



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:44 AM GMT

PDB ID : 3FVC
Title : Crystal structure of a trimeric variant of the Epstein-Barr virus glycoprotein B
Authors : Backovic, M.
Deposited on : 2009-01-15
Resolution : 3.20 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
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

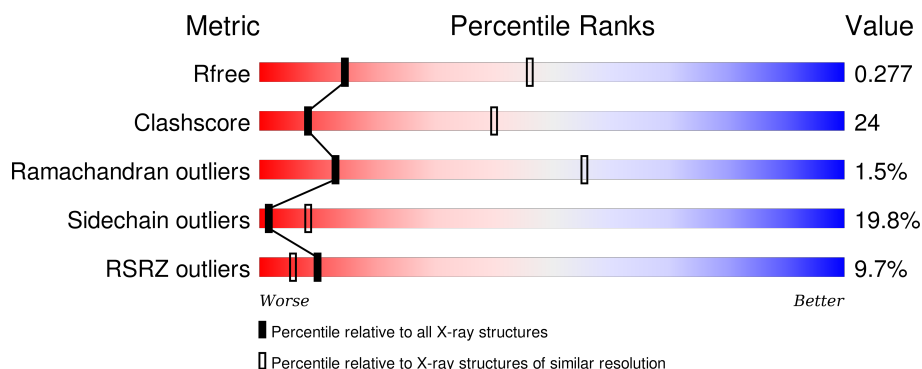
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 ≥ 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	663	

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	A	687	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4552 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.

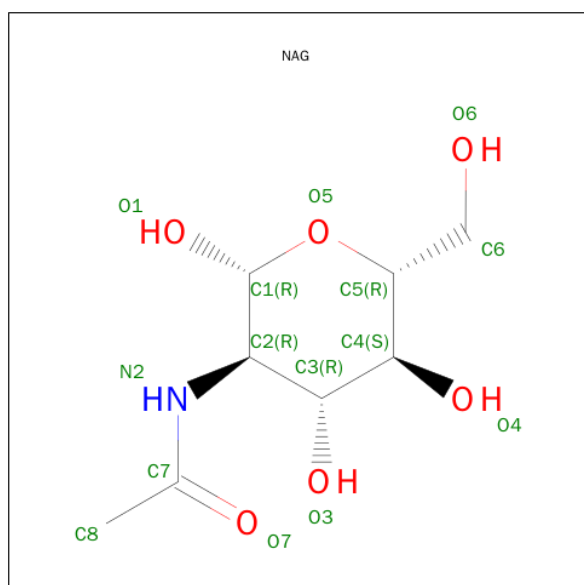
- Molecule 1 is a protein called Glycoprotein GP110.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4501	2833	775	872	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	HIS	TRP	ENGINEERED	UNP P03188
A	113	ARG	TYR	ENGINEERED	UNP P03188
A	193	ARG	TRP	ENGINEERED	UNP P03188
A	194	VAL	LEU	ENGINEERED	UNP P03188
A	195	GLU	ILE	ENGINEERED	UNP P03188
A	196	ALA	TRP	ENGINEERED	UNP P03188

- 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		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.80Å 106.80Å 210.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.61 – 3.20 26.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (26.61-3.20) 98.4 (26.61-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.283 0.238 , 0.277	Depositor DCC
R_{free} test set	2153 reflections (10.19%)	DCC
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.2	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23299 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4552	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.79	0/4590	0.85	2/6209 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	187	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	A	82	LEU	CA-CB-CG	-5.02	103.76	115.30

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	4501	0	4362	217	0
2	A	42	0	39	2	0
3	A	9	0	0	0	0
All	All	4552	0	4401	217	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 24.

