wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 02:36 PM EDT

PDB ID	:	4MAF
Title	:	Soybean ATP Sulfurylase
Authors	:	Herrmann, J.; Ravilious, G.E.; McKinney, S.E.; Westfall, C.S.; Lee, S.G.; Krishnan, H.B.; Jez, J.M.
Deposited on	:	2013-08-16
Resolution	:	2.48 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 (i)) were used in the production of this report:

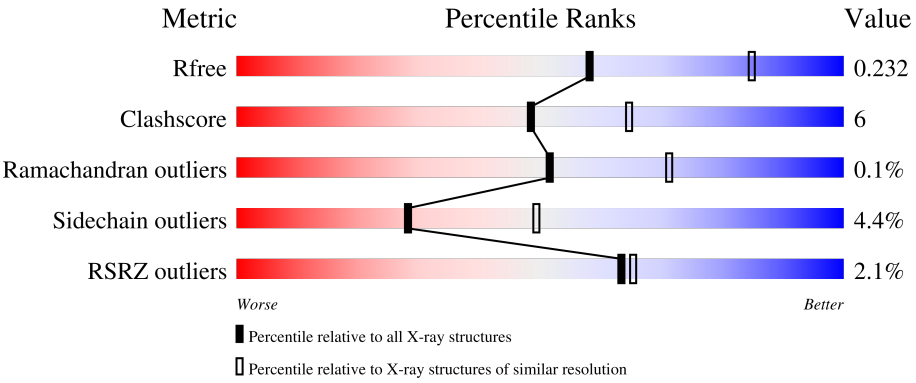
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	404	81% 17%
1	B	404	86% 14%
1	C	404	87% 12%
1	D	404	83% 14%
1	E	404	86% 12%

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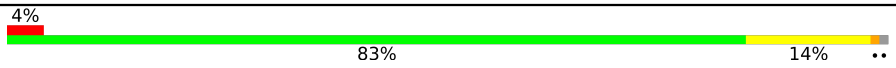
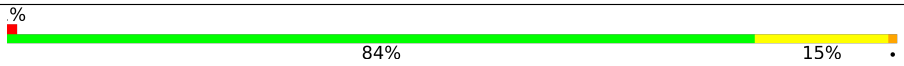
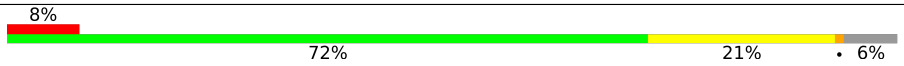
Mol	Chain	Length	Quality of chain
1	F	404	
1	G	404	
1	H	404	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26495 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 ATP sulfurylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3197	2045	558	581	13			
1	B	404	Total	C	N	O	S	0	2	0
			3219	2059	560	587	13			
1	C	403	Total	C	N	O	S	0	0	0
			3205	2051	559	582	13			
1	D	401	Total	C	N	O	S	0	0	0
			3190	2040	557	580	13			
1	E	403	Total	C	N	O	S	0	0	0
			3205	2051	559	582	13			
1	F	401	Total	C	N	O	S	0	0	0
			3190	2040	557	580	13			
1	G	404	Total	C	N	O	S	0	0	0
			3211	2054	560	584	13			
1	H	381	Total	C	N	O	S	0	0	0
			3037	1948	528	550	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	MET	-	initiating methionine	UNP Q8SAG1
A	450	LEU	-	expression tag	UNP Q8SAG1
A	451	SER	-	expression tag	UNP Q8SAG1
B	48	MET	-	initiating methionine	UNP Q8SAG1
B	450	LEU	-	expression tag	UNP Q8SAG1
B	451	SER	-	expression tag	UNP Q8SAG1
C	48	MET	-	initiating methionine	UNP Q8SAG1
C	450	LEU	-	expression tag	UNP Q8SAG1
C	451	SER	-	expression tag	UNP Q8SAG1
D	48	MET	-	initiating methionine	UNP Q8SAG1
D	450	LEU	-	expression tag	UNP Q8SAG1
D	451	SER	-	expression tag	UNP Q8SAG1
E	48	MET	-	initiating methionine	UNP Q8SAG1

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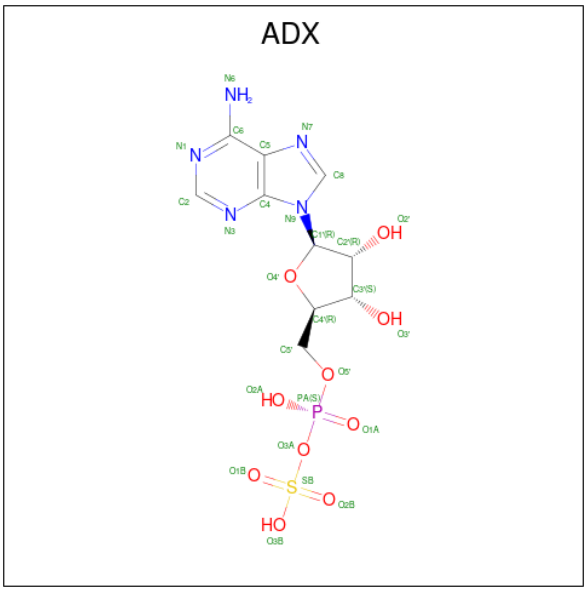
Chain	Residue	Modelled	Actual	Comment	Reference
E	450	LEU	-	expression tag	UNP Q8SAG1
E	451	SER	-	expression tag	UNP Q8SAG1
F	48	MET	-	initiating methionine	UNP Q8SAG1
F	450	LEU	-	expression tag	UNP Q8SAG1
F	451	SER	-	expression tag	UNP Q8SAG1
G	48	MET	-	initiating methionine	UNP Q8SAG1
G	450	LEU	-	expression tag	UNP Q8SAG1
G	451	SER	-	expression tag	UNP Q8SAG1
H	48	MET	-	initiating methionine	UNP Q8SAG1
H	450	LEU	-	expression tag	UNP Q8SAG1
H	451	SER	-	expression tag	UNP Q8SAG1

- Molecule 2 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: $C_{10}H_{14}N_5O_{10}PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	E	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	G	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	H	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		

- Molecule 3 is water.

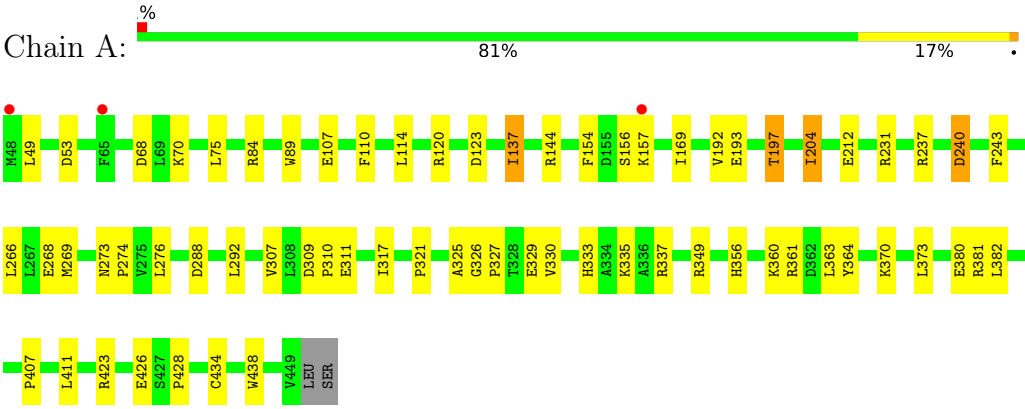
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	146	Total	O	0	0
			146	146		
3	C	167	Total	O	0	0
			167	167		
3	D	122	Total	O	0	0
			122	122		
3	E	136	Total	O	0	0
			136	136		
3	F	57	Total	O	0	0
			57	57		
3	G	106	Total	O	0	0
			106	106		
3	H	24	Total	O	0	0
			24	24		

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.

