



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:54 PM GMT

PDB ID : 4GKL
Title : Crystal structure of a noncanonic maltogenic alpha-amylase AmyB from *Thermotoga neapolitana*
Authors : Ha, N.C.; Jun, S.Y.; Kim, J.S.
Deposited on : 2012-08-13
Resolution : 2.40 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

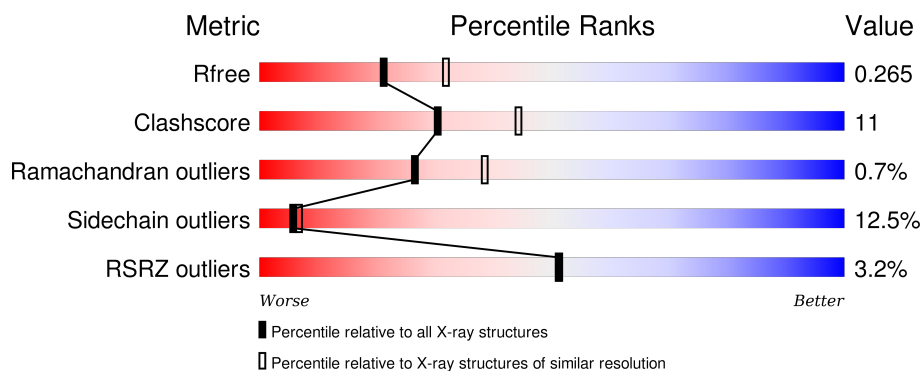
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	422	 4% 65% 27% 6%
1	B	422	 2% 70% 26% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7265 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 Alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3514	2274	600	622	18			
1	B	419	Total	C	N	O	S	0	0	0
			3507	2269	599	621	18			

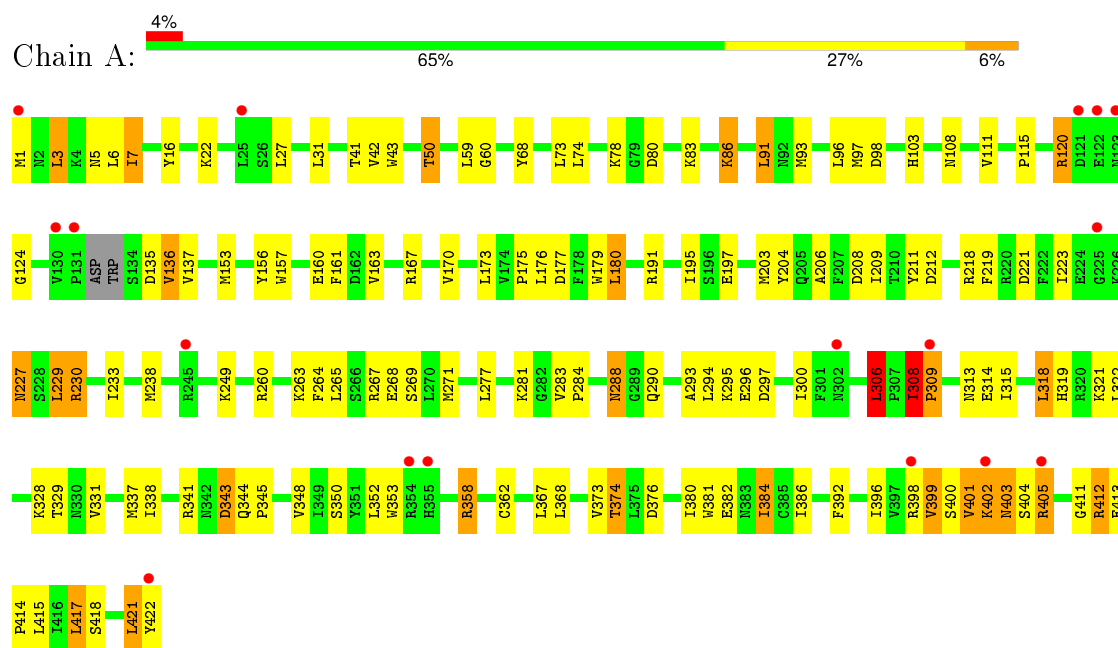
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	117	Total	O	0	0
			117	117		
2	B	127	Total	O	0	0
			127	127		

