



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:16 AM GMT

PDB ID : 3OJO  
Title : Derivative structure of the UDP-N-acetyl-mannosamine dehydrogenase Cap5O from *S. aureus*  
Authors : Nessler, S.; Gruszczyk, J.; Olivares-Illana, V.; Meyer, P.; Morera, S.  
Deposited on : 2010-08-23  
Resolution : 2.50 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 (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

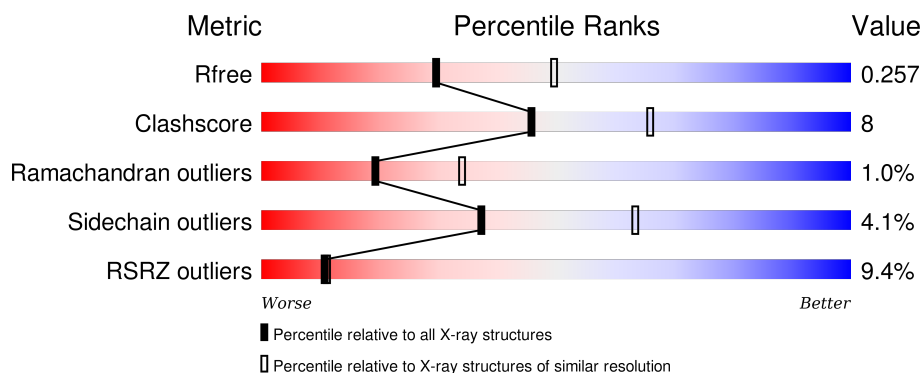
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	431	<div> <div>10%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	B	431	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>• •</div> </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
3	PDC	A	504	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6747 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.

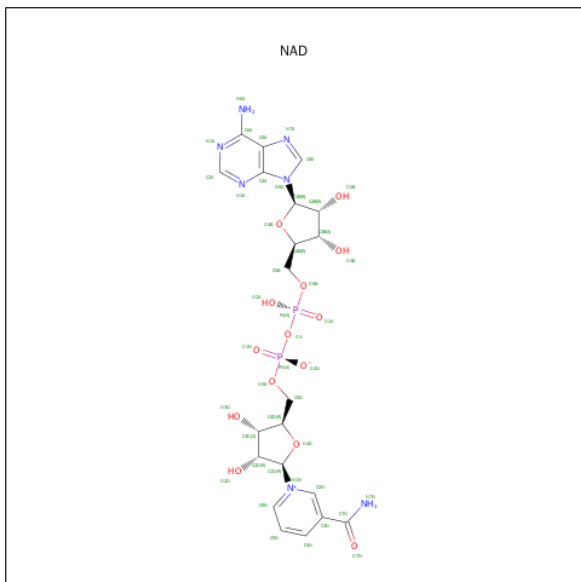
- Molecule 1 is a protein called Cap5O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3194	2026	531	621	16			
1	B	418	Total	C	N	O	S	0	0	0
			3271	2079	541	635	16			

There are 24 discrepancies between the modelled and reference sequences:

