



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 AM UTC

PDB ID : 6TGV / pdb_00006tgv
Title : Crystal structure of Mycobacterium smegmatis CoaBC in complex with CTP and FMN
Authors : Mendes, V.; Blaszczyk, M.; Bryant, O.; Cory-Wright, J.; Blundell, T.L.
Deposited on : 2019-11-18
Resolution : 2.50 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

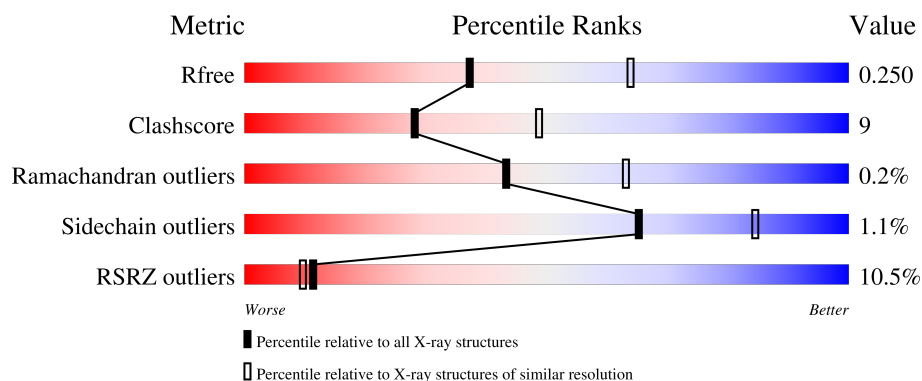
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	415	11% 77% 14% 8%
1	B	415	9% 72% 17% 10%
1	C	415	7% 80% 13% 6%
1	D	415	12% 75% 14% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CTP	A	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10828 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.

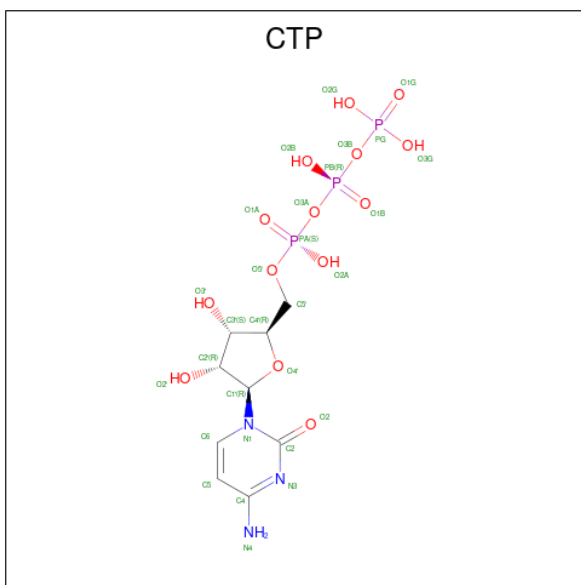
- Molecule 1 is a protein called Coenzyme A biosynthesis bifunctional protein CoaBC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2680	1673	492	506	9			
1	B	372	Total	C	N	O	S	0	0	0
			2559	1600	474	476	9			
1	C	389	Total	C	N	O	S	0	0	0
			2715	1696	498	512	9			
1	D	374	Total	C	N	O	S	0	0	0
			2576	1609	473	484	10			

There are 4 discrepancies between the modelled and reference sequences:

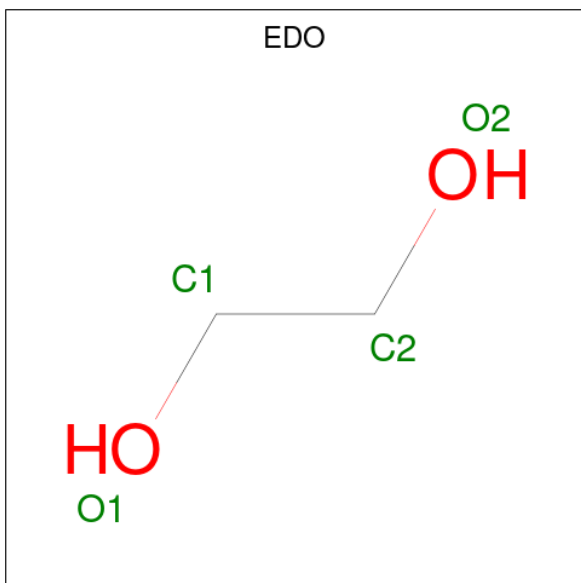
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0QWT2
B	0	SER	-	expression tag	UNP A0QWT2
C	0	SER	-	expression tag	UNP A0QWT2
D	0	SER	-	expression tag	UNP A0QWT2

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 29	C 9	N 3	O 14	P 3	0	0
2	B	1	Total 29	C 9	N 3	O 14	P 3	0	0
2	C	1	Total 29	C 9	N 3	O 14	P 3	0	0
2	D	1	Total 29	C 9	N 3	O 14	P 3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).

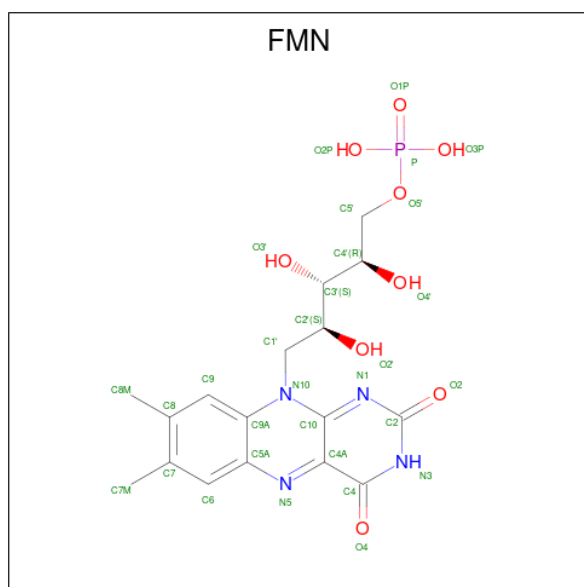


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

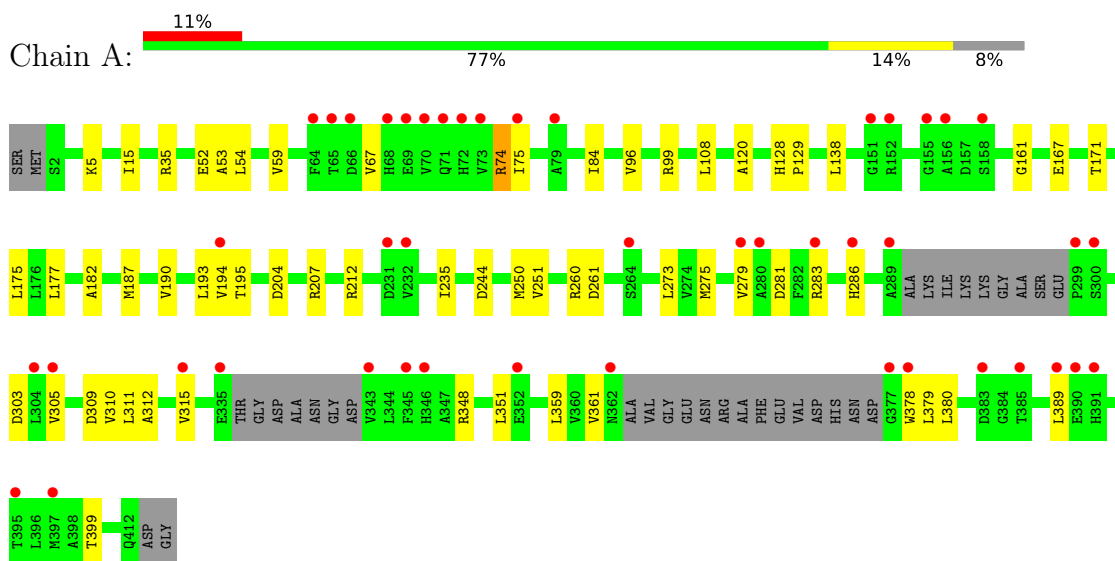
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	6	Total	O	0	0
			6	6		
6	C	5	Total	O	0	0
			5	5		
6	D	10	Total	O	0	0
			10	10		

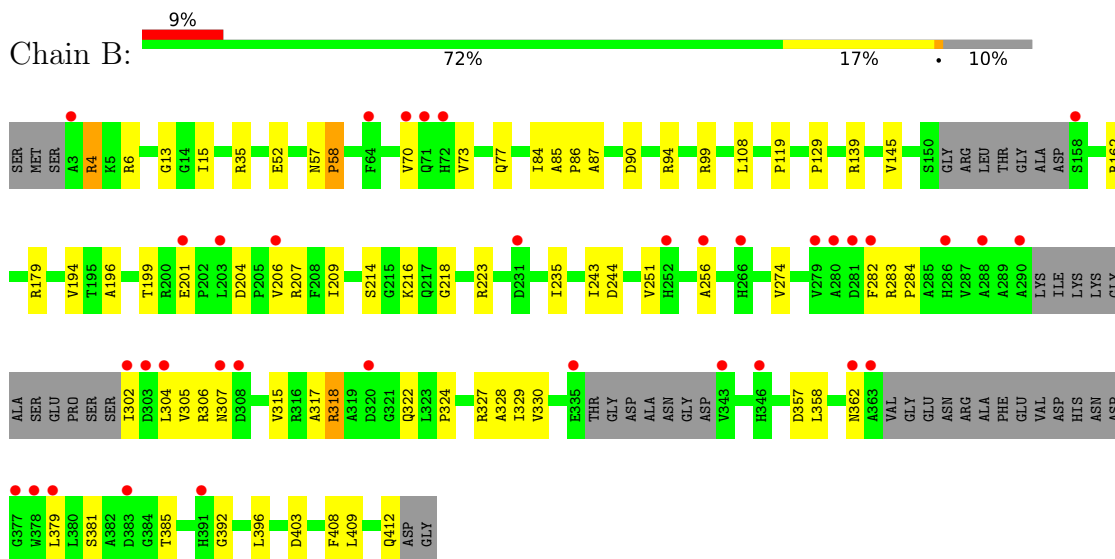
3 Residue-property plots [i](#)

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.

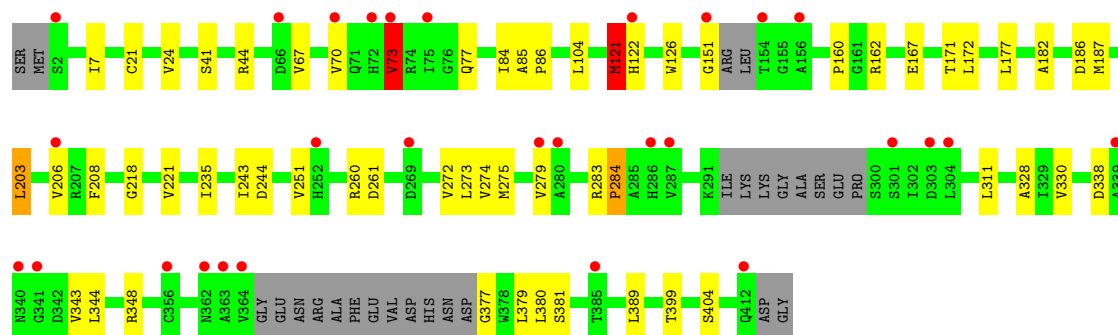
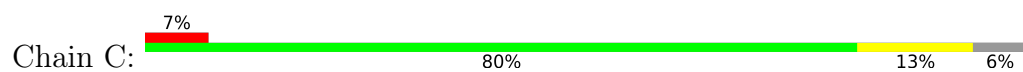
- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



