



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 04:43 AM UTC

PDB ID : 1XNJ / pdb_00001xnj
Title : APS complex of human PAPS synthetase 1
Authors : Harjes, S.; Bayer, P.; Scheidig, A.J.
Deposited on : 2004-10-05
Resolution : 1.98 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

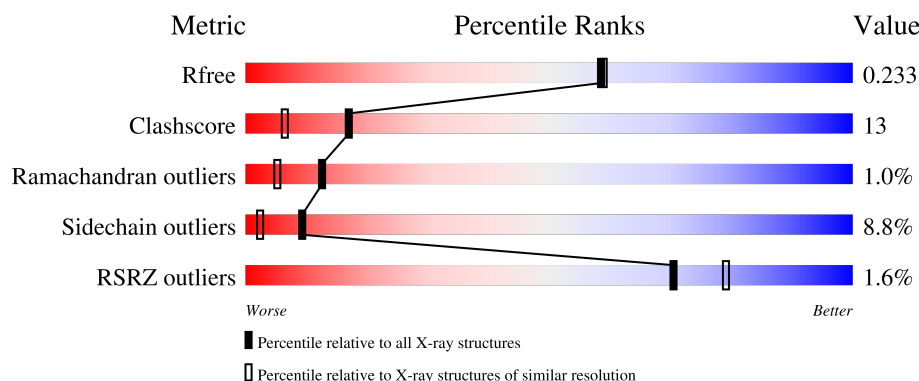
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 $\leq 5\%$. 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	630	2% 56% 26% 6% 11%
1	B	630	% 50% 33% 9% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10000 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 Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	590	Total	C	N	O	S	0	4	0
			4717	2989	830	867	31			
1	A	562	Total	C	N	O	S	0	8	0
			4508	2856	793	827	32			

There are 14 discrepancies between the modelled and reference sequences:

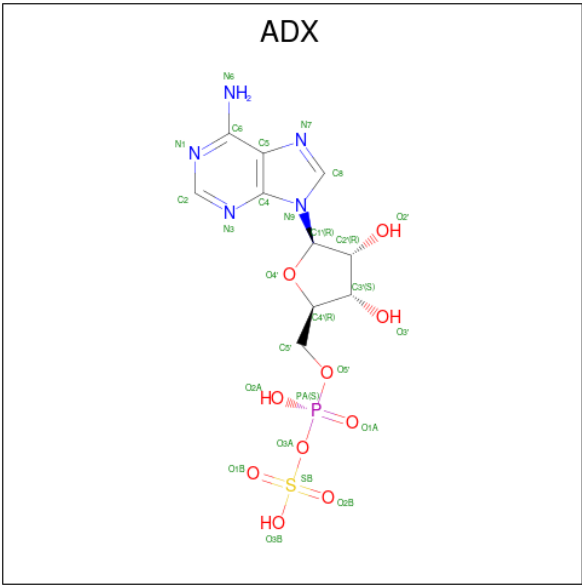
Chain	Residue	Modelled	Actual	Comment	Reference
B	416	SER	PHE	conflict	UNP O43252
B	625	HIS	-	expression tag	UNP O43252
B	626	HIS	-	expression tag	UNP O43252
B	627	HIS	-	expression tag	UNP O43252
B	628	HIS	-	expression tag	UNP O43252
B	629	HIS	-	expression tag	UNP O43252
B	630	HIS	-	expression tag	UNP O43252
A	416	SER	PHE	conflict	UNP O43252
A	625	HIS	-	expression tag	UNP O43252
A	626	HIS	-	expression tag	UNP O43252
A	627	HIS	-	expression tag	UNP O43252
A	628	HIS	-	expression tag	UNP O43252
A	629	HIS	-	expression tag	UNP O43252
A	630	HIS	-	expression tag	UNP O43252

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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

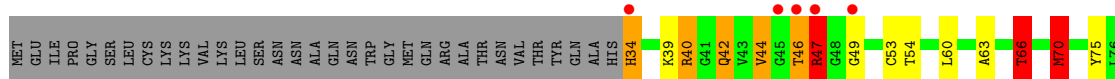


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	B	1	27	10	5	10	1	1	0	0
3	B	1	27	10	5	10	1	1	0	0
3	A	1	27	10	5	10	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	324	Total 324	O 324	0	0
4	A	343	Total 343	O 343	0	0

