



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:44 PM UTC

PDB ID : 8VLQ / pdb_00008vlq
Title : Structure of PmHMGR bound to mevalonate, CoA and NAD 5 minutes after reaction initiation at pH 9
Authors : Purohit, V.; Steussy, C.N.; Stauffacher, C.V.
Deposited on : 2024-01-12
Resolution : 2.07 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

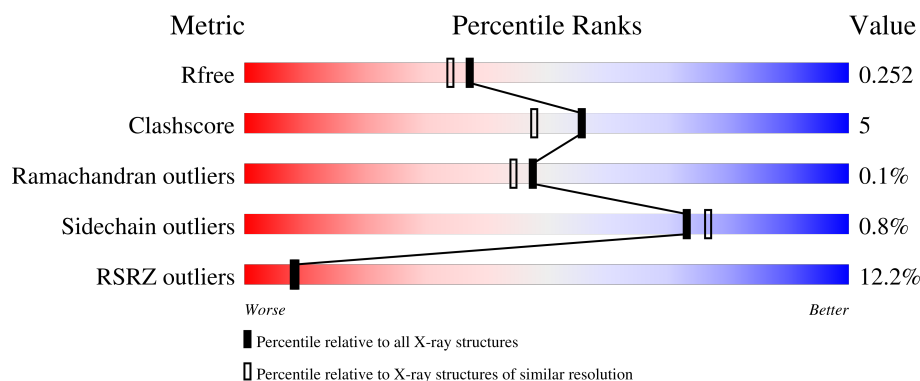
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	14% 85% 13% .
1	B	428	8% 80% 7% 12%

2 Entry composition [i](#)

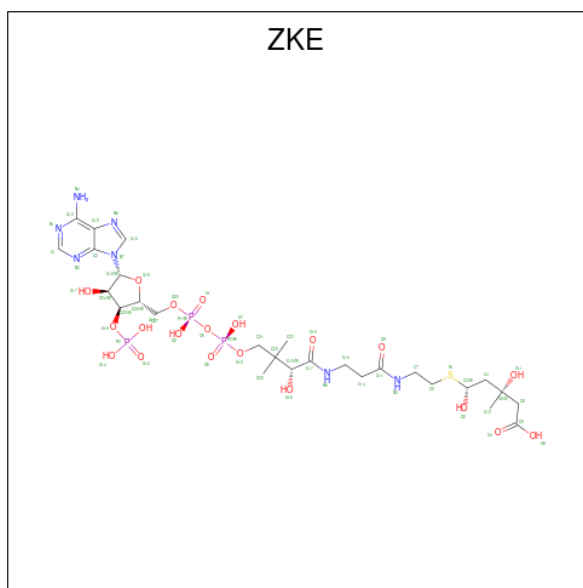
There are 9 unique types of molecules in this entry. The entry contains 6590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

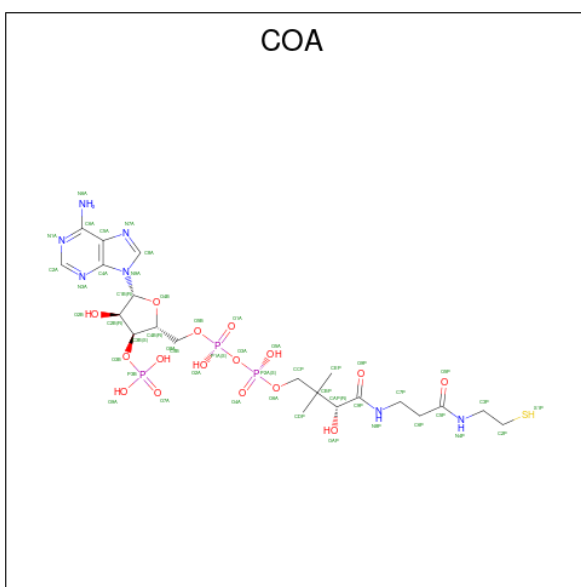
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	3	0
			3151	1967	578	590	16			
1	B	375	Total	C	N	O	S	0	1	0
			2791	1748	504	525	14			

- Molecule 2 is Mevaldyl-Coenzyme A (CCD ID: ZKE) (formula: $C_{27}H_{46}N_7O_{20}P_3S$) (labeled as "Ligand of Interest" by depositor).



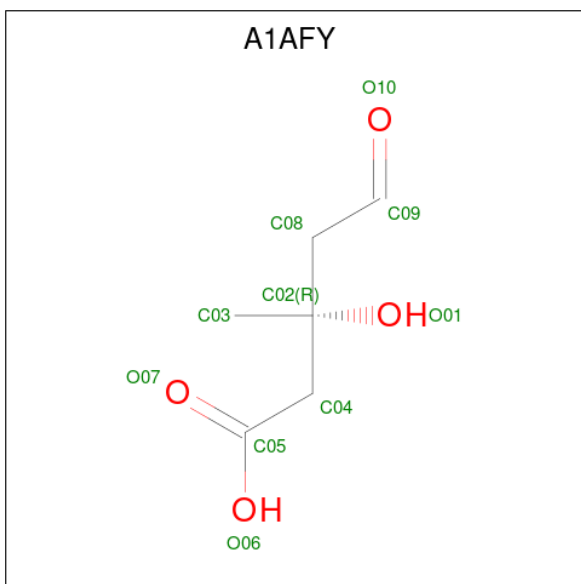
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	1
			58	27	7	20	3 1		

- Molecule 3 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
3	A	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	

- Molecule 4 is (R)-mevaldehyde (CCD ID: A1AFY) (formula: $C_6H_{10}O_4$) (labeled as "Ligand of Interest" by depositor).



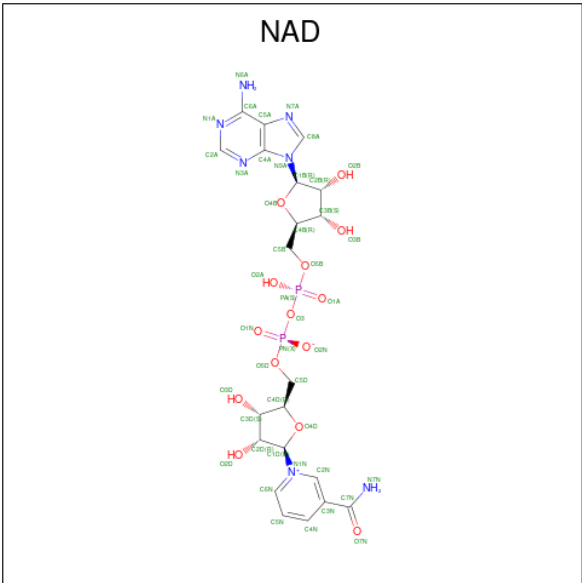
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O		
			10	6	4	0	1

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



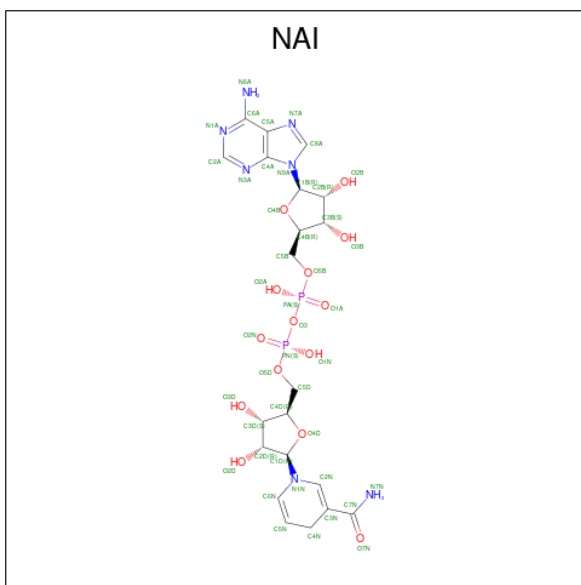
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



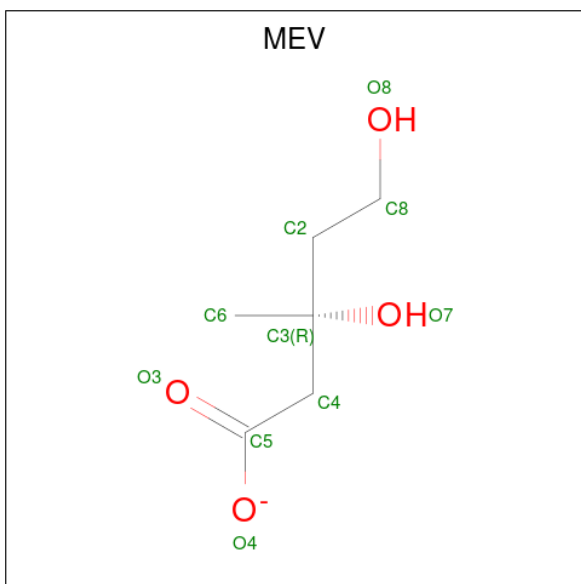
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	1
			44	21	7	14	2		

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

- Molecule 8 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
8	B	1	Total	C	O	0	0
			10	6	4		

