



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 04:34 AM EDT

PDB ID : 7R74  
Title : Crystal structure of llama VHH antibody in complex with HIV-1 HXBC2 gp120 core  
Authors : Zhou, T.; Kwong, P.D.  
Deposited on : 2021-06-24  
Resolution : 2.76 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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) : 2.35.1

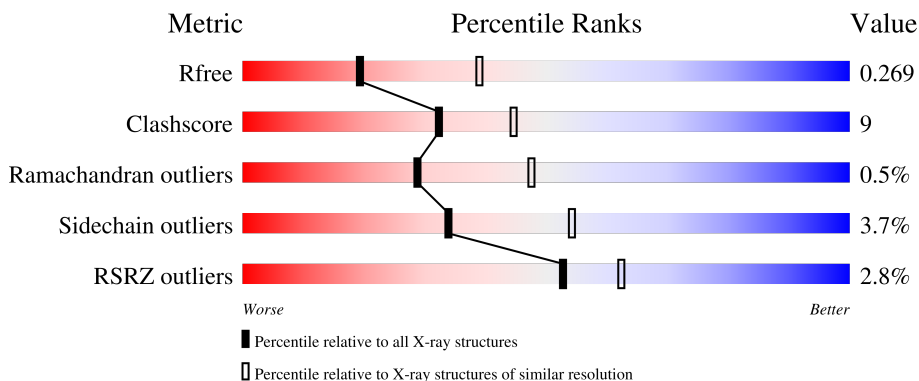
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 of 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	360	
1	C	360	
2	B	118	
2	D	118	

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	503	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6759 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.

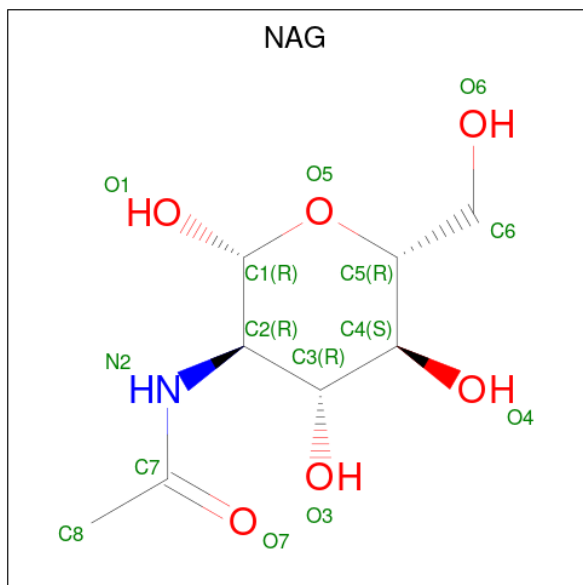
- Molecule 1 is a protein called Glycoprotein 120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	Total 2314	C 1457	N 400	O 438	S 19	0	0	0
1	C	297	Total 2331	C 1469	N 404	O 439	S 19	0	0	0

- Molecule 2 is a protein called Antibody C8 VHH domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	118	Total 891	C 553	N 158	O 176	S 4	0	0	0
2	D	118	Total 890	C 553	N 158	O 175	S 4	0	0	0

- Molecule 3 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
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	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	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	17	Total	O	0	0
			17	17		

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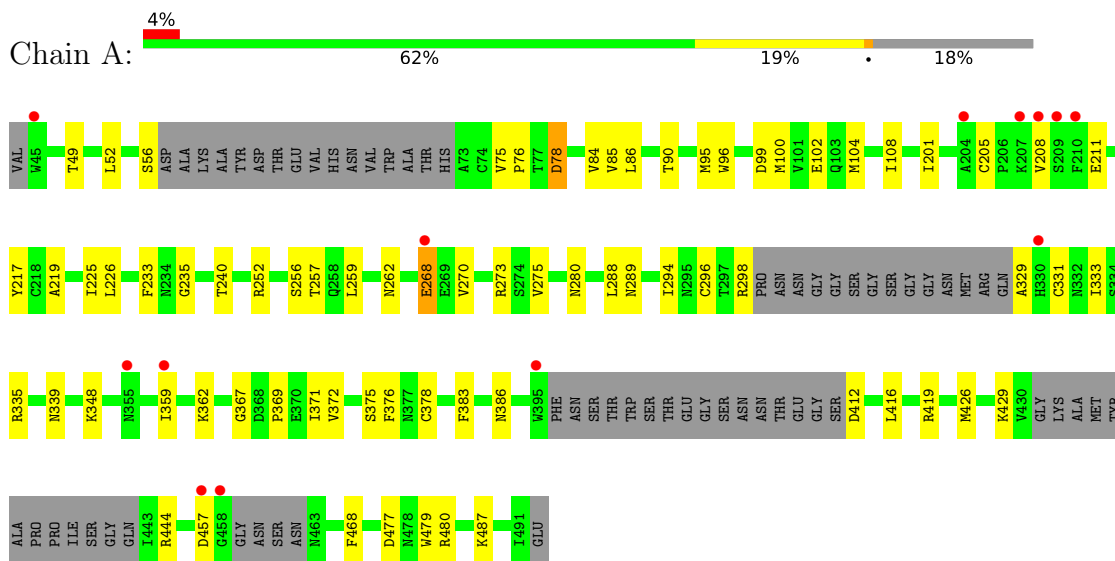
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	21	Total	O	0	0
			21	21		
4	D	13	Total	O	0	0
			13	13		

