Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2021 – 11:38 PM BST

PDB ID	:	6ZTH
Title	:	Phospholipase PlaB from Legionella pneumophila
Authors	:	Diwo, M.G.; Flieger, A.; Blankenfeldt, W.
Deposited on	:	2020-07-20
Resolution	:	2.30 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
https://www.wwpdb.org/validation/2017/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:

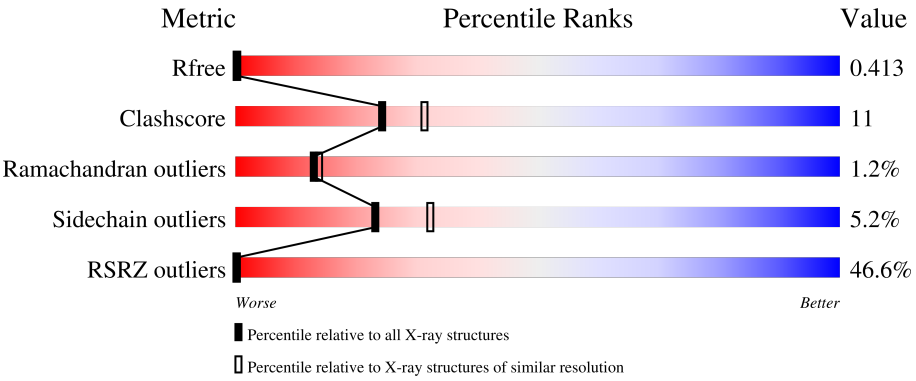
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	489	42% 72% 23%
1	B	489	43% 72% 22%
1	C	489	44% 73% 20%
1	D	489	46% 71% 23%

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
2	NAD	D	501	-	-	-	X
2	NAD	D	502	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30812 atoms, of which 14970 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 PlaB phospholipase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	Se	0	7	0
			7444	2372	3694	661	699	5	13			
1	B	470	Total	C	H	N	O	S	Se	0	1	0
			7417	2360	3683	661	695	5	13			
1	C	467	Total	C	H	N	O	S	Se	0	2	0
			7417	2358	3697	657	687	5	13			
1	D	474	Total	C	H	N	O	S	Se	1	0	0
			7431	2369	3688	658	698	5	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MSE	-	initiating methionine	UNP A0A378K488
A	-13	ALA	-	expression tag	UNP A0A378K488
A	-12	SER	-	expression tag	UNP A0A378K488
A	-11	TRP	-	expression tag	UNP A0A378K488
A	-10	SER	-	expression tag	UNP A0A378K488
A	-9	HIS	-	expression tag	UNP A0A378K488
A	-8	PRO	-	expression tag	UNP A0A378K488
A	-7	GLN	-	expression tag	UNP A0A378K488
A	-6	PHE	-	expression tag	UNP A0A378K488
A	-5	GLU	-	expression tag	UNP A0A378K488
A	-4	LYS	-	expression tag	UNP A0A378K488
A	-3	GLY	-	expression tag	UNP A0A378K488
A	-2	ALA	-	expression tag	UNP A0A378K488
A	-1	GLY	-	expression tag	UNP A0A378K488
A	0	THR	-	expression tag	UNP A0A378K488
A	203	ASN	ASP	conflict	UNP A0A378K488
B	-14	MSE	-	initiating methionine	UNP A0A378K488
B	-13	ALA	-	expression tag	UNP A0A378K488
B	-12	SER	-	expression tag	UNP A0A378K488
B	-11	TRP	-	expression tag	UNP A0A378K488
B	-10	SER	-	expression tag	UNP A0A378K488

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP A0A378K488
B	-8	PRO	-	expression tag	UNP A0A378K488
B	-7	GLN	-	expression tag	UNP A0A378K488
B	-6	PHE	-	expression tag	UNP A0A378K488
B	-5	GLU	-	expression tag	UNP A0A378K488
B	-4	LYS	-	expression tag	UNP A0A378K488
B	-3	GLY	-	expression tag	UNP A0A378K488
B	-2	ALA	-	expression tag	UNP A0A378K488
B	-1	GLY	-	expression tag	UNP A0A378K488
B	0	THR	-	expression tag	UNP A0A378K488
B	203	ASN	ASP	conflict	UNP A0A378K488
C	-14	MSE	-	initiating methionine	UNP A0A378K488
C	-13	ALA	-	expression tag	UNP A0A378K488
C	-12	SER	-	expression tag	UNP A0A378K488
C	-11	TRP	-	expression tag	UNP A0A378K488
C	-10	SER	-	expression tag	UNP A0A378K488
C	-9	HIS	-	expression tag	UNP A0A378K488
C	-8	PRO	-	expression tag	UNP A0A378K488
C	-7	GLN	-	expression tag	UNP A0A378K488
C	-6	PHE	-	expression tag	UNP A0A378K488
C	-5	GLU	-	expression tag	UNP A0A378K488
C	-4	LYS	-	expression tag	UNP A0A378K488
C	-3	GLY	-	expression tag	UNP A0A378K488
C	-2	ALA	-	expression tag	UNP A0A378K488
C	-1	GLY	-	expression tag	UNP A0A378K488
C	0	THR	-	expression tag	UNP A0A378K488
C	203	ASN	ASP	conflict	UNP A0A378K488
D	-14	MSE	-	initiating methionine	UNP A0A378K488
D	-13	ALA	-	expression tag	UNP A0A378K488
D	-12	SER	-	expression tag	UNP A0A378K488
D	-11	TRP	-	expression tag	UNP A0A378K488
D	-10	SER	-	expression tag	UNP A0A378K488
D	-9	HIS	-	expression tag	UNP A0A378K488
D	-8	PRO	-	expression tag	UNP A0A378K488
D	-7	GLN	-	expression tag	UNP A0A378K488
D	-6	PHE	-	expression tag	UNP A0A378K488
D	-5	GLU	-	expression tag	UNP A0A378K488
D	-4	LYS	-	expression tag	UNP A0A378K488
D	-3	GLY	-	expression tag	UNP A0A378K488
D	-2	ALA	-	expression tag	UNP A0A378K488
D	-1	GLY	-	expression tag	UNP A0A378K488
D	0	THR	-	expression tag	UNP A0A378K488

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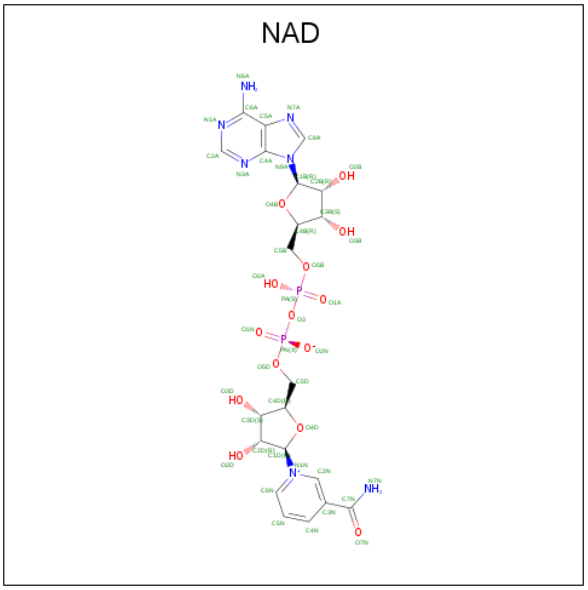
Chain	Residue	Modelled	Actual	Comment	Reference
D	203	ASN	ASP	conflict	UNP A0A378K488

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is water.

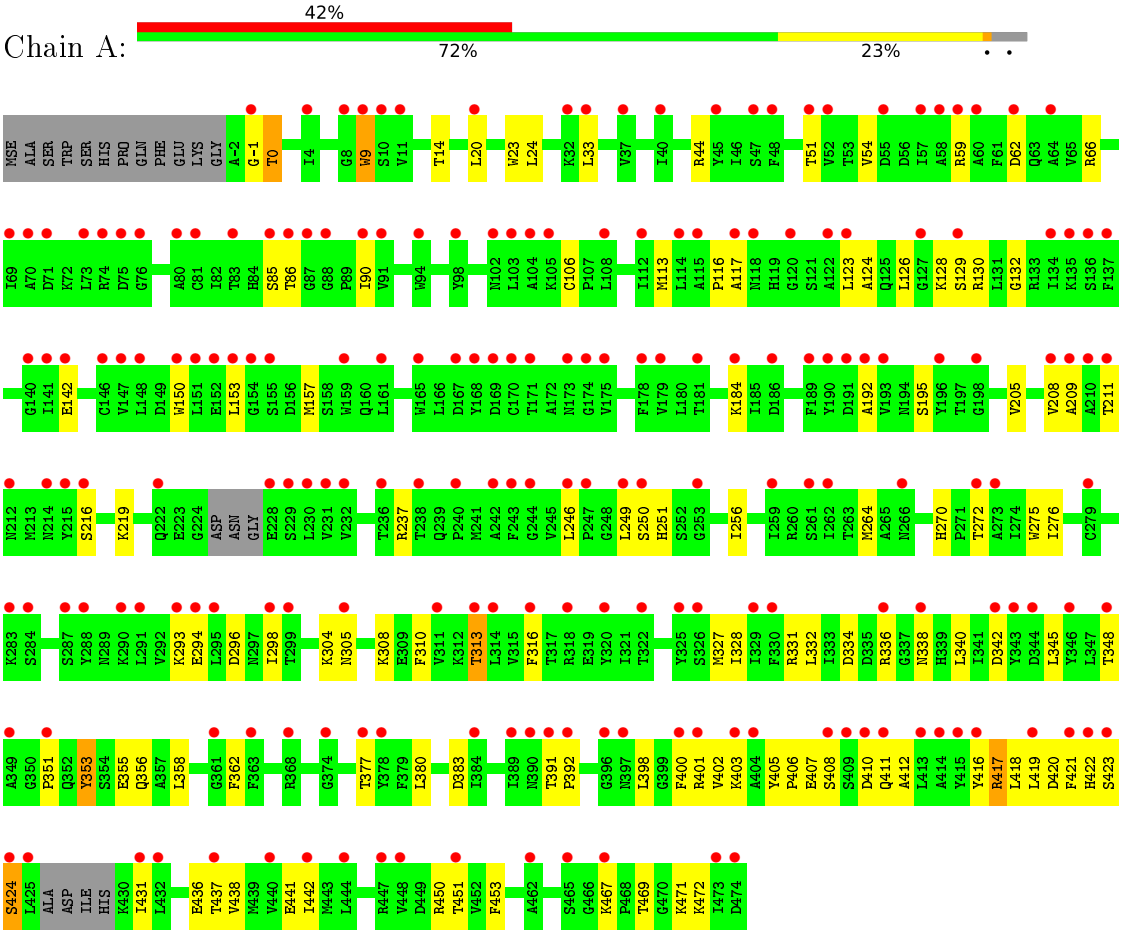
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	131	Total O 131 131	0	0
3	B	125	Total O 125 125	0	0
3	C	148	Total O 148 148	0	0
3	D	139	Total O 139 139	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

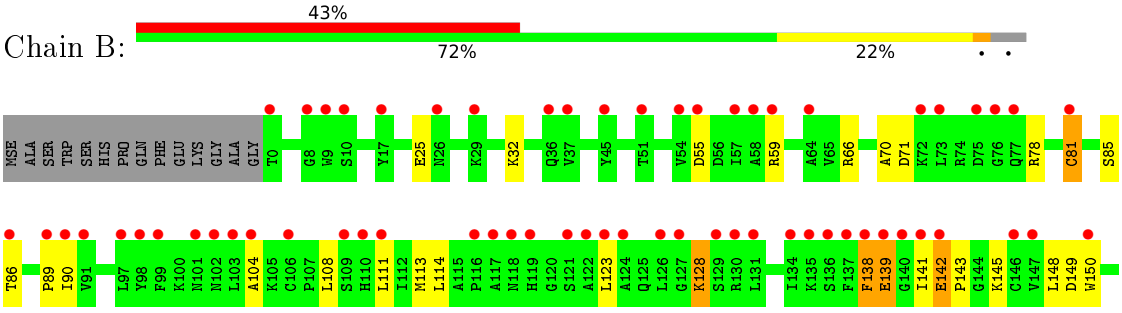
- Molecule 1: PlaB phospholipase

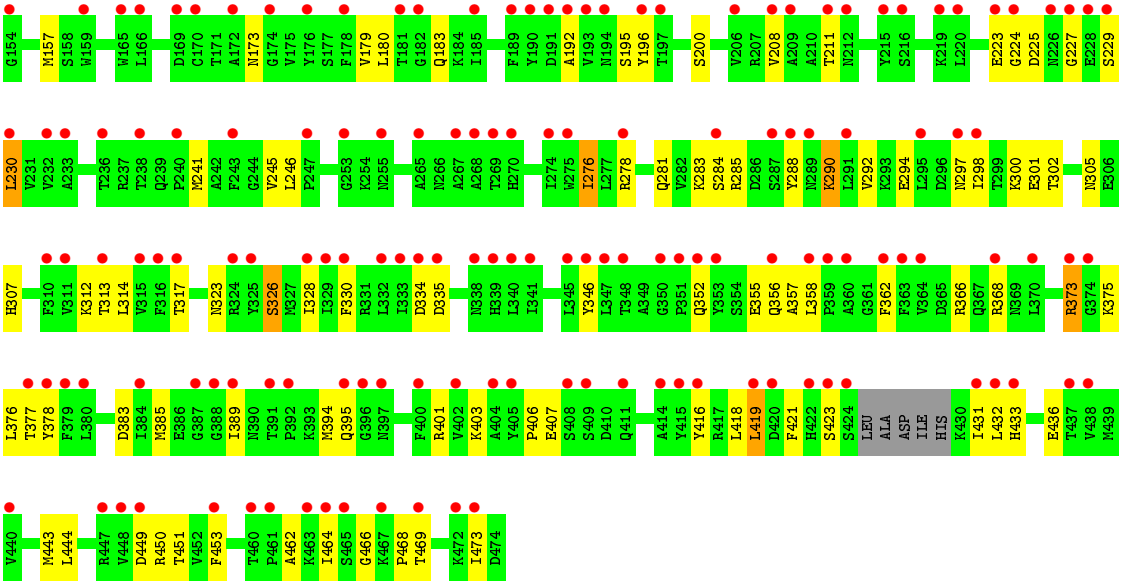
Chain A:



- Molecule 1: PlaB phospholipase

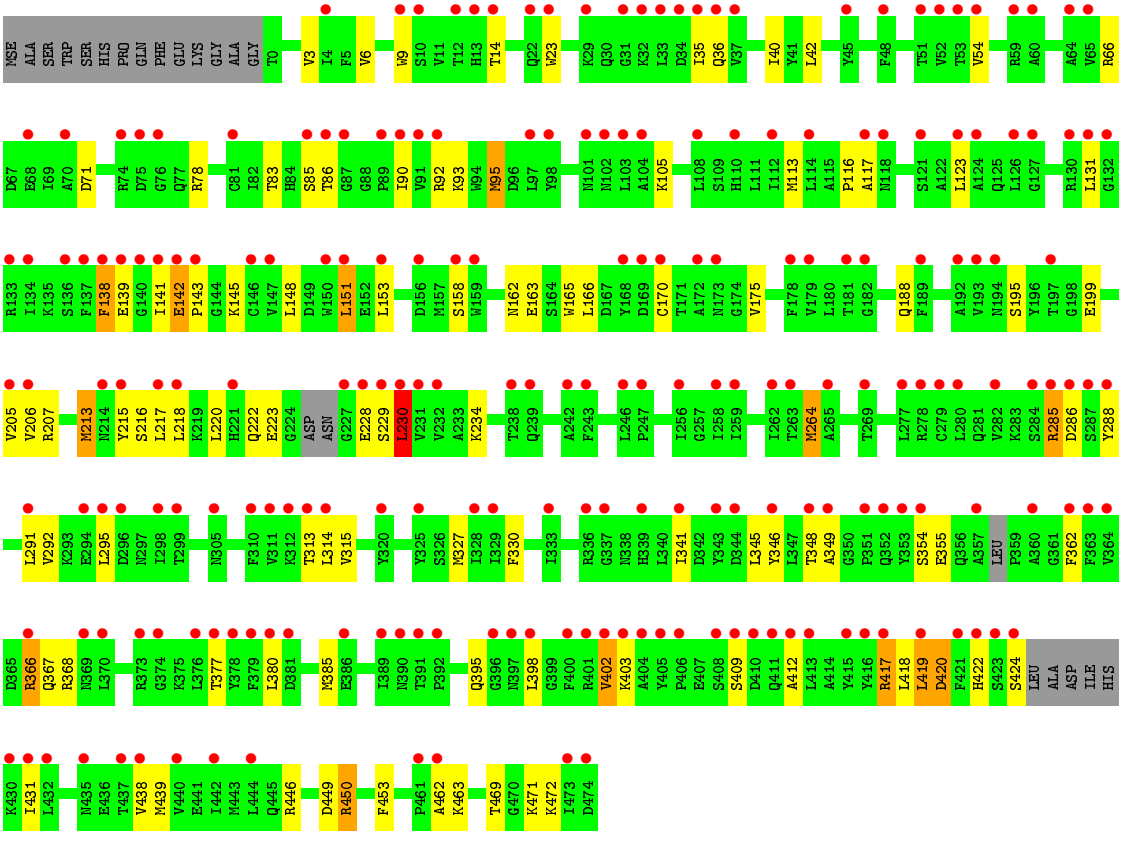
Chain B:





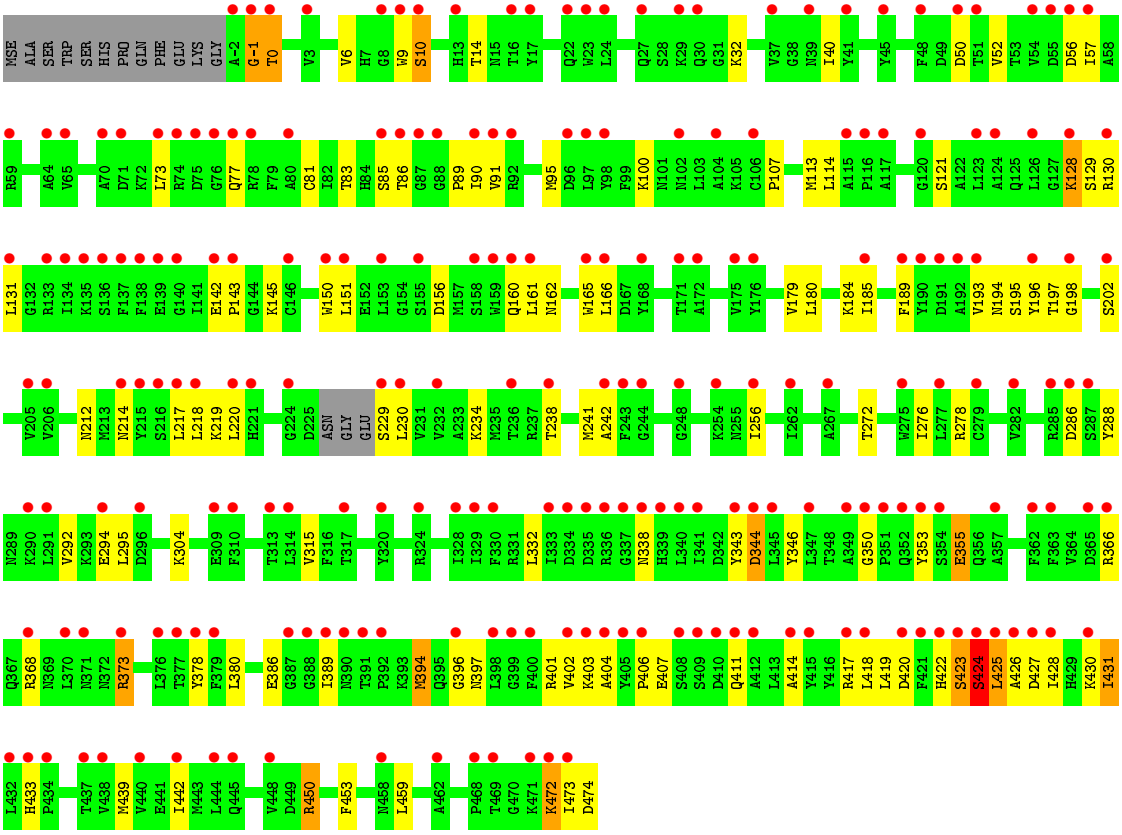
• Molecule 1: PlaB phospholipase

Chain C:



• Molecule 1: PlaB phospholipase

Chain D:


MSE ALA SER TRP SER HIS PRO GLN PHE GLU LYS GLY A-2 G-1 T0 V3 V6 H7 G8 W9 S10 H13 T14 N15 T16 Y17 Q22 W23 L24 Q27 S28 K29 Q30 G31 K32 V37 G38 N39 I40 Y41 Y45 F48 D49 D50 T51 V52 T53 V54 D55 D56 I57 A58
R59 A64 V65 A70 D71 K72 L73 R74 D75 G76 Q77 R78 F79 A80 C81 I82 T83 H84 S85 T86 G87 G88 P89 I90 V91 R92 M95 D96 L97 Y98 F99 K100 N101 N102 L103 A104 K105 C106 P107 M113 L114 A115 P116 A117 G120 S121 A122 L123 A124 Q125 L126 G127 K128 S129 R130
L131 G132 R133 I134 K135 S136 F137 F138 E139 G140 I141 E142 P143 G144 K145 C146 W150 L151 E152 L153 G154 S155 D156 M157 S158 W159 Q160 L161 N162 W165 L166 D167 Y168 T171 A172 V175 Y176 V179 L180 K184 I185 F189 Y190 D191 A192 V193 N194 S195 Y196 T197 G198 S202
V205 V206 N212 N213 N214 Y215 S216 L217 L218 K219 L220 H221 G224 D225 ASN GLY GLU S229 L230 V231 V232 A233 K234 M235 T236 R237 T238 M241 A242 F243 G244 G248 K254 N255 I256 I262 A267 T272 W275 I276 L277 R278 C279 V282 R285 D286 S287 Y288
N289 K290 L291 V292 K293 E294 L295 D296 K304 E309 F310 T313 L314 V315 F316 T317 Y320 R324 I328 I329 F330 R331 L332 I333 D334 D335 R336 G337 N338 H339 L340 I341 D342 Y343 D344 L345 Y346 L347 T348 A349 G350 P351 Q352 Y353 S354 E355 Q356 A357 F362 F363 V364 D365 R366
Q367 R368 N369 L370 N371 N372 R373 L376 T377 Y378 F379 L380 E386 G387 G388 I389 N390 T391 P392 K393 N394 Q395 G396 N397 L398 G399 F400 R401 V402 K403 A404 Y405 P406 E407 S408 S409 D410 Q411 A412 L413 A414 Y415 Y416 R417 L418 L419 D420 F421 H422 S423 S424 L425 A426 D427 I428 H429 K430 I431
L432 H433 P434 T437 V438 M439 V440 E441 T442 M443 L444 Q445 V448 D449 R450 F463 M458 L459 A462 P468 T469 G470 K471 K472 I473 D474

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.81Å 170.58Å 93.48Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	49.24 – 2.30 49.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.24-2.30) 99.7 (49.24-2.30)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_3922	Depositor
R, R_{free}	0.364 , 0.413 0.363 , 0.413	Depositor DCC
R_{free} test set	5247 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	30812	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7605e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/3858	0.47	0/5192
1	B	0.25	0/3800	0.47	0/5115
1	C	0.26	0/3788	0.45	0/5094
1	D	0.49	2/3807 (0.1%)	0.47	1/5130 (0.0%)
All	All	0.33	2/15253 (0.0%)	0.47	1/20531 (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
1	C	0	1
1	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	424	SER	CB-OG	-23.99	1.11	1.42
1	D	431	ILE	CG1-CD1	-8.62	0.91	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	431	ILE	CB-CG1-CD1	6.52	132.16	113.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	SER	Peptide
1	C	230	LEU	Peptide
1	D	424	SER	Peptide

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	3750	3694	3662	79	0
1	B	3734	3683	3700	77	0
1	C	3720	3697	3701	75	0
1	D	3743	3688	3689	106	0
2	A	88	52	51	6	0
2	B	88	52	49	1	0
2	C	88	52	50	4	0
2	D	88	52	52	12	0
3	A	131	0	0	15	0
3	B	125	0	0	11	1
3	C	148	0	0	7	0
3	D	139	0	0	11	1
All	All	15842	14970	14954	333	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (333) 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:D:431:ILE:CD1	1:D:431:ILE:CB	2.24	1.14
1:D:431:ILE:CG1	1:D:431:ILE:HD11	1.53	1.05
1:D:431:ILE:CG1	1:D:431:ILE:HD12	1.53	1.02
1:D:431:ILE:CG1	1:D:431:ILE:HD13	1.53	1.02
1:D:431:ILE:CD1	1:D:431:ILE:HG13	1.48	0.99
1:D:431:ILE:CD1	1:D:431:ILE:HG12	1.48	0.98
1:B:352:GLN:NE2	3:B:702:HOH:O	1.98	0.94
1:D:431:ILE:CD1	1:D:431:ILE:CG1	0.91	0.90
1:B:297:ASN:OD1	1:B:300:LYS:NZ	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLN:O	1:B:283:LYS:NZ	2.06	0.88
1:A:142:GLU:OE2	3:A:601:HOH:O	1.94	0.85
1:A:62:ASP:OD2	1:A:66:ARG:NH1	2.11	0.84
1:B:183:GLN:OE1	3:B:701:HOH:O	1.96	0.82
1:D:286:ASP:OD2	3:D:601:HOH:O	1.99	0.81
1:D:472:LYS:NZ	3:D:602:HOH:O	2.16	0.79
1:B:375:LYS:NZ	3:B:706:HOH:O	2.16	0.78
1:A:272:THR:HG22	1:A:276:ILE:HD12	1.65	0.78
1:C:188:GLN:O	3:C:601:HOH:O	2.01	0.78
1:B:421:PHE:HE1	1:B:431:ILE:HD11	1.48	0.77
1:B:449:ASP:OD1	1:B:450:ARG:N	2.17	0.77
1:D:474:ASP:OD1	3:D:602:HOH:O	2.04	0.76
1:B:431:ILE:O	3:B:703:HOH:O	2.05	0.75
1:C:153:LEU:HD22	1:C:327:MSE:HE1	1.66	0.75
1:D:197:THR:O	3:D:603:HOH:O	2.04	0.75
1:A:451:THR:HG23	1:A:469:THR:HG23	1.68	0.75
1:C:35:ILE:HG21	1:C:40:ILE:HD11	1.69	0.74
1:D:417:ARG:NH2	3:D:611:HOH:O	2.21	0.74
1:B:401:ARG:NH1	3:B:708:HOH:O	2.19	0.74
1:C:431:ILE:O	1:C:438:VAL:HG11	1.88	0.74
1:A:348:THR:O	1:A:398:LEU:HD12	1.88	0.73
1:B:383:ASP:OD2	3:B:705:HOH:O	2.06	0.73
1:C:117:ALA:HB3	1:C:151:LEU:HD21	1.69	0.73
1:B:196:TYR:O	3:B:704:HOH:O	2.05	0.73
1:D:424:SER:O	1:D:426:ALA:N	2.22	0.72
1:C:14:THR:HG21	1:C:42:LEU:HD13	1.71	0.72
1:A:59:ARG:NH1	3:A:608:HOH:O	2.22	0.71
1:B:368:ARG:NH2	1:B:373:ARG:O	2.23	0.71
1:C:420:ASP:N	3:C:606:HOH:O	2.23	0.71
1:D:368:ARG:NH1	1:D:373:ARG:O	2.24	0.71
1:D:100:LYS:O	3:D:605:HOH:O	2.09	0.70
1:B:104:ALA:HB2	1:B:173:ASN:OD1	1.90	0.70
1:D:424:SER:OG	1:D:431:ILE:HD13	1.91	0.69
1:B:301:GLU:OE1	1:B:305:ASN:ND2	2.26	0.68
1:A:437:THR:O	3:A:602:HOH:O	2.11	0.68
1:A:408:SER:OG	1:A:417:ARG:NH1	2.27	0.67
1:D:129:SER:OG	3:D:606:HOH:O	2.12	0.67
1:A:128:LYS:HZ2	1:A:142:GLU:HB2	1.59	0.67
1:C:23:TRP:HA	1:C:264:MSE:HE1	1.77	0.67
1:B:143:PRO:HG2	1:B:148:LEU:HD11	1.77	0.67
1:B:431:ILE:HG22	1:B:432:LEU:HG	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:OD1	3:A:603:HOH:O	2.13	0.66
1:C:6:VAL:HB	1:C:83:THR:HG22	1.78	0.66
1:A:124:ALA:O	3:A:604:HOH:O	2.14	0.65
1:D:52:VAL:HG11	1:D:57:ILE:HD11	1.79	0.65
1:B:355:GLU:OE2	1:B:356:GLN:NE2	2.30	0.65
1:D:420:ASP:O	3:D:609:HOH:O	2.15	0.65
1:A:410:ASP:OD1	3:A:605:HOH:O	2.15	0.65
1:D:423:SER:OG	1:D:424:SER:N	2.30	0.65
1:B:378:TYR:OH	2:D:502:NAD:N6A	2.21	0.65
1:C:395:GLN:O	3:C:602:HOH:O	2.13	0.64
2:D:501:NAD:O1A	2:D:502:NAD:O3D	2.14	0.64
1:B:328:ILE:HG21	1:B:330:PHE:CZ	2.33	0.64
1:D:162:ASN:OD1	3:D:607:HOH:O	2.15	0.64
1:D:52:VAL:CG1	1:D:57:ILE:HD11	2.28	0.64
1:D:344:ASP:OD2	1:D:403:LYS:NZ	2.31	0.64
1:A:327:MSE:HB3	1:A:437:THR:HG22	1.80	0.63
1:A:451:THR:HG21	1:A:467:LYS:O	1.97	0.63
1:B:358:LEU:HD23	1:B:362:PHE:CD2	2.34	0.63
1:A:332:LEU:HG	1:A:340:LEU:HD12	1.81	0.62
1:A:356:GLN:NE2	3:A:614:HOH:O	2.32	0.62
1:D:6:VAL:CG1	1:D:83:THR:HG22	2.30	0.62
1:C:35:ILE:HG21	1:C:40:ILE:CD1	2.30	0.61
1:A:348:THR:HB	1:A:353:TYR:HB3	1.82	0.61
1:D:407:GLU:OE2	3:D:610:HOH:O	2.16	0.61
1:A:451:THR:CG2	1:A:469:THR:HG23	2.31	0.61
1:B:208:VAL:O	1:B:211:THR:OG1	2.14	0.61
1:C:450:ARG:NE	1:C:472:LYS:O	2.34	0.61
1:C:42:LEU:HD11	1:D:459:LEU:HA	1.82	0.60
1:A:411:GLN:OE1	3:A:605:HOH:O	2.15	0.60
1:A:421:PHE:HE2	1:A:431:ILE:HD11	1.67	0.60
1:A:313:THR:HG23	1:A:316:PHE:H	1.67	0.60
1:C:380:LEU:HD13	1:C:385:MSE:HE2	1.82	0.60
1:A:128:LYS:NZ	1:A:142:GLU:HB2	2.15	0.59
1:D:89:PRO:HB3	1:D:150:TRP:CH2	2.36	0.59
1:C:341:ILE:O	1:C:368:ARG:NH1	2.36	0.59
1:A:331:ARG:NH2	3:A:615:HOH:O	2.33	0.59
1:B:223:GLU:N	1:B:230:LEU:O	2.35	0.59
1:D:195:SER:OG	2:D:502:NAD:H4N	2.02	0.59
1:A:250:SER:OG	1:A:251:HIS:N	2.35	0.59
1:A:294:GLU:OE2	3:A:606:HOH:O	2.17	0.59
1:C:71:ASP:N	1:C:71:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ILE:O	1:B:302:THR:HG23	2.02	0.58
1:B:451:THR:OG1	1:B:469:THR:HG23	2.03	0.58
1:C:95:MSE:HE3	1:C:165:TRP:CZ2	2.38	0.58
1:D:128:LYS:HD2	1:D:142:GLU:HB3	1.86	0.58
1:C:66:ARG:NH2	3:C:613:HOH:O	2.37	0.57
1:A:209:ALA:O	1:A:437:THR:HG23	2.03	0.57
1:D:450:ARG:NE	1:D:472:LYS:O	2.37	0.57
1:D:6:VAL:HG12	1:D:83:THR:HG22	1.86	0.57
1:C:195:SER:OG	2:C:501:NAD:H4N	2.04	0.57
1:C:207:ARG:NH1	1:C:327:MSE:HE3	2.19	0.57
1:C:207:ARG:HH11	1:C:327:MSE:HE3	1.69	0.56
1:C:213:MSE:O	3:C:604:HOH:O	2.17	0.56
1:C:327:MSE:HE2	1:C:377:THR:CG2	2.35	0.56
1:A:391:THR:HB	1:A:392:PRO:CD	2.35	0.56
1:D:450:ARG:HG3	1:D:473:ILE:HG22	1.87	0.56
1:A:-1:GLY:O	1:A:0:THR:CB	2.54	0.56
1:C:450:ARG:HE	1:C:472:LYS:C	2.09	0.56
1:D:355:GLU:OE2	1:D:401:ARG:NH1	2.39	0.55
1:B:335:ASP:OD1	1:B:335:ASP:N	2.40	0.55
1:A:113:MSE:HB3	1:A:116:PRO:HG3	1.88	0.55
1:A:419:LEU:HD23	1:A:420:ASP:N	2.22	0.55
1:C:123:LEU:HB3	1:C:131:LEU:HD21	1.87	0.55
1:A:184:LYS:HD3	1:A:256:ILE:HD13	1.89	0.55
1:B:114:LEU:HD21	1:B:276:ILE:HD11	1.89	0.55
1:D:332:LEU:HD13	1:D:343:TYR:CZ	2.42	0.55
1:C:85:SER:OG	1:C:86:THR:N	2.40	0.55
1:A:275:TRP:CZ2	1:A:298:ILE:HG13	2.41	0.54
1:A:342:ASP:OD2	1:A:405:TYR:HB2	2.08	0.54
1:D:218:LEU:HD21	1:D:220:LEU:HD21	1.89	0.54
1:D:272:THR:HG22	1:D:276:ILE:HD12	1.89	0.54
1:D:423:SER:O	1:D:424:SER:HB2	2.07	0.54
1:C:222:GLN:HB2	1:C:419:LEU:HD12	1.89	0.54
1:D:402:VAL:HG12	1:D:419:LEU:HB3	1.90	0.53
1:B:436:GLU:OE1	3:B:707:HOH:O	2.18	0.53
1:B:111:LEU:HD21	1:B:113:MSE:HE2	1.91	0.53
1:C:409:SER:OG	1:C:412:ALA:N	2.41	0.53
1:A:450:ARG:NH2	3:A:625:HOH:O	2.39	0.53
1:B:418:LEU:HD21	3:B:722:HOH:O	2.08	0.53
1:C:417:ARG:NH2	1:C:418:LEU:HB3	2.23	0.53
1:B:85:SER:OG	1:B:86:THR:N	2.42	0.53
1:C:95:MSE:HE3	1:C:165:TRP:HZ2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:HD2	1:A:418:LEU:HD11	1.91	0.52
1:C:213:MSE:HE3	1:C:215:TYR:CE1	2.44	0.52
1:D:420:ASP:OD1	1:D:422:HIS:NE2	2.41	0.52
1:D:353:TYR:CZ	1:D:422:HIS:HB3	2.43	0.52
1:A:421:PHE:CE2	1:A:431:ILE:HD11	2.45	0.52
1:D:278:ARG:NH2	1:D:294:GLU:OE1	2.42	0.52
1:D:-1:GLY:O	1:D:0:THR:CB	2.57	0.52
1:B:326:SER:HB3	1:B:432:LEU:HD22	1.92	0.51
1:C:54:VAL:HG13	1:C:90:ILE:HD13	1.92	0.51
1:D:196:TYR:CE1	2:D:502:NAD:C2N	2.94	0.51
1:A:391:THR:HB	1:A:392:PRO:HD2	1.93	0.51
1:B:394:MSE:HE2	1:D:315:VAL:HG12	1.93	0.51
1:C:313:THR:HG22	1:C:315:VAL:H	1.76	0.51
1:B:385:MSE:O	1:B:389:ILE:HD13	2.11	0.51
1:C:218:LEU:HD21	1:C:220:LEU:HG	1.93	0.51
1:A:195:SER:OG	2:A:501:NAD:H4N	2.11	0.50
1:D:406:PRO:HG2	1:D:414:ALA:O	2.12	0.50
1:A:128:LYS:HZ2	1:A:142:GLU:CB	2.24	0.50
1:C:93:LYS:NZ	3:C:608:HOH:O	2.29	0.50
1:C:217:LEU:HD13	1:C:439:MSE:HB2	1.93	0.50
1:C:349:ALA:O	1:C:354:SER:N	2.44	0.49
1:B:421:PHE:CZ	1:B:423:SER:HB2	2.47	0.49
1:A:24:LEU:HD12	1:A:33:LEU:HD13	1.94	0.49
1:B:195:SER:HB2	2:D:501:NAD:H4N	1.94	0.49
1:C:162:ASN:CB	1:C:439:MSE:HE1	2.43	0.49
1:C:348:THR:O	1:C:398:LEU:HD12	2.12	0.49
1:D:73:LEU:HD23	1:D:77:GLN:O	2.13	0.49
1:C:228:GLU:O	1:C:229:SER:HB3	2.13	0.49
1:A:150:TRP:HA	1:A:157:MSE:HE3	1.95	0.49
1:D:242:ALA:HB1	1:D:295:LEU:HD12	1.94	0.49
1:D:332:LEU:CD2	1:D:402:VAL:HG21	2.43	0.48
1:A:237:ARG:NH2	1:A:436:GLU:OE2	2.46	0.48
1:D:344:ASP:HB2	1:D:403:LYS:NZ	2.27	0.48
1:D:91:VAL:O	1:D:95:MSE:HG3	2.13	0.48
1:A:331:ARG:NH1	3:A:632:HOH:O	2.46	0.48
1:A:403:LYS:NZ	1:A:407:GLU:OE1	2.46	0.48
1:A:345:LEU:HD12	1:A:402:VAL:HG12	1.96	0.48
1:B:358:LEU:HD23	1:B:362:PHE:CE2	2.48	0.48
1:D:189:PHE:CD1	1:D:189:PHE:N	2.81	0.48
1:D:344:ASP:HA	2:D:501:NAD:H2A	1.95	0.48
2:A:502:NAD:O3B	1:C:366:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:GLU:HA	1:D:425:LEU:HD23	1.96	0.48
1:D:431:ILE:HD12	1:D:431:ILE:N	2.29	0.48
1:B:278:ARG:HD2	1:B:281:GLN:NE2	2.29	0.48
1:B:335:ASP:HB3	1:B:443:MSE:HE3	1.96	0.48
1:C:446:ARG:NH1	1:D:56:ASP:OD2	2.46	0.48
1:D:229:SER:C	1:D:230:LEU:HD23	2.35	0.48
1:B:149:ASP:HB3	1:B:157:MSE:HE1	1.96	0.47
1:C:450:ARG:HB2	1:C:469:THR:HG21	1.96	0.47
1:A:123:LEU:HD22	1:A:126:LEU:HD12	1.96	0.47
1:B:224:GLY:O	1:B:227:GLY:N	2.46	0.47
1:C:170:CYS:HB3	1:C:175:VAL:HB	1.95	0.47
1:D:344:ASP:HB2	1:D:403:LYS:HZ2	1.78	0.47
1:B:368:ARG:HD3	2:D:502:NAD:O4B	2.14	0.47
1:B:138:PHE:O	1:B:139:GLU:CB	2.62	0.47
1:C:330:PHE:CE1	1:C:345:LEU:HD21	2.49	0.47
1:B:290:LYS:HD3	1:B:294:GLU:OE1	2.15	0.47
1:A:355:GLU:O	2:C:502:NAD:N6A	2.44	0.47
1:C:54:VAL:HG13	1:C:90:ILE:CD1	2.44	0.47
1:C:123:LEU:HD12	1:C:205:VAL:HG13	1.97	0.47
1:D:220:LEU:HD12	1:D:442:ILE:HD13	1.96	0.47
1:D:366:ARG:NH2	2:D:501:NAD:O1N	2.47	0.47
1:A:24:LEU:HD12	1:A:33:LEU:CD1	2.45	0.47
1:D:85:SER:OG	1:D:86:THR:N	2.47	0.47
2:A:501:NAD:O1A	2:C:501:NAD:O3D	2.24	0.47
1:B:401:ARG:NH1	3:B:722:HOH:O	2.48	0.46
1:B:128:LYS:HD2	1:B:141:ILE:HG23	1.96	0.46
1:C:143:PRO:HG2	1:C:148:LEU:HD11	1.97	0.46
1:C:420:ASP:OD1	1:C:422:HIS:CE1	2.68	0.46
1:C:92:ARG:NH2	1:C:162:ASN:OD1	2.48	0.46
1:C:450:ARG:NH2	1:C:472:LYS:O	2.48	0.46
1:C:213:MSE:HE3	1:C:215:TYR:HE1	1.81	0.46
1:C:449:ASP:OD1	1:C:469:THR:HG22	2.15	0.46
1:D:9:TRP:HZ2	1:D:131:LEU:HD11	1.81	0.46
1:D:50:ASP:OD1	1:D:145:LYS:N	2.42	0.46
1:D:212:ASN:HD21	1:D:214:ASN:HB2	1.79	0.46
1:D:389:ILE:HA	1:D:394:MSE:HG2	1.97	0.46
1:C:3:VAL:HB	1:C:40:ILE:HD12	1.97	0.46
1:A:417:ARG:NH2	1:A:418:LEU:HD13	2.31	0.46
1:B:328:ILE:O	1:B:377:THR:HA	2.16	0.46
1:A:358:LEU:HD23	1:A:362:PHE:CD2	2.50	0.46
1:A:402:VAL:HG22	1:A:419:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:O	3:A:607:HOH:O	2.21	0.46
1:B:288:TYR:O	1:B:292:VAL:HG23	2.15	0.46
1:D:288:TYR:O	1:D:292:VAL:HG13	2.16	0.46
1:C:462:ALA:N	1:D:14:THR:OG1	2.44	0.45
1:D:160:GLN:OE1	1:D:160:GLN:HA	2.16	0.45
1:D:350:GLY:HA3	1:D:394:MSE:HE3	1.97	0.45
2:C:501:NAD:O5D	2:C:501:NAD:H2N	2.17	0.45
1:B:313:THR:HG22	1:B:314:LEU:N	2.32	0.45
1:D:401:ARG:HG3	1:D:418:LEU:HD11	1.98	0.45
1:B:180:LEU:HD22	1:B:246:LEU:HD21	1.97	0.45
1:D:166:LEU:HA	1:D:238:THR:HG22	1.99	0.45
1:B:86:THR:HG22	1:B:90:ILE:HG13	1.98	0.45
1:B:89:PRO:HB3	1:B:150:TRP:CH2	2.52	0.45
1:D:73:LEU:HD22	1:D:107:PRO:HB2	1.99	0.45
1:D:166:LEU:HD21	1:D:217:LEU:HB3	1.98	0.45
1:A:328:ILE:HD11	1:A:380:LEU:HD11	1.99	0.45
2:A:501:NAD:H2N	2:A:501:NAD:O5D	2.16	0.45
1:D:57:ILE:HG21	1:D:90:ILE:HD13	1.99	0.45
1:D:114:LEU:O	1:D:180:LEU:O	2.34	0.44
1:D:131:LEU:HD23	1:D:143:PRO:HG3	1.98	0.44
1:B:334:ASP:OD2	1:B:416:TYR:OH	2.30	0.44
1:D:156:ASP:O	1:D:160:GLN:HG2	2.17	0.44
1:A:85:SER:OG	1:A:86:THR:N	2.50	0.44
1:A:153:LEU:HD13	1:A:377:THR:HG21	2.00	0.44
1:B:355:GLU:O	2:B:602:NAD:N6A	2.47	0.44
1:D:9:TRP:CE3	1:D:143:PRO:HB3	2.52	0.44
1:D:130:ARG:NH2	1:D:194:ASN:OD1	2.46	0.44
1:C:113:MSE:HB3	1:C:116:PRO:HG3	2.00	0.44
1:D:131:LEU:CD2	1:D:143:PRO:HG3	2.47	0.44
1:D:366:ARG:NE	2:D:501:NAD:O2A	2.49	0.44
1:A:23:TRP:HA	1:A:264:MSE:HE1	1.99	0.44
1:A:219:LYS:O	1:A:219:LYS:HG3	2.18	0.44
1:C:288:TYR:O	1:C:292:VAL:HG23	2.17	0.44
1:D:95:MSE:SE	1:D:165:TRP:HH2	2.50	0.44
2:D:502:NAD:O5D	2:D:502:NAD:H2N	2.17	0.44
1:A:334:ASP:OD2	1:A:416:TYR:OH	2.34	0.44
1:B:245:VAL:O	1:B:302:THR:HG21	2.17	0.44
1:C:117:ALA:CB	1:C:151:LEU:HD21	2.43	0.44
1:B:128:LYS:CD	1:B:141:ILE:HG23	2.48	0.44
1:C:142:GLU:HB2	1:C:143:PRO:HD3	1.99	0.44
1:D:217:LEU:C	1:D:217:LEU:HD13	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:MSE:HE3	1:D:179:VAL:HG22	1.99	0.44
1:A:192:ALA:HB3	1:C:346:TYR:HE1	1.82	0.43
1:A:270:HIS:HD2	1:A:272:THR:H	1.64	0.43
1:B:55:ASP:O	1:B:59:ARG:HG3	2.18	0.43
1:B:179:VAL:HG23	1:B:241:MSE:SE	2.68	0.43
1:C:345:LEU:HD12	1:C:402:VAL:HG12	1.99	0.43
1:A:20:LEU:HD21	1:A:276:ILE:HD13	2.00	0.43
1:A:401:ARG:NH1	3:A:634:HOH:O	2.50	0.43
1:B:419:LEU:HD13	1:B:444:LEU:CD2	2.48	0.43
1:B:450:ARG:HG3	1:B:473:ILE:HG22	1.99	0.43
1:C:145:LYS:NZ	3:C:603:HOH:O	2.17	0.43
1:D:9:TRP:CE3	1:D:10:SER:N	2.87	0.43
1:D:424:SER:HB3	1:D:425:LEU:H	1.50	0.43
1:B:81:CYS:HB2	1:B:108:LEU:HD11	2.00	0.43
1:C:380:LEU:HD13	1:C:385:MSE:CE	2.48	0.43
1:A:362:PHE:HD2	1:A:380:LEU:HD22	1.83	0.43
1:B:362:PHE:HB2	1:B:385:MSE:HG3	2.00	0.43
1:C:92:ARG:HA	1:C:95:MSE:HE2	2.01	0.43
1:A:345:LEU:CD1	1:A:402:VAL:HG12	2.48	0.42
1:D:185:ILE:HD12	1:D:198:GLY:HA2	2.01	0.42
1:D:161:LEU:HD11	1:D:165:TRP:HE1	1.84	0.42
1:D:366:ARG:NE	2:D:501:NAD:H8A	2.35	0.42
1:A:419:LEU:HD13	1:A:442:ILE:HG21	2.02	0.42
1:A:246:LEU:HB2	1:A:249:LEU:HD12	2.02	0.42
1:A:313:THR:HG23	1:A:316:PHE:N	2.32	0.42
1:A:362:PHE:CD2	1:A:380:LEU:HD22	2.54	0.42
1:A:400:PHE:CZ	1:A:431:ILE:HD13	2.54	0.42
1:C:162:ASN:HB2	1:C:439:MSE:HE1	2.01	0.42
1:D:353:TYR:CE2	1:D:397:ASN:HB3	2.55	0.42
1:D:426:ALA:HB1	1:D:428:ILE:HD12	2.02	0.42
1:A:14:THR:HG1	1:B:462:ALA:H	1.63	0.42
1:B:326:SER:OG	1:B:433:HIS:O	2.37	0.42
1:A:44:ARG:HB2	1:B:464:ILE:HG23	2.00	0.42
1:B:71:ASP:OD1	1:B:71:ASP:N	2.52	0.42
1:D:128:LYS:CD	1:D:142:GLU:HB3	2.48	0.42
1:A:132:GLY:HA3	1:A:142:GLU:HG2	2.02	0.42
1:B:376:LEU:HD21	2:D:502:NAD:C5A	2.50	0.42
1:D:217:LEU:HD11	1:D:219:LYS:HE2	2.01	0.42
1:D:422:HIS:O	1:D:423:SER:HB2	2.19	0.42
1:D:234:LYS:N	3:D:632:HOH:O	2.52	0.42
1:A:208:VAL:O	1:A:211:THR:OG1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ALA:HB3	1:D:346:TYR:CE2	2.55	0.42
1:D:332:LEU:HD21	1:D:402:VAL:HG21	2.01	0.42
1:C:163:GLU:HA	1:C:166:LEU:HD12	2.01	0.41
1:A:420:ASP:HB3	1:A:422:HIS:CE1	2.55	0.41
1:C:314:LEU:HD12	1:C:314:LEU:H	1.85	0.41
1:A:54:VAL:HG13	1:A:90:ILE:HD13	2.01	0.41
2:A:502:NAD:N6A	1:C:355:GLU:O	2.54	0.41
1:C:291:LEU:HD13	1:C:295:LEU:HG	2.02	0.41
2:A:502:NAD:H5N	3:A:635:HOH:O	2.21	0.41
1:B:312:LYS:HE2	1:B:317:THR:HG23	2.02	0.41
1:C:199:GLU:OE1	1:C:207:ARG:NE	2.48	0.41
1:D:86:THR:CG2	1:D:151:LEU:HD11	2.50	0.41
1:D:378:TYR:HD2	1:D:380:LEU:HD21	1.85	0.41
1:C:223:GLU:O	1:C:230:LEU:HA	2.21	0.41
1:B:466:GLY:O	1:B:468:PRO:HD3	2.20	0.41
1:C:403:LYS:CB	1:C:418:LEU:HD12	2.51	0.41
1:D:389:ILE:HG22	1:D:396:GLY:HA2	2.03	0.41
1:B:142:GLU:HB2	1:B:143:PRO:HD3	2.02	0.41
1:B:346:TYR:CE1	1:D:193:VAL:HG23	2.56	0.41
1:D:217:LEU:HD11	1:D:219:LYS:HG3	2.03	0.41
1:B:66:ARG:O	1:B:70:ALA:HB2	2.21	0.41
1:B:307:HIS:NE2	1:B:323:ASN:OD1	2.54	0.41
1:D:179:VAL:HG23	1:D:241:MSE:SE	2.71	0.41
1:D:430:LYS:HE2	1:D:433:HIS:ND1	2.35	0.41
1:A:51:THR:HG21	1:B:406:PRO:HG2	2.03	0.40
1:D:184:LYS:HD3	1:D:256:ILE:CD1	2.51	0.40
1:B:357:ALA:HB2	3:B:702:HOH:O	2.22	0.40
1:C:285[A]:ARG:HD3	1:C:285[A]:ARG:H	1.87	0.40
1:D:332:LEU:HD22	1:D:343:TYR:CD2	2.57	0.40
1:D:162:ASN:CB	1:D:439:MSE:HE1	2.51	0.40
1:A:405:TYR:HB3	1:A:406:PRO:HA	2.03	0.40
1:B:403:LYS:NZ	1:B:407:GLU:OE2	2.52	0.40
1:C:291:LEU:O	1:C:295:LEU:HG	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:790:HOH:O	3:D:652:HOH:O[1_655]	2.15	0.05

