



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:24 PM GMT

PDB ID : 1TGO
Title : THERMOSTABLE B TYPE DNA POLYMERASE FROM THERMOCOCCUS GORGONARIUS
Authors : Hopfner, K.-P.; Eichinger, A.; Engh, R.A.; Laue, F.; Ankenbauer, W.; Huber, R.; Angerer, B.
Deposited on : 1999-02-23
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
<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

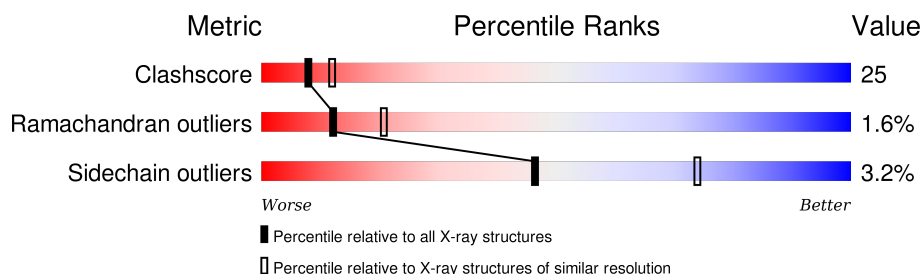
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	773	 59% 38% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6667 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 PROTEIN (THERMOSTABLE B DNA POLYMERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	135	0	0
			6328	4079	1066	1170	13			

- Molecule 2 is water.

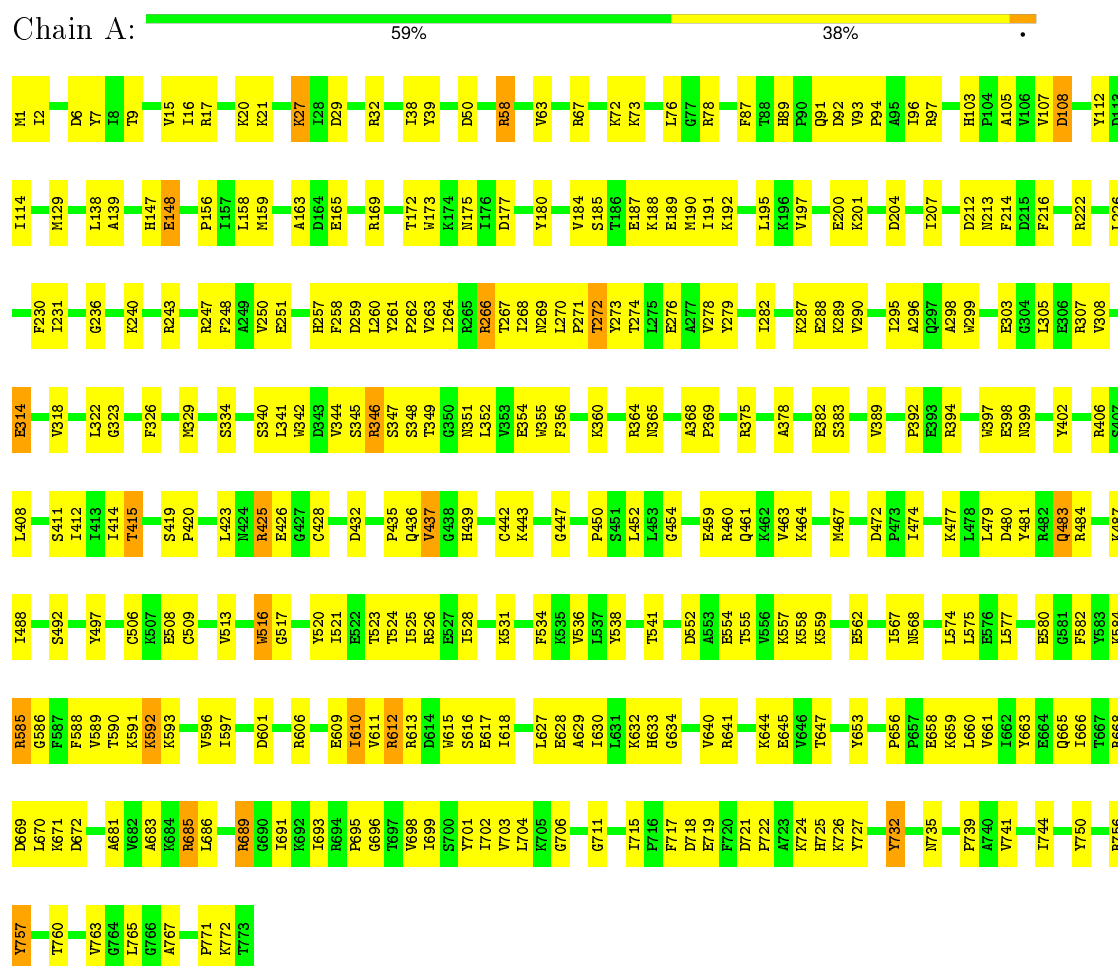
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	339	Total	O	0	0
			339	339		

3 Residue-property plots

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.

