



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:04 AM UTC

PDB ID : 8GDN / pdb_00008gdn
Title : Structure of PmHMGR bound to mevalonate, CoA and NAD.
Authors : Purohit, V.; Steussy, C.N.; Stauffacher, C.V.
Deposited on : 2023-03-06
Resolution : 1.99 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

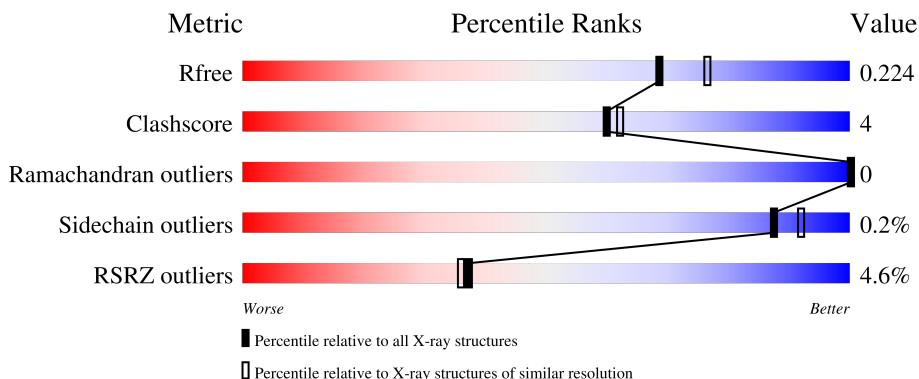
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	6% 89% 10% .
1	B	428	2% 81% 8% 12%

2 Entry composition [i](#)

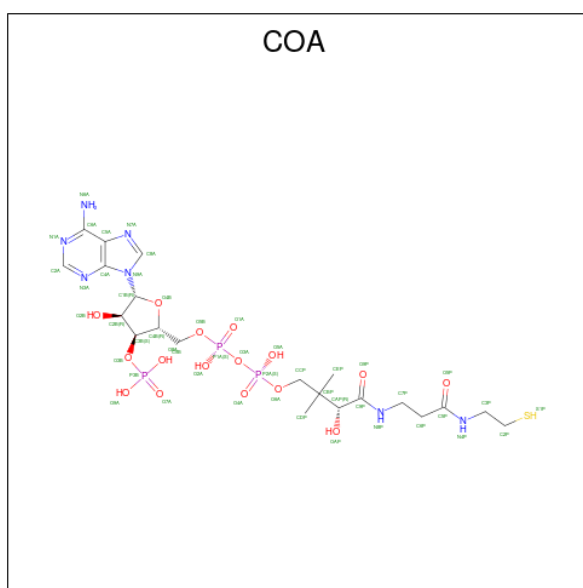
There are 6 unique types of molecules in this entry. The entry contains 6664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

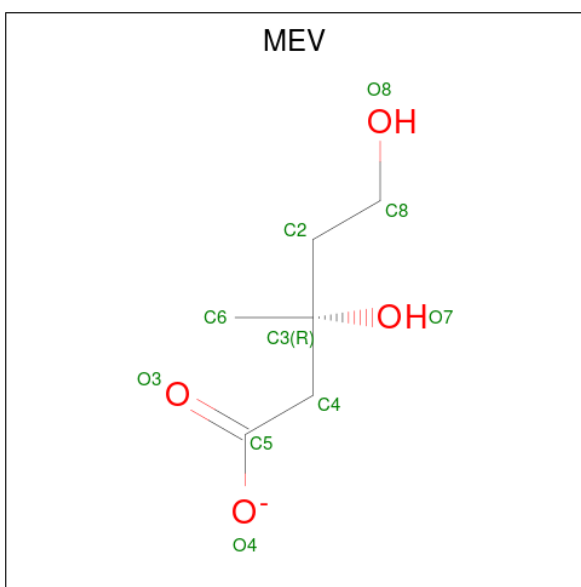
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	7	5	0
			3174	1981	581	596	16			
1	B	378	Total	C	N	O	S	2	5	0
			2842	1778	514	534	16			

- 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
			96	42	14	32	6 2		

- Molecule 3 is (R)-MEVALONATE (CCD ID: MEV) (formula: $C_6H_{11}O_4$) (labeled as "Ligand of Interest" by depositor).



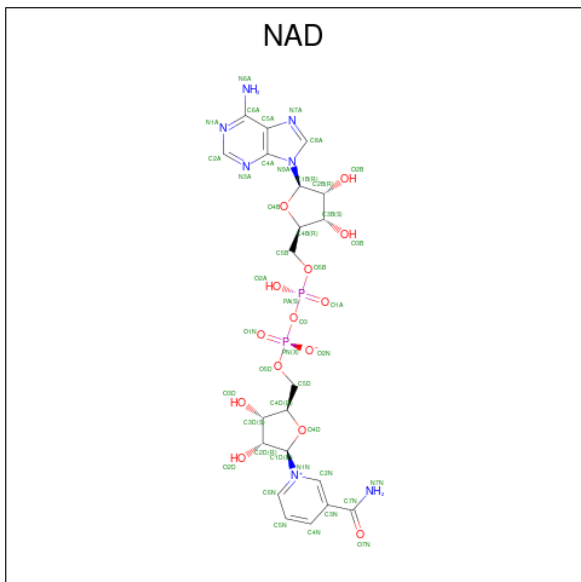
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

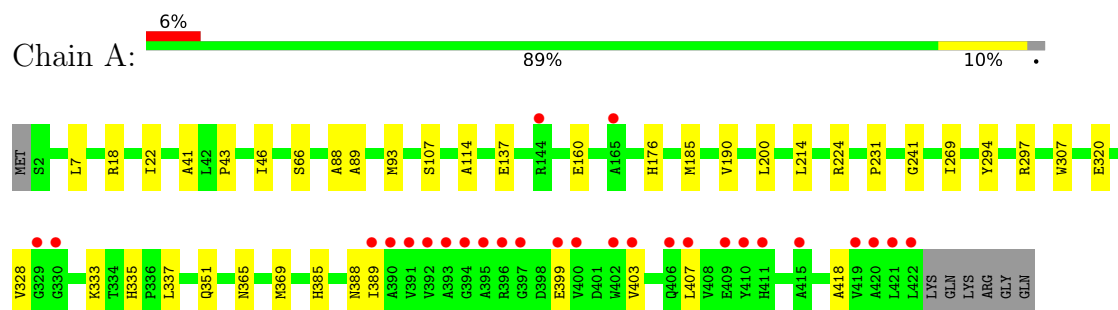
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	271	Total O 271 271	0	0
6	B	207	Total O 207 207	0	0

