



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:01 PM UTC

PDB ID : 2DHT / pdb_00002dht
Title : Crystal structure of isocitrate dehydrogenase from Sulfolobus tokodaii strain7
Authors : Kondo, H.; Murakami, M.; Ihara, K.; Suzuki, S.; Kouyama, T.
Deposited on : 2006-03-25
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 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

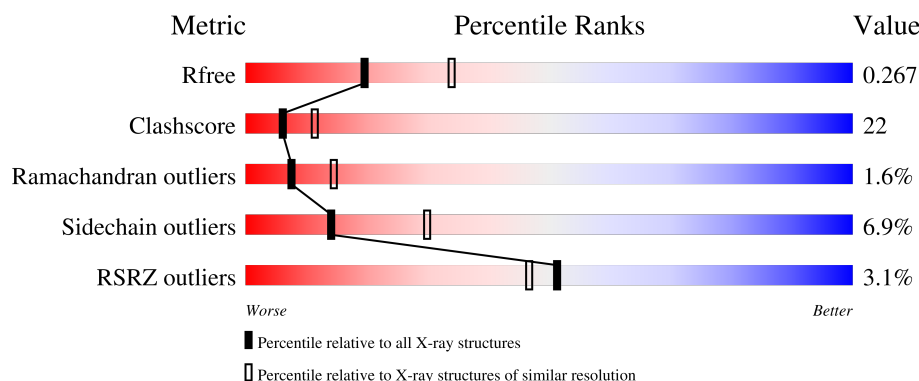
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	409	2% 56% 35% 7% .
1	B	409	4% 54% 38% 6% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6484 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 409aa long hypothetical NADP-dependent isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3223	2063	545	600	15			
1	B	403	Total	C	N	O	S	0	0	0
			3223	2063	545	600	15			

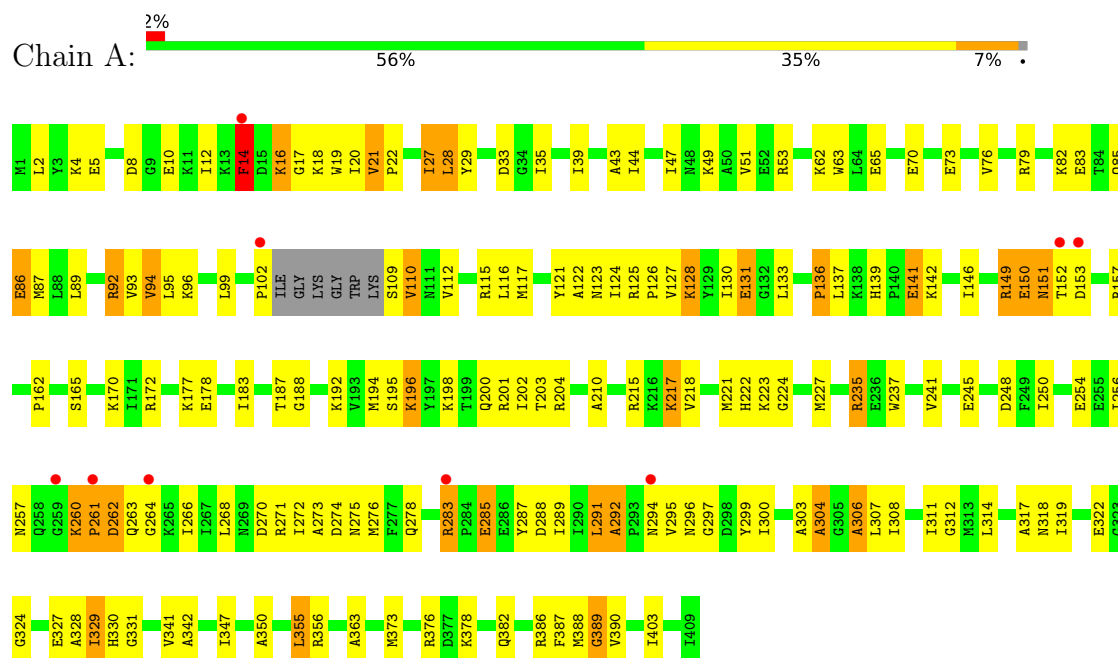
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	20	Total	O	0	0
			20	20		

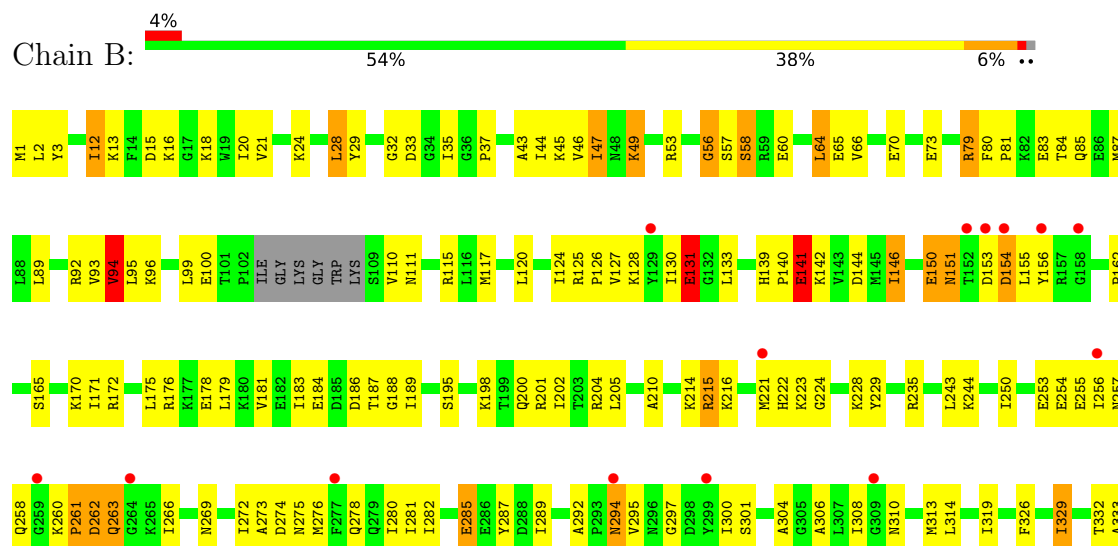
3 Residue-property plots

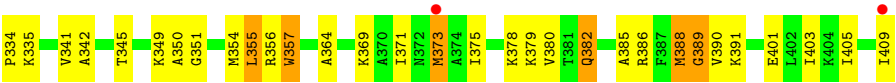
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 409aa long hypothetical NADP-dependent isocitrate dehydrogenase



- Molecule 1: 409aa long hypothetical NADP-dependent 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	73.98Å 88.09Å 76.22Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-2.50) 98.0 (15.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.51Å)	Xtriage
Refinement program	XTALVIEW, CNS 1.0	Depositor
R, R_{free}	0.241 , 0.272 0.241 , 0.267	Depositor DCC
R_{free} test set	1474 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for l,k,-h 0.086 for h,-k,-l 0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6484	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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	0.50	0/3279	1.06	23/4410 (0.5%)
1	B	0.47	0/3279	1.03	25/4410 (0.6%)
All	All	0.48	0/6558	1.04	48/8820 (0.5%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	PHE	CA-C-N	11.32	131.44	119.90
1	B	80	PHE	C-N-CA	11.32	131.44	119.90
