



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:48 am GMT

PDB ID : 1NM5  
Title : R. rubrum transhydrogenase (dI.Q132N)2(dIII)1 asymmetric complex  
Authors : Van Boxel, G.I.; Quirk, P.G.; Cotton, N.P.; White, S.A.; Jackson, J.B.  
Deposited on : 2003-01-09  
Resolution : 2.40 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

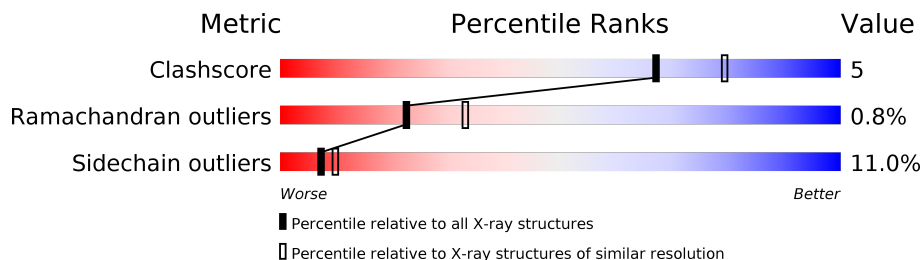
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	384	
1	B	384	
2	C	203	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6785 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 NAD(P) transhydrogenase subunit alpha part 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	1	0
			2649	1674	458	500	17			
1	B	358	Total	C	N	O	S	0	1	0
			2634	1667	457	494	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ASN	GLN	ENGINEERED	UNP Q60164
B	132	ASN	GLN	ENGINEERED	UNP Q60164

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

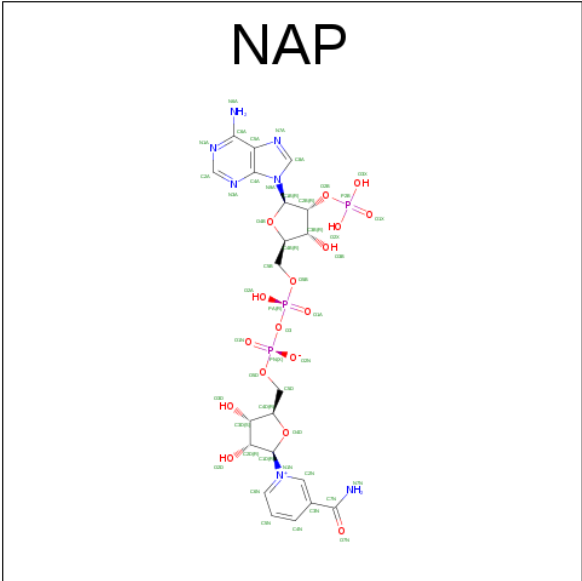
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1310	830	217	252	11			

- Molecule 3 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
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
			27	10	5	10	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

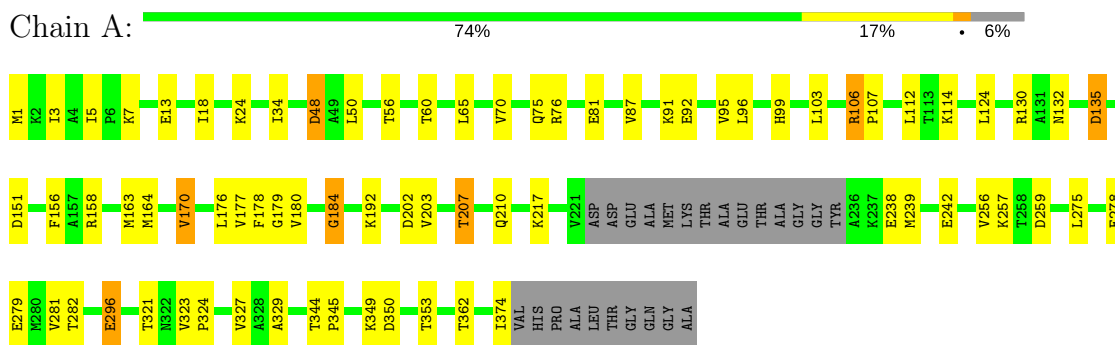
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	31	Total	O	0	0
			31	31		
6	C	8	Total	O	0	0
			8	8		

