



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2024 – 12:05 AM EST

PDB ID : 4GX1  
Title : Crystal structure of the GsuK bound to ADP  
Authors : Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.;  
Jiang, Y.  
Deposited on : 2012-09-03  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

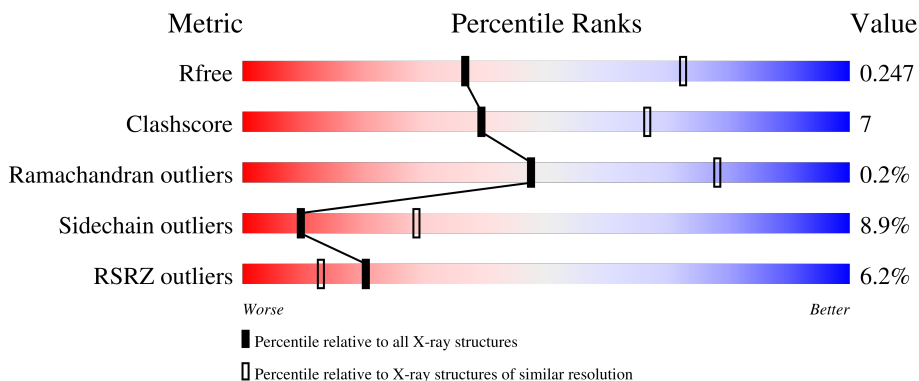
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	565	 2% 54% 11% 33%
1	B	565	 11% 74% 20%
1	C	565	 5% 76% 19%
1	D	565	 2% 52% 12% 33%

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	K	B	602	-	-	-	X
2	K	B	603	-	-	-	X
7	PO4	C	610	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14702 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	376	Total 2931	C 1885	N 507	O 528	S 11	0	0	0
1	B	547	Total 4197	C 2687	N 725	O 770	S 15	0	0	0
1	C	546	Total 4188	C 2682	N 723	O 768	S 15	0	0	0
1	D	376	Total 2928	C 1883	N 507	O 527	S 11	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q74FS9
A	5	GLN	-	expression tag	UNP Q74FS9
A	6	ARG	-	expression tag	UNP Q74FS9
A	7	GLY	-	expression tag	UNP Q74FS9
A	8	SER	-	expression tag	UNP Q74FS9
A	52	ALA	GLU	engineered mutation	UNP Q74FS9
A	77	GLU	GLN	engineered mutation	UNP Q74FS9
A	97	ASP	LEU	engineered mutation	UNP Q74FS9
A	565	LEU	-	expression tag	UNP Q74FS9
A	566	VAL	-	expression tag	UNP Q74FS9
A	567	PRO	-	expression tag	UNP Q74FS9
A	568	ARG	-	expression tag	UNP Q74FS9
B	4	MET	-	expression tag	UNP Q74FS9
B	5	GLN	-	expression tag	UNP Q74FS9
B	6	ARG	-	expression tag	UNP Q74FS9
B	7	GLY	-	expression tag	UNP Q74FS9
B	8	SER	-	expression tag	UNP Q74FS9
B	52	ALA	GLU	engineered mutation	UNP Q74FS9
B	77	GLU	GLN	engineered mutation	UNP Q74FS9
B	97	ASP	LEU	engineered mutation	UNP Q74FS9
B	565	LEU	-	expression tag	UNP Q74FS9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	566	VAL	-	expression tag	UNP Q74FS9
B	567	PRO	-	expression tag	UNP Q74FS9
B	568	ARG	-	expression tag	UNP Q74FS9
C	4	MET	-	expression tag	UNP Q74FS9
C	5	GLN	-	expression tag	UNP Q74FS9
C	6	ARG	-	expression tag	UNP Q74FS9
C	7	GLY	-	expression tag	UNP Q74FS9
C	8	SER	-	expression tag	UNP Q74FS9
C	52	ALA	GLU	engineered mutation	UNP Q74FS9
C	77	GLU	GLN	engineered mutation	UNP Q74FS9
C	97	ASP	LEU	engineered mutation	UNP Q74FS9
C	565	LEU	-	expression tag	UNP Q74FS9
C	566	VAL	-	expression tag	UNP Q74FS9
C	567	PRO	-	expression tag	UNP Q74FS9
C	568	ARG	-	expression tag	UNP Q74FS9
D	4	MET	-	expression tag	UNP Q74FS9
D	5	GLN	-	expression tag	UNP Q74FS9
D	6	ARG	-	expression tag	UNP Q74FS9
D	7	GLY	-	expression tag	UNP Q74FS9
D	8	SER	-	expression tag	UNP Q74FS9
D	52	ALA	GLU	engineered mutation	UNP Q74FS9
D	77	GLU	GLN	engineered mutation	UNP Q74FS9
D	97	ASP	LEU	engineered mutation	UNP Q74FS9
D	565	LEU	-	expression tag	UNP Q74FS9
D	566	VAL	-	expression tag	UNP Q74FS9
D	567	PRO	-	expression tag	UNP Q74FS9
D	568	ARG	-	expression tag	UNP Q74FS9

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total K 3 3	0	0
2	B	3	Total K 3 3	0	0
2	C	3	Total K 3 3	0	0
2	D	2	Total K 2 2	0	0