All (217) 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:623:GLN:HG3	1:A:625:PHE:CE1	1.71	1.25
1:A:660:ILE:C	1:A:660:ILE:HD12	1.67	1.12
1:A:533:GLN:NE2	1:A:533:GLN:HA	1.64	1.08
1:A:361:ARG:HH11	1:A:361:ARG:HG2	0.98	1.08
1:A:533:GLN:HE21	1:A:533:GLN:CA	1.69	1.06
1:A:554:ARG:HB2	1:A:571:GLN:HE21	1.24	0.99
1:A:361:ARG:HG2	1:A:361:ARG:NH1	1.76	0.96
1:A:533:GLN:HE21	1:A:533:GLN:HA	0.80	0.96
1:A:538:LEU:HA	1:A:557:VAL:HG12	1.47	0.93
1:A:592:SER:OG	1:A:607:ASP:HA	1.72	0.90
1:A:238:GLY:O	1:A:239:LYS:HB2	1.73	0.87
1:A:259:ILE:HD11	1:A:274:ARG:NE	1.90	0.85
1:A:323:THR:O	1:A:323:THR:HG23	1.76	0.85
1:A:602:ILE:HD12	1:A:619:ILE:HD12	1.58	0.85
1:A:623:GLN:CG	1:A:625:PHE:CE1	2.58	0.84
1:A:81:LEU:HD12	1:A:383:LEU:HD11	1.59	0.84
1:A:361:ARG:HH11	1:A:361:ARG:CG	1.87	0.83
1:A:632:LEU:H	1:A:632:LEU:HD23	1.42	0.83
1:A:554:ARG:HB2	1:A:571:GLN:NE2	1.94	0.83
1:A:259:ILE:HD11	1:A:274:ARG:CZ	2.09	0.82
1:A:660:ILE:O	1:A:660:ILE:HD12	1.79	0.82
1:A:542:MET:HB2	1:A:608:TYR:HB3	1.63	0.81
1:A:47:PRO:O	1:A:49:ARG:HG3	1.81	0.80
1:A:605:TYR:CD2	1:A:610:HIS:HA	2.17	0.80
1:A:106:ILE:HD11	1:A:187:LEU:HD11	1.62	0.80
1:A:184:GLN:OE1	1:A:184:GLN:HA	1.81	0.78
1:A:672:ALA:HB1	1:A:675:ARG:NH1	1.99	0.77
1:A:374:THR:HG22	1:A:376:GLY:H	1.49	0.76
1:A:237:ASP:N	1:A:237:ASP:OD1	2.17	0.76
1:A:184:GLN:CA	1:A:184:GLN:OE1	2.34	0.75
1:A:232:MET:HE1	1:A:244:PHE:HE2	1.51	0.74
1:A:330:THR:HG21	1:A:372:PHE:HD2	1.50	0.74
1:A:71:PHE:HD2	1:A:71:PHE:C	1.91	0.74
1:A:334:ILE:HB	1:A:370:THR:HB	1.70	0.72
1:A:188:TYR:CE2	1:A:201:ARG:HD2	2.24	0.72
1:A:71:PHE:C	1:A:71:PHE:CD2	2.62	0.72
1:A:574:THR:O	1:A:575:ASP:HB2	1.89	0.71
1:A:232:MET:HE2	1:A:244:PHE:CD2	2.25	0.71
1:A:160:ASP:OD1	1:A:202:THR:HB	1.92	0.70
1:A:295:CYS:SG	1:A:296:PRO:HD2	2.32	0.70
1:A:168:LEU:CD2	1:A:183:SER:HB3	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ILE:HD13	1:A:383:LEU:HB3	1.75	0.69
1:A:192:GLY:HA3	1:A:199:ARG:HD3	1.75	0.69
1:A:623:GLN:HG3	1:A:625:PHE:HE1	1.51	0.68
1:A:672:ALA:HB1	1:A:675:ARG:HH11	1.57	0.68
1:A:554:ARG:CB	1:A:571:GLN:HE21	2.05	0.68
1:A:81:LEU:HG	1:A:385:LEU:HD11	1.75	0.68
1:A:61:ARG:HG3	1:A:62:PHE:N	2.09	0.67
1:A:605:TYR:CE2	1:A:610:HIS:HB2	2.29	0.67
1:A:330:THR:HG21	1:A:372:PHE:CD2	2.28	0.67
1:A:323:THR:O	1:A:323:THR:CG2	2.43	0.66
