



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 10:09 AM EDT

PDB ID : 9ZW9 / pdb_00009zw9
Title : Structure of the HMG-CoA reductase from *Borrelia burgdorferi* bound to CoA and Mevalonate
Authors : Paddy, I.; Dassma, L.M.K.
Deposited on : 2026-01-01
Resolution : 2.20 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

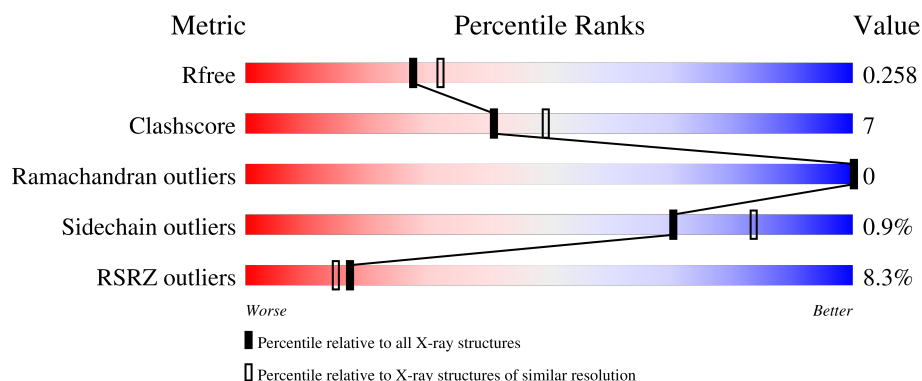
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	436	8% 78% 13% 9%
1	B	436	7% 80% 14% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6757 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.

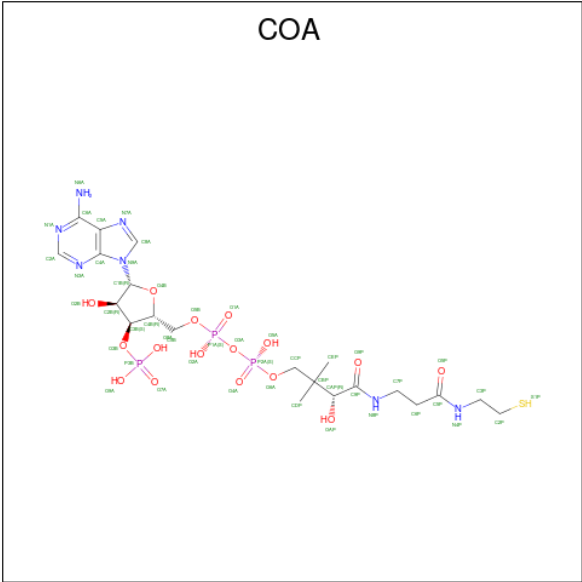
- Molecule 1 is a protein called Probable 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3142	2031	521	579	11			
1	B	412	Total	C	N	O	S	0	0	0
			3290	2129	543	605	13			

There are 10 discrepancies between the modelled and reference sequences:

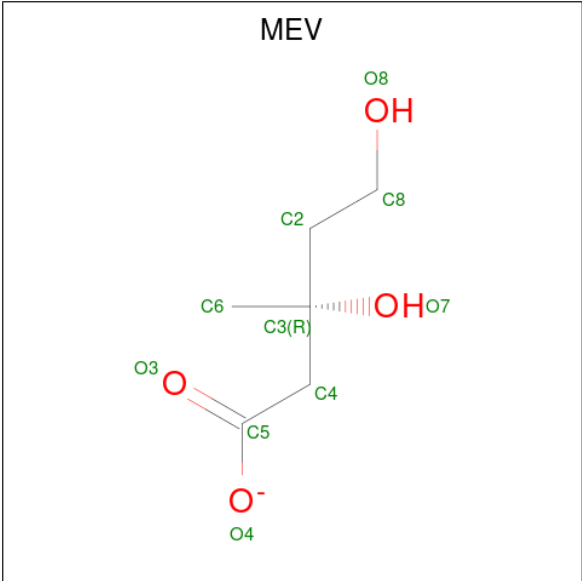
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP O51628
A	-3	HIS	-	expression tag	UNP O51628
A	-2	HIS	-	expression tag	UNP O51628
A	-1	HIS	-	expression tag	UNP O51628
A	0	HIS	-	expression tag	UNP O51628
B	-4	HIS	-	expression tag	UNP O51628
B	-3	HIS	-	expression tag	UNP O51628
B	-2	HIS	-	expression tag	UNP O51628
B	-1	HIS	-	expression tag	UNP O51628
B	0	HIS	-	expression tag	UNP O51628

- 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		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is (R)-MEVALONATE (CCD ID: MEV) (formula: C₆H₁₁O₄) (labeled as "Ligand of Interest" by depositor).



