

wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 04:03 pm BST

PDB ID : 1SQ5

Title : Crystal Structure of E. coli Pantothenate kinase

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Deposited on : 2004-03-17

Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 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)

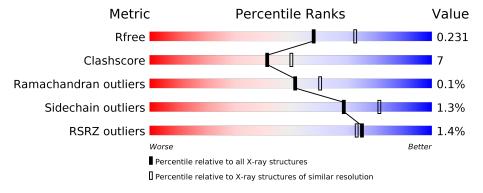
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	308	79%	19%	
1	В	308	81%	16%	
1	С	308	81%	15%	•
1	D	308	81%	17%	



2 Entry composition (i)

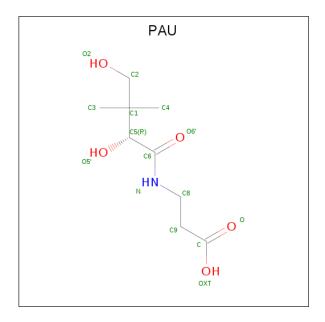
There are 4 unique types of molecules in this entry. The entry contains 10703 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pantothenate kinase.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	302	Total	С	N	О	S	0	0	0
1	A	302	2414	1555	411	442	6	0	U	
1	В	302	Total	С	N	О	S	0	0	
1	Б	302	2418	1558	411	444	5		0	
1	С	298	Total	С	N	О	S	0	0	0
1		290	2391	1541	404	440	6	0	0	
1	1 D	D 204	Total	С	N	О	S	0	0	0
1	ש	304	2427	1564	412	445	6	U	U	U

• Molecule 2 is PANTOTHENOIC ACID (three-letter code: PAU) (formula: C₉H₁₇NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total				0	0	
_	11	_	15	9	1	5	Ŭ.		
9	D	1	Total	\mathbf{C}	N	Ο	0	0	
	Б	1	15	9	1	5	0	0	

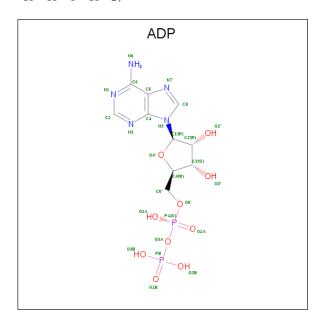
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	С	1	Total 15				0	0
2	D	1	Total 15	C 9		O 5	0	0

• 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	Δ	1	Total	С	N	О	Р	0	0	
,	Λ	1	27	10	5	10	2	0		
3	В	1	Total	С	N	О	Р	0	0	
,	Б	1	27	10	5	10	2	0		
2	3 C	C	1	Total	С	N	О	Р	0	0
3		1	27	10	5	10	2	U		
2	2 D	1	Total	С	N	О	Р	0	0	
3	ש	1	27	10	5	10	2	U	U	

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	235	Total O 235 235	0	0
4	В	191	Total O 191 191	0	0
4	С	230	Total O 230 230	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	229	Total O 229 229	0	0

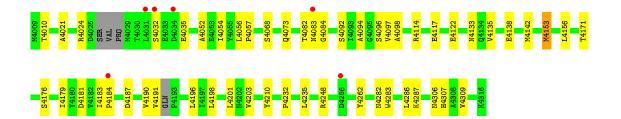


3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Pantothenate kinase Chain A: • Molecule 1: Pantothenate kinase Chain B: 81% 16% • Molecule 1: Pantothenate kinase Chain C: 81% 15% • Molecule 1: Pantothenate kinase Chain D: 81%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	181.20Å 181.66Å 47.42Å	Danasitan
a, b, c, α , β , γ	90.00° 104.79° 90.00°	Depositor
Resolution (Å)	20.00 - 2.20	Depositor
rtesoration (A)	40.82 - 2.00	EDS
% Data completeness	99.2 (20.00-2.20)	Depositor
(in resolution range)	88.7 (40.82-2.00)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$2.75~({\rm at}~2.00{\rm \AA})$	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.187 , 0.225	Depositor
	0.195 , 0.231	DCC
R_{free} test set	8528 reflections $(8.87%)$	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 45.4	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
	$0.000 { m for} k{+}l,\!h{+}l,\!-l$	
Estimated twinning fraction	$0.000 { m for} { m -k+l,-h-l,-l}$	Xtriage
	0.024 for -h-2*l,-k,l	
F_o, F_c correlation	0.94	EDS
Total number of atoms	10703	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.64% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: PAU, 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		
IVIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.34	0/2468	0.58	0/3349	
1	В	0.33	0/2475	0.57	0/3364	
1	С	0.35	0/2442	0.57	0/3309	
1	D	0.33	0/2483	0.57	0/3374	
All	All	0.34	0/9868	0.57	0/13396	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2414	0	2381	39	0
1	В	2418	0	2392	32	0
1	С	2391	0	2370	35	1
1	D	2427	0	2400	33	0
2	A	15	0	16	0	0
2	В	15	0	16	0	0
2	С	15	0	16	1	0
2	D	15	0	16	1	0
3	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	27	0	12	0	0
3	С	27	0	12	0	0
3	D	27	0	12	0	0
4	A	235	0	0	6	0
4	В	191	0	0	5	0
4	С	230	0	0	8	0
4	D	229	0	0	5	0
All	All	10703	0	9655	136	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 7.