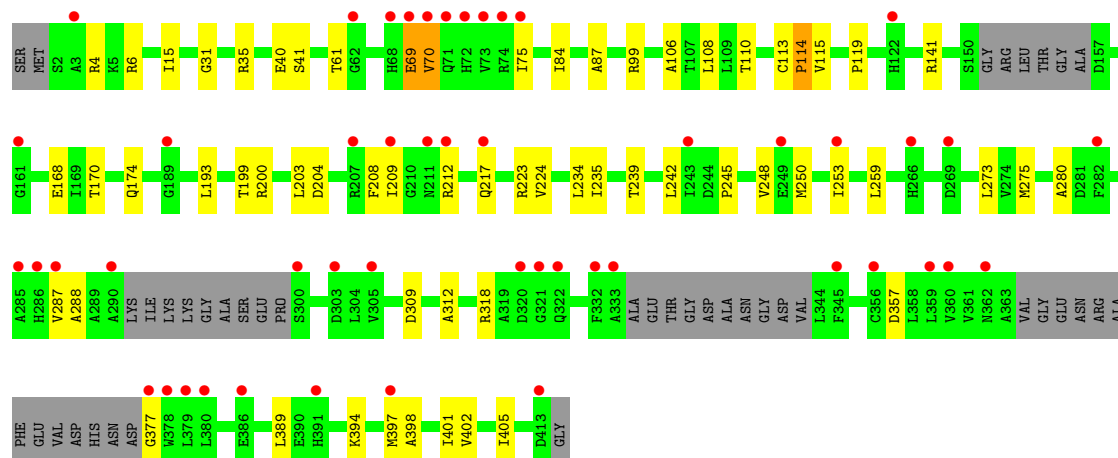
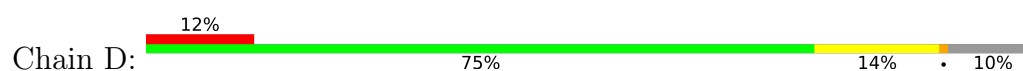
- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



• Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	195.13Å 195.13Å 373.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.67 – 2.50 62.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.67-2.50) 99.9 (62.67-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.245 0.211 , 0.250	Depositor DCC
R_{free} test set	4765 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 94.3	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	0.95	EDS
Total number of atoms	10828	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: FMN, EDO, CTP, MG

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	0.49	0/2717	0.70	2/3708 (0.1%)
1	B	0.55	1/2590 (0.0%)	0.70	3/3541 (0.1%)
1	C	0.50	2/2752 (0.1%)	0.73	2/3760 (0.1%)
1	D	0.46	2/2610 (0.1%)	0.67	1/3568 (0.0%)
All	All	0.50	5/10669 (0.0%)	0.70	8/14577 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	PRO	C-O	-7.43	1.15	1.23
1	B	58	PRO	C-O	-6.49	1.16	1.23
1	D	115	VAL	C-O	-6.25	1.17	1.24
1	C	160	PRO	C-O	-5.68	1.17	1.23
1	C	121	MET	C-O	-5.12	1.18	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	LEU	N-CA-C	-5.47	104.85	112.45
1	B	385	THR	CB-CA-C	-5.37	100.80	109.72
1	D	69	GLU	CB-CG-CD	5.34	121.69	112.60
1	C	73	VAL	N-CA-C	-5.27	107.69	112.12
1	B	317	ALA	N-CA-C	-5.24	105.98	112.38
1	B	318	ARG	N-CA-C	-5.10	105.42	110.97
1	A	281	ASP	CA-C-N	-5.04	114.15	121.76
1	A	281	ASP	C-N-CA	-5.04	114.15	121.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2680	0	2629	55	0
1	B	2559	0	2481	52	0
1	C	2715	0	2647	45	0
1	D	2576	0	2479	45	0
2	A	29	0	12	10	0
2	B	29	0	12	0	0
2	C	29	0	12	1	0
2	D	29	0	12	2	0
3	A	12	0	18	0	0
3	B	8	0	12	3	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	1	0	0	0	0
5	A	31	0	19	1	0
5	B	31	0	19	2	0
5	C	31	0	19	1	0
5	D	31	0	19	3	0
6	A	8	0	0	1	0
6	B	6	0	0	3	0
6	C	5	0	0	0	0
6	D	10	0	0	0	0
All	All	10828	0	10402	188	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 9.

All (188) 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:C:283:ARG:HG2	1:C:284:PRO:HD2	1.21	1.17
1:C:283:ARG:HG2	1:C:284:PRO:CD	1.75	1.15
1:A:279:VAL:HG21	2:A:501:CTP:C4	1.85	1.11
1:D:113:CYS:HB2	1:D:114:PRO:HD2	1.41	0.98
1:B:315:VAL:O	1:B:318:ARG:HB3	1.66	0.95
1:A:279:VAL:CG2	2:A:501:CTP:C4	2.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG21	2:A:501:CTP:N3	1.91	0.85
1:A:351:LEU:HD22	1:A:380:LEU:HD13	1.58	0.84
1:B:235:ILE:HG22	1:B:251:VAL:HB	1.59	0.83
1:B:328:ALA:HB2	1:B:409:LEU:HD21	1.64	0.80
1:A:15:ILE:HB	5:A:506:FMN:H6	1.65	0.79
1:A:379:LEU:HD23	1:A:389:LEU:HD21	1.67	0.76
1:A:279:VAL:CG2	2:A:501:CTP:C5	2.69	0.75
1:C:203:LEU:HD11	1:D:209:ILE:HD12	1.69	0.75
1:B:15:ILE:HB	5:B:504:FMN:H6	1.69	0.74
1:A:244:ASP:CG	1:A:250:MET:HE2	2.12	0.74
1:B:379:LEU:HD12	1:B:379:LEU:O	1.88	0.74
1:A:303:ASP:HA	1:B:302:ILE:HG13	1.70	0.72
1:B:379:LEU:HD12	1:B:379:LEU:C	2.14	0.72
1:C:283:ARG:CG	1:C:284:PRO:CD	2.62	0.72
1:B:204:ASP:HB3	1:B:207:ARG:H	1.55	0.70
1:B:13:GLY:N	5:B:504:FMN:O1P	2.23	0.70
1:A:279:VAL:CG2	2:A:501:CTP:C6	2.74	0.70
1:C:283:ARG:HG2	1:C:284:PRO:HD3	1.68	0.70
1:A:74:ARG:HH11	1:A:74:ARG:HG2	1.57	0.70
1:A:167:GLU:O	1:A:171:THR:HG23	1.92	0.69
1:C:338:ASP:HB3	1:C:343:VAL:HG13	1.73	0.68
1:A:279:VAL:HG21	2:A:501:CTP:C5	2.29	0.67
1:C:41:SER:O	1:C:44:ARG:HG2	1.94	0.67
1:D:203:LEU:O	1:D:287:VAL:HA	1.95	0.66
1:A:359:LEU:HB3	1:A:380:LEU:HD11	1.77	0.66
1:D:113:CYS:HB2	1:D:114:PRO:CD	2.21	0.64
1:A:74:ARG:HH11	1:A:74:ARG:CG	2.11	0.64
1:D:309:ASP:HB3	1:D:312:ALA:HB3	1.81	0.63
1:C:7:ILE:HD11	1:C:177:LEU:HD11	1.81	0.62
1:D:203:LEU:HD13	1:D:208:PHE:HA	1.81	0.62
1:A:275:MET:HG3	1:A:311:LEU:HB2	1.82	0.62
1:D:377:GLY:N	1:D:389:LEU:O	2.33	0.62
1:D:275:MET:HG3	2:D:501:CTP:O2'	2.01	0.60
1:D:204:ASP:HB3	1:D:288:ALA:HB3	1.83	0.60
1:A:244:ASP:OD1	1:A:250:MET:CE	2.48	0.60
1:B:283:ARG:O	1:B:305:VAL:N	2.32	0.60
1:A:187:MET:HE3	1:A:190:VAL:HG21	1.84	0.59
1:D:35:ARG:HD2	1:D:75:ILE:CD1	2.33	0.59
1:C:283:ARG:CG	1:C:284:PRO:HD2	2.14	0.58
1:B:99:ARG:NH1	6:B:601:HOH:O	2.37	0.58
1:B:214:SER:HB2	1:B:216:LYS:HG3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:HD2	1:D:75:ILE:HD13	1.84	0.57
1:A:204:ASP:OD1	1:A:207:ARG:N	2.32	0.57
1:D:199:THR:HG21	1:D:280:ALA:H	1.70	0.57
1:D:273:LEU:HD21	1:D:275:MET:HE2	1.87	0.57
1:C:344:LEU:HD22	1:C:380:LEU:HD21	1.87	0.56
1:D:40:GLU:OE1	1:D:61:THR:HG21	2.06	0.56
1:B:235:ILE:HA	1:B:251:VAL:O	2.07	0.55
1:C:235:ILE:HA	1:C:251:VAL:HG13	1.89	0.55
1:D:84:ILE:HD11	1:D:108:LEU:HD21	1.89	0.54
1:D:318:ARG:NH2	1:D:357:ASP:OD2	2.35	0.54
1:B:327:ARG:O	1:B:412:GLN:NE2	2.41	0.54
1:B:392:GLY:HA3	1:B:396:LEU:HD23	1.88	0.54
1:C:273:LEU:CD2	1:C:275:MET:HG2	2.38	0.54
1:A:212:ARG:HG3	1:B:206:VAL:O	2.08	0.53
1:B:90:ASP:OD1	1:D:99:ARG:HD2	2.07	0.53
1:D:41:SER:OG	5:D:503:FMN:O2P	2.25	0.53
1:B:84:ILE:HD11	1:B:108:LEU:HD21	1.91	0.53
1:A:283:ARG:N	1:A:305:VAL:O	2.41	0.52
1:C:41:SER:OG	5:C:503:FMN:O1P	2.28	0.52
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.74	0.52
1:C:273:LEU:HD21	1:C:275:MET:HG2	1.90	0.52
1:A:244:ASP:OD1	1:A:250:MET:HE2	2.08	0.52
1:D:203:LEU:CD1	1:D:203:LEU:N	2.72	0.52
1:B:139:ARG:NH1	1:B:145:VAL:O	2.41	0.52
1:A:99:ARG:NH2	6:A:601:HOH:O	2.38	0.52
1:D:217:GLN:H	1:D:217:GLN:CD	2.18	0.51
1:A:244:ASP:CG	1:A:250:MET:CE	2.83	0.51
1:C:274:VAL:HA	1:C:330:VAL:HG13	1.93	0.51
1:D:253:ILE:HD13	1:D:259:LEU:HB2	1.92	0.51
1:A:279:VAL:HG21	2:A:501:CTP:C2	2.45	0.50
1:B:73:VAL:HG12	1:B:77:GLN:CD	2.36	0.50
1:B:162:ARG:HA	3:B:503:EDO:H12	1.93	0.50
1:D:234:LEU:HD23	1:D:250:MET:SD	2.51	0.50
1:C:279:VAL:HB	2:C:501:CTP:C5	2.47	0.50
1:A:96:VAL:HG12	1:A:138:LEU:HG	1.94	0.50
1:A:279:VAL:HG22	2:A:501:CTP:C6	2.46	0.50
1:B:94:ARG:NH2	6:B:602:HOH:O	2.41	0.50
1:B:196:ALA:HB2	1:B:218:GLY:HA3	1.94	0.50
1:A:5:LYS:HG3	1:A:177:LEU:HD22	1.94	0.49
1:A:359:LEU:HB3	1:A:380:LEU:CD1	2.42	0.49
1:A:279:VAL:HG21	2:A:501:CTP:C6	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ALA:O	1:D:110:THR:HG23	2.11	0.49
1:D:401:ILE:O	1:D:405:ILE:HG13	2.13	0.49
1:B:6:ARG:HB3	3:B:502:EDO:H11	1.94	0.49
1:B:315:VAL:O	1:B:318:ARG:CB	2.51	0.49
1:D:15:ILE:HB	5:D:503:FMN:H6	1.94	0.49
1:D:245:PRO:HB2	1:D:248:VAL:HG21	1.95	0.49
1:A:74:ARG:CG	1:A:74:ARG:NH1	2.73	0.48
1:C:21:CYS:O	1:C:24:VAL:HG22	2.13	0.48
1:D:200:ARG:HD2	1:D:208:PHE:CE1	2.48	0.48
1:B:282:PHE:HA	1:B:306:ARG:HA	1.96	0.48
1:D:193:LEU:HD21	1:D:235:ILE:HD12	1.95	0.48
1:C:379:LEU:HD23	1:C:404:SER:OG	2.14	0.48
1:B:358:LEU:HB3	1:B:381:SER:HA	1.96	0.48
1:C:348:ARG:NH2	1:C:381:SER:O	2.47	0.48
1:A:250:MET:HB3	1:A:250:MET:HE3	1.65	0.48
1:C:272:VAL:HG22	1:C:328:ALA:HB3	1.95	0.47
1:A:128:HIS:CG	1:A:129:PRO:HD2	2.50	0.47
1:A:279:VAL:HG23	2:A:501:CTP:C5	2.48	0.47
1:C:206:VAL:O	1:D:212:ARG:HG3	2.14	0.47
1:A:35:ARG:HD3	1:A:75:ILE:HD11	1.96	0.47
1:A:361:VAL:CG1	1:A:378:TRP:HB2	2.45	0.47
1:C:283:ARG:CG	1:C:284:PRO:HD3	2.40	0.47
1:D:4:ARG:NH2	1:D:31:GLY:O	2.48	0.47
1:A:260:ARG:HB3	1:A:310:VAL:HG22	1.96	0.47
1:D:217:GLN:HB2	1:D:397:MET:HE1	1.97	0.47
1:C:84:ILE:CD1	1:C:104:LEU:HD11	2.45	0.47
1:C:151:GLY:HA3	1:C:162:ARG:HH21	1.80	0.47
1:B:194:VAL:HG13	1:B:274:VAL:HG13	1.96	0.46
1:B:214:SER:CB	1:B:216:LYS:HG3	2.45	0.46
1:B:129:PRO:HB2	1:D:141:ARG:HD3	1.97	0.46
1:B:256:ALA:HB3	1:B:307:ASN:ND2	2.30	0.46
1:D:398:ALA:O	1:D:402:VAL:HG23	2.15	0.46
1:B:330:VAL:HA	1:B:358:LEU:O	2.15	0.46
1:A:52:GLU:HG2	1:A:59:VAL:HG23	1.98	0.45
1:B:243:ILE:HD12	1:B:244:ASP:H	1.81	0.45
1:A:175:LEU:HD11	1:A:399:THR:HG21	1.98	0.45
1:D:394:LYS:O	1:D:397:MET:HG3	2.16	0.45
1:B:57:ASN:HB3	1:B:58:PRO:HD2	1.98	0.45
1:D:170:THR:O	1:D:174:GLN:HG3	2.17	0.45
1:B:73:VAL:CG1	1:B:77:GLN:CD	2.90	0.45
1:C:260:ARG:HG3	1:C:261:ASP:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:GLY:HA3	1:C:389:LEU:HB2	1.99	0.45
1:B:199:THR:HG21	1:B:256:ALA:HB2	1.99	0.44
1:B:284:PRO:HA	1:B:304:LEU:HA	2.00	0.44
1:A:235:ILE:HG22	1:A:251:VAL:HB	1.98	0.44
1:C:203:LEU:CD1	1:D:209:ILE:HD12	2.42	0.44
1:A:53:ALA:HB1	1:B:15:ILE:HD12	2.00	0.44
1:A:84:ILE:HD11	1:A:108:LEU:HD21	1.98	0.44
1:A:193:LEU:HD23	1:A:194:VAL:N	2.33	0.44
1:B:357:ASP:HB3	1:B:408:PHE:CZ	2.52	0.44
1:A:261:ASP:OD2	1:A:261:ASP:N	2.51	0.44
1:C:379:LEU:CD2	1:C:404:SER:OG	2.66	0.44
1:C:85:ALA:HA	1:C:86:PRO:HA	1.80	0.43
1:B:4:ARG:O	1:B:4:ARG:HG2	2.18	0.43
1:B:194:VAL:HG22	1:B:274:VAL:CG1	2.49	0.43
5:D:503:FMN:H9	5:D:503:FMN:H1'1	1.81	0.43
1:A:35:ARG:HD3	1:A:75:ILE:CD1	2.49	0.43
1:B:94:ARG:NE	6:B:602:HOH:O	2.37	0.43
1:B:179:ARG:NH2	1:B:403:ASP:OD2	2.45	0.43
1:C:208:PHE:HE2	1:D:212:ARG:HG2	1.83	0.43
1:B:322:GLN:C	1:B:324:PRO:HD3	2.43	0.43
1:A:309:ASP:HB3	1:A:312:ALA:HB3	2.00	0.42
1:C:275:MET:HG3	1:C:311:LEU:HB2	2.01	0.42
1:B:85:ALA:HA	1:B:86:PRO:HA	1.90	0.42
1:B:362:ASN:OD1	1:B:362:ASN:N	2.52	0.42
1:C:172:LEU:HD23	1:C:172:LEU:HA	1.87	0.42
1:A:312:ALA:HA	1:A:315:VAL:HG12	2.01	0.42
1:B:201:GLU:HB2	1:B:209:ILE:HG23	2.01	0.42
1:D:6:ARG:HE	1:D:6:ARG:HB2	1.69	0.42
1:A:195:THR:HG21	1:A:275:MET:SD	2.60	0.42
1:C:70:VAL:HG13	1:C:70:VAL:O	2.20	0.42
1:C:73:VAL:HG22	1:C:77:GLN:CD	2.45	0.42
1:C:221:VAL:HG21	1:C:274:VAL:HG11	2.01	0.42
1:A:120:ALA:HA	1:A:161:GLY:O	2.21	0.41
1:A:273:LEU:CD1	1:A:275:MET:HG2	2.50	0.41
1:B:35:ARG:HD2	3:B:502:EDO:C2	2.50	0.41
1:C:121:MET:HG3	1:C:126:TRP:HB2	2.02	0.41
1:D:168:GLU:HG3	1:D:223:ARG:HE	1.86	0.41
2:D:501:CTP:H6	2:D:501:CTP:O2A	2.04	0.41
1:A:182:ALA:HB1	1:A:399:THR:HG21	2.02	0.41
1:B:379:LEU:C	1:B:379:LEU:CD1	2.85	0.41
1:C:243:ILE:HD12	1:C:244:ASP:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ALA:O	1:B:119:PRO:HA	2.21	0.41
1:A:15:ILE:O	1:A:15:ILE:HG12	2.21	0.41
1:C:182:ALA:HB1	1:C:399:THR:HG21	2.02	0.41
1:C:186:ASP:OD1	1:C:187:MET:HG2	2.21	0.41
1:D:224:VAL:HG12	1:D:402:VAL:HG21	2.03	0.41
1:C:218:GLY:O	1:C:221:VAL:HG22	2.21	0.41
1:D:168:GLU:CD	1:D:223:ARG:HE	2.28	0.41
1:C:203:LEU:HD11	1:D:209:ILE:CD1	2.47	0.40
1:C:284:PRO:CD	1:C:284:PRO:O	2.69	0.40
1:D:239:THR:HB	1:D:242:LEU:HG	2.03	0.40
1:A:348:ARG:HA	1:A:348:ARG:HD3	1.89	0.40
1:C:167:GLU:O	1:C:171:THR:HG23	2.21	0.40
1:D:87:ALA:O	1:D:119:PRO:HA	2.21	0.40
1:A:244:ASP:OD1	1:A:250:MET:HE1	2.20	0.40
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.83	0.40
1:B:318:ARG:NH1	1:B:329:ILE:HD12	2.36	0.40
1:C:84:ILE:HD12	1:C:104:LEU:HD11	2.04	0.40
1:C:203:LEU:CD1	1:D:209:ILE:CD1	2.99	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	373/415 (90%)	356 (95%)	16 (4%)	1 (0%)	36	55
1	B	362/415 (87%)	352 (97%)	10 (3%)	0	100	100
1	C	381/415 (92%)	368 (97%)	12 (3%)	1 (0%)	36	55
1	D	364/415 (88%)	348 (96%)	15 (4%)	1 (0%)	36	55
All	All	1480/1660 (89%)	1424 (96%)	53 (4%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	70	VAL
1	A	286	HIS
1	C	284	PRO