- Molecule 1: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1



V77	C78	H79	G80	I81	P82	C83	Y84	D89	R92	Q93	G94	L95	N96	K97	N98	L99	R106	E107	E108	N109	V110	R111	R112	I113	A114	K118	L119	F120	A121	V126	G127	I128	I129	S130	P134	D138	S150	P161	HIS	VAL	CYS	GLU	GLN	ARG	ASP	VAL	LYS	GLY	LEU		
TYR	LYS	LYS	ALA	ARG	ALA	GLY	GLU	ILE	LYS	GLY	PHE	THR	GLY	ILE	ASP	SER	E191	Y192	E196	A197	S206	C207	Q214	E222	I225	V226	P227	V228	D229	A230	S231	V232	E233	V234	K235	E236	V239	P240	E241	V242	K243	L244	H245	L246	K247	T249	N264	Q265	V266	V267	Q268
L270	A271	M368	A275	N279	R283	E284	R285	C290	L291	H292	L384	I302	D385	R386	L304	P307	I308	H314	E315	D316	K317	D321	Y330	R333	R334	I337	R340	P341	E342	F343	F344	E345	H346	R347	K348	R351	C352	A353	R354	Q355	W356	G357	T358	T359	C360	R361	R362	H363			
I366	K367	M368	M370	E371	W375	L376	I377	G378	Q382	V383	L384	D385	R386	G392	Q395	Y396	T401	E402	L403	K404	Q405	K408	D409	M410	N411	A414	V415	S416	L420	P423	H428	M432	T435	H436	L439	L440	E441	R445	B446	P447	V448	L449									
H452	P453	L454	G455	G456	W457	D460	P464	L465	M466	Q471	H472	L476	A489	T490	F491	M496	M496	Y497	A498	T501	E502	H506	C507	R508	A509	R510	M511	G514	Y518	R522	D523	P524	A525	H529	P530	E531	K534	E538	P539	S540	H541	M548	A549								
L553	T554	L555	E556	I557	R561	K568	K569	K570	R571	M572	S577	E578	H579	H580	E581	D582	I586	M591	R592	A595	R596	E597	K609	L614	L621	A624	HIS	HIS	HIS	HIS	HIS	HIS	HIS	K534	E538	P539	S540	H541	M548	A549											

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.50Å 82.50Å 133.00Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	129.10 – 1.98 128.47 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.0 (129.10-1.98) 97.6 (128.47-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.184 , 0.239 (Not available) , 0.233	Depositor DCC
R_{free} test set	5581 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10000	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 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADX, ADP

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	1.99	101/4663 (2.2%)	1.57	48/6321 (0.8%)
1	B	2.08	138/4846 (2.8%)	1.64	52/6563 (0.8%)
All	All	2.04	239/9509 (2.5%)	1.60	100/12884 (0.8%)

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	A	0	2
1	B	0	2
All	All	0	4

The worst 5 of 239 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	ASN	CA-C	-14.25	1.44	1.53
1	B	329	MET	SD-CE	11.66	2.08	1.79
1	A	70	MET	SD-CE	11.08	2.07	1.79
1	B	491	PHE	CA-C	-10.93	1.41	1.52
1	B	433	GLN	CA-C	-10.04	1.39	1.52

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	PRO	CA-C-O	-10.21	109.82	121.36
1	B	102	SER	CA-C-N	9.17	131.30	119.84
1	B	102	SER	C-N-CA	9.17	131.30	119.84
1	B	525	ALA	CA-C-N	-8.80	113.24	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	525	ALA	C-N-CA	-8.80	113.24	122.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	VAL	Peptide
1	A	229	ASP	Peptide
1	B	102	SER	Peptide
1	B	506	HIS	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4508	0	4420	103	0
1	B	4717	0	4653	137	0
2	B	27	0	12	1	0
3	A	27	0	11	0	0
3	B	54	0	25	6	0
4	A	343	0	0	27	0
4	B	324	0	0	28	0
All	All	10000	0	9121	235	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 13.

