



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:36 AM UTC

PDB ID : 1V94 / pdb_00001v94
Title : Crystal structure of isocitrate dehydrogenase from *Aeropyrum pernix*
Authors : Jeong, J.-J.; Sonoda, T.; Fushinobu, S.; Shoun, H.; Wakagi, T.
Deposited on : 2004-01-20
Resolution : 2.28 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

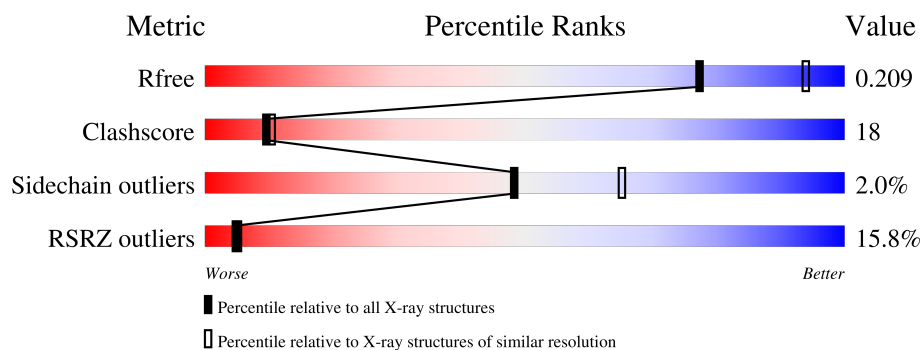
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	435	6% 74% 22% ..
1	B	435	26% 60% 36% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6860 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 isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3330	2111	590	616	13			
1	B	423	Total	C	N	O	S	0	0	0
			3287	2085	580	609	13			

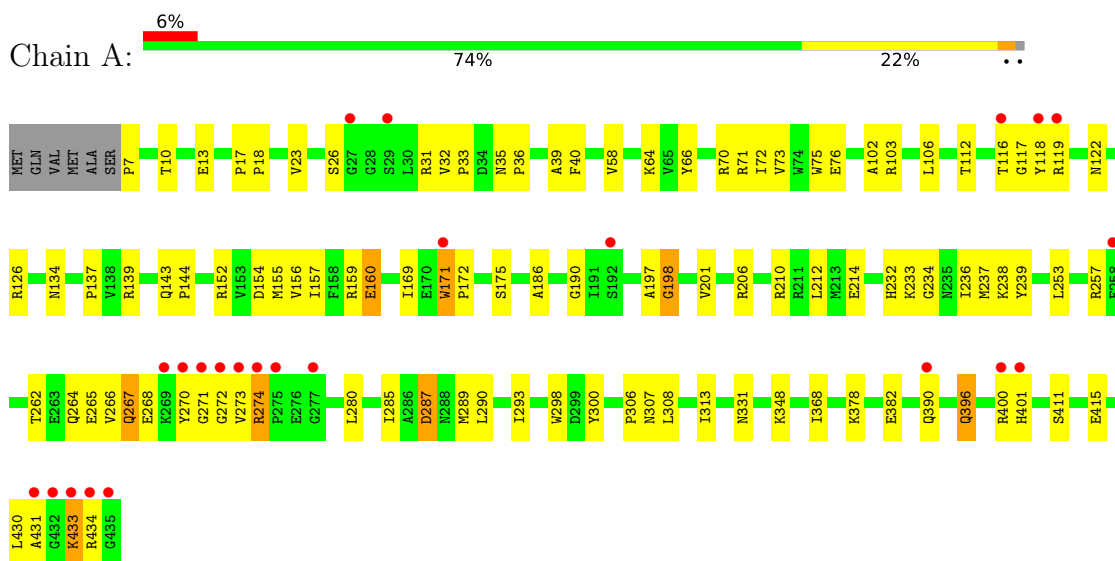
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	163	Total	O	0	0
			163	163		
2	B	80	Total	O	0	0
			80	80		

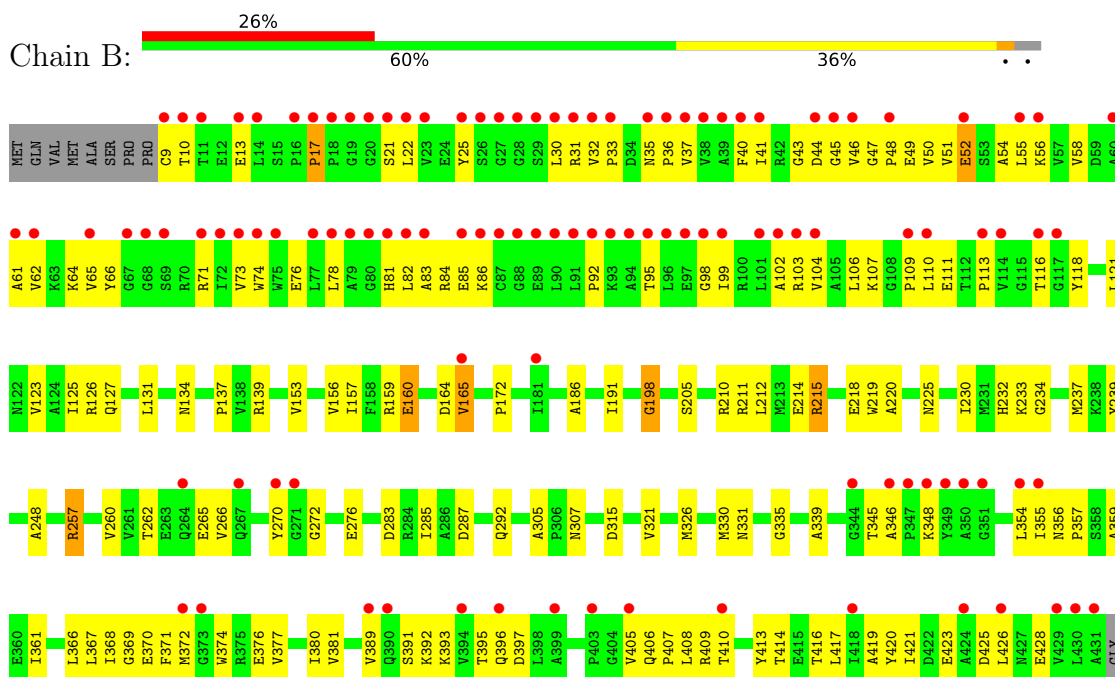
3 Residue-property plots

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: isocitrate dehydrogenase



- Molecule 1: isocitrate dehydrogenase



LYS
ARG
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.86Å 107.86Å 172.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.98 – 2.28 45.98 – 2.28	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.98-2.28) 99.7 (45.98-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.256 0.217 , 0.209	Depositor DCC
