



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:31 PM UTC

PDB ID : 4GKL / pdb_00004gkl
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

<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
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

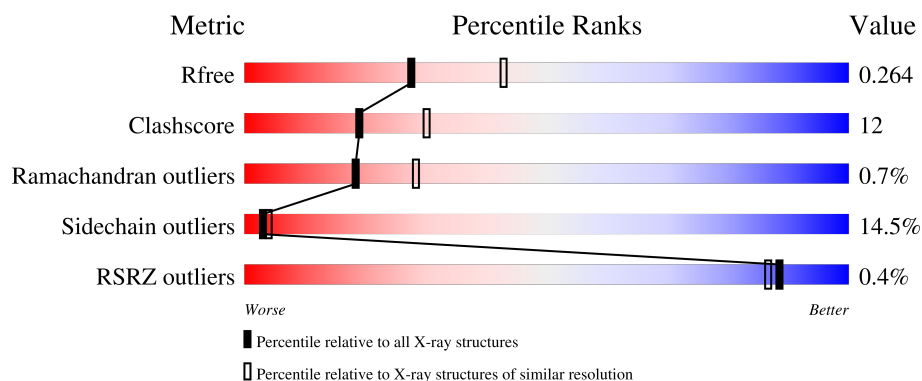
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	422	 64% 28% 7%
1	B	422	 67% 27% . .

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			

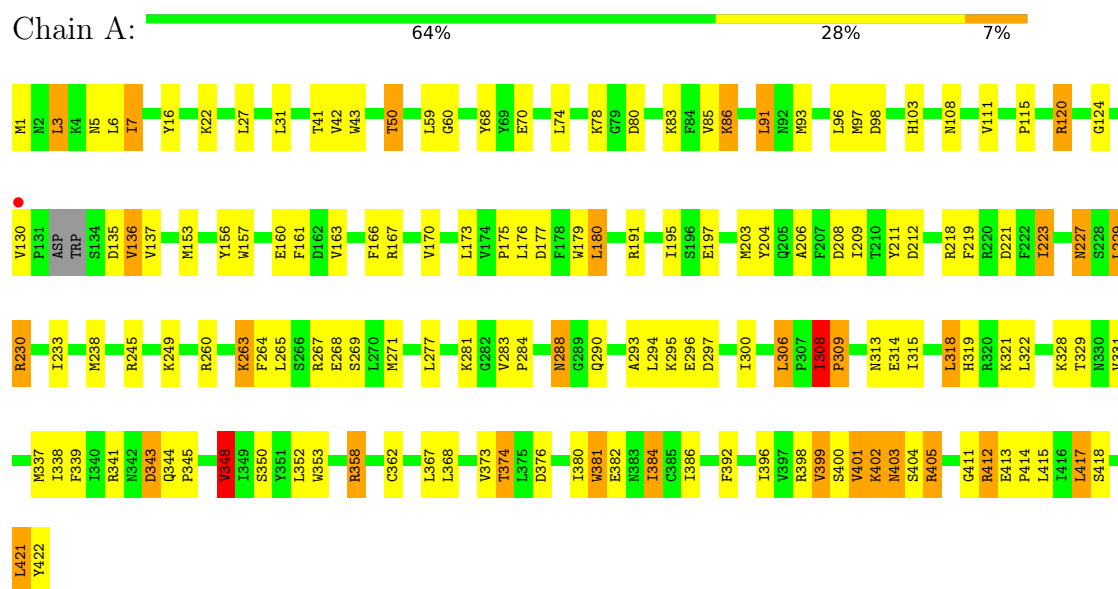
- Molecule 2 is water.