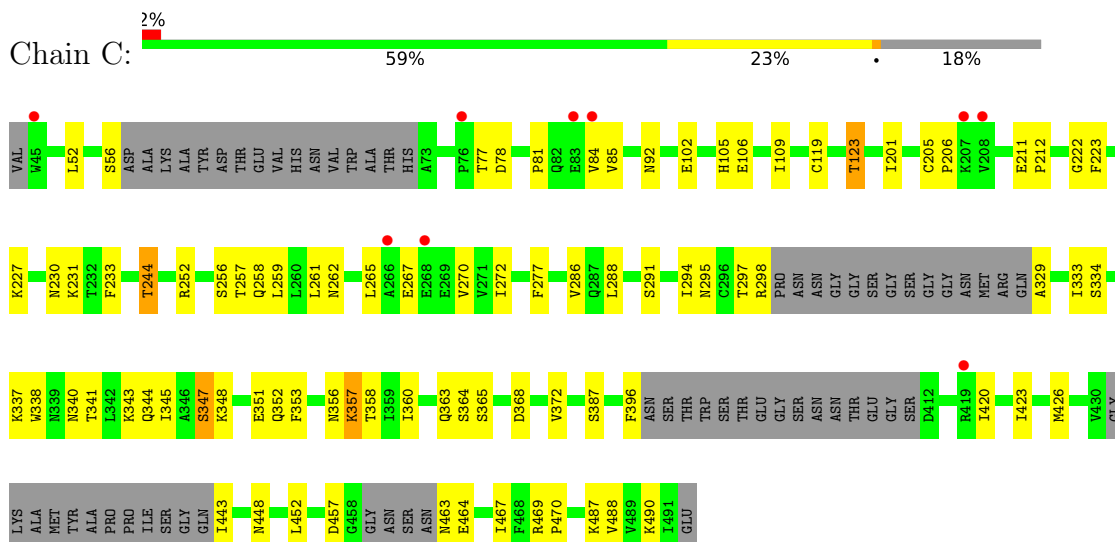
### 3 Residue-property plots i

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: Glycoprotein 120



• Molecule 1: Glycoprotein 120



• Molecule 2: Antibody C8 VHH domain





- Molecule 2: Antibody C8 VHH domain

Chain D: 83% 17%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.08Å 87.40Å 91.58Å 90.00° 109.12° 90.00°	Depositor
Resolution (Å)	49.56 – 2.76 49.56 – 2.76	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.56-2.76) 93.2 (49.56-2.76)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.19-4092	Depositor
R, $R_{free}$	0.212 , 0.270 0.210 , 0.269	Depositor DCC
$R_{free}$ test set	1103 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtrriage
Anisotropy	0.575	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4362e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/2357	0.48	0/3195
1	C	0.26	0/2374	0.51	0/3215
2	B	0.26	0/906	0.54	0/1227
2	D	0.27	0/905	0.54	0/1227
All	All	0.26	0/6542	0.51	0/8864

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	C	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	C	78	ASP	Peptide

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2314	0	2266	41	0
1	C	2331	0	2285	56	0
2	B	891	0	872	14	0
2	D	890	0	872	9	0
3	A	126	0	117	1	1
3	C	126	0	117	2	0
4	A	30	0	0	4	0
4	B	17	0	0	1	0
4	C	21	0	0	7	0
4	D	13	0	0	1	0
All	All	6759	0	6529	116	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 9.

