.10	1.06
1:A:389:ASP:CB	1:A:403:THR:HG21	1.86	1.06
1:A:81:PRO:HA	1:A:82:GLN:CB	1.86	1.05
1:A:395:TYR:HD2	1:A:399:THR:HB	0.92	1.05
1:A:241:ASN:OD1	3:A:741:NAG:H2	1.54	1.03
1:A:389:ASP:OD1	1:A:403:THR:CG2	2.06	1.02
1:A:81:PRO:CA	1:A:82:GLN:HB3	1.91	1.01
1:A:419:LYS:HD3	1:A:420:ILE:H	1.28	0.96
1:A:82:GLN:HG2	1:A:82:GLN:O	1.66	0.94
1:A:389:ASP:HA	1:A:403:THR:HG21	1.44	0.94
1:A:395:TYR:OH	1:A:401:ASN:HB2	1.70	0.91
1:A:389:ASP:HA	1:A:403:THR:CG2	2.03	0.88
1:A:395:TYR:HD2	1:A:399:THR:CB	1.83	0.88
1:A:241:ASN:OD1	3:A:741:NAG:C2	2.07	0.85
1:A:420:ILE:HG22	1:A:421:LYS:H	1.40	0.85
1:A:382:PHE:HB2	1:A:421:LYS:HG3	1.59	0.84
1:A:83:GLU:HG2	1:A:245:VAL:HG12	1.59	0.83
1:A:45:TRP:N	1:A:491:ILE:HA	1.94	0.82
1:A:90:THR:HG22	1:A:240:ARG:HG3	1.66	0.78
1:A:421:LYS:O	1:A:422:GLN:HB2	1.87	0.75
1:A:419:LYS:HD3	1:A:420:ILE:N	2.01	0.73
1:A:64:GLU:HA	1:A:209:SER:HB2	1.69	0.72
1:A:389:ASP:HB3	1:A:403:THR:HG21	1.71	0.71
1:A:358:THR:HB	1:A:465:THR:HG22	1.73	0.71
1:A:95:MET:SD	1:A:273:ARG:HD2	2.32	0.70
1:A:389:ASP:CB	1:A:403:THR:CG2	2.67	0.70
1:A:404:GLY:H	3:A:892:NAG:H62	1.57	0.70
1:A:234:ASN:O	1:A:273:ARG:HG2	1.92	0.69
1:A:229:ASN:CG	3:A:741:NAG:O6	2.31	0.69
1:A:420:ILE:HG22	1:A:421:LYS:N	2.08	0.68
1:A:79:PRO:C	1:A:81:PRO:HD3	2.15	0.68
1:A:79:PRO:O	1:A:81:PRO:HD3	1.94	0.67
1:A:110:SER:O	1:A:114:GLU:HG2	1.95	0.66
1:A:64:GLU:OE1	1:A:66:HIS:HB2	1.96	0.65
1:A:272:ILE:HG12	1:A:352:HIS:CE1	2.31	0.65
1:A:474:ASP:OD1	1:A:476:ARG:HG3	1.97	0.64
1:A:217:TYR:O	1:A:248:THR:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:HA	1:A:489:VAL:HG12	1.81	0.62
1:A:259:LEU:HD13	1:A:449:ILE:HD13	1.82	0.61
1:A:270:ILE:HB	1:A:348:GLU:HG3	1.82	0.61
1:A:335:GLU:HG3	1:A:413:THR:HA	1.83	0.61
1:A:64:GLU:HB3	1:A:67:ASN:HD22	1.65	0.61
1:A:389:ASP:CG	1:A:403:THR:CG2	2.69	0.61
1:A:297:THR:HB	1:A:444:THR:HB	1.83	0.60
1:A:64:GLU:OE2	1:A:66:HIS:HD2	1.84	0.60
1:A:386:ASN:OD1	1:A:388:SER:OG	2.18	0.60
1:A:263:GLY:O	1:A:450:THR:HG21	2.02	0.60
1:A:363:PRO:HG3	1:A:388:SER:HA	1.85	0.59
2:B:3:GLN:HB2	2:B:25:SER:OG	2.02	0.59
1:A:272:ILE:HG12	1:A:352:HIS:HE1	1.68	0.59
1:A:260:LEU:HD12	1:A:451:GLY:HA3	1.85	0.58
2:B:2:VAL:CG1	2:B:24:ALA:HB1	2.33	0.58
1:A:420:ILE:CG2	1:A:421:LYS:H	2.16	0.57
1:A:349:LEU:HD13	1:A:468:PHE:CE2	2.40	0.57
1:A:53:PHE:CZ	1:A:218:CYS:HB2	2.40	0.57
1:A:389:ASP:CG	1:A:403:THR:HG22	2.25	0.57
