



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:11 am BST

PDB ID : 1QHT
Title : DNA POLYMERASE FROM THERMOCOCCUS SP. 9ON-7 ARCHAEON
Authors : Park, H.-W.; Rodriguez, A.C.; Beese, L.S.
Deposited on : 1999-05-26
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

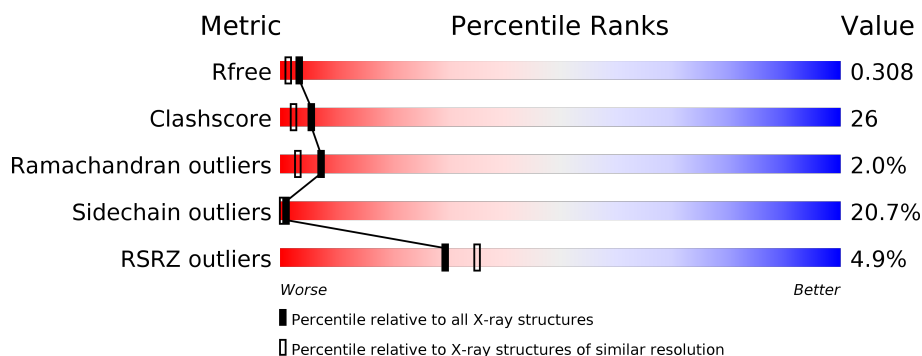
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	775	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5912 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 (DNA POLYMERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5803	3745	987	1056	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	ENGINEERED MUTATION	UNP Q56366
A	143	ALA	GLU	ENGINEERED MUTATION	UNP Q56366

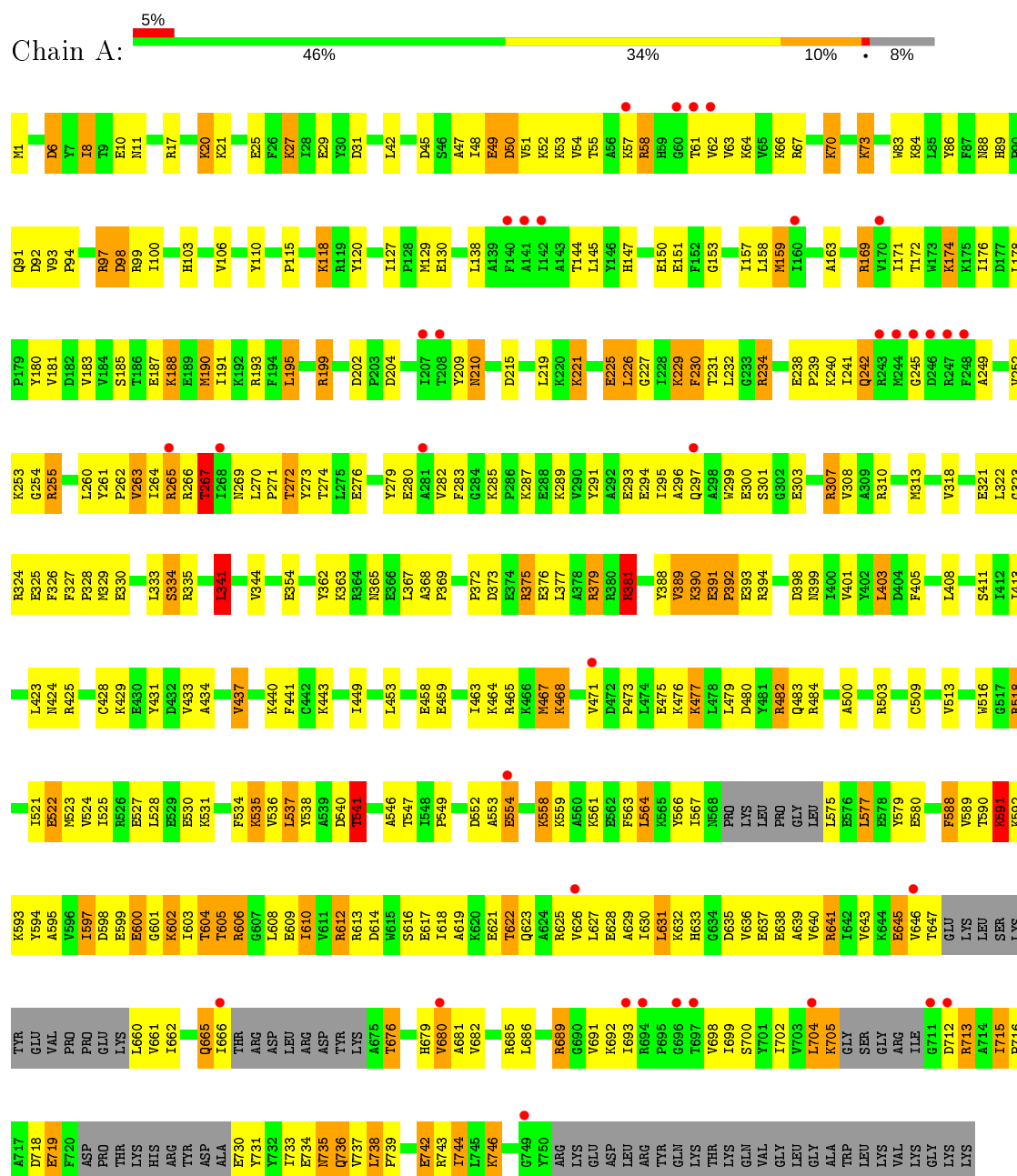
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total	O	0	0
			109	109		

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 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: PROTEIN (DNA POLYMERASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.30Å 98.70Å 112.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 24.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.5 (25.00-2.10) 89.3 (24.45-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.245 , 0.312 0.250 , 0.308	Depositor DCC
R_{free} test set	2822 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5912	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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 [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	0.43	0/5929	0.62	1/7991 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LEU	CA-CB-CG	5.73	128.48	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	5803	0	5850	301	0
2	A	109	0	0	7	0
All	All	5912	0	5850	301	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 26.

All (301) 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:159:MET:HA	1:A:190:MET:HE2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:CYS:HB2	1:A:431:TYR:CZ	2.04	0.92
1:A:610:ILE:HD12	1:A:610:ILE:H	1.36	0.91
1:A:480:ASP:O	1:A:484:ARG:HG3	1.73	0.89
1:A:147:HIS:O	1:A:150:GLU:HB2	1.75	0.86
1:A:334:SER:HA	1:A:344:VAL:HG21	1.59	0.84
1:A:178:LEU:HB2	1:A:181:VAL:HG23	1.57	0.84
1:A:733:ILE:HG23	1:A:734:GLU:HG2	1.59	0.83