R_{free} test set	2384 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6860	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.43	0/3400	0.94	10/4610 (0.2%)
1	B	0.38	0/3355	0.90	10/4552 (0.2%)
All	All	0.40	0/6755	0.92	20/9162 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	GLY	N-CA-C	-8.08	101.06	112.37
1	A	32	VAL	N-CA-C	7.90	116.06	107.60
1	B	305	ALA	N-CA-C	7.49	114.96	108.22
1	B	198	GLY	N-CA-C	-6.53	103.81	112.82
1	B	98	GLY	N-CA-C	-5.78	107.49	114.66
1	A	7	PRO	CA-C-N	5.70	126.14	119.99
1	A	7	PRO	C-N-CA	5.70	126.14	119.99
1	B	260	VAL	N-CA-C	5.68	117.09	108.80
1	A	308	LEU	N-CA-C	5.63	117.10	111.07
1	A	23	VAL	N-CA-C	-5.52	102.46	109.80
1	B	307	ASN	N-CA-C	5.48	117.71	111.02
1	A	396	GLN	N-CA-C	5.44	118.71	111.75
1	B	292	GLN	N-CA-C	5.41	117.94	111.71
1	A	238	LYS	N-CA-C	5.30	117.06	111.28
1	B	17	PRO	CA-C-N	5.28	125.58	119.93
1	B	17	PRO	C-N-CA	5.28	125.58	119.93
1	A	160	GLU	N-CA-C	-5.27	101.84	109.59
1	B	160	GLU	N-CA-C	-5.11	102.34	109.96
1	B	84	ARG	N-CA-C	-5.09	106.58	112.89
1	A	64	LYS	N-CA-C	5.04	116.78	111.28

There are no chirality outliers.

There are no planarity outliers.

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	3330	0	3351	88	0
1	B	3287	0	3304	158	0
2	A	163	0	0	5	0
2	B	80	0	0	0	0
All	All	6860	0	6655	236	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 18.