1:A:232:THR:HG22	1:A:232:THR:O	2.04	0.56
2:B:95:LYS:HD2	2:B:100(I):ASP:O	2.07	0.55
1:A:347:GLU:O	1:A:351:LYS:HG3	2.07	0.55
1:A:464:ASP:OD2	1:A:465:THR:HG23	2.06	0.55
1:A:268:GLU:O	1:A:289:ASN:ND2	2.40	0.54
1:A:75:VAL:CG1	1:A:76:PRO:HD2	2.38	0.54
1:A:84:MET:HB2	1:A:244:THR:HB	1.90	0.54
1:A:67:ASN:O	1:A:71:THR:HG23	2.08	0.54
1:A:373:THR:HB	1:A:385:CYS:O	2.08	0.54
1:A:360:LYS:HE3	1:A:465:THR:HG21	1.90	0.53
2:B:48:VAL:HG13	2:B:63:VAL:HG21	1.90	0.53
1:A:85:VAL:C	1:A:86:LEU:HD23	2.28	0.53
2:B:63:VAL:HG13	2:B:67:PHE:HB2	1.89	0.53
1:A:474:ASP:HB2	2:B:101:TYR:CE1	2.44	0.52
1:A:94:ASN:ND2	1:A:97:LYS:HB2	2.23	0.52
1:A:83:GLU:HG2	1:A:245:VAL:CG1	2.38	0.51
1:A:272:ILE:O	1:A:272:ILE:HD12	2.11	0.51
1:A:386:ASN:O	1:A:416:LEU:HB3	2.10	0.51
1:A:451:GLY:C	1:A:452:LEU:HD12	2.31	0.51
1:A:64:GLU:OE2	1:A:66:HIS:CD2	2.64	0.50
1:A:381:GLU:HB2	1:A:383:PHE:CE2	2.46	0.50
1:A:391:PHE:CD1	1:A:470:PRO:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:HB2	1:A:456:ARG:O	2.11	0.50
1:A:335:GLU:HG3	1:A:413:THR:CA	2.41	0.50
1:A:364:SER:HB3	1:A:372:THR:HA	1.93	0.50
1:A:86:LEU:HB3	1:A:89:VAL:HG11	1.94	0.50
2:B:52:SER:HB2	2:B:100(C):ASP:O	2.12	0.50
2:B:61:ASP:HA	2:B:64:LYS:HE2	1.93	0.50
1:A:259:LEU:HB2	1:A:374:HIS:CE1	2.47	0.50
1:A:338:TRP:CZ2	1:A:390:LEU:HG	2.47	0.49
1:A:377:ASN:C	1:A:377:ASN:OD1	2.50	0.49
1:A:349:LEU:HD13	1:A:468:PHE:HE2	1.78	0.49
1:A:456:ARG:HD3	1:A:468:PHE:HE1	1.76	0.49
1:A:297:THR:CB	1:A:444:THR:HB	2.42	0.49
1:A:268:GLU:O	3:A:789:NAG:H83	2.13	0.49
1:A:333:ILE:HD12	1:A:390:LEU:HD13	1.93	0.49
1:A:65:VAL:HG13	1:A:209:SER:O	2.13	0.48
1:A:381:GLU:HB2	1:A:383:PHE:HE2	1.77	0.48
1:A:400:TYR:N	1:A:400:TYR:CD2	2.81	0.48
2:B:22:CYS:HB3	2:B:78:VAL:HG12	1.96	0.48
1:A:363:PRO:CG	1:A:388:SER:HA	2.44	0.48
1:A:297:THR:HB	1:A:444:THR:HA	1.96	0.48
1:A:389:ASP:C	1:A:403:THR:HG21	2.31	0.47
1:A:374:HIS:CD2	1:A:376:PHE:CD1	3.02	0.47
1:A:223:PHE:CE1	1:A:490:GLU:HB3	2.49	0.47
1:A:45:TRP:N	1:A:490:GLU:O	2.47	0.47
1:A:391:PHE:CG	1:A:470:PRO:HG3	2.50	0.47
1:A:216:HIS:CE1	1:A:250:GLY:N	2.83	0.47
1:A:389:ASP:HA	1:A:403:THR:HG23	1.93	0.47
1:A:257:THR:O	1:A:258:GLN:HB2	2.15	0.47
2:B:31:SER:HB3	2:B:97:ARG:O	2.15	0.47
1:A:105:HIS:O	1:A:109:ILE:HG13	2.15	0.46
1:A:45:TRP:O	1:A:45:TRP:CG	2.68	0.46
1:A:59:LYS:HD2	1:A:62:GLU:OE2	2.15	0.46
