



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:47 PM GMT

PDB ID : 1D1S  
Title : WILD-TYPE HUMAN SIGMA (CLASS IV) ALCOHOL DEHYDROGE-  
NASE  
Authors : Xie, P.T.; Hurley, T.D.  
Deposited on : 1999-09-21  
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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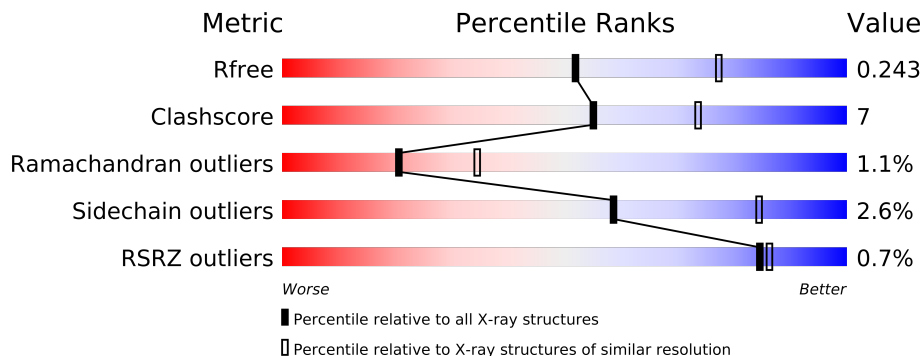
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
1	C	373	
1	D	373	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	A	501	-	X
3	ACT	A	502	-	X
3	ACT	A	513	-	X
3	ACT	B	506	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	B	507	-	X
3	ACT	D	508	-	X
3	ACT	D	511	-	X
3	ACT	D	512	-	X
3	ACT	D	514	-	X
4	CAC	A	554	X	-
4	CAC	B	555	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11836 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

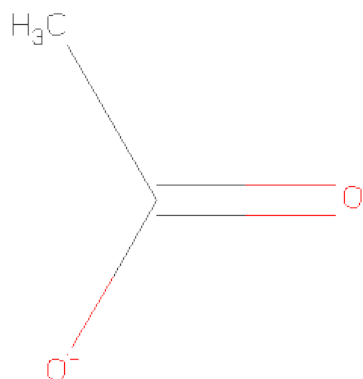
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	B	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	C	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	D	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

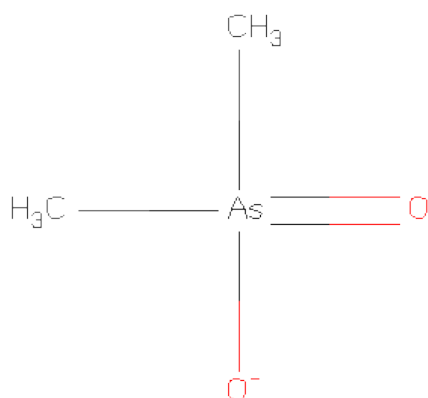
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	6	Total	Zn	0	0
			6	6		
2	D	5	Total	Zn	0	0
			5	5		
2	C	3	Total	Zn	0	0
			3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



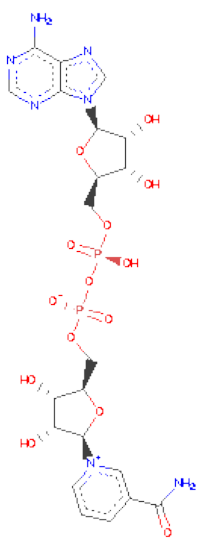
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total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

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is water.

