



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:30 AM GMT

PDB ID : 2X9M  
Title : HENDRA VIRUS ATTACHMENT GLYCOPROTEIN  
Authors : Bowden, T.A.; Crispin, M.; Harvey, D.; Jones, E.Y.; Stuart, D.I.  
Deposited on : 2010-03-23  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

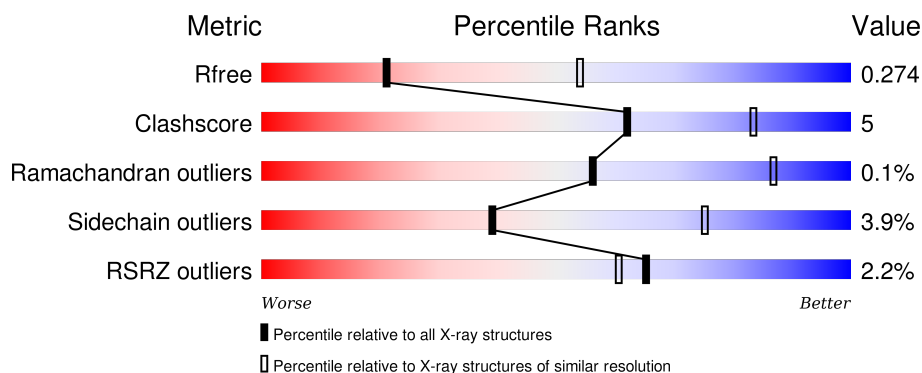
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	<div> <div>2%</div> <div>85%</div> <div>15%</div> </div>
1	B	420	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	420	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	420	<div> <div>3%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1607	-	-	-	X

## 2 Entry composition [i](#)

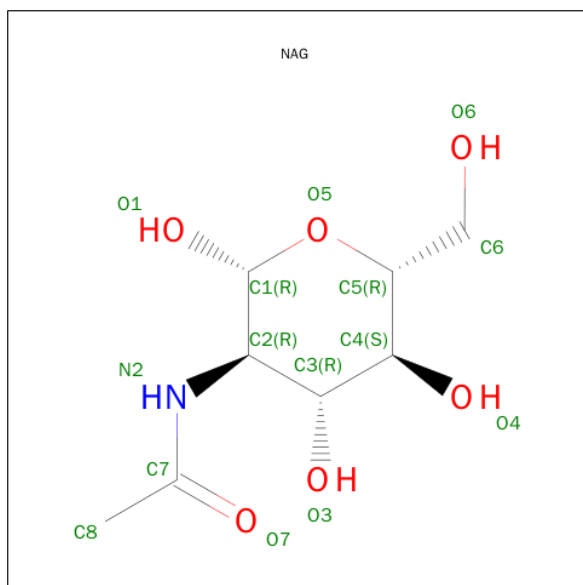
There are 3 unique types of molecules in this entry. The entry contains 13464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3311	2109	556	627	19			
1	B	418	Total	C	N	O	S	0	0	0
			3304	2104	555	626	19			
1	C	417	Total	C	N	O	S	0	0	0
			3296	2100	553	624	19			
1	D	417	Total	C	N	O	S	0	0	0
			3296	2100	553	624	19			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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		

*Continued on next page...*

*Continued from previous page...*

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		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

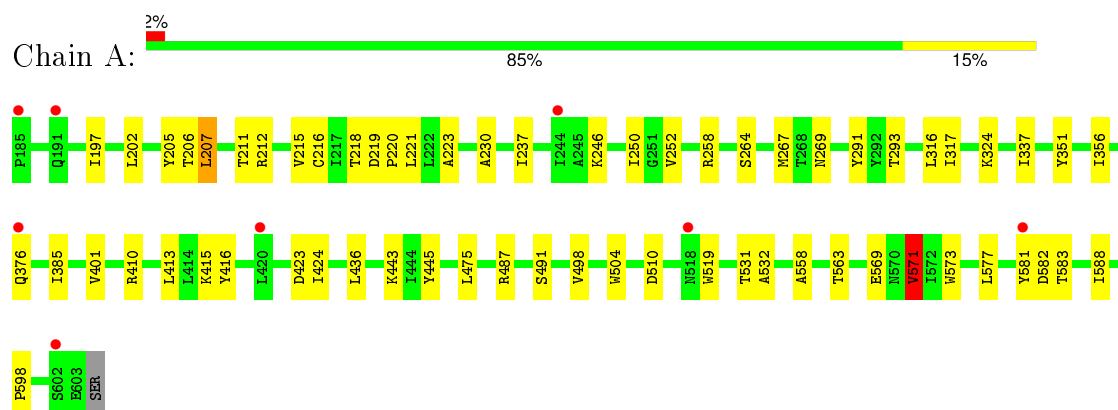
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	30	Total	O	0	0
			30	30		
3	C	34	Total	O	0	0
			34	34		
3	D	23	Total	O	0	0
			23	23		