All (116) 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:C:258:GLN:HG2	1:C:470:PRO:HB2	1.65	0.78
1:A:90:THR:HG22	1:A:240:THR:HA	1.65	0.77
1:A:270:VAL:HG22	1:A:288:LEU:HA	1.72	0.71
1:C:231:LYS:HB3	1:C:267:GLU:HB2	1.70	0.71
1:C:102:GLU:OE1	4:C:602:HOH:O	2.08	0.71
3:C:501:NAG:O7	4:C:601:HOH:O	2.08	0.70
1:C:360:ILE:HB	1:C:467:ILE:HD13	1.76	0.68
1:A:78:ASP:OD1	4:A:602:HOH:O	2.14	0.66
1:A:99:ASP:HA	1:A:102:GLU:HG2	1.78	0.66
1:A:256:SER:OG	4:A:601:HOH:O	2.14	0.66
1:C:463:ASN:OD1	1:C:464:GLU:N	2.29	0.66
1:C:298:ARG:HE	1:C:443:ILE:HG21	1.60	0.65
1:C:105:HIS:O	4:C:603:HOH:O	2.15	0.64
1:C:341:THR:O	1:C:345:ILE:HG13	2.01	0.61
1:C:272:ILE:HG22	1:C:286:VAL:HG22	1.84	0.60
1:C:270:VAL:HG22	1:C:288:LEU:HA	1.84	0.60
1:C:52:LEU:HD21	1:C:488:VAL:HG21	1.82	0.59
1:C:227:LYS:NZ	4:C:607:HOH:O	2.35	0.59
2:D:71:ARG:NE	2:D:73:ASN:OD1	2.36	0.58
1:A:96:TRP:CD2	1:A:275:VAL:HG22	2.39	0.58
1:A:298:ARG:HA	1:A:329:ALA:HA	1.86	0.57
2:B:90:THR:HG23	2:B:115:THR:HA	1.87	0.57
1:C:109:ILE:N	4:C:603:HOH:O	2.27	0.57
2:B:32:ASN:O	4:B:201:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.87	0.56
1:A:52:LEU:HD11	1:A:100:MET:HG2	1.88	0.55
1:C:102:GLU:O	1:C:106:GLU:HG3	2.06	0.55
1:A:85:VAL:HB	1:C:85:VAL:HB	1.89	0.55
1:A:268:GLU:O	1:A:289:ASN:ND2	2.40	0.55
1:A:369:PRO:HA	1:A:372:VAL:HG22	1.90	0.54
1:A:84:VAL:HG13	1:C:84:VAL:HB	1.89	0.54
1:A:386:ASN:O	1:A:416:LEU:HG	2.08	0.54
1:C:352:GLN:OE1	4:C:604:HOH:O	2.19	0.53
1:C:230:ASN:HB3	1:C:233:PHE:HB2	1.91	0.53
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.91	0.52
1:A:335:ARG:HH12	1:A:412:ASP:N	2.07	0.52
1:A:426:MET:HG2	2:D:53:GLY:HA2	1.90	0.52
2:B:87:PRO:HA	2:B:116:VAL:HG13	1.91	0.52
2:B:34:MET:HG3	1:C:426:MET:SD	2.50	0.52
1:C:252:ARG:NH1	1:C:262:ASN:HD22	2.08	0.52
2:B:40:ALA:HB3	2:B:43:LYS:HE2	1.91	0.51
2:B:12:VAL:HG11	2:B:18:LEU:HG	1.93	0.51
1:A:359:ILE:HD12	1:A:468:PHE:HE2	1.75	0.51
1:A:95:MET:SD	1:A:235:GLY:HA3	2.51	0.51
1:C:298:ARG:HB3	1:C:443:ILE:HG21	1.92	0.51
1:A:201:ILE:HD13	1:A:429:LYS:HB2	1.93	0.51
1:C:368:ASP:O	1:C:372:VAL:HG23	2.11	0.51
1:A:335:ARG:O	1:A:339:ASN:HB2	2.12	0.49
1:A:52:LEU:HD13	1:A:217:TYR:HB3	1.93	0.49
1:A:211:GLU:N	4:A:606:HOH:O	2.35	0.49
2:B:20:LEU:HD12	2:B:80:LEU:HD23	1.94	0.49
1:C:298:ARG:HD3	1:C:420:ILE:HD12	1.94	0.49
1:C:223:PHE:CZ	1:C:490:LYS:HD3	2.48	0.49
1:A:75:VAL:HG12	1:A:76:PRO:O	2.13	0.48
1:A:375:SER:HA	1:A:383:PHE:O	2.13	0.48
1:A:86:LEU:O	4:A:603:HOH:O	2.20	0.48
1:C:297:THR:O	1:C:329:ALA:HA	2.13	0.48
1:C:347:SER:O	1:C:351:GLU:HG2	2.14	0.48
1:C:294:ILE:HD12	1:C:333:ILE:HD11	1.94	0.47
