Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 08:30 pm BST

PDB ID	:	4PFP
Title	:	Myosin VI motor domain in the Pi release state (with Pi) space group P21
Authors	:	Isabet, T.; Benisty, H.; Llinas, P.; Sweeney, H.L.; Houdusse, A.
Deposited on	:	2014-04-30
Resolution	:	2.32 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

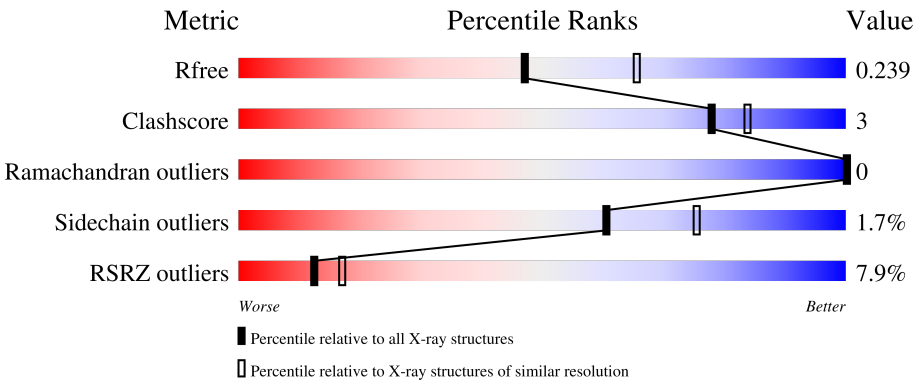
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 >=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	788	10% 88% 8% • •
1	C	788	5% 91% 6% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12526 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.

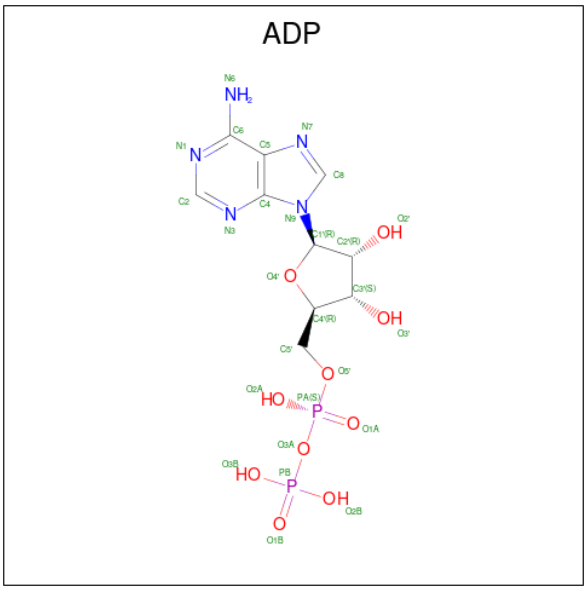
- Molecule 1 is a protein called Unconventional myosin-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	760	5988	3822	1032	1105	29	0	6	0
1	C	766	6051	3854	1035	1132	30	0	4	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

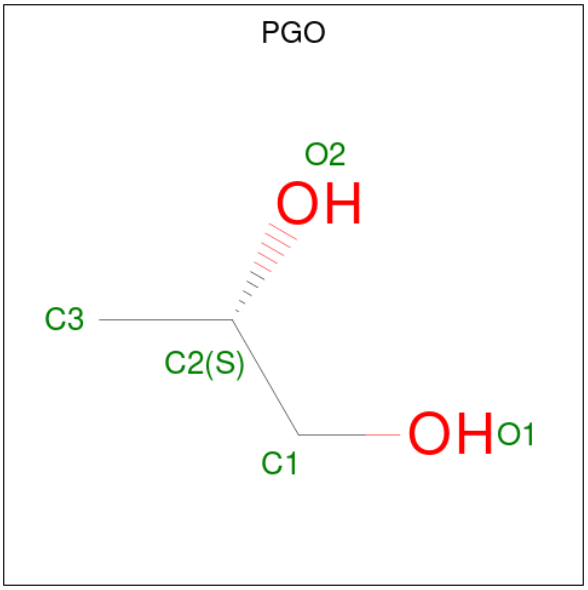
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	C	1	1	1	0	0