Note EDS was not executed.

- Molecule 1: PROTEIN (THERMOSTABLE B DNA POLYMERASE)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.11Å 105.22Å 154.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	91.0 (25.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.209 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6667	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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	0.41	0/6469	0.66	1/8724 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	771	PRO	N-CA-CB	5.28	109.64	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	732	TYR	Sidechain

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	6328	0	6351	305	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	339	0	0	29	0
All	All	6667	0	6351	305	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 25.

All (305) 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:693:ILE:HG21	1:A:699:ILE:HD11	1.33	1.09
1:A:612:ARG:HH11	1:A:612:ARG:HB3	1.25	0.99
1:A:612:ARG:NH1	1:A:613:ARG:H	1.62	0.98
1:A:647:THR:HG21	1:A:756:ARG:HG3	1.45	0.98
1:A:108:ASP:HB2	2:A:1087:HOH:O	1.66	0.94
1:A:272:THR:HG22	1:A:613:ARG:HG2	1.50	0.93
1:A:612:ARG:HH11	1:A:613:ARG:H	1.04	0.90
1:A:411:SER:O	1:A:415:THR:HG23	1.72	0.90
1:A:689:ARG:HD3	2:A:922:HOH:O	1.71	0.90
1:A:612:ARG:NH1	1:A:612:ARG:HB3	1.89	0.86
1:A:72:LYS:HE3	2:A:1017:HOH:O	1.76	0.85
1:A:342:TRP:O	1:A:346:ARG:HD2	1.77	0.84
1:A:428:CYS:HG	1:A:442:CYS:HG	0.81	0.79
1:A:346:ARG:HH11	1:A:346:ARG:HG2	1.48	0.78
1:A:666:ILE:HG13	1:A:695:PRO:HA	1.68	0.76
1:A:1:MET:HB2	1:A:129:MET:HA	1.67	0.75
1:A:724:LYS:O	1:A:724:LYS:HD3	1.88	0.74
1:A:129:MET:HB2	2:A:1085:HOH:O	1.86	0.74
1:A:653:TYR:HA	1:A:727:TYR:OH	1.88	0.73
1:A:87:PHE:CE2	1:A:96:ILE:HG21	2.23	0.73
1:A:617:GLU:HG2	2:A:833:HOH:O	1.86	0.73
1:A:517:GLY:O	1:A:521:ILE:HD13	1.88	0.72
1:A:612:ARG:HH11	1:A:613:ARG:N	1.84	0.72
1:A:15:VAL:HG22	1:A:32:ARG:HG2	1.71	0.72
1:A:630:ILE:O	1:A:634:GLY:HA2	1.91	0.71
1:A:464:LYS:HG3	1:A:483:GLN:HG3	1.73	0.70
1:A:628:GLU:HG3	1:A:632:LYS:HD2	1.74	0.70
1:A:93:VAL:HG12	1:A:97:ARG:CD	2.22	0.69
1:A:703:VAL:HG11	1:A:711:GLY:HA2	1.73	0.69