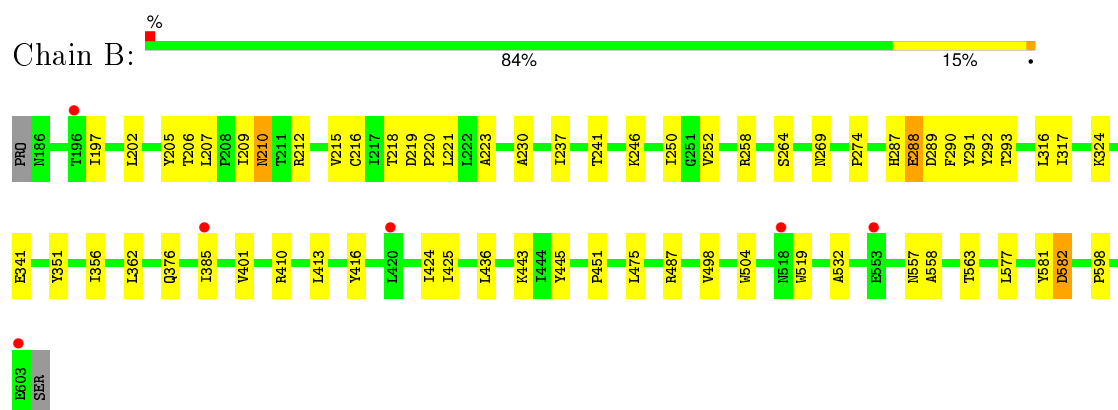
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

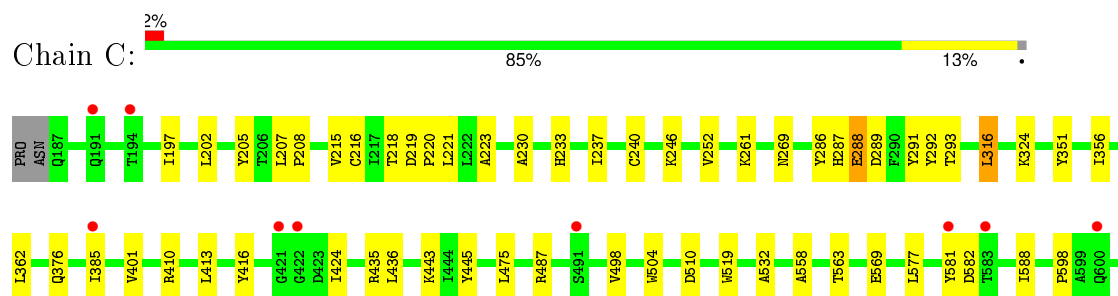
#### • Molecule 1: GLYCOPROTEIN G



#### • Molecule 1: GLYCOPROTEIN G

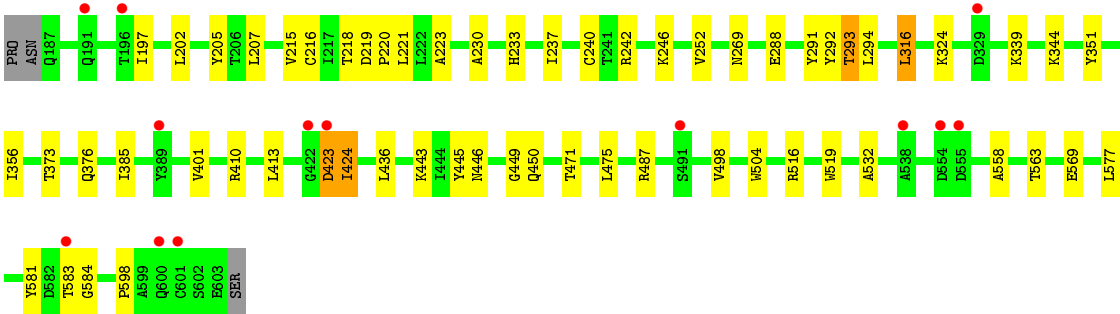
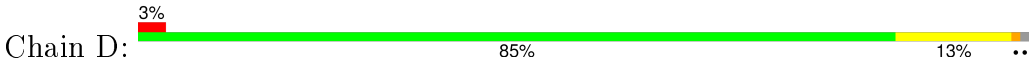