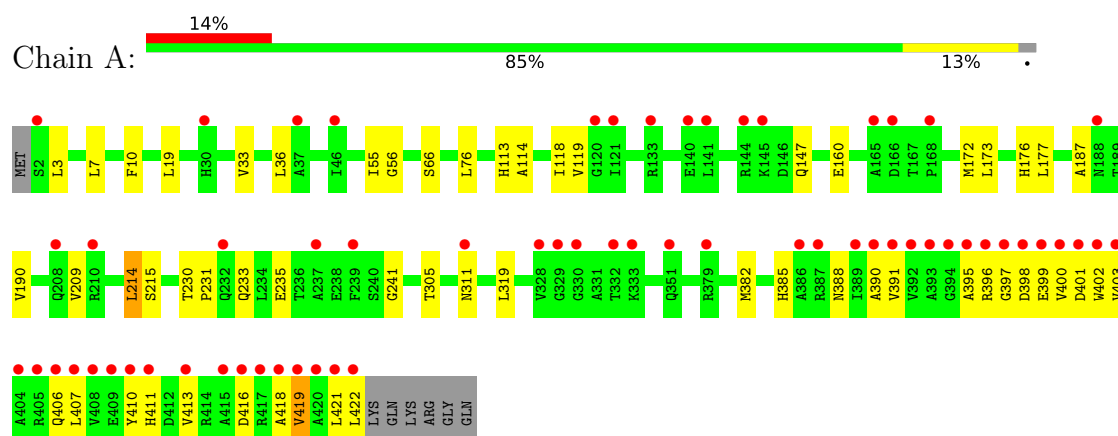
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	227	Total 227	O 227	0	0
9	B	202	Total 202	O 202	0	0

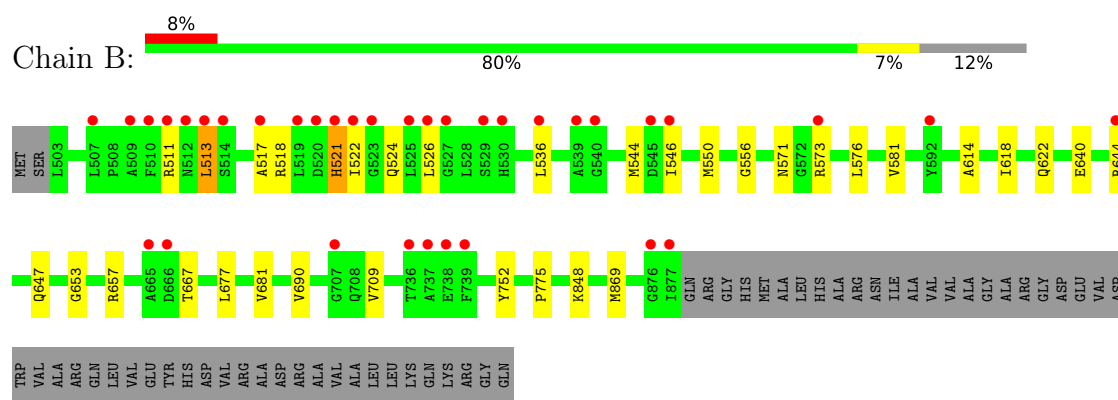
3 Residue-property plots

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	225.99Å 225.99Å 225.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.07 48.18 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.18-2.07) 99.0 (48.18-2.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.36 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.215 , 0.248 0.220 , 0.252	Depositor DCC
R_{free} test set	2994 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6590	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: ZKE, A1AFY, SO4, NAD, COA, MEV, NAI

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	0.20	0/3200	0.35	0/4353
1	B	0.16	0/2834	0.32	0/3855
All	All	0.18	0/6034	0.34	0/8208

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 [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	3151	0	3174	39	0
1	B	2791	0	2832	23	0
2	A	58	0	0	0	0
3	A	48	0	32	1	0
4	A	10	0	0	0	0
5	A	5	0	0	0	0
6	B	44	0	25	1	0
7	B	44	0	27	0	0
8	B	10	0	11	0	0
9	A	227	0	0	3	0
9	B	202	0	0	0	0
All	All	6590	0	6101	58	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 5.

All (58) 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)
3:A:502[Y]:COA:O4B	3:A:502[Y]:COA:C1B	1.65	1.21
1:A:114:ALA:HB2	1:A:190:VAL:HB	1.72	0.71
1:A:235:GLU:HG2	1:A:241:GLY:H	1.56	0.71
1:A:395:ALA:HB1	1:A:399:GLU:HB2	1.76	0.67
1:A:416:ASP:OD2	1:B:647:GLN:N	2.26	0.65
1:A:388:ASN:ND2	9:A:603:HOH:O	2.27	0.61
1:A:187:ALA:HA	1:A:214:LEU:HD13	1.82	0.60
1:A:399:GLU:HB3	1:A:421:LEU:HD11	1.82	0.60
1:A:407:LEU:HD21	1:A:418:ALA:HB2	1.84	0.60
1:A:235:GLU:HG2	1:A:241:GLY:N	2.17	0.59
1:B:653:GLY:O	1:B:657:ARG:NH2	2.36	0.57
1:A:114:ALA:HB3	1:A:177:LEU:HB2	1.87	0.56
1:B:614:ALA:HB2	1:B:690:VAL:HB	1.89	0.55
1:B:521:HIS:O	1:B:524:GLN:N	2.39	0.54
1:A:118:ILE:HD12	1:A:173:LEU:HD22	1.90	0.54
1:A:160:GLU:HG2	1:A:176:HIS:HB2	1.90	0.54
1:B:618:ILE:HG12	1:B:709:VAL:HG22	1.90	0.54
1:A:55:ILE:HG22	1:B:518:ARG:HB3	1.91	0.53
1:A:419:VAL:HG22	1:A:422:LEU:HD13	1.91	0.53
1:B:544:MET:HE1	1:B:556:GLY:HA2	1.90	0.52
1:A:391:VAL:HG13	1:A:396:ARG:CB	2.40	0.52
1:B:752:TYR:HB2	1:B:869:MET:HE1	1.93	0.51
1:A:407:LEU:HD22	1:A:413:VAL:HA	1.93	0.51
1:A:147:GLN:NE2	9:A:611:HOH:O	2.45	0.50
1:A:390:ALA:HB3	1:A:400:VAL:HG23	1.92	0.50
1:A:118:ILE:HG12	1:A:209:VAL:HG22	1.93	0.50
1:B:518:ARG:O	1:B:522:ILE:HG12	2.11	0.50
1:A:416:ASP:OD2	1:B:647:GLN:HB2	2.12	0.50
1:B:571:ASN:HB2	1:B:573:ARG:HH12	1.77	0.49
1:B:614:ALA:HB3	1:B:677:LEU:HB2	1.95	0.48
1:B:681:VAL:O	6:B:1001[X]:NAD:H2A	2.14	0.48
1:A:311:ASN:OD1	9:A:601:HOH:O	2.19	0.47
1:A:19:LEU:HG	1:A:33:VAL:HG23	1.96	0.47
1:A:36:LEU:HD22	1:B:556:GLY:HA3	1.97	0.47
1:A:230:THR:HG1	1:A:233:GLN:HG3	1.80	0.47
1:A:385:HIS:CE1	1:A:388:ASN:HD22	2.33	0.47
1:A:3:LEU:HD21	1:A:76:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:GLU:O	1:B:644:ARG:HG3	2.15	0.46
1:A:231:PRO:O	1:A:241:GLY:HA3	2.15	0.46
1:A:56:GLY:HA3	1:B:536:LEU:HD22	1.97	0.46
1:A:7:LEU:HD12	1:A:66:SER:HB3	1.98	0.45
1:A:400:VAL:HG22	1:A:401:ASP:H	1.82	0.45
1:A:7:LEU:HB3	1:A:10:PHE:HB2	1.99	0.45
1:A:410:TYR:O	1:A:411:HIS:C	2.60	0.44
1:A:119:VAL:HG12	1:A:172:MET:HG2	1.98	0.44
1:B:513:LEU:HG	1:B:517:ALA:HB3	1.99	0.44
1:B:511:ARG:O	1:B:518:ARG:NH2	2.38	0.43
1:B:546:ILE:O	1:B:550:MET:HG3	2.18	0.43
1:A:382:MET:HB3	1:A:413:VAL:HB	2.00	0.43
1:B:848:LYS:HA	1:B:848:LYS:HD2	1.94	0.42
1:A:403:VAL:HA	1:A:406:GLN:HG2	2.02	0.42
1:B:526:LEU:HD11	1:B:576:LEU:HD12	2.01	0.42
1:A:305:THR:HG22	1:A:319:LEU:HB2	2.01	0.41
1:B:581:VAL:HB	1:B:775:PRO:HG3	2.03	0.41
1:B:622:GLN:O	1:B:622:GLN:HG3	2.21	0.40
1:A:113:HIS:HB2	1:A:215:SER:HB3	2.02	0.40
1:A:397:GLY:O	1:A:400:VAL:HG12	2.21	0.40
1:A:400:VAL:C	1:A:402:TRP:H	2.30	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	422/428 (99%)	401 (95%)	21 (5%)	0	100	100
1	B	374/428 (87%)	361 (96%)	12 (3%)	1 (0%)	36	30
All	All	796/856 (93%)	762 (96%)	33 (4%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	HIS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/327 (98%)	319 (99%)	3 (1%)	70	74
1	B	288/327 (88%)	286 (99%)	2 (1%)	76	79
All	All	610/654 (93%)	605 (99%)	5 (1%)	73	77