1:A:243:ARG:HG3	1:A:247:ARG:O	1.93	0.69
1:A:299:TRP:HB2	2:A:1108:HOH:O	1.92	0.69
1:A:329:MET:HE2	1:A:488:ILE:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:CD2	1:A:91:GLN:H	2.11	0.68
1:A:506:CYS:HG	1:A:509:CYS:HG	1.38	0.68
1:A:213:ASN:HD21	1:A:248:PHE:H	1.39	0.68
1:A:20:LYS:HB2	1:A:27:LYS:HD2	1.76	0.67
1:A:287:LYS:HD3	1:A:288:GLU:N	2.11	0.66
1:A:261:TYR:HB3	1:A:262:PRO:HD3	1.77	0.66
1:A:177:ASP:HA	2:A:1026:HOH:O	1.95	0.66
1:A:63:VAL:HG11	1:A:92:ASP:HB3	1.78	0.66
1:A:521:ILE:HG12	1:A:541:THR:O	1.95	0.65
1:A:612:ARG:HH11	1:A:612:ARG:CB	2.05	0.65
1:A:63:VAL:CG1	1:A:92:ASP:HB3	2.27	0.65
1:A:216:PHE:HB2	1:A:250:VAL:HG21	1.78	0.65
1:A:670:LEU:HB3	1:A:683:ALA:HB2	1.79	0.64
1:A:213:ASN:HD21	1:A:247:ARG:HB3	1.62	0.64
1:A:251:GLU:HG3	2:A:1016:HOH:O	1.96	0.64
1:A:685:ARG:HD2	1:A:715:ILE:HG22	1.80	0.64
1:A:289:LYS:HD2	1:A:663:TYR:CE1	2.33	0.64
1:A:322:LEU:O	1:A:326:PHE:HD1	1.81	0.64
1:A:668:ARG:HG2	1:A:669:ASP:N	2.12	0.64
1:A:89:HIS:HD2	1:A:91:GLN:H	1.46	0.64
1:A:436:GLN:O	1:A:437:VAL:HG23	1.96	0.64
1:A:647:THR:CG2	1:A:756:ARG:HG3	2.25	0.63
1:A:589:VAL:O	1:A:590:THR:HG23	1.99	0.63
1:A:6:ASP:OD1	1:A:17:ARG:HB2	1.98	0.63
1:A:329:MET:CE	1:A:488:ILE:HD12	2.28	0.62
1:A:279:TYR:CD1	1:A:318:VAL:HG13	2.35	0.62
1:A:656:PRO:HG2	1:A:659:LYS:HD2	1.83	0.61
1:A:258:PHE:HE1	1:A:263:VAL:HG21	1.66	0.61
1:A:39:TYR:CZ	1:A:73:LYS:HE3	2.36	0.61
1:A:93:VAL:HB	1:A:94:PRO:HD3	1.82	0.60
1:A:477:LYS:HE2	1:A:481:TYR:OH	2.01	0.60
1:A:524:THR:HG21	1:A:577:LEU:HD22	1.83	0.60
1:A:240:LYS:HG2	2:A:1100:HOH:O	2.02	0.60
1:A:271:PRO:HB3	1:A:611:VAL:O	2.02	0.60
1:A:334:SER:HA	1:A:344:VAL:HG21	1.83	0.60
1:A:159:MET:HE2	1:A:299:TRP:HH2	1.66	0.60
1:A:414:ILE:HD13	1:A:454:GLY:HA2	1.83	0.59
1:A:272:THR:HG21	2:A:826:HOH:O	2.02	0.59
1:A:612:ARG:NH1	1:A:613:ARG:N	2.42	0.59
1:A:436:GLN:C	1:A:437:VAL:HG23	2.23	0.59
1:A:138:LEU:HD12	1:A:163:ALA:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:LYS:HD2	1:A:592:LYS:N	2.17	0.59
1:A:107:VAL:O	1:A:108:ASP:HB3	2.02	0.59
1:A:715:ILE:HD13	1:A:725:HIS:HD2	1.67	0.59
1:A:259:ASP:O	1:A:262:PRO:HD2	2.03	0.59
1:A:641:ARG:HG2	1:A:645:GLU:OE2	2.03	0.59