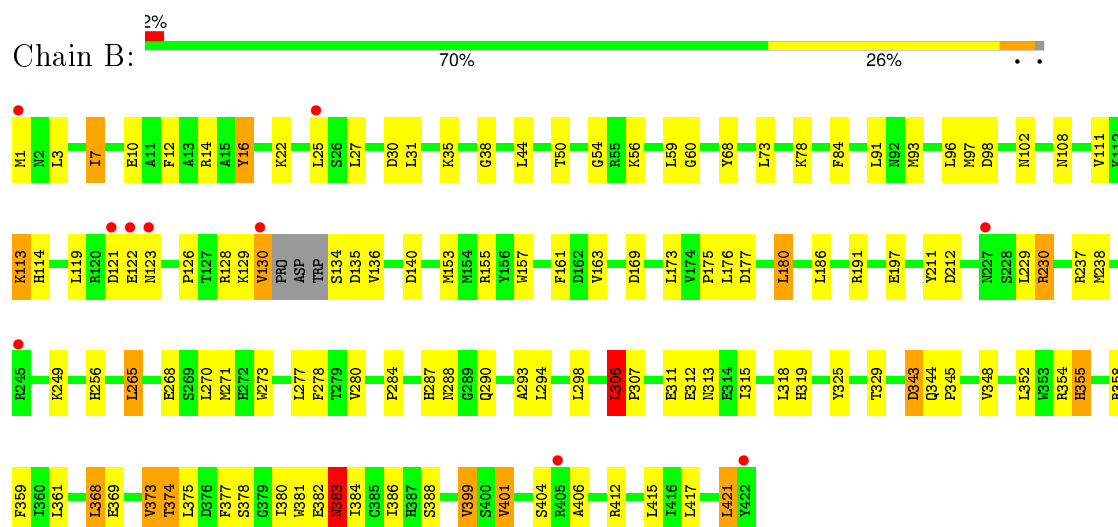
3 Residue-property plots [i](#)

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: Alpha-amylase



• Molecule 1: Alpha-amylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.88Å 74.45Å 108.90Å 90.00° 107.77° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.9 (19.98-2.40) 94.0 (19.98-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.197 , 0.263 0.200 , 0.265	Depositor DCC
R_{free} test set	1981 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.4	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 37658 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7265	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.36% 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](#)

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	0.42	0/3608	0.63	1/4874 (0.0%)
1	B	0.42	0/3600	0.62	1/4862 (0.0%)
All	All	0.42	0/7208	0.63	2/9736 (0.0%)

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	A	0	1

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	306	LEU	CA-CB-CG	6.65	130.59	115.30
1	B	306	LEU	CA-CB-CG	5.62	128.22	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	308	ILE	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	3514	0	3467	84	0
1	B	3507	0	3460	70	0
2	A	117	0	0	5	0
2	B	127	0	0	5	0
All	All	7265	0	6927	154	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 11.

