



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:33 AM UTC

PDB ID : 6ZTH / pdb_00006zth
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

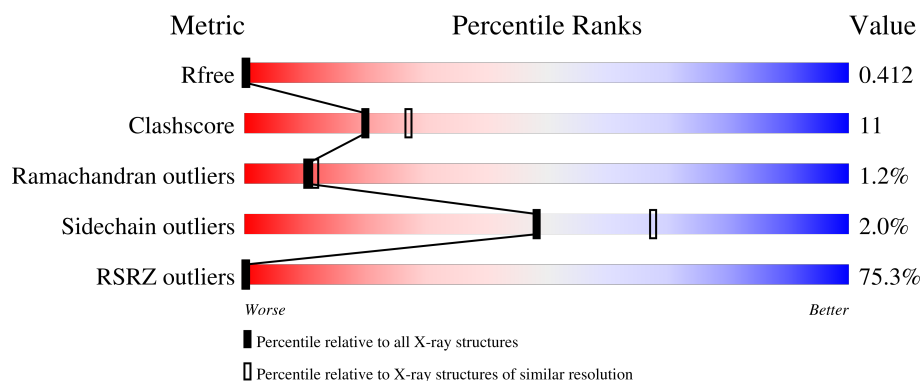
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	489	68% 74% 21% ..
1	B	489	69% 73% 22% ..
1	C	489	71% 74% 20% ..
1	D	489	74% 73% 22% ..

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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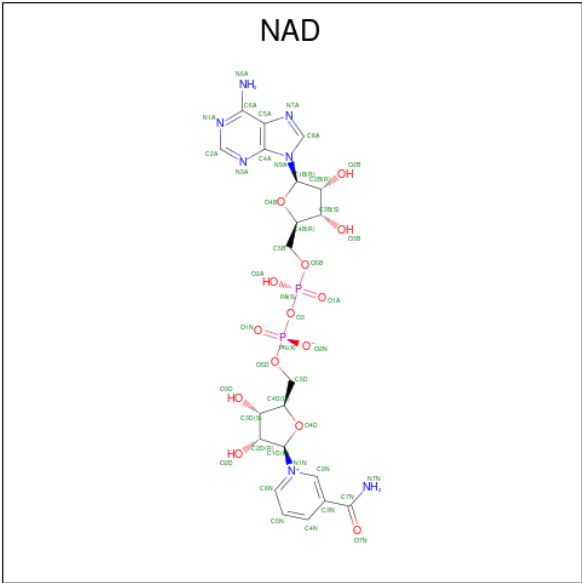
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP A0A378K488
B	-8	PRO	-	expression tag	UNP A0A378K488
B	-7	GLN	-	expression tag	UNP A0A378K488
B	-6	PHE	-	expression tag	UNP A0A378K488
B	-5	GLU	-	expression tag	UNP A0A378K488
B	-4	LYS	-	expression tag	UNP A0A378K488
B	-3	GLY	-	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 (CCD ID: 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 131	O 131	0	0
3	B	125	Total 125	O 125	0	0
3	C	148	Total 148	O 148	0	0
3	D	139	Total 139	O 139	0	0

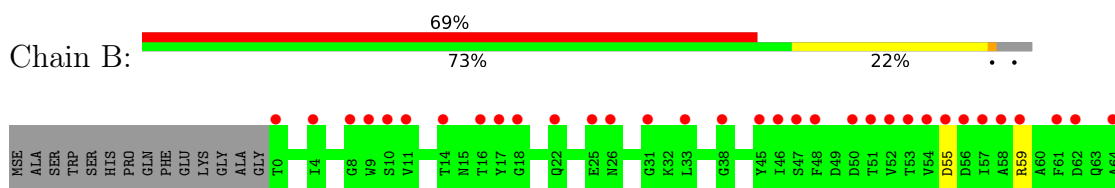
3 Residue-property plots

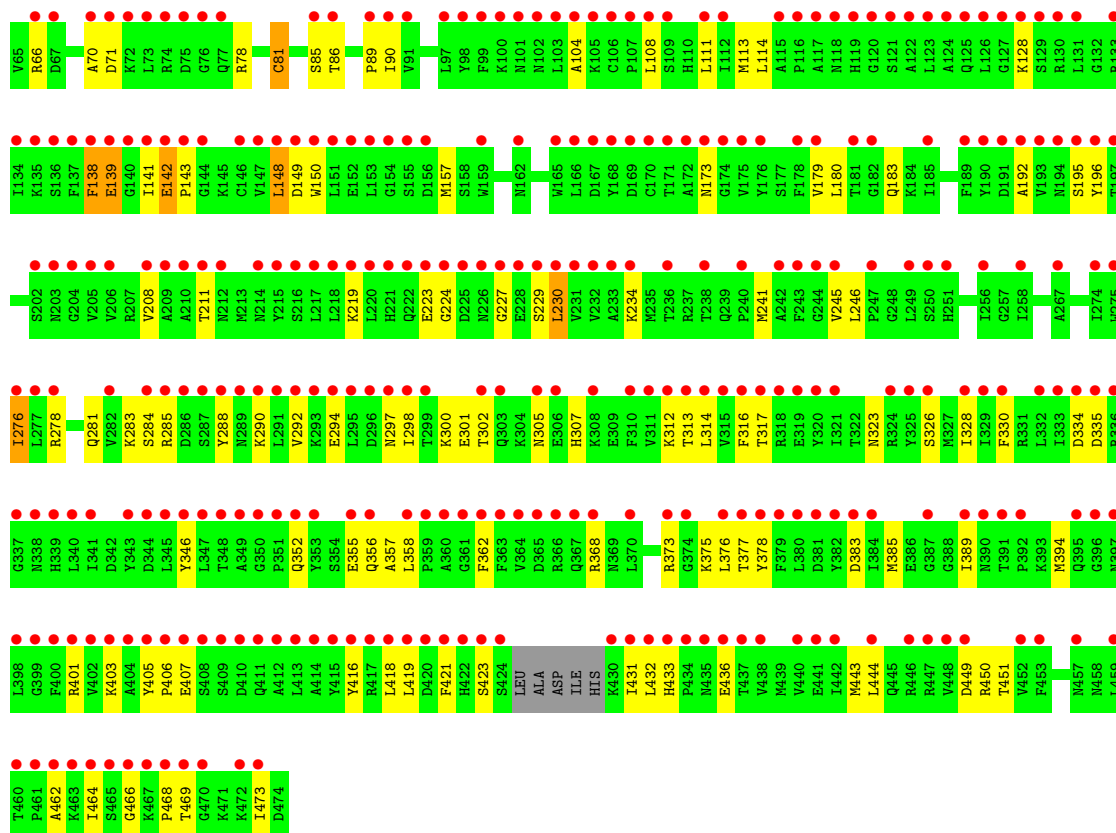
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

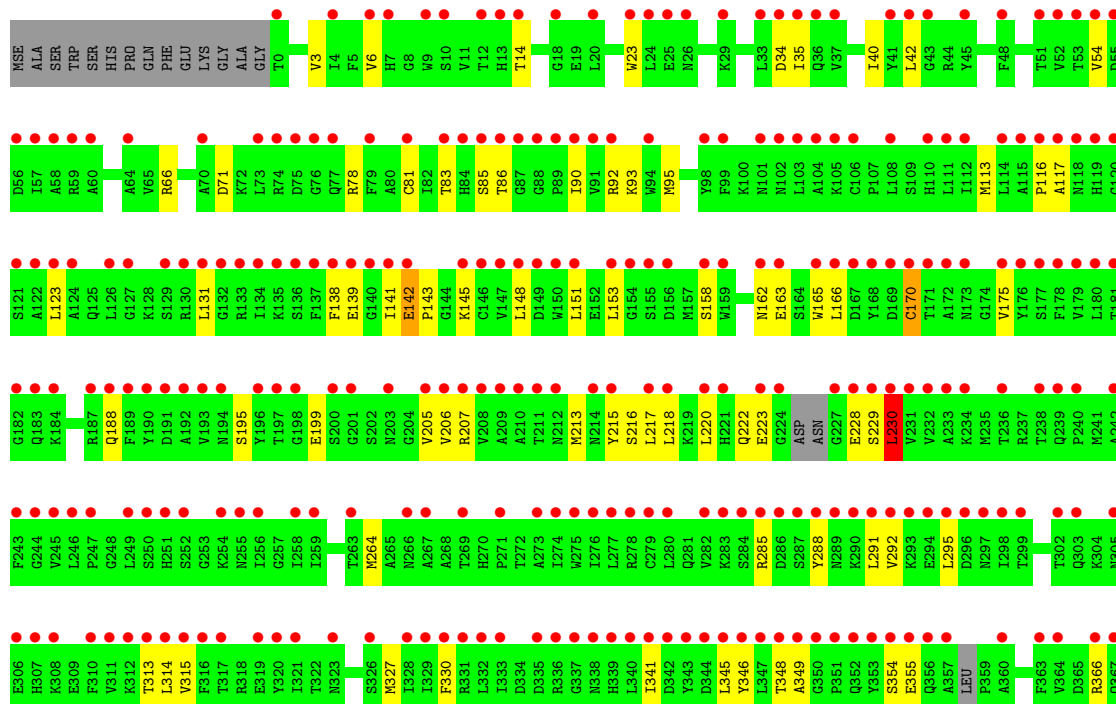
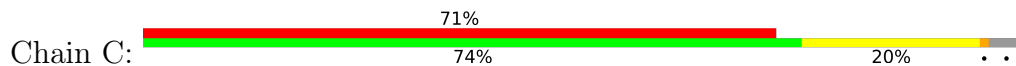


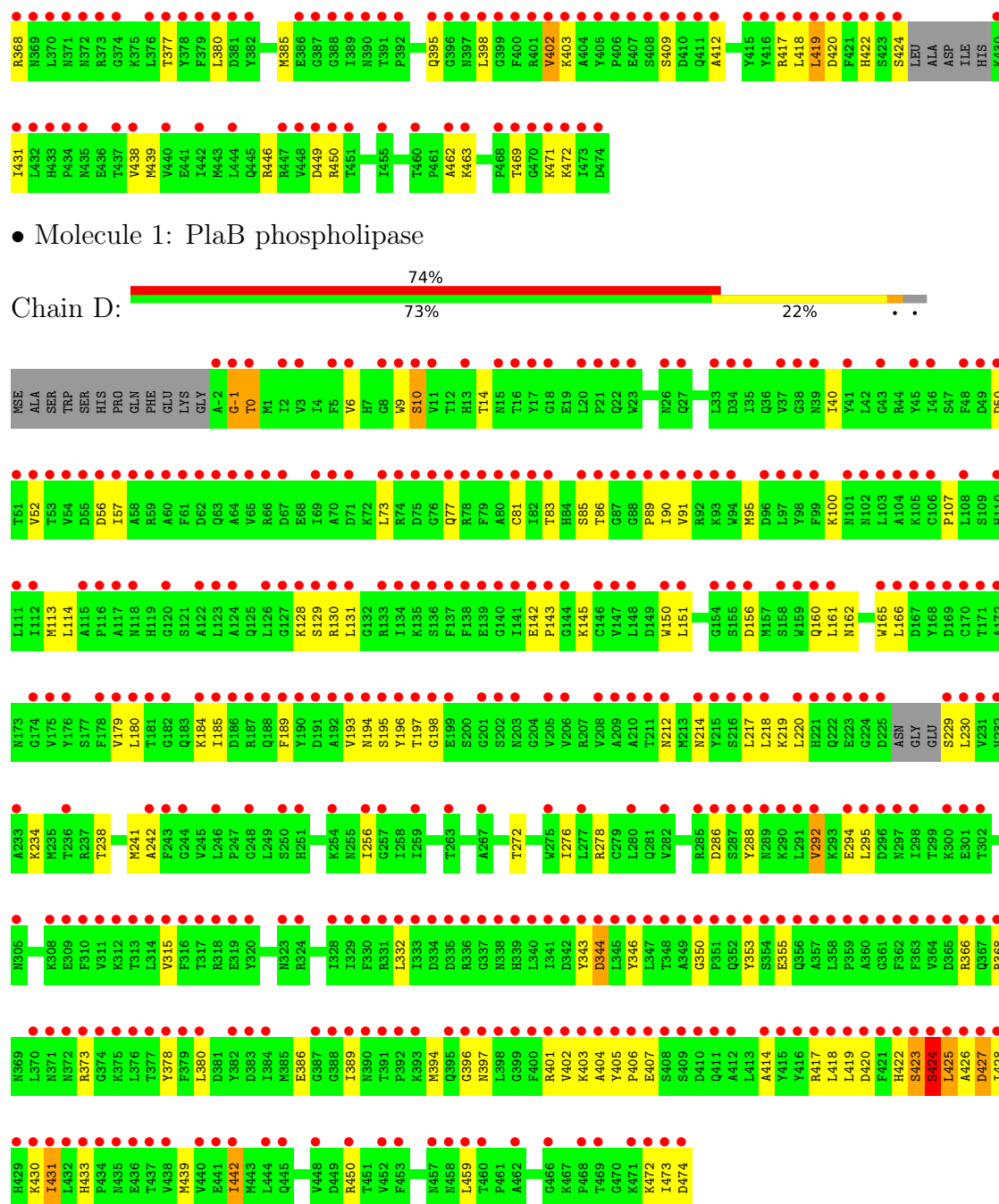
• Molecule 1: PlaB phospholipase





● Molecule 1: PlaB phospholipase





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_3922	Depositor
R, R_{free}	0.364 , 0.413 0.363 , 0.412	Depositor DCC
R_{free} test set	5257 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)	0.37 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.81	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.19	0/3858	0.36	0/5192
1	B	0.14	0/3800	0.35	0/5115
1	C	0.16	0/3788	0.33	0/5094
1	D	0.38	2/3807 (0.1%)	0.35	2/5130 (0.0%)
All	All	0.24	2/15253 (0.0%)	0.35	2/20531 (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	431	ILE	CG1-CD1	-15.59	0.91	1.51
1	D	424	SER	CB-OG	-15.54	1.11	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	431	ILE	CB-CG1-CD1	8.74	132.16	113.80
1	D	424	SER	CA-CB-OG	5.34	121.78	111.10

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

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	82	0
1	B	3734	3683	3700	82	0
1	C	3720	3697	3701	78	0
1	D	3743	3688	3689	109	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	13	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	346	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 (346) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:129:SER:OG	3:D:604:HOH:O	2.08	0.69
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:208:VAL:O	1:B:211:THR:OG1	2.14	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: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:C:450:ARG:HE	1:C:472:LYS:C	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:229:SER:C	1:D:230:LEU:HD23	2.35	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:B:378:TYR:HH	2:D:502:NAD:H61A	1.53	0.49
1:A:150:TRP:HA	1:A:157:MSE:HE3	1.95	0.49
1:C:228:GLU:O	1:C:229:SER:HB3	2.13	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:D:217:LEU:C	1:D:217:LEU:HD13	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:14:THR:HG1	1:B:462:ALA:H	1.61	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:A:405:TYR:HA	1:A:406:PRO:C	2.42	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:A:208:VAL:O	1:A:211:THR:OG1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:393:LYS:NZ	1:C:314:LEU:O	2.50	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:B:405:TYR:HA	1:B:406:PRO:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:419:LEU:C	1:C:419:LEU:HD23	2.44	0.42
1:B:352:GLN:CD	1:B:352:GLN:H	2.28	0.42
1:C:34:ASP:O	1:C:34:ASP:CG	2.62	0.42
1:D:217:LEU:HD11	1:D:219:LYS:HE2	2.01	0.42
1:D:344:ASP:OD2	1:D:405:TYR:OH	2.31	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: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:B:219:LYS:HZ2	1:B:234:LYS:HD2	1.85	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:B:316:PHE:CD1	1:B:316:PHE:C	2.98	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:405:TYR:HA	1:D:406:PRO:C	2.46	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:A:350:GLY:O	1:A:351:PRO:C	2.65	0.40
1:B:357:ALA:HB2	3:B:702:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:427:ASP:OD1	1:D:427:ASP:C	2.63	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

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	471/489 (96%)	445 (94%)	22 (5%)	4 (1%)	16	20
1	B	467/489 (96%)	434 (93%)	27 (6%)	6 (1%)	9	10
1	C	461/489 (94%)	437 (95%)	18 (4%)	6 (1%)	9	10
1	D	470/489 (96%)	439 (93%)	25 (5%)	6 (1%)	9	10
All	All	1869/1956 (96%)	1755 (94%)	92 (5%)	22 (1%)	10	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	THR
1	A	412	ALA
1	B	139	GLU

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Mol	Chain	Res	Type
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 ⓘ

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%)	396 (97%)	11 (3%)	39	58
1	B	403/408 (99%)	398 (99%)	5 (1%)	63	79
1	C	402/408 (98%)	391 (97%)	11 (3%)	39	58
1	D	401/408 (98%)	393 (98%)	8 (2%)	48	67
All	All	1613/1632 (99%)	1578 (98%)	35 (2%)	48	65

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	CYS
1	A	129	SER

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Mol	Chain	Res	Type
1	A	305	ASN
1	A	313	THR
1	A	341[A]	ILE
1	A	341[B]	ILE
1	A	402	VAL
1	A	418	LEU
1	A	432	LEU
1	A	438	VAL
1	A	441	GLU
1	B	81	CYS
1	B	148	LEU
1	B	276	ILE
1	B	285[A]	ARG
1	B	285[B]	ARG
1	C	81	CYS
1	C	158	SER
1	C	170	CYS
1	C	206	VAL
1	C	216	SER
1	C	402	VAL
1	C	419	LEU
1	C	424	SER
1	C	463[A]	LYS
1	C	463[B]	LYS
1	C	471	LYS
1	D	10	SER
1	D	40	ILE
1	D	81	CYS
1	D	292	VAL
1	D	344	ASP
1	D	424	SER
1	D	427	ASP
1	D	442	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	270	HIS
1	A	303	GLN
1	A	411	GLN
1	A	433	HIS

