



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:58 AM UTC

PDB ID : 5XEB / pdb_00005xeb
Title : Structure of the envelope glycoprotein of Dhori virus
Authors : Peng, R.; Shi, Y.; Qi, J.; Gao, G.F.
Deposited on : 2017-04-03
Resolution : 2.50 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

<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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

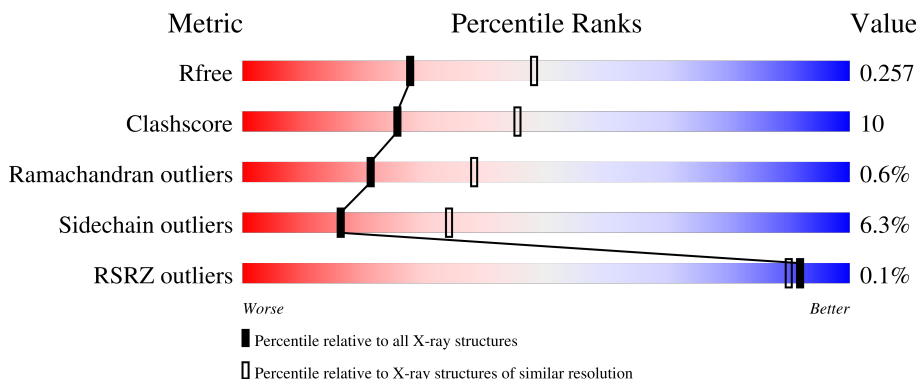
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	474	 65% 16% • 18%
1	B	474	 66% 15% • 18%
1	C	474	 59% 20% • 18%

2 Entry composition [i](#)

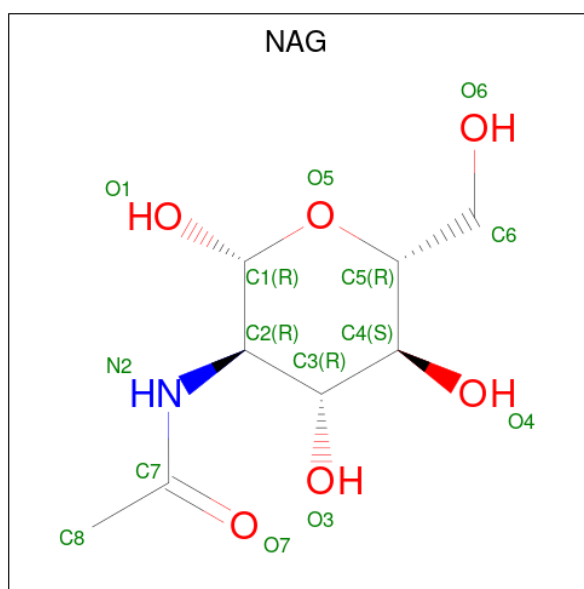
There are 3 unique types of molecules in this entry. The entry contains 9601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3114	1982	532	580	20			
1	B	390	Total	C	N	O	S	0	0	0
			3114	1982	532	580	20			
1	C	389	Total	C	N	O	S	0	1	0
			3116	1983	533	581	19			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

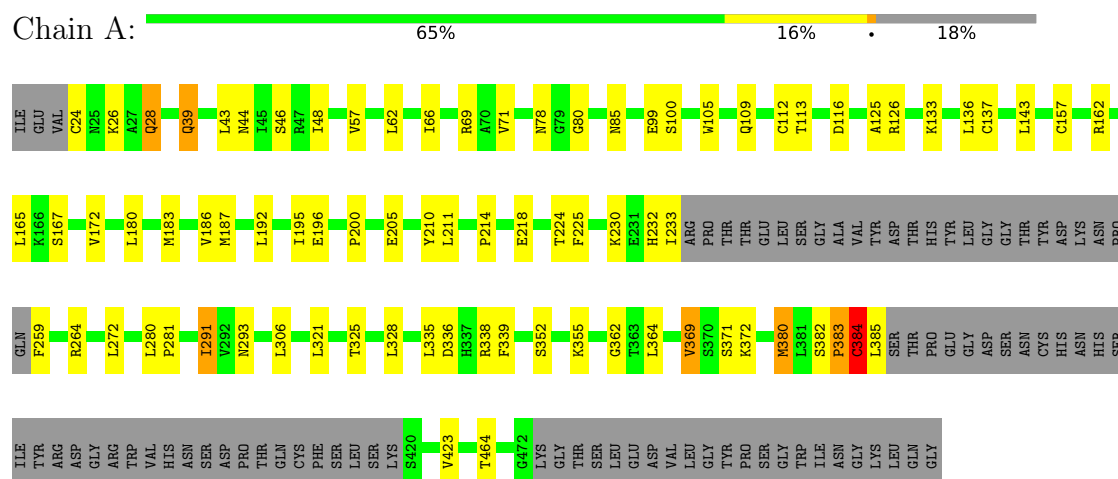
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	72	Total	O	0	0
			72	72		
3	C	24	Total	O	0	0
			24	24		