All (236) 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:172:PRO:HG2	1:A:175:SER:HB3	1.44	0.99
1:A:274:ARG:HD2	1:A:274:ARG:O	1.64	0.96
1:B:330:MET:HE1	1:B:367:LEU:HA	1.56	0.87
1:B:354:LEU:HB3	1:B:396:GLN:HE21	1.39	0.86
1:B:71:ARG:HH12	1:B:73:VAL:HG22	1.40	0.85
1:B:330:MET:HE3	1:B:366:LEU:HG	1.60	0.82
1:B:368:ILE:HA	1:B:372:MET:HE3	1.68	0.74
1:B:232:HIS:HD2	1:B:234:GLY:H	1.36	0.73
1:A:390:GLN:HG2	2:A:583:HOH:O	1.90	0.72
1:B:81:HIS:CD2	1:B:82:LEU:HG	2.26	0.71
1:B:41:ILE:HG22	1:B:43:GLY:H	1.56	0.70
1:B:58:VAL:O	1:B:62:VAL:HG23	1.91	0.70
1:A:267:GLN:HA	1:A:272:GLY:HA2	1.75	0.69
1:A:433:LYS:O	1:A:434:ARG:HG3	1.93	0.69
1:B:45:GLY:O	1:B:48:PRO:HD2	1.93	0.69
1:B:54:ALA:O	1:B:58:VAL:HG23	1.93	0.68
1:B:61:ALA:HA	1:B:421:ILE:HG21	1.74	0.68
1:A:232:HIS:HD2	1:A:234:GLY:H	1.41	0.67
1:B:330:MET:HE2	1:B:339:ALA:HB2	1.76	0.67
1:B:51:VAL:O	1:B:55:LEU:HG	1.95	0.66
1:B:116:THR:HG23	1:B:118:TYR:H	1.59	0.66
1:B:257:ARG:HA	1:B:257:ARG:HH11	1.61	0.66
1:A:237:MET:SD	1:B:165:VAL:HG21	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PRO:HG2	1:A:73:VAL:HG12	1.77	0.65
1:B:71:ARG:NH1	1:B:73:VAL:HG22	2.10	0.64
1:A:232:HIS:CD2	1:A:234:GLY:H	2.15	0.63
1:B:354:LEU:HB3	1:B:396:GLN:NE2	2.12	0.63
1:B:25:TYR:H	1:B:103:ARG:NH1	1.97	0.63
1:B:107:LYS:HZ1	1:B:110:LEU:HG	1.64	0.62
1:B:232:HIS:CD2	1:B:234:GLY:H	2.16	0.62
1:A:274:ARG:O	1:A:274:ARG:CD	2.46	0.62
1:B:419:ALA:O	1:B:423:GLU:HG2	1.99	0.62
1:B:367:LEU:HG	1:B:372:MET:HE2	1.81	0.61
1:B:393:LYS:HG3	1:B:408:LEU:HD11	1.82	0.61
1:A:152:ARG:HG2	1:A:298:TRP:HE3	1.66	0.61
1:B:113:PRO:O	1:B:116:THR:HG22	2.00	0.61
1:B:210:ARG:O	1:B:214:GLU:HG3	2.00	0.61
1:B:47:GLY:O	1:B:50:VAL:HG22	2.01	0.60
1:B:354:LEU:HD13	1:B:396:GLN:HE22	1.66	0.60
1:B:377:VAL:O	1:B:381:VAL:HG23	2.02	0.59
1:B:366:LEU:O	1:B:370:GLU:HB2	2.03	0.59
1:A:119:ARG:HG2	1:A:119:ARG:HH21	1.68	0.59
1:B:78:LEU:HD22	1:B:82:LEU:O	2.03	0.59
1:A:26:SER:OG	1:A:31:ARG:HD2	2.03	0.58
1:B:25:TYR:CD2	1:B:335:GLY:HA3	2.38	0.58
1:A:66:TYR:CD2	1:A:70:ARG:HD2	2.39	0.58
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.67	0.58
1:B:215:ARG:CA	1:B:215:ARG:HH11	2.16	0.58
1:B:113:PRO:CG	1:B:121:LEU:HG	2.33	0.57
1:A:116:THR:HG22	1:A:117:GLY:H	1.69	0.57
1:B:21:SER:O	1:B:33:PRO:HG3	2.04	0.57