1:A:636:VAL:O	1:A:640:VAL:HG23	1.79	0.82
1:A:666:ILE:HD11	1:A:699:ILE:HG23	1.62	0.81
1:A:617:GLU:O	1:A:621:GLU:HG2	1.81	0.81
1:A:392:PRO:HG3	1:A:538:TYR:HD1	1.46	0.78
1:A:262:PRO:O	1:A:266:ARG:HD2	1.83	0.78
1:A:590:THR:HG22	1:A:591:LYS:N	1.99	0.77
1:A:45:ASP:OD1	1:A:70:LYS:HE3	1.84	0.77
1:A:403:LEU:HD11	1:A:564:LEU:HD11	1.65	0.77
1:A:643:VAL:O	1:A:647:THR:HG22	1.84	0.77
1:A:742:GLU:HG3	1:A:743:ARG:N	1.98	0.76
1:A:622:THR:OG1	1:A:646:VAL:HG11	1.86	0.76
1:A:575:LEU:HD12	1:A:575:LEU:O	1.87	0.75
1:A:665:GLN:HG2	1:A:698:VAL:HG22	1.69	0.75
1:A:48:ILE:HG23	1:A:49:GLU:H	1.53	0.72
1:A:93:VAL:HB	1:A:94:PRO:HD3	1.69	0.72
1:A:145:LEU:HB2	1:A:158:LEU:HD21	1.69	0.72
1:A:638:GLU:O	1:A:641:ARG:HG3	1.88	0.72
1:A:388:TYR:HD1	1:A:518:ARG:HG2	1.53	0.72
1:A:252:VAL:HG12	1:A:255:ARG:HG3	1.70	0.72
1:A:270:LEU:HB3	1:A:271:PRO:HD2	1.73	0.71
1:A:601:GLY:O	1:A:603:ILE:HD12	1.90	0.71
1:A:730:GLU:O	1:A:733:ILE:HG22	1.90	0.71
1:A:475:GLU:OE2	1:A:479:LEU:HD11	1.91	0.70
1:A:705:LYS:CD	1:A:713:ARG:HD2	2.21	0.70
1:A:327:PHE:CE1	1:A:341:LEU:HD21	2.27	0.70
1:A:341:LEU:O	1:A:341:LEU:HD12	1.92	0.70
1:A:590:THR:CG2	1:A:591:LYS:H	2.05	0.69
1:A:590:THR:CG2	1:A:591:LYS:N	2.55	0.69
1:A:465:ARG:HA	1:A:468:LYS:HD2	1.73	0.69
1:A:375:ARG:HD3	1:A:379:ARG:NH2	2.08	0.68
1:A:392:PRO:HA	1:A:537:LEU:O	1.94	0.68
1:A:392:PRO:HB3	1:A:588:PHE:HB2	1.74	0.68
1:A:521:ILE:O	1:A:525:ILE:HG13	1.93	0.68
1:A:541:THR:HG23	2:A:1079:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLU:HG3	1:A:27:LYS:HZ2	1.59	0.67
1:A:424:ASN:HD21	1:A:440:LYS:H	1.43	0.67
1:A:48:ILE:HG23	1:A:49:GLU:N	2.09	0.67
1:A:51:VAL:HG22	1:A:103:HIS:CD2	2.29	0.67
1:A:715:ILE:HG12	1:A:719:GLU:O	1.94	0.67
1:A:172:THR:HA	1:A:190:MET:HE3	1.77	0.67
1:A:159:MET:CA	1:A:190:MET:HE2	2.22	0.66
1:A:637:GLU:CD	1:A:637:GLU:H	1.97	0.65
1:A:169:ARG:NH1	1:A:180:TYR:HA	2.11	0.65
1:A:327:PHE:N	1:A:328:PRO:HD2	2.11	0.65
1:A:49:GLU:OE1	1:A:52:LYS:HE2	1.97	0.65
1:A:392:PRO:HG3	1:A:538:TYR:CD1	2.31	0.65
1:A:647:THR:HG23	1:A:647:THR:O	1.95	0.65
1:A:733:ILE:O	1:A:738:LEU:HB2	1.96	0.65
1:A:191:ILE:O	1:A:195:LEU:HD12	1.97	0.64
1:A:408:LEU:CD2	1:A:575:LEU:HD13	2.27	0.64
1:A:705:LYS:HD2	1:A:713:ARG:HD2	1.80	0.64
1:A:676:THR:HG23	1:A:679:HIS:CG	2.33	0.64
1:A:597:ILE:HD11	1:A:601:GLY:HA2	1.79	0.63
