



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:32 PM UTC

PDB ID : 2HYX / pdb_00002hyx
Title : Structure of the C-terminal domain of DipZ from Mycobacterium tuberculosis
Authors : Goldstone, D.; Baker, E.N.; Metcalf, P.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2006-08-08
Resolution : 1.90 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

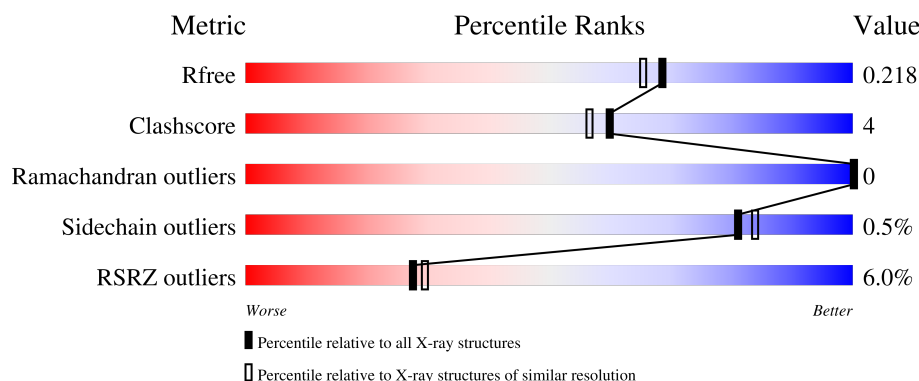
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	352	3% 83% 11% • 5%
1	B	352	14% 79% 13% • 7%
1	C	352	3% 86% 8% • 5%
1	D	352	3% 84% 9% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10818 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 Protein dipZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2503	1592	425	481	5			
1	B	328	Total	C	N	O	S	0	0	0
			2434	1549	410	470	5			
1	C	333	Total	C	N	O	S	0	0	0
			2501	1590	425	481	5			
1	D	329	Total	C	N	O	S	0	0	0
			2481	1578	424	474	5			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	cloning artifact	UNP Q10801
A	-21	ARG	-	cloning artifact	UNP Q10801
A	-20	GLY	-	cloning artifact	UNP Q10801
A	-19	SER	-	cloning artifact	UNP Q10801
A	-18	HIS	-	cloning artifact	UNP Q10801
A	-17	HIS	-	cloning artifact	UNP Q10801
A	-16	HIS	-	cloning artifact	UNP Q10801
A	-15	HIS	-	cloning artifact	UNP Q10801
A	-14	HIS	-	cloning artifact	UNP Q10801
A	-13	HIS	-	cloning artifact	UNP Q10801
A	-12	GLY	-	cloning artifact	UNP Q10801
A	-11	SER	-	cloning artifact	UNP Q10801
A	-10	GLU	-	cloning artifact	UNP Q10801
A	-9	ASN	-	cloning artifact	UNP Q10801
A	-8	LEU	-	cloning artifact	UNP Q10801
A	-7	TYR	-	cloning artifact	UNP Q10801
A	-6	PHE	-	cloning artifact	UNP Q10801
A	-5	GLN	-	cloning artifact	UNP Q10801
A	-4	SER	-	cloning artifact	UNP Q10801
A	-3	GLY	-	cloning artifact	UNP Q10801
A	-2	ALA	-	cloning artifact	UNP Q10801