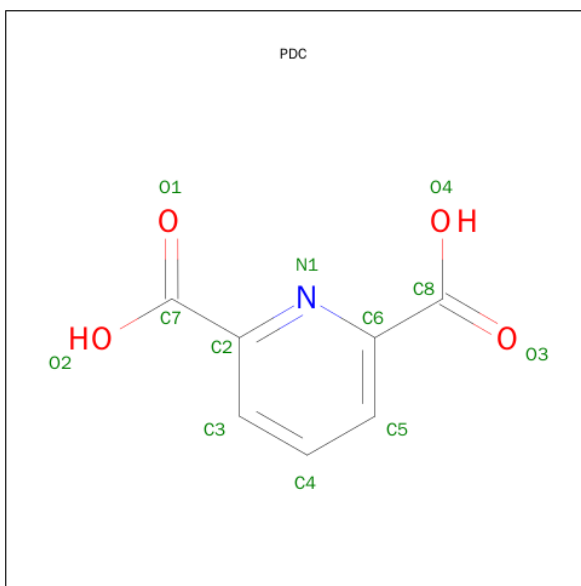
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P95708
A	-9	ARG	-	EXPRESSION TAG	UNP P95708
A	-8	GLY	-	EXPRESSION TAG	UNP P95708
A	-7	SER	-	EXPRESSION TAG	UNP P95708
A	-6	HIS	-	EXPRESSION TAG	UNP P95708
A	-5	HIS	-	EXPRESSION TAG	UNP P95708
A	-4	HIS	-	EXPRESSION TAG	UNP P95708
A	-3	HIS	-	EXPRESSION TAG	UNP P95708
A	-2	HIS	-	EXPRESSION TAG	UNP P95708
A	-1	HIS	-	EXPRESSION TAG	UNP P95708
A	0	GLY	-	EXPRESSION TAG	UNP P95708
A	1	SER	-	EXPRESSION TAG	UNP P95708
B	-10	MET	-	EXPRESSION TAG	UNP P95708
B	-9	ARG	-	EXPRESSION TAG	UNP P95708
B	-8	GLY	-	EXPRESSION TAG	UNP P95708
B	-7	SER	-	EXPRESSION TAG	UNP P95708
B	-6	HIS	-	EXPRESSION TAG	UNP P95708
B	-5	HIS	-	EXPRESSION TAG	UNP P95708
B	-4	HIS	-	EXPRESSION TAG	UNP P95708
B	-3	HIS	-	EXPRESSION TAG	UNP P95708
B	-2	HIS	-	EXPRESSION TAG	UNP P95708
B	-1	HIS	-	EXPRESSION TAG	UNP P95708
B	0	GLY	-	EXPRESSION TAG	UNP P95708
B	1	SER	-	EXPRESSION TAG	UNP P95708

- 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		

- Molecule 3 is PYRIDINE-2,6-DICARBOXYLIC ACID (three-letter code: PDC) (formula:  $C_7H_5NO_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 12 7 1 4	0	0
3	A	1	Total C N O 12 7 1 4	0	0
3	A	1	Total C N O 12 7 1 4	0	0
3	B	1	Total C N O 12 7 1 4	0	0
3	B	1	Total C N O 12 7 1 4	0	0
3	B	1	Total C N O 12 7 1 4	0	0

- Molecule 4 is EUROPIUM ION (three-letter code: EU) (formula: Eu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Eu 1 1	0	0
4	A	1	Total Eu 1 1	0	0

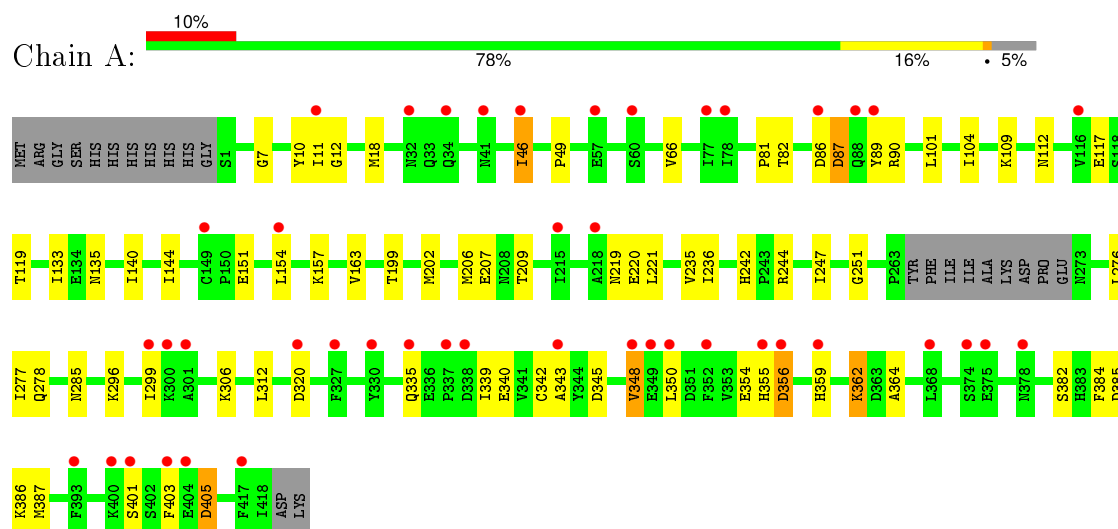
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	57	Total O 57 57	0	0
5	B	63	Total O 63 63	0	0

