



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:32 AM UTC

PDB ID : 8JRB / pdb_00008jrb
Title : Structure of DNA polymerase 1 from Aquifex pyrophilus
Authors : Clement, P.; Nair, D.T.
Deposited on : 2023-06-16
Resolution : 2.20 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

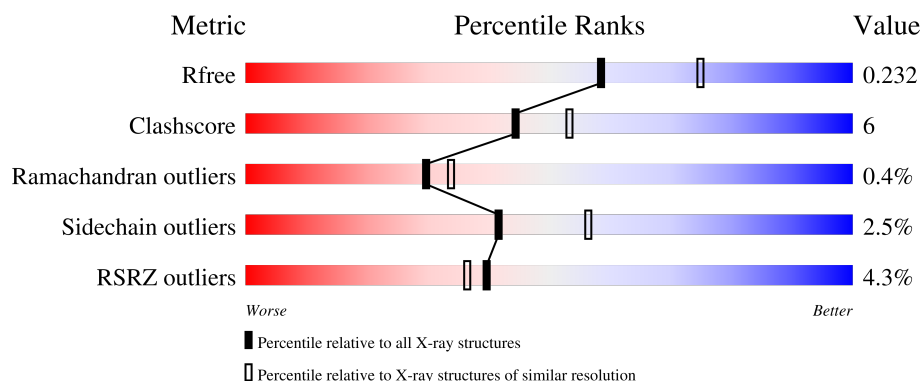
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	597	
1	B	597	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9698 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 DNA polymerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	0	0
			4642	2980	799	853	10			
1	B	574	Total	C	N	O	S	0	0	0
			4645	2981	800	854	10			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q8GHE9
A	-21	HIS	-	expression tag	UNP Q8GHE9
A	-20	HIS	-	expression tag	UNP Q8GHE9
A	-19	HIS	-	expression tag	UNP Q8GHE9
A	-18	HIS	-	expression tag	UNP Q8GHE9
A	-17	HIS	-	expression tag	UNP Q8GHE9
A	-16	HIS	-	expression tag	UNP Q8GHE9
A	-15	LEU	-	expression tag	UNP Q8GHE9
A	-14	GLU	-	expression tag	UNP Q8GHE9
A	-13	VAL	-	expression tag	UNP Q8GHE9
A	-12	LEU	-	expression tag	UNP Q8GHE9
A	-11	PHE	-	expression tag	UNP Q8GHE9
A	-10	GLN	-	expression tag	UNP Q8GHE9
A	-9	GLY	-	expression tag	UNP Q8GHE9
A	-8	PRO	-	expression tag	UNP Q8GHE9
A	-7	LEU	-	expression tag	UNP Q8GHE9
A	-6	GLY	-	expression tag	UNP Q8GHE9
A	-5	SER	-	expression tag	UNP Q8GHE9
A	-4	GLU	-	expression tag	UNP Q8GHE9
A	-3	PHE	-	expression tag	UNP Q8GHE9
A	-2	ARG	-	expression tag	UNP Q8GHE9
A	-1	ALA	-	expression tag	UNP Q8GHE9
A	0	GLY	-	expression tag	UNP Q8GHE9
A	28	ALA	ASP	conflict	UNP Q8GHE9
A	30	ALA	GLU	conflict	UNP Q8GHE9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	initiating methionine	UNP Q8GHE9
B	-21	HIS	-	expression tag	UNP Q8GHE9
B	-20	HIS	-	expression tag	UNP Q8GHE9
B	-19	HIS	-	expression tag	UNP Q8GHE9
B	-18	HIS	-	expression tag	UNP Q8GHE9
B	-17	HIS	-	expression tag	UNP Q8GHE9
B	-16	HIS	-	expression tag	UNP Q8GHE9
B	-15	LEU	-	expression tag	UNP Q8GHE9
B	-14	GLU	-	expression tag	UNP Q8GHE9
B	-13	VAL	-	expression tag	UNP Q8GHE9
B	-12	LEU	-	expression tag	UNP Q8GHE9
B	-11	PHE	-	expression tag	UNP Q8GHE9
B	-10	GLN	-	expression tag	UNP Q8GHE9
B	-9	GLY	-	expression tag	UNP Q8GHE9
B	-8	PRO	-	expression tag	UNP Q8GHE9
B	-7	LEU	-	expression tag	UNP Q8GHE9
B	-6	GLY	-	expression tag	UNP Q8GHE9
B	-5	SER	-	expression tag	UNP Q8GHE9
B	-4	GLU	-	expression tag	UNP Q8GHE9
B	-3	PHE	-	expression tag	UNP Q8GHE9
B	-2	ARG	-	expression tag	UNP Q8GHE9
B	-1	ALA	-	expression tag	UNP Q8GHE9
B	0	GLY	-	expression tag	UNP Q8GHE9
B	28	ALA	ASP	conflict	UNP Q8GHE9
B	30	ALA	GLU	conflict	UNP Q8GHE9