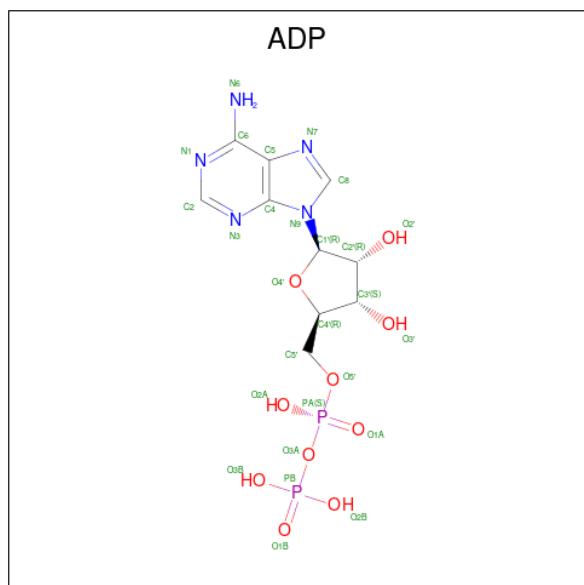
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	2	Total Ca 2 2	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



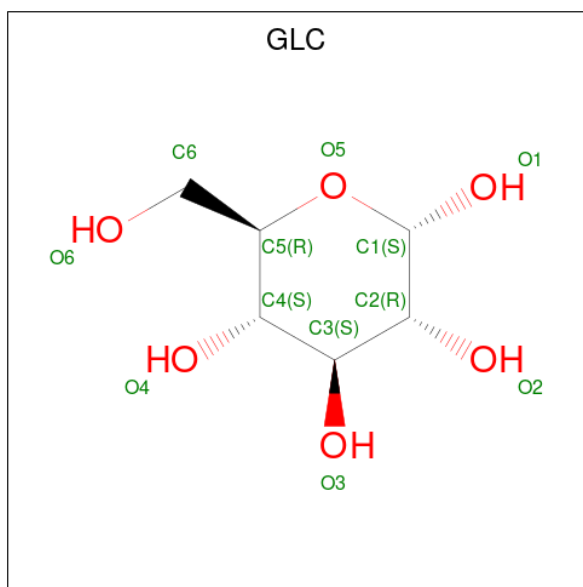
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 27 10 5 10 2	0	0
5	B	1	Total C N O P 27 10 5 10 2	0	0

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

- Molecule 6 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

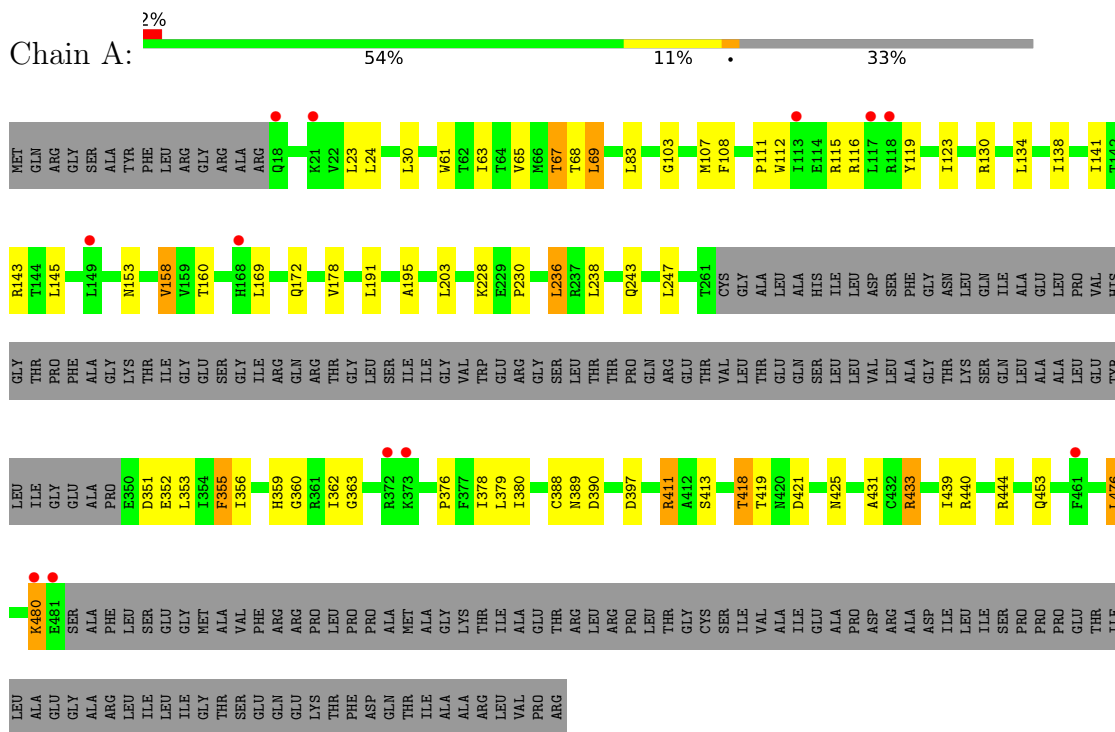
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total	O	0	0
			49	49		
8	B	91	Total	O	0	0
			91	91		
8	C	83	Total	O	0	0
			83	83		
8	D	50	Total	O	0	0
			50	50		