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

Mol	Chain	Res	Type
1	A	214	LEU
1	A	398	ASP
1	A	419	VAL
1	B	513	LEU
1	B	667	THR

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	115	GLN
1	A	147	GLN
1	A	150	ASN
1	A	388	ASN
1	A	411	HIS
1	B	567	ASN
1	B	569	GLN
1	B	600	ASN
1	B	662	HIS

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 ⓘ

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$
4	A1AFY	A	503[Z]	-	8,9,9	1.72	3 (37%)	10,12,12	1.05	0
2	ZKE	A	501[X]	-	54,60,60	2.42	18 (33%)	78,90,90	2.24	17 (21%)
5	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.06	0
3	COA	A	502[Y]	-	47,50,50	3.22	19 (40%)	69,75,75	1.80	15 (21%)
8	MEV	B	1003	-	8,9,9	1.31	1 (12%)	7,12,12	1.14	0
6	NAD	B	1001[X]	-	46,48,48	4.01	21 (45%)	64,73,73	2.01	15 (23%)
7	NAI	B	1002[Y]	-	47,48,48	1.52	8 (17%)	64,73,73	1.57	12 (18%)

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
4	A1AFY	A	503[Z]	-	-	2/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZKE	A	501[X]	-	-	8/59/77/77	0/3/3/3
3	COA	A	502[Y]	-	-	6/48/64/64	0/3/3/3
8	MEV	B	1003	-	-	5/9/9/9	-
6	NAD	B	1001[X]	-	-	5/30/62/62	0/5/5/5
7	NAI	B	1002[Y]	-	-	7/29/72/72	0/5/5/5

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1001[X]	NAD	C2D-C3D	-10.45	1.25	1.53
6	B	1001[X]	NAD	C3B-C4B	-10.34	1.26	1.53
3	A	502[Y]	COA	O4B-C1B	10.22	1.65	1.42
6	B	1001[X]	NAD	C2B-C1B	-8.25	1.27	1.53
6	B	1001[X]	NAD	C7N-N7N	8.13	1.47	1.33
3	A	502[Y]	COA	P2A-O3A	7.33	1.67	1.59
6	B	1001[X]	NAD	O4D-C1D	7.32	1.50	1.40
3	A	502[Y]	COA	P1A-O3A	7.30	1.67	1.59
3	A	502[Y]	COA	C9P-N8P	6.63	1.49	1.33
6	B	1001[X]	NAD	O4D-C4D	-6.47	1.30	1.45
3	A	502[Y]	COA	C5P-N4P	6.21	1.48	1.33
3	A	502[Y]	COA	O4B-C4B	-6.19	1.31	1.45
3	A	502[Y]	COA	C2B-C1B	-6.18	1.34	1.53
2	A	501[X]	ZKE	C10-N5	6.17	1.50	1.39
6	B	1001[X]	NAD	PA-O3	6.10	1.66	1.59
6	B	1001[X]	NAD	O4B-C1B	5.63	1.55	1.42
6	B	1001[X]	NAD	C6A-N6A	5.41	1.48	1.34
2	A	501[X]	ZKE	P1-O5	5.37	1.65	1.59
2	A	501[X]	ZKE	P2-O5	5.31	1.65	1.59
6	B	1001[X]	NAD	C2B-C3B	5.27	1.67	1.53
2	A	501[X]	ZKE	C11-N3	5.11	1.45	1.33
2	A	501[X]	ZKE	C17-N6	5.06	1.45	1.33
6	B	1001[X]	NAD	C3D-C4D	5.05	1.65	1.53
6	B	1001[X]	NAD	PN-O3	4.72	1.64	1.59
3	A	502[Y]	COA	C6A-N6A	4.63	1.46	1.34
6	B	1001[X]	NAD	O4B-C4B	4.59	1.55	1.45
2	A	501[X]	ZKE	C13-N4	4.46	1.45	1.34
2	A	501[X]	ZKE	C16-N7	-4.35	1.30	1.37
6	B	1001[X]	NAD	C3N-C7N	3.89	1.56	1.50
6	B	1001[X]	NAD	O2D-C2D	3.77	1.52	1.43
7	B	1002[Y]	NAI	PA-O3	3.63	1.63	1.59
2	A	501[X]	ZKE	C2-N7	-3.56	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[X]	ZKE	O19-C18	3.44	1.50	1.42
6	B	1001[X]	NAD	O7N-C7N	-3.40	1.17	1.24
7	B	1002[Y]	NAI	PN-O3	3.36	1.63	1.59
2	A	501[X]	ZKE	P3-O18	3.29	1.65	1.59
3	A	502[Y]	COA	O3B-C3B	-3.18	1.33	1.44
4	A	503[Z]	A1AFY	O01-C02	-3.12	1.40	1.44
3	A	502[Y]	COA	P3B-O3B	3.12	1.65	1.59
7	B	1002[Y]	NAI	PA-O5B	3.11	1.71	1.59
2	A	501[X]	ZKE	C24-C25	-3.11	1.46	1.53
7	B	1002[Y]	NAI	PN-O5D	2.98	1.71	1.59
3	A	502[Y]	COA	C5A-C4A	-2.86	1.34	1.39
2	A	501[X]	ZKE	O11-C6	-2.79	1.40	1.44
8	B	1003	MEV	O7-C3	-2.69	1.40	1.44
6	B	1001[X]	NAD	C5A-C4A	-2.66	1.34	1.39
3	A	502[Y]	COA	C5A-N7A	-2.57	1.34	1.39
4	A	503[Z]	A1AFY	C03-C02	2.44	1.55	1.52
6	B	1001[X]	NAD	O3D-C3D	2.43	1.49	1.43
7	B	1002[Y]	NAI	C8A-N9A	2.37	1.41	1.37
3	A	502[Y]	COA	OAP-CAP	-2.35	1.38	1.42
3	A	502[Y]	COA	C3B-C4B	2.31	1.58	1.52
2	A	501[X]	ZKE	C10-C2	2.31	1.43	1.39
3	A	502[Y]	COA	P2A-O6A	2.29	1.68	1.59
2	A	501[X]	ZKE	O15-C17	-2.28	1.19	1.23
6	B	1001[X]	NAD	C5B-C4B	2.24	1.58	1.51
2	A	501[X]	ZKE	P3-O14	-2.24	1.46	1.54
2	A	501[X]	ZKE	P3-O13	-2.22	1.46	1.54
6	B	1001[X]	NAD	C5A-N7A	-2.18	1.35	1.39
3	A	502[Y]	COA	O9P-C9P	-2.18	1.19	1.23
2	A	501[X]	ZKE	O9-C11	-2.18	1.18	1.23
7	B	1002[Y]	NAI	O3B-C3B	-2.17	1.37	1.43
7	B	1002[Y]	NAI	O3D-C3D	-2.16	1.37	1.43
3	A	502[Y]	COA	C8A-N9A	-2.14	1.33	1.37
3	A	502[Y]	COA	O5P-C5P	-2.12	1.19	1.23
2	A	501[X]	ZKE	C10-C13	-2.08	1.35	1.41
6	B	1001[X]	NAD	C8A-N9A	-2.06	1.34	1.37
3	A	502[Y]	COA	O2B-C2B	2.03	1.48	1.43
4	A	503[Z]	A1AFY	C04-C05	2.03	1.56	1.50
7	B	1002[Y]	NAI	O4B-C4B	-2.03	1.40	1.45

