



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:57 PM GMT

PDB ID : 1HYH  
Title : CRYSTAL STRUCTURE OF L-2-HYDROXYISOCAPROATE DEHYDROGENASE FROM LACTOBACILLUS CONFUSUS AT 2.2 ANGSTROMS RESOLUTION-AN EXAMPLE OF STRONG ASYMMETRY BETWEEN SUBUNITS  
Authors : Niefind, K.; Hecht, H.-J.; Schomburg, D.  
Deposited on : 1995-06-05  
Resolution : 2.20 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

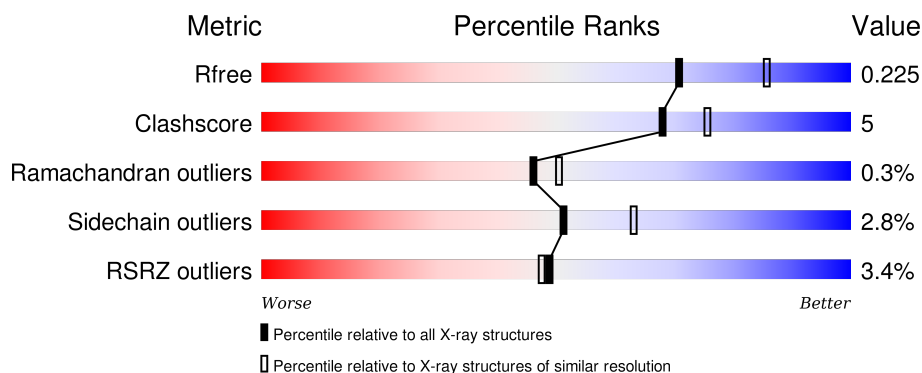
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	309	<div> <div>2%</div> <div>81% 14% . .</div> </div>
1	B	309	<div> <div>3%</div> <div>76% 17% . 5%</div> </div>
1	C	309	<div> <div>2%</div> <div>82% 13% . .</div> </div>
1	D	309	<div> <div>%</div> <div>83% 12% . .</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	331	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9318 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 L-2-HYDROXYISOCAPROATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	1	0
			2217	1397	381	432	7			
1	B	294	Total	C	N	O	S	0	1	0
			2184	1376	374	427	7			
1	C	297	Total	C	N	O	S	0	0	0
			2207	1389	378	433	7			
1	D	297	Total	C	N	O	S	0	0	0
			2205	1389	376	433	7			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



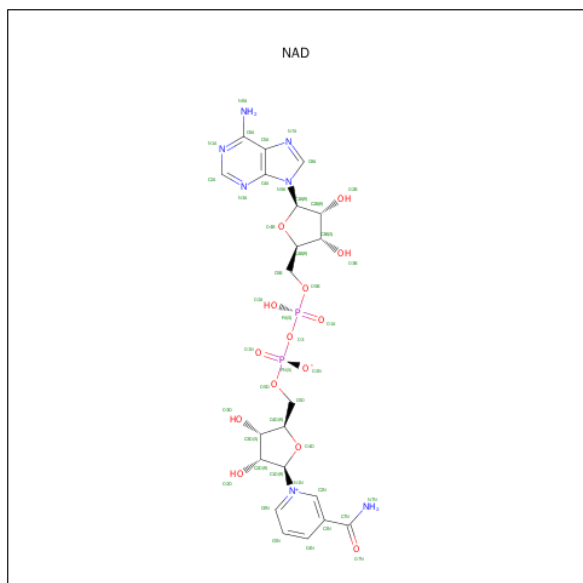
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	70	Total	O	0	0
			70	70		
4	C	79	Total	O	0	0
			79	79		