#### • Molecule 1: GLYCOPROTEIN G





● Molecule 1: GLYCOPROTEIN G



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.88Å 84.78Å 91.55Å 103.39° 99.63° 108.62°	Depositor
Resolution (Å)	44.20 – 2.90 43.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.20-2.90) 87.4 (43.57-2.90)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.233 , 0.273 0.236 , 0.274	Depositor DCC
$R_{free}$ test set	1891 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 22.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 38059 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.53 % 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 1.8148e-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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/3392	0.59	1/4619 (0.0%)
1	B	0.41	0/3384	0.57	0/4608
1	C	0.42	0/3376	0.59	0/4597
1	D	0.44	2/3376 (0.1%)	0.58	0/4597
All	All	0.42	2/13528 (0.0%)	0.58	1/18421 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	446	ASN	CG-ND2	-6.23	1.17	1.32
1	D	446	ASN	CG-OD1	-5.81	1.11	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	VAL	CG1-CB-CG2	8.18	123.99	110.90

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	3311	0	3249	40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3304	0	3241	40	2
1	C	3296	0	3238	34	1
1	D	3296	0	3238	35	1
2	A	56	0	52	2	0
2	B	56	0	52	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	30	0	0	1	0
3	B	30	0	0	4	0
3	C	34	0	0	1	0
3	D	23	0	0	2	0
All	All	13464	0	13096	143	2

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 5.