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q10801
B	-22	MET	-	cloning artifact	UNP Q10801
B	-21	ARG	-	cloning artifact	UNP Q10801
B	-20	GLY	-	cloning artifact	UNP Q10801
B	-19	SER	-	cloning artifact	UNP Q10801
B	-18	HIS	-	cloning artifact	UNP Q10801
B	-17	HIS	-	cloning artifact	UNP Q10801
B	-16	HIS	-	cloning artifact	UNP Q10801
B	-15	HIS	-	cloning artifact	UNP Q10801
B	-14	HIS	-	cloning artifact	UNP Q10801
B	-13	HIS	-	cloning artifact	UNP Q10801
B	-12	GLY	-	cloning artifact	UNP Q10801
B	-11	SER	-	cloning artifact	UNP Q10801
B	-10	GLU	-	cloning artifact	UNP Q10801
B	-9	ASN	-	cloning artifact	UNP Q10801
B	-8	LEU	-	cloning artifact	UNP Q10801
B	-7	TYR	-	cloning artifact	UNP Q10801
B	-6	PHE	-	cloning artifact	UNP Q10801
B	-5	GLN	-	cloning artifact	UNP Q10801
B	-4	SER	-	cloning artifact	UNP Q10801
B	-3	GLY	-	cloning artifact	UNP Q10801
B	-2	ALA	-	cloning artifact	UNP Q10801
B	-1	MET	-	cloning artifact	UNP Q10801
C	-22	MET	-	cloning artifact	UNP Q10801
C	-21	ARG	-	cloning artifact	UNP Q10801
C	-20	GLY	-	cloning artifact	UNP Q10801
C	-19	SER	-	cloning artifact	UNP Q10801
C	-18	HIS	-	cloning artifact	UNP Q10801
C	-17	HIS	-	cloning artifact	UNP Q10801
C	-16	HIS	-	cloning artifact	UNP Q10801
C	-15	HIS	-	cloning artifact	UNP Q10801
C	-14	HIS	-	cloning artifact	UNP Q10801
C	-13	HIS	-	cloning artifact	UNP Q10801
C	-12	GLY	-	cloning artifact	UNP Q10801
C	-11	SER	-	cloning artifact	UNP Q10801
C	-10	GLU	-	cloning artifact	UNP Q10801
C	-9	ASN	-	cloning artifact	UNP Q10801
C	-8	LEU	-	cloning artifact	UNP Q10801
C	-7	TYR	-	cloning artifact	UNP Q10801
C	-6	PHE	-	cloning artifact	UNP Q10801
C	-5	GLN	-	cloning artifact	UNP Q10801
C	-4	SER	-	cloning artifact	UNP Q10801

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	cloning artifact	UNP Q10801
C	-2	ALA	-	cloning artifact	UNP Q10801
C	-1	MET	-	cloning artifact	UNP Q10801
D	-22	MET	-	cloning artifact	UNP Q10801
D	-21	ARG	-	cloning artifact	UNP Q10801
D	-20	GLY	-	cloning artifact	UNP Q10801
D	-19	SER	-	cloning artifact	UNP Q10801
D	-18	HIS	-	cloning artifact	UNP Q10801
D	-17	HIS	-	cloning artifact	UNP Q10801
D	-16	HIS	-	cloning artifact	UNP Q10801
D	-15	HIS	-	cloning artifact	UNP Q10801
D	-14	HIS	-	cloning artifact	UNP Q10801
D	-13	HIS	-	cloning artifact	UNP Q10801
D	-12	GLY	-	cloning artifact	UNP Q10801
D	-11	SER	-	cloning artifact	UNP Q10801
D	-10	GLU	-	cloning artifact	UNP Q10801
D	-9	ASN	-	cloning artifact	UNP Q10801
D	-8	LEU	-	cloning artifact	UNP Q10801
D	-7	TYR	-	cloning artifact	UNP Q10801
D	-6	PHE	-	cloning artifact	UNP Q10801
D	-5	GLN	-	cloning artifact	UNP Q10801
D	-4	SER	-	cloning artifact	UNP Q10801
D	-3	GLY	-	cloning artifact	UNP Q10801
D	-2	ALA	-	cloning artifact	UNP Q10801
D	-1	MET	-	cloning artifact	UNP Q10801

- Molecule 2 is water.