1:A:240:LYS:HE2	1:A:242:GLN:HE22	1.64	0.63
1:A:178:LEU:HB2	1:A:181:VAL:CG2	2.29	0.62
1:A:733:ILE:HG23	1:A:734:GLU:N	2.14	0.62
1:A:388:TYR:CD1	1:A:518:ARG:HG2	2.33	0.62
1:A:375:ARG:HD3	1:A:379:ARG:CZ	2.29	0.62
1:A:535:LYS:HB2	1:A:549:PRO:HD3	1.81	0.62
1:A:153:GLY:HA3	1:A:221:LYS:HD2	1.81	0.62
1:A:522:GLU:OE1	1:A:522:GLU:HA	2.00	0.62
1:A:202:ASP:OD1	1:A:255:ARG:NH2	2.32	0.62
1:A:379:ARG:O	1:A:381:ARG:HG3	2.00	0.62
1:A:705:LYS:HD3	1:A:713:ARG:HD2	1.82	0.61
1:A:373:ASP:O	1:A:377:LEU:HB2	1.99	0.61
1:A:264:ILE:HA	1:A:267:THR:HG23	1.81	0.60
1:A:269:ASN:HA	1:A:273:TYR:OH	2.01	0.60
1:A:408:LEU:HD23	1:A:575:LEU:HD13	1.82	0.60
1:A:424:ASN:ND2	1:A:440:LYS:H	1.99	0.60
1:A:261:TYR:O	1:A:265:ARG:HB2	2.02	0.60
1:A:388:TYR:O	1:A:540:ASP:HA	2.01	0.60
1:A:736:GLN:H	1:A:739:PRO:HD2	1.65	0.60
1:A:689:ARG:NH1	1:A:691:VAL:HG21	2.17	0.59
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.16	0.59
1:A:260:LEU:HD21	1:A:323:GLY:HA2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:HE1	1:A:322:LEU:HD23	1.66	0.59
1:A:597:ILE:HG13	1:A:598:ASP:N	2.17	0.59
1:A:8:ILE:HD13	1:A:17:ARG:NH1	2.17	0.58
1:A:434:ALA:CB	1:A:437:VAL:HG23	2.33	0.58
1:A:354:GLU:CD	1:A:503:ARG:HG3	2.23	0.58
1:A:188:LYS:HD3	1:A:226:LEU:HB3	1.85	0.58
1:A:590:THR:HG22	1:A:591:LYS:H	1.68	0.58
1:A:635:ASP:HB3	1:A:638:GLU:HB3	1.85	0.58
1:A:362:TYR:HB2	2:A:1018:HOH:O	2.03	0.58
1:A:295:ILE:HD13	1:A:308:VAL:HG13	1.86	0.58
1:A:110:TYR:HB2	1:A:367:LEU:HD11	1.84	0.57
1:A:646:VAL:HG12	1:A:646:VAL:O	2.04	0.57
1:A:225:GLU:C	1:A:227:GLY:H	2.06	0.57
1:A:595:ALA:HB2	1:A:608:LEU:HD11	1.85	0.57
1:A:307:ARG:HG2	1:A:310:ARG:HH21	1.69	0.57
1:A:405:PHE:HA	2:A:1020:HOH:O	2.04	0.57
1:A:20:LYS:HE2	1:A:29:GLU:HB2	1.86	0.57
1:A:610:ILE:CD1	1:A:610:ILE:H	2.11	0.57
1:A:301:SER:OG	1:A:303:GLU:HB2	2.05	0.57
1:A:638:GLU:OE1	1:A:638:GLU:HA	2.04	0.57
1:A:593:LYS:HA	1:A:606:ARG:O	2.06	0.56
1:A:263:VAL:HG12	1:A:267:THR:HG21	1.87	0.56
1:A:297:GLN:O	1:A:301:SER:HB3	2.06	0.56
1:A:174:LYS:HB2	1:A:299:TRP:CH2	2.41	0.56
1:A:230:PHE:O	1:A:238:GLU:HG2	2.05	0.56
1:A:55:THR:O	1:A:99:ARG:NE	2.38	0.55
1:A:390:LYS:HD3	1:A:391:GLU:O	2.06	0.55
1:A:612:ARG:HH21	1:A:736:GLN:HE22	1.54	0.55
1:A:145:LEU:HD11	1:A:296:ALA:HA	1.88	0.54
1:A:225:GLU:OE1	1:A:225:GLU:HA	2.06	0.54