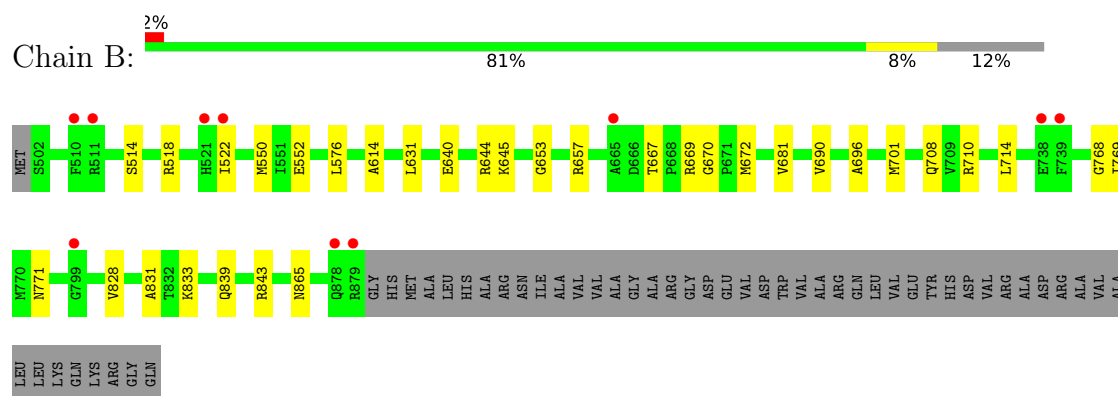
3 Residue-property plots [i](#)

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

- Molecule 1: 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	226.04Å 226.04Å 226.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.19 – 1.99 48.19 – 1.99	Depositor EDS
% Data completeness (in resolution range)	82.9 (48.19-1.99) 82.9 (48.19-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.10 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.181 , 0.225 0.181 , 0.224	Depositor DCC
R_{free} test set	2824 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6664	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD, COA, MEV

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	0.38	0/3223	0.59	1/4383 (0.0%)
1	B	0.36	0/2892	0.60	0/3931
All	All	0.37	0/6115	0.59	1/8314 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	MET	CA-CB-CG	-6.85	100.39	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3174	0	3196	25	0
1	B	2842	0	2882	23	0
2	A	96	0	64	6	0
3	A	10	0	11	2	0
3	B	10	0	11	0	0
4	A	10	0	0	0	0
5	B	44	0	24	2	0
6	A	271	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	207	0	0	0	0
All	All	6664	0	6188	53	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 (53) 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:501[B]:COA:C1B	2:A:501[B]:COA:O4B	1.65	1.26
2:A:501[A]:COA:O4B	2:A:501[A]:COA:C1B	1.65	1.26
1:B:667:THR:HG22	1:B:669:ARG:H	1.52	0.74
1:B:667:THR:HG21	1:B:672:MET:HE3	1.73	0.69
3:A:502:MEV:H81	5:B:1001:NAD:C4N	2.25	0.66
1:A:328:VAL:HA	1:A:333:LYS:HD3	1.78	0.65
1:A:7:LEU:HD12	1:A:66:SER:HB3	1.81	0.62
1:A:307:TRP:NE1	1:A:369:MET:HE1	2.16	0.61
1:A:407:LEU:HD11	1:A:418:ALA:HB2	1.86	0.58
1:B:667:THR:HB	1:B:670:GLY:O	2.04	0.57
1:A:114:ALA:HB2	1:A:190:VAL:HB	1.87	0.57
1:B:667:THR:HG22	1:B:669:ARG:N	2.19	0.57
1:A:307:TRP:CD1	1:A:369:MET:HE1	2.40	0.56
1:B:708:GLN:CD	1:B:710:ARG:HH12	2.14	0.56
1:B:640:GLU:HG3	1:B:644:ARG:HH12	1.71	0.56
1:B:667:THR:CG2	1:B:669:ARG:H	2.20	0.55
1:B:640:GLU:HG3	1:B:644:ARG:NH1	2.24	0.53
1:B:614:ALA:HA	1:B:714:LEU:HA	1.91	0.52
2:A:501[A]:COA:S1P	3:A:502:MEV:H82	2.51	0.51
1:B:514:SER:O	1:B:518:ARG:HG3	2.11	0.50
1:B:828:VAL:HG12	1:B:833:LYS:HE3	1.94	0.49
1:B:769:ILE:HG12	1:B:865:ASN:HB2	1.94	0.49
1:A:89:ALA:HB2	2:A:501[B]:COA:H61	1.95	0.48
1:B:614:ALA:HB2	1:B:690:VAL:HB	1.95	0.48
1:A:107:SER:HB2	1:A:351:GLN:HE21	1.78	0.48
1:A:399:GLU:O	1:A:403:VAL:HG22	2.14	0.48
1:B:667:THR:HG21	1:B:672:MET:CE	2.42	0.48
2:A:501[B]:COA:O5B	2:A:501[B]:COA:H8A	2.16	0.46
1:A:137[B]:GLU:HG2	1:A:200:LEU:HD21	1.98	0.45
1:B:631:LEU:HD21	1:B:701:MET:HG2	1.99	0.45
1:A:269:ILE:HG12	1:A:365:ASN:HB2	1.99	0.45
1:A:224:ARG:HD3	1:A:320:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160[A]:GLU:HG3	1:A:176:HIS:HB2	1.99	0.44
1:A:294:TYR:O	1:A:297:ARG:HG2	2.17	0.44
1:A:335:HIS:CE1	1:A:337:LEU:HB2	2.52	0.44
1:B:550[B]:MET:HE2	1:B:831:ALA:HB1	2.00	0.44
1:A:43:PRO:HG2	1:A:46:ILE:HG13	1.99	0.43
1:B:839:GLN:O	1:B:843:ARG:HG3	2.18	0.43
1:B:653:GLY:O	1:B:657:ARG:NH2	2.44	0.43
1:A:185:MET:HE1	6:A:779:HOH:O	2.18	0.42
2:A:501[A]:COA:O4B	2:A:501[A]:COA:C8A	2.68	0.42
1:A:88:ALA:HB2	1:B:552:GLU:HG2	2.02	0.42
1:B:522:ILE:HD12	1:B:576:LEU:HD13	2.01	0.42
1:B:681:VAL:O	5:B:1001:NAD:H2A	2.19	0.42
1:A:107:SER:HB2	1:A:351:GLN:NE2	2.35	0.41
1:A:385:HIS:CE1	1:A:388:ASN:HB2	2.55	0.41
1:A:18:ARG:O	1:A:22:ILE:HG12	2.20	0.41
1:A:41:ALA:O	1:A:43:PRO:HD3	2.21	0.41
1:A:231:PRO:O	1:A:241:GLY:HA3	2.21	0.41
1:B:645:LYS:HD2	1:B:696:ALA:HB2	2.03	0.40
1:B:768:GLY:O	1:B:771:ASN:HB2	2.22	0.40
1:A:385:HIS:CD2	1:A:389:ILE:HG12	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/428 (99%)	407 (96%)	17 (4%)	0	100	100
1	B	381/428 (89%)	371 (97%)	10 (3%)	0	100	100
All	All	805/856 (94%)	778 (97%)	27 (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	325/327 (99%)	324 (100%)	1 (0%)	86	91
1	B	295/327 (90%)	295 (100%)	0	100	100
All	All	620/654 (95%)	619 (100%)	1 (0%)	87	92

