



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 09:00 am BST

PDB ID : 1XFW
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin and 3'5' cyclic AMP (cAMP)
Authors : Shen, Y.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.
Deposited on : 2004-09-15
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

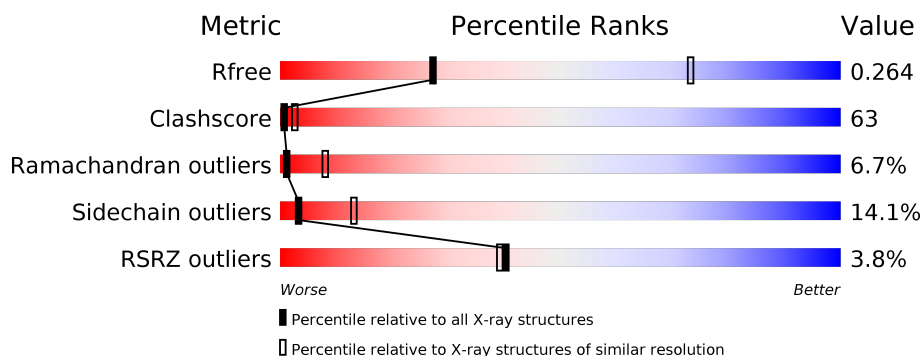
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



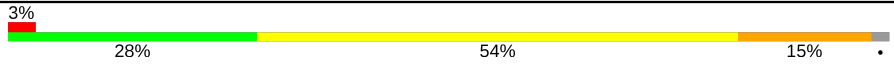

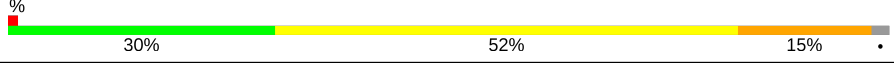
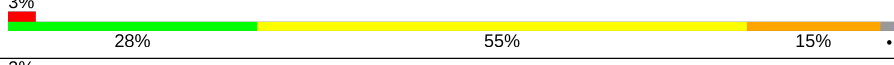
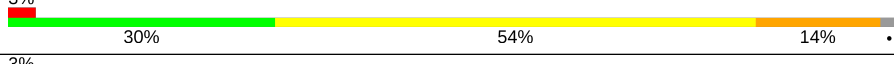

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on 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	777	<div> <div>4%</div> <div>27% 55% 12% • 5%</div> </div>
1	B	777	<div> <div>4%</div> <div>27% 54% 12% • 5%</div> </div>
1	C	777	<div> <div>4%</div> <div>27% 54% 12% • 5%</div> </div>
1	D	777	<div> <div>4%</div> <div>28% 54% 12% • 5%</div> </div>
1	E	777	<div> <div>3%</div> <div>27% 54% 12% • 5%</div> </div>
1	F	777	<div> <div>4%</div> <div>26% 55% 12% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	O	149	
2	P	149	
2	Q	149	
2	R	149	
2	S	149	
2	T	149	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 42990 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 Calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	B	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	C	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	D	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	E	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	F	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	INITIATING METHIONINE	UNP P40136
A	25	HIS	-	EXPRESSION TAG	UNP P40136
A	26	HIS	-	EXPRESSION TAG	UNP P40136
A	27	HIS	-	EXPRESSION TAG	UNP P40136
A	28	HIS	-	EXPRESSION TAG	UNP P40136
A	29	HIS	-	EXPRESSION TAG	UNP P40136
A	30	HIS	-	EXPRESSION TAG	UNP P40136
A	31	ALA	-	CLONING ARTIFACT	UNP P40136
A	32	ALA	-	CLONING ARTIFACT	UNP P40136
B	24	MET	-	INITIATING METHIONINE	UNP P40136
B	25	HIS	-	EXPRESSION TAG	UNP P40136
B	26	HIS	-	EXPRESSION TAG	UNP P40136
B	27	HIS	-	EXPRESSION TAG	UNP P40136
B	28	HIS	-	EXPRESSION TAG	UNP P40136
B	29	HIS	-	EXPRESSION TAG	UNP P40136
B	30	HIS	-	EXPRESSION TAG	UNP P40136
B	31	ALA	-	CLONING ARTIFACT	UNP P40136

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	ALA	-	CLONING ARTIFACT	UNP P40136
C	24	MET	-	INITIATING METHIONINE	UNP P40136
C	25	HIS	-	EXPRESSION TAG	UNP P40136
C	26	HIS	-	EXPRESSION TAG	UNP P40136
C	27	HIS	-	EXPRESSION TAG	UNP P40136
C	28	HIS	-	EXPRESSION TAG	UNP P40136
C	29	HIS	-	EXPRESSION TAG	UNP P40136
C	30	HIS	-	EXPRESSION TAG	UNP P40136
C	31	ALA	-	CLONING ARTIFACT	UNP P40136
C	32	ALA	-	CLONING ARTIFACT	UNP P40136
D	24	MET	-	INITIATING METHIONINE	UNP P40136
D	25	HIS	-	EXPRESSION TAG	UNP P40136
D	26	HIS	-	EXPRESSION TAG	UNP P40136
D	27	HIS	-	EXPRESSION TAG	UNP P40136
D	28	HIS	-	EXPRESSION TAG	UNP P40136
D	29	HIS	-	EXPRESSION TAG	UNP P40136
D	30	HIS	-	EXPRESSION TAG	UNP P40136
D	31	ALA	-	CLONING ARTIFACT	UNP P40136
D	32	ALA	-	CLONING ARTIFACT	UNP P40136
E	24	MET	-	INITIATING METHIONINE	UNP P40136
E	25	HIS	-	EXPRESSION TAG	UNP P40136
E	26	HIS	-	EXPRESSION TAG	UNP P40136
E	27	HIS	-	EXPRESSION TAG	UNP P40136
E	28	HIS	-	EXPRESSION TAG	UNP P40136
E	29	HIS	-	EXPRESSION TAG	UNP P40136
E	30	HIS	-	EXPRESSION TAG	UNP P40136
E	31	ALA	-	CLONING ARTIFACT	UNP P40136
E	32	ALA	-	CLONING ARTIFACT	UNP P40136
F	24	MET	-	INITIATING METHIONINE	UNP P40136
F	25	HIS	-	EXPRESSION TAG	UNP P40136
F	26	HIS	-	EXPRESSION TAG	UNP P40136
F	27	HIS	-	EXPRESSION TAG	UNP P40136
F	28	HIS	-	EXPRESSION TAG	UNP P40136
F	29	HIS	-	EXPRESSION TAG	UNP P40136
F	30	HIS	-	EXPRESSION TAG	UNP P40136
F	31	ALA	-	CLONING ARTIFACT	UNP P40136
F	32	ALA	-	CLONING ARTIFACT	UNP P40136

- Molecule 2 is a protein called Calmodulin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			