*Continued on next page...*

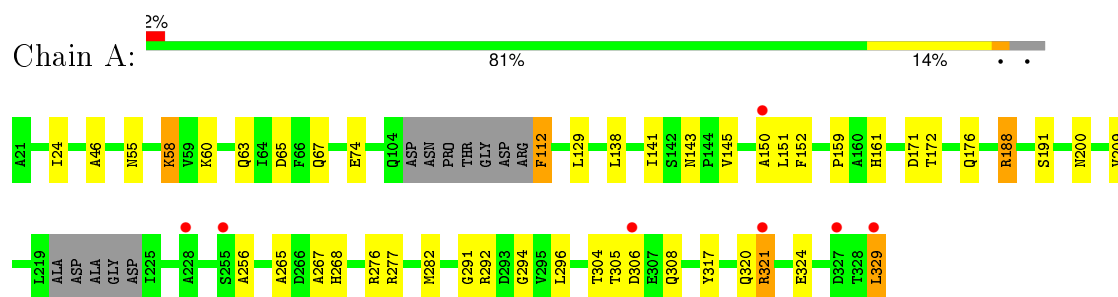
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	73	Total	O	0	0
			73	73		

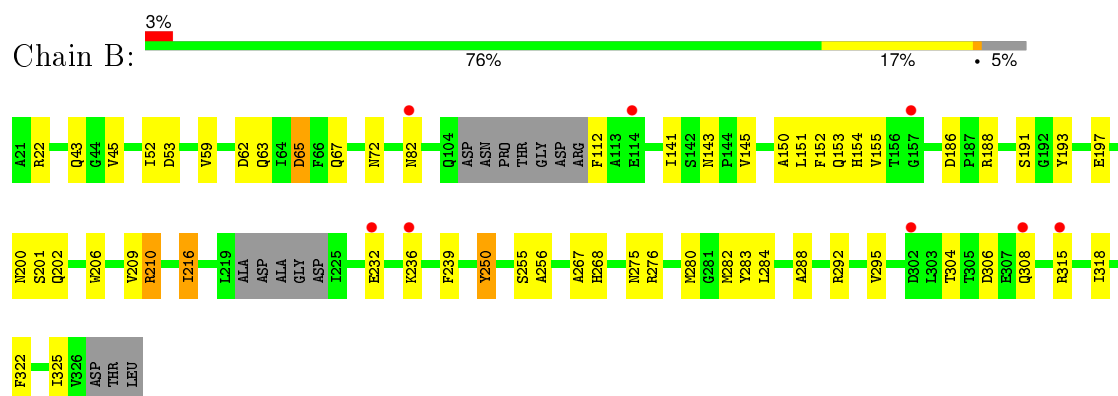
### 3 Residue-property plots

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.

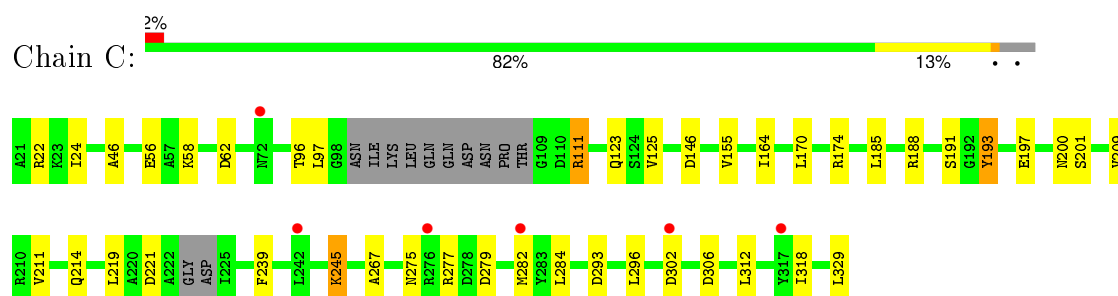
- Molecule 1: L-2-HYDROXYISOCAPROATE DEHYDROGENASE



