



# Full wwPDB X-ray Structure Validation Report

Oct 12, 2014 – 10:35 PM EDT

PDB ID : 1CWU  
Title : BRASSICA NAPUS ENOYL ACP REDUCTASE A138G MUTANT COM-  
PLEXED WITH NAD<sup>+</sup> AND THIENODIAZABORINE  
Authors : Roujeinikova, A.; Rafferty, J.B.; Rice, D.W.  
Deposited on : 1999-08-26  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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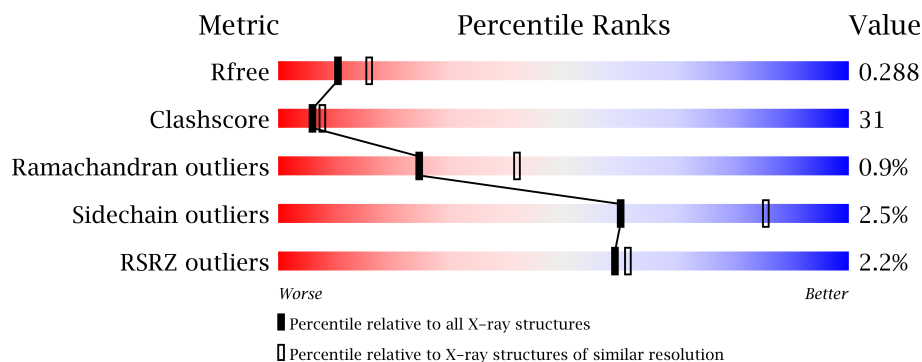
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
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) : stable23828

# 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	296	
1	B	296	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4554 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.

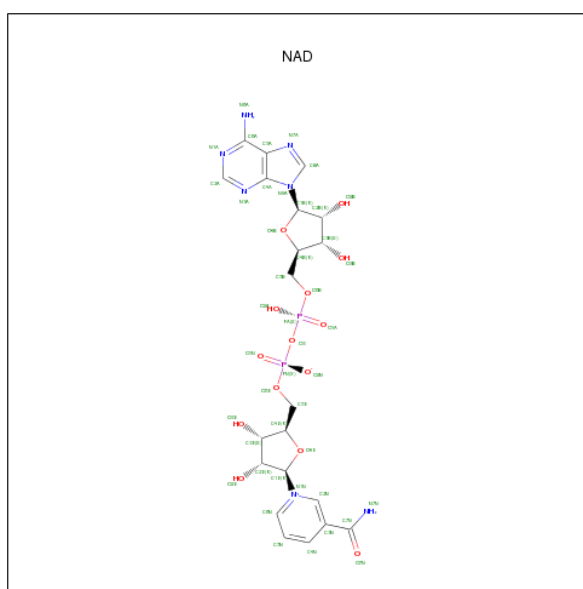
- Molecule 1 is a protein called ENOYL ACP REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2174	1380	368	420	6			
1	B	296	Total	C	N	O	S	0	0	0
			2145	1366	358	415	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	GLY	ENGINEERED	UNP P80030
B	41	ALA	GLY	ENGINEERED	UNP P80030

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



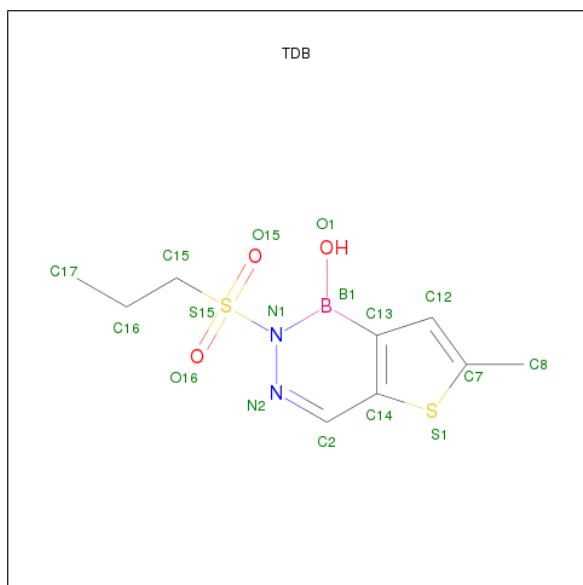
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 3 is 6-METHYL-2(PROPANE-1-SULFONYL)-2H-THIENO[3,2-D][1,2,3]DIAZABORININ-1-OL (three-letter code: TDB) (formula:  $C_9H_{13}BN_2O_3S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	S	0
			17	1	9	2	3	2	
3	B	1	Total	B	C	N	O	S	0
			17	1	9	2	3	2	

- Molecule 4 is water.