All (59) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[X]	ZKE	C2-N7-C16	13.16	119.56	105.74
2	A	501[X]	ZKE	C10-C2-N7	-6.58	98.64	105.81
3	A	502[Y]	COA	N6A-C6A-N1A	-5.94	105.16	118.38
3	A	502[Y]	COA	N3A-C2A-N1A	-5.62	120.07	128.58
6	B	1001[X]	NAD	N3A-C2A-N1A	-5.45	120.33	128.58
3	A	502[Y]	COA	C5A-C4A-N3A	-4.99	119.85	126.72
6	B	1001[X]	NAD	C4D-O4D-C1D	-4.78	105.55	109.92
6	B	1001[X]	NAD	N9A-C8A-N7A	-4.72	107.24	113.94
3	A	502[Y]	COA	C5A-C6A-N6A	4.66	134.83	123.29
6	B	1001[X]	NAD	C5A-C4A-N3A	-4.66	120.30	126.72
2	A	501[X]	ZKE	N2-C2-N7	4.63	135.04	127.17
7	B	1002[Y]	NAI	O3-PN-O2N	-4.49	97.20	110.70
6	B	1001[X]	NAD	C1B-N9A-C8A	-4.35	117.43	127.09
3	A	502[Y]	COA	N9A-C8A-N7A	-4.08	108.14	113.94
2	A	501[X]	ZKE	N2-C1-N1	-3.98	122.56	128.58
7	B	1002[Y]	NAI	O1N-PN-O3	3.95	117.94	107.27
6	B	1001[X]	NAD	N6A-C6A-N1A	-3.87	109.75	118.38
3	A	502[Y]	COA	C2A-N3A-C4A	3.40	120.14	111.83
6	B	1001[X]	NAD	C4A-N9A-C8A	3.32	109.22	105.74
6	B	1001[X]	NAD	N3A-C4A-N9A	3.22	132.65	127.17
2	A	501[X]	ZKE	C18-N7-C16	-3.22	119.95	127.09
6	B	1001[X]	NAD	C2A-N3A-C4A	3.20	119.64	111.83
7	B	1002[Y]	NAI	O2A-PA-O1A	3.19	127.27	112.44
6	B	1001[X]	NAD	C4B-O4B-C1B	-3.16	102.48	109.47
3	A	502[Y]	COA	C6P-C7P-N8P	-3.16	105.27	112.00
7	B	1002[Y]	NAI	O1N-PN-O2N	3.08	126.77	112.44
7	B	1002[Y]	NAI	O5B-PA-O1A	-3.07	96.75	108.94
3	A	502[Y]	COA	N3A-C4A-N9A	3.02	132.30	127.17
7	B	1002[Y]	NAI	O2A-PA-O3	3.02	115.43	107.27
6	B	1001[X]	NAD	C5A-N7A-C8A	3.00	108.17	103.45
6	B	1001[X]	NAD	C3B-C2B-C1B	2.95	107.04	101.46
6	B	1001[X]	NAD	C4A-N9A-C1B	2.87	133.35	126.63
3	A	502[Y]	COA	C5A-N7A-C8A	2.83	107.90	103.45
6	B	1001[X]	NAD	C5A-C6A-N6A	2.82	130.26	123.29
2	A	501[X]	ZKE	C14-C15-N6	-2.80	106.03	112.00
2	A	501[X]	ZKE	C10-N5-C16	-2.68	99.24	103.45
7	B	1002[Y]	NAI	PA-O5B-C5B	-2.68	106.00	121.35
2	A	501[X]	ZKE	C2-N7-C18	-2.62	120.49	126.63
3	A	502[Y]	COA	C2P-C3P-N4P	-2.62	106.37	112.31
7	B	1002[Y]	NAI	C3N-C2N-N1N	-2.53	119.49	123.20
2	A	501[X]	ZKE	C25-C24-C18	2.49	105.37	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1002[Y]	NAI	O5D-PN-O2N	-2.44	99.25	108.94
2	A	501[X]	ZKE	O2-P1-O1	-2.42	101.18	112.44
2	A	501[X]	ZKE	O7-P2-O8	-2.39	101.35	112.44
6	B	1001[X]	NAD	C6N-N1N-C2N	-2.23	119.98	121.88
2	A	501[X]	ZKE	P3-O18-C25	-2.22	117.50	123.43
2	A	501[X]	ZKE	C13-C10-C2	-2.22	114.15	117.18
7	B	1002[Y]	NAI	PN-O5D-C5D	-2.21	108.71	121.35
7	B	1002[Y]	NAI	O3-PA-O1A	-2.15	104.23	110.70
3	A	502[Y]	COA	C4A-C5A-N7A	-2.15	108.12	110.58
2	A	501[X]	ZKE	N7-C16-N5	-2.15	110.89	113.94
3	A	502[Y]	COA	C4A-N9A-C8A	2.14	107.99	105.74
2	A	501[X]	ZKE	O13-P3-O18	2.14	114.18	105.85
2	A	501[X]	ZKE	O14-P3-O18	2.14	114.17	105.85
3	A	502[Y]	COA	C3B-C2B-C1B	2.11	104.54	99.89
7	B	1002[Y]	NAI	N3A-C4A-N9A	2.08	130.70	127.17
2	A	501[X]	ZKE	C5-C7-N3	-2.05	108.12	112.41
3	A	502[Y]	COA	P3B-O3B-C3B	-2.00	118.08	123.43
3	A	502[Y]	COA	C6A-C5A-C4A	2.00	119.91	117.18

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[Y]	COA	CDP-CBP-CCP-O6A
3	A	502[Y]	COA	CEP-CBP-CCP-O6A
3	A	502[Y]	COA	CAP-CBP-CCP-O6A
3	A	502[Y]	COA	S1P-C2P-C3P-N4P
4	A	503[Z]	A1AFY	O01-C02-C08-C09
6	B	1001[X]	NAD	O4D-C1D-N1N-C2N
6	B	1001[X]	NAD	O4D-C1D-N1N-C6N
6	B	1001[X]	NAD	C2D-C1D-N1N-C6N
7	B	1002[Y]	NAI	C2D-C1D-N1N-C2N
7	B	1002[Y]	NAI	C2N-C3N-C7N-O7N
8	B	1003	MEV	C3-C2-C8-O8
8	B	1003	MEV	C8-C2-C3-C4
8	B	1003	MEV	C8-C2-C3-C6
7	B	1002[Y]	NAI	C2D-C1D-N1N-C6N
7	B	1002[Y]	NAI	C2N-C3N-C7N-N7N
6	B	1001[X]	NAD	PN-O3-PA-O1A
2	A	501[X]	ZKE	C23-C20-C21-O10
4	A	503[Z]	A1AFY	C04-C02-C08-C09
2	A	501[X]	ZKE	C25-O18-P3-O13

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Mol	Chain	Res	Type	Atoms
6	B	1001[X]	NAD	C2D-C1D-N1N-C2N
7	B	1002[Y]	NAI	O4D-C1D-N1N-C2N
2	A	501[X]	ZKE	C25-O18-P3-O12
3	A	502[Y]	COA	P1A-O3A-P2A-O5A
7	B	1002[Y]	NAI	C3B-C4B-C5B-O5B
8	B	1003	MEV	C3-C4-C5-O4
2	A	501[X]	ZKE	C3-C4-C6-C12
2	A	501[X]	ZKE	C25-O18-P3-O14
3	A	502[Y]	COA	C3B-O3B-P3B-O9A
2	A	501[X]	ZKE	C22-C20-C21-O10
8	B	1003	MEV	C3-C4-C5-O3
2	A	501[X]	ZKE	C3-C4-C6-O11
2	A	501[X]	ZKE	O3-C3-C4-C6
7	B	1002[Y]	NAI	PN-O3-PA-O2A

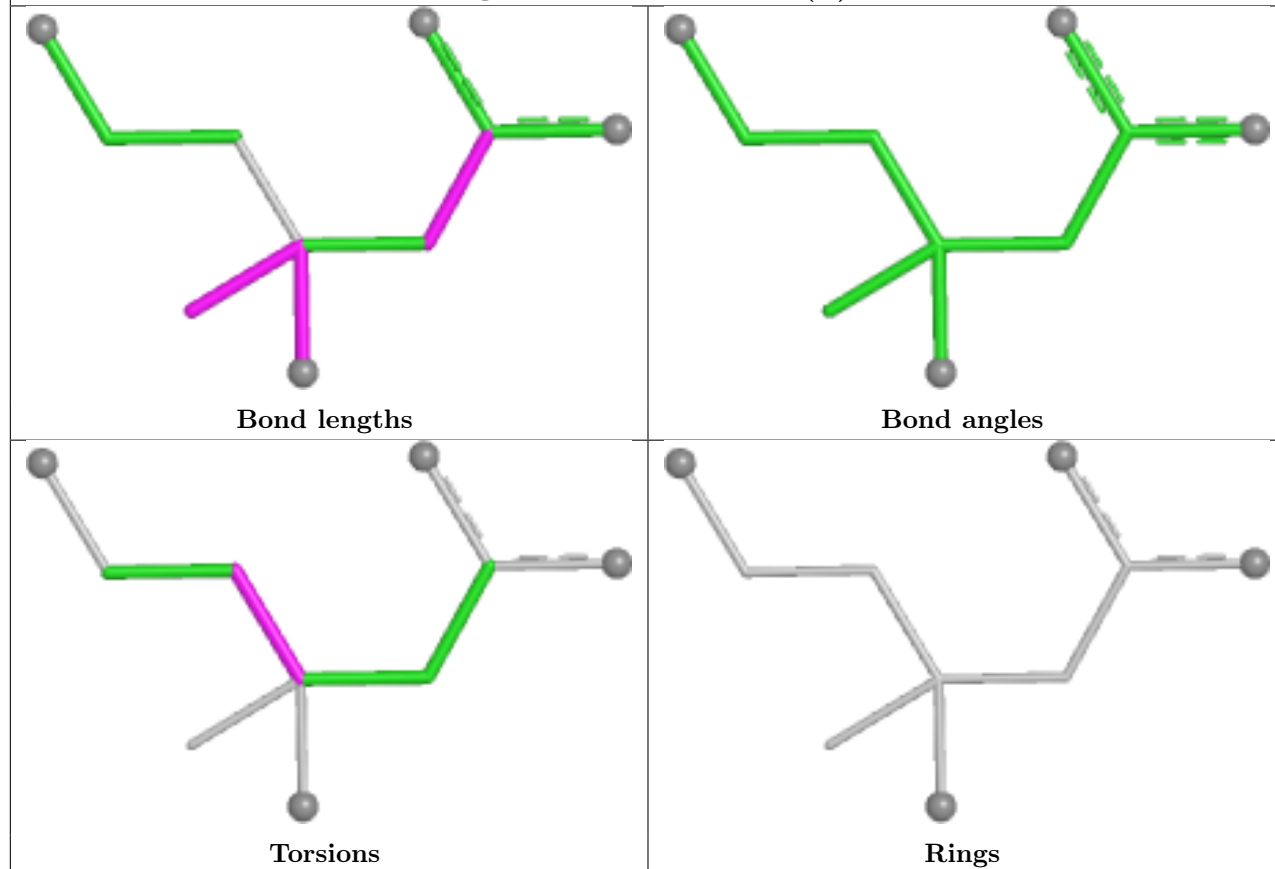
There are no ring outliers.

