



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 01:59 PM EDT

PDB ID : 1Y7W / pdb\_00001y7w  
Title : Crystal structure of a halotolerant carbonic anhydrase from *Dunaliella salina*  
Authors : Premkumar, L.; Greenblatt, H.M.; Bageshwar, U.K.; Savchenko, T.; Gokhman, I.; Sussman, J.L.; Zamir, A.; Israel Structural Proteomics Center (ISPC)  
Deposited on : 2004-12-10  
Resolution : 1.86 Å(reported)

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<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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

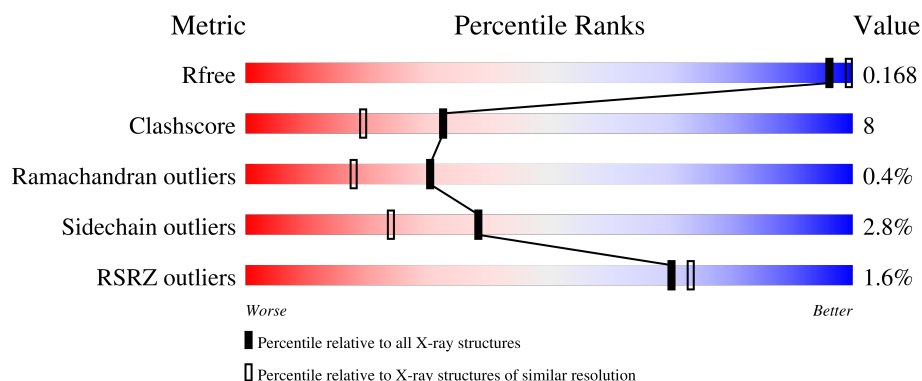
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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))
$R_{free}$	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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  $\geq 3$ , 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	291	
1	B	291	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4790 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 Halotolerant alpha-type carbonic anhydrase (dCA II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	3	0
			2129	1329	359	429	12			
1	B	274	Total	C	N	O	S	0	2	0
			2121	1325	358	427	11			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		


- Molecule 5 is water.

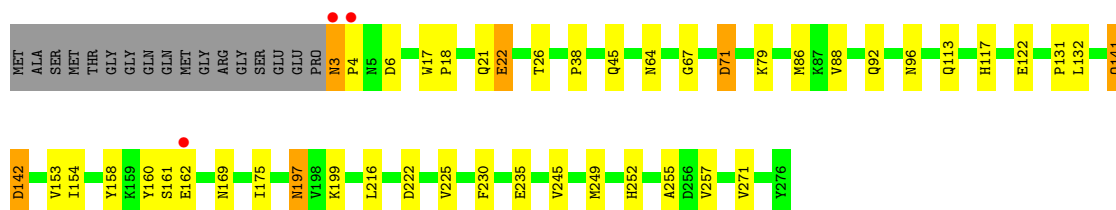
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total	O	0	0
			265	265		
5	B	262	Total	O	0	0
			262	262		

### 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.

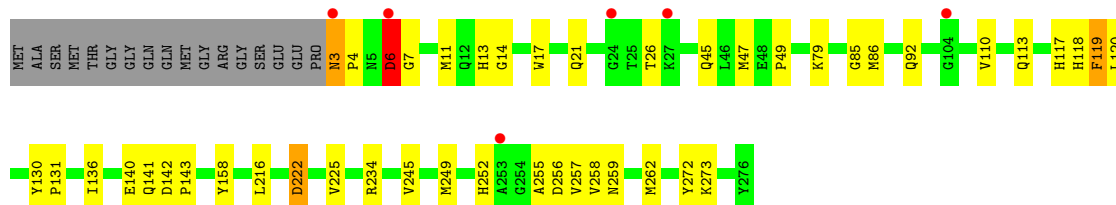
- Molecule 1: Halotolerant alpha-type carbonic anhydrase (dCA II)

Chain A: 



- Molecule 1: Halotolerant alpha-type carbonic anhydrase (dCA II)

