



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2016 – 07:45 PM EDT

PDB ID : 4Z6K  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

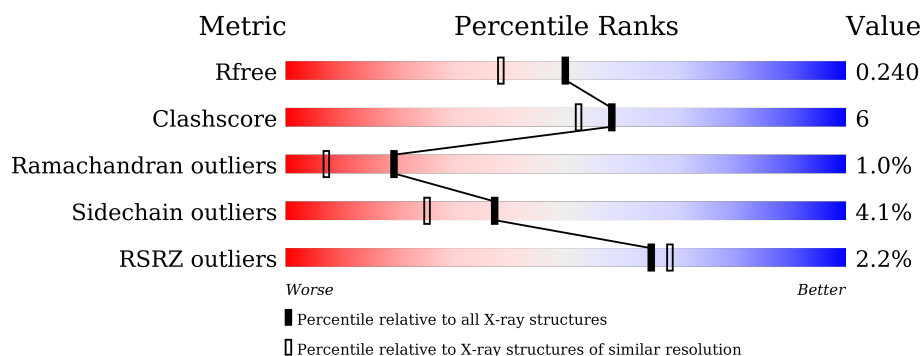
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	B	346	<div> <div>%</div> <div>85%</div> <div>10%</div> <div>..</div> </div>
1	C	346	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	D	346	<div> <div>%</div> <div>86%</div> <div>9%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	401	-	-	-	X
2	ZN	B	401	-	-	-	X
2	ZN	B	403	-	-	-	X
2	ZN	D	403	-	-	-	X

## 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 (three-letter code: ZN) (formula: Zn).

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

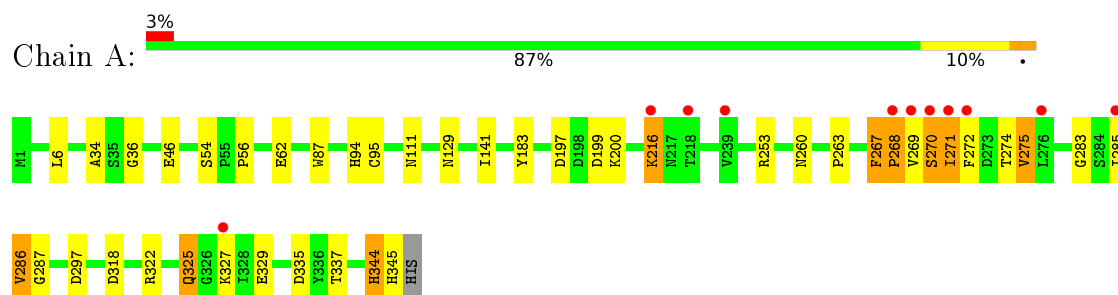
- Molecule 3 is water.

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

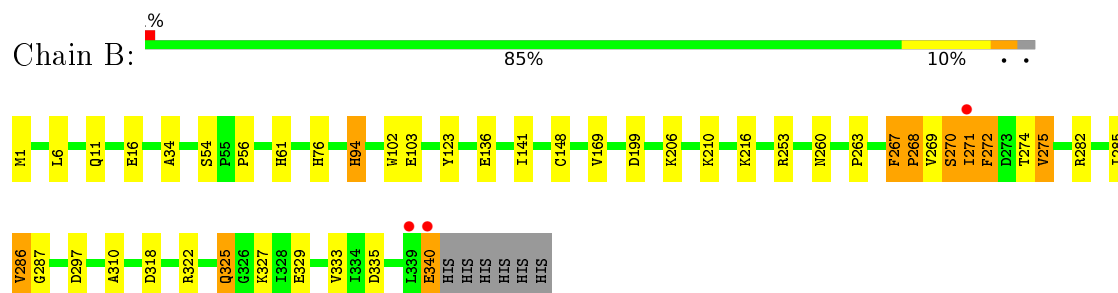
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

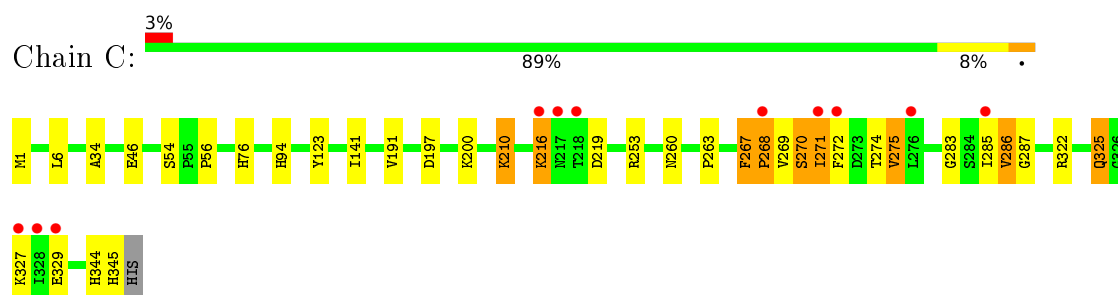
#### • Molecule 1: Alcohol dehydrogenase