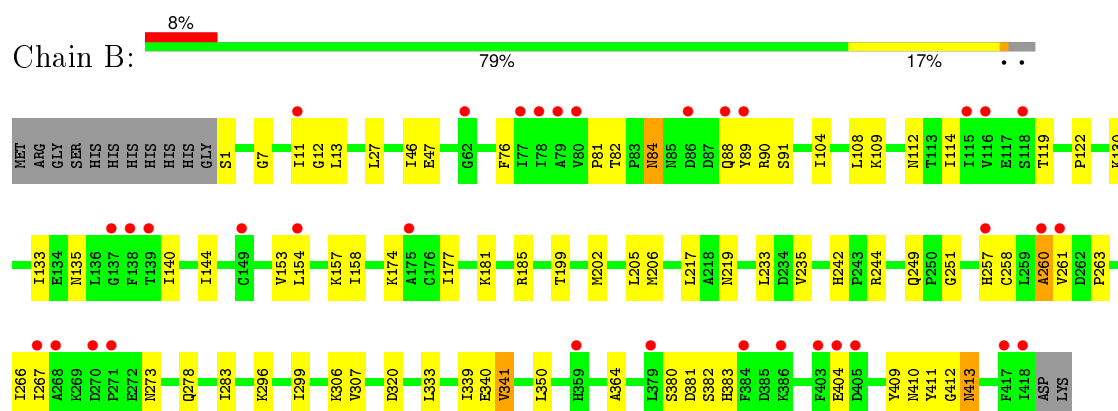
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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: Cap5O



#### • Molecule 1: Cap5O



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.22Å 131.50Å 158.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.50 29.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.63-2.50) 99.7 (29.43-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.201 , 0.246 0.206 , 0.257	Depositor DCC
$R_{free}$ test set	1525 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 30007 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: EU, PDC, 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	0.50	0/3250	0.75	2/4408 (0.0%)
1	B	0.48	0/3331	0.72	0/4520
All	All	0.49	0/6581	0.73	2/8928 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	C-N-CA	5.58	135.64	121.70
1	A	86	ASP	C-N-CA	5.55	135.59	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3194	0	3198	55	0
1	B	3271	0	3274	58	0
2	A	44	0	26	3	0
2	B	44	0	26	2	0
3	A	36	0	11	3	0
3	B	36	0	10	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	57	0	0	2	0
5	B	63	0	0	0	0
All	All	6747	0	6545	100	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 8.