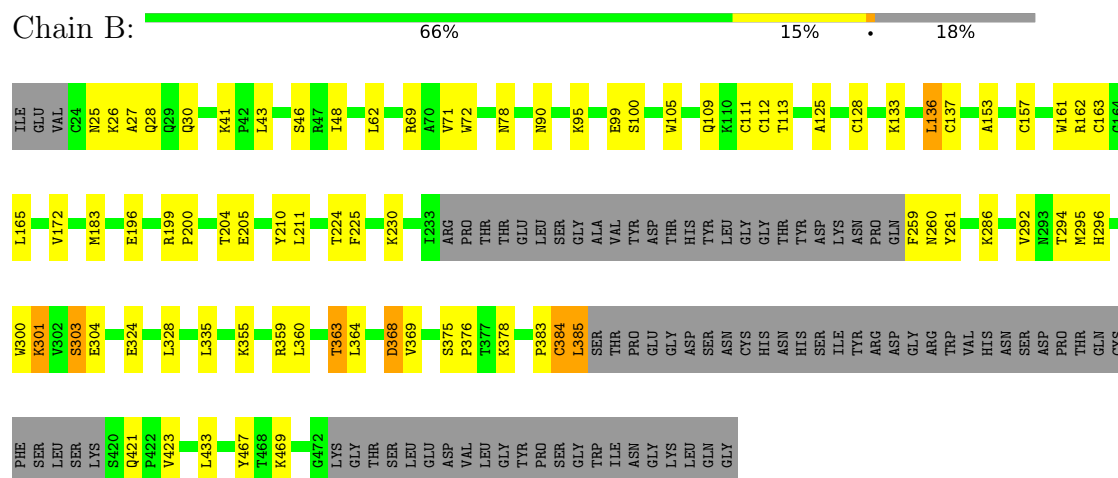
3 Residue-property plots

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: Envelope glycoprotein



• Molecule 1: Envelope glycoprotein



• Molecule 1: Envelope glycoprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	106.73Å 106.73Å 134.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.94 – 2.50 34.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	72.3 (34.94-2.50) 72.4 (34.94-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.231 , 0.257 0.228 , 0.257	Depositor DCC
R_{free} test set	2170 reflections (3.65%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 20.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.407 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9601	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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 35.02 % 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 6.2255e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.14	0/3192	0.37	0/4330
1	B	0.13	0/3192	0.37	0/4330
1	C	0.16	0/3194	0.44	0/4333
All	All	0.15	0/9578	0.39	0/12993

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	43	LEU	Peptide

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	3114	0	3036	48	1
1	B	3114	0	3037	53	0
1	C	3116	0	3037	77	0
2	A	28	0	26	1	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
3	A	105	0	0	23	1
3	B	72	0	0	15	0
3	C	24	0	0	5	0
All	All	9601	0	9162	178	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 10.