All (143) 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:206:THR:O	1:A:207:LEU:HD22	1.77	0.83
1:D:344:LYS:HG2	3:D:2011:HOH:O	1.81	0.78
1:A:415:LYS:HE2	2:A:1604:NAG:H81	1.69	0.74
1:C:218:THR:HG21	1:C:240:CYS:HB3	1.69	0.74
1:A:293:THR:HG22	1:A:317:ILE:O	1.92	0.69
1:B:212:ARG:NH2	1:B:246:LYS:HZ2	1.90	0.68
1:B:209:ILE:HG13	1:D:207:LEU:HD13	1.76	0.67
1:A:416:TYR:CE2	1:A:424:ILE:HG13	2.31	0.66
1:D:293:THR:HG23	3:D:2008:HOH:O	1.96	0.66
1:C:401:VAL:HG22	1:C:504:TRP:CE2	2.31	0.65
1:D:401:VAL:HG22	1:D:504:TRP:CE2	2.32	0.64
1:A:571:VAL:HG22	1:A:573:TRP:CD1	2.32	0.64
1:D:218:THR:HG21	1:D:240:CYS:HB3	1.78	0.64
1:B:416:TYR:CE2	1:B:424:ILE:HG13	2.34	0.63
1:B:401:VAL:HG22	1:B:504:TRP:CE2	2.35	0.62
1:C:288:GLU:N	1:C:288:GLU:OE1	2.33	0.61
1:C:424:ILE:HG23	1:C:424:ILE:O	2.00	0.60
1:A:401:VAL:HG22	1:A:504:TRP:CE2	2.37	0.60
1:A:385:ILE:N	1:A:385:ILE:HD13	2.18	0.59
1:D:450:GLN:HE21	1:D:516:ARG:CZ	2.16	0.58
1:B:293:THR:HG22	1:B:317:ILE:O	2.03	0.58
1:A:218:THR:HG22	1:A:581:TYR:OH	2.02	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ILE:N	1:C:385:ILE:HD13	2.19	0.58
1:D:385:ILE:N	1:D:385:ILE:HD13	2.20	0.57
1:B:385:ILE:HD13	1:B:385:ILE:N	2.19	0.57
1:C:292:TYR:HB3	1:C:316:LEU:HD11	1.86	0.56
1:A:581:TYR:O	1:A:583:THR:HG23	2.05	0.55
1:A:206:THR:C	1:A:207:LEU:HD22	2.26	0.55
1:A:415:LYS:CE	2:A:1604:NAG:H81	2.36	0.55
1:D:205:TYR:CE1	1:D:207:LEU:HD11	2.42	0.55
1:D:223:ALA:HB3	1:D:230:ALA:HB3	1.89	0.55
1:B:205:TYR:CE1	1:B:207:LEU:HD11	2.42	0.54
1:B:250:ILE:HG21	1:B:293:THR:HG21	1.89	0.54
1:B:212:ARG:CZ	1:B:246:LYS:NZ	2.71	0.54
1:C:223:ALA:HB3	1:C:230:ALA:HB3	1.88	0.54
1:C:205:TYR:CE1	1:C:207:LEU:HD11	2.42	0.54
1:D:216:CYS:SG	1:D:218:THR:HG23	2.47	0.54
1:B:401:VAL:HG13	1:B:504:TRP:CE3	2.43	0.54
1:C:410:ARG:HD2	1:C:436:LEU:HD11	1.89	0.54
1:B:288:GLU:O	1:B:289:ASP:HB2	2.08	0.53
1:D:532:ALA:HB1	1:D:558:ALA:O	2.08	0.53
1:B:498:VAL:HG12	1:B:498:VAL:O	2.09	0.53
1:D:205:TYR:CD1	1:D:207:LEU:HD11	2.43	0.53
1:C:532:ALA:HB1	1:C:558:ALA:O	2.08	0.53
1:A:250:ILE:HG21	1:A:293:THR:HG21	1.90	0.52
1:A:498:VAL:HG12	1:A:498:VAL:O	2.08	0.52
1:C:205:TYR:CD1	1:C:207:LEU:HD11	2.45	0.52
1:B:205:TYR:CD1	1:B:207:LEU:HD11	2.44	0.52
1:B:532:ALA:HB1	1:B:558:ALA:O	2.10	0.52
1:C:288:GLU:OE1	1:C:288:GLU:CA	2.58	0.52
1:D:443:LYS:NZ	1:D:563:THR:O	2.43	0.52
1:A:207:LEU:HD13	1:A:267:MET:HE1	1.93	0.51
1:B:410:ARG:HD2	1:B:436:LEU:HD11	1.92	0.51
1:A:356:ILE:CG2	1:A:445:TYR:HA	2.41	0.51
1:C:216:CYS:SG	1:C:218:THR:HG23	2.50	0.51
1:A:531:THR:HG23	1:D:449:GLY:O	2.11	0.51
1:C:287:HIS:HB2	1:C:362:LEU:HD21	1.91	0.51
1:B:287:HIS:HB2	1:B:362:LEU:HD21	1.92	0.51
1:A:401:VAL:HG13	1:A:504:TRP:CE3	2.46	0.51
1:A:577:LEU:HD23	1:A:577:LEU:C	2.32	0.50
1:B:223:ALA:HB3	1:B:230:ALA:HB3	1.94	0.50
1:D:356:ILE:CG2	1:D:445:TYR:HA	2.42	0.50
1:B:356:ILE:CG2	1:B:445:TYR:HA	2.42	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ARG:HD2	1:A:436:LEU:HD11	1.93	0.50
1:C:288:GLU:O	1:C:289:ASP:HB2	2.12	0.49
1:C:413:LEU:HG	1:C:475:LEU:HD22	1.94	0.49
1:A:532:ALA:HB1	1:A:558:ALA:O	2.13	0.49
1:C:356:ILE:CG2	1:C:445:TYR:HA	2.42	0.49
1:D:410:ARG:HD2	1:D:436:LEU:HD11	1.94	0.49
1:B:425:ILE:HG22	3:B:2021:HOH:O	2.12	0.49
1:C:443:LYS:NZ	1:C:563:THR:O	2.45	0.49
1:B:443:LYS:NZ	1:B:563:THR:O	2.46	0.49