1:C:265:LEU:HD11	1:C:291:SER:HB3	1.96	0.47
1:A:49:THR:OG1	1:A:99:ASP:OD1	2.24	0.47
3:A:505:NAG:H81	1:C:81:PRO:HB2	1.97	0.47
2:D:39:GLN:HA	4:D:201:HOH:O	2.15	0.46
1:C:56:SER:N	1:C:77:THR:OG1	2.49	0.46
1:A:457:ASP:OD1	1:A:457:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ARG:HB3	2:B:83:ASN:O	2.16	0.46
2:D:48:VAL:HA	2:D:60:ILE:HG12	1.98	0.46
1:A:104:MET:SD	1:A:479:TRP:HB3	2.57	0.45
2:B:4:LEU:HD22	2:B:24:VAL:HG12	1.97	0.45
1:A:257:THR:O	1:A:259:LEU:N	2.46	0.45
2:D:12:VAL:HG23	2:D:116:VAL:HG23	1.99	0.45
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.49	0.45
1:C:211:GLU:OE1	1:C:211:GLU:N	2.48	0.45
1:C:353:PHE:O	1:C:357:LYS:HD3	2.17	0.45
1:C:340:ASN:O	1:C:344:GLN:HG3	2.17	0.45
1:C:358:THR:HG22	1:C:396:PHE:HA	1.99	0.45
1:C:457:ASP:HB3	1:C:467:ILE:HB	1.99	0.44
1:C:363:GLN:O	1:C:469:ARG:NH1	2.47	0.44
1:C:295:ASN:ND2	3:C:501:NAG:O7	2.50	0.44
2:D:66:ARG:HB3	2:D:83:ASN:O	2.17	0.44
1:C:261:LEU:HA	1:C:448:ASN:O	2.18	0.44
1:A:233:PHE:O	1:A:273:ARG:NH2	2.43	0.44
1:C:298:ARG:HB3	1:C:443:ILE:CG2	2.48	0.43
1:C:334:SER:HB3	1:C:337:LYS:HB2	2.01	0.43
1:A:289:ASN:OD1	1:A:289:ASN:N	2.50	0.43
1:C:338:TRP:HH2	1:C:452:LEU:HD11	1.83	0.43
2:D:20:LEU:HD12	2:D:80:LEU:HD23	2.00	0.43
2:D:60:ILE:HG13	2:D:63:VAL:HG22	2.00	0.43
1:A:104:MET:O	1:A:108:ILE:HG12	2.19	0.43
1:A:252:ARG:NH1	1:A:262:ASN:HD22	2.17	0.43
1:A:376:PHE:CE2	1:A:378:CYS:HB2	2.53	0.42
2:B:4:LEU:HB3	2:B:95:CYS:SG	2.59	0.42
1:C:84:VAL:HG23	1:C:244:THR:HG23	2.01	0.42
1:C:109:ILE:HG13	4:C:603:HOH:O	2.19	0.42
1:C:348:LYS:HD3	1:C:348:LYS:HA	1.82	0.42
1:A:296:CYS:HA	1:A:331:CYS:HA	2.02	0.42
1:C:364:SER:HB3	1:C:372:VAL:HG13	2.01	0.42
2:B:100:LEU:HD23	2:B:100:LEU:HA	1.90	0.42
1:C:298:ARG:NE	1:C:443:ILE:HG21	2.32	0.42
1:C:298:ARG:HE	1:C:298:ARG:HB3	1.70	0.42
1:A:362:LYS:HE3	1:A:362:LYS:HB2	1.69	0.42
1:C:222:GLY:O	1:C:490:LYS:HD2	2.19	0.42
2:B:42:GLY:C	2:B:43:LYS:HD3	2.40	0.42
1:C:92:ASN:O	1:C:487:LYS:NZ	2.42	0.42
2:B:32:ASN:OD1	2:B:98:ARG:NH2	2.49	0.42
1:A:226:LEU:HB2	1:A:487:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:SER:OG	1:C:259:LEU:O	2.38	0.41
1:C:123:THR:HG21	1:C:201:ILE:HD11	2.03	0.41
1:C:277:PHE:CG	1:C:352:GLN:HG2	2.55	0.41
1:C:423:ILE:HD13	1:C:423:ILE:HA	1.96	0.41
1:C:344:GLN:HE21	1:C:344:GLN:HB3	1.57	0.41
2:B:50:ARG:O	2:B:57:THR:HA	2.21	0.41
1:A:348:LYS:HD3	1:A:348:LYS:HA	1.90	0.40
1:A:426:MET:SD	2:D:34:MET:HG3	2.61	0.40
1:C:211:GLU:HA	1:C:212:PRO:HD3	1.88	0.40
1:C:257:THR:O	1:C:259:LEU:N	2.55	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)
3:A:508:NAG:O4	3:A:508:NAG:O4[2_555]	2.18	0.02