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

Mol	Chain	Res	Type
1	A	214	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	67	ASN
1	A	100	ASN
1	A	115	GLN
1	A	150	ASN
1	A	351	GLN
1	B	524	GLN
1	B	569	GLN
1	B	626	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	COA	A	501[A]	-	47,50,50	3.09	17 (36%)	69,75,75	2.03	16 (23%)
2	COA	A	501[B]	-	47,50,50	3.19	19 (40%)	69,75,75	1.82	12 (17%)
5	NAD	B	1001	-	46,48,48	3.98	20 (43%)	64,73,73	2.12	20 (31%)
4	SO4	A	504	-	4,4,4	0.32	0	6,6,6	0.17	0
4	SO4	A	503	-	4,4,4	0.21	0	6,6,6	0.27	0
3	MEV	B	1002	-	8,9,9	1.33	1 (12%)	7,12,12	1.36	1 (14%)
3	MEV	A	502	-	8,9,9	1.43	1 (12%)	7,12,12	0.82	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
2	COA	A	501[A]	-	-	4/48/64/64	0/3/3/3
2	COA	A	501[B]	-	-	16/48/64/64	0/3/3/3
5	NAD	B	1001	-	-	7/30/62/62	0/5/5/5
3	MEV	B	1002	-	-	2/9/9/9	-
3	MEV	A	502	-	-	0/9/9/9	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	NAD	C3B-C4B	-10.29	1.26	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	COA	O4B-C1B	10.25	1.65	1.42
2	A	501[A]	COA	O4B-C1B	9.98	1.65	1.42
5	B	1001	NAD	C2D-C3D	-9.86	1.26	1.53
5	B	1001	NAD	C7N-N7N	8.89	1.49	1.33
5	B	1001	NAD	O4D-C1D	8.44	1.52	1.40
5	B	1001	NAD	C2B-C1B	-7.80	1.29	1.53
2	A	501[A]	COA	P1A-O3A	7.50	1.67	1.59
2	A	501[B]	COA	P1A-O3A	7.07	1.67	1.59
2	A	501[B]	COA	P2A-O3A	7.03	1.67	1.59
5	B	1001	NAD	PA-O3	7.02	1.67	1.59
2	A	501[A]	COA	P2A-O3A	6.88	1.66	1.59
2	A	501[B]	COA	C9P-N8P	6.71	1.49	1.33
2	A	501[A]	COA	C9P-N8P	6.32	1.48	1.33
2	A	501[B]	COA	C2B-C1B	-6.17	1.34	1.53
2	A	501[B]	COA	C5P-N4P	6.16	1.48	1.33
2	A	501[A]	COA	O4B-C4B	-6.12	1.31	1.45
2	A	501[B]	COA	O4B-C4B	-6.10	1.31	1.45
2	A	501[A]	COA	C2B-C1B	-5.95	1.34	1.53
5	B	1001	NAD	O4D-C4D	-5.77	1.32	1.45
2	A	501[A]	COA	C5P-N4P	5.46	1.46	1.33
5	B	1001	NAD	C6A-N6A	5.24	1.47	1.34
5	B	1001	NAD	O4B-C1B	5.09	1.53	1.42
5	B	1001	NAD	C2B-C3B	5.08	1.67	1.53
5	B	1001	NAD	C3D-C4D	5.00	1.65	1.53
5	B	1001	NAD	PN-O3	4.68	1.64	1.59
2	A	501[B]	COA	C6A-N6A	4.60	1.46	1.34
2	A	501[A]	COA	C6A-N6A	4.50	1.45	1.34
5	B	1001	NAD	O4B-C4B	4.44	1.54	1.45
5	B	1001	NAD	O2D-C2D	3.68	1.52	1.43
5	B	1001	NAD	C3N-C7N	3.42	1.55	1.50
2	A	501[A]	COA	O3B-C3B	-3.32	1.32	1.44
2	A	501[B]	COA	P3B-O3B	3.29	1.65	1.59
2	A	501[B]	COA	O3B-C3B	-3.09	1.33	1.44
2	A	501[B]	COA	C5A-C4A	-2.77	1.34	1.39
5	B	1001	NAD	O3D-C3D	2.74	1.49	1.43
2	A	501[A]	COA	P3B-O3B	2.71	1.64	1.59
2	A	501[A]	COA	OAP-CAP	-2.69	1.37	1.42
2	A	501[B]	COA	C5A-N7A	-2.56	1.34	1.39
3	A	502	MEV	O7-C3	-2.44	1.41	1.44
2	A	501[A]	COA	P2A-O6A	2.43	1.68	1.59
5	B	1001	NAD	C5A-C4A	-2.42	1.34	1.39
2	A	501[B]	COA	OAP-CAP	-2.41	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	MEV	O7-C3	-2.38	1.41	1.44
2	A	501[A]	COA	C5A-C4A	-2.38	1.34	1.39
2	A	501[B]	COA	C3B-C4B	2.35	1.59	1.52
2	A	501[B]	COA	P2A-O6A	2.31	1.68	1.59
