



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:40 pm GMT

PDB ID : 2ZTV  
Title : The binary complex of D-3-hydroxybutyrate dehydrogenase with NAD+  
Authors : Nakashima, K.; Nakajima, Y.; Ito, K.; Yoshimoto, T.  
Deposited on : 2008-10-09  
Resolution : 1.95 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

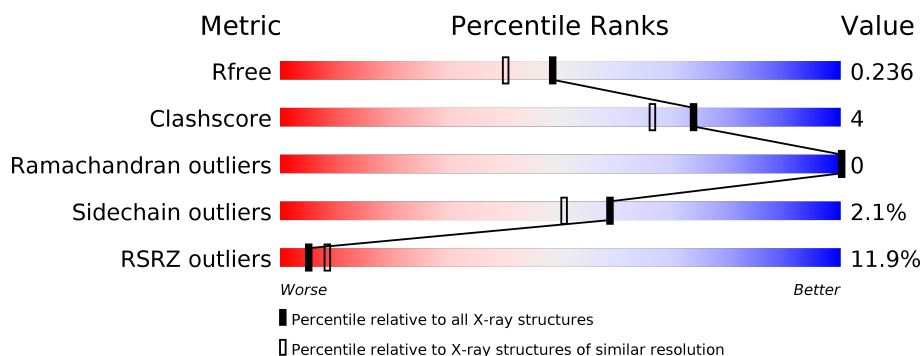
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	260	
1	B	260	
1	C	260	
1	D	260	

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	NAD	C	300	-	-	-	X

## 2 Entry composition [i](#)

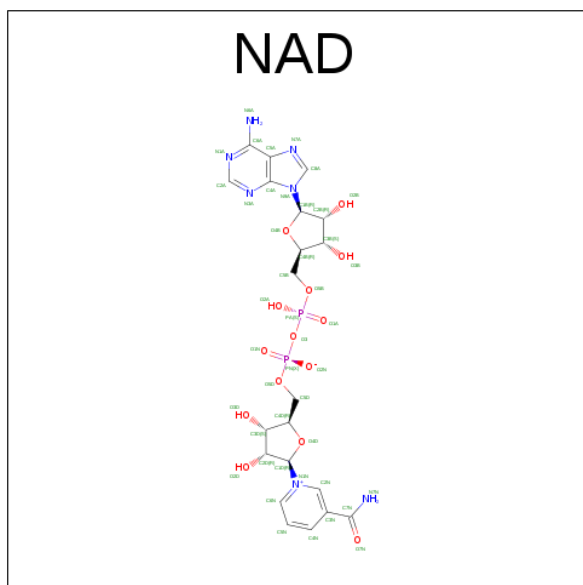
There are 5 unique types of molecules in this entry. The entry contains 7981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D(-)-3-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	1	0
			1877	1181	334	358	4			
1	B	246	Total	C	N	O	S	0	0	0
			1713	1080	302	327	4			
1	C	255	Total	C	N	O	S	0	0	0
			1804	1134	322	344	4			
1	D	253	Total	C	N	O	S	0	0	0
			1825	1147	324	350	4			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

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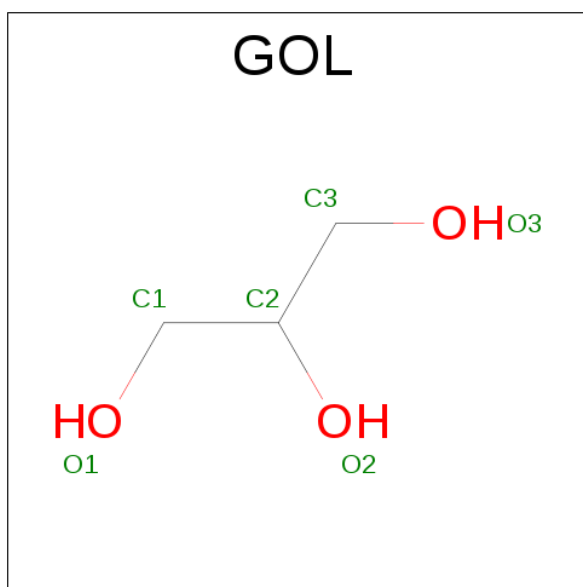
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	148	Total	O	0	0
			148	148		
5	B	86	Total	O	0	0
			86	86		