1:A:647:ASP:N	1:A:647:ASP:OD2	2.24	0.66
1:A:101:LYS:HD3	1:A:145:VAL:HG22	1.77	0.66
1:A:632:LEU:CD2	1:A:632:LEU:H	2.08	0.66
1:A:374:THR:CG2	1:A:376:GLY:H	2.09	0.65
1:A:383:LEU:HD13	1:A:383:LEU:O	1.97	0.65
1:A:601:GLU:HB3	1:A:615:GLU:HA	1.79	0.65
1:A:660:ILE:CD1	1:A:660:ILE:C	2.48	0.64
1:A:348:ASN:HD22	1:A:348:ASN:C	2.00	0.64
1:A:593:GLN:O	1:A:594:TYR:HD2	1.80	0.64
1:A:232:MET:HE1	1:A:244:PHE:CE2	2.32	0.63
1:A:168:LEU:HD23	1:A:183:SER:HB3	1.78	0.63
1:A:46:PHE:CD2	1:A:46:PHE:N	2.68	0.62
1:A:112:HIS:HB2	1:A:195:GLU:OE2	2.00	0.61
1:A:559:PHE:HE2	1:A:561:PHE:CE2	2.18	0.61
1:A:128:ASP:O	1:A:132:THR:HG23	2.00	0.61
1:A:232:MET:CE	1:A:244:PHE:CE2	2.83	0.61
1:A:509:ILE:HG13	1:A:510:TYR:N	2.15	0.61
1:A:168:LEU:HD12	1:A:208:ILE:HD12	1.82	0.61
1:A:81:LEU:HD12	1:A:383:LEU:CD1	2.31	0.61
1:A:124:LYS:O	1:A:281:THR:HA	2.00	0.61
1:A:626:ILE:HD12	1:A:626:ILE:H	1.66	0.61
1:A:448:LYS:HD2	1:A:449:SER:H	1.66	0.60
1:A:374:THR:HG22	1:A:376:GLY:N	2.15	0.60
1:A:101:LYS:HD3	1:A:145:VAL:CG2	2.32	0.60
1:A:273:ARG:CZ	1:A:288:LEU:HD23	2.31	0.60
1:A:671:ILE:HA	1:A:674:LEU:HD22	1.83	0.59
1:A:138:ILE:O	1:A:139:TYR:HB2	2.02	0.59
1:A:168:LEU:HD12	1:A:208:ILE:CD1	2.33	0.59
1:A:50:VAL:HG13	1:A:50:VAL:O	2.02	0.58
1:A:325:SER:OG	1:A:462:GLN:HG3	2.03	0.58
1:A:542:MET:CB	1:A:608:TYR:HB3	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:O	1:A:69:PRO:HD3	2.04	0.58
1:A:48:PHE:HZ	1:A:599:GLY:H	1.52	0.58
1:A:348:ASN:C	1:A:348:ASN:ND2	2.57	0.58
1:A:626:ILE:N	1:A:626:ILE:HD12	2.19	0.57
1:A:559:PHE:HE2	1:A:561:PHE:CZ	2.22	0.57
1:A:645:SER:O	1:A:649:GLN:HG2	2.04	0.57
1:A:486:GLU:O	1:A:490:GLN:HG2	2.05	0.57
1:A:605:TYR:CE2	1:A:610:HIS:HA	2.39	0.56
1:A:658:GLU:HG3	1:A:662:ARG:HD3	1.86	0.56
1:A:660:ILE:HD12	1:A:661:PHE:N	2.18	0.56
1:A:259:ILE:CD1	1:A:274:ARG:CZ	2.82	0.55
1:A:313:LYS:O	1:A:331:THR:CG2	2.55	0.55
1:A:672:ALA:CB	1:A:675:ARG:HH11	2.19	0.55
1:A:57:GLY:O	1:A:58:ASP:OD1	2.26	0.54
1:A:354:LYS:HD3	1:A:354:LYS:N	2.23	0.53
1:A:46:PHE:HD2	1:A:46:PHE:H	1.56	0.53
1:A:80:GLY:HA2	1:A:385:LEU:HD12	1.89	0.53
1:A:560:SER:OG	1:A:561:PHE:N	2.42	0.53
1:A:656:ASP:O	1:A:657:LEU:C	2.43	0.53
1:A:188:TYR:CD2	1:A:201:ARG:HB3	2.44	0.53
1:A:99:TYR:C	1:A:100:THR:HG22	2.28	0.52
1:A:678:LEU:O	1:A:679:ASP:C	2.47	0.52
1:A:331:THR:O	1:A:332:VAL:HB	2.10	0.52