1:A:588:PHE:CD1	1:A:588:PHE:N	2.76	0.54
1:A:171:ILE:HD13	1:A:193:ARG:HG3	1.89	0.54
1:A:276:GLU:HG3	1:A:287:LYS:HB3	1.88	0.54
1:A:428:CYS:HB2	1:A:431:TYR:CE1	2.43	0.53
1:A:603:ILE:HG22	1:A:604:THR:N	2.22	0.53
1:A:158:LEU:O	1:A:190:MET:HE1	2.08	0.53
1:A:685:ARG:HG2	1:A:716:PRO:HD2	1.89	0.53
1:A:283:PHE:O	1:A:285:LYS:HE3	2.09	0.53
1:A:705:LYS:HD2	1:A:713:ARG:HH11	1.72	0.53
1:A:705:LYS:HD2	1:A:713:ARG:NH1	2.22	0.53
1:A:241:ILE:N	1:A:241:ILE:HD12	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:LEU:HD11	1:A:744:ILE:CD1	2.39	0.53
1:A:509:CYS:O	1:A:513:VAL:HG23	2.08	0.53
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.74	0.53
1:A:115:PRO:HB2	1:A:118:LYS:HG2	1.90	0.52
1:A:682:VAL:O	1:A:686:LEU:HG	2.09	0.52
1:A:73:LYS:HB3	1:A:365:ASN:OD1	2.09	0.52
1:A:405:PHE:HB2	1:A:408:LEU:HG	1.91	0.52
1:A:138:LEU:HD12	1:A:163:ALA:O	2.09	0.52
1:A:733:ILE:CG2	1:A:734:GLU:HG2	2.36	0.52
1:A:629:ALA:O	1:A:633:HIS:HB2	2.10	0.52
1:A:25:GLU:HG3	1:A:27:LYS:NZ	2.23	0.52
1:A:176:ILE:HB	1:A:181:VAL:HG11	1.92	0.51
1:A:229:LYS:HD2	1:A:231:THR:CG2	2.40	0.51
1:A:547:THR:O	1:A:549:PRO:HD3	2.11	0.51
1:A:58:ARG:NH1	1:A:92:ASP:OD1	2.43	0.51
1:A:598:ASP:HB2	2:A:1081:HOH:O	2.10	0.51
1:A:614:ASP:N	1:A:614:ASP:OD1	2.43	0.51
1:A:612:ARG:NH2	1:A:736:GLN:HE22	2.09	0.51
1:A:159:MET:HA	1:A:190:MET:CE	2.30	0.51
1:A:187:GLU:OE1	1:A:226:LEU:HD11	2.11	0.51
1:A:593:LYS:O	1:A:594:TYR:HB3	2.11	0.51
1:A:225:GLU:O	1:A:227:GLY:N	2.44	0.50
1:A:270:LEU:HB3	1:A:271:PRO:CD	2.40	0.50
1:A:42:LEU:HG	1:A:83:TRP:CD1	2.47	0.50
1:A:597:ILE:CG2	1:A:631:LEU:HB3	2.41	0.50
1:A:680:VAL:HG12	1:A:681:ALA:N	2.25	0.50
1:A:735:ASN:OD1	1:A:735:ASN:O	2.29	0.50
1:A:279:TYR:HE1	1:A:321:GLU:OE1	1.94	0.50
1:A:399:ASN:OD1	1:A:553:ALA:HB2	2.11	0.50
1:A:661:VAL:HG12	1:A:662:ILE:H	1.76	0.50
1:A:219:LEU:HD13	1:A:230:PHE:CZ	2.46	0.50
1:A:618:ILE:HG23	1:A:619:ALA:N	2.26	0.50
1:A:401:VAL:HG13	1:A:579:TYR:CE1	2.46	0.50
1:A:733:ILE:CG2	1:A:734:GLU:N	2.74	0.50
1:A:1:MET:HG3	1:A:129:MET:HA	1.94	0.49
1:A:225:GLU:C	1:A:227:GLY:N	2.65	0.49
1:A:603:ILE:CG2	1:A:604:THR:N	2.76	0.49
1:A:199:ARG:CG	1:A:199:ARG:HH11	2.24	0.49
1:A:434:ALA:HB1	1:A:437:VAL:HG23	1.94	0.49
1:A:475:GLU:O	1:A:479:LEU:HG	2.12	0.49
1:A:738:LEU:CB	1:A:739:PRO:HD3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ASP:HB3	1:A:638:GLU:CB	2.43	0.49
