



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:00 AM UTC

PDB ID : 9DCP / pdb_00009dcp
Title : Structure of PmHMGR bound to mevalonate, CoA and NAD 1 minute after reaction initiation at pH 9
Authors : Purohit, V.; Stauffacher, C.V.
Deposited on : 2024-08-27
Resolution : 2.06 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

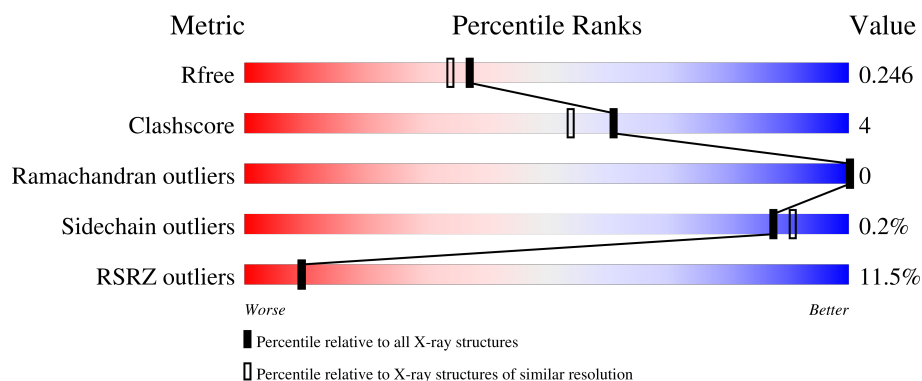
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	428	<div> <div>14%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
1	B	428	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>12%</div> </div> </div>

2 Entry composition [i](#)

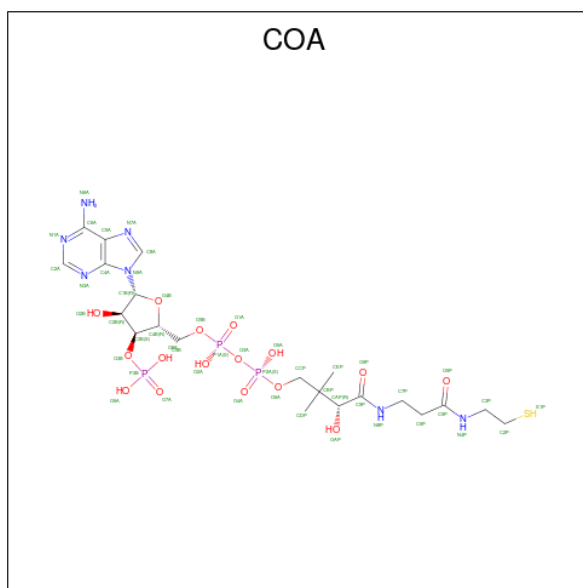
There are 7 unique types of molecules in this entry. The entry contains 6432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

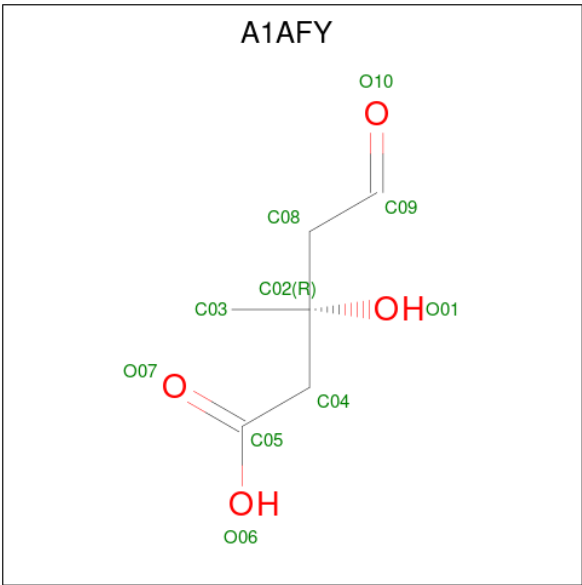
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	22	5	0
			3152	1974	576	586	16			
1	B	377	Total	C	N	O	S	14	2	0
			2792	1752	502	523	15			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



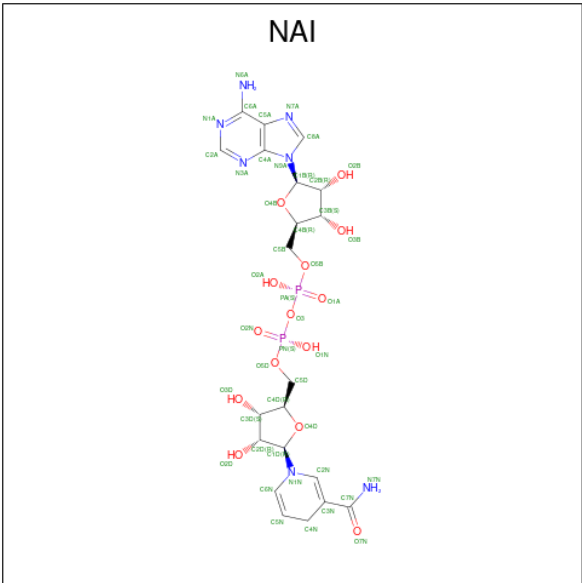
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	1
			48	21	7	16	3 1		
2	A	1	Total	C	N	O	P S	0	1
			48	21	7	16	3 1		

- Molecule 3 is (R)-mevaldehyde (CCD ID: A1AFY) (formula: $C_6H_{10}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			10	6	4		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



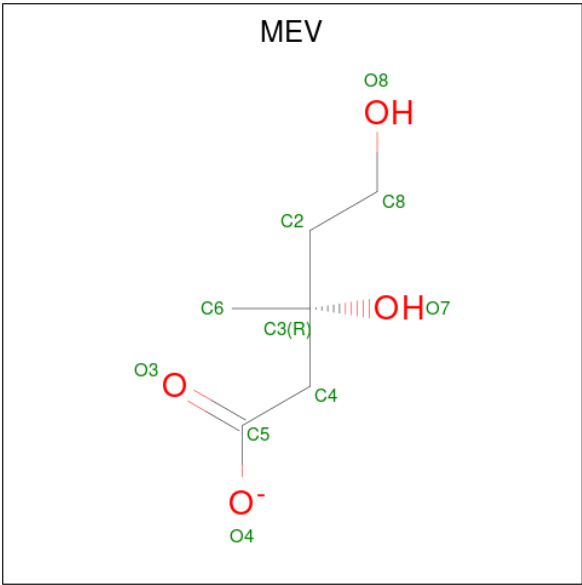
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			44	21	7	14		

- Molecule 5 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
5	B	1	Total	C	N	O	P	0	1
			44	21	7	14	2		

- Molecule 6 is (R)-MEVALONATE (CCD ID: MEV) (formula: C₆H₁₁O₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C O	0	0
			10	6 4		

