Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 10:05 AM EST

PDB ID	:	1FNC
Title	:	REFINED CRYSTAL STRUCTURE OF SPINACH FERREDOXIN REDUCTASE AT 1.7 ANGSTROMS RESOLUTION: OXIDIZED, REDUCED, AND 2'-PHOSPHO-5'-AMP BOUND STATES
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Deposited on	:	1995-01-05
Resolution	:	2.00 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 (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 (i)) were used in the production of this report:

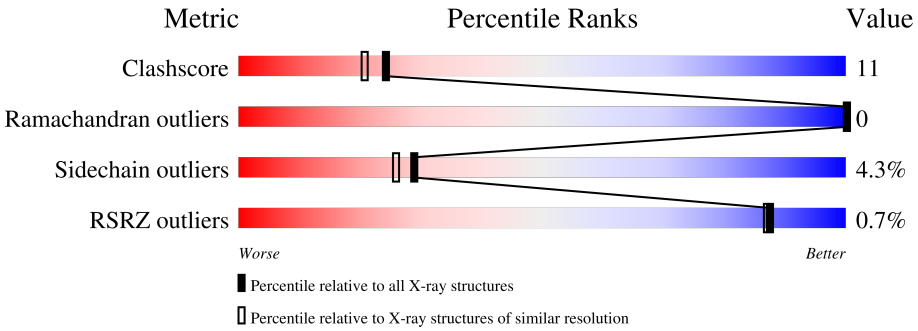
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	A	314	% 64% 25% 5% 6%

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	SO4	A	317	-	-	X	-

2 Entry composition (i)

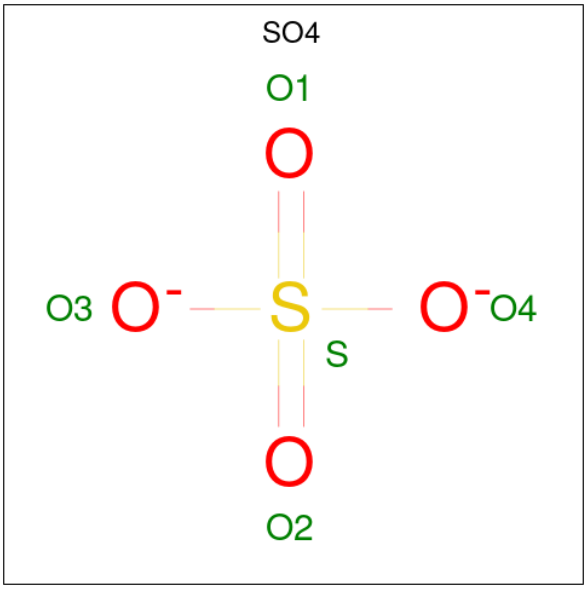
There are 5 unique types of molecules in this entry. The entry contains 2680 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FERREDOXIN-NADP+ REDUCTASE.

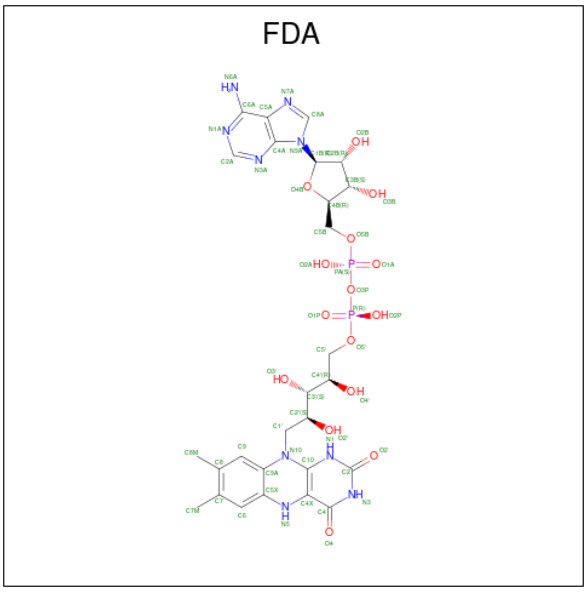
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2352	1506	388	440	18	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



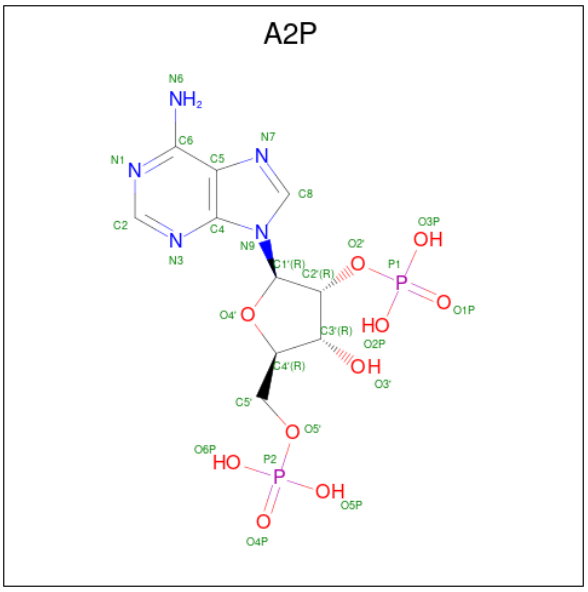
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0