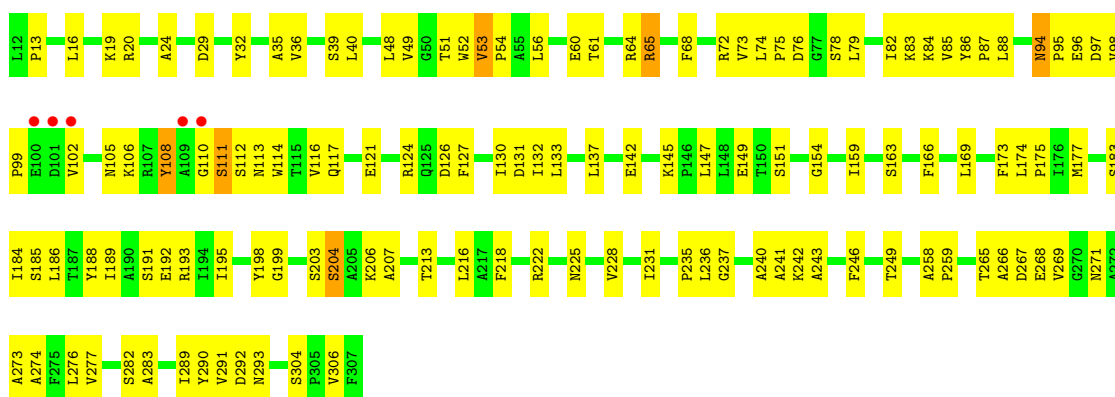
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	49	Total	O	0	0
			49	49		

### 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.

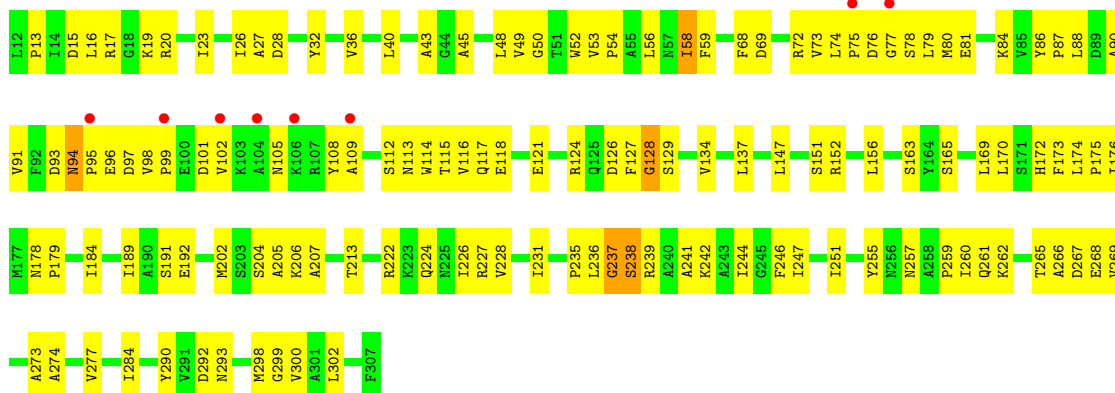
#### • Molecule 1: ENOYL ACP REDUCTASE

Chain A: 



#### • Molecule 1: ENOYL ACP REDUCTASE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.58Å 104.58Å 283.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 19.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (10.00-2.50) 92.9 (19.79-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.04 (at 2.50Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.211 , 0.314 0.199 , 0.288	Depositor DCC
$R_{free}$ test set	1305 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25739 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: TDB, 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	0.67	0/2217	0.81	3/3018 (0.1%)
1	B	0.64	0/2188	0.79	0/2984
All	All	0.65	0/4405	0.80	3/6002 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	267	ASP	N-CA-CB	-6.43	99.03	110.60
1	A	106	LYS	N-CA-C	5.85	126.78	111.00
1	A	110	GLY	N-CA-C	5.31	126.38	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	TYR	Sidechain

## 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	2174	0	2144	120	0
1	B	2145	0	2098	154	0
2	A	44	0	24	6	0
2	B	44	0	24	3	0
3	A	17	0	13	3	0
3	B	17	0	13	6	0
4	A	64	0	0	3	0
4	B	49	0	0	2	0
All	All	4554	0	4316	271	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 31.