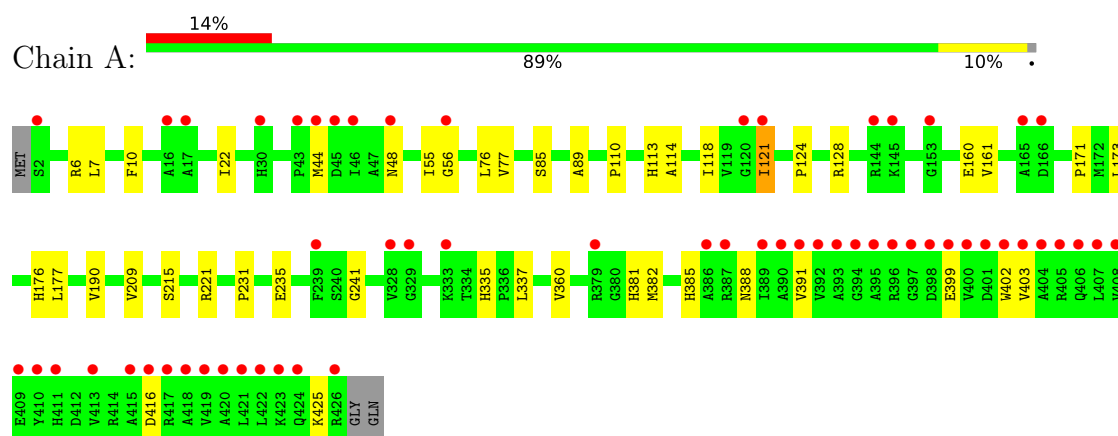
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	135	Total 135	O 135	0	0
7	B	149	Total 149	O 149	0	0

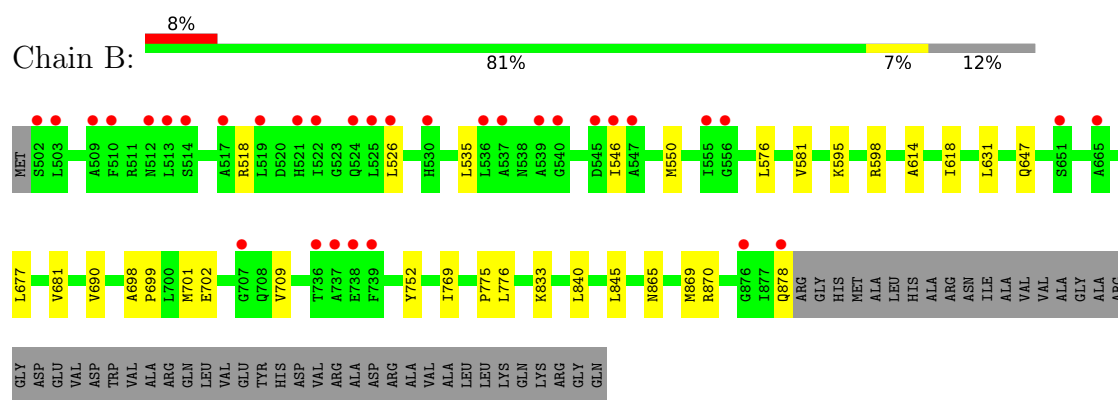
3 Residue-property plots

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: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	225.77Å 225.77Å 225.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 2.06 48.13 – 2.06	Depositor EDS
% Data completeness (in resolution range)	89.9 (48.13-2.06) 89.9 (48.13-2.06)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.07Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286)	Depositor
R, R_{free}	0.214 , 0.241 0.218 , 0.246	Depositor DCC
R_{free} test set	2723 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6432	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: COA, NAI, A1AFY, MEV, 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	0.12	0/3206	0.30	0/4363
1	B	0.12	0/2838	0.28	0/3862
All	All	0.12	0/6044	0.29	0/8225

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3152	0	3173	29	0
1	B	2792	0	2831	24	0
2	A	96	0	64	3	0
3	A	10	0	0	0	0
4	B	44	0	27	0	0
5	B	44	0	26	1	0
6	B	10	0	11	0	0
7	A	135	0	0	3	0
7	B	149	0	0	1	0
All	All	6432	0	6132	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (51) 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)
2:A:502[Y]:COA:O4B	2:A:502[Y]:COA:C1B	1.65	1.25
2:A:501[X]:COA:O4B	2:A:501[X]:COA:C1B	1.65	1.22
1:A:114:ALA:HB2	1:A:190:VAL:HB	1.70	0.74
1:A:160[A]:GLU:HG3	1:A:176:HIS:HB2	1.75	0.68
1:A:114:ALA:HB3	1:A:177:LEU:HB2	1.81	0.63
1:A:48:ASN:OD1	1:B:518:ARG:NH2	2.34	0.61
1:A:391:VAL:HG12	1:B:833:LYS:HD3	1.83	0.60
1:B:631:LEU:HD11	1:B:701:MET:HG2	1.85	0.58
1:B:878:GLN:N	1:B:878:GLN:OE1	2.40	0.54
1:A:118:ILE:HD12	1:A:173:LEU:HD22	1.90	0.53
1:A:44:MET:HE1	1:A:56:GLY:HA2	1.90	0.53
1:A:6:ARG:NH1	7:A:607:HOH:O	2.40	0.53
1:A:85[A]:SER:OG	1:A:381:HIS:HA	2.09	0.52
1:A:382:MET:HA	1:A:382:MET:HE2	1.92	0.51
1:B:614:ALA:HB2	1:B:690:VAL:HB	1.94	0.50
1:A:89:ALA:HB2	2:A:501[X]:COA:H61	1.93	0.50
1:A:118:ILE:HG12	1:A:209:VAL:HG22	1.93	0.50
1:A:416:ASP:OD2	1:B:647:GLN:N	2.31	0.50
1:A:385:HIS:CE1	1:A:388:ASN:HD22	2.30	0.49
1:B:769:ILE:HG12	1:B:865:ASN:HB2	1.95	0.48
1:A:381:HIS:CD2	1:A:382:MET:HE3	2.48	0.48
1:B:698:ALA:HB1	1:B:709:VAL:HG11	1.96	0.47
1:A:402:TRP:CZ3	1:A:425:LYS:HB2	2.50	0.47
1:A:231:PRO:O	1:A:241:GLY:HA3	2.15	0.47
1:A:7:LEU:HB3	1:A:10:PHE:HB2	1.96	0.46
1:B:681:VAL:O	5:B:1002[Y]:NAD:H2A	2.16	0.46
7:A:609:HOH:O	1:B:833:LYS:NZ	2.49	0.46
1:B:546:ILE:O	1:B:550:MET:HG3	2.16	0.46
1:B:870:ARG:HH11	1:B:870:ARG:HB3	1.81	0.46
1:A:124:PRO:HG3	1:A:171:PRO:HB2	1.98	0.45
1:B:526:LEU:HD21	1:B:576:LEU:HD12	1.98	0.45
1:B:618[B]:ILE:HG12	1:B:709:VAL:HG22	1.98	0.45
1:A:22:ILE:HD12	1:A:76:LEU:HD13	1.98	0.45
1:A:128:ARG:HG3	1:A:161:VAL:HB	1.99	0.44
1:A:55:ILE:HG22	1:B:518:ARG:HB3	1.98	0.44
1:B:581:VAL:HB	1:B:775:PRO:HG3	2.00	0.44
1:B:618[A]:ILE:HG12	1:B:709:VAL:HG22	1.98	0.44
1:A:110:PRO:HA	1:A:221:ARG:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:LYS:O	1:B:598:ARG:HG2	2.19	0.43
1:A:121:ILE:HD12	1:A:124:PRO:HA	2.01	0.42
1:B:535:LEU:HD12	1:B:840:LEU:HD22	2.01	0.42
1:A:335:HIS:CE1	1:A:337:LEU:HB2	2.55	0.41
1:A:399:GLU:O	1:A:403:VAL:HG22	2.19	0.41
1:B:614:ALA:HB3	1:B:677:LEU:HB2	2.02	0.41
1:B:699:PRO:HG2	7:B:1169:HOH:O	2.21	0.41
1:B:752:TYR:HB2	1:B:869:MET:HE1	2.02	0.41
1:B:776:LEU:HD11	1:B:845:LEU:HD11	2.02	0.41
1:A:235:GLU:OE1	7:A:601:HOH:O	2.20	0.41
1:B:702:GLU:HG3	1:B:709:VAL:HG23	2.03	0.40
1:A:77:VAL:HG11	1:A:360:VAL:HG21	2.03	0.40
1:A:113:HIS:HB2	1:A:215:SER:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/428 (100%)	413 (96%)	15 (4%)	0	100	100
1	B	377/428 (88%)	366 (97%)	11 (3%)	0	100	100
All	All	805/856 (94%)	779 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	318/327 (97%)	317 (100%)	1 (0%)	86	89
1	B	287/327 (88%)	287 (100%)	0	100	100
All	All	605/654 (92%)	604 (100%)	1 (0%)	87	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	188	ASN
1	A	351	GLN
1	A	388	ASN
1	B	615	GLN
1	B	839	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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
5	NAD	B	1002[Y]	-	46,48,48	4.11	21 (45%)	64,73,73	1.98	16 (25%)
3	A1AFY	A	503[J]	-	8,9,9	1.73	2 (25%)	10,12,12	1.06	0
2	COA	A	501[X]	-	47,50,50	3.20	20 (42%)	69,75,75	1.80	12 (17%)
2	COA	A	502[Y]	-	47,50,50	3.22	19 (40%)	69,75,75	1.82	13 (18%)
4	NAI	B	1001[X]	-	47,48,48	1.59	8 (17%)	64,73,73	1.53	11 (17%)
6	MEV	B	1003	-	8,9,9	1.31	1 (12%)	7,12,12	1.07	0