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

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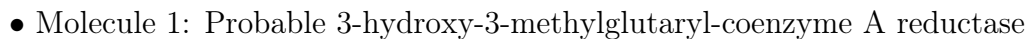
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total	O	0	0
			99	99		
4	B	110	Total	O	0	0
			110	110		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.44Å 109.17Å 139.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 2.20 24.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.89-2.20) 98.7 (24.89-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.19Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.211 , 0.257 0.211 , 0.258	Depositor DCC
R_{free} test set	1747 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6757	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEV, 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	0.22	0/3199	0.60	1/4302 (0.0%)
1	B	0.22	0/3352	0.56	1/4505 (0.0%)
All	All	0.22	0/6551	0.58	2/8807 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	395	ASP	N-CA-C	-7.80	101.81	112.03
1	B	397	GLU	N-CA-C	-6.41	105.10	114.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3142	0	3204	40	0
1	B	3290	0	3340	52	0
2	A	48	0	32	1	0
2	B	48	0	32	1	0
3	A	10	0	11	1	0
3	B	10	0	11	0	0
4	A	99	0	0	2	0
4	B	110	0	0	3	0
All	All	6757	0	6630	86	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 7.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASP:HB2	1:B:258:VAL:HG11	1.52	0.91
1:A:285:SER:HB3	1:A:318:GLN:HE21	1.46	0.80
1:A:211:ASN:O	1:A:318:GLN:NE2	2.19	0.75
1:B:380:VAL:HG21	1:B:410:ILE:HD13	1.73	0.71
1:B:10:MET:HE1	1:B:28:ILE:HG23	1.74	0.69
1:B:407:ARG:HG2	1:B:408:MET:H	1.56	0.68
1:A:47:ASP:OD2	1:B:382:LYS:NZ	2.22	0.68
1:B:391:TYR:CD2	1:B:393:ILE:HG22	2.32	0.65
1:B:398:LYS:O	1:B:402:LEU:HG	1.99	0.62
1:A:184:LEU:HB2	1:B:407:ARG:NH1	2.15	0.62
1:B:407:ARG:CG	1:B:408:MET:H	2.12	0.61
1:B:380:VAL:HG21	1:B:410:ILE:CD1	2.30	0.61
1:A:143:LEU:HD23	1:B:405:MET:HE2	1.82	0.61
1:A:77:TYR:CE2	1:A:350:ILE:HD11	2.35	0.60
1:B:213:ILE:HD13	1:B:318:GLN:HB3	1.85	0.58
1:B:387:LEU:HB2	1:B:388:LYS:HD2	1.86	0.56
1:B:7:SER:N	4:B:602:HOH:O	2.37	0.56
1:B:401:LEU:HD21	1:B:410:ILE:HG12	1.88	0.54
1:A:151:GLY:HA3	1:A:177:CYS:SG	2.47	0.54
1:B:180:MET:HA	1:B:180:MET:HE2	1.89	0.54
1:A:393:ILE:HD12	1:A:398:LYS:HG2	1.90	0.54
1:B:244:GLU:HG3	1:B:303:TYR:HA	1.89	0.53
1:B:407:ARG:HG2	1:B:408:MET:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:ND2	1:B:404:GLU:OE1	2.42	0.53
1:B:382:LYS:O	1:B:386:LEU:HG	2.09	0.52
1:B:141:GLU:O	1:B:145:THR:HG23	2.10	0.52
1:A:399:ASP:OD1	1:A:401:LEU:HG	2.09	0.52
1:A:301:LYS:NZ	4:A:602:HOH:O	2.31	0.50
1:A:220:ALA:HB3	1:A:313:ILE:HG22	1.94	0.50
3:A:502:MEV:H81	4:B:601:HOH:O	2.11	0.49
1:A:213:ILE:HD13	1:A:318:GLN:HG2	1.94	0.49
1:A:387:LEU:HB3	1:A:389:THR:HG23	1.95	0.49
1:B:237:TRP:O	1:B:241:LYS:HG2	2.13	0.49
1:A:147:MET:HG3	1:A:150:ARG:HA	1.94	0.49
