



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:15 AM GMT

PDB ID : 3OJL
Title : Native structure of the UDP-N-acetyl-mannosamine dehydrogenase Cap5O from *Staphylococcus aureus*
Authors : Nessler, S.; Gruszczyk, J.; Olivares-Illana, V.; Meyer, P.; Morera, S.; Grangeasse, C.; Fleurie, A.
Deposited on : 2010-08-23
Resolution : 2.80 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

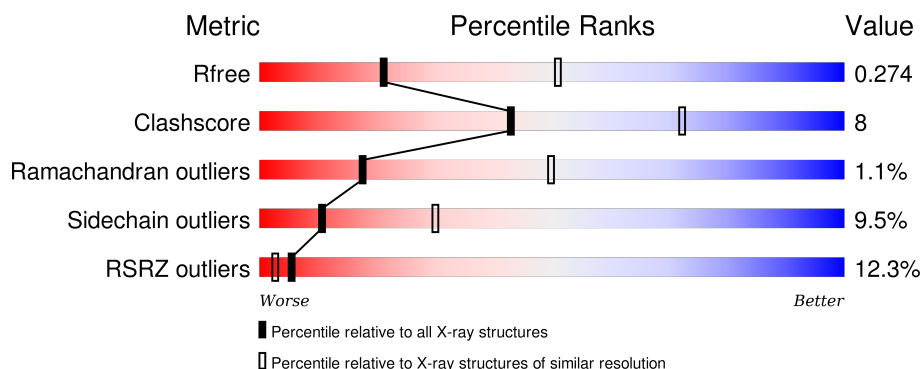
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 ≥ 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	
1	B	431	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6627 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.

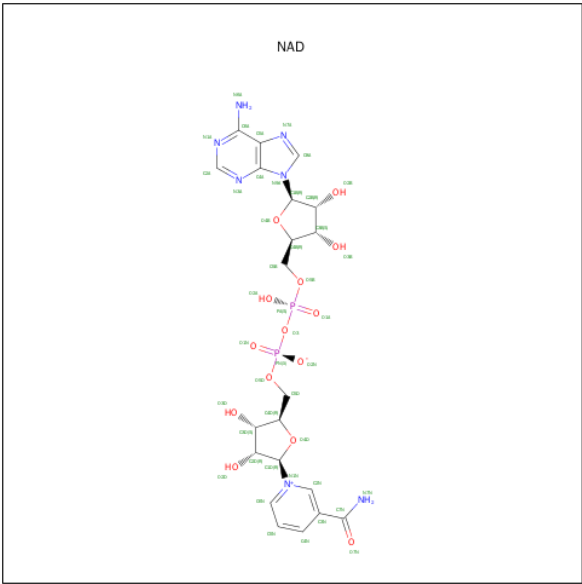
- Molecule 1 is a protein called Cap5O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3271	2079	541	635	16			
1	B	412	Total	C	N	O	S	0	0	0
			3225	2048	534	627	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: C₂₁H₂₇N₇O₁₄P₂).



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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	28	Total	O	0	0
			28	28		

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.

Chain A:

16% 71% 23%

MET ARG GLY SER HIS THR ASP LYS

T313 G316 D317 V318 D319 D320 D321 D322 D323 S324 P325 A326 F327 D328 P331 L332 L333 L334 Q335 Q336 P337 D338 L339 E340 E341 C342 R347 V348 E349 L350 D351 F352 S358 V361 K362 D363 A364 S365 L366 V367 L368 L369 L370 S374 E375 V378 L379 S380 D381 S382 R383 F384

N85 D86 D87 Q88 Y89 R90 S91 C92 S95 L96 Y97 M98 L101 L102 D103 S103 L104 L105 L108 T113 L114 L115 V116 E117 L118 T119 P122 L133 L136 I144 C149 P150 E151 L154 P155 G156 L159 E160 L162 M165 M166 R167 K174 I177 V181

