



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 10:07 pm BST

PDB ID : 2IV0
Title : Thermal stability of isocitrate dehydrogenase from *Archaeoglobus fulgidus* studied by crystal structure analysis and engineering of chimeras
Authors : Stokke, R.; Karlstrom, M.; Yang, N.; Leiros, I.; Ladenstein, R.; Birkeland, N.K.; Steen, I.H.
Deposited on : 2006-06-08
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

<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

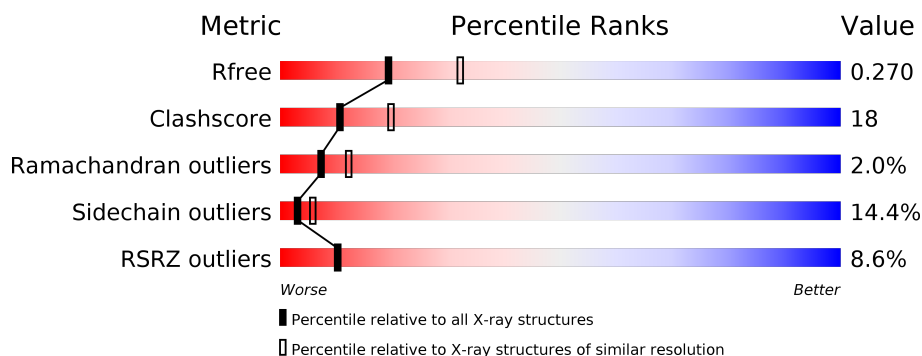
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	412	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>26%</div> <div>7%</div> </div> </div>
1	B	412	<div> <div>13%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6557 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	412	Total	C	N	O	S	0	0	0
			3228	2070	542	607	9			
1	B	412	Total	C	N	O	S	0	0	0
			3223	2065	542	607	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	4	Total	Zn	0	0
			4	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	2	Total	Cl	0	0
			2	2		

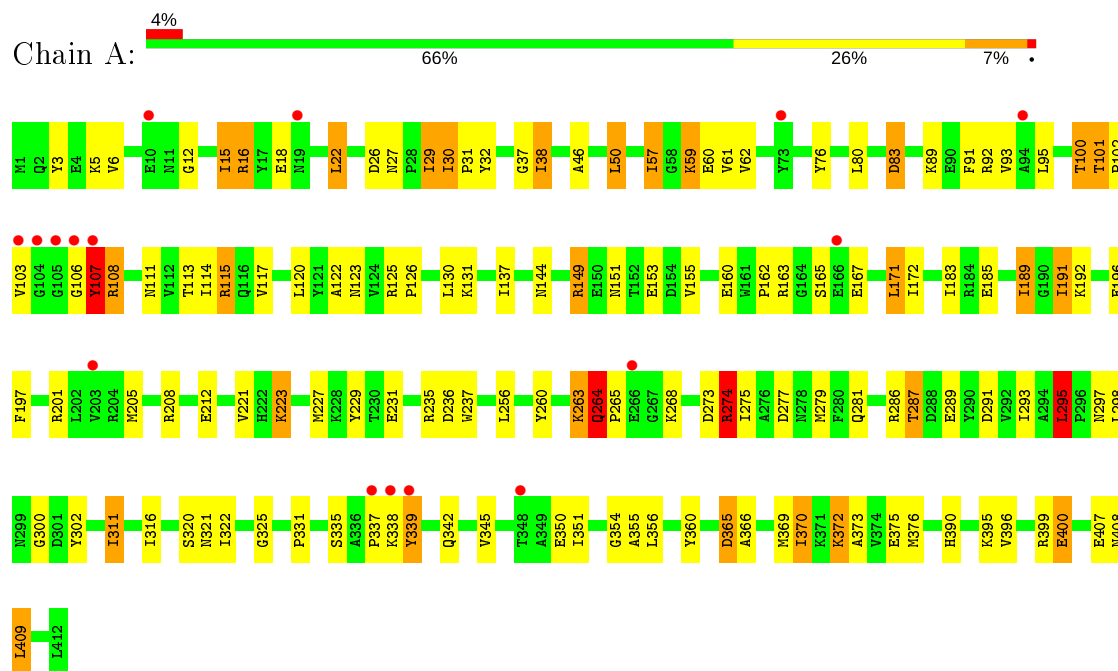
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	28	Total	O	0	0
			28	28		

