



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:39 AM UTC

PDB ID : 4Z6K / pdb_00004z6k
Title : Alcohol dehydrogenase from the antarctic psychrophile Moraxella sp. TAE 123
Authors : Papanikolau, Y.; Bouriotis, V.; Petratos, K.
Deposited on : 2015-04-05
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

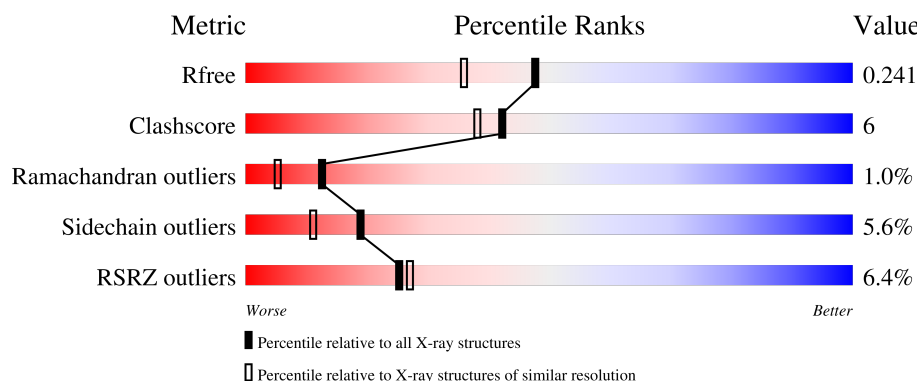
1 Overall quality at a glance

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	346	6% 84% 12% ..
1	B	346	8% 83% 12% ..
1	C	346	6% 84% 13% ..
1	D	346	6% 83% 10% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11196 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 Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	2	0
			2577	1627	442	492	16			
1	B	340	Total	C	N	O	S	0	2	0
			2521	1593	427	485	16			
1	C	345	Total	C	N	O	S	0	1	0
			2567	1621	441	489	16			
1	D	340	Total	C	N	O	S	0	2	0
			2526	1596	428	486	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	LEU	-	expression tag	UNP Q8GIX7
A	340	GLU	-	expression tag	UNP Q8GIX7
A	341	HIS	-	expression tag	UNP Q8GIX7
A	342	HIS	-	expression tag	UNP Q8GIX7
A	343	HIS	-	expression tag	UNP Q8GIX7
A	344	HIS	-	expression tag	UNP Q8GIX7
A	345	HIS	-	expression tag	UNP Q8GIX7
A	346	HIS	-	expression tag	UNP Q8GIX7
B	339	LEU	-	expression tag	UNP Q8GIX7
B	340	GLU	-	expression tag	UNP Q8GIX7
B	341	HIS	-	expression tag	UNP Q8GIX7
B	342	HIS	-	expression tag	UNP Q8GIX7
B	343	HIS	-	expression tag	UNP Q8GIX7
B	344	HIS	-	expression tag	UNP Q8GIX7
B	345	HIS	-	expression tag	UNP Q8GIX7
B	346	HIS	-	expression tag	UNP Q8GIX7
C	339	LEU	-	expression tag	UNP Q8GIX7
C	340	GLU	-	expression tag	UNP Q8GIX7
C	341	HIS	-	expression tag	UNP Q8GIX7
C	342	HIS	-	expression tag	UNP Q8GIX7
C	343	HIS	-	expression tag	UNP Q8GIX7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	344	HIS	-	expression tag	UNP Q8GIX7
C	345	HIS	-	expression tag	UNP Q8GIX7
C	346	HIS	-	expression tag	UNP Q8GIX7
D	339	LEU	-	expression tag	UNP Q8GIX7
D	340	GLU	-	expression tag	UNP Q8GIX7
D	341	HIS	-	expression tag	UNP Q8GIX7
D	342	HIS	-	expression tag	UNP Q8GIX7
D	343	HIS	-	expression tag	UNP Q8GIX7
D	344	HIS	-	expression tag	UNP Q8GIX7
D	345	HIS	-	expression tag	UNP Q8GIX7
D	346	HIS	-	expression tag	UNP Q8GIX7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	3	Total Zn 3 3	0	0
2	C	2	Total Zn 2 2	0	0
2	D	3	Total Zn 3 3	0	0