1:A:2:ILE:O	1:A:129:MET:HG3	2.03	0.58
1:A:744:ILE:HG13	2:A:926:HOH:O	2.02	0.58
1:A:76:LEU:HD23	1:A:78:ARG:HE	1.67	0.58
1:A:398:GLU:HA	1:A:584:LYS:O	2.04	0.58
1:A:364:ARG:HD3	2:A:985:HOH:O	2.04	0.58
1:A:270:LEU:N	1:A:270:LEU:HD23	2.17	0.58
1:A:420:PRO:HG3	1:A:506:CYS:HB2	1.86	0.58
1:A:276:GLU:CD	1:A:290:VAL:HG23	2.23	0.58
1:A:472:ASP:OD2	1:A:474:ILE:HB	2.03	0.57
1:A:702:ILE:HD11	1:A:717:PHE:CD1	2.38	0.57
1:A:593:LYS:HA	1:A:606:ARG:O	2.05	0.57
1:A:158:LEU:HD13	1:A:299:TRP:CD2	2.39	0.57
1:A:685:ARG:CD	1:A:715:ILE:HG22	2.35	0.57
1:A:346:ARG:HG2	1:A:346:ARG:NH1	2.18	0.56
1:A:169:ARG:NH1	1:A:180:TYR:HA	2.21	0.56
1:A:156:PRO:HA	1:A:222:ARG:HH11	1.70	0.56
1:A:260:LEU:HD21	1:A:323:GLY:HA2	1.88	0.56
1:A:184:VAL:HG21	1:A:189:GLU:HB3	1.87	0.56
1:A:606:ARG:HH11	1:A:606:ARG:HG2	1.68	0.56
1:A:660:LEU:HD22	1:A:732:TYR:CD2	2.40	0.56
1:A:89:HIS:HD2	1:A:91:GLN:HB2	1.71	0.56
1:A:94:PRO:HA	1:A:97:ARG:HD3	1.88	0.56
1:A:437:VAL:CG1	1:A:439:HIS:NE2	2.69	0.56
1:A:212:ASP:CG	1:A:346:ARG:HH12	2.10	0.56
1:A:103:HIS:CD2	1:A:105:ALA:H	2.22	0.56
1:A:272:THR:CG2	1:A:613:ARG:HA	2.35	0.55
1:A:437:VAL:HG11	1:A:439:HIS:NE2	2.20	0.55
1:A:27:LYS:HE2	1:A:29:ASP:OD1	2.07	0.55
1:A:763:VAL:O	1:A:763:VAL:HG12	2.06	0.55
1:A:158:LEU:HD13	1:A:299:TRP:CE2	2.42	0.55
1:A:187:GLU:OE2	1:A:222:ARG:HD3	2.07	0.55
1:A:425:ARG:HG2	1:A:425:ARG:HH11	1.71	0.54
1:A:269:ASN:HA	1:A:273:TYR:OH	2.07	0.54
1:A:329:MET:HE2	1:A:488:ILE:CD1	2.37	0.54
1:A:484:ARG:O	1:A:488:ILE:HG13	2.08	0.54
1:A:364:ARG:NH2	1:A:452:LEU:HD23	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ARG:HD2	2:A:862:HOH:O	2.06	0.54
1:A:195:LEU:HD21	1:A:230:PHE:CE1	2.42	0.54
1:A:341:LEU:O	1:A:341:LEU:HD23	2.07	0.54
1:A:258:PHE:CE1	1:A:263:VAL:HG21	2.43	0.54
1:A:724:LYS:HD2	1:A:725:HIS:CE1	2.42	0.54
1:A:538:TYR:OH	1:A:592:LYS:N	2.38	0.54
1:A:342:TRP:O	1:A:346:ARG:CD	2.52	0.53
1:A:73:LYS:HE2	2:A:856:HOH:O	2.06	0.53
1:A:406:ARG:HD3	2:A:814:HOH:O	2.08	0.53
1:A:666:ILE:HG23	1:A:699:ILE:HD13	1.90	0.53
1:A:103:HIS:CD2	1:A:105:ALA:HB3	2.43	0.53
1:A:644:LYS:HB3	1:A:757:TYR:CE2	2.43	0.53
1:A:397:TRP:O	1:A:585:ARG:HA	2.08	0.53
1:A:197:VAL:O	1:A:200:GLU:HB3	2.09	0.53
