

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 31, 2023 - 04:53 PM EDT

PDB ID	:	3JQQ
Title	:	Crystal structure of the H286K mutant of Ferredoxin-NADP+ reductase from
		Plasmodium falciparum in complex with 2'P-AMP
Authors	:	Canevari, G.; Milani, M.; Bolognesi, M.
Deposited on	:	2009-09-07
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

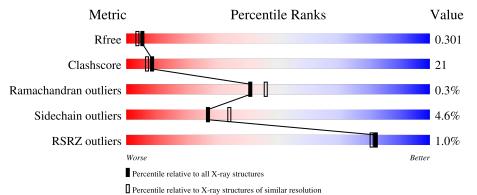
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	А	316	% 61%	20%	·	17%				
1	В	316	% 62%	19%	•	17%				
1	С	316	% 64%	19%	•	16%				
1	D	316	60%	19%	5%	16%				
1	Е	316	57%	21%	•	20%				



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Mol	Chain	Length	Quality	of chain		
1	F	216	2%			
	Г	310	51%	28%	•	20%



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14736 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	261	Total	С	Ν	Ο	S	0	0	0
1	Л	201	2188	1421	360	398	9	0	0	0
1	В	263	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	D	200	2207	1436	361	401	9	0	0	0
1	С	267	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	U	201	2227	1443	367	408	9	0	0	0
1	D	267	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	D	201	2227	1443	366	409	9	0	0	0
1	Е	253	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	Ľ	200	2121	1382	346	384	9	0	0	0
1	F	254	Total	С	Ν	Ο	S	0	0	0
		254	2126	1382	348	387	9		0	0

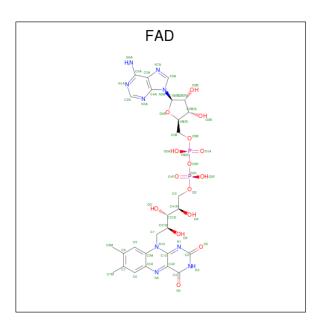
• Molecule 1 is a protein called Ferredoxin NADP reductase.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LYS	HIS	engineered mutation	UNP C6KT68
В	286	LYS	HIS	engineered mutation	UNP C6KT68
С	286	LYS	HIS	engineered mutation	UNP C6KT68
D	286	LYS	HIS	engineered mutation	UNP C6KT68
Е	286	LYS	HIS	engineered mutation	UNP C6KT68
F	286	LYS	HIS	engineered mutation	UNP C6KT68

• Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

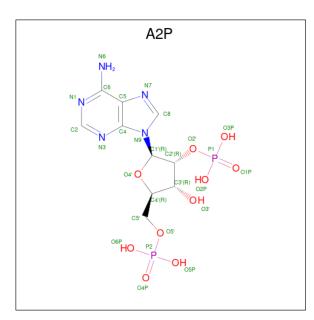




Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
2	А	1	Total	С	Ν	Ο	Р	0	0
	A	1	53	27	9	15	2	0	0
2	В	1	Total	С	Ν	Ο	Р	0	0
	D	1	53	27	9	15	2	0	0
2	С	1	Total	С	Ν	Ο	Р	0	0
	U	1	53	27	9	15	2	0	0
2	D	1	Total	С	Ν	Ο	Р	0	0
	D	1	53	27	9	15	2	0	0
2	Е	1	Total	С	Ν	Ο	Р	0	0
	Ľ	1	53	27	9	15	2	0	0
2	F	1	Total	С	Ν	Ο	Р	0	0
	T,	1	53	27	9	15	2	0	0

• Molecule 3 is ADENOSINE-2'-5'-DIPHOSPHATE (three-letter code: A2P) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
3	А	1	Total	С	Ν	Ο	Р	0	0
5	A	1	27	10	5	10	2	0	0
3	В	1	Total	С	Ν	Ο	Р	0	0
5	D	1	27	10	5	10	2	0	0
3	С	1	Total	С	Ν	Ο	Р	0	0
5	U	T	27	10	5	10	2	0	0
3	Л	1	Total	С	Ν	Ο	Р	0	0
0	D	T	27	10	5	10	2	0	0
3	Е	1	Total	С	Ν	Ο	Р	0	0
0	Ľ	I	27	10	5	10	2	0	0
3	F	1	Total	С	Ν	Ō	Р	0	0
	Ľ	1	27	10	5	10	2	0	0

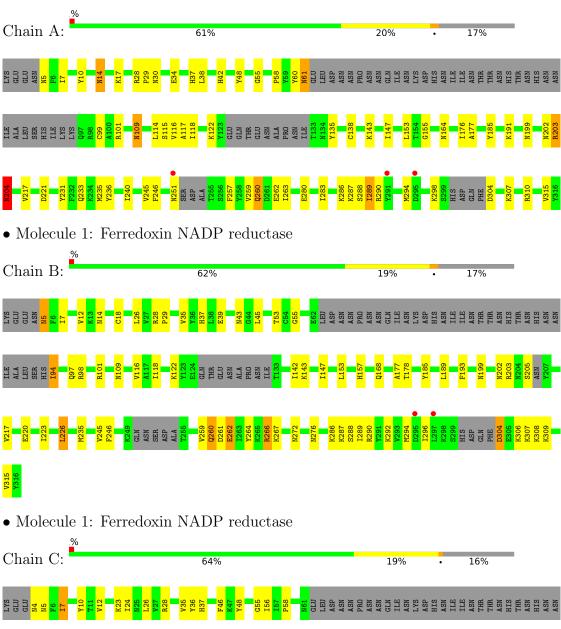
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	194	Total O 194 194	0	0
4	В	223	Total         O           223         223	0	0
4	С	221	Total         O           221         221	0	0
4	D	198	Total O 198 198	0	0
4	Е	152	Total O 152 152	0	0
4	F	172	Total O 172 172	0	0



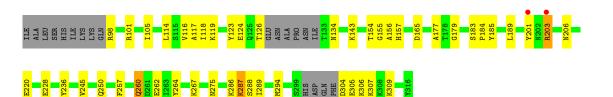
# 3 Residue-property plots (i)

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.