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	471/489 (96%)	445 (94%)	22 (5%)	4 (1%)	19	23
1	B	467/489 (96%)	434 (93%)	27 (6%)	6 (1%)	12	12
1	C	461/489 (94%)	437 (95%)	18 (4%)	6 (1%)	12	12
1	D	470/489 (96%)	439 (93%)	25 (5%)	6 (1%)	12	12
All	All	1869/1956 (96%)	1755 (94%)	92 (5%)	22 (1%)	13	14

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	THR
1	A	412	ALA
1	B	139	GLU
1	B	229	SER
1	C	138	PHE
1	D	424	SER
1	D	425	LEU
1	B	142	GLU
1	D	0	THR
1	A	424	SER
1	B	138	PHE
1	B	230	LEU
1	C	78	ARG
1	C	139	GLU
1	C	142	GLU
1	C	230	LEU
1	D	-1	GLY
1	D	404	ALA
1	D	423	SER
1	A	351	PRO
1	B	78	ARG
1	C	141	ILE

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	407/408 (100%)	385 (95%)	22 (5%)	22	30
1	B	403/408 (99%)	385 (96%)	18 (4%)	27	39
1	C	402/408 (98%)	374 (93%)	28 (7%)	15	19
1	D	401/408 (98%)	382 (95%)	19 (5%)	26	37
All	All	1613/1632 (99%)	1526 (95%)	87 (5%)	23	30

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TRP
1	A	106	CYS
1	A	129	SER
1	A	130	ARG
1	A	216	SER
1	A	293	LYS
1	A	296	ASP
1	A	304	LYS
1	A	305	ASN
1	A	308	LYS
1	A	310	PHE
1	A	313	THR
1	A	336	ARG
1	A	353	TYR
1	A	383	ASP
1	A	417	ARG
1	A	424	SER
1	A	438	VAL
1	A	441	GLU
1	A	453	PHE
1	A	471	LYS
1	A	472	LYS
1	B	25	GLU
1	B	32	LYS

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Mol	Chain	Res	Type
1	B	81	CYS
1	B	123	LEU
1	B	128	LYS
1	B	145	LYS
1	B	200	SER
1	B	225	ASP
1	B	276	ILE
1	B	285[A]	ARG
1	B	285[B]	ARG
1	B	290	LYS
1	B	326	SER
1	B	366	ARG
1	B	373	ARG
1	B	395	GLN
1	B	419	LEU
1	B	453	PHE
1	C	9	TRP
1	C	36	GLN
1	C	95	MSE
1	C	105	LYS
1	C	138	PHE
1	C	151	LEU
1	C	158	SER
1	C	206	VAL
1	C	213	MSE
1	C	216	SER
1	C	234	LYS
1	C	264	MSE
1	C	285[A]	ARG
1	C	285[B]	ARG
1	C	286	ASP
1	C	362	PHE
1	C	366	ARG
1	C	367	GLN
1	C	402	VAL
1	C	417	ARG
1	C	419	LEU
1	C	420	ASP
1	C	424	SER
1	C	450	ARG
1	C	453	PHE
1	C	463[A]	LYS

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Mol	Chain	Res	Type
1	C	463[B]	LYS
1	C	471	LYS
1	D	10	SER
1	D	32	LYS
1	D	40	ILE
1	D	81	CYS
1	D	121	SER
1	D	128	LYS
1	D	202	SER
1	D	304	LYS
1	D	338	ASN
1	D	344	ASP
1	D	355	GLU
1	D	373	ARG
1	D	394	MSE
1	D	411	GLN
1	D	424	SER
1	D	427	ASP
1	D	450	ARG
1	D	453	PHE
1	D	472	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	270	HIS
1	A	356	GLN
1	B	281	GLN
1	C	305	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	D	501	-	42,48,48	4.70	19 (45%)	50,73,73	1.76	7 (14%)
2	NAD	C	502	-	42,48,48	5.04	19 (45%)	50,73,73	1.82	9 (18%)
2	NAD	B	602	-	42,48,48	4.83	19 (45%)	50,73,73	1.75	9 (18%)
2	NAD	B	601	-	42,48,48	4.85	19 (45%)	50,73,73	1.76	10 (20%)
2	NAD	A	502	-	42,48,48	5.05	19 (45%)	50,73,73	1.80	10 (20%)
2	NAD	C	501	-	42,48,48	4.73	19 (45%)	50,73,73	1.77	6 (12%)
2	NAD	D	502	-	42,48,48	4.71	19 (45%)	50,73,73	1.82	11 (22%)
2	NAD	A	501	-	42,48,48	4.72	19 (45%)	50,73,73	1.81	10 (20%)