All (100) 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:133:ILE:HG21	1:B:144:ILE:HD11	1.46	0.96
1:A:11:ILE:HG22	2:A:500:NAD:O2N	1.68	0.93
1:A:221:LEU:HD21	1:B:206:MET:SD	2.10	0.90
1:A:355:HIS:HB2	1:A:359:HIS:HB3	1.58	0.85
1:A:312:LEU:HD21	1:A:343:ALA:HB1	1.61	0.82
1:A:219:ASN:HD21	1:A:251:GLY:H	1.28	0.80
1:B:219:ASN:HD21	1:B:251:GLY:H	1.29	0.79
1:A:384:PHE:HB3	1:A:387:MET:CE	2.13	0.78
1:B:242:HIS:HD2	1:B:244:ARG:H	1.34	0.75
1:A:90:ARG:HH12	1:A:285:ASN:HD21	1.36	0.74
1:A:242:HIS:HD2	1:A:244:ARG:H	1.35	0.74
1:A:384:PHE:HB3	1:A:387:MET:HE2	1.70	0.73
1:A:362:LYS:HA	1:A:386:LYS:HB3	1.71	0.71
1:B:409:TYR:HA	1:B:413:ASN:HD21	1.55	0.71
1:B:108:LEU:HD21	1:B:114:ILE:HD11	1.73	0.70
1:B:89:TYR:HB3	1:B:261:VAL:HG21	1.74	0.70
1:B:82:THR:HG21	1:B:119:THR:O	1.91	0.69
1:A:235:VAL:HG12	1:B:206:MET:SD	2.32	0.69
1:A:82:THR:HG21	1:A:119:THR:O	1.93	0.69
1:B:333:LEU:HB3	1:B:341:VAL:HG11	1.77	0.67
1:A:209:THR:HG22	1:B:217:LEU:HD11	1.77	0.65
1:B:133:ILE:HG21	1:B:144:ILE:CD1	2.25	0.65
1:A:209:THR:CG2	1:B:217:LEU:HD11	2.29	0.63
1:A:206:MET:SD	1:B:235:VAL:HG12	2.39	0.62
1:A:133:ILE:HG21	1:A:140:ILE:HD11	1.82	0.62
1:A:81:PRO:HG3	2:A:500:NAD:H51A	1.81	0.61
1:A:18:MET:CE	1:A:163:VAL:HG23	2.30	0.61
1:B:81:PRO:HG3	2:B:500:NAD:H51A	1.83	0.61
1:B:122:PRO:HD3	1:B:205:LEU:HD12	1.83	0.59
1:A:306:LYS:HB3	1:A:364:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HA	1:B:177:ILE:HD12	1.85	0.59
1:A:89:TYR:CE1	1:A:278:GLN:HB2	2.38	0.58
1:A:11:ILE:HG13	1:A:151:GLU:HG2	1.87	0.57
1:A:18:MET:CE	1:A:163:VAL:CG2	2.83	0.56
1:B:306:LYS:HB3	1:B:364:ALA:HA	1.86	0.56
1:B:119:THR:OG1	2:B:500:NAD:H6N	2.05	0.56
1:B:130:LYS:HG3	1:B:140:ILE:HD13	1.87	0.56
1:A:133:ILE:CG2	1:A:140:ILE:HD11	2.35	0.56
1:A:247:ILE:HD13	1:B:206:MET:HE3	1.87	0.55
1:A:384:PHE:HB3	1:A:387:MET:HE3	1.86	0.55
1:A:221:LEU:CD2	1:B:206:MET:SD	2.90	0.55
1:A:18:MET:HE1	1:A:163:VAL:HG23	1.88	0.55
1:B:296:LYS:HG2	1:B:339:ILE:HD11	1.87	0.55
1:A:209:THR:HG23	1:A:277:ILE:HG12	1.88	0.55
1:B:410:ASN:HB3	1:B:412:GLY:H	1.72	0.54
1:A:236:ILE:HA	1:B:206:MET:HE1	1.90	0.54
1:A:296:LYS:HG2	1:A:339:ILE:HD11	1.90	0.54
1:A:119:THR:OG1	2:A:500:NAD:H6N	2.08	0.54
1:A:11:ILE:HG23	5:A:467:HOH:O	2.09	0.52
1:A:11:ILE:HD11	1:A:117:GLU:HB3	1.93	0.51
1:B:261:VAL:HA	1:B:266:ILE:HD11	1.92	0.51
1:A:202:MET:HG3	1:B:235:VAL:HG11	1.93	0.51
1:A:242:HIS:CD2	1:A:244:ARG:H	2.23	0.51
1:B:154:LEU:HD22	1:B:157:LYS:HB2	1.92	0.51
1:B:413:ASN:C	1:B:413:ASN:HD22	2.14	0.50
1:B:84:ASN:HD21	1:B:258:CYS:HB3	1.76	0.50
1:A:154:LEU:HD22	1:A:157:LYS:HG3	1.94	0.49
1:A:235:VAL:HG11	1:B:202:MET:HG3	1.95	0.49
1:B:380:SER:H	1:B:383:HIS:CD2	2.31	0.49
1:B:333:LEU:HB3	1:B:341:VAL:CG1	2.42	0.48
1:A:89:TYR:HE1	1:A:278:GLN:HB2	1.78	0.48
1:B:11:ILE:HD13	1:B:153:VAL:HG13	1.95	0.48
1:B:89:TYR:CE1	1:B:278:GLN:HB2	2.48	0.48
1:B:242:HIS:CD2	1:B:244:ARG:H	2.24	0.48
1:A:355:HIS:HB2	1:A:359:HIS:CB	2.38	0.48
1:A:11:ILE:HD11	1:A:151:GLU:HB3	1.95	0.47
1:B:153:VAL:HB	1:B:158:ILE:HG12	1.96	0.47
1:A:109:LYS:H	1:A:112:ASN:ND2	2.13	0.47
1:B:181:LYS:O	1:B:185:ARG:HB2	2.14	0.46
1:B:333:LEU:CB	1:B:341:VAL:HG11	2.43	0.46
3:B:504:PDC:O2	3:B:503:PDC:O4	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:O	3:A:504:PDC:H4	2.17	0.45
1:B:109:LYS:H	1:B:112:ASN:ND2	2.15	0.45
1:B:307:VAL:HG11	1:B:333:LEU:HD13	1.99	0.44
1:A:306:LYS:HA	1:A:340:GLU:O	2.18	0.44
1:A:220:GLU:HG3	1:B:273:ASN:O	2.18	0.44
1:A:10:TYR:CE2	1:A:46:ILE:HG13	2.51	0.44
1:B:263:PRO:HA	1:B:267:ILE:HD12	1.99	0.43
1:B:13:LEU:HD23	1:B:46:ILE:HG12	1.99	0.43
1:A:7:GLY:O	1:A:12:GLY:HA3	2.17	0.43
1:A:199:THR:HG23	1:B:235:VAL:HG22	2.01	0.43
1:A:11:ILE:CD1	1:A:151:GLU:HB3	2.49	0.43
1:A:247:ILE:HD13	1:B:206:MET:CE	2.49	0.42
1:B:205:LEU:HB3	1:B:260:ALA:HA	2.00	0.42
1:B:90:ARG:O	1:B:90:ARG:HG3	2.19	0.42
3:A:504:PDC:O1	1:B:244:ARG:NH1	2.52	0.42
1:B:84:ASN:ND2	1:B:258:CYS:HB3	2.34	0.42
1:A:320:ASP:HA	5:A:443:HOH:O	2.20	0.42
1:A:101:LEU:HD11	1:A:133:ILE:HD11	2.01	0.42
1:A:276:LEU:HB2	1:B:283:ILE:CD1	2.49	0.42
1:B:7:GLY:O	1:B:12:GLY:HA3	2.20	0.41
1:A:235:VAL:HG22	1:B:199:THR:HG23	2.01	0.41
1:A:345:ASP:HB3	1:A:348:VAL:HG22	2.02	0.41
1:A:112:ASN:HB2	1:A:144:ILE:HD13	2.03	0.41
1:B:88:GLN:CD	1:B:88:GLN:H	2.24	0.41
3:A:502:PDC:O4	3:A:504:PDC:O4	2.39	0.41
1:B:306:LYS:HA	1:B:340:GLU:O	2.21	0.41
1:B:233:LEU:HD22	1:B:249:GLN:HE22	1.86	0.41
1:B:205:LEU:HB3	1:B:260:ALA:CA	2.51	0.40
1:B:76:PHE:CD1	1:B:104:ILE:HG12	2.56	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	405/431 (94%)	386 (95%)	13 (3%)	6 (2%)	13	22
1	B	416/431 (96%)	397 (95%)	17 (4%)	2 (0%)	34	55
All	All	821/862 (95%)	783 (95%)	30 (4%)	8 (1%)	19	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
1	A	356	ASP
1	A	362	LYS
1	B	257	HIS
1	A	354	GLU
1	A	405	ASP
1	A	87	ASP
1	B	260	ALA