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
5	NAD	B	1002[Y]	-	-	11/30/62/62	0/5/5/5
3	A1AFY	A	503[J]	-	-	2/9/9/9	-
2	COA	A	501[X]	-	-	13/48/64/64	0/3/3/3
2	COA	A	502[Y]	-	-	13/48/64/64	0/3/3/3
4	NAI	B	1001[X]	-	-	7/29/72/72	0/5/5/5
6	MEV	B	1003	-	-	3/9/9/9	-

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1002[Y]	NAD	C2D-C3D	-10.74	1.24	1.53
2	A	501[X]	COA	O4B-C1B	10.26	1.65	1.42
2	A	502[Y]	COA	O4B-C1B	10.25	1.65	1.42
5	B	1002[Y]	NAD	C3B-C4B	-10.12	1.27	1.53
5	B	1002[Y]	NAD	C2B-C1B	-8.25	1.27	1.53
5	B	1002[Y]	NAD	C7N-N7N	8.21	1.48	1.33
5	B	1002[Y]	NAD	O4D-C1D	7.85	1.51	1.40
2	A	502[Y]	COA	P1A-O3A	7.36	1.67	1.59
2	A	501[X]	COA	P1A-O3A	7.24	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502[Y]	COA	P2A-O3A	7.12	1.67	1.59
2	A	501[X]	COA	P2A-O3A	7.03	1.67	1.59
5	B	1002[Y]	NAD	PA-O3	6.85	1.66	1.59
2	A	502[Y]	COA	C9P-N8P	6.68	1.49	1.33
2	A	501[X]	COA	C9P-N8P	6.64	1.49	1.33
5	B	1002[Y]	NAD	O4D-C4D	-6.33	1.30	1.45
2	A	502[Y]	COA	C5P-N4P	6.25	1.48	1.33
2	A	501[X]	COA	C5P-N4P	6.19	1.48	1.33
2	A	501[X]	COA	O4B-C4B	-6.17	1.31	1.45
2	A	501[X]	COA	C2B-C1B	-6.16	1.34	1.53
2	A	502[Y]	COA	C2B-C1B	-6.13	1.34	1.53
2	A	502[Y]	COA	O4B-C4B	-6.11	1.31	1.45
5	B	1002[Y]	NAD	O4B-C1B	6.01	1.55	1.42
5	B	1002[Y]	NAD	C6A-N6A	5.55	1.48	1.34
5	B	1002[Y]	NAD	PN-O3	5.21	1.65	1.59
5	B	1002[Y]	NAD	C3D-C4D	5.19	1.66	1.53
5	B	1002[Y]	NAD	C2B-C3B	5.07	1.67	1.53
5	B	1002[Y]	NAD	O4B-C4B	4.92	1.55	1.45
2	A	502[Y]	COA	C6A-N6A	4.64	1.46	1.34
2	A	501[X]	COA	C6A-N6A	4.62	1.46	1.34
5	B	1002[Y]	NAD	C3N-C7N	4.08	1.56	1.50
5	B	1002[Y]	NAD	O2D-C2D	3.84	1.52	1.43
4	B	1001[X]	NAI	PN-O5D	3.82	1.74	1.59
4	B	1001[X]	NAI	PA-O5B	3.65	1.73	1.59
4	B	1001[X]	NAI	PA-O3	3.58	1.63	1.59
4	B	1001[X]	NAI	PN-O3	3.33	1.63	1.59
5	B	1002[Y]	NAD	O7N-C7N	-3.27	1.18	1.24
2	A	502[Y]	COA	P3B-O3B	3.20	1.65	1.59
2	A	501[X]	COA	O3B-C3B	-3.19	1.33	1.44
3	A	503[J]	A1AFY	O01-C02	-3.13	1.40	1.44
2	A	502[Y]	COA	O3B-C3B	-3.11	1.33	1.44
2	A	501[X]	COA	P3B-O3B	3.07	1.64	1.59
2	A	501[X]	COA	C5A-C4A	-2.82	1.34	1.39
2	A	502[Y]	COA	C5A-C4A	-2.80	1.34	1.39
4	B	1001[X]	NAI	C8A-N9A	2.79	1.42	1.37
6	B	1003	MEV	O7-C3	-2.63	1.40	1.44
3	A	503[J]	A1AFY	C03-C02	2.60	1.55	1.52
2	A	502[Y]	COA	C5A-N7A	-2.57	1.34	1.39
2	A	501[X]	COA	C5A-N7A	-2.55	1.34	1.39
5	B	1002[Y]	NAD	C5B-C4B	2.54	1.59	1.51
5	B	1002[Y]	NAD	O3D-C3D	2.51	1.49	1.43
5	B	1002[Y]	NAD	C5A-C4A	-2.44	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502[Y]	COA	C3B-C4B	2.41	1.59	1.52
2	A	501[X]	COA	OAP-CAP	-2.40	1.38	1.42
2	A	502[Y]	COA	OAP-CAP	-2.34	1.38	1.42
2	A	502[Y]	COA	P2A-O6A	2.33	1.68	1.59
2	A	501[X]	COA	P2A-O6A	2.32	1.68	1.59
2	A	501[X]	COA	C3B-C4B	2.29	1.58	1.52
4	B	1001[X]	NAI	C5A-C4A	2.25	1.43	1.39
5	B	1002[Y]	NAD	C5A-N7A	-2.20	1.35	1.39
4	B	1001[X]	NAI	C4A-N3A	2.20	1.38	1.34
2	A	501[X]	COA	O9P-C9P	-2.17	1.19	1.23
2	A	502[Y]	COA	O9P-C9P	-2.16	1.19	1.23
2	A	502[Y]	COA	O5P-C5P	-2.14	1.19	1.23