All (178) 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:B:128:CYS:SG	3:B:725:HOH:O	2.29	0.91
1:B:199:ARG:HD2	1:B:200:PRO:HD2	1.61	0.82
1:C:111:CYS:SG	1:C:141:LYS:NZ	2.54	0.78
1:C:45:ILE:HD11	1:C:229:PHE:HB3	1.70	0.73
1:B:384:CYS:SG	1:B:385:LEU:N	2.58	0.72
1:A:336:ASP:OD1	3:A:701:HOH:O	2.08	0.71
1:A:26:LYS:HE3	1:A:28:GLN:H	1.56	0.70
1:A:44:ASN:HD22	2:A:602:NAG:C7	2.05	0.69
1:B:300:TRP:O	3:B:701:HOH:O	2.11	0.68
1:C:97:PRO:O	1:C:202:TYR:OH	2.14	0.66
1:A:464:THR:OG1	3:A:702:HOH:O	2.13	0.66
1:C:280:LEU:HD22	1:C:285:TYR:HE2	1.60	0.65
1:A:80:GLY:N	3:A:703:HOH:O	2.30	0.65
1:B:375:SER:HB3	1:B:378:LYS:HB2	1.77	0.65
1:B:95:LYS:HB2	3:B:704:HOH:O	1.97	0.64
1:C:287:ARG:NH1	3:C:704:HOH:O	2.29	0.64
1:B:78:ASN:OD1	3:B:702:HOH:O	2.15	0.64
1:C:138:HIS:HB3	1:C:141:LYS:HE3	1.79	0.64
1:A:78:ASN:OD1	3:A:703:HOH:O	2.16	0.63
1:C:115:PRO:O	1:C:161:TRP:NE1	2.29	0.63
1:C:64:PHE:CE2	1:C:66:ILE:HD11	2.35	0.62
1:C:110:LYS:HE3	1:C:137:CYS:HB2	1.82	0.62
1:B:230:LYS:O	3:B:703:HOH:O	2.16	0.62
1:C:359:ARG:NH2	1:C:368:ASP:OD1	2.33	0.61
1:B:172:VAL:HG11	1:B:183:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:SER:O	3:A:704:HOH:O	2.16	0.60
1:B:95:LYS:O	3:B:704:HOH:O	2.17	0.60
1:A:369:VAL:HA	1:A:382:SER:O	2.02	0.59
1:C:270:PHE:HE1	1:C:272:LEU:HD23	1.67	0.59
1:A:39:GLN:OE1	3:A:705:HOH:O	2.17	0.59
1:A:24:CYS:N	3:A:733:HOH:O	2.35	0.59
1:A:232:HIS:HA	1:A:259:PHE:HA	1.85	0.58
1:A:172:VAL:HG11	1:A:183:MET:HE2	1.85	0.58
1:B:112:CYS:HA	1:B:137:CYS:HA	1.86	0.58
1:B:368:ASP:HB3	1:B:385:LEU:HA	1.86	0.58
1:B:69:ARG:HA	1:B:162:ARG:O	2.05	0.57
1:C:78:ASN:HD22	1:C:150[B]:ASN:HA	1.70	0.56
1:B:28:GLN:O	1:B:30:GLN:N	2.36	0.56
1:C:375:SER:HG	1:C:378:LYS:H	1.54	0.56
1:A:371:SER:HA	1:A:380:MET:O	2.06	0.55
1:A:113:THR:HG22	1:A:136:LEU:O	2.06	0.55
1:A:339:PHE:HB2	3:A:701:HOH:O	2.07	0.55
1:A:187:MET:SD	3:A:709:HOH:O	2.58	0.55
1:A:362:GLY:HA2	1:A:369:VAL:HG12	1.88	0.55
1:B:421:GLN:N	3:B:708:HOH:O	2.39	0.54
1:A:109:GLN:OE1	3:A:706:HOH:O	2.18	0.54
1:A:48:ILE:HG12	3:A:708:HOH:O	2.08	0.54
1:A:116:ASP:OD2	3:A:707:HOH:O	2.19	0.53
1:B:69:ARG:HG3	1:B:163:CYS:HB3	1.90	0.53
1:C:66:ILE:O	1:C:165:LEU:HA	2.08	0.53
1:C:138:HIS:C	1:C:141:LYS:HE3	2.34	0.52
1:C:186:VAL:O	3:C:701:HOH:O	2.19	0.52
1:C:265:ASP:OD2	1:C:285:TYR:OH	2.17	0.52
1:C:76:CYS:SG	3:C:714:HOH:O	2.58	0.52
1:B:99:GLU:HG3	1:B:211:LEU:HD13	1.93	0.51
1:C:71:VAL:HG23	1:C:93:ILE:HB	1.92	0.51
1:A:230:LYS:NZ	3:A:741:HOH:O	2.44	0.51
1:C:147:SER:HB3	1:C:468:THR:HG21	1.93	0.51
1:A:66:ILE:HG12	1:A:210:TYR:HD1	1.76	0.50
1:A:99:GLU:HG3	1:A:211:LEU:HD13	1.94	0.50