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Mol	Chain	Res	Type
1	A	435	ASN
1	A	445	GLN
1	B	26	ASN
1	B	338	ASN
1	B	352	GLN
1	C	84	HIS
1	C	239	GLN
1	C	305	ASN
1	C	411	GLN
1	D	338	ASN
1	D	458	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	46,48,48	4.06	21 (45%)	64,73,73	1.82	16 (25%)
2	NAD	A	502	-	46,48,48	4.17	21 (45%)	64,73,73	1.84	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	601	-	46,48,48	4.09	21 (45%)	64,73,73	1.82	14 (21%)
2	NAD	A	501	-	46,48,48	4.05	20 (43%)	64,73,73	1.88	16 (25%)
2	NAD	B	602	-	46,48,48	4.07	21 (45%)	64,73,73	1.81	15 (23%)
2	NAD	C	502	-	46,48,48	4.16	21 (45%)	64,73,73	1.83	17 (26%)
2	NAD	D	502	-	46,48,48	4.08	21 (45%)	64,73,73	1.87	18 (28%)
2	NAD	C	501	-	46,48,48	4.06	20 (43%)	64,73,73	1.83	15 (23%)

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	-	-	2/30/62/62	0/5/5/5
2	NAD	A	502	-	-	6/30/62/62	0/5/5/5
2	NAD	B	601	-	-	6/30/62/62	0/5/5/5
2	NAD	A	501	-	-	4/30/62/62	0/5/5/5
2	NAD	B	602	-	-	4/30/62/62	0/5/5/5
2	NAD	C	502	-	-	7/30/62/62	0/5/5/5
2	NAD	D	502	-	-	3/30/62/62	0/5/5/5
2	NAD	C	501	-	-	3/30/62/62	0/5/5/5

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAD	C2D-C3D	-10.75	1.24	1.53
2	C	501	NAD	C2D-C3D	-10.72	1.24	1.53
2	D	502	NAD	C2D-C3D	-10.69	1.24	1.53
2	B	602	NAD	C2D-C3D	-10.67	1.24	1.53
2	D	501	NAD	C2D-C3D	-10.67	1.24	1.53
2	A	501	NAD	C2D-C3D	-10.66	1.24	1.53
2	B	601	NAD	C2D-C3D	-10.59	1.24	1.53
2	A	502	NAD	C2D-C3D	-10.57	1.24	1.53
2	D	502	NAD	C3B-C4B	-10.34	1.26	1.53
2	B	602	NAD	C3B-C4B	-10.33	1.26	1.53
2	C	502	NAD	C3B-C4B	-10.29	1.26	1.53
2	A	502	NAD	C3B-C4B	-10.27	1.26	1.53
2	C	501	NAD	C3B-C4B	-10.26	1.27	1.53
2	D	501	NAD	C3B-C4B	-10.24	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	C3B-C4B	-10.23	1.27	1.53
2	A	501	NAD	C3B-C4B	-10.21	1.27	1.53
2	C	502	NAD	C2B-C1B	-8.85	1.25	1.53
2	A	502	NAD	C2B-C1B	-8.76	1.26	1.53
2	D	502	NAD	O4D-C1D	8.55	1.52	1.40
2	B	601	NAD	C2B-C1B	-8.27	1.27	1.53
2	C	502	NAD	C7N-N7N	8.25	1.48	1.33
2	A	502	NAD	C7N-N7N	8.20	1.48	1.33
2	B	602	NAD	C2B-C1B	-8.19	1.27	1.53
2	B	601	NAD	C7N-N7N	8.18	1.48	1.33
2	A	502	NAD	O4D-C1D	8.16	1.51	1.40
2	B	602	NAD	C7N-N7N	8.14	1.48	1.33
2	D	501	NAD	O4D-C1D	8.14	1.51	1.40
2	D	502	NAD	C7N-N7N	8.13	1.47	1.33
2	C	501	NAD	C7N-N7N	8.13	1.47	1.33
2	A	501	NAD	C7N-N7N	8.13	1.47	1.33
2	D	501	NAD	C7N-N7N	8.10	1.47	1.33
2	B	601	NAD	O4D-C1D	8.01	1.51	1.40
2	C	501	NAD	O4D-C1D	8.01	1.51	1.40
2	A	501	NAD	O4D-C1D	7.97	1.51	1.40
2	B	602	NAD	O4D-C1D	7.92	1.51	1.40
2	C	501	NAD	C2B-C1B	-7.81	1.28	1.53
2	C	502	NAD	O4D-C1D	7.80	1.51	1.40
2	A	501	NAD	C2B-C1B	-7.75	1.29	1.53
2	D	501	NAD	C2B-C1B	-7.72	1.29	1.53
2	D	502	NAD	C2B-C1B	-7.71	1.29	1.53
2	A	502	NAD	O4B-C1B	7.16	1.58	1.42
2	C	502	NAD	O4B-C1B	7.04	1.58	1.42
2	D	501	NAD	PA-O3	6.61	1.66	1.59
2	A	502	NAD	PA-O3	6.55	1.66	1.59
2	A	502	NAD	O4D-C4D	-6.53	1.30	1.45
2	B	602	NAD	O4D-C4D	-6.53	1.30	1.45
2	C	502	NAD	PA-O3	6.49	1.66	1.59
2	B	601	NAD	O4D-C4D	-6.48	1.30	1.45
2	C	502	NAD	O4D-C4D	-6.48	1.30	1.45
2	A	501	NAD	PA-O3	6.47	1.66	1.59
2	C	501	NAD	O4D-C4D	-6.41	1.30	1.45
2	C	501	NAD	PA-O3	6.36	1.66	1.59
2	D	502	NAD	O4D-C4D	-6.36	1.30	1.45
2	A	501	NAD	O4D-C4D	-6.36	1.30	1.45
2	D	502	NAD	PA-O3	6.34	1.66	1.59
2	D	501	NAD	O4D-C4D	-6.29	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAD	PA-O3	6.21	1.66	1.59
2	B	601	NAD	PA-O3	6.16	1.66	1.59
2	B	601	NAD	O4B-C1B	5.97	1.55	1.42
2	B	602	NAD	O4B-C1B	5.92	1.55	1.42
2	C	501	NAD	O4B-C1B	5.62	1.55	1.42
2	A	501	NAD	O4B-C1B	5.61	1.55	1.42
2	C	501	NAD	C6A-N6A	5.57	1.48	1.34
2	C	502	NAD	C6A-N6A	5.55	1.48	1.34
2	D	502	NAD	C6A-N6A	5.53	1.48	1.34
2	A	502	NAD	C6A-N6A	5.50	1.48	1.34
2	B	602	NAD	C6A-N6A	5.49	1.48	1.34
2	B	601	NAD	C6A-N6A	5.49	1.48	1.34
2	D	501	NAD	C6A-N6A	5.48	1.48	1.34
2	A	501	NAD	C6A-N6A	5.47	1.48	1.34
2	D	501	NAD	O4B-C1B	5.45	1.54	1.42
2	D	502	NAD	O4B-C1B	5.40	1.54	1.42
2	A	501	NAD	C3D-C4D	5.25	1.66	1.53
2	D	501	NAD	C3D-C4D	5.22	1.66	1.53
2	A	502	NAD	O4B-C4B	5.19	1.56	1.45
2	C	502	NAD	C3D-C4D	5.17	1.66	1.53
2	D	502	NAD	C3D-C4D	5.16	1.66	1.53
2	A	501	NAD	O4B-C4B	5.15	1.56	1.45
2	D	501	NAD	O4B-C4B	5.15	1.56	1.45
2	B	601	NAD	C3D-C4D	5.14	1.66	1.53
2	C	501	NAD	C3D-C4D	5.14	1.66	1.53
2	B	601	NAD	C2B-C3B	5.13	1.67	1.53
2	B	601	NAD	O4B-C4B	5.13	1.56	1.45
2	A	502	NAD	C3D-C4D	5.12	1.66	1.53
2	D	502	NAD	O4B-C4B	5.12	1.56	1.45
2	B	602	NAD	O4B-C4B	5.11	1.56	1.45
2	B	602	NAD	C3D-C4D	5.11	1.65	1.53
2	C	501	NAD	C2B-C3B	5.07	1.67	1.53
2	B	602	NAD	C2B-C3B	5.07	1.67	1.53
2	C	501	NAD	O4B-C4B	5.07	1.56	1.45
2	C	502	NAD	O4B-C4B	5.06	1.56	1.45
2	A	502	NAD	C2B-C3B	5.05	1.67	1.53
2	C	502	NAD	C2B-C3B	5.04	1.67	1.53
2	A	501	NAD	C2B-C3B	5.02	1.67	1.53
2	D	501	NAD	C2B-C3B	5.00	1.66	1.53
2	D	501	NAD	PN-O3	4.91	1.64	1.59
2	D	502	NAD	C2B-C3B	4.88	1.66	1.53
2	D	502	NAD	PN-O3	4.87	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAD	PN-O3	4.87	1.64	1.59
2	C	502	NAD	PN-O3	4.80	1.64	1.59
2	C	501	NAD	PN-O3	4.80	1.64	1.59
2	A	501	NAD	PN-O3	4.71	1.64	1.59
2	B	601	NAD	PN-O3	4.58	1.64	1.59
2	B	602	NAD	PN-O3	4.33	1.64	1.59
2	A	501	NAD	C3N-C7N	4.21	1.56	1.50
2	D	502	NAD	C3N-C7N	4.15	1.56	1.50
2	C	501	NAD	C3N-C7N	4.10	1.56	1.50
2	D	501	NAD	C3N-C7N	4.08	1.56	1.50
2	B	601	NAD	C3N-C7N	4.07	1.56	1.50
2	A	502	NAD	C3N-C7N	3.96	1.56	1.50
2	B	602	NAD	C3N-C7N	3.94	1.56	1.50
2	C	502	NAD	C3N-C7N	3.88	1.56	1.50
2	C	502	NAD	O2D-C2D	3.81	1.52	1.43
2	B	601	NAD	O2D-C2D	3.81	1.52	1.43
2	A	502	NAD	O2D-C2D	3.78	1.52	1.43
2	B	602	NAD	O2D-C2D	3.71	1.52	1.43
2	D	502	NAD	O2D-C2D	3.70	1.52	1.43
2	C	501	NAD	O2D-C2D	3.66	1.52	1.43
2	A	501	NAD	O2D-C2D	3.64	1.52	1.43
2	D	501	NAD	O2D-C2D	3.57	1.51	1.43
2	A	502	NAD	O7N-C7N	-3.29	1.18	1.24
2	C	502	NAD	O7N-C7N	-3.28	1.18	1.24
2	B	601	NAD	O7N-C7N	-3.27	1.18	1.24
2	B	602	NAD	O7N-C7N	-3.21	1.18	1.24
2	C	501	NAD	O7N-C7N	-3.21	1.18	1.24
2	A	501	NAD	O7N-C7N	-3.20	1.18	1.24
2	D	501	NAD	O7N-C7N	-3.17	1.18	1.24
2	D	502	NAD	O7N-C7N	-3.15	1.18	1.24
2	A	502	NAD	O3D-C3D	2.69	1.49	1.43
2	B	601	NAD	O3D-C3D	2.68	1.49	1.43
2	D	502	NAD	O3D-C3D	2.67	1.49	1.43
2	B	602	NAD	O3D-C3D	2.64	1.49	1.43
2	B	602	NAD	C5A-C4A	-2.63	1.34	1.39
2	D	502	NAD	C5A-C4A	-2.63	1.34	1.39
2	C	502	NAD	O3D-C3D	2.63	1.49	1.43
2	D	501	NAD	C5A-C4A	-2.61	1.34	1.39
2	C	501	NAD	O3D-C3D	2.60	1.49	1.43
2	D	501	NAD	O3D-C3D	2.59	1.49	1.43
2	C	501	NAD	C5B-C4B	2.58	1.59	1.51
2	A	501	NAD	C5A-C4A	-2.57	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAD	C5A-C4A	-2.57	1.34	1.39
2	D	501	NAD	C5B-C4B	2.56	1.59	1.51
2	A	501	NAD	C5B-C4B	2.56	1.59	1.51
2	B	601	NAD	C5A-C4A	-2.56	1.34	1.39
2	A	501	NAD	O3D-C3D	2.56	1.49	1.43
2	A	502	NAD	C5A-C4A	-2.56	1.34	1.39
2	D	502	NAD	C5B-C4B	2.50	1.59	1.51
2	C	501	NAD	C5A-C4A	-2.46	1.34	1.39
2	B	602	NAD	C5B-C4B	2.46	1.59	1.51
2	A	502	NAD	C5B-C4B	2.45	1.58	1.51
2	C	502	NAD	C5B-C4B	2.44	1.58	1.51
2	B	601	NAD	C5B-C4B	2.44	1.58	1.51
2	B	602	NAD	C5A-N7A	-2.29	1.34	1.39
2	D	502	NAD	C5A-N7A	-2.29	1.34	1.39
2	C	501	NAD	C5A-N7A	-2.29	1.34	1.39
2	D	502	NAD	C8A-N9A	-2.25	1.33	1.37
2	C	502	NAD	C5A-N7A	-2.22	1.35	1.39
2	B	601	NAD	C5A-N7A	-2.20	1.35	1.39
2	A	502	NAD	C5A-N7A	-2.20	1.35	1.39
2	B	601	NAD	C1B-N9A	2.18	1.52	1.46
2	C	502	NAD	C1B-N9A	2.17	1.52	1.46
2	A	501	NAD	C5A-N7A	-2.16	1.35	1.39
2	D	501	NAD	C5A-N7A	-2.13	1.35	1.39
2	A	502	NAD	C1B-N9A	2.13	1.52	1.46
2	B	602	NAD	C1B-N9A	2.09	1.52	1.46
2	D	501	NAD	C8A-N9A	-2.02	1.34	1.37