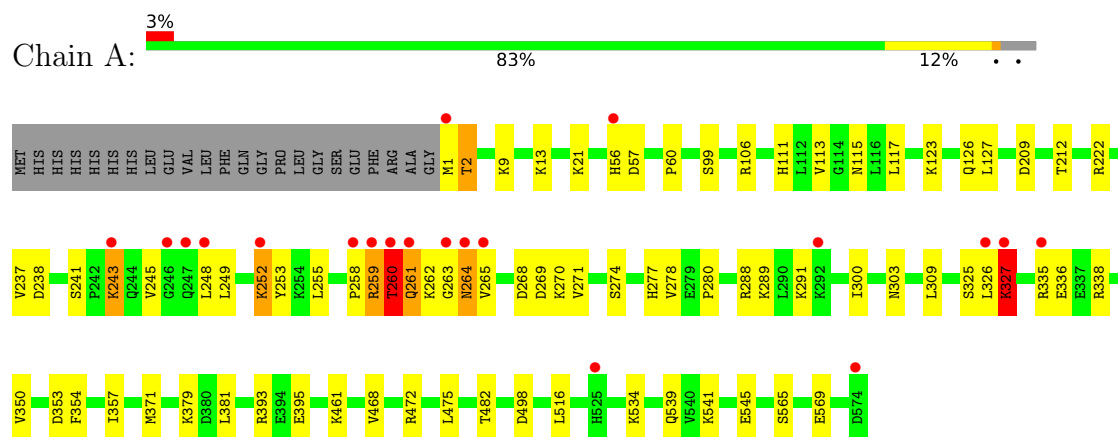
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	244	Total O 244 244	0	0
2	B	167	Total O 167 167	0	0

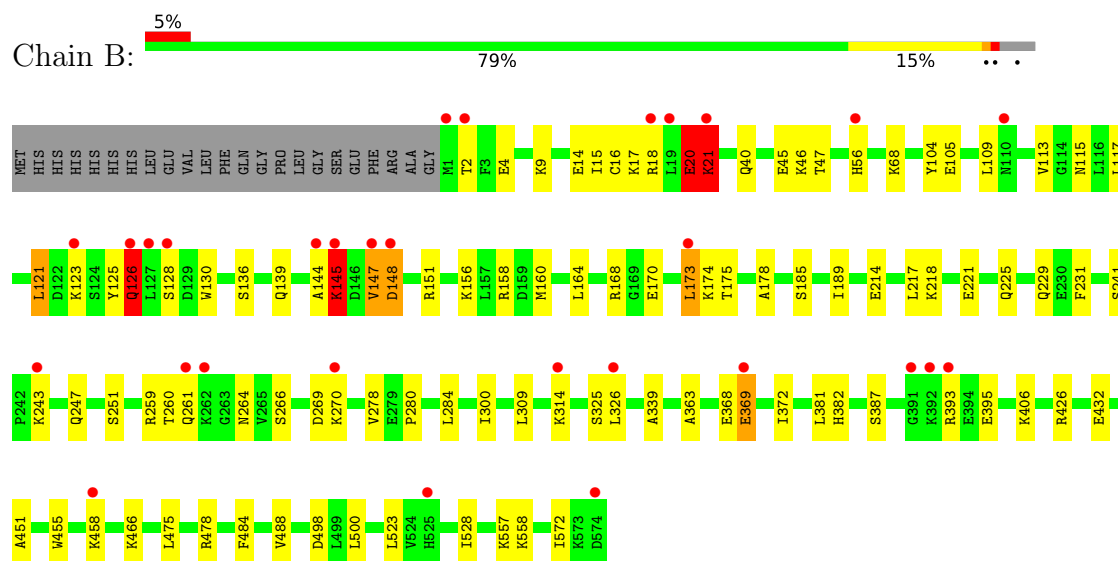
3 Residue-property plots [i](#)