1:A:223:ALA:HB3	1:A:230:ALA:HB3	1.95	0.49
1:D:498:VAL:HG12	1:D:498:VAL:O	2.14	0.48
1:A:337:ILE:CD1	1:A:424:ILE:HG12	2.43	0.48
1:B:274:PRO:HD2	3:B:2008:HOH:O	2.13	0.48
1:A:337:ILE:HD12	1:A:424:ILE:HG12	1.95	0.48
1:B:293:THR:HG23	1:B:317:ILE:HB	1.96	0.48
1:D:413:LEU:HG	1:D:475:LEU:HD22	1.96	0.48
1:A:424:ILE:HG22	3:A:2019:HOH:O	2.14	0.47
1:A:443:LYS:NZ	1:A:563:THR:O	2.48	0.47
1:A:443:LYS:NZ	1:A:510:ASP:OD2	2.35	0.47
1:B:252:VAL:HG22	1:B:269:ASN:HB3	1.97	0.47
1:C:581:TYR:CD1	1:C:588:ILE:HG21	2.50	0.47
1:B:577:LEU:C	1:B:577:LEU:HD23	2.35	0.47
1:A:413:LEU:HG	1:A:475:LEU:HD22	1.97	0.47
1:C:401:VAL:HG13	1:C:504:TRP:CE3	2.50	0.46
1:D:401:VAL:HG13	1:D:504:TRP:CE3	2.51	0.46
1:C:219:ASP:N	1:C:220:PRO:HD3	2.30	0.46
1:B:237:ILE:HD11	1:B:246:LYS:HD2	1.97	0.46
1:A:237:ILE:HD11	1:A:246:LYS:HD2	1.97	0.46
1:B:413:LEU:HG	1:B:475:LEU:HD22	1.97	0.46
1:C:498:VAL:O	1:C:498:VAL:HG12	2.14	0.46
1:D:577:LEU:C	1:D:577:LEU:HD23	2.36	0.46
1:A:216:CYS:SG	1:A:218:THR:HG23	2.55	0.46
1:A:219:ASP:N	1:A:220:PRO:HD3	2.30	0.46
1:B:219:ASP:N	1:B:220:PRO:HD3	2.30	0.46
1:B:293:THR:CG2	1:B:317:ILE:O	2.64	0.45
1:C:435:ARG:HG3	3:C:2026:HOH:O	2.15	0.45
1:D:339:LYS:HD2	1:D:423:ASP:HB2	1.98	0.45
1:A:491:SER:OG	1:D:471:THR:HA	2.17	0.45
1:D:219:ASP:N	1:D:220:PRO:HD3	2.32	0.45
1:B:451:PRO:HD2	3:B:2026:HOH:O	2.16	0.45
1:A:252:VAL:HG22	1:A:269:ASN:HB3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ASN:ND2	1:B:582:ASP:OD2	2.48	0.45
1:B:206:THR:HA	1:D:207:LEU:O	2.17	0.44
1:B:197:ILE:HD12	1:B:598:PRO:HG2	1.99	0.44
1:C:237:ILE:HD11	1:C:246:LYS:HD2	2.00	0.44
1:A:197:ILE:HD12	1:A:598:PRO:HG2	1.98	0.44
1:A:581:TYR:HD1	1:A:588:ILE:HG21	1.81	0.44
1:C:197:ILE:HD12	1:C:598:PRO:HG2	1.99	0.44
1:A:211:THR:O	1:A:211:THR:HG22	2.17	0.44
1:D:424:ILE:H	1:D:424:ILE:HD12	1.83	0.44
1:D:294:LEU:HD13	1:D:316:LEU:HD23	2.00	0.44
1:D:292:TYR:HB3	1:D:316:LEU:HD11	2.01	0.43
1:C:205:TYR:CE1	1:C:207:LEU:CD1	3.01	0.43
1:B:218:THR:HG22	1:B:581:TYR:OH	2.19	0.43
1:D:583:THR:O	1:D:584:GLY:C	2.56	0.43
1:A:206:THR:HA	1:C:207:LEU:O	2.18	0.43
1:C:416:TYR:CE2	1:C:424:ILE:HG13	2.53	0.43
1:D:450:GLN:HE21	1:D:516:ARG:NH2	2.17	0.43
1:D:197:ILE:HD12	1:D:598:PRO:HG2	2.01	0.43
1:D:205:TYR:CE1	1:D:207:LEU:CD1	3.01	0.43
1:A:571:VAL:HG22	1:A:573:TRP:NE1	2.33	0.43
1:B:205:TYR:CE1	1:B:207:LEU:CD1	3.02	0.42
1:C:261:LYS:HE3	1:C:569:GLU:CG	2.48	0.42
1:C:252:VAL:HG22	1:C:269:ASN:HB3	2.00	0.42
1:B:216:CYS:SG	1:B:218:THR:HG23	2.60	0.42
1:D:581:TYR:N	1:D:581:TYR:CD2	2.87	0.42
1:D:237:ILE:HD11	1:D:246:LYS:HD2	2.02	0.42
1:D:252:VAL:HG22	1:D:269:ASN:HB3	2.02	0.41
1:B:212:ARG:CZ	1:B:246:LYS:HZ2	2.30	0.41
1:C:577:LEU:HD23	1:C:577:LEU:C	2.39	0.41
1:B:210:ASN:HD21	1:B:212:ARG:NE	2.19	0.41
1:A:258:ARG:HB3	1:A:264:SER:OG	2.21	0.41
1:C:443:LYS:NZ	1:C:510:ASP:OD2	2.48	0.41
1:D:216:CYS:SG	1:D:218:THR:CG2	3.09	0.41
1:A:581:TYR:CD1	1:A:588:ILE:HG21	2.56	0.41
1:B:258:ARG:HB3	1:B:264:SER:OG	2.21	0.40
1:C:286:TYR:CE2	1:C:288:GLU:OE1	2.74	0.40
1:B:425:ILE:CG2	3:B:2021:HOH:O	2.69	0.40
1:A:205:TYR:O	1:C:208:PRO:HA	2.21	0.40
1:B:290:PHE:HB2	1:B:292:TYR:CE2	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:OE2	1:D:373:THR:OG1[1_556]	1.92	0.28
1:B:582:ASP:OD2	1:C:288:GLU:OE2[1_565]	2.13	0.07