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	N3A-C2A-N1A	-5.52	120.22	128.58
2	A	501	NAD	N3A-C2A-N1A	-5.50	120.26	128.58
2	C	502	NAD	N3A-C2A-N1A	-5.47	120.30	128.58
2	B	602	NAD	N3A-C2A-N1A	-5.46	120.32	128.58
2	A	502	NAD	N3A-C2A-N1A	-5.44	120.35	128.58
2	D	502	NAD	N3A-C2A-N1A	-5.39	120.43	128.58
2	D	501	NAD	N3A-C2A-N1A	-5.37	120.45	128.58
2	C	501	NAD	N3A-C2A-N1A	-5.36	120.46	128.58
2	B	601	NAD	C5A-C4A-N3A	-4.77	120.15	126.72
2	B	602	NAD	C5A-C4A-N3A	-4.76	120.16	126.72
2	A	501	NAD	C5A-C4A-N3A	-4.72	120.22	126.72
2	A	502	NAD	C5A-C4A-N3A	-4.71	120.23	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C5A-C4A-N3A	-4.59	120.39	126.72
2	D	502	NAD	N9A-C8A-N7A	-4.57	107.46	113.94
2	A	501	NAD	N9A-C8A-N7A	-4.51	107.53	113.94
2	D	501	NAD	N9A-C8A-N7A	-4.49	107.57	113.94
2	C	502	NAD	C5A-C4A-N3A	-4.49	120.54	126.72
2	C	502	NAD	N9A-C8A-N7A	-4.35	107.76	113.94
2	C	501	NAD	N9A-C8A-N7A	-4.34	107.78	113.94
2	A	502	NAD	N9A-C8A-N7A	-4.30	107.83	113.94
2	B	602	NAD	N9A-C8A-N7A	-4.27	107.87	113.94
2	B	601	NAD	N9A-C8A-N7A	-4.26	107.90	113.94
2	D	501	NAD	C5A-C4A-N3A	-4.21	120.93	126.72
2	D	502	NAD	C4D-O4D-C1D	-4.20	106.08	109.92
2	D	501	NAD	N6A-C6A-N1A	-4.11	109.22	118.38
2	B	602	NAD	C4D-O4D-C1D	-4.11	106.16	109.92
2	C	502	NAD	C4D-O4D-C1D	-4.10	106.17	109.92
2	C	502	NAD	N6A-C6A-N1A	-4.08	109.29	118.38
2	A	501	NAD	N6A-C6A-N1A	-4.06	109.33	118.38
2	D	502	NAD	C5A-C4A-N3A	-4.05	121.14	126.72
2	C	501	NAD	N6A-C6A-N1A	-4.05	109.36	118.38
2	C	501	NAD	C4D-O4D-C1D	-4.02	106.24	109.92
2	D	502	NAD	N6A-C6A-N1A	-4.02	109.43	118.38
2	B	602	NAD	N6A-C6A-N1A	-4.01	109.45	118.38
2	D	501	NAD	C4D-O4D-C1D	-4.00	106.26	109.92
2	A	502	NAD	N6A-C6A-N1A	-3.98	109.52	118.38
2	B	601	NAD	N6A-C6A-N1A	-3.96	109.56	118.38
2	B	601	NAD	C4D-O4D-C1D	-3.91	106.34	109.92
2	A	502	NAD	C4D-O4D-C1D	-3.84	106.41	109.92
2	A	501	NAD	C4D-O4D-C1D	-3.75	106.49	109.92
2	A	501	NAD	C1B-N9A-C8A	-3.66	118.98	127.09
2	D	502	NAD	C1B-N9A-C8A	-3.41	119.53	127.09
2	C	501	NAD	C1B-N9A-C8A	-3.37	119.62	127.09
2	B	601	NAD	C2A-N3A-C4A	3.26	119.78	111.83
2	A	501	NAD	C2A-N3A-C4A	3.23	119.72	111.83
2	D	502	NAD	C5A-C6A-N6A	3.22	131.25	123.29
2	A	502	NAD	C2A-N3A-C4A	3.21	119.67	111.83
2	C	502	NAD	C5A-C6A-N6A	3.21	131.23	123.29
2	B	602	NAD	C2A-N3A-C4A	3.20	119.66	111.83
2	D	501	NAD	C5A-C6A-N6A	3.19	131.19	123.29
2	C	501	NAD	C5A-C6A-N6A	3.14	131.07	123.29
2	C	502	NAD	C2A-N3A-C4A	3.10	119.41	111.83
2	C	501	NAD	C2A-N3A-C4A	3.07	119.33	111.83
2	A	501	NAD	C5A-N7A-C8A	3.03	108.21	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	C2A-N3A-C4A	3.01	119.17	111.83
2	A	501	NAD	N3A-C4A-N9A	3.00	132.26	127.17
2	A	502	NAD	C5A-N7A-C8A	2.98	108.14	103.45
2	C	502	NAD	C5A-N7A-C8A	2.98	108.14	103.45
2	A	501	NAD	C5A-C6A-N6A	2.98	130.66	123.29
2	D	501	NAD	C5A-N7A-C8A	2.97	108.12	103.45
2	C	501	NAD	C5A-N7A-C8A	2.97	108.12	103.45
2	B	602	NAD	C5A-C6A-N6A	2.97	130.65	123.29
2	A	502	NAD	C5A-C6A-N6A	2.96	130.61	123.29
2	B	601	NAD	C5A-N7A-C8A	2.96	108.09	103.45
2	D	502	NAD	C4A-N9A-C8A	2.94	108.83	105.74
2	D	502	NAD	C5A-N7A-C8A	2.94	108.07	103.45
2	B	602	NAD	C1B-N9A-C8A	-2.93	120.59	127.09
2	B	602	NAD	C5A-N7A-C8A	2.93	108.05	103.45
2	D	502	NAD	C2A-N3A-C4A	2.92	118.97	111.83
2	B	601	NAD	C5A-C6A-N6A	2.92	130.50	123.29
2	A	502	NAD	C1B-N9A-C8A	-2.89	120.67	127.09
2	B	601	NAD	N3A-C4A-N9A	2.87	132.05	127.17
2	B	601	NAD	C1B-N9A-C8A	-2.85	120.77	127.09
2	B	602	NAD	N3A-C4A-N9A	2.84	132.00	127.17
2	C	502	NAD	C1B-N9A-C8A	-2.82	120.83	127.09
2	D	501	NAD	C1B-N9A-C8A	-2.81	120.86	127.09
2	C	501	NAD	N3A-C4A-N9A	2.80	131.93	127.17
2	A	501	NAD	C4A-N9A-C8A	2.78	108.66	105.74
2	A	502	NAD	N3A-C4A-N9A	2.78	131.89	127.17
2	D	501	NAD	C4A-N9A-C8A	2.66	108.53	105.74
2	D	501	NAD	C4A-C5A-N7A	-2.60	107.61	110.58
2	A	502	NAD	C6N-N1N-C2N	-2.57	119.69	121.88
2	B	601	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
2	C	502	NAD	N3A-C4A-N9A	2.49	131.41	127.17
2	C	501	NAD	C4A-N9A-C8A	2.47	108.33	105.74
2	D	502	NAD	C3N-C7N-N7N	2.45	120.76	117.74
2	A	501	NAD	C4A-N9A-C1B	2.45	132.36	126.63
2	D	502	NAD	C4B-O4B-C1B	-2.44	104.08	109.47
2	B	602	NAD	C6N-N1N-C2N	-2.42	119.82	121.88
2	D	502	NAD	C4A-C5A-N7A	-2.40	107.84	110.58
2	C	502	NAD	C4A-C5A-N7A	-2.36	107.88	110.58
2	D	501	NAD	O4B-C1B-N9A	2.35	112.60	108.09
2	C	502	NAD	C6N-N1N-C2N	-2.35	119.88	121.88
2	C	501	NAD	C4A-N9A-C1B	2.31	132.04	126.63
2	D	501	NAD	C4B-O4B-C1B	-2.31	104.37	109.47
2	C	502	NAD	C4A-N9A-C8A	2.30	108.16	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	NAD	C3B-C2B-C1B	2.30	105.81	101.46
2	D	502	NAD	N3A-C4A-N9A	2.29	131.06	127.17
2	B	602	NAD	C4A-N9A-C8A	2.29	108.14	105.74
2	B	601	NAD	C4A-N9A-C8A	2.29	108.14	105.74
2	A	502	NAD	C4A-N9A-C8A	2.28	108.13	105.74
2	A	502	NAD	C4A-C5A-N7A	-2.25	108.01	110.58
2	A	501	NAD	C3N-C7N-N7N	2.21	120.46	117.74
2	B	601	NAD	C4A-C5A-N7A	-2.20	108.06	110.58
2	D	501	NAD	N3A-C4A-N9A	2.20	130.90	127.17
2	C	501	NAD	C4A-C5A-N7A	-2.19	108.08	110.58
2	A	501	NAD	C4A-C5A-N7A	-2.19	108.08	110.58
2	A	502	NAD	C3B-C2B-C1B	2.18	105.59	101.46
2	B	602	NAD	C4A-C5A-N7A	-2.18	108.09	110.58
2	D	501	NAD	C5A-C4A-N9A	2.17	108.17	105.81
2	D	502	NAD	C2B-C3B-C4B	2.15	106.77	102.61
2	A	501	NAD	C2B-C3B-C4B	2.14	106.75	102.61
2	D	502	NAD	C4A-N9A-C1B	2.14	131.64	126.63
2	A	502	NAD	C2D-C3D-C4D	2.13	106.73	102.61
2	B	602	NAD	C2D-C3D-C4D	2.13	106.73	102.61
2	D	502	NAD	C2D-C3D-C4D	2.11	106.69	102.61
2	C	502	NAD	C2D-C3D-C4D	2.09	106.65	102.61
2	D	501	NAD	C3N-C7N-N7N	2.07	120.29	117.74
2	C	502	NAD	C5A-C4A-N9A	2.06	108.06	105.81
2	C	501	NAD	C6A-C5A-C4A	2.05	119.97	117.18
2	A	502	NAD	C4B-O4B-C1B	-2.04	104.96	109.47
2	A	501	NAD	C4B-O4B-C1B	-2.04	104.97	109.47
2	B	601	NAD	C2D-C3D-C4D	2.04	106.54	102.61
2	C	502	NAD	C4B-O4B-C1B	-2.03	104.99	109.47
2	D	502	NAD	O7N-C7N-N7N	-2.02	119.70	122.62
2	B	602	NAD	C6A-C5A-C4A	2.02	119.93	117.18
2	C	501	NAD	C2D-C3D-C4D	2.01	106.50	102.61

There are no chirality outliers.

All (35) 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-O3
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

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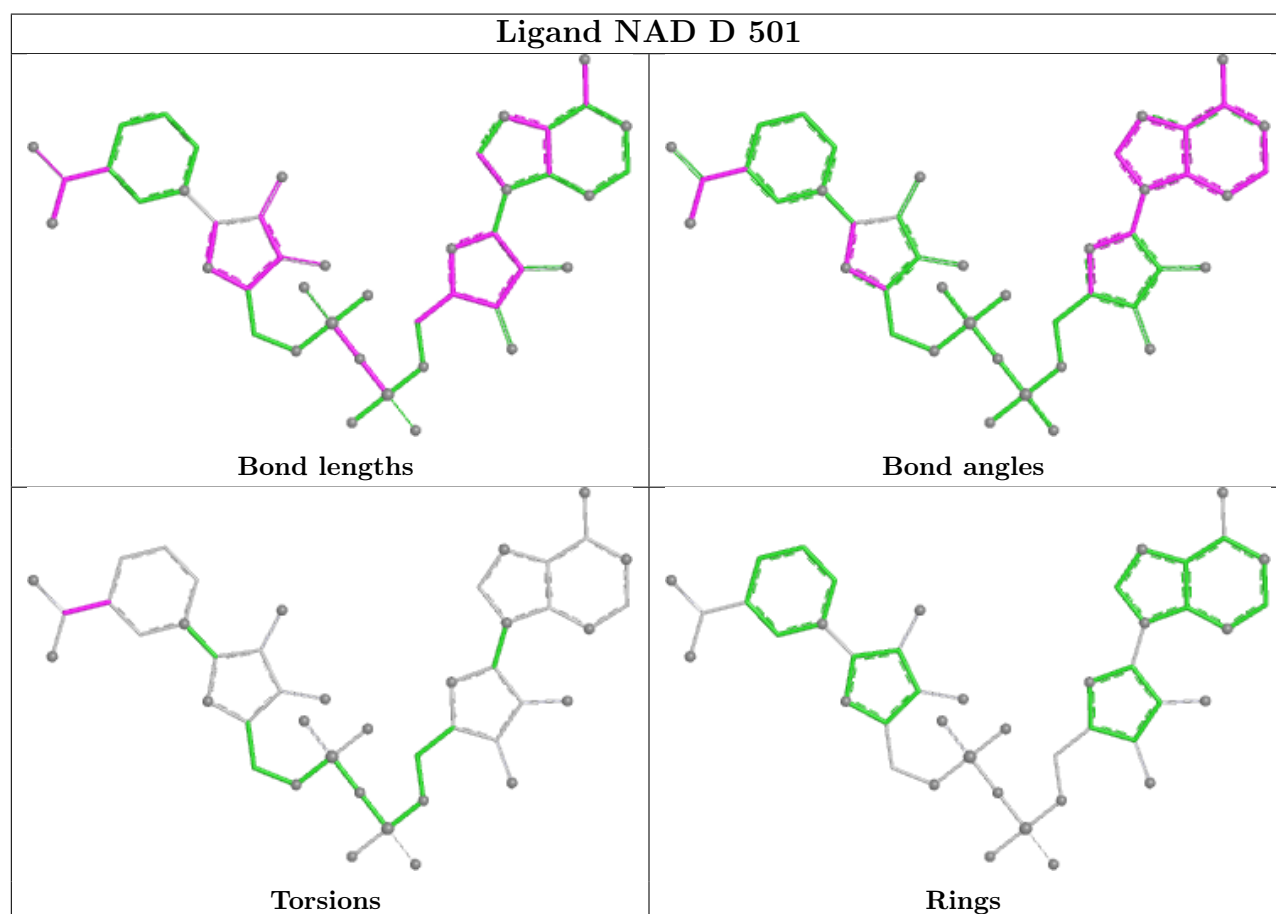
Mol	Chain	Res	Type	Atoms
2	B	601	NAD	O4D-C1D-N1N-C6N
2	B	602	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	PN-O3-PA-O5B
2	C	502	NAD	PA-O3-PN-O5D
2	C	502	NAD	C5D-O5D-PN-O3
2	C	502	NAD	C5D-O5D-PN-O1N
2	C	502	NAD	O4D-C1D-N1N-C6N
2	D	502	NAD	O4D-C4D-C5D-O5D
2	A	502	NAD	PA-O3-PN-O5D
2	B	601	NAD	PA-O3-PN-O5D
2	D	502	NAD	PN-O3-PA-O5B
2	D	502	NAD	C3D-C4D-C5D-O5D
2	A	501	NAD	O4D-C4D-C5D-O5D
2	A	502	NAD	O4D-C1D-N1N-C2N
2	B	601	NAD	O4D-C1D-N1N-C2N
2	B	602	NAD	O4D-C1D-N1N-C2N
2	B	602	NAD	O4D-C1D-N1N-C6N
2	C	502	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	C4N-C3N-C7N-N7N
2	A	501	NAD	C4N-C3N-C7N-O7N
2	C	501	NAD	C4N-C3N-C7N-N7N
2	C	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	D	501	NAD	C4N-C3N-C7N-O7N
2	B	601	NAD	C2B-C1B-N9A-C8A
2	A	502	NAD	PN-O3-PA-O2A
2	B	602	NAD	PN-O3-PA-O2A

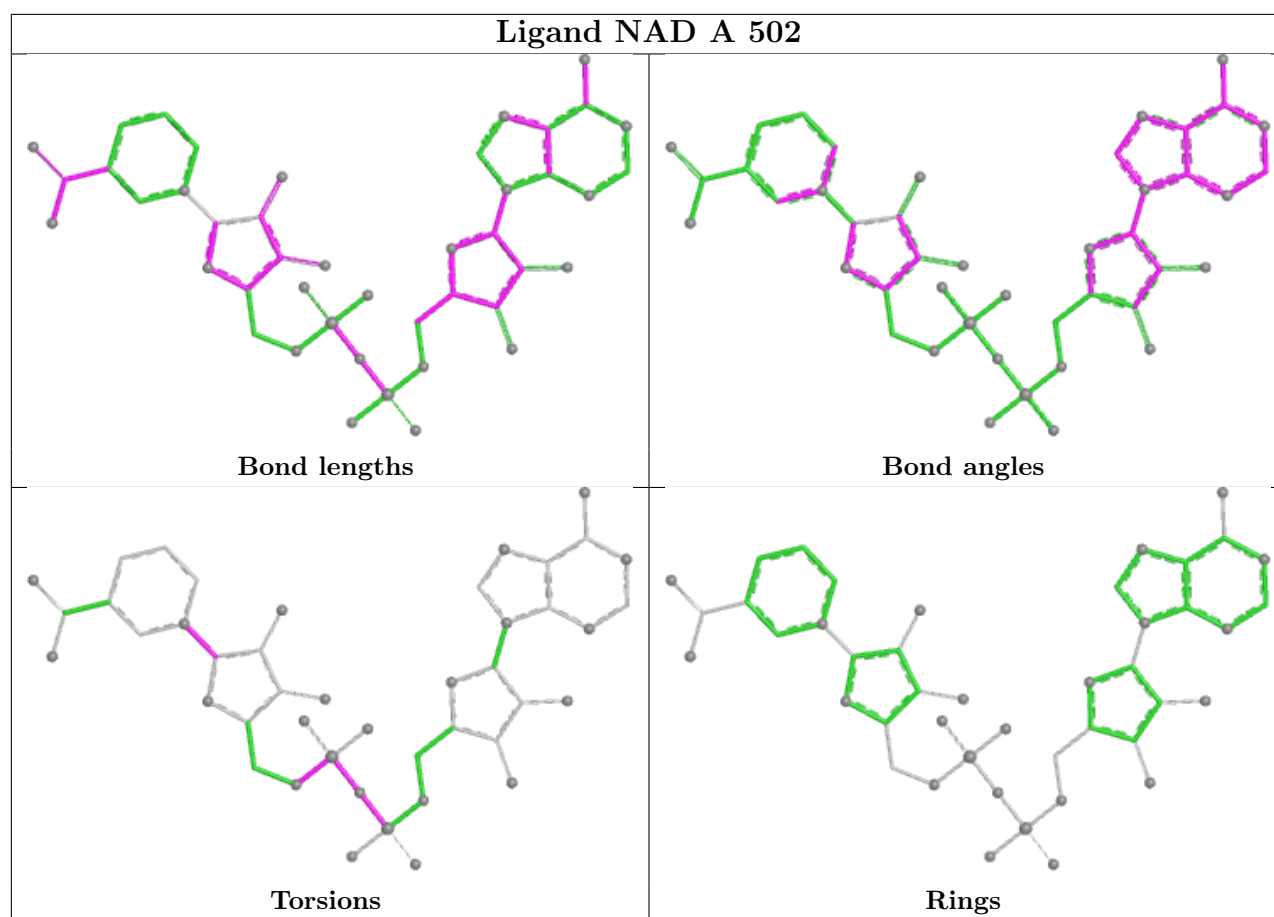
There are no ring outliers.