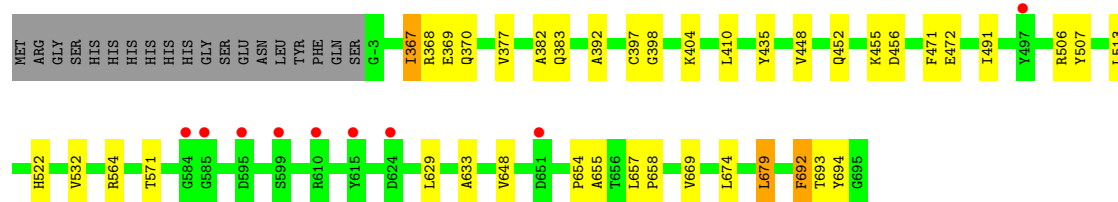
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	228	Total O 228 228	0	0
2	B	167	Total O 167 167	0	0
2	C	247	Total O 247 247	0	0
2	D	257	Total O 257 257	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

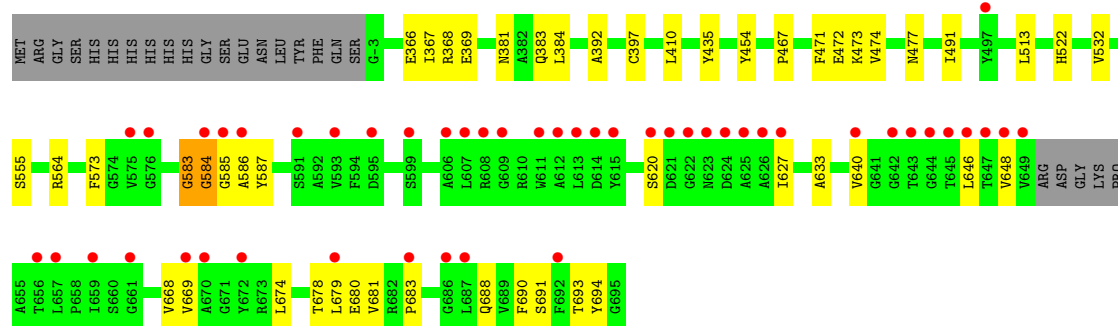
• Molecule 1: Protein dipZ

Chain A: 



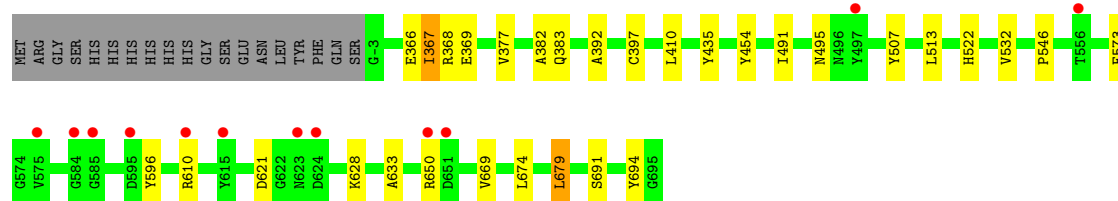
• Molecule 1: Protein dipZ

Chain B: 

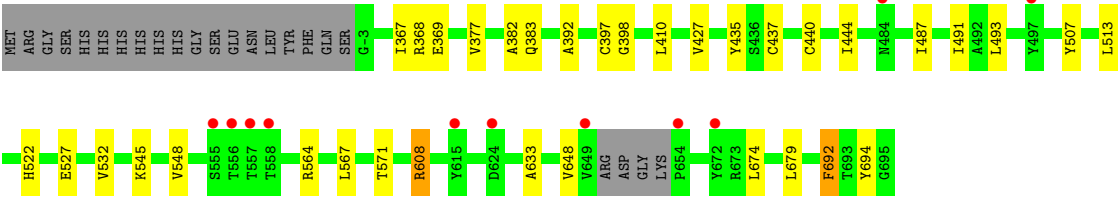
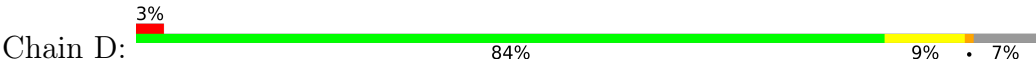