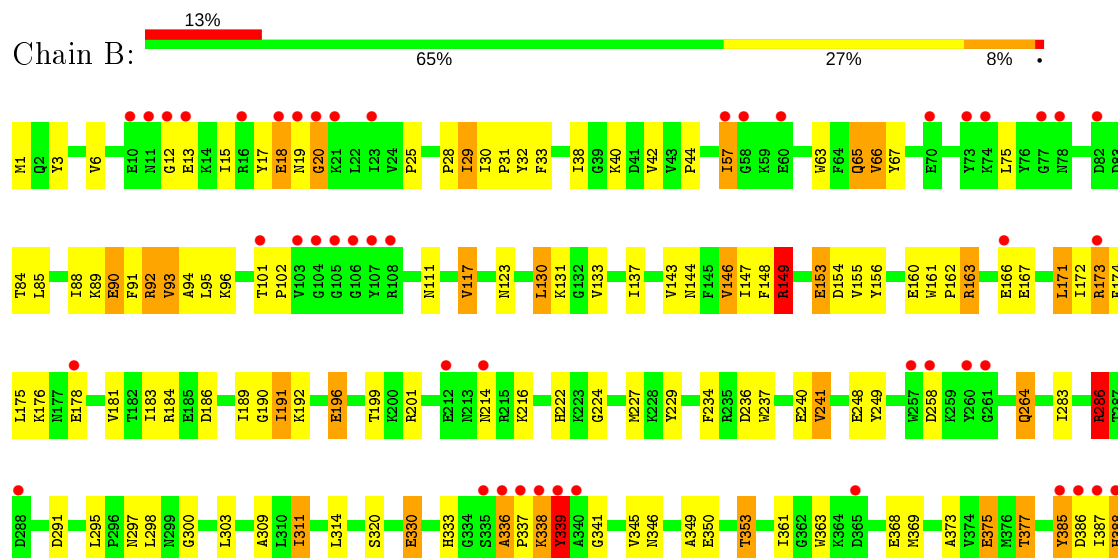
3 Residue-property plots

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: ISOCITRATE DEHYDROGENASE



• Molecule 1: ISOCITRATE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 65.41Å 87.18Å 90.00° 95.28° 90.00°	Depositor
Resolution (Å)	86.71 – 2.50 19.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (86.71-2.50) 100.0 (19.96-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.254 0.223 , 0.270	Depositor DCC
R_{free} test set	1607 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL

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	0.82	0/3299	0.94	7/4468 (0.2%)
1	B	0.69	0/3294	0.80	4/4460 (0.1%)
All	All	0.76	0/6593	0.88	11/8928 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	295	LEU	CA-CB-CG	8.33	134.47	115.30
1	A	274	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	A	409	LEU	CA-CB-CG	6.64	130.56	115.30
1	A	125	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	314	LEU	CA-CB-CG	6.01	129.11	115.30
1	B	201	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	286	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	107	TYR	N-CA-C	5.57	126.05	111.00
1	B	149	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	201	ARG	NE-CZ-NH2	-5.09	117.76	120.30