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	D	501	-	-	2/26/62/62	0/5/5/5
2	NAD	C	502	-	-	6/26/62/62	0/5/5/5
2	NAD	B	602	-	-	2/26/62/62	0/5/5/5
2	NAD	B	601	-	-	4/26/62/62	0/5/5/5
2	NAD	A	502	-	-	4/26/62/62	0/5/5/5
2	NAD	C	501	-	-	3/26/62/62	0/5/5/5
2	NAD	D	502	-	-	3/26/62/62	0/5/5/5
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAD	C2B-C1B	-18.51	1.25	1.53
2	A	502	NAD	C2B-C1B	-18.32	1.26	1.53
2	B	601	NAD	C2B-C1B	-17.30	1.27	1.53
2	B	602	NAD	C2B-C1B	-17.15	1.27	1.53
2	C	501	NAD	C2B-C1B	-16.37	1.28	1.53
2	A	501	NAD	C2B-C1B	-16.23	1.29	1.53
2	D	501	NAD	C2B-C1B	-16.18	1.29	1.53
2	D	502	NAD	C2B-C1B	-16.15	1.29	1.53
2	A	502	NAD	O4B-C1B	12.52	1.58	1.41
2	C	502	NAD	O4B-C1B	12.32	1.58	1.41
2	C	502	NAD	C2D-C3D	-10.63	1.24	1.53
2	C	501	NAD	C2D-C3D	-10.60	1.24	1.53
2	D	502	NAD	C2D-C3D	-10.58	1.24	1.53
2	B	602	NAD	C2D-C3D	-10.56	1.24	1.53
2	D	501	NAD	C2D-C3D	-10.55	1.24	1.53
2	B	601	NAD	O4B-C1B	10.55	1.55	1.41
2	A	501	NAD	C2D-C3D	-10.54	1.24	1.53
2	B	601	NAD	C2D-C3D	-10.47	1.24	1.53
2	B	602	NAD	O4B-C1B	10.46	1.55	1.41
2	A	502	NAD	C2D-C3D	-10.46	1.24	1.53
2	D	502	NAD	C3B-C4B	-10.27	1.26	1.53
2	B	602	NAD	C3B-C4B	-10.25	1.26	1.53
2	C	502	NAD	C3B-C4B	-10.22	1.26	1.53
2	A	502	NAD	C3B-C4B	-10.20	1.26	1.53
2	C	501	NAD	C3B-C4B	-10.19	1.27	1.53
2	D	501	NAD	C3B-C4B	-10.16	1.27	1.53
2	B	601	NAD	C3B-C4B	-10.15	1.27	1.53
2	A	501	NAD	C3B-C4B	-10.13	1.27	1.53
2	C	501	NAD	O4B-C1B	9.98	1.55	1.41
2	A	501	NAD	O4B-C1B	9.96	1.55	1.41
2	D	501	NAD	O4B-C1B	9.68	1.54	1.41
2	D	502	NAD	O4B-C1B	9.60	1.54	1.41
2	C	502	NAD	C7N-N7N	7.96	1.48	1.33
2	A	502	NAD	C7N-N7N	7.91	1.48	1.33
2	D	502	NAD	O4D-C1D	7.90	1.52	1.41
2	B	601	NAD	C7N-N7N	7.89	1.48	1.33
2	B	602	NAD	C7N-N7N	7.85	1.48	1.33
2	D	502	NAD	C7N-N7N	7.84	1.47	1.33
2	C	501	NAD	C7N-N7N	7.84	1.47	1.33
2	A	501	NAD	C7N-N7N	7.84	1.47	1.33
2	D	501	NAD	C7N-N7N	7.81	1.47	1.33
2	A	502	NAD	O4D-C1D	7.54	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	O4D-C1D	7.52	1.51	1.41
2	B	601	NAD	O4D-C1D	7.40	1.51	1.41
2	C	501	NAD	O4D-C1D	7.40	1.51	1.41
2	A	501	NAD	O4D-C1D	7.36	1.51	1.41
2	B	602	NAD	O4D-C1D	7.32	1.51	1.41
2	C	502	NAD	O4D-C1D	7.21	1.51	1.41
2	A	502	NAD	O4D-C4D	-6.50	1.30	1.45
2	B	602	NAD	O4D-C4D	-6.50	1.30	1.45
2	B	601	NAD	O4D-C4D	-6.45	1.30	1.45
2	C	502	NAD	O4D-C4D	-6.45	1.30	1.45
2	C	501	NAD	O4D-C4D	-6.38	1.30	1.45
2	D	502	NAD	O4D-C4D	-6.33	1.30	1.45
2	A	501	NAD	O4D-C4D	-6.32	1.30	1.45
2	D	501	NAD	O4D-C4D	-6.26	1.31	1.45
2	A	501	NAD	C3D-C4D	5.21	1.66	1.53
2	D	501	NAD	C3D-C4D	5.19	1.66	1.53
2	A	502	NAD	O4B-C4B	5.16	1.56	1.45
2	C	502	NAD	C3D-C4D	5.14	1.66	1.53
2	A	501	NAD	O4B-C4B	5.12	1.56	1.45
2	D	501	NAD	O4B-C4B	5.12	1.56	1.45
2	D	502	NAD	C3D-C4D	5.12	1.66	1.53
2	B	601	NAD	C3D-C4D	5.11	1.66	1.53
2	B	601	NAD	O4B-C4B	5.10	1.56	1.45
2	C	501	NAD	C3D-C4D	5.10	1.66	1.53
2	B	601	NAD	C2B-C3B	5.09	1.67	1.53
2	D	502	NAD	O4B-C4B	5.09	1.56	1.45
2	A	502	NAD	C3D-C4D	5.09	1.66	1.53
2	B	602	NAD	O4B-C4B	5.08	1.56	1.45
2	B	602	NAD	C3D-C4D	5.07	1.65	1.53
2	C	501	NAD	O4B-C4B	5.04	1.56	1.45
2	C	501	NAD	C2B-C3B	5.03	1.67	1.53
2	C	502	NAD	O4B-C4B	5.03	1.56	1.45
2	B	602	NAD	C2B-C3B	5.03	1.67	1.53
2	A	502	NAD	C2B-C3B	5.01	1.67	1.53
2	C	502	NAD	C2B-C3B	5.00	1.67	1.53
2	A	501	NAD	C2B-C3B	4.98	1.67	1.53
2	D	501	NAD	C2B-C3B	4.96	1.66	1.53
2	D	502	NAD	C2B-C3B	4.84	1.66	1.53
2	A	501	NAD	C3N-C7N	4.18	1.56	1.50
2	D	502	NAD	C3N-C7N	4.12	1.56	1.50
2	C	501	NAD	C3N-C7N	4.08	1.56	1.50
2	D	501	NAD	C3N-C7N	4.06	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	C3N-C7N	4.05	1.56	1.50
2	D	501	NAD	C2D-C1D	4.01	1.59	1.53
2	C	502	NAD	O2D-C2D	4.00	1.52	1.43
2	B	601	NAD	C2D-C1D	4.00	1.59	1.53
2	B	601	NAD	O2D-C2D	4.00	1.52	1.43
2	B	602	NAD	C2D-C1D	3.99	1.59	1.53
2	A	501	NAD	C2D-C1D	3.99	1.59	1.53
2	A	502	NAD	C2D-C1D	3.97	1.59	1.53
2	A	502	NAD	O2D-C2D	3.97	1.52	1.43
2	C	502	NAD	C2D-C1D	3.95	1.59	1.53
2	C	501	NAD	C6A-N6A	3.94	1.48	1.34
2	A	502	NAD	C3N-C7N	3.94	1.56	1.50
2	C	502	NAD	C6A-N6A	3.92	1.48	1.34
2	B	602	NAD	C3N-C7N	3.92	1.56	1.50
2	D	502	NAD	C6A-N6A	3.91	1.48	1.34
2	B	602	NAD	O2D-C2D	3.90	1.52	1.43
2	A	502	NAD	C6A-N6A	3.89	1.48	1.34
2	B	602	NAD	C6A-N6A	3.88	1.48	1.34
2	B	601	NAD	C6A-N6A	3.88	1.48	1.34
2	D	502	NAD	O2D-C2D	3.88	1.52	1.43
2	D	501	NAD	C6A-N6A	3.88	1.48	1.34
2	A	501	NAD	C6A-N6A	3.87	1.48	1.34
2	C	502	NAD	C3N-C7N	3.86	1.56	1.50
2	C	501	NAD	O2D-C2D	3.84	1.52	1.43
2	A	501	NAD	O2D-C2D	3.82	1.52	1.43
2	C	501	NAD	C2D-C1D	3.79	1.59	1.53
2	D	501	NAD	O2D-C2D	3.74	1.51	1.43
2	D	502	NAD	C2D-C1D	3.49	1.59	1.53
2	A	502	NAD	O7N-C7N	-3.21	1.18	1.24
2	C	502	NAD	O7N-C7N	-3.20	1.18	1.24
2	B	601	NAD	O7N-C7N	-3.19	1.18	1.24
2	B	602	NAD	O7N-C7N	-3.13	1.18	1.24
2	C	501	NAD	O7N-C7N	-3.13	1.18	1.24
2	A	501	NAD	O7N-C7N	-3.12	1.18	1.24
2	D	501	NAD	O7N-C7N	-3.10	1.18	1.24
2	D	502	NAD	O7N-C7N	-3.08	1.18	1.24
2	B	601	NAD	C2A-N3A	2.86	1.36	1.32
2	A	502	NAD	C2A-N3A	2.83	1.36	1.32
2	A	502	NAD	O3D-C3D	2.82	1.49	1.43
2	B	601	NAD	O3D-C3D	2.81	1.49	1.43
2	D	502	NAD	O3D-C3D	2.80	1.49	1.43
2	C	501	NAD	C2A-N3A	2.79	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C2A-N3A	2.78	1.36	1.32
2	B	602	NAD	O3D-C3D	2.77	1.49	1.43
2	B	602	NAD	C2A-N3A	2.76	1.36	1.32
2	C	502	NAD	O3D-C3D	2.75	1.49	1.43
2	C	501	NAD	O3D-C3D	2.72	1.49	1.43
2	D	501	NAD	O3D-C3D	2.71	1.49	1.43
2	D	501	NAD	C2A-N3A	2.69	1.36	1.32
2	D	502	NAD	C2A-N3A	2.68	1.36	1.32
2	A	501	NAD	O3D-C3D	2.68	1.49	1.43
2	C	502	NAD	C2A-N3A	2.61	1.36	1.32
2	B	602	NAD	C5A-C4A	-2.47	1.34	1.40
2	C	501	NAD	C5B-C4B	2.47	1.59	1.51
2	D	502	NAD	C5A-C4A	-2.47	1.34	1.40
2	D	501	NAD	C5B-C4B	2.46	1.59	1.51
2	A	501	NAD	C5B-C4B	2.46	1.59	1.51
2	D	501	NAD	C5A-C4A	-2.45	1.34	1.40
2	A	501	NAD	C5A-C4A	-2.43	1.34	1.40
2	C	502	NAD	C5A-C4A	-2.43	1.34	1.40
2	B	601	NAD	C5A-C4A	-2.42	1.34	1.40
2	A	502	NAD	C5A-C4A	-2.42	1.34	1.40
2	D	502	NAD	C5B-C4B	2.40	1.59	1.51
2	B	602	NAD	C5B-C4B	2.36	1.59	1.51
2	C	501	NAD	C5A-C4A	-2.35	1.34	1.40
2	A	502	NAD	C5B-C4B	2.35	1.58	1.51
2	C	502	NAD	C5B-C4B	2.34	1.58	1.51
2	B	601	NAD	C5B-C4B	2.34	1.58	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502	NAD	C5A-C6A-N6A	7.17	131.25	120.35
2	C	502	NAD	C5A-C6A-N6A	7.16	131.23	120.35
2	D	501	NAD	C5A-C6A-N6A	7.13	131.19	120.35
2	C	501	NAD	C5A-C6A-N6A	7.05	131.07	120.35
2	A	501	NAD	C5A-C6A-N6A	6.78	130.66	120.35
2	B	602	NAD	C5A-C6A-N6A	6.78	130.65	120.35
2	A	502	NAD	C5A-C6A-N6A	6.75	130.61	120.35
2	B	601	NAD	C5A-C6A-N6A	6.68	130.50	120.35
2	B	601	NAD	N3A-C2A-N1A	-5.41	120.22	128.68
2	A	501	NAD	N3A-C2A-N1A	-5.39	120.26	128.68
2	C	502	NAD	N3A-C2A-N1A	-5.36	120.30	128.68
2	B	602	NAD	N3A-C2A-N1A	-5.35	120.32	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	NAD	N3A-C2A-N1A	-5.33	120.35	128.68
2	D	502	NAD	N3A-C2A-N1A	-5.28	120.43	128.68
2	D	501	NAD	N3A-C2A-N1A	-5.27	120.45	128.68
2	C	501	NAD	N3A-C2A-N1A	-5.26	120.46	128.68
2	D	501	NAD	N6A-C6A-N1A	-4.51	109.22	118.57
2	C	502	NAD	N6A-C6A-N1A	-4.47	109.29	118.57
2	A	501	NAD	N6A-C6A-N1A	-4.45	109.33	118.57
2	C	501	NAD	N6A-C6A-N1A	-4.44	109.36	118.57
2	D	502	NAD	N6A-C6A-N1A	-4.41	109.43	118.57
2	B	602	NAD	N6A-C6A-N1A	-4.40	109.45	118.57
2	A	502	NAD	N6A-C6A-N1A	-4.36	109.52	118.57
2	B	601	NAD	N6A-C6A-N1A	-4.34	109.56	118.57
2	A	501	NAD	C1B-N9A-C4A	3.26	132.36	126.64
2	C	502	NAD	C3B-C2B-C1B	3.21	105.81	100.98
2	C	501	NAD	C1B-N9A-C4A	3.08	132.04	126.64
2	A	502	NAD	C3B-C2B-C1B	3.07	105.59	100.98
2	A	501	NAD	PN-O3-PA	-2.88	122.94	132.83
2	D	502	NAD	C1B-N9A-C4A	2.85	131.64	126.64
2	C	501	NAD	PN-O3-PA	-2.70	123.57	132.83
2	B	602	NAD	C1B-N9A-C4A	2.63	131.26	126.64
2	A	502	NAD	C1B-N9A-C4A	2.59	131.19	126.64
2	D	501	NAD	PN-O3-PA	-2.59	123.94	132.83
2	D	502	NAD	O4B-C1B-C2B	-2.55	103.20	106.93
2	B	601	NAD	PN-O3-PA	-2.54	124.11	132.83
2	B	601	NAD	C1B-N9A-C4A	2.53	131.08	126.64
2	C	502	NAD	C3D-C2D-C1D	2.52	104.77	100.98
2	B	602	NAD	PN-O3-PA	-2.51	124.21	132.83
2	A	502	NAD	C6N-N1N-C2N	-2.51	119.69	121.97
2	D	502	NAD	C3N-C7N-N7N	2.51	120.76	117.75
2	C	502	NAD	C1B-N9A-C4A	2.48	131.00	126.64
2	B	601	NAD	C6N-N1N-C2N	-2.44	119.75	121.97
2	B	602	NAD	C6N-N1N-C2N	-2.36	119.82	121.97
2	D	502	NAD	PN-O3-PA	-2.34	124.79	132.83
2	A	502	NAD	PN-O3-PA	-2.32	124.86	132.83
2	C	502	NAD	C6N-N1N-C2N	-2.29	119.88	121.97
2	D	501	NAD	C1B-N9A-C4A	2.26	130.62	126.64
2	B	602	NAD	C3D-C2D-C1D	2.26	104.38	100.98
2	A	501	NAD	C3N-C7N-N7N	2.26	120.46	117.75
2	B	601	NAD	O4D-C1D-C2D	-2.20	103.71	106.93
2	B	602	NAD	O4D-C1D-C2D	-2.20	103.71	106.93
2	A	502	NAD	O4D-C1D-C2D	-2.18	103.74	106.93
2	C	501	NAD	C3B-C2B-C1B	2.16	104.23	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	NAD	C3D-C2D-C1D	2.14	104.21	100.98
2	A	501	NAD	C3B-C2B-C1B	2.14	104.19	100.98
2	D	501	NAD	O4D-C1D-C2D	-2.14	103.80	106.93
2	D	502	NAD	C2B-C3B-C4B	2.12	106.77	102.64
2	A	501	NAD	C2B-C3B-C4B	2.11	106.75	102.64
2	D	501	NAD	C3N-C7N-N7N	2.11	120.29	117.75
2	A	502	NAD	C2D-C3D-C4D	2.11	106.73	102.64
2	B	602	NAD	C2D-C3D-C4D	2.10	106.73	102.64
2	B	601	NAD	C3D-C2D-C1D	2.10	104.14	100.98
2	B	601	NAD	C3B-C2B-C1B	2.09	104.13	100.98
2	D	502	NAD	C2D-C3D-C4D	2.08	106.69	102.64
2	A	501	NAD	O4B-C1B-C2B	-2.08	103.89	106.93
2	A	501	NAD	O4D-C1D-C2D	-2.07	103.91	106.93
2	C	502	NAD	C2D-C3D-C4D	2.06	106.65	102.64
2	C	502	NAD	PN-O3-PA	-2.05	125.80	132.83
2	D	502	NAD	O4D-C1D-C2D	-2.04	103.95	106.93
2	D	502	NAD	O7N-C7N-N7N	-2.03	119.70	122.58
2	B	601	NAD	C2D-C3D-C4D	2.01	106.54	102.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	PN-O3-PA-O5B
2	A	502	NAD	C5D-O5D-PN-O1N
2	A	502	NAD	O4D-C1D-N1N-C6N
2	B	601	NAD	C5D-O5D-PN-O3
2	B	601	NAD	C5D-O5D-PN-O1N
2	B	601	NAD	O4D-C1D-N1N-C6N
2	B	602	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	PN-O3-PA-O5B
2	C	502	NAD	PA-O3-PN-O5D
2	C	502	NAD	C5D-O5D-PN-O1N
2	C	502	NAD	O4D-C1D-N1N-C6N
2	D	502	NAD	O4D-C4D-C5D-O5D
2	D	502	NAD	C3D-C4D-C5D-O5D
2	A	502	NAD	PA-O3-PN-O5D
2	B	601	NAD	PA-O3-PN-O5D
2	D	502	NAD	PN-O3-PA-O5B
2	A	501	NAD	O4D-C4D-C5D-O5D
2	A	501	NAD	C4N-C3N-C7N-N7N
2	A	501	NAD	C4N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
2	C	501	NAD	C4N-C3N-C7N-N7N
2	C	501	NAD	C4N-C3N-C7N-O7N
2	A	502	NAD	C5D-O5D-PN-O3
2	B	602	NAD	C5D-O5D-PN-O3
2	C	502	NAD	C5D-O5D-PN-O3
2	D	501	NAD	C4N-C3N-C7N-O7N
2	D	501	NAD	C4N-C3N-C7N-N7N
2	C	502	NAD	PN-O3-PA-O1A
2	C	502	NAD	PN-O3-PA-O2A
2	A	501	NAD	C3D-C4D-C5D-O5D

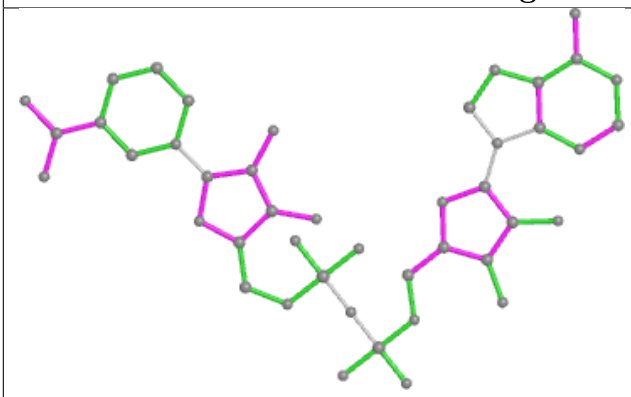
There are no ring outliers.