1:A:666:ILE:HD11	1:A:699:ILE:CG2	2.39	0.49
1:A:373:ASP:OD1	1:A:376:GLU:N	2.43	0.49
1:A:8:ILE:HA	1:A:8:ILE:HD12	1.65	0.49
1:A:99:ARG:HD2	2:A:1063:HOH:O	2.11	0.49
1:A:55:THR:O	1:A:99:ARG:NH2	2.46	0.49
1:A:48:ILE:CG2	1:A:49:GLU:H	2.23	0.48
1:A:635:ASP:CG	1:A:638:GLU:HB2	2.33	0.48
1:A:272:THR:HG23	1:A:274:THR:HG23	1.95	0.48
1:A:49:GLU:OE1	1:A:49:GLU:HA	2.11	0.48
1:A:600:GLU:OE1	1:A:602:LYS:HD2	2.14	0.48
1:A:645:GLU:OE1	1:A:646:VAL:HG23	2.14	0.48
1:A:130:GLU:OE1	1:A:335:ARG:NH1	2.46	0.48
1:A:702:ILE:HG22	1:A:704:LEU:HD23	1.96	0.48
1:A:646:VAL:O	1:A:646:VAL:CG1	2.61	0.48
1:A:291:TYR:HD1	1:A:294:GLU:OE2	1.97	0.47
1:A:398:ASP:HB3	1:A:399:ASN:ND2	2.29	0.47
1:A:616:SER:OG	1:A:618:ILE:HG22	2.13	0.47
1:A:605:THR:HB	1:A:608:LEU:CD1	2.44	0.47
1:A:463:ILE:HG23	1:A:479:LEU:HB3	1.96	0.47
1:A:626:VAL:O	1:A:630:ILE:HG13	2.14	0.47
1:A:54:VAL:O	1:A:64:LYS:HG3	2.15	0.47
1:A:647:THR:OG1	1:A:733:ILE:HD11	2.14	0.47
1:A:733:ILE:HG23	1:A:734:GLU:CG	2.39	0.47
1:A:327:PHE:N	1:A:328:PRO:CD	2.78	0.47
1:A:48:ILE:CG2	1:A:49:GLU:N	2.78	0.47
1:A:66:LYS:HE3	1:A:88:ASN:ND2	2.30	0.47
1:A:265:ARG:HD2	1:A:265:ARG:HA	1.63	0.46
1:A:84:LYS:HD3	1:A:86:TYR:CZ	2.49	0.46
1:A:232:LEU:O	1:A:255:ARG:NH1	2.46	0.46
1:A:289:LYS:NZ	1:A:291:TYR:HA	2.30	0.46
1:A:685:ARG:HG2	1:A:716:PRO:CD	2.46	0.46
1:A:234:ARG:HB2	1:A:254:GLY:HA3	1.96	0.46
1:A:552:ASP:OD1	1:A:554:GLU:HB3	2.15	0.46
1:A:689:ARG:HH11	1:A:691:VAL:HG21	1.77	0.46
1:A:42:LEU:HG	1:A:83:TRP:HD1	1.80	0.46
1:A:174:LYS:HB2	1:A:299:TRP:CZ3	2.51	0.46
1:A:326:PHE:CD1	1:A:326:PHE:N	2.81	0.46
1:A:434:ALA:HB3	1:A:437:VAL:HG23	1.96	0.46
1:A:627:LEU:HD11	1:A:744:ILE:HD11	1.97	0.46
1:A:145:LEU:CD1	1:A:296:ALA:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HA	1:A:567:ILE:HG22	1.97	0.46
1:A:689:ARG:HH11	1:A:691:VAL:CG2	2.28	0.46
1:A:605:THR:HB	1:A:608:LEU:HD12	1.97	0.45
1:A:693:ILE:HG22	1:A:693:ILE:O	2.16	0.45
1:A:174:LYS:HE3	1:A:299:TRP:CE2	2.52	0.45
1:A:465:ARG:HA	1:A:468:LYS:CD	2.46	0.45
1:A:372:PRO:HG3	1:A:500:ALA:O	2.17	0.45
1:A:629:ALA:HB3	1:A:639:ALA:HB2	1.97	0.45
1:A:423:LEU:HB2	1:A:441:PHE:CE1	2.52	0.45
1:A:50:ASP:O	1:A:53:LYS:HB2	2.17	0.45
1:A:392:PRO:CB	1:A:588:PHE:HB2	2.44	0.45
1:A:323:GLY:O	1:A:327:PHE:HB2	2.17	0.45
