



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 AM UTC

PDB ID : 1UJQ / pdb_00001ujq
Title : Crystal structure of 2-methylisocitrate lyase (PrpB) from *Salmonella enterica* serovar typhimurium
Authors : Simanshu, D.K.; Murthy, M.R.N.
Deposited on : 2003-08-11
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

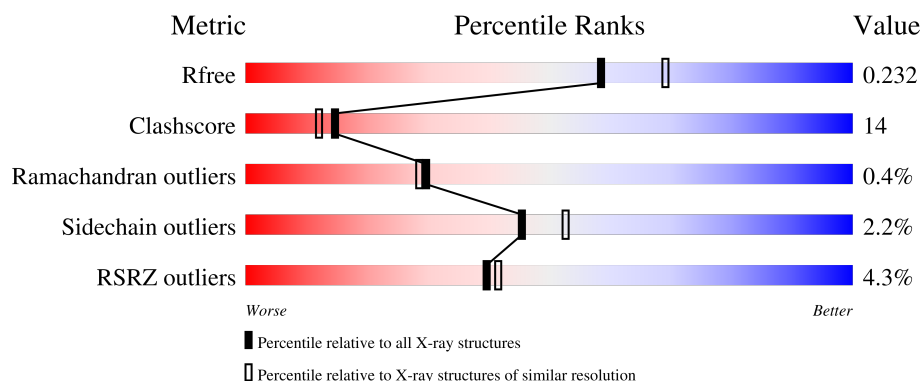
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	305	 3% 69% 18% • 11%
1	B	305	 % 71% 15% • 12%
1	C	305	 4% 62% 26% • 10%
1	D	305	 7% 62% 25% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8785 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 Probable methylisocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	1	0
			2068	1303	358	399	8			
1	B	268	Total	C	N	O	S	0	1	0
			2038	1284	353	393	8			
1	C	275	Total	C	N	O	S	0	0	0
			2087	1316	362	401	8			
1	D	268	Total	C	N	O	S	0	0	0
			2027	1279	354	386	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q56062
A	0	ALA	-	cloning artifact	UNP Q56062
A	1	SER	-	cloning artifact	UNP Q56062
A	296	LEU	-	expression tag	UNP Q56062
A	297	GLU	-	expression tag	UNP Q56062
A	298	HIS	-	expression tag	UNP Q56062
A	299	HIS	-	expression tag	UNP Q56062
A	300	HIS	-	expression tag	UNP Q56062
A	301	HIS	-	expression tag	UNP Q56062
A	302	HIS	-	expression tag	UNP Q56062
A	303	HIS	-	expression tag	UNP Q56062
B	-1	MET	-	cloning artifact	UNP Q56062
B	0	ALA	-	cloning artifact	UNP Q56062
B	1	SER	-	cloning artifact	UNP Q56062
B	296	LEU	-	expression tag	UNP Q56062
B	297	GLU	-	expression tag	UNP Q56062
B	298	HIS	-	expression tag	UNP Q56062
B	299	HIS	-	expression tag	UNP Q56062
B	300	HIS	-	expression tag	UNP Q56062
B	301	HIS	-	expression tag	UNP Q56062
B	302	HIS	-	expression tag	UNP Q56062

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	expression tag	UNP Q56062
C	-1	MET	-	cloning artifact	UNP Q56062
C	0	ALA	-	cloning artifact	UNP Q56062
C	1	SER	-	cloning artifact	UNP Q56062
C	296	LEU	-	expression tag	UNP Q56062
C	297	GLU	-	expression tag	UNP Q56062
C	298	HIS	-	expression tag	UNP Q56062
C	299	HIS	-	expression tag	UNP Q56062
C	300	HIS	-	expression tag	UNP Q56062
C	301	HIS	-	expression tag	UNP Q56062
C	302	HIS	-	expression tag	UNP Q56062
C	303	HIS	-	expression tag	UNP Q56062
D	-1	MET	-	cloning artifact	UNP Q56062
D	0	ALA	-	cloning artifact	UNP Q56062
D	1	SER	-	cloning artifact	UNP Q56062
D	296	LEU	-	expression tag	UNP Q56062
D	297	GLU	-	expression tag	UNP Q56062
D	298	HIS	-	expression tag	UNP Q56062
D	299	HIS	-	expression tag	UNP Q56062
D	300	HIS	-	expression tag	UNP Q56062
D	301	HIS	-	expression tag	UNP Q56062
D	302	HIS	-	expression tag	UNP Q56062
D	303	HIS	-	expression tag	UNP Q56062