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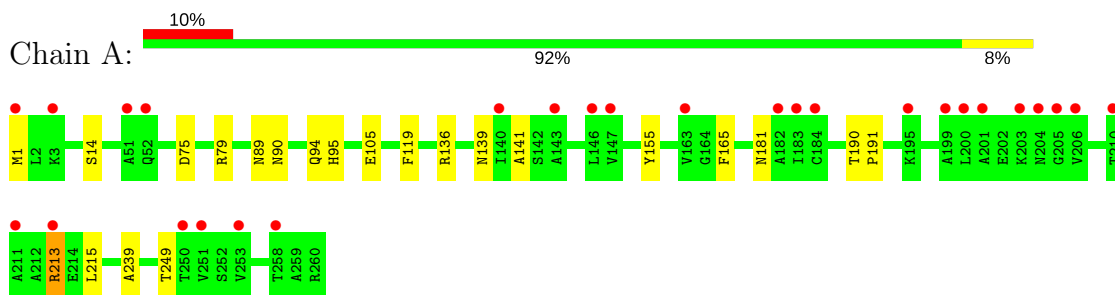
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	179	Total 179	O 179	0	0
5	D	165	Total 165	O 165	0	0

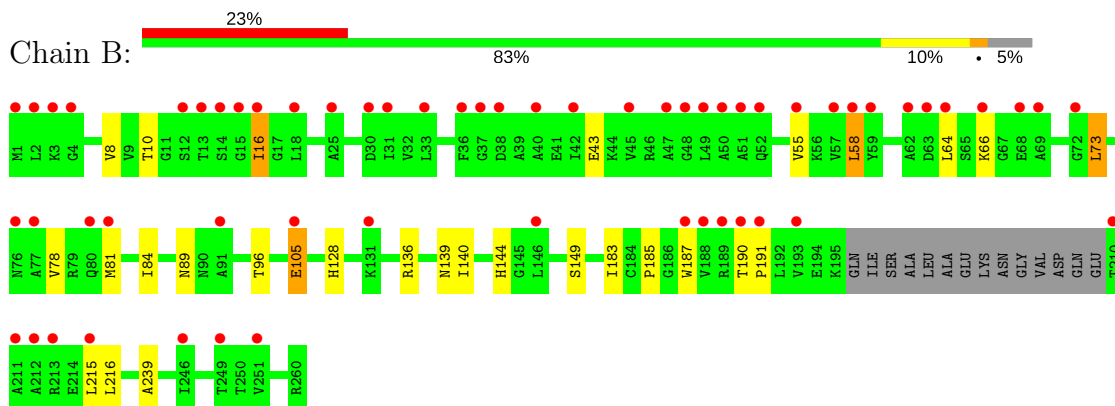
### 3 Residue-property plots

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

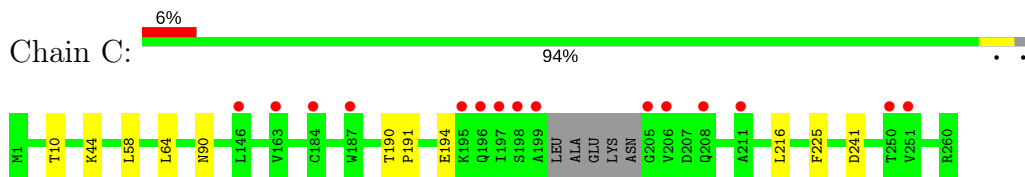
- Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase



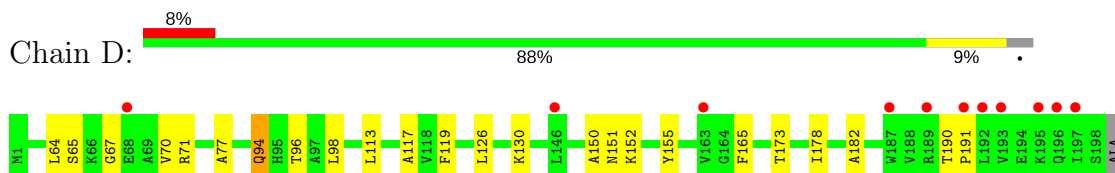
- Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase

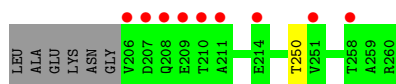


- Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase



- Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.23Å 106.79Å 163.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 48.54 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.95) 99.4 (48.54-1.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.53 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.236 0.202 , 0.236	Depositor DCC
$R_{free}$ test set	4666 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: GOL, MG, 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	0.84	0/1906	0.75	0/2586
1	B	0.78	0/1738	0.66	0/2365
1	C	0.94	0/1829	0.77	1/2484 (0.0%)
1	D	0.92	1/1850 (0.1%)	0.81	0/2510
All	All	0.87	1/7323 (0.0%)	0.75	1/9945 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	ALA	CA-CB	6.66	1.66	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ASP	CB-CG-OD2	5.82	123.53	118.30

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	1877	0	1915	14	0
1	B	1713	0	1690	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1804	0	1802	6	0
1	D	1825	0	1849	13	0
2	A	44	0	26	2	0
2	B	44	0	26	2	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	D	6	0	8	0	0
5	A	148	0	0	1	0
5	B	86	0	0	2	0
5	C	179	0	0	0	0
5	D	165	0	0	0	1
All	All	7981	0	7368	56	1

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 4.

All (56) 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:16:ILE:HD11	1:B:140:ILE:HG21	1.51	0.92
1:B:190:THR:HB	1:B:191:PRO:HD2	1.57	0.87
1:B:96:THR:HG22	5:B:1535:HOH:O	1.95	0.66
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.61	0.65
1:A:89:ASN:HB2	1:A:139:ASN:HD22	1.62	0.65
1:B:105:GLU:CD	1:B:105:GLU:H	2.01	0.64
1:B:78:VAL:HG21	1:B:128:HIS:ND1	2.14	0.62
1:B:58:LEU:HB2	1:B:81:MET:CE	2.29	0.62
1:A:94:GLN:HE21	1:A:95:HIS:H	1.48	0.62
1:B:144:HIS:NE2	1:B:149:SER:OG	2.27	0.61
1:B:190:THR:HB	1:B:191:PRO:CD	2.30	0.61
1:D:67:GLY:O	1:D:71:ARG:HG3	2.00	0.60