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

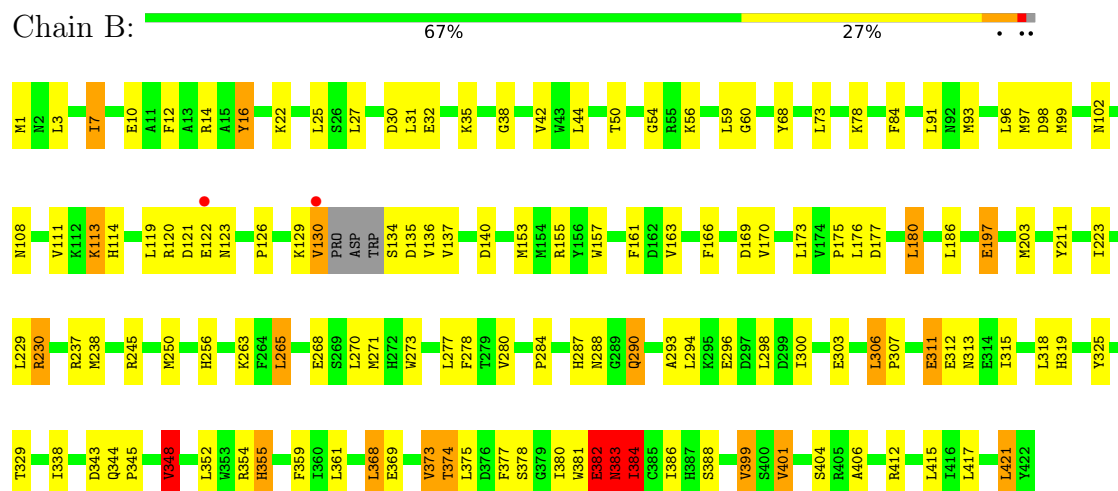
3 Residue-property plots

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: 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) 93.9 (19.98-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.197 , 0.263 0.198 , 0.264	Depositor DCC
R_{free} test set	1981 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	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 18.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.52	0/3608	0.91	4/4874 (0.1%)
1	B	0.52	0/3600	0.90	5/4862 (0.1%)
All	All	0.52	0/7208	0.91	9/9736 (0.1%)

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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	245	ARG	N-CA-C	6.95	118.51	111.07
1	B	384	ILE	N-CA-C	6.86	120.28	108.90
1	A	223	ILE	CB-CA-C	-6.72	103.22	112.02
1	A	245	ARG	N-CA-C	6.55	118.08	111.07
1	B	348	VAL	N-CA-C	6.20	117.51	108.53
1	B	382	GLU	CA-C-N	5.74	132.03	121.70
1	B	382	GLU	C-N-CA	5.74	132.03	121.70
1	A	130	VAL	N-CA-C	5.32	113.73	107.77
1	A	348	VAL	N-CA-C	5.05	116.62	108.85

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

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	89	0
1	B	3507	0	3460	76	0
2	A	117	0	0	5	0
2	B	127	0	0	5	0
All	All	7265	0	6927	165	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 12.