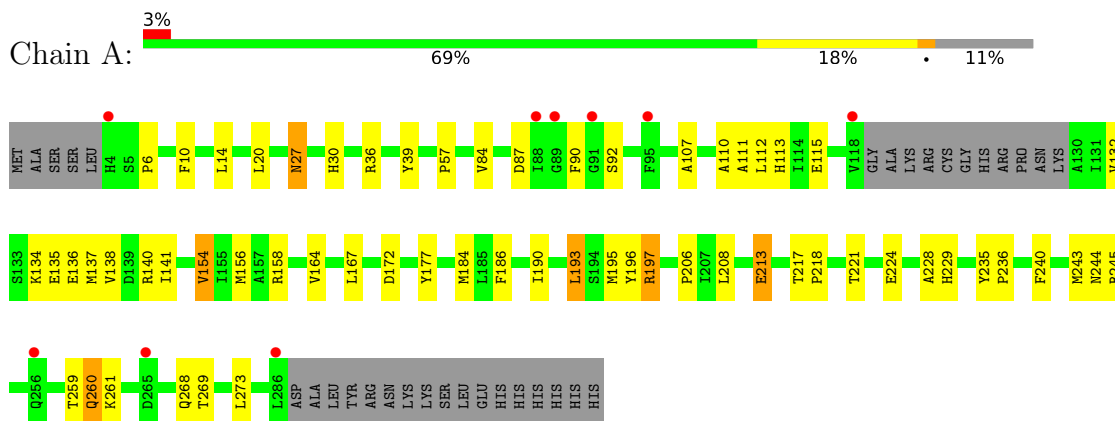
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	179	Total O 179 179	0	0
2	B	175	Total O 175 175	0	0
2	C	121	Total O 121 121	0	0
2	D	90	Total O 90 90	0	0

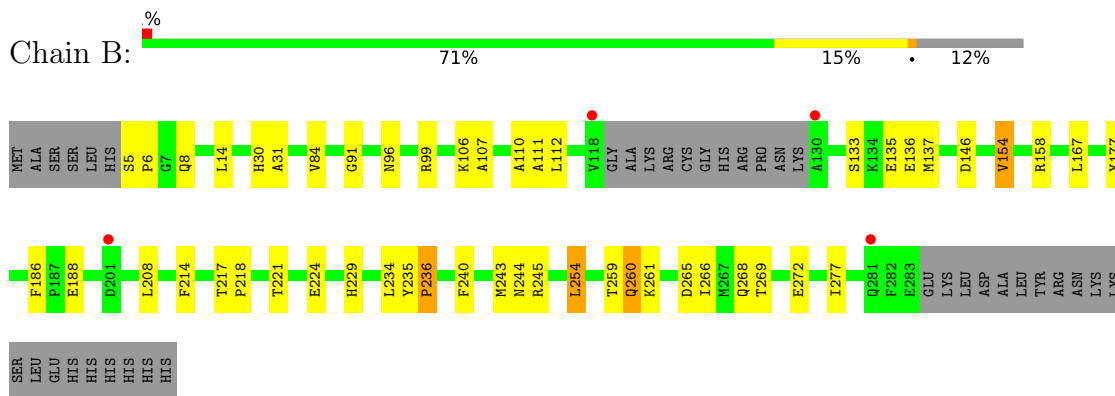
3 Residue-property plots

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.

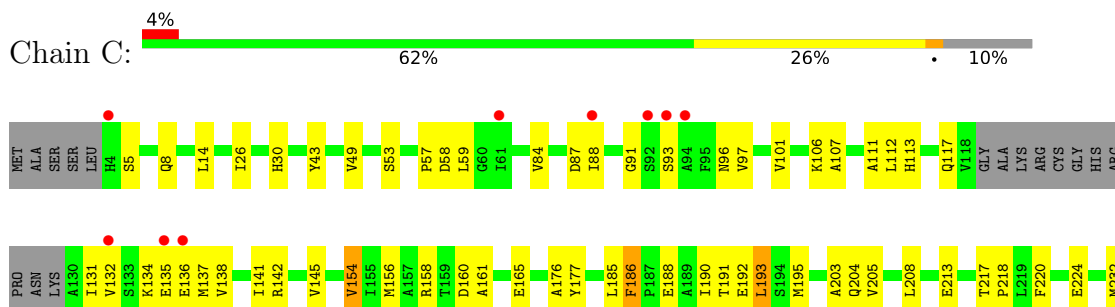
- Molecule 1: Probable methylisocitrate lyase