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



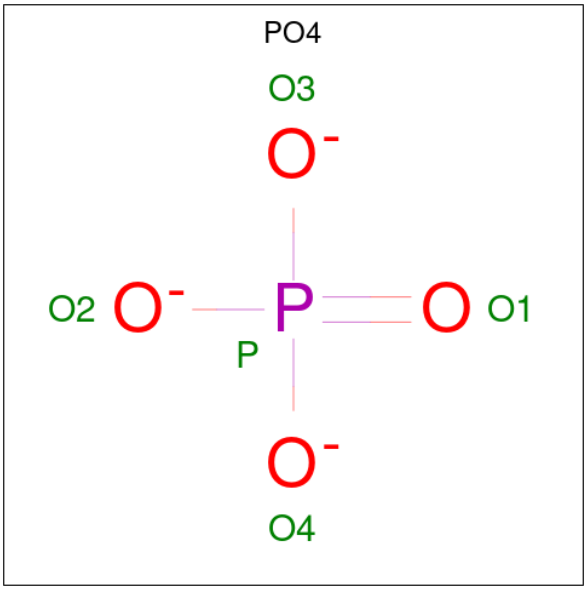
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	C	1	27	10	5	10	2	0	0

- Molecule 4 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	5	3	2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

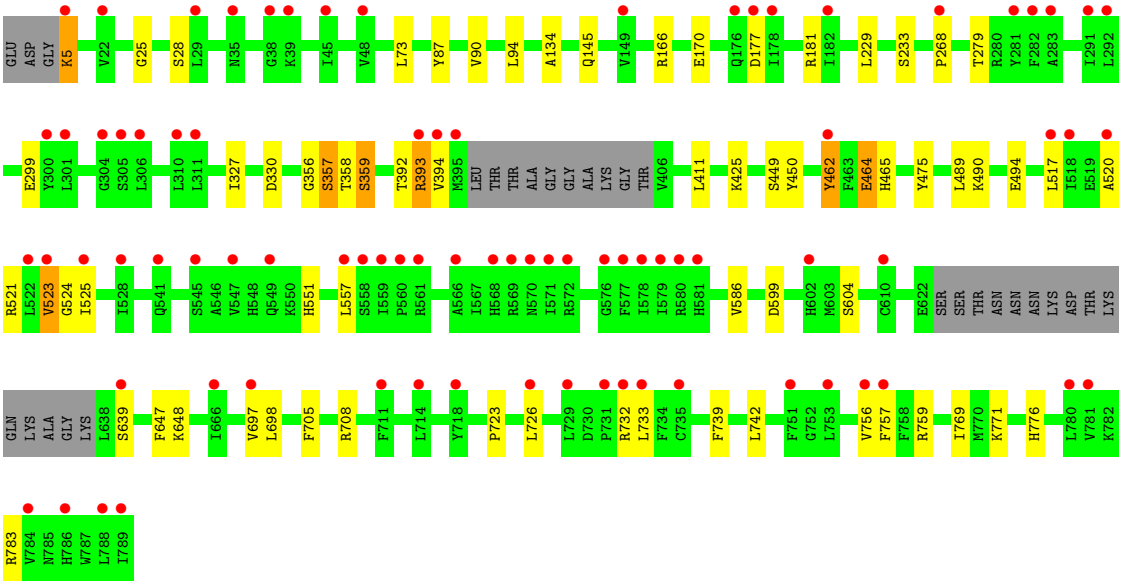
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	170	170	170	0	0
			Total	O		
6	C	241	241	241	0	0

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.

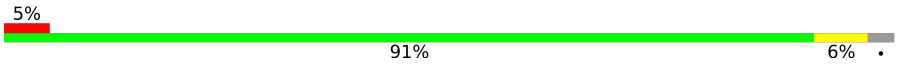
- Molecule 1: Unconventional myosin-VI

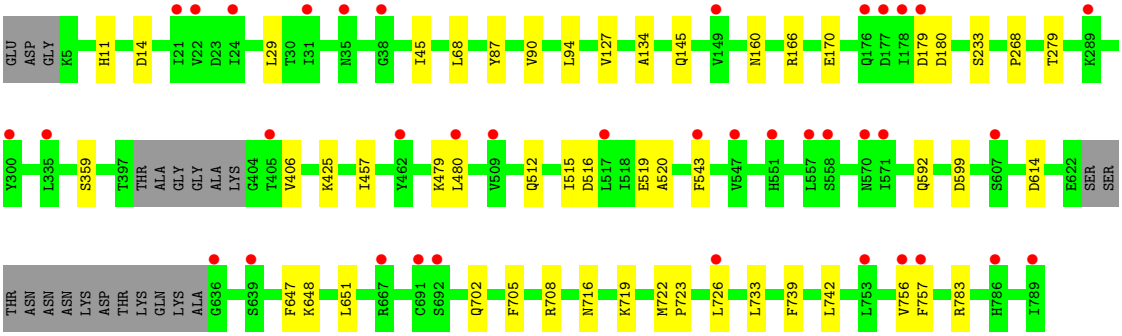
Chain A:



- Molecule 1: Unconventional myosin-VI

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.65Å 94.89Å 97.30Å 90.00° 99.55° 90.00°	Depositor
Resolution (Å)	23.39 – 2.32 43.98 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.39-2.32) 99.8 (43.98-2.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.189 , 0.229 0.199 , 0.239	Depositor DCC
R_{free} test set	3902 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12526	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.74 % 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 7.6209e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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, PGO, MG

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	0.55	3/6121 (0.0%)	0.67	4/8270 (0.0%)
1	C	0.52	0/6175	0.66	1/8340 (0.0%)
All	All	0.54	3/12296 (0.0%)	0.67	5/16610 (0.0%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	THR	C-N	-17.98	0.92	1.34
1	A	393	ARG	C-N	8.50	1.53	1.34
1	A	5	LYS	C-N	-7.92	1.19	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	LYS	O-C-N	-8.81	104.36	121.10
1	A	5	LYS	CA-C-N	8.22	140.12	117.10
1	A	25	GLY	C-N-CD	5.99	140.97	128.40
1	A	90	VAL	N-CA-C	-5.11	97.20	111.00
1	C	90	VAL	N-CA-C	-5.08	97.30	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	LYS	Mainchain

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	5988	0	5795	43	0
1	C	6051	0	5862	25	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	12	0	0
3	C	27	0	12	0	0
4	A	5	0	8	0	0
5	A	10	0	0	0	0
5	C	5	0	0	0	0
6	A	170	0	0	2	0
6	C	241	0	0	3	0
All	All	12526	0	11689	68	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 3.