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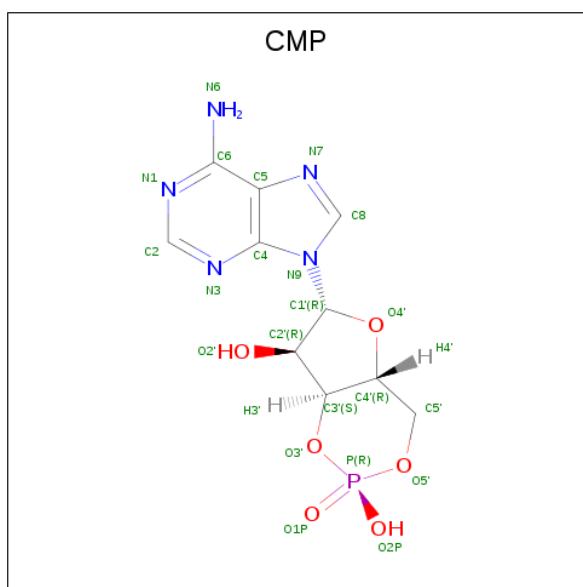
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			
2	Q	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			
2	R	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			
2	S	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			
2	T	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C₁₀H₁₂N₅O₆P).



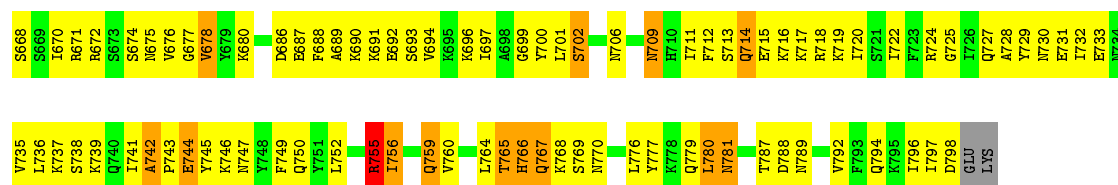
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

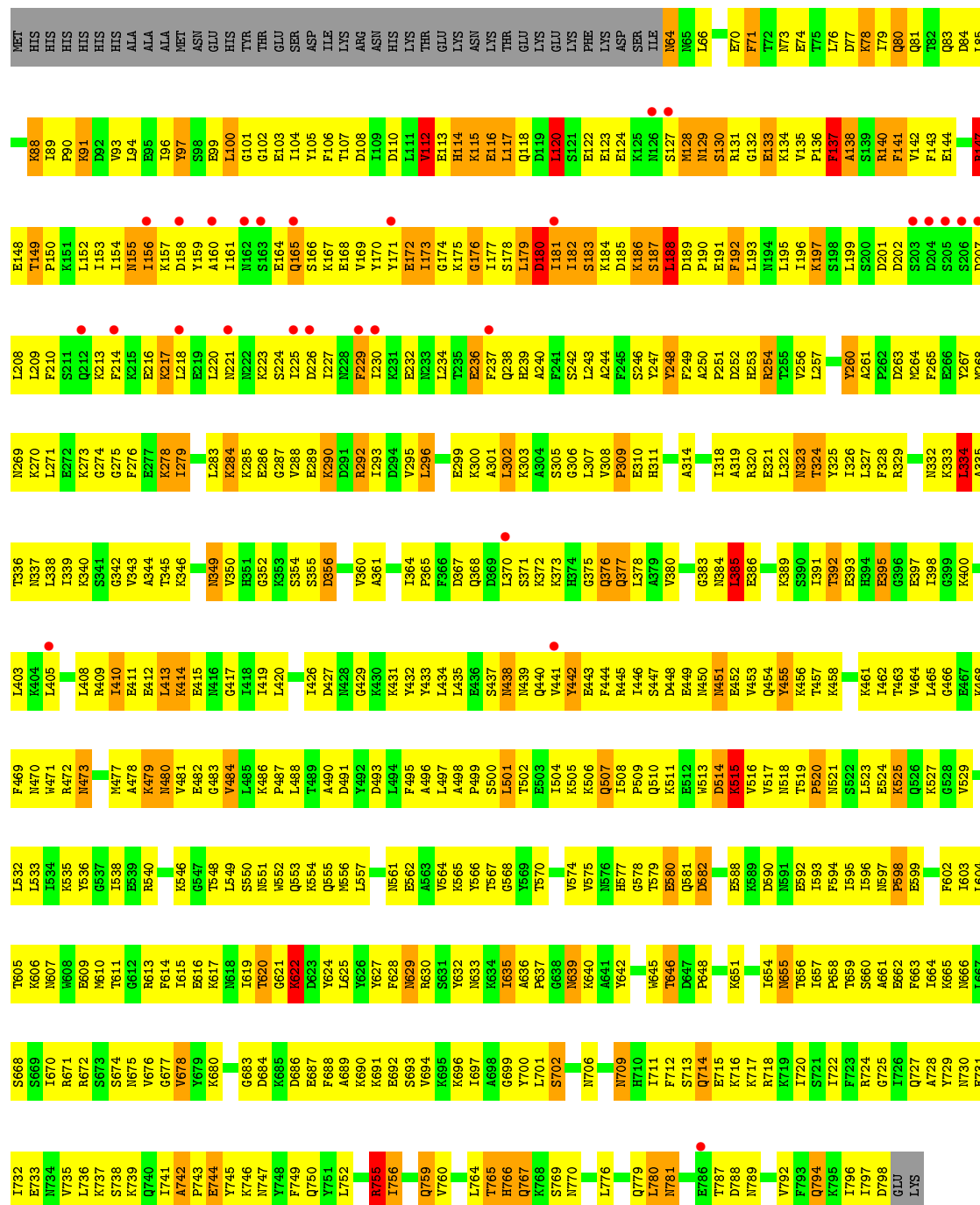
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	3	Total	Ca	0	0
			3	3		
5	Q	3	Total	Ca	0	0
			3	3		
5	T	3	Total	Ca	0	0
			3	3		
5	O	3	Total	Ca	0	0
			3	3		
5	R	3	Total	Ca	0	0
			3	3		
5	S	3	Total	Ca	0	0
			3	3		