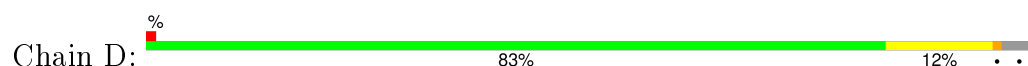
- Molecule 1: L-2-HYDROXYISOCAPROATE DEHYDROGENASE

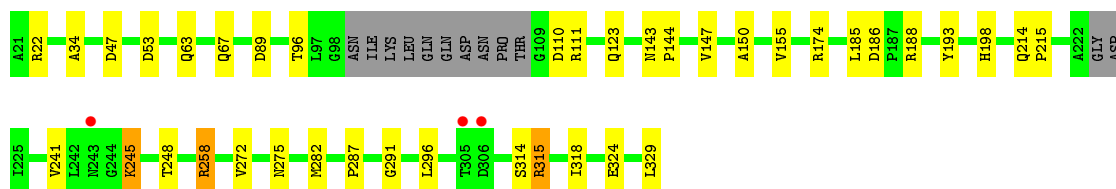


- Molecule 1: L-2-HYDROXYISOCAPROATE DEHYDROGENASE



- Molecule 1: L-2-HYDROXYISOCAPROATE DEHYDROGENASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.90Å 135.90Å 205.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.2 (8.00-2.20) 96.9 (8.00-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.21Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.210 , 0.250 0.193 , 0.225	Depositor DCC
$R_{free}$ test set	10596 reflections (11.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 65.3	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 105711 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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, 0.375 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: SO4, NAD

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	0.91	1/2253 (0.0%)	1.26	10/3054 (0.3%)
1	B	0.79	2/2220 (0.1%)	1.27	12/3011 (0.4%)
1	C	0.80	1/2238 (0.0%)	1.27	14/3035 (0.5%)
1	D	0.82	1/2236 (0.0%)	1.29	11/3033 (0.4%)
All	All	0.83	5/8947 (0.1%)	1.27	47/12133 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	LEU	C-OXT	20.33	1.61	1.23
1	D	329	LEU	C-OXT	13.65	1.49	1.23
1	B	255[A]	SER	CB-OG	8.05	1.52	1.42
1	B	255[B]	SER	CB-OG	8.05	1.52	1.42
1	C	329	LEU	C-OXT	6.52	1.35	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	292	ARG	NE-CZ-NH2	9.80	125.20	120.30
1	C	188	ARG	CD-NE-CZ	9.35	136.69	123.60
1	A	277	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	D	315	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	D	193	TYR	CB-CG-CD1	-8.41	115.95	121.00
1	C	188	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	D	188	ARG	CD-NE-CZ	7.95	134.72	123.60
1	B	292	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	B	210	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	188	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	D	245	LYS	CA-CB-CG	7.43	129.75	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASP	CB-CG-OD2	7.32	124.89	118.30
1	C	277	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	292	ARG	NE-CZ-NH1	-7.21	116.69	120.30
1	A	276	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	D	185	LEU	CA-CB-CG	7.03	131.46	115.30
1	C	185	LEU	CA-CB-CG	6.74	130.81	115.30
1	D	22	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	277	ARG	CD-NE-CZ	6.49	132.69	123.60
1	C	22	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	D	258	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	146	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	276	ARG	CD-NE-CZ	6.24	132.33	123.60
1	B	250	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	D	89	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	65	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	193	TYR	CB-CA-C	-5.98	98.44	110.40
1	B	250	TYR	CB-CG-CD1	5.94	124.57	121.00
1	A	276	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	239	PHE	CB-CG-CD2	-5.89	116.68	120.80
1	B	284	LEU	CA-CB-CG	5.85	128.76	115.30
1	C	56	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	B	188	ARG	CD-NE-CZ	5.74	131.63	123.60
1	A	276	ARG	CD-NE-CZ	5.70	131.58	123.60
1	C	111	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	188	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	B	22	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	221	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	306	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	C	193	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	B	188	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
1	C	306	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	D	315	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	D	174	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	C	245	LYS	CA-CB-CG	5.19	124.81	113.40
1	A	292	ARG	CD-NE-CZ	5.00	130.60	123.60