7 monomers are involved in 22 short contacts:

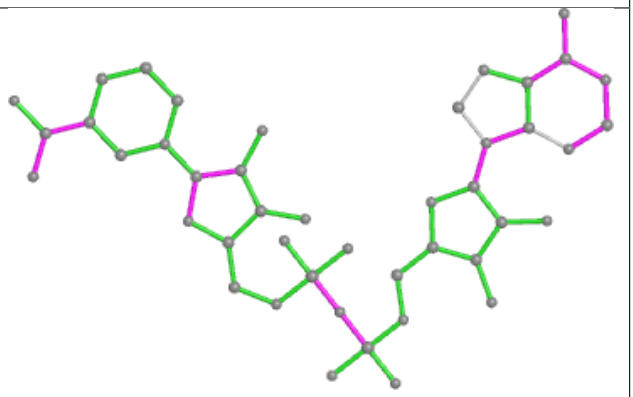
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	NAD	6	0
2	C	502	NAD	1	0
2	B	602	NAD	1	0
2	A	502	NAD	3	0
2	C	501	NAD	3	0
2	D	502	NAD	7	0
2	A	501	NAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

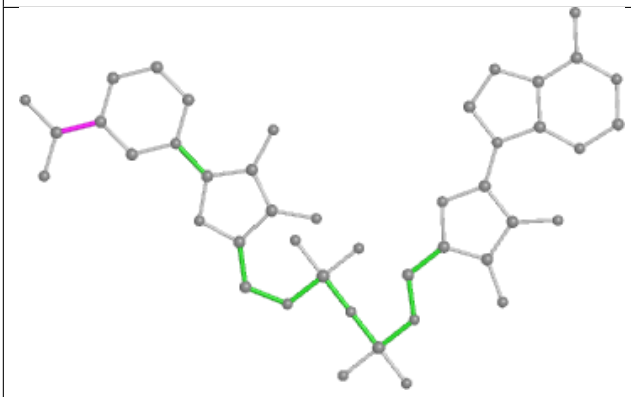
Ligand NAD D 501



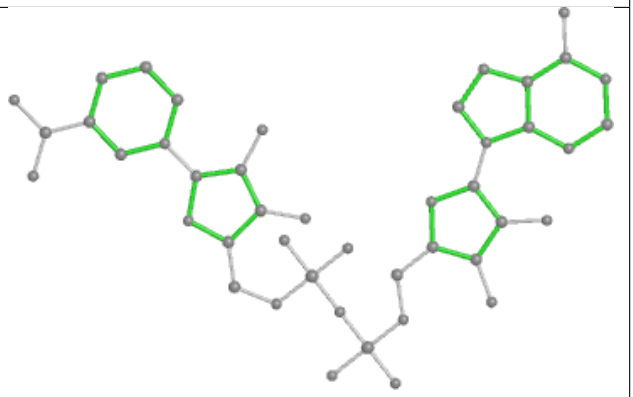
Bond lengths



Bond angles

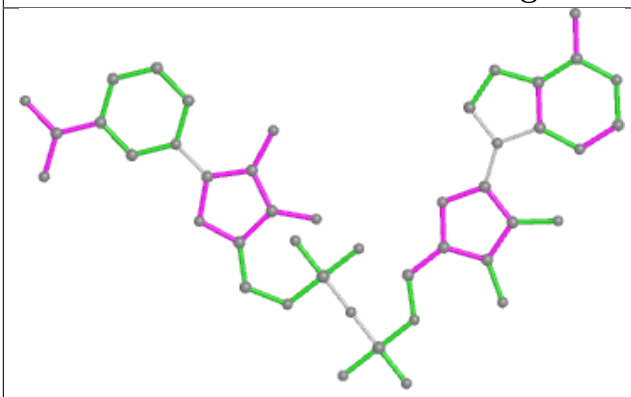


Torsions



Rings

Ligand NAD C 502



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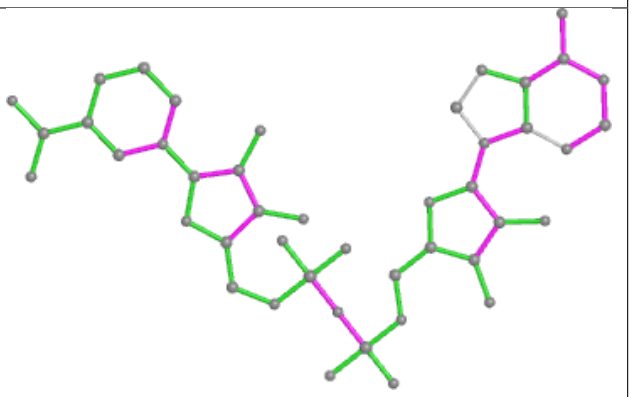

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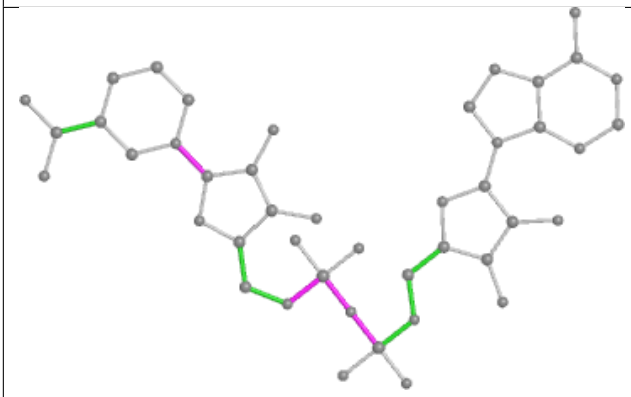
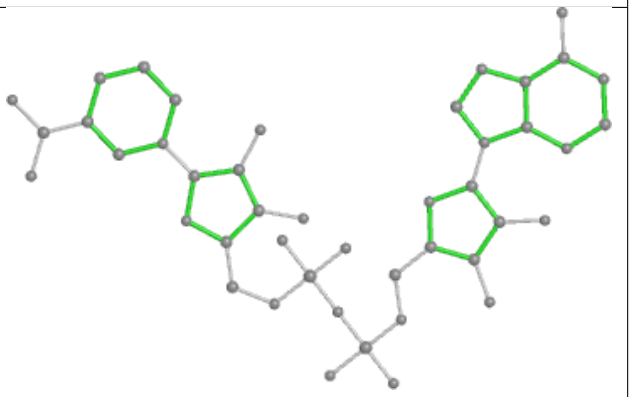
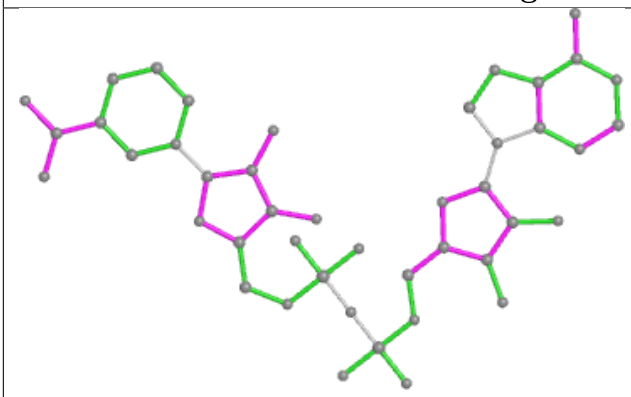


Torsions

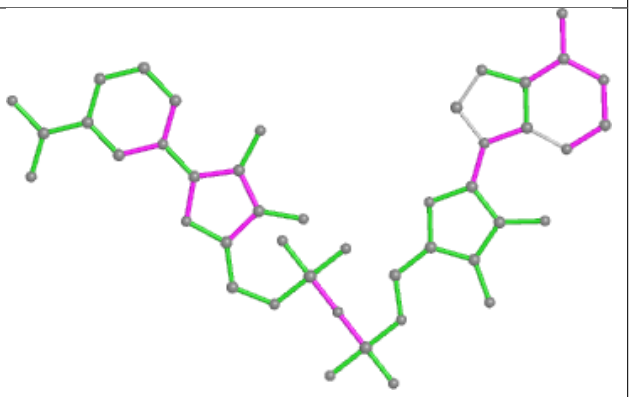


Rings

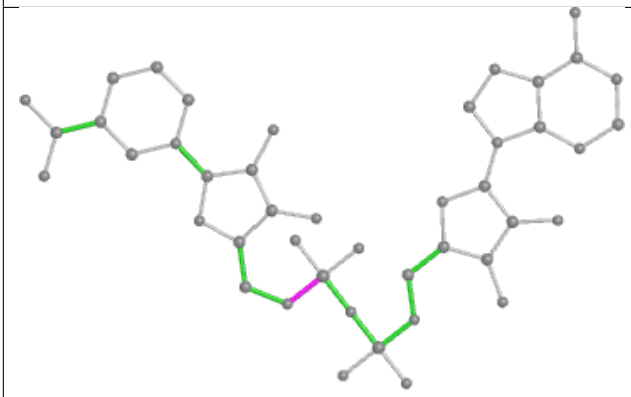
Ligand NAD B 602



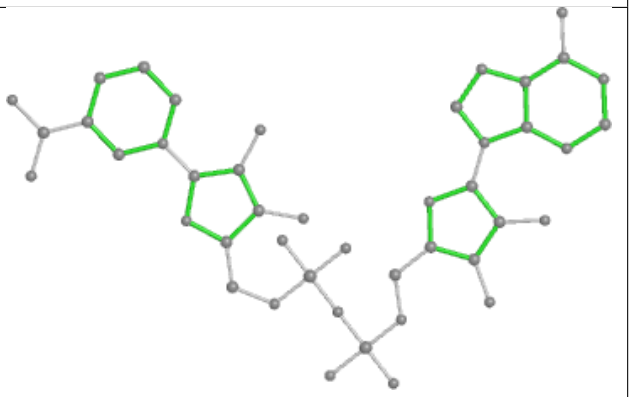
Bond lengths



Bond angles



Torsions



Rings

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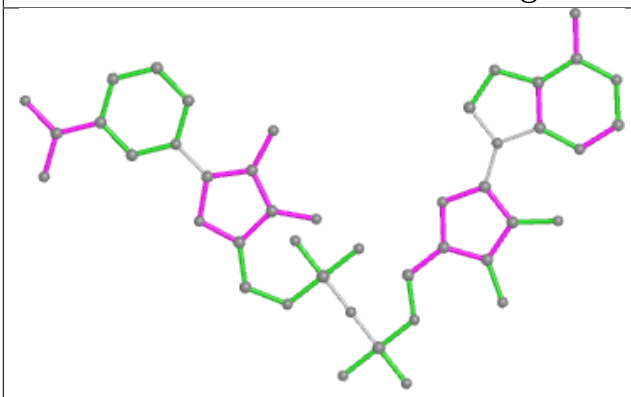
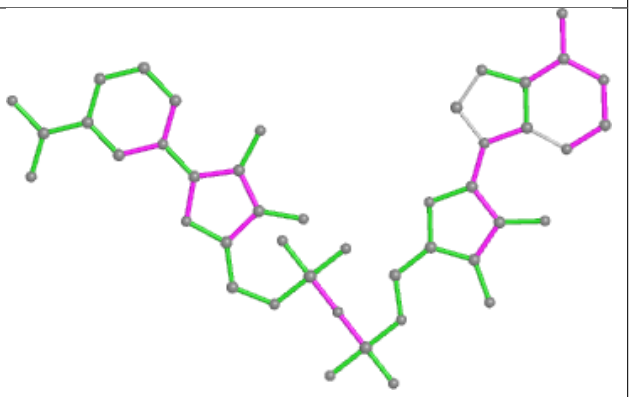
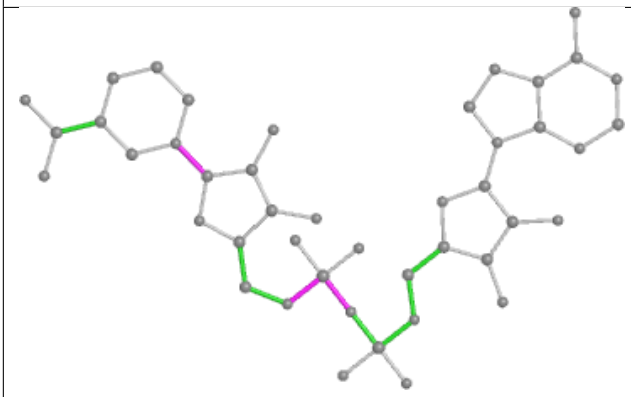


Bond lengths



Bond angles



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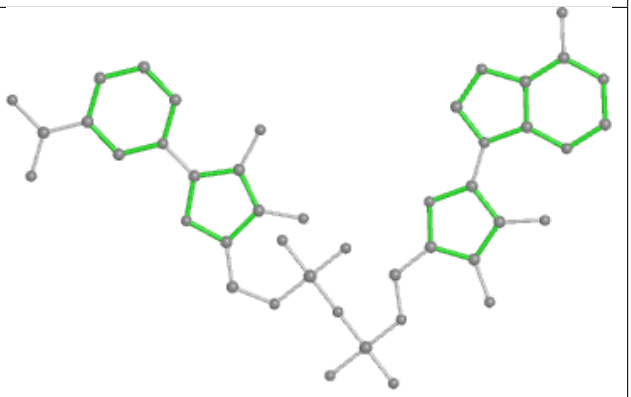
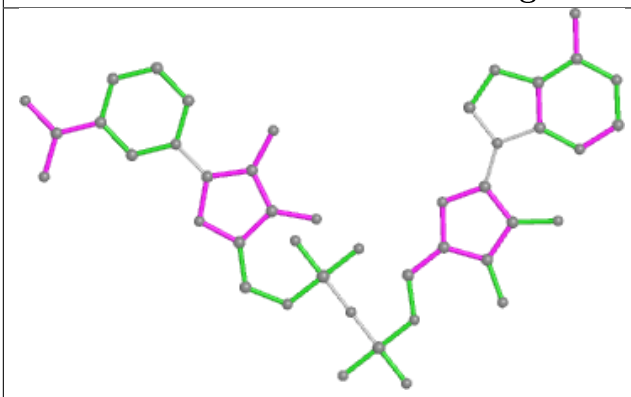


Rings

Ligand NAD A 502



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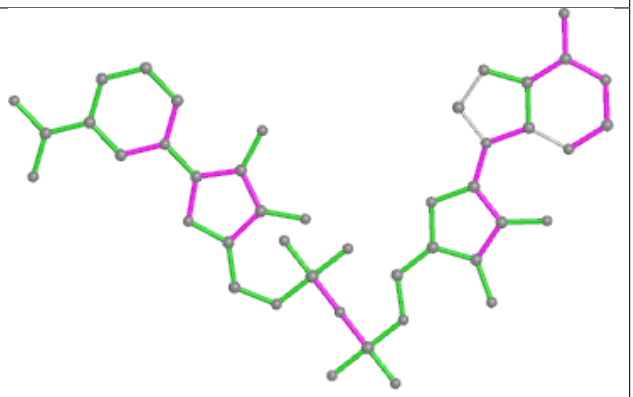

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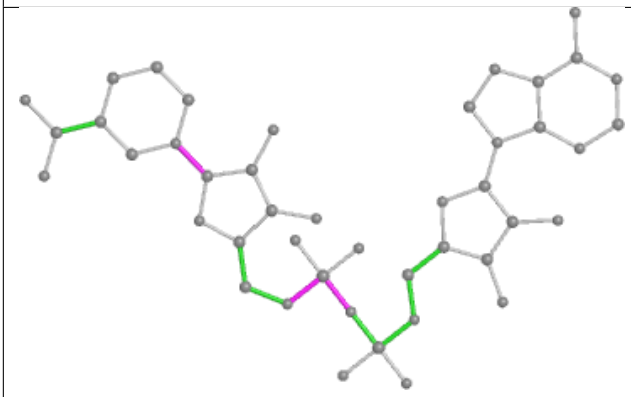

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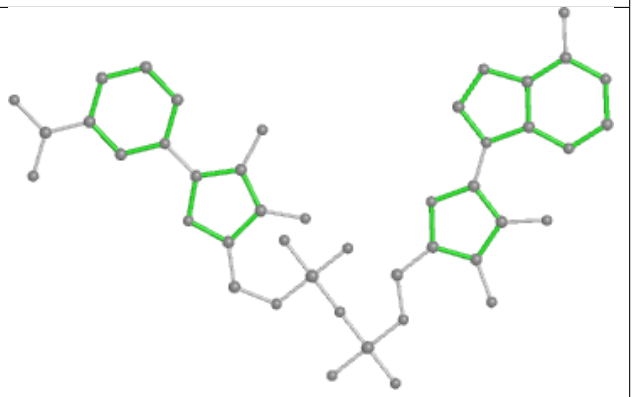
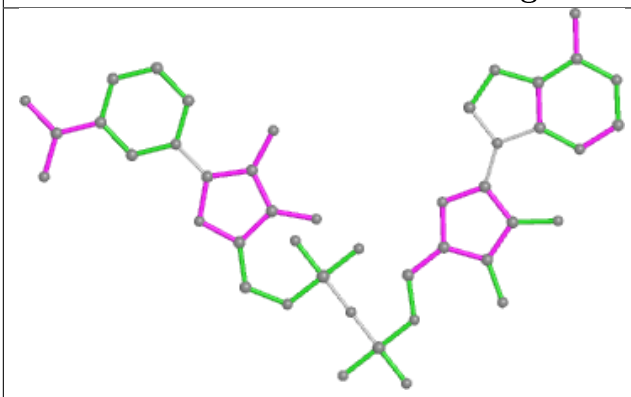
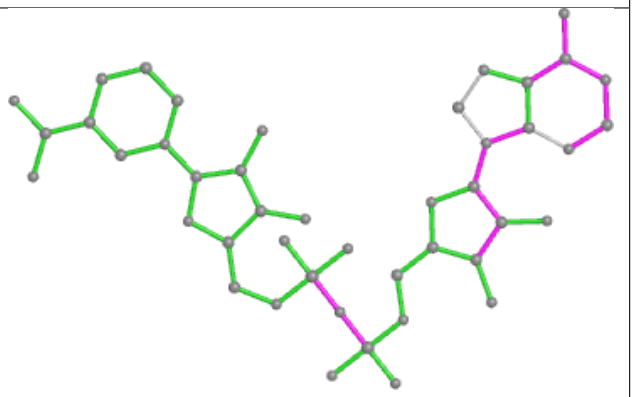


Rings

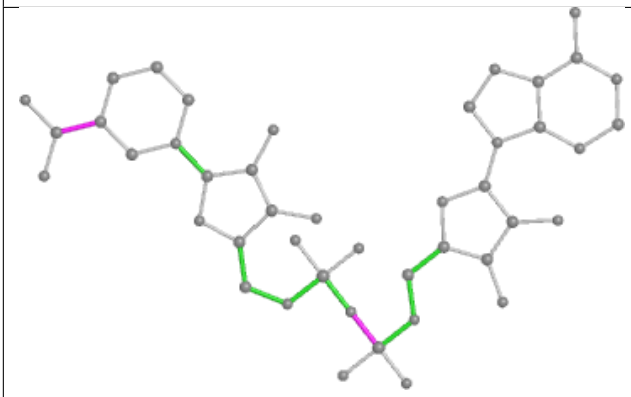
Ligand NAD C 501



Bond lengths



Bond angles



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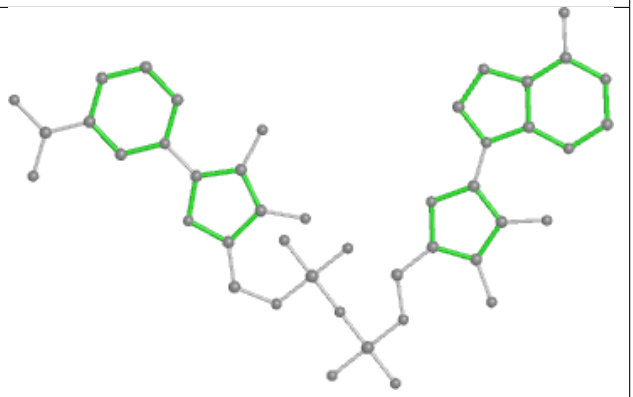
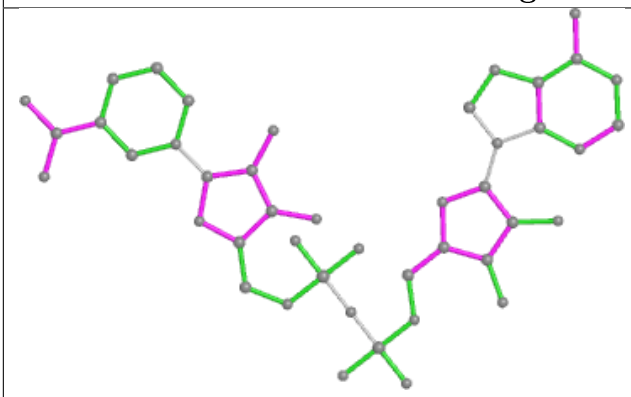
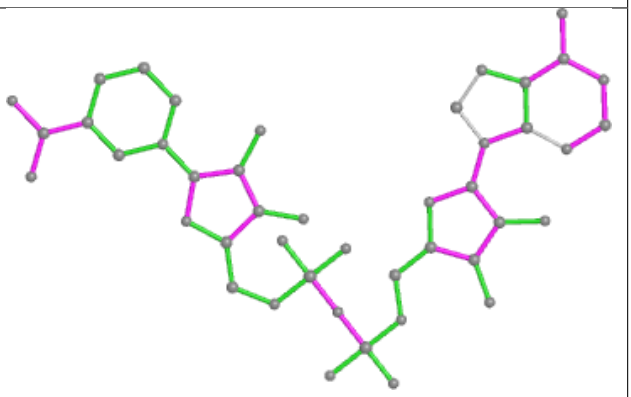