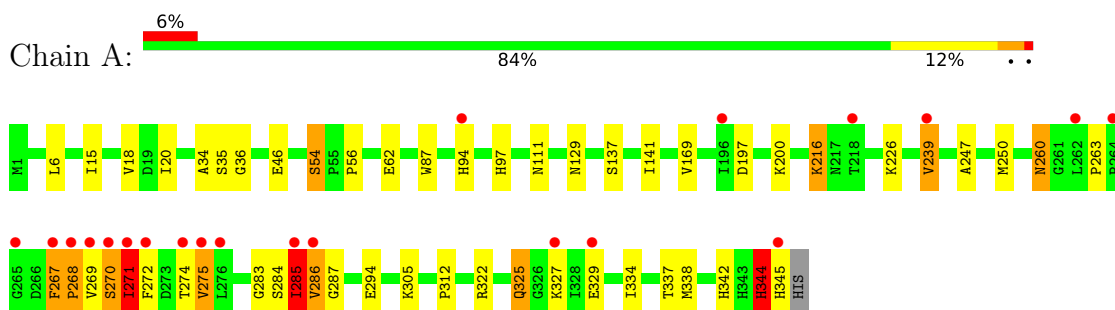
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	260	Total O 260 260	0	0
3	B	269	Total O 269 269	0	0
3	C	230	Total O 230 230	0	0
3	D	236	Total O 236 236	0	0

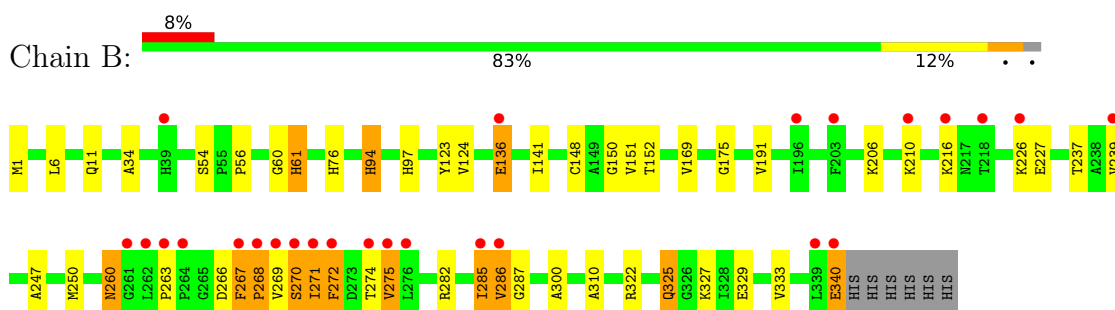
3 Residue-property plots [i](#)

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.