All (68) 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:356:GLY:O	1:A:358:THR:HG23	1.78	0.83
1:C:68:LEU:HD12	1:C:702:GLN:HG2	1.64	0.79
1:C:723:PRO:HD2	1:C:726:LEU:HD12	1.67	0.77
1:A:299:GLU:CD	6:A:901:HOH:O	2.26	0.73
1:C:457:ILE:HD13	1:C:480:LEU:HD12	1.69	0.72
1:A:356:GLY:C	1:A:358:THR:HG23	2.09	0.71
1:A:357:SER:HA	1:A:358:THR:C	2.10	0.71
1:A:357:SER:HA	1:A:358:THR:HG23	1.77	0.65
1:A:358:THR:OG1	1:A:359:SER:N	2.33	0.60
1:A:357:SER:CA	1:A:358:THR:HG23	2.33	0.58
1:A:449:SER:C	1:A:450:TYR:HA	2.23	0.58
1:C:592:GLN:HA	6:C:1072:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:O	1:A:181:ARG:HG3	2.04	0.57
1:A:357:SER:CA	1:A:358:THR:CG2	2.85	0.54
1:A:739:PHE:CE2	1:A:756:VAL:HG21	2.45	0.52
1:C:512:GLN:HA	1:C:515:ILE:HD12	1.91	0.52
1:A:73:LEU:HD22	1:A:698:LEU:HD21	1.92	0.52
1:A:464:GLU:HG2	1:A:465:HIS:CD2	2.45	0.51
1:C:515:ILE:HD11	6:C:905:HOH:O	2.10	0.51
1:A:357:SER:HA	1:A:358:THR:CG2	2.41	0.50
1:A:394:VAL:HG12	1:A:604:SER:HB3	1.92	0.50
1:C:739:PHE:CE2	1:C:756:VAL:HG21	2.47	0.50
1:A:489:LEU:HD21	1:A:697:VAL:HG12	1.94	0.49
1:C:127:VAL:HG11	1:C:160:ASN:OD1	2.12	0.49
1:A:87:TYR:HB3	1:A:94:LEU:HD11	1.95	0.48
1:C:716:ASN:O	1:C:719:LYS:HG2	2.13	0.48
1:A:551:HIS:HB2	1:A:557:LEU:HD22	1.95	0.48
1:A:393:ARG:HB2	1:A:411:LEU:HD21	1.96	0.48
1:A:705:PHE:HB3	1:A:757:PHE:HB3	1.95	0.48
1:C:87:TYR:HB3	1:C:94:LEU:HD11	1.95	0.48
1:C:516:ASP:O	1:C:520:ALA:HB2	2.16	0.46
1:C:739:PHE:HE2	1:C:756:VAL:HG21	1.80	0.46
1:C:11:HIS:HD2	1:C:14:ASP:H	1.64	0.46
1:A:134:ALA:O	1:A:145:GLN:HG3	2.15	0.46
1:C:134:ALA:O	1:C:145:GLN:HG3	2.16	0.46
1:C:268:PRO:HB2	1:C:279:THR:HB	1.98	0.45
1:C:68:LEU:CD1	1:C:702:GLN:HG2	2.40	0.45
1:C:166:ARG:O	1:C:170:GLU:HB2	2.18	0.44
1:A:166:ARG:O	1:A:170:GLU:HB2	2.18	0.44
1:A:449:SER:C	1:A:450:TYR:CA	2.86	0.44
1:A:357:SER:CA	1:A:358:THR:C	2.85	0.44
1:A:517:LEU:O	1:A:525:ILE:HG13	2.17	0.44
1:A:268:PRO:HB2	1:A:279:THR:HB	2.00	0.44
1:A:357:SER:N	1:A:358:THR:HG23	2.32	0.43
1:A:520:ALA:O	1:A:524:GLY:HA3	2.18	0.43
1:A:521:ARG:O	1:A:523:VAL:N	2.48	0.43
1:C:647:PHE:CE2	1:C:651:LEU:HD11	2.53	0.43
1:A:723:PRO:HD2	1:A:726:LEU:HD12	2.00	0.43
1:A:771:LYS:HB3	1:A:776:HIS:CD2	2.54	0.43
1:C:705:PHE:HB3	1:C:757:PHE:HB3	1.99	0.43
1:C:233:SER:HA	1:C:425:LYS:HE2	2.00	0.43
1:A:490:LYS:O	1:A:494:GLU:HG3	2.20	0.42
1:A:742:LEU:HD22	1:A:783:ARG:HH11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:LEU:HD22	1:C:783:ARG:HH11	1.84	0.42
1:A:229:LEU:HD11	1:A:647:PHE:CE2	2.54	0.42
1:A:742:LEU:HD12	1:A:769:ILE:HD11	2.01	0.42
1:A:181:ARG:HG2	1:A:327:ILE:HG22	2.02	0.42
1:C:519:GLU:HB2	1:C:648:LYS:HE3	2.01	0.42
1:C:29:LEU:HG	1:C:45:ILE:HG12	2.00	0.42
1:A:462:TYR:CD2	1:A:586:VAL:HG22	2.54	0.42
1:A:759:ARG:HD3	6:A:909:HOH:O	2.18	0.42
1:A:475:TYR:OH	1:A:648:LYS:HG3	2.21	0.41
1:A:233:SER:HA	1:A:425:LYS:HE2	2.02	0.41
1:A:357:SER:C	1:A:358:THR:HG22	2.41	0.41
1:A:739:PHE:HE2	1:A:756:VAL:HG21	1.84	0.41
1:C:719:LYS:HA	1:C:722:MET:HG2	2.01	0.41
1:C:479:LYS:HA	6:C:905:HOH:O	2.21	0.41
1:A:356:GLY:C	1:A:358:THR:CG2	2.86	0.40

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	758/788 (96%)	745 (98%)	13 (2%)	0	100	100
1	C	764/788 (97%)	751 (98%)	13 (2%)	0	100	100
All	All	1522/1576 (97%)	1496 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	630/696 (90%)	618 (98%)	12 (2%)	57	73
1	C	644/696 (92%)	635 (99%)	9 (1%)	67	80
All	All	1274/1392 (92%)	1253 (98%)	21 (2%)	60	77

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	330	ASP
1	A	357	SER
1	A	359	SER
1	A	462	TYR
1	A	464	GLU
1	A	523	VAL
1	A	599	ASP
1	A	639	SER
1	A	708	ARG
1	A	732	ARG
1	A	733	LEU
1	C	179	ASP
1	C	180	ASP
1	C	359	SER
1	C	406	VAL
1	C	543	PHE
1	C	599	ASP
1	C	614	ASP
1	C	708	ARG
1	C	733	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	507	HIS
1	A	716	ASN
1	C	11	HIS
1	C	482	GLN