1:A:609:GLU:HG2	1:A:610:ILE:HG12	1.91	0.53
1:A:250:VAL:O	1:A:257:HIS:HD2	1.92	0.52
1:A:89:HIS:CD2	1:A:91:GLN:HB2	2.44	0.52
1:A:213:ASN:ND2	1:A:248:PHE:H	2.06	0.52
1:A:212:ASP:OD2	1:A:346:ARG:NH1	2.42	0.52
1:A:274:THR:O	1:A:278:VAL:HG23	2.09	0.52
1:A:616:SER:OG	1:A:618:ILE:HG22	2.10	0.52
1:A:188:LYS:CA	1:A:226:LEU:HD23	2.39	0.52
1:A:93:VAL:HG12	1:A:97:ARG:HD3	1.92	0.52
1:A:408:LEU:O	1:A:412:ILE:HG13	2.08	0.52
1:A:159:MET:HE2	1:A:299:TRP:CH2	2.43	0.52
1:A:93:VAL:HG12	1:A:97:ARG:HD2	1.90	0.52
1:A:428:CYS:HG	1:A:442:CYS:CB	2.20	0.51
1:A:436:GLN:HA	2:A:874:HOH:O	2.10	0.51
1:A:704:LEU:HA	1:A:727:TYR:HA	1.92	0.51
1:A:156:PRO:HA	1:A:222:ARG:NH1	2.25	0.51
1:A:760:THR:HG22	1:A:760:THR:O	2.11	0.51
1:A:609:GLU:HG2	1:A:610:ILE:H	1.75	0.51
1:A:757:TYR:HB2	1:A:760:THR:OG1	2.11	0.51
1:A:264:ILE:HD13	1:A:278:VAL:HG11	1.92	0.51
1:A:197:VAL:HG13	1:A:201:LYS:HE2	1.92	0.51
1:A:295:ILE:HG12	1:A:308:VAL:HG13	1.91	0.51
1:A:76:LEU:O	1:A:425:ARG:NH2	2.43	0.51
1:A:231:ILE:HD12	1:A:236:GLY:O	2.11	0.51
1:A:629:ALA:HA	1:A:633:HIS:CD2	2.46	0.51
1:A:314:GLU:HG2	2:A:1067:HOH:O	2.10	0.51
1:A:272:THR:HG21	1:A:613:ARG:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ARG:NH2	1:A:487:LYS:HD2	2.26	0.50
1:A:552:ASP:HB3	1:A:555:THR:OG1	2.11	0.50
1:A:685:ARG:HG2	1:A:719:GLU:OE1	2.11	0.50
1:A:287:LYS:HD3	1:A:288:GLU:O	2.11	0.50
1:A:356:PHE:CZ	1:A:360:LYS:HE3	2.47	0.50
1:A:9:THR:OG1	1:A:89:HIS:HE1	1.94	0.50
1:A:665:GLN:HG3	1:A:696:GLY:O	2.10	0.50
1:A:558:LYS:O	1:A:562:GLU:HG3	2.11	0.50
1:A:765:LEU:C	1:A:767:ALA:H	2.15	0.50
1:A:681:ALA:HB1	1:A:685:ARG:NH1	2.27	0.50
1:A:609:GLU:HG2	1:A:610:ILE:N	2.27	0.49
1:A:477:LYS:O	1:A:480:ASP:HB3	2.13	0.49
1:A:419:SER:HB3	1:A:450:PRO:HD3	1.95	0.49
1:A:351:ASN:ND2	1:A:355:TRP:CZ2	2.81	0.49
1:A:557:LYS:HE2	1:A:582:PHE:CG	2.46	0.49
1:A:399:ASN:HA	1:A:582:PHE:CZ	2.46	0.49
1:A:698:VAL:HG11	2:A:1031:HOH:O	2.12	0.49
1:A:415:THR:CG2	1:A:574:LEU:H	2.25	0.49
1:A:216:PHE:HE2	1:A:257:HIS:CE1	2.31	0.49
1:A:169:ARG:HH12	1:A:180:TYR:HA	1.78	0.48
1:A:7:TYR:HB3	1:A:16:ILE:HD13	1.95	0.48
1:A:461:GLN:HA	1:A:461:GLN:HE21	1.78	0.48
1:A:520:TYR:CD2	1:A:575:LEU:CD2	2.96	0.48
