



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2025 – 02:08 PM JST

PDB ID : 9ISH / pdb\_00009ish  
Title : Crystal structure of nanobody 32 in complex with HSV-2 gD  
Authors : Hu, J.; Jin, T.C.  
Deposited on : 2024-07-17  
Resolution : 2.88 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

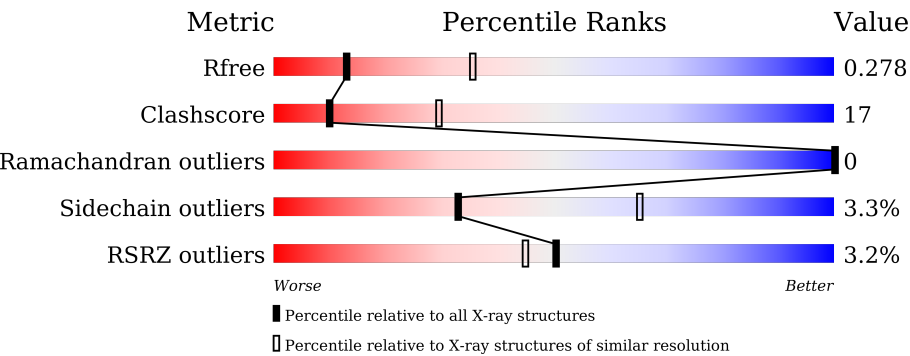
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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))
$R_{free}$	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

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	275	
1	C	275	
2	B	131	
2	D	131	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	301	-	-	X	-
3	NAG	B	201	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6443 atoms, of which 1655 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.

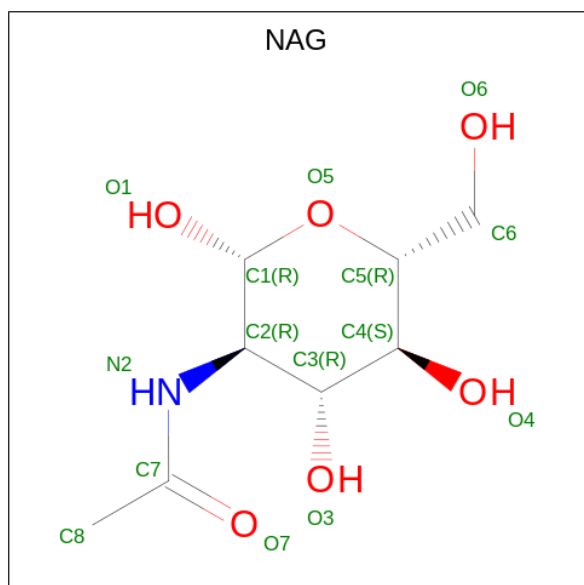
- Molecule 1 is a protein called Glycoprotein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	178	Total	C	N	O	S	0	1	0
			1397	902	234	253	8			
1	A	178	Total	C	N	O	S	0	0	0
			1370	882	229	251	8			

- Molecule 2 is a protein called Nanobody 32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	131	Total	C	H	N	O	S	0	0
			1799	613	819	168	194	5		
2	B	131	Total	C	H	N	O	S	0	0
			1821	617	836	169	194	5		