The worst 5 of 235 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:553:ILE:CG1	1:B:553:ILE:CD1	1.75	1.63
1:B:466:MET:CE	1:B:466:MET:SD	2.04	1.46
1:A:466:MET:CE	1:A:466:MET:SD	2.04	1.44
1:A:70:MET:CE	1:A:70:MET:SD	2.07	1.41
1:B:329:MET:CE	1:B:329:MET:SD	2.08	1.41

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	566/630 (90%)	547 (97%)	17 (3%)	2 (0%)	30	20
1	B	591/630 (94%)	557 (94%)	24 (4%)	10 (2%)	7	1
All	All	1157/1260 (92%)	1104 (95%)	41 (4%)	12 (1%)	12	5

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	SER
1	B	103	PRO
1	B	183	LYS
1	B	579	HIS
1	A	230	ALA

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	489/538 (91%)	450 (92%)	39 (8%)	11	3
1	B	507/538 (94%)	458 (90%)	49 (10%)	8	1
All	All	996/1076 (93%)	908 (91%)	88 (9%)	9	2

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	MET
1	A	386	ARG
1	A	93	GLN
1	A	214	GLN
1	A	508	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	579	HIS
1	A	422	ASN
1	B	422	ASN
1	A	140	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
2	ADP	B	2800	-	28,29,29	1.57	3 (10%)	43,45,45	2.11	14 (32%)
3	ADX	B	2700	-	29,29,29	1.82	7 (24%)	42,45,45	3.05	19 (45%)
3	ADX	A	2900	-	29,29,29	1.81	7 (24%)	42,45,45	2.32	15 (35%)
3	ADX	B	2805	-	29,29,29	1.46	5 (17%)	42,45,45	2.93	19 (45%)

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	ADP	B	2800	-	-	2/16/32/32	0/3/3/3
3	ADX	B	2700	-	-	2/10/32/32	0/3/3/3
3	ADX	A	2900	-	-	2/10/32/32	0/3/3/3
3	ADX	B	2805	-	-	3/10/32/32	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2900	ADX	C8-N7	4.36	1.40	1.31
2	B	2800	ADP	C8-N7	4.36	1.40	1.31
3	B	2700	ADX	C8-N7	4.20	1.39	1.31
3	B	2700	ADX	C2-N1	3.99	1.41	1.33
3	A	2900	ADX	C8-N9	3.57	1.43	1.37

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2700	ADX	O3B-SB-O2B	8.70	139.01	108.56
3	B	2805	ADX	N3-C2-N1	-7.90	116.63	128.58
3	A	2900	ADX	N3-C2-N1	-7.32	117.50	128.58
3	B	2700	ADX	O3B-SB-O3A	-6.83	91.38	106.02
3	B	2805	ADX	N9-C8-N7	-6.80	104.29	113.94

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2805	ADX	C5'-O5'-PA-O1A
3	A	2900	ADX	C5'-O5'-PA-O1A