All (271) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:260:ILE:HD12	1:B:262:LYS:HD3	1.16	1.15
1:B:53:VAL:HG13	1:B:54:PRO:HD3	1.27	1.14
1:B:241:ALA:HB1	1:B:247:ILE:HG21	1.34	1.03
1:B:53:VAL:CG1	1:B:54:PRO:HD3	1.97	0.93
1:A:133:LEU:HD11	1:A:169:LEU:HD23	1.50	0.91
1:B:172:HIS:O	1:B:175:PRO:HD2	1.70	0.90
1:B:273:ALA:O	1:B:277:VAL:HG22	1.72	0.90
1:B:58:ILE:HD12	1:B:58:ILE:H	1.36	0.89
1:A:56:LEU:HD22	1:A:87:PRO:HB3	1.55	0.87
1:B:58:ILE:N	1:B:58:ILE:HD12	1.90	0.85
1:A:94:ASN:HB2	1:A:95:PRO:CD	2.07	0.84
1:B:98:VAL:HG13	1:B:99:PRO:HD2	1.59	0.83
1:B:237:GLY:HA2	1:B:247:ILE:HD12	1.59	0.82
1:B:238:SER:O	1:B:242:LYS:HG2	1.79	0.82
1:B:58:ILE:CD1	1:B:58:ILE:H	1.93	0.81
1:A:133:LEU:HD11	1:A:169:LEU:CD2	2.12	0.80
1:B:99:PRO:HG2	1:B:102:VAL:HG23	1.65	0.78
1:B:260:ILE:CD1	1:B:262:LYS:HD3	2.08	0.78
1:A:56:LEU:CD2	1:A:87:PRO:HB3	2.14	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:PRO:HG2	1:A:102:VAL:CB	2.15	0.77
1:B:255:TYR:O	1:B:261:GLN:HG3	1.85	0.77
1:A:111:SER:HB3	4:A:534:HOH:O	1.83	0.77
1:B:213:THR:HG23	1:B:228:VAL:HG12	1.68	0.76
1:A:231:ILE:HG23	1:A:291:VAL:HG23	1.67	0.75
1:B:260:ILE:HD12	1:B:262:LYS:CD	2.09	0.75
1:A:60:GLU:O	1:A:64:ARG:HD3	1.87	0.75
1:B:16:LEU:HD12	1:B:43:ALA:HB3	1.69	0.74
1:A:94:ASN:HB2	1:A:95:PRO:HD2	1.69	0.73
1:B:56:LEU:O	1:B:56:LEU:HD12	1.89	0.72
2:B:503:NAD:H2D	3:B:504:TDB:N1	2.04	0.72
1:B:56:LEU:HD22	1:B:87:PRO:HA	1.71	0.72
1:B:52:TRP:HA	1:B:88:LEU:O	1.91	0.71
1:A:48:LEU:HD23	1:A:83:LYS:HB3	1.72	0.71
1:B:99:PRO:HG2	1:B:102:VAL:CG2	2.19	0.71
1:B:32:TYR:CE1	1:B:266:ALA:HA	2.26	0.71
1:A:273:ALA:O	1:A:277:VAL:HG22	1.91	0.70
1:A:73:VAL:HG22	1:A:79:LEU:HD21	1.74	0.70
1:A:108:TYR:HD2	1:A:114:TRP:CZ2	2.08	0.70
1:A:32:TYR:CE1	1:A:269:VAL:HG21	2.27	0.69
1:A:304:SER:OG	1:A:306:VAL:HG22	1.91	0.69
1:B:241:ALA:CB	1:B:247:ILE:HD13	2.23	0.69
1:A:13:PRO:HA	1:B:13:PRO:HA	1.72	0.69
1:B:94:ASN:C	1:B:94:ASN:HD22	1.96	0.69
1:A:159:ILE:O	1:A:163:SER:HB3	1.93	0.68
1:B:90:ALA:HB1	1:B:165:SER:HB2	1.75	0.68
1:A:102:VAL:O	1:A:105:ASN:HB3	1.93	0.68
1:B:98:VAL:CG1	1:B:99:PRO:HD2	2.24	0.67
1:B:124:ARG:O	1:B:128:GLY:N	2.25	0.66
1:B:32:TYR:CE1	1:B:269:VAL:HG21	2.30	0.66
1:B:56:LEU:CD2	1:B:87:PRO:HB3	2.26	0.66
1:A:32:TYR:O	1:A:36:VAL:HG23	1.96	0.66
1:A:265:THR:OG1	1:A:268:GLU:HG3	1.96	0.65
1:B:127:PHE:O	1:B:129:SER:N	2.30	0.65
1:B:189:ILE:HD13	1:B:290:TYR:HE1	1.62	0.64
1:B:53:VAL:HG13	1:B:54:PRO:CD	2.16	0.64
1:B:99:PRO:CG	1:B:102:VAL:HG23	2.27	0.64
1:A:24:ALA:O	1:A:137:LEU:HD23	1.98	0.64
1:A:61:THR:O	1:A:65:ARG:HG2	1.99	0.64
1:A:53:VAL:HG13	1:A:54:PRO:HD3	1.80	0.63
1:B:241:ALA:HB1	1:B:247:ILE:HD13	1.80	0.63
1:A:39:SER:HB3	1:A:274:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:169:LEU:CD2	1:B:173:PHE:HE2	2.12	0.63
1:B:76:ASP:C	1:B:78:SER:H	2.01	0.63
1:B:16:LEU:O	1:B:19:LYS:HB2	1.99	0.62
1:B:244:ILE:HD11	3:B:504:TDB:C17	2.29	0.62
1:B:16:LEU:HD12	1:B:43:ALA:CB	2.28	0.62
1:A:68:PHE:O	1:A:72:ARG:HG3	1.98	0.62
1:A:56:LEU:O	1:A:60:GLU:HG3	1.99	0.62
