



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:38 PM UTC

PDB ID : 9DG2 / pdb_00009dg2
Title : PmHMGR bound to mevalonate, CoA, and NAD, buffer-exchanged to ammonium acetate environment at pH 6.7
Authors : Purohit, V.; Steussy, C.N.; Schmidt, T.; Stauffacher, C.V.; Rushton, P.
Deposited on : 2024-09-01
Resolution : 1.93 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

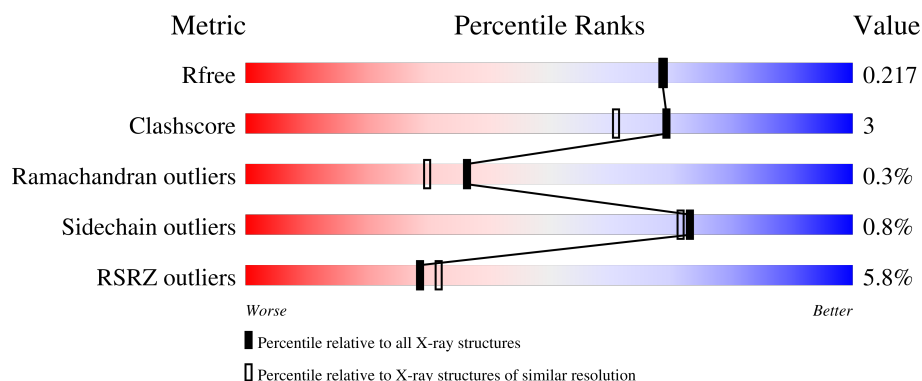
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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>8%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	B	428	<div> <div>3%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>

2 Entry composition [i](#)

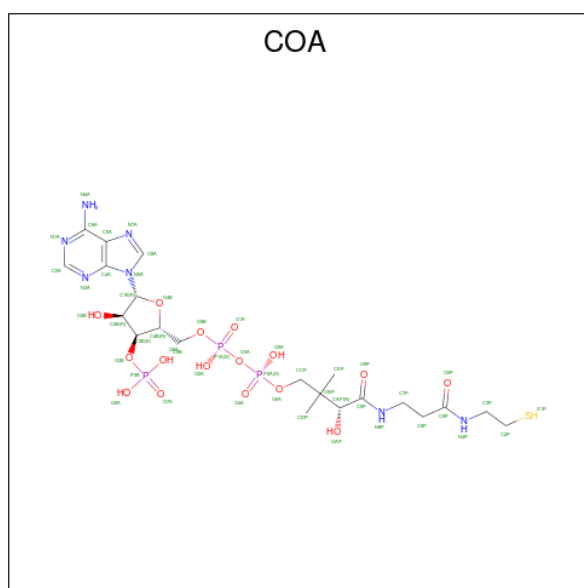
There are 6 unique types of molecules in this entry. The entry contains 6479 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

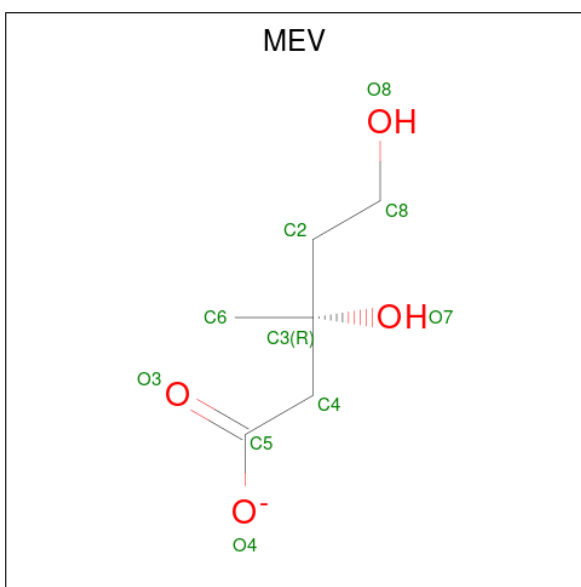
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	16	5	0
			3123	1949	573	585	16			
1	B	377	Total	C	N	O	S	9	0	0
			2791	1748	502	527	14			

- 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).



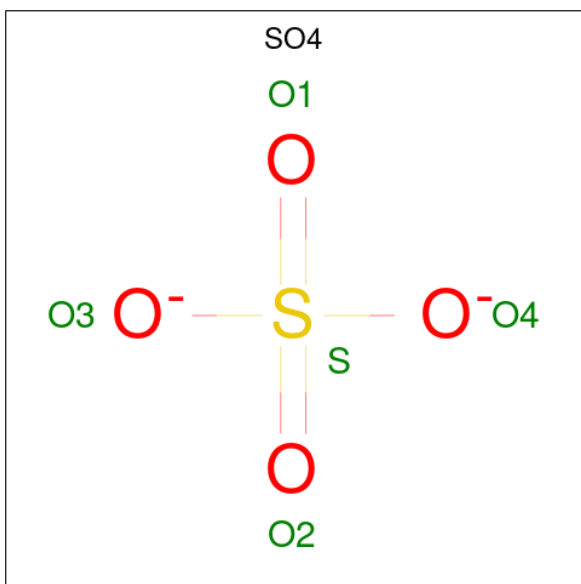
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

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



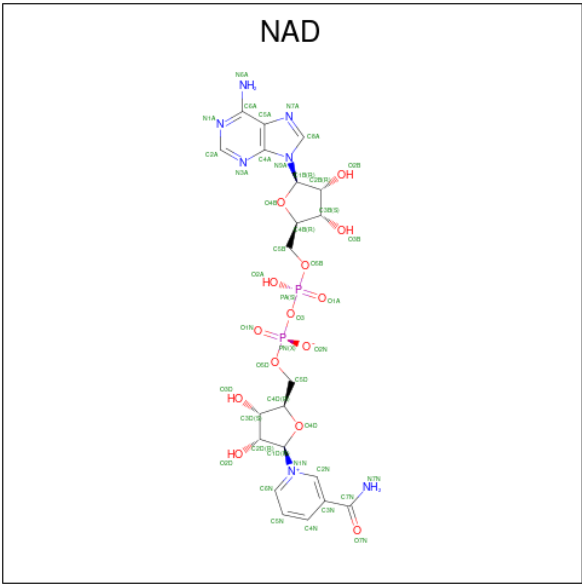
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (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		