1:A:347:VAL:HG12	1:A:348:ASN:N	2.25	0.52
1:A:600:ASN:C	1:A:601:GLU:HG3	2.30	0.52
1:A:348:ASN:HD22	1:A:349:LYS:N	2.08	0.52
1:A:533:GLN:NE2	1:A:533:GLN:CA	2.44	0.52
1:A:623:GLN:HG3	1:A:625:PHE:CZ	2.36	0.51
1:A:380:LEU:N	1:A:380:LEU:HD12	2.26	0.51
1:A:361:ARG:NH1	1:A:361:ARG:CG	2.54	0.51
1:A:144:ALA:CB	2:A:1:NAG:H82	2.41	0.51
1:A:55:SER:O	1:A:56:HIS:C	2.48	0.51
1:A:465:TYR:CD1	1:A:465:TYR:C	2.84	0.51
1:A:380:LEU:N	1:A:380:LEU:CD1	2.74	0.51
1:A:334:ILE:HG22	1:A:372:PHE:CZ	2.46	0.51
1:A:554:ARG:NH1	1:A:572:LEU:O	2.43	0.50
1:A:232:MET:HE2	1:A:244:PHE:HD2	1.73	0.50
1:A:593:GLN:NE2	1:A:595:TYR:OH	2.43	0.50
1:A:152:LEU:N	1:A:152:LEU:HD23	2.27	0.50
1:A:672:ALA:HA	1:A:675:ARG:HD3	1.94	0.50
1:A:247:ARG:HB2	1:A:250:SER:OG	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:MET:HB2	1:A:608:TYR:CB	2.40	0.50
1:A:559:PHE:CE2	1:A:561:PHE:CE2	3.00	0.50
1:A:237:ASP:OD1	1:A:240:ASN:HB2	2.11	0.49
1:A:215:SER:HB2	1:A:222:PHE:HB3	1.94	0.49
1:A:249:ASP:OD1	1:A:249:ASP:N	2.44	0.49
1:A:478:ASP:OD1	1:A:478:ASP:N	2.43	0.49
1:A:295:CYS:SG	1:A:296:PRO:CD	3.00	0.49
1:A:531:VAL:HG12	1:A:561:PHE:CE1	2.47	0.49
1:A:80:GLY:HA3	1:A:382:TRP:CH2	2.48	0.49
1:A:351:MET:SD	1:A:383:LEU:HD12	2.53	0.49
1:A:71:PHE:CZ	1:A:477:GLY:HA2	2.48	0.48
1:A:617:ASP:OD1	1:A:617:ASP:N	2.47	0.48
1:A:529:VAL:O	1:A:529:VAL:HG13	2.14	0.48
1:A:144:ALA:HB3	2:A:1:NAG:H82	1.95	0.48
1:A:450:LEU:H	1:A:450:LEU:HD12	1.79	0.48
1:A:656:ASP:O	1:A:660:ILE:HG23	2.12	0.48
1:A:605:TYR:CZ	1:A:610:HIS:HB2	2.49	0.47
1:A:343:ILE:O	1:A:344:GLU:C	2.52	0.47
1:A:505:VAL:O	1:A:509:ILE:HG23	2.14	0.47
1:A:129:SER:HA	1:A:132:THR:HG23	1.96	0.47
1:A:232:MET:CE	1:A:244:PHE:CD2	2.97	0.47
1:A:372:PHE:HB2	1:A:380:LEU:HB2	1.95	0.47
1:A:505:VAL:O	1:A:509:ILE:CG2	2.63	0.47
1:A:379:LEU:HB2	1:A:450:LEU:HD23	1.96	0.47
1:A:60:PHE:CD1	1:A:60:PHE:N	2.81	0.47
1:A:575:ASP:O	1:A:576:ASN:HB2	2.14	0.47
1:A:238:GLY:O	1:A:239:LYS:CB	2.49	0.47
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.77	0.47
1:A:232:MET:HE2	1:A:244:PHE:CE2	2.48	0.47
1:A:181:TYR:O	1:A:207:LEU:HD23	2.16	0.46
1:A:259:ILE:HG21	1:A:259:ILE:HD12	1.71	0.46
1:A:328:THR:OG1	1:A:330:THR:HG23	2.16	0.46
1:A:232:MET:HE3	1:A:246:GLU:HG3	1.97	0.46
1:A:448:LYS:HD2	1:A:449:SER:N	2.32	0.45