1:B:56:LEU:C	1:B:56:LEU:HD12	2.21	0.62
1:A:292:ASP:O	1:A:293:ASN:HB2	2.00	0.61
1:A:40:LEU:HD21	1:A:277:VAL:HG21	1.82	0.61
1:B:32:TYR:HE1	1:B:266:ALA:HA	1.66	0.61
1:B:192:GLU:OE2	1:B:290:TYR:OH	2.16	0.60
1:B:76:ASP:O	1:B:78:SER:N	2.33	0.60
1:B:72:ARG:O	1:B:80:MET:N	2.33	0.60
1:A:94:ASN:HB2	1:A:95:PRO:HD3	1.83	0.60
1:A:142:GLU:OE2	1:A:151:SER:OG	2.21	0.59
1:B:84:LYS:NZ	1:B:126:ASP:OD2	2.25	0.59
1:A:191:SER:HB3	1:A:206:LYS:HB2	1.83	0.59
1:B:56:LEU:HD23	1:B:87:PRO:HB3	1.85	0.59
1:B:184:ILE:HD11	1:B:231:ILE:HG13	1.85	0.58
1:A:276:LEU:HD11	1:A:289:ILE:HG13	1.85	0.58
1:A:51:THR:HB	1:A:56:LEU:HD13	1.86	0.58
1:B:74:LEU:HB3	1:B:75:PRO:HD2	1.85	0.57
1:B:99:PRO:CG	1:B:102:VAL:CG2	2.83	0.57
1:B:73:VAL:HA	1:B:79:LEU:HD23	1.87	0.57
1:B:244:ILE:HD11	3:B:504:TDB:H173	1.86	0.57
1:A:32:TYR:CZ	1:A:269:VAL:HG21	2.40	0.56
1:B:137:LEU:HD12	1:B:137:LEU:C	2.25	0.56
1:B:121:GLU:HA	1:B:121:GLU:OE2	2.05	0.56
1:B:178:ASN:O	1:B:179:PRO:C	2.42	0.56
1:B:94:ASN:HB2	1:B:95:PRO:CD	2.35	0.56
1:A:48:LEU:CD2	1:A:83:LYS:HB3	2.34	0.56
1:A:133:LEU:O	1:A:183:SER:HA	2.05	0.56
1:B:20:ARG:HD2	1:B:129:SER:O	2.05	0.56
1:A:29:ASP:OD1	1:A:29:ASP:N	2.39	0.56
1:B:239:ARG:O	1:B:242:LYS:HB2	2.06	0.55
1:B:74:LEU:N	1:B:78:SER:O	2.23	0.55
1:B:241:ALA:HB1	1:B:247:ILE:CG2	2.24	0.55
1:A:166:PHE:HE2	1:A:216:LEU:HD13	1.70	0.55
1:A:84:LYS:HD3	1:A:86:TYR:CZ	2.42	0.55
1:A:16:LEU:CD1	1:A:40:LEU:HD22	2.37	0.55
1:A:20:ARG:HD3	1:A:48:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:235:PRO:HB2	1:B:251:ILE:HG13	1.86	0.55
1:B:265:THR:OG1	1:B:267:ASP:HB3	2.07	0.55
1:A:56:LEU:HD22	1:A:87:PRO:CB	2.30	0.54
1:B:23:ILE:HG23	1:B:134:VAL:HB	1.88	0.54
1:B:32:TYR:CE1	1:B:236:LEU:HD22	2.43	0.54
1:B:299:GLY:O	1:B:300:VAL:HG13	2.08	0.54
1:A:198:TYR:OH	1:A:206:LYS:HE2	2.08	0.54
1:B:76:ASP:C	1:B:78:SER:N	2.61	0.54
1:A:112:SER:O	1:A:113:ASN:HB2	2.08	0.54
1:A:142:GLU:OE2	1:A:154:GLY:HA3	2.08	0.54
1:B:189:ILE:CD1	1:B:290:TYR:HE1	2.21	0.54
1:A:236:LEU:N	2:A:501:NAD:O7N	2.39	0.53
1:B:299:GLY:O	1:B:300:VAL:CG1	2.56	0.53
1:B:170:LEU:O	1:B:174:LEU:HB2	2.07	0.53
1:A:94:ASN:HB3	1:A:117:GLN:NE2	2.23	0.53
1:A:49:VAL:HG23	1:A:82:ILE:HG23	1.90	0.53
1:A:73:VAL:HA	1:A:79:LEU:HD23	1.91	0.53
1:B:152:ARG:O	1:B:156:LEU:HG	2.09	0.53
1:B:169:LEU:HD23	1:B:173:PHE:HE2	1.74	0.53
1:A:192:GLU:C	1:A:193:ARG:HG2	2.29	0.53
1:A:265:THR:N	1:A:268:GLU:OE1	2.42	0.53
1:B:112:SER:O	1:B:113:ASN:HB2	2.10	0.53
1:A:73:VAL:HG22	1:A:79:LEU:CD2	2.37	0.52
1:B:15:ASP:OD1	1:B:17:ARG:HG3	2.09	0.52
1:B:56:LEU:HD22	1:B:87:PRO:CA	2.39	0.52
2:A:501:NAD:H2D	3:A:502:TDB:N1	2.23	0.52
1:B:32:TYR:CE1	1:B:269:VAL:CG2	2.92	0.52
2:A:501:NAD:C2D	3:A:502:TDB:N1	2.71	0.52
1:B:257:ASN:O	1:B:298:MET:HG3	2.09	0.52
1:B:169:LEU:CD2	1:B:173:PHE:CE2	2.93	0.52
1:A:94:ASN:ND2	1:A:96:GLU:HG2	2.25	0.52
1:B:213:THR:CG2	1:B:228:VAL:HG12	2.38	0.52
1:A:145:LYS:HD3	1:A:149:GLU:O	2.09	0.52
1:A:231:ILE:HG23	1:A:291:VAL:CG2	2.36	0.52
1:A:32:TYR:CE1	1:A:269:VAL:CG2	2.92	0.52