• Molecule 1: Protein dipZ

Chain C: 



• Molecule 1: Protein dipZ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.07Å 117.92Å 123.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-1.90) 97.6 (30.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.219 0.195 , 0.218	Depositor DCC
R_{free} test set	12569 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10818	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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	0/2566	0.90	7/3507 (0.2%)
1	B	0.66	10/2494 (0.4%)	0.96	11/3415 (0.3%)
1	C	0.37	0/2564	0.91	6/3505 (0.2%)
1	D	0.38	0/2543	0.91	8/3473 (0.2%)
All	All	0.46	10/10167 (0.1%)	0.92	32/13900 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	ALA	CA-CB	-12.15	1.33	1.53
1	B	584	GLY	C-O	-10.86	1.12	1.23
1	B	585	GLY	C-O	-9.80	1.12	1.23
1	B	586	ALA	C-O	-6.80	1.14	1.23
1	B	587	TYR	C-O	-6.73	1.14	1.23
1	B	584	GLY	CA-C	-6.24	1.45	1.52
1	B	583	GLY	C-O	-6.17	1.13	1.23
1	B	583	GLY	C-N	-5.82	1.27	1.33
1	B	587	TYR	CE1-CZ	-5.73	1.24	1.38
1	B	587	TYR	CG-CD1	-5.31	1.28	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	586	ALA	N-CA-C	9.85	123.33	110.43
1	B	585	GLY	CA-C-O	-9.81	114.77	122.52
1	B	583	GLY	CA-C-N	-8.10	112.05	120.31
1	B	583	GLY	C-N-CA	-8.10	112.05	120.31
1	D	507	TYR	N-CA-C	7.03	119.85	109.24
1	C	694	TYR	N-CA-C	6.93	119.47	109.14
1	D	694	TYR	N-CA-C	6.79	119.72	109.41
1	A	694	TYR	N-CA-C	6.71	119.61	109.41
1	B	435	TYR	N-CA-C	6.62	119.33	111.71
1	C	507	TYR	N-CA-C	6.51	119.06	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	367	ILE	N-CA-C	-6.50	99.08	108.17
1	B	454	TYR	N-CA-C	6.27	121.87	113.72
1	A	435	TYR	N-CA-C	6.15	118.78	111.71
1	B	564	ARG	N-CA-C	-6.11	101.37	110.23
1	C	435	TYR	N-CA-C	6.11	118.74	111.71
1	B	584	GLY	CA-C-N	-5.89	112.65	122.43
1	B	584	GLY	C-N-CA	-5.89	112.65	122.43
1	D	435	TYR	N-CA-C	5.83	119.50	112.38
1	B	694	TYR	N-CA-C	5.75	117.71	109.14
1	D	692	PHE	N-CA-C	-5.68	100.14	109.40
1	C	367	ILE	N-CA-C	-5.61	100.32	108.17
1	D	427	VAL	N-CA-C	-5.57	101.64	109.21
1	A	398	GLY	N-CA-C	5.54	119.86	112.65
1	A	564	ARG	N-CA-C	-5.47	102.30	110.23
1	C	454	TYR	N-CA-C	5.46	120.83	113.72
1	A	507	TYR	N-CA-C	5.42	117.43	109.24
1	D	398	GLY	N-CA-C	5.35	121.17	112.61
1	A	367	ILE	N-CA-C	-5.33	100.70	108.17
1	D	564	ARG	N-CA-C	-5.30	102.55	110.23
1	B	584	GLY	CA-C-O	-5.13	116.97	121.58
1	C	495	ASN	N-CA-C	5.09	118.96	112.34
1	A	692	PHE	N-CA-C	-5.08	101.12	109.40

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	2503	0	2434	24	0
1	B	2434	0	2331	26	0
1	C	2501	0	2430	17	0
1	D	2481	0	2421	17	0
2	A	228	0	0	2	0
2	B	167	0	0	2	0
2	C	247	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	257	0	0	1	0
All	All	10818	0	9616	83	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 4.