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: DNA polymerase I



• Molecule 1: DNA polymerase I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.83Å 74.72Å 129.56Å 90.00° 108.25° 90.00°	Depositor
Resolution (Å)	46.26 – 2.20 46.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (46.26-2.20) 97.2 (46.26-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.233 0.192 , 0.232	Depositor DCC
R_{free} test set	4086 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9698	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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	0.28	0/4719	0.60	11/6344 (0.2%)
1	B	0.32	2/4722 (0.0%)	0.74	22/6348 (0.3%)
All	All	0.30	2/9441 (0.0%)	0.67	33/12692 (0.3%)

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	4
1	B	0	5
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	LYS	CD-CE	-5.79	1.35	1.52
1	B	21	LYS	C-O	-5.09	1.17	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LYS	CA-CB-CG	12.36	138.82	114.10
1	B	21	LYS	CB-CG-CD	10.81	136.17	111.30
1	B	21	LYS	CA-CB-CG	10.58	135.26	114.10
1	B	21	LYS	CG-CD-CE	-10.11	88.05	111.30
1	B	314	LYS	CG-CD-CE	-10.07	88.14	111.30
1	B	20	GLU	CA-C-N	-9.68	108.40	122.44
1	B	20	GLU	C-N-CA	-9.68	108.40	122.44
1	A	327	LYS	CB-CA-C	-9.16	92.12	110.17
1	B	270	LYS	CG-CD-CE	9.03	132.06	111.30
1	A	252	LYS	CB-CG-CD	8.63	131.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	LYS	CB-CG-CD	8.47	130.79	111.30
1	B	270	LYS	CB-CG-CD	8.15	130.04	111.30
1	B	314	LYS	CA-CB-CG	7.90	129.90	114.10
1	B	270	LYS	N-CA-C	-7.76	101.66	112.45
1	B	21	LYS	CD-CE-NZ	7.75	136.72	111.90
1	A	260	THR	N-CA-C	-7.41	103.32	113.18
1	B	270	LYS	CD-CE-NZ	-7.37	88.32	111.90
1	B	270	LYS	CA-CB-CG	-6.96	100.18	114.10
1	B	314	LYS	CD-CE-NZ	6.94	134.11	111.90
1	A	259	ARG	CB-CG-CD	6.91	127.19	111.30
1	B	270	LYS	CA-C-N	6.67	128.97	120.56
1	B	270	LYS	C-N-CA	6.67	128.97	120.56
1	B	144	ALA	CA-C-N	-6.54	114.27	123.03
1	B	144	ALA	C-N-CA	-6.54	114.27	123.03
1	A	258	PRO	CA-C-N	6.28	131.81	121.39
1	A	258	PRO	C-N-CA	6.28	131.81	121.39
1	B	123	LYS	CD-CE-NZ	6.19	131.71	111.90
1	B	369	GLU	CA-CB-CG	6.15	126.40	114.10
1	A	327	LYS	N-CA-C	5.71	122.43	109.81
1	B	145	LYS	CA-CB-CG	5.46	125.02	114.10
1	A	259	ARG	CG-CD-NE	-5.28	100.38	112.00
1	A	259	ARG	CA-CB-CG	5.16	124.41	114.10
1	A	252	LYS	CG-CD-CE	-5.02	99.75	111.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ARG	Sidechain
1	A	259	ARG	Peptide
1	A	263	GLY	Peptide
1	A	264	ASN	Peptide
1	B	126	GLN	Peptide
1	B	145	LYS	Peptide
1	B	20	GLU	Peptide
1	B	21	LYS	Peptide
1	B	269	ASP	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	4642	0	4816	50	0
1	B	4645	0	4820	64	0
2	A	244	0	0	7	0
2	B	167	0	0	6	0
All	All	9698	0	9636	113	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 6.