1:B:257:ASN:OD1	1:B:302:LEU:N	2.43	0.51
1:A:191:SER:HB2	1:A:207:ALA:HA	1.91	0.51
1:A:243:ALA:HB3	4:A:529:HOH:O	2.10	0.51
1:B:127:PHE:C	1:B:129:SER:H	2.13	0.51
1:B:20:ARG:NH1	1:B:129:SER:O	2.33	0.51
1:B:99:PRO:HG2	1:B:102:VAL:CB	2.40	0.51
1:B:299:GLY:C	1:B:300:VAL:HG13	2.31	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:ILE:HD11	1:A:231:ILE:HG13	1.91	0.51
1:B:36:VAL:O	1:B:40:LEU:HG	2.10	0.51
1:A:174:LEU:HA	1:A:177:MET:HG3	1.92	0.51
1:B:94:ASN:C	1:B:94:ASN:ND2	2.64	0.51
1:A:191:SER:HB2	1:A:207:ALA:CA	2.41	0.51
1:A:56:LEU:HD11	1:A:85:VAL:HG12	1.93	0.51
1:B:163:SER:OG	1:B:205:ALA:O	2.27	0.51
1:A:192:GLU:OE1	1:A:290:TYR:OH	2.28	0.50
1:B:93:ASP:O	1:B:117:GLN:HB2	2.11	0.50
1:B:202:MET:CE	3:B:504:TDB:H161	2.41	0.50
1:B:20:ARG:HD3	1:B:48:LEU:HD11	1.93	0.50
1:B:189:ILE:HD13	1:B:290:TYR:CE1	2.43	0.50
1:B:206:LYS:NZ	4:B:530:HOH:O	2.41	0.50
1:B:32:TYR:CZ	1:B:269:VAL:HG21	2.46	0.50
1:A:39:SER:OG	1:A:271:ASN:ND2	2.43	0.50
1:A:84:LYS:NZ	1:A:126:ASP:OD2	2.30	0.50
1:A:20:ARG:CZ	1:A:127:PHE:HB3	2.42	0.50
1:A:258:ALA:O	1:B:222:ARG:NH2	2.39	0.50
1:A:174:LEU:N	1:A:175:PRO:CD	2.75	0.49
1:B:91:VAL:O	1:B:91:VAL:HG12	2.12	0.49
1:B:86:TYR:HH	1:B:127:PHE:HE2	1.61	0.49
2:B:503:NAD:O2D	3:B:504:TDB:O1	2.30	0.49
1:B:27:ALA:O	1:B:28:ASP:HB3	2.13	0.49
1:B:191:SER:HB2	1:B:207:ALA:N	2.28	0.49
1:B:94:ASN:HB2	1:B:95:PRO:HD3	1.94	0.49
1:A:166:PHE:CE2	1:A:216:LEU:HD13	2.48	0.49
2:A:501:NAD:H2N	2:A:501:NAD:O1N	2.13	0.48
1:B:99:PRO:HG2	1:B:102:VAL:HB	1.95	0.48
1:B:292:ASP:O	1:B:293:ASN:HB2	2.12	0.48
1:B:16:LEU:HG	1:B:43:ALA:HB1	1.93	0.48
1:A:121:GLU:HA	1:A:121:GLU:OE2	2.13	0.48
1:A:20:ARG:N	1:A:131:ASP:OD2	2.43	0.48
1:B:242:LYS:HD3	1:B:247:ILE:HD11	1.94	0.48
1:B:69:ASP:HB2	4:B:511:HOH:O	2.13	0.48
1:A:213:THR:HG23	1:A:228:VAL:HG12	1.95	0.48
1:B:227:ARG:HD2	1:B:284:ILE:O	2.12	0.48
1:B:93:ASP:O	1:B:117:GLN:CB	2.61	0.48
1:A:52:TRP:HA	1:A:88:LEU:O	2.14	0.47
1:A:173:PHE:C	1:A:175:PRO:HD2	2.34	0.47
1:A:116:VAL:HG13	1:A:169:LEU:HD12	1.95	0.47
1:A:249:THR:HG23	4:A:512:HOH:O	2.14	0.47
1:B:99:PRO:C	1:B:101:ASP:N	2.68	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:TYR:OH	1:B:127:PHE:HE2	1.98	0.47
1:A:132:ILE:HG12	1:A:277:VAL:HB	1.97	0.47
1:B:235:PRO:HB2	1:B:251:ILE:CG1	2.44	0.47
1:B:237:GLY:O	1:B:242:LYS:HE2	2.15	0.47
1:B:53:VAL:HG11	1:B:108:TYR:CE2	2.50	0.47
1:A:108:TYR:HD2	1:A:114:TRP:CH2	2.33	0.46
1:B:202:MET:O	1:B:205:ALA:HB3	2.14	0.46
1:B:32:TYR:CD1	1:B:236:LEU:HD22	2.51	0.46
1:A:237:GLY:O	1:A:242:LYS:HE3	2.16	0.46
1:A:40:LEU:HD21	1:A:277:VAL:CG2	2.45	0.46
1:B:124:ARG:HG3	1:B:176:ILE:HG21	1.97	0.46
1:A:203:SER:OG	1:A:204:SER:N	2.49	0.46
1:B:95:PRO:O	1:B:97:ASP:N	2.48	0.46
1:A:56:LEU:CD1	1:A:85:VAL:HG12	2.46	0.45
1:A:189:ILE:HG23	1:A:195:ILE:HD11	1.97	0.45
1:B:172:HIS:C	1:B:175:PRO:HD2	2.33	0.45
1:A:94:ASN:CB	1:A:95:PRO:CD	2.77	0.45
1:A:282:SER:HG	1:B:268:GLU:HG2	1.82	0.45
1:B:32:TYR:CD1	1:B:266:ALA:HA	2.51	0.45
1:A:130:ILE:O	1:A:177:MET:HA	2.17	0.45