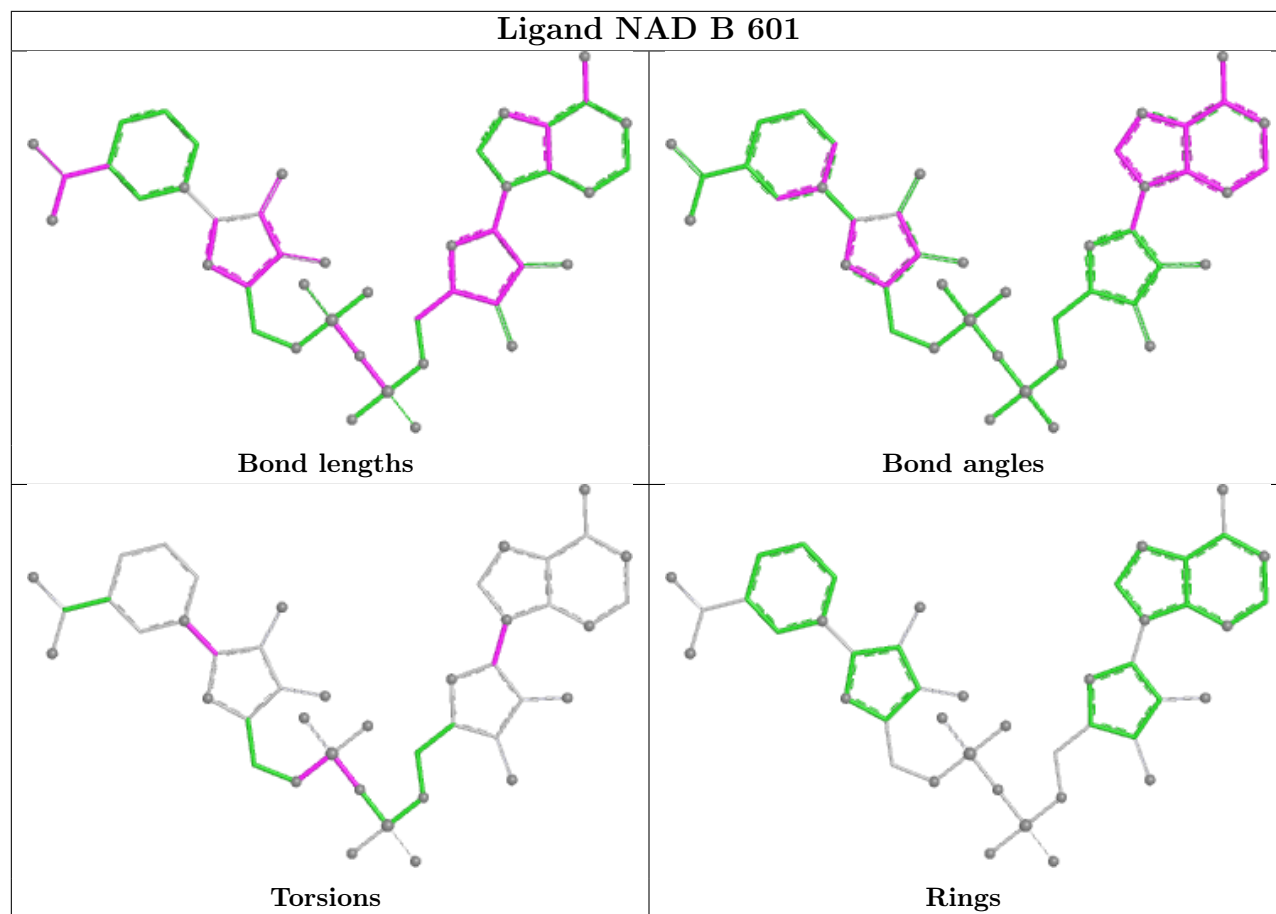
7 monomers are involved in 23 short contacts:

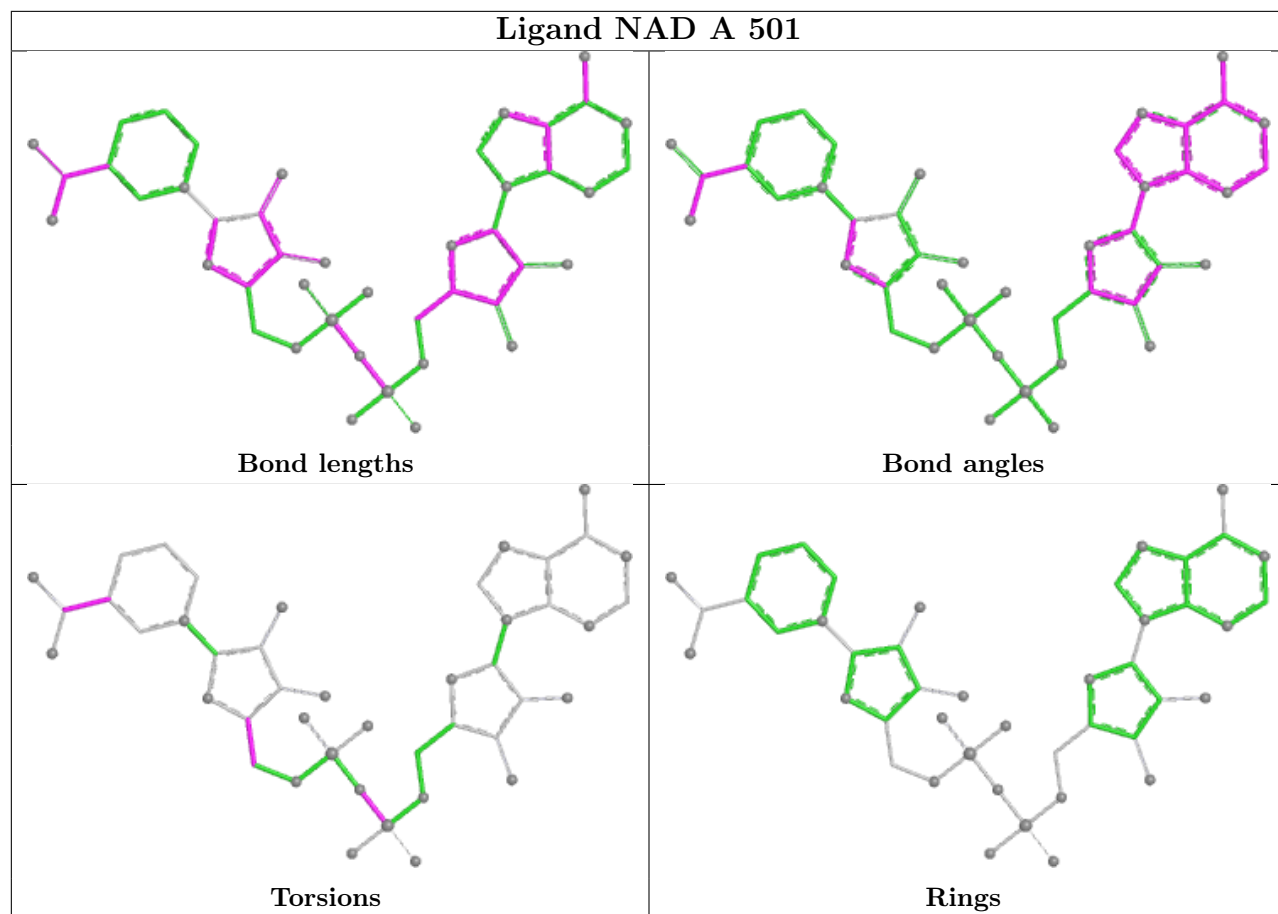
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	NAD	6	0
2	A	502	NAD	3	0
2	A	501	NAD	3	0
2	B	602	NAD	1	0
2	C	502	NAD	1	0
2	D	502	NAD	8	0
2	C	501	NAD	3	0

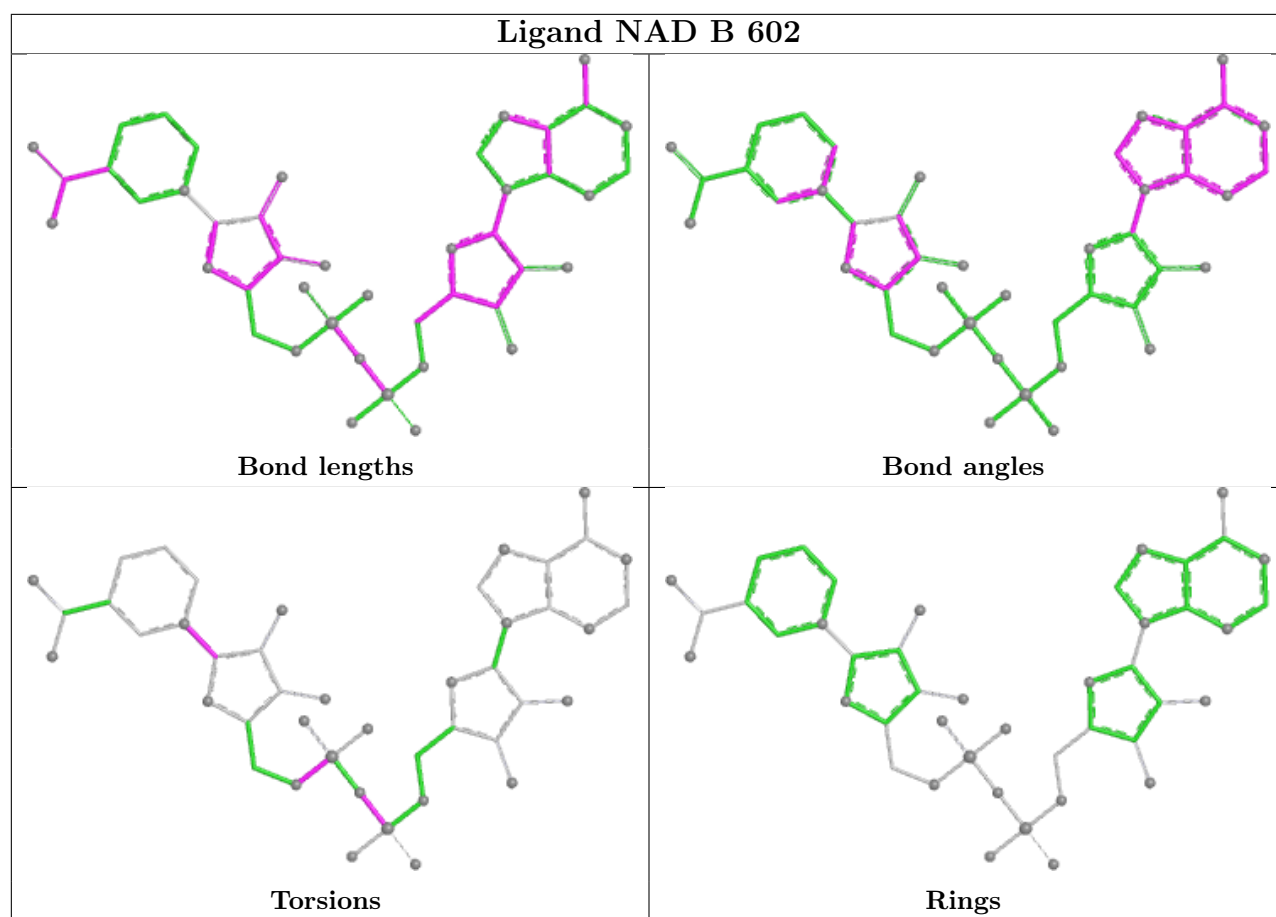
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