- Molecule 1: Probable methylisocitrate lyase

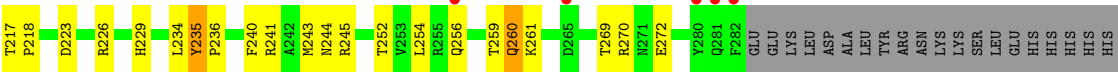
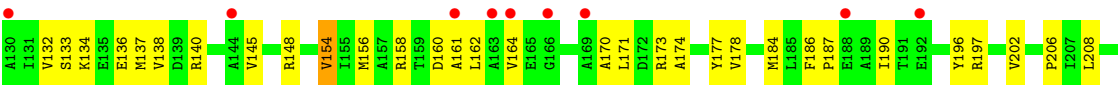
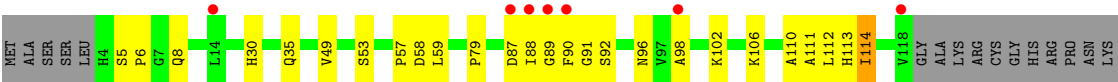


- Molecule 1: Probable methylisocitrate lyase





● Molecule 1: Probable methylisocitrate lyase



HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.81Å 99.09Å 201.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.10 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-2.10) 92.9 (19.99-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.232 0.204 , 0.232	Depositor DCC
R_{free} test set	3515 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.5	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	8785	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/2098	0.87	9/2848 (0.3%)
1	B	0.40	0/2068	0.88	7/2809 (0.2%)
1	C	0.37	1/2118 (0.0%)	0.84	5/2876 (0.2%)
1	D	0.34	0/2058	0.82	3/2795 (0.1%)
All	All	0.37	1/8342 (0.0%)	0.85	24/11328 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	MET	SD-CE	-5.95	1.64	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	TYR	CA-C-N	7.66	127.20	119.24
1	D	235	TYR	C-N-CA	7.66	127.20	119.24
1	C	235	TYR	CA-C-N	7.29	127.64	119.32
1	C	235	TYR	C-N-CA	7.29	127.64	119.32
1	C	154	VAL	N-CA-C	6.99	118.12	108.89
1	B	154	VAL	N-CA-C	6.72	117.76	108.89
1	A	235	TYR	CA-C-N	6.65	126.90	119.32
1	A	235	TYR	C-N-CA	6.65	126.90	119.32
1	B	236	PRO	N-CA-C	6.49	123.42	113.75
1	A	236	PRO	N-CA-C	6.33	123.19	113.75
1	B	235	TYR	CA-C-N	6.15	126.33	119.32
1	B	235	TYR	C-N-CA	6.15	126.33	119.32
1	A	164	VAL	N-CA-C	6.01	116.07	110.42
1	A	154	VAL	N-CA-C	5.78	116.90	108.58
1	C	236	PRO	N-CA-C	5.77	122.34	113.75
1	B	268	GLN	N-CA-C	-5.49	102.15	110.28
1	A	268	GLN	N-CA-C	-5.49	101.73	109.96
1	A	167	LEU	N-CA-C	5.40	116.85	111.07
1	A	84	VAL	N-CA-C	5.29	116.20	108.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	VAL	N-CA-C	5.24	116.12	108.53
1	C	84	VAL	N-CA-C	5.17	115.92	108.48
1	D	154	VAL	N-CA-C	5.12	115.95	108.58
1	A	196	TYR	N-CA-C	-5.07	105.83	111.36
1	B	31	ALA	N-CA-C	-5.05	105.85	111.36

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	2068	0	2066	48	0
1	B	2038	0	2035	37	0
1	C	2087	0	2089	90	0
1	D	2027	0	2030	79	0
2	A	179	0	0	3	0
2	B	175	0	0	4	0
2	C	121	0	0	5	0
2	D	90	0	0	4	0
All	All	8785	0	8220	229	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 14.

