



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 11:35 PM EDT

PDB ID : 1YP4  
Title : Crystal structure of potato tuber ADP-glucose pyrophosphorylase in complex with ADP-glucose  
Authors : Jin, X.; Ballicora, M.A.; Preiss, J.; Geiger, J.H.  
Deposited on : 2005-01-29  
Resolution : 2.30 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

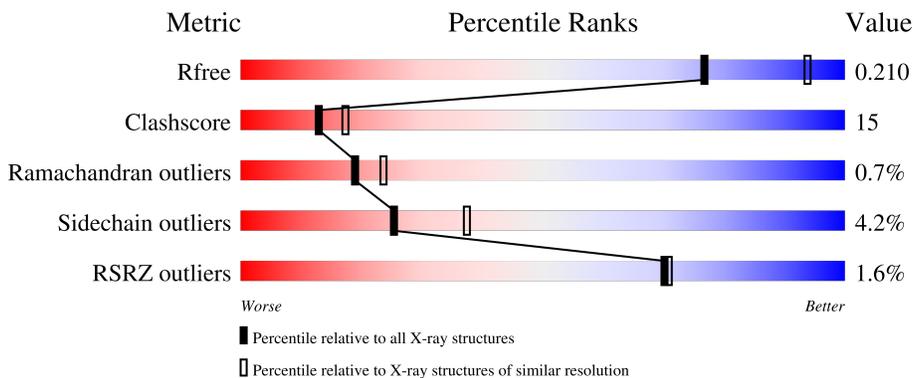
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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  $\geq 3$ , 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	451	 2% 70% 24% . .
1	B	451	 2% 64% 31% . .
1	C	451	 2% 68% 26% . .
1	D	451	 2% 64% 29% . 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	B	1021	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14021 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 Glucose-1-phosphate adenylyltransferase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	432	3356	2136	568	636	16	0	0	0
1	B	433	3350	2125	570	639	16	0	0	0
1	C	434	3371	2144	570	641	16	0	0	0
1	D	426	3301	2099	560	626	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P23509
B	1	MET	-	initiating methionine	UNP P23509
C	1	MET	-	initiating methionine	UNP P23509
D	1	MET	-	initiating methionine	UNP P23509

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



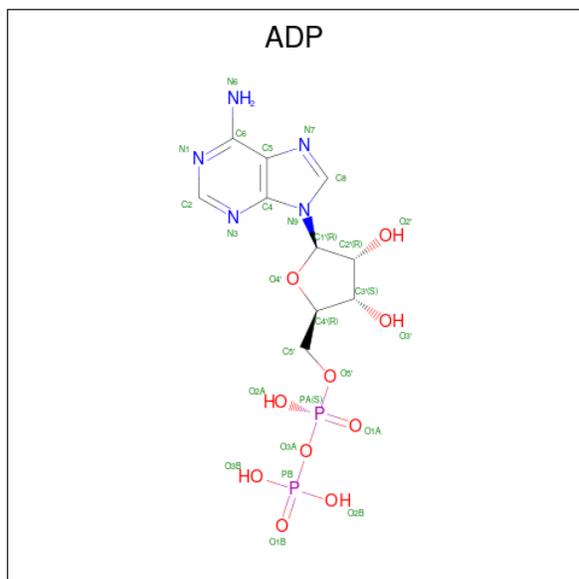
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