All (165) 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:97:MET:HE1	1:A:157:TRP:HB3	1.46	0.98
1:B:97:MET:HE1	1:B:157:TRP:HB3	1.47	0.96
1:B:50:THR:HG21	1:B:60:GLY:HA3	1.59	0.85
1:B:68:TYR:HB3	1:B:153:MET:HE3	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:68:TYR:HB3	1:A:153:MET:HE3	1.61	0.80
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:A:97:MET:HE2	1:A:163:VAL:HG11	1.73	0.70
1:B:111:VAL:HG23	1:B:126:PRO:HG2	1.76	0.68
1:A:91:LEU:HB3	1:A:93:MET:HE2	1.75	0.67
1:B:97:MET:HE2	1:B:163:VAL:HG21	1.77	0.67
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:260:ARG:H	1:A:263:LYS:HZ3	1.45	0.64
1:A:376:ASP:HA	1:A:405:ARG:HD2	1.80	0.63
1:B:153:MET:HE2	1:B:157:TRP:HE1	1.62	0.63
1:A:219:PHE:CZ	1:A:223:ILE:HD11	2.33	0.62
1:A:358:ARG:NH1	1:A:418:SER:OG	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:HE2	1:A:163:VAL:HG21	1.83	0.60
1:A:50:THR:HG21	1:A:60:GLY:HA3	1.84	0.59
1:A:411:GLY:O	1:A:413:GLU:N	2.32	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: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:31:LEU:HB3	1:A:93:MET:HE1	1.86	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:170:VAL:HG11	1:B:203:MET:HE2	1.85	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
1:A:381:TRP:H	1:A:381:TRP:CD1	2.22	0.56
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:134:SER:N	2:B:606:HOH:O	2.39	0.55
1:B:311:GLU:O	1:B:313:ASN:N	2.40	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:B:97:MET:HE2	1:B:163:VAL:HG11	1.89	0.54
1:A:170:VAL:HG11	1:A:203:MET:HE2	1.89	0.54
1:A:212:ASP:OD2	1:A:249:LYS:NZ	2.37	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:O	1:A:288:ASN:ND2	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:97:MET:HE1	1:B:157:TRP:CB	2.30	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:B:99:MET:HE1	1:B:153:MET:HE1	1.92	0.52
1:B:265:LEU:HD21	1:B:273:TRP:CD1	2.45	0.51
1:A:293:ALA:HB2	1:A:315:ILE:HG13	1.91	0.51
1:A:97:MET:HE1	1:A:157:TRP:CB	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:OG	1:A:402:LYS:NZ	2.43	0.51
1:B:325:TYR:O	1:B:329:THR:HG22	2.10	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:A:170:VAL:HG11	1:A:203:MET:CE	2.40	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:B:378:SER:HA	1:B:404:SER:HB3	1.93	0.50
1:B:230:ARG:HD3	1:B:345:PRO:O	2.12	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
1:A:412:ARG:HB2	1:A:412:ARG:NH1	2.28	0.48
1:B:56:LYS:O	1:B:60:GLY:HA2	2.13	0.48
1:B:7:ILE:HG12	1:B:38:GLY:O	2.14	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:153:MET:HE2	1:B:157:TRP:NE1	2.27	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: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:HA	1:B:230:ARG:HD2	1.53	0.46
1:A:269:SER:HA	1:A:368:LEU:HD21	1.98	0.46
1:A:344:GLN:HG3	1:A:373:VAL:HG22	1.97	0.46
1:B:16:TYR:OH	1:B:30:ASP:OD1	2.16	0.46
1:B:268:GLU:HA	1:B:271:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASP:C	1:B:123:ASN:H	2.25	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:97:MET:HE3	1:A:166:PHE:HE1	1.81	0.45
1:A:401:VAL:HA	1:A:405:ARG:O	2.16	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:B:35:LYS:HB2	1:B:93:MET:HE2	1.99	0.44
1:A:197:GLU:HB2	1:A:211:TYR:CZ	2.52	0.44
1:A:421:LEU:O	1:A:422:TYR:HB2	2.17	0.44
1:A:91:LEU:CB	1:A:93:MET:HE2	2.45	0.44
1:A:68:TYR:HB3	1:A:153:MET:CE	2.40	0.44
1:B:54:GLY:O	1:B:135:ASP:HB3	2.18	0.44
1:B:97:MET:HE3	1:B:166:PHE:HE1	1.83	0.44
1:B:315:ILE:O	1:B:319:HIS:HD2	2.00	0.44
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:404:SER:C	1:A:405:ARG:HD3	2.43	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:31:LEU:O	1:B:93:MET:HE1	2.18	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:280:VAL:O	2:B:524:HOH:O	2.21	0.43
1:B:361:LEU:O	1:B:417:LEU:HB2	2.19	0.43
1:A:281:LYS:HB3	1:A:281:LYS:HE3	1.74	0.42
1:B:68:TYR:HB3	1:B:153:MET:CE	2.42	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:97:MET:CE	1:B:163:VAL:HG21	2.47	0.42
1:B:293:ALA:HB2	1:B:315:ILE:HG13	2.01	0.42
1:A:5:ASN:ND2	2:A:535:HOH:O	2.37	0.42
1:A:337:MET:HG3	1:A:353:TRP:NE1	2.34	0.42
1:B:7:ILE:CD1	1:B:278:PHE:HE1	2.32	0.42
1:A:6:LEU:HD22	1:A:41:THR:OG1	2.20	0.42
1:A:31:LEU:HD22	1:A:93:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:OE2	1:A:412:ARG:HG2	2.20	0.42
1:B:155:ARG:HB2	1:B:186:LEU:HD21	2.01	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: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:413:GLU:HA	1:A:414:PRO:HD2	1.95	0.41
1:B:97:MET:HE3	1:B:97:MET:HB2	1.79	0.41
1:A:308:ILE:HD12	1:A:308:ILE:HA	1.51	0.41
1:A:350:SER:HA	1:A:362:CYS:O	2.20	0.41
1:B:354:ARG:O	1:B:355:HIS:HB2	2.19	0.41
1:A:93:MET:HE3	1:A:93:MET:HB2	1.87	0.41
1:B:375:LEU:HD12	1:B:377:PHE:CZ	2.56	0.41
1:B:344:GLN:HB2	1:B:348:VAL:HG13	2.04	0.40
1:B:368:LEU:HD12	1:B:412:ARG:HA	2.04	0.40
1:B:211:TYR:CD2	1:B:250:MET:HE2	2.56	0.40
1:A:267:ARG:HH21	1:A:314:GLU:HG2	1.86	0.40
1:A:337:MET:HE1	1:A:339:PHE:CE2	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	416/422 (99%)	394 (95%)	19 (5%)	3 (1%)	18	28
1	B	415/422 (98%)	393 (95%)	19 (5%)	3 (1%)	18	28
All	All	831/844 (98%)	787 (95%)	38 (5%)	6 (1%)	18	28