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

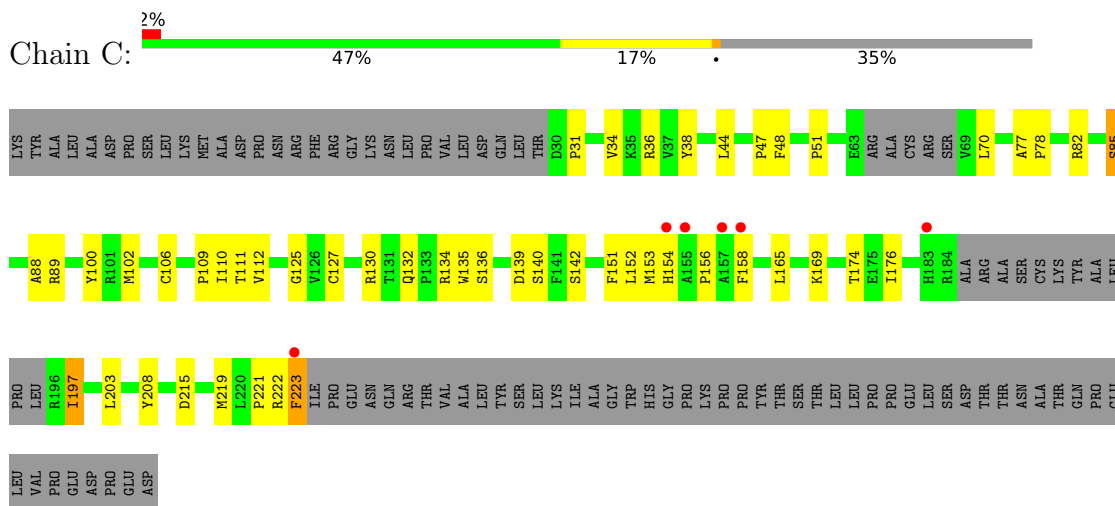


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

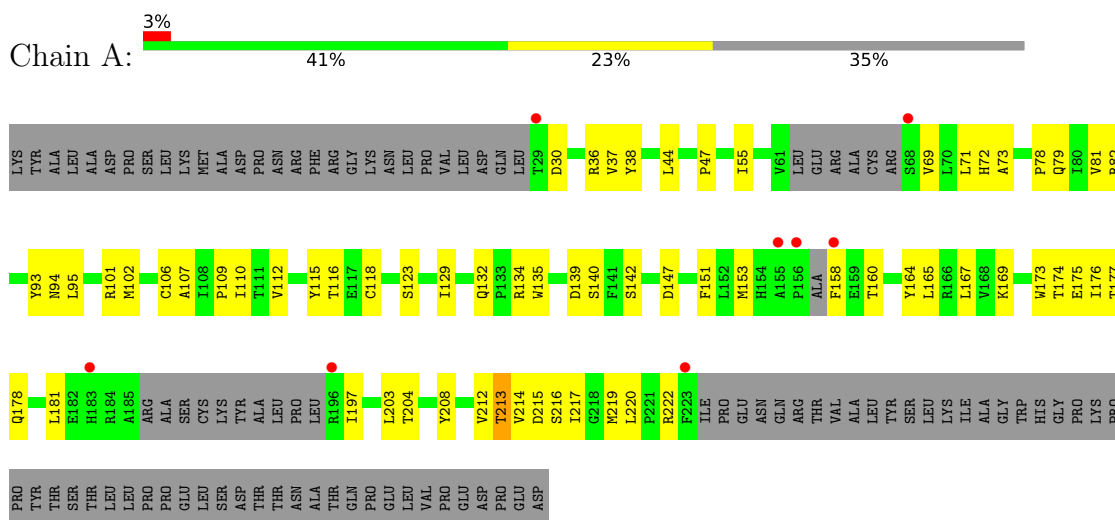
### 3 Residue-property plots [i](#)

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: Glycoprotein D

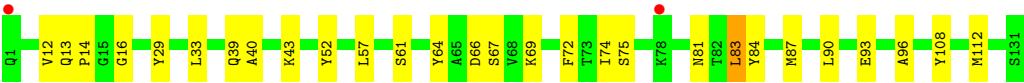


#### • Molecule 1: Glycoprotein D

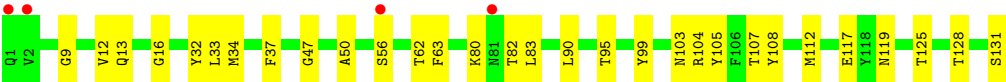
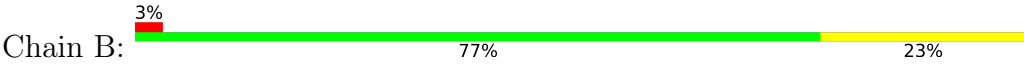