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

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

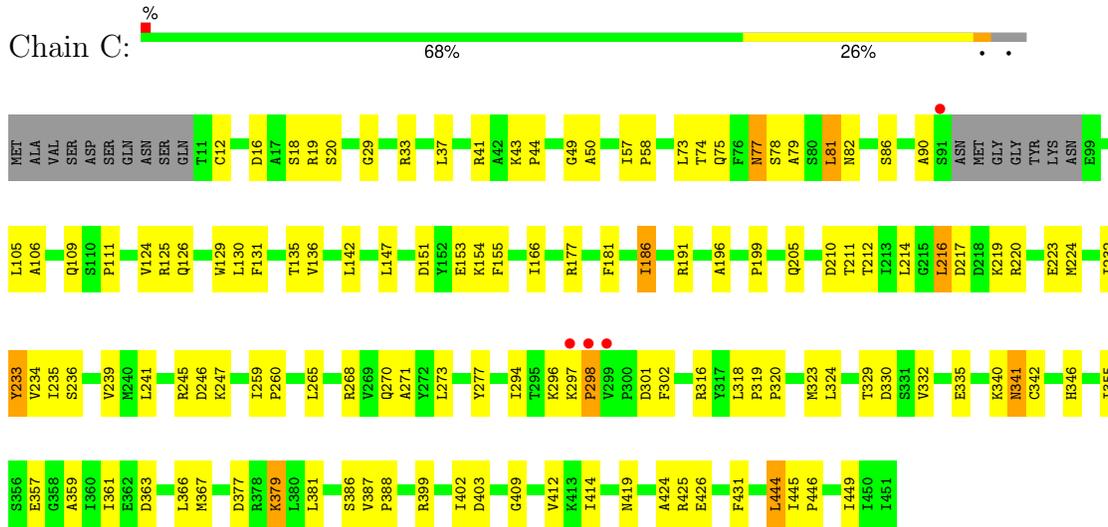


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

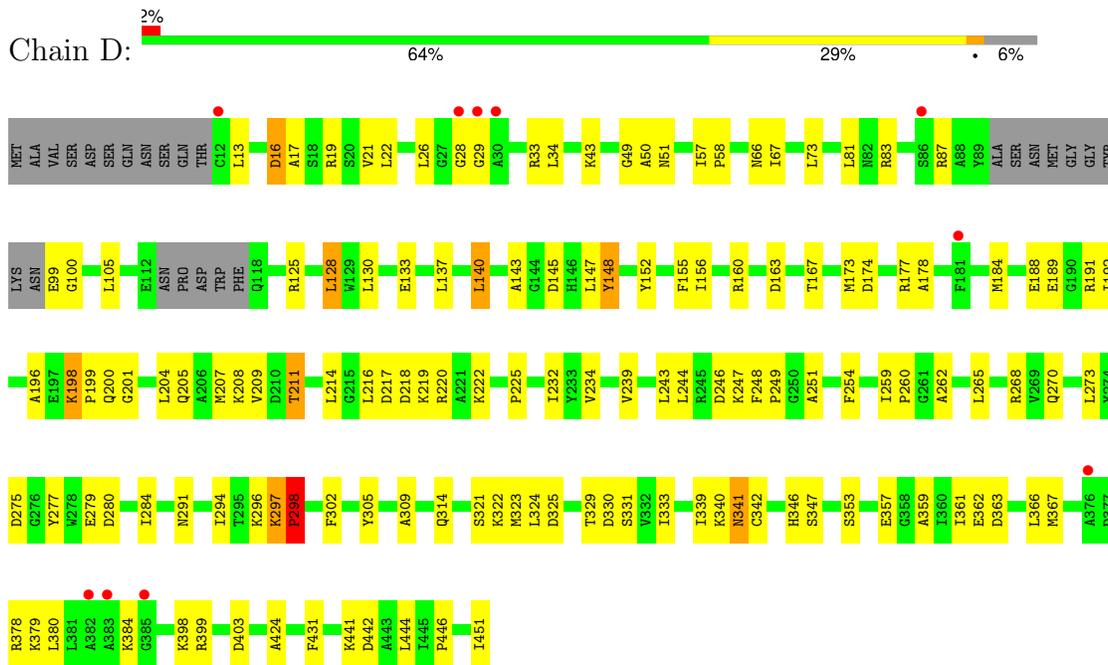
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: ADQ) (formula:  $C_{16}H_{25}N_5O_{15}P_2$ ).







• Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.86Å 137.96Å 90.83Å 90.00° 112.91° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-2.30) 98.4 (19.99-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.31Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.183 , 0.244 0.205 , 0.210	Depositor DCC
$R_{free}$ test set	3933 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtrriage
Anisotropy	0.370	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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: ADP, ADQ, SO4

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	0.38	0/3420	0.64	0/4629
1	B	0.37	0/3409	0.63	0/4610
1	C	0.38	0/3435	0.65	0/4649
1	D	0.35	0/3360	0.62	0/4543
All	All	0.37	0/13624	0.63	0/18431

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3356	0	3372	85	0
1	B	3350	0	3360	120	0
1	C	3371	0	3383	113	0
1	D	3301	0	3324	99	0
2	A	20	0	0	0	0
2	B	20	0	0	3	0
2	C	20	0	0	1	0
2	D	20	0	0	2	0
3	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	27	0	12	0	0
4	B	38	0	22	4	0
5	A	130	0	0	6	0
5	B	106	0	0	6	1
5	C	142	0	0	12	1
5	D	93	0	0	5	0
All	All	14021	0	13485	399	1

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 15.

The worst 5 of 399 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:D:297:LYS:HB3	1:D:298:PRO:HD2	1.27	1.11
1:B:268:ARG:HH11	1:B:268:ARG:HB3	1.06	1.10
1:D:125:ARG:HA	1:D:128:LEU:HD23	1.47	0.97
1:B:268:ARG:HB3	1:B:268:ARG:NH1	1.83	0.91
1:A:12:CYS:HB2	1:C:12:CYS:SG	2.10	0.91

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1123:HOH:O	5:C:1158:HOH:O[2_657]	2.19	0.01

## 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	428/451 (95%)	401 (94%)	26 (6%)	1 (0%)	44 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	427/451 (95%)	393 (92%)	30 (7%)	4 (1%)	14	17
1	C	430/451 (95%)	406 (94%)	23 (5%)	1 (0%)	44	55
1	D	420/451 (93%)	386 (92%)	28 (7%)	6 (1%)	9	9
All	All	1705/1804 (94%)	1586 (93%)	107 (6%)	12 (1%)	19	23

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	ASP
1	D	297	LYS
1	D	298	PRO
1	B	28	GLY
1	B	218	ASP

### 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	359/375 (96%)	345 (96%)	14 (4%)	27	41
1	B	358/375 (96%)	341 (95%)	17 (5%)	22	32
1	C	361/375 (96%)	349 (97%)	12 (3%)	33	48
1	D	353/375 (94%)	336 (95%)	17 (5%)	21	32
All	All	1431/1500 (95%)	1371 (96%)	60 (4%)	25	37

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	341	ASN
1	D	244	LEU
1	C	186	ILE
1	D	211	THR
1	D	399	ARG

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

Mol	Chain	Res	Type
1	C	126	GLN
1	C	396	HIS
1	C	146	HIS
1	C	252	ASN
1	D	66	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](#)

19 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	SO4	B	1009	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	D	1011	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	C	1022	-	4,4,4	0.31	0	6,6,6	0.20	0
2	SO4	A	1000	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	A	1007	-	4,4,4	0.41	0	6,6,6	0.09	0
2	SO4	D	1003	-	4,4,4	0.44	0	6,6,6	0.29	0
3	ADP	C	558	-	24,29,29	1.08	2 (8%)	29,45,45	1.65	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	A	557	-	24,29,29	1.27	2 (8%)	29,45,45	1.57	4 (13%)
2	SO4	B	1001	-	4,4,4	0.29	0	6,6,6	0.20	0
2	SO4	C	1010	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	B	1021	-	4,4,4	0.37	0	6,6,6	0.03	0
2	SO4	A	1008	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	D	1004	-	4,4,4	0.40	0	6,6,6	0.06	0
2	SO4	C	1005	-	4,4,4	0.40	0	6,6,6	0.05	0
2	SO4	A	1020	-	4,4,4	0.32	0	6,6,6	0.15	0
2	SO4	C	1002	-	4,4,4	0.26	0	6,6,6	0.29	0
2	SO4	B	1006	-	4,4,4	0.36	0	6,6,6	0.12	0
4	ADQ	B	506	-	36,41,41	2.00	10 (27%)	46,63,63	3.36	9 (19%)
2	SO4	D	1023	-	4,4,4	0.40	0	6,6,6	0.09	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	ADP	A	557	-	-	3/12/32/32	0/3/3/3
4	ADQ	B	506	-	-	10/19/59/59	0/4/4/4
3	ADP	C	558	-	-	3/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	506	ADQ	C2-N3	4.16	1.38	1.32
4	B	506	ADQ	PB-O3A	-4.04	1.55	1.59
4	B	506	ADQ	PB-O3B	-3.95	1.47	1.59
4	B	506	ADQ	C1D-N9	3.67	1.59	1.49
4	B	506	ADQ	C4-N3	3.30	1.40	1.35