## 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	417/420 (99%)	395 (95%)	21 (5%)	1 (0%)	52	84
1	B	416/420 (99%)	393 (94%)	23 (6%)	0	100	100
1	C	415/420 (99%)	392 (94%)	23 (6%)	0	100	100
1	D	415/420 (99%)	386 (93%)	28 (7%)	1 (0%)	52	84
All	All	1663/1680 (99%)	1566 (94%)	95 (6%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	GLU
1	D	288	GLU

### 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	376/377 (100%)	361 (96%)	15 (4%)	38	74
1	B	375/377 (100%)	361 (96%)	14 (4%)	41	77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	374/377 (99%)	360 (96%)	14 (4%)	41	77
1	D	374/377 (99%)	358 (96%)	16 (4%)	35	71
All	All	1499/1508 (99%)	1440 (96%)	59 (4%)	39	75

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	LEU
1	A	207	LEU
1	A	212	ARG
1	A	215	VAL
1	A	221	LEU
1	A	291	TYR
1	A	316	LEU
1	A	324	LYS
1	A	351	TYR
1	A	376	GLN
1	A	423	ASP
1	A	487	ARG
1	A	519	TRP
1	A	571	VAL
1	A	582	ASP
1	B	202	LEU
1	B	210	ASN
1	B	215	VAL
1	B	221	LEU
1	B	241	THR
1	B	288	GLU
1	B	291	TYR
1	B	316	LEU
1	B	324	LYS
1	B	351	TYR
1	B	376	GLN
1	B	487	ARG
1	B	519	TRP
1	B	582	ASP
1	C	202	LEU
1	C	215	VAL
1	C	221	LEU
1	C	233	HIS
1	C	288	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	291	TYR
1	C	293	THR
1	C	316	LEU
1	C	324	LYS
1	C	351	TYR
1	C	376	GLN
1	C	487	ARG
1	C	519	TRP
1	C	582	ASP
1	D	202	LEU
1	D	215	VAL
1	D	221	LEU
1	D	233	HIS
1	D	242	ARG
1	D	291	TYR
1	D	293	THR
1	D	316	LEU
1	D	324	LYS
1	D	351	TYR
1	D	376	GLN
1	D	423	ASP
1	D	424	ILE
1	D	487	ARG
1	D	519	TRP
1	D	569	GLU