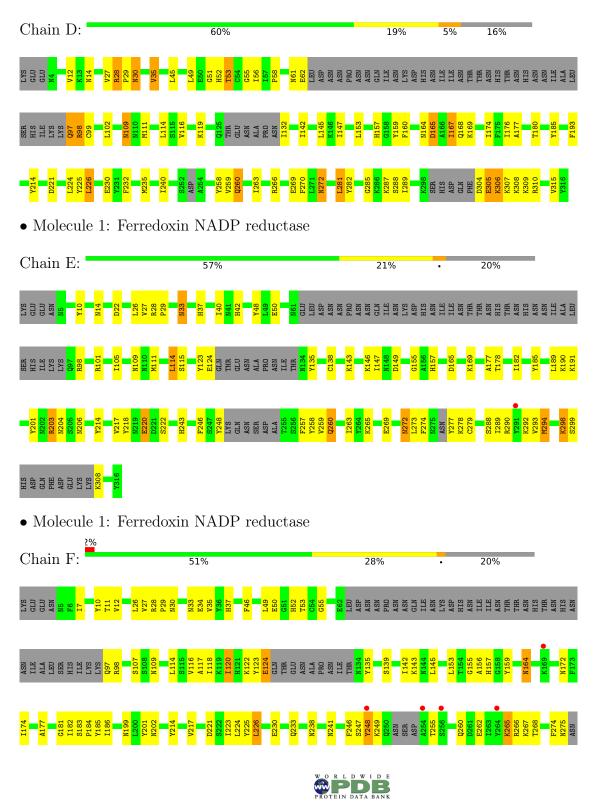


• Molecule 1: Ferredoxin NADP reductase





• Molecule 1: Ferredoxin NADP reductase







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants	124.24Å $124.24$ Å $134.25$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	62.12 - 2.20	Depositor
Resolution (A)	62.12 - 2.20	EDS
% Data completeness	100.0 (62.12-2.20)	Depositor
(in resolution range)	$100.0\ (62.12-2.20)$	EDS
R <sub>merge</sub>	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.96 (at 2.20 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
D D	0.256 , $0.308$	Depositor
$R, R_{free}$	0.254 , $0.301$	DCC
$R_{free}$ test set	5894 reflections $(5.01\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.0	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, $32.7$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
	0.000 for -h,-k,l	
Estimated twinning fraction	0.458 for h,-h-k,-l	Xtriage
	0.000 for -k,-h,-l	
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14736	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 37.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4690e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD,  $\rm A2P$ 

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	Bo	nd lengths	Bond angles		
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.36	0/2240	0.47	0/3019	
1	В	0.32	0/2258	0.47	0/3039	
1	С	0.41	1/2280~(0.0%)	0.48	0/3076	
1	D	0.34	0/2279	0.49	0/3073	
1	Е	0.32	0/2172	0.46	0/2928	
1	F	0.34	0/2177	0.47	0/2934	
All	All	0.35	1/13406~(0.0%)	0.47	0/18069	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	236	TYR	CD2-CE2	-5.62	1.30	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

#### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2188	0	2154	73	0
1	В	2207	0	2182	81	0
1	С	2227	0	2183	75	0
1	D	2227	0	2178	101	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
1	Ε	2121	0	2083	105	0		
1	F	2126	0	2076	134	0		
2	А	53	0	31	1	0		
2	В	53	0	31	0	0		
2	С	53	0	31	1	0		
2	D	53	0	31	0	0		
2	Ε	53	0	31	0	0		
2	F	53	0	31	0	0		
3	А	27	0	11	4	0		
3	В	27	0	11	4	0		
3	С	27	0	11	5	0		
3	D	27	0	11	2	0		
3	Ε	27	0	11	7	0		
3	F	27	0	11	1	0		
4	А	194	0	0	10	0		
4	В	223	0	0	22	0		
4	$\mathbf{C}$	221	0	0	12	0		
4	D	198	0	0	12	0		
4	Ε	152	0	0	17	0		
4	F	172	0	0	24	0		
All	All	14736	0	13108	556	0		

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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 21.

The worst 5 of 556 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:E:294:MET:CE	1:E:294:MET:HA	1.60	1.32
1:D:305:GLU:CG	1:D:307:LYS:HG3	1.66	1.25
1:F:294:MET:O	1:F:295:ASP:OD1	1.65	1.12
1:C:305:GLU:HG2	1:C:306:LYS:N	1.44	1.12
1:D:306:LYS:CG	1:D:309:LYS:HD3	1.79	1.12

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	Perce	ntiles
1	А	251/316~(79%)	241 (96%)	8(3%)	2(1%)	19	19
1	В	251/316~(79%)	240 (96%)	11 (4%)	0	100	100
1	С	259/316~(82%)	249 (96%)	10 (4%)	0	100	100
1	D	257/316~(81%)	247 (96%)	8(3%)	2(1%)	19	19
1	Е	241/316~(76%)	236~(98%)	5(2%)	0	100	100
1	F	242/316~(77%)	231 (96%)	11 (4%)	0	100	100
All	All	1501/1896~(79%)	1444 (96%)	53~(4%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	305	GLU
1	А	204	ASN
1	D	306	LYS
1	А	289	ILE