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	2217	0	2187	23	0
1	B	2184	0	2139	27	0
1	C	2207	0	2167	18	0
1	D	2205	0	2162	24	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	0	0
3	C	44	0	26	2	0
3	D	44	0	26	3	0
4	A	87	0	0	1	0
4	B	70	0	0	0	0
4	C	79	0	0	1	0
4	D	73	0	0	2	0
All	All	9318	0	8759	84	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 5.

All (84) 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:62:ASP:OD1	1:D:245:LYS:HE3	1.85	0.77
1:B:141:ILE:HD11	1:B:256:ALA:HB2	1.69	0.74
1:D:123:GLN:HA	1:D:155:VAL:HG11	1.71	0.73
1:C:123:GLN:HA	1:C:155:VAL:HG11	1.72	0.71
1:C:282:MET:HE2	1:C:318:ILE:HG22	1.76	0.67
1:A:151:LEU:HD22	1:A:329:LEU:HD11	1.78	0.66
1:A:150:ALA:HB2	1:A:282:MET:HE3	1.77	0.65
1:A:65:ASP:OD2	1:C:245:LYS:NZ	2.30	0.63
1:B:65:ASP:OD2	1:D:245:LYS:NZ	2.33	0.62
1:C:197:GLU:OE1	1:C:200:ASN:HB3	2.01	0.61
1:B:197:GLU:HB2	1:B:318:ILE:HD11	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PRO:HG2	1:D:147:VAL:HB	1.85	0.59
1:C:96:THR:O	3:C:330:NAD:H4D	2.04	0.58
1:B:280:MET:O	1:B:315:ARG:HD2	2.04	0.58
1:A:141:ILE:HD11	1:A:256:ALA:HB2	1.87	0.57
1:A:112:PHE:HZ	1:A:321:ARG:HG3	1.69	0.57
1:B:191:SER:OG	1:B:210:ARG:HG3	2.05	0.57
1:C:282:MET:CE	1:C:318:ILE:HG22	2.35	0.57
1:D:248:THR:HB	4:D:368:HOH:O	2.06	0.56
1:B:150:ALA:HB2	1:B:282:MET:HE3	1.88	0.56
1:B:52:ILE:HG12	1:B:82:ASN:HA	1.89	0.55
1:B:143:ASN:HA	1:B:145:VAL:N	2.22	0.54
1:B:191:SER:O	1:B:209:VAL:HA	2.08	0.54
1:B:322:PHE:O	1:B:325:ILE:HG22	2.08	0.53
1:B:288:ALA:HB1	1:B:295:VAL:HG13	1.91	0.52
1:B:197:GLU:O	1:B:202:GLN:HB3	2.10	0.52
1:A:191:SER:O	1:A:209:VAL:HA	2.10	0.52
1:B:197:GLU:HB3	1:B:201:SER:OG	2.10	0.51
1:D:282:MET:HE2	1:D:318:ILE:HG22	1.92	0.51
1:B:63:GLN:O	1:B:67:GLN:HG3	2.10	0.50
1:A:188:ARG:HD3	4:C:343:HOH:O	2.10	0.50
1:A:265:ALA:HA	1:D:47:ASP:HB3	1.93	0.49
1:D:291:GLY:HA3	1:D:296:LEU:HD11	1.93	0.49
1:D:63:GLN:O	1:D:67:GLN:HG3	2.13	0.49
1:A:317:TYR:O	1:A:321:ARG:HG2	2.13	0.49
1:A:143:ASN:HA	1:A:145:VAL:N	2.28	0.48
1:B:267:ALA:O	1:B:268:HIS:HB2	2.12	0.48
1:A:291:GLY:HA3	1:A:296:LEU:HD11	1.96	0.48
1:A:304:THR:O	1:A:308:GLN:HG3	2.14	0.47
1:A:172:THR:O	1:A:176:GLN:HG3	2.13	0.47
1:D:53:ASP:OD2	3:D:330:NAD:H1B	2.13	0.47
1:B:72:ASN:OD1	1:D:258:ARG:NH1	2.42	0.47
4:A:361:HOH:O	1:C:245:LYS:HE3	2.15	0.46
1:B:151:LEU:O	1:B:155:VAL:HG23	2.16	0.46
1:A:129:LEU:HD21	1:A:138:LEU:HD13	1.99	0.45
1:B:206:TRP:HE3	1:B:216:ILE:HG21	1.81	0.45
1:A:112:PHE:CZ	1:A:321:ARG:HG3	2.51	0.45
1:A:320:GLN:O	1:A:324:GLU:HG3	2.17	0.45
1:B:232:GLU:HG3	1:B:236:LYS:NZ	2.32	0.45
1:D:282:MET:CE	1:D:318:ILE:HG22	2.47	0.44