- Molecule 3 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is ADENOSINE-2'-5'-DIPHOSPHATE (three-letter code: A2P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	22	1
			54	20	10	20	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	216	Total	O	0	0
			216	216		

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

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.70Å 57.70Å 68.10Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 34.51 – 1.96	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 85.6 (34.51-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	TNT 5A	Depositor
R, R_{free}	0.149 , (Not available) 0.140 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 141.1	EDS
L-test for twinning[1]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2680	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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: A2P, SO4, FDA

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	1.16	17/2406 (0.7%)	1.41	34/3236 (1.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CD-OE2	7.96	1.34	1.25
1	A	240	GLU	CD-OE2	7.11	1.33	1.25
1	A	24	GLU	CD-OE2	6.83	1.33	1.25
1	A	187	GLU	CD-OE1	6.67	1.32	1.25
1	A	214	GLU	CD-OE1	6.66	1.32	1.25
1	A	25	GLU	CD-OE2	6.58	1.32	1.25
1	A	243	GLU	CD-OE1	6.49	1.32	1.25
1	A	278	GLU	CD-OE1	6.48	1.32	1.25
1	A	144	GLU	CD-OE2	6.42	1.32	1.25
1	A	257	GLU	CD-OE2	6.10	1.32	1.25
1	A	56	GLU	CD-OE1	6.02	1.32	1.25
1	A	298	GLU	CD-OE2	-5.89	1.19	1.25
1	A	67	GLU	CD-OE1	5.83	1.32	1.25
1	A	307	GLU	CD-OE1	5.56	1.31	1.25
1	A	292	GLU	CD-OE2	5.41	1.31	1.25
1	A	217	GLU	CD-OE2	-5.12	1.20	1.25
1	A	65	GLU	CD-OE2	-5.05	1.20	1.25