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Percentiles		
1	А	243/295~(82%)	234~(96%)	9~(4%)	34 43	
1	В	245/295~(83%)	231 (94%)	14 (6%)	20 24	
1	С	246/295~(83%)	237~(96%)	9~(4%)	34 43	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	D	246/295~(83%)	230~(94%)	16 (6%)	17 19		
1	Ε	235/295~(80%)	224~(95%)	11 (5%)	26 33		
1	F	234/295~(79%)	226~(97%)	8 (3%)	37 47		
All	All	1449/1770~(82%)	1382~(95%)	67 (5%)	27 34		

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5 of 67 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	Ε	298	LYS
1	F	120	ILE
1	F	248	TYR
1	С	28	ARG
1	С	7	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	D	8	ASN
1	Е	8	ASN
1	D	41	ASN
1	D	241	ASN
1	Е	33	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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

12 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	Turne	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
	Type	Chain	in nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	A2P	D	416	-	$25,\!29,\!29$	0.96	1 (4%)	31,45,45	1.24	2 (6%)
3	A2P	F	416	-	$25,\!29,\!29$	0.93	1 (4%)	31,45,45	1.28	3 (9%)
3	A2P	А	416	-	25,29,29	0.93	1 (4%)	31,45,45	1.21	1 (3%)
2	FAD	D	415	-	$53,\!58,\!58$	1.17	4 (7%)	68,89,89	1.31	11 (16%)
2	FAD	А	415	-	$53,\!58,\!58$	1.13	4 (7%)	68,89,89	1.37	11 (16%)
2	FAD	F	415	-	$53,\!58,\!58$	1.13	4 (7%)	68,89,89	1.32	10 (14%)
2	FAD	В	415	-	$53,\!58,\!58$	1.13	4 (7%)	68,89,89	1.40	10 (14%)
2	FAD	С	415	-	$53,\!58,\!58$	1.16	4 (7%)	68,89,89	1.38	11 (16%)
3	A2P	В	416	-	25,29,29	0.95	1 (4%)	31,45,45	1.26	2 (6%)
3	A2P	С	416	-	25,29,29	0.96	1 (4%)	31,45,45	1.28	2 (6%)
2	FAD	Е	415	-	$53,\!58,\!58$	1.14	4 (7%)	68,89,89	1.35	9 (13%)
3	A2P	Е	416	-	25,29,29	0.95	1 (4%)	31,45,45	1.31	2 (6%)

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	A2P	D	416	-	-	2/11/31/31	0/3/3/3
3	A2P	F	416	-	-	2/11/31/31	0/3/3/3
3	A2P	А	416	-	-	2/11/31/31	0/3/3/3
2	FAD	D	415	-	-	1/30/50/50	0/6/6/6
2	FAD	А	415	-	-	2/30/50/50	0/6/6/6
2	FAD	F	415	-	-	3/30/50/50	0/6/6/6
2	FAD	В	415	-	-	4/30/50/50	0/6/6/6
2	FAD	С	415	-	-	4/30/50/50	0/6/6/6



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2P	В	416	-	-	3/11/31/31	0/3/3/3
3	A2P	С	416	-	-	2/11/31/31	0/3/3/3
2	FAD	Е	415	-	-	0/30/50/50	0/6/6/6
3	A2P	Е	416	-	-	0/11/31/31	0/3/3/3

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The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	415	FAD	C2A-N3A	4.34	1.39	1.32
2	С	415	FAD	C4X-N5	4.01	1.38	1.30
2	С	415	FAD	C2A-N3A	4.01	1.38	1.32
2	А	415	FAD	C4X-N5	3.97	1.38	1.30
2	Ε	415	FAD	C2A-N3A	3.96	1.38	1.32

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	415	FAD	N3A-C2A-N1A	-5.51	120.06	128.68
2	С	415	FAD	N3A-C2A-N1A	-5.50	120.08	128.68
2	Е	415	FAD	N3A-C2A-N1A	-5.49	120.09	128.68
2	F	415	FAD	N3A-C2A-N1A	-5.40	120.24	128.68
2	В	415	FAD	N3A-C2A-N1A	-5.36	120.29	128.68

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	415	FAD	C1'-C2'-C3'-C4'
2	С	415	FAD	C1'-C2'-C3'-C4'
3	А	416	A2P	C2'-O2'-P1-O1P
3	В	416	A2P	C2'-O2'-P1-O1P
3	D	416	A2P	C2'-O2'-P1-O1P

There are no ring outliers.

8 monomers are involved in 25 short contacts:

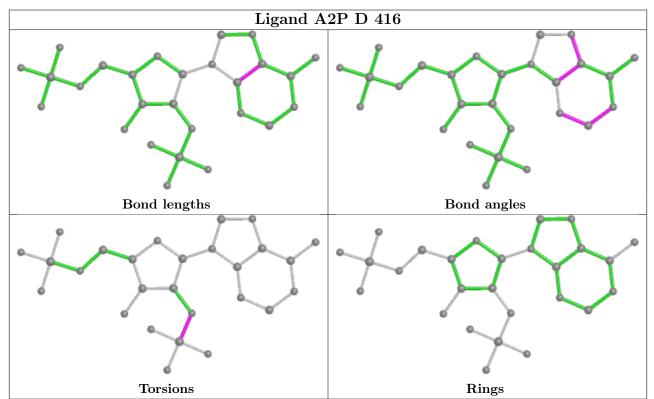
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	416	A2P	2	0
3	F	416	A2P	1	0
3	А	416	A2P	4	0