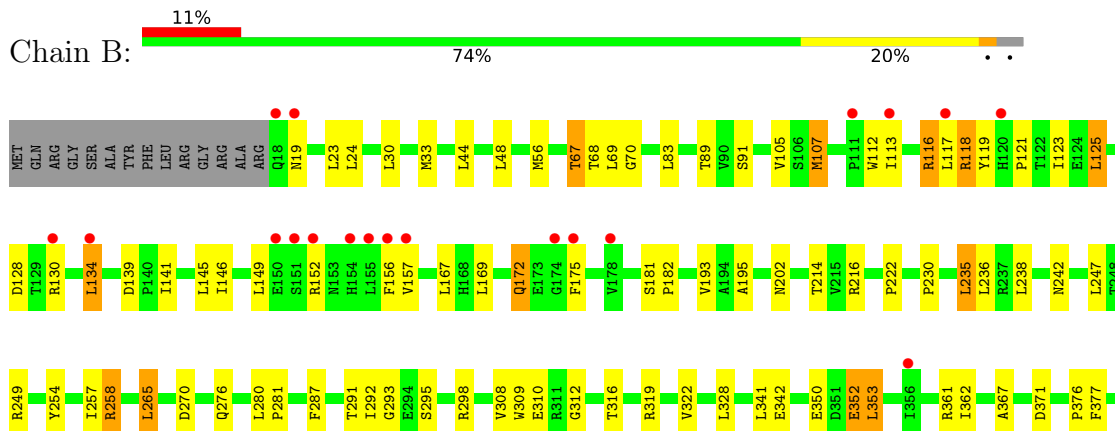
### 3 Residue-property plots [i](#)

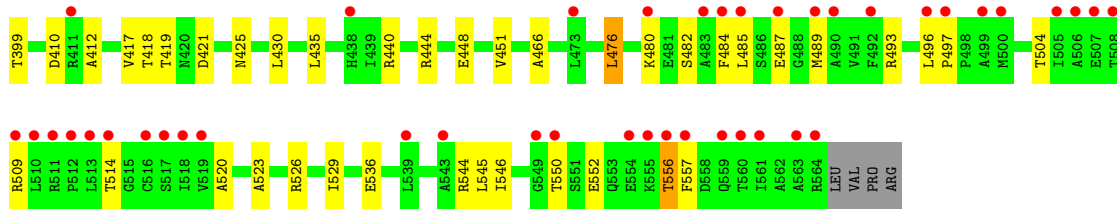
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: TrkA domain protein

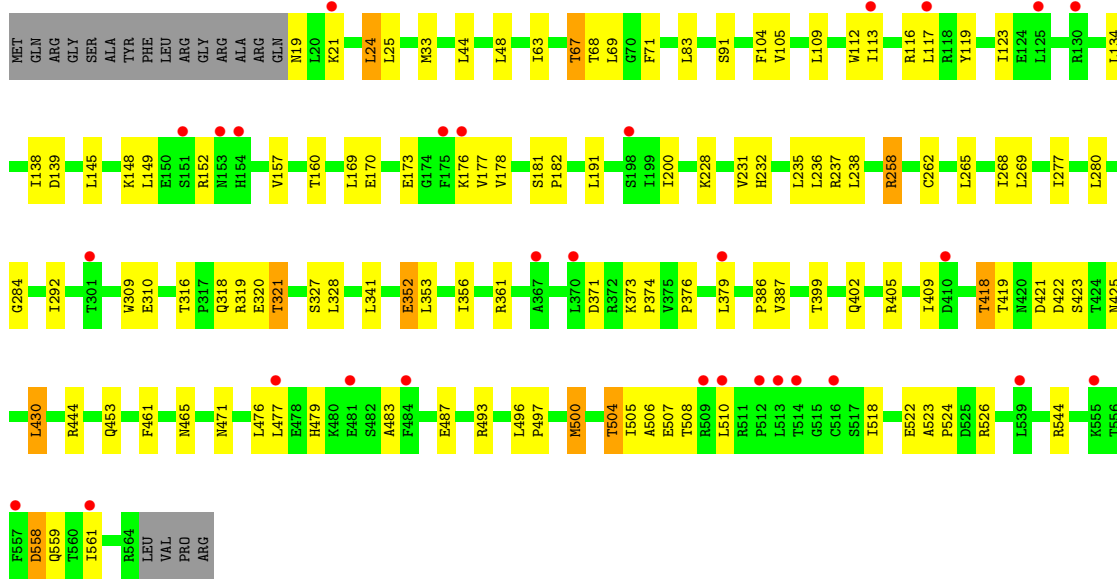
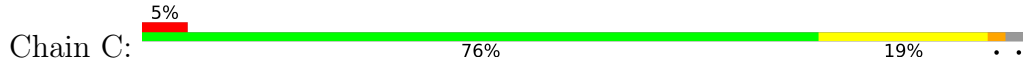