#### • Molecule 2: Nanobody 32





● Molecule 2: Nanobody 32



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.64Å 136.22Å 136.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.28 – 2.88 19.28 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.28-2.88) 99.5 (19.28-2.88)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.88Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.216 , 0.276 0.217 , 0.278	Depositor DCC
$R_{free}$ test set	22108 reflections (8.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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	0.61	0/1410	0.79	0/1933
1	C	0.53	0/1442	0.76	0/1975
2	B	0.43	0/1009	0.64	0/1365
2	D	0.51	0/1004	0.73	1/1360 (0.1%)
All	All	0.53	0/4865	0.74	1/6633 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	83	LEU	N-CA-C	-5.80	100.24	109.76

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	1370	0	1296	74	0
1	C	1397	0	1341	34	0
2	B	985	836	924	19	0
2	D	980	819	911	25	0
3	A	14	0	13	8	0
3	B	14	0	13	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	14	0	13	4	0
3	D	14	0	13	5	0
All	All	4788	1655	4524	159	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 17.

All (159) 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:214:VAL:HG22	1:A:219:MET:HB2	1.36	1.04
1:A:214:VAL:HG23	1:A:219:MET:HE2	1.33	1.03
3:C:301:NAG:O4	3:D:201:NAG:O3	1.77	1.02
3:A:301:NAG:O4	3:B:201:NAG:H3	1.64	0.98
1:A:94:ASN:OD1	3:A:301:NAG:C1	2.23	0.87
1:C:169:LYS:HE3	1:C:174:THR:OG1	1.75	0.86
1:A:214:VAL:CG2	1:A:219:MET:HE2	2.08	0.84
1:A:158:PHE:HB2	1:A:197:ILE:HD11	1.60	0.83
2:D:13:GLN:HG3	2:D:14:PRO:HD2	1.62	0.82
1:A:213:THR:CG2	1:A:216:SER:H	1.92	0.82
1:A:153:MET:HE3	1:A:160:THR:HG22	1.62	0.81
1:A:213:THR:HG22	1:A:216:SER:HB3	1.62	0.80
2:D:39:GLN:O	2:D:96:ALA:HB1	1.81	0.78
3:A:301:NAG:H61	3:B:201:NAG:C8	2.14	0.77
1:C:85:SER:HB2	1:C:88:ALA:H	1.51	0.75
1:A:158:PHE:CD2	1:A:197:ILE:HD11	2.23	0.74
1:A:102:MET:HE3	1:A:165:LEU:HB2	1.71	0.73
1:A:220:LEU:HD12	1:A:220:LEU:O	1.89	0.73
2:D:75:SER:HB2	2:D:84:TYR:HB2	1.69	0.73
1:A:102:MET:CE	1:A:165:LEU:HB2	2.20	0.71
1:C:109:PRO:HB2	1:C:219:MET:HE3	1.73	0.70
1:A:102:MET:HE3	1:A:165:LEU:HD13	1.73	0.70
1:A:213:THR:HG22	1:A:216:SER:CB	2.23	0.69
1:C:139:ASP:O	1:C:222:ARG:NH2	2.26	0.68
1:C:139:ASP:OD1	1:C:142:SER:HB2	1.93	0.68