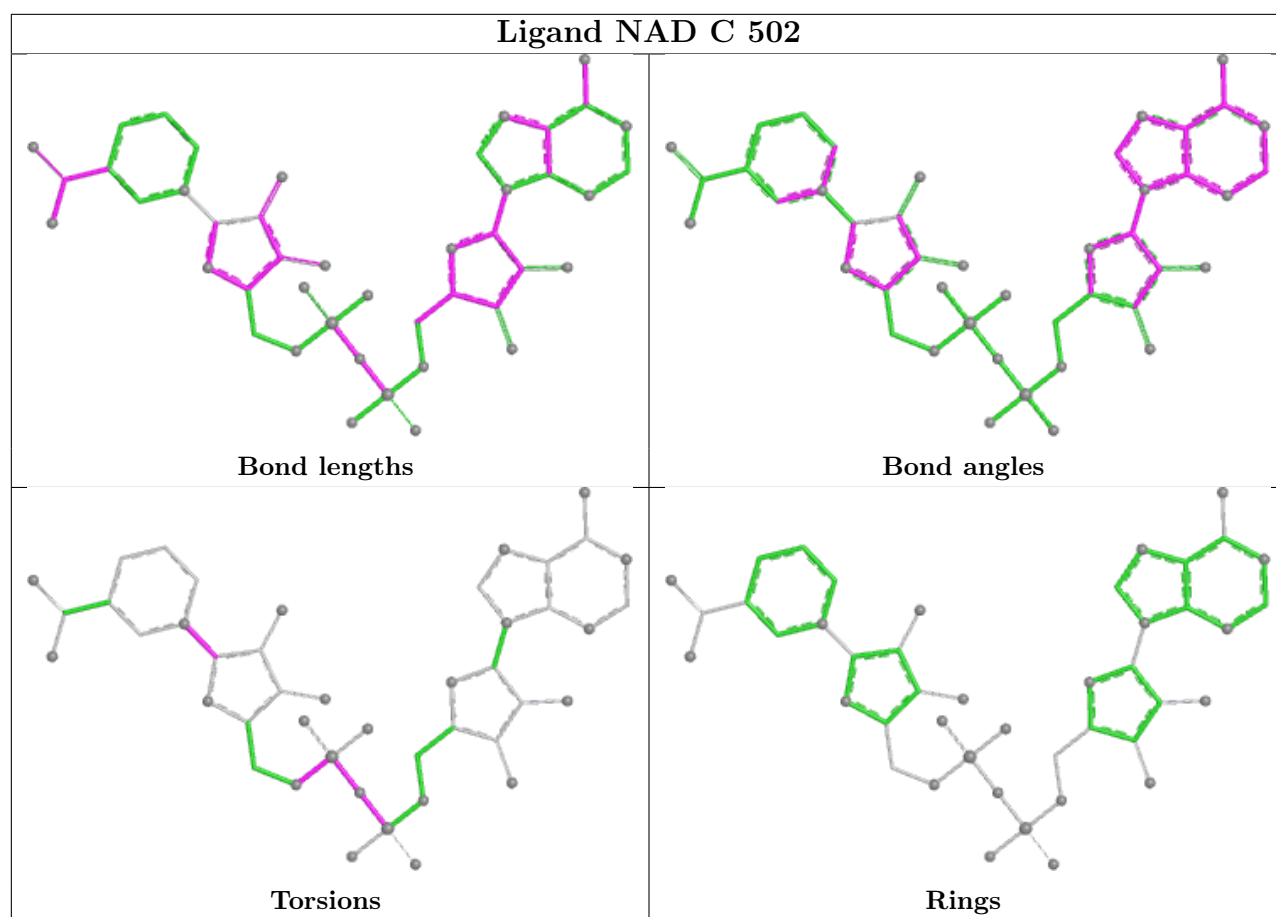


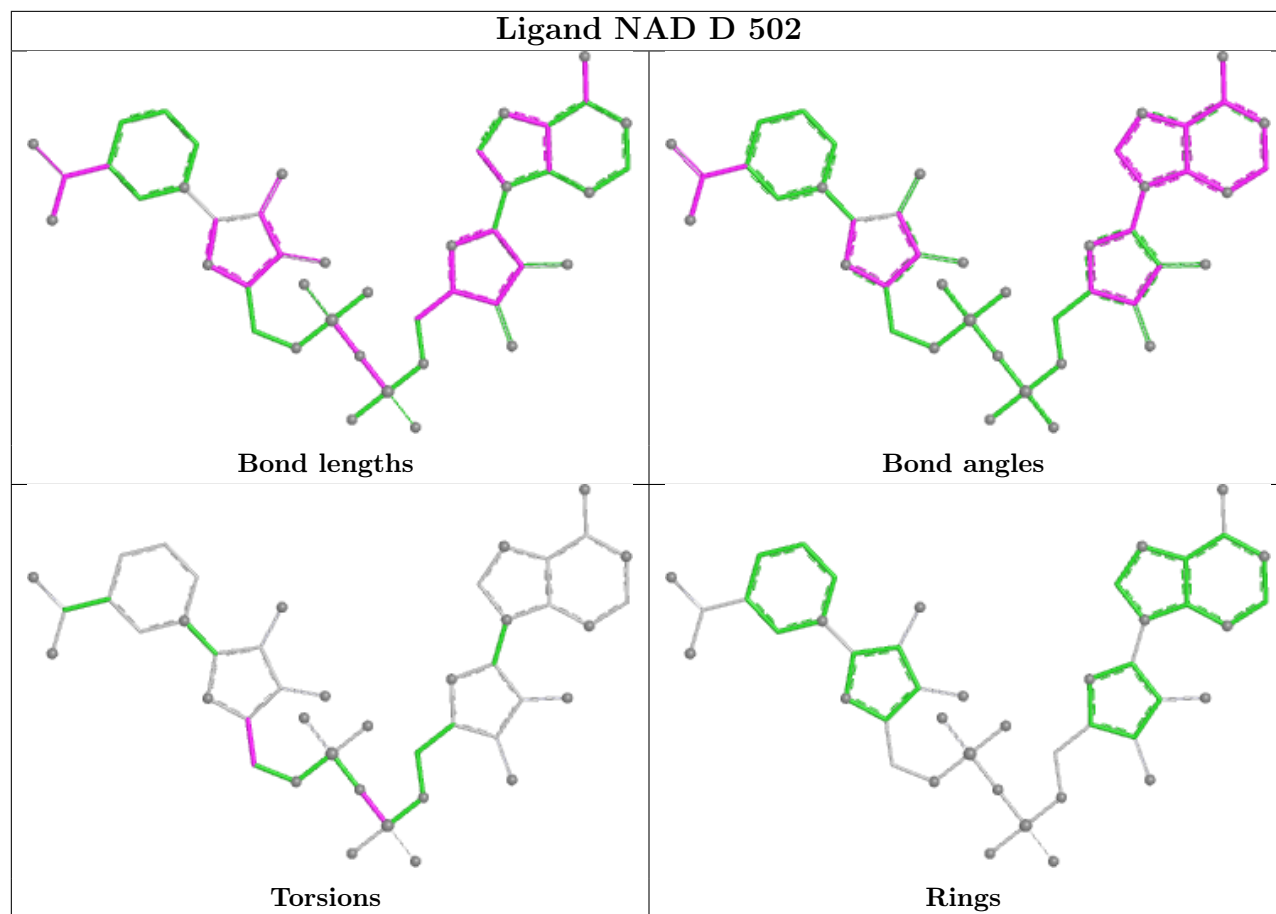


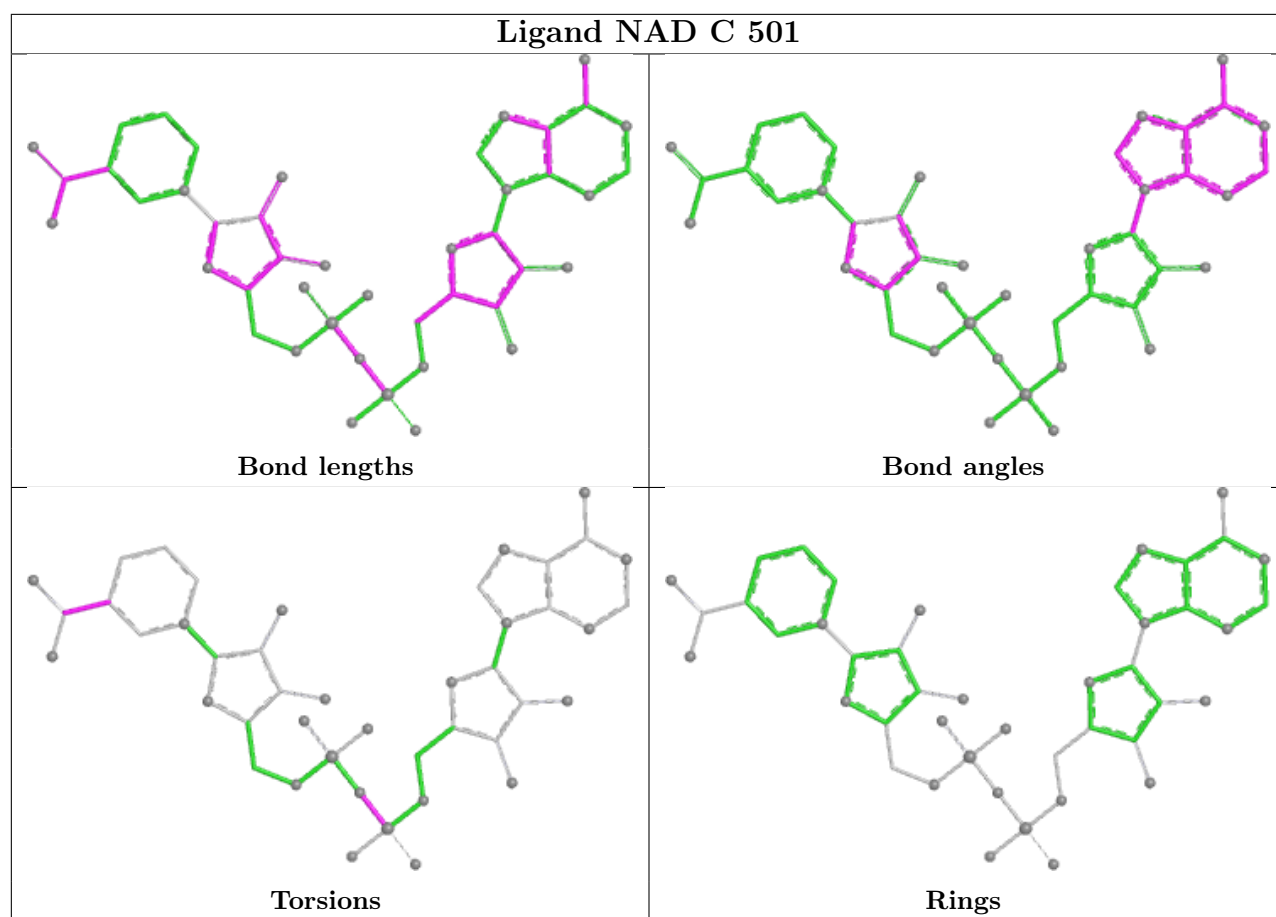












5.7 Other polymers [i](#)

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	457/489 (93%)	2.85	333 (72%) 0 0	19, 35, 56, 82	3 (0%)
1	B	457/489 (93%)	2.98	336 (73%) 0 0	17, 39, 65, 91	1 (0%)
1	C	454/489 (92%)	3.03	346 (76%) 0 0	22, 37, 61, 98	2 (0%)
1	D	461/489 (94%)	3.19	362 (78%) 0 0	25, 41, 65, 97	0
All	All	1829/1956 (93%)	3.01	1377 (75%) 0 0	17, 38, 62, 98	6 (0%)

All (1377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	GLY	11.8
1	B	138	PHE	11.7
1	C	424	SER	11.1
1	D	427	ASP	10.7
1	D	399	GLY	9.6
1	A	136	SER	9.4
1	B	136	SER	9.3
1	D	136	SER	9.3
1	D	424	SER	9.2
1	D	412	ALA	9.0
1	C	10	SER	8.6
1	D	137	PHE	8.6
1	D	425	LEU	8.2
1	B	137	PHE	8.2
1	D	343	TYR	8.1
1	D	140	GLY	8.1
1	D	396	GLY	8.0
1	B	141	ILE	7.8
1	D	428	ILE	7.7
1	C	104	ALA	7.6
1	C	229	SER	7.6