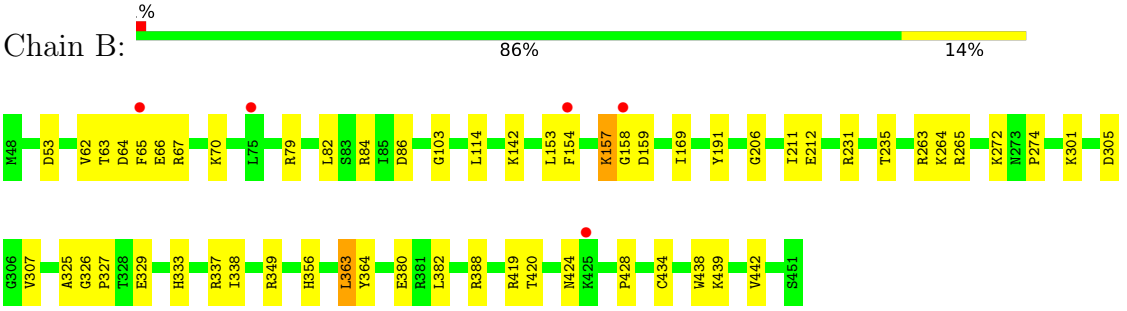
• Molecule 1: ATP sulfurylase

Chain A:



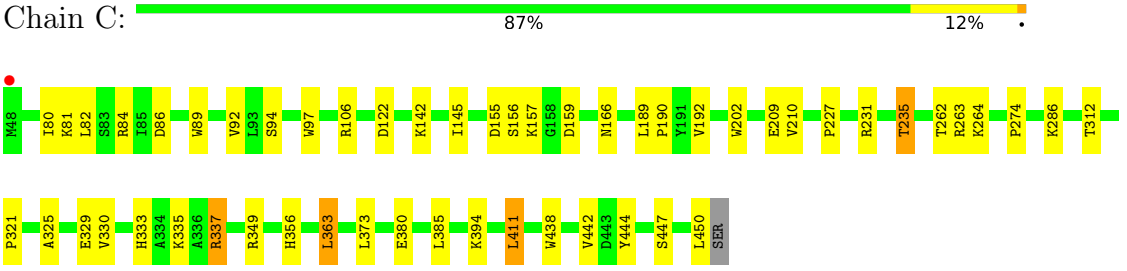
• Molecule 1: ATP sulfurylase

Chain B:



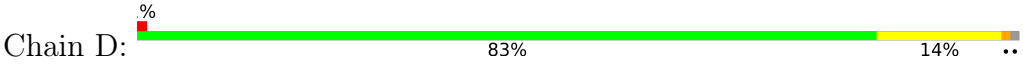
• Molecule 1: ATP sulfurylase

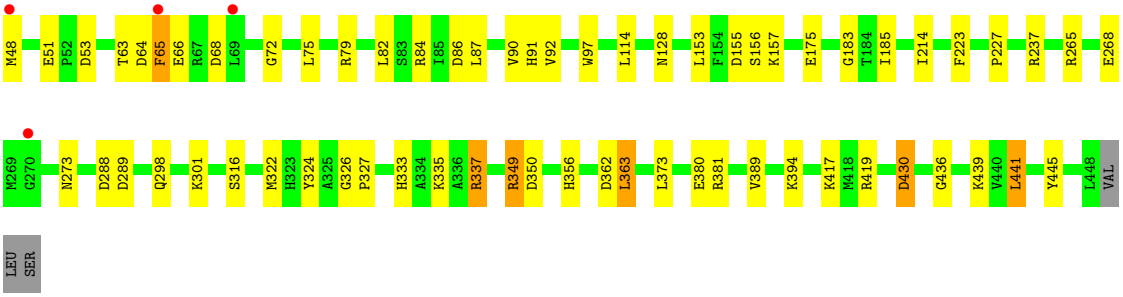
Chain C:



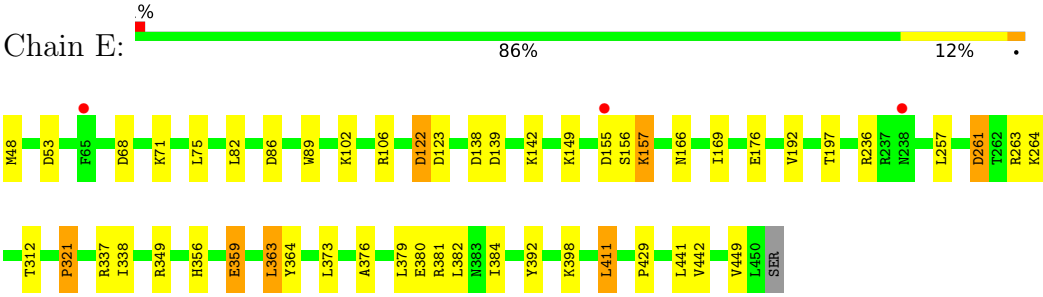
• Molecule 1: ATP sulfurylase

Chain D:

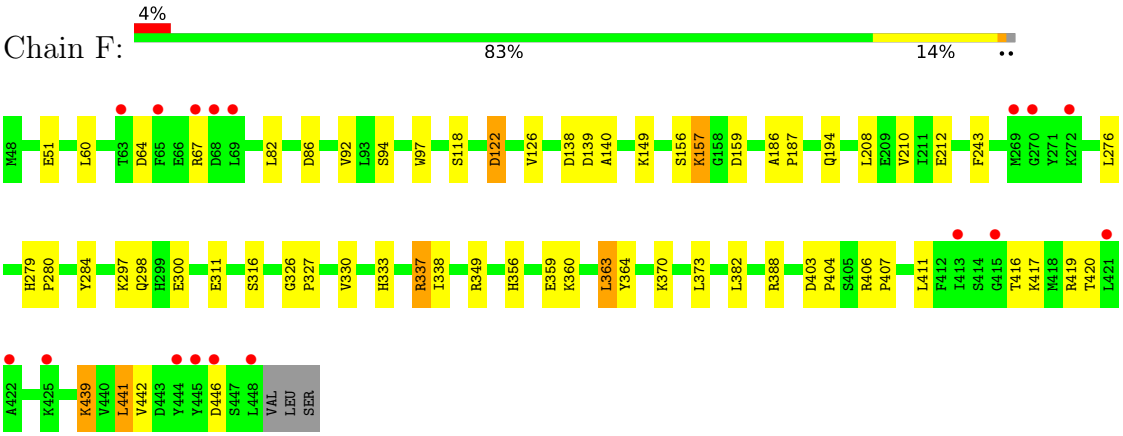




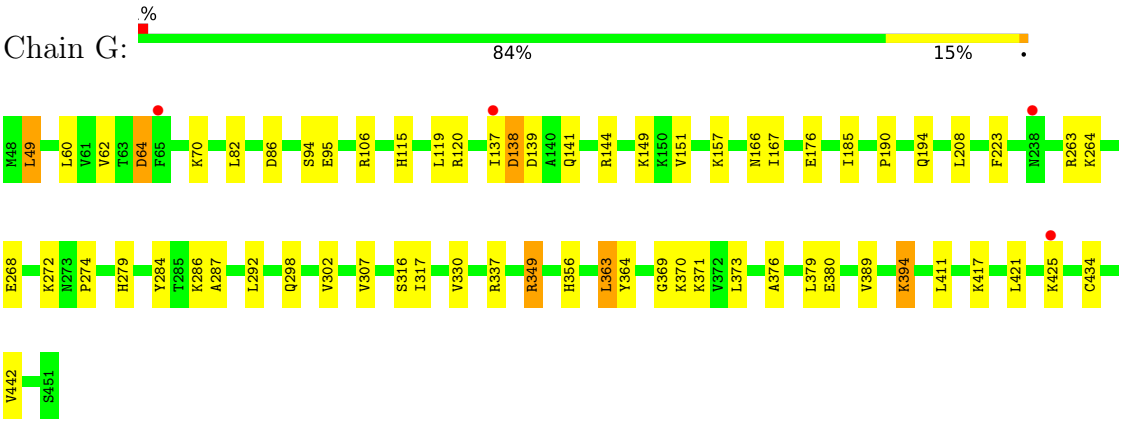
• Molecule 1: ATP sulfurylase



• Molecule 1: ATP sulfurylase

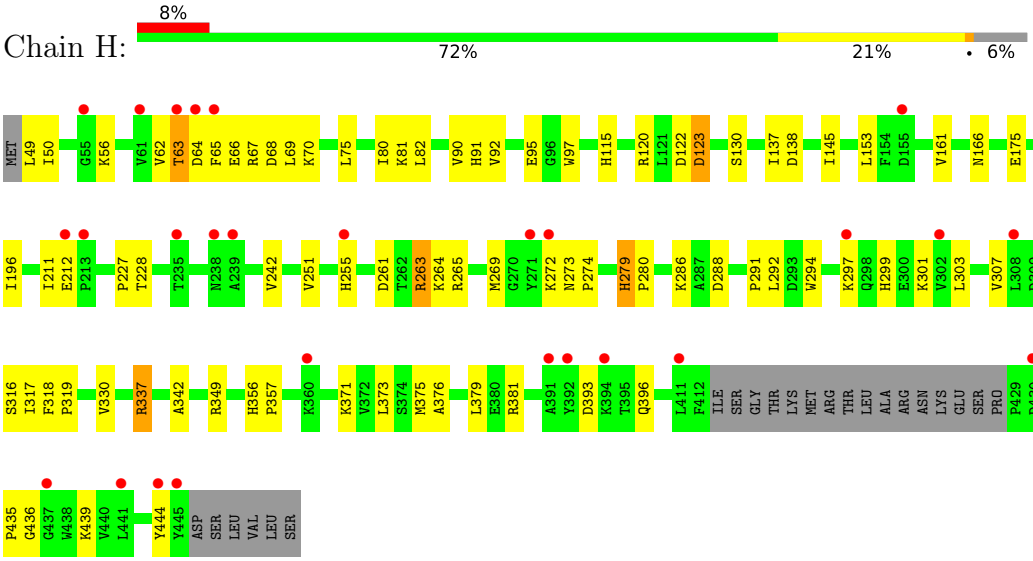


• Molecule 1: ATP sulfurylase



• Molecule 1: ATP sulfurylase

Chain H:


8%
72%
21%
6%
MET L49 I50 G55 K56 V61 V62 T63 D64 F65 E66 R67 D68 L69 K70 L75 I80 K81 L82 V90 H91 V92 E95 G96 W97 H115 R120 L121 D122 D123 S130 I137 D138 I145 L153 F154 D155 V161 N166 E175 I185 Q194 T195
I196 I211 E212 P213 P227 T228 T235 N238 A239 V242 V251 H265 D261 T262 R263 K264 R265 M269 G270 Y271 K272 N273 P274 H279 P280 K286 A287 D288 P291 L292 D293 W294 K297 Q298 H299 E300 K301 V302 L303 V307 L308 D309 P310 E311 T312
S316 I317 F318 P319 V330 R337 A342 R349 H356 P357 K360 K371 V372 L373 S374 M375 A376 L379 E380 R381 A391 Y392 D393 K394 T395 Q396 L411 F412 ILE SER GLY THR LYS MET ARG THR LEU ALA ARG ASN LYS GLU SER PRO P429 D430 G431 F432 M433 C434
P435 G436 G437 W438 K439 V440 L441 Y444 Y445 ASP SER LEU VAL LEU SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	204.27Å 230.75Å 159.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 2.48 48.55 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.5 (48.21-2.48) 88.6 (48.55-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.173 , 0.222 0.185 , 0.232	Depositor DCC
R_{free} test set	6239 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26495	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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 29.77 % 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 1.4649e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] 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: ADX

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	0.37	0/3278	0.56	0/4447
1	B	0.39	0/3306	0.57	0/4485
1	C	0.44	0/3286	0.59	0/4458
1	D	0.42	0/3271	0.58	0/4437
1	E	0.42	0/3286	0.59	0/4458
1	F	0.35	0/3271	0.54	0/4437
1	G	0.42	0/3292	0.57	0/4466
1	H	0.30	0/3116	0.51	0/4228
All	All	0.39	0/26106	0.56	0/35416

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	122	ASP	Peptide

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	3197	0	3190	47	0
1	B	3219	0	3215	33	0
1	C	3205	0	3201	33	0
1	D	3190	0	3181	37	0
1	E	3205	0	3201	34	0
1	F	3190	0	3181	33	0
1	G	3211	0	3206	41	0
1	H	3037	0	3018	57	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
3	A	67	0	0	8	0
3	B	146	0	0	5	0
3	C	167	0	0	3	0
3	D	122	0	0	8	0
3	E	136	0	0	2	0
3	F	57	0	0	2	0
3	G	106	0	0	8	0
3	H	24	0	0	4	0
All	All	26495	0	25489	306	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 6.

The worst 5 of 306 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:356:HIS:O	3:C:1010:HOH:O	1.80	0.98
1:A:423:ARG:NH2	3:A:1028:HOH:O	2.08	0.85
1:E:156:SER:H	1:E:157:LYS:HB3	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:ASN:ND2	3:H:1022:HOH:O	2.13	0.82
1:D:349:ARG:NH1	3:D:1073:HOH:O	2.13	0.81

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	400/404 (99%)	394 (98%)	6 (2%)	0	100	100
1	B	404/404 (100%)	397 (98%)	5 (1%)	2 (0%)	29	46
1	C	401/404 (99%)	396 (99%)	5 (1%)	0	100	100
1	D	399/404 (99%)	388 (97%)	10 (2%)	1 (0%)	41	59
1	E	401/404 (99%)	396 (99%)	5 (1%)	0	100	100
1	F	399/404 (99%)	390 (98%)	9 (2%)	0	100	100
1	G	402/404 (100%)	392 (98%)	10 (2%)	0	100	100
1	H	377/404 (93%)	360 (96%)	16 (4%)	1 (0%)	41	59
All	All	3183/3232 (98%)	3113 (98%)	66 (2%)	4 (0%)	51	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	156	SER
1	H	195	THR
1	B	157	LYS
1	B	158	GLY

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	344/346 (99%)	329 (96%)	15 (4%)	28	49
1	B	348/346 (101%)	336 (97%)	12 (3%)	37	61
1	C	345/346 (100%)	337 (98%)	8 (2%)	50	74
1	D	343/346 (99%)	325 (95%)	18 (5%)	23	41
1	E	345/346 (100%)	326 (94%)	19 (6%)	21	39
1	F	343/346 (99%)	326 (95%)	17 (5%)	24	43
1	G	346/346 (100%)	330 (95%)	16 (5%)	27	47
1	H	325/346 (94%)	309 (95%)	16 (5%)	25	44
All	All	2739/2768 (99%)	2618 (96%)	121 (4%)	28	49

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	138	ASP
1	H	228	THR
1	E	449	VAL
1	H	212	GLU
1	H	337	ARG

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

Mol	Chain	Res	Type
1	D	323	HIS
1	H	115	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
2	ADX	B	900	-	25,29,29	1.54	5 (20%)	26,45,45	1.50	5 (19%)
2	ADX	F	900	-	25,29,29	1.73	7 (28%)	26,45,45	1.37	3 (11%)
2	ADX	E	900	-	25,29,29	1.53	5 (20%)	26,45,45	1.43	5 (19%)
2	ADX	C	900	-	25,29,29	1.52	4 (16%)	26,45,45	1.40	5 (19%)
2	ADX	D	900	-	25,29,29	1.64	7 (28%)	26,45,45	1.48	5 (19%)
2	ADX	H	900	-	25,29,29	1.65	6 (24%)	26,45,45	1.41	4 (15%)
2	ADX	G	900	-	25,29,29	1.60	5 (20%)	26,45,45	1.38	2 (7%)
2	ADX	A	900	-	25,29,29	1.69	7 (28%)	26,45,45	1.42	4 (15%)

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
2	ADX	B	900	-	-	1/6/32/32	0/3/3/3
2	ADX	F	900	-	-	3/6/32/32	0/3/3/3
2	ADX	E	900	-	-	2/6/32/32	0/3/3/3
2	ADX	C	900	-	-	3/6/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADX	D	900	-	-	1/6/32/32	0/3/3/3
2	ADX	H	900	-	-	3/6/32/32	0/3/3/3
2	ADX	G	900	-	-	0/6/32/32	0/3/3/3
2	ADX	A	900	-	-	0/6/32/32	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	900	ADX	C2'-C1'	-4.09	1.47	1.53
2	G	900	ADX	C2'-C1'	-3.98	1.47	1.53
2	A	900	ADX	C2'-C1'	-3.65	1.48	1.53
2	H	900	ADX	C2'-C1'	-3.61	1.48	1.53
2	B	900	ADX	C2'-C1'	-3.46	1.48	1.53

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	900	ADX	N3-C2-N1	-4.64	121.43	128.68
2	H	900	ADX	N3-C2-N1	-4.61	121.47	128.68
2	B	900	ADX	N3-C2-N1	-4.55	121.57	128.68
2	F	900	ADX	N3-C2-N1	-4.51	121.62	128.68
2	A	900	ADX	N3-C2-N1	-4.50	121.64	128.68

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	900	ADX	C5'-O5'-PA-O1A
2	F	900	ADX	C5'-O5'-PA-O1A
2	F	900	ADX	C5'-O5'-PA-O3A
2	H	900	ADX	C5'-O5'-PA-O1A
2	H	900	ADX	C5'-O5'-PA-O2A