All (229) 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:260:GLN:H	1:A:260:GLN:HE21	1.09	0.97
1:C:260:GLN:H	1:C:260:GLN:HE21	0.98	0.96
1:B:260:GLN:H	1:B:260:GLN:HE21	0.98	0.94
1:C:260:GLN:HE21	1:C:260:GLN:N	1.66	0.93
1:D:260:GLN:HE21	1:D:260:GLN:N	1.67	0.92
1:C:243:MET:HG3	1:D:243:MET:HB2	1.50	0.91
1:C:30:HIS:NE2	1:C:243:MET:HE3	1.84	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:MET:HE2	1:D:243:MET:HE3	1.56	0.88
1:C:192:GLU:H	1:C:195:MET:HE3	1.37	0.87
1:C:260:GLN:H	1:C:260:GLN:NE2	1.72	0.87
1:B:146:ASP:HB2	2:B:462:HOH:O	1.75	0.86
1:D:260:GLN:HE21	1:D:260:GLN:H	0.91	0.86
1:C:250:VAL:HG22	1:C:263:VAL:HG11	1.58	0.84
1:B:260:GLN:HE21	1:B:260:GLN:N	1.75	0.84
1:C:26:ILE:HG21	1:C:243:MET:HE1	1.58	0.83
1:C:93:SER:HB3	1:C:96:ASN:ND2	1.95	0.82
1:A:132:VAL:HB	1:A:136:GLU:HG2	1.62	0.81
1:A:137:MET:HE3	1:A:140:ARG:HB2	1.63	0.80
1:C:192:GLU:N	1:C:195:MET:HE3	1.97	0.79
1:A:197:ARG:HD3	1:A:228:ALA:HA	1.67	0.77
1:C:243:MET:HE2	1:D:243:MET:CE	2.15	0.77
1:D:114:ILE:HD13	1:D:114:ILE:H	1.49	0.77
1:D:260:GLN:H	1:D:260:GLN:NE2	1.76	0.75
1:D:252:THR:O	1:D:256:GLN:HG3	1.89	0.73
1:D:57:PRO:HB2	1:D:59:LEU:HD13	1.70	0.73
1:D:132:VAL:CG1	1:D:136:GLU:HB3	2.19	0.72
1:C:57:PRO:HB2	1:C:59:LEU:HD13	1.73	0.71
1:D:269:THR:OG1	1:D:272:GLU:HG3	1.92	0.70
1:C:269:THR:OG1	1:C:272:GLU:HG3	1.93	0.69
1:A:27:ASN:C	1:A:27:ASN:HD22	2.02	0.68
1:D:137:MET:HE3	1:D:140:ARG:HB3	1.75	0.67
1:D:91:GLY:HA3	1:D:96:ASN:HB3	1.77	0.66
1:D:223:ASP:HA	1:D:226:ARG:NH1	2.10	0.66
1:A:260:GLN:HE21	1:A:260:GLN:N	1.90	0.65
1:C:281:GLN:HB2	2:C:365:HOH:O	1.95	0.65
1:C:245:ARG:HD3	2:D:334:HOH:O	1.98	0.64
1:A:193:LEU:HG	1:A:228:ALA:HB2	1.80	0.63
1:A:244:ASN:ND2	1:B:30:HIS:HE1	1.95	0.63
1:A:259:THR:OG1	1:A:261:LYS:HG3	1.99	0.62
1:D:112:LEU:HD12	1:D:112:LEU:C	2.25	0.61
1:D:208:LEU:C	1:D:208:LEU:HD23	2.25	0.61
1:D:111:ALA:HB2	1:D:154:VAL:HB	1.82	0.61
1:A:134:LYS:O	1:A:138:VAL:HG23	2.01	0.61
1:C:191:THR:OG1	1:C:195:MET:HE1	2.01	0.61
1:D:223:ASP:HA	1:D:226:ARG:HH12	1.65	0.61
1:C:132:VAL:HB	1:C:136:GLU:HG2	1.81	0.61
1:D:134:LYS:O	1:D:138:VAL:HG23	2.01	0.60
1:A:244:ASN:HD22	1:B:30:HIS:HE1	1.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:C	1:A:112:LEU:HD12	2.27	0.60
1:D:6:PRO:HB2	1:D:110:ALA:HB2	1.83	0.60
1:D:89:GLY:C	1:D:91:GLY:H	2.09	0.59
1:C:30:HIS:NE2	1:C:243:MET:CE	2.62	0.59
1:C:252:THR:CG2	1:C:256:GLN:HE21	2.16	0.59
1:B:112:LEU:HD12	1:B:112:LEU:C	2.28	0.59
1:B:259:THR:OG1	1:B:261:LYS:HG3	2.03	0.59
1:D:132:VAL:HG11	1:D:136:GLU:HB3	1.85	0.58
1:B:234:LEU:HG	1:B:236:PRO:HD3	1.86	0.57
1:C:192:GLU:HG3	2:C:362:HOH:O	2.05	0.57
1:B:269:THR:OG1	1:B:272:GLU:HG3	2.05	0.56
1:C:26:ILE:CG2	1:C:243:MET:HE1	2.34	0.56
1:D:111:ALA:CB	1:D:154:VAL:HB	2.35	0.56
1:A:107:ALA:O	1:D:106:LYS:HE2	2.04	0.56
1:A:221:THR:OG1	1:A:224:GLU:HG3	2.05	0.56
1:A:30:HIS:HE1	1:B:244:ASN:ND2	2.03	0.56
1:A:115:GLU:HA	1:A:158:ARG:O	2.06	0.55
1:A:240:PHE:O	1:A:243:MET:HG2	2.06	0.55
1:C:158:ARG:NH2	1:C:188:GLU:HG3	2.21	0.55
1:B:5:SER:OG	1:B:8:GLN:HG3	2.06	0.55
1:C:14:LEU:HD21	1:C:232:MET:CG	2.37	0.55
1:C:213:GLU:CD	1:C:213:GLU:H	2.15	0.55
1:B:188:GLU:HG2	2:B:409:HOH:O	2.07	0.54
1:C:203:ALA:O	1:C:204:GLN:HB2	2.07	0.54
1:A:243:MET:HB2	1:B:243:MET:HB2	1.87	0.54
1:A:27:ASN:ND2	1:A:30:HIS:H	2.05	0.54
1:C:30:HIS:HE1	1:D:244:ASN:HD22	1.56	0.54
1:D:186:PHE:CD2	1:D:186:PHE:C	2.85	0.54
1:A:132:VAL:HB	1:A:136:GLU:CG	2.37	0.54
1:D:187:PRO:HB2	1:D:190:ILE:HD11	1.89	0.54