1:C:267:ALA:O	1:D:186:ASP:HB2	2.17	0.44
1:B:304:THR:O	1:B:308:GLN:HG3	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:O	1:A:67:GLN:HG3	2.17	0.44
1:D:150:ALA:CB	1:D:282:MET:HE1	2.47	0.44
1:D:248:THR:CB	4:D:368:HOH:O	2.65	0.43
1:C:191:SER:O	1:C:209:VAL:HA	2.16	0.43
1:A:55:ASN:ND2	1:A:58:LYS:HB2	2.32	0.43
1:B:53:ASP:HB3	1:B:59:VAL:HB	1.99	0.43
1:C:58:LYS:NZ	1:C:62:ASP:OD2	2.46	0.43
1:A:267:ALA:O	1:B:186:ASP:HB2	2.17	0.43
1:D:96:THR:O	3:D:330:NAD:H4D	2.18	0.43
1:D:198:HIS:NE2	3:D:330:NAD:O7N	2.51	0.43
1:B:43:GLN:HB2	1:B:45:VAL:HG23	1.99	0.43
1:C:214:GLN:CB	1:C:219:LEU:HD21	2.49	0.43
1:C:24:ILE:HD12	1:C:46:ALA:HB2	2.01	0.42
1:D:272:VAL:HA	1:D:287:PRO:HA	2.01	0.42
1:B:250:TYR:OH	1:D:34:ALA:HB1	2.20	0.42
3:A:330:NAD:H71N	3:A:330:NAD:H2N	1.67	0.42
1:D:143:ASN:HA	1:D:144:PRO:HA	1.86	0.42
1:D:214:GLN:HA	1:D:215:PRO:HD3	1.81	0.42
1:C:97:LEU:HD21	3:C:330:NAD:C4A	2.50	0.41
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.85	0.41
1:A:161:HIS:O	1:A:294:GLY:HA3	2.21	0.41
1:B:236:LYS:HA	1:B:239:PHE:CD2	2.56	0.41
1:C:170:LEU:O	1:C:174:ARG:HG3	2.20	0.41
1:C:97:LEU:CD1	1:C:125:VAL:HG21	2.50	0.41
1:A:267:ALA:O	1:A:268:HIS:HB2	2.20	0.41
1:C:302:ASP:CG	1:D:214:GLN:HE22	2.24	0.41
1:A:159:PRO:HB2	1:A:161:HIS:CD2	2.56	0.40
1:A:24:ILE:HD12	1:A:46:ALA:HB2	2.03	0.40
1:D:241:VAL:CG1	1:D:248:THR:HG22	2.51	0.40
1:D:111:ARG:NH2	1:D:324:GLU:OE1	2.53	0.40
1:B:153:GLN:HG3	1:B:283:TYR:OH	2.21	0.40
1:C:293:ASP:HB2	1:C:296:LEU:HD21	2.04	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	292/309 (94%)	282 (97%)	9 (3%)	1 (0%)	46	50
1	B	289/309 (94%)	280 (97%)	8 (3%)	1 (0%)	46	50
1	C	291/309 (94%)	285 (98%)	5 (2%)	1 (0%)	46	50
1	D	291/309 (94%)	284 (98%)	7 (2%)	0	100	100
All	All	1163/1236 (94%)	1131 (97%)	29 (2%)	3 (0%)	46	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	ASN
1	A	200	ASN
1	C	201	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	229/243 (94%)	222 (97%)	7 (3%)	47	59
1	B	224/243 (92%)	217 (97%)	7 (3%)	47	59
1	C	226/243 (93%)	219 (97%)	7 (3%)	47	59
1	D	225/243 (93%)	221 (98%)	4 (2%)	66	79
All	All	904/972 (93%)	879 (97%)	25 (3%)	51	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	60	LYS
1	A	74	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	112	PHE
1	A	152	PHE
1	A	305	THR
1	A	321	ARG
1	B	112	PHE
1	B	152	PHE
1	B	154	HIS
1	B	193	TYR
1	B	216	ILE
1	B	275	ASN
1	B	306	ASP
1	C	111	ARG
1	C	164	ILE
1	C	193	TYR
1	C	211	VAL
1	C	275	ASN
1	C	279	ASP
1	C	284	LEU
1	D	110	ASP
1	D	275	ASN
1	D	314	SER
1	D	315	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	243	ASN
1	B	319	GLN
1	C	214	GLN
1	D	67	GLN