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	252/307 (82%)	250 (99%)	2 (1%)	73	88
1	B	227/307 (74%)	224 (99%)	3 (1%)	61	82
1	C	251/307 (82%)	247 (98%)	4 (2%)	55	79
1	D	232/307 (76%)	230 (99%)	2 (1%)	70	87
All	All	962/1228 (78%)	951 (99%)	11 (1%)	65	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	74	ARG
1	B	4	ARG
1	B	52	GLU
1	B	70	VAL
1	C	67	VAL
1	C	73	VAL
1	C	121	MET
1	C	122	HIS
1	D	69	GLU
1	D	70	VAL

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	238	ASN
1	A	362	ASN
1	B	60	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	238	ASN
1	C	72	HIS
1	D	266	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FMN	A	506	-	33,33,33	1.16	2 (6%)	48,50,50	1.39	9 (18%)
3	EDO	B	503	-	3,3,3	0.57	0	2,2,2	0.09	0
3	EDO	A	504	-	3,3,3	0.43	0	2,2,2	0.39	0
5	FMN	C	503	-	33,33,33	2.24	15 (45%)	48,50,50	1.51	11 (22%)
3	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.28	0
2	CTP	D	501	-	29,30,30	1.09	2 (6%)	43,47,47	0.93	2 (4%)
5	FMN	B	504	-	33,33,33	1.05	2 (6%)	48,50,50	1.36	8 (16%)
5	FMN	D	503	-	33,33,33	1.11	2 (6%)	48,50,50	1.53	10 (20%)
3	EDO	B	502	-	3,3,3	0.56	0	2,2,2	0.04	0
3	EDO	D	502	-	3,3,3	0.56	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	503	-	3,3,3	0.67	0	2,2,2	0.05	0
2	CTP	B	501	-	29,30,30	1.12	2 (6%)	43,47,47	0.86	2 (4%)
2	CTP	C	501	-	29,30,30	0.99	0	43,47,47	0.98	2 (4%)
2	CTP	A	501	4	29,30,30	1.01	1 (3%)	43,47,47	0.87	0
3	EDO	A	502	-	3,3,3	0.50	0	2,2,2	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FMN	A	506	-	-	7/18/18/18	0/3/3/3
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
5	FMN	C	503	-	-	5/18/18/18	0/3/3/3
3	EDO	C	502	-	-	0/1/1/1	-
2	CTP	D	501	-	-	4/22/38/38	0/2/2/2
5	FMN	B	504	-	-	4/18/18/18	0/3/3/3
5	FMN	D	503	-	-	9/18/18/18	0/3/3/3
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	D	502	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
2	CTP	B	501	-	-	10/22/38/38	0/2/2/2
2	CTP	C	501	-	-	8/22/38/38	0/2/2/2
2	CTP	A	501	4	-	6/22/38/38	0/2/2/2
3	EDO	A	502	-	-	0/1/1/1	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	FMN	P-O2P	-4.86	1.36	1.54
5	C	503	FMN	C5A-N5	-4.31	1.31	1.39
5	C	503	FMN	C4-N3	-4.22	1.30	1.38
5	C	503	FMN	C2-N3	-3.66	1.30	1.39
5	C	503	FMN	C9A-C5A	3.65	1.47	1.41
5	B	504	FMN	C4A-N5	3.46	1.38	1.30
5	D	503	FMN	C4A-N5	3.39	1.38	1.30
5	A	506	FMN	C4A-N5	3.00	1.37	1.30
5	C	503	FMN	P-O3P	-2.99	1.43	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	FMN	C6-C5A	-2.87	1.35	1.40
5	A	506	FMN	C10-N1	2.81	1.38	1.33
2	D	501	CTP	PB-O3B	2.81	1.62	1.59
2	B	501	CTP	PA-O3A	2.68	1.62	1.59
5	D	503	FMN	C10-N1	2.68	1.38	1.33
5	B	504	FMN	C10-N1	2.65	1.38	1.33
5	C	503	FMN	C6-C7	-2.48	1.36	1.39
5	C	503	FMN	C9-C9A	-2.41	1.35	1.39
2	A	501	CTP	PB-O3B	2.37	1.62	1.59
5	C	503	FMN	P-O1P	-2.37	1.43	1.50
5	C	503	FMN	C9-C8	-2.36	1.36	1.39
2	B	501	CTP	PB-O3A	2.36	1.62	1.59
5	C	503	FMN	P-O5'	-2.35	1.52	1.60
2	D	501	CTP	C4-N3	2.17	1.38	1.34
5	C	503	FMN	C2'-C3'	-2.10	1.49	1.53
5	C	503	FMN	C4'-C3'	-2.07	1.49	1.53
5	C	503	FMN	C9A-N10	-2.05	1.37	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	503	FMN	O4-C4-C4A	-3.39	117.59	126.53
5	A	506	FMN	C7M-C7-C6	-3.32	113.73	119.57
5	D	503	FMN	C4-N3-C2	-3.23	119.91	125.64
5	D	503	FMN	O4'-C4'-C3'	3.19	116.72	109.25
5	D	503	FMN	C2'-C1'-N10	3.10	124.87	110.20
5	D	503	FMN	C4A-C10-N10	3.03	120.82	116.48
5	C	503	FMN	O2P-P-O5'	-2.99	98.88	106.67
5	D	503	FMN	C5A-C9A-N10	2.92	120.61	117.97
5	C	503	FMN	O5'-P-O1P	-2.77	98.97	106.44
5	A	506	FMN	C4-N3-C2	-2.74	120.77	125.64
5	B	504	FMN	O4-C4-C4A	-2.71	119.38	126.53
5	A	506	FMN	C4A-C10-N10	2.69	120.34	116.48
5	C	503	FMN	C4A-C4-N3	2.68	120.08	113.25
5	B	504	FMN	C4-N3-C2	-2.66	120.92	125.64
5	B	504	FMN	C4A-C10-N10	2.61	120.21	116.48
5	B	504	FMN	O3'-C3'-C4'	2.58	114.79	108.93
5	A	506	FMN	C10-C4A-N5	-2.57	119.56	124.81
5	C	503	FMN	C4A-C10-N1	-2.49	118.49	124.59
5	A	506	FMN	O4-C4-C4A	-2.48	119.98	126.53
5	D	503	FMN	C4A-C4-N3	2.47	119.55	113.25
2	C	501	CTP	O2A-PA-O3A	2.42	113.81	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	506	FMN	C4-C4A-C10	2.42	121.08	116.93
5	D	503	FMN	O4-C4-C4A	-2.40	120.19	126.53
5	B	504	FMN	C4'-C3'-C2'	-2.40	109.58	113.57
5	C	503	FMN	C10-N1-C2	2.37	121.97	116.85
5	B	504	FMN	C4A-C4-N3	2.27	119.04	113.25
2	C	501	CTP	O2-C2-N3	-2.27	118.76	122.33
5	D	503	FMN	C4A-C10-N1	-2.26	119.05	124.59
5	C	503	FMN	C9A-N10-C10	-2.20	117.40	120.75
5	B	504	FMN	C10-C4A-N5	-2.19	120.34	124.81
2	D	501	CTP	O2B-PB-O3B	2.17	113.14	107.27
2	B	501	CTP	C6-N1-C2	-2.13	116.87	120.46
5	A	506	FMN	C4'-C3'-C2'	-2.12	110.04	113.57
5	C	503	FMN	C4A-C10-N10	2.11	119.50	116.48
5	C	503	FMN	O2-C2-N1	-2.11	118.30	121.80
5	B	504	FMN	C5A-C9A-N10	2.10	119.87	117.97
5	A	506	FMN	C4A-C10-N1	-2.10	119.44	124.59
2	D	501	CTP	C5-C6-N1	-2.08	118.45	121.84
5	D	503	FMN	C1'-C2'-C3'	2.08	115.30	109.66
5	C	503	FMN	C4-C4A-N5	2.05	121.04	118.21
5	C	503	FMN	C4-N3-C2	-2.04	122.01	125.64
5	D	503	FMN	C4-C4A-C10	2.04	120.44	116.93
5	A	506	FMN	C4A-C4-N3	2.04	118.44	113.25
2	B	501	CTP	C4-N3-C2	-2.04	117.06	120.26