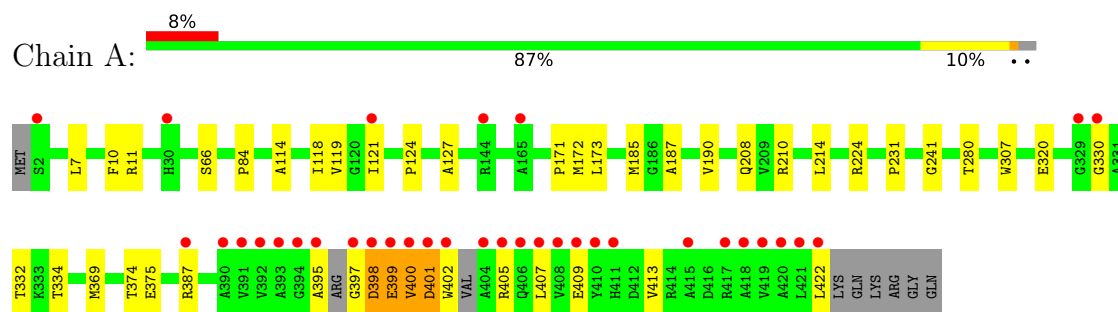
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	236	Total	O	0	0
			236	236		
6	B	212	Total	O	0	0
			212	212		

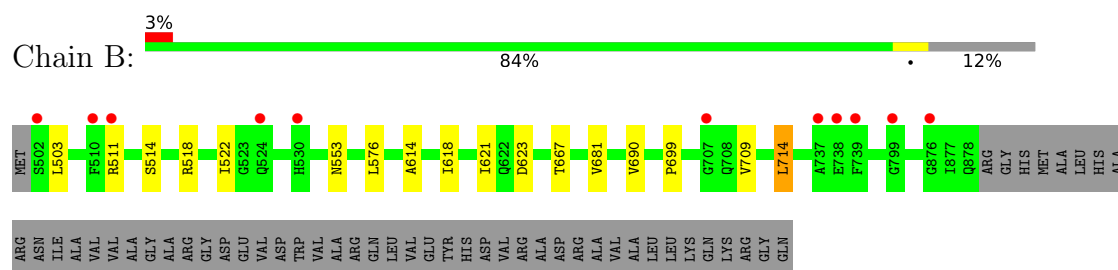
3 Residue-property plots

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



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4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	225.67Å 225.67Å 225.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 1.93 48.11 – 1.93	Depositor EDS
% Data completeness (in resolution range)	85.8 (48.11-1.93) 85.8 (48.11-1.93)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.178 , 0.217 0.178 , 0.217	Depositor DCC
R_{free} test set	3077 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	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	0.95	EDS
Total number of atoms	6479	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, MEV, NAD, COA

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	0.35	0/3168	0.55	4/4308 (0.1%)
1	B	0.30	0/2834	0.50	0/3856
All	All	0.33	0/6002	0.53	4/8164 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	GLU	CB-CA-C	-6.30	109.32	116.63
1	A	398	ASP	N-CA-C	6.03	117.71	108.42
1	A	84	PRO	CA-C-N	5.01	131.11	121.54
1	A	84	PRO	C-N-CA	5.01	131.11	121.54

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	3123	0	3132	27	0
1	B	2791	0	2827	10	0
2	A	48	0	32	6	0
3	A	10	0	11	3	0
3	B	10	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
5	B	44	0	25	2	0
6	A	236	0	0	0	0
6	B	212	0	0	2	0
All	All	6479	0	6038	42	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 3.

All (42) 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:COA:O4B	2:A:501:COA:C1B	1.65	1.27
1:B:511:ARG:NH1	6:B:1101:HOH:O	2.21	0.73
1:A:114:ALA:HB2	1:A:190:VAL:HB	1.74	0.70
1:A:185:MET:HE1	1:A:187:ALA:HB2	1.79	0.64
1:A:397:GLY:HA2	1:A:422:LEU:HD13	1.81	0.63
2:A:501:COA:S1P	3:A:502:MEV:H82	2.40	0.62
1:A:118:ILE:HD12	1:A:173:LEU:HD22	1.82	0.61
1:A:400:VAL:O	1:A:401:ASP:C	2.45	0.59
3:A:502:MEV:H81	5:B:1001:NAD:C4N	2.31	0.59
1:A:407:LEU:HB3	1:A:413:VAL:HG22	1.85	0.57
1:A:11:ARG:HB3	2:A:501:COA:C2A	2.39	0.53
1:A:307:TRP:NE1	1:A:369:MET:HE1	2.24	0.52
1:A:280:THR:O	1:A:332:THR:HG22	2.09	0.52
1:A:121:ILE:HD11	1:A:127:ALA:HB2	1.91	0.52
1:B:618:ILE:HG12	1:B:709:VAL:HG22	1.93	0.51
1:A:231:PRO:O	1:A:241:GLY:HA3	2.11	0.51
1:B:514:SER:O	1:B:518:ARG:HG3	2.10	0.51
1:B:614:ALA:HB2	1:B:690:VAL:HB	1.93	0.49
1:A:185:MET:HE3	1:A:185:MET:HB3	1.64	0.48
1:A:402:TRP:O	1:A:405:ARG:N	2.46	0.48
1:A:330:GLY:O	1:A:334:THR:HG23	2.14	0.47
1:A:119:VAL:HG12	1:A:172:MET:HG2	1.97	0.47
1:A:395:ALA:HB1	1:A:399:GLU:O	2.14	0.47
1:A:208:GLN:CD	1:A:210:ARG:HH12	2.23	0.46
1:A:224:ARG:HD3	1:A:320:GLU:OE1	2.15	0.46
1:A:398:ASP:H	1:A:422:LEU:HD22	1.81	0.46
1:B:621:ILE:HG22	1:B:623:ASP:H	1.80	0.45
1:A:400:VAL:O	1:A:402:TRP:N	2.50	0.45
2:A:501:COA:H2A	1:B:553:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:COA:C2P	3:A:502:MEV:H82	2.47	0.44
1:A:124:PRO:HG3	1:A:171:PRO:HB2	2.00	0.44
1:A:374:THR:OG1	1:A:375:GLU:N	2.50	0.44
2:A:501:COA:O4B	2:A:501:COA:C8A	2.66	0.43
1:B:681:VAL:O	5:B:1001:NAD:H2A	2.18	0.43
1:A:7:LEU:HD12	1:A:66:SER:HB3	2.00	0.43
1:A:307:TRP:CD1	1:A:369:MET:HE1	2.55	0.41
1:B:699:PRO:HG2	6:B:1153:HOH:O	2.20	0.41
1:A:405:ARG:O	1:A:409:GLU:HG2	2.21	0.41
1:B:614:ALA:HA	1:B:714:LEU:HA	2.02	0.41
1:B:522:ILE:HD12	1:B:576:LEU:HD13	2.02	0.41
1:A:7:LEU:HB3	1:A:10:PHE:HB2	2.03	0.41
1:A:307:TRP:CE2	1:A:369:MET:HE1	2.56	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	418/428 (98%)	400 (96%)	16 (4%)	2 (0%)	24	15
1	B	375/428 (88%)	366 (98%)	9 (2%)	0	100	100
All	All	793/856 (93%)	766 (97%)	25 (3%)	2 (0%)	36	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	VAL
1	A	401	ASP