2 monomers are involved in 2 short contacts:

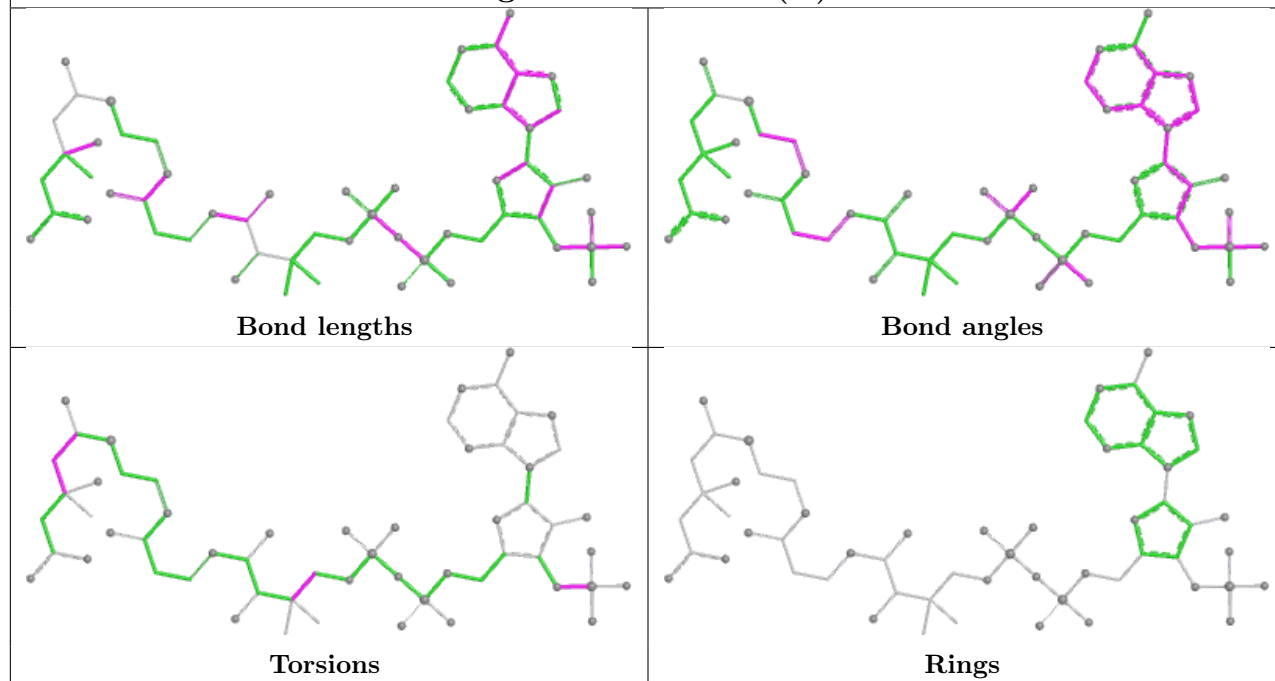
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[Y]	COA	1	0
6	B	1001[X]	NAD	1	0

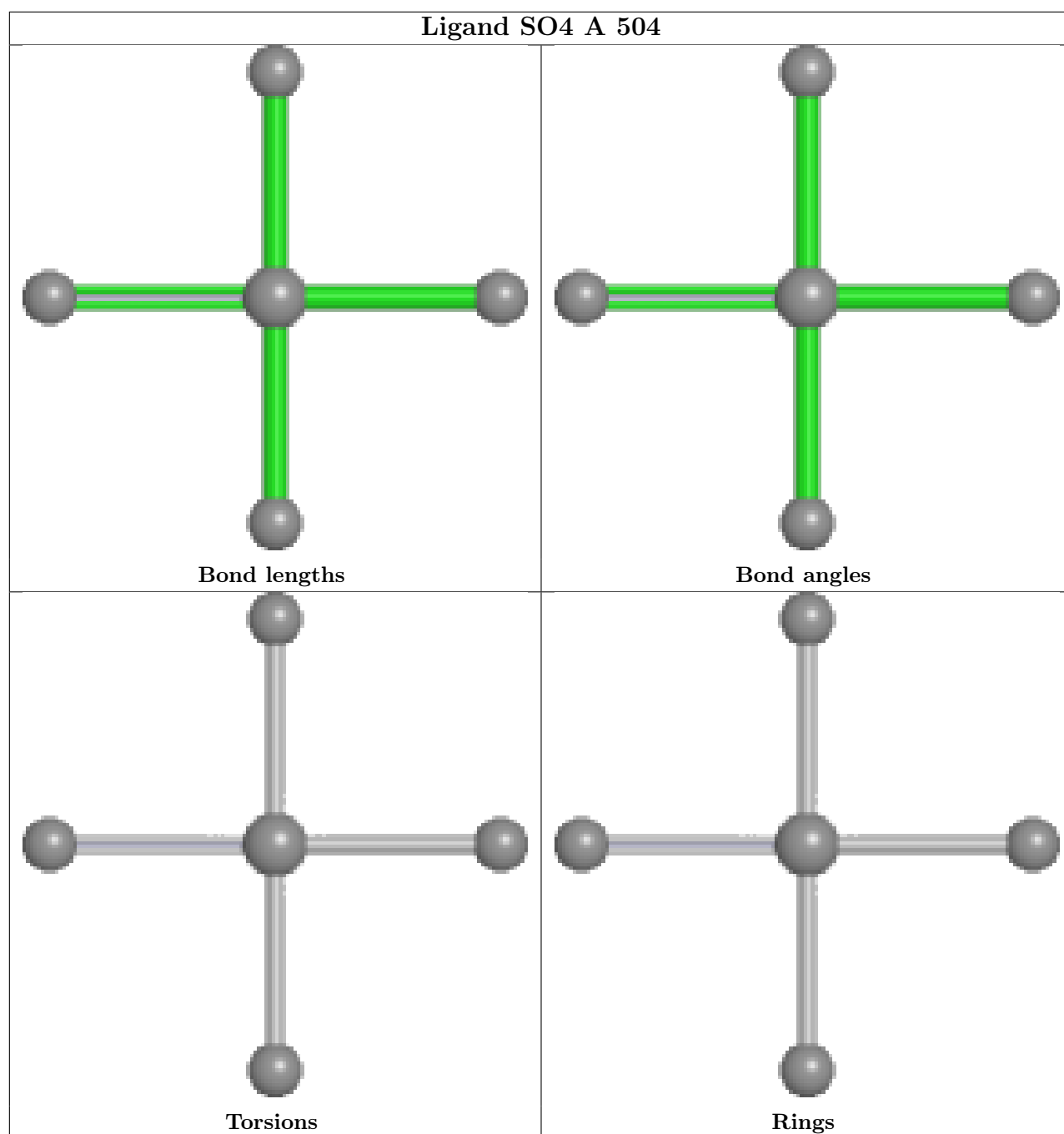
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

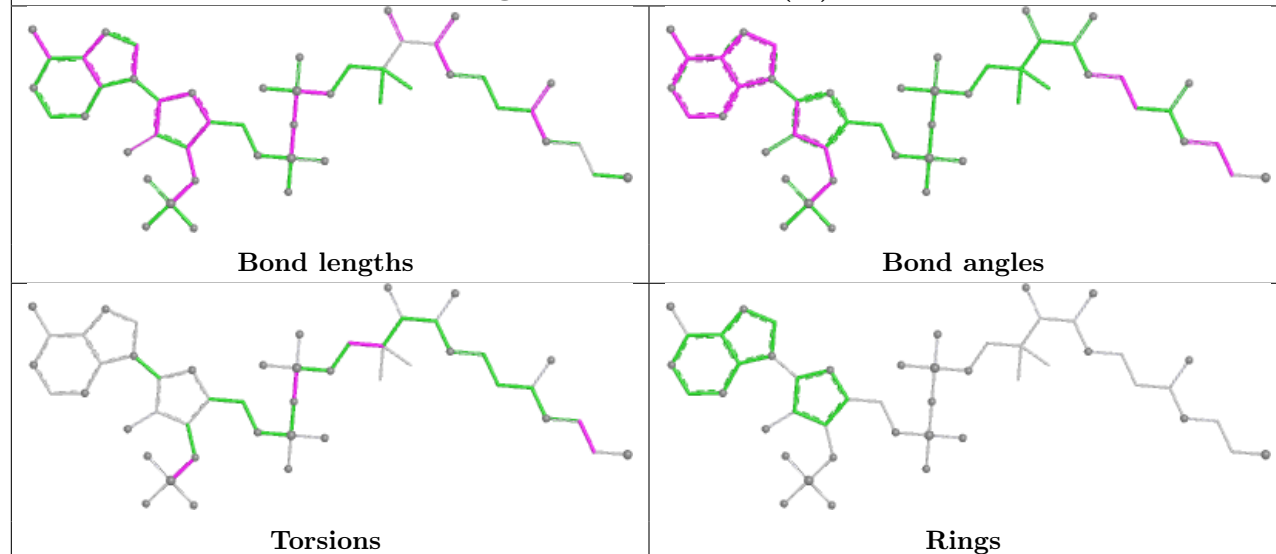


Ligand ZKE A 501 (X)