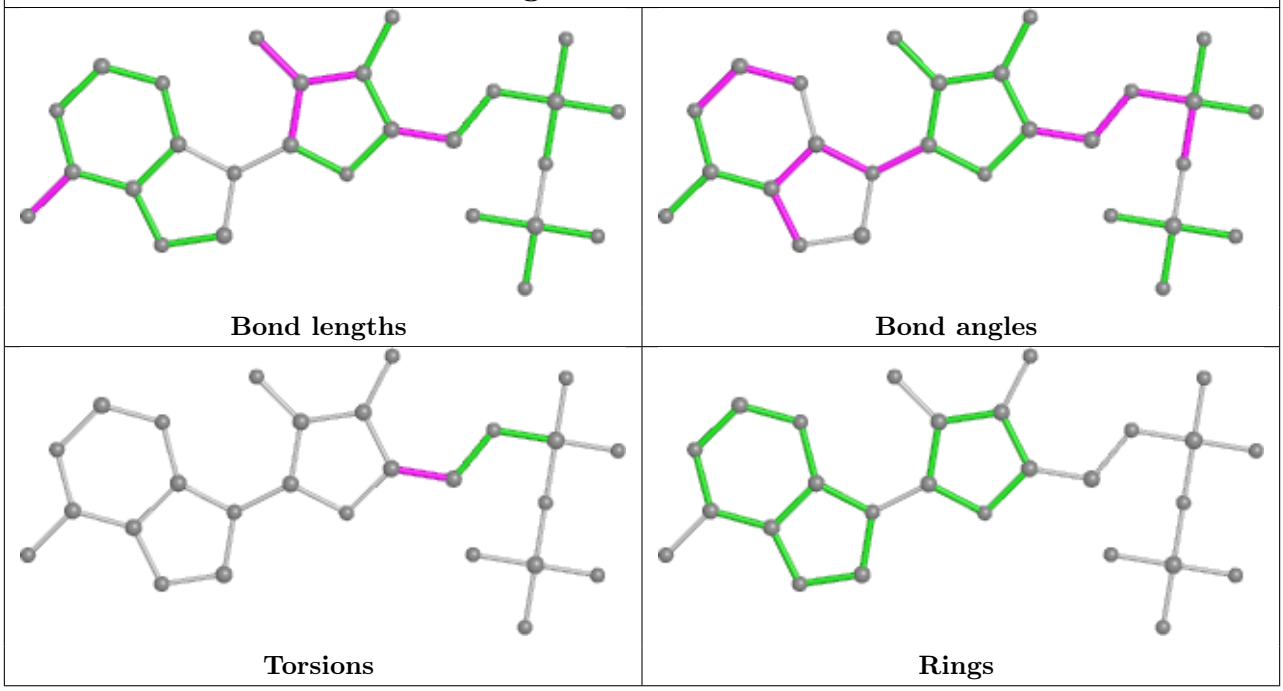
There are no ring outliers.

No monomer is involved in short contacts.

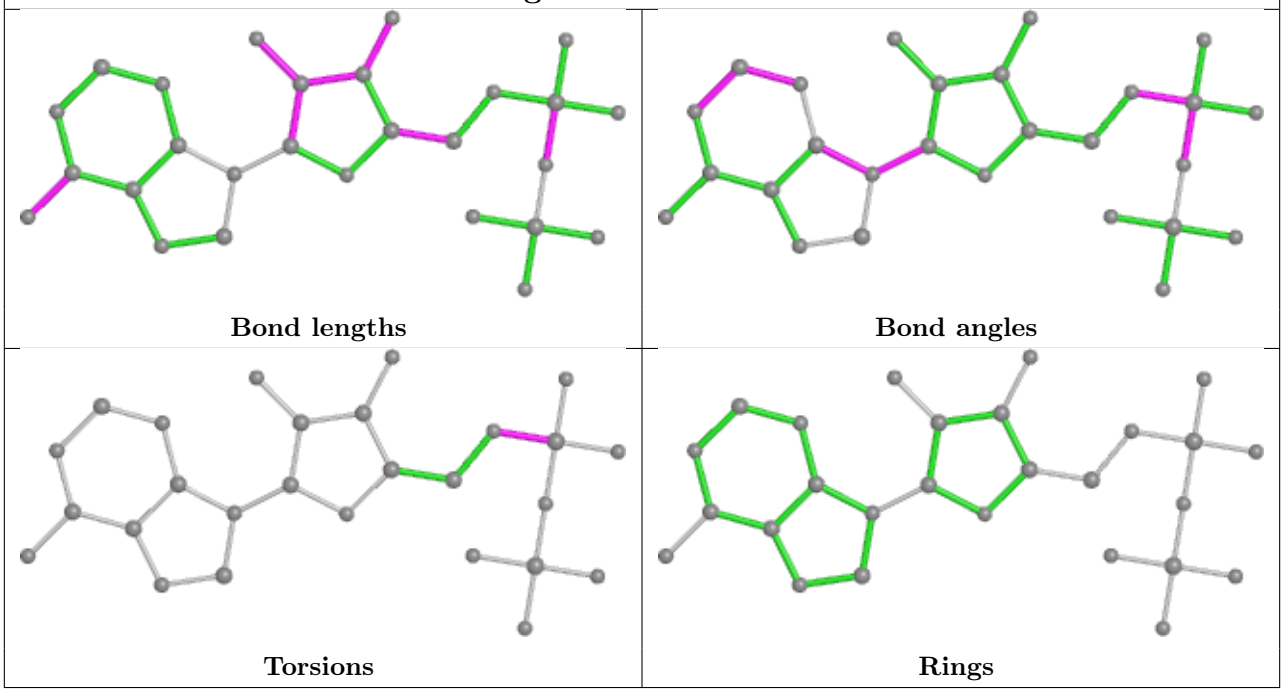
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

