



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 06:07 am BST

PDB ID : 2GOY
Title : Crystal structure of assimilatory adenosine 5'-phosphosulfate reductase with bound APS
Authors : Chartron, J.; Carroll, K.S.; Shiau, C.; Gao, H.; Leary, J.A.; Bertozzi, C.R.; Stout, C.D.
Deposited on : 2006-04-14
Resolution : 2.70 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

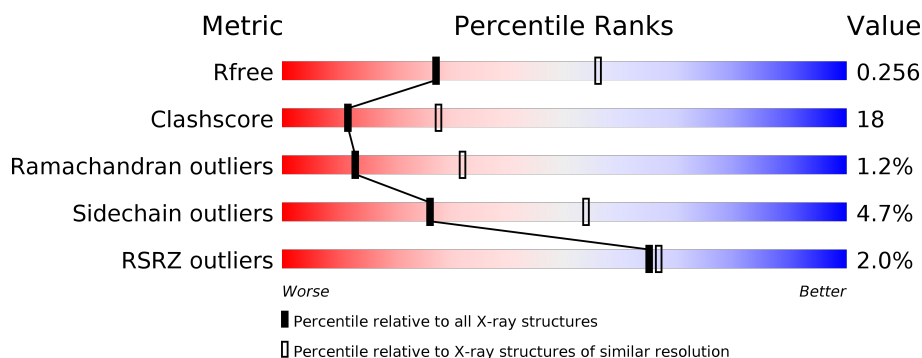
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 54%, green 24%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 54% 24% • 19% </div> </div>
1	B	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 50%, green 29%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 50% 29% • 19% </div> </div>
1	C	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 53%, green 25%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 53% 25% • 19% </div> </div>
1	D	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 50%, green 28%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 50% 28% • 19% </div> </div>
1	E	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 55%, green 24%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 55% 24% • 19% </div> </div>
1	F	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 50%, green 28%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 50% 28% • 19% </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	275	
1	H	275	

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	SF4	G	307	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14727 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 adenosine phosphosulfate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1797	1149	314	327	7			
1	B	223	Total	C	N	O	S	0	0	0
			1804	1154	315	328	7			
1	C	222	Total	C	N	O	S	0	0	0
			1797	1149	314	327	7			
1	D	223	Total	C	N	O	S	0	0	0
			1804	1154	315	328	7			
1	E	222	Total	C	N	O	S	0	0	0
			1797	1149	314	327	7			
1	F	223	Total	C	N	O	S	0	0	0
			1804	1154	315	328	7			
1	G	222	Total	C	N	O	S	0	0	0
			1797	1149	314	327	7			
1	H	223	Total	C	N	O	S	0	0	0
			1804	1154	315	328	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	LEU	-	CLONING ARTIFACT	UNP O05927
A	269	GLU	-	CLONING ARTIFACT	UNP O05927
A	270	HIS	-	EXPRESSION TAG	UNP O05927
A	271	HIS	-	EXPRESSION TAG	UNP O05927
A	272	HIS	-	EXPRESSION TAG	UNP O05927
A	273	HIS	-	EXPRESSION TAG	UNP O05927
A	274	HIS	-	EXPRESSION TAG	UNP O05927
A	275	HIS	-	EXPRESSION TAG	UNP O05927
B	268	LEU	-	CLONING ARTIFACT	UNP O05927
B	269	GLU	-	CLONING ARTIFACT	UNP O05927
B	270	HIS	-	EXPRESSION TAG	UNP O05927
B	271	HIS	-	EXPRESSION TAG	UNP O05927
B	272	HIS	-	EXPRESSION TAG	UNP O05927