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	316/327 (97%)	314 (99%)	2 (1%)	78	78
1	B	288/327 (88%)	285 (99%)	3 (1%)	68	64
All	All	604/654 (92%)	599 (99%)	5 (1%)	73	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	LEU
1	A	387	ARG
1	B	503	LEU
1	B	667	THR
1	B	714	LEU

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	69	GLN
1	A	150	ASN
1	A	162	HIS
1	B	615	GLN
1	B	626	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
3	MEV	B	1002	-	8,9,9	1.22	1 (12%)	7,12,12	1.25	1 (14%)
2	COA	A	501	-	47,50,50	3.20	17 (36%)	69,75,75	1.90	12 (17%)
3	MEV	A	502	-	8,9,9	1.26	1 (12%)	7,12,12	0.94	0
4	SO4	A	503	-	4,4,4	0.71	0	6,6,6	0.20	0
5	NAD	B	1001	-	46,48,48	3.99	20 (43%)	64,73,73	2.08	19 (29%)

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
3	MEV	B	1002	-	-	0/9/9/9	-
2	COA	A	501	-	-	4/48/64/64	0/3/3/3
3	MEV	A	502	-	-	1/9/9/9	-
5	NAD	B	1001	-	-	7/30/62/62	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	COA	O4B-C1B	10.31	1.65	1.42
5	B	1001	NAD	C3B-C4B	-10.28	1.26	1.53
5	B	1001	NAD	C2D-C3D	-9.71	1.27	1.53
5	B	1001	NAD	C7N-N7N	8.56	1.48	1.33
5	B	1001	NAD	O4D-C1D	8.17	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	NAD	C2B-C1B	-7.96	1.28	1.53
2	A	501	COA	P1A-O3A	7.84	1.68	1.59
2	A	501	COA	P2A-O3A	7.72	1.67	1.59
5	B	1001	NAD	PA-O3	6.73	1.66	1.59
2	A	501	COA	C9P-N8P	6.50	1.48	1.33
2	A	501	COA	O4B-C4B	-6.02	1.31	1.45
5	B	1001	NAD	O4D-C4D	-5.94	1.31	1.45
2	A	501	COA	C2B-C1B	-5.83	1.35	1.53
2	A	501	COA	C5P-N4P	5.50	1.46	1.33
5	B	1001	NAD	O4B-C1B	5.44	1.54	1.42
5	B	1001	NAD	C6A-N6A	5.34	1.47	1.34
5	B	1001	NAD	C2B-C3B	5.25	1.67	1.53
5	B	1001	NAD	PN-O3	5.17	1.65	1.59
5	B	1001	NAD	C3D-C4D	4.77	1.65	1.53
2	A	501	COA	C6A-N6A	4.71	1.46	1.34
5	B	1001	NAD	O4B-C4B	4.40	1.54	1.45
5	B	1001	NAD	O2D-C2D	3.84	1.52	1.43
5	B	1001	NAD	C3N-C7N	3.59	1.55	1.50
2	A	501	COA	O3B-C3B	-3.41	1.32	1.44
2	A	501	COA	P3B-O3B	2.79	1.64	1.59
5	B	1001	NAD	O7N-C7N	-2.77	1.19	1.24
5	B	1001	NAD	C5A-C4A	-2.63	1.34	1.39
5	B	1001	NAD	O3D-C3D	2.59	1.49	1.43
2	A	501	COA	C5A-C4A	-2.54	1.34	1.39
2	A	501	COA	P2A-O6A	2.40	1.68	1.59
2	A	501	COA	O2B-C2B	2.37	1.48	1.43
3	A	502	MEV	O7-C3	-2.32	1.41	1.44
2	A	501	COA	C5A-N7A	-2.25	1.35	1.39
2	A	501	COA	OAP-CAP	-2.22	1.38	1.42
2	A	501	COA	C3B-C4B	2.22	1.58	1.52
2	A	501	COA	O5P-C5P	-2.19	1.18	1.23
3	B	1002	MEV	O7-C3	-2.07	1.41	1.44
5	B	1001	NAD	C2N-N1N	2.06	1.37	1.35
5	B	1001	NAD	C5B-C4B	2.02	1.57	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	NAD	N3A-C2A-N1A	-5.86	119.72	128.58
2	A	501	COA	N3A-C2A-N1A	-5.75	119.87	128.58
2	A	501	COA	C2P-C3P-N4P	-5.37	100.12	112.31
2	A	501	COA	N6A-C6A-N1A	-5.18	106.83	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	NAD	N9A-C8A-N7A	-4.81	107.11	113.94
5	B	1001	NAD	C5A-C4A-N3A	-4.55	120.45	126.72
5	B	1001	NAD	C4D-O4D-C1D	-4.47	105.83	109.92
5	B	1001	NAD	C1B-N9A-C8A	-4.46	117.20	127.09
2	A	501	COA	C5A-C4A-N3A	-4.42	120.62	126.72
2	A	501	COA	C6P-C7P-N8P	-4.23	102.99	112.00
2	A	501	COA	C5A-C6A-N6A	4.22	133.73	123.29
2	A	501	COA	N9A-C8A-N7A	-4.01	108.25	113.94
5	B	1001	NAD	N6A-C6A-N1A	-3.86	109.79	118.38
5	B	1001	NAD	C4A-N9A-C8A	3.65	109.57	105.74
5	B	1001	NAD	C2A-N3A-C4A	3.39	120.11	111.83
5	B	1001	NAD	C6N-N1N-C2N	-3.30	119.07	121.88
5	B	1001	NAD	N3A-C4A-N9A	3.27	132.73	127.17
2	A	501	COA	C2A-N3A-C4A	3.14	119.51	111.83
5	B	1001	NAD	C3B-C2B-C1B	3.08	107.28	101.46
2	A	501	COA	N3A-C4A-N9A	3.03	132.32	127.17
5	B	1001	NAD	C4B-O4B-C1B	-2.99	102.87	109.47
2	A	501	COA	P3B-O3B-C3B	-2.88	115.75	123.43
5	B	1001	NAD	C5A-N7A-C8A	2.83	107.89	103.45
5	B	1001	NAD	C4A-N9A-C1B	2.82	133.23	126.63
5	B	1001	NAD	C5A-C6A-N6A	2.63	129.79	123.29
2	A	501	COA	C5A-N7A-C8A	2.59	107.52	103.45
2	A	501	COA	C4A-N9A-C8A	2.47	108.33	105.74
5	B	1001	NAD	C2N-C3N-C4N	2.39	121.04	118.26
3	B	1002	MEV	C6-C3-C4	-2.12	108.70	111.30
5	B	1001	NAD	O2N-PN-O3	2.04	112.78	107.27
5	B	1001	NAD	O3D-C3D-C4D	-2.04	105.24	111.08
5	B	1001	NAD	C2N-N1N-C1D	2.03	123.61	119.13