All (83) 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:C:610:ARG:HG2	1:C:621:ASP:HB3	1.72	0.70
1:D:633:ALA:HA	1:D:674:LEU:CD1	2.23	0.69
1:B:679:LEU:C	1:B:679:LEU:HD12	2.20	0.66
1:A:448:VAL:O	1:A:452:GLN:HG3	1.95	0.66
1:C:679:LEU:HD12	1:C:679:LEU:C	2.23	0.64
1:C:383:GLN:O	1:C:397:CYS:HB2	2.00	0.62
1:C:650:ARG:HD2	1:C:669:VAL:HG22	1.82	0.61
1:D:633:ALA:HA	1:D:674:LEU:HD12	1.83	0.60
1:A:404:LYS:HE3	2:A:838:HOH:O	2.01	0.60
1:D:368:ARG:O	1:D:369:GLU:HB2	2.01	0.60
1:A:679:LEU:C	1:A:679:LEU:HD23	2.28	0.59
1:D:383:GLN:O	1:D:397:CYS:HB2	2.02	0.59
1:B:633:ALA:HA	1:B:674:LEU:HD13	1.87	0.57
1:A:383:GLN:O	1:A:397:CYS:HB2	2.05	0.56
1:A:368:ARG:O	1:A:369:GLU:HB2	2.06	0.56
1:A:410:LEU:HD22	1:C:546:PRO:HB2	1.88	0.56
1:C:368:ARG:O	1:C:369:GLU:HB2	2.08	0.54
1:B:474:VAL:HB	1:B:477:ASN:ND2	2.23	0.54
1:D:633:ALA:HA	1:D:674:LEU:HD11	1.90	0.53
1:C:573:PHE:HD1	1:C:691:SER:HA	1.73	0.52
1:D:437:CYS:SG	1:D:440:CYS:SG	3.08	0.52
1:A:633:ALA:HA	1:A:674:LEU:CD1	2.40	0.52
1:B:640:VAL:HG23	1:B:688:GLN:O	2.10	0.51
1:C:377:VAL:HG13	1:C:382:ALA:HA	1.93	0.51
1:A:669:VAL:CG2	1:A:679:LEU:HD12	2.41	0.51
1:A:633:ALA:HA	1:A:674:LEU:HD13	1.92	0.50
1:B:383:GLN:O	1:B:397:CYS:HB2	2.11	0.50
1:D:444:ILE:HD13	1:D:487:ILE:HD11	1.93	0.50
1:A:513:LEU:HB3	1:A:522:HIS:HB3	1.92	0.50
1:D:545:LYS:HE3	1:D:548:VAL:HG23	1.93	0.50
1:B:693:THR:HG21	2:B:739:HOH:O	2.10	0.49
1:C:513:LEU:HB3	1:C:522:HIS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:O	1:A:370:GLN:HB2	2.13	0.49
1:B:410:LEU:HB2	1:B:491:ILE:HB	1.95	0.48
1:D:608:ARG:C	1:D:608:ARG:HD3	2.39	0.48
1:B:668:VAL:HG23	1:B:669:VAL:HG23	1.94	0.48
1:B:633:ALA:HA	1:B:674:LEU:CD1	2.43	0.48
1:D:377:VAL:HG13	1:D:382:ALA:HA	1.96	0.48
1:B:513:LEU:HB3	1:B:522:HIS:HB3	1.96	0.47
1:D:527:GLU:HA	2:D:771:HOH:O	2.15	0.47
1:B:646:LEU:C	1:B:646:LEU:HD23	2.39	0.47
1:B:679:LEU:HD12	1:B:679:LEU:O	2.14	0.47
1:D:567:LEU:CD2	1:D:674:LEU:HD11	2.44	0.47
1:A:629:LEU:HB3	1:A:679:LEU:HD22	1.97	0.46
1:C:532:VAL:HG23	2:C:851:HOH:O	2.13	0.46
1:C:573:PHE:CD1	1:C:691:SER:HA	2.50	0.46
1:A:455:LYS:HG3	1:A:456:ASP:N	2.30	0.45