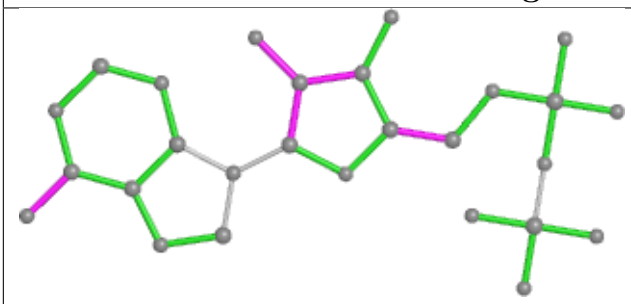
Ligand ADX B 900



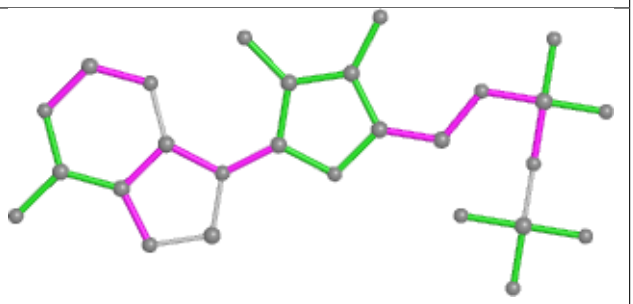
Ligand ADX F 900



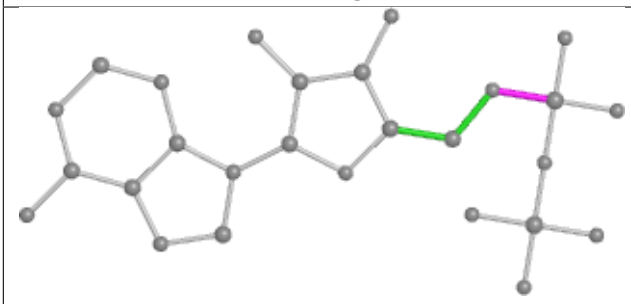
Ligand ADX E 900



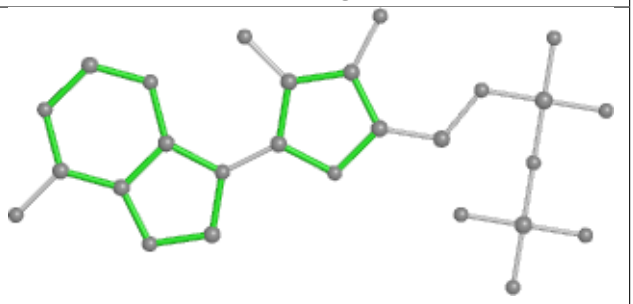
Bond lengths



Bond angles

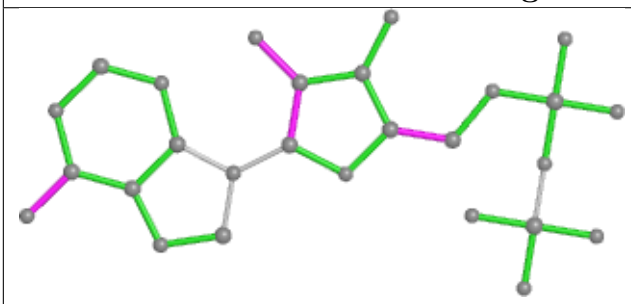


Torsions

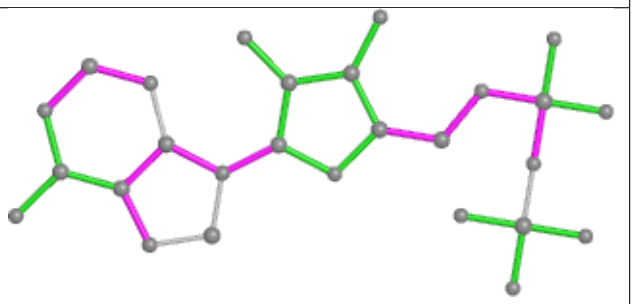


Rings

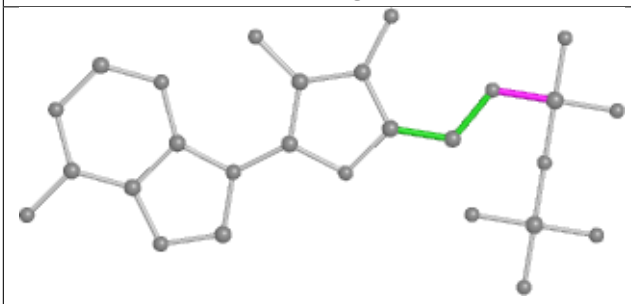
Ligand ADX C 900



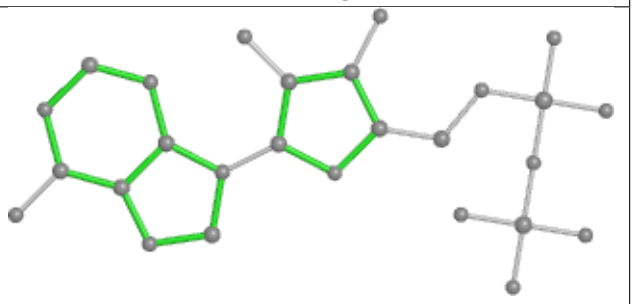
Bond lengths



Bond angles

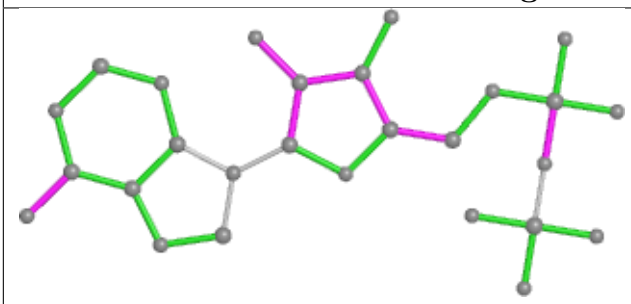


Torsions

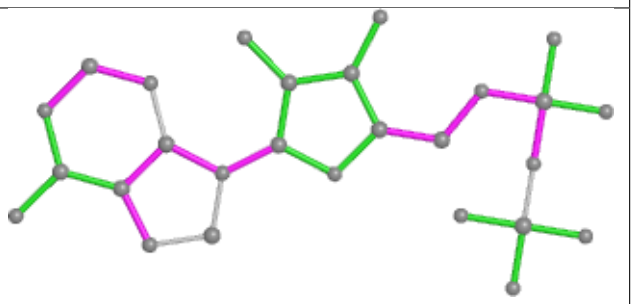


Rings

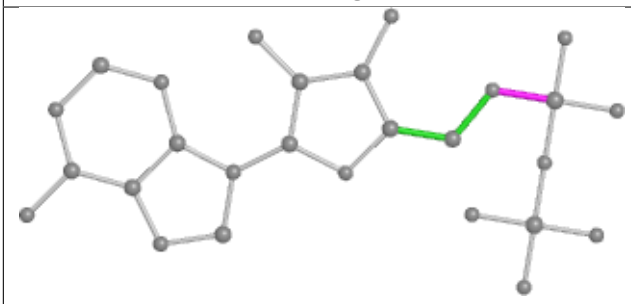
Ligand ADX D 900



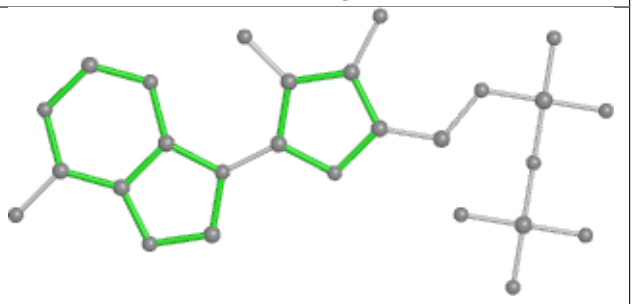
Bond lengths



Bond angles

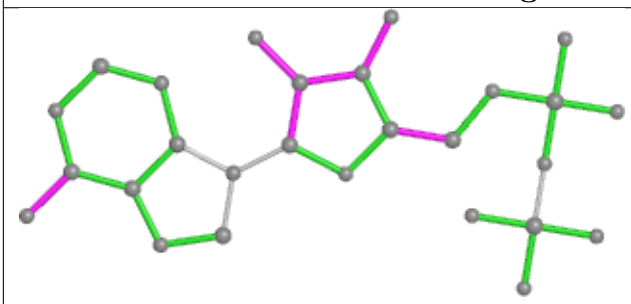


Torsions

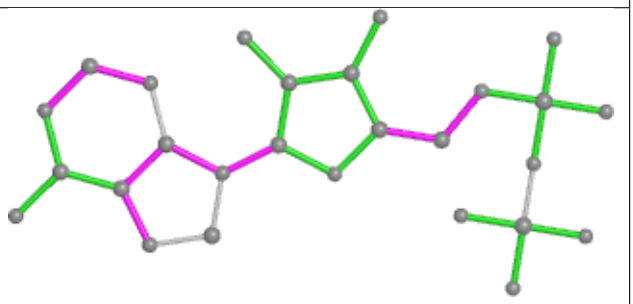


Rings

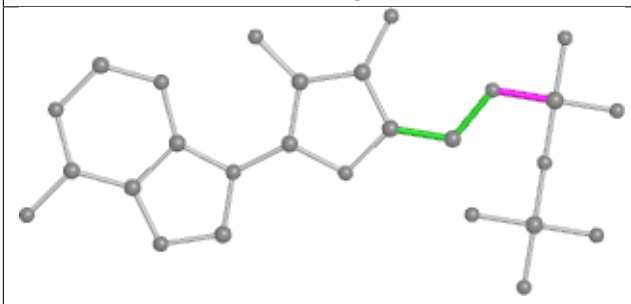
Ligand ADX H 900



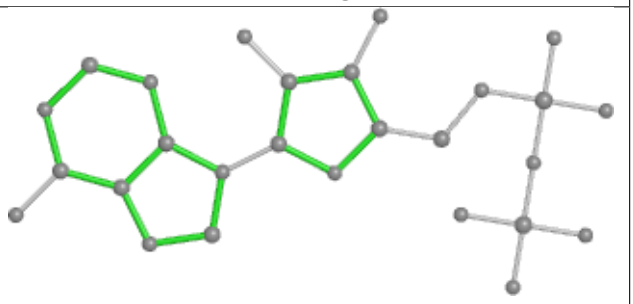
Bond lengths



Bond angles

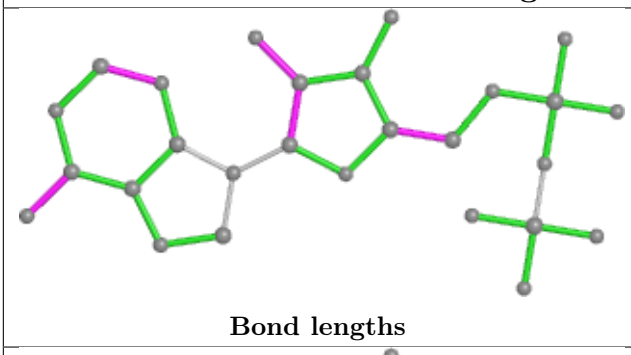


Torsions

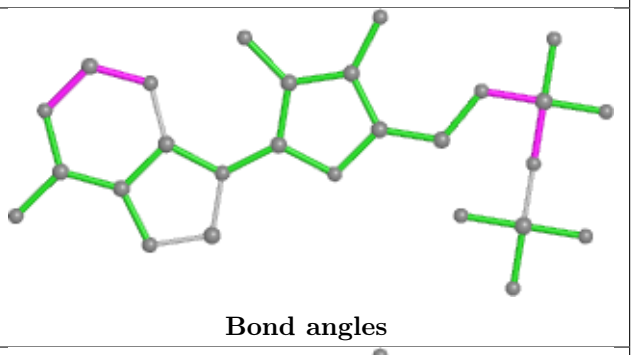


Rings

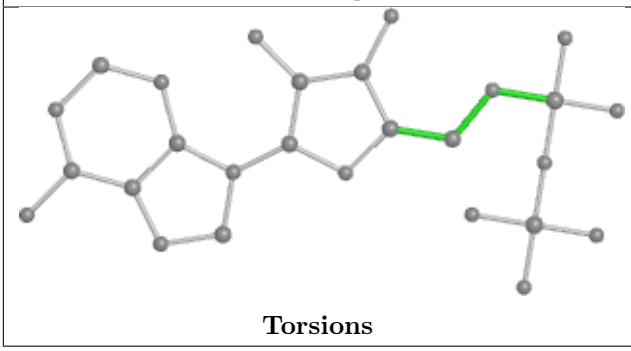
Ligand ADX G 900



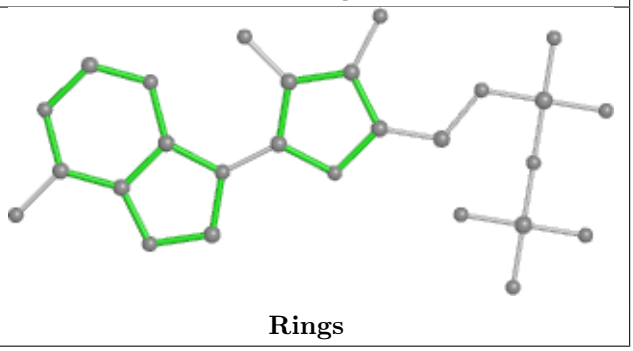
Bond lengths



Bond angles

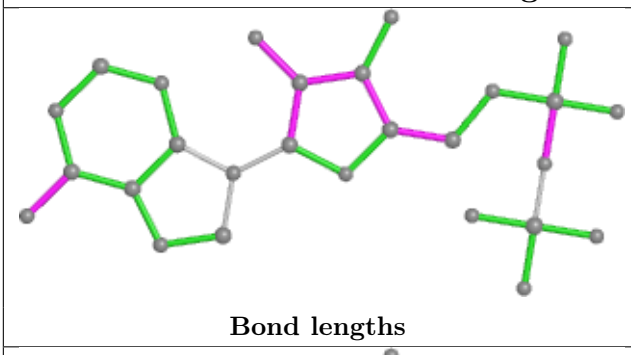


Torsions

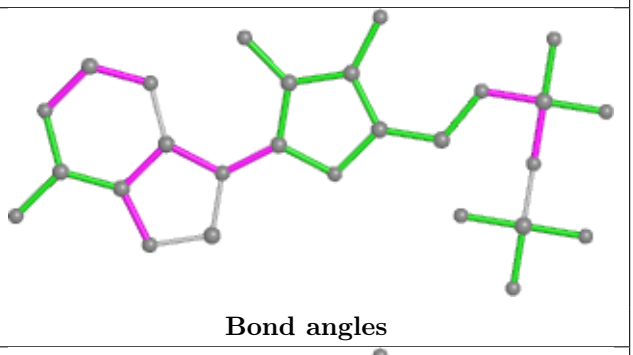


Rings

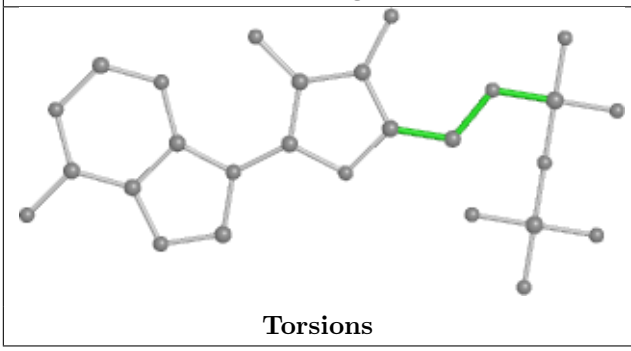