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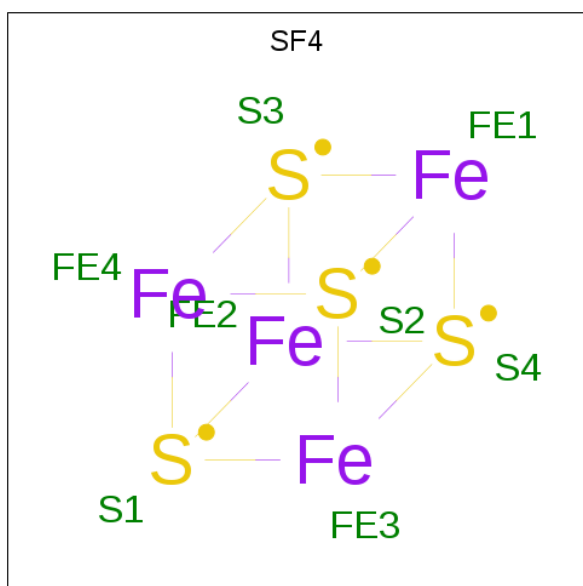
Chain	Residue	Modelled	Actual	Comment	Reference
B	273	HIS	-	EXPRESSION TAG	UNP O05927
B	274	HIS	-	EXPRESSION TAG	UNP O05927
B	275	HIS	-	EXPRESSION TAG	UNP O05927
C	268	LEU	-	CLONING ARTIFACT	UNP O05927
C	269	GLU	-	CLONING ARTIFACT	UNP O05927
C	270	HIS	-	EXPRESSION TAG	UNP O05927
C	271	HIS	-	EXPRESSION TAG	UNP O05927
C	272	HIS	-	EXPRESSION TAG	UNP O05927
C	273	HIS	-	EXPRESSION TAG	UNP O05927
C	274	HIS	-	EXPRESSION TAG	UNP O05927
C	275	HIS	-	EXPRESSION TAG	UNP O05927
D	268	LEU	-	CLONING ARTIFACT	UNP O05927
D	269	GLU	-	CLONING ARTIFACT	UNP O05927
D	270	HIS	-	EXPRESSION TAG	UNP O05927
D	271	HIS	-	EXPRESSION TAG	UNP O05927
D	272	HIS	-	EXPRESSION TAG	UNP O05927
D	273	HIS	-	EXPRESSION TAG	UNP O05927
D	274	HIS	-	EXPRESSION TAG	UNP O05927
D	275	HIS	-	EXPRESSION TAG	UNP O05927
E	268	LEU	-	CLONING ARTIFACT	UNP O05927
E	269	GLU	-	CLONING ARTIFACT	UNP O05927
E	270	HIS	-	EXPRESSION TAG	UNP O05927
E	271	HIS	-	EXPRESSION TAG	UNP O05927
E	272	HIS	-	EXPRESSION TAG	UNP O05927
E	273	HIS	-	EXPRESSION TAG	UNP O05927
E	274	HIS	-	EXPRESSION TAG	UNP O05927
E	275	HIS	-	EXPRESSION TAG	UNP O05927
F	268	LEU	-	CLONING ARTIFACT	UNP O05927
F	269	GLU	-	CLONING ARTIFACT	UNP O05927
F	270	HIS	-	EXPRESSION TAG	UNP O05927
F	271	HIS	-	EXPRESSION TAG	UNP O05927
F	272	HIS	-	EXPRESSION TAG	UNP O05927
F	273	HIS	-	EXPRESSION TAG	UNP O05927
F	274	HIS	-	EXPRESSION TAG	UNP O05927
F	275	HIS	-	EXPRESSION TAG	UNP O05927
G	268	LEU	-	CLONING ARTIFACT	UNP O05927
G	269	GLU	-	CLONING ARTIFACT	UNP O05927
G	270	HIS	-	EXPRESSION TAG	UNP O05927
G	271	HIS	-	EXPRESSION TAG	UNP O05927
G	272	HIS	-	EXPRESSION TAG	UNP O05927
G	273	HIS	-	EXPRESSION TAG	UNP O05927
G	274	HIS	-	EXPRESSION TAG	UNP O05927

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Chain	Residue	Modelled	Actual	Comment	Reference
G	275	HIS	-	EXPRESSION TAG	UNP O05927
H	268	LEU	-	CLONING ARTIFACT	UNP O05927
H	269	GLU	-	CLONING ARTIFACT	UNP O05927
H	270	HIS	-	EXPRESSION TAG	UNP O05927
H	271	HIS	-	EXPRESSION TAG	UNP O05927
H	272	HIS	-	EXPRESSION TAG	UNP O05927
H	273	HIS	-	EXPRESSION TAG	UNP O05927
H	274	HIS	-	EXPRESSION TAG	UNP O05927
H	275	HIS	-	EXPRESSION TAG	UNP O05927

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



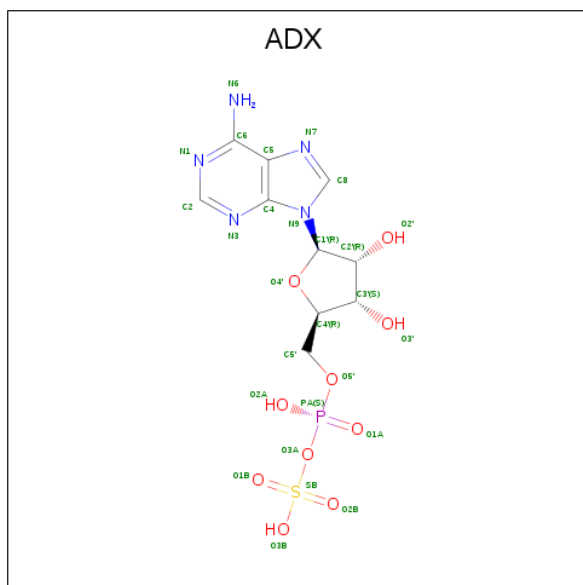
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		
2	G	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: $C_{10}H_{14}N_5O_{10}PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	D	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	F	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
3	H	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		

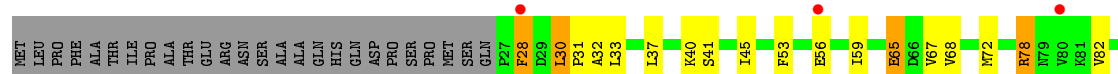
- Molecule 4 is water.

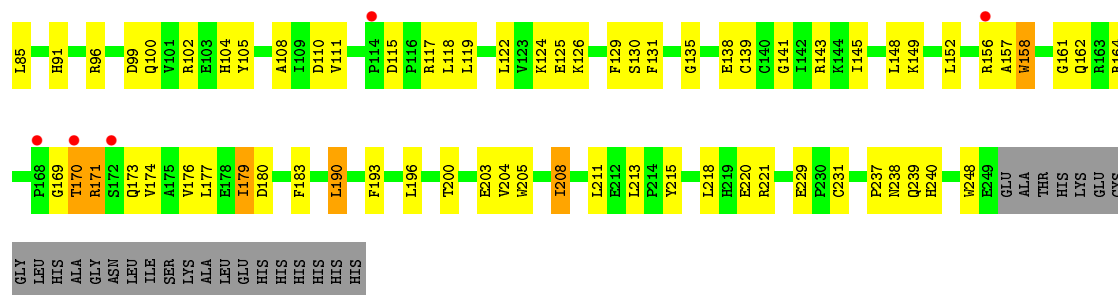
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	8	Total	O	0	0
			8	8		
4	C	24	Total	O	0	0
			24	24		
4	D	15	Total	O	0	0
			15	15		