1	A	283	ARG	CA-C-N	9.65	129.27	119.82
1	A	283	ARG	C-N-CA	9.65	129.27	119.82
1	A	306	ALA	N-CA-C	-9.23	102.03	113.20
1	A	151	ASN	N-CA-C	8.31	123.04	113.15
1	B	257	ASN	N-CA-C	-8.29	104.19	112.97
1	B	151	ASN	N-CA-C	8.25	122.70	113.21
1	A	304	ALA	N-CA-C	-7.95	100.04	110.53
1	B	228	LYS	N-CA-C	7.78	119.76	111.28
1	B	21	VAL	N-CA-C	7.75	117.19	108.05
1	B	92	ARG	N-CA-C	7.65	122.33	113.38
1	A	21	VAL	N-CA-C	7.50	116.17	107.77
1	A	292	ALA	N-CA-C	7.43	114.91	108.22
1	A	92	ARG	N-CA-C	7.11	125.93	110.80
1	A	389	GLY	N-CA-C	7.07	129.93	113.18
1	B	58	SER	N-CA-C	-6.62	105.17	113.18
1	A	187	THR	N-CA-C	6.47	118.95	108.41
1	A	188	GLY	N-CA-C	-6.45	103.83	112.14
1	A	141	GLU	N-CA-C	6.38	118.77	111.11
1	B	95	LEU	N-CA-C	-6.32	96.81	107.99
1	B	131	GLU	N-CA-C	6.15	123.90	110.80
1	B	294	ASN	N-CA-C	6.07	118.40	111.11
1	A	350	ALA	N-CA-C	-6.00	104.82	111.36
1	B	216	LYS	N-CA-C	5.92	120.52	113.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	ILE	N-CA-C	-5.89	101.97	109.80
1	B	382	GLN	N-CA-C	5.83	119.22	111.75
1	B	188	GLY	N-CA-C	-5.81	101.34	111.62
1	A	17	GLY	N-CA-C	-5.75	107.31	115.30
1	B	187	THR	N-CA-C	5.68	118.74	109.59
1	B	350	ALA	N-CA-C	-5.57	104.84	111.69
1	B	150	GLU	N-CA-C	-5.52	100.11	108.67
1	A	150	GLU	N-CA-C	-5.44	100.93	109.25
1	B	260	LYS	CA-C-N	5.43	126.63	119.84
1	B	260	LYS	C-N-CA	5.43	126.63	119.84
1	B	94	VAL	CB-CA-C	-5.42	102.16	110.50
1	B	110	VAL	N-CA-C	-5.39	105.28	110.72
1	A	96	LYS	N-CA-C	5.36	117.83	108.76
1	A	125	ARG	CA-C-N	-5.30	113.09	120.25
1	A	125	ARG	C-N-CA	-5.30	113.09	120.25
1	A	122	ALA	N-CA-C	5.27	117.11	108.52
1	B	215	ARG	N-CA-C	-5.26	102.73	110.52
1	B	189	ILE	N-CA-C	5.21	115.40	108.11
1	A	136	PRO	N-CA-C	-5.16	107.31	114.27
1	B	342	ALA	N-CA-C	5.14	116.92	110.24
1	A	273	ALA	N-CA-C	5.04	117.67	111.82
1	A	260	LYS	CA-C-N	5.03	126.13	119.84
1	A	260	LYS	C-N-CA	5.03	126.13	119.84

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	3223	0	3299	154	0
1	B	3223	0	3299	148	0
2	A	18	0	0	3	0
2	B	20	0	0	1	0
All	All	6484	0	6598	293	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 22.