1:B:40:LEU:HD21	1:B:274:ALA:HA	1.98	0.45
1:A:145:LYS:O	1:A:199:GLY:HA3	2.17	0.45
1:A:121:GLU:OE1	1:A:124:ARG:NH2	2.36	0.45
1:A:185:SER:O	1:A:186:LEU:HD23	2.16	0.44
1:A:191:SER:HB3	1:A:206:LYS:CB	2.47	0.44
1:B:169:LEU:HD23	1:B:173:PHE:CE2	2.50	0.44
1:A:218:PHE:HE1	1:B:302:LEU:HD11	1.82	0.44
1:B:88:LEU:HD11	1:B:116:VAL:HG22	1.99	0.44
1:A:225:ASN:ND2	1:A:225:ASN:O	2.50	0.44
1:A:73:VAL:HA	1:A:79:LEU:CD2	2.48	0.44
1:A:56:LEU:CD1	1:A:85:VAL:CG1	2.96	0.44
1:B:80:MET:CG	1:B:81:GLU:N	2.80	0.44
1:A:147:LEU:HA	1:A:147:LEU:HD23	1.83	0.44
1:A:240:ALA:O	1:A:243:ALA:HB3	2.17	0.44
1:A:94:ASN:CB	1:A:95:PRO:HD3	2.43	0.44
2:B:503:NAD:C2D	3:B:504:TDB:N1	2.78	0.44
1:B:98:VAL:CG1	1:B:99:PRO:CD	2.96	0.44
1:A:218:PHE:CE1	1:B:302:LEU:HD11	2.53	0.44
1:B:174:LEU:N	1:B:175:PRO:CD	2.81	0.43
1:B:94:ASN:CB	1:B:95:PRO:CD	2.95	0.43
1:B:241:ALA:C	1:B:247:ILE:HD13	2.39	0.43
1:A:283:ALA:HA	1:B:293:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:49:VAL:HG12	1:B:50:GLY:N	2.33	0.43
1:A:282:SER:OG	1:B:268:GLU:HG2	2.17	0.43
1:B:105:ASN:O	1:B:109:ALA:N	2.52	0.43
1:B:260:ILE:HG13	1:B:260:ILE:O	2.19	0.43
1:A:74:LEU:HB3	1:A:75:PRO:HD2	2.01	0.43
1:A:76:ASP:OD1	1:A:78:SER:OG	2.26	0.43
1:B:91:VAL:O	1:B:91:VAL:CG1	2.67	0.43
1:A:283:ALA:O	1:B:293:ASN:N	2.42	0.43
1:A:99:PRO:O	1:A:102:VAL:N	2.52	0.43
1:B:174:LEU:HB3	1:B:175:PRO:HD3	2.01	0.43
1:B:124:ARG:O	1:B:128:GLY:CA	2.67	0.43
1:A:235:PRO:HA	2:A:501:NAD:O7N	2.19	0.42
1:B:53:VAL:HG11	1:B:108:TYR:CD2	2.54	0.42
1:B:191:SER:HB3	1:B:206:LYS:CB	2.49	0.42
1:A:16:LEU:O	1:A:19:LYS:HB2	2.19	0.42
1:A:32:TYR:CE1	1:A:266:ALA:HA	2.55	0.42
1:B:74:LEU:CB	1:B:75:PRO:HD2	2.45	0.42
1:B:94:ASN:C	1:B:115:THR:HG21	2.40	0.42
1:A:188:TYR:CG	3:A:502:TDB:H81	2.55	0.42
1:A:94:ASN:O	1:A:97:ASP:HB2	2.20	0.42
1:B:113:ASN:HA	1:B:118:GLU:CD	2.40	0.42
1:B:112:SER:HA	1:B:114:TRP:CD1	2.55	0.42
1:A:98:VAL:HG13	1:A:99:PRO:HD2	2.01	0.42
1:B:124:ARG:O	1:B:128:GLY:HA2	2.19	0.41
1:B:247:ILE:O	1:B:251:ILE:N	2.32	0.41
1:B:68:PHE:O	1:B:72:ARG:HG3	2.19	0.41
1:B:26:ILE:HG22	1:B:59:PHE:CE1	2.55	0.41
1:B:49:VAL:CG1	1:B:50:GLY:N	2.83	0.41
1:A:258:ALA:HB1	1:A:259:PRO:HD2	2.02	0.41
1:A:241:ALA:HB2	2:A:501:NAD:N7N	2.35	0.41
1:A:51:THR:HG21	1:A:56:LEU:HA	2.02	0.41
1:B:147:LEU:HD23	1:B:147:LEU:HA	1.98	0.41
1:B:16:LEU:HB3	1:B:45:ALA:HB2	2.03	0.41
1:A:191:SER:HB2	1:A:207:ALA:N	2.36	0.41
1:B:86:TYR:OH	1:B:127:PHE:CE2	2.73	0.41
1:A:222:ARG:HG2	1:B:259:PRO:O	2.21	0.40
1:A:265:THR:O	1:A:268:GLU:N	2.54	0.40
1:A:56:LEU:HD11	1:A:85:VAL:CG1	2.50	0.40
1:A:94:ASN:ND2	1:A:96:GLU:CD	2.75	0.40
1:B:224:GLN:HB3	1:B:226:ILE:HG12	2.03	0.40
1:B:26:ILE:HG22	1:B:27:ALA:N	2.35	0.40
1:A:35:ALA:HB2	1:A:266:ALA:HB1	2.03	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	294/296 (99%)	274 (93%)	20 (7%)	0	100	100
1	B	294/296 (99%)	266 (90%)	23 (8%)	5 (2%)	14	22
All	All	588/592 (99%)	540 (92%)	43 (7%)	5 (1%)	25	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	128	GLY
1	B	96	GLU
1	B	77	GLY
1	B	238	SER
1	B	237	GLY