- Molecule 1: TrkA domain protein

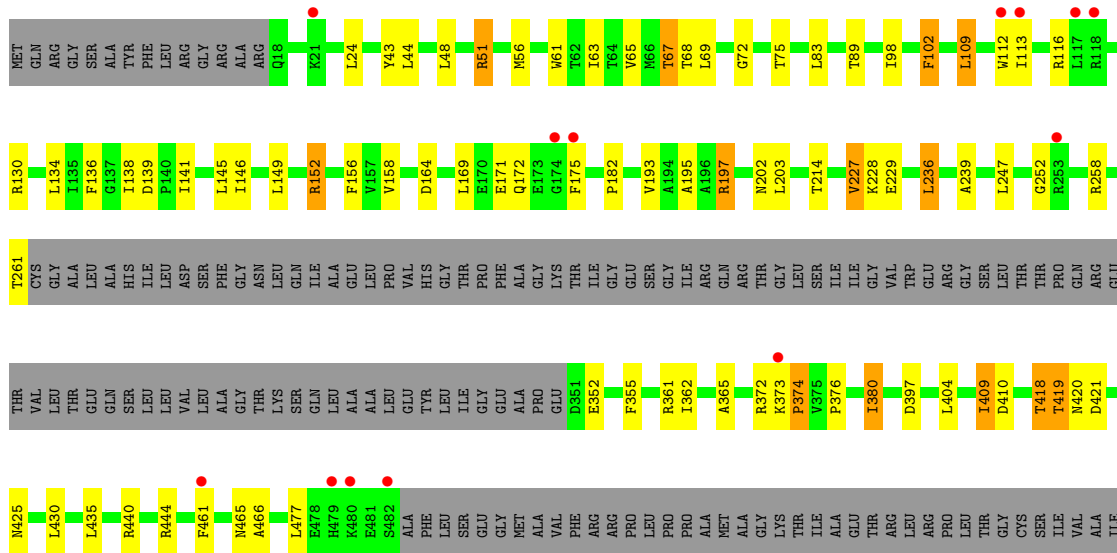




• Molecule 1: TrkA domain protein



• Molecule 1: TrkA domain protein



GLU  
ALA  
PRO  
ASP  
ARG  
ALA  
ASP  
ILE  
LEU  
ILE  
SER  
PRO  
PRO  
GLU  
THR  
THR  
ILE  
LEU  
ALA  
GLU  
GLY  
ALA  
ALA  
ARG  
ARG  
LEU  
ILE  
LEU  
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GLY  
THR  
SER  
SER  
GLU  
GLN  
GLU  
LYS  
THR  
PHE  
ASP  
GLN  
THR  
ILE  
ILE  
ALA  
ALA  
ARG  
LEU  
VAL  
PRO  
ARG

## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	234.32Å 111.44Å 164.74Å 90.00° 134.93° 90.00°	Depositor
Resolution (Å)	41.47 – 2.80 49.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (41.47-2.80) 96.8 (49.53-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.212 , 0.255 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	3624 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtrriage
Anisotropy	0.354	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.089 for -h-2*k,h+1 0.015 for -h,-k,h+1 0.023 for -h-2*k,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.14 % 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 1.3762e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, PO4, ZN, CA, K, GLC

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	0.34	0/2991	0.49	0/4072
1	B	0.31	0/4280	0.47	0/5829
1	C	0.28	0/4271	0.47	0/5817
1	D	0.29	0/2988	0.47	0/4068
All	All	0.31	0/14530	0.48	0/19786

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	2931	0	2961	43	0
1	B	4197	0	4267	73	0
1	C	4188	0	4259	64	0
1	D	2928	0	2960	48	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	27	0	12	6	0
5	B	27	0	12	2	0
5	C	27	0	12	1	0
5	D	27	0	12	5	0
6	B	12	0	11	0	0
6	C	24	0	22	0	0
6	D	12	0	11	0	0
7	B	5	0	0	0	0
7	C	5	0	0	2	0
8	A	49	0	0	0	0
8	B	91	0	0	1	0
8	C	83	0	0	4	0
8	D	50	0	0	0	0
All	All	14702	0	14539	213	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 7.

The worst 5 of 213 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:THR:HG22	1:A:421:ASP:H	1.36	0.90
1:C:112:TRP:HE1	1:C:116:ARG:HH11	1.24	0.84
1:C:419:THR:HG22	1:C:421:ASP:H	1.43	0.83
1:C:493:ARG:HD2	1:C:544:ARG:HD3	1.63	0.80
1:C:419:THR:HB	1:C:425:ASN:HD21	1.45	0.80

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	372/565 (66%)	356 (96%)	15 (4%)	1 (0%)	41	72
1	B	545/565 (96%)	527 (97%)	18 (3%)	0	100	100
1	C	544/565 (96%)	522 (96%)	20 (4%)	2 (0%)	34	66
1	D	372/565 (66%)	357 (96%)	14 (4%)	1 (0%)	41	72
All	All	1833/2260 (81%)	1762 (96%)	67 (4%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	524	PRO
1	C	374	PRO
1	D	374	PRO
1	A	230	PRO

### 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	314/463 (68%)	286 (91%)	28 (9%)	9	28
1	B	448/463 (97%)	411 (92%)	37 (8%)	11	32
1	C	447/463 (96%)	405 (91%)	42 (9%)	8	26
1	D	314/463 (68%)	285 (91%)	29 (9%)	9	27
All	All	1523/1852 (82%)	1387 (91%)	136 (9%)	9	28

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	134	LEU
1	D	164	ASP
1	D	410	ASP
1	B	265	LEU
1	B	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	172	GLN
1	C	425	ASN
1	C	465	ASN
1	D	465	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 19 are monoatomic - leaving 10 for Mogul analysis.

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
5	ADP	D	604	-	24,29,29	1.51	4 (16%)	29,45,45	1.82	5 (17%)
6	GLC	C	609	-	12,12,12	1.74	2 (16%)	17,17,17	1.16	1 (5%)
7	PO4	B	608	-	4,4,4	0.94	0	6,6,6	0.44	0
5	ADP	A	606	-	24,29,29	1.52	5 (20%)	29,45,45	1.59	2 (6%)
6	GLC	D	605	-	12,12,12	1.72	2 (16%)	17,17,17	1.15	2 (11%)
6	GLC	C	608	-	12,12,12	1.73	2 (16%)	17,17,17	1.18	1 (5%)
7	PO4	C	610	-	4,4,4	0.92	0	6,6,6	0.35	0
5	ADP	C	607	-	24,29,29	1.55	4 (16%)	29,45,45	1.72	4 (13%)
6	GLC	B	607	-	12,12,12	1.77	2 (16%)	17,17,17	1.20	0
5	ADP	B	606	-	24,29,29	1.60	5 (20%)	29,45,45	1.84	5 (17%)