2	A	501[X]	COA	O5P-C5P	-2.14	1.19	1.23
2	A	502[Y]	COA	C8A-N9A	-2.13	1.33	1.37
5	B	1002[Y]	NAD	C1B-N9A	2.11	1.52	1.46
2	A	501[X]	COA	C8A-N9A	-2.10	1.34	1.37
4	B	1001[X]	NAI	C2A-N1A	2.09	1.37	1.33
2	A	501[X]	COA	O2B-C2B	2.05	1.48	1.43
2	A	502[Y]	COA	O2B-C2B	2.04	1.48	1.43
2	A	501[X]	COA	CCP-CBP	2.00	1.55	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502[Y]	COA	N6A-C6A-N1A	-5.96	105.10	118.38
2	A	501[X]	COA	N6A-C6A-N1A	-5.94	105.14	118.38
2	A	502[Y]	COA	N3A-C2A-N1A	-5.60	120.11	128.58
2	A	501[X]	COA	N3A-C2A-N1A	-5.60	120.11	128.58
5	B	1002[Y]	NAD	N3A-C2A-N1A	-5.52	120.23	128.58
2	A	502[Y]	COA	C5A-C4A-N3A	-5.16	119.61	126.72
5	B	1002[Y]	NAD	C5A-C4A-N3A	-4.98	119.85	126.72
2	A	501[X]	COA	C5A-C4A-N3A	-4.93	119.92	126.72
5	B	1002[Y]	NAD	C1B-N9A-C8A	-4.80	116.44	127.09
2	A	502[Y]	COA	C5A-C6A-N6A	4.70	134.92	123.29
2	A	501[X]	COA	C5A-C6A-N6A	4.69	134.91	123.29
5	B	1002[Y]	NAD	N9A-C8A-N7A	-4.50	107.55	113.94
5	B	1002[Y]	NAD	N6A-C6A-N1A	-4.04	109.37	118.38
2	A	501[X]	COA	N9A-C8A-N7A	-4.04	108.21	113.94
2	A	502[Y]	COA	N9A-C8A-N7A	-3.97	108.31	113.94
4	B	1001[X]	NAI	O3-PN-O2N	-3.96	98.78	110.70
4	B	1001[X]	NAI	O1N-PN-O3	3.89	117.78	107.27
5	B	1002[Y]	NAD	C4D-O4D-C1D	-3.73	106.51	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001[X]	NAI	O2A-PA-O3	3.62	117.06	107.27
5	B	1002[Y]	NAD	C4A-N9A-C1B	3.53	134.89	126.63
2	A	502[Y]	COA	C2A-N3A-C4A	3.46	120.28	111.83
2	A	501[X]	COA	C6P-C7P-N8P	-3.43	104.70	112.00
2	A	501[X]	COA	C2A-N3A-C4A	3.38	120.08	111.83
5	B	1002[Y]	NAD	C2A-N3A-C4A	3.36	120.04	111.83
5	B	1002[Y]	NAD	N3A-C4A-N9A	3.34	132.85	127.17
2	A	502[Y]	COA	N3A-C4A-N9A	3.17	132.56	127.17
5	B	1002[Y]	NAD	C3B-C2B-C1B	3.09	107.31	101.46
5	B	1002[Y]	NAD	C5A-N7A-C8A	3.08	108.29	103.45
4	B	1001[X]	NAI	O2A-PA-O1A	3.06	126.66	112.44
2	A	502[Y]	COA	C3B-C2B-C1B	3.05	106.60	99.89
5	B	1002[Y]	NAD	C5A-C6A-N6A	2.94	130.57	123.29
4	B	1001[X]	NAI	O1N-PN-O2N	2.91	125.99	112.44
2	A	501[X]	COA	N3A-C4A-N9A	2.89	132.08	127.17
2	A	502[Y]	COA	C5A-N7A-C8A	2.84	107.92	103.45
2	A	501[X]	COA	C5A-N7A-C8A	2.82	107.88	103.45
5	B	1002[Y]	NAD	C4A-N9A-C8A	2.79	108.67	105.74
4	B	1001[X]	NAI	PA-O5B-C5B	-2.78	105.39	121.35
4	B	1001[X]	NAI	O3-PA-O1A	-2.73	102.48	110.70
4	B	1001[X]	NAI	O5B-PA-O1A	-2.73	98.13	108.94
5	B	1002[Y]	NAD	C6N-N1N-C2N	-2.60	119.66	121.88
4	B	1001[X]	NAI	O5D-PN-O2N	-2.52	98.95	108.94
4	B	1001[X]	NAI	PN-O5D-C5D	-2.40	107.60	121.35
5	B	1002[Y]	NAD	C2B-C3B-C4B	2.31	107.07	102.61
2	A	501[X]	COA	C4A-C5A-N7A	-2.23	108.03	110.58
2	A	502[Y]	COA	C6P-C7P-N8P	-2.18	107.35	112.00
2	A	502[Y]	COA	C4A-C5A-N7A	-2.17	108.10	110.58
2	A	502[Y]	COA	C6A-C5A-C4A	2.10	120.05	117.18
5	B	1002[Y]	NAD	C4A-C5A-N7A	-2.08	108.20	110.58
4	B	1001[X]	NAI	N3A-C4A-N9A	2.06	130.67	127.17
2	A	501[X]	COA	C4A-N9A-C8A	2.06	107.90	105.74
2	A	502[Y]	COA	C4A-N9A-C8A	2.01	107.85	105.74
2	A	501[X]	COA	C6A-C5A-C4A	2.00	119.91	117.18