1:C:243:MET:CG	1:D:243:MET:HB2	2.33	0.54
1:C:244:ASN:HD22	1:D:30:HIS:HE1	1.56	0.54
1:D:240:PHE:O	1:D:243:MET:HG2	2.08	0.54
1:C:138:VAL:O	1:C:142:ARG:HG3	2.07	0.53
1:B:106:LYS:HE2	1:C:107:ALA:O	2.08	0.53
1:C:277:ILE:HD12	1:D:57:PRO:HA	1.91	0.53
1:D:145:VAL:HG13	1:D:148:ARG:NH2	2.24	0.53
1:B:111:ALA:CB	1:B:154:VAL:HB	2.39	0.53
1:C:5:SER:HB3	1:C:8:GLN:OE1	2.08	0.52
1:C:250:VAL:HG22	1:C:263:VAL:CG1	2.33	0.52
1:D:197:ARG:HG2	1:D:229:HIS:HD2	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LEU:HD23	1:C:208:LEU:C	2.34	0.52
1:D:132:VAL:HG12	1:D:136:GLU:HB3	1.92	0.52
1:A:111:ALA:HB2	1:A:154:VAL:HB	1.91	0.52
1:C:111:ALA:CB	1:C:154:VAL:HB	2.40	0.52
1:C:235:TYR:CG	1:D:254:LEU:HD21	2.44	0.52
1:A:113:HIS:HA	1:A:156:MET:O	2.09	0.52
1:A:57:PRO:HA	1:B:277:ILE:HD12	1.91	0.51
1:C:137:MET:HG2	1:C:177:TYR:CZ	2.45	0.51
1:A:30:HIS:HE1	1:B:244:ASN:HD22	1.56	0.51
1:C:30:HIS:HE1	1:D:244:ASN:ND2	2.08	0.51
1:D:114:ILE:HD13	1:D:114:ILE:N	2.21	0.51
1:D:197:ARG:HG2	1:D:229:HIS:CD2	2.46	0.51
1:B:265:ASP:OD1	1:B:266:ILE:HG23	2.10	0.51
1:C:193:LEU:HD21	1:C:224:GLU:HB3	1.92	0.51
1:D:186:PHE:C	1:D:186:PHE:HD2	2.19	0.51
1:D:187:PRO:HB2	1:D:190:ILE:CD1	2.40	0.51
1:C:58:ASP:C	1:C:59:LEU:HD12	2.36	0.51
1:A:36:ARG:HG3	2:A:471:HOH:O	2.10	0.51
1:A:137:MET:CE	1:A:140:ARG:HB2	2.39	0.51
1:D:113:HIS:HA	1:D:156:MET:O	2.11	0.51
1:D:171:LEU:HD22	1:D:202:VAL:HG21	1.91	0.51
1:A:134:LYS:HE2	1:A:172:ASP:OD1	2.11	0.51
1:C:113:HIS:HA	1:C:156:MET:O	2.11	0.51
1:A:30:HIS:HD2	2:A:397:HOH:O	1.94	0.50
2:C:372:HOH:O	1:D:245:ARG:HD3	2.11	0.50
1:D:5:SER:HB3	1:D:8:GLN:NE2	2.26	0.50
1:C:117:GLN:HE21	1:C:160:ASP:CG	2.19	0.50
1:C:186:PHE:C	1:C:186:PHE:CD2	2.90	0.50
1:C:252:THR:HG22	1:C:256:GLN:HE21	1.75	0.50
1:D:132:VAL:HG21	1:D:140:ARG:NH2	2.27	0.50
1:C:30:HIS:CD2	1:C:243:MET:HE3	2.46	0.50
1:D:114:ILE:HD13	1:D:156:MET:O	2.11	0.50
1:C:185:LEU:HD23	1:C:205:VAL:HG21	1.92	0.50
1:C:185:LEU:HD23	1:C:205:VAL:CG2	2.42	0.49
1:C:263:VAL:HG12	1:C:263:VAL:O	2.13	0.49
1:D:145:VAL:HG13	1:D:148:ARG:HH21	1.78	0.49
1:D:137:MET:HG2	1:D:177:TYR:CZ	2.48	0.49
1:B:137:MET:HG2	1:B:177:TYR:CZ	2.47	0.49
1:A:184:MET:HG2	1:A:206:PRO:HB2	1.95	0.48
1:C:112:LEU:C	1:C:112:LEU:HD12	2.39	0.48
1:D:88:ILE:HD11	2:D:383:HOH:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HG3	1:A:229:HIS:CE1	2.48	0.48
1:B:208:LEU:C	1:B:208:LEU:HD23	2.38	0.48
1:D:87:ASP:O	1:D:114:ILE:HA	2.13	0.48
1:C:93:SER:H	1:C:96:ASN:HD22	1.61	0.48
1:C:234:LEU:HG	1:C:236:PRO:HD3	1.95	0.48
2:C:310:HOH:O	1:D:241:ARG:HG2	2.12	0.48
1:D:113:HIS:HB3	1:D:156:MET:HB3	1.94	0.48
1:A:111:ALA:CB	1:A:154:VAL:HB	2.43	0.48
1:C:30:HIS:HD2	2:C:356:HOH:O	1.96	0.48
1:D:161:ALA:CB	1:D:173:ARG:HD2	2.44	0.48
1:B:91:GLY:HA3	1:B:96:ASN:CB	2.44	0.48
1:A:213:GLU:CD	1:A:213:GLU:H	2.21	0.48
1:D:98:ALA:O	1:D:102:LYS:HG3	2.13	0.48
1:D:5:SER:HB3	1:D:8:GLN:HE21	1.77	0.47
1:C:111:ALA:HB2	1:C:154:VAL:HB	1.96	0.47
1:D:132:VAL:HG12	1:D:133:SER:N	2.29	0.47
1:D:174:ALA:O	1:D:178:VAL:HG23	2.13	0.47
1:B:260:GLN:H	1:B:260:GLN:NE2	1.83	0.47
1:C:87:ASP:OD2	1:C:88:ILE:HG12	2.14	0.47
1:C:263:VAL:HG13	1:C:266:ILE:HD11	1.97	0.47
1:A:186:PHE:C	1:A:186:PHE:CD2	2.93	0.47
1:C:186:PHE:C	1:C:186:PHE:HD2	2.22	0.47
1:D:259:THR:OG1	1:D:261:LYS:HG3	2.14	0.47
1:D:89:GLY:O	1:D:91:GLY:N	2.47	0.47
1:A:137:MET:HE3	1:A:137:MET:O	2.15	0.47
1:A:137:MET:HE2	1:A:141:ILE:HG13	1.97	0.47
1:B:111:ALA:HB2	1:B:154:VAL:HB	1.96	0.47
1:C:14:LEU:HD21	1:C:232:MET:HG2	1.97	0.47