All (113) 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:145:LYS:HD2	1:B:148:ASP:HB2	1.47	0.96
1:B:218:LYS:NZ	2:B:601:HOH:O	2.06	0.89
1:A:270:LYS:H	1:A:270:LYS:HD2	1.44	0.82
1:B:178:ALA:HB2	1:B:189:ILE:HD13	1.64	0.79
1:B:126:GLN:HA	1:B:128:SER:H	1.48	0.78
1:A:9:LYS:HE3	1:A:57:ASP:H	1.49	0.78
1:B:9:LYS:HD2	1:B:9:LYS:H	1.52	0.74
1:A:475:LEU:HD12	1:A:498:ASP:HB3	1.70	0.72
1:B:475:LEU:HD12	1:B:498:ASP:HB3	1.71	0.71
1:B:21:LYS:HB3	1:B:68:LYS:HZ1	1.57	0.69
1:B:455:TRP:O	1:B:458:LYS:HB3	1.93	0.69
1:B:20:GLU:O	1:B:68:LYS:NZ	2.24	0.68
1:B:17:LYS:HA	1:B:20:GLU:HG3	1.76	0.67
1:A:270:LYS:HD2	1:A:270:LYS:N	2.10	0.67
1:A:106:ARG:NH2	2:A:606:HOH:O	2.29	0.66
1:B:368:GLU:HB2	1:B:451:ALA:HB3	1.79	0.64
1:B:4:GLU:OE2	2:B:602:HOH:O	2.15	0.64
1:B:170:GLU:O	1:B:173:LEU:HB2	1.96	0.63
1:B:164:LEU:HD22	1:B:478:ARG:HE	1.64	0.63
1:B:21:LYS:HB3	1:B:68:LYS:NZ	2.14	0.62
1:A:393:ARG:NH1	1:A:395:GLU:OE2	2.32	0.62
1:B:113:VAL:HG12	1:B:117:LEU:HD12	1.81	0.62
1:A:123:LYS:O	1:A:126:GLN:HG2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLU:O	1:B:218:LYS:HE2	2.01	0.61
1:B:136:SER:OG	1:B:139:GLN:HG3	2.01	0.60
1:A:237:VAL:HG21	1:A:248:LEU:HD22	1.83	0.60
1:A:335:ARG:NH1	1:A:338:ARG:HH11	2.00	0.60
1:A:252:LYS:HB3	1:A:253:TYR:CD1	2.37	0.59
1:B:156:LYS:O	1:B:160:MET:HG3	2.03	0.59
1:B:229:GLN:NE2	2:B:605:HOH:O	2.35	0.58
1:B:426:ARG:HH21	1:B:432:GLU:CD	2.10	0.58
1:B:185:SER:O	1:B:189:ILE:HG13	2.03	0.58
1:B:363:ALA:O	1:B:372:ILE:HD11	2.05	0.57
1:B:104:TYR:HE2	1:B:115:ASN:HD22	1.52	0.56
1:A:13:LYS:HE2	1:A:60:PRO:HG3	1.87	0.56
1:B:557:LYS:NZ	2:B:607:HOH:O	2.38	0.56
1:B:14:GLU:O	1:B:18:ARG:HB2	2.06	0.56
1:B:47:THR:OG1	1:B:148:ASP:OD1	2.22	0.56
1:B:113:VAL:HG21	1:B:121:LEU:HG	1.88	0.56
1:B:259:ARG:HD3	1:B:264:ASN:C	2.32	0.55
1:A:126:GLN:HG3	1:A:127:LEU:HD22	1.88	0.55
1:A:9:LYS:NZ	2:A:614:HOH:O	2.36	0.55
1:B:14:GLU:HG3	1:B:18:ARG:CZ	2.36	0.55
1:B:125:TYR:C	1:B:126:GLN:HG3	2.32	0.54
1:B:387:SER:HB2	1:B:393:ARG:HA	1.90	0.53
1:A:541:LYS:HE2	1:A:565:SER:OG	2.07	0.53
1:A:300:ILE:HG23	1:A:309:LEU:HD11	1.92	0.52
1:A:260:THR:OG1	1:A:261:GLN:N	2.39	0.52
1:A:461:LYS:HE2	2:A:609:HOH:O	2.09	0.52
1:B:125:TYR:O	1:B:126:GLN:HG3	2.09	0.52
1:A:268:ASP:OD1	1:A:271:VAL:HG23	2.09	0.51
1:B:9:LYS:HG2	1:B:56:HIS:CE1	2.46	0.51
1:B:148:ASP:HB3	1:B:151:ARG:NH1	2.26	0.51
1:B:109:LEU:O	1:B:113:VAL:HG22	2.11	0.50
1:A:336:GLU:H	1:A:336:GLU:CD	2.20	0.50
1:B:164:LEU:CD2	1:B:478:ARG:HE	2.24	0.50
1:B:126:GLN:HG2	1:B:130:TRP:HZ2	1.77	0.49
1:B:217:LEU:HD23	2:B:601:HOH:O	2.13	0.49
1:A:353:ASP:OD2	2:A:601:HOH:O	2.20	0.49
1:A:371:MET:HG2	1:A:381:LEU:HD21	1.93	0.49