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	506	ADQ	O3B-C1'-C2'	14.47	134.89	108.38
4	B	506	ADQ	O5'-C1'-O3B	-10.98	97.01	111.36
4	B	506	ADQ	PB-O3B-C1'	8.03	153.90	121.21
4	B	506	ADQ	N3-C2-N1	-7.67	118.26	128.67
3	C	558	ADP	N3-C2-N1	-4.08	123.13	128.67

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

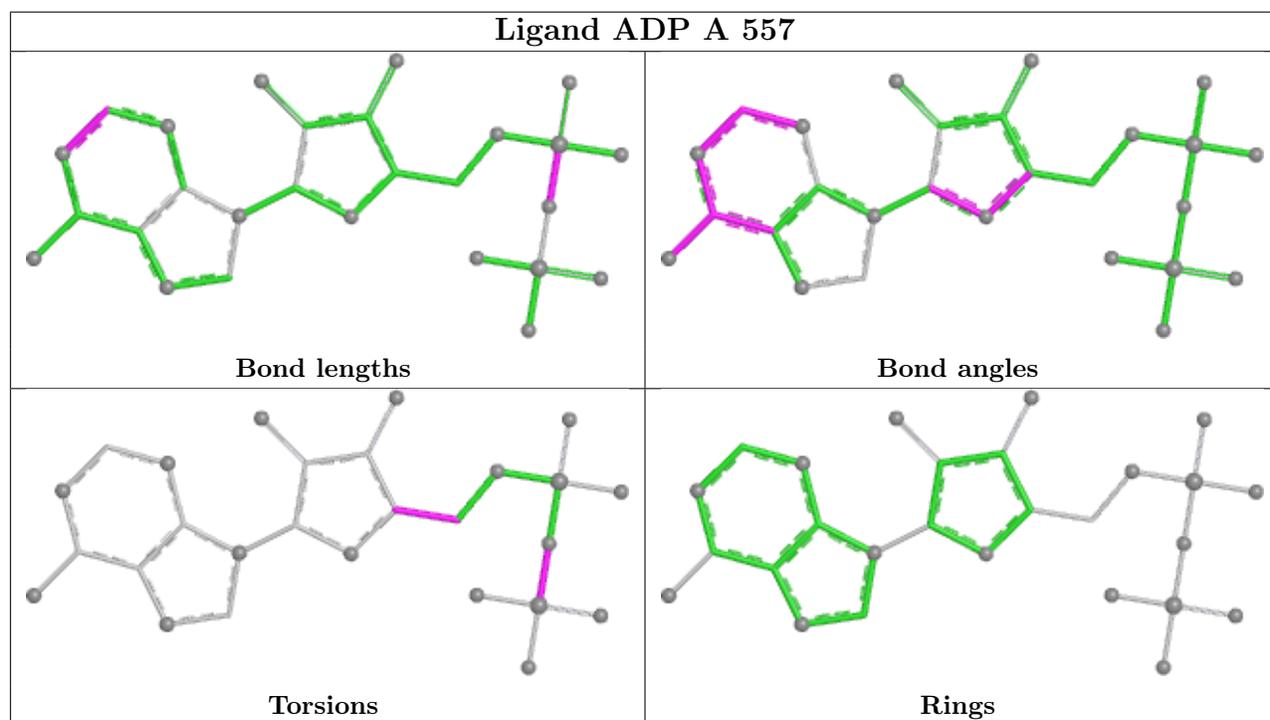
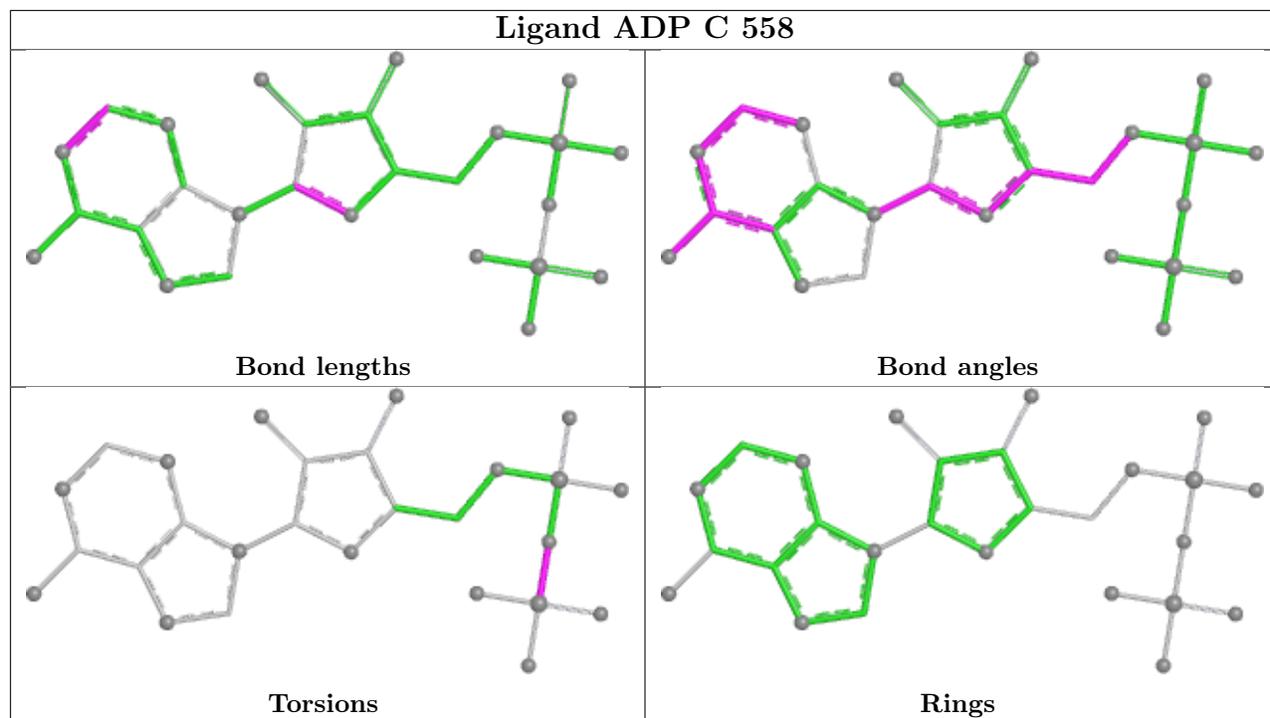
Mol	Chain	Res	Type	Atoms
3	A	557	ADP	PA-O3A-PB-O3B
3	C	558	ADP	PA-O3A-PB-O3B
4	B	506	ADQ	C1'-O3B-PB-O3A
4	B	506	ADQ	C2'-C1'-O3B-PB
4	B	506	ADQ	O5'-C1'-O3B-PB