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CTP	O4'-C4'-C5'-O5'
2	A	501	CTP	C5'-O5'-PA-O1A
2	A	501	CTP	C5'-O5'-PA-O2A
2	A	501	CTP	C5'-O5'-PA-O3A
2	B	501	CTP	C5'-O5'-PA-O1A
2	B	501	CTP	PB-O3B-PG-O3G
2	C	501	CTP	O4'-C4'-C5'-O5'
2	C	501	CTP	C5'-O5'-PA-O1A
2	C	501	CTP	C5'-O5'-PA-O2A
2	C	501	CTP	PB-O3B-PG-O3G
5	A	506	FMN	O3'-C3'-C4'-C5'
5	A	506	FMN	C5'-O5'-P-O1P
5	A	506	FMN	C5'-O5'-P-O3P
5	B	504	FMN	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

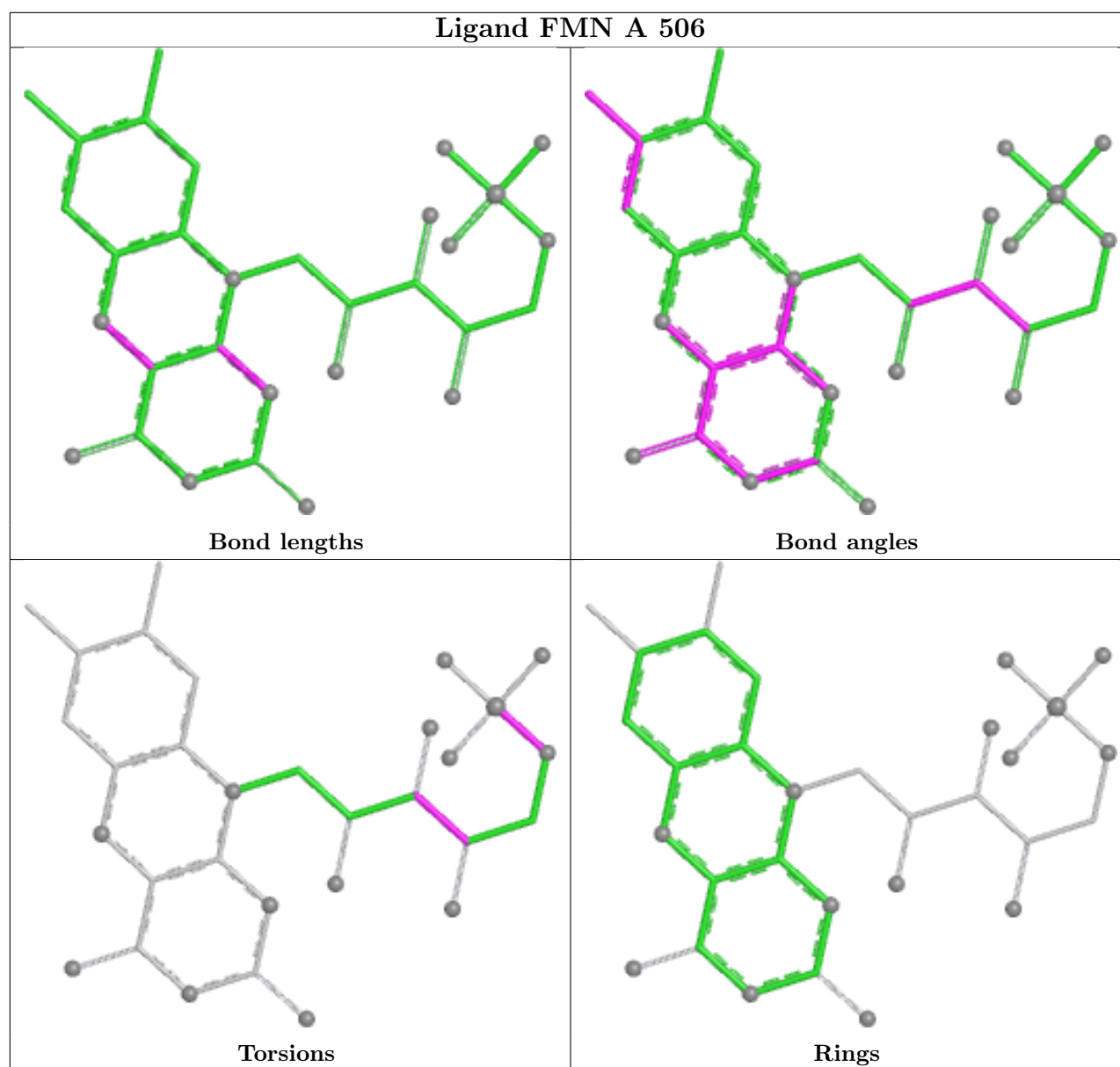
Mol	Chain	Res	Type	Atoms
5	B	504	FMN	O4'-C4'-C5'-O5'
5	B	504	FMN	C5'-O5'-P-O2P
5	B	504	FMN	C5'-O5'-P-O3P
5	C	503	FMN	O4'-C4'-C5'-O5'
5	C	503	FMN	C5'-O5'-P-O2P
5	C	503	FMN	C5'-O5'-P-O3P
5	D	503	FMN	N10-C1'-C2'-O2'
5	D	503	FMN	N10-C1'-C2'-C3'
5	D	503	FMN	C5'-O5'-P-O2P
5	D	503	FMN	C5'-O5'-P-O3P
5	D	503	FMN	O3'-C3'-C4'-O4'
5	D	503	FMN	C2'-C3'-C4'-O4'
2	B	501	CTP	C3'-C4'-C5'-O5'
2	B	501	CTP	O4'-C4'-C5'-O5'
2	C	501	CTP	C3'-C4'-C5'-O5'
5	D	503	FMN	O3'-C3'-C4'-C5'
5	A	506	FMN	C2'-C3'-C4'-C5'
5	D	503	FMN	C2'-C3'-C4'-C5'
5	A	506	FMN	C2'-C3'-C4'-O4'
5	A	506	FMN	O3'-C3'-C4'-O4'
2	A	501	CTP	C3'-C4'-C5'-O5'
5	C	503	FMN	C5'-O5'-P-O1P
5	D	503	FMN	C5'-O5'-P-O1P
2	D	501	CTP	PG-O3B-PB-O1B
2	B	501	CTP	PB-O3A-PA-O5'
5	A	506	FMN	C5'-O5'-P-O2P
2	B	501	CTP	PB-O3B-PG-O2G
2	D	501	CTP	PB-O3B-PG-O2G
2	A	501	CTP	PB-O3A-PA-O1A
2	C	501	CTP	C5'-O5'-PA-O3A
2	D	501	CTP	PA-O3A-PB-O1B
2	B	501	CTP	PA-O3A-PB-O3B
3	A	504	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
2	B	501	CTP	C4'-C5'-O5'-PA
2	B	501	CTP	PB-O3B-PG-O1G
2	C	501	CTP	PB-O3B-PG-O1G
2	C	501	CTP	PB-O3B-PG-O2G
3	D	502	EDO	O1-C1-C2-O2
5	C	503	FMN	C3'-C4'-C5'-O5'
2	B	501	CTP	PA-O3A-PB-O1B
2	D	501	CTP	PG-O3B-PB-O2B

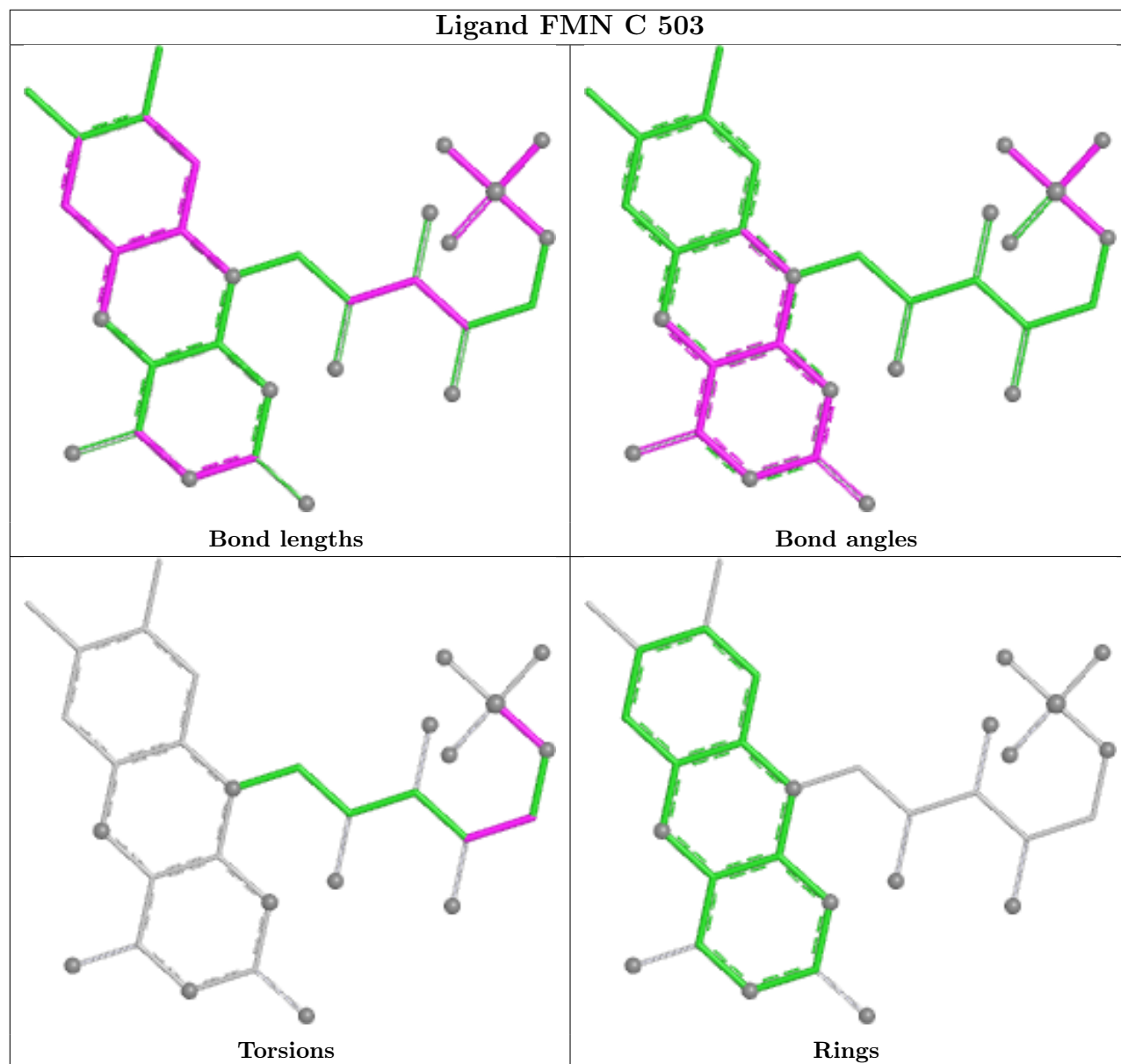
There are no ring outliers.