1:A:197:VAL:CG1	1:A:201:LYS:HE2	2.43	0.48
1:A:567:ILE:HG23	1:A:568:ASN:N	2.28	0.48
1:A:612:ARG:NH1	1:A:613:ARG:HB2	2.29	0.48
1:A:666:ILE:CG1	1:A:695:PRO:HA	2.41	0.47
1:A:340:SER:O	1:A:344:VAL:HG23	2.14	0.47
1:A:188:LYS:HA	1:A:226:LEU:HD23	1.97	0.47
1:A:741:VAL:HG12	1:A:741:VAL:O	2.14	0.47
1:A:107:VAL:O	1:A:108:ASP:CB	2.62	0.47
1:A:586:GLY:HA3	1:A:596:VAL:HG12	1.95	0.47
1:A:344:VAL:HG13	1:A:352:LEU:CD2	2.45	0.47
1:A:349:THR:HA	1:A:352:LEU:HD12	1.96	0.47
1:A:432:ASP:OD2	1:A:443:LYS:HD2	2.14	0.47
1:A:715:ILE:HD13	1:A:725:HIS:CD2	2.50	0.46
1:A:264:ILE:HG21	1:A:278:VAL:HG13	1.97	0.46
1:A:139:ALA:HA	1:A:207:ILE:O	2.15	0.46
1:A:459:GLU:O	1:A:463:VAL:HG23	2.14	0.46
1:A:329:MET:CE	1:A:488:ILE:CD1	2.93	0.46
1:A:148:GLU:OE2	1:A:669:ASP:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:TRP:HZ3	1:A:617:GLU:OE1	1.98	0.46
1:A:276:GLU:OE1	1:A:287:LYS:HD2	2.16	0.46
1:A:58:ARG:NH1	2:A:907:HOH:O	2.47	0.46
1:A:509:CYS:O	1:A:513:VAL:HG23	2.16	0.46
1:A:461:GLN:NE2	2:A:939:HOH:O	2.42	0.46
1:A:437:VAL:HG12	1:A:439:HIS:CE1	2.51	0.46
1:A:447:GLY:C	1:A:450:PRO:HD2	2.36	0.46
1:A:78:ARG:NH2	1:A:425:ARG:HE	2.12	0.46
1:A:268:ILE:HD13	1:A:282:ILE:HD11	1.99	0.46
1:A:299:TRP:HE3	1:A:299:TRP:HA	1.81	0.45
1:A:686:LEU:O	1:A:689:ARG:HB2	2.16	0.45
1:A:299:TRP:CE3	1:A:299:TRP:HA	2.52	0.45
1:A:165:GLU:HA	1:A:165:GLU:OE1	2.16	0.45
1:A:266:ARG:NH2	1:A:348:SER:HA	2.30	0.45
1:A:63:VAL:HG13	1:A:92:ASP:HB3	1.99	0.45
1:A:435:PRO:HD3	1:A:516:TRP:CE2	2.52	0.45
1:A:666:ILE:HD11	1:A:693:ILE:HG22	1.98	0.45
1:A:699:ILE:HG22	1:A:701:TYR:HD2	1.80	0.45
1:A:187:GLU:HG2	1:A:226:LEU:HD21	1.98	0.45
1:A:588:PHE:CD1	1:A:588:PHE:N	2.84	0.45
1:A:347:SER:OG	1:A:351:ASN:HB3	2.16	0.45
1:A:538:TYR:HE1	1:A:591:LYS:HA	1.82	0.45
1:A:508:GLU:CD	1:A:508:GLU:H	2.20	0.45
1:A:668:ARG:HG2	1:A:669:ASP:H	1.80	0.45
1:A:264:ILE:HG21	1:A:278:VAL:CG1	2.47	0.45
1:A:412:ILE:HD13	1:A:516:TRP:HB3	1.99	0.44
1:A:21:LYS:HD3	1:A:204:ASP:OD1	2.17	0.44
1:A:20:LYS:HD2	1:A:27:LYS:HD2	1.99	0.44
1:A:425:ARG:HG2	1:A:425:ARG:NH1	2.32	0.44
1:A:184:VAL:CG2	1:A:189:GLU:HB3	2.46	0.44
1:A:114:ILE:N	1:A:114:ILE:HD12	2.32	0.44
1:A:520:TYR:CD2	1:A:575:LEU:HD21	2.53	0.44