All (293) 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:47:ILE:HD13	1:B:355:LEU:HD21	1.45	0.97
1:B:49:LYS:HG3	1:B:403:ILE:HG23	1.46	0.97
1:A:49:LYS:HG3	1:A:403:ILE:HG23	1.63	0.79
1:A:295:VAL:HG12	2:A:506:HOH:O	1.83	0.79
1:B:198:LYS:HA	1:B:201:ARG:HD2	1.65	0.79
1:A:223:LYS:HE3	1:A:274:ASP:HB3	1.65	0.78
1:A:8:ASP:HB3	1:A:62:LYS:NZ	1.99	0.77
1:A:297:GLY:HA2	1:A:300:ILE:HG22	1.65	0.77
1:B:378:LYS:HG3	1:B:388:MET:HE3	1.66	0.77
1:A:222:HIS:HD2	1:A:224:GLY:H	1.30	0.77
1:B:162:PRO:HG2	1:B:165:SER:HB3	1.65	0.76
1:A:14:PHE:HB3	1:A:19:TRP:HA	1.70	0.74
1:A:172:ARG:HG2	1:A:183:ILE:HD12	1.69	0.74
1:A:341:VAL:HG13	1:A:382:GLN:HG2	1.68	0.74
1:A:153:ASP:H	1:A:294:ASN:HD22	1.34	0.74
1:B:47:ILE:CD1	1:B:355:LEU:HD21	2.18	0.73
1:B:349:LYS:HE2	1:B:371:ILE:HD13	1.70	0.73
1:B:130:ILE:HD11	1:B:133:LEU:HG	1.71	0.73
1:B:221:MET:HB3	1:B:292:ALA:HB2	1.70	0.72
1:A:123:ASN:ND2	1:A:149:ARG:HH21	1.88	0.71
1:A:221:MET:HB3	1:A:292:ALA:HB2	1.72	0.71
1:B:221:MET:HB2	1:B:276:MET:HE2	1.73	0.71
1:A:196:LYS:HB3	1:B:186:ASP:HB2	1.72	0.70
1:A:124:ILE:HD13	1:A:319:ILE:HD13	1.73	0.70
1:A:271:ARG:HB2	1:A:276:MET:HE3	1.72	0.69
1:A:123:ASN:HD22	1:A:149:ARG:HH21	1.40	0.69
1:B:250:ILE:HG22	1:B:266:ILE:HB	1.75	0.67
1:A:27:ILE:HD12	1:A:93:VAL:HG23	1.76	0.67
1:B:341:VAL:HG13	1:B:382:GLN:HG2	1.77	0.67
1:A:308:ILE:HD11	1:A:314:LEU:HD21	1.75	0.66
1:A:222:HIS:CD2	1:A:224:GLY:H	2.13	0.66
1:B:85:GLN:HB3	1:B:117:MET:HE1	1.77	0.66
1:B:222:HIS:HD2	1:B:224:GLY:H	1.44	0.66
1:B:351:GLY:O	1:B:355:LEU:HD22	1.96	0.66
1:B:142:LYS:HG2	1:B:285:GLU:HB3	1.77	0.65
1:B:382:GLN:O	1:B:386:ARG:HG3	1.96	0.65
1:A:8:ASP:HB3	1:A:62:LYS:HZ2	1.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:SER:HB3	1:B:198:LYS:HB2	1.80	0.64
1:B:53:ARG:HE	1:B:409:ILE:HG13	1.62	0.64
1:A:304:ALA:HA	1:A:307:LEU:HD13	1.79	0.63
1:A:128:LYS:HE3	1:A:128:LYS:H	1.63	0.63
1:B:297:GLY:HA2	1:B:300:ILE:HG22	1.80	0.63
1:A:295:VAL:HG11	2:B:508:HOH:O	1.98	0.62
1:B:335:LYS:H	1:B:335:LYS:HD2	1.64	0.62
1:A:2:LEU:HD23	1:A:2:LEU:H	1.65	0.62
1:A:149:ARG:HG3	1:A:297:GLY:HA3	1.81	0.62
1:B:263:GLN:H	1:B:263:GLN:NE2	1.98	0.62
1:B:45:LYS:HG2	1:B:403:ILE:HD11	1.83	0.61
1:B:111:ASN:HB3	1:B:115:ARG:HH21	1.66	0.61
1:A:33:ASP:OD2	1:A:70:GLU:HG2	2.01	0.61
1:A:329:ILE:O	1:A:329:ILE:HD13	2.01	0.61
1:A:16:LYS:HD2	1:A:16:LYS:N	2.16	0.61
1:A:123:ASN:HD22	1:A:149:ARG:NH2	1.98	0.60
1:B:308:ILE:O	1:B:308:ILE:HG13	2.01	0.60
1:B:20:ILE:O	1:B:20:ILE:HG13	2.00	0.60
1:B:3:TYR:CE2	1:B:66:VAL:HA	2.37	0.60
1:B:329:ILE:HD13	1:B:329:ILE:O	2.01	0.60