### 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	364/383 (95%)	349 (96%)	15 (4%)	37	63
1	B	372/383 (97%)	357 (96%)	15 (4%)	38	64
All	All	736/766 (96%)	706 (96%)	30 (4%)	37	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	66	VAL
1	A	87	ASP
1	A	104	ILE
1	A	135	ASN
1	A	299	ILE
1	A	335	GLN
1	A	342	CYS

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Mol	Chain	Res	Type
1	A	348	VAL
1	A	350	LEU
1	A	382	SER
1	A	385	ASP
1	A	401	SER
1	A	403	PHE
1	A	405	ASP
1	B	1	SER
1	B	27	LEU
1	B	47	GLU
1	B	84	ASN
1	B	91	SER
1	B	135	ASN
1	B	299	ILE
1	B	320	ASP
1	B	341	VAL
1	B	350	LEU
1	B	381	ASP
1	B	382	SER
1	B	404	GLU
1	B	411	TYR
1	B	413	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	40	GLN
1	A	52	GLN
1	A	112	ASN
1	A	208	ASN
1	A	214	ASN
1	A	219	ASN
1	A	226	ASN
1	A	242	HIS
1	A	248	HIS
1	A	285	ASN
1	A	383	HIS
1	B	22	HIS
1	B	40	GLN
1	B	52	GLN
1	B	84	ASN