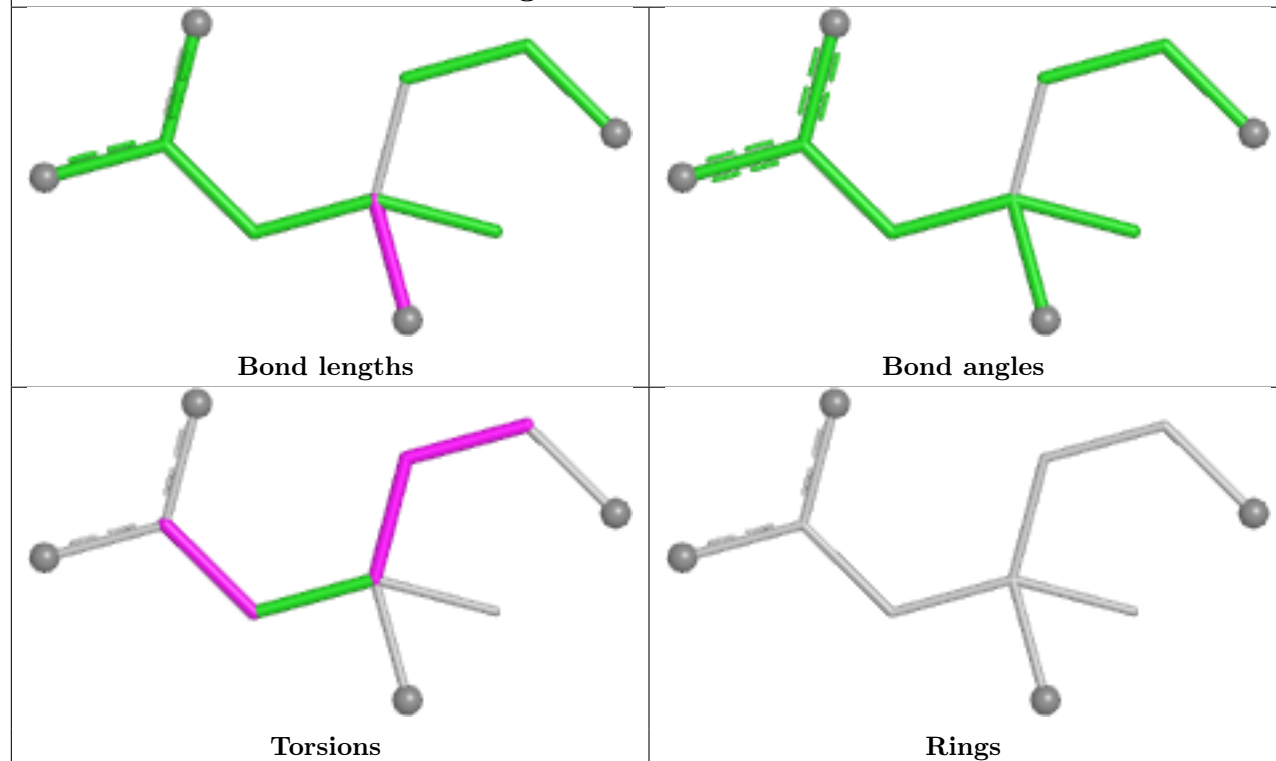


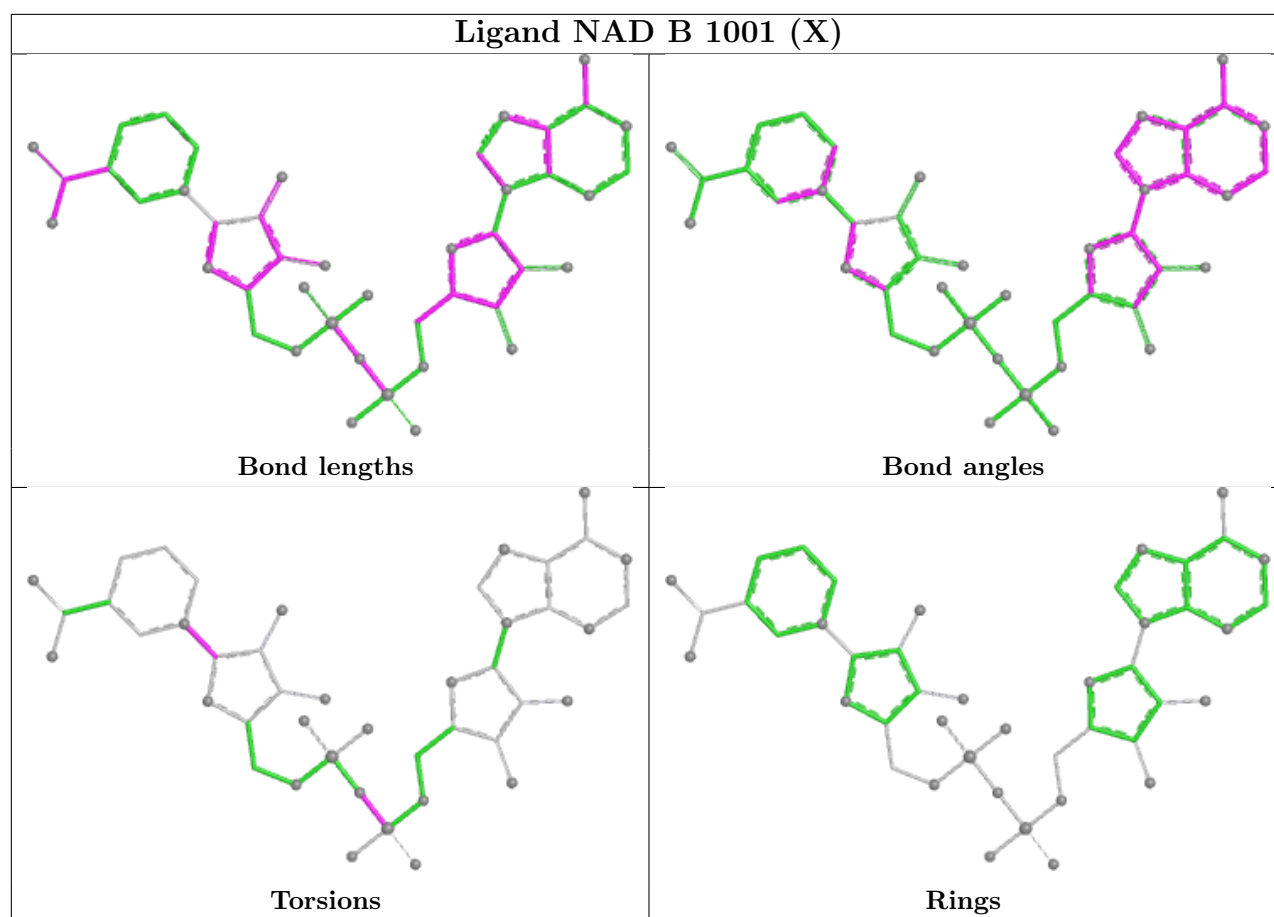


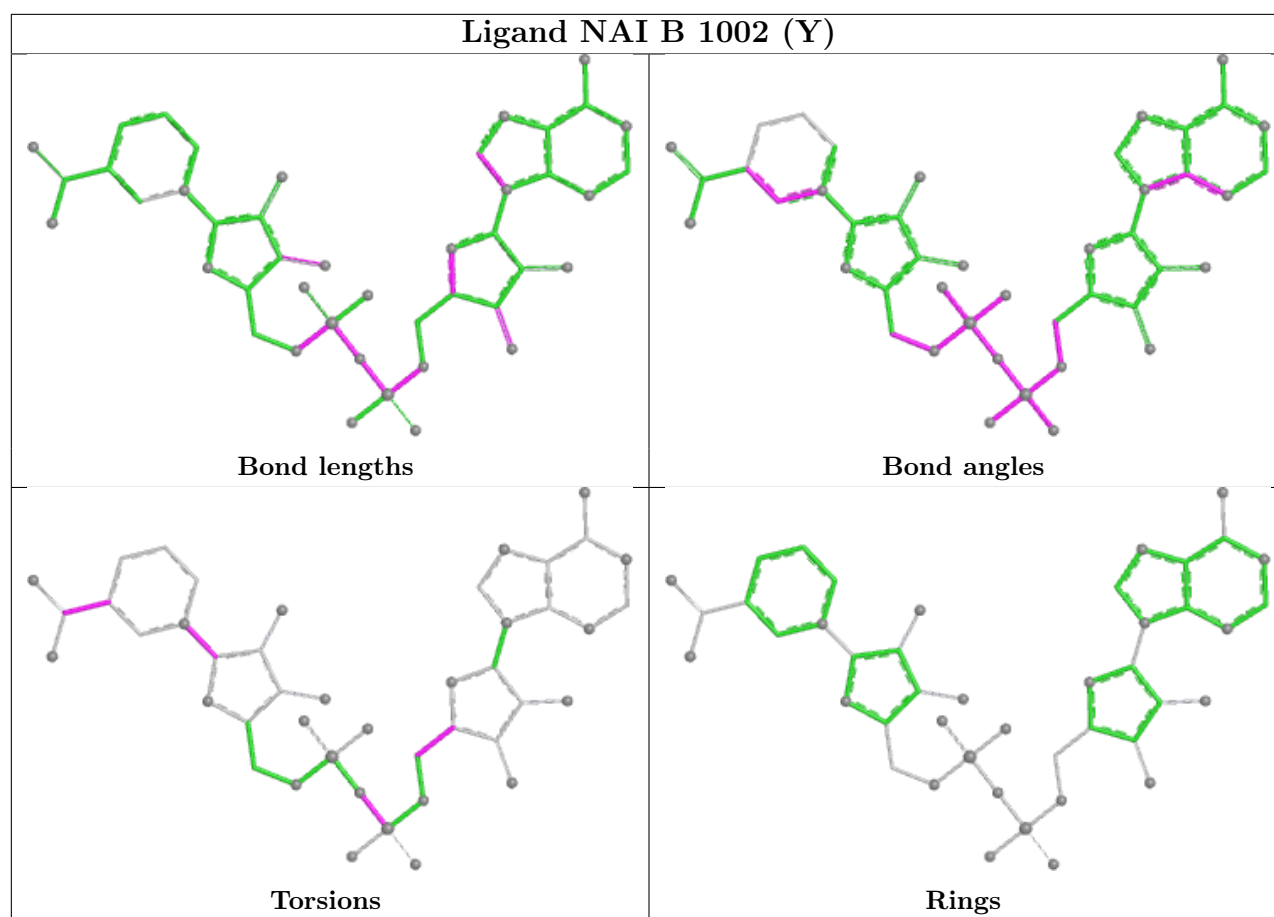
Ligand COA A 502 (Y)