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Mol	Chain	Res	Type	RSRZ
1	C	402	VAL	7.5
1	A	189	PHE	7.5
1	C	419	LEU	7.5
1	D	104	ALA	7.4
1	D	138	PHE	7.3
1	C	221	HIS	7.3
1	D	400	PHE	7.3
1	C	378	TYR	7.2
1	B	174	GLY	7.1
1	D	229	SER	7.1
1	B	379	PHE	7.1
1	A	-1	GLY	7.0
1	C	412	ALA	7.0
1	A	425	LEU	7.0
1	D	317	THR	6.9
1	D	350	GLY	6.9
1	A	229	SER	6.9
1	A	415	TYR	6.9
1	A	408	SER	6.9
1	D	429	HIS	6.8
1	D	134	ILE	6.7
1	C	231	VAL	6.7
1	A	104	ALA	6.7
1	B	424	SER	6.6
1	A	378	TYR	6.5
1	D	402	VAL	6.5
1	B	423	SER	6.5
1	D	10	SER	6.5
1	D	438	VAL	6.5
1	B	57	ILE	6.5
1	C	140	GLY	6.5
1	B	352	GLN	6.4
1	A	87	GLY	6.4
1	A	127	GLY	6.4
1	C	230	LEU	6.3
1	A	192	ALA	6.3
1	D	344	ASP	6.2
1	D	9	TRP	6.2
1	D	426	ALA	6.2
1	B	348	THR	6.2
1	C	139	GLU	6.1
1	A	414	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	134	ILE	6.1
1	B	316	PHE	6.1
1	A	424	SER	6.0
1	A	118	ASN	6.0
1	C	438	VAL	6.0
1	D	198	GLY	6.0
1	C	282	VAL	6.0
1	D	440	VAL	6.0
1	C	218	LEU	6.0
1	D	143	PRO	5.9
1	A	174	GLY	5.9
1	A	-2	ALA	5.9
1	D	423	SER	5.9
1	B	206	VAL	5.9
1	D	193	VAL	5.9
1	A	142	GLU	5.9
1	C	431	ILE	5.9
1	B	229	SER	5.8
1	D	98	TYR	5.8
1	D	422	HIS	5.8
1	B	311	VAL	5.8
1	D	409	SER	5.8
1	B	140	GLY	5.8
1	C	137	PHE	5.8
1	D	189	PHE	5.8
1	C	141	ILE	5.8
1	A	342	ASP	5.7
1	A	396	GLY	5.7
1	A	409	SER	5.7
1	C	0	THR	5.7
1	C	404	ALA	5.7
1	B	363	PHE	5.7
1	D	414	ALA	5.6
1	C	314	LEU	5.6
1	C	9	TRP	5.6
1	A	295	LEU	5.6
1	D	165	TRP	5.6
1	B	135	LYS	5.6
1	B	438	VAL	5.5
1	A	298	ILE	5.5
1	D	430	LYS	5.5
1	D	159	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	396	GLY	5.5
1	B	189	PHE	5.5
1	D	139	GLU	5.5
1	C	170	CYS	5.5
1	D	230	LEU	5.4
1	B	350	GLY	5.4
1	C	348	THR	5.4
1	D	349	ALA	5.4
1	C	151	LEU	5.4
1	C	444	LEU	5.4
1	D	340	LEU	5.4
1	C	86	THR	5.4
1	C	146	CYS	5.4
1	C	74	ARG	5.3
1	C	285[A]	ARG	5.3
1	A	8	GLY	5.3
1	B	230	LEU	5.3
1	C	390	ASN	5.3
1	B	233	ALA	5.3
1	D	332	LEU	5.3
1	D	421	PHE	5.3
1	C	305	ASN	5.3
1	B	91	VAL	5.3
1	D	310	PHE	5.3
1	B	378	TYR	5.3
1	C	343	TYR	5.3
1	D	-2	ALA	5.3
1	C	227	GLY	5.2
1	A	397	ASN	5.2
1	D	387	GLY	5.2
1	B	0	THR	5.2
1	A	9	TRP	5.2
1	A	70	ALA	5.2
1	C	354	SER	5.2
1	D	432	LEU	5.2
1	B	102	ASN	5.2
1	B	165	TRP	5.1
1	C	409	SER	5.1
1	D	161	LEU	5.1
1	C	410	ASP	5.1
1	A	423	SER	5.1
1	B	227	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	5.1
1	D	339	HIS	5.1
1	A	86	THR	5.1
1	C	344	ASP	5.1
1	C	232	VAL	5.1
1	B	120	GLY	5.1
1	A	141	ILE	5.1
1	C	341	ILE	5.1
1	A	447	ARG	5.1
1	B	345	LEU	5.1
1	C	474	ASP	5.1
1	B	208	VAL	5.1
1	C	396	GLY	5.1
1	D	248	GLY	5.1
1	B	359	PRO	5.0
1	A	211	THR	5.0
1	C	411	GLN	5.0
1	C	320	TYR	5.0
1	B	76	GLY	5.0
1	C	75	ASP	5.0
1	B	405	TYR	5.0
1	D	244	GLY	5.0
1	B	317	THR	5.0
1	B	315	VAL	4.9
1	B	387	GLY	4.9
1	D	330	PHE	4.9
1	B	310	PHE	4.9
1	B	130	ARG	4.9
1	D	410	ASP	4.9
1	A	242	ALA	4.9
1	A	244	GLY	4.9
1	D	378	TYR	4.9
1	C	339	HIS	4.9
1	B	55	ASP	4.9
1	D	102	ASN	4.9
1	D	218	LEU	4.9
1	A	88	GLY	4.9
1	B	353	TYR	4.9
1	D	215	TYR	4.9
1	D	126	LEU	4.8
1	C	228	GLU	4.8
1	B	154	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	51	THR	4.8
1	A	75	ASP	4.8
1	B	380	LEU	4.8
1	C	430	LYS	4.8
1	D	357	ALA	4.8
1	C	422	HIS	4.8
1	D	363	PHE	4.8
1	A	33	LEU	4.8
1	A	117	ALA	4.8
1	C	179	VAL	4.8
1	D	448	VAL	4.8
1	C	172	ALA	4.8
1	C	54	VAL	4.8
1	D	341	ILE	4.7
1	A	108	LEU	4.7
1	B	340	LEU	4.7
1	C	295	LEU	4.7
1	A	288	TYR	4.7
1	A	410	ASP	4.7
1	C	437	THR	4.7
1	D	296	ASP	4.7
1	D	418	LEU	4.7
1	A	143	PRO	4.7
1	D	115	ALA	4.7
1	C	102	ASN	4.7
1	C	350	GLY	4.7
1	D	368	ARG	4.7
1	C	313	THR	4.7
1	D	0	THR	4.7
1	D	86	THR	4.7
1	B	126	LEU	4.7
1	B	131	LEU	4.7
1	B	228	GLU	4.7
1	D	191	ASP	4.6
1	B	341	ILE	4.6
1	C	76	GLY	4.6
1	B	129	SER	4.6
1	C	136	SER	4.6
1	D	354	SER	4.6
1	C	103	LEU	4.6
1	A	140	GLY	4.6
1	A	129	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	240	PRO	4.6
1	B	178	PHE	4.6
1	C	92	ARG	4.6
1	D	150	TRP	4.6
1	D	337	GLY	4.6
1	D	135	LYS	4.6
1	B	289	ASN	4.6
1	A	152	GLU	4.6
1	D	142	GLU	4.6
1	B	123	LEU	4.6
1	D	374	GLY	4.5
1	C	423	SER	4.5
1	A	444	LEU	4.5
1	B	368	ARG	4.5
1	C	135	LYS	4.5
1	D	120	GLY	4.5
1	D	158	SER	4.5
1	B	437	THR	4.5
1	B	103	LEU	4.5
1	A	11	VAL	4.5
1	A	208	VAL	4.5
1	B	75	ASP	4.5
1	A	135	LYS	4.5
1	A	413	LEU	4.5
1	A	228	GLU	4.5
1	B	172	ALA	4.5
1	A	51	THR	4.4
1	B	211	THR	4.4
1	B	346	TYR	4.4
1	C	51	THR	4.4
1	B	440	VAL	4.4
1	C	258	ILE	4.4
1	C	448	VAL	4.4
1	D	185	ILE	4.4
1	B	182	GLY	4.4
1	C	421	PHE	4.4
1	B	415	TYR	4.4
1	B	147	VAL	4.4
1	C	374	GLY	4.4
1	B	121	SER	4.4
1	A	330	PHE	4.4
1	D	404	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	231	VAL	4.4
1	B	179	VAL	4.4
1	C	87	GLY	4.4
1	C	403	LYS	4.4
1	D	366	ARG	4.4
1	D	23	TRP	4.4
1	D	52	VAL	4.4
1	B	169	ASP	4.4
1	C	34	ASP	4.4
1	A	230	LEU	4.3
1	D	285	ARG	4.3
1	B	9	TRP	4.3
1	C	389	ILE	4.3
1	B	287	SER	4.3
1	C	366	ARG	4.3
1	D	331	ARG	4.3
1	C	238	THR	4.3
1	D	391	THR	4.3
1	D	469	THR	4.3
1	B	442	ILE	4.3
1	D	112	ILE	4.3
1	B	397	ASN	4.3
1	B	240	PRO	4.3
1	D	411	GLN	4.3
1	D	431	ILE	4.3
1	D	91	VAL	4.3
1	D	232	VAL	4.3
1	A	10	SER	4.3
1	A	305	ASN	4.3
1	C	189	PHE	4.3
1	A	103	LEU	4.3
1	A	411	GLN	4.3
1	A	361	GLY	4.3
1	A	147	VAL	4.2
1	B	448	VAL	4.2
1	D	85	SER	4.2
1	B	422	HIS	4.2
1	A	138	PHE	4.2
1	C	351	PRO	4.2
1	D	351	PRO	4.2
1	C	33	LEU	4.2
1	A	81	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	329	ILE	4.2
1	C	171	THR	4.2
1	D	-1	GLY	4.2
1	A	102	ASN	4.2
1	C	193	VAL	4.2
1	C	364	VAL	4.2
1	D	205	VAL	4.2
1	D	334	ASP	4.2
1	C	98	TYR	4.2
1	C	415	TYR	4.2
1	D	168	TYR	4.2
1	D	243	PHE	4.2
1	C	131	LEU	4.2
1	C	291	LEU	4.2
1	B	313	THR	4.2
1	A	120	GLY	4.1
1	B	433	HIS	4.1
1	B	170	CYS	4.1
1	B	297	ASN	4.1
1	C	85	SER	4.1
1	B	176	TYR	4.1
1	A	246	LEU	4.1
1	A	76	GLY	4.1
1	A	167	ASP	4.1
1	D	408	SER	4.1
1	B	193	VAL	4.1
1	B	351	PRO	4.1
1	B	104	ALA	4.1
1	A	419	LEU	4.1
1	C	469	THR	4.1
1	D	437	THR	4.1
1	A	224	GLY	4.1
1	A	422	HIS	4.1
1	B	275	TRP	4.1
1	D	57	ILE	4.1
1	A	179	VAL	4.1
1	C	355	GLU	4.1
1	D	58	ALA	4.1
1	C	398	LEU	4.1
1	A	137	PHE	4.1
1	C	363	PHE	4.1
1	A	442	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	389	ILE	4.1
1	A	250	SER	4.1
1	B	54	VAL	4.1
1	D	131	LEU	4.0
1	C	299	THR	4.0
1	B	373	ARG	4.0
1	D	225	ASP	4.0
1	B	284	SER	4.0
1	A	351	PRO	4.0
1	D	348	THR	4.0
1	C	417	ARG	4.0
1	C	118	ASN	4.0
1	C	284	SER	4.0
1	C	333	ILE	4.0
1	D	315	VAL	4.0
1	D	221	HIS	4.0
1	B	360	ALA	4.0
1	B	324	ARG	4.0
1	B	325	TYR	4.0
1	A	284	SER	4.0
1	B	298	ILE	4.0
1	B	150	TRP	4.0
1	B	117	ALA	4.0
1	C	243	PHE	4.0
1	A	465	SER	4.0
1	D	324	ARG	3.9
1	A	218	LEU	3.9
1	D	217	LEU	3.9
1	B	391	THR	3.9
1	D	316	PHE	3.9
1	B	435	ASN	3.9
1	C	342	ASP	3.9
1	C	298	ILE	3.9
1	C	416	TYR	3.9
1	D	328	ILE	3.9
1	D	433	HIS	3.9
1	B	285[A]	ARG	3.9
1	D	347	LEU	3.9
1	B	462	ALA	3.9
1	C	399	GLY	3.9
1	D	172	ALA	3.9
1	B	197	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	471	LYS	3.9
1	D	342	ASP	3.9
1	A	401	ARG	3.9
1	A	247	PRO	3.9
1	C	405	TYR	3.9
1	A	123	LEU	3.9
1	B	398	LEU	3.9
1	B	419	LEU	3.9
1	D	444	LEU	3.9
1	C	23	TRP	3.9
1	B	53	THR	3.9
1	B	414	ALA	3.9
1	B	118	ASN	3.9
1	B	194	ASN	3.9
1	C	435	ASN	3.9
1	D	101	ASN	3.9
1	D	130	ARG	3.9
1	D	141	ILE	3.9
1	B	196	TYR	3.9
1	B	343	TYR	3.9
1	C	346	TYR	3.9
1	A	114	LEU	3.9
1	C	312	LYS	3.9
1	A	204	GLY	3.9
1	B	204	GLY	3.9
1	B	101	ASN	3.9
1	C	401	ARG	3.9
1	D	92	ARG	3.9
1	D	435	ASN	3.9
1	C	408	SER	3.8
1	D	329	ILE	3.8
1	A	249	LEU	3.8
1	C	337	GLY	3.8
1	D	295	LEU	3.8
1	D	314	LEU	3.8
1	A	169	ASP	3.8
1	D	338	ASN	3.8
1	A	421	PHE	3.8
1	D	415	TYR	3.8
1	D	54	VAL	3.8
1	D	206	VAL	3.8
1	A	154	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	358	LEU	3.8
1	B	370	LEU	3.8
1	A	451	THR	3.8
1	A	390	ASN	3.8
1	B	338	ASN	3.8
1	B	390	ASN	3.8
1	C	150	TRP	3.8
1	C	89	PRO	3.8
1	A	151[A]	LEU	3.8
1	A	432	LEU	3.8
1	B	86	THR	3.8
1	C	377	THR	3.8
1	D	236	THR	3.8
1	C	223	GLU	3.8
1	A	184	LYS	3.8
1	A	403	LYS	3.8
1	B	409	SER	3.8
1	D	406	PRO	3.8
1	A	363	PHE	3.8
1	B	421	PHE	3.8
1	B	432	LEU	3.8
1	D	8	GLY	3.8
1	B	58	ALA	3.7
1	C	214	ASN	3.7
1	D	59	ARG	3.7
1	A	329	ILE	3.7
1	C	90	ILE	3.7
1	B	332	LEU	3.7
1	D	345	LEU	3.7
1	A	196	TYR	3.7
1	D	434	PRO	3.7
1	A	243	PHE	3.7
1	D	90	ILE	3.7
1	A	73	LEU	3.7
1	B	364	VAL	3.7
1	A	348	THR	3.7
1	D	420	ASP	3.7
1	C	373	ARG	3.7
1	B	392	PRO	3.7
1	C	392	PRO	3.7
1	A	275	TRP	3.7
1	D	106	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	126	LEU	3.7
1	C	182	GLY	3.7
1	D	257	GLY	3.7
1	B	452	VAL	3.7
1	A	302	THR	3.7
1	C	117	ALA	3.7
1	D	176	TYR	3.7
1	B	216	SER	3.7
1	B	339	HIS	3.7
1	B	330	PHE	3.6
1	B	159	TRP	3.6
1	C	217	LEU	3.6
1	C	311	VAL	3.6
1	A	171	THR	3.6
1	D	51	THR	3.6
1	A	100	LYS	3.6
1	B	10	SER	3.6
1	B	464	ILE	3.6
1	C	138	PHE	3.6
1	D	442	ILE	3.6
1	B	146	CYS	3.6
1	B	410	ASP	3.6
1	C	159	TRP	3.6
1	D	15	ASN	3.6
1	B	205	VAL	3.6
1	D	242	ALA	3.6
1	A	134	ILE	3.6
1	A	316	PHE	3.6
1	C	316	PHE	3.6
1	A	392	PRO	3.6
1	C	349	ALA	3.6
1	D	233	ALA	3.6
1	C	130	ARG	3.6
1	B	466	GLY	3.6
1	C	127	GLY	3.6
1	D	48	PHE	3.6
1	A	186	ASP	3.6
1	A	191	ASP	3.6
1	B	139	GLU	3.6
1	B	356	GLN	3.5
1	D	373	ARG	3.5
1	A	168	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	416	TYR	3.5
1	B	288	TYR	3.5
1	C	280	LEU	3.5
1	D	194	ASN	3.5
1	C	181	THR	3.5
1	D	16	THR	3.5
1	D	377	THR	3.5
1	C	147	VAL	3.5
1	C	315	VAL	3.5
1	B	329	ILE	3.5
1	A	400	PHE	3.5
1	B	314	LEU	3.5
1	C	108	LEU	3.5
1	C	166	LEU	3.5
1	A	173	ASN	3.5
1	B	420	ASP	3.5
1	A	301	GLU	3.5
1	D	171	THR	3.5
1	B	292	VAL	3.5
1	B	402	VAL	3.5
1	B	349	ALA	3.5
1	A	216	SER	3.5
1	D	405	TYR	3.5
1	A	182	GLY	3.5
1	B	399	GLY	3.5
1	D	384	ILE	3.5
1	B	286	ASP	3.5
1	C	101	ASN	3.5
1	C	212	ASN	3.5
1	B	407	GLU	3.5
1	A	0	THR	3.5
1	D	133	ARG	3.5
1	A	412	ALA	3.5
1	C	357	ALA	3.5
1	D	88	GLY	3.5
1	A	289	ASN	3.5
1	A	291	LEU	3.5
1	C	114	LEU	3.5
1	D	291	LEU	3.5
1	C	178	PHE	3.5
1	B	411	GLN	3.5
1	A	193	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	6	VAL	3.4
1	D	216	SER	3.4
1	B	142	GLU	3.4
1	D	309	GLU	3.4
1	B	185	ILE	3.4
1	A	24	LEU	3.4
1	A	161	LEU	3.4
1	A	166	LEU	3.4
1	D	196	TYR	3.4
1	D	379	PHE	3.4
1	D	128	LYS	3.4
1	B	366	ARG	3.4
1	B	166	LEU	3.4
1	B	347	LEU	3.4
1	C	57	ILE	3.4
1	D	151	LEU	3.4
1	D	335	ASP	3.4
1	D	352	GLN	3.4
1	C	463[A]	LYS	3.4
1	C	406	PRO	3.4
1	A	313	THR	3.4
1	D	302	THR	3.4
1	C	91	VAL	3.4
1	D	452	VAL	3.4
1	A	122	ALA	3.4
1	C	192	ALA	3.4
1	D	124	ALA	3.4
1	B	447	ARG	3.4
1	C	77	GLN	3.4
1	A	420	ASP	3.4
1	B	389	ILE	3.4
1	C	297	ASN	3.4
1	D	166	LEU	3.4
1	D	254	LYS	3.4
1	D	372	ASN	3.4
1	B	400	PHE	3.4
1	C	288	TYR	3.4
1	D	320	TYR	3.4
1	D	353	TYR	3.4
1	B	181	THR	3.4
1	C	451	THR	3.4
1	A	311	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	349	ALA	3.4
1	C	336	ARG	3.4
1	D	192	ALA	3.4
1	A	279[A]	CYS	3.4
1	C	293	LYS	3.4
1	D	76	GLY	3.4
1	D	118	ASN	3.4
1	C	148	LEU	3.3
1	C	418	LEU	3.3
1	C	442	ILE	3.3
1	D	73	LEU	3.3
1	C	310	PHE	3.3
1	C	330	PHE	3.3
1	C	400	PHE	3.3
1	A	336	ARG	3.3
1	C	142	GLU	3.3
1	D	223	GLU	3.3
1	C	273	ALA	3.3
1	D	403	LYS	3.3
1	B	212	ASN	3.3
1	D	75	ASP	3.3
1	C	53	THR	3.3
1	A	150	TRP	3.3
1	A	176	TYR	3.3
1	D	346	TYR	3.3
1	A	315	VAL	3.3
1	D	356	GLN	3.3
1	A	214	ASN	3.3
1	B	167	ASP	3.3
1	D	390	ASN	3.3
1	A	347	LEU	3.3
1	C	468	PRO	3.3
1	A	299	THR	3.3
1	B	171	THR	3.3
1	B	243	PHE	3.3
1	C	48	PHE	3.3
1	B	109	SER	3.3
1	D	129	SER	3.3
1	A	58	ALA	3.3
1	A	448	VAL	3.3
1	C	70	ALA	3.3
1	A	212	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	191	ASP	3.3
1	B	226	ASN	3.3
1	B	334	ASP	3.3
1	A	332	LEU	3.3
1	C	153	LEU	3.3
1	D	370	LEU	3.3
1	A	74	ARG	3.3
1	B	251	HIS	3.3
1	B	395	GLN	3.3
1	A	45	TYR	3.3
1	B	416	TYR	3.3
1	C	215	TYR	3.3
1	B	344	ASP	3.2
1	D	39	ASN	3.2
1	D	371	ASN	3.2
1	D	336	ARG	3.2
1	D	97	LEU	3.2
1	A	105	LYS	3.2
1	A	464	ILE	3.2
1	B	100	LYS	3.2
1	B	384	ILE	3.2
1	C	197	THR	3.2
1	A	99	PHE	3.2
1	A	354	SER	3.2
1	D	190	TYR	3.2
1	A	52	VAL	3.2
1	A	440	VAL	3.2
1	C	52	VAL	3.2
1	D	388	GLY	3.2
1	B	467	LYS	3.2
1	A	148	LEU	3.2
1	B	277	LEU	3.2
1	C	376	LEU	3.2
1	D	419	LEU	3.2
1	A	343	TYR	3.2
1	A	368	ARG	3.2
1	A	374	GLY	3.2
1	C	208	VAL	3.2
1	A	55	ASP	3.2
1	D	436	GLU	3.2
1	D	472	LYS	3.2
1	D	123	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	468	PRO	3.2
1	B	299	THR	3.2
1	C	379	PHE	3.2
1	A	47	SER	3.2
1	B	219	LYS	3.2
1	C	290	LYS	3.2
1	B	320	TYR	3.2
1	C	88	GLY	3.2
1	C	191	ASP	3.2
1	C	296	ASP	3.2
1	D	311	VAL	3.2
1	D	416	TYR	3.2
1	C	275	TRP	3.2
1	A	116	PRO	3.2
1	B	247	PRO	3.2
1	D	103	LEU	3.2
1	A	379	PHE	3.1
1	A	119	HIS	3.1
1	B	8	GLY	3.1
1	A	286	ASP	3.1
1	A	338	ASN	3.1
1	B	225	ASP	3.1
1	C	369	ASN	3.1
1	C	381	ASP	3.1
1	D	55	ASP	3.1
1	D	117	ALA	3.1
1	D	65	VAL	3.1
1	A	353	TYR	3.1
1	C	353	TYR	3.1
1	A	217	LEU	3.1
1	D	160	GLN	3.1
1	C	35	ILE	3.1
1	D	99	PHE	3.1
1	A	337	GLY	3.1
1	C	224	GLY	3.1
1	B	124	ALA	3.1
1	C	267	ALA	3.1
1	D	62	ASP	3.1
1	D	267	ALA	3.1
1	D	323	ASN	3.1
1	C	175	VAL	3.1
1	D	231	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	395	GLN	3.1
1	C	370	LEU	3.1
1	A	2	ILE	3.1
1	D	275	TRP	3.1
1	C	169	ASP	3.1
1	C	470	GLY	3.1
1	A	222	GLN	3.1
1	A	267	ALA	3.1
1	C	188	GLN	3.1
1	C	239	GLN	3.1
1	C	395	GLN	3.1
1	B	245	VAL	3.1
1	D	376	LEU	3.1
1	D	392	PRO	3.1
1	C	450	ARG	3.1
1	D	78	ARG	3.1
1	C	473	ILE	3.1
1	D	333	ILE	3.1
1	D	13	HIS	3.1
1	B	465	SER	3.1
1	B	31	GLY	3.1
1	B	361	GLY	3.1
1	B	374	GLY	3.1
1	C	289	ASN	3.1
1	D	56	ASP	3.1
1	A	115	ALA	3.1
1	C	122	ALA	3.1
1	B	232	VAL	3.1
1	C	440	VAL	3.1
1	B	376	LEU	3.1
1	A	190	TYR	3.0
1	A	355	GLU	3.0
1	A	112	ILE	3.0
1	C	112	ILE	3.0
1	D	473	ILE	3.0
1	B	236	THR	3.0
1	B	244	GLY	3.0
1	D	169	ASP	3.0
1	A	170	CYS	3.0
1	A	285	ARG	3.0
1	B	417	ARG	3.0
1	D	290	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	345	LEU	3.0
1	B	413	LEU	3.0
1	B	444	LEU	3.0
1	C	42	LEU	3.0
1	D	208	VAL	3.0
1	C	190	TYR	3.0
1	A	53	THR	3.0
1	D	181	THR	3.0
1	A	165	TRP	3.0
1	A	293	LYS	3.0
1	C	59	ARG	3.0
1	C	79	PHE	3.0
1	D	116	PRO	3.0
1	A	402	VAL	3.0
1	B	90	ILE	3.0
1	C	328	ILE	3.0
1	A	322	THR	3.0
1	A	36	GLN	3.0
1	C	36	GLN	3.0
1	D	367	GLN	3.0
1	A	393	LYS	3.0
1	C	133	ARG	3.0
1	D	318	ARG	3.0
1	A	155	SER	3.0
1	C	121	SER	3.0
1	C	287	SER	3.0
1	B	355	GLU	3.0
1	B	406	PRO	3.0
1	B	111	LEU	3.0
1	D	3	VAL	3.0
1	B	328	ILE	3.0
1	B	190	TYR	3.0
1	C	14	THR	3.0
1	C	155	SER	3.0
1	C	26	ASN	3.0
1	A	306	GLU	3.0
1	B	362	PHE	2.9
1	C	180	LEU	2.9
1	D	220	LEU	2.9
1	A	82	ILE	2.9
1	A	258	ILE	2.9
1	D	2	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	256	ILE	2.9
1	D	298	ILE	2.9
1	A	236	THR	2.9
1	B	302	THR	2.9
1	A	163[A]	GLU	2.9
1	C	173	ASN	2.9
1	A	159[A]	TRP	2.9
1	B	48	PHE	2.9
1	D	453	PHE	2.9
1	B	108	LEU	2.9
1	D	360	ALA	2.9
1	D	398	LEU	2.9
1	B	77	GLN	2.9
1	A	473	ILE	2.9
1	A	101	ASN	2.9
1	A	177	SER	2.9
1	C	420	ASP	2.9
1	D	155	SER	2.9
1	B	312	LYS	2.9
1	A	314	LEU	2.9
1	B	404	ALA	2.9
1	C	73	LEU	2.9
1	C	124	ALA	2.9
1	D	122	ALA	2.9
1	D	445	GLN	2.9
1	C	81	CYS	2.9
1	A	238	THR	2.9
1	A	294	GLU	2.9
1	C	449	ASP	2.9
1	D	50	ASP	2.9
1	A	346	TYR	2.9
1	B	89	PRO	2.9
1	D	312	LYS	2.9
1	A	310	PHE	2.9
1	C	340	LEU	2.9
1	D	459	LEU	2.9
1	A	276	ILE	2.9
1	D	46	ILE	2.9
1	D	26	ASN	2.9
1	D	156	ASP	2.9
1	D	214	ASN	2.9
1	B	128	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	472	LYS	2.8
1	A	271	PRO	2.8
1	A	320	TYR	2.8
1	B	221	HIS	2.8
1	C	187	ARG	2.8
1	C	271	PRO	2.8
1	A	126	LEU	2.8
1	A	91	VAL	2.8
1	A	282	VAL	2.8
1	C	205	VAL	2.8
1	B	436	GLU	2.8
1	B	441	GLU	2.8
1	A	181	THR	2.8
1	B	333	ILE	2.8
1	A	297	ASN	2.8
1	B	26	ASN	2.8
1	B	173	ASN	2.8
1	D	87	GLY	2.8
1	B	461	PRO	2.8
1	C	176	TYR	2.8
1	A	180	LEU	2.8
1	A	370	LEU	2.8
1	B	33	LEU	2.8
1	A	178	PHE	2.8
1	B	412	ALA	2.8
1	B	52	VAL	2.8
1	D	300	LYS	2.8
1	A	256	ILE	2.8
1	A	272	THR	2.8
1	A	106	CYS	2.8
1	B	59	ARG	2.8
1	D	313	THR	2.8
1	D	212	ASN	2.8
1	C	200	SER	2.8
1	B	434	PRO	2.8
1	C	64	ALA	2.8
1	D	210	ALA	2.8
1	A	232	VAL	2.8
1	C	206	VAL	2.8
1	D	292	VAL	2.8
1	A	384	ILE	2.8
1	B	214	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	144	GLY	2.8
1	B	155	SER	2.8
1	B	202	SER	2.8
1	D	146	CYS	2.8
1	C	294	GLU	2.8
1	B	295	LEU	2.8
1	B	382	TYR	2.8
1	C	184	LYS	2.8
1	D	60	ALA	2.8
1	B	336	ARG	2.8
1	A	377	THR	2.7
1	B	50	ASP	2.7
1	B	276	ILE	2.7
1	C	335	ASP	2.7
1	D	67	ASP	2.7
1	D	365	ASP	2.7
1	A	94	TRP	2.7
1	C	177	SER	2.7
1	C	252	SER	2.7
1	C	306	GLU	2.7
1	A	219	LYS	2.7
1	B	97	LEU	2.7
1	B	218	LEU	2.7
1	D	20	LEU	2.7
1	B	446	ARG	2.7
1	A	175	VAL	2.7
1	C	6	VAL	2.7
1	D	37	VAL	2.7
1	C	236	THR	2.7
1	A	431	ILE	2.7
1	D	82	ILE	2.7
1	D	286	ASP	2.7
1	C	18	GLY	2.7
1	C	129	SER	2.7
1	B	143	PRO	2.7
1	D	21	PRO	2.7
1	D	89	PRO	2.7
1	B	306	GLU	2.7
1	C	254	LYS	2.7
1	A	130	ARG	2.7
1	D	187	ARG	2.7
1	B	209	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	339	HIS	2.7
1	C	119	HIS	2.7
1	D	61	PHE	2.7
1	A	245	VAL	2.7
1	A	34	ASP	2.7
1	A	194	ASN	2.7
1	B	377	THR	2.7
1	C	12	THR	2.7
1	C	391	THR	2.7
1	D	53	THR	2.7
1	D	71	ASP	2.7
1	A	399	GLY	2.7
1	D	43	GLY	2.7
1	B	326	SER	2.7
1	B	463	LYS	2.7
1	C	308	LYS	2.7
1	A	318	ARG	2.7
1	B	106	CYS	2.7
1	B	133	ARG	2.7
1	C	432	LEU	2.7
1	A	273	ALA	2.7
1	D	64	ALA	2.7
1	B	168	TYR	2.7
1	A	206	VAL	2.7
1	C	105	LYS	2.7
1	C	162	ASN	2.7
1	C	211	THR	2.7
1	D	49	ASP	2.7
1	D	364	VAL	2.7
1	A	391	THR	2.7
1	C	386	GLU	2.7
1	D	199	GLU	2.7
1	B	258	ILE	2.7
1	A	434	PRO	2.7
1	D	287	SER	2.7
1	A	153	LEU	2.7
1	C	220	LEU	2.7
1	A	124	ALA	2.6
1	A	395	GLN	2.6
1	B	22	GLN	2.6
1	A	6	VAL	2.6
1	B	203	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	163	GLU	2.6
1	C	319	GLU	2.6
1	B	282	VAL	2.6
1	C	245	VAL	2.6
1	C	198	GLY	2.6
1	B	74	ARG	2.6
1	A	85	SER	2.6
1	A	340	LEU	2.6
1	C	123	LEU	2.6
1	D	111	LEU	2.6
1	D	380	LEU	2.6
1	B	222	GLN	2.6
1	D	375	LYS	2.6
1	C	99	PHE	2.6
1	C	196	TYR	2.6
1	C	323	ASN	2.6
1	D	383	ASP	2.6
1	A	278[A]	ARG	2.6
1	C	368	ARG	2.6
1	C	447	ARG	2.6
1	B	224	GLY	2.6
1	B	460	THR	2.6
1	C	302	THR	2.6
1	D	361	GLY	2.6
1	A	326	SER	2.6
1	D	69	ILE	2.6
1	A	358	LEU	2.6
1	D	180	LEU	2.6
1	D	246	LEU	2.6
1	A	209	ALA	2.6
1	C	462	ALA	2.6
1	A	366	ARG	2.6
1	A	435	ASN	2.6
1	B	56	ASP	2.6
1	B	67	ASP	2.6
1	D	167	ASP	2.6
1	D	45	TYR	2.6
1	D	144	GLY	2.6
1	D	466	GLY	2.6
1	B	85	SER	2.6
1	C	276	ILE	2.6
1	D	202	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	24	LEU	2.6
1	B	210	ALA	2.6
1	C	165	TRP	2.6
1	A	71[A]	ASP	2.6
1	A	296	ASP	2.6
1	A	344	ASP	2.6
1	B	296	ASP	2.6
1	B	381	ASP	2.6
1	C	149	ASP	2.6
1	C	286	ASP	2.6
1	D	397	ASN	2.6
1	B	99	PHE	2.6
1	B	453	PHE	2.6
1	C	132	GLY	2.6
1	D	182	GLY	2.6
1	A	195	SER	2.6
1	A	252	SER	2.6
1	A	287	SER	2.6
1	D	17	TYR	2.6
1	B	472	LYS	2.6
1	D	108	LEU	2.5
1	D	74	ARG	2.5
1	C	94	TRP	2.5
1	A	89	PRO	2.5
1	A	461	PRO	2.5
1	B	107	PRO	2.5
1	C	434	PRO	2.5
1	D	174	GLY	2.5
1	B	290	LYS	2.5
1	A	281	GLN	2.5
1	A	382	TYR	2.5
1	C	41	TYR	2.5
1	C	45	TYR	2.5
1	B	294	GLU	2.5
1	A	450	ARG	2.5
1	A	20	LEU	2.5
1	C	277	LEU	2.5
1	C	380	LEU	2.5
1	A	56	ASP	2.5
1	B	64	ALA	2.5
1	B	71	ASP	2.5
1	B	115	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	233	ALA	2.5
1	D	209	ALA	2.5
1	A	32	LYS	2.5
1	A	467	LYS	2.5
1	B	72	LYS	2.5
1	B	430	LYS	2.5
1	C	116	PRO	2.5
1	D	38	GLY	2.5
1	D	308	LYS	2.5
1	A	269	THR	2.5
1	C	84	HIS	2.5
1	D	197	THR	2.5
1	D	362	PHE	2.5
1	A	438	VAL	2.5
1	B	175	VAL	2.5
1	D	179	VAL	2.5
1	B	321	ILE	2.5
1	A	133	ARG	2.5
1	A	280	LEU	2.5
1	A	398	LEU	2.5
1	B	151	LEU	2.5
1	B	220	LEU	2.5
1	B	291	LEU	2.5
1	C	345	LEU	2.5
1	C	347	LEU	2.5
1	A	255	ASN	2.5
1	A	449	ASP	2.5
1	B	293	LYS	2.5
1	B	365	ASP	2.5
1	C	234	LYS	2.5
1	C	360	ALA	2.5
1	C	397	ASN	2.5
1	C	471	LYS	2.5
1	C	303	GLN	2.5
1	A	364	VAL	2.5
1	C	25	GLU	2.5
1	B	274	ILE	2.5
1	A	325	TYR	2.5
1	D	382	TYR	2.5
1	A	277	LEU	2.5
1	B	148	LEU	2.5
1	C	194	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	297	ASN	2.5
1	A	201	GLY	2.5
1	B	38	GLY	2.5
1	B	337	GLY	2.5
1	C	201	GLY	2.5
1	D	18	GLY	2.5
1	D	359	PRO	2.5
1	A	59	ARG	2.4
1	A	146	CYS	2.4
1	D	81	CYS	2.4
1	C	158	SER	2.4
1	A	54	VAL	2.4
1	D	79	PHE	2.4
1	B	112	ILE	2.4
1	C	259	ILE	2.4
1	A	131	LEU	2.4
1	A	376	LEU	2.4
1	D	41	TYR	2.4
1	A	335	ASP	2.4
1	B	305	ASN	2.4
1	C	203	ASN	2.4
1	C	266	ASN	2.4
1	D	203	ASN	2.4
1	D	289	ASN	2.4
1	A	22	GLN	2.4
1	B	303	GLN	2.4
1	A	207	ARG	2.4
1	C	60	ALA	2.4
1	B	319	GLU	2.4
1	C	331	ARG	2.4
1	B	238	THR	2.4
1	C	460	THR	2.4
1	A	90	ILE	2.4
1	B	11	VAL	2.4
1	B	61	PHE	2.4
1	C	37	VAL	2.4
1	C	283	LYS	2.4
1	B	149	ASP	2.4
1	B	335	ASP	2.4
1	D	63	GLN	2.4
1	D	186	ASP	2.4
1	B	223	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	209	ALA	2.4
1	C	387	GLY	2.4
1	C	106	CYS	2.4
1	A	259	ILE	2.4
1	B	473	ILE	2.4
1	D	11	VAL	2.4
1	D	282	VAL	2.4
1	B	249	LEU	2.4
1	C	168	TYR	2.4
1	C	356	GLN	2.4
1	C	167	ASP	2.4
1	D	319	GLU	2.4
1	A	359	PRO	2.4
1	D	224	GLY	2.4
1	B	250	SER	2.4
1	B	231	VAL	2.4
1	C	292	VAL	2.4
1	C	249	LEU	2.4
1	A	446	ARG	2.4
1	A	303	GLN	2.4
1	C	156	ASP	2.3
1	C	372	ASN	2.3
1	D	305	ASN	2.3
1	D	468	PRO	2.3
1	A	60	ALA	2.3
1	A	404	ALA	2.3
1	C	242	ALA	2.3
1	D	80	ALA	2.3
1	A	437	THR	2.3
1	C	274	ILE	2.3
1	C	207	ARG	2.3
1	A	188	GLN	2.3
1	B	73	LEU	2.3
1	C	111	LEU	2.3
1	C	367	GLN	2.3
1	D	188	GLN	2.3
1	A	471	LYS	2.3
1	B	45	TYR	2.3
1	B	18	GLY	2.3
1	C	120	GLY	2.3
1	C	244	GLY	2.3
1	D	462	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	16	THR	2.3
1	B	318	ARG	2.3
1	C	251	HIS	2.3
1	A	48	PHE	2.3
1	B	367	GLN	2.3
1	D	77	GLN	2.3
1	A	418	LEU	2.3
1	A	62	ASP	2.3
1	A	371	ASN	2.3
1	D	34	ASP	2.3
1	B	116	PRO	2.3
1	A	215	TYR	2.3
1	B	242	ALA	2.3
1	C	317	THR	2.3
1	B	401	ARG	2.3
1	D	401	ARG	2.3
1	D	27	GLN	2.3
1	B	256	ILE	2.3
1	C	256	ILE	2.3
1	C	321	ILE	2.3
1	D	280	LEU	2.3
1	C	55	ASP	2.3
1	A	198	GLY	2.3
1	A	80	ALA	2.3
1	B	278	ARG	2.3
1	D	450	ARG	2.3
1	B	469	THR	2.3
1	D	211	THR	2.3
1	A	202	SER	2.3
1	A	270	HIS	2.3
1	B	47	SER	2.3
1	C	7	HIS	2.3
1	C	183	GLN	2.3
1	D	407	GLU	2.3
1	A	4	ILE	2.3
1	A	42	LEU	2.2
1	A	79	PHE	2.2
1	D	170	CYS	2.2
1	D	474	ASP	2.2
1	A	12	THR	2.2
1	A	469	THR	2.2
1	B	25	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	70	ALA	2.2
1	C	210	ALA	2.2
1	C	83	THR	2.2
1	C	110	HIS	2.2
1	D	251	HIS	2.2
1	D	294	GLU	2.2
1	D	355	GLU	2.2
1	B	195	SER	2.2
1	A	472	LYS	2.2
1	A	328	ILE	2.2
1	B	4	ILE	2.2
1	D	358	LEU	2.2
1	A	453	PHE	2.2
1	A	474	ASP	2.2
1	B	62	ASP	2.2
1	B	383	ASP	2.2
1	A	417	ARG	2.2
1	C	247	PRO	2.2
1	C	388	GLY	2.2
1	C	307	HIS	2.2
1	D	301	GLU	2.2
1	B	105	LYS	2.2
1	D	70	ALA	2.2
1	A	98	TYR	2.2
1	D	288	TYR	2.2
1	A	321	ILE	2.2
1	A	389	ILE	2.2
1	B	46	ILE	2.2
1	C	455	ILE	2.2
1	D	35	ILE	2.2
1	B	418	LEU	2.2
1	D	5	PHE	2.2
1	A	39	ASN	2.2
1	A	373	ARG	2.2
1	B	470	GLY	2.2
1	D	201	GLY	2.2
1	A	125	GLN	2.2
1	A	254	LYS	2.2
1	B	119	HIS	2.2
1	C	407	GLU	2.2
1	D	441	GLU	2.2
1	D	22	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	105	LYS	2.2
1	D	222	GLN	2.2
1	A	360	ALA	2.2
1	B	122	ALA	2.2
1	C	250	SER	2.2
1	D	250	SER	2.2
1	A	405	TYR	2.2
1	C	382	TYR	2.2
1	A	220	LEU	2.2
1	A	274	ILE	2.2
1	B	66	ARG	2.2
1	B	217	LEU	2.2
1	C	246	LEU	2.2
1	C	278	ARG	2.2
1	D	33	LEU	2.2
1	D	277	LEU	2.2
1	A	452	VAL	2.2
1	B	457	ASN	2.2
1	C	56	ASP	2.2
1	D	96	ASP	2.2
1	D	457	ASN	2.2
1	A	107	PRO	2.2
1	A	468	PRO	2.2
1	D	127	GLY	2.2
1	B	14	THR	2.2
1	C	58	ALA	2.2
1	D	263	THR	2.2
1	A	237	ARG	2.1
1	B	215	TYR	2.1
1	D	417	ARG	2.1
1	B	153	LEU	2.1
1	C	145	LYS	2.1
1	C	240	PRO	2.1
1	D	178	PHE	2.1
1	C	13	HIS	2.1
1	C	433	HIS	2.1
1	D	110	HIS	2.1
1	A	248	GLY	2.1
1	A	265	ALA	2.1
1	B	134	ILE	2.1
1	B	403	LYS	2.1
1	C	20	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	393	LYS	2.1
1	A	292	VAL	2.1
1	D	94	TRP	2.1
1	C	352	GLN	2.1
1	C	43	GLY	2.1
1	C	279	CYS	2.1
1	A	197	THR	2.1
1	B	408	SER	2.1
1	C	269	THR	2.1
1	C	326	SER	2.1
1	D	195	SER	2.1
1	A	234	LYS	2.1
1	A	283	LYS	2.1
1	B	308	LYS	2.1
1	C	29	LYS	2.1
1	D	93	LYS	2.1
1	B	156	ASP	2.1
1	C	338	ASN	2.1
1	C	154	GLY	2.1
1	B	192	ALA	2.1
1	A	97	LEU	2.1
1	B	125	GLN	2.1
1	C	4	ILE	2.1
1	C	255	ASN	2.1
1	D	259	ILE	2.1
1	A	406	PRO	2.1
1	B	17	TYR	2.1
1	A	23	TRP	2.1
1	B	234	LYS	2.0
1	D	83	THR	2.0
1	B	152	GLU	2.0
1	A	111	LEU	2.0
1	A	380	LEU	2.0
1	B	459	LEU	2.0
1	D	458	ASN	2.0
1	B	98	TYR	2.0
1	D	147	VAL	2.0
1	D	175	VAL	2.0
1	A	470	GLY	2.0
1	D	154	GLY	2.0
1	A	5	PHE	2.0
1	A	362	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	304	LYS	2.0
1	C	263	THR	2.0
1	D	460	THR	2.0
1	B	267	ALA	2.0
1	C	115	ALA	2.0
1	B	162	ASN	2.0
1	B	449	ASP	2.0
1	C	332	LEU	2.0
1	C	371	ASN	2.0
1	D	148	LEU	2.0
1	D	66	ARG	2.0
1	D	184	LYS	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 oligosaccharides in this entry.