R185 T186 Q189 M202 L205 M206 P211 N219 E220 L221 N226 M231 D234 V235 R242 P243 R244 V245 N246 L247 R248 G251 G256 H257 C258 L259 A260 V261 T266 K269 R281 V292 T295 L298 S303 G304 N305 K306 V307 T308

T4 T5 V6 L8 G9 Y10 I11 G12 L13 P14 T15 S16 V26 L27 I31 Q34 R41 Q42 Q43 V54 E57 V58 L59 G62 K63 L64 E71 E75 F76 I77 I78 A79 V80 P81 T82 R83 N84

Chain B:

7% 71% 23%

0.00 0.05 0.10 0.15

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400

MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY S1 K2 L3 T4 V5 V6 G7 L8 I11 G12 L13 P14 T15 S16 I17 K21 H22 V26 L27 G28 I31 E47 E48 P49 Q52 E53 V54 E57 V58 L64 V75 I77 I78 A79 V80 P81 T82 P83 N84 T85 D86 D87 Q88 Y89 A90 S91 L96 L101 D102 L105 T113 T114 I115 V116 E117 T119 I183 L136 G137 F138 T139 D143 I144 G149 P150 E151 R152 V153 L154 P155 G156 L159 E160 E161 L162 V163 H164 R167 K174 I177 K181 V183 P184 R185 F187 V188 Q189 M202 S203 K204 L205 M206 N219 E220 L221 N226 V235 H242 P243 R244 V245 N246 I247 H248 G251 G256 H257 C258 F263 Y264 F265 ILE ILE ALA LYS ASP P80 N273 R281 V292 T295 I298 S303 K306 L312 T313 L314 D319 D320 I321 Y330 L333 D338 I339 E340 A343 E349 L350 S358 H359 A364 S365 L366 V367 L368 L379 S380 D381 S382 H383 F384 D385 K390 F393 S402 D405 V406 N410 L414 F415 N416 F417 D418 D419 LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.90 Å 87.26 Å 131.58 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.12 – 2.80 29.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.12-2.80) 98.3 (29.06-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.80 Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.217 , 0.263 0.228 , 0.274	Depositor DCC
R_{free} test set	810 reflections (3.77%)	DCC
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 71.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 22319 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6627	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	0/3331	0.73	0/4520
1	B	0.50	0/3283	0.74	0/4453
All	All	0.50	0/6614	0.73	0/8973

There are no bond length outliers.

There are no bond angle outliers.