1:B:215:ARG:HH11	1:B:215:ARG:HA	1.69	0.57
1:B:392:LYS:HD3	1:B:405:VAL:HG22	1.85	0.57
1:A:253:LEU:O	1:A:257:ARG:HB2	2.05	0.56
1:A:17:PRO:HG2	1:A:73:VAL:CG1	2.35	0.56
1:B:369:GLY:HA2	1:B:374:TRP:O	2.05	0.56
1:A:159:ARG:HD2	1:A:307:ASN:O	2.05	0.56
1:B:41:ILE:HG22	1:B:43:GLY:N	2.20	0.56
1:B:81:HIS:HD2	1:B:82:LEU:H	1.53	0.56
1:A:237:MET:HE2	1:B:165:VAL:HG11	1.87	0.56
1:B:215:ARG:HH11	1:B:215:ARG:N	2.03	0.55
1:B:10:THR:OG1	1:B:13:GLU:HG3	2.07	0.55
1:A:390:GLN:NE2	1:A:390:GLN:HA	2.20	0.55
1:B:326:MET:HA	1:B:359:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ALA:HA	1:B:205:SER:HA	1.89	0.55
1:B:30:LEU:O	1:B:31:ARG:HG3	2.06	0.55
1:A:40:PHE:CZ	1:A:76:GLU:HB2	2.42	0.55
1:B:380:ILE:HD13	1:B:421:ILE:HG23	1.89	0.55
1:B:123:VAL:O	1:B:127:GLN:HG3	2.07	0.54
1:B:81:HIS:CD2	1:B:82:LEU:N	2.75	0.54
1:A:206:ARG:HG2	1:A:210:ARG:HD2	1.87	0.54
1:B:46:VAL:HB	1:B:355:ILE:HG21	1.90	0.54
1:B:164:ASP:CG	1:B:165:VAL:H	2.15	0.54
1:B:257:ARG:HH11	1:B:257:ARG:CA	2.21	0.54
1:B:78:LEU:HB3	1:B:83:ALA:HB2	1.90	0.54
1:B:376:GLU:CD	1:B:376:GLU:H	2.16	0.54
1:B:61:ALA:O	1:B:65:VAL:HG22	2.08	0.54
1:B:160:GLU:HB2	1:B:212:LEU:HD22	1.89	0.54
1:A:262:THR:O	1:A:266:VAL:HG23	2.07	0.54
1:A:411:SER:O	1:A:415:GLU:HG2	2.08	0.54
1:A:400:ARG:HG2	2:A:574:HOH:O	2.07	0.53
1:A:271:GLY:O	1:A:273:VAL:HG23	2.08	0.53
1:B:164:ASP:OD1	1:B:165:VAL:N	2.38	0.53
1:A:58:VAL:HG11	1:A:368:ILE:CD1	2.39	0.53
1:A:232:HIS:O	1:A:285:ILE:HA	2.09	0.53
1:B:232:HIS:HE1	1:B:283:ASP:OD2	1.91	0.53
1:A:267:GLN:HG3	1:A:268:GLU:H	1.74	0.53
1:B:113:PRO:HB2	1:B:116:THR:CG2	2.39	0.53
1:B:35:ASN:N	1:B:36:PRO:CD	2.72	0.53
1:A:10:THR:OG1	1:A:13:GLU:HG3	2.09	0.52
1:B:416:THR:HG22	1:B:420:TYR:CE2	2.44	0.52
1:B:157:ILE:N	1:B:157:ILE:HD12	2.25	0.52
1:B:262:THR:OG1	1:B:265:GLU:HG3	2.11	0.51
1:A:264:GLN:O	1:A:267:GLN:HG3	2.09	0.51
1:B:49:GLU:O	1:B:52:GLU:HB3	2.11	0.51
1:B:113:PRO:HB2	1:B:116:THR:HG21	1.91	0.51
1:B:233:LYS:HB3	1:B:237:MET:HE3	1.93	0.51
1:B:47:GLY:O	1:B:51:VAL:HG23	2.10	0.50
1:B:95:THR:O	1:B:99:ILE:HG13	2.12	0.50
1:B:348:LYS:HB2	1:B:348:LYS:NZ	2.25	0.50
1:B:40:PHE:CZ	1:B:76:GLU:HB2	2.46	0.50
1:A:152:ARG:CG	1:A:298:TRP:HB3	2.42	0.50
1:A:287:ASP:HB2	1:B:315:ASP:OD2	2.12	0.50
1:A:266:VAL:O	1:A:270:TYR:HB2	2.12	0.50