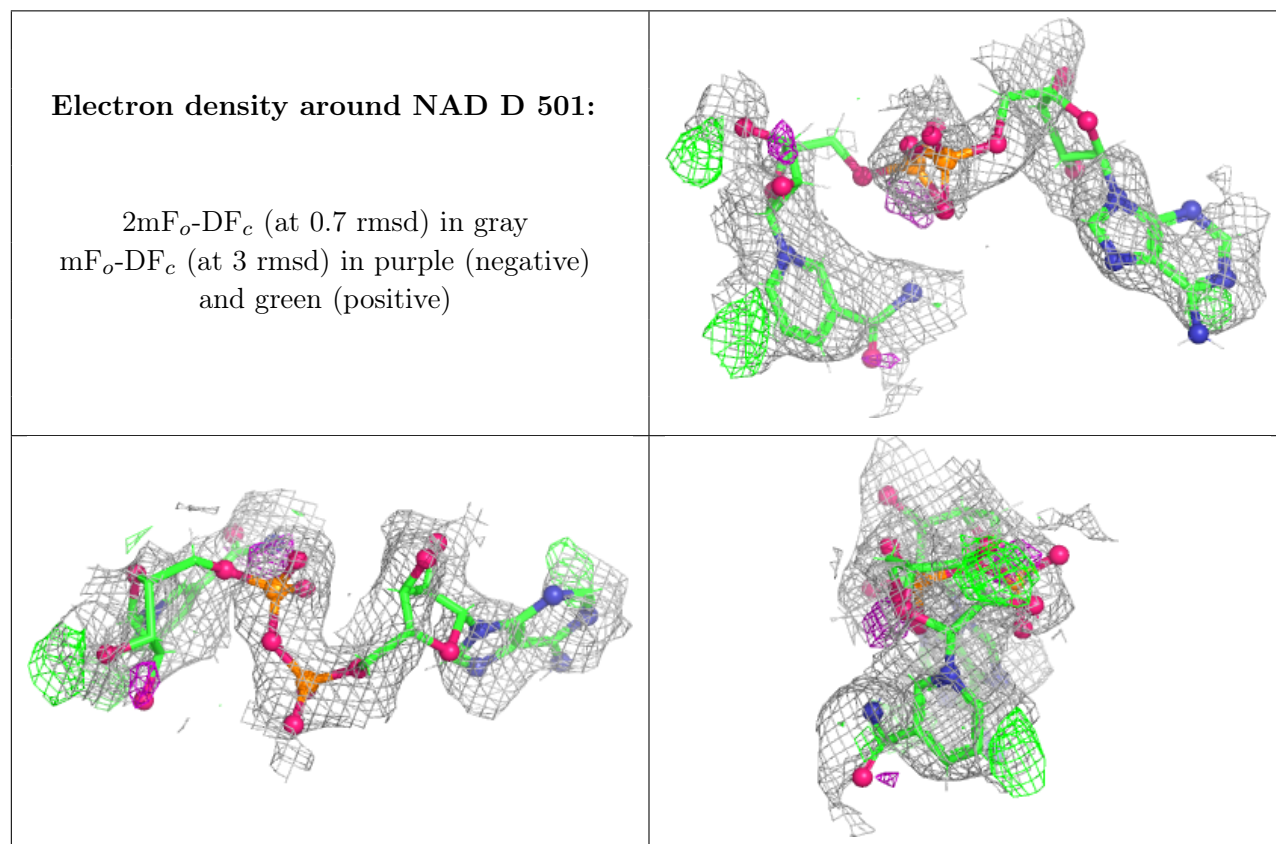
6.4 Ligands [i](#)