1:A:476:ARG:NH2	2:B:102:ASP:OD1	2.49	0.46
1:A:113:ASP:OD2	2:B:27:ARG:NH2	2.48	0.46
3:A:892:NAG:H83	3:A:892:NAG:H2	1.80	0.46
2:B:67:PHE:CE1	2:B:82:MET:HB3	2.51	0.46
1:A:368:ASP:O	1:A:372:THR:HG23	2.16	0.46
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.84	0.46
1:A:262:ASN:OD1	1:A:447:SER:HB2	2.15	0.46
1:A:400:TYR:HD2	1:A:400:TYR:N	2.13	0.46
2:B:83:LYS:HB3	2:B:85:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:HA	1:A:71:THR:HG21	1.98	0.46
1:A:85:VAL:O	1:A:86:LEU:HD23	2.16	0.46
1:A:484:TYR:H	1:A:484:TYR:HD1	1.64	0.45
2:B:84:PRO:HA	2:B:111:VAL:HB	1.97	0.45
2:B:51:ILE:HA	2:B:56:THR:O	2.17	0.45
1:A:383:PHE:CD2	1:A:383:PHE:N	2.84	0.45
1:A:68:VAL:HG12	1:A:69:TRP:N	2.31	0.45
1:A:112:TRP:CZ3	2:B:98:PRO:HB2	2.52	0.45
1:A:397:ASN:OD1	3:A:897:NAG:C7	2.65	0.45
1:A:55:ALA:HA	1:A:75:VAL:O	2.17	0.45
1:A:47:GLU:CA	1:A:489:VAL:HG12	2.46	0.45
1:A:258:GLN:HG2	1:A:470:PRO:HB2	1.99	0.44
1:A:84:MET:SD	1:A:84:MET:N	2.90	0.44
1:A:66:HIS:CE1	1:A:212:PRO:HA	2.52	0.44
1:A:255:VAL:HG13	1:A:475:MET:SD	2.58	0.44
1:A:104:MET:O	1:A:108:ILE:HG12	2.18	0.44
1:A:283:THR:HG22	1:A:284:ILE:N	2.32	0.44
1:A:295:VAL:HG13	1:A:446:ASN:OD1	2.18	0.44
1:A:387:THR:HG23	1:A:387:THR:O	2.18	0.43
1:A:270:ILE:H	3:A:789:NAG:H61	1.82	0.43
1:A:58:ALA:HB1	1:A:71:THR:HG23	2.00	0.43
1:A:87:ALA:C	1:A:89:VAL:H	2.21	0.43
2:B:3:GLN:HB2	2:B:25:SER:CB	2.48	0.43
2:B:3:GLN:O	2:B:24:ALA:HA	2.18	0.43
1:A:101:VAL:HG13	1:A:479:TRP:HB2	2.00	0.43
1:A:87:ALA:O	1:A:88:ASN:HB2	2.19	0.42
2:B:54:GLY:HA3	2:B:100(C):ASP:OD1	2.19	0.42
1:A:452:LEU:HD12	1:A:452:LEU:N	2.34	0.42
1:A:369:LEU:HD23	2:B:100(A):TYR:HB2	2.01	0.42
1:A:447:SER:HB3	3:A:762:NAG:HN2	1.85	0.42
1:A:255:VAL:HG13	1:A:475:MET:HG3	2.02	0.42
1:A:75:VAL:HG13	1:A:76:PRO:HD2	2.01	0.42
1:A:289:ASN:ND2	3:A:789:NAG:C7	2.76	0.41
1:A:90:THR:HA	1:A:239:CYS:O	2.20	0.41
2:B:63:VAL:CG1	2:B:67:PHE:HB2	2.50	0.41
1:A:341:THR:O	1:A:345:VAL:HG23	2.20	0.41
1:A:348:GLU:HA	1:A:351:LYS:HG3	2.03	0.41
1:A:295:VAL:HG22	1:A:446:ASN:CG	2.41	0.41
1:A:403:THR:HG22	1:A:404:GLY:N	2.36	0.41
1:A:78:ASP:HA	1:A:79:PRO:HD3	1.90	0.41
2:B:100:ARG:HG3	2:B:100:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASN:OD1	1:A:337:LYS:HG3	2.20	0.41
1:A:349:LEU:HD22	1:A:468:PHE:CE2	2.55	0.41
1:A:396:ARG:HG3	1:A:397:ASN:N	2.35	0.41
2:B:24:ALA:CB	2:B:28:ILE:HD11	2.51	0.40