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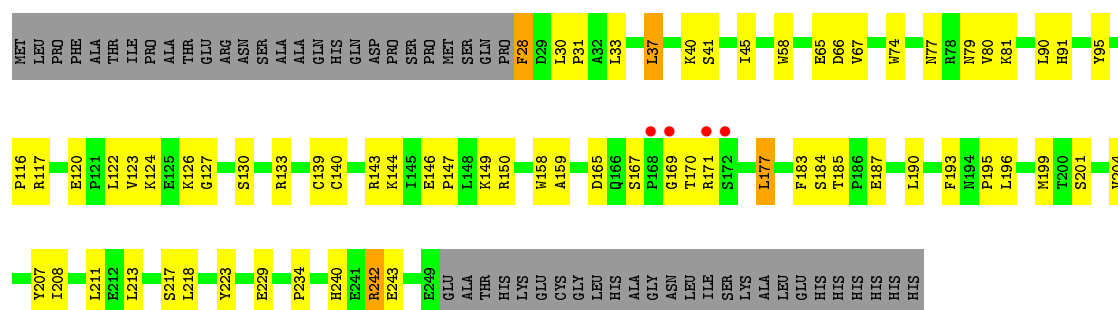
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	30	Total 30	O 30	0	0
4	F	14	Total 14	O 14	0	0
4	G	28	Total 28	O 28	0	0
4	H	12	Total 12	O 12	0	0

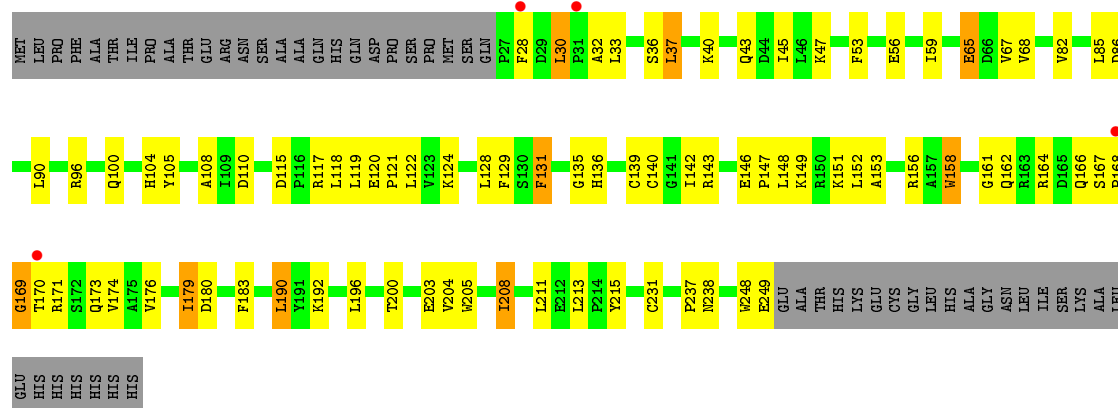




- Molecule 1: adenosine phosphosulfate reductase



- Molecule 1: adenosine phosphosulfate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.03Å 102.79Å 139.37Å 90.10° 102.57° 89.95°	Depositor
Resolution (Å)	38.68 – 2.70 68.02 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.5 (38.68-2.70) 94.8 (68.02-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.265 0.222 , 0.256	Depositor DCC
R_{free} test set	4181 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-h-l 0.387 for -h,k,-l 0.387 for -h,-k,h+l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14727	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0.35	0/1848	0.60	1/2506 (0.0%)
1	B	0.32	0/1856	0.57	0/2517
1	C	0.36	0/1848	0.61	0/2506
1	D	0.32	0/1856	0.56	0/2517
1	E	0.36	0/1848	0.61	0/2506
1	F	0.31	0/1856	0.56	0/2517
1	G	0.35	0/1848	0.58	0/2506
1	H	0.32	0/1856	0.57	0/2517
All	All	0.34	0/14816	0.58	1/20092 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLN	CB-CA-C	5.29	120.98	110.40

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	1797	0	1753	54	0
1	B	1804	0	1761	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1797	0	1753	55	0
1	D	1804	0	1761	76	0
1	E	1797	0	1753	56	0
1	F	1804	0	1761	84	0
1	G	1797	0	1753	53	0
1	H	1804	0	1761	68	0
2	A	8	0	0	1	0
2	B	8	0	0	1	0
2	C	8	0	0	1	0
2	D	8	0	0	1	0
2	E	8	0	0	1	0
2	F	8	0	0	1	0
2	G	8	0	0	2	0
2	H	8	0	0	1	0
3	B	27	0	13	5	0
3	D	27	0	13	6	0
3	F	27	0	13	4	0
3	H	27	0	13	3	0
4	A	20	0	0	1	0
4	B	8	0	0	1	0
4	C	24	0	0	2	0
4	D	15	0	0	1	0
4	E	30	0	0	4	0
4	F	14	0	0	2	0
4	G	28	0	0	0	0
4	H	12	0	0	0	0
All	All	14727	0	14108	503	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 18.