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	191	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	A	107	ASP	CB-CG-OD1	8.74	126.17	118.30
1	A	265	ASP	CB-CG-OD1	-8.46	110.69	118.30
1	A	301	ARG	NE-CZ-NH1	8.39	124.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	A	107	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	A	84	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	178	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	84	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	93	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	191	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	282	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	230	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	52	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	71	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	52	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	265	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	270	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	190	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	253	GLN	N-CA-CB	-5.82	100.12	110.60
1	A	104	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	295	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	123	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	178	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	51	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	225	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	222	LYS	CB-CA-C	-5.43	99.53	110.40
1	A	295	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	250	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	157	MET	CG-SD-CE	5.19	108.51	100.20
1	A	282	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	71	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	270	TYR	CB-CG-CD2	5.04	124.03	121.00
1	A	51	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2352	0	2342	53	0
2	A	5	0	0	2	0
3	A	53	0	33	0	0
4	A	54	0	22	0	0
5	A	216	0	0	5	0
All	All	2680	0	2397	53	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 11.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:HB1	1:A:288:LEU:HD21	1.48	0.92
1:A:285:MET:HA	1:A:285:MET:HE3	1.57	0.84
1:A:33:LYS:HB3	1:A:34:PRO:HD2	1.65	0.78
1:A:35:LYS:HG3	5:A:480:HOH:O	1.84	0.77
1:A:274:LEU:O	1:A:277:MET:HG2	1.94	0.66
1:A:257:GLU:HB2	5:A:719:HOH:O	1.95	0.65
1:A:121:THR:HA	1:A:126:GLU:O	1.97	0.65
1:A:239:ASN:O	1:A:242:GLY:N	2.30	0.65
1:A:238:THR:HA	1:A:243:GLU:O	2.00	0.61
1:A:90:HIS:HA	2:A:317:SO4:O1	2.00	0.61
1:A:285:MET:HE3	1:A:285:MET:CA	2.28	0.60
1:A:20:SER:O	1:A:159:LYS:NZ	2.28	0.60
1:A:239:ASN:ND2	1:A:243:GLU:OE1	2.31	0.59
1:A:47:LYS:HD2	1:A:56:GLU:HB3	1.85	0.59
1:A:239:ASN:OD1	1:A:243:GLU:N	2.29	0.58
1:A:246:TYR:O	1:A:249:THR:HB	2.04	0.57
1:A:259:TRP:NE1	1:A:263:LYS:HE3	2.19	0.57
1:A:84:ASP:N	1:A:88:LYS:O	2.32	0.57
1:A:27:ILE:HG22	1:A:71:ARG:HD2	1.87	0.55
1:A:264:LYS:NZ	5:A:741:HOH:O	2.39	0.55
1:A:90:HIS:ND1	2:A:317:SO4:O1	2.29	0.54
1:A:296:TRP:CZ2	1:A:300:LYS:HG3	2.43	0.54
1:A:252:ALA:HB2	1:A:284:ILE:HD12	1.89	0.54
1:A:284:ILE:HG22	1:A:288:LEU:HD12	1.88	0.53
1:A:274:LEU:N	1:A:274:LEU:HD12	2.23	0.53
1:A:157:MET:CE	1:A:183:LYS:HD3	2.39	0.53
1:A:27:ILE:HD11	1:A:153:LYS:CG	2.39	0.53
1:A:195:ASN:HB2	5:A:522:HOH:O	2.08	0.53
1:A:120:TYR:O	1:A:128:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:SER:O	1:A:244:LYS:HG2	2.11	0.50
1:A:99:SER:HB3	1:A:112:SER:HB2	1.93	0.50
1:A:250:ARG:O	1:A:253:GLN:HB3	2.11	0.50
1:A:223:ALA:HB1	1:A:226:ASN:HB2	1.96	0.47
1:A:157:MET:HE1	1:A:183:LYS:HD3	1.95	0.47
1:A:118:LEU:C	1:A:119:ILE:HG12	2.36	0.46
1:A:241:LYS:HG2	1:A:241:LYS:O	2.15	0.46
1:A:245:MET:SD	1:A:249:THR:HG22	2.56	0.45
1:A:282:ASP:O	1:A:286:VAL:HG23	2.18	0.44
1:A:204:VAL:HG21	1:A:210:LEU:HD23	1.98	0.44
1:A:241:LYS:HB3	1:A:243:GLU:HG3	1.99	0.44
1:A:246:TYR:HD1	1:A:246:TYR:HA	1.51	0.43
1:A:274:LEU:HD12	1:A:274:LEU:H	1.84	0.42
1:A:306:ALA:O	1:A:307:GLU:HB2	2.18	0.42
1:A:210:LEU:HD22	1:A:231:PHE:CD1	2.55	0.42
1:A:157:MET:HE1	1:A:183:LYS:CD	2.50	0.42
1:A:25:GLU:OE2	1:A:159:LYS:HE2	2.20	0.42
1:A:33:LYS:HB3	1:A:34:PRO:CD	2.44	0.42
1:A:176:PRO:O	1:A:179:SER:HB3	2.20	0.42
1:A:65:GLU:HA	5:A:516:HOH:O	2.19	0.42
1:A:274:LEU:H	1:A:274:LEU:CD1	2.32	0.41
1:A:259:TRP:CD1	1:A:263:LYS:HE3	2.55	0.41
1:A:42:CYS:HA	1:A:62:PHE:HD1	1.85	0.41
1:A:27:ILE:CG2	1:A:71:ARG:HD2	2.50	0.40

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	294/314 (94%)	284 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	253/267 (95%)	242 (96%)	11 (4%)	29 26