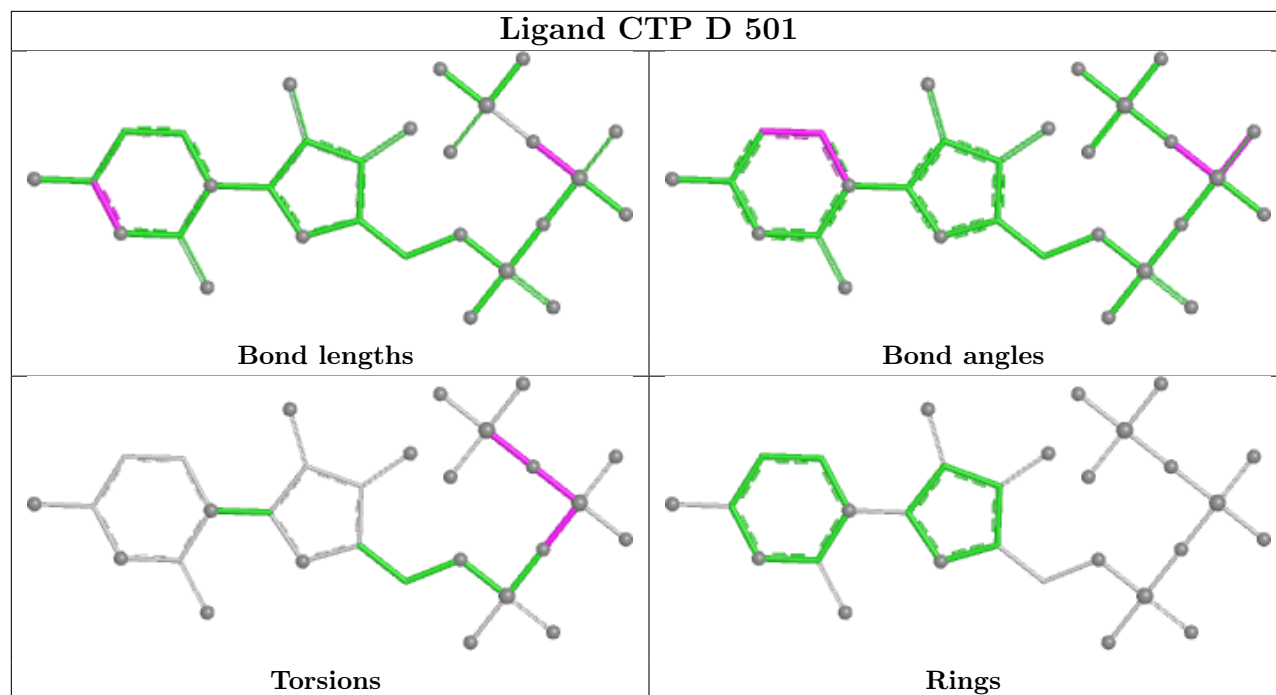
9 monomers are involved in 23 short contacts:

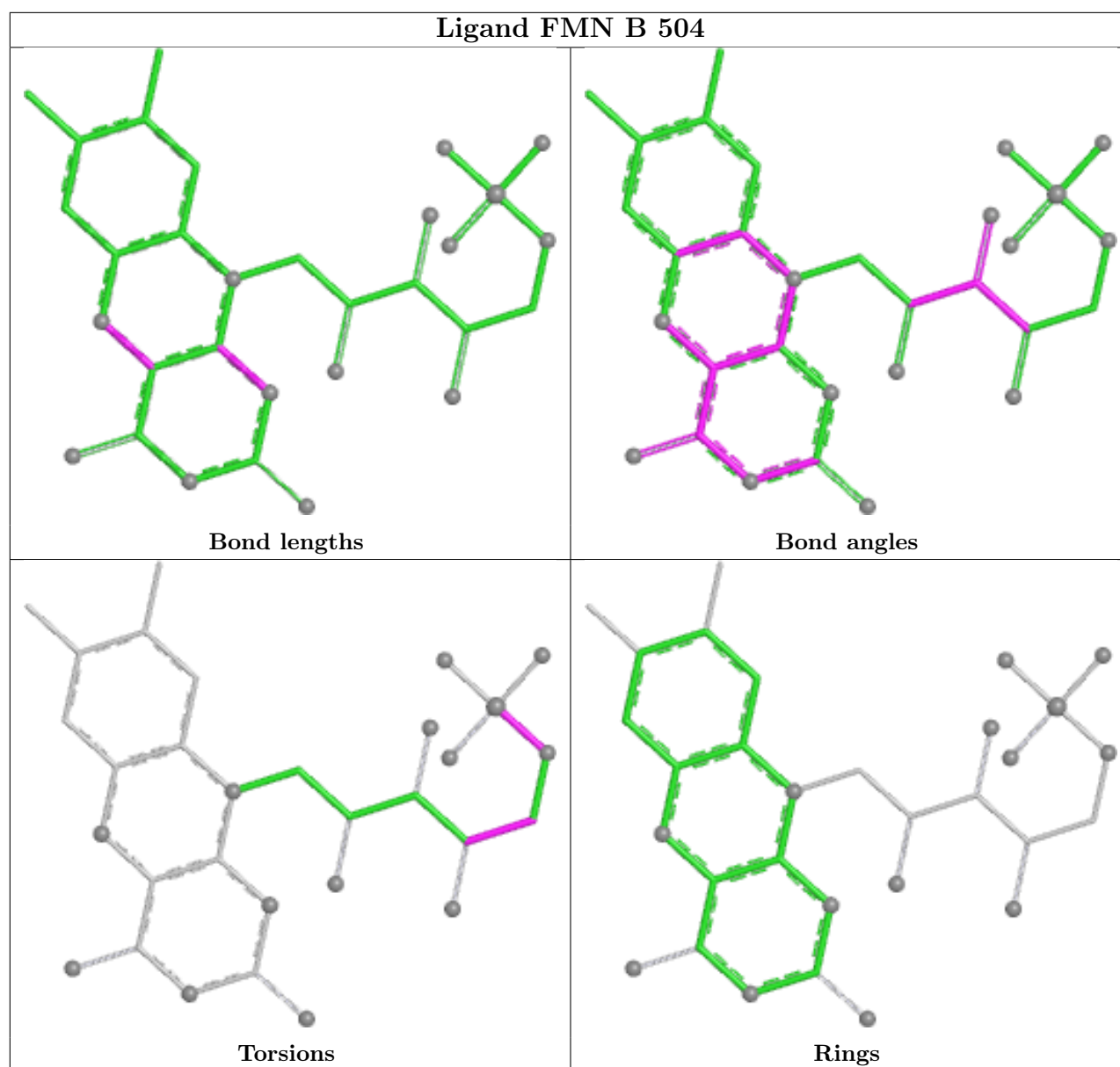
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	FMN	1	0
3	B	503	EDO	1	0
5	C	503	FMN	1	0
2	D	501	CTP	2	0
5	B	504	FMN	2	0
5	D	503	FMN	3	0
3	B	502	EDO	2	0
2	C	501	CTP	1	0
2	A	501	CTP	10	0

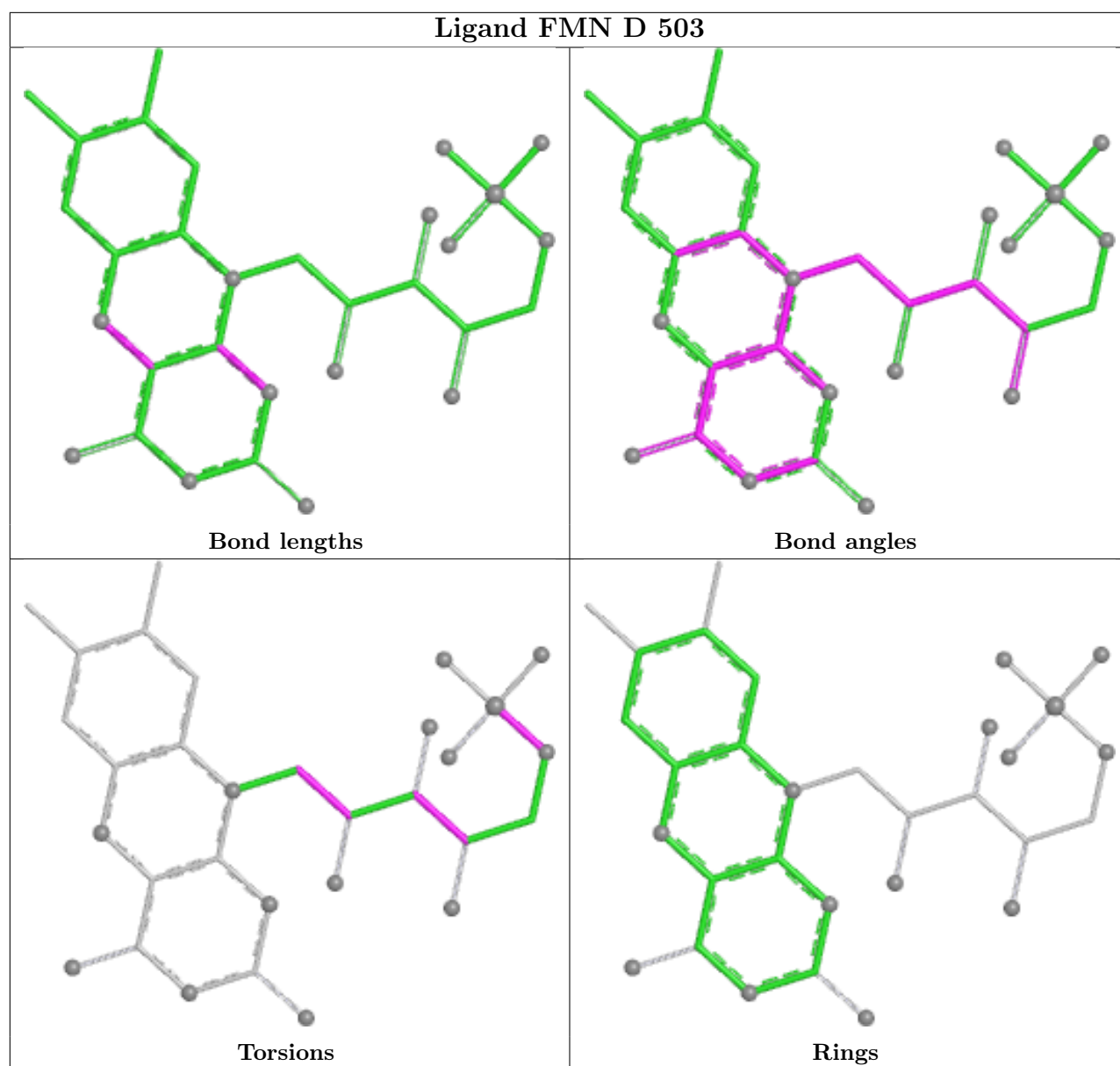
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