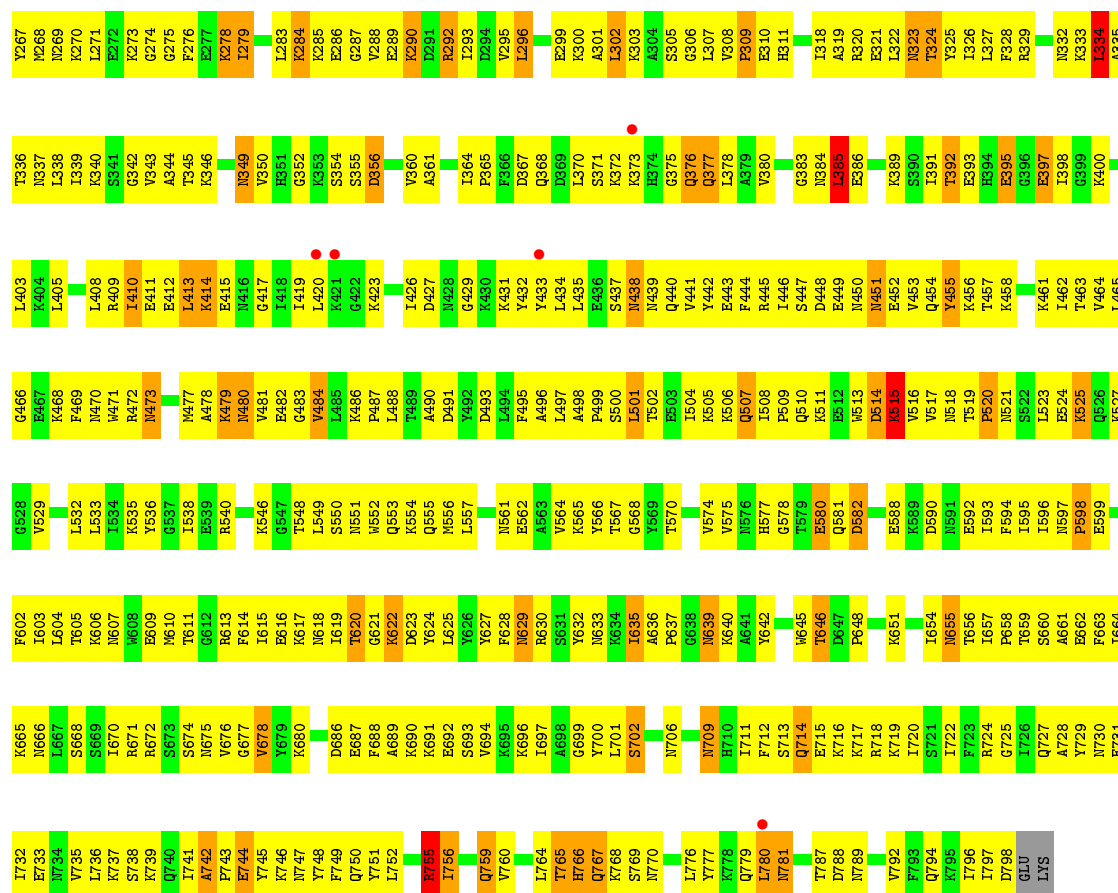
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		
6	E	1	Total	O	0	0
			1	1		
6	F	1	Total	O	0	0
			1	1		



• Molecule 1: Calmodulin-sensitive adenylate cyclase



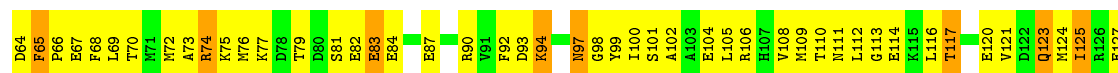


• Molecule 2: Calmodulin 2

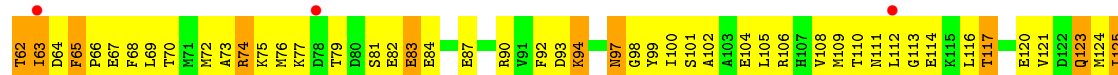
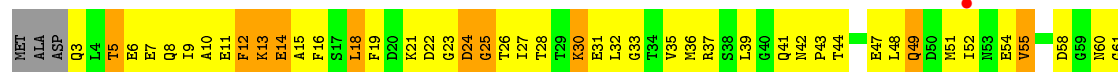




• Molecule 2: Calmodulin 2



• Molecule 2: Calmodulin 2

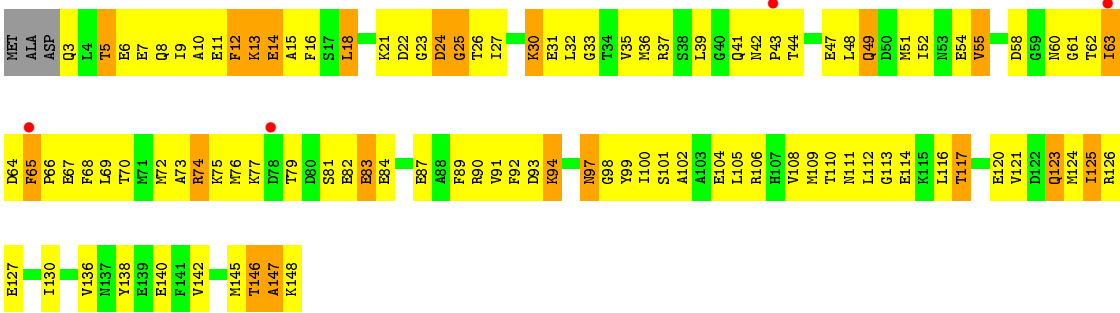


• Molecule 2: Calmodulin 2



• Molecule 2: Calmodulin 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	320.50Å 185.04Å 142.45Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	29.68 – 3.40 30.56 – 3.28	Depositor EDS
% Data completeness (in resolution range)	93.6 (29.68-3.40) 87.9 (30.56-3.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.266 , 0.283 0.248 , 0.264	Depositor DCC
R_{free} test set	6075 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	92.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.448 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.449 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.438 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.440 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.440 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	42990	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: CA, MG, CMP

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	0.54	0/6104	0.80	8/8208 (0.1%)
1	B	0.54	0/6104	0.82	10/8208 (0.1%)
1	C	0.57	3/6104 (0.0%)	0.81	7/8208 (0.1%)
1	D	0.55	0/6104	0.82	9/8208 (0.1%)
1	E	0.54	0/6104	0.81	9/8208 (0.1%)
1	F	0.55	0/6104	0.81	8/8208 (0.1%)
2	O	0.61	1/1158 (0.1%)	0.78	0/1553
2	P	0.61	1/1158 (0.1%)	0.78	0/1553
2	Q	0.61	1/1158 (0.1%)	0.79	0/1553
2	R	0.60	1/1158 (0.1%)	0.78	0/1553
2	S	0.61	1/1158 (0.1%)	0.79	0/1553
2	T	0.61	1/1158 (0.1%)	0.78	0/1553
All	All	0.56	9/43572 (0.0%)	0.81	51/58566 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	GLU	C-N	-6.32	1.19	1.34
1	C	261	ALA	C-N	5.87	1.45	1.34
2	S	42	ASN	N-CA	-5.57	1.35	1.46
2	T	42	ASN	N-CA	-5.55	1.35	1.46
2	P	42	ASN	N-CA	-5.54	1.35	1.46

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	188	LEU	N-CA-C	-7.80	89.94	111.00
1	D	188	LEU	N-CA-C	-7.80	89.95	111.00
1	A	188	LEU	N-CA-C	-7.79	89.96	111.00
1	C	188	LEU	N-CA-C	-7.79	89.97	111.00
1	E	188	LEU	N-CA-C	-7.79	89.98	111.00

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	5992	0	6010	790	0
1	B	5992	0	6010	797	0
1	C	5992	0	6009	781	0
1	D	5992	0	6010	781	0
1	E	5992	0	6010	784	0
1	F	5992	0	6010	782	0
2	O	1146	0	1071	138	0
2	P	1146	0	1071	144	0
2	Q	1146	0	1071	142	0
2	R	1146	0	1071	141	0
2	S	1146	0	1071	140	0
2	T	1146	0	1071	146	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	22	0	11	4	0
4	B	22	0	11	4	0
4	C	22	0	11	4	0
4	D	22	0	11	4	0
4	E	22	0	11	4	0
4	F	22	0	11	4	0
5	O	3	0	0	0	0
5	P	3	0	0	0	0
5	Q	3	0	0	0	0
5	R	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	42990	0	42551	5408	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 63.