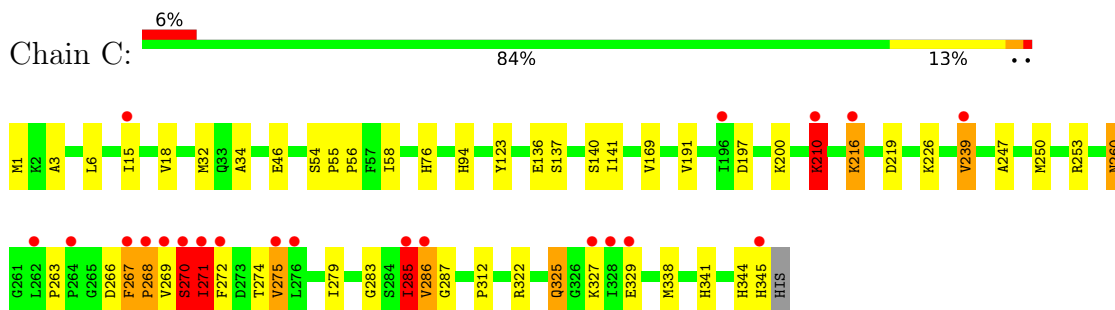
- Molecule 1: Alcohol dehydrogenase



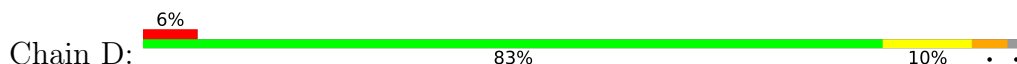
- Molecule 1: Alcohol dehydrogenase

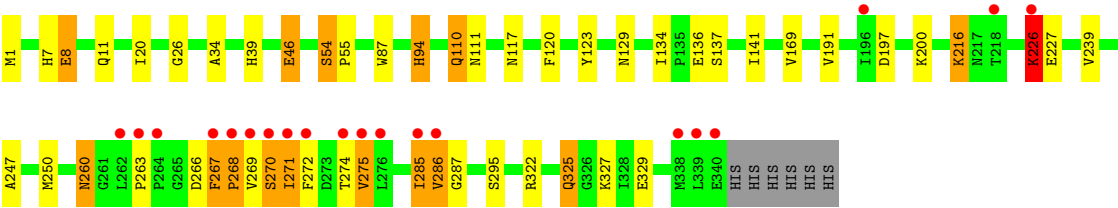


- Molecule 1: Alcohol dehydrogenase



- Molecule 1: Alcohol dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.57Å 136.57Å 210.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	118.34 – 1.90 118.28 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (118.34-1.90) 96.6 (118.28-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.210 , 0.233 0.218 , 0.241	Depositor DCC
R_{free} test set	8905 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11196	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0011e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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

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	1.38	11/2631 (0.4%)	1.23	9/3576 (0.3%)
1	B	1.40	9/2579 (0.3%)	1.26	11/3505 (0.3%)
1	C	1.29	11/2625 (0.4%)	1.19	13/3568 (0.4%)
1	D	1.33	9/2579 (0.3%)	1.22	13/3505 (0.4%)
All	All	1.35	40/10414 (0.4%)	1.23	46/14154 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	ASN	CA-C	-8.62	1.41	1.52
1	C	260	ASN	CA-C	-8.15	1.41	1.52
1	B	151	VAL	N-CA	7.83	1.55	1.46
1	A	97	HIS	N-CA	-7.68	1.37	1.46
1	A	344	HIS	CA-C	-7.28	1.43	1.53
1	C	239	VAL	CA-C	7.21	1.59	1.53
1	A	239	VAL	CA-C	7.14	1.59	1.53
1	B	61	HIS	N-CA	7.00	1.56	1.46
1	D	55	PRO	C-O	-6.95	1.19	1.25
1	B	97	HIS	N-CA	-6.39	1.38	1.46
1	A	342	HIS	CA-C	-6.15	1.44	1.52
1	D	137	SER	C-O	-6.12	1.16	1.24
1	B	150	GLY	C-N	-6.11	1.26	1.34
1	A	137	SER	C-O	-6.07	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	260	ASN	CA-C	-6.06	1.43	1.52
1	B	266	ASP	CA-C	-5.97	1.45	1.53
1	C	341	HIS	N-CA	-5.95	1.39	1.46
1	C	55	PRO	C-O	-5.93	1.20	1.25
1	A	305	LYS	N-CA	-5.91	1.38	1.46
1	C	344	HIS	CA-C	-5.88	1.44	1.52
1	C	266	ASP	CA-C	-5.87	1.45	1.53
1	D	20	ILE	CA-C	-5.77	1.47	1.53
1	A	271	ILE	C-O	-5.77	1.17	1.24
1	D	266	ASP	CA-C	-5.58	1.45	1.53
1	B	260	ASN	CA-C	-5.54	1.44	1.52
1	C	279	ILE	N-CA	5.54	1.52	1.46
1	D	110[A]	GLN	N-CA	5.50	1.52	1.45
1	D	110[B]	GLN	N-CA	5.50	1.52	1.45
1	B	124	VAL	C-O	-5.44	1.18	1.24
1	C	271	ILE	C-O	-5.40	1.17	1.24
1	C	58	ILE	CA-C	-5.40	1.48	1.53