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	MEV	C3-C2-C8-O8
5	B	1001	NAD	O4D-C1D-N1N-C2N
5	B	1001	NAD	O4D-C1D-N1N-C6N
5	B	1001	NAD	C2D-C1D-N1N-C6N
2	A	501	COA	P1A-O3A-P2A-O6A
2	A	501	COA	CDP-CBP-CCP-O6A
2	A	501	COA	CEP-CBP-CCP-O6A
5	B	1001	NAD	C2D-C1D-N1N-C2N
5	B	1001	NAD	O4B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
2	A	501	COA	CBP-CCP-O6A-P2A
5	B	1001	NAD	C2B-C1B-N9A-C8A
5	B	1001	NAD	PN-O3-PA-O2A

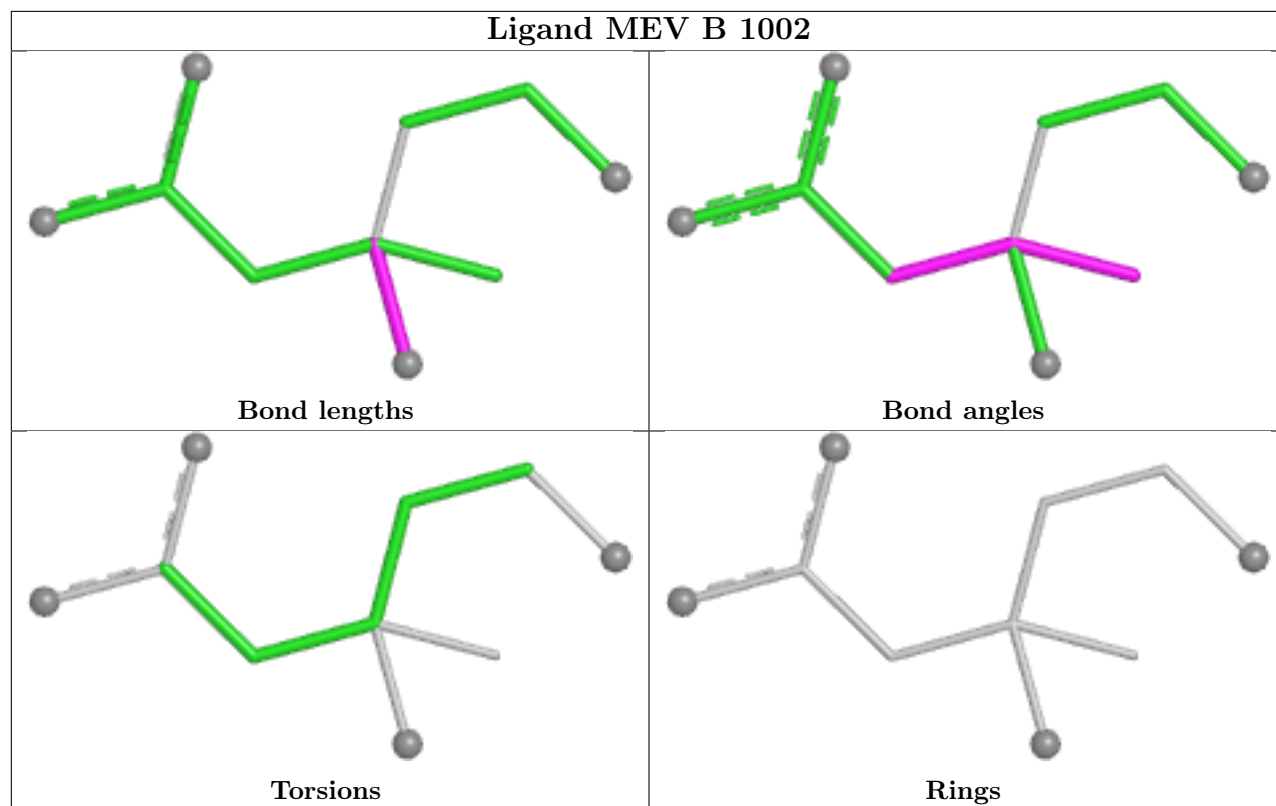
There are no ring outliers.

3 monomers are involved in 8 short contacts:

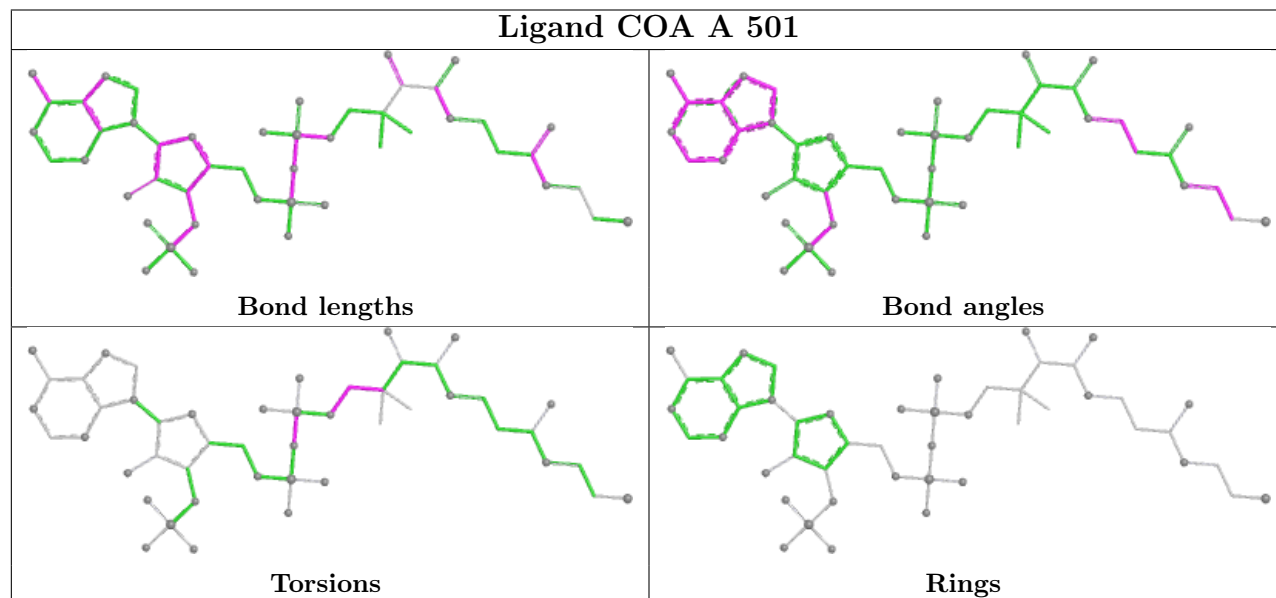
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	COA	6	0
3	A	502	MEV	3	0
5	B	1001	NAD	2	0

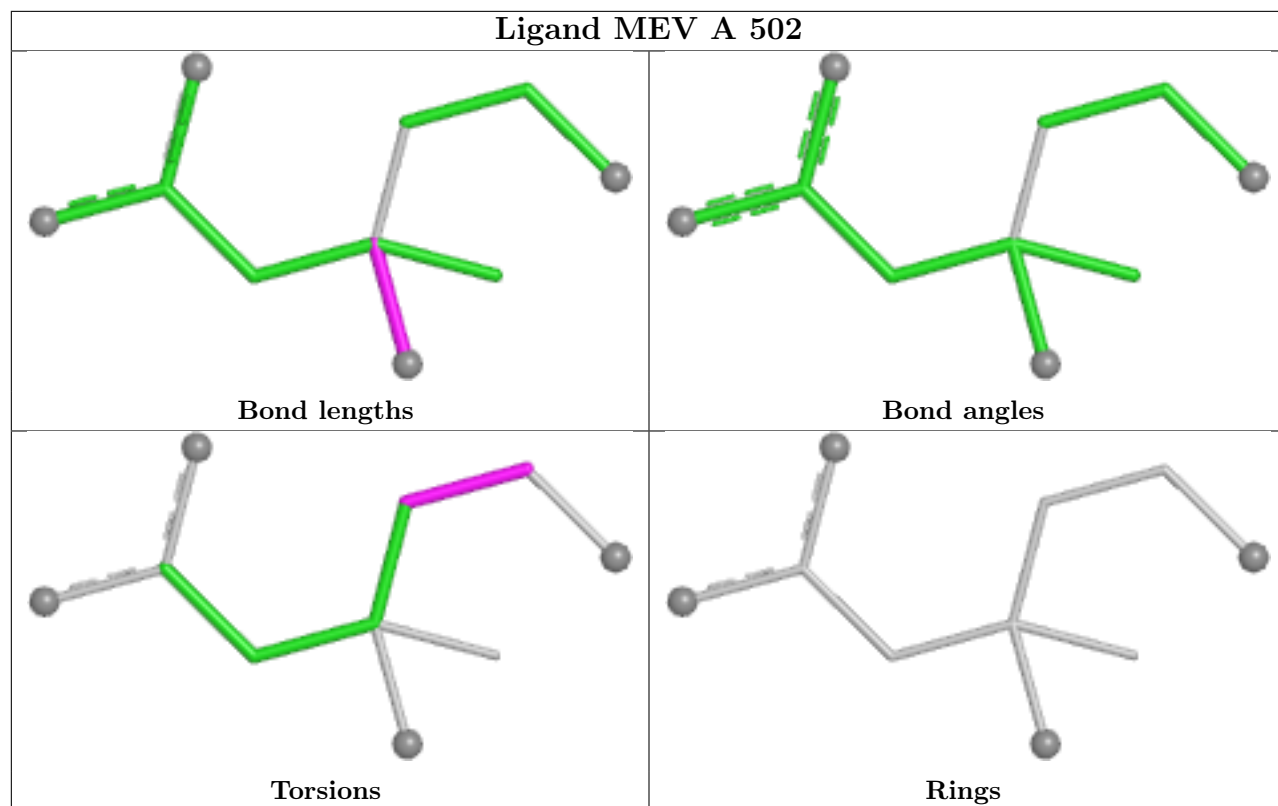
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