1:A:421:LYS:HB3	1:A:421:LYS:HE3	1.97	0.40
1:A:364:SER:CB	1:A:372:THR:HA	2.52	0.40
1:A:232:THR:CG2	1:A:232:THR:O	2.70	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	280/382 (73%)	253 (90%)	24 (9%)	3 (1%)	14	30
2	B	125/143 (87%)	118 (94%)	6 (5%)	1 (1%)	19	39
All	All	405/525 (77%)	371 (92%)	30 (7%)	4 (1%)	15	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	354	PRO
1	A	396	ARG
2	B	100(I)	ASP

#### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/334 (78%)	240 (92%)	20 (8%)	13	25
2	B	101/117 (86%)	98 (97%)	3 (3%)	41	67
All	All	361/451 (80%)	338 (94%)	23 (6%)	17	35

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	68	VAL
1	A	82	GLN
1	A	84	MET
1	A	89	VAL
1	A	90	THR
1	A	209	SER
1	A	233	PHE
1	A	242	VAL
1	A	257	THR
1	A	267	GLU
1	A	341	THR
1	A	364	SER
1	A	383	PHE
1	A	385	CYS
1	A	387	THR
1	A	400	TYR
1	A	418	CYS
1	A	444	THR
1	A	467	THR
2	B	25	SER
2	B	70	SER
2	B	110	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	67	ASN
1	A	82	GLN
1	A	246	GLN

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Mol	Chain	Res	Type
1	A	374	HIS
2	B	76	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	776	1	14,14,15	0.40	0	17,19,21	2.00	3 (17%)
3	NAG	A	734	1	14,14,15	0.40	0	17,19,21	1.92	2 (11%)
3	NAG	A	897	1	14,14,15	0.60	0	17,19,21	1.20	3 (17%)
3	NAG	A	789	1	14,14,15	0.45	0	17,19,21	0.93	1 (5%)
3	NAG	A	741	1	14,14,15	0.72	0	17,19,21	1.33	2 (11%)
3	NAG	A	762	1	14,14,15	0.55	0	17,19,21	1.05	1 (5%)
3	NAG	A	886	1	14,14,15	0.56	0	17,19,21	0.95	0
3	NAG	A	892	-	14,14,15	0.45	0	17,19,21	1.31	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	776	1	-	3/6/23/26	0/1/1/1
3	NAG	A	734	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	A	897	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	789	1	-	4/6/23/26	0/1/1/1
3	NAG	A	741	1	-	0/6/23/26	0/1/1/1
3	NAG	A	762	1	-	2/6/23/26	0/1/1/1
3	NAG	A	886	1	-	4/6/23/26	0/1/1/1
3	NAG	A	892	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	776	NAG	C1-O5-C5	5.96	120.27	112.19
3	A	734	NAG	C1-O5-C5	5.90	120.19	112.19
3	A	734	NAG	O5-C1-C2	4.17	117.87	111.29
3	A	892	NAG	C1-O5-C5	3.52	116.95	112.19
3	A	741	NAG	O5-C1-C2	-3.32	106.04	111.29
3	A	776	NAG	C4-C3-C2	-3.21	106.31	111.02
3	A	776	NAG	O5-C1-C2	3.20	116.34	111.29
3	A	741	NAG	C1-O5-C5	-3.07	108.03	112.19
3	A	897	NAG	C1-O5-C5	2.66	115.80	112.19