1:B:40:PHE:HA	1:B:106:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TYR:HB3	1:B:103:ARG:NH1	2.27	0.50
1:A:40:PHE:HA	1:A:106:LEU:O	2.12	0.49
1:A:116:THR:HG22	1:A:117:GLY:N	2.26	0.49
1:A:17:PRO:HD3	1:A:75:TRP:CD1	2.48	0.49
1:B:392:LYS:HD3	1:B:405:VAL:CG2	2.42	0.49
1:B:45:GLY:C	1:B:47:GLY:H	2.18	0.49
1:A:239:TYR:O	1:B:198:GLY:HA3	2.13	0.49
1:B:25:TYR:CG	1:B:335:GLY:HA3	2.48	0.48
1:A:266:VAL:HG21	1:A:280:LEU:HD13	1.95	0.48
1:B:113:PRO:HG2	1:B:121:LEU:HG	1.93	0.48
1:A:144:PRO:HG3	1:A:401:HIS:HB2	1.96	0.48
1:A:119:ARG:HG2	1:A:119:ARG:NH2	2.28	0.48
1:A:137:PRO:HA	1:A:156:VAL:HA	1.96	0.48
1:B:64:LYS:HE3	1:B:426:LEU:HG	1.96	0.48
1:A:210:ARG:O	1:A:214:GLU:HG3	2.14	0.47
1:B:30:LEU:C	1:B:31:ARG:HG3	2.39	0.47
1:B:104:VAL:HG12	1:B:371:PHE:HE2	1.79	0.47
1:A:139:ARG:HD2	1:A:154:ASP:OD2	2.15	0.47
1:B:270:TYR:C	1:B:272:GLY:H	2.21	0.47
1:A:17:PRO:CG	1:A:73:VAL:HG12	2.44	0.47
1:A:117:GLY:O	1:A:118:TYR:C	2.56	0.47
1:A:233:LYS:HE3	1:A:236:ILE:HG13	1.96	0.47
1:B:102:ALA:O	1:B:103:ARG:HB2	2.14	0.47
1:B:417:LEU:O	1:B:421:ILE:HG13	2.13	0.47
1:B:56:LYS:NZ	1:B:414:THR:HG21	2.29	0.47
1:B:81:HIS:NE2	1:B:82:LEU:HG	2.29	0.47
1:B:215:ARG:N	1:B:215:ARG:NH1	2.62	0.47
1:A:171:TRP:CD1	1:A:171:TRP:N	2.83	0.47
1:B:81:HIS:HD2	1:B:82:LEU:N	2.10	0.47
1:B:211:ARG:O	1:B:215:ARG:HG2	2.15	0.47
1:B:425:ASP:HB2	1:B:428:GLU:HG2	1.95	0.47
1:A:306:PRO:HG2	2:A:442:HOH:O	2.14	0.47
1:B:104:VAL:HG12	1:B:371:PHE:CE2	2.50	0.47
1:B:9:CYS:SG	1:B:86:LYS:HG2	2.55	0.46
1:B:380:ILE:CD1	1:B:421:ILE:HG23	2.45	0.46
1:B:413:TYR:CE1	1:B:417:LEU:HD11	2.51	0.46
1:B:137:PRO:HA	1:B:156:VAL:HA	1.98	0.46
1:B:233:LYS:HE3	1:B:287:ASP:OD2	2.15	0.46
1:A:267:GLN:HG3	1:A:268:GLU:N	2.31	0.46
1:B:156:VAL:HG11	1:B:219:TRP:CZ3	2.50	0.46
1:B:109:PRO:O	1:B:345:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:O	1:B:346:ALA:C	2.59	0.46
1:B:58:VAL:HG11	1:B:368:ILE:CD1	2.45	0.46
1:B:71:ARG:HH12	1:B:73:VAL:CG2	2.19	0.46
1:A:237:MET:SD	1:B:165:VAL:CG2	3.03	0.46
1:B:21:SER:O	1:B:22:LEU:C	2.59	0.46
1:B:32:VAL:HG23	1:B:36:PRO:HB3	1.98	0.45
1:A:152:ARG:HG2	1:A:298:TRP:CE3	2.47	0.45
1:B:406:GLN:HE21	1:B:407:PRO:HD2	1.81	0.45
1:A:122:ASN:O	1:A:126:ARG:HG3	2.16	0.45
1:A:134:ASN:HD22	1:A:331:ASN:ND2	2.14	0.45
1:A:290:LEU:HD23	1:A:313:ILE:HD12	1.99	0.45
1:B:56:LYS:NZ	1:B:56:LYS:HB2	2.32	0.45