1:C:213:GLU:HG2	1:C:241:ARG:NE	2.30	0.47
1:A:137:MET:HG2	1:A:177:TYR:CZ	2.50	0.47
1:C:244:ASN:ND2	1:D:30:HIS:HE1	2.12	0.46
1:D:162:LEU:HD13	1:D:162:LEU:C	2.41	0.46
1:D:184:MET:HG2	1:D:206:PRO:HB2	1.96	0.46
1:C:91:GLY:HA3	1:C:96:ASN:HB3	1.96	0.46
1:D:158:ARG:HA	1:D:186:PHE:HB3	1.98	0.46
1:D:162:LEU:HA	1:D:170:ALA:HB2	1.98	0.46
1:C:134:LYS:O	1:C:138:VAL:HG23	2.16	0.46
1:A:208:LEU:C	1:A:208:LEU:HD23	2.41	0.46
1:C:253:VAL:O	1:C:257:GLU:HG3	2.16	0.46
1:A:39:TYR:OH	1:B:254:LEU:HB3	2.15	0.46
1:D:160:ASP:O	1:D:164:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASN:C	1:A:27:ASN:ND2	2.74	0.45
1:A:135:GLU:CD	1:A:135:GLU:H	2.23	0.45
1:C:213:GLU:HG2	1:C:241:ARG:HE	1.80	0.45
1:A:6:PRO:HB2	1:A:110:ALA:HB2	1.99	0.45
1:C:243:MET:HE2	1:D:243:MET:SD	2.55	0.45
1:D:58:ASP:C	1:D:59:LEU:HD12	2.41	0.45
1:C:235:TYR:CE2	1:D:254:LEU:HD11	2.51	0.45
1:C:135:GLU:H	1:C:135:GLU:CD	2.25	0.45
1:B:135:GLU:CD	1:B:135:GLU:H	2.25	0.45
1:A:132:VAL:CB	1:A:136:GLU:HG2	2.41	0.45
1:B:186:PHE:C	1:B:186:PHE:CD2	2.94	0.45
1:C:278:ASN:O	1:C:282:PHE:HD1	2.00	0.44
1:D:89:GLY:C	1:D:91:GLY:N	2.72	0.44
1:B:217:THR:HA	1:B:218:PRO:HD3	1.81	0.44
1:B:240:PHE:O	1:B:243:MET:HG2	2.17	0.44
1:C:253:VAL:HG11	1:C:263:VAL:HG23	1.99	0.44
1:B:107:ALA:O	1:C:106:LYS:HE2	2.17	0.44
1:D:190:ILE:HD12	1:D:196:TYR:CE1	2.52	0.44
1:A:269:THR:HA	1:B:214:PHE:CE2	2.53	0.44
1:C:193:LEU:HD13	1:C:220:PHE:CE2	2.53	0.44
1:C:91:GLY:HA3	1:C:96:ASN:CB	2.47	0.44
1:D:30:HIS:HD2	2:D:310:HOH:O	2.01	0.44
1:B:91:GLY:HA3	1:B:96:ASN:HB3	2.00	0.44
1:C:141:ILE:O	1:C:145:VAL:HG23	2.18	0.44
1:A:10:PHE:O	1:A:14:LEU:HD23	2.17	0.43
1:D:5:SER:CB	1:D:8:GLN:HE21	2.32	0.43
1:C:43:TYR:CG	1:C:234:LEU:HD11	2.54	0.43
1:D:234:LEU:HG	1:D:236:PRO:HD3	1.99	0.43
1:C:49:VAL:O	1:C:53:SER:HB2	2.19	0.43
1:C:281:GLN:O	1:C:284:GLU:HB2	2.19	0.43
1:C:5:SER:HB3	1:C:8:GLN:HG3	2.00	0.43
1:C:161:ALA:O	1:C:165:GLU:N	2.51	0.43
1:D:49:VAL:O	1:D:53:SER:HB2	2.18	0.42
1:D:270:ARG:NH2	2:D:352:HOH:O	2.50	0.42
1:C:93:SER:HB3	1:C:96:ASN:HD22	1.77	0.42
1:C:254:LEU:HD21	1:D:235:TYR:CG	2.54	0.42
1:A:87[B]:ASP:HB3	2:A:477:HOH:O	2.19	0.42
1:C:5:SER:HB3	1:C:8:GLN:CD	2.45	0.42
1:B:6:PRO:HB2	1:B:110:ALA:HA	2.02	0.42
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.90	0.42
1:A:217:THR:HA	1:A:218:PRO:HD3	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:OG1	1:B:224:GLU:HG3	2.20	0.42
1:C:254:LEU:HD13	1:C:260:GLN:HB3	2.02	0.42
1:D:35:GLN:HE22	1:D:79:PRO:HG2	1.85	0.42
1:B:99:ARG:HG2	2:B:375:HOH:O	2.20	0.41
1:D:217:THR:HA	1:D:218:PRO:HD3	1.93	0.41
1:B:133:SER:OG	1:B:136:GLU:HG3	2.20	0.41
1:C:5:SER:HB3	1:C:8:GLN:CG	2.50	0.41
1:A:190:ILE:HG23	1:A:195:MET:HB3	2.01	0.41
1:C:134:LYS:HD3	1:C:176:ALA:HB2	2.02	0.41
1:C:131:ILE:HD13	1:C:161:ALA:HA	2.03	0.41
1:B:158:ARG:HA	1:B:186:PHE:HB3	2.03	0.41
1:C:190:ILE:HG23	1:C:195:MET:HB2	2.03	0.41
1:A:14:LEU:HD22	1:A:20:LEU:CD2	2.51	0.41
1:B:229:HIS:NE2	2:B:404:HOH:O	2.33	0.41
1:C:217:THR:HA	1:C:218:PRO:HD3	1.96	0.41
1:C:243:MET:CE	1:D:243:MET:HE3	2.38	0.41
1:C:97:VAL:O	1:C:101:VAL:HG23	2.21	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	269/305 (88%)	260 (97%)	7 (3%)	2 (1%)	18	15
1	B	265/305 (87%)	262 (99%)	3 (1%)	0	100	100
1	C	271/305 (89%)	259 (96%)	12 (4%)	0	100	100
1	D	264/305 (87%)	259 (98%)	3 (1%)	2 (1%)	16	12
All	All	1069/1220 (88%)	1040 (97%)	25 (2%)	4 (0%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	90	PHE
1	A	90	PHE
1	A	92	SER
1	D	92	SER