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	3228	0	3219	119	0
1	B	3223	0	3208	126	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	1	0
4	A	66	0	0	7	0
4	B	28	0	0	3	0
All	All	6557	0	6427	237	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 (237) 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:192:LYS:HE2	1:B:227:MET:CE	1.63	1.28
1:A:263:LYS:HG3	1:A:264:GLN:N	1.67	1.08
1:A:263:LYS:CG	1:A:264:GLN:H	1.66	1.06
1:B:130:LEU:O	1:B:133:VAL:HG12	1.58	1.04
1:B:192:LYS:HE2	1:B:227:MET:HE1	1.41	1.00
1:A:263:LYS:HG3	1:A:264:GLN:H	0.83	0.98
1:A:192:LYS:HE2	1:A:227:MET:CE	1.98	0.94
1:A:274:ARG:HB3	1:A:279:MET:HE1	1.51	0.92
1:B:156:TYR:HE1	1:B:298:LEU:HD13	1.36	0.91
3:B:1418:CL:CL	4:B:2023:HOH:O	2.26	0.90
1:B:149:ARG:CG	1:B:300:GLY:HA3	2.03	0.89
1:A:221:VAL:HB	1:A:295:LEU:HD13	1.55	0.89
1:B:156:TYR:CE1	1:B:298:LEU:HD13	2.10	0.86
1:A:274:ARG:CB	1:A:279:MET:HE1	2.06	0.85
1:A:373:ALA:HA	1:A:376:MET:HE3	1.55	0.85
1:B:173:ARG:HG2	1:B:173:ARG:HH11	1.42	0.85
1:A:192:LYS:HE2	1:A:227:MET:HE3	1.57	0.84
1:B:192:LYS:CE	1:B:227:MET:HE1	2.08	0.83
1:B:192:LYS:CE	1:B:227:MET:CE	2.53	0.83
1:B:216:LYS:HG3	1:B:264:GLN:NE2	1.95	0.81
1:B:12:GLY:HA3	1:B:29:ILE:HG22	1.65	0.79
1:B:42:VAL:HG23	1:B:350:GLU:HG3	1.65	0.79
1:B:149:ARG:HG3	1:B:300:GLY:HA3	1.62	0.79
1:A:274:ARG:HB3	1:A:279:MET:CE	2.13	0.79
1:B:222:HIS:HD2	1:B:224:GLY:H	1.30	0.79
1:B:236:ASP:O	1:B:240:GLU:HG3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HG	1:A:300:GLY:HA2	1.64	0.77
1:B:38:ILE:HG13	1:B:339:TYR:HD2	1.50	0.76
1:A:50:LEU:HD21	1:A:354:GLY:HA3	1.66	0.75
1:A:274:ARG:CB	1:A:279:MET:CE	2.65	0.75
1:B:130:LEU:O	1:B:133:VAL:CG1	2.35	0.74
1:A:373:ALA:HA	1:A:376:MET:CE	2.18	0.74
1:B:222:HIS:CD2	1:B:224:GLY:H	2.05	0.73
1:B:395:LYS:O	1:B:396:VAL:HB	1.88	0.73
1:A:149:ARG:NH1	1:A:297:ASN:OD1	2.22	0.71
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.54	0.71
1:B:339:TYR:HD1	1:B:341:GLY:O	1.74	0.71
1:B:339:TYR:CD1	1:B:341:GLY:O	2.44	0.71
1:B:192:LYS:HE2	1:B:227:MET:HE2	1.65	0.70
1:B:66:VAL:HG11	1:B:84:THR:HA	1.73	0.70
1:A:101:THR:HG21	1:A:107:TYR:O	1.92	0.70
1:A:29:ILE:HG12	1:A:91:PHE:CE1	2.27	0.69
1:B:349:ALA:O	1:B:353:THR:CG2	2.40	0.69
1:B:149:ARG:HG2	1:B:300:GLY:HA3	1.75	0.69
1:A:287:THR:HG21	4:A:2024:HOH:O	1.92	0.69
1:B:192:LYS:HE2	1:B:227:MET:HE3	1.72	0.68
1:A:15:ILE:CD1	1:A:22:LEU:HG	2.25	0.67
1:A:100:THR:HG23	1:A:335:SER:OG	1.94	0.66
1:B:15:ILE:HD11	1:B:92:ARG:HB2	1.77	0.66
1:B:173:ARG:CG	1:B:173:ARG:HH11	2.08	0.66
1:A:57:ILE:HG12	1:A:365:ASP:OD2	1.97	0.65
1:B:349:ALA:O	1:B:353:THR:HG22	1.95	0.65
1:B:286:ARG:HH11	1:B:286:ARG:CG	2.10	0.65
1:A:29:ILE:HG12	1:A:91:PHE:CD1	2.31	0.65
1:B:286:ARG:HH11	1:B:286:ARG:HG2	1.60	0.64
1:B:155:VAL:HG13	1:B:192:LYS:HG3	1.80	0.64