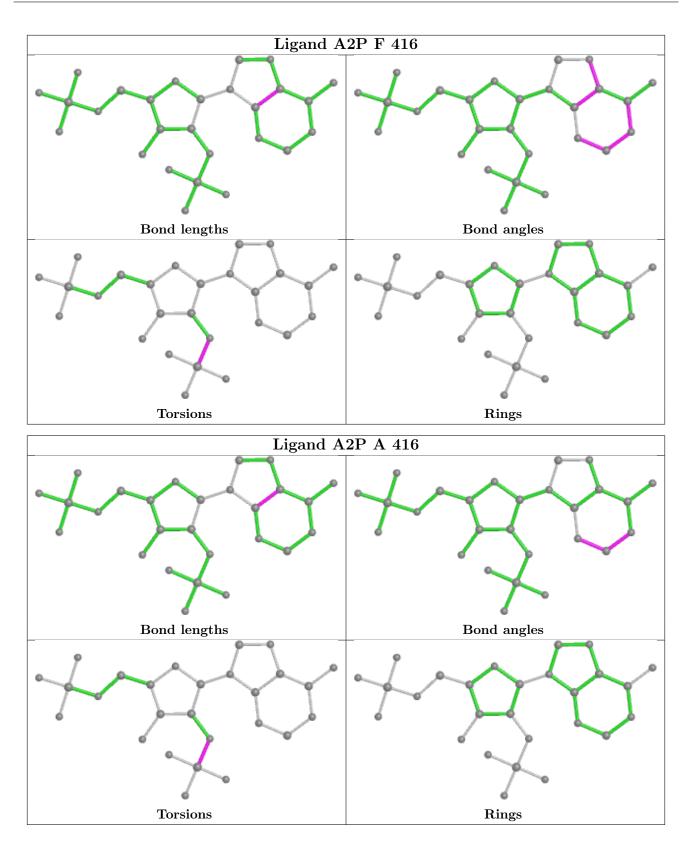
	5	1	1 5		
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	415	FAD	1	0
2	С	415	FAD	1	0
3	В	416	A2P	4	0
3	С	416	A2P	5	0
3	Е	416	A2P	7	0

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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 then 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.