1:D:64:LEU:HD22	1:D:70:VAL:HG22	1.85	0.58
1:B:187:TRP:HD1	1:B:216:LEU:HD23	1.69	0.56
1:C:190:THR:HB	1:C:191:PRO:HD2	1.88	0.55
1:A:213:ARG:NH1	1:A:213:ARG:HG2	2.23	0.54
1:C:90:ASN:O	2:C:300:NAD:H4D	2.08	0.53
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.21	0.53
1:B:8:VAL:HG23	1:B:84:ILE:HD12	1.93	0.51
1:B:64:LEU:HD21	1:B:73:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:GLN:NE2	1:D:96:THR:HG22	2.26	0.51
1:B:183:ILE:O	1:B:185:PRO:HD3	2.11	0.51
1:B:10:THR:HB	1:B:64:LEU:HD11	1.93	0.51
1:B:136:ARG:HG3	1:B:239:ALA:HA	1.93	0.49
1:B:89:ASN:HB2	1:B:139:ASN:HD22	1.77	0.49
1:B:43:GLU:HA	1:B:43:GLU:OE1	2.12	0.48
1:D:190:THR:HB	1:D:191:PRO:HD2	1.95	0.48
1:B:16:ILE:CD1	1:B:140:ILE:HG21	2.32	0.47
1:D:126:LEU:O	1:D:130:LYS:HG3	2.13	0.47
1:B:8:VAL:CG2	1:B:84:ILE:HD12	2.45	0.47
1:A:181:ASN:OD1	1:A:249:THR:HG22	2.15	0.46
1:B:105:GLU:CD	1:B:105:GLU:N	2.69	0.46
1:A:119:PHE:HA	1:A:165:PHE:CZ	2.52	0.45
1:B:187:TRP:CD1	1:B:216:LEU:HD23	2.50	0.45
1:B:10:THR:HB	1:B:64:LEU:CD1	2.46	0.45
1:D:119:PHE:HA	1:D:165:PHE:CZ	2.52	0.45
1:D:94:GLN:OE1	1:D:155:TYR:HB2	2.17	0.45
1:A:141:ALA:O	2:A:300:NAD:H6N	2.16	0.44
1:A:94:GLN:HE22	1:A:155:TYR:HB2	1.82	0.44
1:A:136:ARG:HG3	1:A:239:ALA:HA	1.98	0.44
1:C:191:PRO:O	1:C:194:GLU:HB3	2.18	0.44
2:B:300:NAD:O2N	5:B:1241:HOH:O	2.21	0.43
1:A:190:THR:HB	1:A:191:PRO:HD2	1.99	0.43
1:D:98:LEU:HD23	1:D:151:ASN:OD1	2.18	0.43
1:D:173:THR:HB	1:D:178:ILE:HB	1.99	0.42
1:D:150:ALA:O	1:D:151:ASN:HB2	2.18	0.42
1:D:182:ALA:HB3	1:D:250:THR:HG22	2.00	0.42
1:C:10:THR:HB	1:C:64:LEU:HD11	2.01	0.41
1:C:44:LYS:HB2	1:C:44:LYS:HE3	1.91	0.41
1:B:16:ILE:HG12	2:B:300:NAD:H51N	2.02	0.41
1:A:75:ASP:HB3	1:A:79:ARG:NH2	2.35	0.41
1:A:213:ARG:HD2	5:A:1572:HOH:O	2.20	0.41
1:A:90:ASN:O	2:A:300:NAD:H4D	2.21	0.41
1:D:113:LEU:O	1:D:117:ALA:HB3	2.21	0.40
1:C:216:LEU:HD11	1:C:225:PHE:CE1	2.56	0.40
1:D:94:GLN:HE22	1:D:152:LYS:HG2	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1336:HOH:O	5:D:1498:HOH:O[4_455]	2.04	0.16