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[X]	COA	C5B-O5B-P1A-O2A
2	A	501[X]	COA	C5B-O5B-P1A-O3A
2	A	501[X]	COA	CCP-O6A-P2A-O4A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	501[X]	COA	CCP-O6A-P2A-O5A
2	A	501[X]	COA	CDP-CBP-CCP-O6A
2	A	501[X]	COA	CEP-CBP-CCP-O6A
2	A	501[X]	COA	CAP-CBP-CCP-O6A
2	A	502[Y]	COA	O4B-C4B-C5B-O5B
2	A	502[Y]	COA	C5B-O5B-P1A-O2A
2	A	502[Y]	COA	C5B-O5B-P1A-O3A
2	A	502[Y]	COA	N8P-C9P-CAP-OAP
3	A	503[J]	A1AFY	O01-C02-C08-C09
4	B	1001[X]	NAI	C5D-O5D-PN-O2N
4	B	1001[X]	NAI	C2D-C1D-N1N-C2N
5	B	1002[Y]	NAD	O4D-C1D-N1N-C6N
5	B	1002[Y]	NAD	C2D-C1D-N1N-C6N
6	B	1003	MEV	C8-C2-C3-C4
4	B	1001[X]	NAI	C2D-C1D-N1N-C6N
5	B	1002[Y]	NAD	O4B-C4B-C5B-O5B
5	B	1002[Y]	NAD	C3B-C4B-C5B-O5B
2	A	502[Y]	COA	C3B-C4B-C5B-O5B
2	A	501[X]	COA	C3B-C4B-C5B-O5B
4	B	1001[X]	NAI	PA-O3-PN-O5D
5	B	1002[Y]	NAD	PN-O3-PA-O5B
2	A	501[X]	COA	O4B-C4B-C5B-O5B
2	A	502[Y]	COA	P2A-O3A-P1A-O1A
5	B	1002[Y]	NAD	PA-O3-PN-O2N
2	A	502[Y]	COA	O9P-C9P-CAP-OAP
6	B	1003	MEV	C8-C2-C3-C6
2	A	501[X]	COA	CCP-O6A-P2A-O3A
2	A	502[Y]	COA	C5B-O5B-P1A-O1A
2	A	502[Y]	COA	CCP-O6A-P2A-O3A
2	A	502[Y]	COA	CCP-O6A-P2A-O4A
2	A	502[Y]	COA	CCP-O6A-P2A-O5A
3	A	503[J]	A1AFY	C04-C02-C08-C09
4	B	1001[X]	NAI	C5D-O5D-PN-O1N
5	B	1002[Y]	NAD	C2B-C1B-N9A-C8A
5	B	1002[Y]	NAD	C2D-C1D-N1N-C2N
5	B	1002[Y]	NAD	C2B-C1B-N9A-C4A
4	B	1001[X]	NAI	O4D-C1D-N1N-C2N
5	B	1002[Y]	NAD	O4D-C1D-N1N-C2N
2	A	501[X]	COA	C3B-O3B-P3B-O7A
5	B	1002[Y]	NAD	O4B-C1B-N9A-C8A
2	A	502[Y]	COA	OAP-CAP-CBP-CDP
2	A	502[Y]	COA	P2A-O3A-P1A-O2A

Continued on next page...

Continued from previous page...

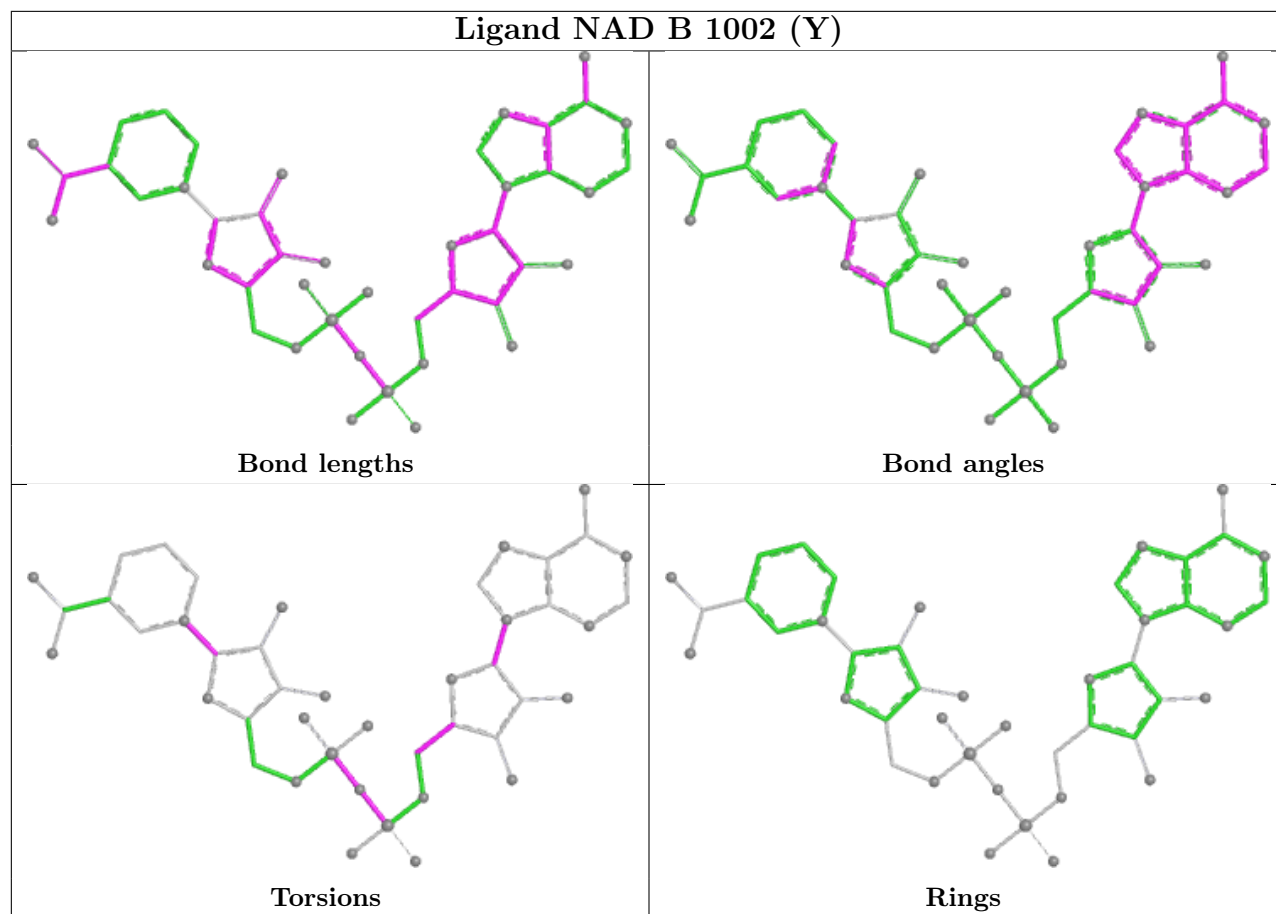
Mol	Chain	Res	Type	Atoms
6	B	1003	MEV	C3-C2-C8-O8
2	A	501[X]	COA	C3B-O3B-P3B-O8A
2	A	501[X]	COA	CBP-CCP-O6A-P2A
4	B	1001[X]	NAI	PN-O3-PA-O2A

There are no ring outliers.