1	A	294	GLU	CA-C	5.39	1.59	1.52
1	C	3	ALA	N-CA	5.36	1.52	1.45
1	D	120	PHE	N-CA	5.28	1.52	1.46
1	A	334	ILE	N-CA	5.23	1.52	1.46
1	D	295	SER	N-CA	5.23	1.52	1.46
1	B	300	ALA	C-O	-5.22	1.17	1.24
1	A	284	SER	C-N	-5.17	1.29	1.33
1	C	137	SER	C-O	-5.15	1.17	1.24
1	B	60	GLY	C-O	5.11	1.30	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	HIS	N-CA-C	8.13	121.08	110.43
1	B	191	VAL	N-CA-C	6.58	117.38	108.17
1	B	266	ASP	N-CA-C	-6.38	102.30	110.53
1	A	285	ILE	CA-C-N	-6.24	110.73	121.97
1	A	285	ILE	C-N-CA	-6.24	110.73	121.97
1	B	152	THR	N-CA-C	6.17	117.67	111.07
1	C	285	ILE	CA-C-N	-6.12	110.96	121.97
1	C	285	ILE	C-N-CA	-6.12	110.96	121.97
1	A	15	ILE	N-CA-C	-6.11	99.49	108.54
1	A	344	HIS	CA-C-N	6.09	132.67	121.70
1	A	344	HIS	C-N-CA	6.09	132.67	121.70
1	D	191	VAL	N-CA-C	6.03	116.61	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ILE	N-CA-C	-5.93	103.53	108.63
1	C	15	ILE	N-CA-C	-5.92	99.17	108.23
1	A	35	SER	N-CA-C	5.90	118.02	108.34
1	B	285	ILE	CA-C-N	-5.84	111.47	121.97
1	B	285	ILE	C-N-CA	-5.84	111.47	121.97
1	D	120	PHE	N-CA-C	-5.82	106.80	112.97
1	B	175	GLY	N-CA-C	-5.71	105.87	112.50
1	D	26	GLY	N-CA-C	-5.70	107.78	115.36
1	D	285	ILE	CA-C-N	-5.68	111.75	121.97
1	D	285	ILE	C-N-CA	-5.68	111.75	121.97
1	A	54	SER	CB-CA-C	-5.66	104.55	110.33
1	B	227	GLU	N-CA-C	5.65	117.25	111.14
1	C	344	HIS	CA-C-N	5.62	131.82	121.70
1	C	344	HIS	C-N-CA	5.62	131.82	121.70
1	C	266	ASP	N-CA-C	-5.55	103.59	110.41
1	B	11	GLN	CB-CA-C	-5.54	100.14	109.83
1	C	270	SER	N-CA-C	5.51	122.53	110.80
1	D	117	ASN	N-CA-C	5.48	117.97	110.24
1	B	282	ARG	N-CA-CB	-5.46	101.37	111.53
1	D	266	ASP	N-CA-C	-5.42	103.74	110.41
1	C	140	SER	N-CA-C	5.38	117.14	111.28
1	D	54	SER	CB-CA-C	-5.36	104.86	110.33
1	C	136	GLU	CB-CA-C	-5.36	101.85	110.74
1	D	295	SER	CB-CA-C	-5.28	102.58	110.88
1	C	210	LYS	N-CA-CB	5.27	119.26	110.41
1	B	237	THR	N-CA-C	-5.22	107.08	113.50
1	C	344	HIS	CB-CA-C	-5.15	100.18	110.42
1	D	227	GLU	N-CA-C	5.13	116.87	111.28
1	D	134	ILE	N-CA-C	5.12	113.03	108.63
1	D	226	LYS	CG-CD-CE	5.09	123.02	111.30
1	C	344	HIS	N-CA-C	5.09	121.64	110.80
1	D	46	GLU	N-CA-C	-5.07	107.10	113.28
1	B	136	GLU	CB-CA-C	-5.05	102.73	110.81
1	C	253	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	HIS	Peptide