1:A:536:VAL:HA	1:A:546:ALA:HB2	1.99	0.45
1:A:733:ILE:CG2	1:A:734:GLU:H	2.30	0.45
1:A:597:ILE:HG21	1:A:631:LEU:HB3	1.99	0.44
1:A:21:LYS:NZ	1:A:204:ASP:OD2	2.44	0.44
1:A:225:GLU:OE1	1:A:225:GLU:CA	2.65	0.44
1:A:393:GLU:HG2	1:A:535:LYS:HE3	1.99	0.44
1:A:661:VAL:HG12	1:A:662:ILE:N	2.32	0.44
1:A:93:VAL:O	1:A:97:ARG:HB2	2.17	0.44
1:A:115:PRO:HB2	1:A:118:LYS:CG	2.47	0.44
1:A:373:ASP:OD1	1:A:373:ASP:C	2.55	0.44
1:A:10:GLU:O	1:A:11:ASN:HB2	2.17	0.44
1:A:590:THR:O	1:A:592:LYS:N	2.51	0.44
1:A:704:LEU:O	1:A:704:LEU:HD12	2.17	0.44
1:A:733:ILE:HG23	1:A:734:GLU:H	1.81	0.44
1:A:589:VAL:HB	1:A:593:LYS:HB2	1.99	0.44
1:A:590:THR:HG23	1:A:591:LYS:H	1.83	0.44
1:A:21:LYS:HD3	1:A:204:ASP:OD1	2.18	0.43
1:A:178:LEU:HD12	1:A:181:VAL:HG21	1.99	0.43
1:A:50:ASP:HA	1:A:53:LYS:HD2	2.00	0.43
1:A:558:LYS:O	1:A:561:LYS:HB2	2.19	0.43
1:A:242:GLN:O	1:A:249:ALA:N	2.50	0.43
1:A:527:GLU:OE1	1:A:566:TYR:OH	2.28	0.43
1:A:209:TYR:O	1:A:210:ASN:CB	2.66	0.43
1:A:127:ILE:O	1:A:130:GLU:HG2	2.18	0.43
1:A:6:ASP:C	1:A:6:ASP:OD1	2.57	0.43
1:A:70:LYS:HG3	1:A:83:TRP:CZ2	2.54	0.43
1:A:742:GLU:OE2	1:A:746:LYS:HE3	2.19	0.43
1:A:296:ALA:O	1:A:300:GLU:HG3	2.19	0.43
1:A:528:LEU:HD13	1:A:563:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:HD21	1:A:577:LEU:HD21	1.99	0.43
1:A:252:VAL:CG1	1:A:255:ARG:HG3	2.46	0.42
1:A:411:SER:OG	1:A:575:LEU:HB3	2.19	0.42
1:A:11:ASN:HD22	1:A:11:ASN:HA	1.68	0.42
1:A:279:TYR:CE1	1:A:318:VAL:HG22	2.55	0.42
1:A:389:VAL:CG1	1:A:591:LYS:HG3	2.50	0.42
1:A:471:VAL:O	1:A:473:PRO:HD3	2.19	0.42
1:A:398:ASP:HB3	1:A:399:ASN:HD22	1.83	0.42
1:A:294:GLU:HA	1:A:297:GLN:OE1	2.20	0.42
1:A:42:LEU:HD23	1:A:106:VAL:HG22	2.01	0.42
1:A:47:ALA:O	1:A:51:VAL:HG23	2.19	0.42
1:A:685:ARG:NE	1:A:719:GLU:OE1	2.53	0.42
1:A:325:GLU:HG2	1:A:326:PHE:CE1	2.54	0.42
1:A:554:GLU:O	1:A:558:LYS:HB2	2.20	0.42
1:A:103:HIS:ND1	1:A:103:HIS:C	2.73	0.42
1:A:31:ASP:OD2	1:A:120:TYR:OH	2.27	0.42
1:A:369:PRO:O	1:A:503:ARG:HB3	2.20	0.42
1:A:376:GLU:HA	1:A:379:ARG:HD2	2.01	0.42
1:A:597:ILE:CD1	1:A:601:GLY:HA2	2.49	0.42
1:A:433:VAL:HG22	1:A:440:LYS:HD3	2.01	0.42
1:A:443:LYS:HE2	1:A:443:LYS:HB3	1.61	0.42
1:A:591:LYS:O	1:A:592:LYS:HD3	2.20	0.42
1:A:715:ILE:HG23	1:A:715:ILE:O	2.19	0.42
1:A:467:MET:HB3	1:A:467:MET:HE2	1.74	0.41