1:B:44:ASP:OD1	1:B:111:GLU:HB2	2.16	0.45
1:B:214:GLU:C	1:B:215:ARG:NH1	2.75	0.45
1:B:92:PRO:HG2	1:B:95:THR:OG1	2.16	0.45
1:B:55:LEU:HD22	1:B:74:TRP:CE3	2.52	0.45
1:B:357:PRO:O	1:B:361:ILE:HG13	2.16	0.45
1:A:17:PRO:HA	1:A:18:PRO:HD3	1.87	0.44
1:B:33:PRO:HD2	1:B:36:PRO:HB3	1.99	0.44
1:B:389:VAL:C	1:B:391:SER:H	2.26	0.44
1:B:354:LEU:HD13	1:B:396:GLN:NE2	2.32	0.44
1:A:262:THR:OG1	1:A:265:GLU:HG3	2.17	0.44
1:B:131:LEU:HB3	1:B:331:ASN:HB3	1.98	0.44
1:B:220:ALA:HA	1:B:225:ASN:HD22	1.83	0.44
1:B:61:ALA:HB2	1:B:421:ILE:HD13	2.00	0.44
1:A:58:VAL:HG11	1:A:368:ILE:HD13	2.00	0.44
1:A:233:LYS:HB3	1:A:237:MET:HE3	2.00	0.44
1:A:33:PRO:O	1:A:36:PRO:HD3	2.18	0.44
1:A:143:GLN:HB2	1:A:144:PRO:HD2	1.99	0.44
1:A:232:HIS:HD2	1:A:234:GLY:N	2.11	0.43
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.32	0.43
1:B:45:GLY:C	1:B:47:GLY:N	2.76	0.43
1:B:113:PRO:HG3	1:B:121:LEU:HG	1.98	0.43
1:A:144:PRO:HG3	2:A:574:HOH:O	2.18	0.43
1:B:232:HIS:HD2	1:B:234:GLY:N	2.12	0.43
1:A:233:LYS:HE3	1:A:236:ILE:CG1	2.49	0.43
1:A:239:TYR:CE1	1:B:172:PRO:HG3	2.53	0.43
1:B:126:ARG:HG3	1:B:126:ARG:HH11	1.83	0.43
1:B:64:LYS:HG2	1:B:421:ILE:O	2.18	0.43
1:A:152:ARG:HG2	1:A:298:TRP:HB3	1.99	0.43
1:A:237:MET:CE	1:B:165:VAL:HG11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:HIS:O	1:B:85:GLU:HG3	2.17	0.43
1:B:409:ARG:HB2	1:B:409:ARG:NH1	2.34	0.43
1:B:214:GLU:O	1:B:218:GLU:HG3	2.18	0.43
1:B:214:GLU:CB	1:B:215:ARG:HH12	2.32	0.43
1:B:230:ILE:HD13	1:B:248:ALA:HB3	2.01	0.43
1:A:198:GLY:HA3	1:B:239:TYR:O	2.19	0.42
1:B:257:ARG:O	1:B:257:ARG:NH1	2.51	0.42
1:A:157:ILE:N	1:A:157:ILE:HD12	2.34	0.42
1:B:121:LEU:O	1:B:125:ILE:HG13	2.19	0.42
1:A:169:ILE:CG2	1:A:201:VAL:HB	2.48	0.42
1:B:233:LYS:HA	1:B:233:LYS:HD2	1.86	0.42
1:B:408:LEU:O	1:B:409:ARG:C	2.63	0.42
1:B:423:GLU:O	1:B:423:GLU:HG3	2.20	0.42
1:A:39:ALA:HA	1:A:75:TRP:O	2.20	0.42
1:A:237:MET:SD	1:B:165:VAL:HG11	2.59	0.42
1:B:17:PRO:HG2	1:B:73:VAL:CG1	2.50	0.42
1:B:22:LEU:HD23	1:B:37:VAL:HB	2.01	0.42
1:B:25:TYR:H	1:B:103:ARG:HH12	1.65	0.42
1:A:118:TYR:CG	1:A:119:ARG:N	2.88	0.42
1:A:119:ARG:NE	2:A:498:HOH:O	2.47	0.42
1:A:430:LEU:O	1:A:431:ALA:C	2.63	0.42
1:A:72:ILE:HD11	1:A:368:ILE:HD13	2.01	0.42
1:B:35:ASN:HA	1:B:71:ARG:O	2.20	0.41
1:B:65:VAL:HG23	1:B:66:TYR:CD2	2.55	0.41