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Mol	Chain	Res	Type
1	B	112	ASN
1	B	214	ASN
1	B	219	ASN
1	B	226	ASN
1	B	242	HIS
1	B	248	HIS
1	B	249	GLN
1	B	278	GLN
1	B	383	HIS
1	B	410	ASN
1	B	413	ASN

### 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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	500	-	38,48,48	1.75	3 (7%)	47,73,73	1.94	3 (6%)
3	PDC	A	502	4	6,12,12	1.40	0	8,16,16	1.29	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PDC	A	503	4	6,12,12	1.31	1 (16%)	8,16,16	1.35	1 (12%)
3	PDC	A	504	4	6,12,12	0.32	0	8,16,16	2.62	5 (62%)
2	NAD	B	500	-	38,48,48	1.72	3 (7%)	47,73,73	2.15	5 (10%)
3	PDC	B	502	4	6,12,12	0.91	0	8,16,16	1.12	0
3	PDC	B	503	4	6,12,12	1.69	1 (16%)	8,16,16	4.27	5 (62%)
3	PDC	B	504	4	6,12,12	1.70	2 (33%)	8,16,16	2.00	3 (37%)

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	500	-	-	0/22/62/62	0/5/5/5
3	PDC	A	502	4	-	0/0/8/8	0/1/1/1
3	PDC	A	503	4	-	0/0/8/8	0/1/1/1
3	PDC	A	504	4	-	0/0/8/8	0/1/1/1
2	NAD	B	500	-	-	0/22/62/62	0/5/5/5
3	PDC	B	502	4	-	0/0/8/8	0/1/1/1
3	PDC	B	503	4	-	0/0/8/8	0/1/1/1
3	PDC	B	504	4	-	0/0/8/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	PDC	C6-N1	-3.48	1.30	1.34
3	B	504	PDC	C3-C2	2.05	1.43	1.38
3	B	504	PDC	C2-N1	2.41	1.38	1.34
3	A	503	PDC	C3-C2	2.67	1.45	1.38
2	B	500	NAD	C2A-N1A	2.70	1.39	1.33
2	A	500	NAD	C2A-N1A	3.06	1.39	1.33
2	B	500	NAD	C2A-N3A	3.61	1.38	1.32
2	A	500	NAD	C2A-N3A	3.70	1.38	1.32
2	B	500	NAD	O7N-C7N	8.32	1.41	1.24
2	A	500	NAD	O7N-C7N	8.48	1.42	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAD	N3A-C2A-N1A	-11.79	119.86	128.89
2	A	500	NAD	N3A-C2A-N1A	-10.34	120.98	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	PDC	C3-C2-N1	-3.49	117.20	122.01
2	B	500	NAD	PN-O3-PA	-3.19	123.78	132.73
2	A	500	NAD	PN-O3-PA	-3.18	123.79	132.73
3	B	504	PDC	C5-C6-N1	-3.15	117.66	122.01
3	A	504	PDC	C3-C2-N1	-2.86	118.07	122.01
3	A	503	PDC	C3-C2-C7	-2.58	117.17	120.15
3	A	504	PDC	C4-C5-C6	-2.57	115.44	118.88
3	B	503	PDC	C5-C6-N1	-2.05	119.18	122.01
2	B	500	NAD	C2B-C1B-N9A	-2.05	111.17	114.29
2	B	500	NAD	C3N-C7N-N7N	2.03	120.04	117.82
3	A	502	PDC	C5-C6-C8	2.20	122.69	120.15
3	A	502	PDC	C6-N1-C2	2.26	120.73	117.99
3	A	504	PDC	C3-C2-C7	2.82	123.41	120.15
3	B	504	PDC	C6-N1-C2	2.89	121.50	117.99
3	A	504	PDC	C5-C6-C8	2.91	123.50	120.15
3	B	504	PDC	C4-C5-C6	2.98	122.86	118.88
3	A	504	PDC	C6-N1-C2	4.40	123.33	117.99
2	A	500	NAD	O4D-C1D-N1N	4.97	113.59	108.13
2	B	500	NAD	O4D-C1D-N1N	5.12	113.75	108.13
3	B	503	PDC	C5-C6-C8	5.34	126.31	120.15
3	B	503	PDC	C3-C2-C7	5.52	126.52	120.15
3	B	503	PDC	C6-N1-C2	8.10	127.83	117.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAD	3	0
3	A	502	PDC	1	0
3	A	504	PDC	3	0
2	B	500	NAD	2	0
3	B	503	PDC	1	0
3	B	504	PDC	1	0