Ligand ADX A 900



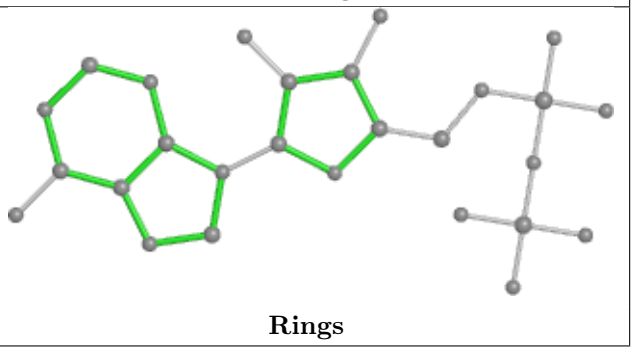
Bond lengths



Bond angles



Torsions



Rings

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	402/404 (99%)	-0.29	3 (0%)	87	89	29, 47, 76, 106	0
1	B	404/404 (100%)	-0.33	5 (1%)	79	80	18, 39, 68, 103	0
1	C	403/404 (99%)	-0.54	1 (0%)	95	95	16, 30, 56, 70	0
1	D	401/404 (99%)	-0.23	4 (0%)	82	84	21, 43, 76, 110	0
1	E	403/404 (99%)	-0.24	3 (0%)	87	89	19, 37, 68, 99	0
1	F	401/404 (99%)	-0.06	17 (4%)	36	38	31, 53, 82, 104	0
1	G	404/404 (100%)	-0.18	4 (0%)	82	84	24, 39, 71, 108	0
1	H	381/404 (94%)	0.46	31 (8%)	12	11	47, 84, 117, 146	0
All	All	3199/3232 (98%)	-0.18	68 (2%)	63	65	16, 44, 91, 146	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	445	TYR	5.2
1	H	445	TYR	5.0
1	A	48	MET	5.0
1	H	65	PHE	4.6
1	F	425	LYS	4.5

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 (i)

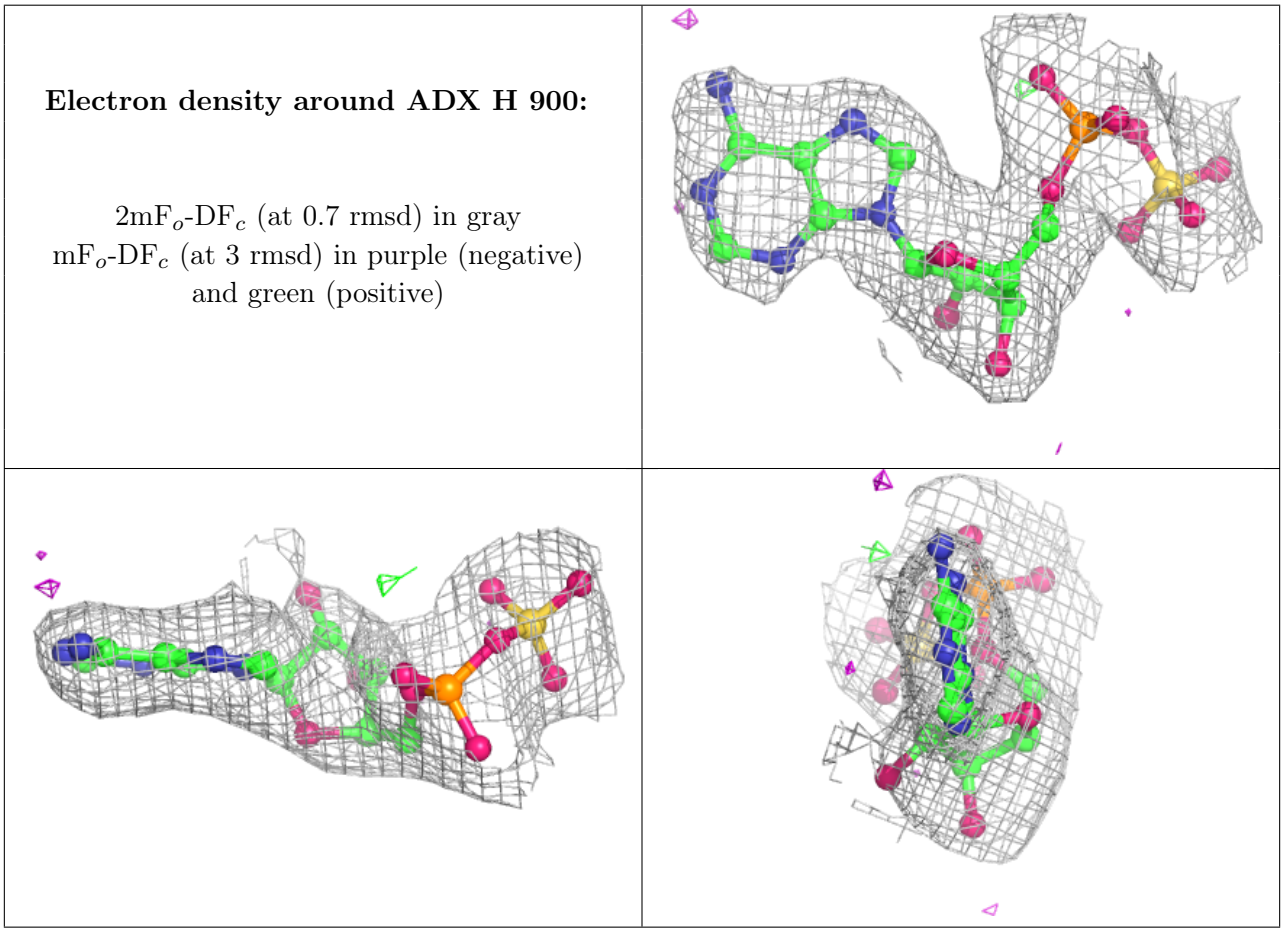
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADX	H	900	27/27	0.96	0.14	71,78,84,91	0
2	ADX	F	900	27/27	0.98	0.13	39,48,53,56	0
2	ADX	G	900	27/27	0.98	0.12	20,27,33,35	0
2	ADX	E	900	27/27	0.98	0.13	21,29,34,37	0
2	ADX	A	900	27/27	0.99	0.10	27,32,36,38	0
2	ADX	B	900	27/27	0.99	0.13	22,29,34,38	0
2	ADX	C	900	27/27	0.99	0.12	17,23,30,32	0
2	ADX	D	900	27/27	0.99	0.13	21,28,30,32	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.