The worst 5 of 5408 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)
4:A:901:CMP:C2	4:A:901:CMP:H2	0.97	1.49
4:D:904:CMP:C2	4:D:904:CMP:H2	0.97	1.49
4:B:902:CMP:H2	4:B:902:CMP:C2	0.97	1.48
4:C:903:CMP:H2	4:C:903:CMP:C2	0.97	1.48
4:F:906:CMP:H2	4:F:906:CMP:C2	0.97	1.47

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/777 (94%)	512 (70%)	172 (24%)	49 (7%)	1	8
1	B	733/777 (94%)	512 (70%)	172 (24%)	49 (7%)	1	8
1	C	733/777 (94%)	510 (70%)	172 (24%)	51 (7%)	1	7
1	D	733/777 (94%)	516 (70%)	168 (23%)	49 (7%)	1	8
1	E	733/777 (94%)	512 (70%)	171 (23%)	50 (7%)	1	8
1	F	733/777 (94%)	513 (70%)	169 (23%)	51 (7%)	1	7
2	O	144/149 (97%)	100 (69%)	35 (24%)	9 (6%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	144/149 (97%)	102 (71%)	33 (23%)	9 (6%)	1	9
2	Q	144/149 (97%)	102 (71%)	33 (23%)	9 (6%)	1	9
2	R	144/149 (97%)	102 (71%)	33 (23%)	9 (6%)	1	9
2	S	144/149 (97%)	102 (71%)	33 (23%)	9 (6%)	1	9
2	T	144/149 (97%)	100 (69%)	35 (24%)	9 (6%)	1	9
All	All	5262/5556 (95%)	3683 (70%)	1226 (23%)	353 (7%)	1	8

5 of 353 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PHE
1	A	183	SER
1	A	377	GLN
1	A	510	GLN
1	A	787	THR

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	664/705 (94%)	575 (87%)	89 (13%)	4	15
1	B	664/705 (94%)	569 (86%)	95 (14%)	3	13
1	C	664/705 (94%)	574 (86%)	90 (14%)	3	14
1	D	664/705 (94%)	572 (86%)	92 (14%)	3	13
1	E	664/705 (94%)	571 (86%)	93 (14%)	3	13
1	F	664/705 (94%)	570 (86%)	94 (14%)	3	13
2	O	123/127 (97%)	104 (85%)	19 (15%)	2	11
2	P	123/127 (97%)	104 (85%)	19 (15%)	2	11
2	Q	123/127 (97%)	104 (85%)	19 (15%)	2	11
2	R	123/127 (97%)	104 (85%)	19 (15%)	2	11
2	S	123/127 (97%)	105 (85%)	18 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	123/127 (97%)	105 (85%)	18 (15%)	3	12
All	All	4722/4992 (95%)	4057 (86%)	665 (14%)	3	13

5 of 665 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	186	LYS
1	E	114	HIS
2	R	30	LYS
1	D	254	ARG
1	D	501	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 199 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	785	ASN
1	D	576	ASN
1	F	781	ASN
1	C	794	GLN
1	D	337	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 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
4	CMP	D	904	3	22,25,25	3.06	7 (31%)	24,39,39	1.90	5 (20%)
4	CMP	F	906	3	22,25,25	3.03	6 (27%)	24,39,39	1.96	6 (25%)
4	CMP	A	901	-	22,25,25	3.02	6 (27%)	24,39,39	1.99	7 (29%)
4	CMP	B	902	3	22,25,25	3.06	7 (31%)	24,39,39	1.90	7 (29%)
4	CMP	E	905	3	22,25,25	3.09	7 (31%)	24,39,39	1.94	5 (20%)
4	CMP	C	903	3	22,25,25	3.06	6 (27%)	24,39,39	1.90	5 (20%)

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	CMP	D	904	3	-	0/0/31/31	0/4/4/4
4	CMP	F	906	3	-	0/0/31/31	0/4/4/4
4	CMP	A	901	-	-	0/0/31/31	0/4/4/4
4	CMP	B	902	3	-	0/0/31/31	0/4/4/4
4	CMP	E	905	3	-	0/0/31/31	0/4/4/4
4	CMP	C	903	3	-	0/0/31/31	0/4/4/4

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	905	CMP	P-O5'	11.97	1.71	1.57
4	D	904	CMP	P-O5'	11.95	1.71	1.57
4	C	903	CMP	P-O5'	11.89	1.71	1.57
4	B	902	CMP	P-O5'	11.82	1.71	1.57
4	A	901	CMP	P-O5'	11.63	1.70	1.57

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	CMP	O3'-C3'-C4'	5.59	114.93	110.71
4	F	906	CMP	O3'-C3'-C4'	5.48	114.84	110.71
4	E	905	CMP	O3'-C3'-C4'	5.40	114.78	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	CMP	O3'-C3'-C4'	5.27	114.69	110.71
4	D	904	CMP	O3'-C3'-C4'	5.24	114.67	110.71

There are no chirality outliers.