2	A	501[A]	COA	O5P-C5P	-2.26	1.18	1.23
2	A	501[B]	COA	O9P-C9P	-2.19	1.19	1.23
2	A	501[B]	COA	O5P-C5P	-2.18	1.18	1.23
2	A	501[B]	COA	C8A-N9A	-2.11	1.34	1.37
5	B	1001	NAD	C2N-N1N	2.09	1.37	1.35
2	A	501[A]	COA	C3B-C4B	2.07	1.58	1.52
5	B	1001	NAD	O7N-C7N	-2.06	1.20	1.24
2	A	501[A]	COA	C5A-N7A	-2.04	1.35	1.39
5	B	1001	NAD	C8A-N7A	2.03	1.35	1.31
2	A	501[A]	COA	O2B-C2B	2.03	1.48	1.43
2	A	501[B]	COA	O2B-C2B	2.02	1.48	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[B]	COA	N6A-C6A-N1A	-6.07	104.87	118.38
2	A	501[A]	COA	N3A-C2A-N1A	-6.04	119.44	128.58
2	A	501[A]	COA	N6A-C6A-N1A	-5.97	105.08	118.38
5	B	1001	NAD	N3A-C2A-N1A	-5.80	119.80	128.58
2	A	501[B]	COA	N3A-C2A-N1A	-5.71	119.94	128.58
2	A	501[A]	COA	C2P-C3P-N4P	-5.30	100.27	112.31
5	B	1001	NAD	N9A-C8A-N7A	-5.19	106.57	113.94
2	A	501[B]	COA	C5A-C4A-N3A	-4.93	119.92	126.72
2	A	501[A]	COA	C5A-C4A-N3A	-4.89	119.99	126.72
2	A	501[B]	COA	C5A-C6A-N6A	4.80	135.16	123.29
2	A	501[A]	COA	C5A-C6A-N6A	4.70	134.93	123.29
5	B	1001	NAD	C1B-N9A-C8A	-4.42	117.28	127.09
5	B	1001	NAD	C5A-C4A-N3A	-4.41	120.64	126.72
5	B	1001	NAD	C4D-O4D-C1D	-4.40	105.89	109.92
2	A	501[A]	COA	C6P-C7P-N8P	-4.38	102.68	112.00
5	B	1001	NAD	N6A-C6A-N1A	-4.32	108.77	118.38
2	A	501[B]	COA	N9A-C8A-N7A	-4.09	108.13	113.94
2	A	501[A]	COA	N9A-C8A-N7A	-3.99	108.28	113.94
5	B	1001	NAD	C4A-N9A-C8A	3.84	109.77	105.74
2	A	501[A]	COA	C2A-N3A-C4A	3.55	120.51	111.83
2	A	501[B]	COA	C2A-N3A-C4A	3.42	120.19	111.83
5	B	1001	NAD	C3B-C2B-C1B	3.36	107.81	101.46
5	B	1001	NAD	C2A-N3A-C4A	3.32	119.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[A]	COA	CDP-CBP-CAP	3.29	114.38	108.77
5	B	1001	NAD	C5A-N7A-C8A	3.23	108.52	103.45
2	A	501[A]	COA	N3A-C4A-N9A	3.07	132.39	127.17
5	B	1001	NAD	N3A-C4A-N9A	3.07	132.39	127.17
5	B	1001	NAD	C4B-O4B-C1B	-3.07	102.69	109.47
5	B	1001	NAD	C5A-C6A-N6A	2.97	130.65	123.29
2	A	501[B]	COA	N3A-C4A-N9A	2.91	132.12	127.17
2	A	501[B]	COA	C5A-N7A-C8A	2.89	107.99	103.45
5	B	1001	NAD	C2N-C3N-C4N	2.86	121.58	118.26
5	B	1001	NAD	C6N-N1N-C2N	-2.83	119.47	121.88
2	A	501[B]	COA	C6P-C7P-N8P	-2.82	106.00	112.00
2	A	501[A]	COA	C5A-N7A-C8A	2.78	107.82	103.45
5	B	1001	NAD	C4A-N9A-C1B	2.70	132.95	126.63
5	B	1001	NAD	O3D-C3D-C4D	-2.41	104.16	111.08
3	B	1002	MEV	O4-C5-C4	2.37	121.85	114.35
5	B	1001	NAD	O4B-C4B-C5B	-2.31	101.92	109.33
2	A	501[B]	COA	C4A-C5A-N7A	-2.28	107.98	110.58
5	B	1001	NAD	O2N-PN-O3	2.26	113.37	107.27
2	A	501[A]	COA	C4A-N9A-C8A	2.21	108.06	105.74
2	A	501[A]	COA	O5A-P2A-O3A	2.21	113.23	107.27
2	A	501[A]	COA	O6A-CCP-CBP	-2.17	107.05	110.55
2	A	501[B]	COA	C3B-C2B-C1B	2.15	104.63	99.89
2	A	501[A]	COA	C3B-C2B-C1B	2.12	104.55	99.89
5	B	1001	NAD	C4A-C5A-N7A	-2.11	108.17	110.58
2	A	501[B]	COA	C4A-N9A-C8A	2.10	107.94	105.74
2	A	501[A]	COA	C4A-C5A-N7A	-2.06	108.23	110.58