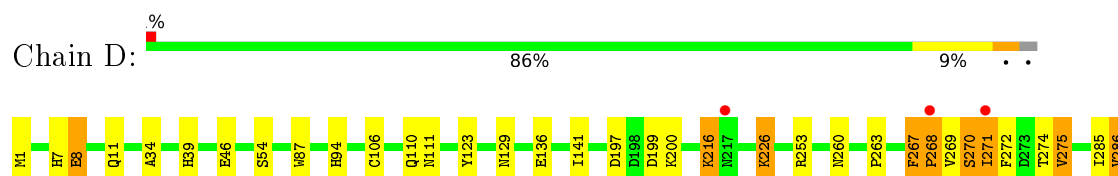
#### • Molecule 1: Alcohol dehydrogenase



#### • 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, $\alpha$ , $\beta$ , $\gamma$	136.57Å 136.57Å 210.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	118.34 – 1.90 78.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (118.34-1.90) 96.6 (78.70-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.78 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.210 , 0.233 0.218 , 0.240	Depositor DCC
$R_{free}$ test set	8613 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.6	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	2 of 171943 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.00	2/2631 (0.1%)	0.98	5/3576 (0.1%)
1	B	1.04	5/2579 (0.2%)	1.02	7/3505 (0.2%)
1	C	0.93	0/2625	0.97	2/3568 (0.1%)
1	D	0.99	1/2579 (0.0%)	0.99	4/3505 (0.1%)
All	All	0.99	8/10414 (0.1%)	0.99	18/14154 (0.1%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	GLU	CG-CD	6.88	1.62	1.51
1	A	95	CYS	CB-SG	-6.60	1.71	1.82
1	B	103	GLU	CD-OE1	6.57	1.32	1.25
1	B	102	TRP	CB-CG	-6.06	1.39	1.50
1	D	106	CYS	CB-SG	-5.63	1.72	1.81
1	B	340	GLU	CD-OE2	5.60	1.31	1.25
1	B	16	GLU	CD-OE1	5.30	1.31	1.25
1	A	183	TYR	CE1-CZ	-5.03	1.32	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	ASP	CB-CG-OD2	8.28	125.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	318	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	199	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	297	ASP	CB-CG-OD1	6.57	124.22	118.30
1	A	297	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	335	ASP	CB-CG-OD1	5.73	123.46	118.30
1	D	253	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	A	253	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	D	297	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	199	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	253	ARG	NE-CZ-NH2	5.23	122.91	120.30
1	D	318	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	11	GLN	CB-CA-C	-5.13	100.14	110.40
1	B	282	ARG	N-CA-CB	-5.13	101.37	110.60
1	C	344	HIS	CB-CA-C	-5.11	100.18	110.40
1	A	335	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	318	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	36	0
1	B	2521	0	2510	32	0
1	C	2567	0	2541	34	0
1	D	2526	0	2513	39	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	269	0	0	9	0
3	C	230	0	0	4	0
3	D	236	0	0	4	0
All	All	11196	0	10112	119	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 (119) 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
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:270:SER:O	1:A:272:PHE:N	2.26	0.68
1:A:263:PRO:HG3	1:C:271:ILE:HG21	1.75	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
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: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:C:191:VAL:H	1:C:210:LYS:HZ3	1.46	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:C:191:VAL:H	1:C:210:LYS:NZ	1.96	0.62
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:94[A]:HIS:ND1	3:B:502:HOH:O	2.32	0.55
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:D:270:SER:O	1:D:271:ILE:C	2.47	0.53
1:B:267:PHE:O	1:B:269:VAL:HG23	2.08	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:A:216:LYS:HE3	1:A:216:LYS:HA	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
1:B:327:LYS:CE	1:B:327:LYS:HA	2.40	0.51
1:A:283:GLY:HA3	1:C:275:VAL:HA	1.92	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:C:216:LYS:HA	1:C:216:LYS:HE3	1.91	0.51
1:D:327:LYS:HE2	1:D:327:LYS:HA	1.92	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:B:270:SER:O	1:B:271:ILE:C	2.49	0.49
1:A:270:SER:O	1:A:271:ILE:C	2.51	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:C:270:SER:O	1:C:271:ILE:C	2.53	0.47
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:CE	1:A:327:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1:D:327:LYS:HA	2.44	0.46
1:A:94[B]:HIS:HE2	1:D:129:ASN:CG	2.17	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:CE	1:C:327:LYS:HA	2.46	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:322:ARG:HG2	1:B:327:LYS:HB2	1.99	0.44
1:B:310:ALA:HA	1:B:333:VAL:O	2.17	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: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:B:6:LEU:O	1:B:56:PRO:HA	2.19	0.43
1:D:226:LYS:HA	1:D:226:LYS:HD3	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:CA	1:A:216:LYS:HE3	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:HA	1:A:271:ILE:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:O	1:C:56:PRO:HA	2.20	0.41
1:B:340:GLU:C	3:B:546:HOH:O	2.60	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:A:216:LYS:CE	1:A:216:LYS:HA	2.50	0.40
1:A:6:LEU:O	1:A:56:PRO:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/346 (100%)	327 (95%)	15 (4%)	3 (1%)	21	9
1	B	340/346 (98%)	324 (95%)	12 (4%)	4 (1%)	16	5
1	C	344/346 (99%)	328 (95%)	13 (4%)	3 (1%)	21	9
1	D	340/346 (98%)	326 (96%)	11 (3%)	3 (1%)	21	9
All	All	1369/1384 (99%)	1305 (95%)	51 (4%)	13 (1%)	19	9