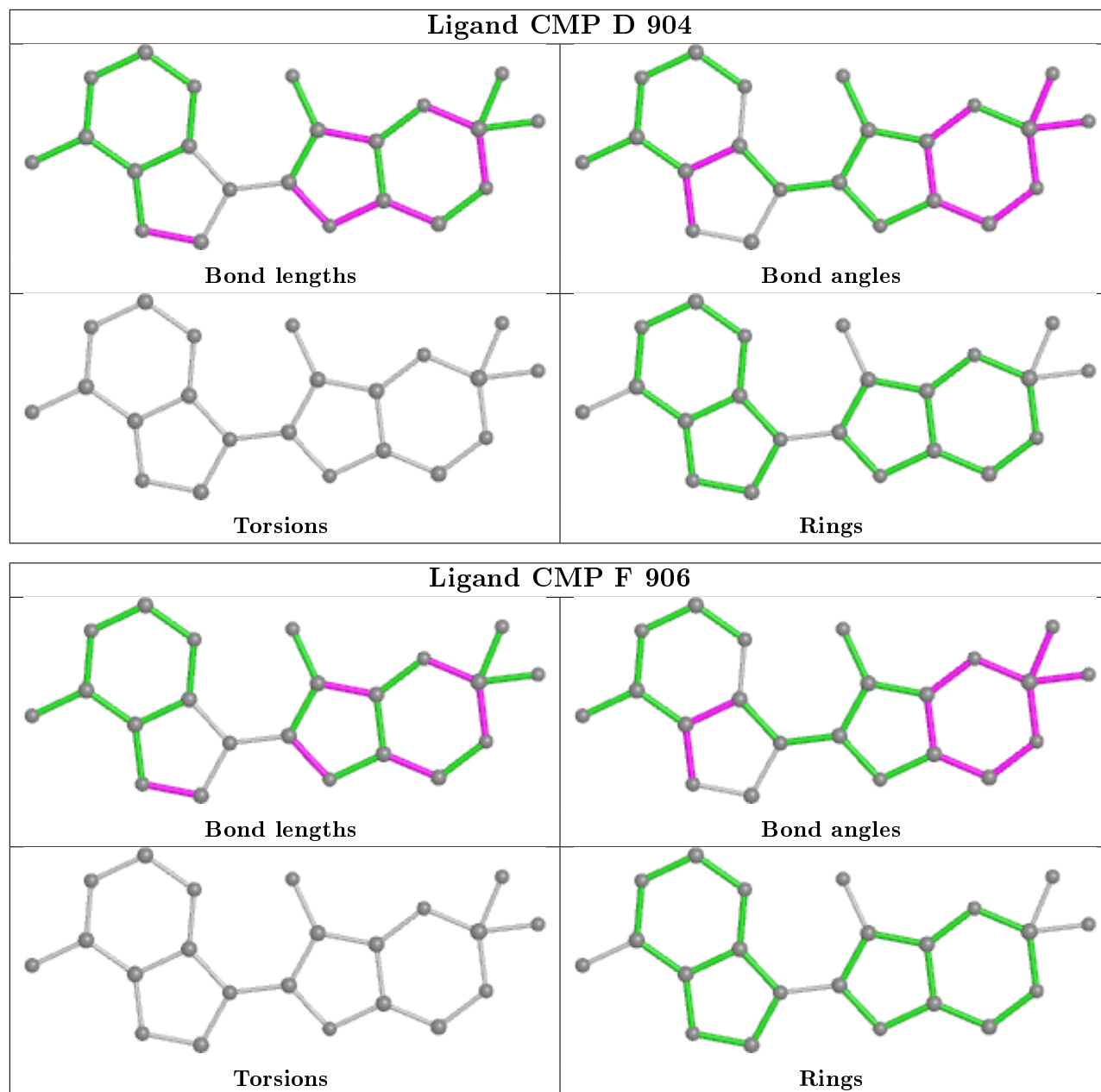
There are no torsion outliers.

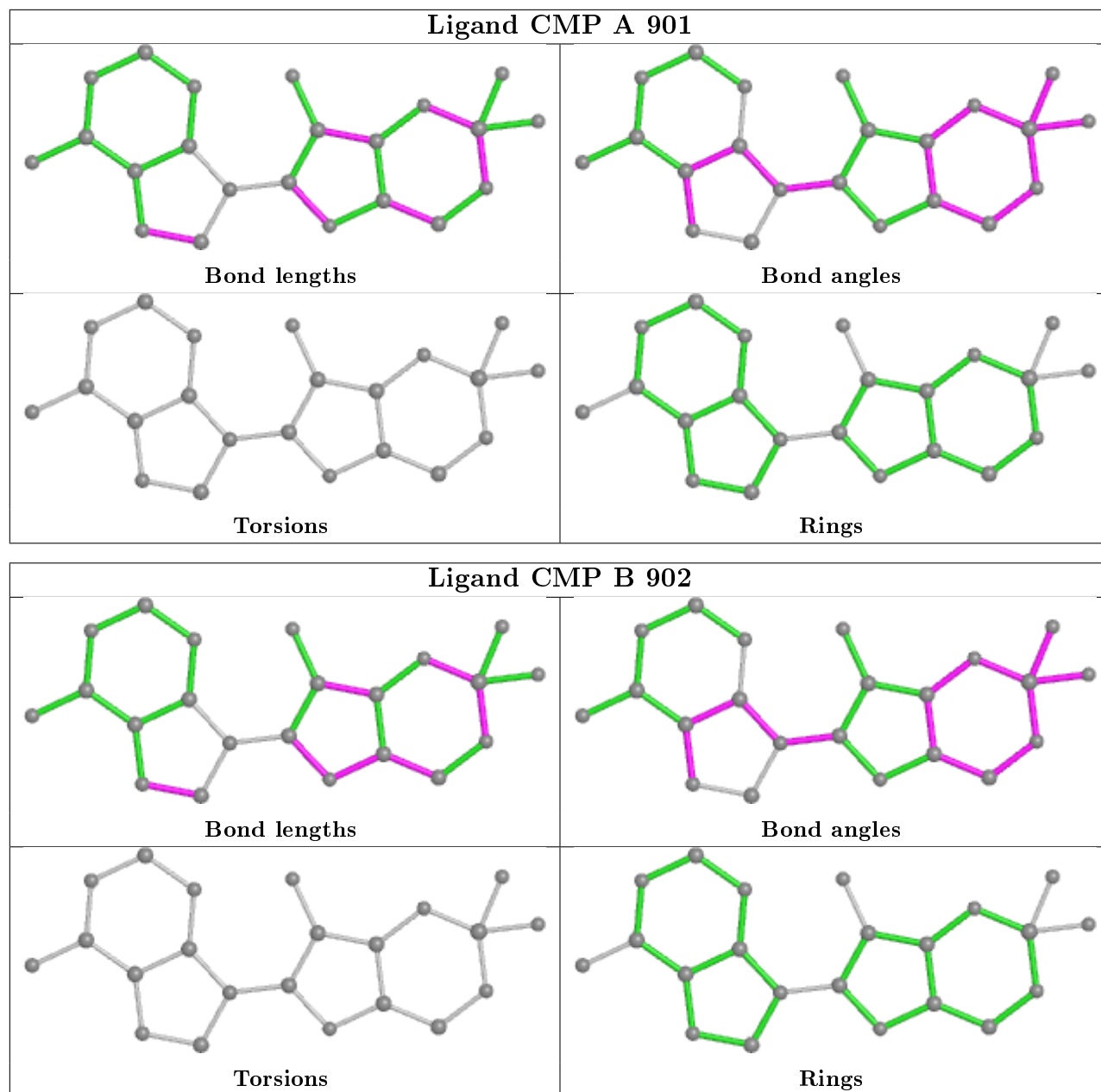
There are no ring outliers.