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	2577	0	2548	38	0
1	B	2521	0	2510	32	0
1	C	2567	0	2541	40	0
1	D	2526	0	2513	40	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
3	A	260	0	0	3	0
3	B	269	0	0	8	0
3	C	230	0	0	5	0
3	D	236	0	0	4	0
All	All	11196	0	10112	128	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 6.

All (128) 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:94[B]:HIS:HD2	3:C:677:HOH:O	1.34	1.08
1:C:219:ASP:HA	3:C:633:HOH:O	1.55	1.05
1:C:191:VAL:H	1:C:210:LYS:HZ3	1.18	0.90
3:B:687:HOH:O	1:C:94[B]:HIS:HD2	1.57	0.87
3:B:687:HOH:O	1:C:94[B]:HIS:CD2	2.34	0.79
1:B:271:ILE:HG21	1:D:263:PRO:HG3	1.66	0.78
1:C:94[A]:HIS:ND1	3:C:501:HOH:O	2.23	0.71
1:B:271:ILE:CG2	1:D:263:PRO:HG3	2.20	0.70
1:B:263:PRO:HG3	1:D:271:ILE:HG21	1.73	0.70
1:D:8:GLU:O	1:D:11:GLN:HG2	1.92	0.69
1:A:344:HIS:CD2	3:A:508:HOH:O	2.45	0.69
1:A:263:PRO:HG3	1:C:271:ILE:HG21	1.75	0.68
1:A:270:SER:O	1:A:272:PHE:N	2.26	0.68
1:A:271:ILE:HG21	1:C:263:PRO:HG3	1.76	0.68
1:D:270:SER:O	1:D:272:PHE:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLU:HB2	3:B:658:HOH:O	1.93	0.67
1:A:263:PRO:HG3	1:C:271:ILE:CG2	2.25	0.67
1:C:247:ALA:HA	1:C:250:MET:HE3	1.76	0.67
1:D:94[B]:HIS:ND1	3:D:502:HOH:O	2.26	0.67
1:A:271:ILE:CG2	1:C:263:PRO:HG3	2.25	0.67
1:D:247:ALA:HA	1:D:250:MET:HE3	1.77	0.67
1:A:247:ALA:HA	1:A:250:MET:HE3	1.80	0.64
1:A:94[B]:HIS:NE2	1:D:129:ASN:OD1	2.26	0.64
1:D:7:HIS:HB2	1:D:11:GLN:OE1	1.98	0.64
1:B:263:PRO:HG3	1:D:271:ILE:CG2	2.26	0.64
1:B:247:ALA:HA	1:B:250:MET:HE3	1.79	0.64
1:B:286:VAL:HG22	1:B:287:GLY:H	1.64	0.62
1:D:8:GLU:OE2	1:D:8:GLU:HA	2.00	0.62
1:C:270:SER:O	1:C:272:PHE:N	2.33	0.61
1:B:76:HIS:HD2	3:B:702:HOH:O	1.82	0.61
1:B:210:LYS:HD2	3:B:631:HOH:O	2.01	0.61
1:C:191:VAL:H	1:C:210:LYS:NZ	1.96	0.61
1:A:129:ASN:O	1:D:94[B]:HIS:HE1	1.84	0.60
1:B:270:SER:O	1:B:272:PHE:N	2.35	0.60
1:D:270:SER:O	1:D:271:ILE:C	2.47	0.58
1:A:275:VAL:HG23	1:C:285:ILE:HG23	1.86	0.57
1:B:268:PRO:HG3	1:D:268:PRO:HG3	1.87	0.57
1:A:344:HIS:HD2	3:A:508:HOH:O	1.85	0.57
1:A:325:GLN:O	1:A:327:LYS:HD2	2.06	0.55
1:B:325:GLN:O	1:B:327:LYS:HD2	2.07	0.55
1:B:327:LYS:HA	1:B:327:LYS:HE2	1.89	0.55
1:C:325:GLN:O	1:C:327:LYS:HD2	2.07	0.55
1:A:275:VAL:HA	1:C:283:GLY:HA3	1.88	0.54
1:B:61:HIS:NE2	3:B:501:HOH:O	2.31	0.54
1:B:270:SER:O	1:B:271:ILE:C	2.49	0.54
1:B:267:PHE:O	1:B:269:VAL:HG23	2.08	0.53
1:A:270:SER:O	1:A:271:ILE:C	2.51	0.53
1:D:267:PHE:O	1:D:269:VAL:HG23	2.09	0.53
1:D:325:GLN:O	1:D:327:LYS:HD2	2.08	0.53
1:A:285:ILE:HG23	1:C:275:VAL:HG23	1.91	0.53
1:C:267:PHE:O	1:C:269:VAL:HG23	2.09	0.52
1:C:270:SER:O	1:C:271:ILE:C	2.53	0.52
1:A:216:LYS:HA	1:A:216:LYS:HE3	1.91	0.52
1:A:267:PHE:O	1:A:269:VAL:HG23	2.09	0.52
1:D:7:HIS:O	1:D:8:GLU:OE2	2.27	0.52
1:A:327:LYS:HA	1:A:327:LYS:HE2	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLY:HA3	1:C:275:VAL:HA	1.92	0.51
1:B:327:LYS:HA	1:B:327:LYS:CE	2.40	0.51
1:D:216:LYS:HE3	1:D:216:LYS:HA	1.92	0.51
1:D:271:ILE:O	1:D:274:THR:HB	2.10	0.51
1:B:271:ILE:O	1:B:274:THR:HB	2.11	0.51
1:A:94[B]:HIS:HE2	1:D:129:ASN:CG	2.17	0.51
1:C:216:LYS:HE3	1:C:216:LYS:HA	1.91	0.51
1:D:327:LYS:HE2	1:D:327:LYS:HA	1.92	0.50
1:A:312:PRO:HD3	1:A:338:MET:HE2	1.93	0.50