1:A:155:MET:HE2	1:A:300:TYR:HB2	2.01	0.41
1:B:270:TYR:O	1:B:272:GLY:N	2.48	0.41
1:A:186:ALA:O	1:A:190:GLY:HA2	2.20	0.41
1:B:409:ARG:O	1:B:410:THR:C	2.63	0.41
1:A:273:VAL:HG12	1:A:274:ARG:N	2.34	0.41
1:A:285:ILE:HG22	1:A:287:ASP:OD1	2.20	0.41
1:B:186:ALA:HA	1:B:191:ILE:O	2.20	0.41
1:A:289:MET:HE2	1:A:293:ILE:HG23	2.02	0.41
1:A:378:LYS:O	1:A:382:GLU:HG3	2.21	0.41
1:A:160:GLU:HB2	1:A:212:LEU:HD22	2.02	0.41
1:B:64:LYS:HE3	1:B:426:LEU:CG	2.51	0.41
1:B:134:ASN:HD22	1:B:159:ARG:HD3	1.85	0.41
1:B:356:ASN:HB2	1:B:397:ASP:CG	2.45	0.41
1:B:266:VAL:HA	1:B:270:TYR:HD2	1.85	0.41
1:B:368:ILE:CA	1:B:372:MET:HE3	2.45	0.41
1:A:35:ASN:HA	1:A:71:ARG:O	2.20	0.41
1:B:153:VAL:HB	1:B:321:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:HG3	1:A:298:TRP:HB3	2.03	0.41
1:B:44:ASP:OD2	1:B:44:ASP:C	2.64	0.41
1:B:232:HIS:O	1:B:285:ILE:HA	2.21	0.41
1:B:21:SER:O	1:B:22:LEU:O	2.38	0.40
1:B:17:PRO:HG2	1:B:73:VAL:HG12	2.02	0.40
1:B:56:LYS:HZ1	1:B:414:THR:HG21	1.87	0.40
1:A:102:ALA:O	1:A:103:ARG:HB2	2.21	0.40
1:A:433:LYS:O	1:A:433:LYS:HG2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	345/350 (99%)	337 (98%)	8 (2%)	44	60
1	B	341/350 (97%)	335 (98%)	6 (2%)	51	68
All	All	686/700 (98%)	672 (98%)	14 (2%)	48	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	A	171	TRP
1	A	267	GLN
1	A	274	ARG
1	A	287	ASP

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Mol	Chain	Res	Type
1	A	348	LYS
1	A	396	GLN
1	A	433	LYS
1	B	52	GLU
1	B	165	VAL
1	B	215	ARG
1	B	257	ARG
1	B	276	GLU
1	B	395	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	147	HIS
1	A	232	HIS
1	A	331	ASN
1	A	390	GLN
1	A	406	GLN
1	B	81	HIS
1	B	122	ASN
1	B	134	ASN
1	B	161	ASN
1	B	225	ASN
1	B	232	HIS
1	B	259	HIS
1	B	301	GLN
1	B	331	ASN
1	B	390	GLN
1	B	396	GLN
1	B	401	HIS
1	B	406	GLN

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 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 [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	429/435 (98%)	0.04	24 (5%) 30 31	17, 29, 59, 86	0
1	B	423/435 (97%)	1.12	111 (26%) 1 1	21, 47, 89, 100	0
All	All	852/870 (97%)	0.58	135 (15%) 5 5	17, 35, 84, 100	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	ALA	6.4
1	B	28	GLY	5.5
1	B	430	LEU	5.4
1	B	14	LEU	5.3