## 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	284/360 (79%)	260 (92%)	21 (7%)	3 (1%)	14	25
1	C	283/360 (79%)	263 (93%)	19 (7%)	1 (0%)	34	53
2	B	116/118 (98%)	116 (100%)	0	0	100	100
2	D	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
All	All	799/956 (84%)	751 (94%)	44 (6%)	4 (0%)	29	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLU
1	C	206	PRO
1	A	208	VAL
1	A	367	GLY

### 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	266/316 (84%)	259 (97%)	7 (3%)	46	66
1	C	268/316 (85%)	258 (96%)	10 (4%)	34	54
2	B	95/95 (100%)	91 (96%)	4 (4%)	30	49
2	D	95/95 (100%)	89 (94%)	6 (6%)	18	31
All	All	724/822 (88%)	697 (96%)	27 (4%)	34	54

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	78	ASP
1	A	205	CYS
1	A	280	ASN
1	A	371	ILE
1	A	419	ARG
1	A	444	ARG
2	B	21	SER
2	B	25	SER
2	B	73	ASN
2	B	95	CYS
1	C	119	CYS
1	C	123	THR
1	C	205	CYS
1	C	244	THR
1	C	343	LYS
1	C	347	SER
1	C	356	ASN

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Mol	Chain	Res	Type
1	C	357	LYS
1	C	365	SER
1	C	387	SER
2	D	21	SER
2	D	24	VAL
2	D	25	SER
2	D	46	ASP
2	D	50	ARG
2	D	95	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	344	GLN

### 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](#)

18 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	C	502	1	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	C	508	1	14,14,15	0.29	0	17,19,21	0.47	0
3	NAG	A	501	1	14,14,15	0.35	0	17,19,21	0.67	1 (5%)
3	NAG	A	508	1	14,14,15	0.22	0	17,19,21	0.54	0
3	NAG	A	507	1	14,14,15	0.19	0	17,19,21	0.39	0
3	NAG	C	506	1	14,14,15	0.23	0	17,19,21	0.53	0
3	NAG	C	507	1	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	C	509	1	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	A	502	1	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	A	505	1	14,14,15	0.43	0	17,19,21	0.47	0
3	NAG	A	503	1	14,14,15	0.24	0	17,19,21	0.36	0
3	NAG	A	509	1	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	A	506	1	14,14,15	0.33	0	17,19,21	0.52	0
3	NAG	C	501	1	14,14,15	0.38	0	17,19,21	0.52	0
3	NAG	C	503	1	14,14,15	0.23	0	17,19,21	0.36	0
3	NAG	A	504	1	14,14,15	0.19	0	17,19,21	0.37	0
3	NAG	C	505	1	14,14,15	0.30	0	17,19,21	0.57	0
3	NAG	C	504	1	14,14,15	0.20	0	17,19,21	0.46	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
3	NAG	C	502	1	-	1/6/23/26	0/1/1/1
3	NAG	C	508	1	-	2/6/23/26	0/1/1/1
3	NAG	A	501	1	-	2/6/23/26	0/1/1/1
3	NAG	A	508	1	-	2/6/23/26	0/1/1/1
3	NAG	A	507	1	-	4/6/23/26	0/1/1/1
3	NAG	C	506	1	-	0/6/23/26	0/1/1/1
3	NAG	C	507	1	-	0/6/23/26	0/1/1/1
3	NAG	C	509	1	-	2/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	505	1	-	2/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
3	NAG	A	509	1	-	0/6/23/26	0/1/1/1
3	NAG	A	506	1	-	2/6/23/26	0/1/1/1
3	NAG	C	501	1	-	2/6/23/26	0/1/1/1
3	NAG	C	503	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	504	1	-	2/6/23/26	0/1/1/1
3	NAG	C	505	1	-	2/6/23/26	0/1/1/1
3	NAG	C	504	1	-	2/6/23/26	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(°)
3	A	501	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	NAG	O5-C5-C6-O6
3	A	505	NAG	O5-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	C	501	NAG	O5-C5-C6-O6
3	A	506	NAG	C4-C5-C6-O6
3	C	509	NAG	O5-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	A	507	NAG	C4-C5-C6-O6
3	C	503	NAG	C4-C5-C6-O6
3	C	501	NAG	C4-C5-C6-O6
3	C	508	NAG	C4-C5-C6-O6
3	A	507	NAG	C8-C7-N2-C2
3	A	507	NAG	O7-C7-N2-C2
3	C	503	NAG	O5-C5-C6-O6
3	C	505	NAG	O5-C5-C6-O6
3	C	508	NAG	O5-C5-C6-O6
3	C	505	NAG	C4-C5-C6-O6
3	A	505	NAG	C4-C5-C6-O6
3	A	507	NAG	O5-C5-C6-O6
3	C	509	NAG	C4-C5-C6-O6
3	A	508	NAG	C4-C5-C6-O6
3	A	508	NAG	O5-C5-C6-O6
3	C	504	NAG	C4-C5-C6-O6
3	A	504	NAG	C4-C5-C6-O6
3	C	502	NAG	C3-C2-N2-C7
3	C	504	NAG	O5-C5-C6-O6
3	A	504	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	508	NAG	0	1
3	A	505	NAG	1	0
3	C	501	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	124:GLY	C	198:GLY	N	3.35