### 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	223/231 (96%)	217 (97%)	6 (3%)	57	83
1	B	217/231 (94%)	212 (98%)	5 (2%)	63	87
All	All	440/462 (95%)	429 (98%)	11 (2%)	60	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	65	ARG
1	A	94	ASN
1	A	111	SER
1	A	204	SER
1	A	246	PHE
1	B	58	ILE
1	B	94	ASN
1	B	151	SER
1	B	204	SER
1	B	246	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	117	GLN
1	A	225	ASN
1	A	256	ASN
1	A	271	ASN
1	B	94	ASN
1	B	117	GLN
1	B	256	ASN
1	B	261	GLN
1	B	271	ASN

### 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

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$
2	NAD	A	501	3	48,48,48	2.16	17 (35%)	73,73,73	2.58	19 (26%)
3	TDB	A	502	2	18,18,18	3.50	9 (50%)	20,27,27	2.34	8 (40%)
2	NAD	B	503	3	48,48,48	2.05	15 (31%)	73,73,73	2.49	23 (31%)
3	TDB	B	504	2	18,18,18	3.23	7 (38%)	20,27,27	5.03	7 (35%)

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	501	3	-	0/30/62/62	0/5/5/5
3	TDB	A	502	2	-	0/4/23/23	0/2/2/2
2	NAD	B	503	3	-	0/30/62/62	0/5/5/5
3	TDB	B	504	2	-	0/4/23/23	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	TDB	C15-S15	-7.79	1.69	1.78
3	A	502	TDB	C14-S1	-7.12	1.67	1.73
3	B	504	TDB	B1-O1	7.03	1.46	1.36
3	B	504	TDB	O16-S15	6.95	1.51	1.43
2	A	501	NAD	C2N-N1N	6.71	1.43	1.35
3	A	502	TDB	B1-O1	6.43	1.46	1.36
3	B	504	TDB	C15-S15	-5.06	1.72	1.78
3	B	504	TDB	B1-N1	-4.85	1.43	1.47
2	B	503	NAD	C3N-C7N	4.72	1.58	1.50
2	B	503	NAD	C2N-N1N	4.56	1.41	1.35
2	A	501	NAD	C2A-N3A	4.31	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	O2B-C2B	-4.15	1.32	1.43
3	B	504	TDB	C14-S1	-4.06	1.69	1.73
2	A	501	NAD	C3N-C7N	3.97	1.57	1.50
2	B	503	NAD	C2A-N3A	3.83	1.38	1.32
2	B	503	NAD	PN-O3	3.76	1.68	1.60
3	A	502	TDB	O16-S15	3.69	1.47	1.43
2	A	501	NAD	C4A-N9A	3.63	1.43	1.37
3	A	502	TDB	N1-N2	-3.60	1.37	1.40
2	B	503	NAD	O4D-C4D	3.40	1.52	1.45
3	A	502	TDB	O15-S15	3.31	1.47	1.43
2	B	503	NAD	O2B-C2B	-3.24	1.35	1.43
2	B	503	NAD	C4A-N9A	3.24	1.42	1.37
2	A	501	NAD	O4D-C4D	3.11	1.52	1.45
3	A	502	TDB	C7-S1	-3.08	1.68	1.74
3	B	504	TDB	N1-N2	-3.02	1.37	1.40
2	B	503	NAD	C1D-N1N	2.94	1.57	1.48
2	A	501	NAD	PN-O3	2.91	1.66	1.60
2	A	501	NAD	PA-O3	-2.89	1.54	1.59
2	B	503	NAD	O3B-C3B	2.87	1.49	1.43
3	A	502	TDB	B1-N1	-2.84	1.45	1.47
2	A	501	NAD	O4B-C1B	-2.80	1.37	1.41
2	B	503	NAD	O3D-C3D	-2.79	1.36	1.43
2	B	503	NAD	C3B-C4B	2.78	1.60	1.53
2	A	501	NAD	C3B-C4B	2.74	1.60	1.53
2	A	501	NAD	C5N-C4N	2.56	1.44	1.38
2	A	501	NAD	O2D-C2D	-2.53	1.36	1.43
2	A	501	NAD	C3D-C4D	2.52	1.59	1.53
2	B	503	NAD	C8A-N9A	2.46	1.40	1.36
2	B	503	NAD	C3D-C4D	2.45	1.59	1.53
2	A	501	NAD	O3B-C3B	2.33	1.48	1.43
2	A	501	NAD	C4A-N3A	2.32	1.39	1.35
2	A	501	NAD	C6A-N6A	-2.21	1.28	1.34
2	B	503	NAD	O4B-C1B	-2.17	1.38	1.41
2	A	501	NAD	O4B-C4B	2.15	1.50	1.45
3	B	504	TDB	S15-N1	-2.13	1.62	1.67
2	B	503	NAD	C2B-C1B	2.07	1.56	1.53
3	A	502	TDB	C16-C15	-2.02	1.41	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	TDB	B1-N1-N2	14.96	127.34	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	TDB	C13-B1-N1	-11.52	111.78	115.51
2	B	503	NAD	C2N-C3N-C4N	8.93	128.33	118.31
2	A	501	NAD	C2N-C3N-C4N	8.18	127.49	118.31
3	B	504	TDB	O1-B1-N1	-8.02	113.79	123.97