1:A:653:TYR:CG	1:A:726:LYS:HE2	2.52	0.44
1:A:703:VAL:CG1	1:A:711:GLY:HA2	2.42	0.44
1:A:349:THR:HB	1:A:492:SER:OG	2.17	0.44
1:A:461:GLN:HA	1:A:461:GLN:NE2	2.32	0.44
1:A:653:TYR:HA	1:A:727:TYR:CZ	2.53	0.44
1:A:521:ILE:HD12	1:A:521:ILE:N	2.33	0.44
1:A:525:ILE:HG23	1:A:536:VAL:HG21	2.00	0.44
1:A:257:HIS:CD2	1:A:346:ARG:HH22	2.34	0.44
1:A:640:VAL:HG21	1:A:750:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLU:O	1:A:191:ILE:HG13	2.18	0.44
1:A:559:LYS:HG2	2:A:1037:HOH:O	2.17	0.43
1:A:721:ASP:HA	1:A:722:PRO:HD2	1.80	0.43
1:A:617:GLU:O	1:A:618:ILE:C	2.57	0.43
1:A:27:LYS:HE2	1:A:29:ASP:CG	2.38	0.43
1:A:641:ARG:O	1:A:645:GLU:HG3	2.19	0.43
1:A:567:ILE:CG2	1:A:568:ASN:N	2.82	0.43
1:A:402:TYR:HD2	1:A:580:GLU:CB	2.31	0.43
1:A:612:ARG:HH12	1:A:613:ARG:HB2	1.84	0.43
1:A:76:LEU:O	1:A:78:ARG:HG3	2.18	0.43
1:A:528:ILE:HG12	1:A:534:PHE:HB2	2.00	0.43
1:A:158:LEU:HD23	1:A:173:TRP:CZ2	2.54	0.43
1:A:589:VAL:O	1:A:590:THR:CG2	2.67	0.43
1:A:184:VAL:HG22	1:A:185:SER:H	1.84	0.43
1:A:670:LEU:O	1:A:672:ASP:N	2.52	0.42
1:A:658:GLU:HA	1:A:661:VAL:HG23	2.00	0.42
1:A:392:PRO:HB3	1:A:538:TYR:HD1	1.84	0.42
1:A:67:ARG:NH1	2:A:1033:HOH:O	2.52	0.42
1:A:296:ALA:HB1	1:A:691:ILE:HG23	2.01	0.42
1:A:415:THR:HG22	1:A:574:LEU:H	1.84	0.42
1:A:460:ARG:NH2	1:A:483:GLN:OE1	2.48	0.42
1:A:147:HIS:O	1:A:148:GLU:C	2.57	0.42
1:A:591:LYS:O	1:A:592:LYS:HB2	2.19	0.42
1:A:243:ARG:HA	1:A:248:PHE:HA	2.00	0.42
1:A:240:LYS:HD3	2:A:984:HOH:O	2.19	0.42
1:A:38:ILE:HG22	1:A:112:TYR:HA	2.01	0.42
1:A:73:LYS:HG2	1:A:365:ASN:OD1	2.20	0.42
1:A:423:LEU:HD21	1:A:508:GLU:HG2	2.01	0.42
1:A:552:ASP:OD1	1:A:554:GLU:N	2.45	0.42
1:A:276:GLU:HG3	2:A:1031:HOH:O	2.18	0.42
1:A:531:LYS:HD2	1:A:531:LYS:N	2.35	0.42
1:A:735:ASN:O	1:A:739:PRO:HG3	2.19	0.42
1:A:681:ALA:HB1	1:A:685:ARG:HH12	1.85	0.41
1:A:187:GLU:O	1:A:190:MET:HB3	2.20	0.41
1:A:103:HIS:NE2	1:A:105:ALA:HB3	2.35	0.41
1:A:341:LEU:O	1:A:345:SER:HB2	2.20	0.41
1:A:426:GLU:OE1	1:A:426:GLU:HA	2.21	0.41
1:A:497:TYR:HA	1:A:497:TYR:HD1	1.78	0.41
1:A:389:VAL:CG1	1:A:591:LYS:HD3	2.51	0.41
1:A:627:LEU:HD21	1:A:744:ILE:HD13	2.01	0.41