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	3271	0	3276	63	0
1	B	3225	0	3220	53	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
3	A	15	0	0	0	0
3	B	28	0	0	0	0
All	All	6627	0	6548	107	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 (107) 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:A:206:MET:SD	1:B:221:LEU:HD11	2.25	0.77
1:A:235:VAL:HG12	1:B:206:MET:SD	2.30	0.71
1:A:205:LEU:HB3	1:A:266:ILE:HD11	1.72	0.71
1:A:333:LEU:HB3	1:A:341:VAL:HG11	1.75	0.69
1:A:242:HIS:HD2	1:A:244:ARG:H	1.40	0.69
1:B:150:PRO:HB2	1:B:204:LYS:HG3	1.74	0.68
1:A:304:GLY:HA3	1:A:365:SER:OG	1.94	0.68
1:B:298:ILE:HG21	1:B:366:LEU:HD13	1.78	0.65
1:A:306:LYS:HB3	1:A:364:ALA:HA	1.79	0.65
1:B:306:LYS:HB3	1:B:364:ALA:HA	1.79	0.65
1:B:242:HIS:HD2	1:B:244:ARG:H	1.45	0.64
1:A:206:MET:CE	1:B:221:LEU:HD21	2.28	0.64
1:A:133:ILE:HG21	1:A:144:ILE:HG21	1.78	0.64
1:A:84:ASN:HD22	1:A:90:ARG:HB3	1.64	0.61
1:A:226:ASN:HD22	1:A:415:PHE:HD2	1.49	0.61
1:B:219:ASN:HD21	1:B:251:GLY:H	1.49	0.60
1:A:27:LEU:HD12	1:A:71:GLU:HG2	1.83	0.59
1:A:219:ASN:HD21	1:A:251:GLY:H	1.51	0.58
1:B:312:LEU:HB3	1:B:321:ILE:HD11	1.85	0.58
1:A:205:LEU:CB	1:A:266:ILE:HD11	2.34	0.57
1:B:226:ASN:HD22	1:B:415:PHE:HD2	1.51	0.57
1:B:416:ASN:C	1:B:418:ILE:H	2.07	0.57
1:B:183:VAL:O	1:B:186:THR:HG23	2.06	0.56
1:A:211:ARG:HG2	1:A:259:LEU:HD11	1.87	0.55
1:A:231:ASN:HD22	1:A:234:ASP:H	1.54	0.54
1:A:154:LEU:HG	1:A:156:GLY:H	1.72	0.53
1:A:235:VAL:CG1	1:B:206:MET:SD	2.97	0.53
1:B:393:PHE:CE1	1:B:414:ILE:HG12	2.44	0.53
1:B:139:THR:H	1:B:143:ASP:HB2	1.74	0.52
1:A:105:LEU:HG	1:A:136:LEU:HD11	1.92	0.52
1:A:306:LYS:HE2	1:A:342:CYS:HB2	1.91	0.52
1:A:133:ILE:CG2	1:A:144:ILE:HG21	2.39	0.52
1:A:306:LYS:HA	1:A:340:GLU:HB3	1.92	0.52
1:A:321:ILE:HD11	1:A:348:VAL:HG11	1.93	0.51
1:A:101:LEU:HD11	1:A:133:ILE:HD11	1.93	0.51
1:A:206:MET:SD	1:B:221:LEU:HD21	2.52	0.50
1:A:242:HIS:CD2	1:A:244:ARG:H	2.24	0.50
1:A:7:GLY:O	1:A:12:GLY:HA3	2.11	0.50
1:B:242:HIS:CD2	1:B:244:ARG:H	2.29	0.50
1:B:105:LEU:HG	1:B:136:LEU:HD11	1.94	0.49
1:B:7:GLY:O	1:B:12:GLY:HA3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PHE:CD1	1:A:104:ILE:HD12	2.48	0.49
1:A:108:LEU:HD22	1:A:144:ILE:HD11	1.94	0.49
1:B:87:ASP:HB2	1:B:89:TYR:H	1.78	0.48
1:B:174:LYS:HA	1:B:177:ILE:HD12	1.95	0.48
1:A:161:GLU:O	1:A:165:ASN:HB2	2.13	0.48
1:A:174:LYS:HA	1:A:177:ILE:HD12	1.94	0.48
1:B:390:LYS:HB3	1:B:406:VAL:HG22	1.96	0.48
1:A:54:VAL:HG21	1:A:159:LEU:HD21	1.96	0.48
1:A:390:LYS:HB3	1:A:406:VAL:HG22	1.95	0.48
1:A:205:LEU:HB3	1:A:266:ILE:CD1	2.42	0.48
1:A:308:THR:HG23	1:A:367:VAL:HG22	1.95	0.48
1:B:181:LYS:O	1:B:185:ARG:HB2	2.14	0.48
1:B:54:VAL:HG21	1:B:159:LEU:HD21	1.96	0.47