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[B]	COA	C5B-O5B-P1A-O1A
2	A	501[B]	COA	C5B-O5B-P1A-O2A
2	A	501[B]	COA	C5B-O5B-P1A-O3A
2	A	501[B]	COA	CCP-O6A-P2A-O3A
2	A	501[B]	COA	CCP-O6A-P2A-O5A
2	A	501[B]	COA	CDP-CBP-CCP-O6A
2	A	501[B]	COA	CEP-CBP-CCP-O6A
2	A	501[B]	COA	CAP-CBP-CCP-O6A
2	A	501[B]	COA	OAP-CAP-CBP-CCP
2	A	501[B]	COA	OAP-CAP-CBP-CDP
5	B	1001	NAD	O4D-C1D-N1N-C2N

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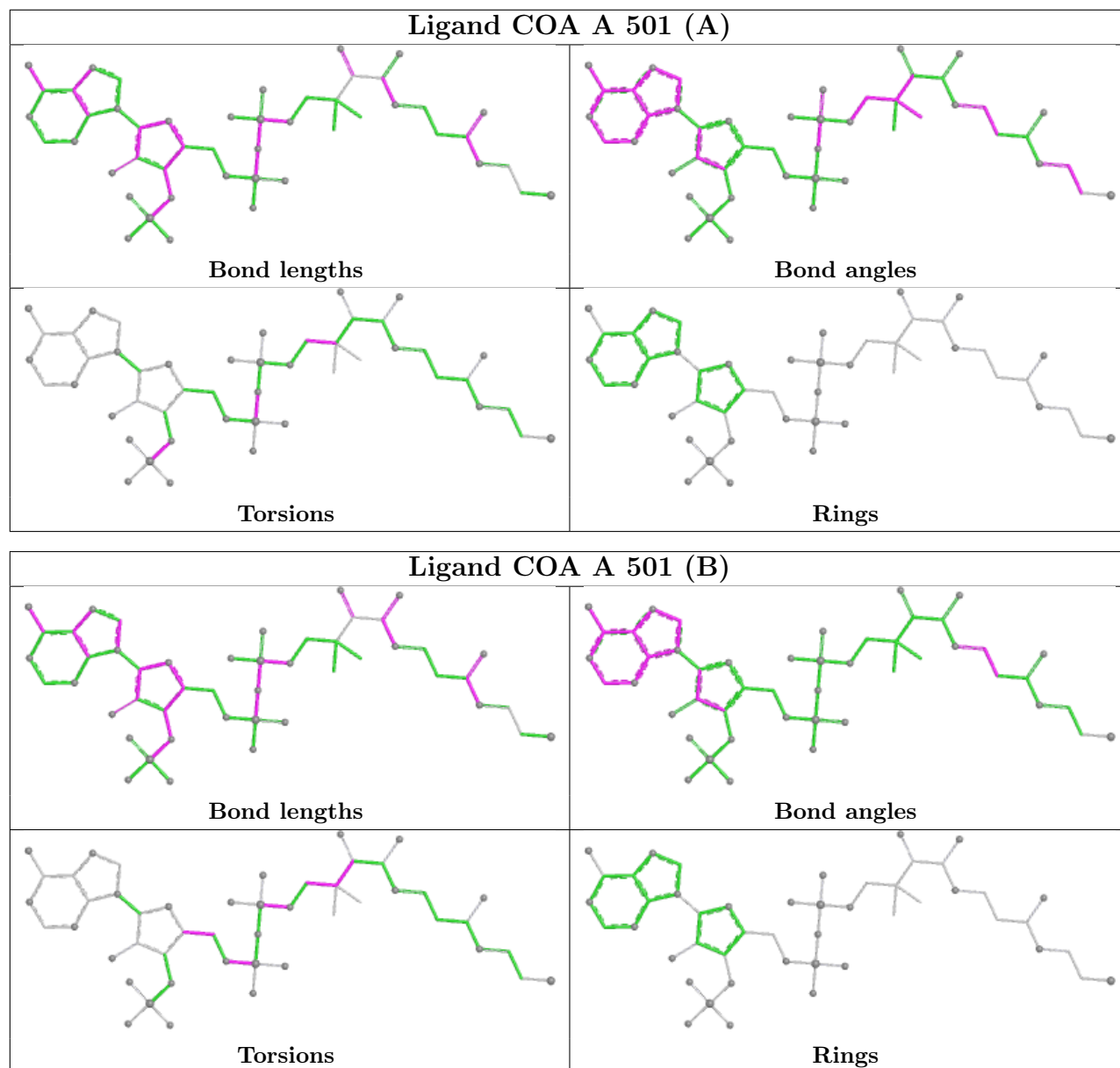
Mol	Chain	Res	Type	Atoms
5	B	1001	NAD	O4D-C1D-N1N-C6N
5	B	1001	NAD	C2D-C1D-N1N-C6N
2	A	501[B]	COA	O4B-C4B-C5B-O5B
2	A	501[B]	COA	OAP-CAP-CBP-CEP
2	A	501[B]	COA	C9P-CAP-CBP-CDP
2	A	501[A]	COA	CEP-CBP-CCP-O6A
2	A	501[B]	COA	C9P-CAP-CBP-CCP
5	B	1001	NAD	C2D-C1D-N1N-C2N
2	A	501[B]	COA	C3B-C4B-C5B-O5B
3	B	1002	MEV	C3-C4-C5-O4
2	A	501[A]	COA	C3B-O3B-P3B-O7A
3	B	1002	MEV	C3-C4-C5-O3
2	A	501[B]	COA	C9P-CAP-CBP-CEP
5	B	1001	NAD	PN-O3-PA-O2A
5	B	1001	NAD	O4B-C1B-N9A-C8A
5	B	1001	NAD	C2B-C1B-N9A-C8A
2	A	501[A]	COA	CDP-CBP-CCP-O6A
2	A	501[A]	COA	P2A-O3A-P1A-O2A

There are no ring outliers.

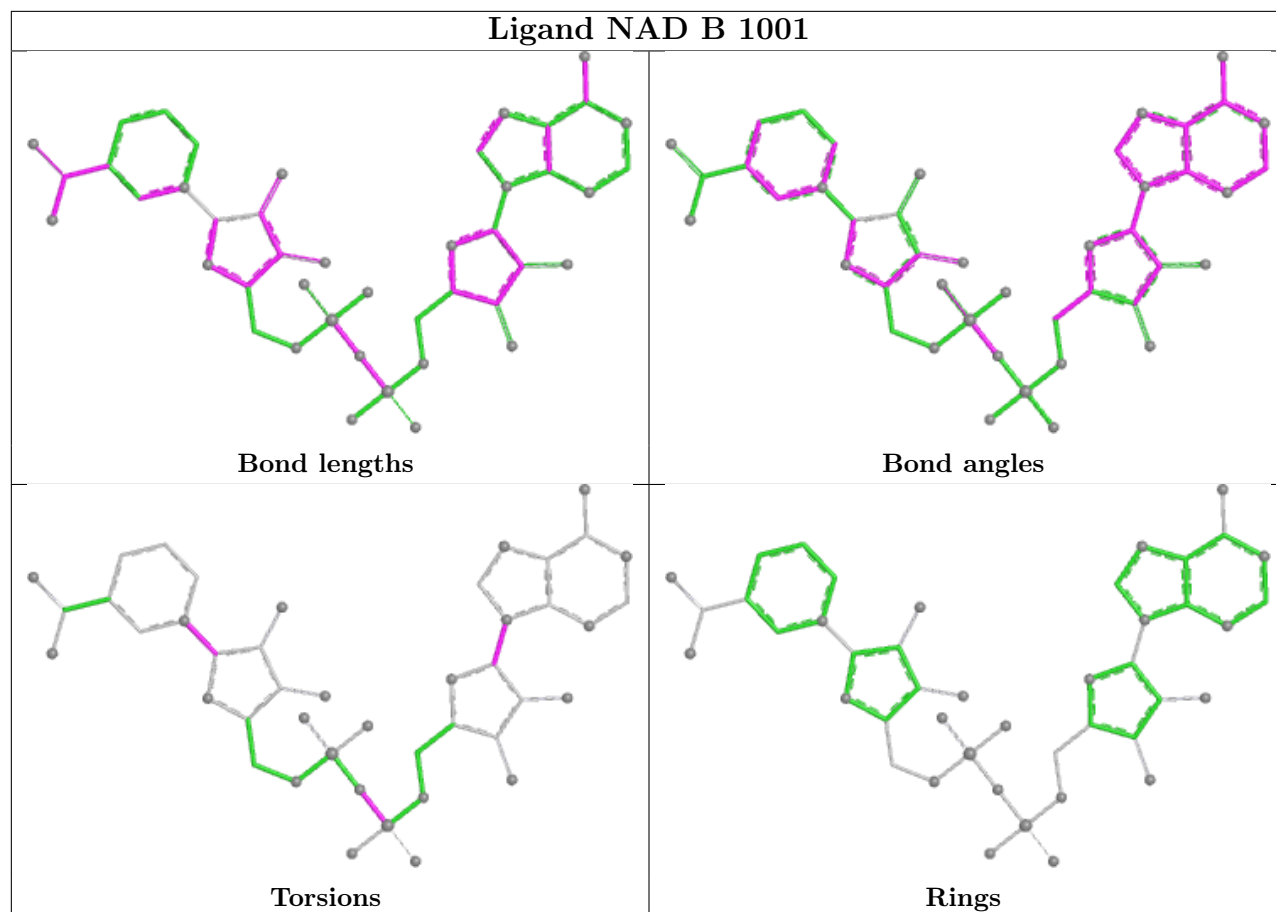
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[A]	COA	3	0
2	A	501[B]	COA	3	0
5	B	1001	NAD	2	0
3	A	502	MEV	2	0