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, 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	B-factors(Å ²)	Q<0.9
2	NAD	D	501	44/44	0.57	0.30	23,48,62,69	70
2	NAD	D	502	44/44	0.61	0.33	22,34,44,53	70
2	NAD	A	501	44/44	0.63	0.23	22,38,52,55	0
2	NAD	C	501	44/44	0.69	0.27	15,30,43,49	70
2	NAD	B	601	44/44	0.72	0.23	21,38,51,57	70
2	NAD	B	602	44/44	0.74	0.23	10,28,39,46	0
2	NAD	A	502	44/44	0.76	0.20	18,31,45,55	70
2	NAD	C	502	44/44	0.86	0.16	6,24,34,41	0

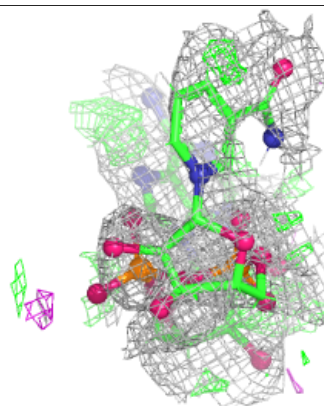
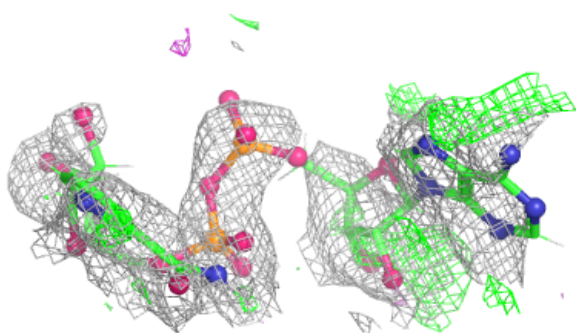
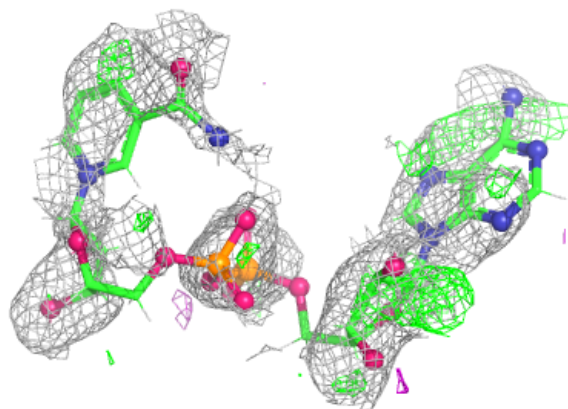
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

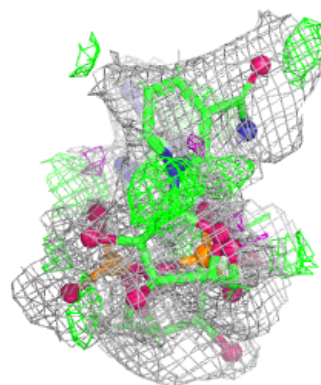
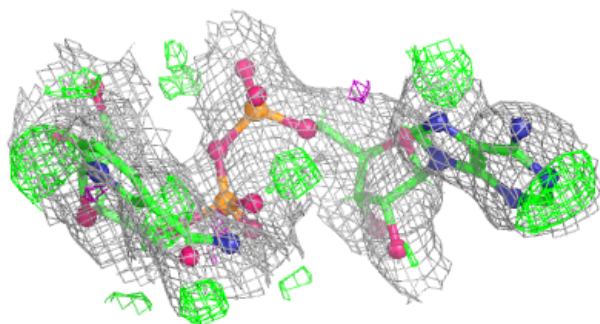
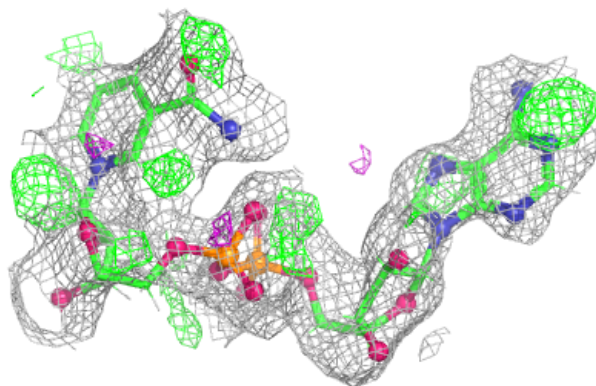


Electron density around NAD D 502:

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

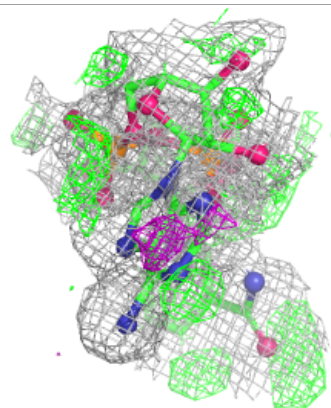
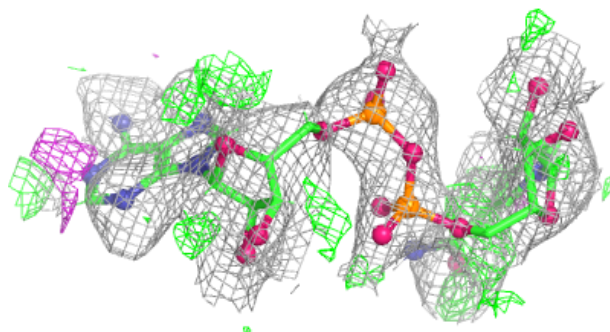
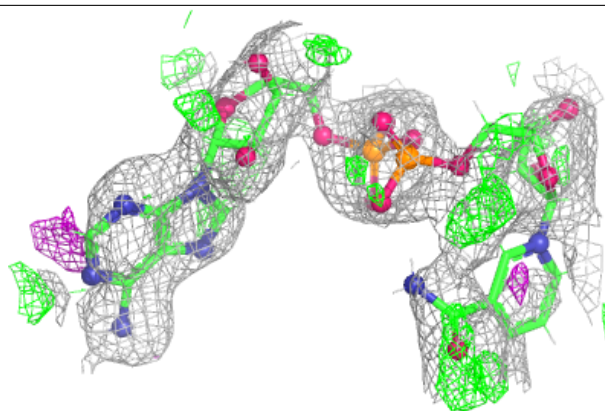
**Electron density around NAD A 501:**

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



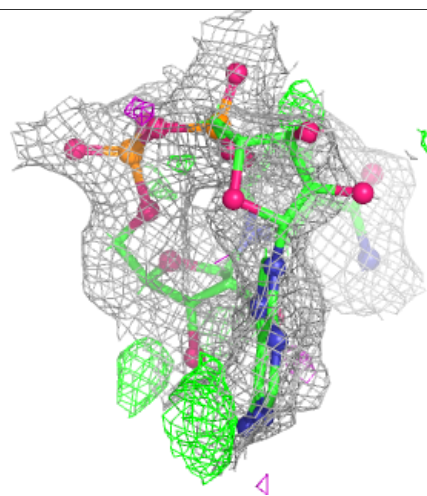
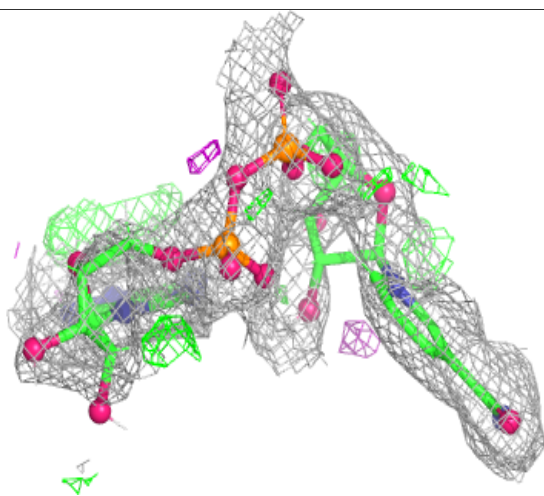
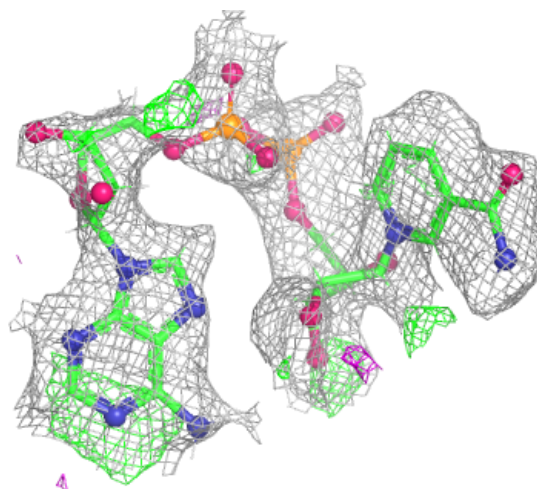
Electron density around NAD C 501:

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



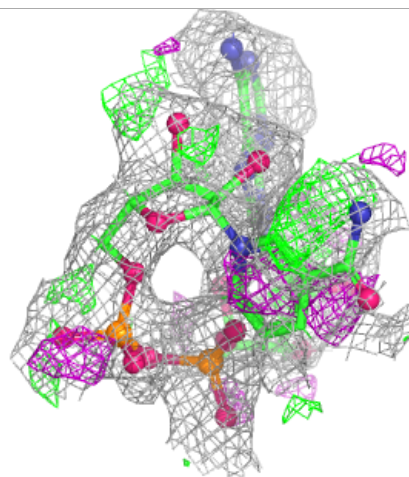
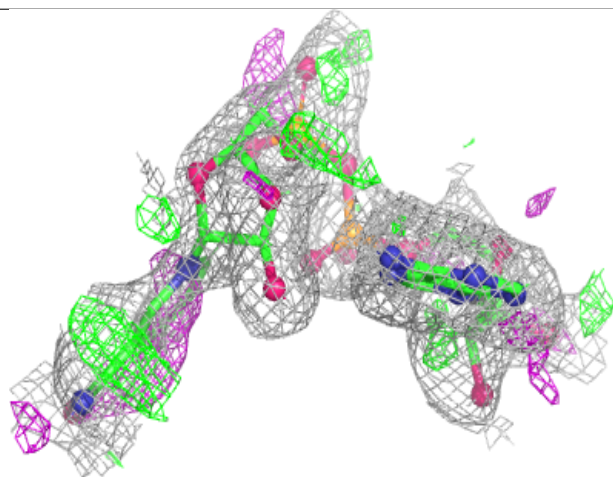
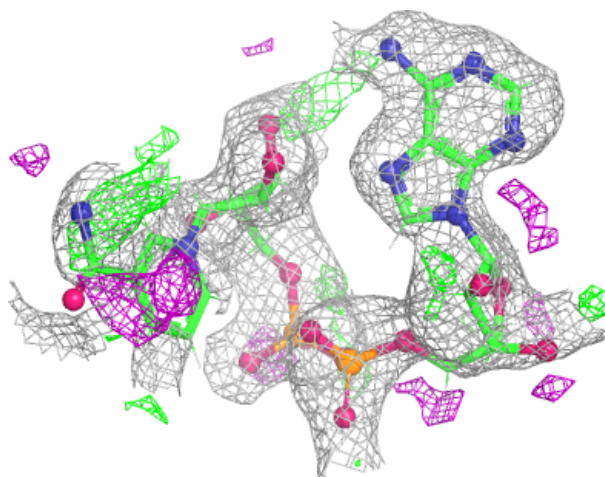
Electron density around NAD B 601:

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



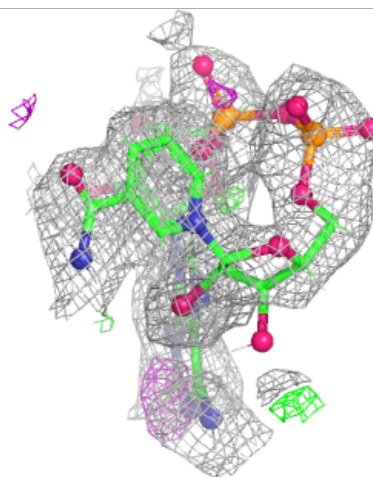
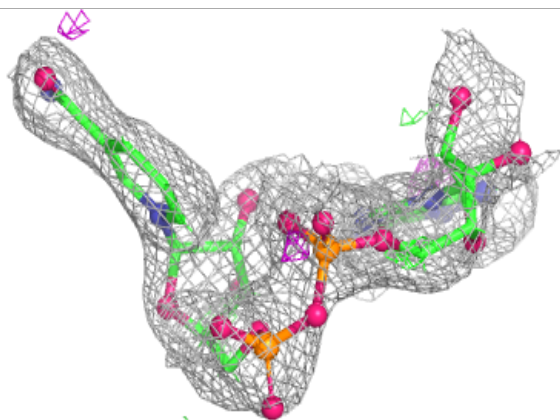
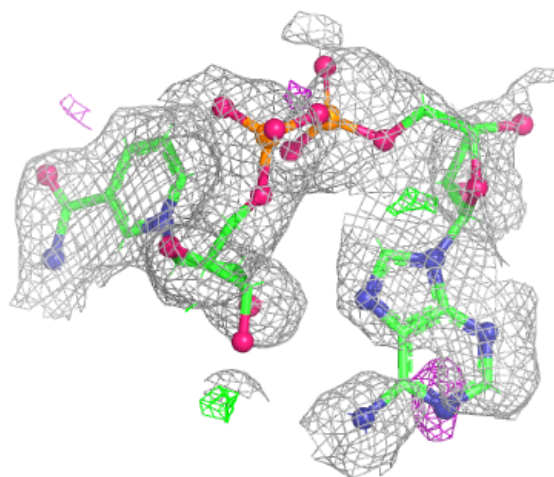
Electron density around NAD B 602:

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



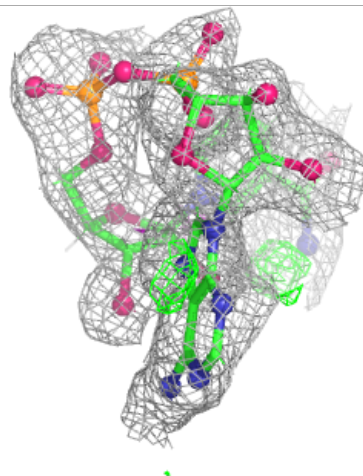
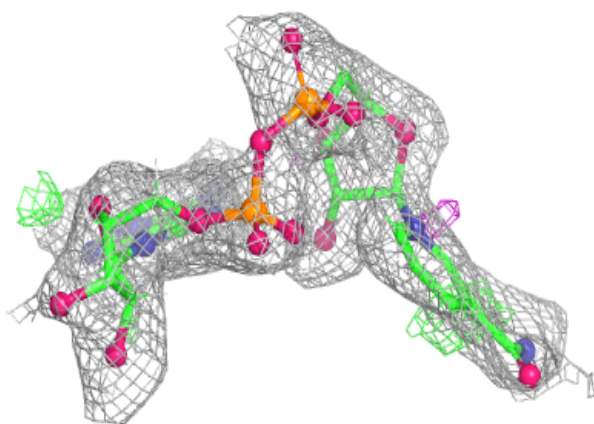
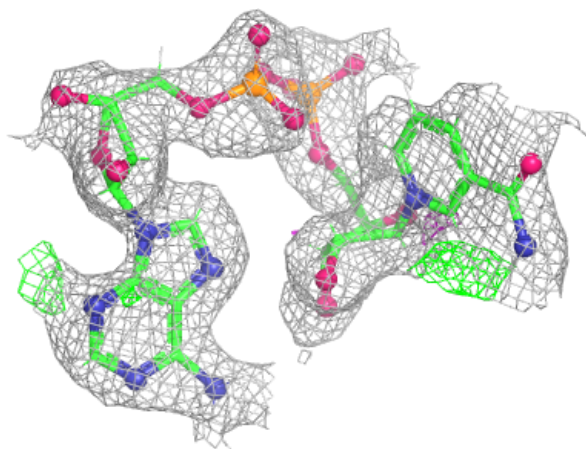
Electron density around NAD A 502:

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



Electron density around NAD C 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 [i](#)

There are no such residues in this entry.