1:A:109:PRO:HG2	1:A:217:ILE:CD1	2.23	0.67
1:A:102:MET:HE1	1:A:165:LEU:HD22	1.77	0.66
1:C:197:ILE:HD12	1:C:197:ILE:O	1.97	0.65
3:C:301:NAG:C4	3:D:201:NAG:O3	2.44	0.65
3:A:301:NAG:H61	3:B:201:NAG:H82	1.80	0.64
1:A:158:PHE:CB	1:A:197:ILE:HD11	2.27	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD23	1:A:176:ILE:HG13	1.79	0.63
2:D:52:TYR:CD2	2:D:57:LEU:HD13	2.34	0.63
3:C:301:NAG:O4	3:D:201:NAG:C3	2.48	0.62
1:A:165:LEU:HD12	1:A:178:GLN:HG2	1.82	0.62
1:A:78:PRO:O	1:A:81:VAL:HG22	2.00	0.61
1:A:213:THR:HG22	1:A:216:SER:H	1.66	0.61
1:A:112:VAL:HG23	1:A:219:MET:HE1	1.83	0.61
1:A:213:THR:HG23	1:A:216:SER:H	1.66	0.61
3:C:301:NAG:C4	3:D:201:NAG:HO3	2.12	0.61
1:C:132:GLN:HG3	2:D:108:TYR:CD2	2.36	0.60
1:A:69:VAL:HG12	1:A:153:MET:HB3	1.82	0.60
1:A:169:LYS:HE3	1:A:174:THR:OG1	2.01	0.60
2:B:32:TYR:HB2	2:B:104:ARG:O	2.02	0.60
3:A:301:NAG:HO4	3:B:201:NAG:H3	1.67	0.59
1:A:214:VAL:HG22	1:A:219:MET:CB	2.24	0.59
2:B:80:LYS:O	2:B:82:THR:HG23	2.04	0.58
1:C:70:LEU:HD13	1:C:152:LEU:HG	1.85	0.57
1:C:44:LEU:CD2	1:C:112:VAL:HG21	2.35	0.57
1:A:142:SER:O	1:A:222:ARG:NH1	2.38	0.57
1:A:158:PHE:HD2	1:A:197:ILE:HD11	1.65	0.57
2:B:103:ASN:CG	2:B:119:ASN:OD1	2.48	0.56
2:D:87:MET:HE3	2:D:90:LEU:HD21	1.86	0.56
1:A:95:LEU:HD23	1:A:115:TYR:CD1	2.40	0.56
1:A:36:ARG:HB3	1:A:132:GLN:HG2	1.87	0.56
1:A:158:PHE:HD1	1:A:158:PHE:O	1.89	0.55
2:B:12:VAL:HG12	2:B:13:GLN:N	2.21	0.55
1:A:102:MET:CE	1:A:165:LEU:HD22	2.36	0.55
1:A:203:LEU:HB2	1:A:208:TYR:CE2	2.42	0.55
1:C:169:LYS:HE3	1:C:174:THR:HG1	1.69	0.54
1:A:101:ARG:CB	1:A:110:ILE:HD11	2.38	0.54
2:B:104:ARG:HD3	2:B:105:TYR:CE2	2.43	0.54
1:C:125:GLY:O	1:C:127:CYS:N	2.41	0.54
1:C:109:PRO:HB2	1:C:219:MET:CE	2.37	0.54
2:D:39:GLN:C	2:D:96:ALA:HB1	2.32	0.53
1:A:158:PHE:CD2	1:A:197:ILE:CD1	2.92	0.53
1:C:47:PRO:HD3	1:C:100:TYR:CE2	2.44	0.53
3:A:301:NAG:C4	3:B:201:NAG:H3	2.39	0.53
1:A:167:LEU:HD23	1:A:176:ILE:CG1	2.40	0.52
2:B:34:MET:HB3	2:B:83:LEU:HD22	1.92	0.52
1:A:106:CYS:HA	1:A:203:LEU:O	2.11	0.50
2:B:95:THR:HG23	2:B:128:THR:HA	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:CE2	2:D:108:TYR:HA	2.46	0.50
1:C:110:ILE:HG21	1:C:151:PHE:CZ	2.47	0.50
2:D:40:ALA:HB3	2:D:43:LYS:HG3	1.94	0.50
2:D:12:VAL:HG21	2:D:16:GLY:HA3	1.94	0.50
2:D:74:ILE:HD11	2:D:83:LEU:HD11	1.93	0.50