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.02Å 119.83Å 58.44Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	32.95 – 1.86 32.95 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.1 (32.95-1.86) 98.1 (32.95-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 1.85Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.167 , 0.202 0.166 , 0.168	Depositor DCC
$R_{free}$ test set	2616 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4790	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	1.01	0/2175	1.18	8/2955 (0.3%)
1	B	1.03	1/2167 (0.0%)	1.19	9/2945 (0.3%)
All	All	1.02	1/4342 (0.0%)	1.18	17/5900 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	MET	SD-CE	6.45	1.95	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ASP	CB-CA-C	-7.93	105.57	111.20
1	A	141	GLN	CA-C-N	-6.63	116.19	124.21
1	A	141	GLN	C-N-CA	-6.63	116.19	124.21
1	A	225	VAL	N-CA-C	6.43	117.12	108.11
1	B	136	ILE	N-CA-C	-6.20	98.94	107.99
1	A	6	ASP	N-CA-C	6.00	120.73	111.56
1	A	117	HIS	N-CA-C	-5.98	97.55	108.02
1	B	234	ARG	N-CA-C	-5.95	100.64	109.86
1	B	216	LEU	N-CA-C	-5.93	102.29	110.35
1	A	216	LEU	N-CA-C	-5.77	102.50	110.35
1	B	117	HIS	N-CA-C	-5.56	98.29	108.02
1	B	245	VAL	CB-CA-C	-5.56	104.73	112.02
1	B	130	TYR	CA-C-N	-5.19	114.44	120.04
1	B	130	TYR	C-N-CA	-5.19	114.44	120.04
1	A	271	VAL	N-CA-C	-5.13	101.09	108.48
1	B	225	VAL	N-CA-C	5.13	115.30	108.11
1	B	259	ASN	N-CA-C	5.09	117.06	110.65

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	2129	0	2025	27	0
1	B	2121	0	2019	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	3	1	0
4	B	4	0	3	0	0
5	A	265	0	0	6	0
5	B	262	0	0	9	0
All	All	4790	0	4050	65	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 8.

All (65) 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:249:MET:HG3	5:B:383:HOH:O	1.37	1.19
1:B:85:GLY:H	1:B:118:HIS:HE1	1.15	0.94
1:B:120:LEU:HD12	5:B:540:HOH:O	1.92	0.70
5:A:482:HOH:O	1:B:262[B]:MET:HE2	1.91	0.69
1:A:92:GLN:HG3	5:A:494:HOH:O	1.91	0.69
1:B:3:ASN:HD22	1:B:3:ASN:N	1.93	0.67
1:B:85:GLY:H	1:B:118:HIS:CE1	2.05	0.66
1:B:256:ASP:OD2	5:B:313:HOH:O	2.16	0.61
1:B:13:HIS:O	1:B:262[A]:MET:HG2	2.01	0.61
1:B:3:ASN:N	1:B:4:PRO:HD3	2.15	0.59
1:B:120:LEU:CD1	5:B:540:HOH:O	2.50	0.59
1:A:67:GLY:H	1:A:197:ASN:HD21	1.50	0.59
1:A:67:GLY:H	1:A:197:ASN:ND2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLN:CG	1:B:110:VAL:HG11	2.35	0.57
1:A:199:LYS:HE2	5:A:486:HOH:O	2.04	0.56
1:B:252:HIS:HB2	1:B:255:ALA:HB2	1.88	0.55
1:A:252:HIS:HD2	5:A:301:HOH:O	1.90	0.54
1:B:49:PRO:HG3	1:B:273:LYS:O	2.08	0.53
1:B:3:ASN:N	1:B:3:ASN:ND2	2.56	0.52
1:A:245:VAL:HG12	1:A:249[B]:MET:HE2	1.91	0.52
1:B:45:GLN:O	1:B:47:MET:HE2	2.10	0.51
1:B:256:ASP:HB3	5:B:545:HOH:O	2.10	0.51
1:B:141:GLN:O	1:B:142:ASP:C	2.52	0.51
1:A:252:HIS:HB2	1:A:255:ALA:HB2	1.94	0.50
1:B:3:ASN:N	1:B:4:PRO:CD	2.75	0.50
1:B:118:HIS:HD2	1:B:257[A]:VAL:O	1.95	0.50
1:B:249:MET:SD	1:B:257[B]:VAL:CG2	3.00	0.49
1:B:120:LEU:HD12	1:B:258:VAL:HG11	1.95	0.49
1:B:92:GLN:HG2	1:B:110:VAL:HG11	1.96	0.48
1:B:140:GLU:HG3	1:B:143:PRO:HB3	1.95	0.48
1:A:3:ASN:N	1:A:4:PRO:HD3	2.29	0.48
1:B:6:ASP:OD2	1:B:6:ASP:N	2.37	0.48
1:A:3:ASN:N	1:A:4:PRO:CD	2.77	0.48
1:A:141:GLN:O	1:A:142:ASP:C	2.55	0.48
1:A:249[A]:MET:SD	1:A:257:VAL:CG2	3.02	0.47
1:B:118:HIS:HD2	1:B:257[B]:VAL:O	1.98	0.47
1:A:199:LYS:CE	5:A:486:HOH:O	2.63	0.47
1:A:153:VAL:HG21	4:A:279:ACY:H2	1.97	0.46
1:A:64:ASN:OD1	1:A:199:LYS:HE2	2.16	0.46
1:B:6:ASP:HB2	1:B:7:GLY:H	1.51	0.46
1:A:21:GLN:HG2	1:A:26:THR:HA	1.97	0.46
1:B:92:GLN:HG3	5:B:544:HOH:O	2.15	0.46
1:B:47:MET:HB2	1:B:272:TYR:CD2	2.50	0.46
1:A:131:PRO:HB3	1:A:160:TYR:CE2	2.51	0.45
1:B:86:MET:HE2	1:B:86:MET:HB3	1.75	0.45
1:B:249:MET:SD	1:B:257[B]:VAL:HG23	2.57	0.45
1:B:21:GLN:HG2	1:B:26:THR:HA	1.99	0.45
1:A:71:ASP:HA	1:A:96:ASN:ND2	2.32	0.45
1:A:3:ASN:HB2	1:A:252:HIS:ND1	2.32	0.45
1:B:79:LYS:HE2	5:B:523:HOH:O	2.15	0.44
1:A:22:GLU:HG3	5:A:396:HOH:O	2.15	0.44
1:A:38:PRO:HG3	1:A:122:GLU:HB3	2.00	0.44
1:A:79:LYS:O	1:A:88:VAL:HA	2.17	0.44
1:A:132:LEU:HB3	1:A:158:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:HIS:HD2	5:B:293:HOH:O	2.02	0.43
1:A:86:MET:HE1	1:A:175:ILE:CD1	2.48	0.43
1:A:197:ASN:C	1:A:197:ASN:HD22	2.26	0.43
1:B:118:HIS:O	1:B:119:PHE:HB2	2.19	0.43
1:A:17:TRP:HB2	1:A:18:PRO:HD3	2.00	0.43
1:B:14:GLY:HA2	1:B:17:TRP:CE2	2.55	0.41
1:B:92:GLN:HA	5:B:544:HOH:O	2.21	0.41
1:B:131:PRO:HD2	1:B:158:TYR:O	2.20	0.41
1:A:154:ILE:HG23	1:A:230:PHE:CE2	2.56	0.40
1:A:161:SER:HB3	1:A:235:GLU:HB3	2.03	0.40
1:B:222:ASP:OD1	1:B:222:ASP:N	2.54	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	275/291 (94%)	269 (98%)	6 (2%)	0	100	100
1	B	274/291 (94%)	263 (96%)	9 (3%)	2 (1%)	19	8
All	All	549/582 (94%)	532 (97%)	15 (3%)	2 (0%)	30	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	ASP
1	B	119	PHE