1:B:65:GLN:OE1	1:B:67:TYR:CZ	2.49	0.64
1:B:172:ILE:CG1	1:B:189:ILE:HD11	2.28	0.63
1:A:263:LYS:CG	1:A:264:GLN:N	2.36	0.63
1:B:373:ALA:O	1:B:377:THR:CG2	2.47	0.63
1:A:274:ARG:HB2	1:A:279:MET:CE	2.29	0.62
1:A:31:PRO:HD2	1:A:93:VAL:O	2.00	0.61
1:B:85:LEU:HD13	1:B:117:VAL:HG21	1.82	0.61
1:B:133:VAL:HG11	4:B:2021:HOH:O	2.01	0.61
1:A:370:ILE:C	1:A:370:ILE:HD12	2.21	0.60
1:A:108:ARG:HG2	1:A:111:ASN:HD22	1.65	0.60
1:B:149:ARG:HG3	1:B:300:GLY:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PRO:HD3	1:A:350:GLU:OE1	2.01	0.60
1:B:199:THR:HG23	1:B:234:PHE:CD1	2.37	0.60
1:A:351:ILE:HG22	1:A:370:ILE:CD1	2.32	0.60
1:B:31:PRO:HD2	1:B:93:VAL:O	2.02	0.59
1:A:370:ILE:O	1:A:370:ILE:HD12	2.02	0.59
1:B:33:PHE:CE1	1:B:96:LYS:HB2	2.37	0.59
1:A:38:ILE:HG13	1:A:345:VAL:HG11	1.85	0.59
1:A:191:ILE:HD11	1:B:183:ILE:HD13	1.84	0.58
1:A:192:LYS:HE2	1:A:227:MET:HE1	1.81	0.58
1:B:156:TYR:CE1	1:B:298:LEU:CD1	2.84	0.58
1:B:160:GLU:HB2	1:B:190:GLY:HA2	1.84	0.58
1:B:373:ALA:O	1:B:377:THR:HG22	2.03	0.58
1:B:161:TRP:CD1	1:B:167:GLU:HG3	2.38	0.58
1:B:38:ILE:HG13	1:B:339:TYR:CD2	2.36	0.57
1:A:185:GLU:OE1	1:A:185:GLU:N	2.26	0.57
1:A:15:ILE:HD11	1:A:22:LEU:HG	1.86	0.57
1:A:351:ILE:CG2	1:A:370:ILE:HD13	2.35	0.56
1:B:29:ILE:HG12	1:B:91:PHE:CE1	2.40	0.56
1:B:96:LYS:HG3	1:B:330:GLU:HB3	1.88	0.56
1:A:338:LYS:O	1:A:339:TYR:CG	2.58	0.56
1:A:372:LYS:HE2	4:A:2060:HOH:O	2.06	0.55
1:B:96:LYS:CG	1:B:330:GLU:HB3	2.36	0.55
1:A:149:ARG:HB2	1:A:300:GLY:HA3	1.88	0.55
1:A:366:ALA:HA	1:A:369:MET:HE2	1.88	0.54
1:A:29:ILE:CG1	1:A:91:PHE:CD1	2.90	0.54
1:B:131:LYS:HB2	1:B:375:GLU:OE1	2.08	0.54
1:B:385:TYR:CG	1:B:386:ASP:N	2.76	0.54
1:B:222:HIS:HD2	1:B:224:GLY:N	2.01	0.54
1:B:248:GLU:OE1	1:B:249:TYR:CD2	2.61	0.54
1:A:191:ILE:HD11	1:B:183:ILE:CD1	2.38	0.54
1:A:3:TYR:HD2	1:A:83:ASP:CB	2.21	0.53
1:A:320:SER:OG	1:A:322:ILE:HD11	2.07	0.53
1:B:40:LYS:O	1:B:44:PRO:HG2	2.08	0.53
1:B:349:ALA:O	1:B:353:THR:HG23	2.07	0.53
1:A:171:LEU:HD13	1:A:189:ILE:HG21	1.90	0.53
1:A:293:ILE:HG22	1:A:295:LEU:HD22	1.90	0.53
1:A:15:ILE:HD13	1:A:22:LEU:HG	1.91	0.53
1:A:46:ALA:HB2	1:A:350:GLU:HB3	1.91	0.52
1:A:355:ALA:HB2	1:A:370:ILE:CG1	2.38	0.52
1:A:172:ILE:HG23	1:A:183:ILE:HB	1.92	0.52
1:B:38:ILE:HD12	1:B:336:ALA:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:NH1	1:A:274:ARG:HG3	2.24	0.52
1:A:12:GLY:HA3	1:A:29:ILE:HG22	1.91	0.52
1:A:273:ASP:O	1:A:274:ARG:HG3	2.09	0.52
1:A:274:ARG:HB2	1:A:279:MET:HE3	1.92	0.51
1:A:137:ILE:HG22	1:B:137:ILE:HG22	1.93	0.51
1:B:18:GLU:O	1:B:19:ASN:HB2	2.10	0.51
1:A:263:LYS:O	1:A:264:GLN:HB2	2.10	0.51
1:A:3:TYR:HD2	1:A:83:ASP:HB3	1.75	0.51
1:B:173:ARG:NH1	1:B:173:ARG:HG2	2.16	0.51
1:B:387:ILE:HG22	1:B:387:ILE:O	2.11	0.51
1:B:29:ILE:O	1:B:29:ILE:HG13	2.10	0.51