1:A:231:ASN:ND2	1:A:234:ASP:H	2.11	0.47
1:B:292:VAL:HG22	1:B:333:LEU:HD13	1.96	0.47
1:B:306:LYS:HA	1:B:340:GLU:HB3	1.95	0.47
1:A:221:LEU:HD22	1:B:206:MET:CE	2.44	0.47
1:A:26:VAL:HG22	1:A:64:LEU:HG	1.97	0.47
1:B:58:VAL:HG13	1:B:64:LEU:HB2	1.98	0.46
1:B:379:LEU:HD13	1:B:384:PHE:HZ	1.81	0.46
1:A:58:VAL:HG13	1:A:64:LEU:HB2	1.99	0.45
1:B:330:TYR:CE1	1:B:343:ALA:HB2	2.52	0.45
1:A:9:GLY:HA3	2:A:500:NAD:O5B	2.16	0.45
1:B:11:ILE:HD12	1:B:151:GLU:HG2	1.98	0.45
1:A:202:MET:HG3	1:B:235:VAL:HG11	1.99	0.45
1:B:380:SER:H	1:B:383:HIS:CD2	2.34	0.45
1:A:13:LEU:HB3	1:A:14:PRO:HD3	1.99	0.45
1:A:181:LYS:O	1:A:185:ARG:HB2	2.16	0.45
1:A:399:VAL:HG11	1:A:403:PHE:HE2	1.81	0.45
1:A:81:PRO:HD2	1:A:96:LEU:HD13	1.99	0.44
1:B:81:PRO:HD2	1:B:96:LEU:HD13	1.98	0.44
1:A:122:PRO:HD2	1:A:269:LYS:HG3	1.98	0.44
1:B:101:LEU:HD11	1:B:133:ILE:HD11	1.99	0.44
1:A:380:SER:H	1:A:383:HIS:CD2	2.35	0.44
1:A:75:VAL:HB	1:A:113:THR:HB	1.98	0.44
1:B:17:ILE:O	1:B:21:LYS:HB2	2.17	0.44
1:B:13:LEU:HB3	1:B:14:PRO:HD3	1.98	0.44
1:A:298:ILE:HG21	1:A:366:LEU:HD13	1.99	0.43
1:A:221:LEU:HD22	1:B:206:MET:HE3	2.00	0.43
1:A:295:THR:HG21	1:A:333:LEU:HD21	2.00	0.43
1:B:314:TYR:CE2	1:B:320:ASP:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:HB	1:B:113:THR:HB	2.00	0.43
1:A:149:CYS:SG	1:A:167:ARG:HG2	2.59	0.43
1:A:242:HIS:HD2	1:A:244:ARG:N	2.13	0.43
1:B:3:LEU:HD21	1:B:77:ILE:HD12	2.00	0.43
1:B:295:THR:HG23	1:B:366:LEU:HD23	2.01	0.42
1:A:81:PRO:HG3	2:A:500:NAD:H51A	2.01	0.42
1:B:138:PHE:HB3	1:B:144:ILE:HG13	2.01	0.42
1:A:235:VAL:HG11	1:B:202:MET:HG3	2.01	0.42
1:B:152:ARG:HE	1:B:152:ARG:HB2	1.71	0.42
1:B:81:PRO:HG3	2:B:500:NAD:H51A	2.01	0.42
1:B:82:THR:HG21	1:B:119:THR:O	2.19	0.42
1:B:22:HIS:CD2	1:B:187:PHE:HB3	2.53	0.42
1:A:379:LEU:HD13	1:A:384:PHE:HZ	1.84	0.42
1:B:133:ILE:CG2	1:B:144:ILE:HD11	2.50	0.42
1:A:324:SER:HA	1:A:325:PRO:HD3	1.98	0.42
1:A:333:LEU:HB3	1:A:341:VAL:CG1	2.47	0.41
1:A:313:THR:HG21	1:A:318:VAL:O	2.19	0.41
1:A:292:VAL:HG22	1:A:333:LEU:HD13	2.01	0.41
1:B:26:VAL:HG22	1:B:64:LEU:HG	2.03	0.41
1:B:8:LEU:HD11	1:B:28:GLY:HA3	2.02	0.41
1:A:308:THR:HG21	1:A:361:VAL:HG12	2.03	0.40
1:A:82:THR:HG21	1:A:119:THR:O	2.21	0.40
1:B:138:PHE:HD2	1:B:143:ASP:HB3	1.87	0.40
1:A:333:LEU:HG	1:A:339:ILE:HG21	2.03	0.40
1:B:333:LEU:HG	1:B:339:ILE:HG21	2.02	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	416/431 (96%)	390 (94%)	21 (5%)	5 (1%)	16 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	408/431 (95%)	380 (93%)	24 (6%)	4 (1%)	19	52
All	All	824/862 (96%)	770 (93%)	45 (6%)	9 (1%)	17	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ARG
1	B	86	ASP
1	A	256	GLY
1	B	49	PRO
1	B	256	GLY
1	B	418	ILE
1	A	87	ASP
1	A	321	ILE
1	A	155	PRO