Rings

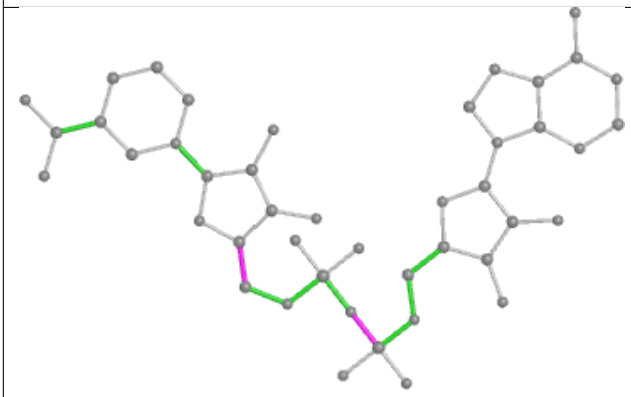
Ligand NAD D 502



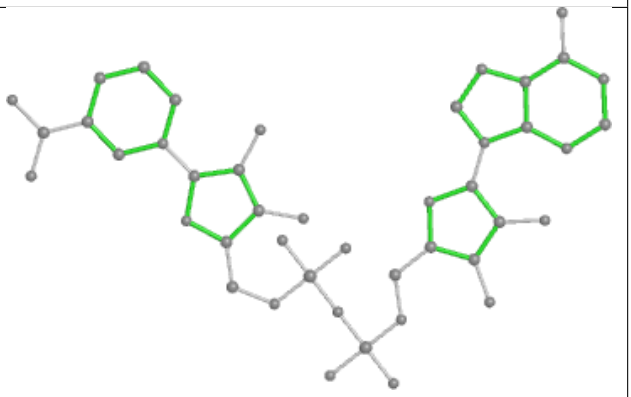
Bond lengths



Bond angles

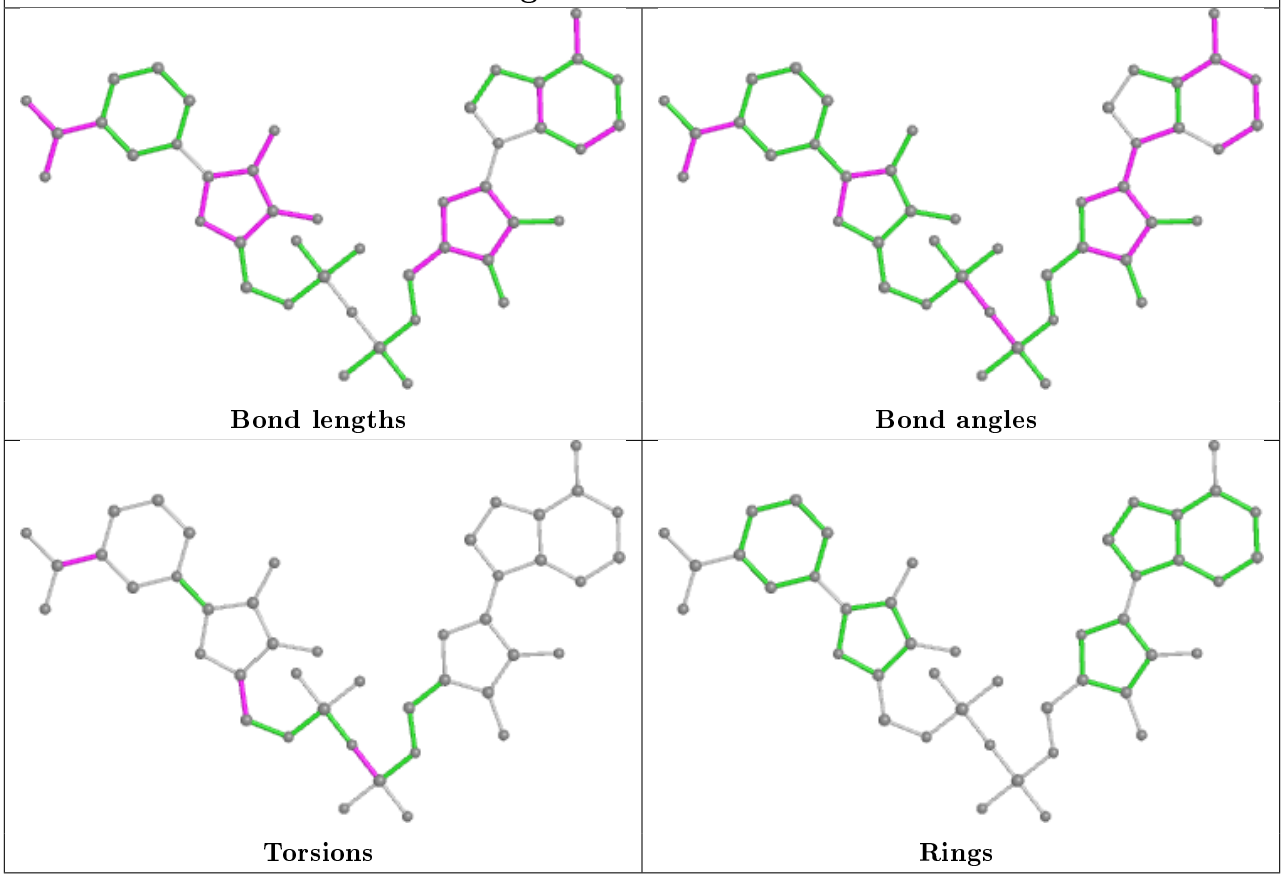


Torsions



Rings

Ligand NAD A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	457/489 (93%)	2.09	204 (44%)	0	0	20, 33, 51, 75	0
1	B	457/489 (93%)	2.10	210 (45%)	0	0	25, 36, 59, 84	0
1	C	454/489 (92%)	2.15	215 (47%)	0	0	22, 34, 56, 87	0
1	D	461/489 (94%)	2.23	224 (48%)	0	0	24, 39, 60, 87	0
All	All	1829/1956 (93%)	2.14	853 (46%)	0	0	20, 35, 57, 87	0