1:A:246:ILE:HD12	1:A:367:ALA:HB2	1.94	0.49
1:B:180:MET:HE3	1:B:319:VAL:O	2.13	0.49
1:B:215:GLU:HG3	4:B:606:HOH:O	2.13	0.49
1:A:81:ILE:HG13	1:A:270:GLY:HA3	1.95	0.48
1:A:359:ASN:ND2	1:A:363:LEU:HD13	2.29	0.48
1:A:222:PHE:CD1	1:A:222:PHE:C	2.92	0.47
1:B:373:LYS:HB2	2:B:501:COA:O5A	2.14	0.47
1:B:407:ARG:CG	1:B:408:MET:N	2.77	0.46
1:B:339:MET:HB3	1:B:341:VAL:HG23	1.97	0.46
1:A:36:TYR:CE1	1:A:37:LYS:HG3	2.50	0.46
1:A:10:MET:HE1	1:A:28:ILE:HG23	1.97	0.46
1:A:116:GLN:HG2	1:A:171:ASN:OD1	2.15	0.46
1:B:126:SER:O	1:B:130:VAL:HG23	2.16	0.46
1:B:359:ASN:ND2	1:B:363:LEU:HD13	2.31	0.45
1:B:401:LEU:HB3	1:B:406:GLU:HG3	1.97	0.45
1:A:378:LEU:HD12	1:A:378:LEU:O	2.17	0.45
1:B:12:LEU:HB2	1:B:68:LYS:HG3	1.98	0.45
1:A:382:LYS:HD2	1:A:400:LYS:HZ2	1.82	0.45
1:B:222:PHE:C	1:B:222:PHE:CD1	2.95	0.45
1:B:227:LYS:HE2	1:B:228:HIS:NE2	2.32	0.44
1:B:401:LEU:HD21	1:B:410:ILE:CG1	2.48	0.44
1:A:146:ASN:HB3	1:B:409:ASN:CG	2.43	0.44
1:A:215:GLU:HG3	4:A:618:HOH:O	2.18	0.43
1:B:94:PHE:CZ	1:B:98:ILE:HD11	2.54	0.43
1:A:59:TYR:CD1	1:A:59:TYR:C	2.97	0.43
1:B:135:LYS:HB3	1:B:139:TRP:CZ2	2.53	0.43
1:A:67:VAL:O	1:A:78:SER:HA	2.19	0.43
1:A:94:PHE:HE2	1:A:364:ARG:NH1	2.17	0.43
1:B:17:ARG:HH12	1:B:377:ARG:NH2	2.17	0.43
1:B:387:LEU:CB	1:B:388:LYS:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:HH12	1:B:377:ARG:HH21	1.66	0.43
1:B:211:ASN:HB3	1:B:318:GLN:HE22	1.84	0.43
2:A:501:COA:O5B	2:A:501:COA:H8A	2.19	0.43
1:B:180:MET:HE3	1:B:319:VAL:C	2.45	0.42
1:B:377:ARG:HA	1:B:377:ARG:HD3	1.88	0.42
1:A:213:ILE:CD1	1:A:318:GLN:HG2	2.50	0.42
1:A:63:PRO:HG2	1:A:83:THR:O	2.20	0.41
1:A:212:ASP:HB2	1:B:258:VAL:CG1	2.37	0.41
1:A:225:ASP:HB3	1:A:228:HIS:ND1	2.36	0.41
1:A:393:ILE:O	1:A:395:ASP:N	2.45	0.41
1:B:220:ALA:HB3	1:B:313:ILE:HG22	2.03	0.41
1:A:184:LEU:HB2	1:B:407:ARG:HH12	1.83	0.41
1:A:29:LYS:O	1:A:33:GLU:N	2.54	0.41
1:A:319:VAL:O	1:A:344:LYS:HD2	2.21	0.41
1:B:116:GLN:HG2	1:B:171:ASN:OD1	2.21	0.41
1:B:213:ILE:CD1	1:B:318:GLN:HB3	2.48	0.41
1:B:77:TYR:CE2	1:B:350:ILE:HG13	2.56	0.41
1:B:19:LYS:HB3	1:B:23:GLU:HB2	2.03	0.40
1:A:393:ILE:C	1:A:395:ASP:N	2.80	0.40
1:B:81:ILE:HG13	1:B:270:GLY:HA3	2.03	0.40
1:B:221:ARG:HA	1:B:311:GLY:O	2.21	0.40
1:A:400:LYS:O	1:A:400:LYS:HG2	2.21	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	393/436 (90%)	370 (94%)	23 (6%)	0	100	100
1	B	410/436 (94%)	392 (96%)	18 (4%)	0	100	100
All	All	803/872 (92%)	762 (95%)	41 (5%)	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	343/383 (90%)	341 (99%)	2 (1%)	78	89
1	B	359/383 (94%)	355 (99%)	4 (1%)	65	79
All	All	702/766 (92%)	696 (99%)	6 (1%)	70	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	207	LYS
1	B	350	ILE
1	B	380	VAL
1	B	390	LYS
1	B	397	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	318	GLN
1	A	342	ASN
1	A	372	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](#)