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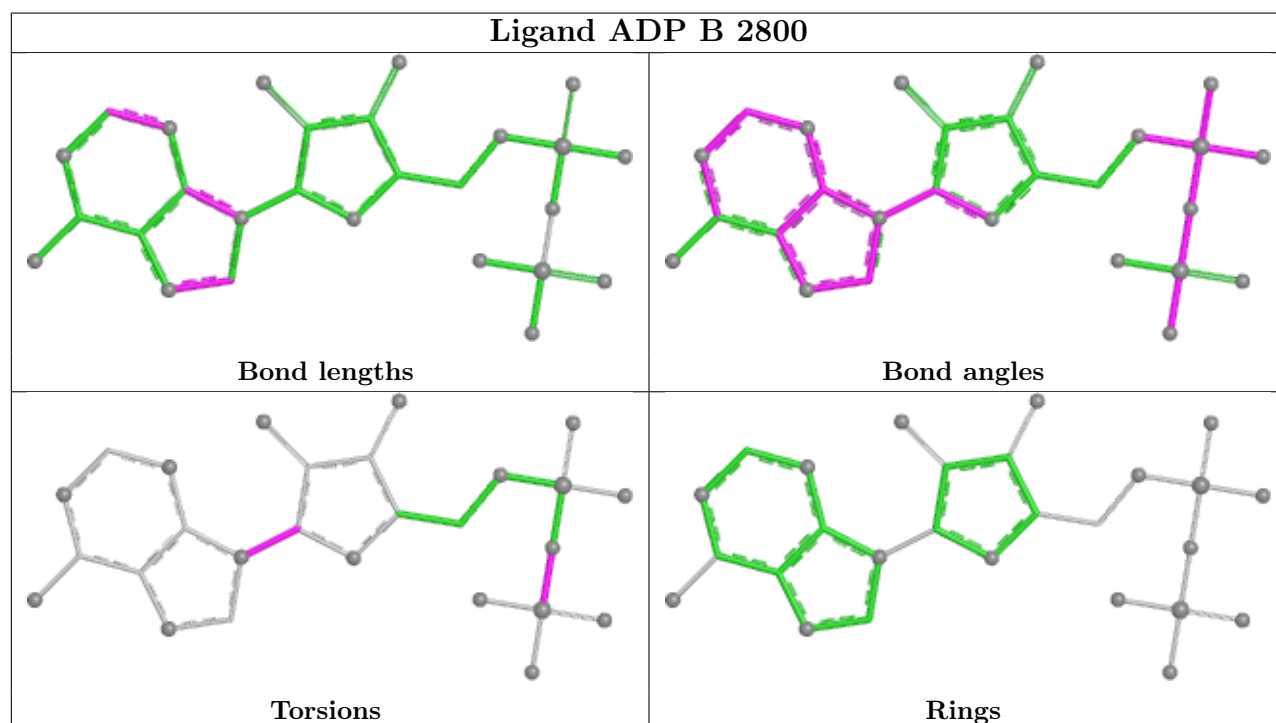
Mol	Chain	Res	Type	Atoms
3	A	2900	ADX	C5'-O5'-PA-O3A
3	B	2805	ADX	C2'-C1'-N9-C4
3	B	2805	ADX	C2'-C1'-N9-C8