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	ADP	A	802	2	24,29,29	0.72	0	29,45,45	0.95	2 (6%)
5	PO4	A	805	-	4,4,4	2.46	1 (25%)	6,6,6	0.84	0
5	PO4	C	802	2	4,4,4	2.50	1 (25%)	6,6,6	0.88	0
4	PGO	A	803	-	3,4,4	0.75	0	1,4,4	0.40	0
5	PO4	A	804	2	4,4,4	2.02	3 (75%)	6,6,6	0.82	0
3	ADP	C	801	2	24,29,29	0.68	0	29,45,45	0.70	1 (3%)

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	802	2	-	2/12/32/32	0/3/3/3
4	PGO	A	803	-	-	0/2/2/2	-
3	ADP	C	801	2	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	802	PO4	P-O1	4.21	1.60	1.50
5	A	805	PO4	P-O1	4.09	1.60	1.50
5	A	804	PO4	P-O1	2.15	1.55	1.50
5	A	804	PO4	P-O2	2.07	1.60	1.54
5	A	804	PO4	P-O4	2.07	1.60	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	ADP	C5-C6-N6	2.36	123.93	120.35
3	C	801	ADP	C5-C6-N6	2.17	123.65	120.35
3	A	802	ADP	O3'-C3'-C4'	2.13	117.21	111.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

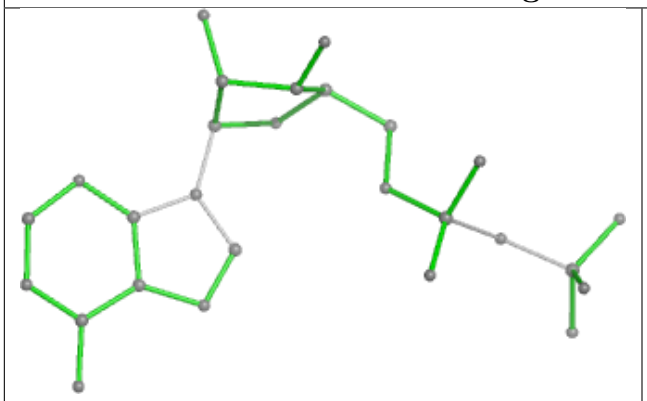
Mol	Chain	Res	Type	Atoms
3	A	802	ADP	PA-O3A-PB-O3B
3	C	801	ADP	PA-O3A-PB-O1B
3	A	802	ADP	PA-O3A-PB-O2B
3	C	801	ADP	PA-O3A-PB-O2B
3	C	801	ADP	PA-O3A-PB-O3B

There are no ring outliers.

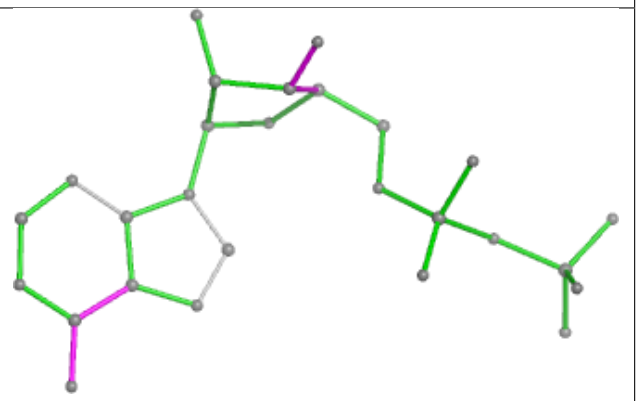
No monomer is involved in short contacts.

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.