### 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](#)

8 ligands are modelled in this entry.

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$
3	NAD	A	330	-	38,48,48	1.56	6 (15%)	47,73,73	2.30	11 (23%)
2	SO4	A	331	-	4,4,4	1.03	0	6,6,6	0.52	0
3	NAD	B	330	-	38,48,48	1.56	6 (15%)	47,73,73	2.57	12 (25%)
2	SO4	B	331	-	4,4,4	1.08	0	6,6,6	0.23	0
3	NAD	C	330	-	38,48,48	1.49	5 (13%)	47,73,73	2.88	17 (36%)
2	SO4	C	331	-	4,4,4	1.08	0	6,6,6	0.22	0
3	NAD	D	330	-	38,48,48	1.63	6 (15%)	47,73,73	2.97	15 (31%)
2	SO4	D	331	-	4,4,4	1.03	0	6,6,6	0.27	0

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
3	NAD	A	330	-	-	0/22/62/62	0/5/5/5
2	SO4	A	331	-	-	0/0/0/0	0/0/0/0
3	NAD	B	330	-	-	0/22/62/62	0/5/5/5
2	SO4	B	331	-	-	0/0/0/0	0/0/0/0
3	NAD	C	330	-	-	0/22/62/62	0/5/5/5
2	SO4	C	331	-	-	0/0/0/0	0/0/0/0
3	NAD	D	330	-	-	0/22/62/62	0/5/5/5
2	SO4	D	331	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	330	NAD	C2N-C3N	-2.64	1.34	1.39
3	C	330	NAD	C5D-C4D	-2.37	1.44	1.51
3	A	330	NAD	O2B-C2B	-2.34	1.37	1.43
3	D	330	NAD	C5D-C4D	-2.27	1.44	1.51
3	B	330	NAD	O2B-C2B	-2.24	1.37	1.43
3	D	330	NAD	O2B-C2B	-2.21	1.37	1.43
3	A	330	NAD	O4B-C1B	-2.15	1.38	1.41
3	C	330	NAD	O2B-C2B	-2.14	1.37	1.43
3	A	330	NAD	C7N-N7N	2.14	1.37	1.33
3	B	330	NAD	C5N-C4N	2.17	1.43	1.38
3	A	330	NAD	C2A-N3A	2.20	1.36	1.32
3	B	330	NAD	C4A-N3A	2.58	1.39	1.35
3	C	330	NAD	O4D-C4D	3.01	1.52	1.45
3	B	330	NAD	C2A-N3A	3.61	1.38	1.32
3	A	330	NAD	O4D-C4D	3.65	1.53	1.45
3	C	330	NAD	C2A-N3A	3.69	1.38	1.32
3	D	330	NAD	O4D-C4D	3.81	1.53	1.45
3	B	330	NAD	O4D-C4D	3.87	1.53	1.45
3	D	330	NAD	C2A-N3A	4.01	1.39	1.32
3	B	330	NAD	C3N-C7N	4.13	1.57	1.50
3	D	330	NAD	C3N-C7N	4.23	1.57	1.50
3	C	330	NAD	C3N-C7N	4.58	1.57	1.50
3	A	330	NAD	C3N-C7N	4.89	1.58	1.50