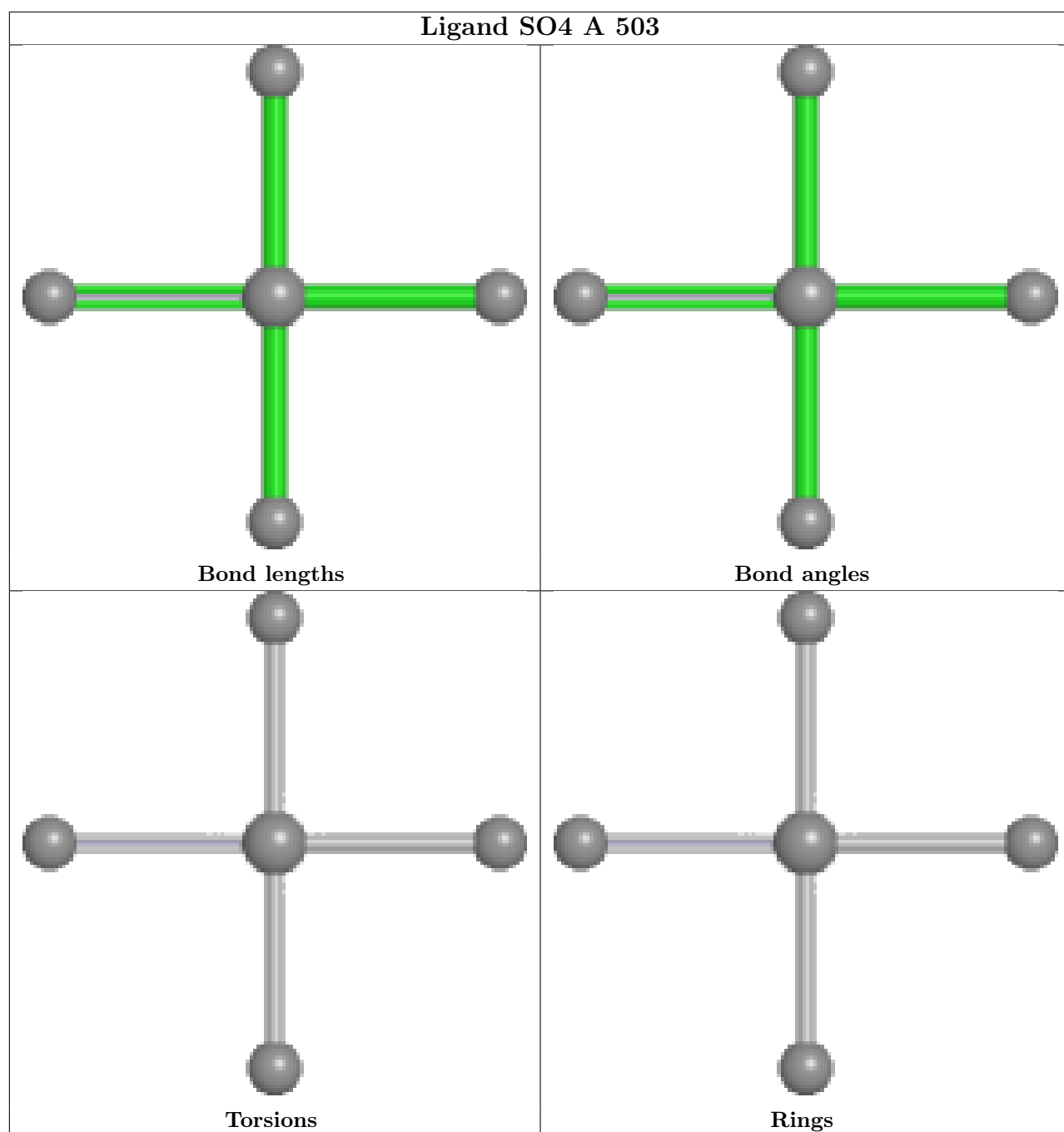
Ligand MEV B 1002

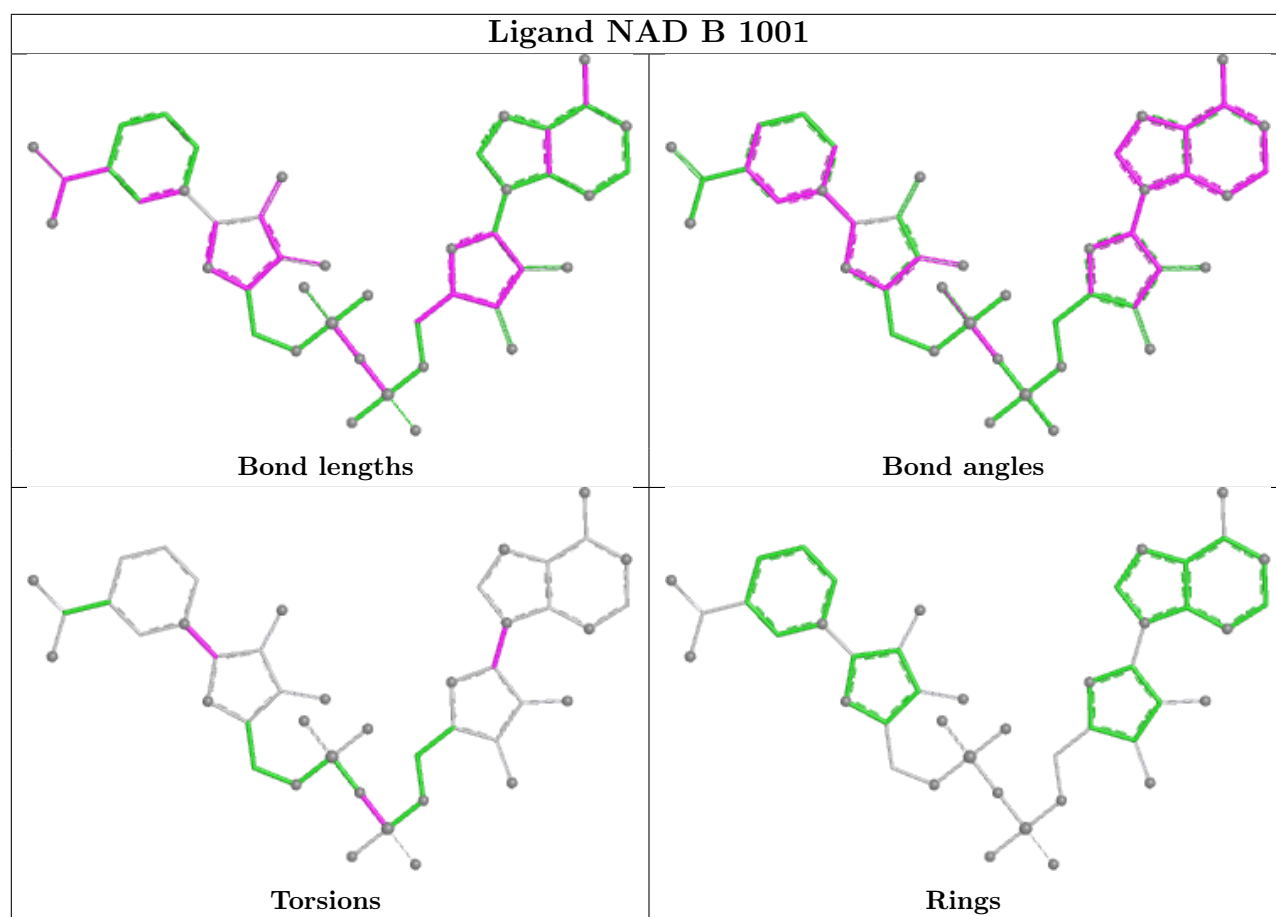


Ligand COA A 501









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	419/428 (97%)	0.12	35 (8%) 17 19	8, 23, 55, 95	14 (3%)
1	B	377/428 (88%)	-0.09	11 (2%) 53 60	11, 22, 42, 62	6 (1%)
All	All	796/856 (92%)	0.02	46 (5%) 29 32	8, 22, 46, 95	20 (2%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	397	GLY	6.2
1	A	398	ASP	6.0
1	A	404	ALA	6.0
1	A	400	VAL	6.0
1	A	399	GLU	5.7
1	A	402	TRP	5.0
1	A	421	LEU	5.0
1	A	422	LEU	4.7
1	A	395	ALA	4.6
1	A	420	ALA	4.5
1	A	393	ALA	4.5
1	A	401	ASP	4.4
1	A	410	TYR	4.4
1	A	407	LEU	4.2
1	A	392	VAL	4.2
1	B	739	PHE	4.1
1	A	387	ARG	4.0
1	A	394	GLY	3.9
1	A	391	VAL	3.9
1	A	415	ALA	3.9
1	B	738	GLU	3.8
1	A	408	VAL	3.8
1	A	419	VAL	3.8
1	A	330	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	390	ALA	3.8
1	A	405	ARG	3.1
1	B	876	GLY	3.1
1	B	502	SER	3.1
1	A	417	ARG	2.8
1	B	707	GLY	2.7
1	A	411	HIS	2.7