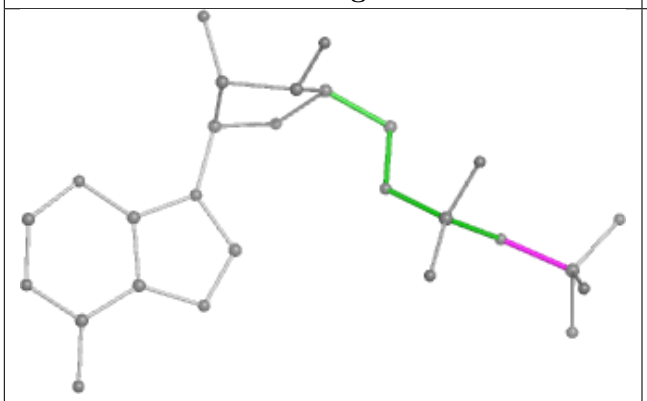
Ligand ADP A 802



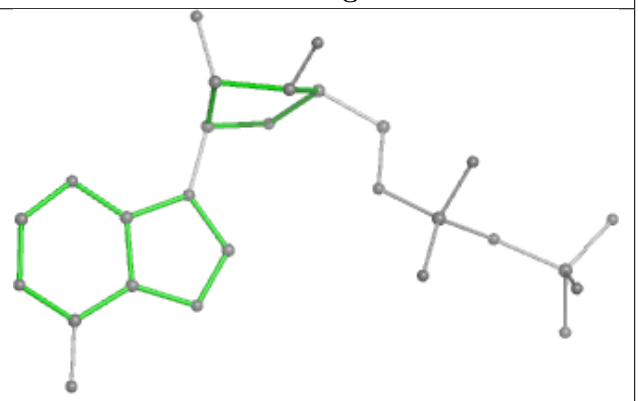
Bond lengths



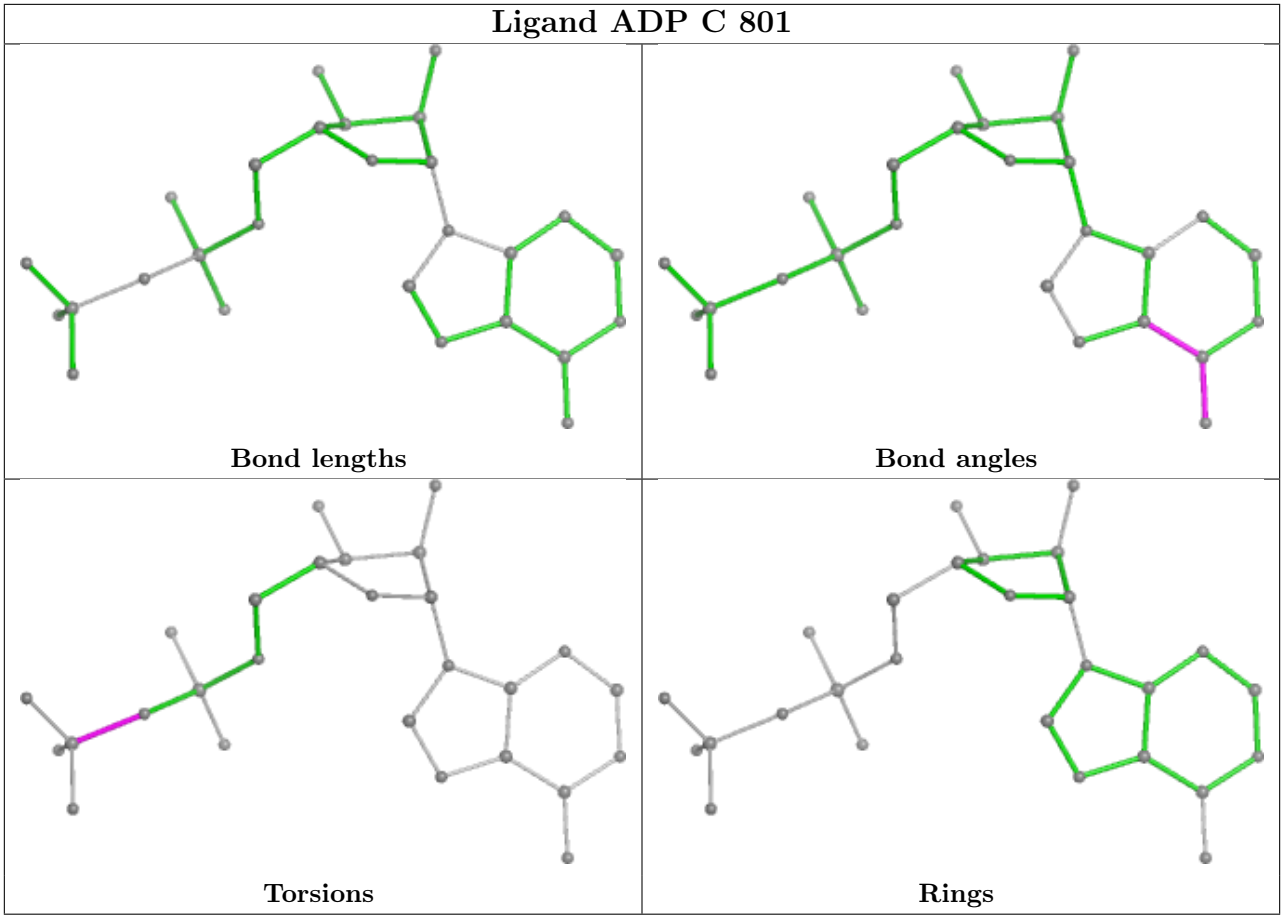
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	449:SER	C	450:TYR	N	2.84
1	A	5:LYS	C	6:PRO	N	1.19
1	A	392:THR	C	393:ARG	N	0.92