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 ⓘ

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%)	323 (85%)	58 (15%)	3	3
1	B	380/383 (99%)	328 (86%)	52 (14%)	3	5
All	All	761/766 (99%)	651 (86%)	110 (14%)	3	4

All (110) 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	70	GLU
1	A	74	LEU
1	A	85	VAL
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

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Mol	Chain	Res	Type
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	263	LYS
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
1	A	328	LYS
1	A	338	ILE
1	A	341	ARG
1	A	343	ASP
1	A	348	VAL
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

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Mol	Chain	Res	Type
1	B	7	ILE
1	B	16	TYR
1	B	22	LYS
1	B	25	LEU
1	B	32	GLU
1	B	42	VAL
1	B	73	LEU
1	B	91	LEU
1	B	96	LEU
1	B	102	ASN
1	B	113	LYS
1	B	120	ARG
1	B	122	GLU
1	B	130	VAL
1	B	136	VAL
1	B	137	VAL
1	B	169	ASP
1	B	173	LEU
1	B	180	LEU
1	B	197	GLU
1	B	223	ILE
1	B	229	LEU
1	B	230	ARG
1	B	238	MET
1	B	263	LYS
1	B	265	LEU
1	B	277	LEU
1	B	288	ASN
1	B	290	GLN
1	B	294	LEU
1	B	296	GLU
1	B	300	ILE
1	B	303	GLU
1	B	306	LEU
1	B	311	GLU
1	B	318	LEU
1	B	338	ILE
1	B	348	VAL
1	B	352	LEU
1	B	368	LEU
1	B	369	GLU
1	B	373	VAL

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Mol	Chain	Res	Type
1	B	374	THR
1	B	380	ILE
1	B	382	GLU
1	B	383	ASN
1	B	384	ILE
1	B	399	VAL
1	B	401	VAL
1	B	421	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	319	HIS
1	A	365	ASN
1	B	357	ASN
1	B	387	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 oligosaccharides 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 [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	420/422 (99%)	-0.26	1 (0%) 91 89	15, 26, 46, 62	0
1	B	419/422 (99%)	-0.26	2 (0%) 87 85	14, 26, 44, 66	0
All	All	839/844 (99%)	-0.26	3 (0%) 88 86	14, 26, 45, 66	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	VAL	2.7
1	B	122	GLU	2.5
1	A	130	VAL	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.