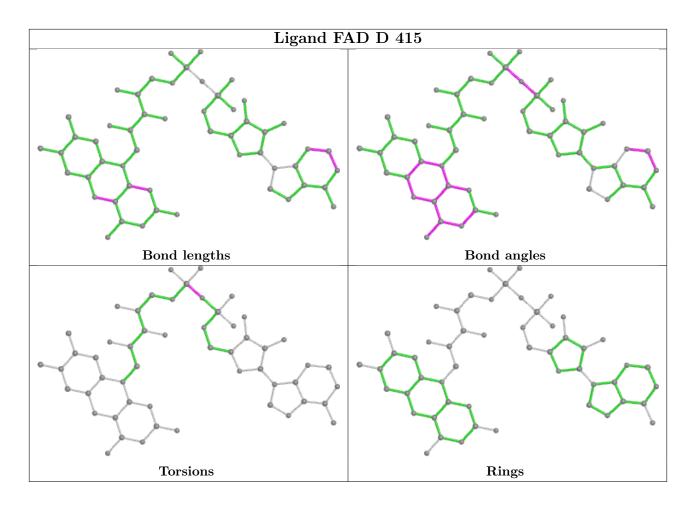






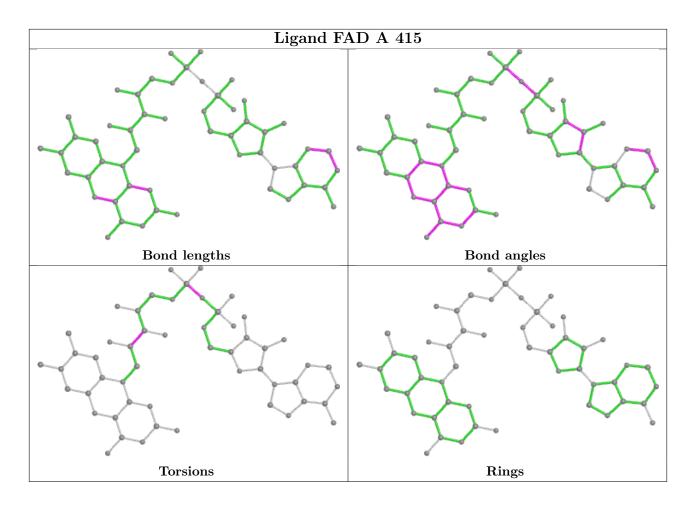






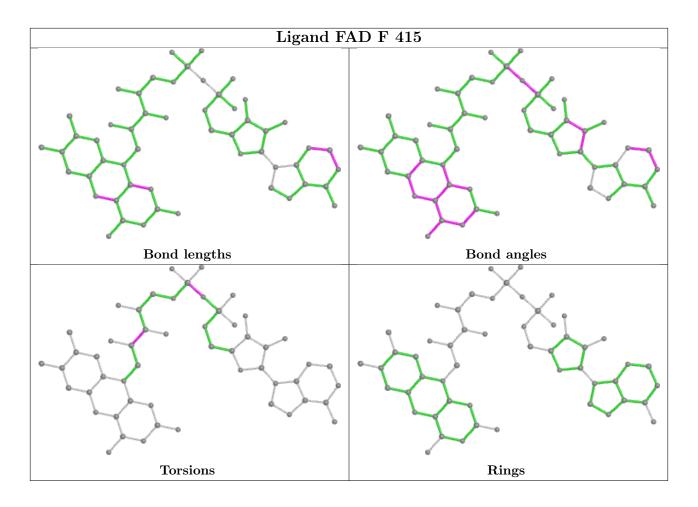






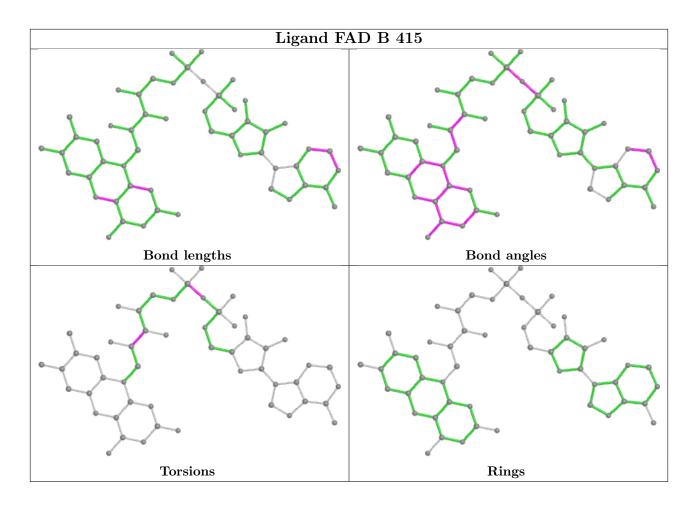






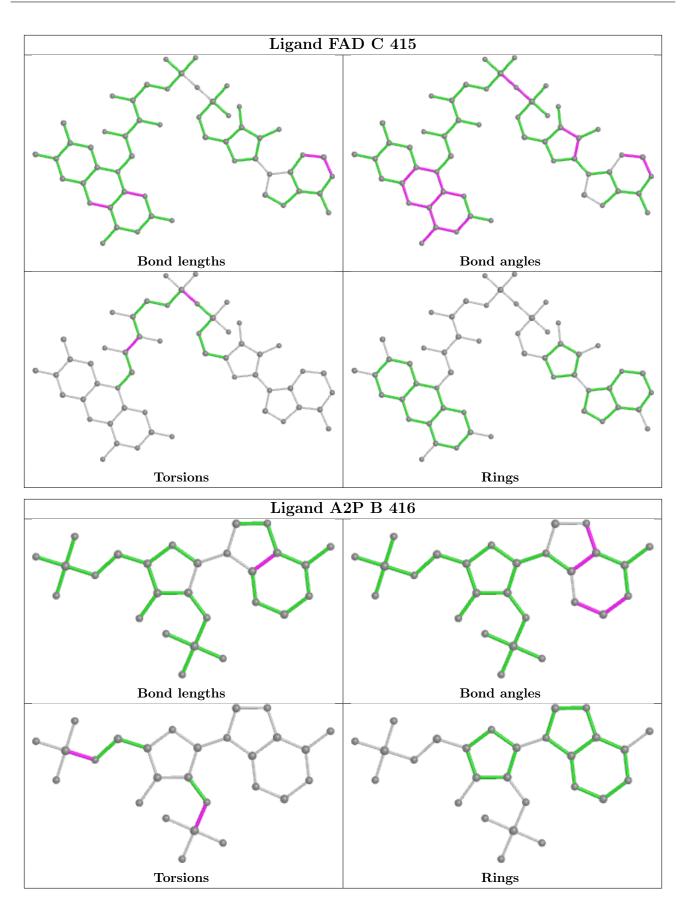




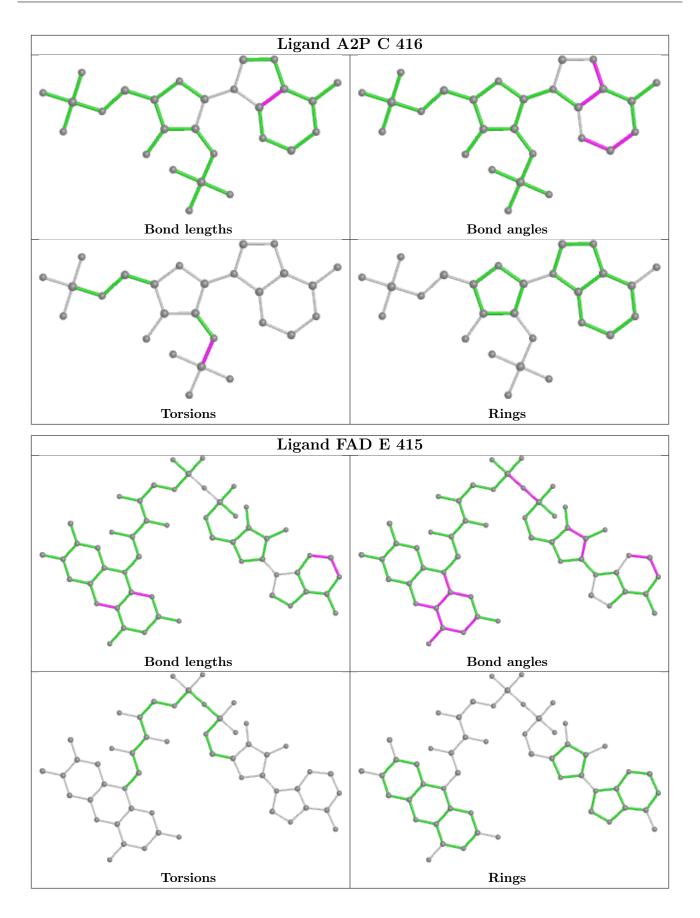




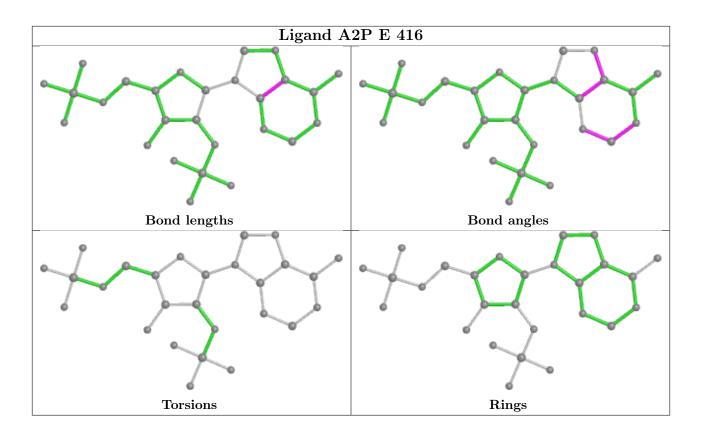












## 5.7 Other polymers (i)

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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(A^2)$	$\mathbf{Q}{<}0.9$
1	А	261/316~(82%)	-0.18	3 (1%) 80 79	17, 27, 47, 56	0
1	В	263/316~(83%)	-0.17	2 (0%) 86 85	17, 30, 53, 67	0
1	С	267/316~(84%)	-0.34	2 (0%) 87 86	14, 25, 44, 54	0
1	D	267/316~(84%)	-0.21	0 100 100	14, 27, 52, 67	0
1	Ε	253/316~(80%)	0.03	1 (0%) 92 91	29, 42, 67, 74	1 (0%)
1	F	254/316~(80%)	0.17	7 (2%) 53 51	35, 48, 68, 77	0
All	All	1565/1896~(82%)	-0.12	15 (0%) 82 81	14,  35,  61,  77	1 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ε	291	TYR	6.6
1	F	254	ALA	3.5
1	В	295	ASP	3.1
1	F	277	TYR	3.0