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	372/383 (97%)	339 (91%)	33 (9%)	12	34
1	B	367/383 (96%)	330 (90%)	37 (10%)	9	27
All	All	739/766 (96%)	669 (90%)	70 (10%)	11	30

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	57	GLU
1	A	58	VAL
1	A	64	LEU
1	A	75	VAL
1	A	95	SER
1	A	98	MET

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Mol	Chain	Res	Type
1	A	102	ASP
1	A	105	LEU
1	A	144	ILE
1	A	151	GLU
1	A	154	LEU
1	A	162	LEU
1	A	167	ARG
1	A	186	THR
1	A	189	GLN
1	A	202	MET
1	A	231	ASN
1	A	246	ASN
1	A	248	HIS
1	A	257	HIS
1	A	258	CYS
1	A	281	ARG
1	A	303	SER
1	A	324	SER
1	A	338	ASP
1	A	350	LEU
1	A	358	SER
1	A	368	LEU
1	A	382	SER
1	A	405	ASP
1	A	411	TYR
1	A	418	ILE
1	B	27	LEU
1	B	31	ILE
1	B	57	GLU
1	B	64	LEU
1	B	75	VAL
1	B	84	ASN
1	B	87	ASP
1	B	88	GLN
1	B	91	SER
1	B	102	ASP
1	B	105	LEU
1	B	151	GLU
1	B	152	ARG
1	B	162	LEU
1	B	167	ARG
1	B	186	THR

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Mol	Chain	Res	Type
1	B	189	GLN
1	B	202	MET
1	B	246	ASN
1	B	248	HIS
1	B	257	HIS
1	B	258	CYS
1	B	262	ASP
1	B	281	ARG
1	B	303	SER
1	B	319	ASP
1	B	321	ILE
1	B	338	ASP
1	B	349	GLU
1	B	350	LEU
1	B	358	SER
1	B	368	LEU
1	B	382	SER
1	B	405	ASP
1	B	410	ASN
1	B	414	ILE
1	B	418	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	219	ASN
1	A	226	ASN
1	A	231	ASN
1	A	242	HIS
1	A	249	GLN
1	A	297	GLN
1	A	334	ASN
1	A	383	HIS
1	B	85	ASN
1	B	219	ASN
1	B	226	ASN
1	B	242	HIS
1	B	249	GLN
1	B	297	GLN
1	B	334	ASN
1	B	383	HIS

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Mol	Chain	Res	Type
1	B	410	ASN
1	B	413	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	500	-	38,48,48	1.72	3 (7%)	47,73,73	1.85	4 (8%)
2	NAD	B	500	-	38,48,48	1.75	3 (7%)	47,73,73	1.94	3 (6%)