All (154) 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:50:THR:HG21	1:B:60:GLY:HA3	1.59	0.85
1:B:383:ASN:HB3	1:B:384:ILE:HG13	1.57	0.85
1:B:7:ILE:HB	1:B:284:PRO:HG2	1.62	0.82
1:B:382:GLU:N	1:B:383:ASN:HB2	1.93	0.82
1:A:308:ILE:HG23	1:A:309:PRO:HD2	1.69	0.75
1:A:386:ILE:HB	1:A:399:VAL:HG13	1.70	0.73
1:A:343:ASP:HB2	1:A:374:THR:H	1.56	0.71
1:B:111:VAL:HG23	1:B:126:PRO:HG2	1.76	0.68
1:A:348:VAL:HG11	1:A:373:VAL:HG21	1.78	0.66
1:B:378:SER:O	2:B:584:HOH:O	2.14	0.65
1:B:329:THR:O	2:B:549:HOH:O	2.14	0.65
1:A:376:ASP:HA	1:A:405:ARG:HD2	1.80	0.63
1:A:219:PHE:CZ	1:A:223:ILE:HD11	2.33	0.62
1:B:97:MET:HE1	1:B:157:TRP:HB3	1.81	0.62
1:A:358:ARG:NH1	1:A:418:SER:OG	2.33	0.61
1:A:260:ARG:H	1:A:263:LYS:HZ3	1.49	0.61
1:A:411:GLY:O	1:A:413:GLU:N	2.32	0.59
1:A:50:THR:HG21	1:A:60:GLY:HA3	1.84	0.59
1:B:386:ILE:HB	1:B:399:VAL:HG13	1.83	0.59
1:A:229:LEU:HD22	1:A:233:ILE:HG12	1.85	0.59
1:B:344:GLN:HG3	1:B:373:VAL:HG13	1.85	0.59
1:A:68:TYR:HB3	1:A:153:MET:HE2	1.84	0.59
1:B:27:LEU:HB3	1:B:84:PHE:CE2	2.39	0.58
1:A:50:THR:HG21	1:A:59:LEU:O	2.04	0.58
1:A:230:ARG:HD3	1:A:345:PRO:O	2.04	0.58
1:A:97:MET:HE1	1:A:157:TRP:HB3	1.85	0.58
1:A:221:ASP:HB3	1:A:227:ASN:HB2	1.85	0.57
1:A:7:ILE:HB	1:A:284:PRO:HG2	1.86	0.57
1:B:382:GLU:H	1:B:383:ASN:HB2	1.68	0.57
1:A:175:PRO:HB2	1:A:177:ASP:OD1	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TYR:HB3	1:B:153:MET:HE2	1.87	0.57
1:B:401:VAL:HG12	1:B:406:ALA:HB2	1.88	0.55
1:A:382:GLU:HA	1:A:404:SER:HA	1.87	0.55
1:B:311:GLU:O	1:B:313:ASN:N	2.40	0.55
1:B:134:SER:N	2:B:606:HOH:O	2.39	0.55
1:A:421:LEU:O	2:A:594:HOH:O	2.18	0.55
1:A:191:ARG:NH2	1:A:208:ASP:OD2	2.40	0.55
1:B:119:LEU:HD23	1:B:140:ASP:HB2	1.89	0.55
1:A:204:TYR:O	2:A:504:HOH:O	2.18	0.54
1:A:31:LEU:HB3	1:A:93:MET:HE1	1.89	0.54
1:B:10:GLU:OE2	1:B:256:HIS:ND1	2.38	0.54
1:B:415:LEU:HB3	1:B:417:LEU:HD13	1.90	0.53
1:A:288:ASN:ND2	1:A:288:ASN:O	2.42	0.53
1:B:44:LEU:O	1:B:98:ASP:HB2	2.09	0.53
1:A:263:LYS:NZ	1:A:297:ASP:OD1	2.33	0.52
1:A:180:LEU:HD13	1:A:206:ALA:HB2	1.91	0.52
1:B:265:LEU:HD23	1:B:270:LEU:HA	1.92	0.52
1:A:267:ARG:NH1	2:A:584:HOH:O	2.28	0.52
1:A:103:HIS:HB2	1:A:136:VAL:HG13	1.90	0.52
1:A:170:VAL:HG11	1:A:203:MET:HE1	1.91	0.52
1:A:68:TYR:HB3	1:A:153:MET:CE	2.40	0.52
1:A:97:MET:CE	1:A:157:TRP:HB3	2.39	0.51
1:B:265:LEU:HD21	1:B:273:TRP:CD1	2.45	0.51
1:A:170:VAL:HG11	1:A:203:MET:CE	2.40	0.51
1:A:293:ALA:HB2	1:A:315:ILE:HG13	1.91	0.51