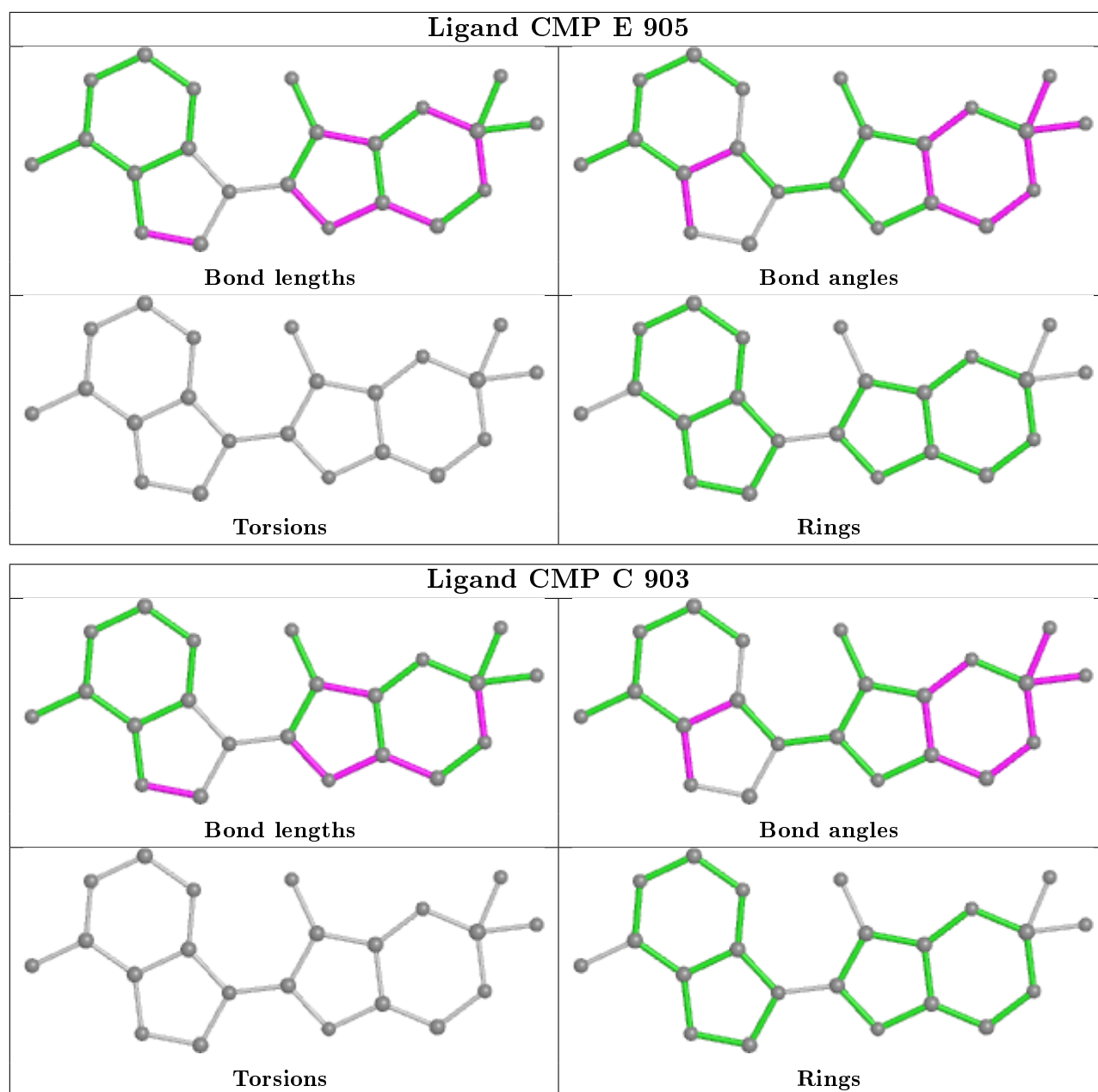
6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	904	CMP	4	0
4	F	906	CMP	4	0
4	A	901	CMP	4	0
4	B	902	CMP	4	0
4	E	905	CMP	4	0
4	C	903	CMP	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	123:GLU	C	124:GLU	N	1.19

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	735/777 (94%)	0.23	31 (4%) 36 35	18, 73, 128, 137	0
1	B	735/777 (94%)	0.23	28 (3%) 40 39	18, 73, 128, 138	0
1	C	735/777 (94%)	0.26	34 (4%) 32 32	17, 73, 128, 138	0
1	D	735/777 (94%)	0.24	30 (4%) 37 36	17, 73, 127, 137	0
1	E	735/777 (94%)	0.23	27 (3%) 41 40	17, 72, 127, 137	0
1	F	735/777 (94%)	0.22	29 (3%) 39 38	19, 73, 127, 138	0
2	O	146/149 (97%)	0.08	4 (2%) 54 53	17, 60, 119, 124	0
2	P	146/149 (97%)	0.09	3 (2%) 63 62	17, 60, 119, 124	0
2	Q	146/149 (97%)	0.08	2 (1%) 75 74	17, 60, 119, 123	0
2	R	146/149 (97%)	0.07	4 (2%) 54 53	16, 60, 119, 123	0
2	S	146/149 (97%)	0.14	4 (2%) 54 53	17, 60, 119, 123	0
2	T	146/149 (97%)	0.10	4 (2%) 54 53	16, 60, 119, 124	0
All	All	5286/5556 (95%)	0.21	200 (3%) 40 39	16, 70, 126, 138	0

The worst 5 of 200 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	ASN	17.4
1	D	162	ASN	9.9
1	A	163	SER	9.5
1	B	204	ASP	8.8
1	F	230	ILE	8.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.