1:C:111:THR:HB	1:C:135:TRP:CE3	2.47	0.49
1:A:71:LEU:HB2	1:A:151:PHE:HB3	1.94	0.49
1:C:102:MET:SD	1:C:165:LEU:HD22	2.52	0.49
1:A:116:THR:CG2	1:A:129:ILE:HB	2.42	0.49
2:D:64:TYR:OH	2:D:74:ILE:HG22	2.13	0.49
1:A:158:PHE:CG	1:A:197:ILE:HD11	2.48	0.49
1:A:208:TYR:HA	1:A:212:VAL:HG23	1.95	0.49
1:A:37:VAL:CG1	1:A:38:TYR:N	2.76	0.49
2:D:33:LEU:HD11	2:D:112:MET:HG2	1.94	0.48
1:A:47:PRO:HG3	1:A:107:ALA:HB3	1.96	0.48
1:A:101:ARG:HD3	1:A:164:TYR:CZ	2.49	0.48
1:A:220:LEU:HD12	1:A:220:LEU:C	2.38	0.48
1:A:134:ARG:HB2	1:A:219:MET:HE3	1.95	0.48
1:A:101:ARG:HB2	1:A:110:ILE:HD11	1.94	0.47
1:A:44:LEU:CD2	1:A:112:VAL:HG21	2.44	0.47
1:A:135:TRP:CD1	1:A:222:ARG:HG3	2.49	0.47
1:C:139:ASP:OD1	1:C:142:SER:CB	2.61	0.47
1:A:153:MET:HE3	1:A:160:THR:CG2	2.40	0.47
1:A:140:SER:H	1:A:222:ARG:HH21	1.62	0.47
1:A:173:TRP:CH2	1:A:175:GLU:HB2	2.50	0.47
2:B:9:GLY:HA3	2:B:125:THR:CG2	2.44	0.47
1:C:106:CYS:HA	1:C:203:LEU:O	2.15	0.47
1:C:154:HIS:C	1:C:156:PRO:HD3	2.40	0.47
1:A:139:ASP:O	1:A:140:SER:CB	2.62	0.47
2:D:64:TYR:CZ	2:D:74:ILE:HG22	2.50	0.46
3:A:301:NAG:H61	3:B:201:NAG:H81	1.95	0.46
1:C:134:ARG:HD2	1:C:221:PRO:HG3	1.96	0.46
2:D:12:VAL:HG11	2:D:90:LEU:HD13	1.98	0.46
2:D:29:TYR:HB2	3:D:201:NAG:HN2	1.81	0.46
1:C:44:LEU:HD22	1:C:112:VAL:HG21	1.97	0.46
2:D:13:GLN:HG3	2:D:14:PRO:CD	2.40	0.46
1:A:158:PHE:O	1:A:158:PHE:CD1	2.69	0.46
2:D:12:VAL:CG2	2:D:16:GLY:HA3	2.45	0.46
1:C:151:PHE:CE2	1:C:153:MET:HG2	2.51	0.46
2:B:33:LEU:HD11	2:B:112:MET:HG2	1.98	0.46
1:A:158:PHE:HD2	1:A:197:ILE:CD1	2.27	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:CG1	2:B:16:GLY:HA3	2.46	0.45
2:B:37:PHE:O	2:B:99:TYR:N	2.43	0.45
1:A:204:THR:O	1:A:208:TYR:HD2	1.99	0.45
1:A:107:ALA:N	1:A:203:LEU:O	2.44	0.45
1:A:140:SER:N	1:A:222:ARG:HH21	2.15	0.45
2:B:50:ALA:HB3	2:B:112:MET:HE2	1.98	0.45
2:D:72:PHE:N	2:D:72:PHE:CD1	2.85	0.45
1:C:36:ARG:HA	1:C:130:ARG:O	2.16	0.44
1:C:31:PRO:HG2	1:C:34:VAL:HG21	1.99	0.44
1:A:139:ASP:O	1:A:140:SER:HB2	2.17	0.44
1:C:36:ARG:HH11	1:C:130:ARG:HB2	1.83	0.44
1:A:79:GLN:HA	1:A:82:ARG:HB2	1.98	0.44
1:C:48:PHE:CE1	1:C:102:MET:HE1	2.53	0.44
1:C:222:ARG:O	1:C:223:PHE:HB2	2.18	0.44
2:B:37:PHE:CD2	2:B:47:GLY:HA2	2.53	0.44
2:B:90:LEU:HD23	2:B:90:LEU:HA	1.80	0.44
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.88	0.43