The worst 5 of 503 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:B:179:ILE:H	1:B:179:ILE:HD12	1.23	1.04
1:F:179:ILE:HD12	1:F:179:ILE:H	1.22	1.03
1:H:179:ILE:H	1:H:179:ILE:HD12	1.27	1.00
1:D:179:ILE:H	1:D:179:ILE:HD12	1.23	0.98
1:A:43:GLN:H	1:A:43:GLN:HE21	1.14	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/275 (80%)	202 (92%)	15 (7%)	3 (1%)	11	28
1	B	221/275 (80%)	195 (88%)	22 (10%)	4 (2%)	8	21
1	C	220/275 (80%)	206 (94%)	12 (6%)	2 (1%)	17	40
1	D	221/275 (80%)	202 (91%)	15 (7%)	4 (2%)	8	21
1	E	220/275 (80%)	206 (94%)	13 (6%)	1 (0%)	29	54
1	F	221/275 (80%)	195 (88%)	22 (10%)	4 (2%)	8	21
1	G	220/275 (80%)	208 (94%)	12 (6%)	0	100	100
1	H	221/275 (80%)	200 (90%)	17 (8%)	4 (2%)	8	21
All	All	1764/2200 (80%)	1614 (92%)	128 (7%)	22 (1%)	13	32

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	171	ARG
1	F	170	THR
1	F	171	ARG
1	F	180	ASP
1	H	170	THR

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	193/237 (81%)	183 (95%)	10 (5%)	23	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	194/237 (82%)	185 (95%)	9 (5%)	27	54
1	C	193/237 (81%)	184 (95%)	9 (5%)	26	54
1	D	194/237 (82%)	182 (94%)	12 (6%)	18	40
1	E	193/237 (81%)	187 (97%)	6 (3%)	40	69
1	F	194/237 (82%)	183 (94%)	11 (6%)	20	44
1	G	193/237 (81%)	187 (97%)	6 (3%)	40	69
1	H	194/237 (82%)	184 (95%)	10 (5%)	23	49
All	All	1548/1896 (82%)	1475 (95%)	73 (5%)	26	54

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	110	ASP
1	E	28	PHE
1	H	110	ASP
1	D	179	ILE
1	E	43	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	219	HIS
1	E	43	GLN
1	H	104	HIS
1	C	240	HIS
1	D	104	HIS

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 carbohydrates 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	B	302	1	0,12,12	0.00	-	-		
3	ADX	H	316	-	25,29,29	1.49	3 (12%)	26,45,45	1.87	5 (19%)
2	SF4	G	307	1	0,12,12	0.00	-	-		
3	ADX	B	310	-	25,29,29	1.59	3 (12%)	26,45,45	1.89	5 (19%)
2	SF4	C	303	1	0,12,12	0.00	-	-		
2	SF4	F	306	1	0,12,12	0.00	-	-		
2	SF4	H	308	1	0,12,12	0.00	-	-		
2	SF4	D	304	1	0,12,12	0.00	-	-		
3	ADX	F	314	-	25,29,29	1.73	3 (12%)	26,45,45	1.90	5 (19%)
2	SF4	E	305	1	0,12,12	0.00	-	-		
3	ADX	D	312	-	25,29,29	1.89	3 (12%)	26,45,45	1.93	5 (19%)
2	SF4	A	301	1	0,12,12	0.00	-	-		

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	SF4	B	302	1	-	-	0/6/5/5
3	ADX	H	316	-	-	0/6/32/32	0/3/3/3
2	SF4	G	307	1	-	-	0/6/5/5
3	ADX	B	310	-	-	0/6/32/32	0/3/3/3
2	SF4	C	303	1	-	-	0/6/5/5
2	SF4	F	306	1	-	-	0/6/5/5
2	SF4	H	308	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	D	304	1	-	-	0/6/5/5
3	ADX	F	314	-	-	0/6/32/32	0/3/3/3
2	SF4	E	305	1	-	-	0/6/5/5
3	ADX	D	312	-	-	0/6/32/32	0/3/3/3
2	SF4	A	301	1	-	-	0/6/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	312	ADX	PA-O3A	6.43	1.64	1.59
3	F	314	ADX	PA-O3A	5.40	1.63	1.59
3	B	310	ADX	PA-O3A	4.45	1.62	1.59
3	H	316	ADX	PA-O3A	4.40	1.62	1.59
3	D	312	ADX	C2'-C1'	4.19	1.60	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	312	ADX	C3'-C2'-C1'	4.71	108.07	100.98
3	H	316	ADX	N3-C2-N1	-4.69	121.35	128.68
3	F	314	ADX	C3'-C2'-C1'	4.67	108.02	100.98
3	B	310	ADX	C3'-C2'-C1'	4.67	108.02	100.98
3	D	312	ADX	N3-C2-N1	-4.62	121.45	128.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 27 short contacts:

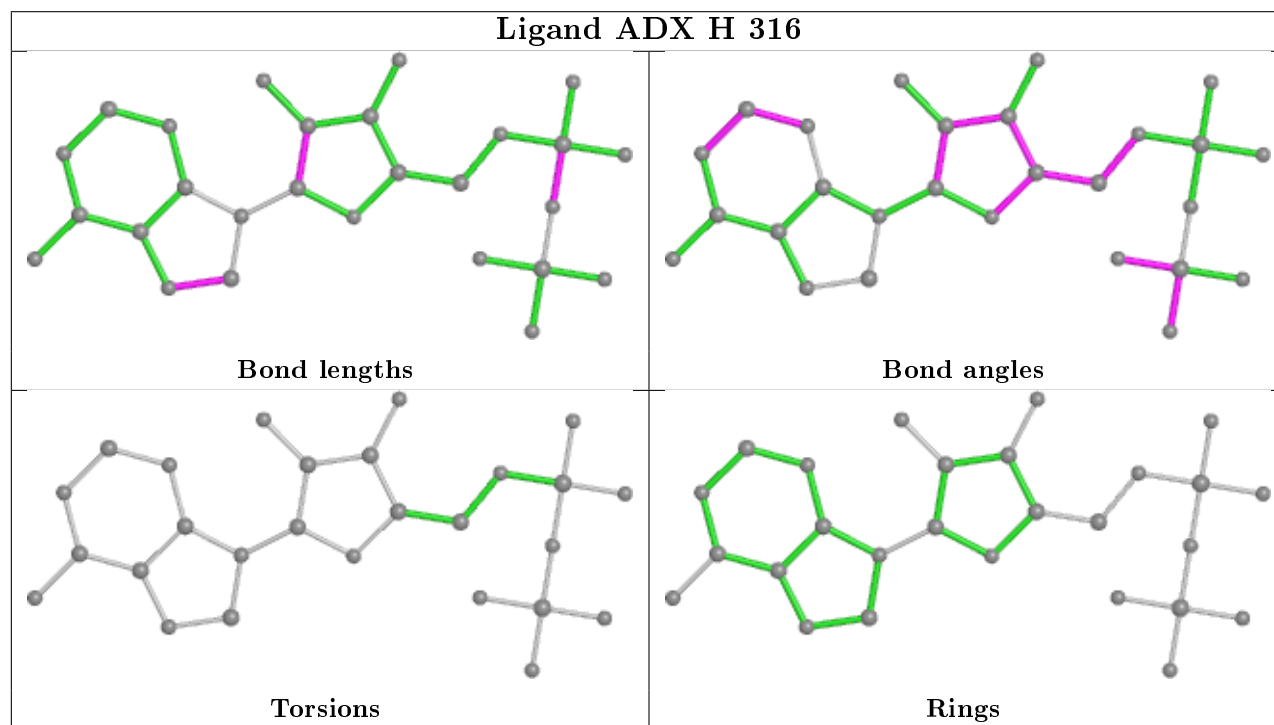
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	SF4	1	0
3	H	316	ADX	3	0
2	G	307	SF4	2	0
3	B	310	ADX	5	0
2	C	303	SF4	1	0
2	F	306	SF4	1	0
2	H	308	SF4	1	0
2	D	304	SF4	1	0
3	F	314	ADX	4	0
2	E	305	SF4	1	0
3	D	312	ADX	6	0