4 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	502	-	8,9,9	0.88	0	7,12,12	0.82	0
2	COA	A	501	-	47,50,50	0.51	0	69,75,75	0.89	3 (4%)
3	MEV	A	502	-	8,9,9	0.87	0	7,12,12	0.90	0
2	COA	B	501	-	47,50,50	0.53	0	69,75,75	0.72	1 (1%)

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	502	-	-	3/9/9/9	-
2	COA	A	501	-	-	10/48/64/64	0/3/3/3
3	MEV	A	502	-	-	2/9/9/9	-
2	COA	B	501	-	-	11/48/64/64	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	COA	P3B-O3B-C3B	-4.37	111.75	123.43
2	B	501	COA	P3B-O3B-C3B	-3.30	114.62	123.43
2	A	501	COA	OAP-CAP-CBP	-2.19	105.10	110.18
2	A	501	COA	O3A-P1A-O1A	-2.17	104.16	110.70

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	COA	OAP-CAP-CBP-CCP
2	A	501	COA	C9P-CAP-CBP-CCP
2	A	501	COA	OAP-CAP-CBP-CDP
2	A	501	COA	C9P-CAP-CBP-CDP
2	A	501	COA	C5P-C6P-C7P-N8P
2	B	501	COA	CCP-O6A-P2A-O3A
2	B	501	COA	CCP-O6A-P2A-O5A
2	B	501	COA	CDP-CBP-CCP-O6A
2	B	501	COA	CEP-CBP-CCP-O6A
2	B	501	COA	CAP-CBP-CCP-O6A
2	B	501	COA	C9P-CAP-CBP-CCP
2	B	501	COA	C5P-C6P-C7P-N8P
3	A	502	MEV	C8-C2-C3-C4
3	B	502	MEV	C8-C2-C3-O7
3	B	502	MEV	C8-C2-C3-C4
3	B	502	MEV	C8-C2-C3-C6
2	A	501	COA	C6P-C7P-N8P-C9P
2	A	501	COA	OAP-CAP-CBP-CEP
2	B	501	COA	P1A-O3A-P2A-O6A
2	B	501	COA	C9P-CAP-CBP-CDP
2	B	501	COA	S1P-C2P-C3P-N4P
3	A	502	MEV	C8-C2-C3-C6
2	A	501	COA	C9P-CAP-CBP-CEP
2	A	501	COA	P1A-O3A-P2A-O4A
2	B	501	COA	N8P-C9P-CAP-OAP
2	A	501	COA	P1A-O3A-P2A-O5A