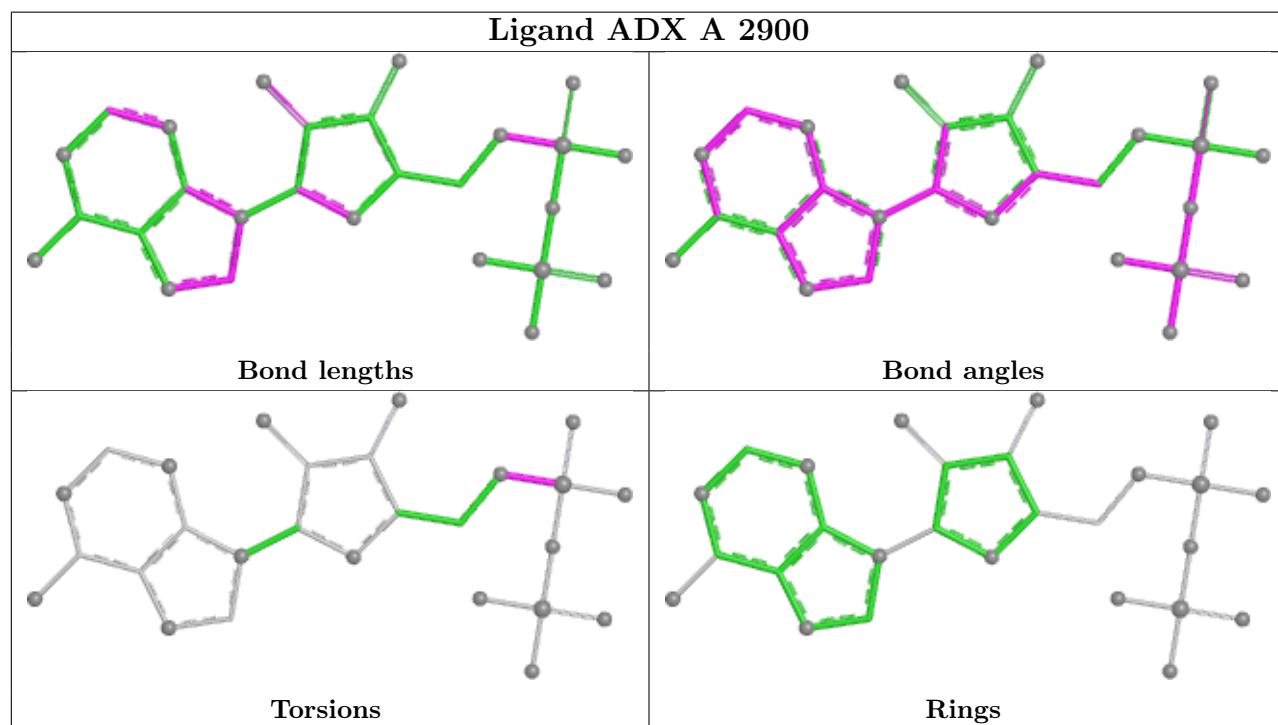
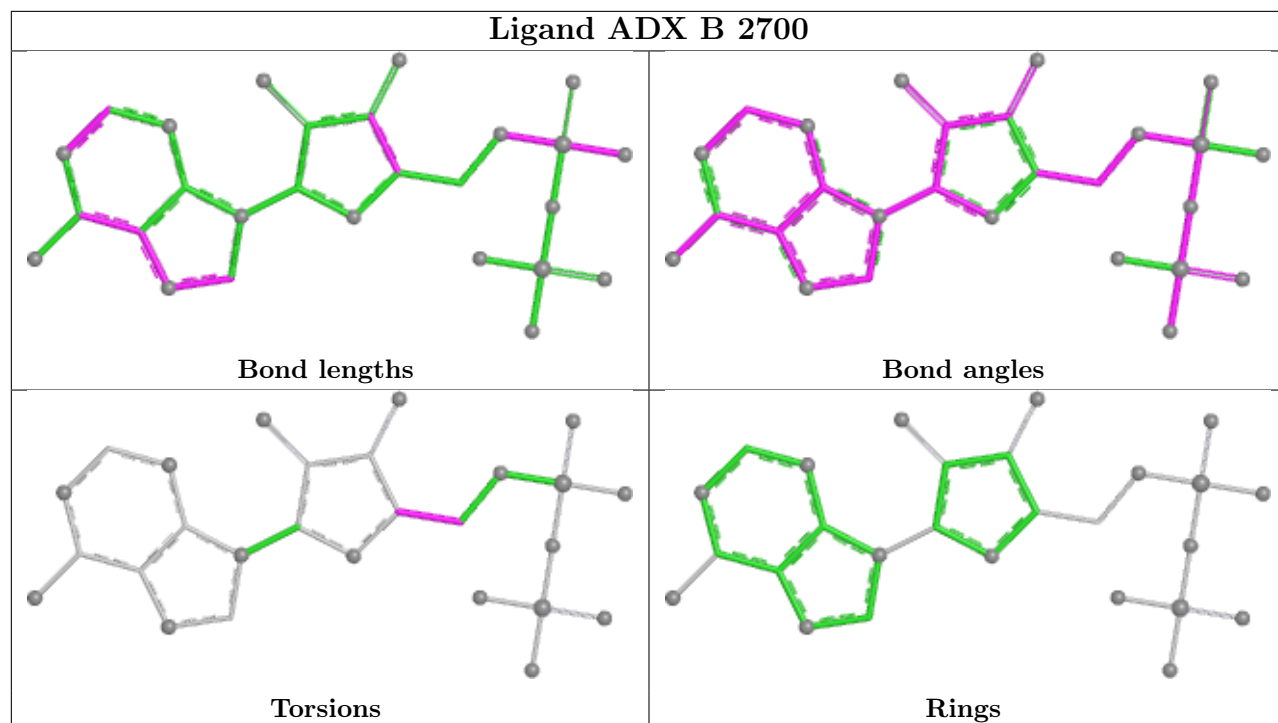
There are no ring outliers.