1:B:3:TYR:HB3	1:B:6:VAL:O	2.09	0.51
1:A:122:ALA:HB3	1:A:205:MET:HE1	1.93	0.51
1:A:26:ASP:OD1	1:A:59:LYS:HE2	2.11	0.51
1:B:29:ILE:HG12	1:B:91:PHE:CD1	2.47	0.50
1:A:162:PRO:HG2	1:A:165:SER:HB3	1.93	0.50
1:A:298:LEU:HD11	1:A:302:TYR:CZ	2.47	0.50
1:A:235:ARG:HD2	1:A:236:ASP:OD1	2.11	0.50
1:B:88:ILE:HG12	1:B:94:ALA:HB2	1.92	0.50
1:A:274:ARG:HH11	1:A:274:ARG:CG	2.23	0.50
1:A:355:ALA:HB2	1:A:370:ILE:HG13	1.94	0.50
1:B:345:VAL:HG22	1:B:346:ASN:N	2.27	0.49
1:A:192:LYS:CE	1:A:227:MET:HE3	2.35	0.49
1:A:29:ILE:HA	1:A:62:VAL:O	2.13	0.49
1:A:3:TYR:HB3	1:A:6:VAL:O	2.13	0.49
1:B:130:LEU:HD12	1:B:375:GLU:HG3	1.95	0.48
1:B:377:THR:HG21	1:B:405:VAL:HA	1.95	0.48
1:A:351:ILE:HG22	1:A:370:ILE:HD13	1.94	0.48
1:B:196:GLU:HG3	1:B:237:TRP:CE2	2.49	0.48
1:B:33:PHE:CZ	1:B:96:LYS:HB2	2.48	0.48
1:A:351:ILE:HG22	1:A:370:ILE:HD11	1.96	0.48
1:A:15:ILE:HD11	1:A:22:LEU:CD1	2.43	0.48
1:A:298:LEU:HD11	1:A:302:TYR:CE1	2.49	0.47
1:B:143:VAL:HB	1:B:311:ILE:HD11	1.95	0.47
1:A:227:MET:HE2	1:A:231:GLU:HG2	1.97	0.47
1:A:286:ARG:HD2	1:A:289:GLU:OE2	2.15	0.47
1:B:13:GLU:O	1:B:28:PRO:HA	2.14	0.47
1:B:1:MET:CE	1:B:90:GLU:HG3	2.45	0.47
1:B:30:ILE:HD11	1:B:63:TRP:CZ3	2.49	0.47
1:A:80:LEU:HD21	1:A:114:ILE:HG13	1.97	0.47
1:B:156:TYR:HE1	1:B:298:LEU:CD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:MET:CE	1:A:408:ASN:HB3	2.45	0.47
1:B:147:ILE:HG23	1:B:295:LEU:CD1	2.45	0.47
1:A:27:ASN:HA	1:A:60:GLU:O	2.15	0.47
1:B:160:GLU:HB2	1:B:189:ILE:O	2.15	0.47
1:B:30:ILE:HD11	1:B:63:TRP:CH2	2.50	0.47
1:B:237:TRP:O	1:B:241:VAL:HG12	2.15	0.46
1:B:388:HIS:CD2	1:B:395:LYS:HE3	2.50	0.46
1:B:66:VAL:HG12	1:B:67:TYR:H	1.80	0.46
1:A:256:LEU:HD11	1:A:263:LYS:O	2.15	0.46
1:B:350:GLU:HA	1:B:353:THR:HG23	1.97	0.46
1:B:387:ILE:O	1:B:387:ILE:CG2	2.63	0.46
1:B:153:GLU:HB2	1:B:154:ASP:H	1.59	0.46
1:A:320:SER:HB2	1:A:356:LEU:HD21	1.98	0.46
1:A:92:ARG:HD3	1:A:325:GLY:O	2.16	0.46
1:B:390:HIS:O	1:B:391:MET:HG2	2.15	0.46
1:B:373:ALA:O	1:B:377:THR:HG23	2.14	0.45
1:A:93:VAL:HG23	1:A:93:VAL:O	2.17	0.45
1:A:260:TYR:HB3	1:A:263:LYS:HG2	1.98	0.45
1:A:339:TYR:O	1:A:342:GLN:CG	2.64	0.45
1:B:283:ILE:HD13	1:B:303:LEU:HD11	1.97	0.45
1:A:126:PRO:HG3	1:A:356:LEU:HD13	1.97	0.45
1:A:221:VAL:CB	1:A:295:LEU:HD13	2.37	0.45
1:A:29:ILE:O	1:A:29:ILE:HG13	2.16	0.45
1:A:229:TYR:HB3	1:B:162:PRO:HA	1.99	0.45
1:B:96:LYS:NZ	1:B:111:ASN:HD21	2.15	0.45
1:B:147:ILE:HG23	1:B:295:LEU:HD11	1.99	0.45
1:B:361:ILE:HG22	1:B:363:TRP:H	1.81	0.44
1:B:396:VAL:HG13	1:B:400:GLU:HB2	1.99	0.44
1:A:15:ILE:HG23	4:A:2003:HOH:O	2.17	0.44
1:A:30:ILE:HA	1:A:31:PRO:HD3	1.88	0.44
1:B:149:ARG:HD3	1:B:297:ASN:O	2.17	0.44
1:B:390:HIS:C	1:B:391:MET:HG2	2.37	0.44
1:A:208:ARG:HD3	4:A:2004:HOH:O	2.17	0.44
1:B:172:ILE:HG12	1:B:189:ILE:HD11	1.99	0.44