## 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	259/260 (100%)	252 (97%)	7 (3%)	0	100	100
1	B	242/260 (93%)	228 (94%)	14 (6%)	0	100	100
1	C	251/260 (96%)	243 (97%)	8 (3%)	0	100	100
1	D	249/260 (96%)	243 (98%)	6 (2%)	0	100	100
All	All	1001/1040 (96%)	966 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	186/187 (100%)	181 (97%)	5 (3%)	50	39
1	B	160/187 (86%)	153 (96%)	7 (4%)	33	18
1	C	172/187 (92%)	171 (99%)	1 (1%)	89	88
1	D	181/187 (97%)	179 (99%)	2 (1%)	78	75
All	All	699/748 (93%)	684 (98%)	15 (2%)	59	50

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	14	SER
1	A	105	GLU
1	A	213	ARG
1	A	215	LEU
1	B	16	ILE
1	B	55	VAL
1	B	58	LEU
1	B	66	LYS
1	B	73	LEU
1	B	105	GLU
1	B	215	LEU
1	C	58	LEU
1	D	65	SER
1	D	94	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	94	GLN
1	A	139	ASN
1	A	208	GLN
1	B	53	HIS
1	B	89	ASN
1	B	139	ASN
1	C	52	GLN
1	C	89	ASN
1	C	94	GLN
1	C	139	ASN
1	C	196	GLN
1	D	89	ASN
1	D	139	ASN
1	D	196	GLN
1	D	208	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z  > 2$
2	NAD	A	300	-	41,48,48	1.52	3 (7%)	43,73,73	2.43	6 (13%)
2	NAD	B	300	-	41,48,48	1.79	3 (7%)	43,73,73	1.68	4 (9%)
2	NAD	C	300	-	41,48,48	1.75	3 (7%)	43,73,73	1.71	2 (4%)
2	NAD	D	300	-	41,48,48	1.75	3 (7%)	43,73,73	1.91	5 (11%)
4	GOL	D	403	-	5,5,5	0.43	0	5,5,5	0.37	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
2	NAD	A	300	-	-	0/22/62/62	0/5/5/5
2	NAD	B	300	-	-	0/22/62/62	0/5/5/5
2	NAD	C	300	-	-	0/22/62/62	0/5/5/5
2	NAD	D	300	-	-	0/22/62/62	0/5/5/5
4	GOL	D	403	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	NAD	C2A-N1A	2.19	1.38	1.33
2	A	300	NAD	C2A-N1A	2.21	1.38	1.33
2	A	300	NAD	C2A-N3A	2.69	1.36	1.32
2	D	300	NAD	C2A-N1A	3.14	1.39	1.33
2	B	300	NAD	C2A-N1A	3.18	1.39	1.33
2	C	300	NAD	C2A-N3A	3.36	1.37	1.32
2	D	300	NAD	C2A-N3A	4.24	1.39	1.32
2	B	300	NAD	C2A-N3A	4.48	1.39	1.32
2	A	300	NAD	O7N-C7N	7.50	1.39	1.24
2	B	300	NAD	O7N-C7N	8.66	1.42	1.24
2	D	300	NAD	O7N-C7N	8.66	1.42	1.24
2	C	300	NAD	O7N-C7N	9.32	1.43	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NAD	N3A-C2A-N1A	-11.88	118.51	128.86
2	D	300	NAD	N3A-C2A-N1A	-10.08	120.08	128.86
2	B	300	NAD	N3A-C2A-N1A	-9.10	120.93	128.86
2	C	300	NAD	N3A-C2A-N1A	-9.09	120.94	128.86
2	A	300	NAD	O7N-C7N-C3N	-4.54	114.32	119.62
2	D	300	NAD	C1B-N9A-C4A	-3.06	121.34	126.64
2	D	300	NAD	C4B-O4B-C1B	-2.68	106.92	109.77
2	D	300	NAD	O7N-C7N-N7N	-2.59	118.90	122.58
2	A	300	NAD	C1B-N9A-C4A	-2.37	122.55	126.64
2	B	300	NAD	C4A-C5A-N7A	-2.34	107.15	109.41
2	C	300	NAD	C1B-N9A-C4A	-2.30	122.66	126.64
2	A	300	NAD	O7N-C7N-N7N	-2.26	119.37	122.58
2	B	300	NAD	O7N-C7N-N7N	-2.02	119.70	122.58
2	D	300	NAD	O4B-C4B-C3B	2.18	109.49	105.17
2	A	300	NAD	C2A-N1A-C6A	2.34	122.87	118.77
2	B	300	NAD	O7N-C7N-C3N	2.61	122.67	119.62
2	A	300	NAD	C3N-C7N-N7N	7.47	126.31	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NAD	2	0
2	B	300	NAD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	NAD	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