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

Mol	Chain	Res	Type
1	A	56	GLU
1	A	85	LYS
1	A	91	LYS
1	A	119	ILE
1	A	191	ASP
1	A	193	LYS
1	A	195	ASN
1	A	209	SER
1	A	214	GLU
1	A	244	LYS
1	A	279	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	162	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FDA	A	315	-	52,58,58	1.72	11 (21%)	60,89,89	1.47	10 (16%)
4	A2P	A	316[A]	-	25,29,29	1.57	3 (12%)	31,45,45	1.46	7 (22%)
4	A2P	A	316[B]	-	25,29,29	2.34	5 (20%)	31,45,45	1.44	7 (22%)
2	SO4	A	317	-	4,4,4	0.73	0	6,6,6	0.25	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
3	FDA	A	315	-	-	2/30/50/50	0/6/6/6
4	A2P	A	316[A]	-	-	6/11/31/31	0/3/3/3
4	A2P	A	316[B]	-	-	3/11/31/31	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	316[B]	A2P	P1-O2'	9.03	1.76	1.59
3	A	315	FDA	C1'-C2'	5.16	1.59	1.52
3	A	315	FDA	O4B-C1B	4.86	1.47	1.41
4	A	316[A]	A2P	O4'-C1'	4.69	1.47	1.41
3	A	315	FDA	C10-N1	-4.58	1.29	1.37
4	A	316[B]	A2P	O4'-C1'	4.48	1.47	1.41
4	A	316[A]	A2P	P2-O6P	-3.60	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	315	FDA	O4-C4	-3.05	1.17	1.23
3	A	315	FDA	C5'-C4'	2.97	1.56	1.51
3	A	315	FDA	C9A-N10	-2.91	1.36	1.41
4	A	316[B]	A2P	O5'-C5'	2.62	1.54	1.44
3	A	315	FDA	C2B-C1B	-2.38	1.50	1.53
3	A	315	FDA	C2-N3	2.33	1.41	1.37
3	A	315	FDA	C4-N3	-2.28	1.34	1.38
3	A	315	FDA	C5X-C9A	2.25	1.43	1.40
3	A	315	FDA	C4X-N5	-2.22	1.31	1.35
4	A	316[A]	A2P	P1-O2'	2.08	1.63	1.59
4	A	316[B]	A2P	P2-O6P	-2.02	1.47	1.54
4	A	316[B]	A2P	P2-O4P	-2.01	1.44	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	315	FDA	C4A-C5A-N7A	3.69	113.24	109.40
4	A	316[B]	A2P	C4-C5-N7	3.05	112.58	109.40
4	A	316[A]	A2P	C4-C5-N7	2.87	112.39	109.40
3	A	315	FDA	O2A-PA-O1A	2.82	126.20	112.24
4	A	316[A]	A2P	P2-O5'-C5'	-2.75	110.72	118.30
3	A	315	FDA	C1B-N9A-C4A	-2.74	121.83	126.64
4	A	316[B]	A2P	C3'-C2'-C1'	-2.61	97.98	102.89
3	A	315	FDA	C2A-N1A-C6A	2.55	123.12	118.75
3	A	315	FDA	C9A-C5X-N5	2.48	122.87	119.56
4	A	316[A]	A2P	C5-C6-N1	-2.44	114.83	120.35
3	A	315	FDA	O4-C4-C4X	-2.43	121.66	127.24
4	A	316[A]	A2P	C2-N1-C6	2.43	122.90	118.75
3	A	315	FDA	C5X-N5-C4X	-2.40	115.34	121.02
4	A	316[B]	A2P	C5-C6-N1	-2.40	114.91	120.35
3	A	315	FDA	N3A-C2A-N1A	-2.37	124.97	128.68
4	A	316[B]	A2P	O5P-P2-O5'	2.33	112.92	106.73
3	A	315	FDA	O2P-P-O1P	2.25	123.38	112.24
4	A	316[B]	A2P	O2'-P1-O1P	-2.24	100.74	109.39
4	A	316[A]	A2P	C5-C6-N6	2.20	123.70	120.35
3	A	315	FDA	C5A-C6A-N1A	-2.19	115.39	120.35
4	A	316[B]	A2P	C2-N1-C6	2.17	122.47	118.75
4	A	316[A]	A2P	O5'-P2-O4P	2.15	112.49	106.47
4	A	316[B]	A2P	O4'-C1'-C2'	-2.14	102.88	106.59
4	A	316[A]	A2P	O6P-P2-O5'	-2.05	101.28	106.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	316[A]	A2P	C5'-O5'-P2-O5P
4	A	316[A]	A2P	C5'-O5'-P2-O6P
4	A	316[A]	A2P	C3'-C4'-C5'-O5'
4	A	316[A]	A2P	O4'-C4'-C5'-O5'
4	A	316[A]	A2P	C5'-O5'-P2-O4P
4	A	316[A]	A2P	C2'-O2'-P1-O1P
4	A	316[B]	A2P	C2'-O2'-P1-O1P
4	A	316[B]	A2P	C2'-O2'-P1-O2P
4	A	316[B]	A2P	O4'-C4'-C5'-O5'
3	A	315	FDA	PA-O3P-P-O1P
3	A	315	FDA	PA-O3P-P-O2P

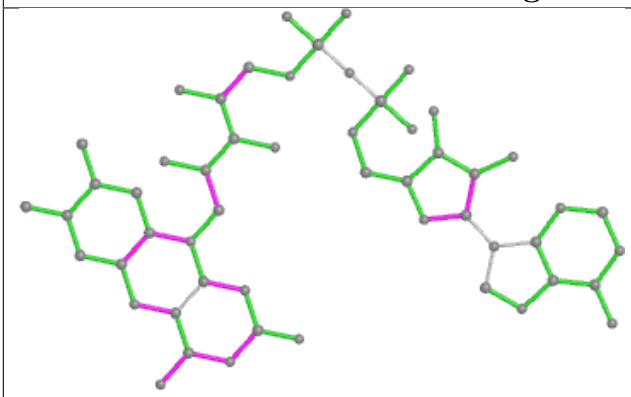
There are no ring outliers.