Ligand MEV B 1003







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%)	0.69	62 (14%) 6 5	11, 31, 68, 110	6 (1%)
1	B	375/428 (87%)	0.47	35 (9%) 14 14	14, 30, 59, 75	3 (0%)
All	All	796/856 (92%)	0.59	97 (12%) 8 8	11, 30, 64, 110	9 (1%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	422	LEU	7.8
1	A	421	LEU	6.1
1	A	403	VAL	6.0
1	A	420	ALA	5.8
1	A	402	TRP	5.2
1	A	395	ALA	4.8
1	A	419	VAL	4.7
1	B	877	ILE	4.6
1	B	513	LEU	4.5
1	A	410	TYR	4.5
1	A	396	ARG	4.4
1	A	400	VAL	4.4
1	A	393	ALA	4.4
1	A	390	ALA	4.2
1	A	401	ASP	4.2
1	B	517	ALA	4.2
1	B	739	PHE	4.2
1	A	407	LEU	4.1
1	A	411	HIS	4.1
1	A	405	ARG	4.0
1	A	166	ASP	3.9
1	A	418	ALA	3.9
1	A	394	GLY	3.6
1	A	144	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	3.5
1	A	416	ASP	3.5
1	B	738	GLU	3.4
1	B	520	ASP	3.4
1	A	387	ARG	3.4
1	B	510	PHE	3.3
1	B	525	LEU	3.3
1	A	406	GLN	3.3
1	B	526	LEU	3.2
1	A	391	VAL	3.2
1	B	530	HIS	3.2
1	A	141	LEU	3.2
1	A	30[A]	HIS	3.1
1	A	232	GLN	3.1
1	A	417	ARG	3.1
1	A	168	PRO	3.1
1	A	145	LYS	3.1
1	A	389	ILE	3.1
1	B	573	ARG	3.0
1	A	328	VAL	3.0
1	A	188	ASN	3.0
1	A	379	ARG	3.0
1	A	404	ALA	3.0
1	A	2	SER	2.9
1	A	386	ALA	2.9
1	B	511	ARG	2.9
1	A	415	ALA	2.9
1	B	519	LEU	2.8
1	A	208	GLN	2.8
1	B	521	HIS	2.8
1	A	409	GLU	2.8
1	B	522	ILE	2.8
1	A	121	ILE	2.7
1	B	512	ASN	2.7
1	B	539	ALA	2.7
1	A	397	GLY	2.7
1	B	665	ALA	2.6
1	B	546	ILE	2.6
1	A	140	GLU	2.6
1	A	165	ALA	2.6
1	A	408	VAL	2.6
1	A	413	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	529	SER	2.6
1	B	876	GLY	2.5
1	B	736	THR	2.5
1	A	237	ALA	2.5
1	A	392	VAL	2.5
1	B	644	ARG	2.5
1	A	398	ASP	2.5
1	B	545	ASP	2.5
1	B	737	ALA	2.5
1	B	527	GLY	2.5
1	B	707	GLY	2.4
1	A	37	ALA	2.3
1	A	330	GLY	2.3
1	A	399	GLU	2.2
1	A	133	ARG	2.2
1	A	311	ASN	2.2
1	A	120	GLY	2.2
1	B	509	ALA	2.2
1	A	351	GLN	2.2
1	A	332	THR	2.2
1	B	592	TYR	2.2
1	B	523	GLY	2.1
1	A	210	ARG	2.1
1	A	46	ILE	2.1
1	B	540	GLY	2.1
1	B	514	SER	2.1
1	B	536	LEU	2.1
1	A	333	LYS	2.1
1	B	507	LEU	2.0
1	A	239	PHE	2.0
1	B	666	ASP	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

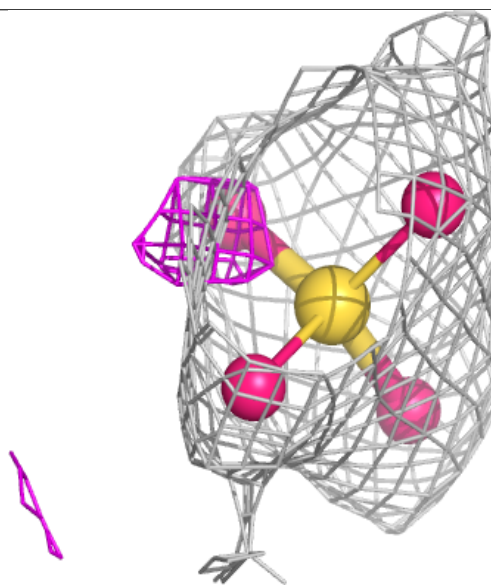
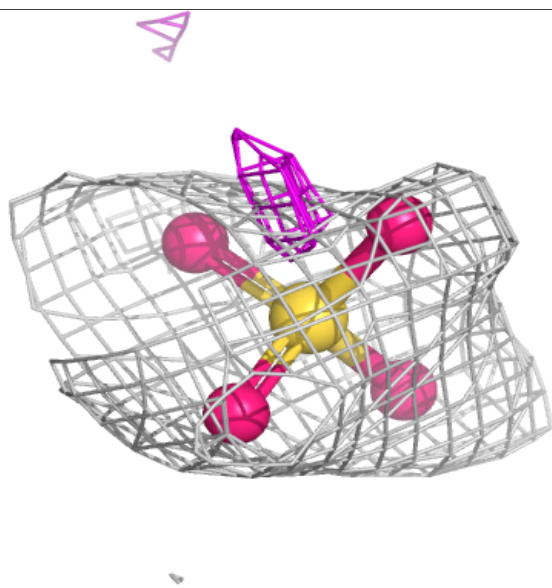
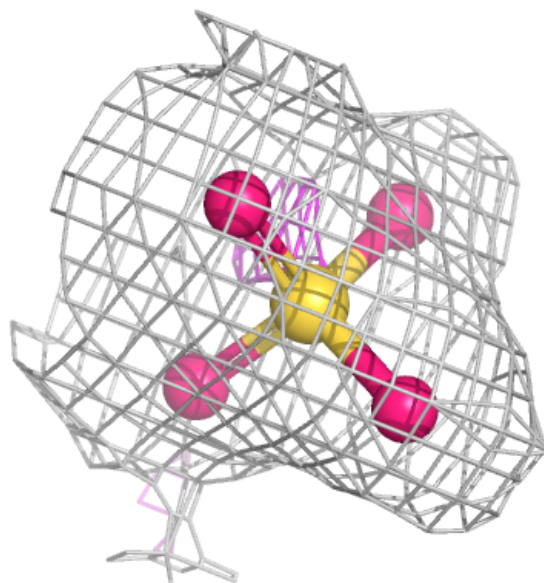
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	504	5/5	0.79	0.14	60,60,74,77	0
6	NAD	B	1001[X]	44/44	0.82	0.18	43,50,55,56	44
2	ZKE	A	501[X]	58/58	0.86	0.15	26,47,60,62	58
3	COA	A	502[Y]	48/48	0.86	0.15	31,48,59,60	48
8	MEV	B	1003	10/10	0.86	0.14	35,40,47,51	0
7	NAI	B	1002[Y]	44/44	0.93	0.09	20,26,30,31	44
4	A1AFY	A	503[Z]	10/10	0.94	0.08	19,23,25,27	10

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.