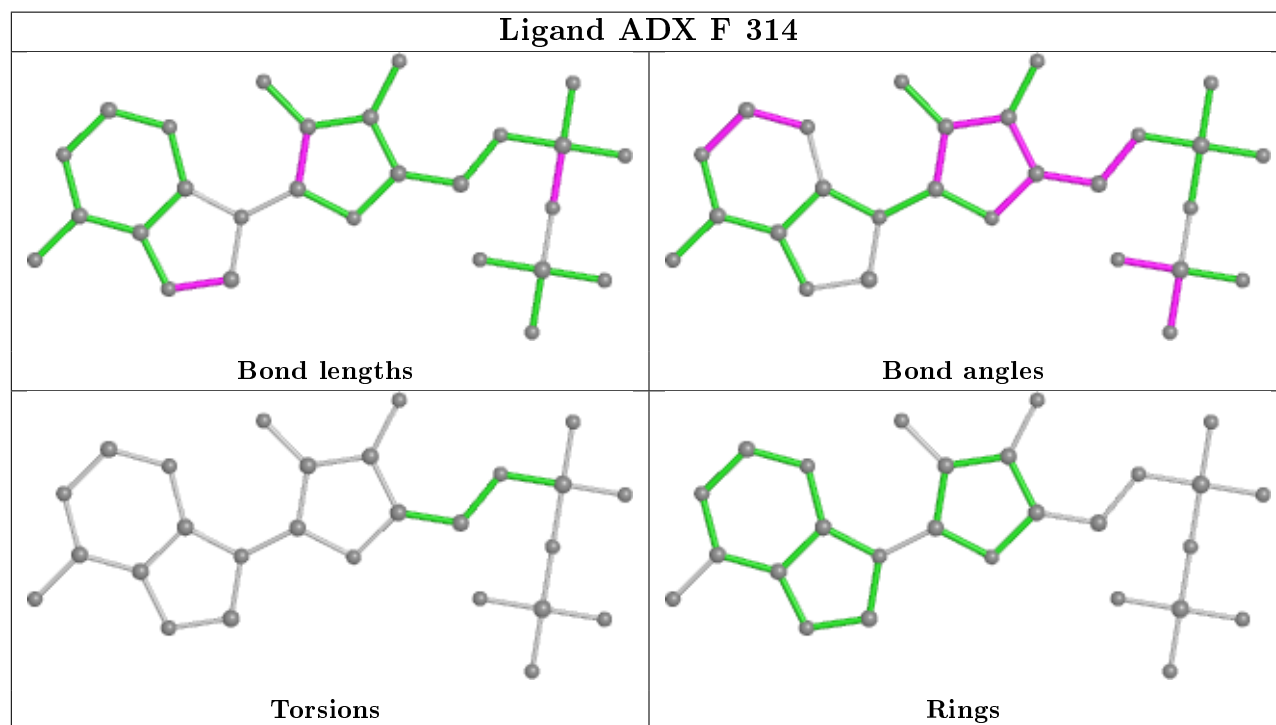
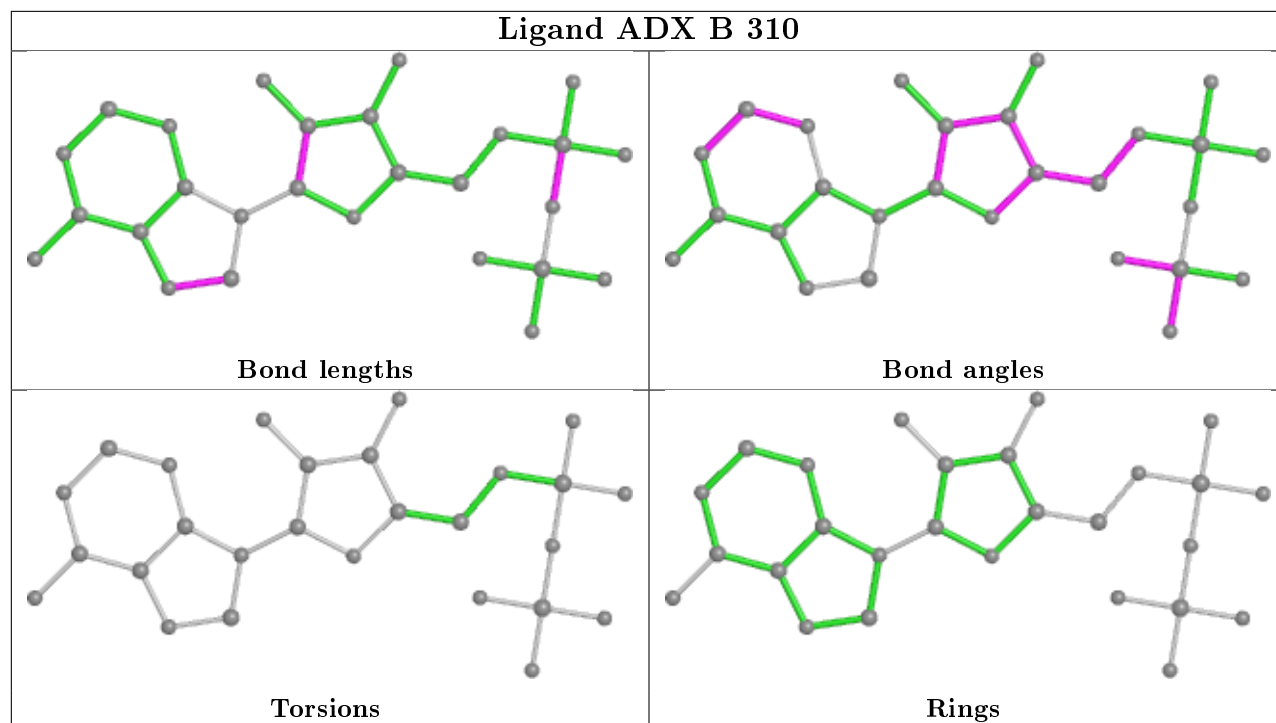
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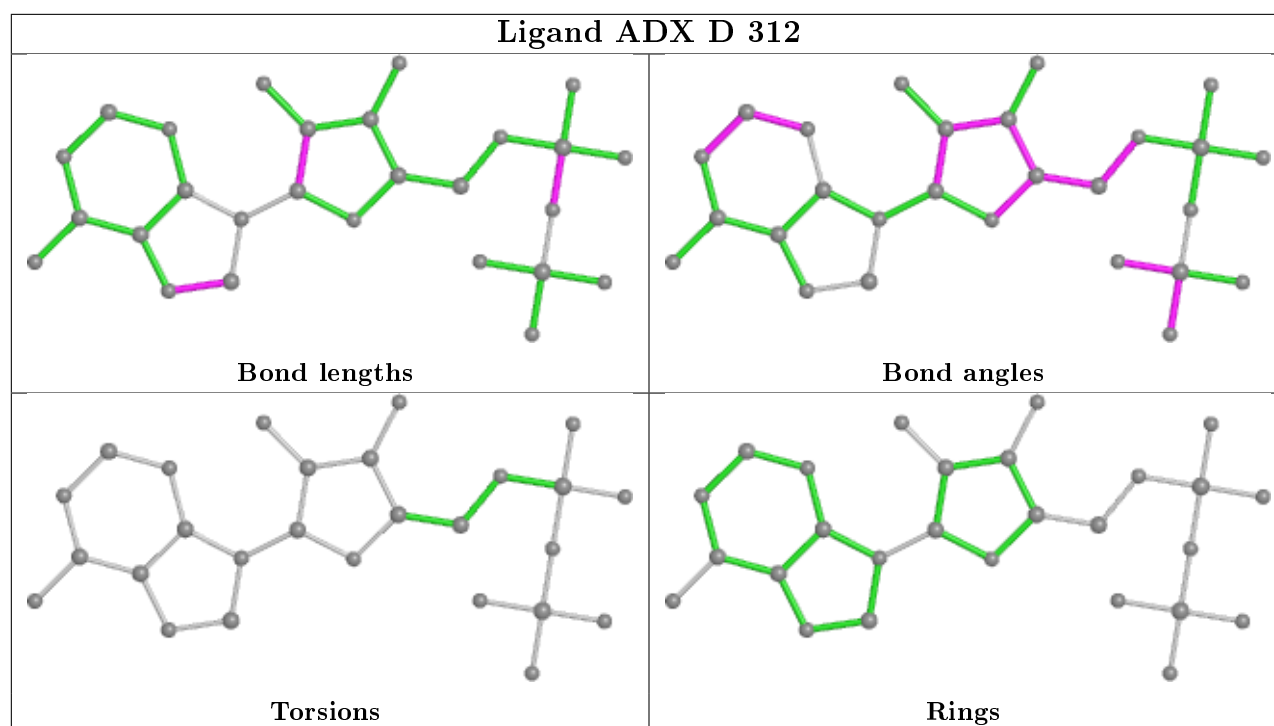
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 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	222/275 (80%)	-0.20	4 (1%) 68 70	9, 29, 54, 90	0
1	B	223/275 (81%)	-0.05	5 (2%) 62 63	24, 42, 75, 101	0
1	C	222/275 (80%)	-0.34	2 (0%) 84 85	12, 25, 50, 87	0
1	D	223/275 (81%)	-0.07	5 (2%) 62 63	15, 41, 73, 106	0
1	E	222/275 (80%)	-0.28	3 (1%) 75 77	13, 25, 49, 90	0
1	F	223/275 (81%)	-0.03	8 (3%) 42 42	15, 43, 77, 100	0
1	G	222/275 (80%)	-0.30	4 (1%) 68 70	14, 29, 50, 88	0
1	H	223/275 (81%)	-0.02	4 (1%) 68 70	21, 42, 74, 100	0
All	All	1780/2200 (80%)	-0.16	35 (1%) 65 67	9, 35, 71, 106	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	170	THR	4.3
1	F	170	THR	4.0
1	A	171	ARG	4.0
1	E	172	SER	4.0
1	E	171	ARG	3.9