1:A:657:LEU:HA	1:A:657:LEU:HD22	1.64	0.45
1:A:313:LYS:O	1:A:331:THR:HG22	2.15	0.45
1:A:138:ILE:HD13	1:A:138:ILE:HG21	1.66	0.45
1:A:108:ILE:HG23	1:A:108:ILE:O	2.17	0.45
1:A:143:ASN:HB2	1:A:158:ASP:HB2	1.98	0.45
1:A:318:VAL:HG11	1:A:470:ARG:HH12	1.82	0.45
1:A:510:TYR:HD2	1:A:514:VAL:HG11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HD11	1:A:274:ARG:CD	2.46	0.44
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.72	0.44
1:A:141:CYS:O	1:A:166:VAL:HG22	2.17	0.44
1:A:66:ILE:CG1	1:A:488:LYS:HA	2.47	0.44
1:A:71:PHE:CE1	1:A:480:ALA:HB2	2.53	0.44
1:A:63:SER:O	1:A:64:SER:C	2.56	0.44
1:A:574:THR:O	1:A:575:ASP:CB	2.62	0.44
1:A:313:LYS:O	1:A:331:THR:HG23	2.18	0.44
1:A:62:PHE:O	1:A:63:SER:C	2.55	0.44
1:A:129:SER:O	1:A:130:TYR:C	2.55	0.44
1:A:518:ARG:HB3	1:A:518:ARG:HE	1.66	0.43
1:A:509:ILE:O	1:A:509:ILE:HD12	2.18	0.43
1:A:257:TYR:CD2	1:A:274:ARG:HD3	2.53	0.43
1:A:306:THR:HG22	1:A:319:THR:HB	2.00	0.43
1:A:554:ARG:HA	1:A:555:PRO:HD3	1.91	0.43
1:A:604:VAL:O	1:A:605:TYR:HD2	2.01	0.43
1:A:498:THR:HG22	1:A:505:VAL:HG11	2.01	0.43
1:A:650:ARG:C	1:A:652:SER:H	2.21	0.43
1:A:193:ARG:H	1:A:193:ARG:HG2	1.69	0.43
1:A:605:TYR:CE2	1:A:610:HIS:CB	2.98	0.43
1:A:140:GLN:HA	1:A:166:VAL:O	2.19	0.43
1:A:184:GLN:N	1:A:205:ASN:OD1	2.40	0.43
1:A:494:LEU:O	1:A:498:THR:HG23	2.19	0.43
1:A:49:ARG:HD3	1:A:513:ALA:HB1	1.99	0.42
1:A:259:ILE:HD13	1:A:259:ILE:HG23	1.76	0.42
1:A:576:ASN:HD21	1:A:598:SER:HA	1.83	0.42
1:A:303:PHE:HB3	1:A:306:THR:CG2	2.49	0.42
1:A:283:THR:HG22	1:A:284:LEU:N	2.33	0.42
1:A:265:ARG:HB2	1:A:265:ARG:HE	1.31	0.42
1:A:217:SER:HA	1:A:219:PHE:N	2.35	0.42
1:A:58:ASP:O	1:A:525:VAL:N	2.52	0.42
1:A:104:THR:HB	1:A:203:THR:HG23	2.02	0.42
1:A:347:VAL:CG1	1:A:348:ASN:N	2.81	0.41
1:A:539:ARG:HD3	1:A:556:LEU:CB	2.49	0.41
1:A:602:ILE:HG22	1:A:603:HIS:N	2.36	0.41
1:A:71:PHE:HZ	1:A:476:LEU:O	2.03	0.41
1:A:576:ASN:HD21	1:A:598:SER:CA	2.33	0.41
1:A:358:VAL:O	1:A:358:VAL:HG13	2.20	0.41
1:A:295:CYS:HA	1:A:296:PRO:HD3	1.69	0.41
1:A:366:GLN:OE1	1:A:384:PRO:HD3	2.20	0.41
1:A:85:PHE:O	1:A:378:LEU:HD12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ARG:O	1:A:652:SER:N	2.54	0.41
1:A:461:ILE:C	1:A:463:PHE:N	2.74	0.41
1:A:360:ASP:N	1:A:360:ASP:OD2	2.53	0.41
1:A:201:ARG:HD3	1:A:201:ARG:HH11	1.68	0.40
1:A:324:SER:HB2	1:A:459:VAL:HG23	2.02	0.40