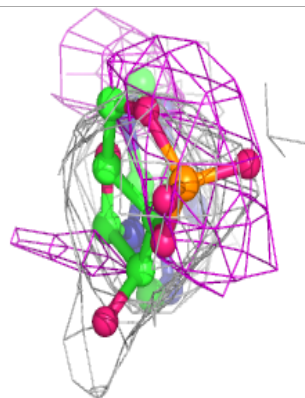
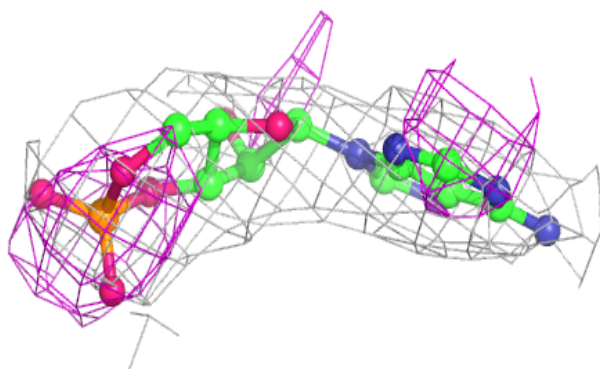
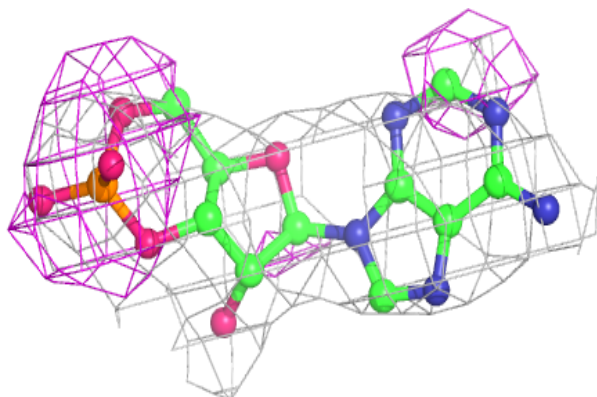
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	Q	705	1/1	0.82	0.15	76,76,76,76	0
4	CMP	F	906	22/22	0.86	0.39	48,63,84,93	0
4	CMP	B	902	22/22	0.88	0.42	49,63,81,89	0
4	CMP	E	905	22/22	0.89	0.39	47,63,84,91	0
4	CMP	A	901	22/22	0.89	0.36	48,65,85,93	0
5	CA	T	711	1/1	0.90	0.11	79,79,79,79	0
4	CMP	D	904	22/22	0.90	0.33	48,62,81,86	0
4	CMP	C	903	22/22	0.90	0.51	48,63,81,92	0
5	CA	O	701	1/1	0.91	0.12	81,81,81,81	0
5	CA	S	709	1/1	0.91	0.08	78,78,78,78	0
5	CA	P	703	1/1	0.94	0.13	76,76,76,76	0
5	CA	O	802	1/1	0.96	0.18	47,47,47,47	0
5	CA	R	707	1/1	0.97	0.11	69,69,69,69	0
5	CA	R	807	1/1	0.97	0.13	29,29,29,29	0
3	MG	E	904	1/1	0.97	0.16	17,17,17,17	0
5	CA	T	811	1/1	0.97	0.14	26,26,26,26	0
3	MG	F	905	1/1	0.97	0.21	15,15,15,15	0
5	CA	Q	806	1/1	0.97	0.19	51,51,51,51	0
5	CA	S	809	1/1	0.97	0.14	26,26,26,26	0
3	MG	D	903	1/1	0.98	0.14	14,14,14,14	0
5	CA	P	803	1/1	0.98	0.17	30,30,30,30	0
5	CA	O	801	1/1	0.98	0.14	27,27,27,27	0
5	CA	T	812	1/1	0.98	0.18	54,54,54,54	0
5	CA	R	808	1/1	0.98	0.16	47,47,47,47	0
3	MG	C	902	1/1	0.98	0.14	17,17,17,17	0
5	CA	Q	805	1/1	0.99	0.19	29,29,29,29	0
3	MG	B	901	1/1	0.99	0.12	27,27,27,27	0
5	CA	P	804	1/1	0.99	0.18	47,47,47,47	0
5	CA	S	810	1/1	0.99	0.17	51,51,51,51	0
3	MG	A	900	1/1	0.99	0.18	13,13,13,13	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.

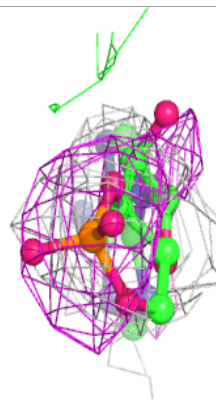
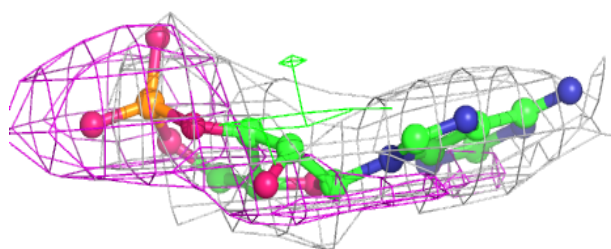
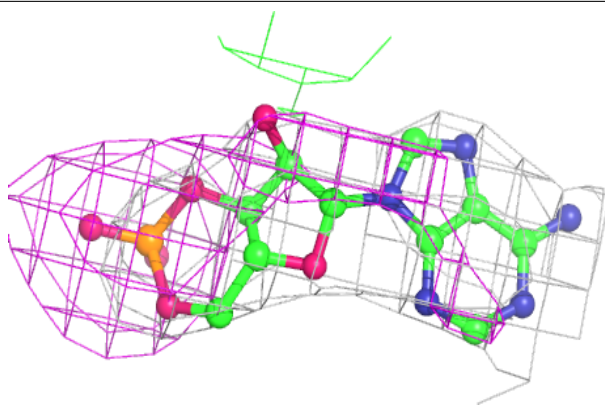
Electron density around CMP F 906:

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

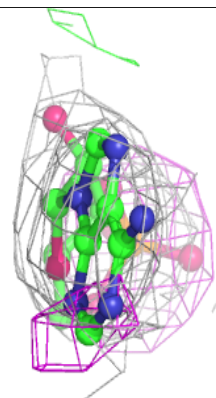
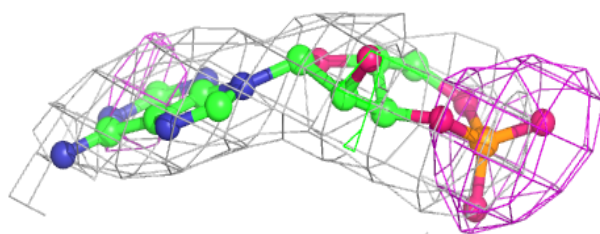
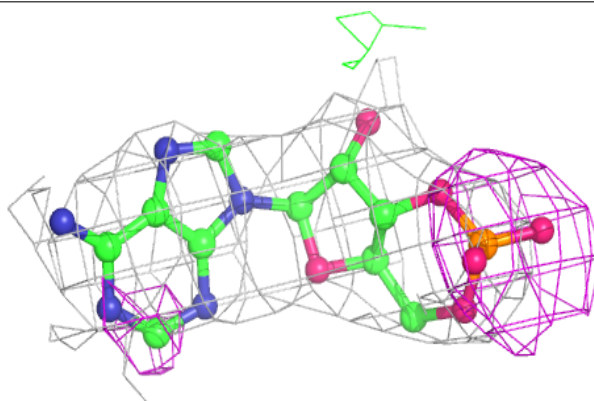


Electron density around CMP B 902:

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

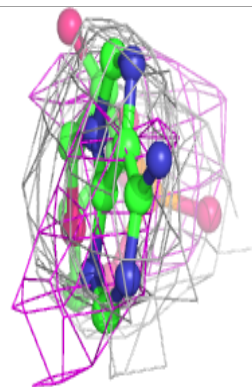
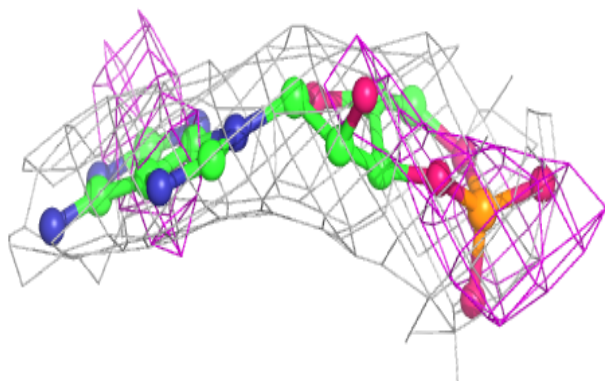
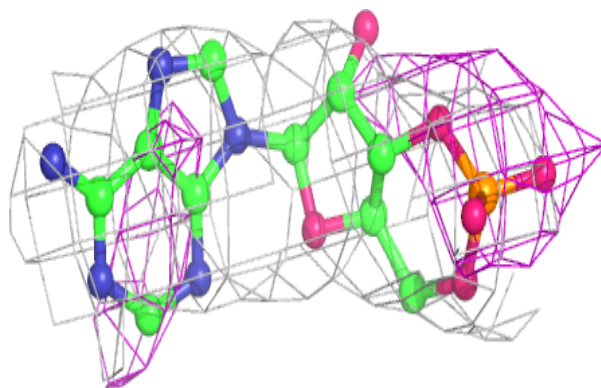
**Electron density around CMP E 905:**

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

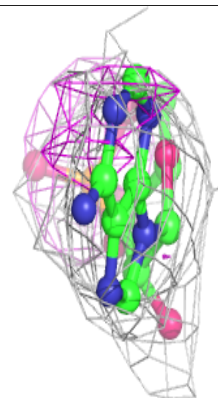
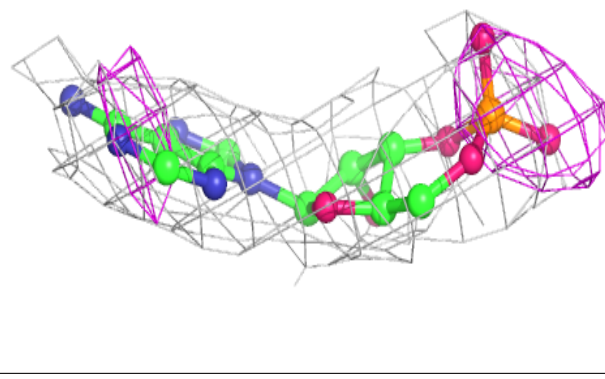
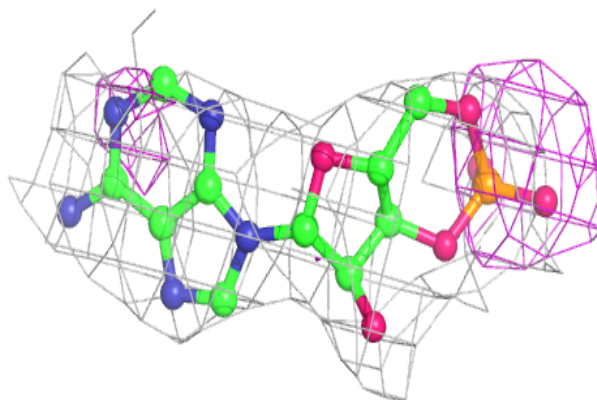


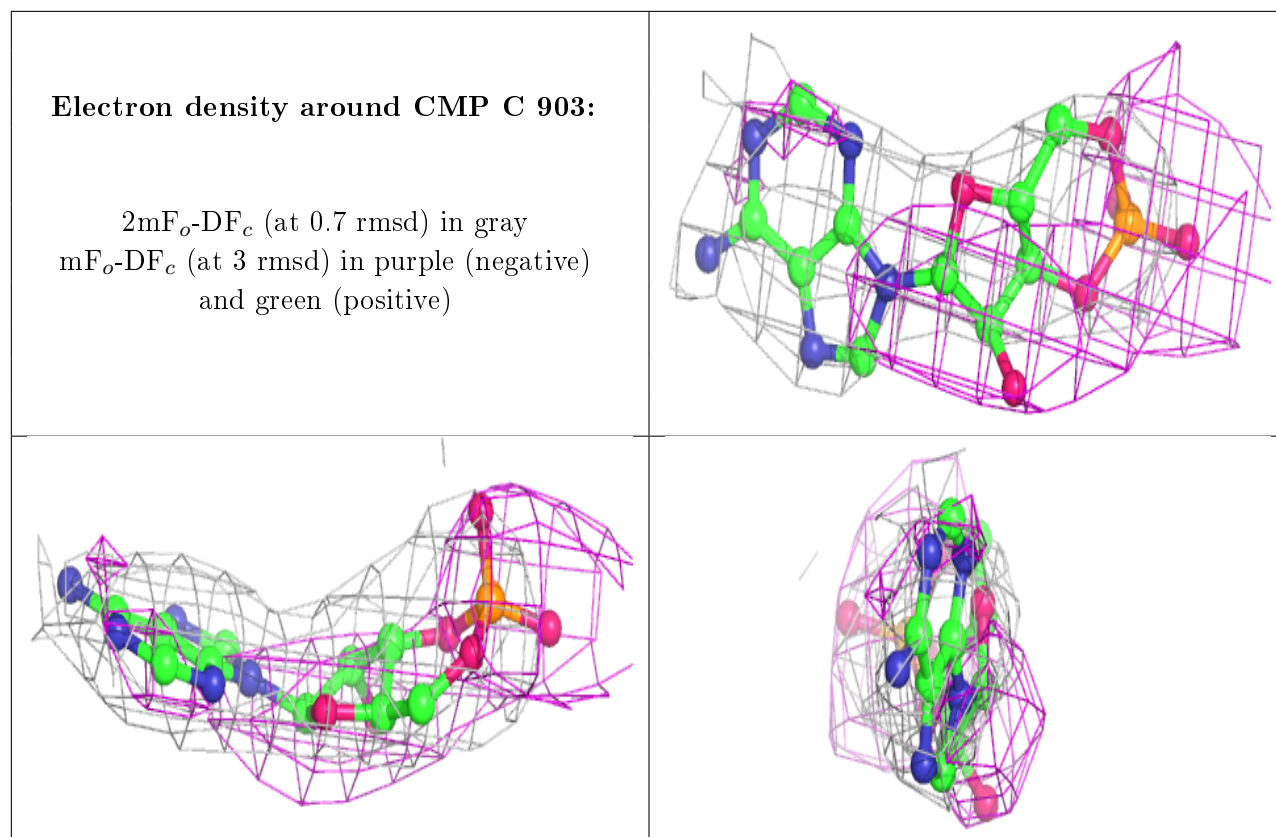
Electron density around CMP A 901:

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

**Electron density around CMP D 904:**

$2mF_o-DF_c$ (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.