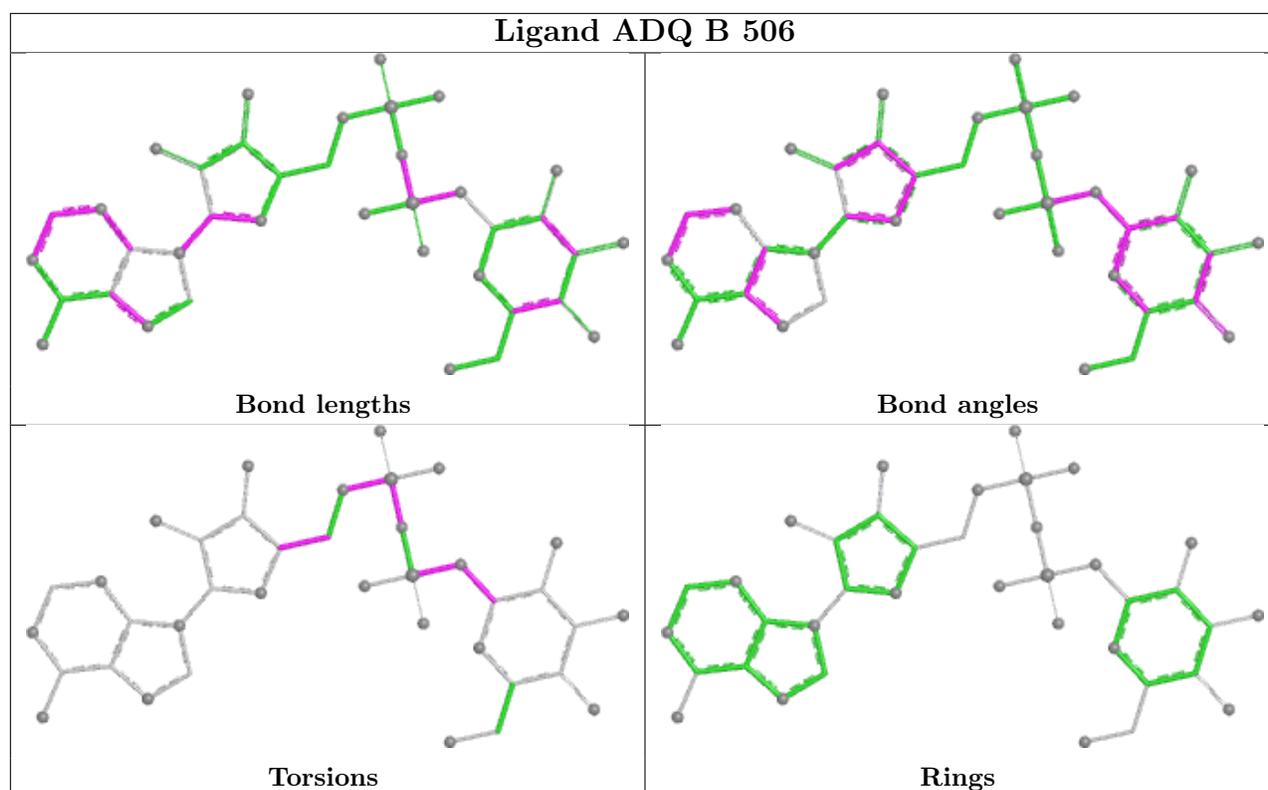
There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1009	SO4	1	0
2	D	1011	SO4	1	0
2	C	1010	SO4	1	0
2	B	1021	SO4	2	0
4	B	506	ADQ	4	0
2	D	1023	SO4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	432/451 (95%)	-0.15	5 (1%) 76 76	23, 42, 72, 91	0
1	B	433/451 (96%)	-0.03	9 (2%) 63 64	22, 45, 81, 91	0
1	C	434/451 (96%)	-0.18	4 (0%) 81 81	20, 40, 71, 91	0
1	D	426/451 (94%)	0.16	10 (2%) 61 62	22, 49, 86, 91	0
All	All	1725/1804 (95%)	-0.05	28 (1%) 70 71	20, 44, 80, 91	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	GLY	3.6
1	C	297	LYS	3.0
1	C	299	VAL	2.9
1	D	181	PHE	2.8
1	D	86	SER	2.8