The worst 5 of 136 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:C:3263:ALA:HB2	4:C:7336:HOH:O	1.89	0.72
1:C:3010:THR:HG22	1:C:3012:TYR:H	1.55	0.72
1:A:1263:ALA:HB2	4:A:7647:HOH:O	1.89	0.71
1:C:3009:MET:HB3	4:C:7474:HOH:O	1.93	0.68
1:D:4021:ALA:O	1:D:4024:ARG:HG2	1.95	0.66

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:C:3014:GLN:NE2	1:C:3014:GLN:NE2[2_555]	2.13	0.07

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	Perce	$_{ m ntiles}$
1	A	293/308~(95%)	287 (98%)	6 (2%)	0	100	100
1	В	298/308~(97%)	288 (97%)	9 (3%)	1 (0%)	41	46
1	С	286/308~(93%)	282 (99%)	4 (1%)	0	100	100
1	D	298/308~(97%)	292 (98%)	6 (2%)	0	100	100
All	All	$1175/1232 \ (95\%)$	1149 (98%)	25 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	2084	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	A	260/277~(94%)	255 (98%)	5 (2%)	57 71		
1	В	261/277 (94%)	258 (99%)	3 (1%)	73 85		
1	С	$260/277 \; (94\%)$	258 (99%)	2 (1%)	81 90		
1	D	$262/277 \; (95\%)$	258 (98%)	4 (2%)	65 78		
All	All	1043/1108 (94%)	1029 (99%)	14 (1%)	69 81		

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	\mathbf{Type}
1	В	2196	LEU
1	В	2218	PHE
1	D	4083	ASN
1	В	2153	MET
1	D	4010	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:



Mol	Chain	Res	Type
1	A	1085	GLN
1	D	4177	HIS
1	D	4018	ASN
1	A	1063	ASN
1	A	1260	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Mol Type Chain		Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	5001	-	24,29,29	0.93	1 (4%)	29,45,45	1.55	4 (13%)
2	PAU	С	6002	-	9,14,14	3.92	4 (44%)	14,19,19	1.28	2 (14%)
3	ADP	D	5004	-	24,29,29	0.99	1 (4%)	29,45,45	1.55	5 (17%)
2	PAU	A	6001	-	9,14,14	3.71	4 (44%)	14,19,19	1.11	2 (14%)
2	PAU	В	6003	-	9,14,14	3.85	4 (44%)	14,19,19	1.19	2 (14%)
3	ADP	С	5003	-	24,29,29	1.15	1 (4%)	29,45,45	1.82	9 (31%)
2	PAU	D	6004	-	9,14,14	4.20	4 (44%)	14,19,19	1.23	3 (21%)
3	ADP	В	5002	-	24,29,29	0.88	1 (4%)	29,45,45	1.59	4 (13%)



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	5001	-	-	3/12/32/32	0/3/3/3
2	PAU	С	6002	-	-	3/17/19/19	-
3	ADP	D	5004	-	-	3/12/32/32	0/3/3/3
2	PAU	A	6001	-	-	0/17/19/19	-
2	PAU	В	6003	_	-	3/17/19/19	-
3	ADP	С	5003	_	-	5/12/32/32	0/3/3/3
2	PAU	D	6004	-	-	5/17/19/19	-
3	ADP	В	5002	-	-	3/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
2	D	6004	PAU	C2-C1	10.78	1.60	1.53
2	С	6002	PAU	C2-C1	9.89	1.59	1.53
2	В	6003	PAU	C2-C1	9.34	1.59	1.53
2	A	6001	PAU	C2-C1	8.79	1.59	1.53
2	A	6001	PAU	O6'-C6	5.35	1.34	1.23

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
3	В	5002	ADP	C5-C6-N6	4.05	126.51	120.35
3	С	5003	ADP	C5-C6-N6	3.95	126.36	120.35
3	A	5001	ADP	C5-C6-N6	3.65	125.90	120.35
3	D	5004	ADP	C5-C6-N6	3.59	125.81	120.35
3	D	5004	ADP	N3-C2-N1	-3.57	123.09	128.68