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 carbohydrates in this entry.

6.4 Ligands

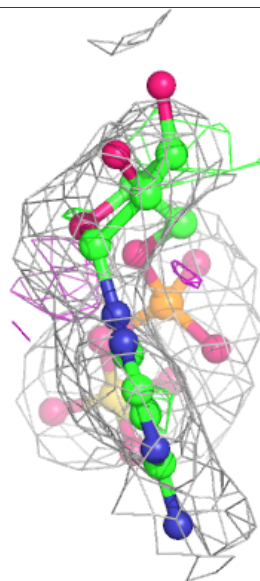
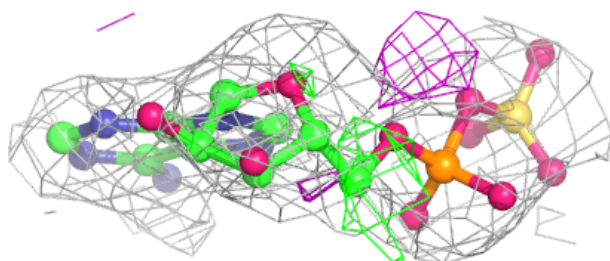
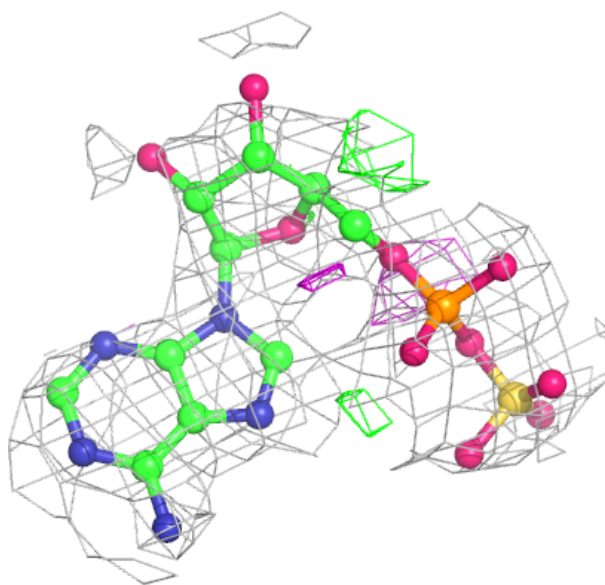
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADX	H	316	27/27	0.79	0.25	100,103,116,117	0
3	ADX	D	312	27/27	0.83	0.31	103,110,115,115	0
3	ADX	F	314	27/27	0.83	0.28	107,111,113,113	0
3	ADX	B	310	27/27	0.88	0.24	106,108,111,113	0
2	SF4	B	302	8/8	0.97	0.14	31,33,34,34	0
2	SF4	D	304	8/8	0.98	0.15	32,33,34,35	0
2	SF4	F	306	8/8	0.98	0.14	31,32,33,33	0
2	SF4	H	308	8/8	0.99	0.14	31,32,34,34	0
2	SF4	C	303	8/8	0.99	0.15	21,22,23,24	0
2	SF4	G	307	8/8	0.99	0.16	18,20,21,22	0
2	SF4	E	305	8/8	0.99	0.14	18,19,22,22	0
2	SF4	A	301	8/8	0.99	0.14	20,21,22,24	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.

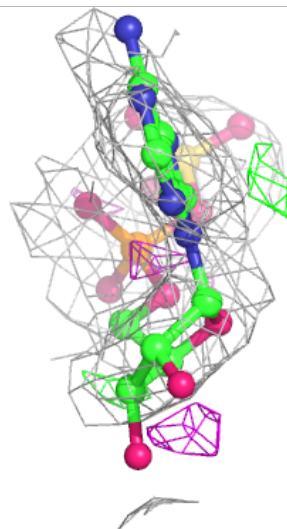
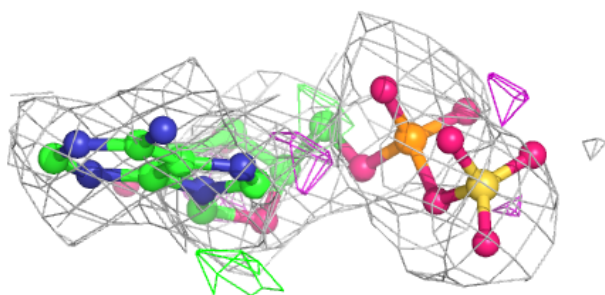
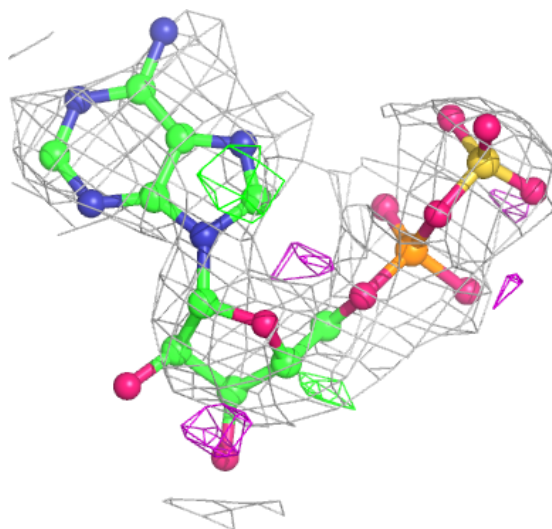
Electron density around ADX H 316:

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



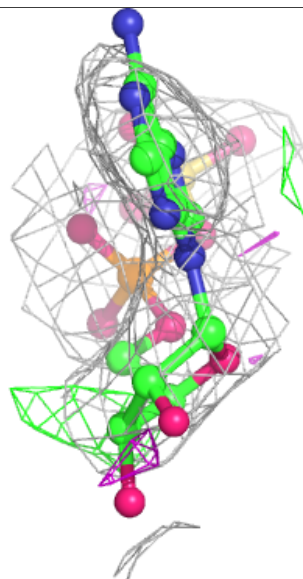
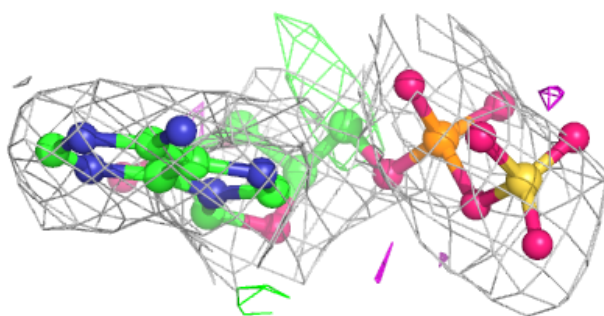
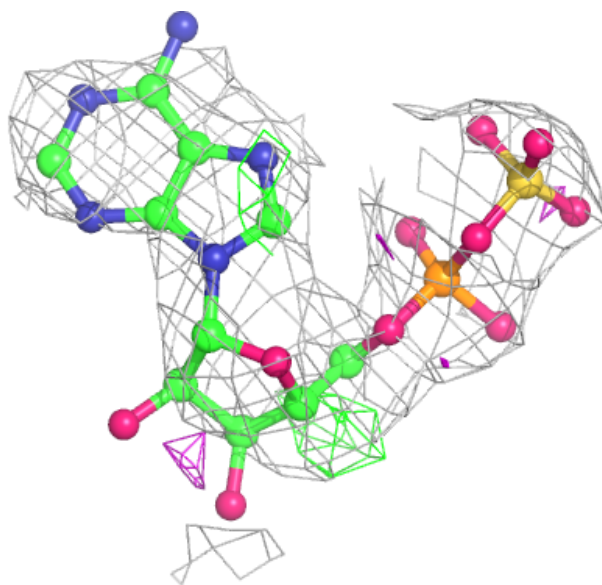
Electron density around ADX D 312:

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



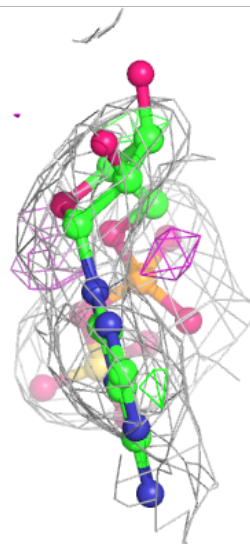
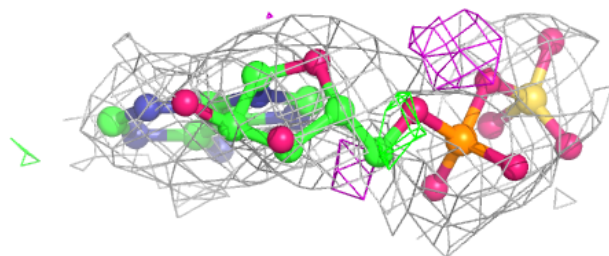
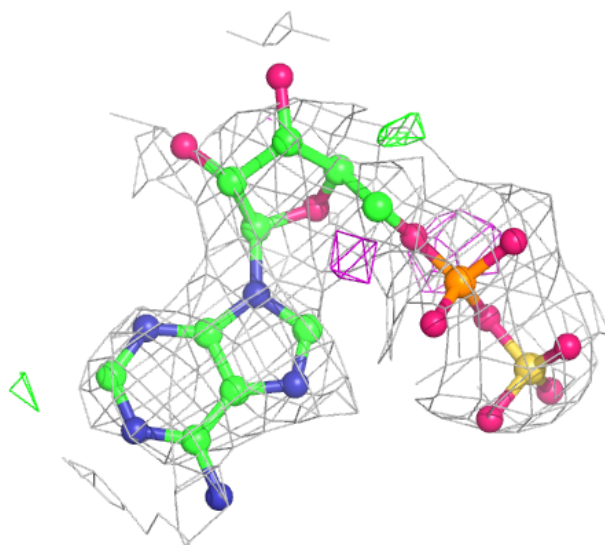
Electron density around ADX F 314:

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



Electron density around ADX B 310:

$2mF_o-DF_c$ (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.