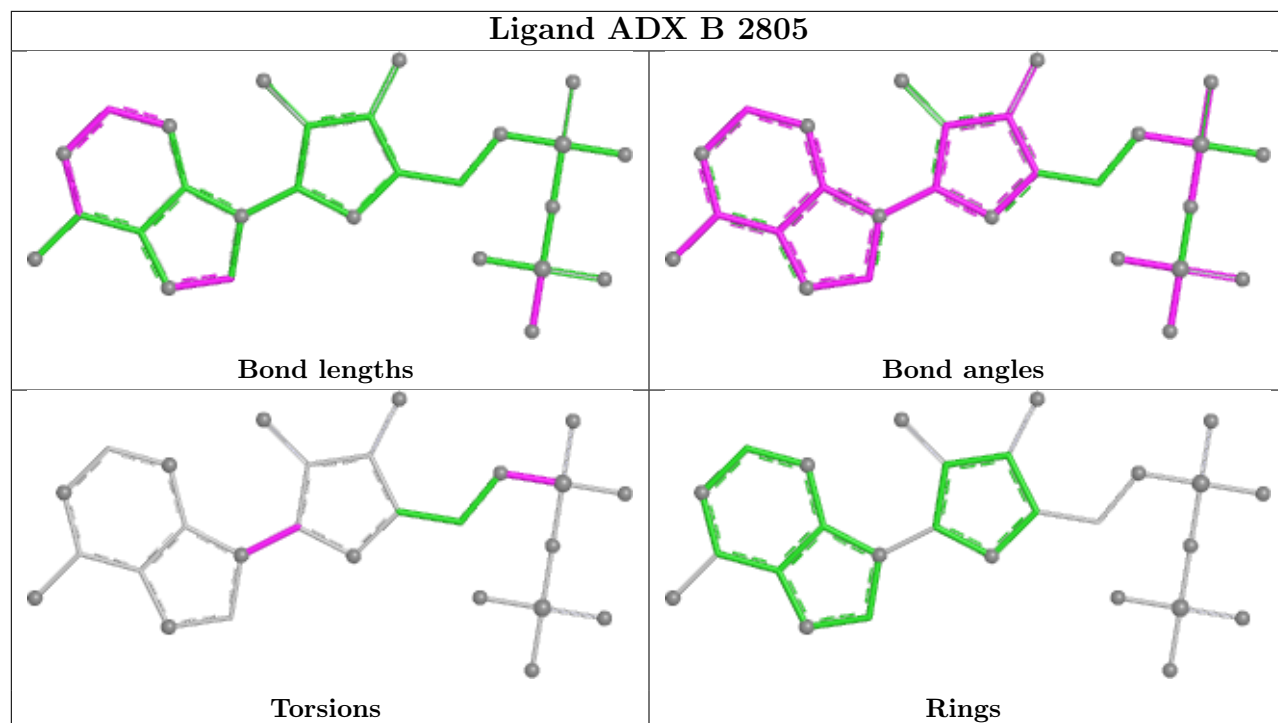
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2800	ADP	1	0
3	B	2805	ADX	6	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	562/630 (89%)	0.03	12 (2%) 63 72	14, 34, 60, 82	10 (1%)
1	B	590/630 (93%)	0.15	6 (1%) 79 86	14, 36, 65, 88	3 (0%)
All	All	1152/1260 (91%)	0.09	18 (1%) 70 79	14, 35, 63, 88	13 (1%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	TYR	4.8
1	A	46	THR	3.9
1	A	34	HIS	3.4
1	A	230	ALA	3.1
1	A	161	PRO	3.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