1 monomer is involved in 2 short contacts:

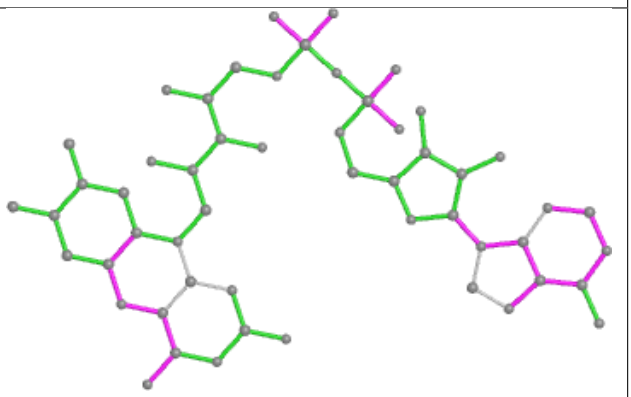
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	317	SO4	2	0

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 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.

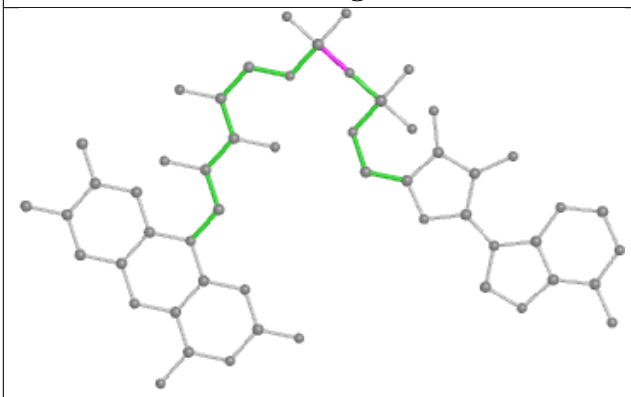
Ligand FDA A 315



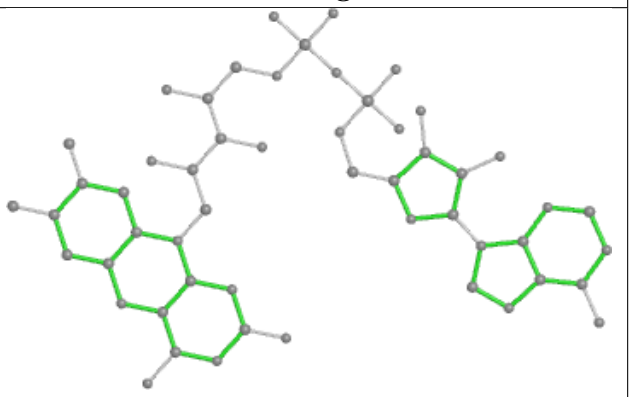
Bond lengths



Bond angles

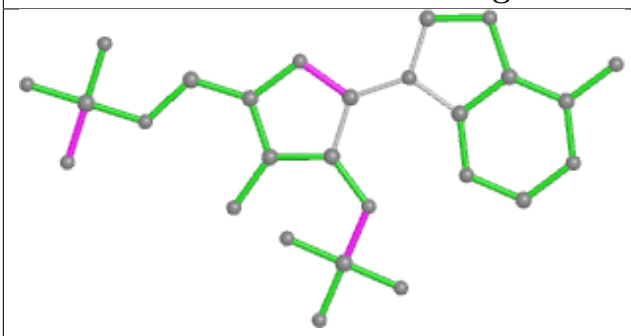


Torsions

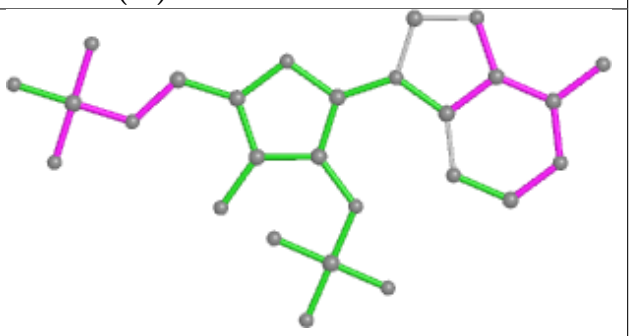


Rings

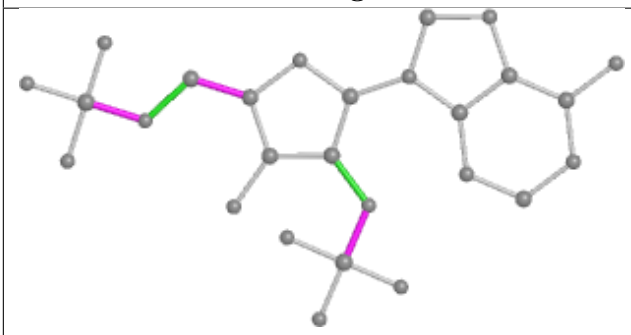
Ligand A2P A 316 (A)