1	F	291	TYR	2.7

### 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 monosaccharides in this entry.



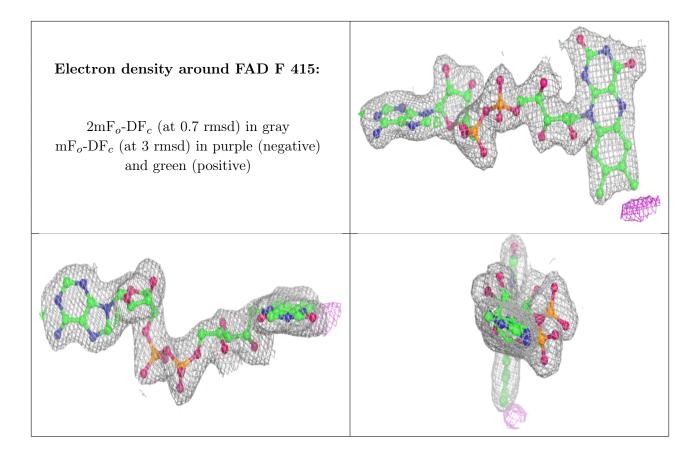
### 6.4 Ligands (i)

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,  $95^{th}$  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.

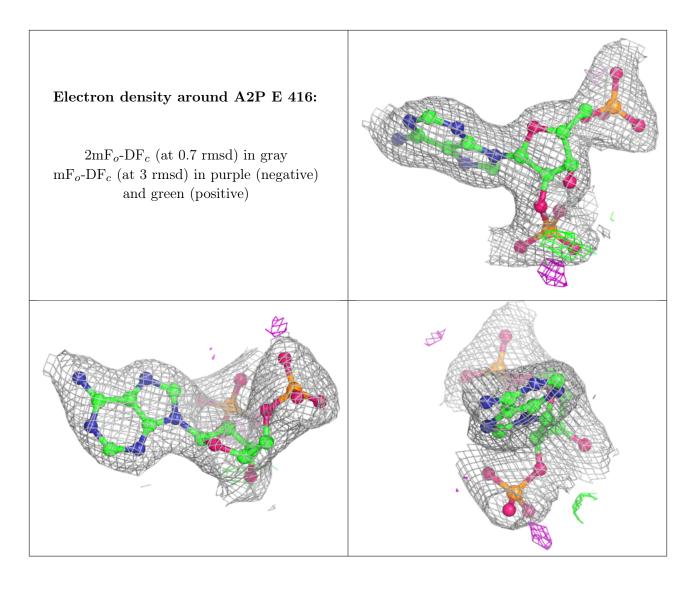
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	FAD	F	415	53/53	0.96	0.12	32,34,34,35	0
3	A2P	Е	416	27/27	0.96	0.12	32,34,38,38	0
3	A2P	F	416	27/27	0.96	0.12	32,33,36,36	0
2	FAD	А	415	53/53	0.97	0.11	9,16,21,22	0
3	A2P	С	416	27/27	0.97	0.09	$16,\!17,\!22,\!23$	0
2	FAD	В	415	53/53	0.97	0.10	$13,\!17,\!22,\!22$	0
2	FAD	Е	415	53/53	0.97	0.10	24,29,36,36	0
3	A2P	В	416	27/27	0.98	0.11	18,20,24,24	0
2	FAD	С	415	53/53	0.98	0.09	$9,\!13,\!17,\!18$	0
3	A2P	D	416	27/27	0.98	0.10	14,16,20,21	0
2	FAD	D	415	53/53	0.98	0.10	$11,\!15,\!19,\!20$	0
3	A2P	A	416	27/27	0.98	0.12	$17,\!19,\!23,\!23$	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.