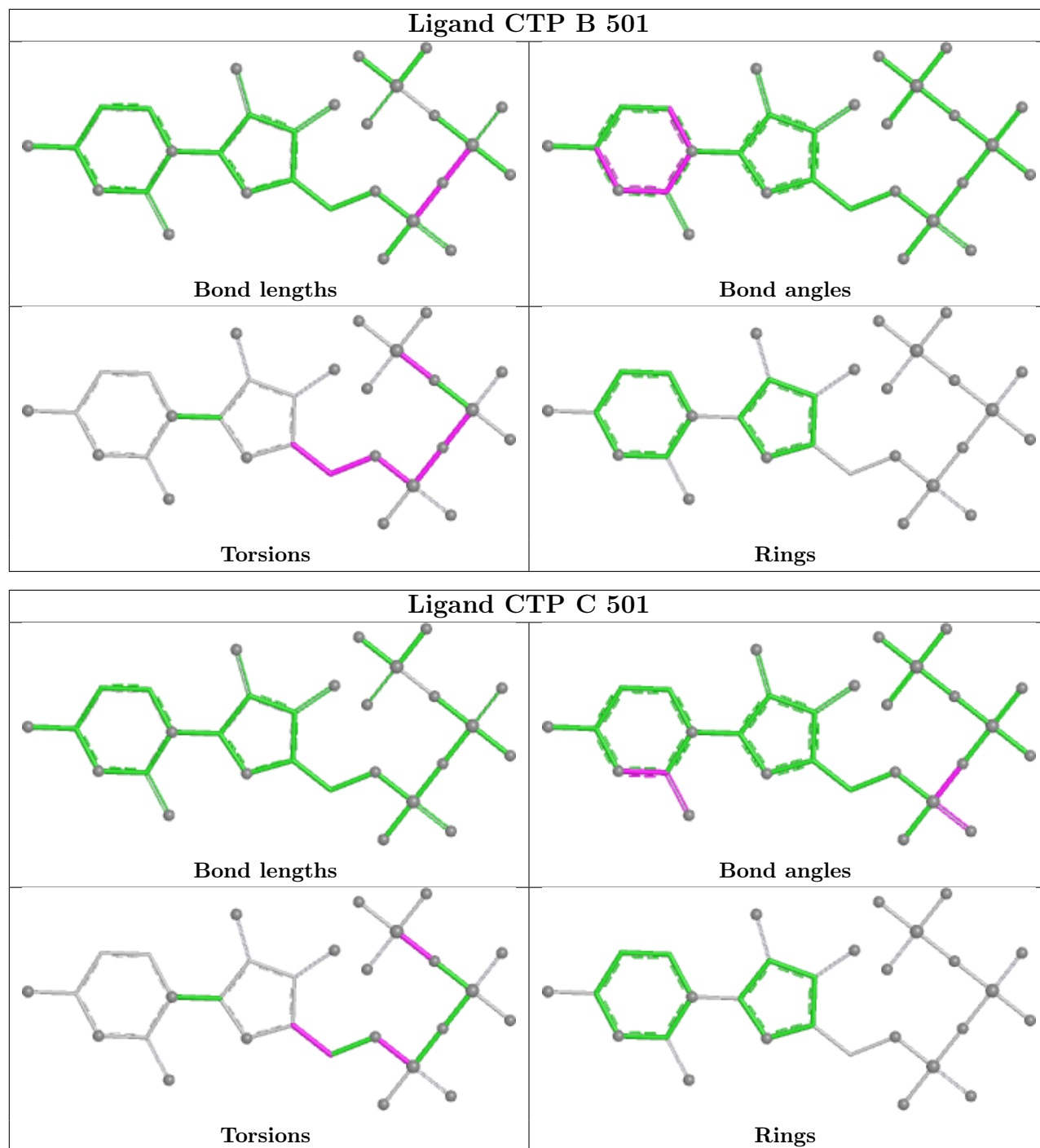


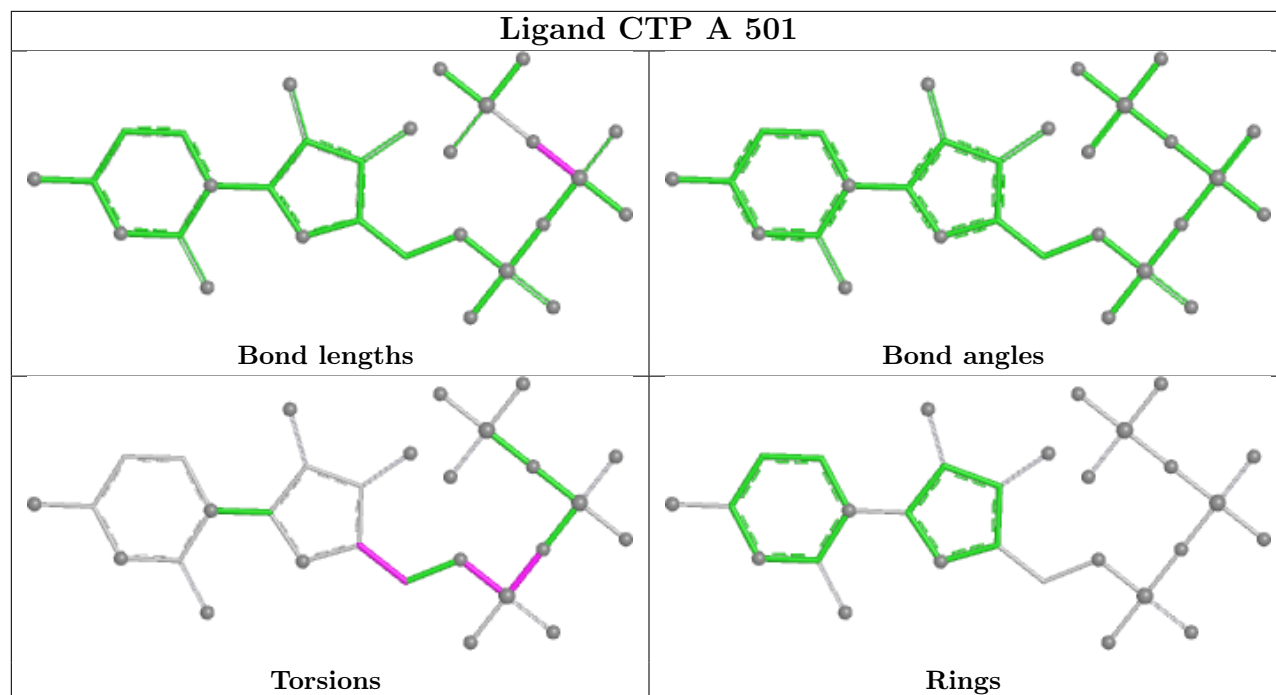












5.7 Other polymers [i](#)

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	381/415 (91%)	0.63	45 (11%) 9 7	59, 112, 167, 200	0
1	B	372/415 (89%)	0.62	36 (9%) 13 11	58, 106, 168, 191	0
1	C	389/415 (93%)	0.49	29 (7%) 20 18	58, 104, 163, 199	0
1	D	374/415 (90%)	0.67	49 (13%) 7 6	57, 110, 167, 191	0
All	All	1516/1660 (91%)	0.60	159 (10%) 11 10	57, 108, 167, 200	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	340	ASN	9.8
1	D	72	HIS	6.5
1	A	343	VAL	6.3
1	D	378	TRP	6.0
1	D	71	GLN	6.0
1	D	73	VAL	5.8
1	B	363	ALA	5.7
1	D	70	VAL	5.6
1	C	363	ALA	5.5
1	B	290	ALA	5.2
1	B	158	SER	5.0
1	B	335	GLU	4.9
1	B	308	ASP	4.8
1	A	299	PRO	4.8
1	A	289	ALA	4.8
1	B	280	ALA	4.7
1	D	290	ALA	4.7
1	D	282	PHE	4.6
1	C	151	GLY	4.6
1	A	73	VAL	4.5
1	A	72	HIS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	320	ASP	4.4
1	C	362	ASN	4.3
1	C	72	HIS	4.2
1	B	343	VAL	4.1
1	D	379	LEU	4.1
1	D	377	GLY	4.1
1	C	286	HIS	4.0
1	D	75	ILE	4.0
1	B	282	PHE	4.0
1	A	300	SER	3.9
1	B	304	LEU	3.9
1	A	391	HIS	3.9
1	D	359	LEU	3.9
1	A	75	ILE	3.9
1	A	346	HIS	3.9
1	B	286	HIS	3.9
1	C	287	VAL	3.7
1	D	74	ARG	3.6
1	C	154	THR	3.6
1	D	362	ASN	3.4
1	C	156	ALA	3.4
1	D	3	ALA	3.3
1	C	70	VAL	3.3
1	D	269	ASP	3.3
1	D	68	HIS	3.3
1	B	281	ASP	3.3
1	B	303	ASP	3.3
1	C	303	ASP	3.3
1	A	70	VAL	3.2
1	A	71	GLN	3.2
1	A	286	HIS	3.2
1	B	72	HIS	3.2
1	D	303	ASP	3.2
1	B	288	ALA	3.1
1	B	378	TRP	3.1
1	B	203	LEU	3.1
1	B	377	GLY	3.1
1	B	71	GLN	3.0
1	C	304	LEU	3.0
1	A	279	VAL	3.0
1	B	302	ILE	3.0
1	D	286	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	304	LEU	3.0
1	C	339	ALA	3.0
1	D	397	MET	2.9
1	B	379	LEU	2.9
1	B	307	ASN	2.9
1	C	279	VAL	2.9
1	A	377	GLY	2.9
1	D	345	PHE	2.9
1	B	279	VAL	2.9
1	D	189	GLY	2.9
1	C	2	SER	2.8
1	D	253	ILE	2.8
1	C	301	SER	2.8
1	D	161	GLY	2.8
1	A	156	ALA	2.8
1	D	391	HIS	2.8
1	C	66	ASP	2.7
1	D	413	ASP	2.7
1	A	385	THR	2.7
1	B	346	HIS	2.7
1	A	158	SER	2.7
1	A	390	GLU	2.7
1	B	3	ALA	2.7
1	B	320	ASP	2.6
1	C	356	CYS	2.6
1	B	391	HIS	2.6
1	B	362	ASN	2.6
1	C	385	THR	2.6
1	A	69	GLU	2.5
1	A	152	ARG	2.5
1	A	155	GLY	2.5
1	A	378	TRP	2.5
1	A	335	GLU	2.5
1	D	122	HIS	2.5
1	C	73	VAL	2.5
1	A	345	PHE	2.5
1	C	206	VAL	2.5
1	A	283	ARG	2.4
1	D	211	ASN	2.4
1	A	383	ASP	2.4
1	C	412	GLN	2.4
1	B	383	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	332	PHE	2.4
1	C	280	ALA	2.4
1	D	285	ALA	2.4
1	D	69	GLU	2.4
1	A	68	HIS	2.4
1	B	266	HIS	2.4
1	D	266	HIS	2.4
1	B	206	VAL	2.4
1	D	380	LEU	2.3
1	A	280	ALA	2.3
1	A	65	THR	2.3
1	B	70	VAL	2.3
1	D	305	VAL	2.3
1	A	151	GLY	2.3
1	C	252	HIS	2.2
1	A	352	GLU	2.2
1	A	64	PHE	2.2
1	A	194	VAL	2.2
1	D	360	VAL	2.2
1	B	256	ALA	2.2
1	D	333	ALA	2.2
1	D	321	GLY	2.2
1	C	75	ILE	2.2
1	B	201	GLU	2.2
1	C	364	VAL	2.2
1	D	62	GLY	2.2
1	D	300	SER	2.2
1	D	287	VAL	2.2
1	D	243	ILE	2.2
1	A	389	LEU	2.1
1	D	212	ARG	2.1
1	A	231	ASP	2.1
1	A	315	VAL	2.1
1	A	362	ASN	2.1
1	A	395	THR	2.1
1	A	66	ASP	2.1
1	A	232	VAL	2.1
1	D	217	GLN	2.1
1	D	356	CYS	2.1
1	A	397	MET	2.1
1	C	341	GLY	2.1
1	D	386	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	209	ILE	2.1
1	A	264	SER	2.1
1	B	252	HIS	2.1
1	D	322	GLN	2.0
1	A	305	VAL	2.0
1	D	207	ARG	2.0
1	C	269	ASP	2.0
1	B	64	PHE	2.0
1	A	79	ALA	2.0
1	D	249	GLU	2.0
1	B	231	ASP	2.0
1	C	122	HIS	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.