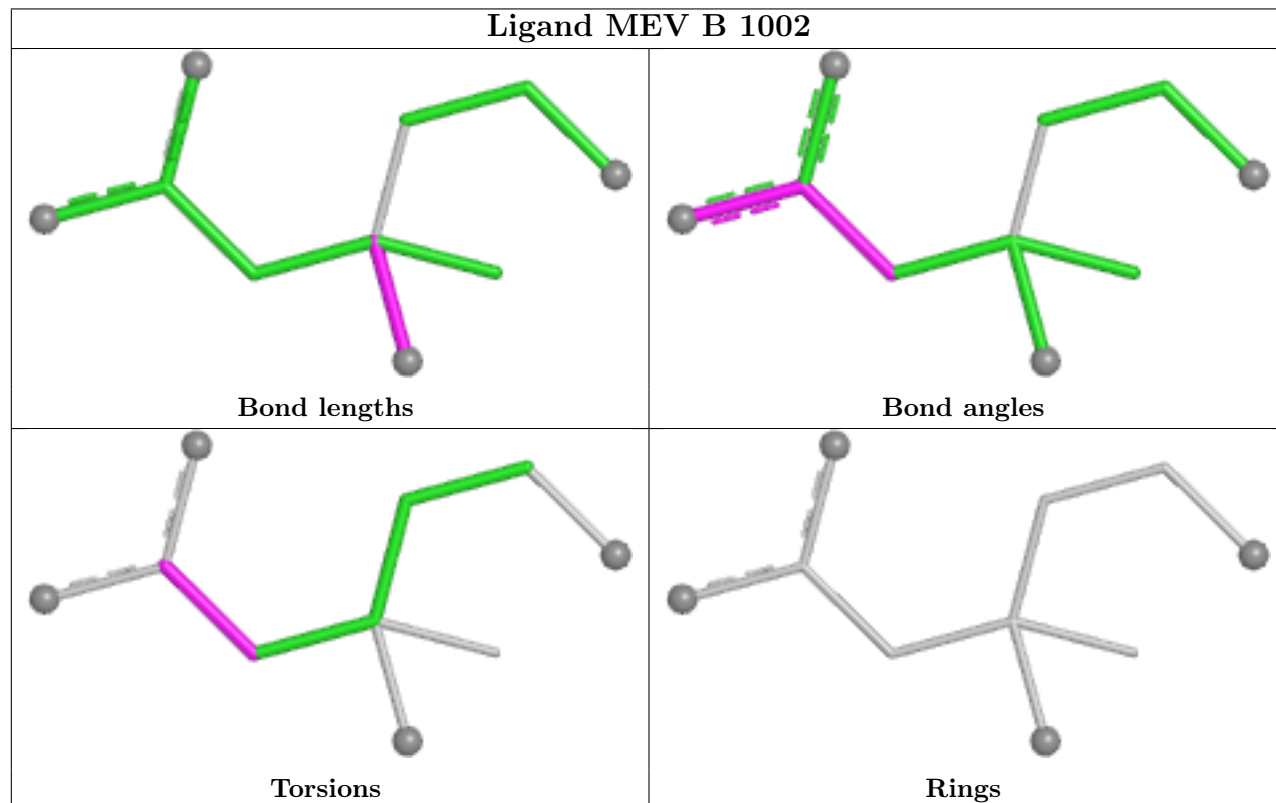
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