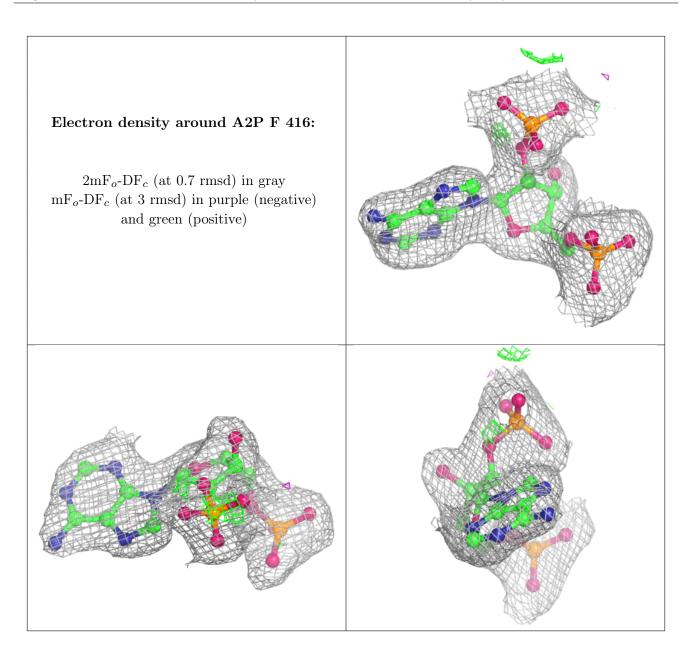




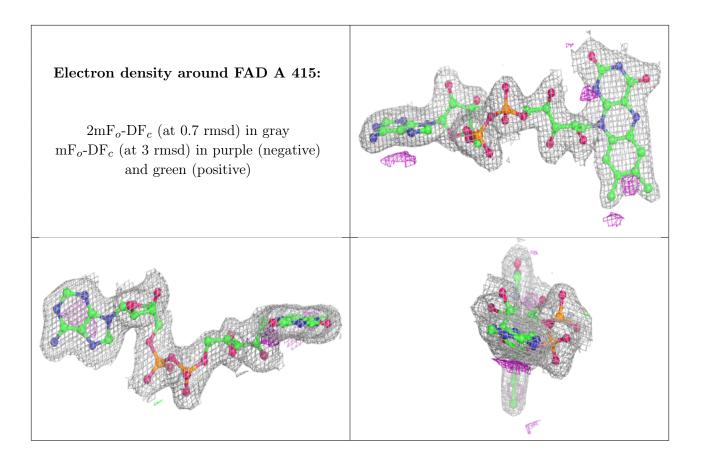




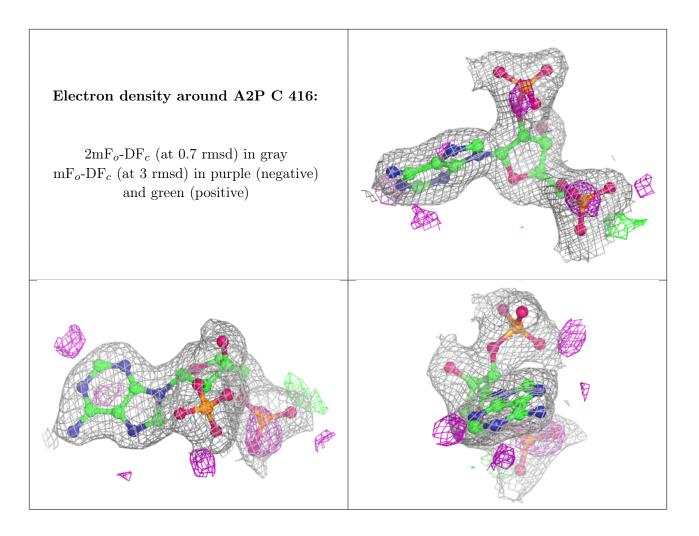




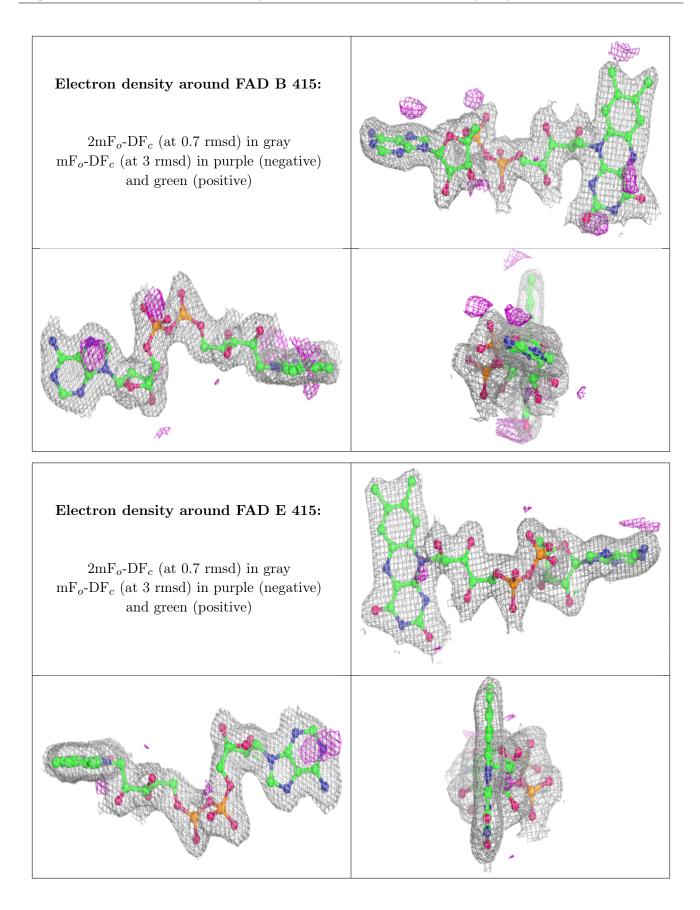




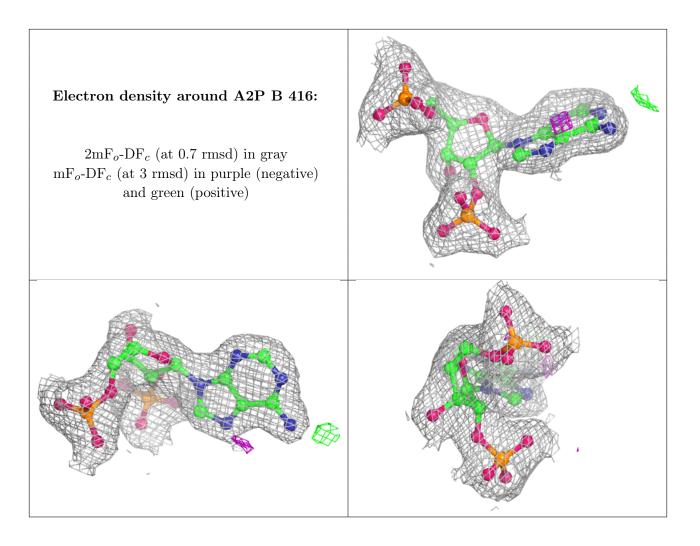