1:B:146:ILE:HG23	1:B:289:ILE:HG12	1.84	0.59
1:B:81:PRO:HG2	1:B:84:THR:OG1	2.02	0.59
1:B:266:ILE:H	1:B:266:ILE:HD12	1.68	0.59
1:B:256:ILE:HA	1:B:261:PRO:HA	1.84	0.58
1:B:154:ASP:HB3	1:B:295:VAL:HG23	1.86	0.58
1:B:33:ASP:OD1	1:B:70:GLU:HG2	2.04	0.58
1:B:222:HIS:CD2	1:B:224:GLY:H	2.20	0.58
1:B:28:LEU:HB3	1:B:94:VAL:HG13	1.86	0.57
1:B:125:ARG:HB3	1:B:125:ARG:NH2	2.20	0.57
1:A:126:PRO:HB3	1:A:146:ILE:HD13	1.86	0.57
1:B:29:TYR:CZ	1:B:65:GLU:HB2	2.39	0.57
1:A:272:ILE:N	1:A:272:ILE:HD12	2.19	0.57
1:B:243:LEU:HD12	1:B:250:ILE:HD11	1.87	0.57
1:A:124:ILE:CG2	1:A:146:ILE:HD11	2.35	0.56
1:B:198:LYS:O	1:B:201:ARG:HG2	2.06	0.56
1:B:369:LYS:HD3	1:B:369:LYS:C	2.30	0.56
1:A:150:GLU:OE1	1:A:153:ASP:HB2	2.05	0.56
1:A:210:ALA:HA	1:A:215:ARG:HB2	1.88	0.56
1:A:314:LEU:O	1:A:329:ILE:HG22	2.06	0.56
1:B:89:LEU:HG	1:B:117:MET:HE2	1.88	0.56
1:A:124:ILE:HG23	1:A:146:ILE:HD11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:HG13	1:A:257:ASN:H	1.70	0.55
1:A:200:GLN:O	1:A:204:ARG:HG3	2.06	0.55
1:A:195:SER:HB3	1:A:198:LYS:HB2	1.88	0.55
1:A:14:PHE:HZ	1:A:92:ARG:HB2	1.72	0.55
1:A:82:LYS:O	1:A:86:GLU:HG2	2.06	0.55
1:B:314:LEU:O	1:B:329:ILE:HG22	2.07	0.55
1:B:125:ARG:HB3	1:B:125:ARG:HH21	1.71	0.55
1:A:27:ILE:HD12	1:A:93:VAL:CG2	2.37	0.55
1:A:83:GLU:HA	1:A:86:GLU:HG3	1.87	0.55
1:A:136:PRO:HG3	1:B:282:ILE:HG22	1.89	0.55
1:A:146:ILE:HG23	1:A:289:ILE:HA	1.88	0.55
1:A:227:MET:HE2	1:B:156:TYR:HE2	1.72	0.55
1:A:126:PRO:HA	1:A:146:ILE:HA	1.89	0.54
1:A:2:LEU:HD23	1:A:2:LEU:N	2.23	0.54
1:A:89:LEU:HG	1:A:117:MET:HE2	1.90	0.54
1:B:154:ASP:HB2	1:B:294:ASN:HB3	1.90	0.54
1:B:183:ILE:HG22	1:B:184:GLU:O	2.07	0.54
1:B:130:ILE:HD12	1:B:375:ILE:HG12	1.89	0.54
1:B:12:ILE:HD12	1:B:93:VAL:HG21	1.90	0.53
1:B:223:LYS:NZ	1:B:274:ASP:HB3	2.24	0.53
1:A:314:LEU:HB2	1:A:329:ILE:CG2	2.37	0.53
1:B:35:ILE:HG12	1:B:332:THR:O	2.09	0.53
1:B:276:MET:O	1:B:280:ILE:HG23	2.08	0.53
1:A:250:ILE:HG22	1:A:266:ILE:HB	1.91	0.53
1:B:390:VAL:HG22	1:B:391:LYS:N	2.23	0.53
1:B:142:LYS:CG	1:B:285:GLU:HB3	2.39	0.53
1:B:297:GLY:HA2	1:B:300:ILE:CG2	2.39	0.52
1:A:8:ASP:HB3	1:A:62:LYS:HZ1	1.74	0.52
1:A:10:GLU:HB2	1:A:22:PRO:HG2	1.91	0.52
1:A:73:GLU:OE1	1:A:79:ARG:HD3	2.10	0.52
1:B:128:LYS:HD3	1:B:144:ASP:CG	2.35	0.52
1:A:28:LEU:CB	1:A:94:VAL:HG13	2.39	0.52
1:B:278:GLN:O	1:B:282:ILE:HG12	2.09	0.52
1:A:306:ALA:HB2	1:B:278:GLN:HG2	1.90	0.52
1:B:133:LEU:HD13	1:B:310:ASN:HD22	1.75	0.51
1:A:272:ILE:HD12	1:A:272:ILE:H	1.74	0.51
1:A:299:TYR:HE1	1:B:273:ALA:HB1	1.76	0.51
1:A:378:LYS:HD2	1:A:378:LYS:N	2.25	0.51