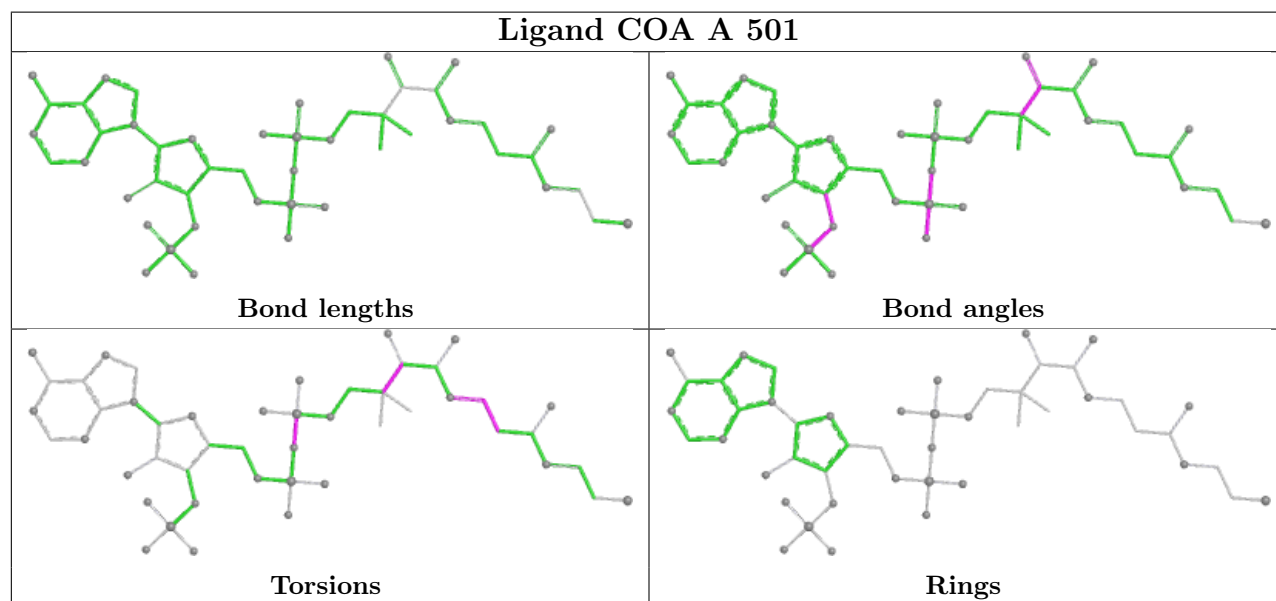
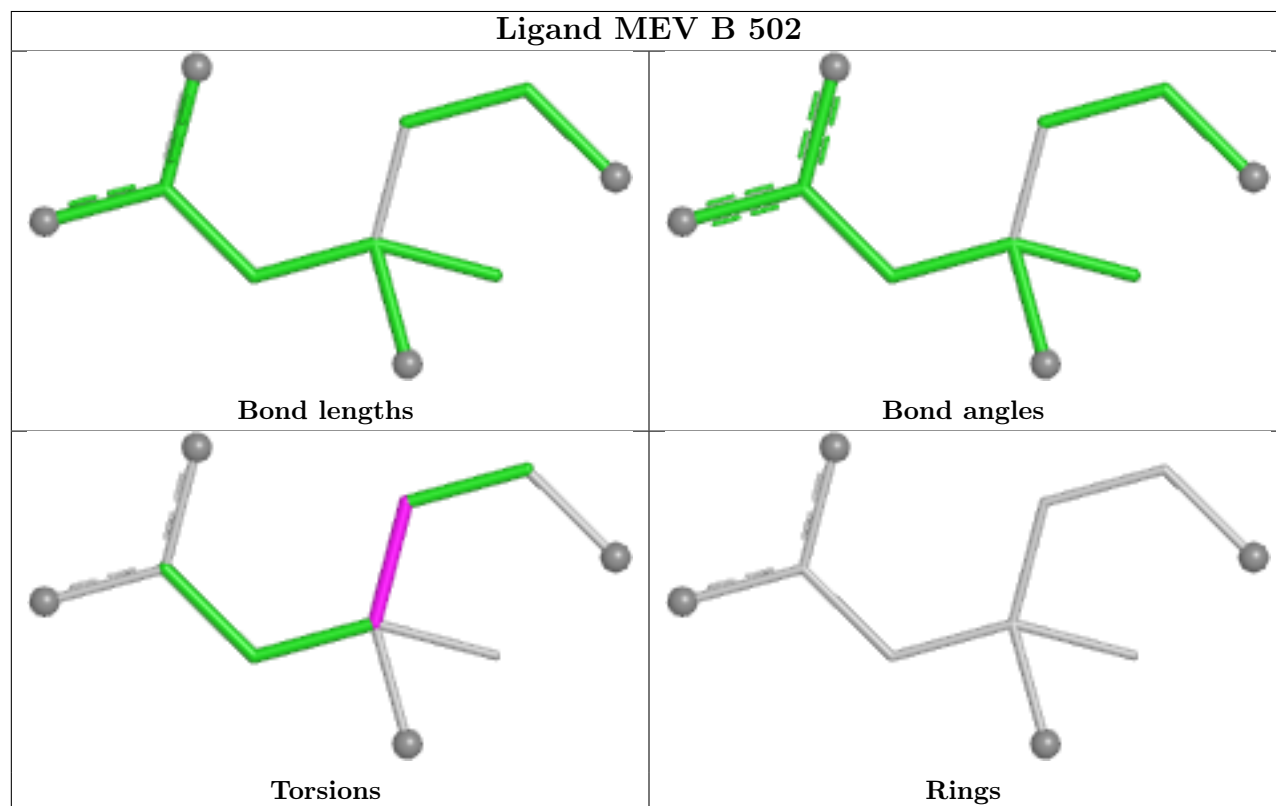
There are no ring outliers.