1:B:372:ILE:HG21	1:B:558:LYS:HB3	1.94	0.49
1:A:106:ARG:NH1	1:A:111:HIS:HB2	2.28	0.49
1:B:221:GLU:O	1:B:225:GLN:HG3	2.14	0.48
1:B:260:THR:HG22	1:B:264:ASN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:SER:O	1:A:326:LEU:HD23	2.14	0.48
1:A:303:ASN:OD1	1:B:125:TYR:OH	2.22	0.48
1:B:9:LYS:H	1:B:9:LYS:CD	2.24	0.48
1:B:278:VAL:HG12	1:B:280:PRO:HD2	1.96	0.48
1:A:326:LEU:O	1:A:327:LYS:HB2	2.14	0.47
1:B:174:LYS:O	1:B:178:ALA:HB3	2.15	0.47
1:B:168:ARG:HG2	1:B:168:ARG:HH11	1.80	0.46
1:B:241:SER:OG	1:B:243:LYS:HG3	2.15	0.46
1:B:147:VAL:HG12	1:B:148:ASP:OD1	2.14	0.46
1:B:523:LEU:CD1	1:B:528:ILE:HG12	2.45	0.46
1:B:300:ILE:HG23	1:B:309:LEU:HD11	1.98	0.46
1:A:209:ASP:OD2	1:A:212:THR:OG1	2.31	0.46
1:A:238:ASP:HB3	1:A:241:SER:HB3	1.97	0.46
1:A:278:VAL:HG12	1:A:280:PRO:HD2	1.98	0.46
1:A:354:PHE:HB3	1:A:357:ILE:HB	1.98	0.46
1:A:516:LEU:HD11	1:A:539:GLN:HG2	1.98	0.45
1:A:277:HIS:CD2	1:A:277:HIS:H	2.33	0.45
1:B:484:PHE:O	1:B:488:VAL:HG22	2.17	0.45
1:A:1:MET:HB3	1:A:2:THR:H	1.61	0.45
1:B:126:GLN:HG2	1:B:130:TRP:CZ2	2.51	0.44
1:B:247:GLN:O	1:B:251:SER:HB3	2.17	0.44
1:A:249:LEU:HB3	1:A:255:LEU:HD12	1.99	0.44
1:B:231:PHE:CE2	1:B:284:LEU:HD12	2.53	0.44
1:B:382:HIS:CD2	1:B:406:LYS:HG3	2.53	0.43
1:B:393:ARG:NH2	1:B:395:GLU:HB2	2.32	0.43
1:A:289:LYS:NZ	2:A:603:HOH:O	2.24	0.43
1:A:379:LYS:NZ	2:A:628:HOH:O	2.51	0.43
1:A:113:VAL:HG13	1:A:117:LEU:HD12	2.01	0.43
1:A:270:LYS:H	1:A:270:LYS:CD	2.23	0.43
1:A:9:LYS:HE2	1:A:56:HIS:CE1	2.54	0.43
1:A:9:LYS:HE3	1:A:57:ASP:N	2.25	0.42
1:B:325:SER:O	1:B:326:LEU:HD22	2.19	0.42
1:B:46:LYS:HD3	2:B:602:HOH:O	2.19	0.42
1:A:241:SER:OG	1:A:243:LYS:HD3	2.20	0.42
1:B:500:LEU:HD23	1:B:500:LEU:HA	1.85	0.42
1:A:248:LEU:HD12	1:A:252:LYS:HB2	2.01	0.41
1:A:241:SER:O	1:A:245:VAL:HG22	2.21	0.41
1:A:350:VAL:HG11	1:A:541:LYS:HA	2.02	0.41
1:A:545:GLU:OE2	1:A:565:SER:OG	2.27	0.41
1:A:534:LYS:NZ	1:A:569:GLU:OE2	2.49	0.41
1:A:269:ASP:OD1	1:A:288:ARG:NH1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:HD2	1:A:291:LYS:HA	1.84	0.41
1:B:104:TYR:HE2	1:B:115:ASN:ND2	2.17	0.41
1:B:145:LYS:HB2	1:B:148:ASP:H	1.86	0.41
1:B:339:ALA:HB2	1:B:572:ILE:HD11	2.03	0.40
1:B:15:ILE:HG13	1:B:16:CYS:N	2.36	0.40
1:A:21:LYS:HB2	1:A:21:LYS:HE2	1.76	0.40
1:A:338:ARG:NH2	2:A:632:HOH:O	2.54	0.40
1:A:468:VAL:HG12	1:A:482:THR:HG22	2.04	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	572/597 (96%)	562 (98%)	8 (1%)	2 (0%)	36	42
1	B	572/597 (96%)	557 (97%)	12 (2%)	3 (0%)	24	27
All	All	1144/1194 (96%)	1119 (98%)	20 (2%)	5 (0%)	30	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	VAL
1	A	264	ASN
1	B	126	GLN
1	B	261	GLN
1	B	175	THR