3	A	897	NAG	O5-C5-C6	2.65	111.35	107.20
3	A	892	NAG	C4-C3-C2	-2.47	107.40	111.02
3	A	762	NAG	C1-O5-C5	2.25	115.23	112.19
3	A	789	NAG	O5-C1-C2	-2.16	107.88	111.29
3	A	897	NAG	O5-C1-C2	2.06	114.54	111.29
3	A	892	NAG	C2-N2-C7	-2.01	120.04	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	734	NAG	C1
3	A	897	NAG	C1

All (17) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	A	789	NAG	C8-C7-N2-C2
3	A	789	NAG	O7-C7-N2-C2
3	A	886	NAG	O7-C7-N2-C2
3	A	892	NAG	C8-C7-N2-C2
3	A	892	NAG	O7-C7-N2-C2
3	A	886	NAG	C8-C7-N2-C2
3	A	886	NAG	O5-C5-C6-O6
3	A	762	NAG	O5-C5-C6-O6
3	A	886	NAG	C4-C5-C6-O6
3	A	789	NAG	O5-C5-C6-O6
3	A	734	NAG	C8-C7-N2-C2
3	A	789	NAG	C4-C5-C6-O6
3	A	734	NAG	O7-C7-N2-C2
3	A	762	NAG	C4-C5-C6-O6
3	A	776	NAG	C8-C7-N2-C2
3	A	776	NAG	O7-C7-N2-C2
3	A	776	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	897	NAG	1	0
3	A	789	NAG	3	0
3	A	741	NAG	3	0
3	A	762	NAG	1	0
3	A	892	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	292/382 (76%)	0.63	32 (10%) <b>5</b> <b>3</b>	65, 135, 201, 256	0
2	B	127/143 (88%)	-0.46	0 <b>100</b> <b>100</b>	47, 81, 113, 132	1 (0%)
All	All	419/525 (79%)	0.30	32 (7%) <b>13</b> <b>10</b>	47, 115, 194, 256	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	8.0
1	A	270	ILE	7.1
1	A	413	THR	6.0
1	A	399	THR	5.1
1	A	389	ASP	4.9
1	A	90	THR	4.7
1	A	62	GLU	4.6
1	A	390	LEU	4.2
1	A	415	THR	3.9
1	A	61	TYR	3.7
1	A	267	GLU	3.6
1	A	422	GLN	3.5
1	A	208	VAL	3.4
1	A	446	ASN	3.2
1	A	240	ARG	3.0
1	A	268	GLU	2.9
1	A	88	ASN	2.8
1	A	265	LEU	2.8
1	A	402	HIS	2.6
1	A	331	CYS	2.5
1	A	226	LEU	2.4
1	A	414	ILE	2.4
1	A	46	LYS	2.4
1	A	269	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	80	ASN	2.3
1	A	332	ASN	2.2
1	A	380	GLY	2.1
1	A	116	LEU	2.1
1	A	444	THR	2.1
1	A	419	LYS	2.1
1	A	417	GLN	2.1
1	A	353	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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
3	NAG	A	897	14/15	0.43	0.47	138,142,148,149	0
3	NAG	A	741	14/15	0.67	0.44	181,209,250,257	0
3	NAG	A	892	14/15	0.71	0.24	122,163,173,174	0
3	NAG	A	734	14/15	0.80	0.33	121,140,148,149	0
3	NAG	A	776	14/15	0.81	0.23	92,128,156,161	0
3	NAG	A	789	14/15	0.82	0.21	117,138,153,156	0
3	NAG	A	886	14/15	0.84	0.18	118,134,152,153	0
3	NAG	A	762	14/15	0.84	0.27	109,144,172,178	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.