1:B:356:ARG:HD2	1:B:364:ALA:HB1	1.91	0.51
1:A:172:ARG:HA	1:A:183:ILE:HD11	1.92	0.51
1:B:13:LYS:HB2	1:B:20:ILE:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HE2	2:A:530:HOH:O	2.10	0.51
1:B:47:ILE:HD12	1:B:47:ILE:O	2.11	0.51
1:A:142:LYS:HB3	1:A:285:GLU:HB3	1.93	0.51
1:A:177:LYS:HE3	1:A:178:GLU:OE2	2.11	0.50
1:A:99:LEU:HD13	1:A:110:VAL:HG21	1.93	0.50
1:A:115:ARG:HD3	1:A:151:ASN:HD21	1.77	0.50
1:A:218:VAL:O	1:A:268:LEU:HD12	2.11	0.50
1:B:150:GLU:HG3	1:B:153:ASP:HB2	1.93	0.50
1:A:14:PHE:CD1	1:A:322:GLU:HB2	2.45	0.50
1:B:73:GLU:OE1	1:B:79:ARG:HB3	2.11	0.50
1:B:326:PHE:CE2	1:B:354:MET:HG3	2.46	0.50
1:A:12:ILE:HD12	1:A:93:VAL:HG21	1.94	0.50
1:A:297:GLY:HA2	1:A:300:ILE:CG2	2.40	0.50
1:A:99:LEU:HD13	1:A:110:VAL:CG2	2.41	0.50
1:B:32:GLY:HA2	1:B:99:LEU:CD2	2.42	0.50
1:B:300:ILE:HG23	1:B:301:SER:N	2.26	0.50
1:A:256:ILE:HG13	1:A:257:ASN:N	2.25	0.50
1:A:304:ALA:C	1:A:306:ALA:H	2.19	0.50
1:A:18:LYS:O	1:A:19:TRP:HB2	2.11	0.50
1:A:373:MET:HA	1:A:376:ARG:HG2	1.94	0.50
1:B:329:ILE:O	1:B:329:ILE:HG23	2.10	0.50
1:B:178:GLU:C	1:B:179:LEU:HD22	2.37	0.49
1:B:255:GLU:HA	1:B:258:GLN:HE21	1.77	0.49
1:A:4:LYS:HD3	1:A:4:LYS:N	2.27	0.49
1:B:200:GLN:O	1:B:204:ARG:HG3	2.11	0.49
1:B:133:LEU:HD13	1:B:310:ASN:ND2	2.27	0.49
1:B:349:LYS:HE2	1:B:371:ILE:CD1	2.41	0.49
1:A:76:VAL:HG12	1:A:76:VAL:O	2.12	0.49
1:A:266:ILE:HD12	1:A:266:ILE:H	1.78	0.49
1:A:16:LYS:HD2	1:A:16:LYS:H	1.77	0.49
1:B:356:ARG:HH21	1:B:356:ARG:HG3	1.77	0.49
1:B:280:ILE:HG22	1:B:287:TYR:CE2	2.47	0.49
1:A:20:ILE:HD12	1:A:20:ILE:N	2.28	0.49
1:B:379:LYS:HB3	1:B:401:GLU:HG2	1.95	0.49
1:A:261:PRO:HG2	1:A:262:ASP:H	1.77	0.48
1:B:256:ILE:C	1:B:258:GLN:H	2.21	0.48
1:A:139:HIS:CD2	1:A:141:GLU:HB2	2.48	0.48
1:B:141:GLU:CD	1:B:141:GLU:H	2.20	0.48
1:A:261:PRO:HB2	1:A:263:GLN:OE1	2.13	0.48
1:A:121:TYR:CE1	1:A:201:ARG:HG3	2.49	0.48
1:A:2:LEU:CD2	1:A:83:GLU:HG2	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ILE:HD12	1:B:124:ILE:N	2.29	0.48
1:B:45:LYS:HG2	1:B:403:ILE:CD1	2.43	0.48
1:B:319:ILE:HG12	1:B:357:TRP:CE2	2.49	0.48
1:B:150:GLU:N	1:B:202:ILE:HD12	2.28	0.48
1:B:378:LYS:N	1:B:378:LYS:HD2	2.28	0.48
1:A:47:ILE:O	1:A:51:VAL:HG23	2.14	0.48
1:A:162:PRO:HA	1:B:229:TYR:HB3	1.95	0.48
1:A:44:ILE:HA	1:A:47:ILE:HG22	1.95	0.48
1:B:87:MET:HE2	1:B:87:MET:HA	1.95	0.48
1:B:115:ARG:HA	1:B:120:LEU:HD12	1.95	0.48
1:A:276:MET:HE2	1:A:287:TYR:CE1	2.49	0.47
1:A:124:ILE:N	1:A:124:ILE:HD12	2.28	0.47
1:A:192:LYS:HD2	1:B:155:LEU:HD11	1.96	0.47
1:A:5:GLU:HG2	1:A:87:MET:HE1	1.95	0.47
1:A:85:GLN:HB3	1:A:117:MET:HE1	1.95	0.47