1:A:16:ARG:NH1	1:A:18:GLU:OE2	2.51	0.44
1:A:265:PRO:HG2	1:A:268:LYS:CG	2.47	0.43
1:B:38:ILE:HG12	1:B:345:VAL:HG11	1.99	0.43
1:A:30:ILE:HG23	1:A:61:VAL:HG13	2.00	0.43
1:A:196:GLU:HG2	1:A:237:TRP:CE2	2.52	0.43
1:A:212:GLU:OE2	4:A:2039:HOH:O	2.20	0.43
1:B:57:ILE:HA	1:B:57:ILE:HD13	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ILE:HD12	1:B:191:ILE:C	2.39	0.43
1:B:42:VAL:CG2	1:B:350:GLU:HG3	2.40	0.43
1:B:345:VAL:HA	1:B:385:TYR:CE1	2.54	0.43
1:A:400:GLU:HG3	4:A:2064:HOH:O	2.17	0.43
1:A:293:ILE:HG22	1:A:295:LEU:CD2	2.47	0.43
1:B:163:ARG:NH1	4:B:2009:HOH:O	2.45	0.43
1:B:171:LEU:O	1:B:175:LEU:HG	2.20	0.42
1:B:160:GLU:CB	1:B:190:GLY:HA2	2.47	0.42
1:B:17:TYR:CE1	1:B:20:GLY:HA2	2.55	0.42
1:B:1:MET:HE3	1:B:90:GLU:HG3	2.00	0.42
1:B:248:GLU:HB3	1:B:249:TYR:CE1	2.55	0.42
1:A:155:VAL:HG11	1:B:192:LYS:HD2	2.01	0.42
1:B:131:LYS:CB	1:B:375:GLU:OE1	2.67	0.42
1:A:160:GLU:HG2	1:B:229:TYR:HD2	1.85	0.42
1:A:281:GLN:HG2	1:B:309:ALA:HB2	2.01	0.42
1:A:223:LYS:NZ	4:A:2040:HOH:O	2.52	0.41
1:B:184:ARG:HB3	1:B:184:ARG:NH1	2.34	0.41
1:B:248:GLU:OE1	1:B:249:TYR:CE2	2.72	0.41
1:A:298:LEU:CD1	1:A:302:TYR:CE1	3.03	0.41
1:B:174:PHE:CE1	1:B:178:GLU:HG3	2.55	0.41
1:B:38:ILE:CD1	1:B:336:ALA:HB3	2.50	0.41
1:B:101:THR:HA	1:B:102:PRO:HD3	1.89	0.41
1:B:32:TYR:HA	1:B:95:LEU:O	2.21	0.41
1:A:122:ALA:CB	1:A:205:MET:CE	2.98	0.41
1:A:32:TYR:HA	1:A:95:LEU:O	2.21	0.41
1:B:172:ILE:HG13	1:B:189:ILE:CD1	2.50	0.41
1:B:146:VAL:HG22	1:B:148:PHE:CE2	2.55	0.41
1:B:338:LYS:O	1:B:339:TYR:CD1	2.74	0.41
1:A:5:LYS:HB2	1:A:76:TYR:CE2	2.56	0.41
1:B:160:GLU:HB2	1:B:190:GLY:CA	2.50	0.41
1:A:229:TYR:HD2	1:B:160:GLU:HG2	1.86	0.41
1:B:29:ILE:CG1	1:B:91:PHE:CD1	3.04	0.41
1:A:376:MET:HE3	1:A:408:ASN:HB3	2.03	0.41
1:A:101:THR:HA	1:A:102:PRO:HD3	1.88	0.41
1:A:131:LYS:HG3	1:A:375:GLU:OE1	2.21	0.41
1:A:275:ILE:HG22	1:A:277:ASP:OD1	2.21	0.41
1:A:355:ALA:HB2	1:A:370:ILE:HG12	2.03	0.41
1:A:3:TYR:CB	1:A:6:VAL:O	2.68	0.41
1:B:32:TYR:CE2	1:B:63:TRP:HB3	2.56	0.40
1:A:197:PHE:HB3	1:B:184:ARG:NH1	2.36	0.40
1:A:321:ASN:C	1:A:322:ILE:HG12	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ILE:HD12	1:A:311:ILE:HA	1.75	0.40
1:A:115:ARG:HB2	1:A:120:LEU:HB2	2.02	0.40
1:A:22:LEU:HD21	1:A:360:TYR:CE2	2.56	0.40
1:B:96:LYS:HZ1	1:B:111:ASN:HD21	1.69	0.40
1:A:38:ILE:HB	1:A:335:SER:O	2.21	0.40
1:A:399:ARG:HB2	1:A:399:ARG:HE	1.56	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	410/412 (100%)	378 (92%)	24 (6%)	8 (2%)	7	12
1	B	410/412 (100%)	366 (89%)	36 (9%)	8 (2%)	7	12
All	All	820/824 (100%)	744 (91%)	60 (7%)	16 (2%)	7	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	A	106	GLY
1	A	263	LYS
1	A	339	TYR
1	B	396	VAL
1	A	107	TYR
1	A	264	GLN
1	B	336	ALA
1	B	339	TYR
1	B	186	ASP
1	B	25	PRO
1	A	37	GLY