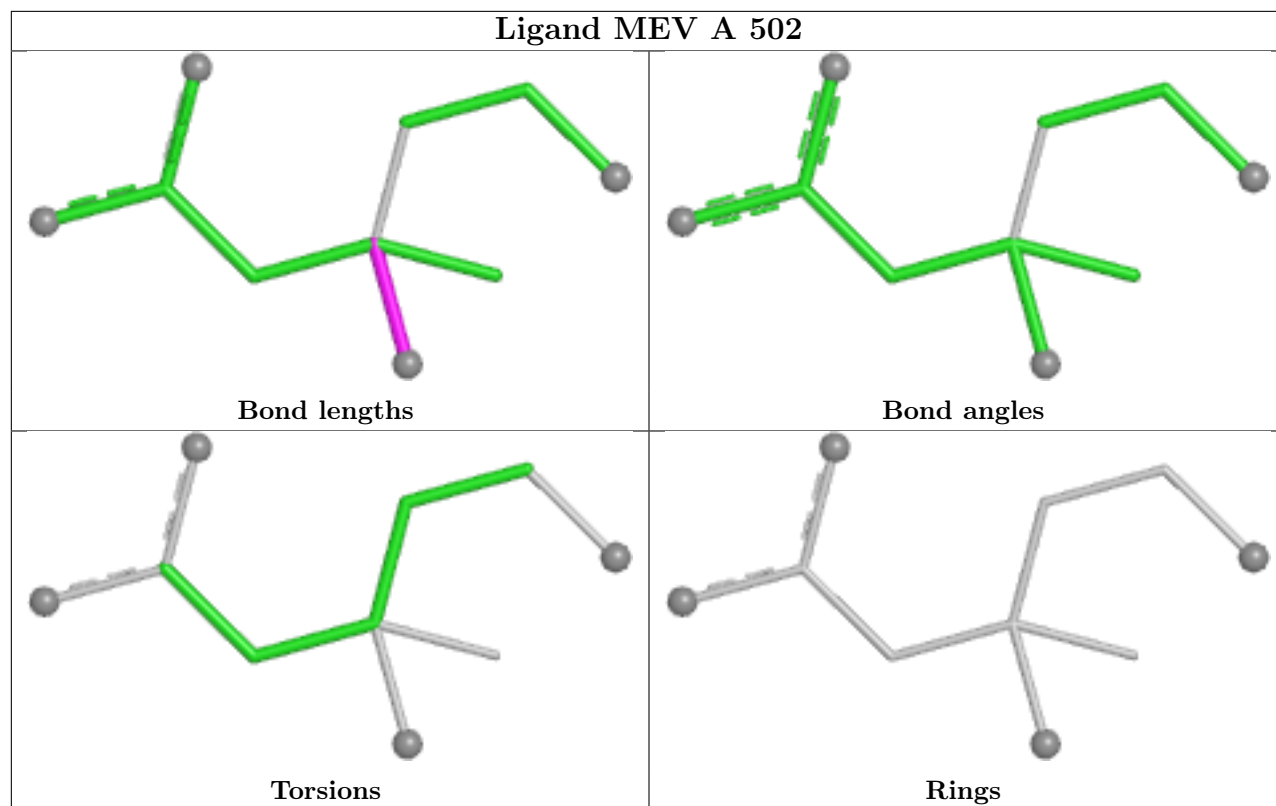


Ligand NAD B 1001



Ligand MEV B 1002





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	421/428 (98%)	0.11	27 (6%) 25 24	13, 30, 64, 103	17 (4%)
1	B	378/428 (88%)	-0.03	10 (2%) 57 56	13, 30, 50, 98	9 (2%)
All	All	799/856 (93%)	0.04	37 (4%) 37 36	13, 30, 55, 103	26 (3%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	TRP	7.0
1	A	403	VAL	5.4
1	A	395	ALA	5.1
1	A	396	ARG	5.0
1	A	422	LEU	4.6
1	A	390	ALA	4.4
1	A	421	LEU	4.2
1	A	397	GLY	4.1
1	A	410	TYR	4.0
1	A	393	ALA	4.0
1	A	420	ALA	3.7
1	A	392	VAL	3.6
1	B	511	ARG	3.4
1	A	394	GLY	3.2
1	A	411	HIS	3.1
1	B	738	GLU	2.9
1	A	391	VAL	2.8
1	A	400	VAL	2.8
1	A	415	ALA	2.8
1	A	419	VAL	2.8
1	B	879	ARG	2.7
1	A	329	GLY	2.6
1	B	799	GLY	2.6
1	B	510	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	144	ARG	2.5
1	B	878	GLN	2.4
1	A	399	GLU	2.4
1	A	409	GLU	2.4
1	A	165	ALA	2.4
1	A	330	GLY	2.3
1	A	407	LEU	2.3
1	B	521[A]	HIS	2.3
1	B	522	ILE	2.2
1	A	389	ILE	2.1
1	B	665	ALA	2.0
1	B	739	PHE	2.0
1	A	406	GLN	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.

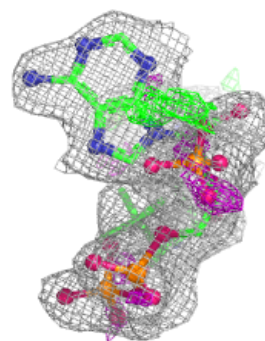
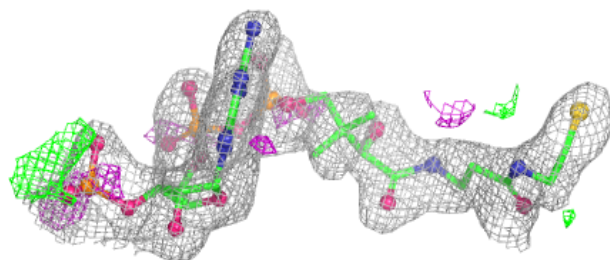
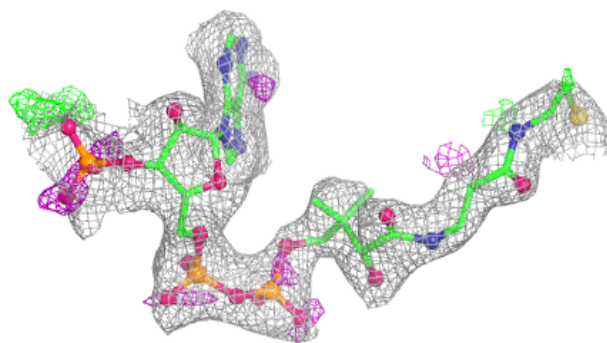
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	504	5/5	0.83	0.11	55,66,75,85	0
2	COA	A	501[B]	48/48	0.93	0.09	28,38,45,46	48
3	MEV	B	1002	10/10	0.93	0.08	21,28,31,32	0
4	SO4	A	503	5/5	0.93	0.09	30,41,45,59	0
2	COA	A	501[A]	48/48	0.93	0.09	27,39,46,48	48
5	NAD	B	1001	44/44	0.95	0.08	20,35,41,45	0
3	MEV	A	502	10/10	0.97	0.06	19,22,27,27	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.

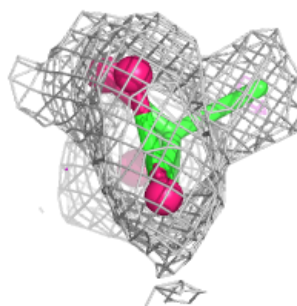
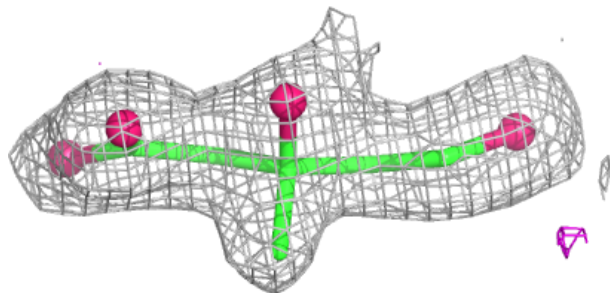
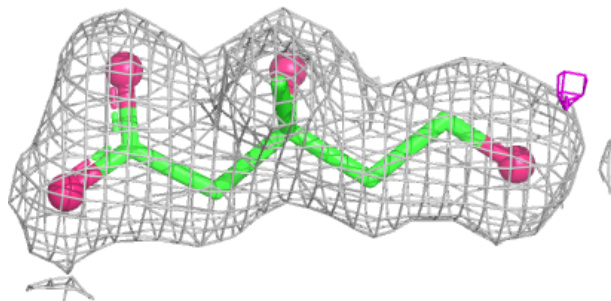
Electron density around COA A 501 (B):