1:B:32:GLY:O	1:B:37:PRO:HD3	2.14	0.47
1:B:155:LEU:HD23	1:B:155:LEU:H	1.79	0.47
1:B:156:TYR:CE2	1:B:295:VAL:HG22	2.49	0.47
1:A:130:ILE:HD12	1:A:133:LEU:HD11	1.97	0.47
1:A:327:GLU:HG2	2:A:511:HOH:O	2.14	0.47
1:B:380:VAL:HG23	1:B:385:ALA:HB2	1.97	0.47
1:A:2:LEU:H	1:A:2:LEU:CD2	2.27	0.47
1:A:43:ALA:O	1:A:47:ILE:HG22	2.15	0.47
1:B:32:GLY:HA2	1:B:99:LEU:HD21	1.96	0.47
1:A:162:PRO:HG2	1:A:165:SER:HB3	1.96	0.47
1:A:378:LYS:HB3	1:A:390:VAL:HG21	1.95	0.47
1:A:262:ASP:C	1:A:264:GLY:H	2.23	0.46
1:A:341:VAL:CG1	1:A:382:GLN:HG2	2.41	0.46
1:B:332:THR:OG1	1:B:334:PRO:HD3	2.16	0.46
1:A:328:ALA:HB2	1:A:347:ILE:N	2.30	0.46
1:A:330:HIS:HD2	1:A:331:GLY:O	1.99	0.46
1:B:272:ILE:HG13	1:B:275:ASN:ND2	2.31	0.46
1:A:306:ALA:CB	1:B:278:GLN:HA	2.46	0.46
1:B:43:ALA:O	1:B:46:VAL:HG22	2.16	0.46
1:B:401:GLU:O	1:B:405:ILE:HG13	2.16	0.46
1:B:378:LYS:HA	1:B:388:MET:HE3	1.98	0.46
1:A:274:ASP:OD1	1:A:275:ASN:N	2.49	0.45
1:A:311:ILE:HD12	1:A:314:LEU:HD12	1.98	0.45
1:B:253:GLU:HB2	1:B:269:ASN:HB3	1.98	0.45
1:A:79:ARG:HH11	1:A:102:PRO:HD3	1.81	0.45
1:B:15:ASP:OD1	1:B:16:LYS:HD3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:VAL:HG22	1:B:391:LYS:H	1.82	0.45
1:A:130:ILE:HB	1:A:133:LEU:HG	1.98	0.45
1:B:139:HIS:HA	1:B:141:GLU:OE2	2.17	0.45
1:A:29:TYR:CZ	1:A:65:GLU:HB2	2.51	0.45
1:A:217:LYS:O	1:A:288:ASP:HB3	2.16	0.45
1:B:53:ARG:HE	1:B:409:ILE:CG1	2.26	0.45
1:B:127:VAL:HG13	1:B:127:VAL:O	2.17	0.45
1:A:28:LEU:HB3	1:A:94:VAL:HG13	1.97	0.45
1:B:254:GLU:O	1:B:258:GLN:HB2	2.17	0.45
1:B:332:THR:O	1:B:333:ALA:C	2.60	0.44
1:A:153:ASP:O	1:A:157:ARG:HD2	2.17	0.44
1:B:150:GLU:CA	1:B:202:ILE:HD12	2.48	0.44
1:B:154:ASP:C	1:B:156:TYR:H	2.25	0.44
1:A:222:HIS:HE1	1:A:270:ASP:HB2	1.82	0.44
1:A:235:ARG:HB3	1:A:235:ARG:NH1	2.33	0.44
1:B:172:ARG:O	1:B:176:ARG:HG3	2.18	0.44
1:B:280:ILE:HG13	1:B:281:ILE:N	2.29	0.44
1:B:130:ILE:CD1	1:B:375:ILE:HG12	2.47	0.44
1:B:378:LYS:HA	1:B:388:MET:CE	2.47	0.44
1:A:150:GLU:CA	1:A:202:ILE:HD12	2.47	0.44
1:A:250:ILE:HA	1:A:266:ILE:O	2.17	0.44
1:A:222:HIS:CE1	1:A:270:ASP:HB2	2.53	0.44
1:B:171:ILE:O	1:B:175:LEU:HG	2.17	0.44
1:A:311:ILE:HG23	1:A:312:GLY:N	2.32	0.43
1:B:127:VAL:HG11	1:B:304:ALA:HB1	2.01	0.43
1:A:130:ILE:O	1:A:131:GLU:HB2	2.17	0.43
1:B:96:LYS:O	1:B:96:LYS:HG3	2.18	0.43
1:A:29:TYR:HA	1:A:95:LEU:O	2.18	0.43
1:A:35:ILE:HG21	1:A:342:ALA:HB2	2.01	0.43
1:B:124:ILE:HG22	1:B:126:PRO:HD3	1.99	0.43
1:B:214:LYS:HA	1:B:214:LYS:HD2	1.88	0.43
1:A:221:MET:HB2	1:A:276:MET:SD	2.59	0.43
1:A:329:ILE:O	1:A:329:ILE:HG23	2.19	0.43