1:B:325:TYR:O	1:B:329:THR:HG22	2.10	0.51
1:A:400:SER:OG	1:A:402:LYS:NZ	2.43	0.51
1:A:156:TYR:CE1	1:A:160:GLU:HG3	2.46	0.51
1:B:175:PRO:HB2	1:B:177:ASP:OD1	2.10	0.51
1:B:78:LYS:HD3	1:B:161:PHE:HZ	1.75	0.51
1:A:86:LYS:HA	1:A:86:LYS:HE3	1.93	0.51
1:B:108:ASN:O	1:B:111:VAL:HG12	2.11	0.50
1:A:290:GLN:HE21	1:A:319:HIS:HE1	1.59	0.50
1:A:31:LEU:HD22	1:A:93:MET:HE3	1.94	0.50
1:B:378:SER:HA	1:B:404:SER:HB3	1.93	0.50
1:B:68:TYR:HB3	1:B:153:MET:CE	2.42	0.50
1:B:212:ASP:OD2	1:B:249:LYS:NZ	2.41	0.49
1:B:230:ARG:HD3	1:B:345:PRO:O	2.12	0.49
1:A:91:LEU:HB3	1:A:93:MET:HE2	1.93	0.49
1:A:108:ASN:O	1:A:111:VAL:HG12	2.12	0.49
1:B:359:PHE:HE2	1:B:421:LEU:HB2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LYS:O	1:B:60:GLY:HA2	2.13	0.48
1:A:412:ARG:HB2	1:A:412:ARG:NH1	2.28	0.48
1:B:7:ILE:HG12	1:B:38:GLY:O	2.14	0.48
1:B:16:TYR:OH	1:B:30:ASP:OD1	2.16	0.48
1:A:321:LYS:NZ	2:A:529:HOH:O	2.31	0.48
1:A:337:MET:HG3	1:A:353:TRP:CE2	2.48	0.48
1:B:97:MET:CE	1:B:157:TRP:HB3	2.43	0.48
1:B:197:GLU:HG3	1:B:211:TYR:CE1	2.49	0.48
1:B:381:TRP:O	1:B:404:SER:HA	2.14	0.48
1:A:78:LYS:HD3	1:A:161:PHE:HZ	1.79	0.48
1:A:3:LEU:HD23	1:A:208:ASP:HB3	1.95	0.48
1:A:415:LEU:HB3	1:A:417:LEU:HD13	1.96	0.48
1:A:392:PHE:CD1	1:A:414:PRO:HG2	2.49	0.47
1:B:35:LYS:HB2	1:B:93:MET:HE2	1.96	0.47
1:B:354:ARG:HG3	1:B:359:PHE:CE1	2.49	0.47
1:A:267:ARG:HH22	1:A:313:ASN:HB2	1.79	0.47
1:B:388:SER:OG	1:B:417:LEU:HG	2.14	0.47
1:B:359:PHE:CE2	1:B:421:LEU:HB2	2.50	0.47
1:A:80:ASP:HA	1:A:83:LYS:HE2	1.96	0.47
1:B:12:PHE:HD2	1:B:298:LEU:HD22	1.80	0.47
1:A:43:TRP:CZ2	1:A:167:ARG:HG3	2.50	0.46
1:B:230:ARG:HD2	1:B:230:ARG:HA	1.53	0.46
1:A:91:LEU:HD23	1:A:93:MET:HE1	1.97	0.46
1:A:344:GLN:HG3	1:A:373:VAL:HG22	1.97	0.46
1:A:269:SER:HA	1:A:368:LEU:HD21	1.98	0.46
1:B:268:GLU:HA	1:B:271:MET:HE2	1.97	0.46
1:A:230:ARG:HD2	1:A:230:ARG:HA	1.37	0.45
1:B:265:LEU:HD21	1:B:273:TRP:HD1	1.81	0.45
1:A:97:MET:CE	1:A:163:VAL:HG21	2.47	0.45
1:A:315:ILE:O	1:A:319:HIS:HD2	1.99	0.45
1:B:14:ARG:HD3	1:B:59:LEU:HD13	1.99	0.45
1:B:343:ASP:HB2	1:B:374:THR:H	1.80	0.45
1:A:401:VAL:HA	1:A:405:ARG:O	2.16	0.45
1:A:68:TYR:O	1:A:153:MET:HE2	2.17	0.45
1:A:223:ILE:HG23	1:A:265:LEU:HD13	1.99	0.45
1:B:176:LEU:HG	1:B:180:LEU:HD22	1.99	0.45
1:A:421:LEU:O	1:A:422:TYR:HB2	2.17	0.44
1:A:197:GLU:HB2	1:A:211:TYR:CZ	2.52	0.44
1:B:54:GLY:O	1:B:135:ASP:HB3	2.18	0.44
1:B:315:ILE:O	1:B:319:HIS:HD2	2.00	0.44