2	A	501	NAD	C3N-C2N-N1N	-6.89	111.17	120.36
2	A	501	NAD	N3A-C2A-N1A	-6.87	122.85	128.89
2	A	501	NAD	C8A-N9A-C4A	-6.82	101.41	106.96
2	B	503	NAD	N3A-C2A-N1A	-6.55	123.13	128.89
2	B	503	NAD	C3N-C2N-N1N	-6.40	111.83	120.36
2	B	503	NAD	C8A-N9A-C4A	-6.18	101.94	106.96
2	B	503	NAD	C5N-C4N-C3N	-5.74	113.18	120.34
3	B	504	TDB	O16-S15-O15	-5.25	113.49	118.92
3	A	502	TDB	O15-S15-N1	5.23	112.79	106.60
2	A	501	NAD	C5A-C4A-N3A	-5.08	121.03	125.98
2	A	501	NAD	C5N-C4N-C3N	-4.84	114.31	120.34
2	B	503	NAD	C2A-N1A-C6A	4.77	127.25	118.76
3	B	504	TDB	O16-S15-N1	4.53	111.96	106.60
2	B	503	NAD	C4B-O4B-C1B	-4.41	104.87	109.72
2	A	501	NAD	C3B-C2B-C1B	-4.21	94.31	100.92
3	A	502	TDB	B1-N1-N2	4.21	123.74	122.33
2	A	501	NAD	O4D-C1D-C2D	4.14	112.72	106.69
2	A	501	NAD	O7N-C7N-C3N	-4.01	115.11	119.59
2	A	501	NAD	C4B-O4B-C1B	-3.98	105.35	109.72
2	A	501	NAD	O4D-C1D-N1N	3.96	112.48	108.13
2	A	501	NAD	C6N-N1N-C1D	-3.83	109.85	119.33
3	B	504	TDB	O16-S15-C15	3.80	114.56	107.91
2	A	501	NAD	C2A-N1A-C6A	3.74	125.42	118.76
2	B	503	NAD	O7N-C7N-C3N	-3.67	115.49	119.59
3	B	504	TDB	C16-C15-S15	3.57	125.41	113.72
2	B	503	NAD	C5A-C4A-N3A	-3.40	122.66	125.98
2	B	503	NAD	C3D-C2D-C1D	-3.39	95.60	100.92
2	A	501	NAD	N3A-C4A-N9A	3.38	131.20	125.39
2	A	501	NAD	C6N-N1N-C2N	3.30	126.10	121.79
2	B	503	NAD	O4D-C1D-N1N	3.29	111.74	108.13
2	A	501	NAD	C6A-C5A-C4A	3.23	121.18	117.55
3	A	502	TDB	C13-B1-N1	-2.99	114.54	115.51
2	B	503	NAD	C6N-N1N-C1D	-2.98	111.94	119.33
3	A	502	TDB	O1-B1-N1	-2.98	120.19	123.97
3	A	502	TDB	O16-S15-O15	-2.94	115.88	118.92
2	B	503	NAD	O4D-C4D-C3D	-2.93	99.20	105.16
3	A	502	TDB	O1-B1-C13	-2.93	114.97	123.72
2	B	503	NAD	C2B-C3B-C4B	2.76	108.15	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	NAD	C8A-N9A-C1B	2.71	131.26	126.15
2	B	503	NAD	O3D-C3D-C4D	-2.64	103.31	111.07
3	A	502	TDB	C15-S15-N1	-2.59	101.09	105.06
3	A	502	TDB	O16-S15-N1	2.57	109.65	106.60
2	B	503	NAD	C6A-C5A-C4A	2.49	120.35	117.55
2	B	503	NAD	C3B-C2B-C1B	-2.49	97.02	100.92
2	B	503	NAD	C5A-C6A-N6A	2.43	126.21	120.72
2	B	503	NAD	N3A-C4A-N9A	2.39	129.50	125.39
2	B	503	NAD	C2N-C3N-C7N	-2.38	112.39	119.32
2	B	503	NAD	C2D-C1D-N1N	2.37	118.21	113.48
2	A	501	NAD	O4D-C4D-C3D	-2.23	100.64	105.16
2	B	503	NAD	C5A-C6A-N1A	-2.17	111.97	119.27
2	A	501	NAD	O3-PN-O1N	-2.15	103.57	108.77
2	A	501	NAD	C8A-N9A-C1B	2.04	129.99	126.15

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	296/296 (100%)	-0.55	5 (1%) 67 69	12, 23, 61, 95	0
1	B	296/296 (100%)	-0.42	8 (2%) 52 54	12, 29, 66, 93	0
All	All	592/592 (100%)	-0.48	13 (2%) 59 61	12, 26, 63, 95	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	4.2
1	B	102	VAL	4.2
1	B	99	PRO	4.0
1	B	77	GLY	3.2
1	B	109	ALA	3.1
1	A	101	ASP	2.7
1	B	104	ALA	2.7
1	A	102	VAL	2.5
1	B	106	LYS	2.5
1	A	100	GLU	2.4
1	A	110	GLY	2.3
1	B	95	PRO	2.1
1	B	75	PRO	2.0

### 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( $\text{\AA}^2$ )	Q<0.9
2	NAD	B	503	44/44	0.10	-0.34	3,32,64,89	0
2	NAD	A	501	44/44	0.09	-0.42	3,20,60,66	0
3	TDB	B	504	17/17	0.10	-0.87	1,22,52,53	0
3	TDB	A	502	17/17	0.08	-0.94	9,15,37,47	0

## 6.5 Other polymers

There are no such residues in this entry.