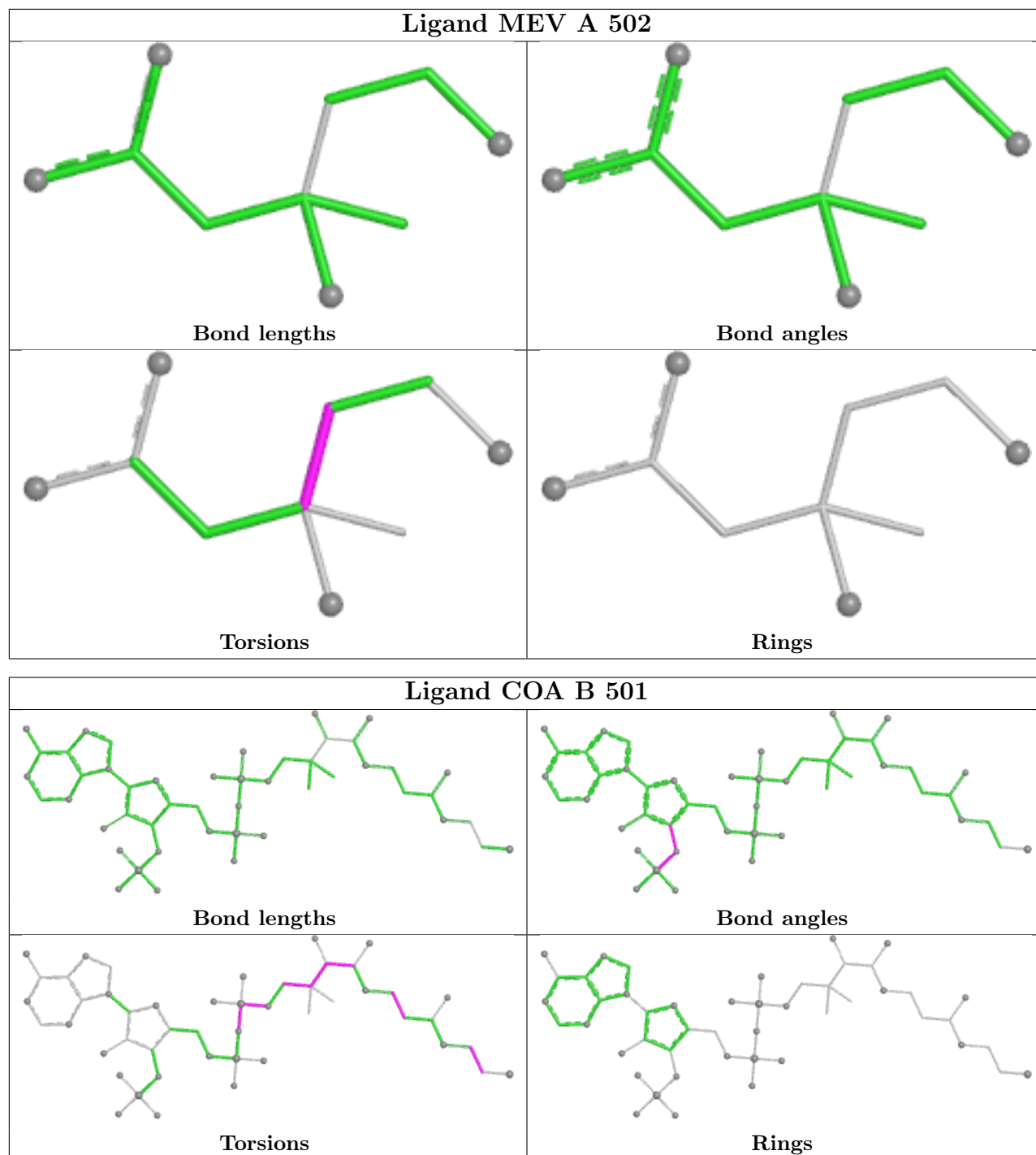
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	COA	1	0
3	A	502	MEV	1	0
2	B	501	COA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	395/436 (90%)	0.29	35 (8%) 15 13	27, 44, 92, 123	0
1	B	412/436 (94%)	0.28	32 (7%) 19 16	28, 43, 68, 109	0
All	All	807/872 (92%)	0.29	67 (8%) 17 15	27, 44, 77, 123	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	TYR	7.5
1	B	410	ILE	6.7
1	A	393	ILE	5.2
1	B	396	PHE	5.1
1	A	378	LEU	5.0
1	A	380	VAL	4.4
1	A	387	LEU	4.3
1	B	417	PHE	4.2
1	B	391	TYR	4.2
1	B	405	MET	4.0
1	A	401	LEU	4.0
1	B	411	TYR	4.0
1	B	407	ARG	3.9
1	B	371	ILE	3.7
1	B	408	MET	3.6
1	A	392	ASN	3.6
1	B	415	PHE	3.6
1	B	149	GLN	3.5
1	B	377	ARG	3.4
1	A	385	HIS	3.4
1	A	384	LEU	3.4
1	B	397	GLU	3.4
1	A	386	LEU	3.3
1	A	381	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	402	LEU	3.2
1	B	413	PHE	3.2
1	A	395	ASP	3.2
1	B	379	HIS	3.2
1	A	379	HIS	3.0
1	B	150	ARG	3.0
1	A	383	ILE	2.9
1	B	143	LEU	2.8
1	A	148	ASN	2.8
1	A	396	PHE	2.8
1	A	389	THR	2.8
1	A	231	PRO	2.8
1	B	145	THR	2.7
1	B	146	ASN	2.7
1	B	370	GLY	2.7
1	A	390	LYS	2.7
1	B	398	LYS	2.7
1	B	404	GLU	2.7
1	A	398	LYS	2.7
1	A	36	TYR	2.6
1	A	399	ASP	2.6
1	B	401	LEU	2.5
1	A	376	MET	2.5
1	A	388	LYS	2.4
1	B	144	LEU	2.4
1	B	380	VAL	2.3
1	A	403	LEU	2.3
1	B	389	THR	2.3
1	A	10	MET	2.2
1	A	404	GLU	2.2
1	B	373	LYS	2.2
1	B	378	LEU	2.2
1	A	31	PHE	2.2
1	A	369	ASN	2.2
1	B	409	ASN	2.2
1	A	128	ILE	2.1
1	A	180	MET	2.1
1	B	390	LYS	2.1
1	A	228	HIS	2.1
1	A	394	SER	2.1
1	A	400	LYS	2.1
1	B	375	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	383	ILE	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](#)