### 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	233/242 (96%)	224 (96%)	9 (4%)	27	13
1	B	232/242 (96%)	228 (98%)	4 (2%)	56	44
All	All	465/484 (96%)	452 (97%)	13 (3%)	38	24

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	22	GLU
1	A	45	GLN
1	A	71	ASP
1	A	113	GLN
1	A	162	GLU
1	A	169	ASN
1	A	197	ASN
1	A	222	ASP
1	B	3	ASN
1	B	6	ASP
1	B	113	GLN
1	B	222	ASP

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	5	ASN
1	A	12	GLN
1	A	84	GLN
1	A	92	GLN
1	A	96	ASN
1	A	141	GLN
1	A	197	ASN
1	B	5	ASN
1	B	44	ASN

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Mol	Chain	Res	Type
1	B	69	GLN
1	B	96	ASN
1	B	118	HIS
1	B	252	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ACY	B	280	3	3,3,3	1.87	1 (33%)	3,3,3	1.34	0
4	ACY	A	279	3	3,3,3	1.53	1 (33%)	3,3,3	1.50	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	280	ACY	O-C	2.71	1.34	1.22
4	A	279	ACY	O-C	2.09	1.31	1.22

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	279	ACY	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	274/291 (94%)	-0.49	3 (1%) 77 81	11, 22, 37, 59	3 (1%)
1	B	274/291 (94%)	-0.34	6 (2%) 62 65	8, 23, 41, 60	3 (1%)
All	All	548/582 (94%)	-0.41	9 (1%) 70 73	8, 22, 41, 60	6 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	LYS	3.6
1	A	4	PRO	2.6
1	A	162	GLU	2.6
1	B	24	GLY	2.4
1	B	6	ASP	2.4
1	B	3	ASN	2.3
1	B	104	GLY	2.3
1	A	3	ASN	2.2
1	B	253	ALA	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	ACY	A	279	4/4	0.90	0.16	39,40,40,40	0
4	ACY	B	280	4/4	0.94	0.14	37,38,40,40	0
2	NA	A	281	1/1	0.98	0.03	23,23,23,23	0
2	NA	B	282	1/1	0.98	0.03	19,19,19,19	0
3	ZN	B	285	1/1	1.00	0.03	19,19,19,19	0
3	ZN	A	283	1/1	1.00	0.02	17,17,17,17	0
3	ZN	B	284	1/1	1.00	0.02	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.