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
5	ADP	D	604	-	-	4/12/32/32	0/3/3/3
6	GLC	C	609	-	-	2/2/22/22	0/1/1/1
5	ADP	A	606	-	-	10/12/32/32	0/3/3/3
6	GLC	D	605	-	-	0/2/22/22	0/1/1/1
6	GLC	C	608	-	-	2/2/22/22	0/1/1/1
5	ADP	C	607	-	-	2/12/32/32	0/3/3/3
6	GLC	B	607	-	-	2/2/22/22	0/1/1/1
5	ADP	B	606	-	-	3/12/32/32	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	607	GLC	C4-C3	-3.95	1.42	1.52
6	C	609	GLC	C4-C3	-3.94	1.42	1.52
6	D	605	GLC	C4-C3	-3.88	1.42	1.52
6	C	608	GLC	C4-C3	-3.86	1.42	1.52
5	A	606	ADP	C2'-C3'	-3.59	1.43	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	ADP	N3-C2-N1	-5.69	119.79	128.68

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	604	ADP	N3-C2-N1	-5.66	119.83	128.68
5	C	607	ADP	N3-C2-N1	-5.47	120.12	128.68
5	A	606	ADP	N3-C2-N1	-5.38	120.27	128.68
5	D	604	ADP	PA-O3A-PB	-4.95	115.83	132.83

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

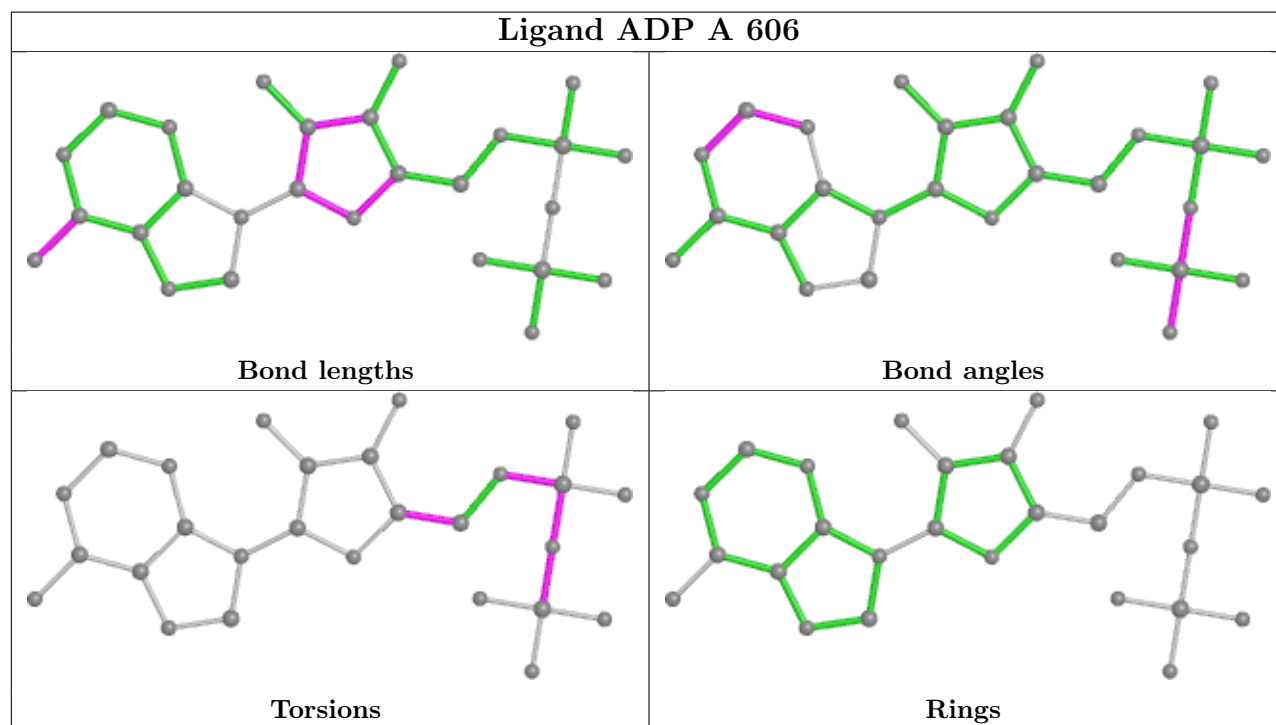
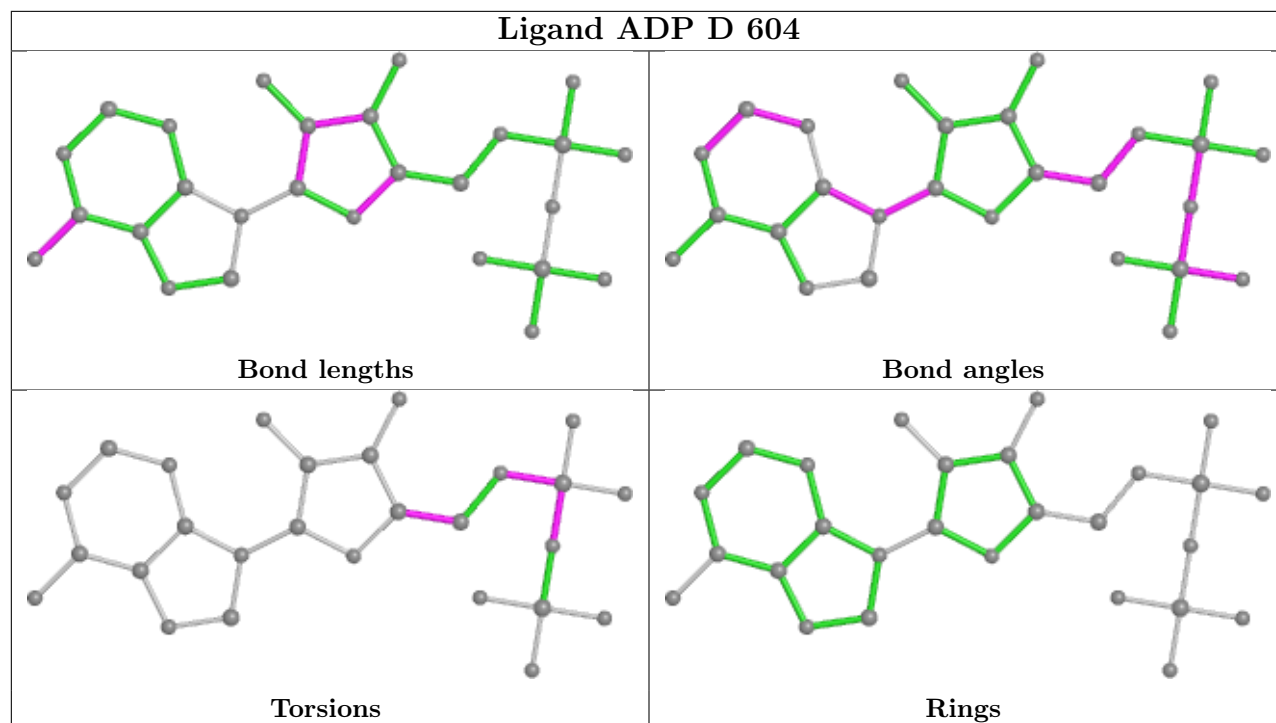
Mol	Chain	Res	Type	Atoms
5	A	606	ADP	PA-O3A-PB-O2B
5	A	606	ADP	C5'-O5'-PA-O1A
5	A	606	ADP	C5'-O5'-PA-O2A
6	C	609	GLC	O5-C5-C6-O6
6	B	607	GLC	O5-C5-C6-O6