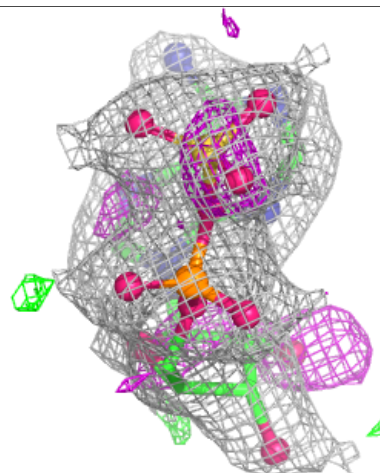
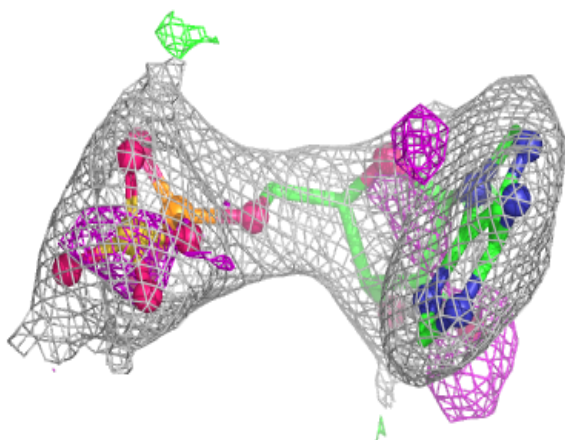
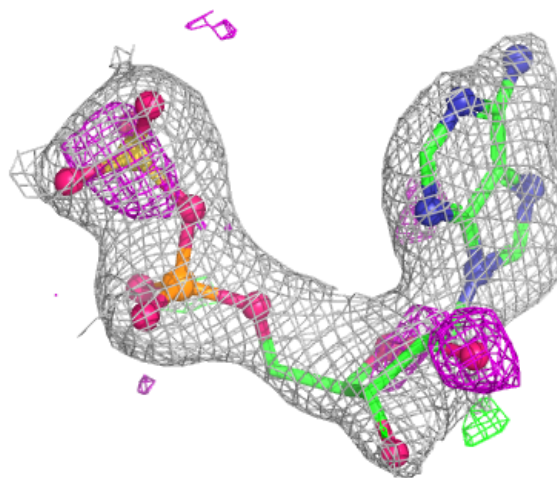
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADX	B	2805	27/27	0.93	0.10	49,61,71,73	0
2	ADP	B	2800	27/27	0.96	0.07	40,46,48,52	0
3	ADX	B	2700	27/27	0.98	0.05	28,34,41,42	0
3	ADX	A	2900	27/27	0.99	0.04	24,30,33,34	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.

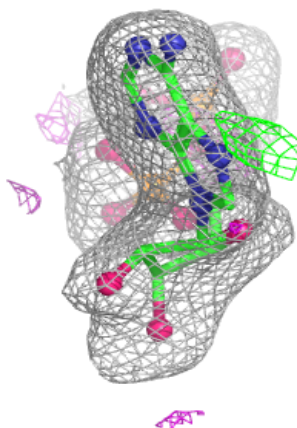
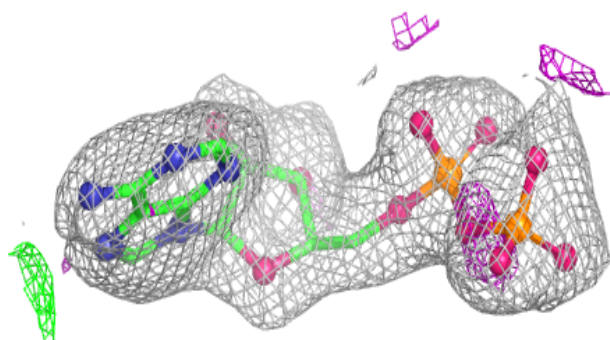
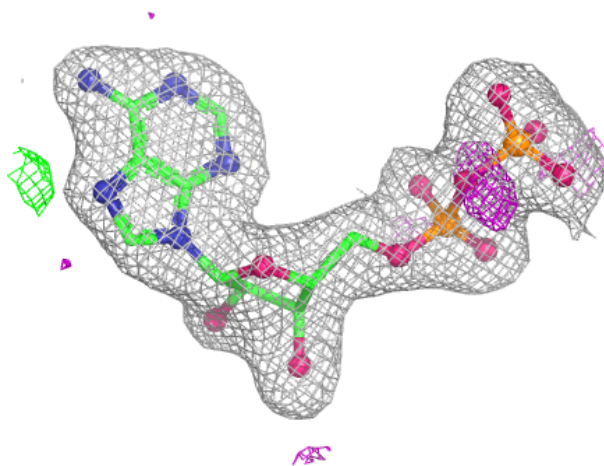
Electron density around ADX B 2805:

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



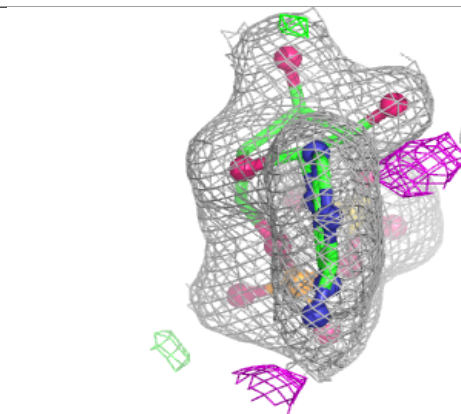
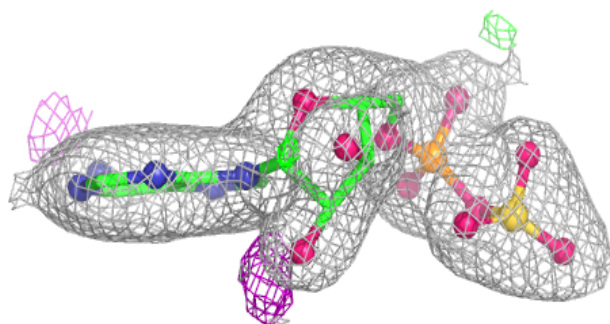
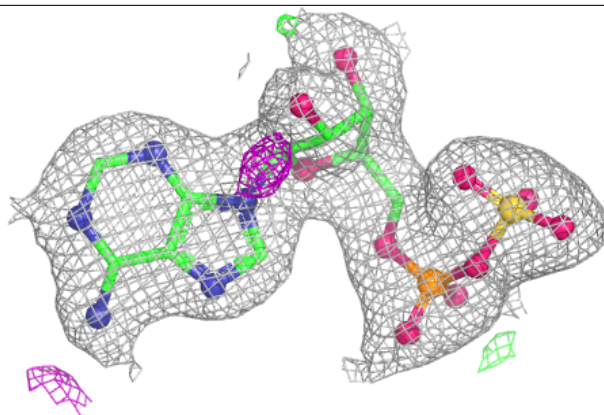
Electron density around ADP B 2800:

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

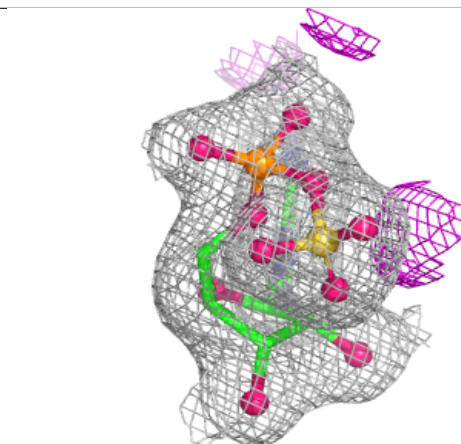
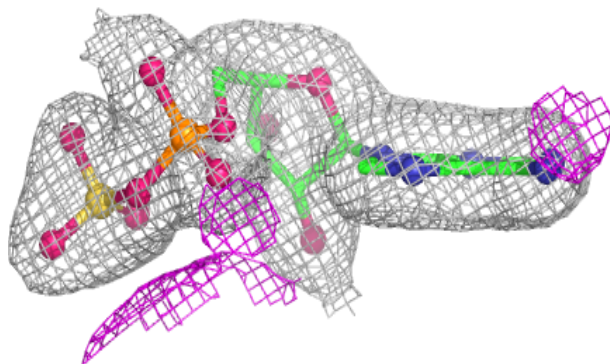
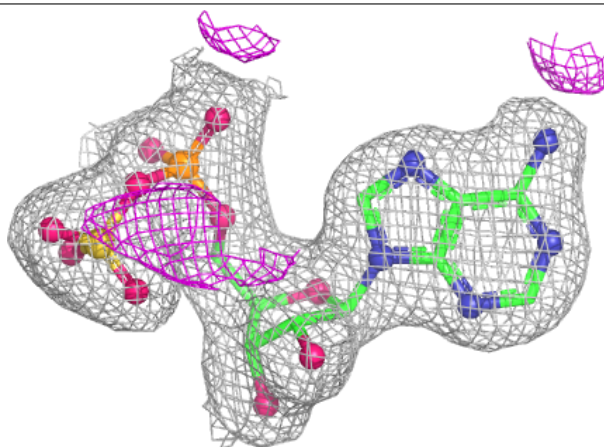


Electron density around ADX B 2700:

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

**Electron density around ADX A 2900:**

$2mF_o-DF_c$ (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.