## 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	296/360 (82%)	0.27	13 (4%) 34 41	29, 50, 81, 103	0
1	C	297/360 (82%)	0.21	9 (3%) 50 59	30, 51, 79, 98	0
2	B	118/118 (100%)	-0.05	1 (0%) 86 90	28, 44, 66, 85	0
2	D	118/118 (100%)	0.10	0 100 100	27, 44, 72, 96	0
All	All	829/956 (86%)	0.18	23 (2%) 53 62	27, 48, 79, 103	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	PHE	6.5
1	A	208	VAL	5.8
1	A	45	TRP	5.0
1	C	45	TRP	4.9
1	A	207	LYS	3.9
1	C	268	GLU	3.1
1	A	209	SER	3.0
1	C	419	ARG	2.8
1	A	458	GLY	2.6
1	C	266	ALA	2.6
1	A	457	ASP	2.6
1	A	355	ASN	2.5
1	A	330	HIS	2.5
1	A	204	ALA	2.5
1	A	359	ILE	2.4
1	A	268	GLU	2.4
1	C	83	GLU	2.3
1	C	208	VAL	2.3
1	C	84	VAL	2.3
1	C	76	PRO	2.2
2	B	42	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	395	TRP	2.1
1	C	207	LYS	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	503	14/15	0.69	0.45	67,98,105,113	0
3	NAG	C	502	14/15	0.73	0.35	71,90,97,102	0
3	NAG	A	505	14/15	0.76	0.24	58,73,81,83	0
3	NAG	A	501	14/15	0.80	0.27	60,78,83,92	0
3	NAG	C	501	14/15	0.82	0.19	51,74,84,84	0
3	NAG	C	505	14/15	0.83	0.34	57,70,86,86	0
3	NAG	A	507	14/15	0.85	0.40	70,79,84,86	0
3	NAG	C	507	14/15	0.85	0.20	48,64,75,80	0
3	NAG	C	503	14/15	0.86	0.37	60,68,76,79	0
3	NAG	A	509	14/15	0.87	0.25	51,63,75,82	0
3	NAG	A	508	14/15	0.88	0.20	58,70,75,83	0
3	NAG	C	509	14/15	0.88	0.26	54,67,79,81	0
3	NAG	C	504	14/15	0.89	0.29	49,61,88,89	0
3	NAG	A	504	14/15	0.89	0.35	70,80,91,96	0
3	NAG	C	508	14/15	0.91	0.16	54,62,71,73	0
3	NAG	A	506	14/15	0.91	0.21	45,56,66,67	0
3	NAG	A	502	14/15	0.92	0.15	48,62,76,76	0
3	NAG	C	506	14/15	0.96	0.12	46,51,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.