1:A:567:ILE:HG13	1:A:567:ILE:O	2.20	0.41
1:A:676:THR:HG23	1:A:679:HIS:HB2	2.02	0.41
1:A:8:ILE:HD13	1:A:17:ARG:HH11	1.84	0.41
1:A:89:HIS:ND1	1:A:91:GLN:HB2	2.35	0.41
1:A:98:ASP:N	1:A:98:ASP:OD1	2.52	0.41
1:A:130:GLU:HB2	2:A:1014:HOH:O	2.20	0.41
1:A:229:LYS:HD2	1:A:231:THR:HG23	2.00	0.41
1:A:291:TYR:O	1:A:295:ILE:HG12	2.21	0.41
1:A:482:ARG:HB3	2:A:1022:HOH:O	2.21	0.41
1:A:178:LEU:HD13	1:A:180:TYR:OH	2.20	0.41
1:A:174:LYS:O	1:A:183:VAL:HG13	2.20	0.41
1:A:434:ALA:HB1	1:A:437:VAL:CG2	2.51	0.41
1:A:645:GLU:C	1:A:647:THR:H	2.23	0.41
1:A:1:MET:SD	1:A:129:MET:HA	2.61	0.41
1:A:401:VAL:HG13	1:A:579:TYR:HE1	1.84	0.41
1:A:477:LYS:HA	1:A:477:LYS:HD2	1.78	0.41
1:A:628:GLU:OE2	1:A:632:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:LEU:HB3	1:A:691:VAL:HB	2.03	0.41
1:A:480:ASP:O	1:A:483:GLN:HG3	2.20	0.41
1:A:84:LYS:HD3	1:A:86:TYR:OH	2.20	0.41
1:A:605:THR:CB	1:A:608:LEU:HD12	2.51	0.41
1:A:735:ASN:O	1:A:736:GLN:HB2	2.21	0.41
1:A:178:LEU:HD12	1:A:181:VAL:CG2	2.51	0.41
1:A:144:THR:HG22	1:A:157:ILE:HG12	2.02	0.40
1:A:389:VAL:HG12	1:A:591:LYS:HG3	2.03	0.40
1:A:230:PHE:O	1:A:239:PRO:HD3	2.22	0.40
1:A:368:ALA:HA	1:A:369:PRO:HD3	1.89	0.40
1:A:713:ARG:HG2	1:A:713:ARG:H	1.61	0.40
1:A:73:LYS:HE2	1:A:365:ASN:OD1	2.21	0.40
1:A:390:LYS:CD	1:A:391:GLU:H	2.34	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	698/775 (90%)	624 (89%)	60 (9%)	14 (2%)	7 3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	ARG
1	A	591	LYS
1	A	736	GLN
1	A	97	ARG
1	A	210	ASN
1	A	245	GLY
1	A	263	VAL
1	A	267	THR

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Mol	Chain	Res	Type
1	A	541	THR
1	A	602	LYS
1	A	735	ASN
1	A	226	LEU
1	A	282	VAL
1	A	392	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	609/666 (91%)	483 (79%)	126 (21%)	1 0

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	8	ILE
1	A	20	LYS
1	A	27	LYS
1	A	49	GLU
1	A	50	ASP
1	A	57	LYS
1	A	58	ARG
1	A	61	THR
1	A	62	VAL
1	A	63	VAL
1	A	67	ARG
1	A	70	LYS
1	A	73	LYS
1	A	98	ASP
1	A	100	ILE
1	A	118	LYS
1	A	151	GLU
1	A	159	MET
1	A	169	ARG

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Mol	Chain	Res	Type
1	A	174	LYS
1	A	185	SER
1	A	188	LYS
1	A	190	MET
1	A	195	LEU
1	A	199	ARG
1	A	215	ASP
1	A	221	LYS
1	A	225	GLU
1	A	229	LYS
1	A	230	PHE
1	A	234	ARG