1:A:150:ASP:C	1:A:152:LEU:H	2.24	0.40
1:A:299:HIS:CG	1:A:346:GLN:HE22	2.40	0.40
1:A:221:PHE:C	1:A:221:PHE:CD2	2.95	0.40
1:A:355:TYR:CD1	1:A:355:TYR:C	2.92	0.40
1:A:63:SER:O	1:A:65:ASP:N	2.55	0.40
1:A:66:ILE:HG12	1:A:488:LYS:HA	2.04	0.40
1:A:85:PHE:CD1	1:A:299:HIS:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/663 (82%)	479 (88%)	60 (11%)	8 (2%)	13	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	VAL
1	A	341	LYS
1	A	651	ALA
1	A	48	PHE
1	A	534	ALA
1	A	503	THR
1	A	358	VAL
1	A	57	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	500/585 (86%)	401 (80%)	99 (20%)	1 8

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	46	PHE
1	A	49	ARG
1	A	51	CYS
1	A	59	LEU
1	A	60	PHE
1	A	64	SER
1	A	71	PHE
1	A	76	ASN
1	A	78	THR
1	A	84	VAL
1	A	86	LYS
1	A	87	ASP
1	A	88	ASN
1	A	96	VAL
1	A	99	TYR
1	A	100	THR
1	A	105	ASN
1	A	107	LEU
1	A	108	ILE
1	A	138	ILE
1	A	148	THR
1	A	153	THR
1	A	157	VAL
1	A	176	ASN
1	A	179	ARG
1	A	184	GLN
1	A	187	LEU
1	A	200	THR
1	A	203	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	207	LEU
1	A	223	VAL
1	A	229	THR
1	A	232	MET
1	A	241	LYS
1	A	242	GLU
1	A	243	THR
1	A	247	ARG
1	A	253	VAL
1	A	255	THR
1	A	258	LYS
1	A	267	THR
1	A	279	LYS
1	A	297	LEU
1	A	302	THR
1	A	304	ASP
1	A	309	THR
1	A	313	LYS
1	A	319	THR
1	A	323	THR
1	A	327	VAL
1	A	334	ILE
1	A	338	ASP
1	A	342	CYS
1	A	347	VAL
1	A	348	ASN
1	A	354	LYS
1	A	358	VAL
1	A	360	ASP
1	A	361	ARG
1	A	378	LEU
1	A	383	LEU
1	A	386	THR
1	A	448	LYS
1	A	450	LEU
1	A	472	ILE
1	A	475	MET
1	A	478	ASP
1	A	479	LEU
1	A	481	ARG
1	A	488	LYS
1	A	489	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	509	ILE
1	A	510	TYR
1	A	533	GLN
1	A	550	MET
1	A	554	ARG
1	A	557	VAL
1	A	567	THR
1	A	569	GLU
1	A	574	THR
1	A	575	ASP
1	A	591	THR
1	A	601	GLU
1	A	614	ILE
1	A	617	ASP
1	A	625	PHE
1	A	632	LEU
1	A	637	ASP
1	A	643	LEU
1	A	647	ASP
1	A	648	GLU
1	A	650	ARG
1	A	652	SER
1	A	657	LEU
1	A	660	ILE
1	A	663	GLU
1	A	674	LEU
1	A	678	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	134	GLN
1	A	228	GLN
1	A	252	HIS
1	A	256	ASN
1	A	329	ASN
1	A	346	GLN
1	A	348	ASN
1	A	460	GLN
1	A	533	GLN
1	A	571	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	576	ASN
1	A	593	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	1	1	14,14,15	0.84	0	15,19,21	2.31	3 (20%)