1:B:97:MET:CE	1:B:163:VAL:HG21	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:HG13	1:A:179:TRP:HE1	1.83	0.44
1:B:35:LYS:HB2	1:B:93:MET:CE	2.48	0.44
1:B:237:ARG:NH1	2:B:551:HOH:O	2.51	0.44
1:A:344:GLN:HB2	1:A:348:VAL:HG13	1.99	0.43
1:A:195:ILE:HA	1:A:209:ILE:O	2.18	0.43
1:B:287:HIS:O	1:B:290:GLN:HB3	2.18	0.43
1:A:212:ASP:OD2	1:A:249:LYS:NZ	2.37	0.43
1:A:115:PRO:O	1:A:120:ARG:HD2	2.17	0.43
1:B:113:LYS:HB2	1:B:114:HIS:CE1	2.53	0.43
1:A:384:ILE:HG12	1:A:401:VAL:HG13	2.01	0.43
1:B:129:LYS:O	1:B:130:VAL:HG22	2.18	0.43
1:B:306:LEU:HA	1:B:307:PRO:HD3	1.74	0.43
1:B:361:LEU:O	1:B:417:LEU:HB2	2.19	0.43
1:B:280:VAL:O	2:B:524:HOH:O	2.21	0.43
1:A:281:LYS:HE3	1:A:281:LYS:HB3	1.74	0.42
1:B:97:MET:HE2	1:B:97:MET:HB2	1.76	0.42
1:A:120:ARG:HG2	1:A:124:GLY:O	2.19	0.42
1:A:223:ILE:HG21	1:A:264:PHE:HB3	2.01	0.42
1:B:293:ALA:HB2	1:B:315:ILE:HG13	2.01	0.42
1:B:7:ILE:CD1	1:B:278:PHE:HE1	2.32	0.42
1:A:337:MET:HG3	1:A:353:TRP:NE1	2.34	0.42
1:A:5:ASN:ND2	2:A:535:HOH:O	2.37	0.42
1:A:268:GLU:OE2	1:A:412:ARG:HG2	2.20	0.42
1:B:31:LEU:O	1:B:93:MET:HE1	2.19	0.42
1:B:155:ARG:HB2	1:B:186:LEU:HD21	2.01	0.42
1:A:6:LEU:HD22	1:A:41:THR:OG1	2.20	0.42
1:A:306:LEU:O	1:A:308:ILE:N	2.52	0.42
1:A:267:ARG:O	1:A:271:MET:HG3	2.19	0.41
1:A:318:LEU:HD22	1:A:322:LEU:HG	2.02	0.41
1:A:413:GLU:HA	1:A:414:PRO:HD2	1.95	0.41
1:A:176:LEU:HG	1:A:180:LEU:HD22	2.01	0.41
1:A:329:THR:OG1	1:A:331:VAL:HG23	2.21	0.41
1:A:308:ILE:HA	1:A:308:ILE:HD12	1.51	0.41
1:B:354:ARG:O	1:B:355:HIS:HB2	2.19	0.41
1:A:350:SER:HA	1:A:362:CYS:O	2.20	0.41
1:B:375:LEU:HD12	1:B:377:PHE:CZ	2.56	0.41
1:B:97:MET:HE2	1:B:163:VAL:HG21	2.02	0.41
1:B:121:ASP:C	1:B:123:ASN:H	2.25	0.41
1:B:344:GLN:HB2	1:B:348:VAL:HG13	2.04	0.40
1:A:97:MET:HE2	1:A:163:VAL:HG21	2.03	0.40
1:B:368:LEU:HD12	1:B:412:ARG:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:HH21	1:A:314:GLU:HG2	1.86	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	416/422 (99%)	394 (95%)	19 (5%)	3 (1%)	26	38
1	B	415/422 (98%)	393 (95%)	19 (5%)	3 (1%)	26	38
All	All	831/844 (98%)	787 (95%)	38 (5%)	6 (1%)	26	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	PRO
1	A	380	ILE
1	B	355	HIS
1	B	383	ASN
1	A	403	ASN
1	B	312	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	381/383 (100%)	326 (86%)	55 (14%)	4	4
1	B	380/383 (99%)	340 (90%)	40 (10%)	8	12
All	All	761/766 (99%)	666 (88%)	95 (12%)	6	7