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5001	ADP	PA-O3A-PB-O3B
2	С	6002	PAU	C5-C6-N-C8
2	С	6002	PAU	O6'-C6-N-C8
3	D	5004	ADP	PA-O3A-PB-O3B
2	В	6003	PAU	C5-C6-N-C8

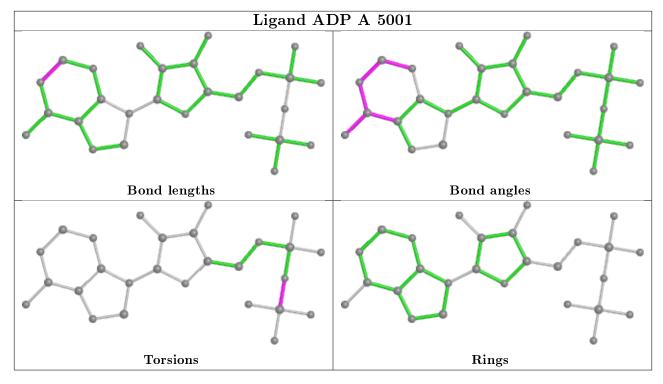


There are no ring outliers.

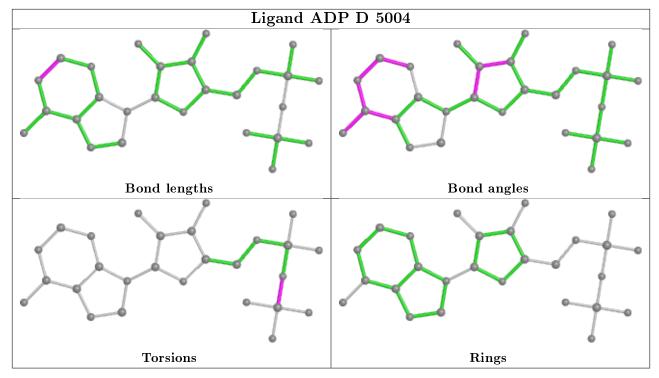
2 monomers are involved in 2 short contacts:

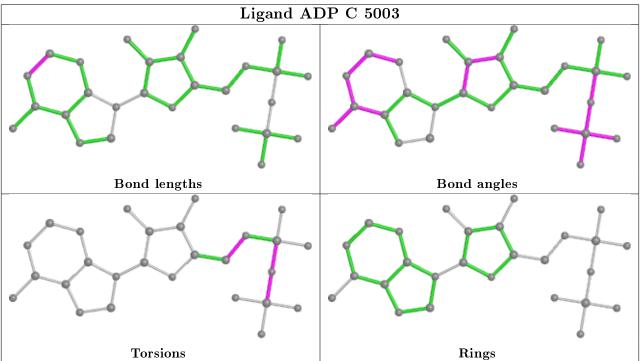
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	6002	PAU	1	0
2	D	6004	PAU	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

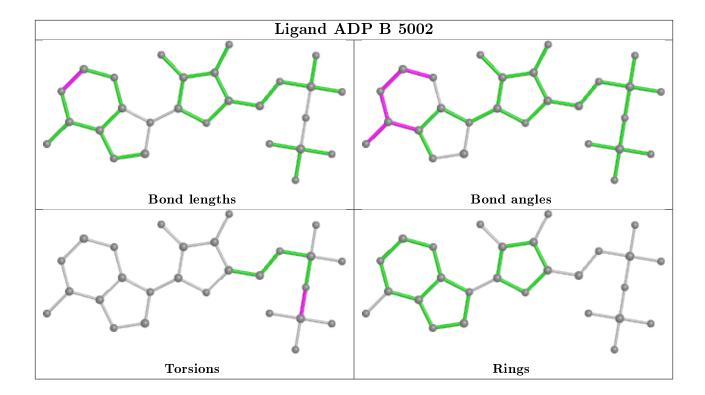












5.7 Other polymers (i)

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	302/308~(98%)	-0.30	3 (0%) 82 81	15, 26, 47, 63	0
1	В	302/308~(98%)	-0.30	4 (1%) 77 75	16, 27, 47, 54	0
1	С	298/308~(96%)	-0.32	4 (1%) 77 75	14, 25, 45, 57	0
1	D	304/308 (98%)	-0.34	6 (1%) 65 63	17, 27, 49, 67	0
All	All	$1206/1232 \ (97\%)$	-0.31	17 (1%) 75 73	14, 26, 48, 67	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4184	PRO	4.0
1	С	3083	ASN	3.6
1	D	4256	ASP	2.9
1	В	2184	PRO	2.8
1	D	4083	ASN	2.7

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 carbohydrates in this entry.