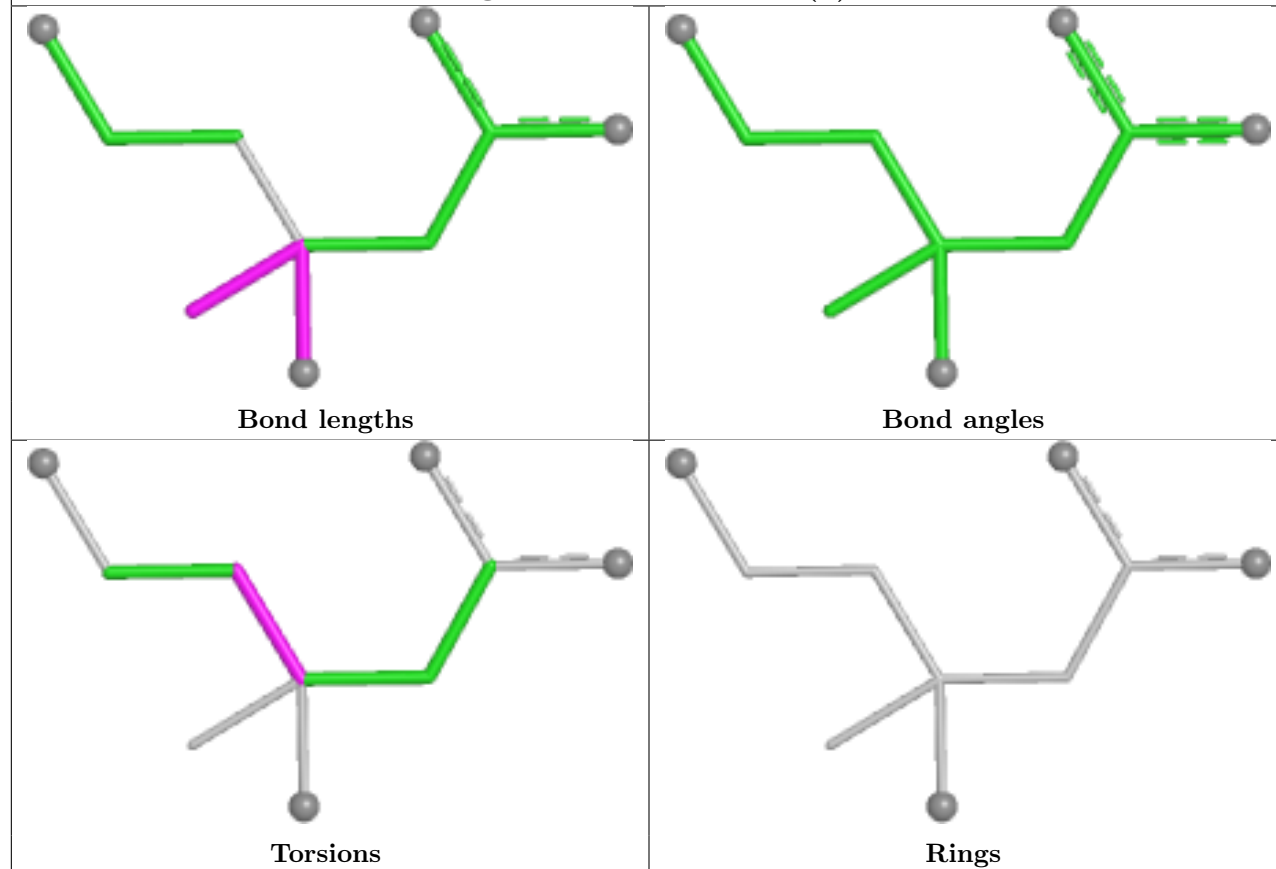
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1002[Y]	NAD	1	0
2	A	501[X]	COA	2	0
2	A	502[Y]	COA	1	0

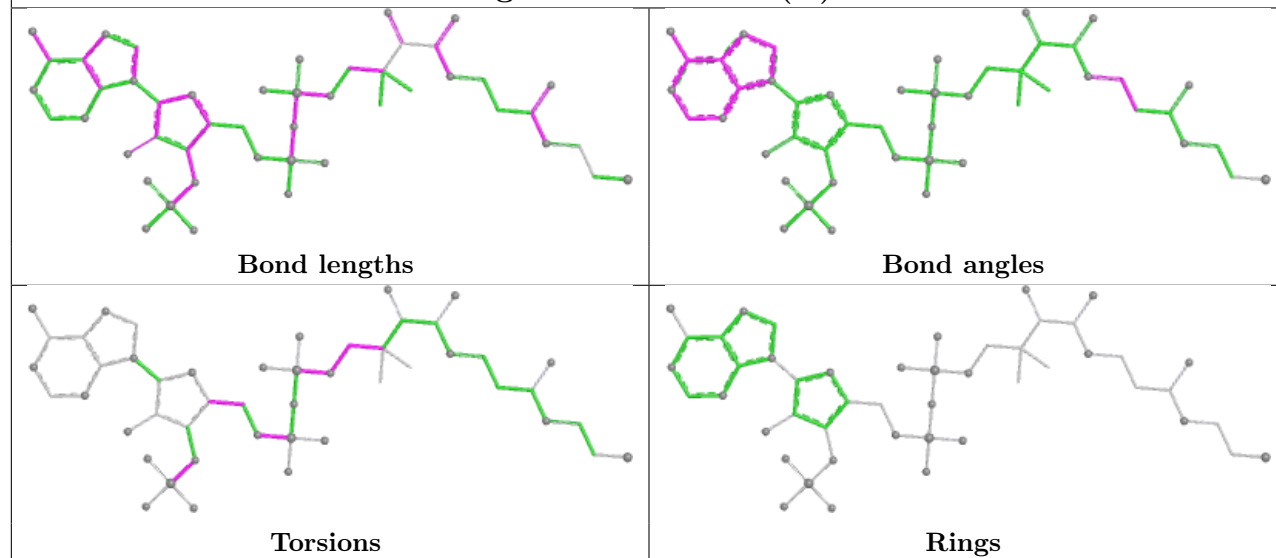
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