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Mol	Chain	Res	Type
1	A	337	PRO
1	B	20	GLY
1	B	393	GLY
1	B	337	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	337/339 (99%)	291 (86%)	46 (14%)	3	7
1	B	336/339 (99%)	285 (85%)	51 (15%)	3	5
All	All	673/678 (99%)	576 (86%)	97 (14%)	3	6

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	16	ARG
1	A	22	LEU
1	A	29	ILE
1	A	30	ILE
1	A	38	ILE
1	A	50	LEU
1	A	57	ILE
1	A	59	LYS
1	A	83	ASP
1	A	89	LYS
1	A	100	THR
1	A	101	THR
1	A	107	TYR
1	A	108	ARG
1	A	113	THR
1	A	115	ARG
1	A	117	VAL
1	A	123	ASN

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Mol	Chain	Res	Type
1	A	130	LEU
1	A	144	ASN
1	A	149	ARG
1	A	151	ASN
1	A	153	GLU
1	A	163	ARG
1	A	167	GLU
1	A	171	LEU
1	A	189	ILE
1	A	191	ILE
1	A	223	LYS
1	A	264	GLN
1	A	274	ARG
1	A	287	THR
1	A	291	ASP
1	A	295	LEU
1	A	311	ILE
1	A	316	ILE
1	A	365	ASP
1	A	370	ILE
1	A	372	LYS
1	A	390	HIS
1	A	395	LYS
1	A	396	VAL
1	A	400	GLU
1	A	407	GLU
1	A	409	LEU
1	B	18	GLU
1	B	29	ILE
1	B	57	ILE
1	B	65	GLN
1	B	66	VAL
1	B	75	LEU
1	B	89	LYS
1	B	90	GLU
1	B	92	ARG
1	B	93	VAL
1	B	117	VAL
1	B	123	ASN
1	B	130	LEU
1	B	144	ASN
1	B	146	VAL