## 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	409/431 (94%)	0.59	44 (10%) <b>8</b> <b>8</b>	32, 54, 89, 101	0
1	B	418/431 (96%)	0.48	34 (8%) <b>15</b> <b>16</b>	31, 55, 84, 99	0
All	All	827/862 (95%)	0.53	78 (9%) <b>11</b> <b>11</b>	31, 55, 87, 101	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	GLN	5.1
1	A	401	SER	5.0
1	A	86	ASP	4.6
1	B	271	PRO	4.6
1	A	88	GLN	4.4
1	B	89	TYR	4.1
1	A	355	HIS	4.0
1	B	261	VAL	3.9
1	A	378	ASN	3.9
1	B	86	ASP	3.9
1	B	138	PHE	3.8
1	A	301	ALA	3.8
1	B	404	GLU	3.7
1	A	404	GLU	3.6
1	B	137	GLY	3.6
1	A	400	LYS	3.6
1	A	349	GLU	3.5
1	B	78	ILE	3.4
1	B	267	ILE	3.4
1	A	348	VAL	3.4
1	A	356	ASP	3.3
1	B	149	CYS	3.3
1	A	403	PHE	3.2
1	B	77	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	89	TYR	3.2
1	A	60	SER	3.1
1	A	368	LEU	3.1
1	A	352	PHE	3.0
1	B	115	ILE	3.0
1	A	350	LEU	2.9
1	A	57	GLU	2.9
1	B	403	PHE	2.9
1	B	116	VAL	2.8
1	B	260	ALA	2.8
1	A	375	GLU	2.8
1	A	149	CYS	2.8
1	B	154	LEU	2.7
1	A	327	PHE	2.7
1	A	338	ASP	2.7
1	B	62	GLY	2.7
1	A	77	ILE	2.7
1	B	257	HIS	2.7
1	A	116	VAL	2.7
1	A	46	ILE	2.6
1	B	79	ALA	2.6
1	B	384	PHE	2.6
1	B	268	ALA	2.5
1	A	78	ILE	2.5
1	A	335	GLN	2.5
1	B	118	SER	2.4
1	A	154	LEU	2.4
1	A	218	ALA	2.4
1	B	379	LEU	2.4
1	B	270	ASP	2.4
1	B	359	HIS	2.4
1	A	300	LYS	2.4
1	B	139	THR	2.4
1	B	88	GLN	2.4
1	A	320	ASP	2.3
1	B	11	ILE	2.2
1	B	405	ASP	2.2
1	A	11	ILE	2.2
1	A	343	ALA	2.2
1	A	393	PHE	2.2
1	A	337	PRO	2.2
1	A	41	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	330	TYR	2.2
1	A	215	ILE	2.2
1	A	374	SER	2.2
1	B	175	ALA	2.1
1	A	359	HIS	2.1
1	A	417	PHE	2.1
1	B	417	PHE	2.1
1	B	418	ILE	2.0
1	B	386	LYS	2.0
1	B	80	VAL	2.0
1	A	299	ILE	2.0
1	A	32	ASN	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
3	PDC	A	504	12/12	0.95	0.21	2.41	36,39,41,43	5
3	PDC	A	503	12/12	0.97	0.18	0.24	36,39,42,42	6
3	PDC	B	503	12/12	0.94	0.15	-0.06	48,51,54,54	0
3	PDC	B	502	12/12	0.98	0.17	-0.26	43,46,50,52	4
2	NAD	B	500	44/44	0.96	0.15	-0.69	33,42,78,79	0
2	NAD	A	500	44/44	0.93	0.14	-1.01	44,60,77,82	0
3	PDC	B	504	12/12	0.98	0.20	-	72,75,78,79	0
4	EU	B	501	1/1	1.00	0.18	-	33,33,33,33	1
4	EU	A	501	1/1	1.00	0.22	-	22,22,22,22	1
3	PDC	A	502	12/12	0.95	0.15	-	48,51,53,55	2

## 6.5 Other polymers ⓘ

There are no such residues in this entry.