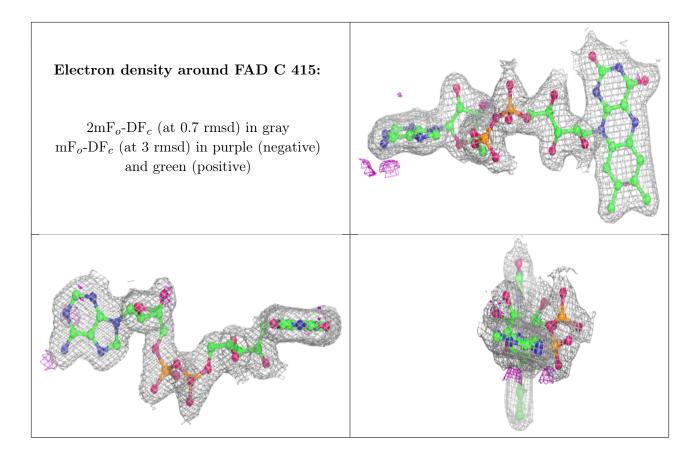




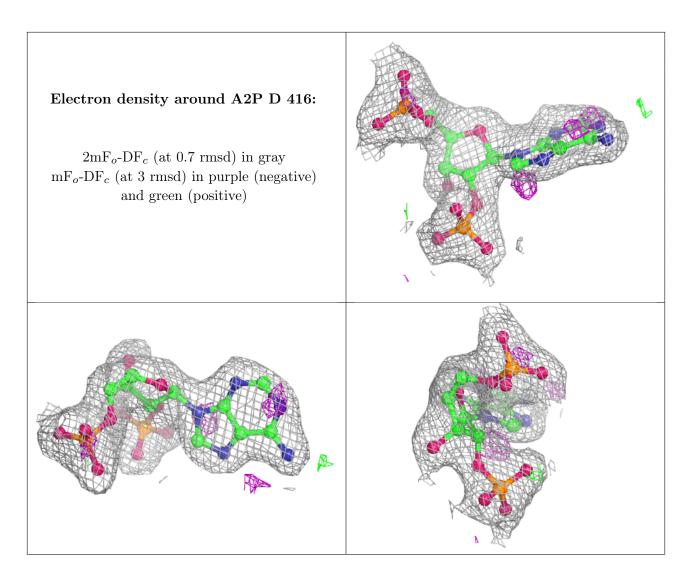




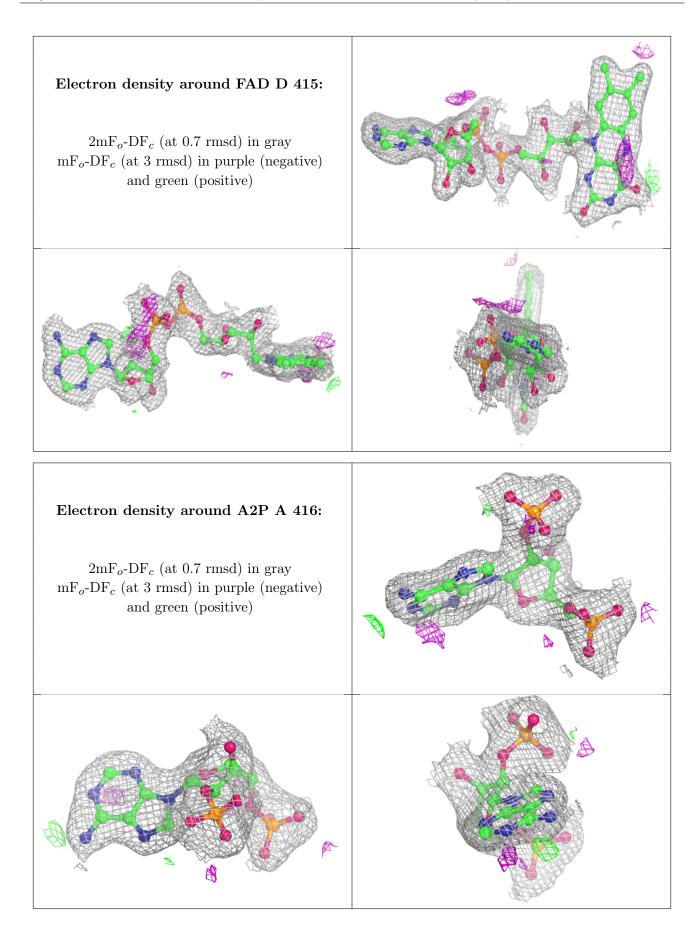














## 6.5 Other polymers (i)

There are no such residues in this entry.