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Mol	Chain	Res	Type
1	B	149	ARG
1	B	153	GLU
1	B	163	ARG
1	B	166	GLU
1	B	171	LEU
1	B	173	ARG
1	B	176	LYS
1	B	181	VAL
1	B	191	ILE
1	B	196	GLU
1	B	214	ASN
1	B	241	VAL
1	B	258	ASP
1	B	264	GLN
1	B	286	ARG
1	B	291	ASP
1	B	311	ILE
1	B	320	SER
1	B	330	GLU
1	B	333	HIS
1	B	338	LYS
1	B	339	TYR
1	B	353	THR
1	B	368	GLU
1	B	369	MET
1	B	375	GLU
1	B	377	THR
1	B	385	TYR
1	B	388	HIS
1	B	389	ARG
1	B	391	MET
1	B	394	THR
1	B	409	LEU
1	B	410	GLN
1	B	411	SER
1	B	412	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	144	ASN

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Mol	Chain	Res	Type
1	A	151	ASN
1	A	321	ASN
1	B	111	ASN
1	B	144	ASN
1	B	151	ASN
1	B	222	HIS
1	B	264	GLN
1	B	408	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	412/412 (100%)	0.26	16 (3%) 39 42	3, 14, 29, 46	0
1	B	412/412 (100%)	0.58	55 (13%) 3 2	2, 15, 36, 55	0
All	All	824/824 (100%)	0.42	71 (8%) 10 10	2, 15, 34, 55	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	PRO	7.8
1	B	104	GLY	7.4
1	B	392	GLY	6.1
1	B	412	LEU	6.1
1	B	105	GLY	6.0
1	B	106	GLY	5.7
1	B	393	GLY	5.7
1	A	105	GLY	5.6
1	B	340	ALA	5.4
1	B	19	ASN	5.3
1	A	106	GLY	5.2
1	B	391	MET	4.8
1	B	394	THR	4.8
1	B	390	HIS	4.7
1	B	10	GLU	4.7
1	B	257	TRP	4.5
1	B	58	GLY	4.4
1	B	107	TYR	4.3
1	B	388	HIS	4.2
1	A	107	TYR	4.2
1	B	21	LYS	4.1
1	B	336	ALA	4.0
1	B	23	ILE	3.8
1	B	103	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	338	LYS	3.7
1	B	389	ARG	3.7
1	A	337	PRO	3.7
1	B	11	ASN	3.7
1	B	260	TYR	3.6
1	B	73	TYR	3.6
1	A	19	ASN	3.4
1	B	12	GLY	3.2
1	A	166	GLU	3.1
1	B	335	SER	3.1
1	A	338	LYS	3.0
1	B	20	GLY	3.0
1	B	214	ASN	3.0
1	B	395	LYS	3.0
1	A	104	GLY	2.9
1	B	60	GLU	2.9
1	A	103	VAL	2.8
1	A	339	TYR	2.8
1	B	101	THR	2.8
1	B	365	ASP	2.8
1	A	73	TYR	2.8
1	B	18	GLU	2.7
1	B	173	ARG	2.7
1	B	108	ARG	2.6
1	A	10	GLU	2.6
1	B	57	ILE	2.6
1	B	16	ARG	2.6
1	B	212	GLU	2.5
1	B	339	TYR	2.5
1	A	94	ALA	2.4
1	B	261	GLY	2.4
1	B	70	GLU	2.4
1	B	288	ASP	2.3
1	B	387	ILE	2.3
1	A	203	VAL	2.3
1	B	386	ASP	2.3
1	B	13	GLU	2.2
1	B	166	GLU	2.2
1	B	82	ASP	2.2
1	B	385	TYR	2.2
1	A	266	GLU	2.2
1	B	77	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	78	ASN	2.1
1	B	74	LYS	2.1
1	B	258	ASP	2.1
1	A	348	THR	2.0
1	B	178	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	1415	1/1	0.88	0.11	49,49,49,49	0
3	CL	A	1418	1/1	0.95	0.07	20,20,20,20	0
2	ZN	A	1414	1/1	0.95	0.07	34,34,34,34	0
3	CL	B	1418	1/1	0.97	0.05	20,20,20,20	0
2	ZN	B	1416	1/1	0.97	0.05	34,34,34,34	0
2	ZN	A	1416	1/1	0.97	0.05	53,53,53,53	0
3	CL	A	1417	1/1	0.97	0.14	14,14,14,14	0
2	ZN	A	1413	1/1	0.98	0.06	11,11,11,11	0
2	ZN	A	1415	1/1	0.99	0.05	15,15,15,15	0
2	ZN	B	1417	1/1	0.99	0.04	19,19,19,19	0
2	ZN	B	1413	1/1	0.99	0.02	24,24,24,24	0
2	ZN	B	1414	1/1	1.00	0.03	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.