1:B:199:ARG:HD2	1:B:200:PRO:CD	2.38	0.50
1:C:66:ILE:HD12	1:C:210:TYR:HD1	1.77	0.50
1:C:61:GLY:O	1:C:169:HIS:ND1	2.45	0.50
1:C:293:ASN:HB3	1:C:295:MET:O	2.12	0.50
1:B:48:ILE:HD13	1:B:230:LYS:HE2	1.94	0.49
1:B:368:ASP:CG	1:B:385:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:GLU:OE1	1:C:210:TYR:OH	2.20	0.49
1:B:205:GLU:HG2	1:B:210:TYR:HE2	1.78	0.49
1:B:324:GLU:OE2	3:B:705:HOH:O	2.19	0.49
1:B:224:THR:OG1	1:B:225:PHE:N	2.46	0.49
1:C:91:ASP:OD2	1:C:93:ILE:HG13	2.12	0.49
1:C:200:PRO:HB3	1:C:211:LEU:HD11	1.94	0.49
1:B:25:ASN:OD1	1:B:26:LYS:N	2.46	0.48
1:C:45:ILE:HD13	1:C:231:GLU:HB2	1.94	0.48
1:C:55:THR:HG21	1:C:181:VAL:HG11	1.96	0.48
1:B:359:ARG:NH2	1:B:368:ASP:OD1	2.42	0.48
1:C:66:ILE:HD12	1:C:210:TYR:CD1	2.49	0.47
1:C:233:ILE:HG13	3:C:713:HOH:O	2.14	0.47
1:B:230:LYS:HA	1:B:260:ASN:O	2.14	0.47
1:C:282:THR:N	3:C:706:HOH:O	2.35	0.47
1:A:264:ARG:NH2	3:A:714:HOH:O	2.43	0.47
1:C:196:GLU:HB2	1:C:198:THR:HG22	1.95	0.47
1:C:105:TRP:CZ3	1:C:111:CYS:HB2	2.50	0.47
1:A:46:SER:O	3:A:708:HOH:O	2.20	0.47
1:C:45:ILE:HG13	1:C:46:SER:N	2.28	0.47
1:C:186:VAL:HG12	1:C:445:VAL:HG11	1.96	0.47
1:A:205:GLU:OE1	3:A:709:HOH:O	2.21	0.47
1:A:383:PRO:HB2	1:A:384:CYS:H	1.53	0.47
1:B:46:SER:OG	3:B:703:HOH:O	2.20	0.47
1:B:133:LYS:HD3	1:B:133:LYS:HA	1.76	0.47
1:B:113:THR:HG22	1:B:136:LEU:O	2.14	0.47
1:C:142:GLU:OE2	1:C:162:ARG:NE	2.47	0.47
1:C:186:VAL:HG11	1:C:445:VAL:HG21	1.97	0.47
1:B:295:MET:HG2	1:B:296:HIS:H	1.79	0.46
1:B:105:TRP:HB3	1:B:165:LEU:HD22	1.96	0.46
1:C:138:HIS:CE1	1:C:139:THR:HG22	2.51	0.46
1:B:125:ALA:HA	1:B:157:CYS:HB3	1.96	0.46
1:C:124:ASP:N	1:C:124:ASP:OD1	2.48	0.46
1:C:25:ASN:OD1	1:C:26:LYS:N	2.49	0.46
1:C:71:VAL:O	1:C:92:LEU:HA	2.16	0.46
1:C:198:THR:HG23	1:C:199:ARG:N	2.30	0.46
1:B:46:SER:N	3:B:703:HOH:O	2.48	0.46
1:C:138:HIS:CG	1:C:139:THR:H	2.34	0.46
1:A:167:SER:OG	3:A:706:HOH:O	2.19	0.46
1:A:291:ILE:H	1:A:291:ILE:HG13	1.55	0.46
1:B:360:LEU:O	1:B:363:THR:HG22	2.16	0.46
1:A:126:ARG:NH2	3:A:723:HOH:O	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LYS:HB2	1:C:162:ARG:HA	1.98	0.45
1:C:45:ILE:HD12	1:C:230:LYS:O	2.17	0.45
1:A:26:LYS:HB3	1:A:28:GLN:HB3	1.97	0.45
1:A:85:ASN:ND2	3:A:736:HOH:O	2.41	0.45
1:A:133:LYS:HD3	1:A:133:LYS:HA	1.82	0.45
1:B:286:LYS:HE3	1:B:292:VAL:HG23	1.99	0.45
1:C:200:PRO:CB	1:C:211:LEU:HD11	2.47	0.45
1:B:71:VAL:HG22	1:B:161:TRP:CZ3	2.52	0.45
1:C:384:CYS:SG	1:C:385:LEU:N	2.89	0.45
1:A:57:VAL:HA	1:A:218:GLU:O	2.17	0.44
1:C:69:ARG:HA	1:C:162:ARG:O	2.16	0.44
1:A:143:LEU:HD12	3:A:702:HOH:O	2.18	0.44
1:A:230:LYS:N	3:A:708:HOH:O	2.40	0.44