1:A:354:GLU:HA	1:A:354:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLY:HA3	2:A:975:HOH:O	2.20	0.41
1:A:159:MET:HG2	1:A:172:THR:HB	2.03	0.41
1:A:73:LYS:HA	1:A:365:ASN:ND2	2.36	0.41
1:A:187:GLU:HG2	1:A:226:LEU:CD2	2.51	0.41
1:A:592:LYS:CD	1:A:592:LYS:N	2.83	0.41
1:A:584:LYS:HD2	2:A:1090:HOH:O	2.20	0.41
1:A:459:GLU:HA	1:A:459:GLU:OE1	2.20	0.41
1:A:270:LEU:N	1:A:270:LEU:CD2	2.84	0.41
1:A:375:ARG:O	1:A:378:ALA:HB3	2.21	0.41
1:A:402:TYR:HD2	1:A:580:GLU:HB3	1.86	0.41
1:A:415:THR:HG21	1:A:575:LEU:HD12	2.03	0.41
1:A:483:GLN:NE2	1:A:484:ARG:HG3	2.35	0.41
1:A:298:ALA:HB1	1:A:305:LEU:HD23	2.03	0.41
1:A:597:ILE:HD11	1:A:601:ASP:HA	2.02	0.41
1:A:264:ILE:HD13	1:A:278:VAL:CG1	2.51	0.41
1:A:368:ALA:HA	1:A:369:PRO:HD3	1.96	0.41
1:A:653:TYR:CD1	1:A:726:LYS:HE2	2.56	0.40
1:A:628:GLU:O	1:A:632:LYS:HB2	2.20	0.40
1:A:158:LEU:CD1	1:A:299:TRP:CE2	3.04	0.40
1:A:437:VAL:CG1	2:A:1040:HOH:O	2.70	0.40
1:A:298:ALA:CB	1:A:308:VAL:HG21	2.51	0.40
1:A:559:LYS:CG	2:A:1037:HOH:O	2.69	0.40
1:A:467:MET:HA	1:A:479:LEU:HD12	2.03	0.40
1:A:91:GLN:O	1:A:94:PRO:HD2	2.21	0.40
1:A:276:GLU:OE1	1:A:290:VAL:HG23	2.20	0.40
1:A:188:LYS:O	1:A:192:LYS:HG3	2.20	0.40
1:A:609:GLU:HG3	2:A:1063:HOH:O	2.21	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	771/773 (100%)	716 (93%)	43 (6%)	12 (2%)	12	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	THR
1	A	437	VAL
1	A	610	ILE
1	A	214	PHE
1	A	382	GLU
1	A	671	LYS
1	A	757	TYR
1	A	108	ASP
1	A	148	GLU
1	A	772	LYS
1	A	267	THR
1	A	383	SER

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	664/670 (99%)	643 (97%)	21 (3%)	46	74

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	50	ASP
1	A	58	ARG
1	A	175	ASN
1	A	266	ARG
1	A	303	GLU
1	A	307	ARG
1	A	314	GLU
1	A	346	ARG

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Mol	Chain	Res	Type
1	A	394	ARG
1	A	415	THR
1	A	425	ARG
1	A	483	GLN
1	A	516	TRP
1	A	523	THR
1	A	585	ARG
1	A	592	LYS
1	A	612	ARG
1	A	685	ARG
1	A	689	ARG
1	A	718	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	91	GLN
1	A	103	HIS
1	A	175	ASN
1	A	213	ASN
1	A	242	GLN
1	A	257	HIS
1	A	285	GLN
1	A	399	ASN
1	A	461	GLN
1	A	491	ASN
1	A	633	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.