1:C:271:ILE:O	1:C:274:THR:HB	2.10	0.50
1:A:271:ILE:O	1:A:274:THR:HB	2.12	0.50
1:B:271:ILE:HG22	1:B:272:PHE:N	2.28	0.49
1:D:285:ILE:HD12	1:D:286:VAL:N	2.26	0.49
1:C:338:MET:HE1	3:C:685:HOH:O	2.13	0.48
1:C:327:LYS:HA	1:C:327:LYS:HE2	1.94	0.48
1:D:136:GLU:HG2	3:D:678:HOH:O	2.12	0.48
1:D:286:VAL:HG22	1:D:287:GLY:H	1.80	0.47
1:A:94[B]:HIS:CE1	1:D:129:ASN:HA	2.50	0.47
1:A:327:LYS:HA	1:A:327:LYS:CE	2.45	0.47
1:B:275:VAL:HG23	1:D:285:ILE:HG23	1.97	0.47
1:D:34:ALA:HB2	1:D:141:ILE:HD13	1.96	0.47
1:D:322:ARG:HD2	3:D:699:HOH:O	2.15	0.47
1:A:34:ALA:HB2	1:A:141:ILE:HD13	1.97	0.46
1:D:327:LYS:HA	1:D:327:LYS:CE	2.44	0.46
1:D:271:ILE:HD13	1:D:271:ILE:HA	1.87	0.46
1:B:34:ALA:HB2	1:B:141:ILE:HD13	1.97	0.46
1:C:327:LYS:HA	1:C:327:LYS:CE	2.46	0.45
1:B:340:GLU:C	3:B:546:HOH:O	2.60	0.45
1:C:312:PRO:HD3	1:C:338:MET:HE2	1.97	0.45
1:B:285:ILE:HG23	1:D:275:VAL:HG23	1.98	0.45
1:C:322:ARG:HG2	1:C:327:LYS:HB2	1.98	0.45
1:A:286:VAL:HG22	1:A:287:GLY:H	1.80	0.45
1:C:286:VAL:HG22	1:C:287:GLY:H	1.81	0.45
1:C:34:ALA:HB2	1:C:141:ILE:HD13	1.98	0.45
1:B:285:ILE:HD12	1:B:286:VAL:N	2.32	0.44
1:B:310:ALA:HA	1:B:333:VAL:O	2.17	0.44
1:B:322:ARG:HG2	1:B:327:LYS:HB2	1.99	0.44
1:A:285:ILE:HD12	1:A:286:VAL:N	2.32	0.44
1:D:110[A]:GLN:OE1	3:D:501:HOH:O	2.21	0.44
1:D:8:GLU:OE2	1:D:8:GLU:CA	2.61	0.44
1:C:267:PHE:O	1:C:268:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ARG:HG2	1:D:327:LYS:HB2	1.99	0.44
1:A:268:PRO:HG3	1:C:268:PRO:HG3	2.00	0.43
1:A:337:THR:HG23	3:A:744:HOH:O	2.18	0.43
1:C:247:ALA:CA	1:C:250:MET:HE3	2.46	0.43
1:B:6:LEU:O	1:B:56:PRO:HA	2.19	0.43
1:D:226:LYS:HD3	1:D:226:LYS:HA	1.61	0.43
1:B:271:ILE:HD13	1:B:271:ILE:HA	1.88	0.43
1:C:197:ASP:HB3	1:C:200:LYS:HD2	2.01	0.42
1:A:322:ARG:HG2	1:A:327:LYS:HB2	2.01	0.42
1:A:216:LYS:HE3	1:A:216:LYS:CA	2.48	0.42
1:D:1:MET:SD	1:D:123:TYR:HB2	2.60	0.42
1:B:148:CYS:SG	3:B:501:HOH:O	2.62	0.42
1:D:197:ASP:HB3	1:D:200:LYS:HD2	2.01	0.42
1:A:271:ILE:HG22	1:C:263:PRO:HG3	2.01	0.42
1:C:216:LYS:HE3	1:C:216:LYS:CA	2.49	0.42
1:C:1:MET:SD	1:C:123:TYR:HB2	2.59	0.41
1:C:76:HIS:HD2	3:C:711:HOH:O	2.01	0.41
1:A:36:GLY:HA3	1:A:62:GLU:OE2	2.21	0.41
1:A:271:ILE:HD13	1:A:271:ILE:HA	1.86	0.41
1:D:216:LYS:HE3	1:D:216:LYS:CA	2.51	0.41
1:D:87:TRP:O	1:D:111:ASN:HA	2.20	0.41
1:A:197:ASP:HB3	1:A:200:LYS:HD2	2.02	0.41
1:B:271:ILE:HG22	1:D:263:PRO:HG3	2.02	0.41
1:B:1:MET:SD	1:B:123:TYR:HB2	2.61	0.41
1:C:6:LEU:O	1:C:56:PRO:HA	2.20	0.41
1:C:285:ILE:HD12	1:C:286:VAL:N	2.36	0.41
1:A:87:TRP:O	1:A:111:ASN:HA	2.21	0.40
1:C:271:ILE:HG22	1:C:272:PHE:N	2.36	0.40
1:C:32:MET:HE2	1:C:32:MET:HA	2.04	0.40
1:A:6:LEU:O	1:A:56:PRO:HA	2.21	0.40
1:A:216:LYS:HA	1:A:216:LYS:CE	2.50	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	345/346 (100%)	327 (95%)	15 (4%)	3 (1%)	14	6
1	B	340/346 (98%)	324 (95%)	12 (4%)	4 (1%)	10	4
1	C	344/346 (99%)	328 (95%)	13 (4%)	3 (1%)	14	6
1	D	340/346 (98%)	326 (96%)	11 (3%)	3 (1%)	14	6
All	All	1369/1384 (99%)	1305 (95%)	51 (4%)	13 (1%)	12	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	SER
1	A	271	ILE
1	B	270	SER
1	B	271	ILE
1	C	270	SER
1	C	271	ILE
1	D	270	SER
1	D	271	ILE
1	B	272	PHE
1	C	286	VAL
1	A	286	VAL
1	D	286	VAL
1	B	286	VAL