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	330	NAD	N3A-C2A-N1A	-8.61	122.31	128.89
3	D	330	NAD	O7N-C7N-C3N	-8.21	110.62	119.59
3	D	330	NAD	N3A-C2A-N1A	-7.64	123.04	128.89
3	D	330	NAD	C3N-C2N-N1N	-7.21	112.05	120.36
3	C	330	NAD	C3N-C2N-N1N	-6.79	112.54	120.36
3	B	330	NAD	N3A-C2A-N1A	-6.59	123.85	128.89
3	A	330	NAD	N3A-C2A-N1A	-6.35	124.03	128.89
3	C	330	NAD	C5N-C4N-C3N	-6.30	112.41	120.33
3	B	330	NAD	C5N-C4N-C3N	-5.73	113.14	120.33
3	A	330	NAD	C3N-C2N-N1N	-5.37	114.17	120.36
3	D	330	NAD	C5N-C4N-C3N	-5.27	113.70	120.33
3	B	330	NAD	O7N-C7N-C3N	-5.14	113.98	119.59
3	B	330	NAD	C3N-C2N-N1N	-4.96	114.65	120.36
3	C	330	NAD	O7N-C7N-C3N	-4.79	114.35	119.59
3	A	330	NAD	C5N-C4N-C3N	-4.62	114.52	120.33
3	A	330	NAD	C2B-C1B-N9A	-4.12	108.00	114.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	330	NAD	C4B-O4B-C1B	-3.69	105.67	109.72
3	D	330	NAD	C4B-O4B-C1B	-3.43	105.95	109.72
3	A	330	NAD	C4D-O4D-C1D	-3.17	106.24	109.72
3	A	330	NAD	C4B-O4B-C1B	-2.90	106.53	109.72
3	C	330	NAD	O3D-C3D-C4D	-2.80	102.65	111.05
3	D	330	NAD	C4N-C3N-C7N	-2.52	114.43	121.09
3	D	330	NAD	C4D-O4D-C1D	-2.51	106.96	109.72
3	A	330	NAD	C2N-C3N-C7N	-2.36	112.45	119.31
3	C	330	NAD	C2N-C3N-C7N	-2.22	112.85	119.31
3	B	330	NAD	O3D-C3D-C4D	-2.09	104.78	111.05
3	C	330	NAD	C4B-O4B-C1B	-2.04	107.48	109.72
3	A	330	NAD	O3D-C3D-C4D	-2.03	104.95	111.05
3	D	330	NAD	O2N-PN-O1N	2.00	123.37	112.53
3	B	330	NAD	C6N-C5N-C4N	2.01	122.48	119.44
3	A	330	NAD	O7N-C7N-N7N	2.02	125.43	122.59
3	C	330	NAD	N6A-C6A-N1A	2.02	123.54	119.20
3	D	330	NAD	N6A-C6A-N1A	2.04	123.58	119.20
3	C	330	NAD	C5D-C4D-C3D	2.15	123.73	115.21
3	D	330	NAD	C2B-C3B-C4B	2.22	107.18	102.61
3	C	330	NAD	O2B-C2B-C3B	2.25	119.16	111.83
3	D	330	NAD	O5D-C5D-C4D	2.30	117.58	109.12
3	C	330	NAD	O2N-PN-O1N	2.45	125.81	112.53
3	C	330	NAD	C2B-C3B-C4B	2.52	107.78	102.61
3	C	330	NAD	C6N-C5N-C4N	2.70	123.52	119.44
3	C	330	NAD	O4D-C1D-N1N	2.72	111.11	108.13
3	B	330	NAD	O7N-C7N-N7N	3.12	126.99	122.59
3	B	330	NAD	C2B-C3B-C4B	3.21	109.22	102.61
3	D	330	NAD	C2A-N1A-C6A	3.61	125.21	118.77
3	B	330	NAD	C2A-N1A-C6A	3.69	125.37	118.77
3	D	330	NAD	O4D-C1D-N1N	3.76	112.26	108.13
3	A	330	NAD	C2A-N1A-C6A	3.89	125.71	118.77
3	C	330	NAD	O7N-C7N-N7N	4.24	128.56	122.59
3	B	330	NAD	O4D-C1D-N1N	4.53	113.11	108.13
3	C	330	NAD	C2A-N1A-C6A	4.59	126.98	118.77
3	D	330	NAD	O7N-C7N-N7N	5.46	130.28	122.59
3	A	330	NAD	C2N-C3N-C4N	7.14	126.24	118.29
3	B	330	NAD	C2N-C3N-C4N	8.04	127.24	118.29
3	D	330	NAD	C2N-C3N-C4N	8.79	128.08	118.29
3	C	330	NAD	C2N-C3N-C4N	8.87	128.16	118.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	330	NAD	1	0
3	C	330	NAD	2	0
3	D	330	NAD	3	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 ⓘ