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

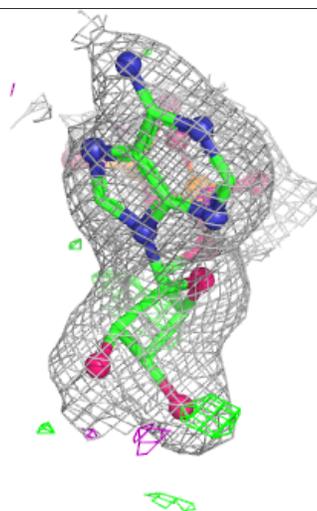
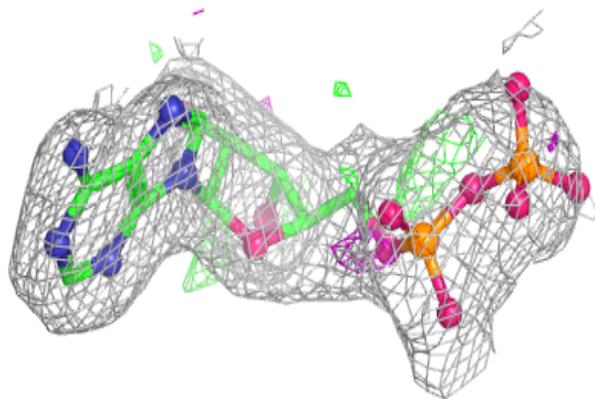
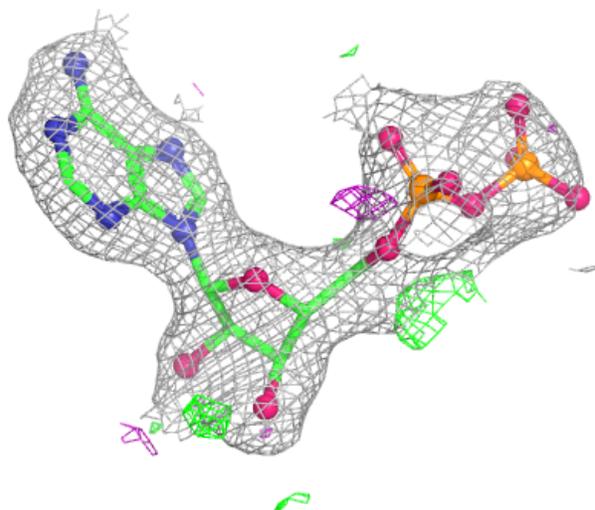
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
2	SO4	D	1023	5/5	0.68	0.12	96,96,96,96	0
2	SO4	B	1006	5/5	0.78	0.14	96,96,96,96	0
2	SO4	C	1022	5/5	0.79	0.17	90,91,91,91	0
2	SO4	B	1021	5/5	0.83	0.14	96,96,96,96	0
2	SO4	D	1004	5/5	0.88	0.12	96,96,96,96	0
2	SO4	C	1005	5/5	0.88	0.11	77,78,79,79	0
3	ADP	A	557	27/27	0.88	0.11	43,50,85,85	0
3	ADP	C	558	27/27	0.88	0.12	42,53,78,79	0
2	SO4	D	1003	5/5	0.89	0.13	43,45,48,49	0
4	ADQ	B	506	38/38	0.89	0.10	47,54,61,62	0
2	SO4	D	1011	5/5	0.91	0.11	62,65,66,67	0
2	SO4	B	1009	5/5	0.93	0.10	62,62,65,66	0
2	SO4	C	1010	5/5	0.93	0.10	54,58,58,58	0
2	SO4	A	1007	5/5	0.94	0.09	70,71,71,71	0
2	SO4	A	1020	5/5	0.95	0.14	66,67,68,69	0
2	SO4	A	1008	5/5	0.96	0.09	54,56,57,59	0
2	SO4	A	1000	5/5	0.98	0.08	43,46,47,49	0
2	SO4	C	1002	5/5	0.98	0.08	38,39,41,41	0
2	SO4	B	1001	5/5	0.98	0.05	36,37,39,41	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.