2:D:12:VAL:HG22	2:D:13:GLN:N	2.33	0.43
2:B:107:THR:HB	2:B:117:GLU:OE1	2.18	0.43
1:A:37:VAL:HG12	1:A:38:TYR:N	2.33	0.43
1:C:77:ALA:HB3	1:C:78:PRO:HD3	2.01	0.43
2:B:13:GLN:OE1	2:B:131:SER:HA	2.18	0.43
1:A:72:HIS:CD2	1:A:73:ALA:N	2.87	0.42
1:C:48:PHE:CE1	1:C:102:MET:CE	3.03	0.42
1:C:36:ARG:HB3	1:C:132:GLN:HG2	2.00	0.42
1:C:51:PRO:HB3	1:C:176:ILE:HD12	2.01	0.42
1:C:82:ARG:O	1:C:89:ARG:NH2	2.52	0.42
1:A:116:THR:HG23	1:A:129:ILE:HB	2.01	0.42
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.57	0.42
2:D:13:GLN:O	2:D:14:PRO:C	2.62	0.42
2:D:61:SER:O	2:D:112:MET:HE1	2.20	0.42
1:C:203:LEU:HB2	1:C:208:TYR:CE2	2.55	0.41
1:A:55:ILE:HG23	1:A:176:ILE:O	2.20	0.41
1:A:109:PRO:HG2	1:A:217:ILE:HD13	2.01	0.41
1:A:132:GLN:HG3	2:B:108:TYR:CG	2.55	0.41
3:A:301:NAG:C6	3:B:201:NAG:H82	2.50	0.41
2:D:57:LEU:HA	2:D:57:LEU:HD12	1.84	0.41
1:A:102:MET:HE3	1:A:165:LEU:CB	2.46	0.41
1:A:214:VAL:CG2	1:A:219:MET:CE	2.89	0.41
1:A:132:GLN:HG3	2:B:108:TYR:CD2	2.56	0.41
1:A:165:LEU:CD1	1:A:178:GLN:HG2	2.48	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:THR:HG22	2:B:63:PHE:N	2.36	0.41
2:D:66:ASP:HA	2:D:69:LYS:HE3	2.03	0.40
1:A:213:THR:HG23	1:A:215:ASP:N	2.36	0.40
1:A:93:TYR:CZ	1:A:118:CYS:HB3	2.57	0.40
2:D:57:LEU:HD23	2:D:112:MET:HE2	2.03	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	170/275 (62%)	156 (92%)	14 (8%)	0	100	100
1	C	173/275 (63%)	158 (91%)	15 (9%)	0	100	100
2	B	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
2	D	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
All	All	601/812 (74%)	561 (93%)	40 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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	144/240 (60%)	139 (96%)	5 (4%)	31	63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	149/240 (62%)	142 (95%)	7 (5%)	22	52
2	B	99/103 (96%)	98 (99%)	1 (1%)	73	90
2	D	98/103 (95%)	95 (97%)	3 (3%)	35	67
All	All	490/686 (71%)	474 (97%)	16 (3%)	33	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	85	SER
1	C	136	SER
1	C	140	SER
1	C	158	PHE
1	C	197	ILE
1	C	215	ASP
1	C	223	PHE
2	D	67	SER
2	D	81	ASN
2	D	93	GLU
1	A	30	ASP
1	A	123	SER
1	A	147	ASP
1	A	177	THR
1	A	213	THR
2	B	56	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	209	GLN
2	D	76	GLN
2	D	81	ASN
1	A	72	HIS
1	A	79	GLN
2	B	3	GLN
2	B	116	GLN