1:C:115:PRO:O	1:C:159:LEU:HD23	2.17	0.44
1:C:168:THR:OG1	1:C:169:HIS:N	2.50	0.44
1:C:138:HIS:ND1	1:C:139:THR:HG22	2.33	0.44
1:C:200:PRO:HA	1:C:214:PRO:HD3	2.00	0.44
1:B:467:TYR:CZ	1:B:469:LYS:HE3	2.53	0.43
1:B:295:MET:HE2	1:B:296:HIS:CE1	2.53	0.43
1:A:205:GLU:HG2	1:A:210:TYR:HE2	1.83	0.43
1:C:99:GLU:OE2	1:C:211:LEU:HD13	2.18	0.43
1:C:69:ARG:HB3	1:C:95:LYS:O	2.18	0.43
1:C:371:SER:HA	1:C:380:MET:O	2.19	0.43
1:A:69:ARG:HA	1:A:162:ARG:O	2.18	0.43
1:A:112:CYS:HA	1:A:137:CYS:HA	2.00	0.43
1:A:321:LEU:O	1:A:325:THR:HG23	2.18	0.43
1:B:303:SER:OG	3:B:707:HOH:O	2.21	0.43
1:C:301:LYS:HD2	1:C:304:GLU:HG3	2.01	0.43
1:B:383:PRO:O	1:B:384:CYS:HB2	2.18	0.43
1:C:92:LEU:HD11	1:C:143:LEU:HD21	2.01	0.43
1:B:196:GLU:O	3:B:706:HOH:O	2.21	0.43
1:C:77:TYR:HB2	1:C:155:HIS:ND1	2.34	0.43
1:B:259:PHE:N	3:B:734:HOH:O	2.52	0.43
1:C:78:ASN:HA	1:C:86:THR:HG23	2.01	0.43
1:C:44:ASN:HB3	1:C:45:ILE:H	1.59	0.42
1:B:300:TRP:H	1:B:300:TRP:CD1	2.37	0.42
1:C:205:GLU:HB2	1:C:210:TYR:CE2	2.54	0.42
1:C:233:ILE:HG12	1:C:260:ASN:OD1	2.19	0.42
1:B:26:LYS:HD2	1:B:27:ALA:H	1.83	0.42
1:C:73:ARG:HB2	1:C:159:LEU:HD12	2.01	0.42
1:C:133:LYS:O	1:C:135:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:HA	1:A:157:CYS:HB3	2.01	0.42
1:A:355:LYS:HB2	3:A:704:HOH:O	2.20	0.42
1:C:201:THR:O	1:C:211:LEU:HD12	2.20	0.42
1:C:295:MET:HG3	1:C:296:HIS:N	2.35	0.42
1:C:296:HIS:N	1:C:297:PRO:HD3	2.35	0.42
1:B:355:LYS:NZ	1:B:376:PRO:HA	2.35	0.42
1:A:224:THR:OG1	1:A:225:PHE:N	2.49	0.41
1:C:105:TRP:HB3	1:C:165:LEU:HD22	2.02	0.41
1:A:105:TRP:HB3	1:A:165:LEU:HD22	2.03	0.41
1:B:230:LYS:HD3	1:B:261:TYR:CE1	2.55	0.41
1:C:93:ILE:H	1:C:93:ILE:HD12	1.85	0.41
1:C:295:MET:HG3	1:C:296:HIS:H	1.84	0.41
1:C:459:GLN:OE1	1:C:462:ILE:HD11	2.20	0.41
1:B:105:TRP:CD2	1:B:111:CYS:HA	2.56	0.41
1:C:276:ARG:NH2	1:C:298:ASN:OD1	2.54	0.41
1:A:200:PRO:HA	1:A:214:PRO:HD3	2.01	0.41
1:B:72:TRP:CH2	1:B:90:ASN:HB3	2.55	0.41
1:B:301:LYS:HB3	1:B:304:GLU:HG3	2.02	0.41
1:B:421:GLN:O	3:B:708:HOH:O	2.22	0.41
1:A:186:VAL:HG22	1:A:192:LEU:HD22	2.02	0.41
1:B:78:ASN:O	1:B:153:ALA:N	2.53	0.41
1:C:103:ARG:HG3	1:C:107:LYS:HZ3	1.86	0.41
1:C:306:LEU:HD23	1:C:445:VAL:HB	2.02	0.41
1:B:368:ASP:OD2	1:B:385:LEU:HD23	2.21	0.41
1:C:43:LEU:HB3	1:C:44:ASN:H	1.69	0.41
1:C:99:GLU:HG2	1:C:202:TYR:CG	2.56	0.41
1:A:280:LEU:O	1:A:281:PRO:C	2.65	0.40
1:B:369:VAL:O	3:B:710:HOH:O	2.22	0.40
1:A:232:HIS:O	3:A:710:HOH:O	2.21	0.40
1:C:29:GLN:O	1:C:31:GLY:N	2.53	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)
1:A:338:ARG:NH1	3:A:701:HOH:O[2_555]	2.11	0.09