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	211/239 (88%)	204 (97%)	7 (3%)	33	37
1	B	208/239 (87%)	203 (98%)	5 (2%)	43	49
1	C	213/239 (89%)	209 (98%)	4 (2%)	50	58
1	D	206/239 (86%)	204 (99%)	2 (1%)	68	76
All	All	838/956 (88%)	820 (98%)	18 (2%)	45	54

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	193	LEU
1	A	197	ARG
1	A	213	GLU
1	A	245	ARG
1	A	260	GLN
1	A	273	LEU
1	B	14	LEU
1	B	167	LEU
1	B	245	ARG
1	B	254	LEU
1	B	260	GLN
1	C	186	PHE
1	C	193	LEU
1	C	260	GLN
1	C	273	LEU
1	D	114	ILE
1	D	260	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	30	HIS
1	A	35	GLN
1	A	117	GLN
1	A	229	HIS
1	A	244	ASN
1	A	260	GLN
1	A	271	ASN
1	A	281	GLN
1	B	30	HIS
1	B	175	GLN
1	B	204	GLN
1	B	244	ASN
1	B	260	GLN
1	B	271	ASN
1	B	281	GLN
1	C	30	HIS
1	C	40	GLN
1	C	96	ASN
1	C	117	GLN
1	C	152	ASN
1	C	175	GLN
1	C	229	HIS
1	C	244	ASN
1	C	256	GLN
1	C	260	GLN
1	C	281	GLN
1	D	8	GLN
1	D	30	HIS
1	D	35	GLN
1	D	117	GLN
1	D	204	GLN
1	D	229	HIS
1	D	244	ASN
1	D	256	GLN
1	D	260	GLN
1	D	271	ASN