1:B:2:LEU:H	1:B:83:GLU:CD	2.27	0.43
1:A:35:ILE:O	1:A:39:ILE:HG12	2.18	0.43
1:B:44:ILE:HA	1:B:47:ILE:CG2	2.49	0.43
1:A:260:LYS:HA	1:A:261:PRO:HD2	1.85	0.42
1:B:13:LYS:HB2	1:B:20:ILE:CG1	2.50	0.42
1:A:196:LYS:HE2	1:A:237:TRP:CD1	2.54	0.42
1:A:378:LYS:HG3	1:A:388:MET:SD	2.58	0.42
1:B:388:MET:O	1:B:389:GLY:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:HB2	1:A:329:ILE:HG21	2.02	0.42
1:B:150:GLU:CG	1:B:153:ASP:HB2	2.49	0.42
1:A:14:PHE:CD1	1:A:14:PHE:N	2.85	0.42
1:A:136:PRO:HD2	1:A:307:LEU:O	2.20	0.42
1:B:155:LEU:HD23	1:B:295:VAL:HG21	2.00	0.42
1:A:79:ARG:NH1	1:A:102:PRO:HD3	2.35	0.42
1:B:154:ASP:CB	1:B:295:VAL:HG23	2.49	0.42
1:A:93:VAL:HA	1:A:324:GLY:O	2.19	0.42
1:A:203:THR:HA	1:A:291:LEU:HD11	2.01	0.42
1:A:355:LEU:HG	1:A:363:ALA:HB3	2.01	0.42
1:A:386:ARG:NH1	1:A:386:ARG:HB2	2.34	0.42
1:A:196:LYS:O	1:A:200:GLN:HG3	2.19	0.42
1:B:201:ARG:HG2	1:B:202:ILE:N	2.34	0.42
1:B:44:ILE:HA	1:B:47:ILE:HG22	2.02	0.42
1:B:18:LYS:HD3	1:B:18:LYS:C	2.45	0.41
1:B:24:LYS:HA	1:B:60:GLU:O	2.20	0.41
1:B:64:LEU:HD22	1:B:65:GLU:N	2.34	0.41
1:A:21:VAL:HA	1:A:22:PRO:HD3	1.90	0.41
1:A:53:ARG:O	1:A:53:ARG:HD3	2.20	0.41
1:A:222:HIS:HD2	1:A:224:GLY:N	2.06	0.41
1:A:202:ILE:O	1:A:202:ILE:HG12	2.21	0.41
1:B:43:ALA:O	1:B:47:ILE:HG22	2.19	0.41
1:B:130:ILE:O	1:B:130:ILE:HG13	2.20	0.41
1:B:140:PRO:C	1:B:142:LYS:H	2.29	0.41
1:A:283:ARG:HG3	1:A:283:ARG:HH21	1.86	0.41
1:B:124:ILE:HG12	1:B:357:TRP:CH2	2.56	0.41
1:A:109:SER:O	1:A:112:VAL:HG12	2.21	0.41
1:A:254:GLU:O	1:A:254:GLU:HG2	2.21	0.41
1:B:56:GLY:C	1:B:58:SER:H	2.29	0.41
1:B:341:VAL:CG1	1:B:382:GLN:HG2	2.49	0.41
1:B:409:ILE:HG13	1:B:409:ILE:H	1.70	0.41
1:A:271:ARG:HB2	1:A:276:MET:CE	2.46	0.41
1:B:261:PRO:O	1:B:262:ASP:C	2.62	0.41
1:A:27:ILE:HG23	1:A:63:TRP:CE3	2.56	0.41
1:A:44:ILE:HA	1:A:47:ILE:CG2	2.50	0.41
1:A:241:VAL:HG23	1:A:245:GLU:CD	2.46	0.41
1:A:303:ALA:O	1:A:306:ALA:HB3	2.21	0.41
1:B:126:PRO:HA	1:B:146:ILE:HA	2.03	0.41
1:B:313:MET:HE2	1:B:345:THR:HG21	2.03	0.41
1:A:150:GLU:HA	1:A:202:ILE:HD12	2.01	0.40
1:A:317:ALA:HB1	1:A:319:ILE:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HG	1:A:117:MET:CE	2.51	0.40
1:A:295:VAL:HG13	1:A:296:ASN:N	2.36	0.40
1:B:115:ARG:HG2	1:B:120:LEU:HB2	2.04	0.40
1:B:369:LYS:HZ1	1:B:373:MET:CG	2.35	0.40
1:A:278:GLN:HA	1:B:306:ALA:HB2	2.03	0.40
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.86	0.40
1:B:263:GLN:H	1:B:263:GLN:CD	2.29	0.40
1:A:386:ARG:HH12	1:A:387:PHE:HE1	1.67	0.40
1:B:179:LEU:HB3	1:B:181:VAL:HG23	2.03	0.40