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	273/272 (100%)	258 (94%)	15 (6%)	19	11
1	B	268/272 (98%)	253 (94%)	15 (6%)	19	11
1	C	272/272 (100%)	256 (94%)	16 (6%)	18	10
1	D	268/272 (98%)	252 (94%)	16 (6%)	17	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1081/1088 (99%)	1019 (94%)	62 (6%)	19	11

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	VAL
1	A	46	GLU
1	A	54	SER
1	A	169	VAL
1	A	216	LYS
1	A	226	LYS
1	A	239	VAL
1	A	260	ASN
1	A	267	PHE
1	A	268	PRO
1	A	275	VAL
1	A	285	ILE
1	A	325	GLN
1	A	329	GLU
1	A	345	HIS
1	B	54	SER
1	B	94[A]	HIS
1	B	94[B]	HIS
1	B	169	VAL
1	B	206	LYS
1	B	216	LYS
1	B	226	LYS
1	B	239	VAL
1	B	260	ASN
1	B	267	PHE
1	B	268	PRO
1	B	275	VAL
1	B	325	GLN
1	B	329	GLU
1	B	340	GLU
1	C	18	VAL
1	C	46	GLU
1	C	54	SER
1	C	169	VAL
1	C	210	LYS
1	C	216	LYS
1	C	226	LYS

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Mol	Chain	Res	Type
1	C	239	VAL
1	C	260	ASN
1	C	267	PHE
1	C	268	PRO
1	C	275	VAL
1	C	285	ILE
1	C	325	GLN
1	C	329	GLU
1	C	345	HIS
1	D	8	GLU
1	D	39	HIS
1	D	46	GLU
1	D	54	SER
1	D	94[A]	HIS
1	D	94[B]	HIS
1	D	169	VAL
1	D	216	LYS
1	D	226	LYS
1	D	239	VAL
1	D	260	ASN
1	D	267	PHE
1	D	268	PRO
1	D	275	VAL
1	D	325	GLN
1	D	329	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	97	HIS
1	A	217	ASN
1	B	76	HIS
1	C	97	HIS
1	C	217	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](#)