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	384/474 (81%)	363 (94%)	19 (5%)	2 (0%)	24	43
1	B	384/474 (81%)	365 (95%)	18 (5%)	1 (0%)	36	55
1	C	384/474 (81%)	353 (92%)	27 (7%)	4 (1%)	12	24
All	All	1152/1422 (81%)	1081 (94%)	64 (6%)	7 (1%)	21	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	PRO
1	B	384	CYS
1	C	43	LEU
1	C	30	GLN
1	C	44	ASN
1	A	384	CYS
1	C	42	PRO

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	344/417 (82%)	321 (93%)	23 (7%)	15	31
1	B	344/417 (82%)	326 (95%)	18 (5%)	21	42
1	C	344/417 (82%)	320 (93%)	24 (7%)	14	29
All	All	1032/1251 (82%)	967 (94%)	65 (6%)	16	34

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	39	GLN
1	A	43	LEU
1	A	62	LEU
1	A	71	VAL
1	A	100	SER
1	A	180	LEU
1	A	195	ILE
1	A	196	GLU
1	A	233	ILE
1	A	272	LEU
1	A	291	ILE
1	A	293	ASN
1	A	306	LEU
1	A	328	LEU
1	A	335	LEU
1	A	364	LEU
1	A	369	VAL
1	A	372	LYS
1	A	380	MET
1	A	384	CYS
1	A	385	LEU
1	A	423	VAL
1	B	41	LYS
1	B	43	LEU
1	B	62	LEU
1	B	100	SER
1	B	109	GLN
1	B	136	LEU
1	B	204	THR
1	B	294	THR
1	B	301	LYS
1	B	303	SER
1	B	328	LEU
1	B	335	LEU
1	B	363	THR
1	B	364	LEU
1	B	368	ASP
1	B	385	LEU
1	B	423	VAL
1	B	433	LEU
1	C	43	LEU

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Mol	Chain	Res	Type
1	C	45	ILE
1	C	60	LYS
1	C	62	LEU
1	C	71	VAL
1	C	73	ARG
1	C	100	SER
1	C	123	SER
1	C	124	ASP
1	C	137	CYS
1	C	141	LYS
1	C	159	LEU
1	C	165	LEU
1	C	186	VAL
1	C	193	ILE
1	C	272	LEU
1	C	292	VAL
1	C	293	ASN
1	C	294	THR
1	C	305	LYS
1	C	335	LEU
1	C	359	ARG
1	C	360	LEU
1	C	439	VAL

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

Mol	Chain	Res	Type
1	A	39	GLN
1	B	148	ASN
1	B	155	HIS
1	B	456	GLN
1	C	78	ASN
1	C	151	HIS

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	$\# Z > 2$
2	NAG	A	601	1	14,14,15	0.32	0	17,19,21	0.41	0
2	NAG	C	601	1	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
2	NAG	B	601	1	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	A	602	1	14,14,15	0.15	0	17,19,21	0.44	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	601	1	-	0/6/23/26	0/1/1/1
2	NAG	C	601	1	-	2/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	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(°)
2	C	601	NAG	C1-O5-C5	2.83	115.97	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	NAG	O5-C5-C6-O6
2	C	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	NAG	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	390/474 (82%)	-1.17	0	100 100	15, 43, 91, 125	0
1	B	390/474 (82%)	-1.16	0	100 100	16, 45, 94, 171	0
1	C	389/474 (82%)	-0.73	1 (0%)	90 87	33, 93, 150, 193	1 (0%)
All	All	1169/1422 (82%)	-1.02	1 (0%)	92 90	15, 58, 128, 193	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	PRO	2.1

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	NAG	A	602	14/15	0.96	0.06	120,123,126,128	0
2	NAG	C	601	14/15	0.97	0.06	77,92,99,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	601	14/15	0.98	0.03	51,63,75,75	0
2	NAG	A	601	14/15	0.99	0.04	57,74,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.