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	301	-	14,14,15	2.63	2 (14%)	17,19,21	2.58	5 (29%)
3	NAG	B	201	-	14,14,15	1.04	2 (14%)	17,19,21	0.78	0
3	NAG	C	301	1	14,14,15	0.91	1 (7%)	17,19,21	0.79	0
3	NAG	D	201	-	14,14,15	0.24	0	17,19,21	1.13	2 (11%)

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	301	-	-	0/6/23/26	0/1/1/1
3	NAG	B	201	-	-	4/6/23/26	0/1/1/1
3	NAG	C	301	1	-	0/6/23/26	0/1/1/1
3	NAG	D	201	-	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	NAG	O5-C1	9.20	1.58	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	NAG	C3-C2	-2.95	1.46	1.52
3	C	301	NAG	O5-C1	-2.88	1.39	1.43
3	B	201	NAG	O5-C1	-2.59	1.39	1.43
3	B	201	NAG	C1-C2	2.33	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	NAG	C1-O5-C5	-6.42	103.50	112.19
3	A	301	NAG	O3-C3-C2	-4.85	99.43	109.47
3	A	301	NAG	O5-C5-C6	3.79	113.14	107.20
3	A	301	NAG	C1-C2-N2	3.21	115.97	110.49
3	A	301	NAG	O4-C4-C3	-3.11	103.15	110.35
3	D	201	NAG	C3-C4-C5	2.27	114.30	110.24
3	D	201	NAG	C4-C3-C2	2.17	114.20	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	NAG	O5-C5-C6-O6
3	B	201	NAG	C4-C5-C6-O6
3	D	201	NAG	C8-C7-N2-C2
3	D	201	NAG	O7-C7-N2-C2
3	B	201	NAG	C8-C7-N2-C2
3	B	201	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAG	8	0
3	B	201	NAG	7	0
3	C	301	NAG	4	0
3	D	201	NAG	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	178/275 (64%)	-0.07	8 (4%) 39 33	31, 49, 73, 107	0
1	C	178/275 (64%)	-0.12	6 (3%) 48 42	31, 46, 78, 103	1 (0%)
2	B	131/131 (100%)	0.03	4 (3%) 51 46	45, 66, 88, 108	0
2	D	131/131 (100%)	-0.06	2 (1%) 71 66	39, 59, 85, 101	0
All	All	618/812 (76%)	-0.06	20 (3%) 50 45	31, 56, 85, 108	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	155	ALA	5.0
2	B	1	GLN	3.7
1	C	157	ALA	3.7
2	B	81	ASN	3.5
1	C	183	HIS	3.5
1	A	156	PRO	3.3
2	D	1	GLN	3.0
1	A	158	PHE	2.9
2	B	2	VAL	2.6
1	A	155	ALA	2.6
2	B	56	SER	2.5
2	D	78	LYS	2.5
1	A	196	ARG	2.4
1	C	223	PHE	2.3
1	A	68	SER	2.3
1	A	29	THR	2.1
1	C	154	HIS	2.1
1	A	223	PHE	2.1
1	C	158	PHE	2.0
1	A	183	HIS	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	201	14/15	0.64	0.23	63,77,86,93	0
3	NAG	D	201	14/15	0.77	0.17	63,72,87,90	0
3	NAG	A	301	14/15	0.88	0.13	51,59,65,69	0
3	NAG	C	301	14/15	0.92	0.09	43,49,53,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.