### 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	260/260 (100%)	0.47	27 (10%) 7 11	18, 30, 61, 74	0
1	B	246/260 (94%)	1.32	59 (23%) 1 0	26, 43, 69, 81	0
1	C	255/260 (98%)	0.17	15 (5%) 23 32	17, 24, 64, 80	0
1	D	253/260 (97%)	0.39	20 (7%) 13 21	19, 28, 58, 77	0
All	All	1014/1040 (97%)	0.58	121 (11%) 5 8	17, 30, 67, 81	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	ILE	8.7
1	B	212	ALA	7.3
1	B	211	ALA	7.0
1	B	40	ALA	6.1
1	B	193	VAL	5.8
1	A	204	ASN	5.2
1	B	51	ALA	5.2
1	D	193	VAL	5.2
1	D	207	ASP	5.1
1	A	210	THR	5.1
1	B	37	GLY	5.1
1	D	206	VAL	5.1
1	C	197	ILE	5.0
1	D	208	GLN	5.0
1	B	36	PHE	4.5
1	D	192	LEU	4.5
1	B	191	PRO	4.4
1	B	215	LEU	4.4
1	D	210	THR	4.4
1	C	206	VAL	4.4
1	C	211	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	4.1
1	B	38	ASP	4.1
1	B	13	THR	4.1
1	C	198	SER	4.0
1	B	48	GLY	4.0
1	B	77	ALA	4.0
1	A	199	ALA	3.9
1	B	47	ALA	3.9
1	B	1	MET	3.9
1	A	146	LEU	3.9
1	B	52	GLN	3.8
1	B	59	TYR	3.7
1	A	163	VAL	3.7
1	A	211	ALA	3.6
1	D	209	GLU	3.4
1	A	200	LEU	3.4
1	D	211	ALA	3.4
1	B	64	LEU	3.4
1	A	1	MET	3.3
1	B	33	LEU	3.3
1	B	105	GLU	3.2
1	A	251	VAL	3.2
1	B	76	ASN	3.1
1	A	201	ALA	3.1
1	B	49	LEU	3.1
1	C	205	GLY	3.1
1	D	191	PRO	3.1
1	A	184	CYS	3.1
1	A	183	ILE	3.0
1	B	31	ILE	3.0
1	B	15	GLY	3.0
1	C	208	GLN	3.0
1	C	146	LEU	2.9
1	B	210	THR	2.9
1	D	214	GLU	2.9
1	A	205	GLY	2.9
1	A	250	THR	2.9
1	A	206	VAL	2.9
1	B	80	GLN	2.8
1	A	143	ALA	2.8
1	B	16	ILE	2.8
1	A	258	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	3	LYS	2.8
1	B	190	THR	2.8
1	B	189	ARG	2.8
1	B	14	SER	2.8
1	D	196	GLN	2.8
1	B	72	GLY	2.7
1	D	195	LYS	2.7
1	B	69	ALA	2.7
1	C	195	LYS	2.7
1	B	25	ALA	2.6
1	B	62	ALA	2.6
1	B	91	ALA	2.6
1	D	146	LEU	2.6
1	B	187	TRP	2.6
1	A	195	LYS	2.6
1	B	246	ILE	2.6
1	B	2	LEU	2.5
1	A	253	VAL	2.5
1	C	199	ALA	2.5
1	C	163	VAL	2.5
1	A	203	LYS	2.5
1	B	4	GLY	2.4
1	B	57	VAL	2.4
1	A	51	ALA	2.4
1	C	251	VAL	2.4
1	C	196	GLN	2.4
1	B	131	LYS	2.4
1	D	187	TRP	2.4
1	D	189	ARG	2.4
1	C	250	THR	2.4
1	D	251	VAL	2.4
1	A	140	ILE	2.3
1	A	147	VAL	2.3
1	A	52	GLN	2.3
1	B	18	LEU	2.3
1	D	68	GLU	2.3
1	B	50	ALA	2.3
1	B	146	LEU	2.3
1	B	42	ILE	2.2
1	C	187	TRP	2.2
1	B	249	THR	2.2
1	B	81	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	184	CYS	2.2
1	B	188	VAL	2.2
1	B	251	VAL	2.2
1	B	66	LYS	2.1
1	A	182	ALA	2.1
1	B	213	ARG	2.1
1	D	258	THR	2.1
1	B	63	ASP	2.1
1	A	3	LYS	2.1
1	B	55	VAL	2.1
1	A	213	ARG	2.0
1	B	45	VAL	2.0
1	D	163	VAL	2.0
1	B	68	GLU	2.0
1	B	30	ASP	2.0
1	B	12	SER	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	NAD	C	300	44/44	0.89	0.18	2.57	33,40,50,52	0
3	MG	A	406	1/1	0.99	0.26	1.94	15,15,15,15	0
3	MG	B	401	1/1	0.99	0.20	1.48	17,17,17,17	0
2	NAD	D	300	44/44	0.84	0.20	1.13	36,48,57,60	0
2	NAD	B	300	44/44	0.82	0.24	0.76	48,62,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	D	403	6/6	0.93	0.11	0.49	29,38,39,42	0
2	NAD	A	300	44/44	0.96	0.10	-0.59	25,28,33,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.