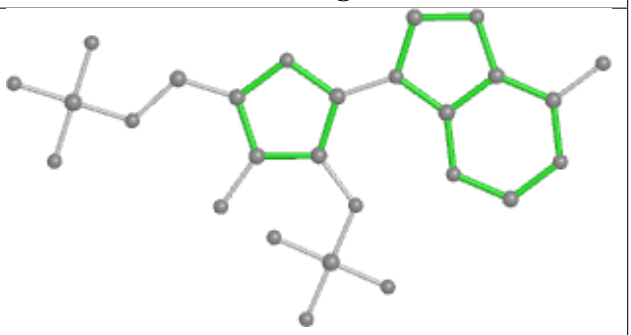
Bond lengths



Bond angles

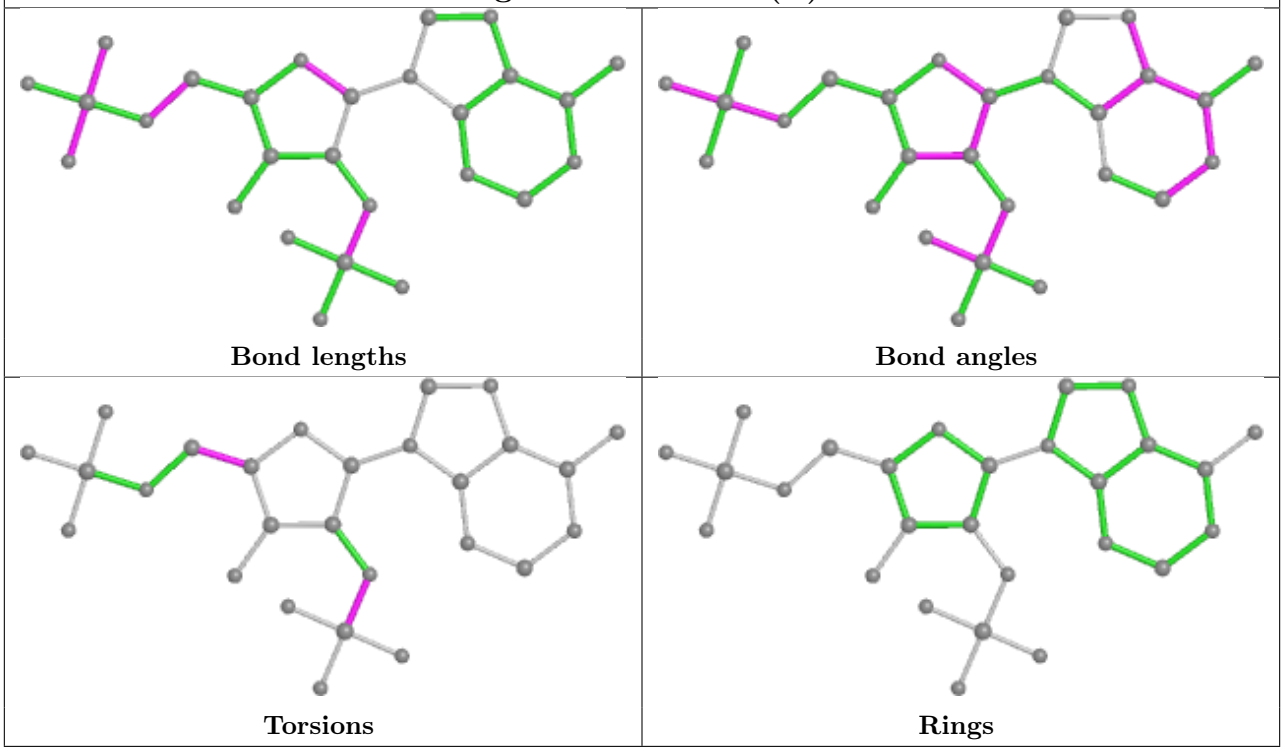


Torsions



Rings

Ligand A2P A 316 (B)



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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	296/314 (94%)	-0.85	2 (0%)	87	87	3, 19, 52, 95	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	HIS	3.9
1	A	242	GLY	2.1

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 monosaccharides 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, 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.