All (853) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	PHE	16.4
1	D	412	ALA	11.5
1	D	427	ASP	10.8
1	D	76	GLY	9.7
1	C	424	SER	9.0
1	D	137	PHE	8.7
1	B	141	ILE	8.2
1	B	136	SER	7.9
1	C	412	ALA	7.7
1	B	227	GLY	7.7
1	A	174	GLY	7.5
1	A	136	SER	7.5
1	D	138	PHE	7.4
1	C	229	SER	7.3
1	D	424	SER	7.2
1	B	127	GLY	7.2
1	B	140	GLY	7.2
1	B	229	SER	7.1
1	D	399	GLY	7.0
1	D	425	LEU	6.8
1	B	137	PHE	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	419	LEU	6.7
1	D	134	ILE	6.6
1	A	229	SER	6.6
1	D	-1	GLY	6.5
1	A	313	THR	6.5
1	D	400	PHE	6.5
1	C	51	THR	6.4
1	C	221	HIS	6.4
1	D	428	ILE	6.3
1	A	408	SER	6.3
1	A	192	ALA	6.3
1	D	140	GLY	6.3
1	B	224	GLY	6.2
1	C	141	ILE	6.2
1	C	146	CYS	6.1
1	D	409	SER	6.0
1	D	136	SER	5.9
1	C	231	VAL	5.9
1	A	189	PHE	5.8
1	B	387	GLY	5.8
1	A	-1	GLY	5.6
1	A	415	TYR	5.6
1	D	411	GLN	5.5
1	A	247	PRO	5.4
1	A	231	VAL	5.4
1	A	314	LEU	5.3
1	C	409	SER	5.3
1	B	230	LEU	5.3
1	D	363	PHE	5.2
1	C	230	LEU	5.2
1	A	414	ALA	5.2
1	A	135	LYS	5.1
1	D	317	THR	5.1
1	C	179	VAL	5.1
1	C	134	ILE	5.1
1	C	10	SER	5.0
1	C	402	VAL	5.0
1	B	379	PHE	5.0
1	A	298	ILE	5.0
1	D	426	ALA	5.0
1	B	409	SER	5.0
1	C	139	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	70	ALA	4.9
1	A	108	LEU	4.9
1	D	51	THR	4.8
1	D	438	VAL	4.8
1	A	409	SER	4.8
1	B	129	SER	4.8
1	C	232	VAL	4.8
1	B	57	ILE	4.8
1	B	348	THR	4.7
1	D	368	ARG	4.7
1	C	343	TYR	4.7
1	D	343	TYR	4.7
1	D	339	HIS	4.7
1	D	402	VAL	4.7
1	D	341	ILE	4.7
1	B	316	PHE	4.7
1	B	415	TYR	4.7
1	D	77	GLN	4.7
1	B	380	LEU	4.7
1	D	126	LEU	4.7
1	A	170	CYS	4.6
1	C	37	VAL	4.6
1	C	410	ASP	4.6
1	D	215	TYR	4.6
1	C	341	ILE	4.6
1	A	423	SER	4.6
1	B	396	GLY	4.5
1	B	363	PHE	4.5
1	A	425	LEU	4.5
1	D	404	ALA	4.4
1	C	282	VAL	4.4
1	C	284	SER	4.4
1	C	35	ILE	4.4
1	C	396	GLY	4.4
1	A	342	ASP	4.4
1	B	391	THR	4.4
1	D	159	TRP	4.4
1	C	287	SER	4.4
1	C	348	THR	4.3
1	D	418	LEU	4.3
1	A	86	THR	4.3
1	B	359	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	352	GLN	4.2
1	B	174	GLY	4.2
1	D	75	ASP	4.2
1	B	360	ALA	4.2
1	D	349	ALA	4.2
1	A	81	CYS	4.2
1	A	413	LEU	4.2
1	B	423	SER	4.2
1	C	404	ALA	4.1
1	C	438	VAL	4.1
1	A	246	LEU	4.1
1	D	432	LEU	4.1
1	D	165	TRP	4.1
1	D	430	LYS	4.1
1	A	118	ASN	4.1
1	A	236	THR	4.1
1	D	143	PRO	4.1
1	C	474	ASP	4.1
1	A	73	LEU	4.1
1	B	233	ALA	4.1
1	C	305	ASN	4.1
1	C	422	HIS	4.1
1	A	447	ARG	4.0
1	C	378	TYR	4.0
1	A	87	GLY	4.0
1	B	424	SER	4.0
1	C	354	SER	4.0
1	D	10	SER	4.0
1	D	333	ILE	4.0
1	C	339	HIS	4.0
1	C	131	LEU	4.0
1	A	141	ILE	4.0
1	C	86	THR	4.0
1	A	432	LEU	3.9
1	D	161	LEU	3.9
1	B	189	PHE	3.9
1	B	247	PRO	3.9
1	B	165	TRP	3.9
1	D	410	ASP	3.9
1	C	280	LEU	3.9
1	D	151	LEU	3.9
1	A	140	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	298	ILE	3.9
1	D	189	PHE	3.9
1	D	422	HIS	3.9
1	A	444	LEU	3.9
1	A	378	TYR	3.8
1	A	88	GLY	3.8
1	D	366	ARG	3.8
1	A	9	TRP	3.8
1	D	23	TRP	3.8
1	B	334	ASP	3.8
1	A	389	ILE	3.8
1	A	397	ASN	3.8
1	D	423	SER	3.8
1	B	123	LEU	3.8
1	C	376	LEU	3.8
1	D	218	LEU	3.8
1	C	286	ASP	3.8
1	C	214	ASN	3.8
1	C	366	ARG	3.8
1	C	218	LEU	3.8
1	A	287	SER	3.8
1	D	267	ALA	3.8
1	C	390	ASN	3.8
1	C	172	ALA	3.7
1	B	448	VAL	3.7
1	C	431	ILE	3.7
1	A	411	GLN	3.7
1	C	444	LEU	3.7
1	D	9	TRP	3.7
1	A	316	PHE	3.7
1	C	320	TYR	3.7
1	D	193	VAL	3.7
1	D	440	VAL	3.7
1	D	73	LEU	3.7
1	D	340	LEU	3.7
1	D	248	GLY	3.7
1	B	405	TYR	3.7
1	D	104	ALA	3.7
1	A	401	ARG	3.7
1	B	275	TRP	3.7
1	A	243	PHE	3.7
1	D	-2	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	422	HIS	3.7
1	C	228	GLU	3.7
1	D	329	ILE	3.7
1	C	247	PRO	3.7
1	A	295	LEU	3.7
1	B	121	SER	3.7
1	A	343	TYR	3.7
1	B	325	TYR	3.7
1	B	346	TYR	3.7
1	A	216	SER	3.6
1	D	414	ALA	3.6
1	C	98	TYR	3.6
1	C	238	THR	3.6
1	A	288	TYR	3.6
1	D	98	TYR	3.6
1	B	194	ASN	3.6
1	A	419	LEU	3.6
1	A	396	GLY	3.6
1	D	396	GLY	3.6
1	C	48	PHE	3.6
1	B	431	ILE	3.6
1	C	337	GLY	3.6
1	C	285[A]	ARG	3.6
1	D	337	GLY	3.5
1	B	126	LEU	3.5
1	D	65	VAL	3.5
1	B	51	THR	3.5
1	D	139	GLU	3.5
1	C	415	TYR	3.5
1	B	339	HIS	3.5
1	B	76	GLY	3.5
1	C	102	ASN	3.5
1	C	423	SER	3.5
1	A	442	ILE	3.5
1	C	398	LEU	3.5
1	C	75	ASP	3.5
1	A	424	SER	3.5
1	B	460	THR	3.5
1	D	310	PHE	3.5
1	C	314	LEU	3.5
1	D	97	LEU	3.5
1	D	131	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	206	VAL	3.5
1	C	140	GLY	3.5
1	D	285	ARG	3.5
1	D	150	TRP	3.4
1	A	240	PRO	3.4
1	D	88	GLY	3.4
1	D	229	SER	3.4
1	B	228	GLU	3.4
1	C	312	LYS	3.4
1	A	249	LEU	3.4
1	D	70	ALA	3.4
1	B	317	THR	3.4
1	B	347	LEU	3.4
1	B	29	LYS	3.4
1	C	373	ARG	3.4
1	A	186	ASP	3.4
1	C	344	ASP	3.4
1	A	134	ILE	3.4
1	D	357	ALA	3.4
1	B	154	GLY	3.4
1	C	153	LEU	3.4
1	A	59	ARG	3.4
1	D	408	SER	3.4
1	D	415	TYR	3.4
1	B	211	THR	3.4
1	C	151	LEU	3.4
1	D	421	PHE	3.4
1	B	402	VAL	3.3
1	A	416	TYR	3.3
1	C	126	LEU	3.3
1	A	228	GLU	3.3
1	D	350	GLY	3.3
1	C	150	TRP	3.3
1	C	74	ARG	3.3
1	C	36	GLN	3.3
1	A	33	LEU	3.3
1	A	403	LYS	3.3
1	A	390	ASN	3.3
1	C	294	GLU	3.3
1	D	243	PHE	3.3
1	A	193	VAL	3.3
1	D	376	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	137	PHE	3.3
1	D	256	ILE	3.3
1	A	284	SER	3.3
1	A	58	ALA	3.3
1	D	370	LEU	3.3
1	C	258	ILE	3.3
1	A	167	ASP	3.3
1	B	135	LYS	3.3
1	C	437	THR	3.3
1	D	473	ILE	3.2
1	C	364	VAL	3.2
1	A	51	THR	3.2
1	B	86	THR	3.2
1	C	12	THR	3.2
1	A	173	ASN	3.2
1	B	414	ALA	3.2
1	B	73	LEU	3.2
1	C	147	VAL	3.2
1	A	142	GLU	3.2
1	C	104	ALA	3.2
1	C	411	GLN	3.2
1	D	176	TYR	3.2
1	B	37	VAL	3.2
1	D	102	ASN	3.2
1	B	447	ARG	3.2
1	A	384	ILE	3.2
1	B	150	TRP	3.2
1	C	215	TYR	3.2
1	A	147	VAL	3.2
1	C	329	ILE	3.2
1	B	91	VAL	3.2
1	D	85	SER	3.2
1	D	279	CYS	3.2
1	B	461	PRO	3.2
1	C	227	GLY	3.2
1	B	134	ILE	3.1
1	D	221	HIS	3.1
1	C	377	THR	3.1
1	A	104	ALA	3.1
1	A	242	ALA	3.1
1	B	368	ARG	3.1
1	A	230	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	112	ILE	3.1
1	B	90	ILE	3.1
1	A	330	PHE	3.1
1	C	189	PHE	3.1
1	C	92	ARG	3.1
1	C	193	VAL	3.1
1	D	472	LYS	3.1
1	C	279	CYS	3.1
1	A	114	LEU	3.1
1	B	324	ARG	3.1
1	B	9	TRP	3.1
1	D	471	LYS	3.1
1	C	277	LEU	3.1
1	B	335	ASP	3.1
1	B	341	ILE	3.1
1	C	333	ILE	3.1
1	A	392	PRO	3.1
1	A	196	TYR	3.1
1	A	325	TYR	3.1
1	B	440	VAL	3.1
1	D	347	LEU	3.1
1	B	58	ALA	3.1
1	A	152	GLU	3.1
1	B	288	TYR	3.1
1	B	378	TYR	3.1
1	D	74	ARG	3.1
1	A	8	GLY	3.1
1	D	387	GLY	3.1
1	C	363	PHE	3.1
1	D	378	TYR	3.0
1	A	94	TRP	3.0
1	D	120	GLY	3.0
1	C	29	LYS	3.0
1	D	371	ASN	3.0
1	C	288	TYR	3.0
1	C	386	GLU	3.0
1	A	322	THR	3.0
1	B	340	LEU	3.0
1	A	410	ASP	3.0
1	B	433	HIS	3.0
1	C	101	ASN	3.0
1	C	421	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	91	VAL	3.0
1	D	91	VAL	3.0
1	B	103	LEU	3.0
1	A	150	TRP	3.0
1	B	389	ILE	3.0
1	B	139	GLU	3.0
1	D	123	LEU	3.0
1	D	291	LEU	3.0
1	A	473	ILE	3.0
1	B	268	ALA	3.0
1	C	262	ILE	3.0
1	A	11	VAL	3.0
1	B	350	GLY	3.0
1	A	211	THR	3.0
1	B	146	CYS	3.0
1	B	166	LEU	3.0
1	B	298	ILE	3.0
1	B	473	ILE	3.0
1	C	259	ILE	3.0
1	A	76	GLY	3.0
1	D	286	ASP	3.0
1	C	9	TRP	3.0
1	B	54	VAL	3.0
1	B	193	VAL	3.0
1	D	469	THR	3.0
1	C	346	TYR	2.9
1	D	168	TYR	2.9
1	D	328	ILE	2.9
1	C	138	PHE	2.9
1	C	403	LYS	2.9
1	B	364	VAL	2.9
1	B	422	HIS	2.9
1	A	151[A]	LEU	2.9
1	C	416	TYR	2.9
1	D	244	GLY	2.9
1	D	205	VAL	2.9
1	C	123	LEU	2.9
1	D	158	SER	2.9
1	D	220	LEU	2.9
1	C	440	VAL	2.9
1	B	287	SER	2.9
1	C	85	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	142	GLU	2.9
1	B	169	ASP	2.9
1	C	299	THR	2.9
1	A	232	VAL	2.9
1	C	408	SER	2.9
1	A	103	LEU	2.9
1	B	419	LEU	2.9
1	C	239	GLN	2.9
1	B	353	TYR	2.9
1	A	55	ASP	2.9
1	C	392	PRO	2.9
1	B	253	GLY	2.9
1	B	397	ASN	2.9
1	B	97	LEU	2.9
1	D	254	LYS	2.9
1	B	117	ALA	2.9
1	A	85	SER	2.8
1	D	330	PHE	2.8
1	B	191	ASP	2.8
1	B	404	ALA	2.8
1	C	328	ILE	2.8
1	D	172	ALA	2.8
1	C	81	CYS	2.8
1	A	45	TYR	2.8
1	A	154	GLY	2.8
1	B	310	PHE	2.8
1	B	330	PHE	2.8
1	C	178	PHE	2.8
1	B	438	VAL	2.8
1	B	131	LEU	2.8
1	D	8	GLY	2.8
1	B	269	THR	2.8
1	D	344	ASP	2.8
1	C	379	PHE	2.8
1	A	311	VAL	2.8
1	A	148	LEU	2.8
1	B	240	PRO	2.8
1	B	102	ASN	2.8
1	A	10	SER	2.8
1	A	75	ASP	2.8
1	A	437	THR	2.8
1	B	170	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	236	THR	2.8
1	A	57	ILE	2.8
1	B	185	ILE	2.8
1	C	90	ILE	2.8
1	C	405	TYR	2.8
1	A	102	ASN	2.8
1	C	192	ALA	2.8
1	D	351	PRO	2.8
1	B	111	LEU	2.8
1	B	216	SER	2.8
1	C	136	SER	2.8
1	D	230	LEU	2.8
1	D	334	ASP	2.8
1	C	112	ILE	2.8
1	C	389	ILE	2.8
1	B	147	VAL	2.7
1	C	52	VAL	2.7
1	C	117	ALA	2.7
1	C	265	ALA	2.7
1	B	17	TYR	2.7
1	A	348	THR	2.7
1	D	377	THR	2.7
1	D	191	ASP	2.7
1	A	105	LYS	2.7
1	D	336	ARG	2.7
1	C	173	ASN	2.7
1	D	389	ILE	2.7
1	B	196	TYR	2.7
1	B	81	CYS	2.7
1	D	434	PRO	2.7
1	B	130	ARG	2.7
1	B	190	TYR	2.7
1	B	215	TYR	2.7
1	A	137	PHE	2.7
1	C	397	ASN	2.7
1	A	181	THR	2.7
1	D	433	HIS	2.7
1	C	132	GLY	2.7
1	C	156	ASP	2.7
1	B	98	TYR	2.7
1	C	313	THR	2.7
1	A	47	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	129	SER	2.6
1	D	392	PRO	2.6
1	A	90	ILE	2.6
1	B	329	ILE	2.6
1	B	333	ILE	2.6
1	A	222	GLN	2.6
1	A	179	VAL	2.6
1	A	253	GLY	2.6
1	D	206	VAL	2.6
1	A	326	SER	2.6
1	B	219	LYS	2.6
1	A	279[A]	CYS	2.6
1	B	411	GLN	2.6
1	A	117	ALA	2.6
1	B	182	GLY	2.6
1	B	374	GLY	2.6
1	C	197	THR	2.6
1	A	363	PHE	2.6
1	D	309	GLU	2.6
1	D	37	VAL	2.6
1	B	118	ASN	2.6
1	B	226	ASN	2.6
1	B	297	ASN	2.6
1	A	146	CYS	2.6
1	D	130	ARG	2.6
1	A	467	LYS	2.6
1	B	243	PHE	2.6
1	C	103	LEU	2.6
1	C	124	ALA	2.6
1	D	117	ALA	2.6
1	A	262	ILE	2.6
1	B	469	THR	2.6
1	A	74	ARG	2.6
1	C	110	HIS	2.6
1	C	473	ILE	2.6
1	B	408	SER	2.6
1	D	86	THR	2.6
1	D	398	LEU	2.6
1	A	52	VAL	2.6
1	B	315	VAL	2.6
1	B	362	PHE	2.6
1	D	3	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	34	ASP	2.6
1	B	172	ALA	2.6
1	C	435	ASN	2.6
1	D	57	ILE	2.6
1	B	313	THR	2.5
1	B	373	ARG	2.5
1	C	181	THR	2.5
1	A	159[A]	TRP	2.5
1	D	116	PRO	2.5
1	D	448	VAL	2.5
1	C	76	GLY	2.5
1	D	290	LYS	2.5
1	A	404	ALA	2.5
1	A	250	SER	2.5
1	D	16	THR	2.5
1	D	90	ILE	2.5
1	B	392	PRO	2.5
1	A	123	LEU	2.5
1	B	295	LEU	2.5
1	B	345	LEU	2.5
1	C	432	LEU	2.5
1	D	166	LEU	2.5
1	A	175	VAL	2.5
1	A	440	VAL	2.5
1	B	467	LYS	2.5
1	D	135	LYS	2.5
1	D	146	CYS	2.5
1	C	357	ALA	2.5
1	A	32	LYS	2.5
1	A	165	TRP	2.5
1	A	198	GLY	2.5
1	C	97	LEU	2.5
1	C	108	LEU	2.5
1	C	206	VAL	2.5
1	B	284	SER	2.5
1	D	106	CYS	2.5
1	B	356	GLN	2.5
1	A	191	ASP	2.5
1	D	324	ARG	2.5
1	C	33	LEU	2.5
1	C	23	TRP	2.5
1	D	379	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	17	TYR	2.5
1	C	53	THR	2.5
1	A	368	ARG	2.5
1	D	185	ILE	2.5
1	D	262	ILE	2.5
1	D	198	GLY	2.5
1	D	338	ASN	2.5
1	C	114	LEU	2.5
1	A	400	PHE	2.5
1	C	159	TRP	2.5
1	D	64	ALA	2.5
1	A	168	TYR	2.5
1	A	391	THR	2.5
1	B	351	PRO	2.5
1	C	118	ASN	2.5
1	B	274	ILE	2.5
1	C	370	LEU	2.5
1	D	54	VAL	2.4
1	B	238	THR	2.4
1	A	190	TYR	2.4
1	B	119	HIS	2.4
1	B	176	TYR	2.4
1	C	182	GLY	2.4
1	A	431	ILE	2.4
1	B	384	ILE	2.4
1	C	256	ILE	2.4
1	C	352	GLN	2.4
1	D	296	ASP	2.4
1	C	401	ARG	2.4
1	C	380	LEU	2.4
1	C	430	LYS	2.4
1	B	208	VAL	2.4
1	B	101	ASN	2.4
1	C	243	PHE	2.4
1	D	362	PHE	2.4
1	A	127	GLY	2.4
1	D	313	THR	2.4
1	A	318	ARG	2.4
1	C	417	ARG	2.4
1	A	184	LYS	2.4
1	C	121	SER	2.4
1	B	358	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	64	ALA	2.4
1	C	349	ALA	2.4
1	D	192	ALA	2.4
1	C	31	GLY	2.4
1	A	329	ILE	2.4
1	B	332	LEU	2.4
1	C	242	ALA	2.4
1	C	269	THR	2.4
1	D	282	VAL	2.4
1	B	328	ILE	2.4
1	D	22	GLN	2.4
1	B	291	LEU	2.4
1	A	80	ALA	2.4
1	B	278	ARG	2.4
1	D	13	HIS	2.4
1	D	388	GLY	2.4
1	A	91	VAL	2.4
1	C	362	PHE	2.4
1	D	48	PHE	2.4
1	C	369	ASN	2.4
1	D	405	TYR	2.4
1	D	78	ARG	2.4
1	D	275	TRP	2.4
1	A	361	GLY	2.4
1	A	161	LEU	2.4
1	D	217	LEU	2.4
1	A	462	ALA	2.4
1	B	104	ALA	2.4
1	D	171	THR	2.4
1	A	421	PHE	2.4
1	D	232	VAL	2.4
1	C	133	ARG	2.3
1	D	442	ILE	2.3
1	A	291	LEU	2.3
1	B	223	GLU	2.3
1	C	54	VAL	2.3
1	D	175	VAL	2.3
1	C	169	ASP	2.3
1	A	122	ALA	2.3
1	A	210	ALA	2.3
1	A	238	THR	2.3
1	B	377	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	420	ASP	2.3
1	D	335	ASP	2.3
1	B	453	PHE	2.3
1	D	406	PRO	2.3
1	B	45	TYR	2.3
1	B	64	ALA	2.3
1	C	70	ALA	2.3
1	C	217	LEU	2.3
1	D	462	ALA	2.3
1	A	272	THR	2.3
1	B	197	THR	2.3
1	B	449	ASP	2.3
1	D	287	SER	2.3
1	B	311	VAL	2.3
1	B	8	GLY	2.3
1	D	87	GLY	2.3
1	B	212	ASN	2.3
1	D	391	THR	2.3
1	B	472	LYS	2.3
1	B	77	GLN	2.3
1	D	160	GLN	2.3
1	A	208	VAL	2.3
1	B	400	PHE	2.3
1	C	130	ARG	2.3
1	B	55	ASP	2.3
1	D	71	ASP	2.3
1	A	155	SER	2.3
1	D	124	ALA	2.3
1	C	413	LEU	2.3
1	A	62	ASP	2.3
1	A	214	ASN	2.3
1	A	305	ASN	2.3
1	D	458	ASN	2.3
1	A	4	ILE	2.3
1	A	40	ILE	2.3
1	A	349	ALA	2.3
1	A	377	THR	2.2
1	A	120	GLY	2.2
1	A	374	GLY	2.2
1	C	59	ARG	2.2
1	B	255	ASN	2.2
1	C	311	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	159	TRP	2.2
1	A	115	ALA	2.2
1	D	59	ARG	2.2
1	C	127	GLY	2.2
1	D	224	GLY	2.2
1	D	437	THR	2.2
1	D	41	TYR	2.2
1	D	294	GLU	2.2
1	B	59	ARG	2.2
1	B	109	SER	2.2
1	B	181	THR	2.2
1	B	464	ILE	2.2
1	C	14	THR	2.2
1	C	246	LEU	2.2
1	C	291	LEU	2.2
1	A	320	TYR	2.2
1	D	45	TYR	2.2
1	B	89	PRO	2.2
1	B	116	PRO	2.2
1	B	232	VAL	2.2
1	C	310	PHE	2.2
1	C	374	GLY	2.2
1	A	294	GLU	2.2
1	D	27	GLN	2.2
1	B	463	LYS	2.2
1	D	190	TYR	2.2
1	D	468	PRO	2.2
1	C	68	GLU	2.2
1	D	56	ASP	2.2
1	C	170	CYS	2.2
1	C	22	GLN	2.2
1	C	4	ILE	2.2
1	A	290	LYS	2.2
1	A	351	PRO	2.2
1	C	89	PRO	2.2
1	A	71[A]	ASP	2.2
1	A	215	TYR	2.2
1	B	75	ASP	2.2
1	D	320	TYR	2.2
1	B	178	PHE	2.2
1	D	214	ASN	2.2
1	D	390	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	273	ALA	2.2
1	C	391	THR	2.2
1	D	238	THR	2.2
1	D	242	ALA	2.2
1	B	370	LEU	2.2
1	D	314	LEU	2.2
1	D	444	LEU	2.2
1	A	261	SER	2.2
1	C	381	ASP	2.2
1	C	325	TYR	2.1
1	D	92	ARG	2.1
1	A	48	PHE	2.1
1	A	178	PHE	2.1
1	B	124	ALA	2.1
1	D	0	THR	2.1
1	A	259	ILE	2.1
1	B	106	CYS	2.1
1	D	153	LEU	2.1
1	D	202	SER	2.1
1	A	266	ASN	2.1
1	D	39	ASN	2.1
1	A	336	ARG	2.1
1	A	448	VAL	2.1
1	C	205	VAL	2.1
1	A	171	THR	2.1
1	B	0	THR	2.1
1	B	122	ALA	2.1
1	B	265	ALA	2.1
1	C	60	ALA	2.1
1	C	64	ALA	2.1
1	C	462	ALA	2.1
1	A	293	LYS	2.1
1	D	29	LYS	2.1
1	D	50	ASP	2.1
1	D	30	GLN	2.1
1	A	212	ASN	2.1
1	B	220	LEU	2.1
1	A	244	GLY	2.1
1	B	289	ASN	2.1
1	C	461	PRO	2.1
1	D	216	SER	2.1
1	C	278	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	373	ARG	2.1
1	D	417	ARG	2.1
1	B	110	HIS	2.1
1	A	60	ALA	2.1
1	A	451	THR	2.1
1	A	338	ASN	2.1
1	C	194	ASN	2.1
1	D	24	LEU	2.1
1	D	345	LEU	2.1
1	A	283	LYS	2.1
1	B	72	LYS	2.1
1	B	270	HIS	2.1
1	C	13	HIS	2.1
1	B	36	GLN	2.1
1	B	267	ALA	2.1
1	C	336	ARG	2.1
1	C	353	TYR	2.1
1	D	80	ALA	2.1
1	A	465	SER	2.1
1	C	143	PRO	2.1
1	A	153	LEU	2.1
1	D	128	LYS	2.1
1	A	474	ASP	2.1
1	D	96	ASP	2.1
1	B	142	GLU	2.1
1	B	437	THR	2.1
1	B	10	SER	2.1
1	C	168	TYR	2.1
1	D	353	TYR	2.1
1	C	406	PRO	2.1
1	A	69	ILE	2.1
1	D	277	LEU	2.1
1	B	26	ASN	2.1
1	D	236	THR	2.1
1	A	209	ALA	2.1
1	C	360	ALA	2.1
1	D	115	ALA	2.1
1	A	37	VAL	2.1
1	B	388	GLY	2.1
1	C	87	GLY	2.1
1	C	351	PRO	2.1
1	C	400	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	142	GLU	2.0
1	D	365	ASP	2.0
1	C	295	LEU	2.0
1	C	442	ILE	2.0
1	C	32	LYS	2.0
1	A	83	THR	2.0
1	B	192	ALA	2.0
1	C	158	SER	2.0
1	A	346	TYR	2.0
1	D	196	TYR	2.0
1	A	20	LEU	2.0
1	B	432	LEU	2.0
1	B	338	ASN	2.0
1	A	299	THR	2.0
1	D	352	GLN	2.0
1	D	354	SER	2.0
1	D	445	GLN	2.0
1	A	169	ASP	2.0
1	A	344	ASP	2.0
1	D	55	ASP	2.0
1	D	133	ARG	2.0
1	C	65	VAL	2.0
1	B	99	PHE	2.0
1	A	98	TYR	2.0
1	B	416	TYR	2.0
1	C	45	TYR	2.0
1	B	395	GLN	2.0
1	B	465	SER	2.0
1	C	263	THR	2.0
1	C	296	ASP	2.0
1	D	155	SER	2.0
1	D	403	LYS	2.0
1	D	420	ASP	2.0
1	B	209	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

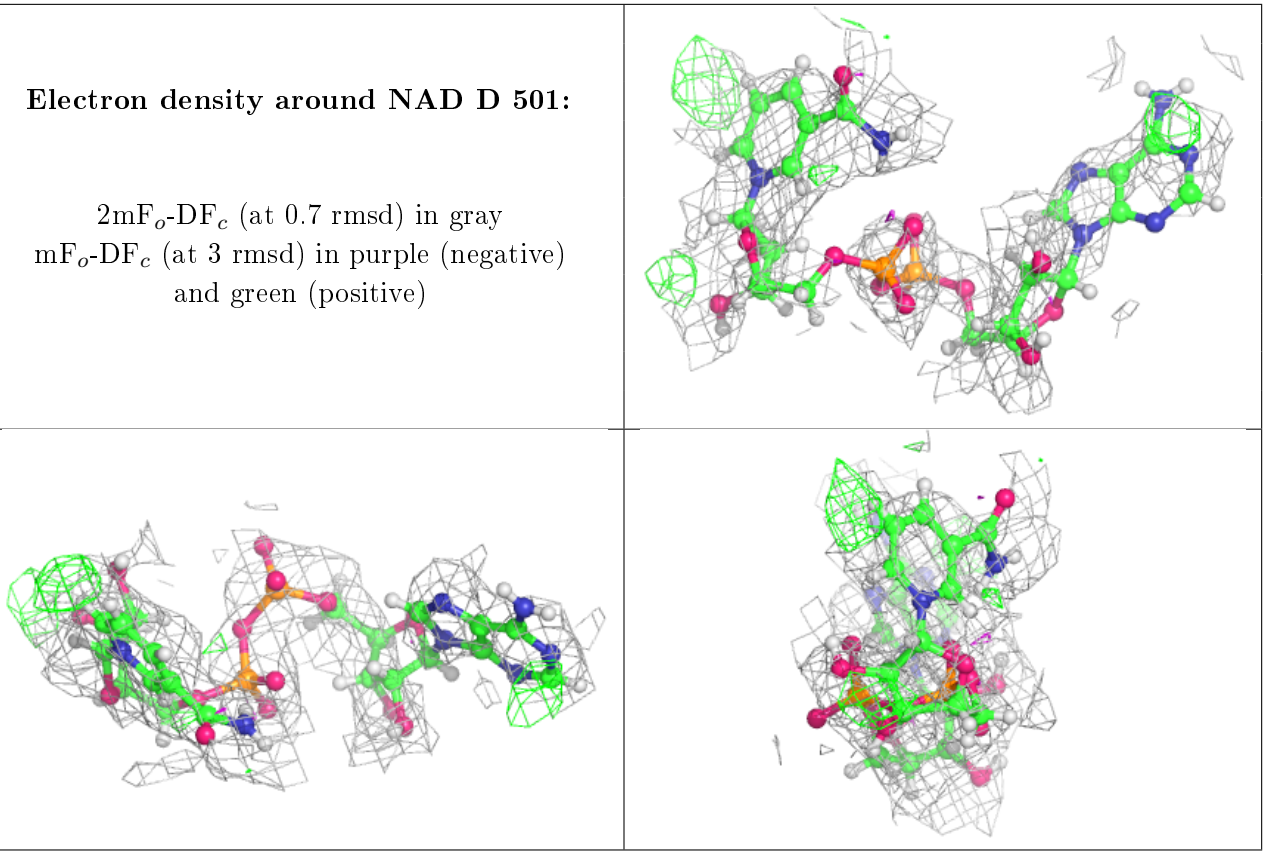
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	D	501	44/44	0.59	0.42	23,48,62,69	70
2	NAD	A	501	44/44	0.66	0.30	22,38,52,55	0
2	NAD	D	502	44/44	0.68	0.44	22,34,44,53	70
2	NAD	A	502	44/44	0.73	0.28	18,31,45,55	70
2	NAD	C	501	44/44	0.73	0.33	15,30,43,49	70
2	NAD	B	602	44/44	0.74	0.33	10,28,39,46	0
2	NAD	B	601	44/44	0.76	0.30	21,38,51,57	70
2	NAD	C	502	44/44	0.82	0.26	6,24,34,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