1	B	799	GLY	2.6
1	B	511	ARG	2.6
1	B	737	ALA	2.5
1	A	144	ARG	2.5
1	B	510	PHE	2.4
1	A	406	GLN	2.4
1	B	530	HIS	2.4
1	A	121	ILE	2.4
1	A	329	GLY	2.4
1	A	165	ALA	2.3
1	B	524	GLN	2.3
1	A	418	ALA	2.2
1	A	30[A]	HIS	2.1
1	A	409	GLU	2.1
1	A	2	SER	2.1

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
2	COA	A	501	48/48	0.84	0.12	28,46,68,72	0

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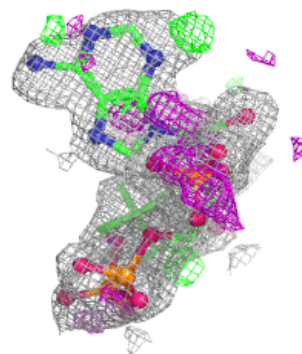
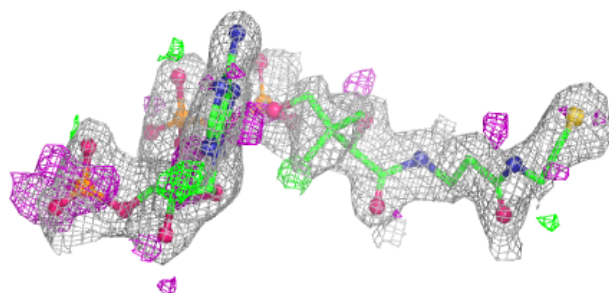
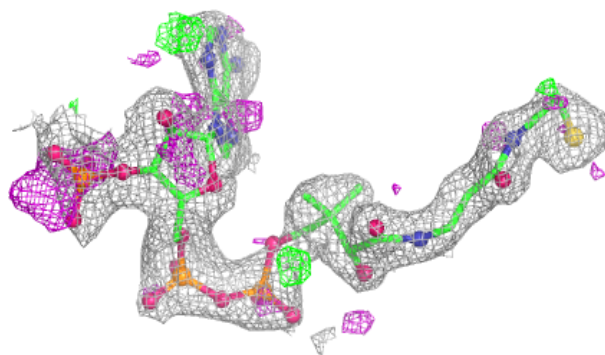
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	503	5/5	0.91	0.10	28,29,34,40	5
3	MEV	B	1002	10/10	0.95	0.07	15,19,22,23	0
5	NAD	B	1001	44/44	0.96	0.07	16,26,34,35	0
3	MEV	A	502	10/10	0.98	0.04	12,15,19,20	0

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.

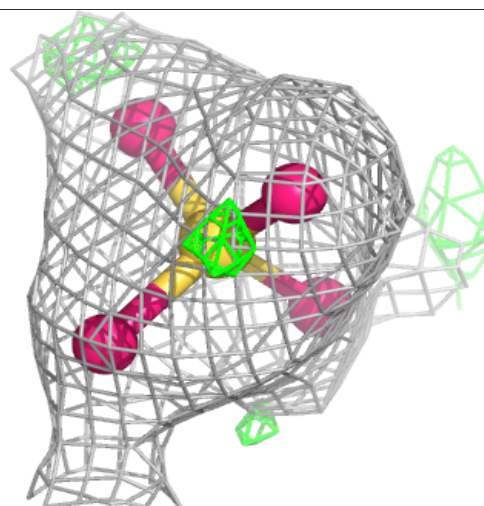
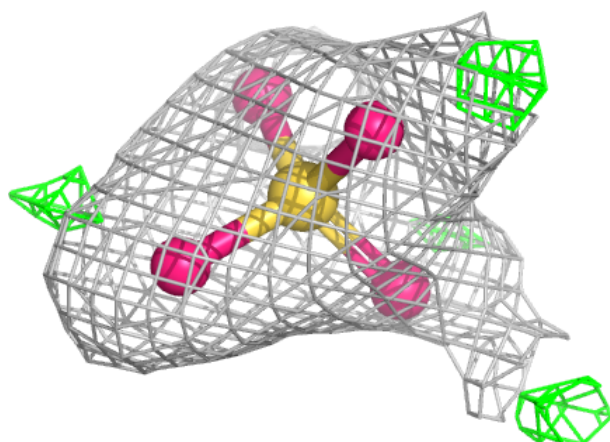
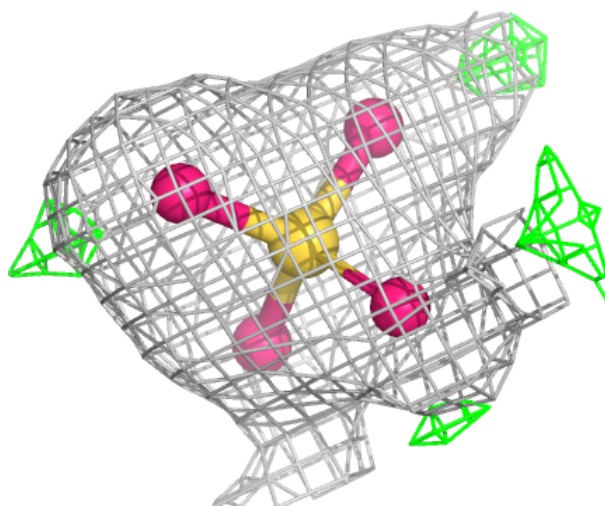
Electron density around COA A 501:

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



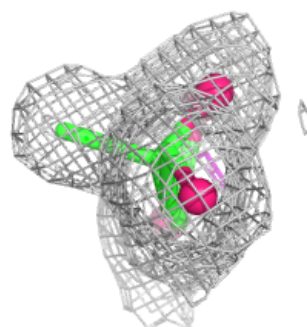
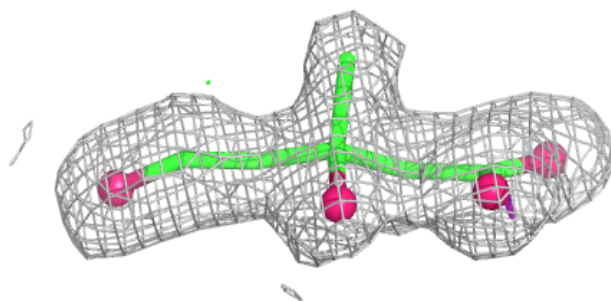
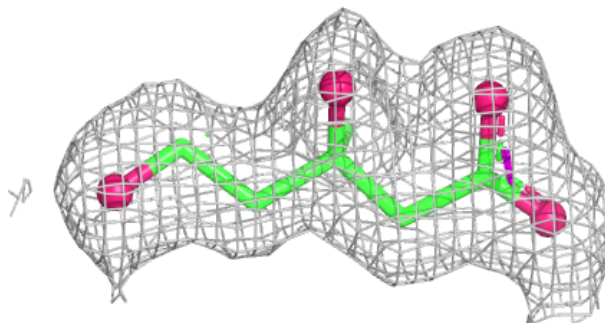
Electron density around SO4 A 503:

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

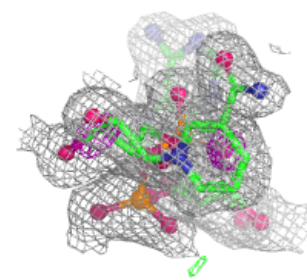
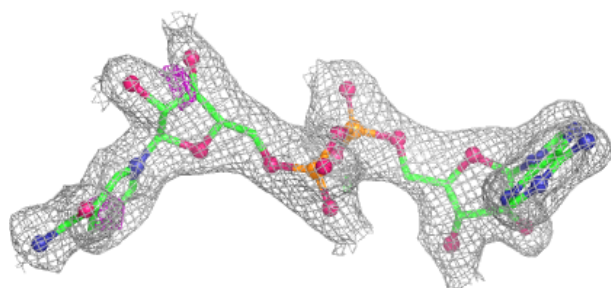
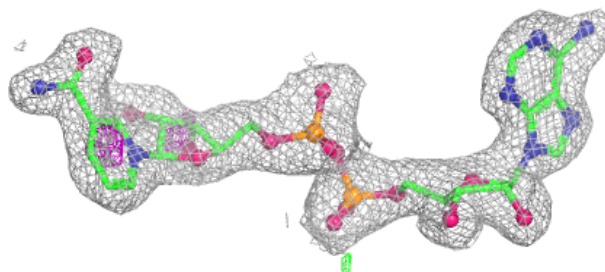


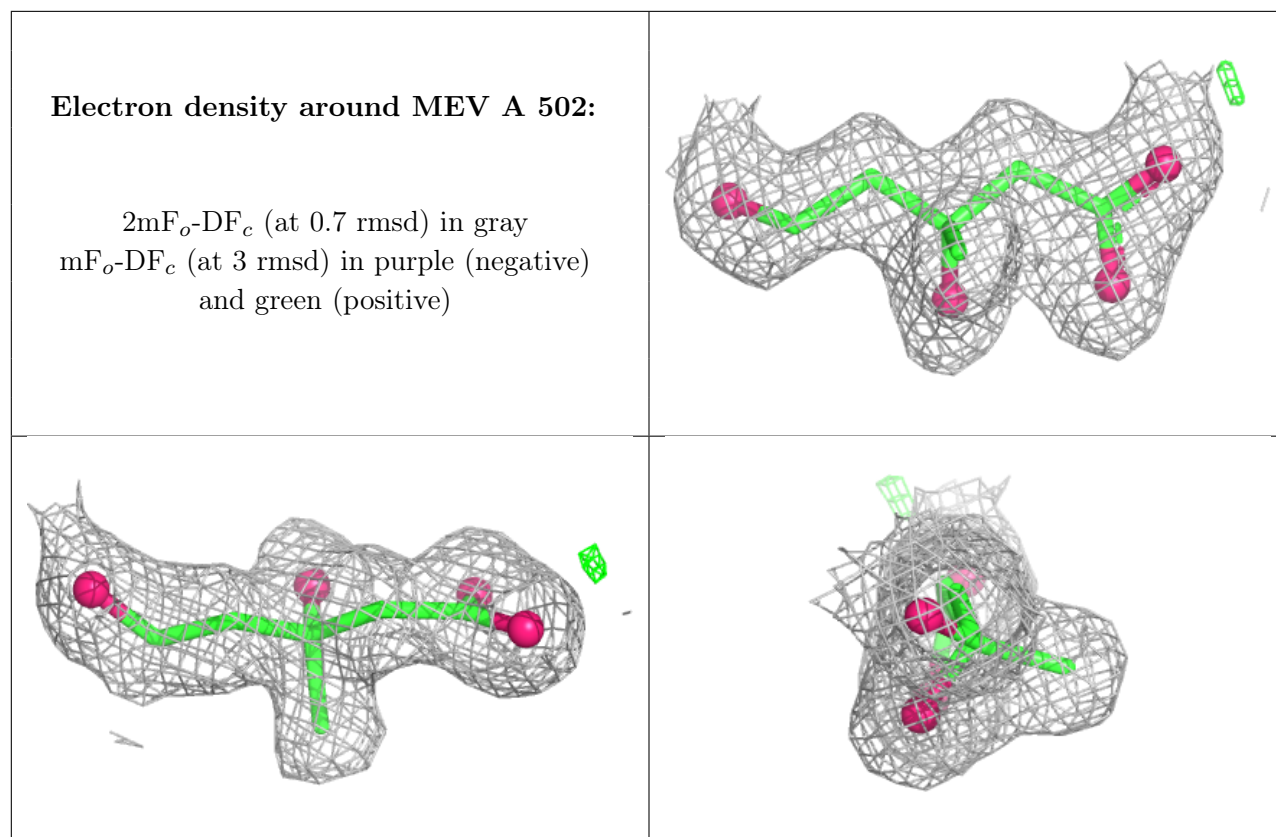
Electron density around MEV B 1002:

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

**Electron density around 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.