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

Mol	Chain	Res	Type
1	D	450	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	1604	1	14,14,15	0.62	0	15,19,21	1.81	2 (13%)
2	NAG	A	1605	1	14,14,15	0.53	0	15,19,21	1.03	1 (6%)
2	NAG	A	1606	1	14,14,15	0.67	0	15,19,21	1.41	3 (20%)
2	NAG	A	1607	1	14,14,15	0.53	0	15,19,21	1.17	0
2	NAG	B	1604	1	14,14,15	0.41	0	15,19,21	1.04	1 (6%)
2	NAG	B	1605	1	14,14,15	0.49	0	15,19,21	1.12	1 (6%)
2	NAG	B	1606	1	14,14,15	0.52	0	15,19,21	1.05	1 (6%)
2	NAG	B	1607	1	14,14,15	0.58	0	15,19,21	0.88	1 (6%)
2	NAG	C	1604	1	14,14,15	0.44	0	15,19,21	1.45	3 (20%)
2	NAG	D	1604	1	14,14,15	0.48	0	15,19,21	1.00	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	1604	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1605	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1606	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1607	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1604	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1605	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1606	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1607	1	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1604	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1604	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1606	NAG	C1-O5-C5	-2.71	108.80	112.25
2	A	1604	NAG	O4-C4-C5	-2.58	102.40	109.24
2	A	1606	NAG	C4-C3-C2	-2.49	107.35	111.23
2	C	1604	NAG	C2-N2-C7	-2.35	120.03	123.04
2	B	1604	NAG	C1-O5-C5	2.06	114.86	112.25
2	B	1606	NAG	C1-O5-C5	2.30	115.17	112.25
2	C	1604	NAG	C3-C4-C5	2.50	114.56	110.20
2	A	1606	NAG	O3-C3-C4	2.51	115.98	110.34
2	B	1607	NAG	C1-O5-C5	2.54	115.47	112.25
2	A	1605	NAG	C1-O5-C5	3.03	116.09	112.25
2	B	1605	NAG	C1-O5-C5	3.21	116.32	112.25
2	C	1604	NAG	C1-O5-C5	3.57	116.78	112.25
2	A	1604	NAG	C1-O5-C5	5.21	118.86	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1604	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	419/420 (99%)	-0.08	8 (1%) 70 66	7, 25, 49, 91	0
1	B	418/420 (99%)	-0.11	6 (1%) 78 76	8, 26, 52, 90	0
1	C	417/420 (99%)	-0.02	9 (2%) 65 60	8, 27, 64, 94	0
1	D	417/420 (99%)	-0.03	13 (3%) 52 45	8, 27, 55, 85	0
All	All	1671/1680 (99%)	-0.06	36 (2%) 65 60	7, 26, 55, 94	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	583	THR	4.6
1	B	420	LEU	3.4
1	C	491	SER	3.4
1	A	420	LEU	3.2
1	D	422	GLY	3.2
1	C	194	THR	3.1
1	B	553	GLU	3.0
1	C	422	GLY	2.9
1	A	518	ASN	2.9
1	D	600	GLN	2.9
1	C	583	THR	2.8
1	B	385	ILE	2.7
1	B	196	THR	2.7
1	A	185	PRO	2.7
1	D	191	GLN	2.6
1	C	385	ILE	2.5
1	B	518	ASN	2.5
1	C	581	TYR	2.5
1	D	554	ASP	2.5
1	A	376	GLN	2.4
1	D	329	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	601	CYS	2.3
1	A	581	TYR	2.3
1	B	603	GLU	2.3
1	D	555	ASP	2.3
1	A	602	SER	2.3
1	D	538	ALA	2.3
1	D	196	THR	2.3
1	D	423	ASP	2.3
1	C	191	GLN	2.2
1	C	600	GLN	2.2
1	A	191	GLN	2.1
1	D	491	SER	2.1
1	A	244	ILE	2.0
1	D	389	TYR	2.0
1	C	421	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	1607	14/15	0.87	0.26	3.36	17,20,22,23	0
2	NAG	D	1604	14/15	0.90	0.26	1.00	14,18,19,20	0
2	NAG	C	1604	14/15	0.85	0.24	0.86	16,18,20,21	0
2	NAG	B	1605	14/15	0.93	0.17	-0.27	7,14,15,17	0
2	NAG	A	1605	14/15	0.94	0.16	-0.34	6,9,11,12	0
2	NAG	A	1604	14/15	0.91	0.16	-0.37	3,8,10,10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	1604	14/15	0.95	0.12	-4.09	9,13,14,14	0
2	NAG	B	1606	14/15	0.82	0.20	-	20,23,24,25	0
2	NAG	A	1607	14/15	0.83	0.29	-	19,20,23,24	0
2	NAG	A	1606	14/15	0.91	0.21	-	18,20,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.