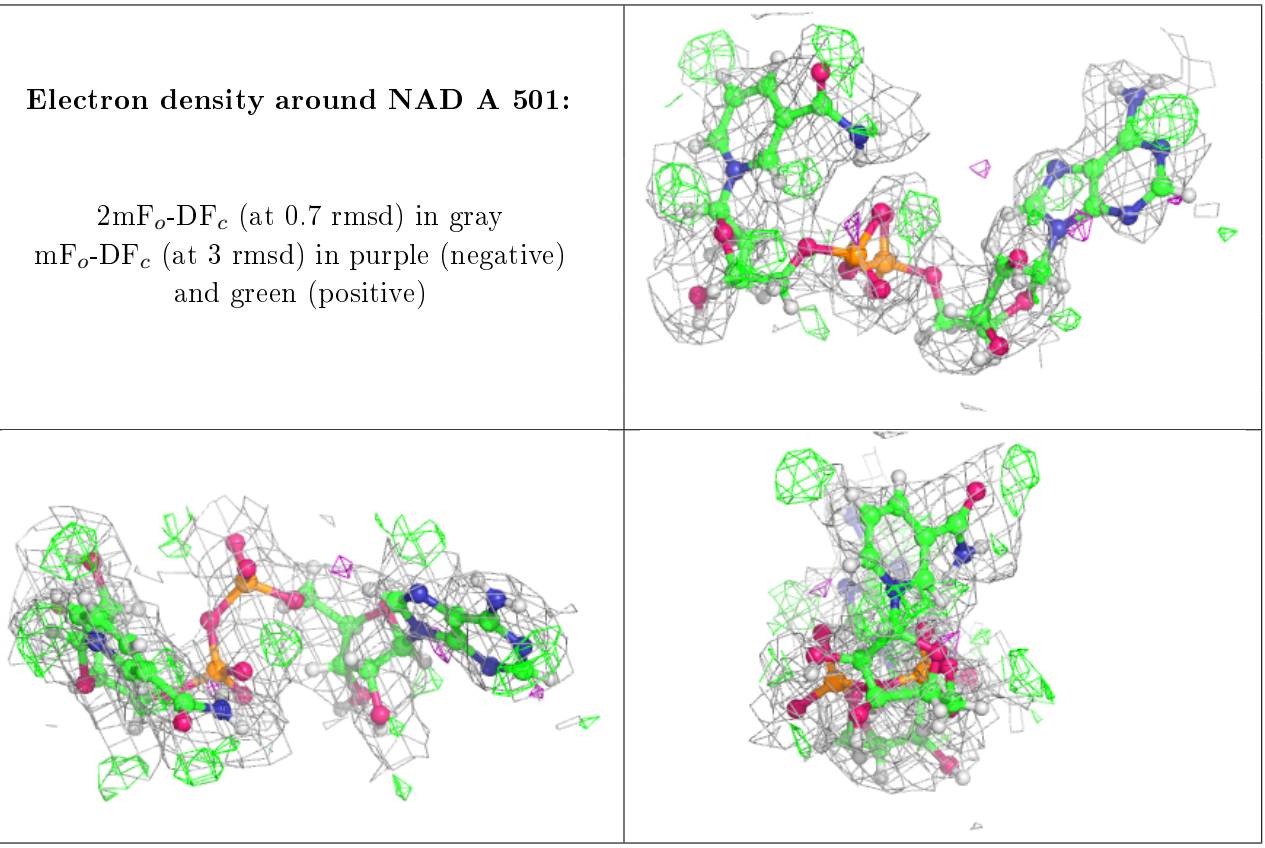
Electron density around NAD D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



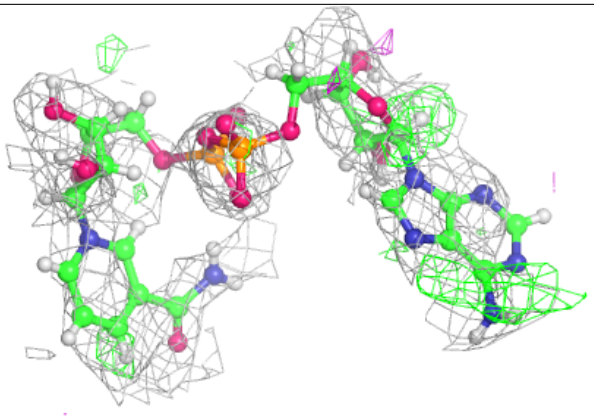
Electron density around NAD A 501:

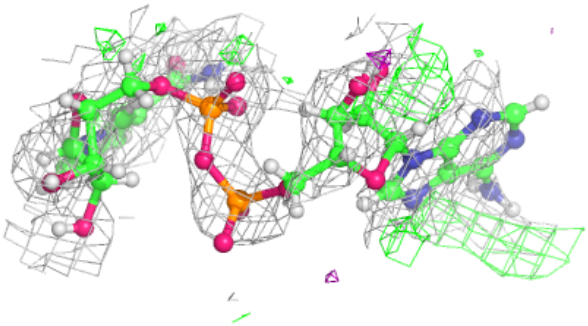
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

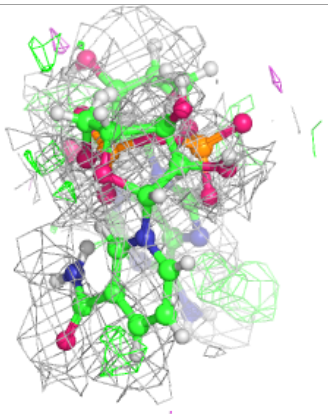


Electron density around NAD D 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

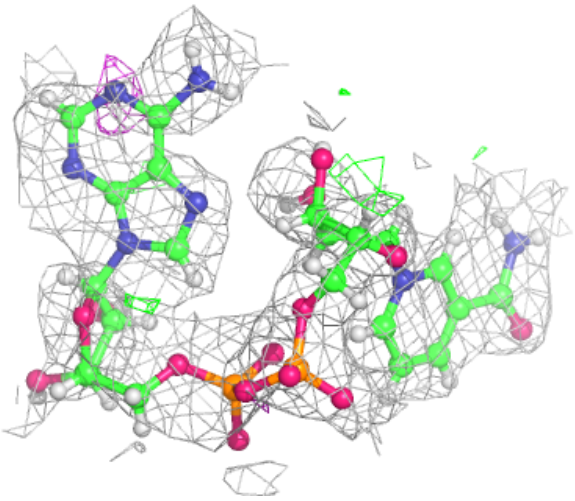


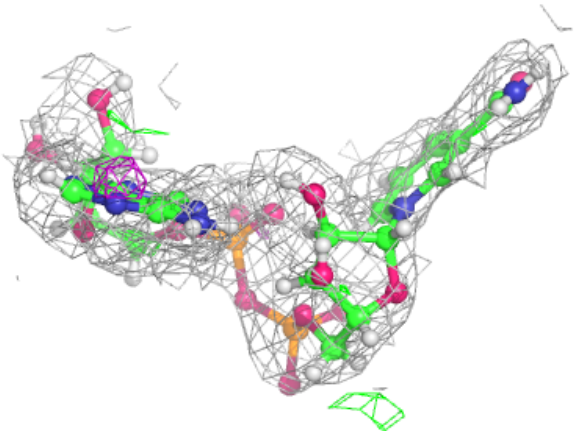


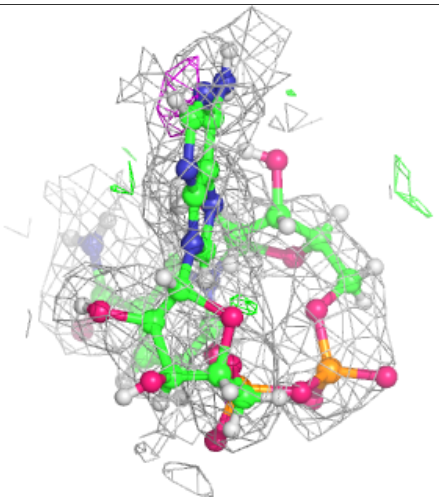


Electron density around NAD A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

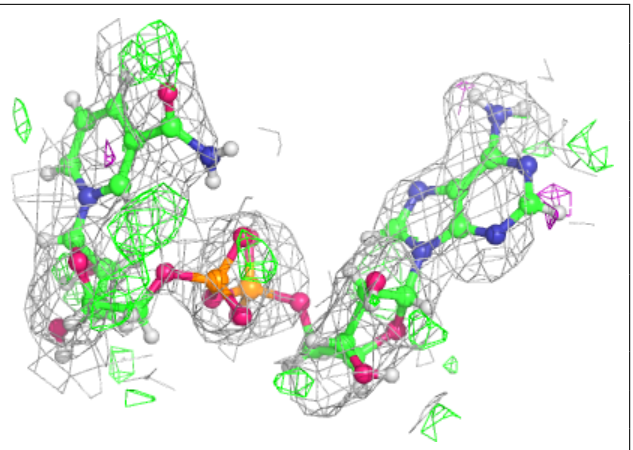


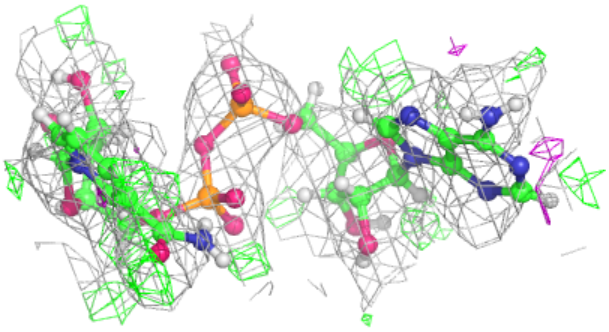


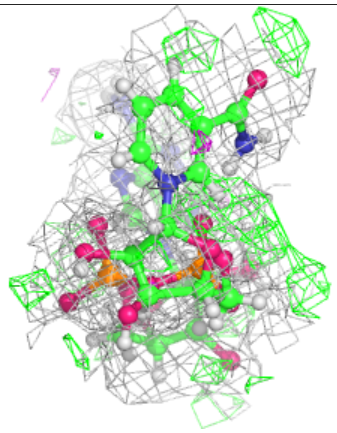


Electron density around NAD C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

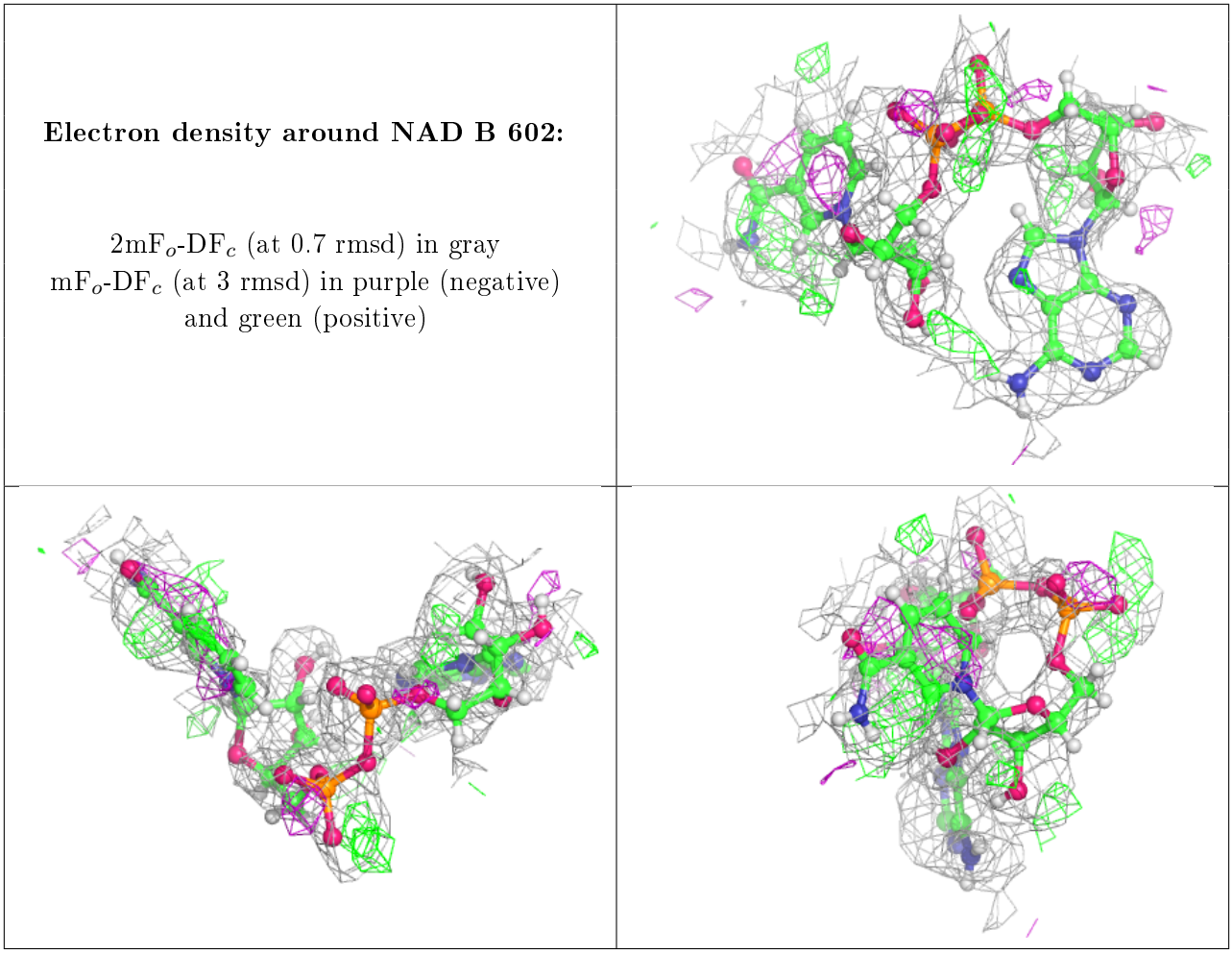






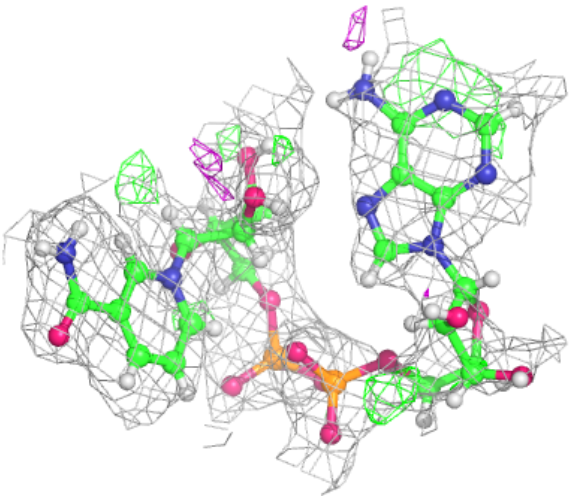
Electron density around NAD B 602:

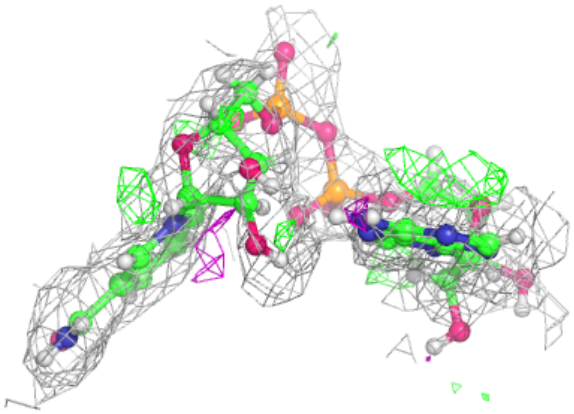
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

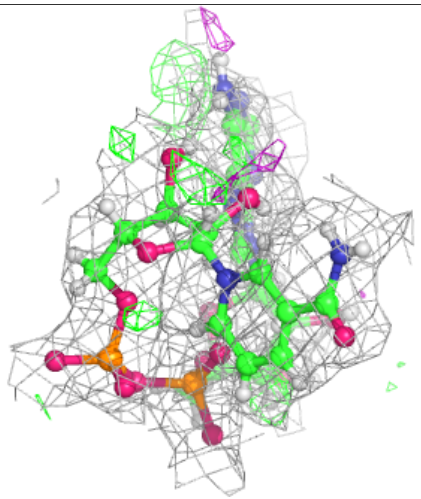


Electron density around NAD B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

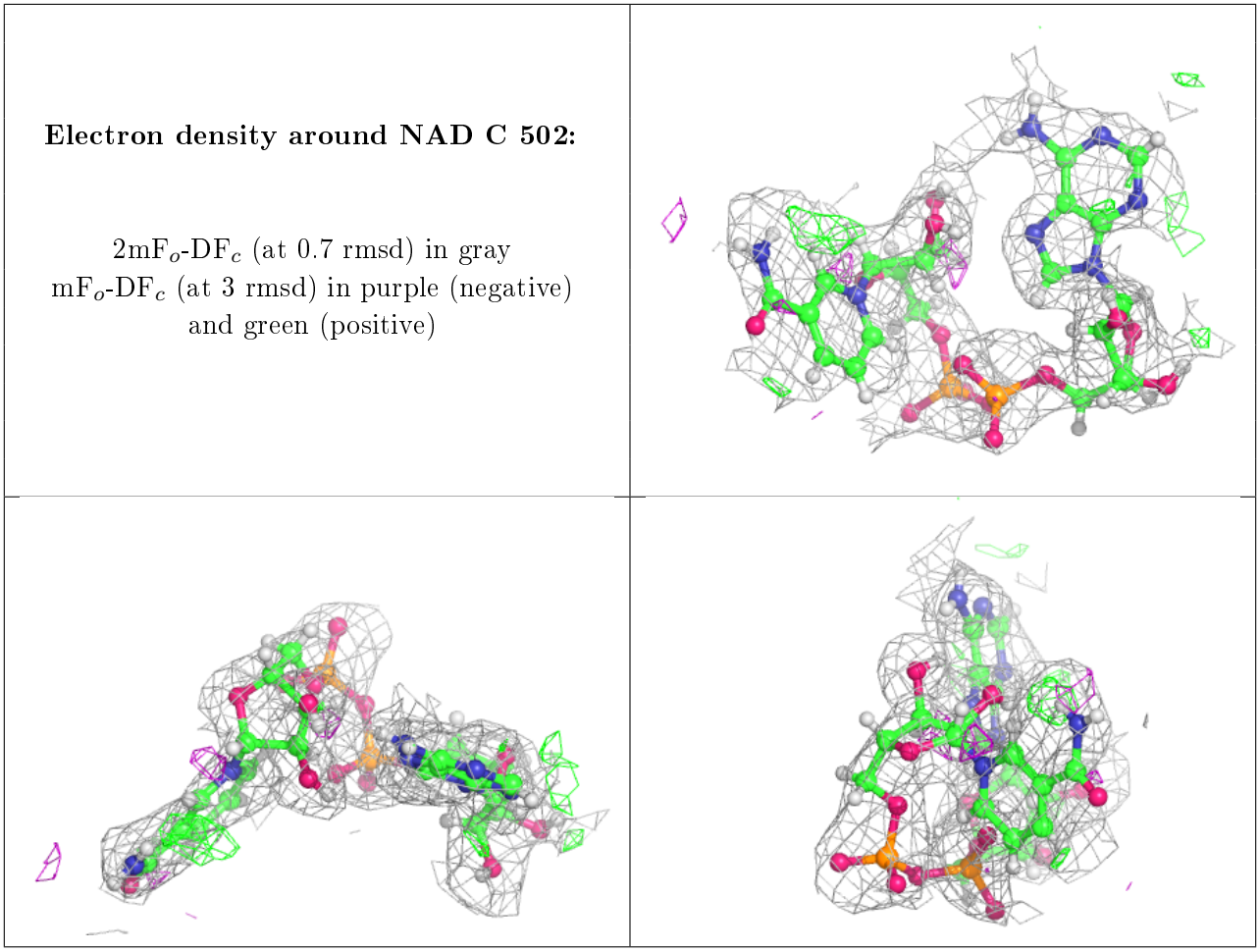






Electron density around NAD C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.