2	NAG	A	686	1	14,14,15	0.96	1 (7%)	15,19,21	1.52	2 (13%)
2	NAG	A	687	1	14,14,15	0.79	1 (7%)	15,19,21	1.31	1 (6%)

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	1	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	A	686	1	-	0/6/23/26	0/1/1/1
2	NAG	A	687	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	687	NAG	C1-C2	2.07	1.55	1.52
2	A	686	NAG	C8-C7	2.45	1.55	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	686	NAG	C4-C3-C2	-3.25	106.18	111.23
2	A	1	NAG	O4-C4-C5	2.44	115.69	109.24
2	A	1	NAG	C2-N2-C7	3.39	127.39	123.04
2	A	686	NAG	O5-C5-C6	3.81	115.59	107.35
2	A	687	NAG	C1-O5-C5	4.32	117.73	112.25
2	A	1	NAG	C1-O5-C5	6.89	121.00	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	1	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, 95th 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 ²)	Q<0.9
1	A	559/663 (84%)	0.37	54 (9%) 10 6	57, 77, 100, 108	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	552	TYR	7.4
1	A	551	CYS	7.1
1	A	550	MET	5.4
1	A	331	THR	5.1
1	A	592	SER	5.1
1	A	535	THR	4.9
1	A	332	VAL	4.5
1	A	68	CYS	4.5
1	A	567	THR	4.3
1	A	543	ARG	4.1
1	A	679	ASP	4.1
1	A	553	SER	3.8
1	A	510	TYR	3.6
1	A	43	GLN	3.5
1	A	532	ASN	3.2
1	A	591	THR	3.2
1	A	609	HIS	3.1
1	A	52	GLU	3.1
1	A	53	LEU	3.1
1	A	67	GLN	3.1
1	A	65	ASP	3.1
1	A	312	GLY	2.9
1	A	267	THR	2.9
1	A	44	THR	2.9
1	A	313	LYS	2.8
1	A	569	GLU	2.8
1	A	531	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	330	THR	2.7
1	A	618	GLY	2.7
1	A	615	GLU	2.7
1	A	389	SER	2.5
1	A	269	PRO	2.5
1	A	613	THR	2.5
1	A	600	ASN	2.5
1	A	542	MET	2.5
1	A	578	ILE	2.4
1	A	603	HIS	2.3
1	A	514	VAL	2.2
1	A	334	ILE	2.2
1	A	536	VAL	2.2
1	A	54	SER	2.2
1	A	270	GLN	2.2
1	A	264	ASN	2.2
1	A	390	LEU	2.1
1	A	561	PHE	2.1
1	A	590	ALA	2.1
1	A	678	LEU	2.1
1	A	620	ALA	2.1
1	A	512	LYS	2.1
1	A	388	ARG	2.1
1	A	621	THR	2.0
1	A	533	GLN	2.0
1	A	367	GLU	2.0
1	A	625	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 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, 95th 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(\AA^2)	Q<0.9
2	NAG	A	687	14/15	0.64	0.69	4.21	102,106,107,107	0
2	NAG	A	1	14/15	0.88	0.20	-0.67	68,69,70,71	0
2	NAG	A	686	14/15	0.66	0.49	-	99,102,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.