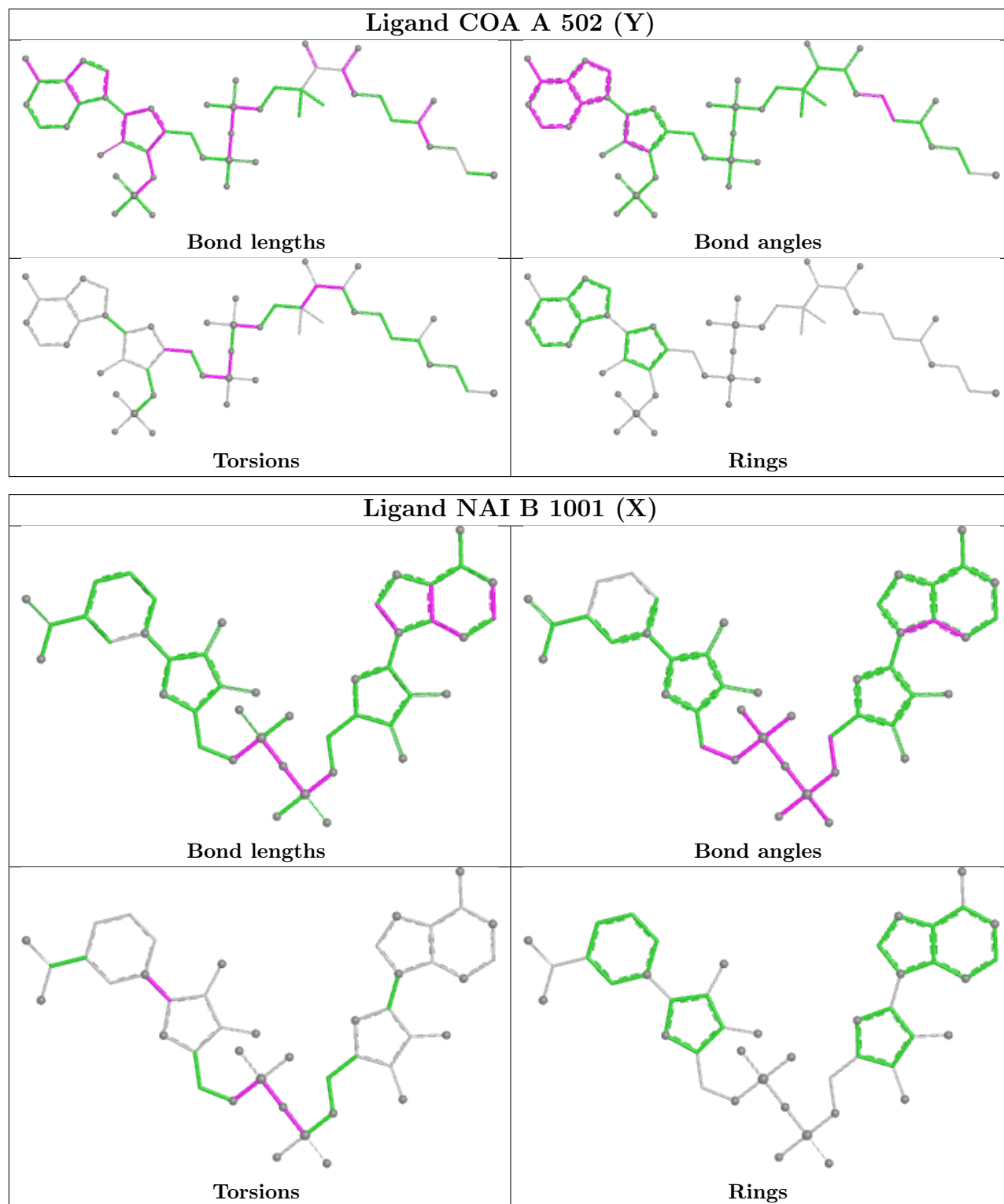


Ligand A1AFY A 503 (J)



Ligand COA A 501 (X)





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	425/428 (99%)	0.67	59 (13%) 6 6	13, 36, 71, 125	15 (3%)
1	B	377/428 (88%)	0.49	33 (8%) 15 16	13, 36, 62, 101	8 (2%)
All	All	802/856 (93%)	0.58	92 (11%) 9 9	13, 36, 64, 125	23 (2%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	502	SER	8.3
1	A	402	TRP	7.2
1	A	399	GLU	6.4
1	A	393	ALA	6.1
1	A	419	VAL	5.5
1	A	400	VAL	5.4
1	A	396	ARG	5.3
1	A	418	ALA	5.2
1	A	390	ALA	5.1
1	A	403	VAL	5.1
1	A	420	ALA	4.6
1	A	395	ALA	4.5
1	A	422	LEU	4.0
1	A	389	ILE	4.0
1	A	392	VAL	3.8
1	B	509	ALA	3.8
1	A	407	LEU	3.7
1	A	391	VAL	3.7
1	B	510	PHE	3.7
1	B	517	ALA	3.7
1	B	503	LEU	3.5
1	A	394	GLY	3.5
1	B	536	LEU	3.4
1	A	406	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	410	TYR	3.4
1	B	739	PHE	3.4
1	A	417	ARG	3.3
1	A	397	GLY	3.3
1	B	530	HIS	3.2
1	A	421	LEU	3.1
1	A	398	ASP	3.1
1	A	409	GLU	3.1
1	A	404	ALA	3.1
1	A	30	HIS	2.9
1	B	512	ASN	2.8
1	A	16	ALA	2.8
1	A	386	ALA	2.8
1	B	521	HIS	2.8
1	B	737	ALA	2.7
1	B	537	ALA	2.7
1	A	56	GLY	2.7
1	B	545	ASP	2.7
1	B	526	LEU	2.6
1	B	546	ILE	2.6
1	A	153	GLY	2.6
1	B	878	GLN	2.6
1	A	46	ILE	2.6
1	A	415	ALA	2.6
1	B	665	ALA	2.6
1	A	45	ASP	2.6
1	A	328	VAL	2.6
1	A	424	GLN	2.6
1	B	522	ILE	2.6
1	B	736	THR	2.6
1	B	707	GLY	2.5
1	A	426	ARG	2.5
1	A	43	PRO	2.5
1	A	423	LYS	2.5
1	B	525	LEU	2.5
1	B	556	GLY	2.5
1	A	17	ALA	2.4
1	A	411	HIS	2.4
1	A	166	ASP	2.4
1	A	413	VAL	2.4
1	B	876	GLY	2.3
1	A	145	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	408	VAL	2.3
1	B	738	GLU	2.3
1	A	405	ARG	2.3
1	B	514	SER	2.3
1	A	329	GLY	2.3
1	A	2	SER	2.2
1	B	555	ILE	2.2
1	B	513	LEU	2.2
1	A	379	ARG	2.2
1	A	239	PHE	2.2
1	A	401	ASP	2.2
1	A	416	ASP	2.2
1	A	121	ILE	2.1
1	B	540	GLY	2.1
1	B	539	ALA	2.1
1	A	44	MET	2.1
1	A	48	ASN	2.1
1	B	524	GLN	2.1
1	A	333	LYS	2.1
1	B	547	ALA	2.1
1	B	651	SER	2.1
1	A	120	GLY	2.0
1	A	165	ALA	2.0
1	B	519	LEU	2.0
1	A	144	ARG	2.0
1	A	387	ARG	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](#)

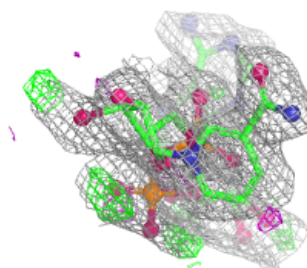
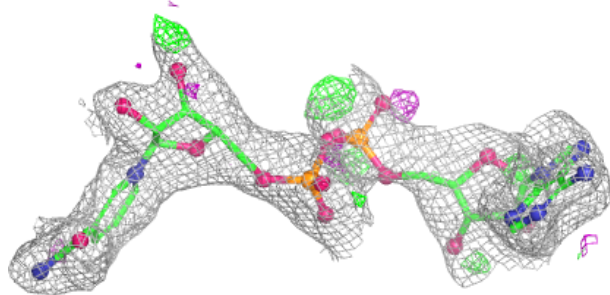
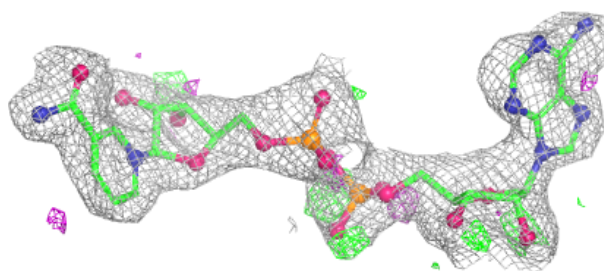
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAD	B	1002[Y]	44/44	0.85	0.14	25,36,43,44	44
2	COA	A	502[Y]	48/48	0.87	0.14	33,46,52,57	48
2	COA	A	501[X]	48/48	0.87	0.14	32,44,53,55	48
4	NAI	B	1001[X]	44/44	0.91	0.11	26,36,43,45	44
3	A1AFY	A	503[J]	10/10	0.94	0.15	26,28,29,33	10
6	MEV	B	1003	10/10	0.94	0.08	31,35,36,37	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.