1	B	431	ALA	5.1
1	B	23	VAL	5.1
1	B	10	THR	4.9
1	A	435	GLY	4.7
1	B	113	PRO	4.6
1	A	434	ARG	4.5
1	A	118	TYR	4.2
1	B	95	THR	4.1
1	B	396	GLN	4.1
1	B	92	PRO	4.1
1	B	22	LEU	4.1
1	B	89	GLU	4.1
1	B	429	VAL	3.9
1	B	82	LEU	3.9
1	B	96	LEU	3.9
1	A	431	ALA	3.9
1	B	72	ILE	3.9
1	B	35	ASN	3.8
1	B	75	TRP	3.8
1	B	77	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	9	CYS	3.7
1	B	350	ALA	3.7
1	B	101	LEU	3.7
1	A	119	ARG	3.7
1	B	90	LEU	3.6
1	B	91	LEU	3.6
1	B	399	ALA	3.6
1	B	116	THR	3.6
1	B	74	TRP	3.6
1	B	65	VAL	3.5
1	B	71	ARG	3.5
1	B	11	THR	3.5
1	B	39	ALA	3.5
1	B	32	VAL	3.4
1	B	73	VAL	3.4
1	A	271	GLY	3.4
1	B	55	LEU	3.4
1	B	403	PRO	3.4
1	B	37	VAL	3.3
1	B	114	VAL	3.3
1	A	400	ARG	3.3
1	B	29	SER	3.3
1	B	346	ALA	3.2
1	B	347	PRO	3.2
1	B	87	CYS	3.1
1	B	13	GLU	3.1
1	B	354	LEU	3.1
1	B	271	GLY	3.1
1	B	110	LEU	3.1
1	B	41	ILE	3.1
1	B	31	ARG	3.0
1	B	86	LYS	3.0
1	B	68	GLY	3.0
1	B	30	LEU	3.0
1	B	38	VAL	3.0
1	B	19	GLY	3.0
1	B	16	PRO	3.0
1	B	79	ALA	2.9
1	B	351	GLY	2.9
1	B	78	LEU	2.9
1	B	424	ALA	2.9
1	B	18	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	274	ARG	2.9
1	B	52	GLU	2.9
1	B	25	TYR	2.8
1	B	426	LEU	2.8
1	A	433	LYS	2.8
1	B	267	GLN	2.8
1	B	99	ILE	2.8
1	B	88	GLY	2.8
1	B	83	ALA	2.8
1	B	165	VAL	2.8
1	B	98	GLY	2.7
1	B	264	GLN	2.7
1	B	390	GLN	2.7
1	A	270	TYR	2.7
1	B	394	VAL	2.7
1	B	40	PHE	2.6
1	A	432	GLY	2.6
1	B	93	LYS	2.6
1	B	17	PRO	2.6
1	B	85	GLU	2.6
1	B	373	GLY	2.6
1	B	60	ALA	2.6
1	B	20	GLY	2.5
1	B	67	GLY	2.5
1	B	69	SER	2.5
1	A	273	VAL	2.5
1	A	390	GLN	2.5
1	B	349	TYR	2.5
1	B	81	HIS	2.5
1	B	26	SER	2.5
1	B	405	VAL	2.5
1	A	401	HIS	2.5
1	B	36	PRO	2.5
1	B	355	ILE	2.4
1	B	102	ALA	2.4
1	B	344	GLY	2.4
1	B	372	MET	2.4
1	B	48	PRO	2.4
1	B	21	SER	2.4
1	B	389	VAL	2.4
1	B	45	GLY	2.3
1	B	80	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	104	VAL	2.3
1	B	46	VAL	2.3
1	B	33	PRO	2.3
1	B	109	PRO	2.3
1	A	269	LYS	2.3
1	B	44	ASP	2.3
1	A	116	THR	2.3
1	B	97	GLU	2.3
1	B	56	LYS	2.3
1	A	272	GLY	2.2
1	B	270	TYR	2.2
1	B	181	ILE	2.2
1	A	192	SER	2.2
1	B	103	ARG	2.2
1	B	27	GLY	2.2
1	A	171	TRP	2.1
1	A	275	PRO	2.1
1	A	277	GLY	2.1
1	B	418	ILE	2.1
1	A	258	GLU	2.1
1	B	62	VAL	2.1
1	A	27	GLY	2.1
1	B	410	THR	2.1
1	B	61	ALA	2.1
1	B	348	LYS	2.1
1	B	117	GLY	2.1
1	A	29	SER	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.