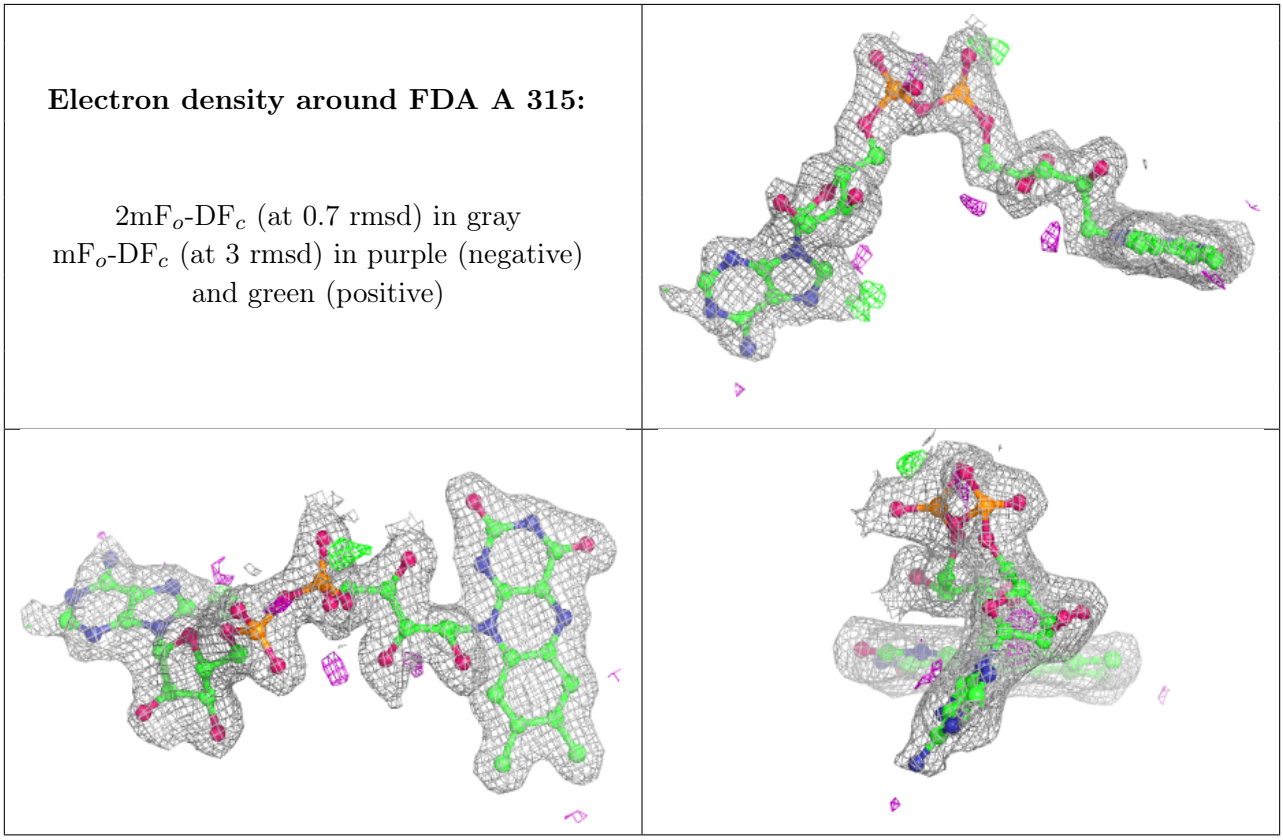
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FDA	A	315	53/53	0.98	0.07	1,15,100,100	0
4	A2P	A	316[A]	27/27	0.98	0.07	10,25,38,100	27
4	A2P	A	316[B]	27/27	0.98	0.07	9,26,36,100	5
2	SO4	A	317	5/5	0.99	0.11	26,37,100,100	0

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.

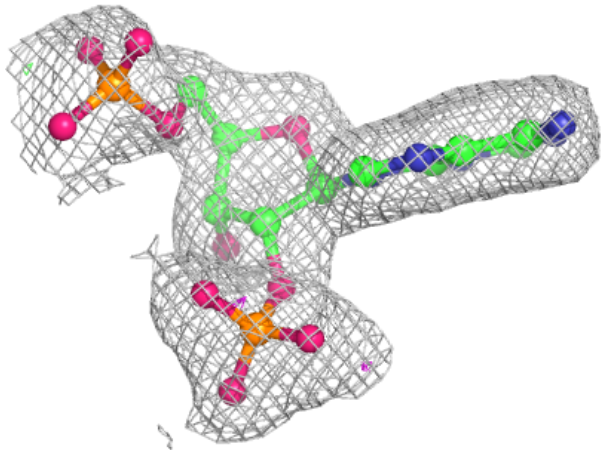
Electron density around FDA A 315:

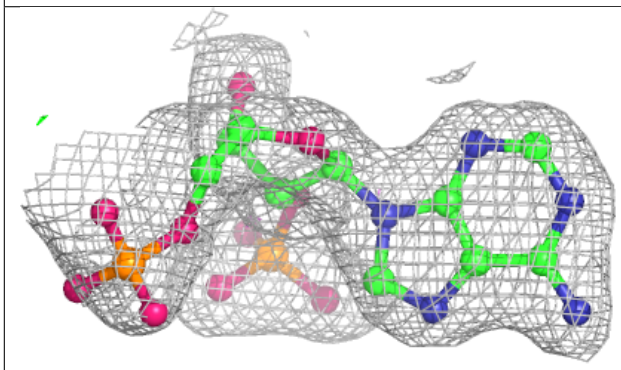
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