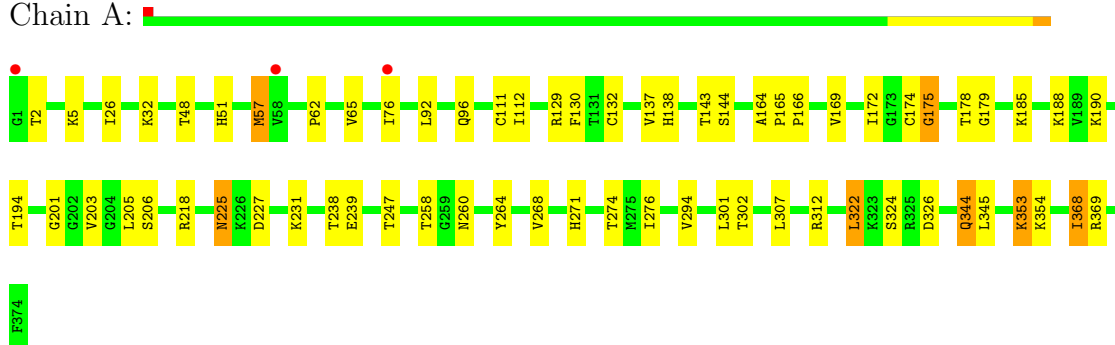
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		
6	B	124	Total	O	0	0
			124	124		
6	C	58	Total	O	0	0
			58	58		
6	D	135	Total	O	0	0
			135	135		

### 3 Residue-property plots

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.

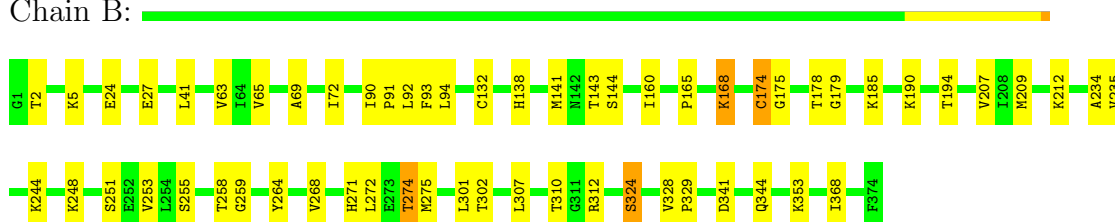
#### • Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain A:



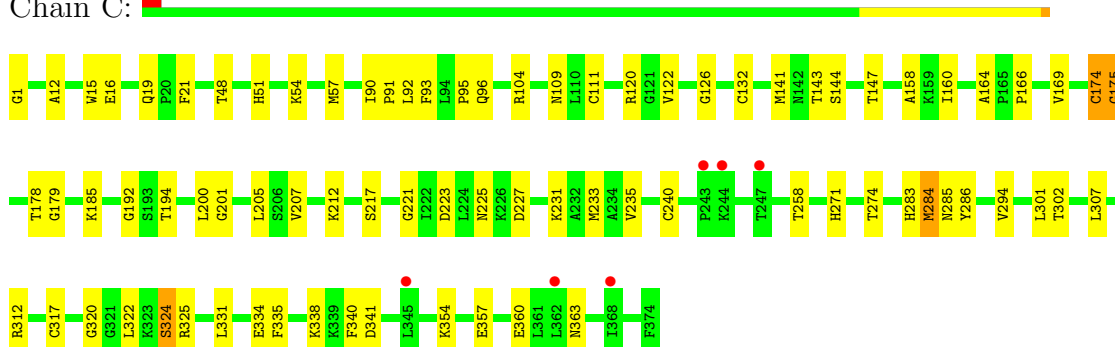
#### • Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain B:



#### • Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain C:

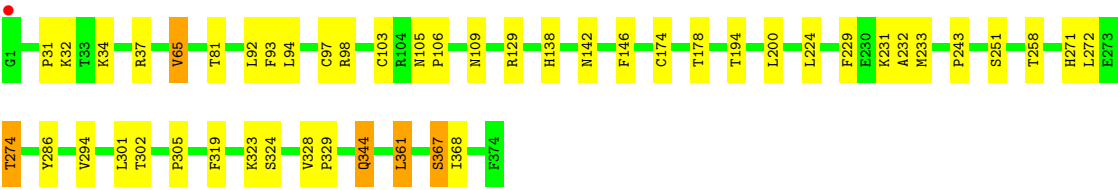


#### • Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

Chain D:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.40Å 90.90Å 121.10Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (50.00-2.50) 87.9 (49.90-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.217 , 0.268 0.198 , 0.243	Depositor DCC
$R_{free}$ test set	3991 reflections (7.62%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 24.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 58662 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.46	0/2840	0.71	2/3839 (0.1%)
1	B	0.50	0/2840	0.73	1/3839 (0.0%)
1	C	0.41	0/2840	0.66	0/3839
1	D	0.49	0/2840	0.73	1/3839 (0.0%)
All	All	0.47	0/11360	0.71	4/15356 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	368	ILE	N-CA-C	-5.57	95.97	111.00
1	D	323	LYS	N-CA-C	-5.22	96.89	111.00
1	A	368	ILE	N-CA-C	-5.20	96.95	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2789	0	2858	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2789	0	2858	32	0
1	C	2789	0	2858	54	0
1	D	2789	0	2858	32	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
3	A	16	0	12	1	0
3	B	8	0	6	2	0
3	C	8	0	6	0	0
3	D	20	0	15	2	0
4	A	5	0	0	0	0
4	B	20	0	0	1	0
5	A	44	0	26	3	0
5	B	44	0	26	2	0
5	C	44	0	26	2	0
5	D	44	0	26	2	0
6	A	91	0	0	3	0
6	B	124	0	0	2	0
6	C	58	0	0	4	0
6	D	135	0	0	5	0
All	All	11836	0	11575	154	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:341:ASP:HB3	1:B:344:GLN:NE2	1.92	0.85
1:A:130:PHE:HB2	1:A:137:VAL:HG23	1.64	0.79
1:C:301:LEU:HB2	1:D:305:PRO:HG3	1.65	0.78
1:B:271:HIS:HB2	1:B:274:THR:OG1	1.84	0.77
1:B:41:LEU:HD11	1:B:72:ILE:HG12	1.69	0.74

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	371/373 (100%)	340 (92%)	27 (7%)	4 (1%)	21	34
1	B	371/373 (100%)	341 (92%)	26 (7%)	4 (1%)	21	34
1	C	371/373 (100%)	331 (89%)	36 (10%)	4 (1%)	21	34
1	D	371/373 (100%)	345 (93%)	22 (6%)	4 (1%)	21	34
All	All	1484/1492 (100%)	1357 (91%)	111 (8%)	16 (1%)	21	34

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	LYS
1	A	174	CYS
1	A	175	GLY
1	B	174	CYS
1	B	324	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/312 (100%)	303 (97%)	9 (3%)	55	81
1	B	312/312 (100%)	301 (96%)	11 (4%)	48	74
1	C	312/312 (100%)	306 (98%)	6 (2%)	69	90
1	D	312/312 (100%)	306 (98%)	6 (2%)	69	90
All	All	1248/1248 (100%)	1216 (97%)	32 (3%)	59	84