1:B:210:ALA:HA	1:B:215:ARG:HB2	2.02	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	399/409 (98%)	359 (90%)	35 (9%)	5 (1%)	9	18
1	B	399/409 (98%)	358 (90%)	33 (8%)	8 (2%)	6	10
All	All	798/818 (98%)	717 (90%)	68 (8%)	13 (2%)	7	14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	PRO
1	A	131	GLU
1	A	261	PRO
1	A	389	GLY
1	B	56	GLY
1	B	131	GLU
1	B	141	GLU
1	B	154	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	389	GLY
1	A	14	PHE
1	A	152	THR
1	B	57	SER
1	B	262	ASP

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	339/343 (99%)	315 (93%)	24 (7%)	13	29
1	B	339/343 (99%)	316 (93%)	23 (7%)	14	31
All	All	678/686 (99%)	631 (93%)	47 (7%)	14	30

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	16	LYS
1	A	27	ILE
1	A	28	LEU
1	A	86	GLU
1	A	94	VAL
1	A	110	VAL
1	A	116	LEU
1	A	127	VAL
1	A	128	LYS
1	A	137	LEU
1	A	149	ARG
1	A	170	LYS
1	A	194	MET
1	A	196	LYS
1	A	217	LYS
1	A	235	ARG
1	A	248	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	262	ASP
1	A	285	GLU
1	A	291	LEU
1	A	318	ASN
1	A	329	ILE
1	A	355	LEU
1	B	1	MET
1	B	28	LEU
1	B	47	ILE
1	B	49	LYS
1	B	64	LEU
1	B	79	ARG
1	B	94	VAL
1	B	100	GLU
1	B	131	GLU
1	B	141	GLU
1	B	146	ILE
1	B	151	ASN
1	B	170	LYS
1	B	205	LEU
1	B	235	ARG
1	B	244	LYS
1	B	263	GLN
1	B	285	GLU
1	B	329	ILE
1	B	355	LEU
1	B	357	TRP
1	B	373	MET
1	B	388	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	85	GLN
1	A	123	ASN
1	A	139	HIS
1	A	151	ASN
1	A	213	HIS
1	A	222	HIS
1	A	278	GLN
1	A	279	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	294	ASN
1	A	310	ASN
1	A	330	HIS
1	A	361	ASN
1	B	23	ASN
1	B	41	ASN
1	B	85	GLN
1	B	111	ASN
1	B	139	HIS
1	B	151	ASN
1	B	208	GLN
1	B	213	HIS
1	B	222	HIS
1	B	258	GLN
1	B	263	GLN
1	B	310	ASN
1	B	318	ASN
1	B	361	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	403/409 (98%)	-0.02	9 (2%) 62 58	25, 48, 80, 112	0
1	B	403/409 (98%)	0.15	16 (3%) 42 38	30, 56, 87, 118	0
All	All	806/818 (98%)	0.07	25 (3%) 51 47	25, 52, 85, 118	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	TYR	4.4
1	B	294	ASN	4.2
1	B	409	ILE	4.0
1	B	154	ASP	3.2
1	B	256	ILE	3.2
1	B	156	TYR	3.2
1	B	277	PHE	3.2
1	B	264	GLY	2.9
1	A	294	ASN	2.8
1	B	152	THR	2.8
1	A	153	ASP	2.8
1	A	14	PHE	2.8
1	B	153	ASP	2.7
1	A	264	GLY	2.5
1	B	309	GLY	2.5
1	A	152	THR	2.4
1	B	129	TYR	2.4
1	A	261	PRO	2.3
1	A	259	GLY	2.2
1	A	102	PRO	2.2
1	B	158	GLY	2.2
1	B	221	MET	2.2
1	B	373	MET	2.2
1	A	283	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	259	GLY	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 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.