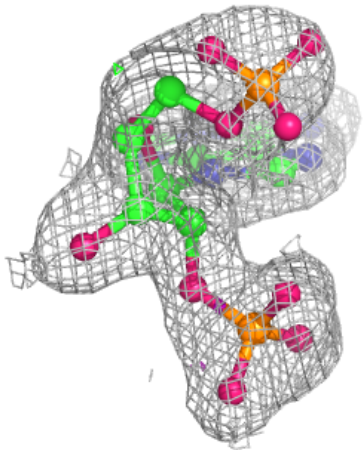


Electron density around A2P A 316 (A):

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

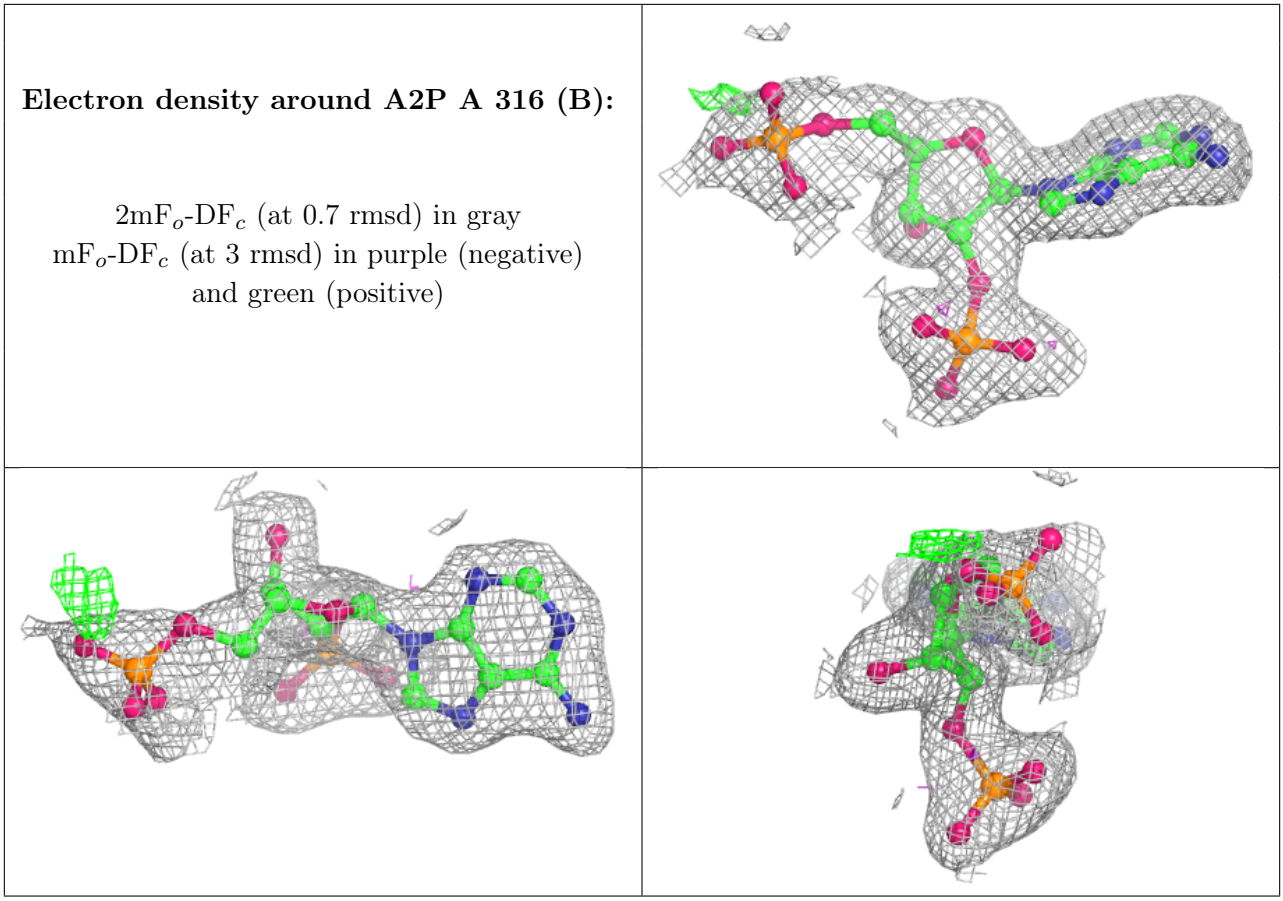






Electron density around A2P A 316 (B):

$2mF_o$-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.