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	244	LYS
1	B	274	THR
1	D	344	GLN
1	B	268	VAL
1	B	310	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	HIS
1	C	260	ASN
1	D	19	GLN
1	B	344	GLN
1	D	17	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 19 are monoatomic - leaving 22 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
5	NAD	A	1377	2	48,48,48	1.70	6 (12%)	73,73,73	1.99	16 (21%)
3	ACT	A	501	2	1,3,3	1.98	0	0,3,3	0.00	-
3	ACT	A	502	2	1,3,3	5.02	1 (100%)	0,3,3	0.00	-
3	ACT	A	504	2	1,3,3	1.76	0	0,3,3	0.00	-
3	ACT	A	513	2	1,3,3	5.32	1 (100%)	0,3,3	0.00	-
4	CAC	A	554	-	4,4,4	2.39	2 (50%)	6,6,6	10.70	3 (50%)
5	NAD	B	2377	2	48,48,48	1.72	7 (14%)	73,73,73	2.14	16 (21%)
3	ACT	B	506	2	1,3,3	0.04	0	0,3,3	0.00	-
3	ACT	B	507	2	1,3,3	1.79	0	0,3,3	0.00	-
4	CAC	B	551	2	4,4,4	1.98	1 (25%)	6,6,6	11.76	1 (16%)
4	CAC	B	552	2	4,4,4	2.72	1 (25%)	6,6,6	11.62	3 (50%)
4	CAC	B	553	2	4,4,4	2.87	1 (25%)	6,6,6	10.42	1 (16%)
4	CAC	B	555	-	4,4,4	2.66	2 (50%)	6,6,6	13.15	2 (33%)
5	NAD	C	3377	2	48,48,48	1.74	9 (18%)	73,73,73	2.06	20 (27%)
3	ACT	C	505	2	1,3,3	1.71	0	0,3,3	0.00	-
3	ACT	C	510	2	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
5	NAD	D	4377	2	48,48,48	1.87	10 (20%)	73,73,73	2.26	19 (26%)
3	ACT	D	508	-	1,3,3	2.19	1 (100%)	0,3,3	0.00	-
3	ACT	D	509	2	1,3,3	0.73	0	0,3,3	0.00	-
3	ACT	D	511	2	1,3,3	0.68	0	0,3,3	0.00	-
3	ACT	D	512	2	1,3,3	0.99	0	0,3,3	0.00	-
3	ACT	D	514	2	1,3,3	0.73	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAD	A	1377	2	-	0/30/62/62	0/3/5/5
3	ACT	A	501	2	-	0/0/0/0	0/0/0/0
3	ACT	A	502	2	-	0/0/0/0	0/0/0/0
3	ACT	A	504	2	-	0/0/0/0	0/0/0/0
3	ACT	A	513	2	-	0/0/0/0	0/0/0/0
4	CAC	A	554	-	-	0/0/0/0	0/0/0/0
5	NAD	B	2377	2	-	0/30/62/62	0/3/5/5
3	ACT	B	506	2	-	0/0/0/0	0/0/0/0
3	ACT	B	507	2	-	0/0/0/0	0/0/0/0
4	CAC	B	551	2	-	0/0/0/0	0/0/0/0
4	CAC	B	552	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAC	B	553	2	-	0/0/0/0	0/0/0/0
4	CAC	B	555	-	-	0/0/0/0	0/0/0/0
5	NAD	C	3377	2	-	0/30/62/62	0/3/5/5
3	ACT	C	505	2	-	0/0/0/0	0/0/0/0
3	ACT	C	510	2	-	0/0/0/0	0/0/0/0
5	NAD	D	4377	2	-	0/30/62/62	0/3/5/5
3	ACT	D	508	-	-	0/0/0/0	0/0/0/0
3	ACT	D	509	2	-	0/0/0/0	0/0/0/0
3	ACT	D	511	2	-	0/0/0/0	0/0/0/0
3	ACT	D	512	2	-	0/0/0/0	0/0/0/0
3	ACT	D	514	2	-	0/0/0/0	0/0/0/0

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	4377	NAD	C3N-C7N	-8.75	1.35	1.50
5	A	1377	NAD	C3N-C7N	-7.87	1.37	1.50
5	C	3377	NAD	C3N-C7N	-6.82	1.38	1.50
5	B	2377	NAD	C3N-C7N	-6.79	1.38	1.50
4	B	553	CAC	O2-AS	-5.35	1.62	1.68

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	555	CAC	O2-AS-O1	-31.99	105.64	112.54
4	B	551	CAC	O2-AS-O1	-28.70	106.35	112.54
4	B	552	CAC	O2-AS-O1	-28.08	106.48	112.54
4	A	554	CAC	O2-AS-O1	-26.00	106.93	112.54
4	B	553	CAC	O2-AS-O1	-25.40	107.06	112.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues

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	373/373 (100%)	-0.23	3 (0%) 83 84	11, 35, 57, 66	0
1	B	373/373 (100%)	-0.33	0 100 100	14, 31, 47, 61	0
1	C	373/373 (100%)	0.18	6 (1%) 68 71	23, 51, 67, 77	0
1	D	373/373 (100%)	-0.39	1 (0%) 91 93	9, 27, 45, 55	0
All	All	1492/1492 (100%)	-0.19	10 (0%) 84 86	9, 34, 61, 77	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	362	LEU	3.6
1	D	1	GLY	2.7
1	A	76	ILE	2.6
1	C	345	LEU	2.5
1	C	243	PRO	2.4

### 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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACT	D	514	4/4	0.34	11.06	52,52,52,53	4
3	ACT	A	513	4/4	0.32	6.75	52,53,53,54	4
3	ACT	B	507	4/4	0.17	5.67	20,28,30,31	0
3	ACT	A	502	4/4	0.26	3.90	46,47,47,47	4
3	ACT	A	501	4/4	0.22	3.79	42,45,45,46	0
3	ACT	D	511	4/4	0.16	3.64	34,34,34,36	0
3	ACT	D	508	4/4	0.18	3.39	18,21,22,23	0
4	CAC	B	555	5/5	0.24	3.07	76,78,80,80	0
3	ACT	B	506	4/4	0.16	2.56	17,27,29,32	0
3	ACT	D	512	4/4	0.22	2.11	25,26,28,31	0
3	ACT	C	505	4/4	0.17	1.55	39,41,42,43	0
4	CAC	A	554	5/5	0.13	1.12	76,77,78,81	0
3	ACT	D	509	4/4	0.17	0.94	13,13,14,16	0
5	NAD	A	1377	44/44	0.12	-0.34	19,25,30,33	0
5	NAD	B	2377	44/44	0.12	-0.58	11,25,31,36	0
5	NAD	C	3377	44/44	0.14	-0.66	20,48,53,55	0
5	NAD	D	4377	44/44	0.11	-0.67	18,24,29,32	0
2	ZN	B	375	1/1	0.09	-0.88	24,24,24,24	0
2	ZN	D	410	1/1	0.14	-1.12	41,41,41,41	1
2	ZN	B	404	1/1	0.09	-1.19	27,27,27,27	0
2	ZN	B	376	1/1	0.11	-1.23	24,24,24,24	0
2	ZN	B	405	1/1	0.08	-1.28	48,48,48,48	0
2	ZN	A	402	1/1	0.12	-1.28	40,40,40,40	1
2	ZN	D	376	1/1	0.09	-1.32	28,28,28,28	0
2	ZN	D	409	1/1	0.09	-1.32	42,42,42,42	0
2	ZN	D	375	1/1	0.09	-1.50	25,25,25,25	0
2	ZN	C	375	1/1	0.08	-1.83	35,35,35,35	0
2	ZN	C	407	1/1	0.05	-1.96	61,61,61,61	0
2	ZN	C	376	1/1	0.08	-2.13	50,50,50,50	0
4	CAC	B	551	5/5	0.10	-2.29	16,31,35,38	0
2	ZN	A	375	1/1	0.06	-2.38	42,42,42,42	0
3	ACT	C	510	4/4	0.07	-2.45	29,32,33,36	0
2	ZN	A	376	1/1	0.07	-2.47	33,33,33,33	0
2	ZN	A	408	1/1	0.07	-2.58	37,37,37,37	0
2	ZN	A	403	1/1	0.11	-2.63	48,48,48,48	0
2	ZN	A	401	1/1	0.07	-3.09	40,40,40,40	0
3	ACT	A	504	4/4	0.12	-4.67	20,20,21,23	0
2	ZN	D	411	1/1	0.05	-5.00	53,53,53,53	0
4	CAC	B	552	5/5	0.09	-13.00	47,49,52,52	0
4	CAC	B	553	5/5	0.08	-17.67	45,46,50,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	406	1/1	0.04	-64.33	43,43,43,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.