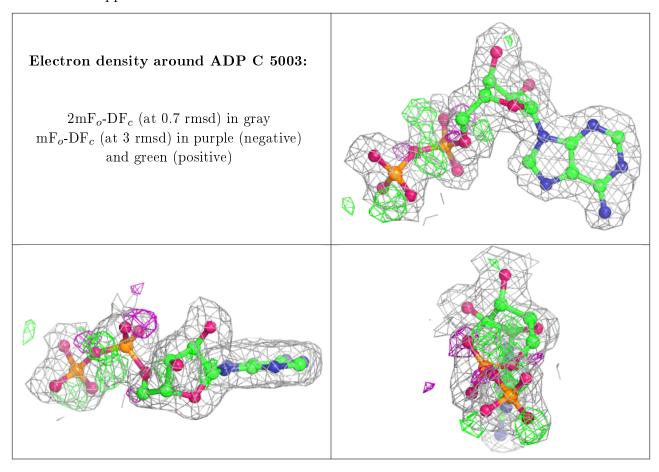
6.4 Ligands (i)

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



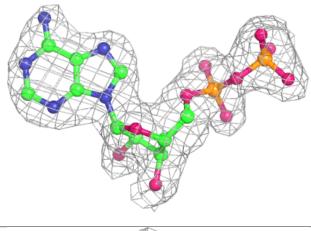
Mol	Type	Chain	${ m Res}$	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
2	PAU	В	6003	15/15	0.85	0.18	30,32,34,35	0
2	PAU	D	6004	15/15	0.88	0.15	30,32,34,35	0
2	PAU	С	6002	15/15	0.92	0.15	23,24,26,29	0
2	PAU	A	6001	15/15	0.93	0.14	22,24,29,29	0
3	ADP	С	5003	27/27	0.95	0.13	21,25,27,31	0
3	ADP	D	5004	27/27	0.96	0.10	21,28,33,35	0
3	ADP	A	5001	27/27	0.97	0.10	15,23,29,31	0
3	ADP	В	5002	27/27	0.97	0.09	16,21,26,26	0

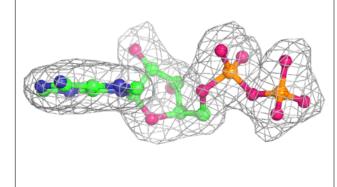
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

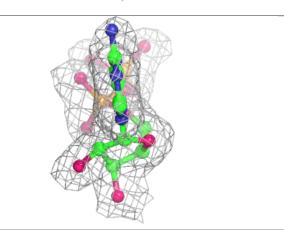




Electron density around ADP D 5004: $2mF_o\text{-}DF_c \text{ (at } 0.7 \text{ rmsd) in gray} \\ mF_o\text{-}DF_c \text{ (at } 3 \text{ rmsd) in purple (negative)} \\ \text{and green (positive)}$

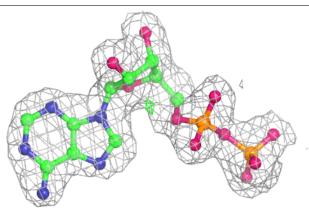


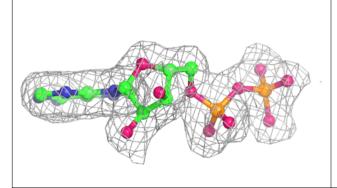


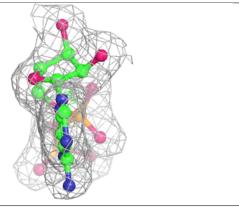


Electron density around ADP A 5001:

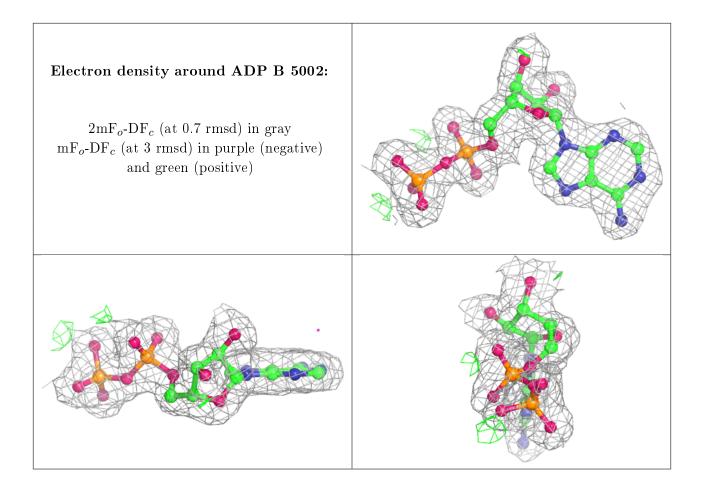
 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