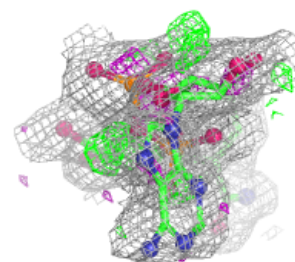
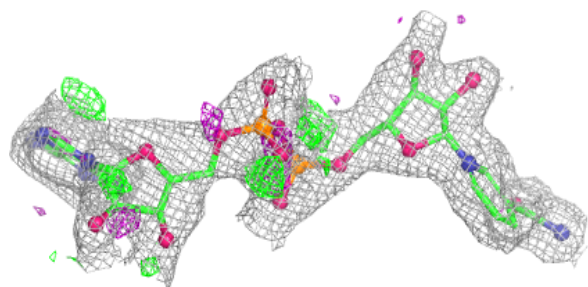
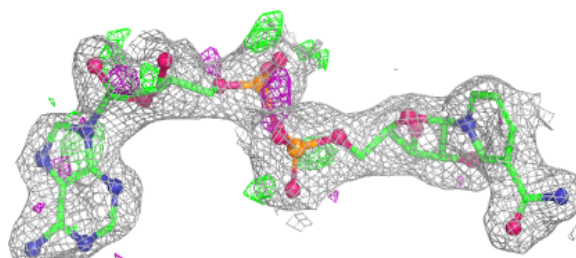
Electron density around SO4 A 504:

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

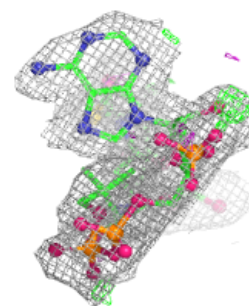
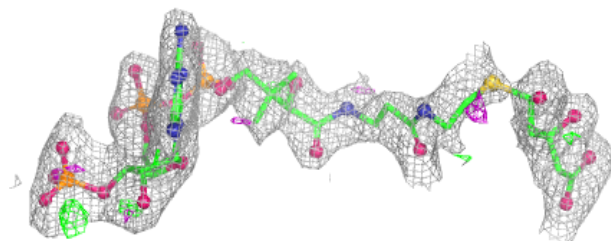
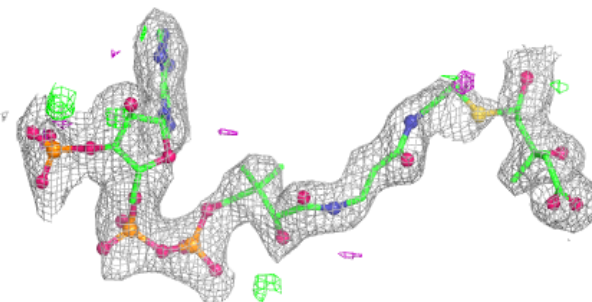


Electron density around NAD B 1001 (X):

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

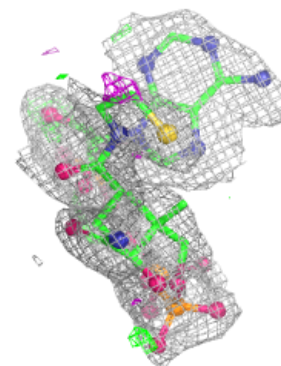
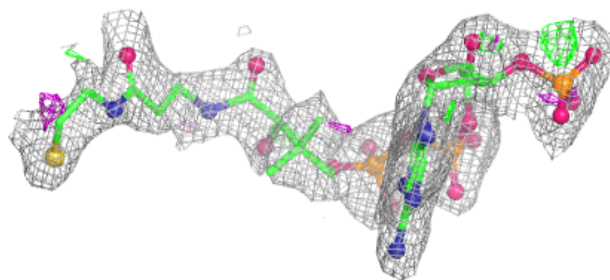
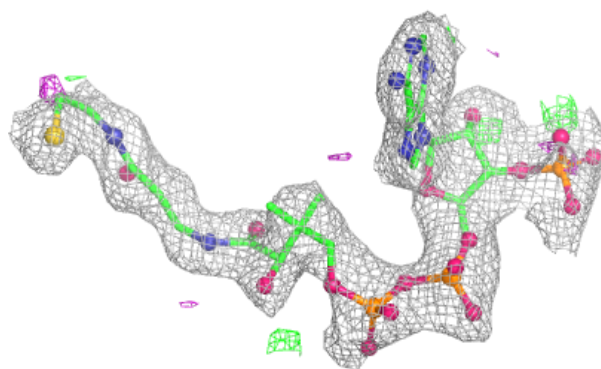
**Electron density around ZKE A 501 (X):**

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

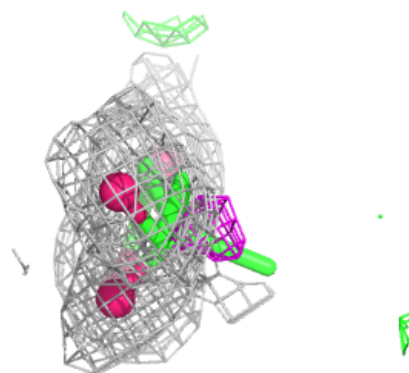
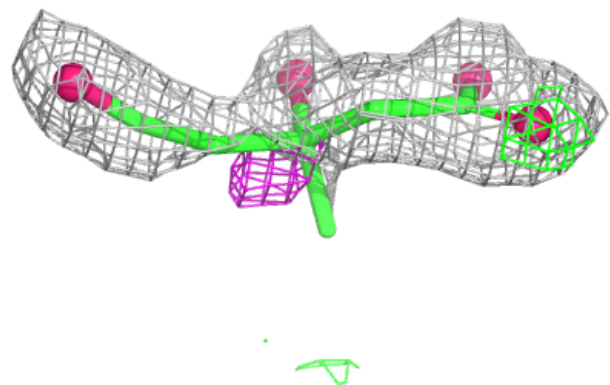
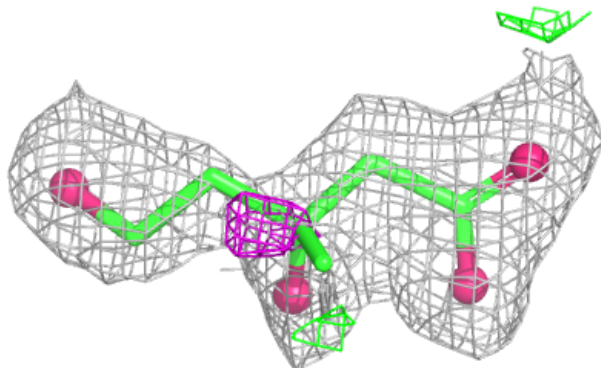


Electron density around COA A 502 (Y):

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

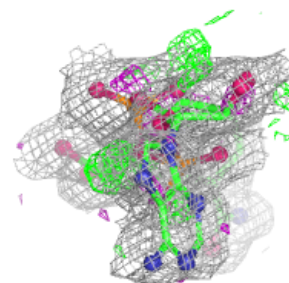
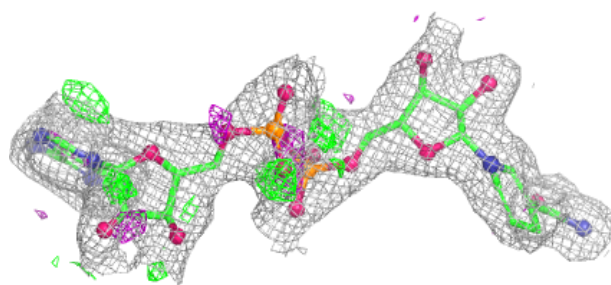
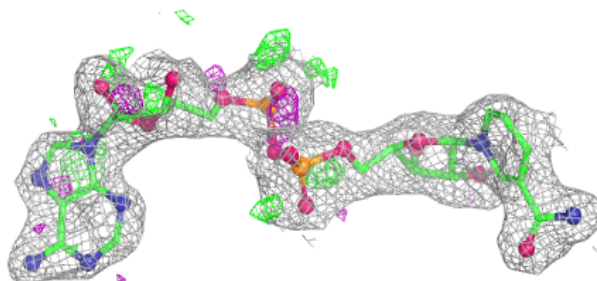
**Electron density around MEV B 1003:**

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

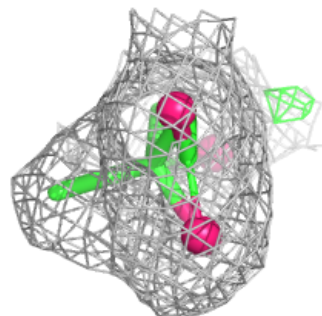
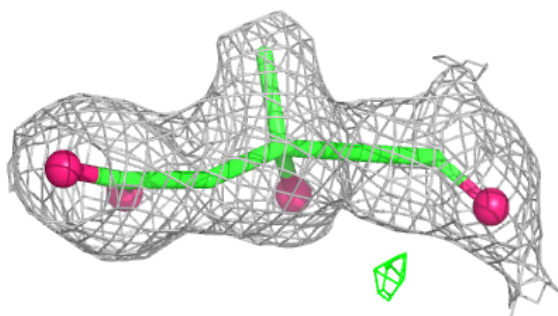
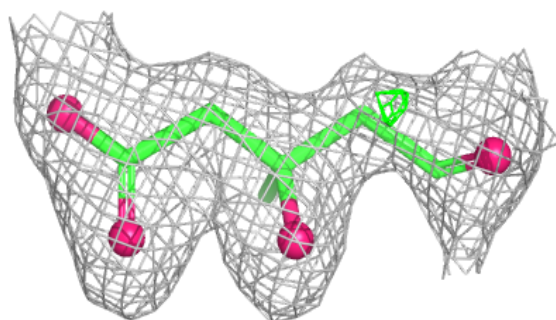


Electron density around NAI B 1002 (Y):

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

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

$2mF_o-DF_c$ (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.