5.3.3 RNA ⓘ

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 [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	272/305 (89%)	-0.03	9 (3%)	49	51	21, 32, 57, 74	1 (0%)
1	B	268/305 (87%)	-0.24	4 (1%)	72	74	19, 29, 43, 70	1 (0%)
1	C	275/305 (90%)	0.28	13 (4%)	36	38	25, 40, 62, 79	0
1	D	268/305 (87%)	0.55	21 (7%)	19	20	25, 45, 68, 93	0
All	All	1083/1220 (88%)	0.14	47 (4%)	40	41	19, 35, 62, 93	2 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	88	ILE	5.0
1	D	282	PHE	4.2
1	C	289	LEU	4.2
1	A	4	HIS	4.0
1	A	91	GLY	3.7
1	A	89	GLY	3.6
1	B	118	VAL	3.6
1	D	90	PHE	3.3
1	C	88	ILE	3.3
1	D	87	ASP	3.2
1	D	169	ALA	3.1
1	D	118	VAL	3.0
1	A	286	LEU	3.0
1	A	88	ILE	2.9
1	C	288	ALA	2.9
1	A	95	PHE	2.8
1	D	265	ASP	2.8
1	D	166	GLY	2.7
1	B	281	GLN	2.7
1	A	118	VAL	2.7
1	D	130	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	188	GLU	2.7
1	D	280	TYR	2.7
1	C	94	ALA	2.6
1	C	4	HIS	2.6
1	C	265	ASP	2.6
1	D	256	GLN	2.4
1	B	130	ALA	2.4
1	D	164	VAL	2.4
1	C	93	SER	2.4
1	D	192	GLU	2.3
1	D	281	GLN	2.3
1	D	14	LEU	2.3
1	A	265	ASP	2.3
1	C	263	VAL	2.3
1	C	135	GLU	2.2
1	C	136	GLU	2.2
1	D	144	ALA	2.2
1	D	163	ALA	2.2
1	C	132	VAL	2.1
1	D	98	ALA	2.1
1	C	92	SER	2.1
1	B	201	ASP	2.1
1	A	256	GLN	2.1
1	D	161	ALA	2.1
1	C	61	ILE	2.0
1	D	89	GLY	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.