1	A	242	GLN
1	A	253	LYS
1	A	255	ARG
1	A	265	ARG
1	A	267	THR
1	A	272	THR
1	A	280	GLU
1	A	293	GLU
1	A	307	ARG
1	A	313	MET
1	A	324	ARG
1	A	329	MET
1	A	330	GLU
1	A	333	LEU
1	A	334	SER
1	A	341	LEU
1	A	363	LYS
1	A	375	ARG
1	A	379	ARG
1	A	381	ARG
1	A	389	VAL
1	A	390	LYS
1	A	391	GLU
1	A	394	ARG
1	A	403	LEU
1	A	413	ILE
1	A	425	ARG
1	A	429	LYS
1	A	437	VAL
1	A	449	ILE

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Mol	Chain	Res	Type
1	A	453	LEU
1	A	458	GLU
1	A	459	GLU
1	A	464	LYS
1	A	467	MET
1	A	468	LYS
1	A	476	LYS
1	A	477	LYS
1	A	482	ARG
1	A	516	TRP
1	A	518	ARG
1	A	522	GLU
1	A	523	MET
1	A	524	VAL
1	A	530	GLU
1	A	531	LYS
1	A	534	PHE
1	A	535	LYS
1	A	537	LEU
1	A	541	THR
1	A	554	GLU
1	A	558	LYS
1	A	559	LYS
1	A	564	LEU
1	A	577	LEU
1	A	580	GLU
1	A	588	PHE
1	A	591	LYS
1	A	597	ILE
1	A	599	GLU
1	A	600	GLU
1	A	604	THR
1	A	605	THR
1	A	606	ARG
1	A	609	GLU
1	A	610	ILE
1	A	612	ARG
1	A	613	ARG
1	A	622	THR
1	A	623	GLN
1	A	625	ARG
1	A	631	LEU

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Mol	Chain	Res	Type
1	A	641	ARG
1	A	645	GLU
1	A	660	LEU
1	A	665	GLN
1	A	676	THR
1	A	680	VAL
1	A	689	ARG
1	A	692	LYS
1	A	700	SER
1	A	704	LEU
1	A	705	LYS
1	A	712	ASP
1	A	713	ARG
1	A	715	ILE
1	A	718	ASP
1	A	719	GLU
1	A	731	TYR
1	A	737	VAL
1	A	738	LEU
1	A	742	GLU
1	A	744	ILE
1	A	746	LYS

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	242	GLN
1	A	424	ASN
1	A	623	GLN
1	A	735	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	710/775 (91%)	0.25	35 (4%)	29 35	14, 40, 65, 84	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ASP	5.3
1	A	243	ARG	4.6
1	A	749	GLY	4.3
1	A	248	PHE	4.2
1	A	471	VAL	4.1
1	A	268	ILE	4.1
1	A	247	ARG	3.9
1	A	60	GLY	3.8
1	A	646	VAL	3.8
1	A	244	MET	3.1
1	A	141	ALA	2.9
1	A	704	LEU	2.8
1	A	626	VAL	2.8
1	A	61	THR	2.8
1	A	712	ASP	2.8
1	A	142	ILE	2.6
1	A	666	ILE	2.6
1	A	57	LYS	2.6
1	A	160	ILE	2.6
1	A	208	THR	2.5
1	A	207	ILE	2.5
1	A	62	VAL	2.5
1	A	170	VAL	2.5
1	A	265	ARG	2.5
1	A	297	GLN	2.4
1	A	697	THR	2.4
1	A	696	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	2.3
1	A	245	GLY	2.3
1	A	711	GLY	2.3
1	A	140	PHE	2.2
1	A	680	VAL	2.2
1	A	693	ILE	2.1
1	A	694	ARG	2.1
1	A	554	GLU	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 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.