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LEU
1	A	7	ILE
1	A	16	TYR
1	A	22	LYS
1	A	27	LEU
1	A	42	VAL
1	A	50	THR
1	A	73	LEU
1	A	74	LEU
1	A	86	LYS
1	A	91	LEU
1	A	96	LEU
1	A	98	ASP
1	A	120	ARG
1	A	135	ASP
1	A	136	VAL
1	A	137	VAL
1	A	173	LEU
1	A	180	LEU
1	A	218	ARG
1	A	227	ASN
1	A	229	LEU
1	A	230	ARG
1	A	238	MET
1	A	277	LEU
1	A	283	VAL
1	A	288	ASN
1	A	294	LEU
1	A	295	LYS
1	A	296	GLU
1	A	300	ILE
1	A	306	LEU
1	A	308	ILE
1	A	318	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	328	LYS
1	A	338	ILE
1	A	341	ARG
1	A	343	ASP
1	A	352	LEU
1	A	358	ARG
1	A	367	LEU
1	A	374	THR
1	A	381	TRP
1	A	384	ILE
1	A	396	ILE
1	A	398	ARG
1	A	399	VAL
1	A	401	VAL
1	A	402	LYS
1	A	403	ASN
1	A	405	ARG
1	A	412	ARG
1	A	417	LEU
1	A	421	LEU
1	B	1	MET
1	B	3	LEU
1	B	7	ILE
1	B	16	TYR
1	B	22	LYS
1	B	25	LEU
1	B	73	LEU
1	B	91	LEU
1	B	96	LEU
1	B	102	ASN
1	B	113	LYS
1	B	122	GLU
1	B	128	ARG
1	B	130	VAL
1	B	136	VAL
1	B	169	ASP
1	B	173	LEU
1	B	180	LEU
1	B	191	ARG
1	B	229	LEU
1	B	230	ARG
1	B	238	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	265	LEU
1	B	277	LEU
1	B	288	ASN
1	B	294	LEU
1	B	306	LEU
1	B	318	LEU
1	B	343	ASP
1	B	352	LEU
1	B	358	ARG
1	B	368	LEU
1	B	369	GLU
1	B	373	VAL
1	B	374	THR
1	B	380	ILE
1	B	383	ASN
1	B	399	VAL
1	B	401	VAL
1	B	421	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	HIS
1	B	319	HIS

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

There are no ligands in this entry.

5.7 Other polymers

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, 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	420/422 (99%)	-0.10	17 (4%) 42 43	15, 26, 46, 62	0
1	B	419/422 (99%)	-0.12	10 (2%) 62 61	14, 26, 44, 66	0
All	All	839/844 (99%)	-0.11	27 (3%) 51 51	14, 26, 45, 66	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	GLU	4.9
1	A	402	LYS	4.6
1	A	130	VAL	4.0
1	B	422	TYR	4.0
1	A	1	MET	3.8
1	B	130	VAL	3.7
1	B	121	ASP	3.6
1	B	123	ASN	3.5
1	A	422	TYR	3.2
1	A	245	ARG	3.1
1	B	245	ARG	3.1
1	A	302	ASN	3.1
1	A	123	ASN	2.9
1	A	25	LEU	2.9
1	A	131	PRO	2.9
1	B	1	MET	2.8
1	A	309	PRO	2.7
1	A	405	ARG	2.5
1	B	405	ARG	2.5
1	B	227	ASN	2.4
1	A	355	HIS	2.2
1	A	225	GLY	2.2
1	A	121	ASP	2.2
1	A	398	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	122	GLU	2.2
1	A	354	ARG	2.2
1	B	25	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.