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
2	NAD	B	500	-	-	0/22/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	C2A-N1A	3.04	1.39	1.33
2	B	500	NAD	C2A-N1A	3.06	1.39	1.33
2	A	500	NAD	C2A-N3A	3.88	1.39	1.32
2	B	500	NAD	C2A-N3A	4.45	1.40	1.32
2	B	500	NAD	O7N-C7N	8.04	1.41	1.24
2	A	500	NAD	O7N-C7N	8.12	1.41	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAD	N3A-C2A-N1A	-10.34	120.98	128.89
2	A	500	NAD	N3A-C2A-N1A	-9.90	121.31	128.89
2	B	500	NAD	PN-O3-PA	-3.56	122.74	132.73
2	A	500	NAD	PN-O3-PA	-3.54	122.79	132.73
2	A	500	NAD	C4A-C5A-N7A	-3.03	106.69	109.48
2	A	500	NAD	O4D-C1D-N1N	4.31	112.86	108.13
2	B	500	NAD	O4D-C1D-N1N	4.96	113.58	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAD	2	0
2	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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	418/431 (96%)	0.72	70 (16%) 2 1	30, 70, 118, 136	0
1	B	412/431 (95%)	0.42	32 (7%) 16 8	30, 66, 94, 117	0
All	All	830/862 (96%)	0.57	102 (12%) 5 3	30, 67, 113, 136	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	SER	6.5
1	A	257	HIS	6.0
1	B	264	TYR	5.0
1	A	43	GLN	4.7
1	A	77	ILE	4.7
1	A	347	HIS	4.5
1	A	156	GLY	4.4
1	A	323	GLU	4.2
1	A	382	SER	4.1
1	A	402	SER	4.0
1	A	335	GLN	4.0
1	A	407	LEU	4.0
1	A	317	ASP	4.0
1	A	5	VAL	4.0
1	B	86	ASP	3.9
1	A	15	THR	3.9
1	A	320	ASP	3.8
1	A	115	ILE	3.6
1	B	77	ILE	3.5
1	A	86	ASP	3.4
1	A	363	ASP	3.4
1	A	395	THR	3.4
1	B	57	GLU	3.3
1	A	89	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	352	PHE	3.2
1	B	156	GLY	3.1
1	B	418	ILE	3.1
1	B	164	HIS	3.1
1	B	12	GLY	3.1
1	A	319	ASP	3.1
1	A	351	ASP	3.0
1	B	88	GLN	3.0
1	A	331	GLU	3.0
1	A	404	GLU	3.0
1	A	78	ILE	2.9
1	A	350	LEU	2.9
1	A	322	ARG	2.9
1	A	59	LEU	2.9
1	A	378	ASN	2.9
1	A	304	GLY	2.8
1	A	303	SER	2.8
1	B	154	LEU	2.8
1	B	155	PRO	2.8
1	B	117	GLU	2.7
1	A	117	GLU	2.7
1	A	349	GLU	2.7
1	B	89	TYR	2.7
1	B	359	HIS	2.7
1	A	42	GLY	2.7
1	A	370	LEU	2.6
1	A	337	PRO	2.6
1	A	11	ILE	2.6
1	A	384	PHE	2.6
1	A	416	ASN	2.6
1	B	53	GLU	2.6
1	A	116	VAL	2.6
1	A	368	LEU	2.5
1	A	31	ILE	2.5
1	A	396	LYS	2.5
1	B	15	THR	2.5
1	B	11	ILE	2.5
1	A	403	PHE	2.5
1	A	418	ILE	2.5
1	A	34	GLN	2.5
1	A	92	CYS	2.5
1	A	4	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	78	ILE	2.4
1	B	118	SER	2.4
1	A	41	ASN	2.4
1	A	79	ALA	2.4
1	A	374	SER	2.4
1	A	85	ASN	2.4
1	A	328	ASP	2.4
1	B	47	GLU	2.4
1	A	62	GLY	2.4
1	A	316	GLY	2.3
1	A	369	ILE	2.3
1	B	265	PHE	2.3
1	B	385	ASP	2.2
1	B	402	SER	2.2
1	B	79	ALA	2.2
1	A	417	PHE	2.2
1	A	332	LEU	2.2
1	A	340	GLU	2.2
1	B	85	ASN	2.2
1	B	115	ILE	2.2
1	A	16	SER	2.1
1	B	160	GLU	2.1
1	A	342	CYS	2.1
1	A	261	VAL	2.1
1	A	327	PHE	2.1
1	A	12	GLY	2.1
1	B	349	GLU	2.1
1	A	149	CYS	2.1
1	B	149	CYS	2.1
1	A	375	GLU	2.0
1	A	365	SER	2.0
1	B	5	VAL	2.0
1	B	189	GLN	2.0
1	A	318	VAL	2.0
1	A	348	VAL	2.0
1	B	52	GLN	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 [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, 95th 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(\AA^2)	Q<0.9
2	NAD	B	500	44/44	0.92	0.24	-0.23	52,63,109,110	0
2	NAD	A	500	44/44	0.92	0.19	-0.81	64,76,90,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.