Of 10 ligands modelled in this entry, 10 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 [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	345/346 (99%)	0.49	21 (6%) 27 29	22, 54, 90, 114	2 (0%)
1	B	340/346 (98%)	0.48	26 (7%) 20 21	32, 53, 89, 116	2 (0%)
1	C	345/346 (99%)	0.61	21 (6%) 27 29	40, 58, 93, 119	1 (0%)
1	D	340/346 (98%)	0.56	20 (5%) 28 30	25, 57, 89, 117	2 (0%)
All	All	1370/1384 (98%)	0.54	88 (6%) 25 27	22, 56, 91, 119	7 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	PRO	5.2
1	A	268	PRO	5.2
1	B	339	LEU	5.1
1	D	268	PRO	4.9
1	C	285	ILE	4.8
1	D	339	LEU	4.8
1	A	271	ILE	4.6
1	A	276	LEU	4.5
1	C	268	PRO	4.5
1	A	269	VAL	4.4
1	A	285	ILE	4.0
1	D	271	ILE	4.0
1	C	276	LEU	4.0
1	A	345	HIS	3.9
1	C	345	HIS	3.8
1	A	272	PHE	3.8
1	C	272	PHE	3.7
1	D	340	GLU	3.7
1	D	276	LEU	3.6
1	B	271	ILE	3.6
1	C	269	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	286	VAL	3.4
1	D	269	VAL	3.4
1	B	264	PRO	3.4
1	D	275	VAL	3.4
1	B	285	ILE	3.4
1	B	276	LEU	3.3
1	B	272	PHE	3.3
1	D	270	SER	3.3
1	C	271	ILE	3.3
1	B	286	VAL	3.2
1	C	239	VAL	3.2
1	D	286	VAL	3.1
1	B	262	LEU	3.0
1	D	262	LEU	3.0
1	D	196	ILE	3.0
1	A	270	SER	3.0
1	A	264	PRO	3.0
1	C	327	LYS	2.9
1	D	264	PRO	2.9
1	B	210	LYS	2.9
1	B	196	ILE	2.9
1	D	274	THR	2.8
1	A	286	VAL	2.8
1	C	264	PRO	2.8
1	C	270	SER	2.8
1	D	285	ILE	2.8
1	C	196	ILE	2.8
1	B	270	SER	2.7
1	B	340	GLU	2.7
1	B	239	VAL	2.7
1	A	196	ILE	2.7
1	D	272	PHE	2.6
1	C	328	ILE	2.6
1	B	226	LYS	2.6
1	D	226	LYS	2.6
1	C	262	LEU	2.6
1	B	275	VAL	2.6
1	A	267	PHE	2.6
1	B	269	VAL	2.6
1	B	267	PHE	2.5
1	A	275	VAL	2.5
1	C	275	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	218	THR	2.5
1	B	274	THR	2.5
1	C	216	LYS	2.5
1	D	267	PHE	2.4
1	A	327	LYS	2.4
1	C	267	PHE	2.4
1	A	218	THR	2.4
1	D	338	MET	2.4
1	A	274	THR	2.3
1	B	263	PRO	2.2
1	B	216	LYS	2.2
1	D	263	PRO	2.2
1	A	239	VAL	2.2
1	D	218	THR	2.2
1	A	265	GLY	2.2
1	C	210	LYS	2.2
1	B	203	PHE	2.1
1	A	262	LEU	2.1
1	A	329	GLU	2.0
1	B	136	GLU	2.0
1	A	94[A]	HIS	2.0
1	B	39	HIS	2.0
1	C	329	GLU	2.0
1	C	15	ILE	2.0
1	B	261	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
2	ZN	B	402	1/1	0.96	0.05	41,41,41,41	0
2	ZN	D	402	1/1	0.96	0.05	40,40,40,40	0
2	ZN	D	401	1/1	0.97	0.07	57,57,57,57	0
2	ZN	B	401	1/1	0.97	0.07	54,54,54,54	0
2	ZN	D	403	1/1	0.97	0.06	59,59,59,59	0
2	ZN	C	401	1/1	0.98	0.06	56,56,56,56	0
2	ZN	C	402	1/1	0.98	0.04	44,44,44,44	0
2	ZN	A	401	1/1	0.98	0.06	53,53,53,53	0
2	ZN	A	402	1/1	0.98	0.04	42,42,42,42	0
2	ZN	B	403	1/1	0.98	0.04	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.