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	502/522 (96%)	492 (98%)	10 (2%)	48 64
1	B	503/522 (96%)	488 (97%)	15 (3%)	36 49
All	All	1005/1044 (96%)	980 (98%)	25 (2%)	42 56

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	99	SER
1	A	115	ASN
1	A	243	LYS
1	A	260	THR
1	A	261	GLN
1	A	262	LYS
1	A	274	SER
1	A	327	LYS
1	A	472	ARG
1	B	2	THR
1	B	21	LYS
1	B	40	GLN
1	B	45	GLU
1	B	105	GLU
1	B	121	LEU
1	B	126	GLN
1	B	147	VAL
1	B	148	ASP
1	B	158	ARG
1	B	173	LEU
1	B	266	SER
1	B	369	GLU
1	B	381	LEU
1	B	466	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	256	ASN
1	A	277	HIS
1	A	403	GLN
1	A	538	ASN
1	A	550	GLN
1	B	40	GLN
1	B	56	HIS
1	B	74	ASN
1	B	115	ASN
1	B	126	GLN
1	B	225	GLN
1	B	277	HIS
1	B	485	ASN
1	B	489	ASN

5.3.3 RNA [i](#)

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](#)

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 ⓘ

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	574/597 (96%)	-0.07	20 (3%)	47 44	27, 47, 78, 158	1 (0%)
1	B	574/597 (96%)	0.29	29 (5%)	33 30	23, 58, 93, 139	1 (0%)
All	All	1148/1194 (96%)	0.11	49 (4%)	40 36	23, 51, 89, 158	2 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	LEU	6.6
1	B	525	HIS	6.3
1	B	128	SER	6.1
1	B	126	GLN	4.9
1	B	1	MET	4.5
1	A	56	HIS	3.6
1	A	1	MET	3.5
1	A	246	GLY	3.5
1	A	326	LEU	3.4
1	B	147	VAL	3.4
1	B	148	ASP	3.4
1	B	145	LYS	3.2
1	B	56	HIS	3.1
1	A	525	HIS	3.1
1	B	262	LYS	3.1
1	A	260	THR	3.0
1	A	264	ASN	3.0
1	A	574	ASP	3.0
1	B	574	ASP	3.0
1	B	458	LYS	3.0
1	A	327	LYS	2.8
1	B	261	GLN	2.8
1	A	259	ARG	2.7
1	B	19	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	173	LEU	2.7
1	B	393	ARG	2.6
1	A	247	GLN	2.6
1	B	123	LYS	2.6
1	B	144	ALA	2.6
1	A	248	LEU	2.5
1	B	2	THR	2.5
1	A	243	LYS	2.5
1	B	18	ARG	2.5
1	B	392	LYS	2.4
1	B	369	GLU	2.4
1	A	252	LYS	2.4
1	A	292	LYS	2.3
1	B	314	LYS	2.3
1	A	263	GLY	2.3
1	A	265	VAL	2.3
1	B	21	LYS	2.2
1	B	326	LEU	2.1
1	B	391	GLY	2.1
1	A	335	ARG	2.1
1	B	270	LYS	2.1
1	B	110	ASN	2.1
1	A	258	PRO	2.1
1	A	261	GLN	2.0
1	B	243	LYS	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 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.