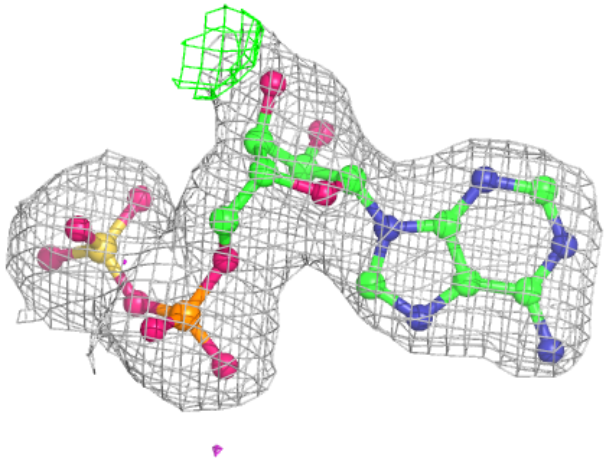
Electron density around ADX H 900:

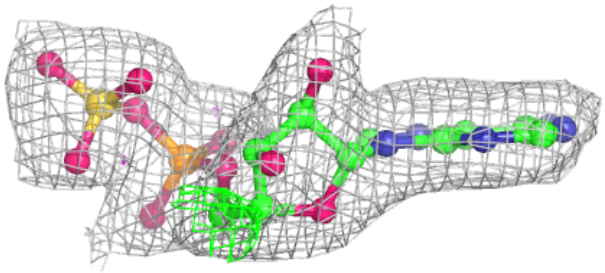
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

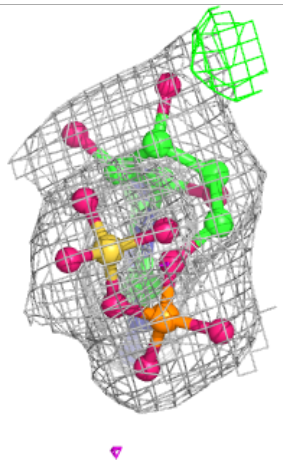


Electron density around ADX F 900:

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

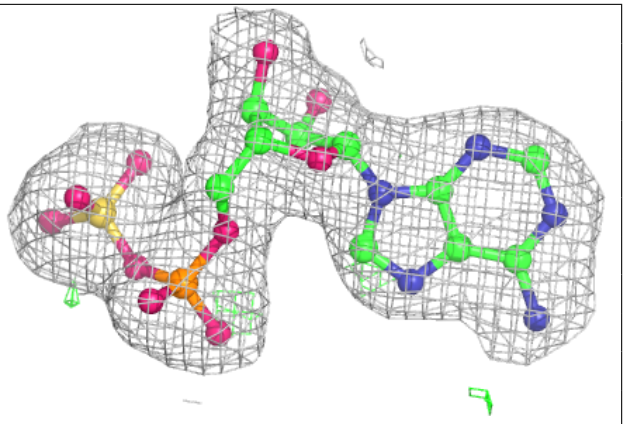


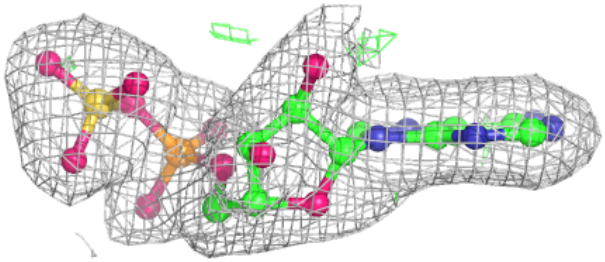


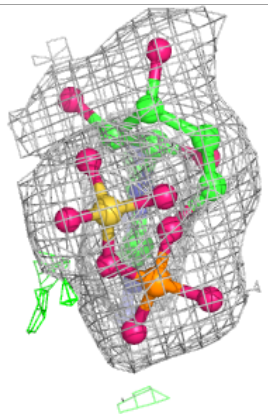


Electron density around ADX G 900:

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

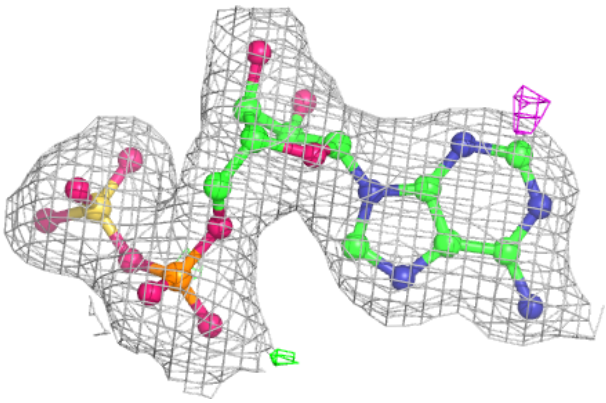


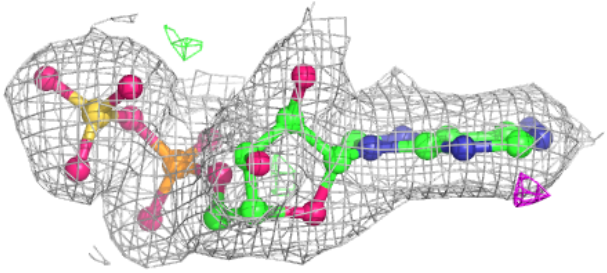


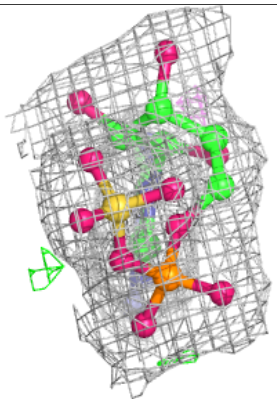


Electron density around ADX E 900:

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

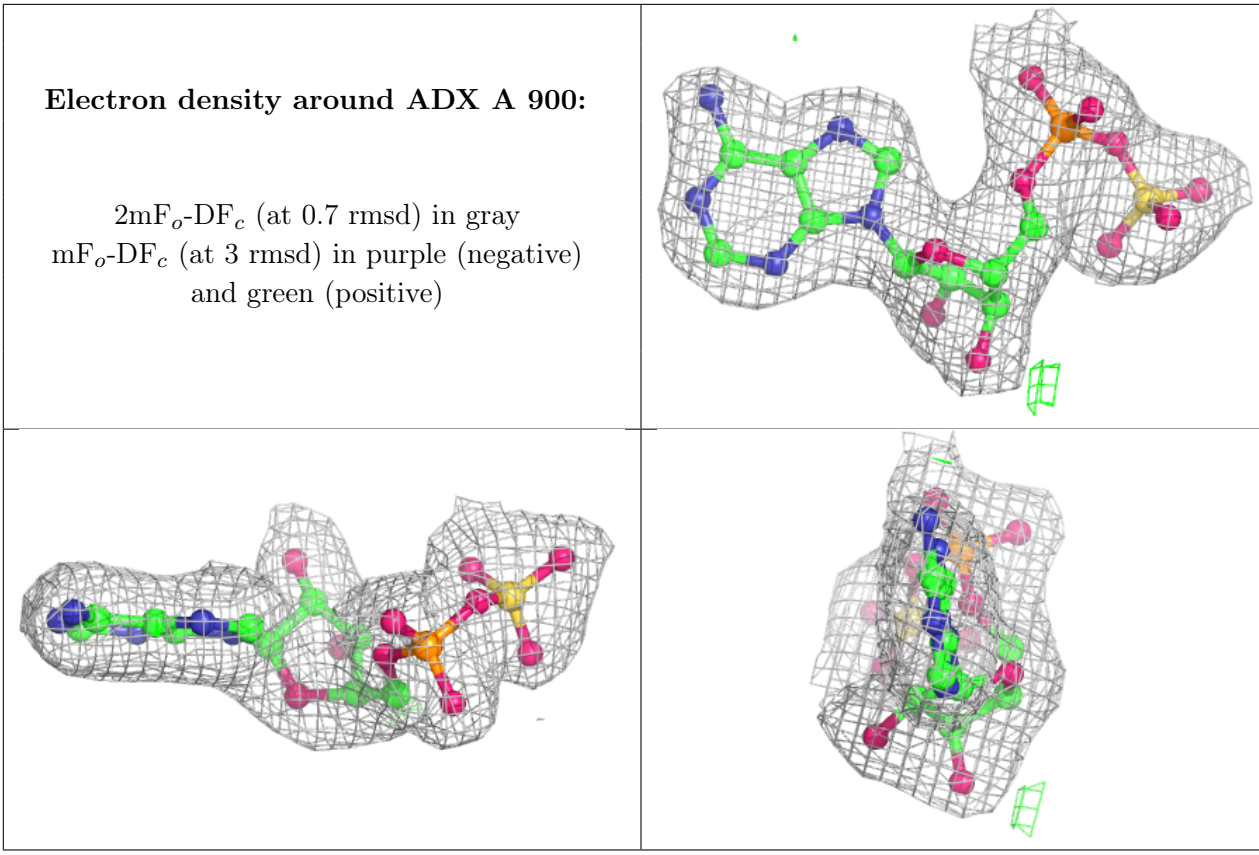






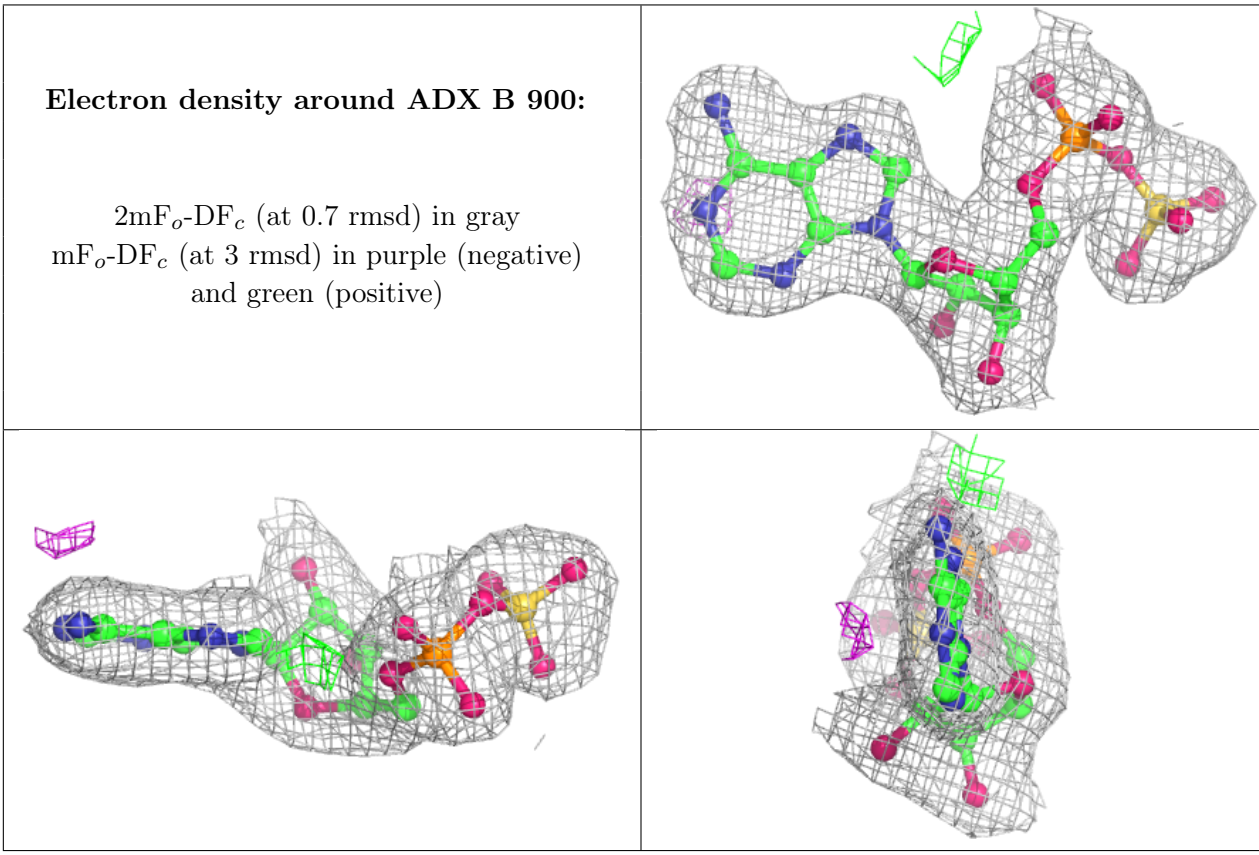
Electron density around ADX A 900:

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



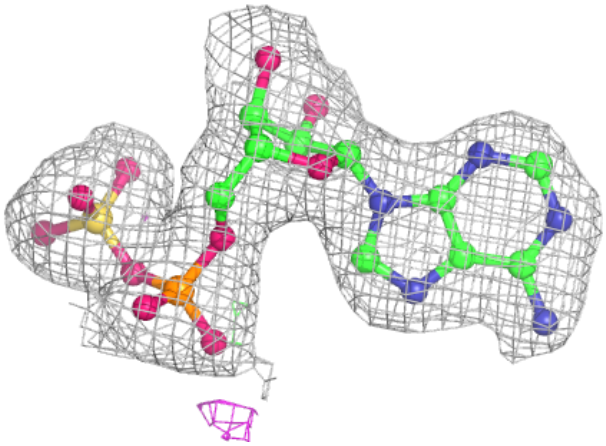
Electron density around ADX B 900:

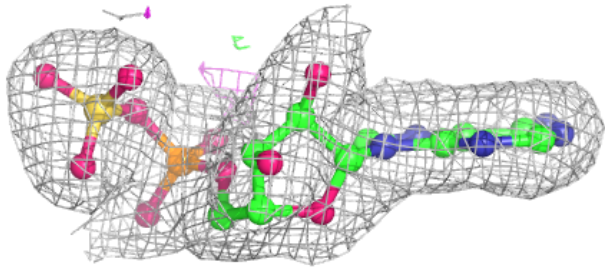
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

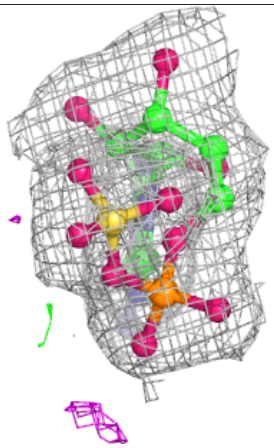


Electron density around ADX C 900:

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

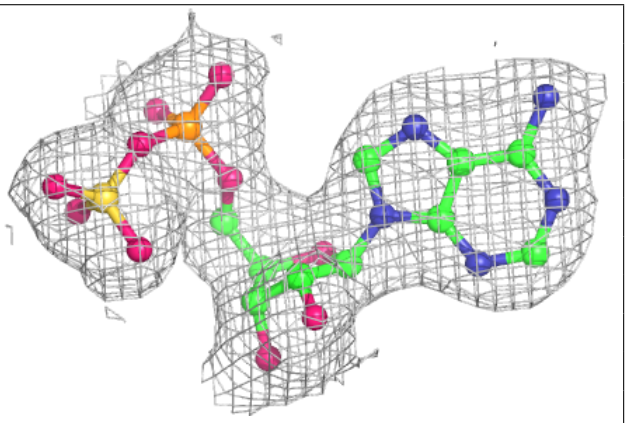


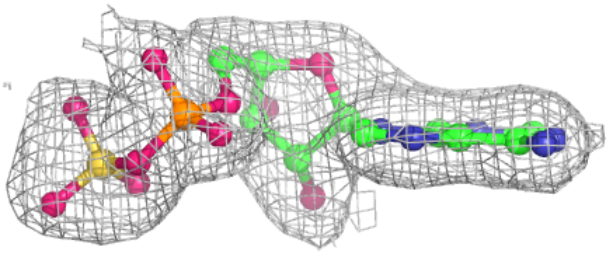


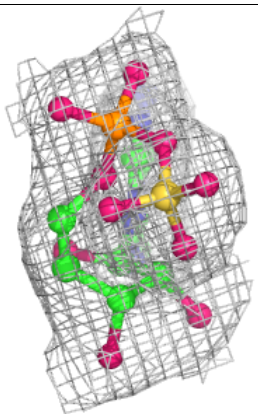


Electron density around ADX D 900:

$2mF_o$-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.