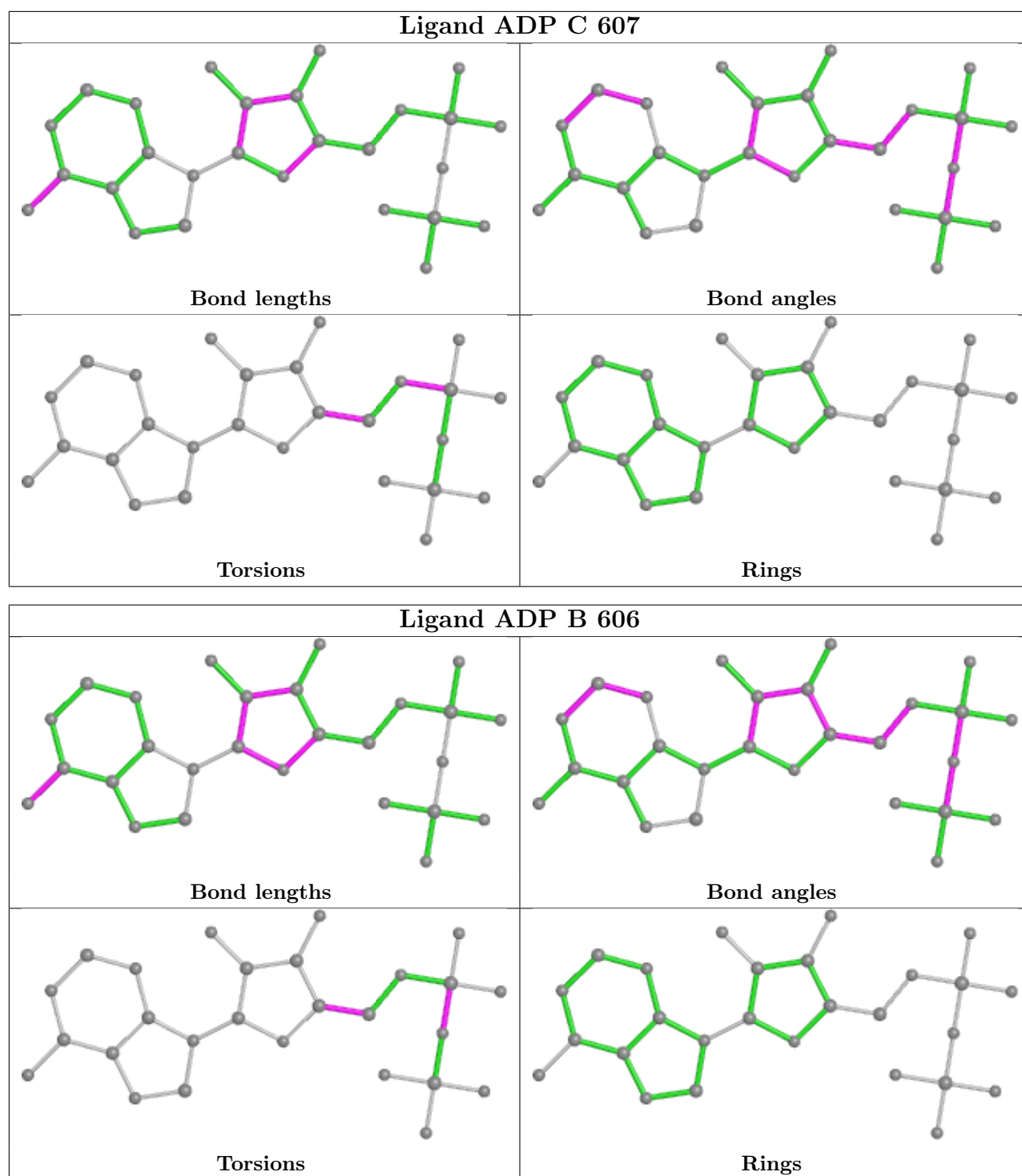
There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	604	ADP	5	0
5	A	606	ADP	6	0
7	C	610	PO4	2	0
5	C	607	ADP	1	0
5	B	606	ADP	2	0