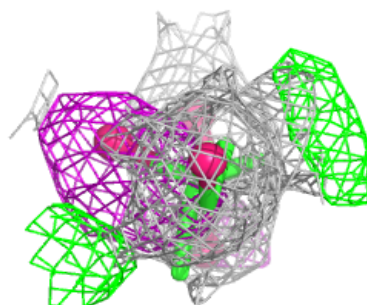
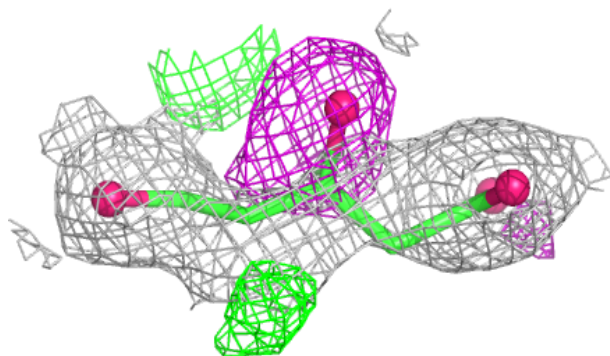
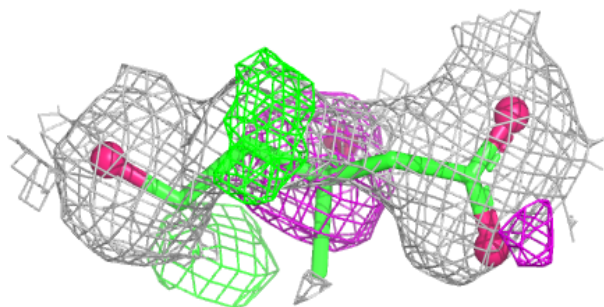
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MEV	B	502	10/10	0.68	0.18	34,47,50,50	0
3	MEV	A	502	10/10	0.78	0.14	30,37,46,58	0
2	COA	A	501	48/48	0.89	0.09	35,45,58,66	0
2	COA	B	501	48/48	0.91	0.09	35,47,64,75	0