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

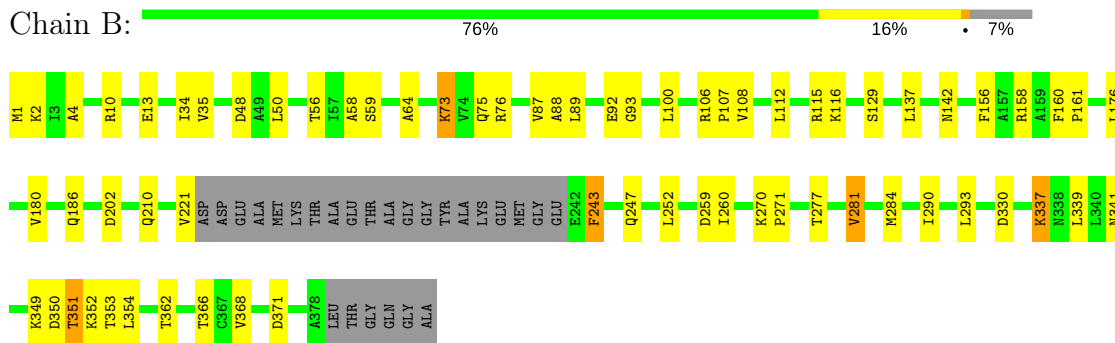
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

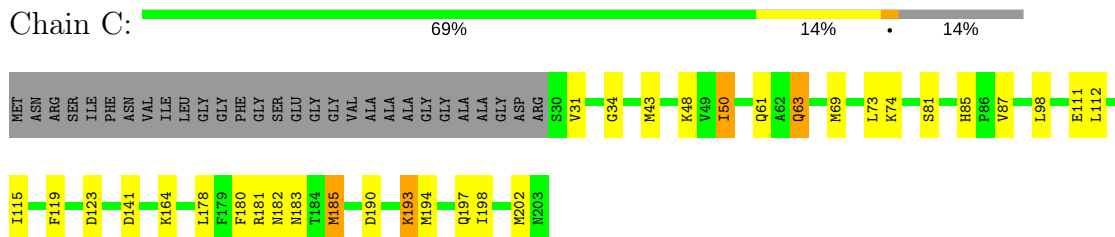
#### • Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



#### • Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



#### • Molecule 2: NAD(P) transhydrogenase subunit beta



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.94 Å 73.89 Å 205.26 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.40	Depositor
% Data completeness (in resolution range)	90.9 (100.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.236 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, 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	0.65	2/2682 (0.1%)	0.77	4/3632 (0.1%)
1	B	0.54	0/2669	0.76	3/3619 (0.1%)
2	C	0.50	0/1333	0.72	3/1803 (0.2%)
All	All	0.58	2/6684 (0.0%)	0.75	10/9054 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	GLY	C-O	12.89	1.44	1.23
1	A	184	GLY	CA-C	5.68	1.60	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	202	ASP	CB-CG-OD2	6.10	123.79	118.30
2	C	190	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	371	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	48	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	350	ASP	CB-CG-OD2	5.71	123.44	118.30
2	C	123	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	151	ASP	CB-CG-OD2	5.59	123.33	118.30
2	C	141	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	48	ASP	CB-CG-OD2	5.32	123.09	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	2649	0	2785	26	0
1	B	2634	0	2771	27	0
2	C	1310	0	1303	11	0
3	A	44	0	26	1	0
3	B	27	0	12	1	0
4	C	48	0	25	0	0
5	B	6	0	8	0	0
6	A	28	0	0	0	0
6	B	31	0	0	0	0
6	C	8	0	0	0	0
All	All	6785	0	6930	62	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 (62) 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:142:ASN:HD21	1:B:186:GLN:HE21	1.03	0.93
1:B:142:ASN:ND2	1:B:186:GLN:HE21	1.82	0.72
1:A:329:ALA:HB3	1:B:158:ARG:HG3	1.72	0.70
1:A:207:THR:HA	1:A:210:GLN:HE21	1.56	0.69
1:B:142:ASN:HD21	1:B:186:GLN:NE2	1.85	0.68
2:C:63:GLN:HG2	2:C:98:LEU:HB3	1.76	0.68
2:C:50:ILE:HG22	2:C:81:SER:HB2	1.76	0.67
1:B:351:THR:O	1:B:351:THR:HG22	2.00	0.62
2:C:50:ILE:HD11	2:C:119:PHE:CD1	2.37	0.59
1:B:10:ARG:NH1	1:B:76:ARG:O	2.37	0.57
1:A:156:PHE:CZ	1:A:259:ASP:HB3	2.40	0.57
1:B:284:MET:HE3	1:B:290:ILE:HD11	1.88	0.55
1:B:156:PHE:CZ	1:B:259:ASP:HB3	2.42	0.54
1:A:3:ILE:HG13	1:A:70:VAL:HG13	1.91	0.53
1:A:5:ILE:HD13	1:A:18:ILE:HD13	1.91	0.52
1:A:203:VAL:HG11	1:A:239:MET:HG3	1.91	0.52
2:C:43:MET:HE3	2:C:73:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLU:OE1	1:A:75:GLN:NE2	2.44	0.50
1:B:13:GLU:OE1	1:B:75:GLN:NE2	2.32	0.49
3:B:500:NAD:H3B	3:B:500:NAD:PA	2.51	0.49
1:A:177:VAL:HG13	1:A:177:VAL:O	2.13	0.49
1:B:87:VAL:HG23	1:B:112:LEU:HD23	1.93	0.48
2:C:193:LYS:HD2	2:C:197:GLN:NE2	2.29	0.48
1:A:135:ASP:OD2	3:A:400:NAD:H4N	2.14	0.48
1:B:156:PHE:CG	1:B:260:ILE:HD11	2.48	0.48
1:A:278:GLU:O	1:A:281:VAL:HG22	2.14	0.48
1:A:87:VAL:HG13	1:A:112:LEU:HD23	1.95	0.47
2:C:85:HIS:CE1	2:C:87:VAL:HG22	2.49	0.47
1:A:178:PHE:HB3	1:A:275:LEU:HD13	1.97	0.47
1:B:4:ALA:HA	1:B:34:ILE:O	2.14	0.46
1:A:106:ARG:N	1:A:107:PRO:CD	2.78	0.46
1:B:284:MET:CE	1:B:290:ILE:HD11	2.46	0.46
1:B:180:VAL:HG12	1:B:180:VAL:O	2.15	0.46
1:A:158:ARG:HB3	1:B:330:ASP:OD2	2.15	0.46
2:C:198:ILE:HG22	2:C:202:MET:HE3	1.99	0.45
1:A:202:ASP:CB	1:A:207:THR:HG21	2.47	0.45
1:B:88:ALA:HA	1:B:115:ARG:NE	2.32	0.45
1:B:337:LYS:HD2	1:B:341:ASN:ND2	2.32	0.44
1:B:2:LYS:HE3	1:B:34:ILE:HD11	1.99	0.44
1:A:180:VAL:HA	1:A:184:GLY:HA3	2.00	0.44
1:A:323:VAL:N	1:A:324:PRO:CD	2.80	0.44
1:A:5:ILE:CD1	1:A:18:ILE:HD13	2.48	0.44
1:B:106:ARG:N	1:B:107:PRO:CD	2.80	0.44
2:C:34:GLY:HA3	2:C:185:MET:SD	2.58	0.43
1:A:163:MET:HB2	1:A:170:VAL:HG13	2.00	0.43
1:A:202:ASP:HB2	1:A:207:THR:HG21	2.01	0.43
1:A:158:ARG:NH1	1:B:330:ASP:OD1	2.51	0.42
2:C:63:GLN:CG	2:C:98:LEU:HB3	2.46	0.42
1:B:270:LYS:HB3	1:B:271:PRO:HD2	2.01	0.42
2:C:69:MET:O	2:C:73:LEU:HB2	2.19	0.42
1:A:103:LEU:HD13	1:A:124:LEU:HD11	2.02	0.42
1:A:296:GLU:OE1	1:A:321:THR:HA	2.20	0.42
1:A:344:THR:N	1:A:345:PRO:CD	2.83	0.42
1:B:93:GLY:HA2	1:B:116:LYS:O	2.20	0.41
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.91	0.41
1:B:160:PHE:N	1:B:161:PRO:HD2	2.36	0.41
1:A:279:GLU:O	1:A:282:THR:HB	2.21	0.41
1:A:374:ILE:O	1:A:374:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:THR:O	1:B:281:VAL:HG13	2.21	0.40
1:B:58:ALA:HB3	1:B:64:ALA:HB2	2.04	0.40
1:B:73:LYS:CB	1:B:73:LYS:NZ	2.84	0.40
2:C:112:LEU:C	2:C:112:LEU:HD23	2.41	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	356/384 (93%)	341 (96%)	14 (4%)	1 (0%)	44	60
1	B	354/384 (92%)	337 (95%)	13 (4%)	4 (1%)	17	23
2	C	172/203 (85%)	165 (96%)	5 (3%)	2 (1%)	15	21
All	All	882/971 (91%)	843 (96%)	32 (4%)	7 (1%)	22	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	PHE
1	B	350	ASP
1	B	351	THR
2	C	182	ASN
1	A	179	GLY
1	B	352	LYS
2	C	31	VAL