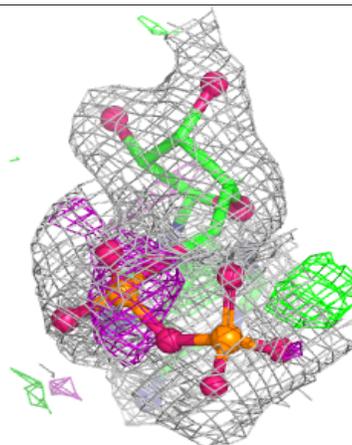
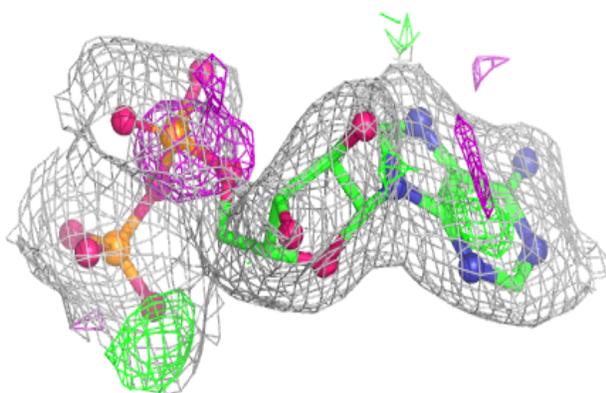
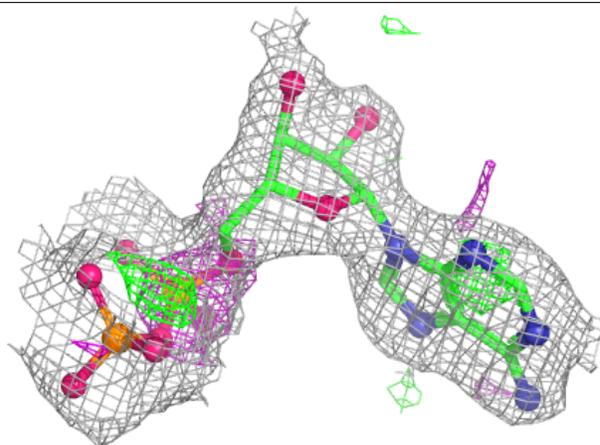
**Electron density around ADP A 557:**

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

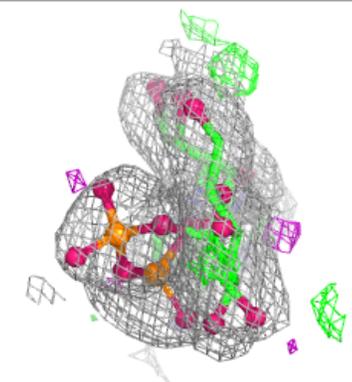
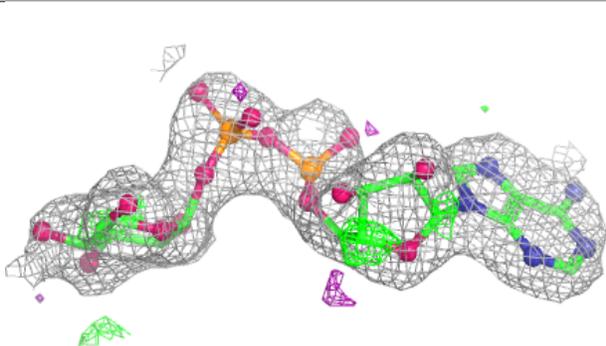
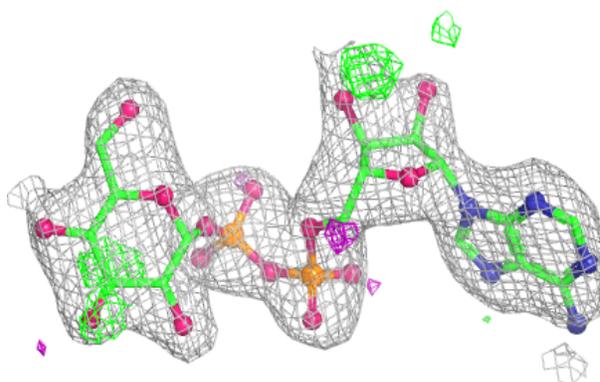


**Electron density around ADP C 558:**

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

**Electron density around ADQ B 506:**

$2mF_o-DF_c$  (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.