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

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	376/565 (66%)	0.19	12 (3%) 47 37	45, 68, 135, 186	0
1	B	547/565 (96%)	0.55	61 (11%) 5 3	49, 81, 190, 249	0
1	C	546/565 (96%)	0.26	29 (5%) 26 17	50, 79, 150, 217	0
1	D	376/565 (66%)	0.18	13 (3%) 44 34	45, 70, 138, 197	0
All	All	1845/2260 (81%)	0.32	115 (6%) 20 13	45, 75, 159, 249	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	CYS	11.5
1	B	509	ARG	9.3
1	B	508	THR	7.2
1	B	561	ILE	7.1
1	B	484	PHE	6.7

### 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](#)

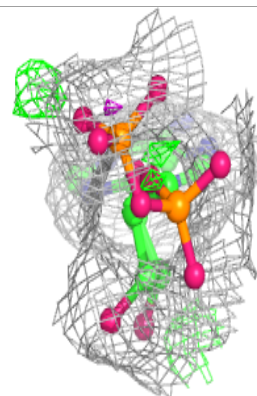
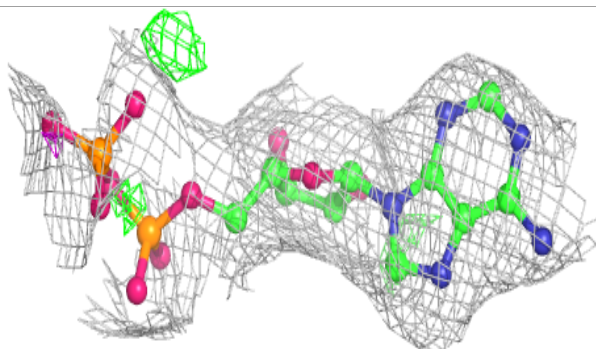
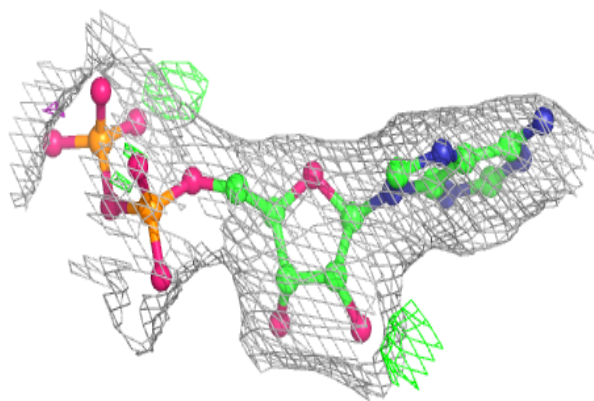
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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	K	B	602	1/1	0.55	0.76	152,152,152,152	1
2	K	B	603	1/1	0.64	1.08	182,182,182,182	1
6	GLC	C	608	12/12	0.69	0.21	118,127,128,128	0
6	GLC	D	605	12/12	0.76	0.26	133,138,139,139	0
6	GLC	C	609	12/12	0.82	0.27	120,127,129,129	0
6	GLC	B	607	12/12	0.84	0.19	148,153,155,155	0
2	K	D	601	1/1	0.85	0.41	127,127,127,127	1
2	K	D	602	1/1	0.85	0.57	121,121,121,121	1
2	K	A	602	1/1	0.85	0.13	47,47,47,47	1
2	K	A	603	1/1	0.87	0.46	127,127,127,127	1
2	K	C	601	1/1	0.87	0.20	54,54,54,54	1
2	K	C	603	1/1	0.91	0.27	71,71,71,71	1
5	ADP	D	604	27/27	0.91	0.17	64,71,124,128	0
2	K	A	601	1/1	0.91	0.17	55,55,55,55	1
5	ADP	A	606	27/27	0.94	0.17	65,71,203,203	0
5	ADP	B	606	27/27	0.95	0.15	62,68,130,155	0
4	CA	B	605	1/1	0.95	0.14	64,64,64,64	0
7	PO4	B	608	5/5	0.96	0.23	80,81,87,87	0
4	CA	A	605	1/1	0.97	0.10	65,65,65,65	0
5	ADP	C	607	27/27	0.97	0.16	48,71,176,177	0
2	K	B	601	1/1	0.97	0.15	75,75,75,75	1
3	ZN	C	604	1/1	0.97	0.18	68,68,68,68	0
7	PO4	C	610	5/5	0.97	0.18	86,91,92,93	0
2	K	C	602	1/1	0.98	0.25	55,55,55,55	1
3	ZN	D	603	1/1	0.98	0.22	68,68,68,68	0
4	CA	C	605	1/1	0.99	0.10	62,62,62,62	0
4	CA	C	606	1/1	0.99	0.17	68,68,68,68	0
3	ZN	A	604	1/1	0.99	0.21	70,70,70,70	0
3	ZN	B	604	1/1	0.99	0.21	73,73,73,73	0