### 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	157/309 (50%)	-0.33	7 (4%)	37	36	13, 27, 52, 63	0
1	B	100/309 (32%)	-0.08	8 (8%)	15	14	15, 31, 57, 73	0
1	C	169/309 (54%)	-0.46	6 (3%)	46	45	12, 21, 46, 65	0
1	D	278/309 (89%)	-0.52	3 (1%)	82	82	10, 23, 50, 64	0
All	All	704/1236 (56%)	-0.40	24 (3%)	49	47	10, 24, 51, 73	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	MET	6.2
1	C	242	LEU	6.2
1	B	114	GLU	4.4
1	B	308	GLN	3.9
1	C	72	ASN	3.7
1	C	276	ARG	3.5
1	A	255[A]	SER	3.5
1	C	317	TYR	3.3
1	B	232	GLU	2.9
1	A	150	ALA	2.8
1	B	315	ARG	2.8
1	C	302	ASP	2.7
1	A	329	LEU	2.4
1	B	82	ASN	2.4
1	D	305	THR	2.4
1	A	321	ARG	2.3
1	B	302	ASP	2.2
1	A	327	ASP	2.2
1	A	306	ASP	2.2
1	B	236	LYS	2.2
1	D	243	ASN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	2.0
1	D	306	ASP	2.0
1	B	157	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 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	SO4	A	331	5/5	0.91	0.17	7.19	82,82,82,82	0
3	NAD	C	330	44/44	0.97	0.10	0.26	32,32,32,32	0
3	NAD	D	330	44/44	0.95	0.11	0.17	35,35,35,35	0
2	SO4	D	331	5/5	0.94	0.12	-0.07	86,86,86,86	0
3	NAD	A	330	44/44	0.99	0.07	-0.32	14,14,14,14	0
3	NAD	B	330	44/44	0.98	0.10	-0.42	33,33,33,33	0
2	SO4	C	331	5/5	-	-	-	78,78,78,78	0
2	SO4	B	331	5/5	-	-	-	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.