1:A:679:LEU:HD23	1:A:679:LEU:O	2.16	0.45
1:B:681:VAL:O	1:B:683:PRO:HD3	2.17	0.45
1:A:471:PHE:CE1	1:A:472:GLU:HG3	2.52	0.45
1:A:392:ALA:HA	1:A:532:VAL:HG13	1.98	0.45
1:B:573:PHE:HD1	1:B:691:SER:HA	1.82	0.44
1:B:392:ALA:HA	1:B:532:VAL:HG13	2.00	0.44
1:B:368:ARG:O	1:B:369:GLU:HB2	2.17	0.44
1:B:555:SER:HB3	2:B:744:HOH:O	2.17	0.44
1:B:583:GLY:O	1:B:584:GLY:C	2.49	0.44
1:A:648:VAL:CG1	1:A:655:ALA:HB3	2.47	0.44
1:A:657:LEU:HA	1:A:658:PRO:HD3	1.88	0.44
1:A:377:VAL:HG13	1:A:382:ALA:HA	2.00	0.43
1:D:392:ALA:HA	1:D:532:VAL:HG13	2.01	0.43
1:D:648:VAL:HG13	1:D:679:LEU:HD11	2.00	0.43
1:D:410:LEU:HB2	1:D:491:ILE:HB	2.01	0.43
1:D:571:THR:HB	1:D:692:PHE:HB2	2.01	0.43
1:A:410:LEU:HB2	1:A:491:ILE:HB	1.99	0.43
1:B:690:PHE:O	1:B:691:SER:HB3	2.19	0.42
1:B:620:SER:HB2	1:B:683:PRO:HB2	2.01	0.42
1:C:679:LEU:C	1:C:679:LEU:CD1	2.92	0.42
1:A:648:VAL:O	1:A:654:PRO:HA	2.18	0.42
1:D:513:LEU:HB3	1:D:522:HIS:HB3	2.00	0.42
1:C:366:GLU:HG2	1:C:367:ILE:N	2.33	0.42
1:C:410:LEU:HB2	1:C:491:ILE:HB	2.00	0.42
1:C:596:TYR:CD1	1:C:628:LYS:HE3	2.55	0.42
1:B:471:PHE:CE1	1:B:472:GLU:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:THR:HB	1:A:692:PHE:HB2	2.02	0.42
1:B:627:ILE:O	1:B:680:GLU:HA	2.20	0.41
1:C:392:ALA:HA	1:C:532:VAL:HG13	2.03	0.41
1:A:693:THR:HG21	2:A:697:HOH:O	2.21	0.41
1:B:381:ASN:HB2	1:B:384:LEU:HD12	2.03	0.41
1:A:506:ARG:O	1:A:506:ARG:HG2	2.20	0.41
1:B:678:THR:HG22	1:B:679:LEU:N	2.37	0.41
1:B:467:PRO:HG3	1:B:473:LYS:HG2	2.03	0.40
1:C:633:ALA:HA	1:C:674:LEU:CD1	2.51	0.40
1:B:366:GLU:HG2	1:B:367:ILE:N	2.36	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	331/352 (94%)	322 (97%)	9 (3%)	0	100	100
1	B	324/352 (92%)	310 (96%)	14 (4%)	0	100	100
1	C	331/352 (94%)	321 (97%)	10 (3%)	0	100	100
1	D	325/352 (92%)	316 (97%)	9 (3%)	0	100	100
All	All	1311/1408 (93%)	1269 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	257/279 (92%)	256 (100%)	1 (0%)	84	87
1	B	245/279 (88%)	244 (100%)	1 (0%)	84	87
1	C	257/279 (92%)	256 (100%)	1 (0%)	84	87
1	D	256/279 (92%)	254 (99%)	2 (1%)	73	75
All	All	1015/1116 (91%)	1010 (100%)	5 (0%)	81	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	679	LEU