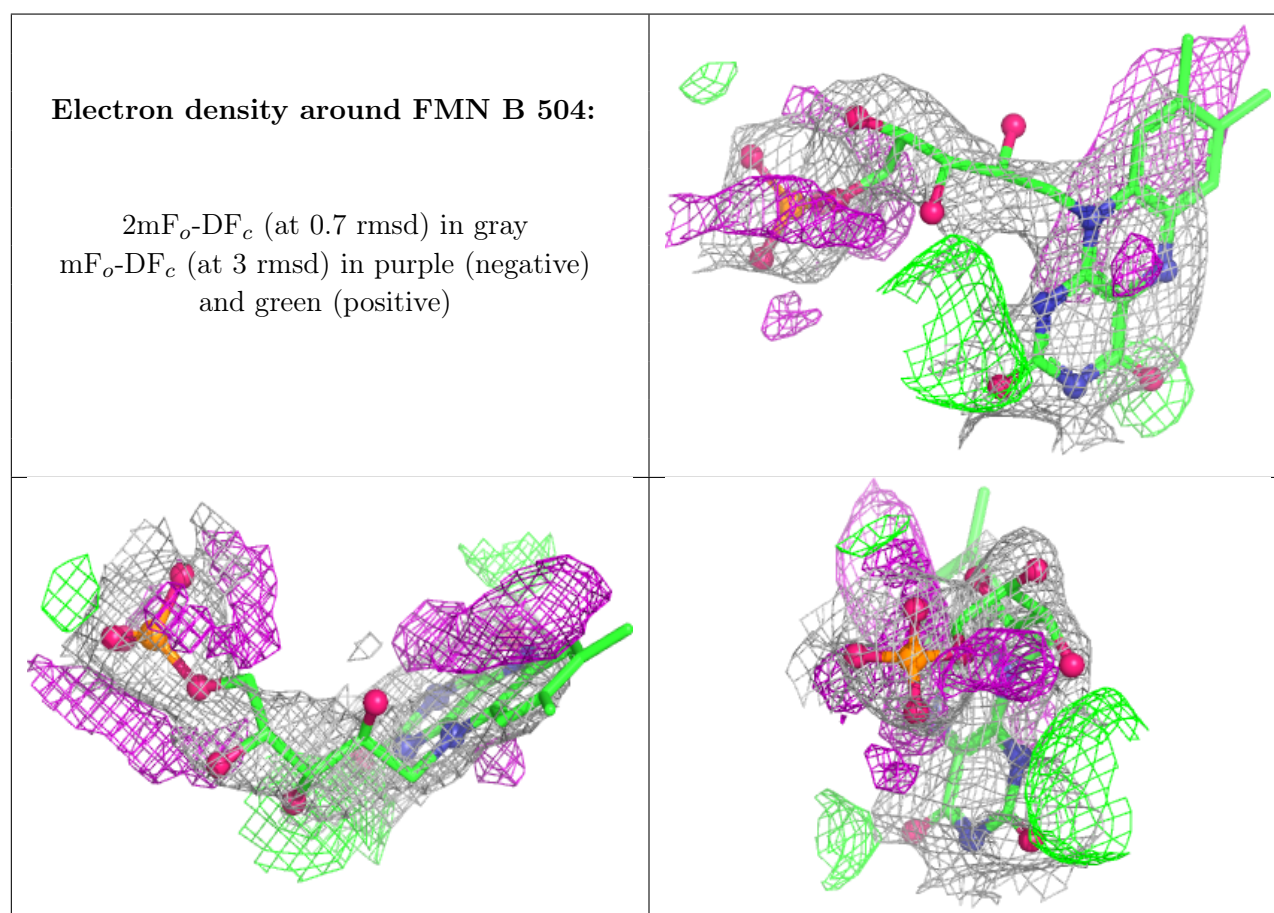
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	D	502	4/4	0.79	0.23	114,121,123,123	0
5	FMN	B	504	31/31	0.80	0.24	121,151,174,175	0
5	FMN	A	506	31/31	0.81	0.22	116,150,164,166	0
2	CTP	D	501	29/29	0.82	0.09	109,141,214,217	0
2	CTP	B	501	29/29	0.83	0.10	165,172,206,207	0
2	CTP	C	501	29/29	0.86	0.10	106,141,197,202	0
4	MG	A	505	1/1	0.87	0.12	125,125,125,125	0
3	EDO	A	502	4/4	0.88	0.18	80,89,100,101	0
5	FMN	D	503	31/31	0.89	0.15	88,110,117,121	0
3	EDO	C	502	4/4	0.90	0.15	95,105,110,113	0
2	CTP	A	501	29/29	0.90	0.09	132,150,204,207	0

Continued on next page...

Continued from previous page...

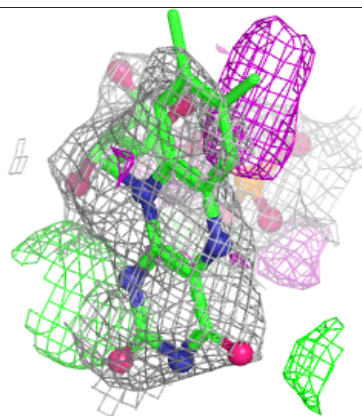
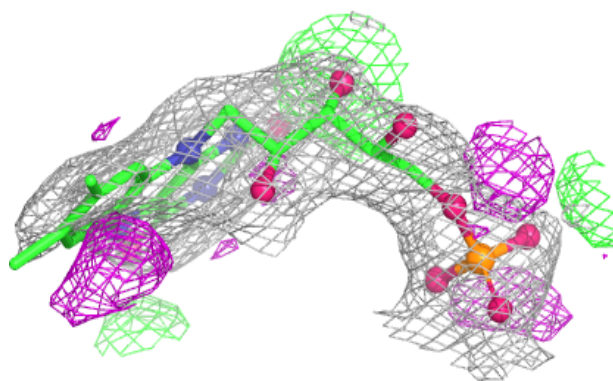
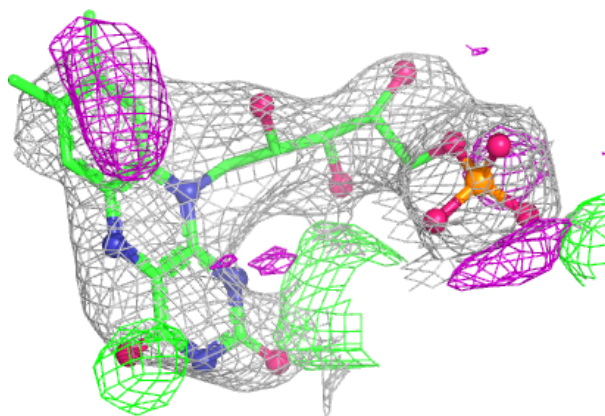
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMN	C	503	31/31	0.90	0.15	84,104,119,120	0
3	EDO	A	504	4/4	0.90	0.17	95,100,107,110	0
3	EDO	B	503	4/4	0.92	0.18	76,91,92,93	0
3	EDO	B	502	4/4	0.92	0.20	105,106,106,107	0
3	EDO	A	503	4/4	0.94	0.17	68,82,94,99	0

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.



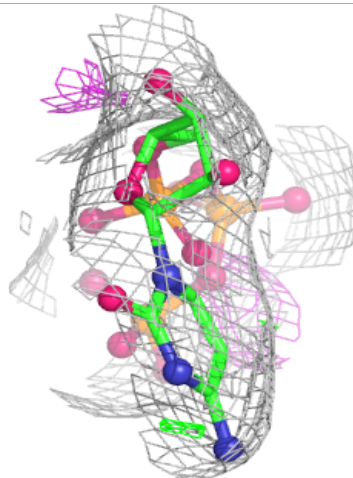
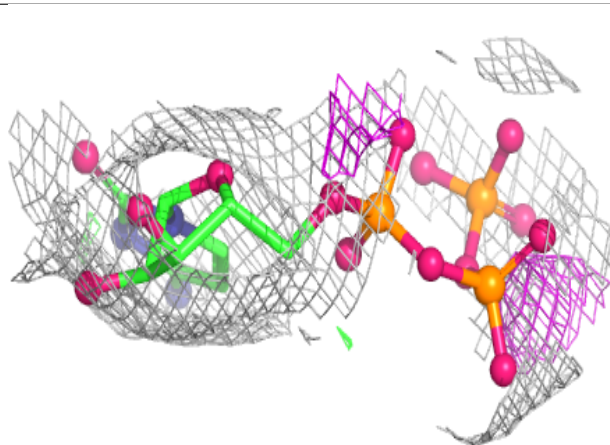
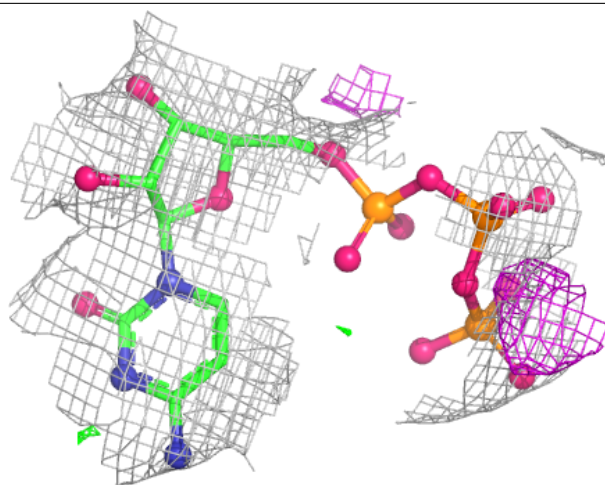
Electron density around FMN A 506:

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



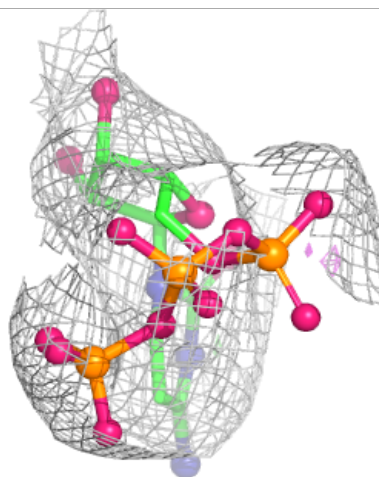
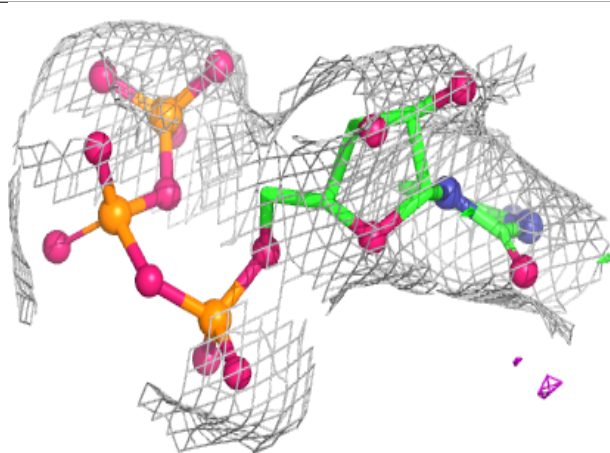
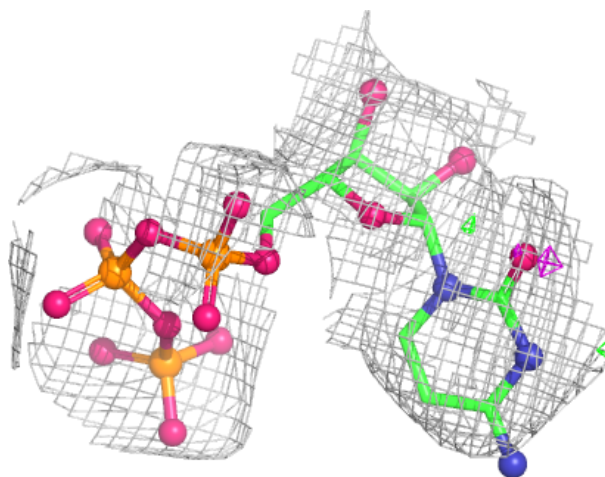
Electron density around CTP D 501:

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



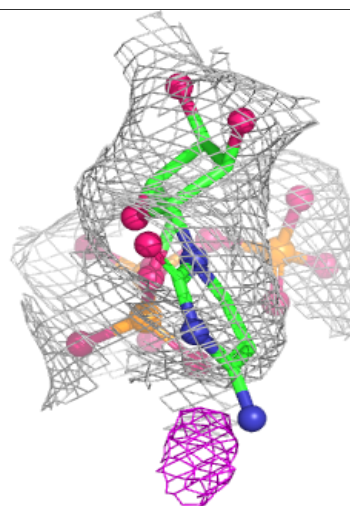
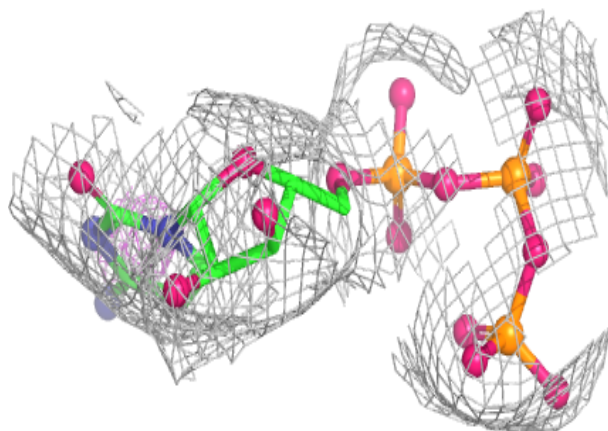
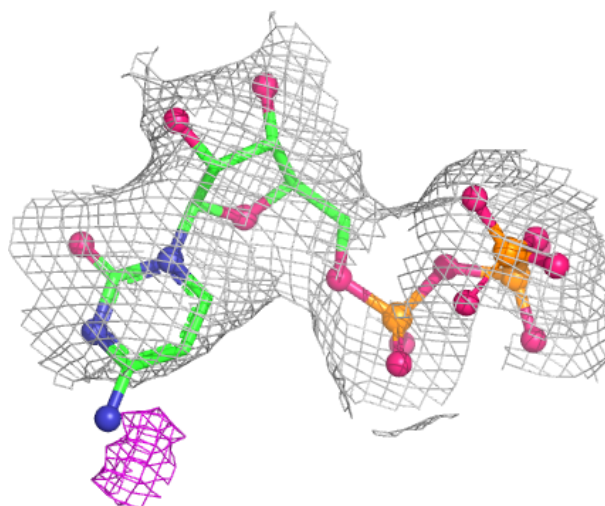
Electron density around CTP B 501:

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



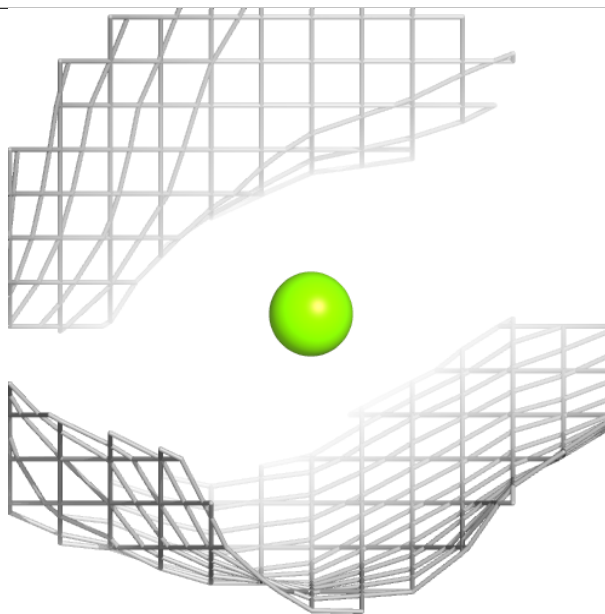
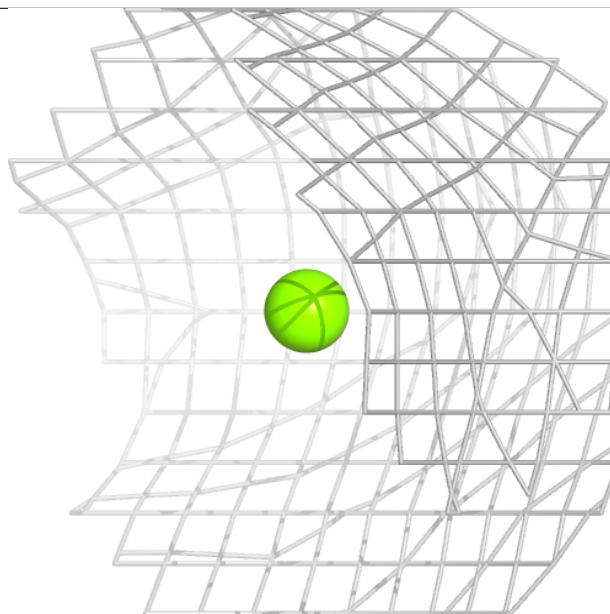
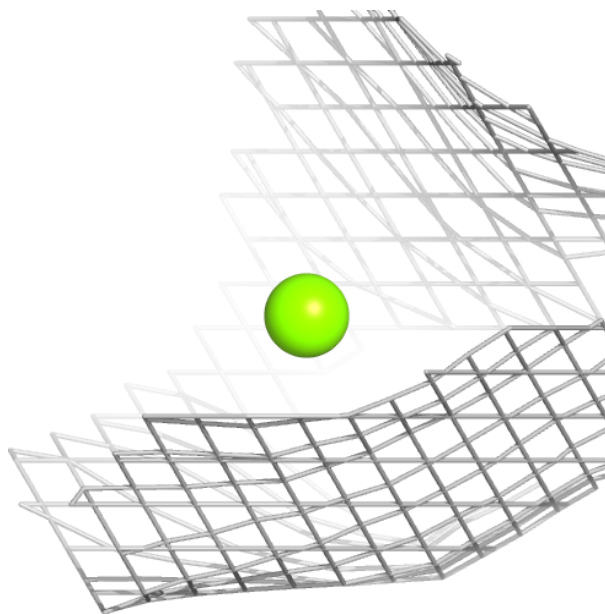
Electron density around CTP C 501:

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



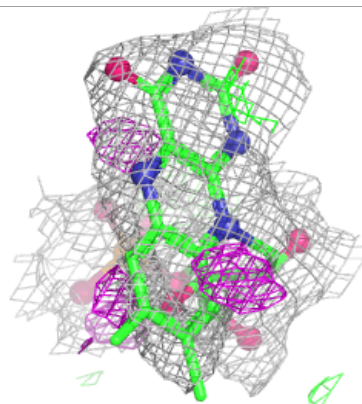
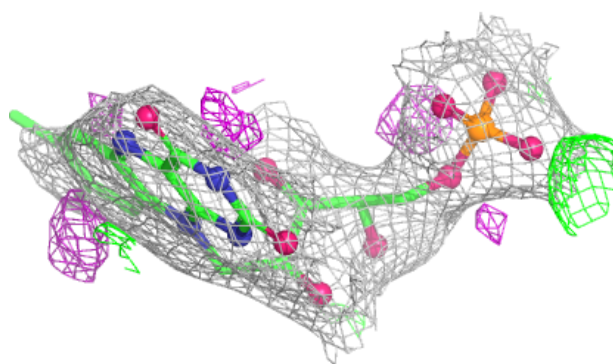
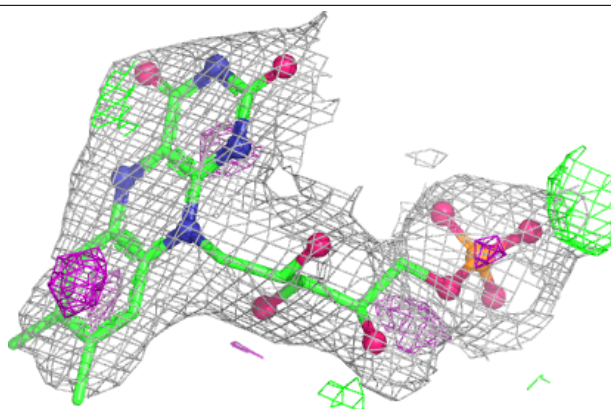
Electron density around MG A 505:

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



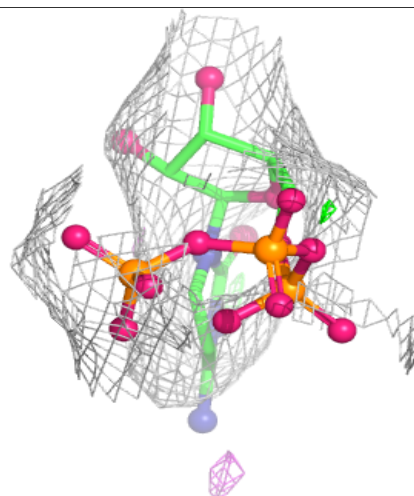
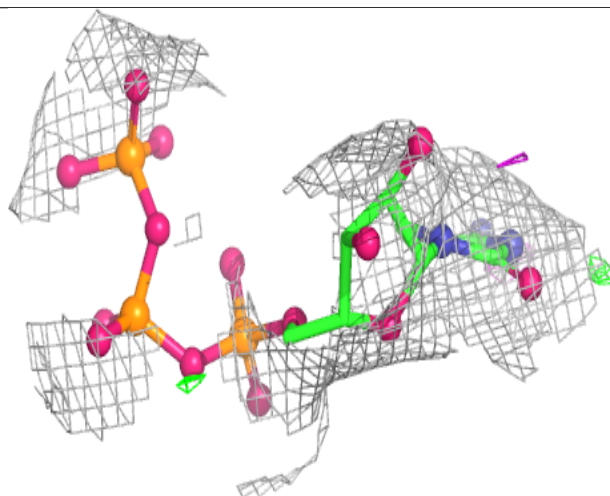
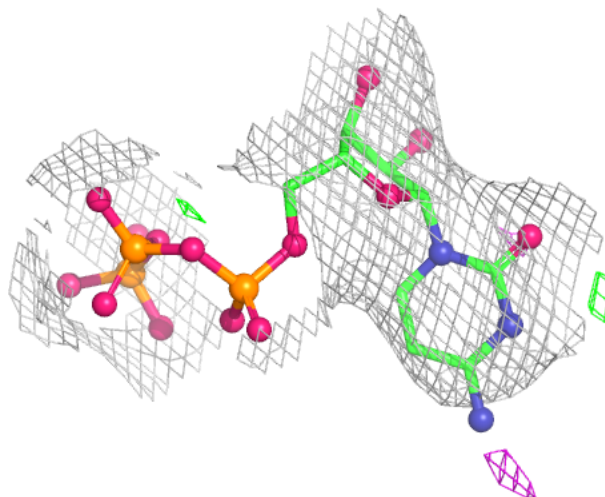
Electron density around FMN D 503:

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



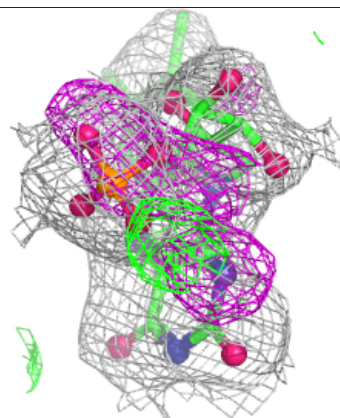
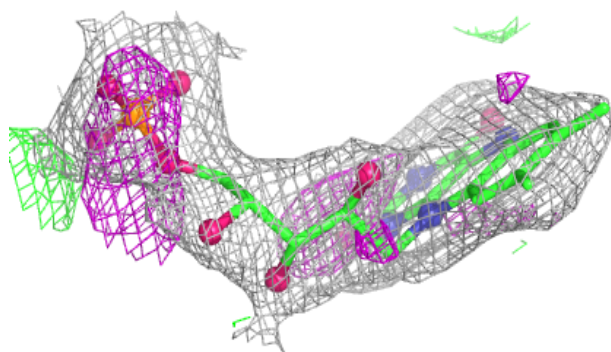
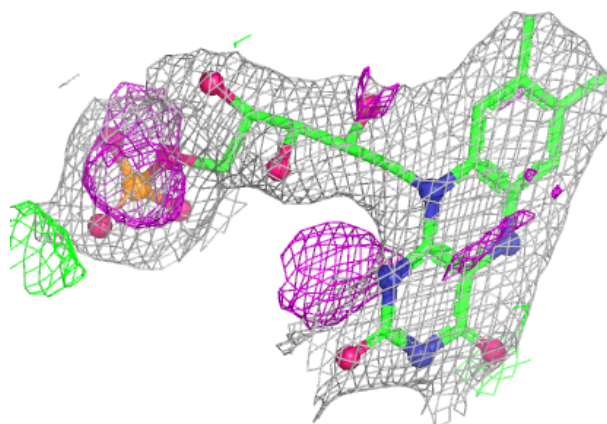
Electron density around CTP A 501:

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



Electron density around FMN C 503:

$2mF_o - DF_c$ (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.