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



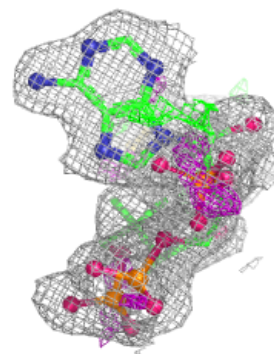
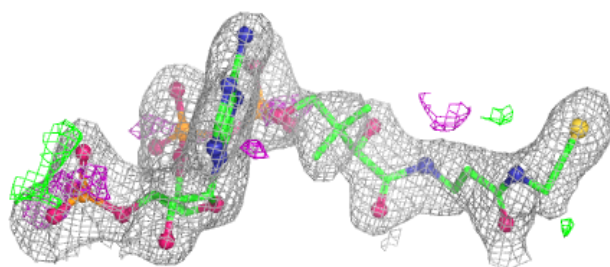
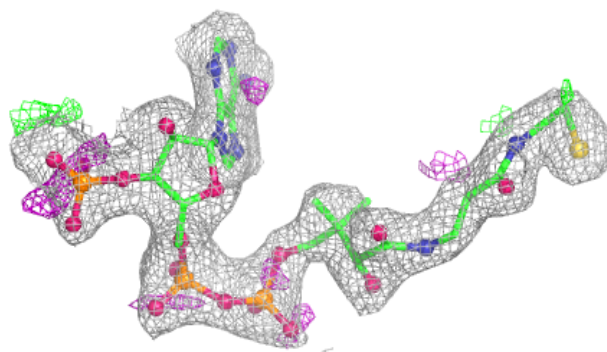
Electron density around MEV B 1002:

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

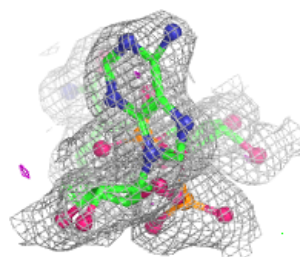
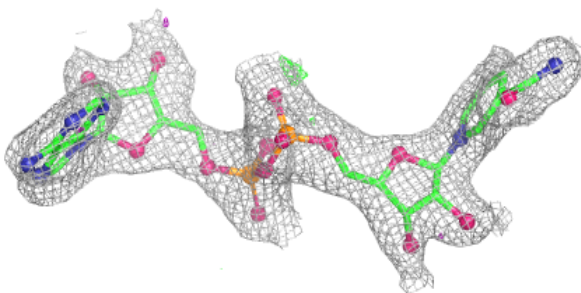
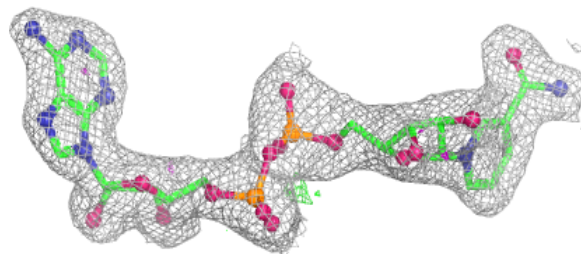


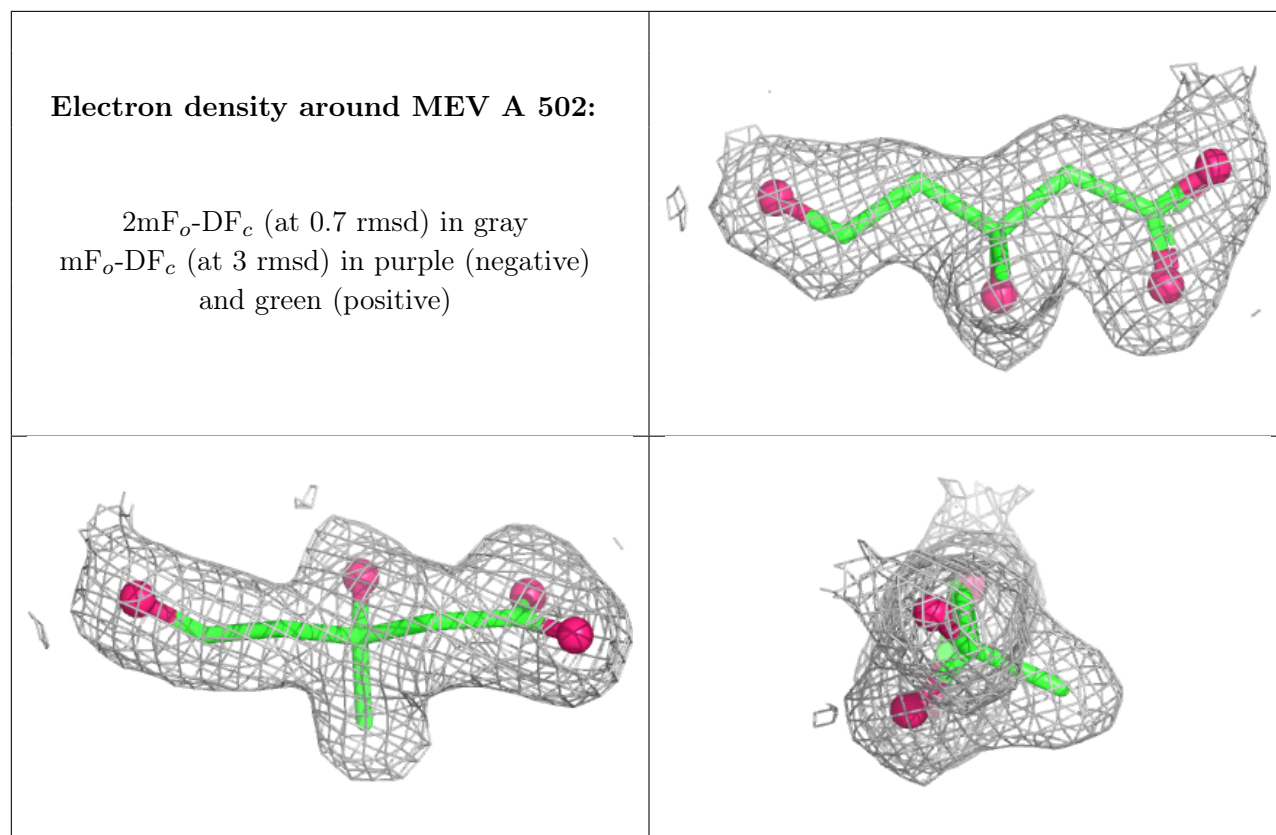
Electron density around COA A 501 (A):

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

**Electron density around NAD B 1001:**

$2mF_o-DF_c$ (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.