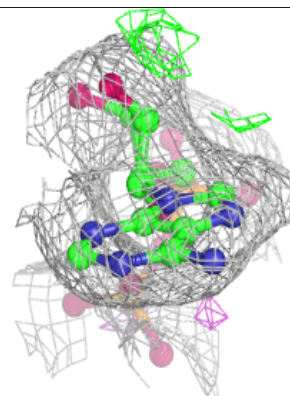
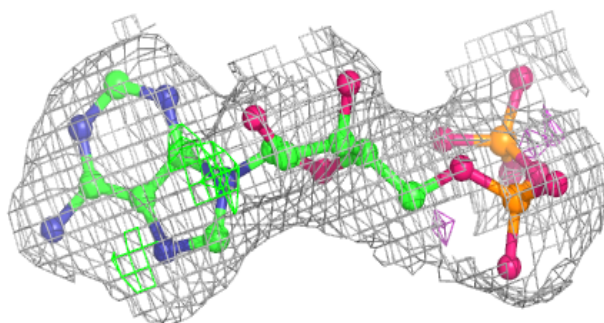
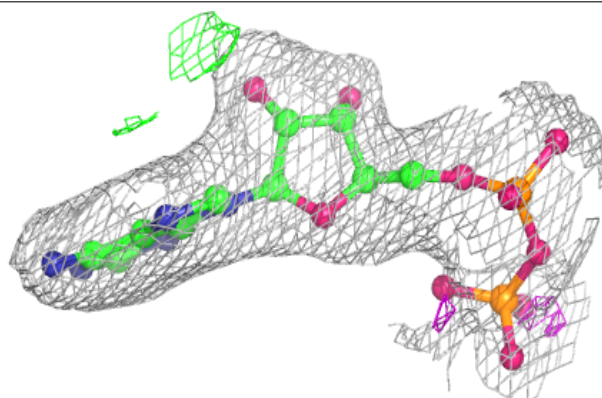
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ADP D 604:**

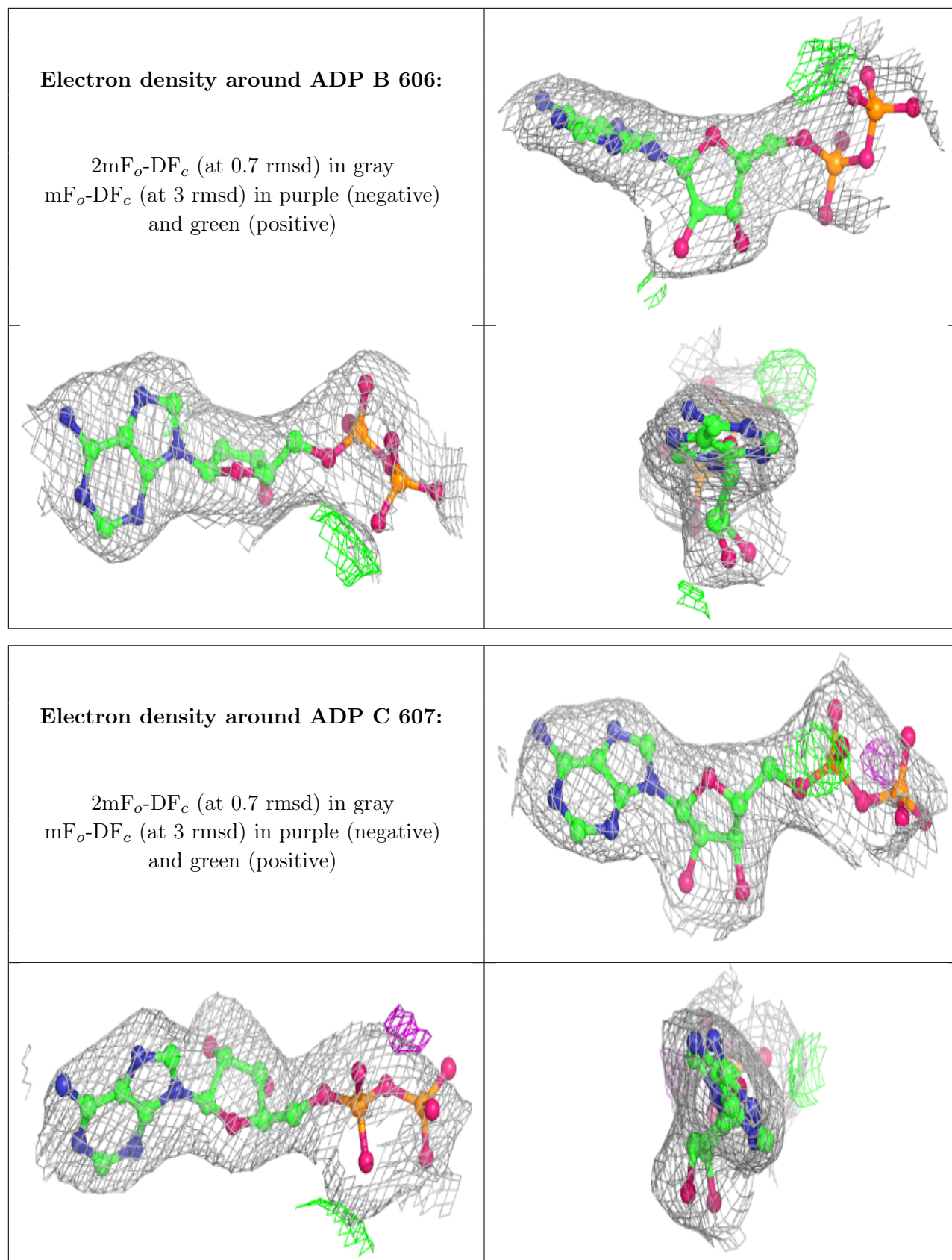
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP A 606:**

$2mF_o-DF_c$  (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.