1	B	648	VAL
1	C	679	LEU
1	D	493	LEU
1	D	608	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	A	383	GLN
1	A	415	ASN
1	A	616	GLN
1	B	452	GLN
1	B	616	GLN
1	C	372	ASN
1	C	383	GLN
1	C	452	GLN
1	C	688	GLN
1	D	372	ASN
1	D	383	GLN
1	D	542	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	333/352 (94%)	0.16	9 (2%) 56 60	11, 23, 35, 41	0
1	B	328/352 (93%)	0.76	48 (14%) 6 6	15, 28, 40, 44	0
1	C	333/352 (94%)	-0.00	12 (3%) 46 49	12, 21, 34, 43	0
1	D	329/352 (93%)	0.11	11 (3%) 49 52	12, 22, 34, 40	0
All	All	1323/1408 (93%)	0.26	80 (6%) 27 29	11, 23, 37, 44	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	584	GLY	4.8
1	D	556	THR	3.9
1	D	557	THR	3.7
1	D	654	PRO	3.5
1	B	645	THR	3.4
1	B	612	ALA	3.4
1	B	608	ARG	3.4
1	C	624	ASP	3.3
1	B	623	ASN	3.2
1	B	640	VAL	3.1
1	B	624	ASP	3.1
1	B	649	VAL	3.0
1	B	625	ALA	3.0
1	B	615	TYR	3.0
1	D	497	TYR	3.0
1	A	651	ASP	2.9
1	C	651	ASP	2.9
1	B	646	LEU	2.9
1	B	609	GLY	2.8
1	B	622	GLY	2.8
1	C	623	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	585	GLY	2.7
1	B	643	THR	2.7
1	B	648	VAL	2.7
1	D	649	VAL	2.7
1	C	615	TYR	2.7
1	B	656	THR	2.7
1	C	584	GLY	2.7
1	B	692	PHE	2.7
1	A	624	ASP	2.6
1	B	621	ASP	2.6
1	B	687	LEU	2.6
1	A	610	ARG	2.5
1	B	614	ASP	2.5
1	C	556	THR	2.5
1	B	642	GLY	2.4
1	B	599	SER	2.4
1	B	586	ALA	2.4
1	B	611	TRP	2.4
1	B	497	TYR	2.4
1	B	591	SER	2.4
1	D	615	TYR	2.4
1	B	644	GLY	2.4
1	D	558	THR	2.4
1	B	661	GLY	2.4
1	B	686	GLY	2.4
1	B	606	ALA	2.3
1	B	585	GLY	2.3
1	B	593	VAL	2.3
1	B	683	PRO	2.3
1	A	615	TYR	2.3
1	C	610	ARG	2.3
1	B	595	ASP	2.3
1	B	575	VAL	2.3
1	B	613	LEU	2.3
1	B	647	THR	2.3
1	B	679	LEU	2.3
1	B	672	TYR	2.2
1	A	595	ASP	2.2
1	B	670	ALA	2.2
1	C	595	ASP	2.2
1	D	672	TYR	2.2
1	B	620	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	484	ASN	2.1
1	A	497	TYR	2.1
1	B	659	ILE	2.1
1	C	585	GLY	2.1
1	B	657	LEU	2.1
1	C	497	TYR	2.1
1	D	624	ASP	2.1
1	B	607	LEU	2.1
1	A	599	SER	2.1
1	C	650	ARG	2.1
1	D	555	SER	2.1
1	A	584	GLY	2.0
1	B	669	VAL	2.0
1	C	575	VAL	2.0
1	B	626	ALA	2.0
1	B	627	ILE	2.0
1	B	576	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.