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

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Mol	Chain	Res	Type
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%)	263 (96%)	10 (4%)	41	29
1	B	268/272 (98%)	256 (96%)	12 (4%)	34	21
1	C	272/272 (100%)	261 (96%)	11 (4%)	38	26
1	D	268/272 (98%)	256 (96%)	12 (4%)	34	21
All	All	1081/1088 (99%)	1036 (96%)	45 (4%)	37	24

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	54	SER
1	A	216	LYS
1	A	260	ASN
1	A	267	PHE
1	A	268	PRO
1	A	275	VAL
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

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Mol	Chain	Res	Type
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	C	46	GLU
1	C	54	SER
1	C	210	LYS
1	C	216	LYS
1	C	260	ASN
1	C	267	PHE
1	C	268	PRO
1	C	275	VAL
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	216	LYS
1	D	226	LYS
1	D	260	ASN
1	D	267	PHE
1	D	268	PRO
1	D	275	VAL
1	D	325	GLN
1	D	329	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	345/346 (99%)	0.13	11 (3%) 51 54	40, 54, 90, 115	0
1	B	340/346 (98%)	0.14	3 (0%) 85 87	40, 53, 89, 116	0
1	C	345/346 (99%)	0.19	11 (3%) 51 54	42, 58, 93, 119	0
1	D	340/346 (98%)	0.10	5 (1%) 76 79	40, 57, 89, 117	0
All	All	1370/1384 (98%)	0.14	30 (2%) 65 68	40, 56, 91, 119	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	PRO	4.9
1	A	268	PRO	4.6
1	B	339	LEU	4.4
1	D	339	LEU	4.1
1	C	218	THR	3.9
1	C	327	LYS	3.7
1	C	285	ILE	3.5
1	A	276	LEU	3.4
1	A	218	THR	3.3
1	C	216	LYS	3.2
1	C	272	PHE	3.1
1	A	216	LYS	3.1
1	A	327	LYS	3.0
1	C	328	ILE	2.9
1	D	271	ILE	2.9
1	C	329	GLU	2.9
1	C	271	ILE	2.9
1	A	269	VAL	2.8
1	D	340	GLU	2.7
1	B	271	ILE	2.7
1	A	270	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	272	PHE	2.6
1	C	276	LEU	2.5
1	B	340	GLU	2.4
1	A	271	ILE	2.4
1	D	268	PRO	2.3
1	C	217	ASN	2.2
1	A	285	ILE	2.2
1	A	239	VAL	2.1
1	D	217	ASN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	B	403	1/1	0.98	0.16	6.13	50,50,50,50	0
2	ZN	D	403	1/1	0.98	0.14	3.31	59,59,59,59	0
2	ZN	A	401	1/1	0.98	0.12	2.31	53,53,53,53	0
2	ZN	B	401	1/1	0.97	0.13	2.02	54,54,54,54	0
2	ZN	C	401	1/1	0.97	0.12	1.91	56,56,56,56	0
2	ZN	B	402	1/1	0.97	0.17	1.82	41,41,41,41	0
2	ZN	A	402	1/1	0.98	0.15	0.80	42,42,42,42	0
2	ZN	C	402	1/1	0.98	0.15	0.70	44,44,44,44	0
2	ZN	D	401	1/1	0.97	0.12	0.68	57,57,57,57	0
2	ZN	D	402	1/1	0.98	0.16	0.65	40,40,40,40	0

## 6.5 Other polymers

There are no such residues in this entry.