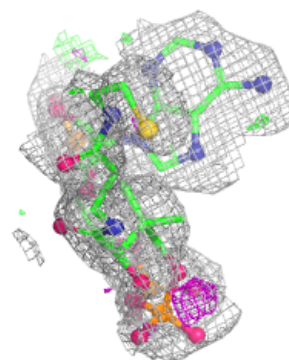
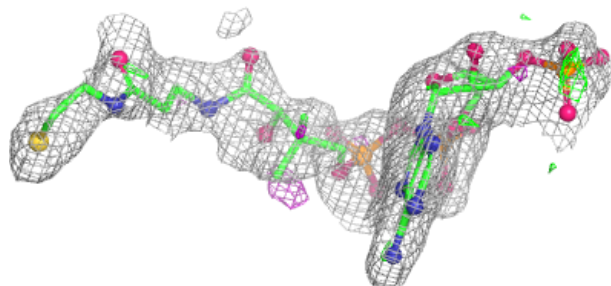
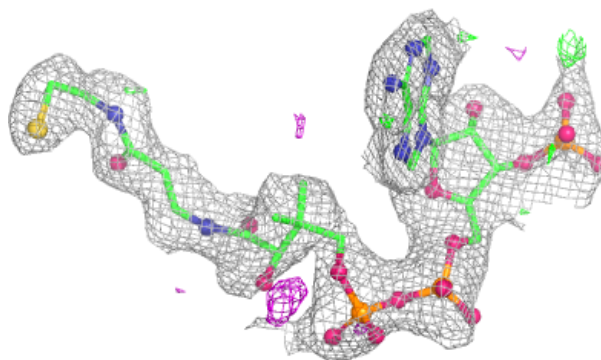
Electron density around NAD B 1002 (Y):

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

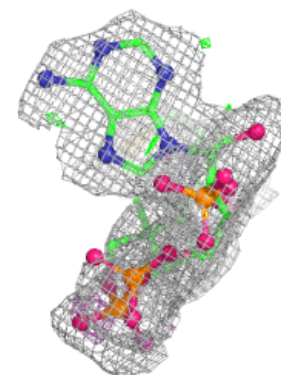
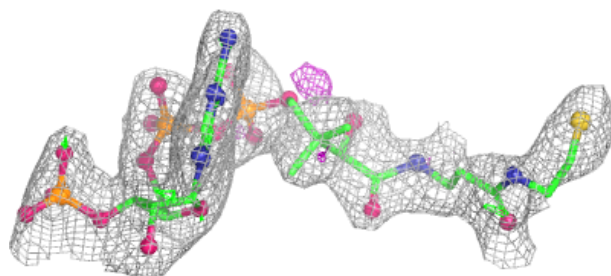
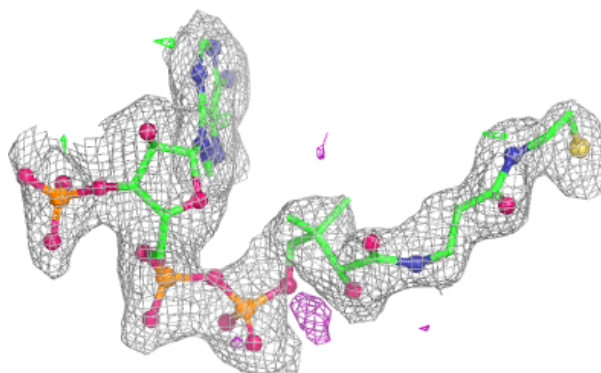


Electron density around COA A 502 (Y):

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

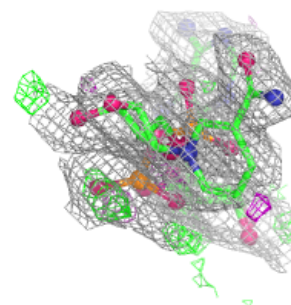
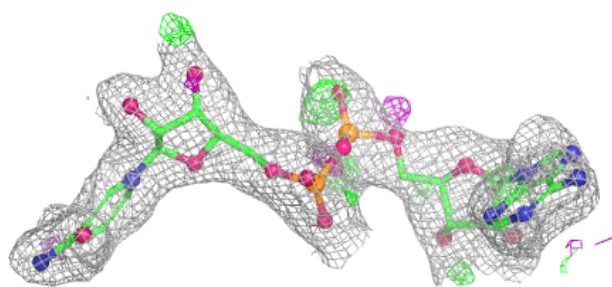
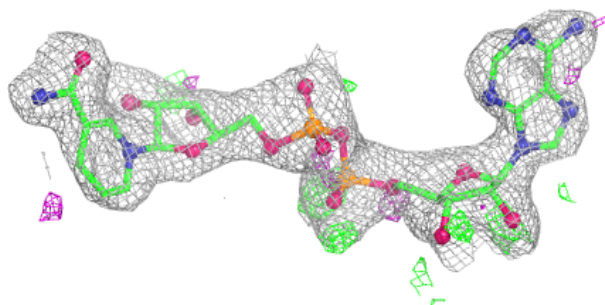
**Electron density around COA A 501 (X):**

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

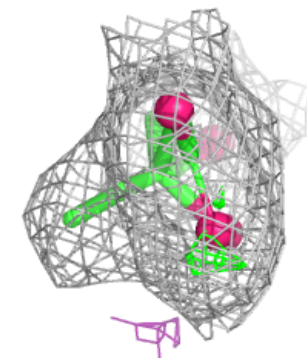
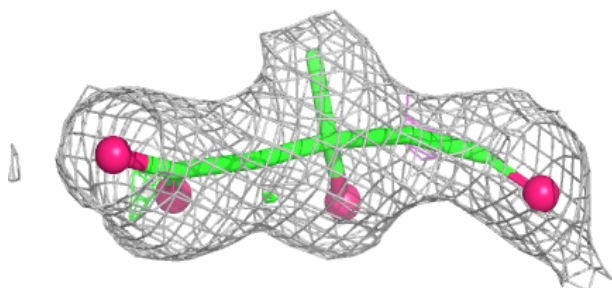
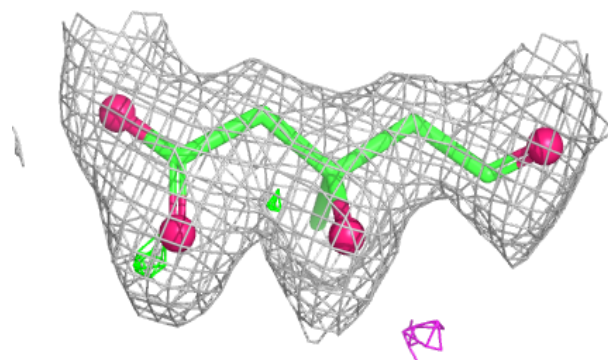


Electron density around NAI B 1001 (X):

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

**Electron density around A1AFY A 503 (J):**

$2mF_o-DF_c$ (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.