### 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	281/296 (95%)	246 (88%)	35 (12%)	5	6
1	B	280/296 (95%)	253 (90%)	27 (10%)	10	14
2	C	138/154 (90%)	123 (89%)	15 (11%)	7	10
All	All	699/746 (94%)	622 (89%)	77 (11%)	7	10

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LYS
1	A	24	LYS
1	A	34	ILE
1	A	48	ASP
1	A	50	LEU
1	A	56	THR
1	A	60	THR
1	A	65	LEU
1	A	76	ARG
1	A	81	GLU
1	A	91	LYS
1	A	92	GLU
1	A	95	VAL
1	A	96	LEU
1	A	99	HIS
1	A	106	ARG
1	A	114	LYS
1	A	130	ARG
1	A	132	ASN
1	A	164	MET
1	A	170	VAL
1	A	176	LEU
1	A	192	LYS
1	A	207	THR
1	A	217	LYS
1	A	238	GLU
1	A	242[A]	GLU
1	A	256	VAL
1	A	257	LYS

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Mol	Chain	Res	Type
1	A	296	GLU
1	A	327	VAL
1	A	349	LYS
1	A	353	THR
1	A	362	THR
1	B	1	MET
1	B	35	VAL
1	B	50	LEU
1	B	56	THR
1	B	59	SER
1	B	73	LYS
1	B	89	LEU
1	B	92	GLU
1	B	100	LEU
1	B	108	VAL
1	B	129	SER
1	B	137	LEU
1	B	176	LEU
1	B	210	GLN
1	B	221	VAL
1	B	243	PHE
1	B	247	GLN
1	B	252	LEU
1	B	281	VAL
1	B	337	LYS
1	B	339	LEU
1	B	349[A]	LYS
1	B	353	THR
1	B	354	LEU
1	B	362	THR
1	B	366	THR
1	B	368	VAL
2	C	48	LYS
2	C	50	ILE
2	C	61	GLN
2	C	63	GLN
2	C	74	LYS
2	C	111	GLU
2	C	115	ILE
2	C	164	LYS
2	C	178	LEU
2	C	180	PHE

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Mol	Chain	Res	Type
2	C	181	ARG
2	C	183	ASN
2	C	185	MET
2	C	193	LYS
2	C	194	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	210	GLN
1	A	300	ASN
1	A	338	ASN
1	B	99	HIS
1	B	132	ASN
1	B	142	ASN
1	B	341	ASN
2	C	45	ASN
2	C	61	GLN
2	C	182	ASN
2	C	183	ASN
2	C	197	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	400	-	41,48,48	1.65	3 (7%)	43,73,73	1.86	4 (9%)
3	NAD	B	500	-	25,29,48	1.30	4 (16%)	24,45,73	2.50	1 (4%)
5	GOL	B	501	-	5,5,5	0.44	0	5,5,5	0.58	0
4	NAP	C	300	-	44,52,52	1.49	3 (6%)	51,80,80	1.59	2 (3%)

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	400	-	-	0/22/62/62	0/5/5/5
3	NAD	B	500	-	-	0/12/32/62	0/3/3/5
5	GOL	B	501	-	-	0/4/4/4	0/0/0/0
4	NAP	C	300	-	-	0/27/67/67	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	NAD	O4B-C1B	2.01	1.44	1.41
3	A	400	NAD	C2A-N1A	2.32	1.38	1.33
3	B	500	NAD	C2A-N1A	2.60	1.38	1.33
4	C	300	NAP	C2A-N1A	2.70	1.39	1.33
3	B	500	NAD	PN-O3	3.01	1.64	1.60
4	C	300	NAP	C2A-N3A	3.39	1.37	1.32
3	B	500	NAD	C2A-N3A	3.87	1.38	1.32
3	A	400	NAD	C2A-N3A	4.27	1.39	1.32
4	C	300	NAP	O7N-C7N	7.61	1.39	1.24
3	A	400	NAD	O7N-C7N	8.40	1.41	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	NAD	N3A-C2A-N1A	-11.42	118.92	128.86

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	NAD	N3A-C2A-N1A	-10.00	120.15	128.86
4	C	300	NAP	N3A-C2A-N1A	-9.61	120.49	128.86
3	A	400	NAD	C4B-O4B-C1B	-2.11	107.53	109.77
3	A	400	NAD	O7N-C7N-N7N	-2.08	119.62	122.58
4	C	300	NAP	C4A-C5A-N7A	-2.07	107.41	109.41
3	A	400	NAD	C3N-C7N-N7N	3.77	122.08	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	NAD	1	0
3	B	500	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.