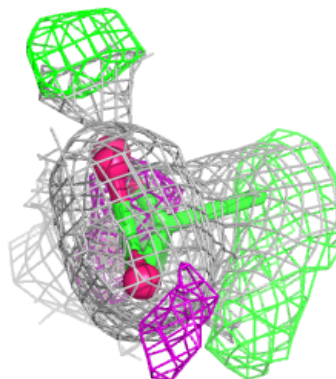
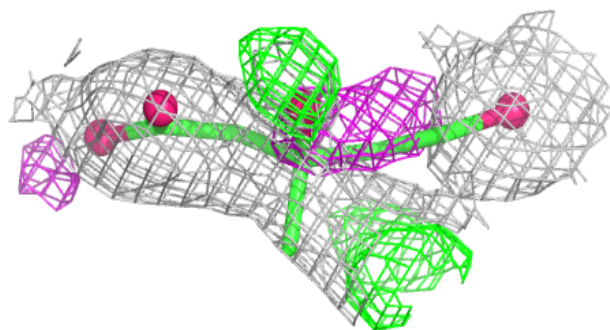
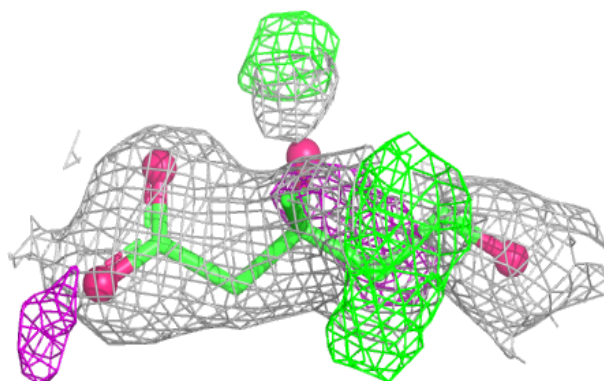
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MEV B 502:

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

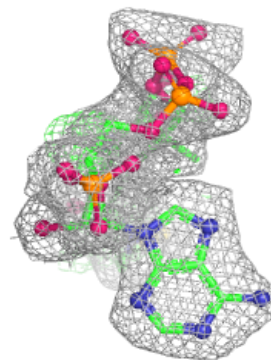
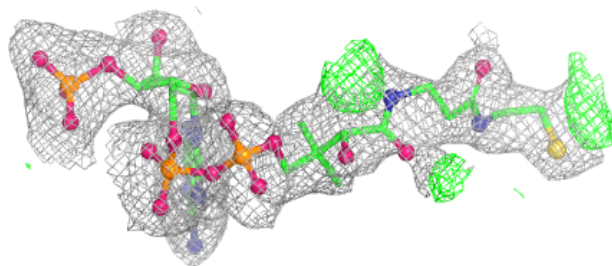
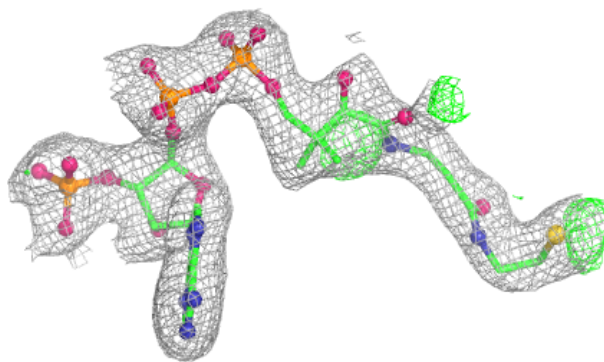
**Electron density around MEV A 502:**

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

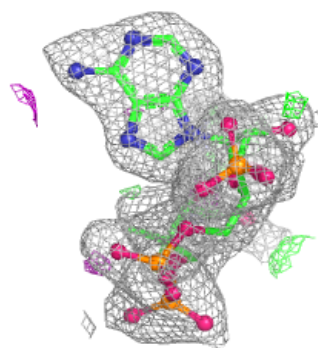
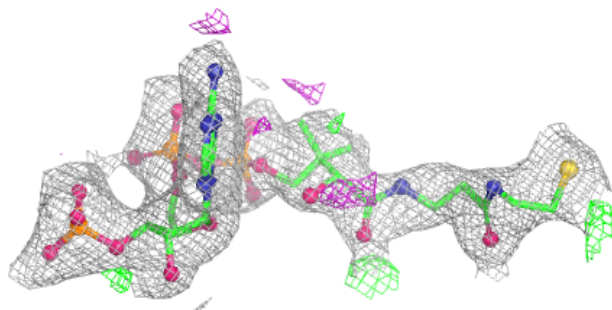
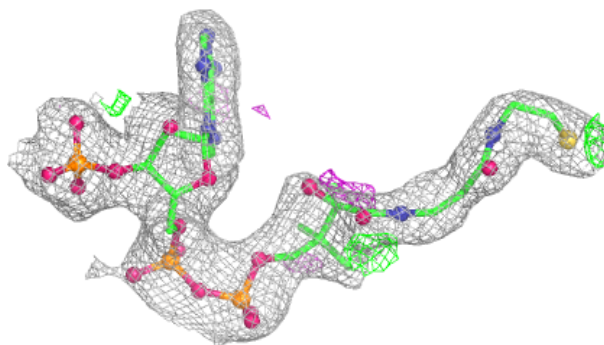


Electron density around COA A 501:

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

**Electron density around COA B 501:**

$2mF_o-DF_c$ (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.