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	760/788 (96%)	0.59	82 (10%)	5	8	29, 57, 86, 114	1 (0%)
1	C	766/788 (97%)	0.37	38 (4%)	28	36	26, 48, 75, 110	0
All	All	1526/1576 (96%)	0.48	120 (7%)	12	17	26, 53, 83, 114	1 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	ASP	7.9
1	C	178	ILE	7.6
1	A	517	LEU	7.3
1	A	177	ASP	6.3
1	A	757	PHE	5.1
1	A	522	LEU	4.8
1	A	572	ARG	4.8
1	C	789	ILE	4.8
1	A	788	LEU	4.8
1	C	38	GLY	4.7
1	A	610	CYS	4.6
1	A	729	LEU	4.4
1	A	545	SER	4.3
1	A	756	VAL	4.2
1	A	786	HIS	4.2
1	A	301	LEU	4.2
1	A	579	ILE	4.2
1	A	781	VAL	4.1
1	A	577	PHE	4.1
1	A	576	GLY	4.1
1	C	753	LEU	4.0
1	C	667[A]	ARG	4.0
1	A	557	LEU	4.0
1	A	560	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	751	PHE	3.9
1	A	310	LEU	3.9
1	A	753	LEU	3.9
1	A	733	LEU	3.8
1	C	24	ILE	3.7
1	A	558	SER	3.7
1	A	300	TYR	3.7
1	A	639	SER	3.6
1	A	393	ARG	3.5
1	C	757	PHE	3.4
1	C	547	VAL	3.4
1	C	405	THR	3.3
1	A	561	ARG	3.3
1	C	509	VAL	3.3
1	A	281	TYR	3.3
1	A	547	VAL	3.2
1	C	179	ASP	3.2
1	A	29	LEU	3.2
1	C	691[A]	CYS	3.2
1	A	5	LYS	3.2
1	A	726	LEU	3.2
1	C	571	ILE	3.1
1	A	304	GLY	3.1
1	A	35	ASN	3.1
1	A	292	LEU	3.1
1	C	35	ASN	3.0
1	A	580	ARG	3.0
1	A	176	GLN	2.9
1	A	559	ILE	2.9
1	A	291	ILE	2.9
1	C	557	LEU	2.9
1	A	39	LYS	2.9
1	A	714	LEU	2.9
1	C	786	HIS	2.8
1	A	306	LEU	2.8
1	A	571	ILE	2.7
1	A	523	VAL	2.7
1	C	480	LEU	2.7
1	A	520	ALA	2.6
1	A	718	TYR	2.6
1	C	517	LEU	2.6
1	C	726	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	462	TYR	2.6
1	A	528	ILE	2.6
1	A	568	HIS	2.6
1	A	22	VAL	2.6
1	C	692	SER	2.6
1	C	22	VAL	2.6
1	C	570	ASN	2.6
1	A	735	CYS	2.5
1	C	176	GLN	2.5
1	A	305	SER	2.5
1	A	311	LEU	2.5
1	A	732	ARG	2.5
1	A	178	ILE	2.4
1	A	149	VAL	2.4
1	C	300	TYR	2.4
1	A	541	GLN	2.4
1	A	581	HIS	2.4
1	A	525	ILE	2.4
1	A	282	PHE	2.3
1	C	543	PHE	2.3
1	A	549	GLN	2.3
1	A	45	ILE	2.3
1	A	182	ILE	2.3
1	A	566	ALA	2.3
1	A	394	VAL	2.2
1	A	38	GLY	2.2
1	C	639	SER	2.2
1	A	666	ILE	2.2
1	A	268	PRO	2.2
1	A	578	ILE	2.2
1	A	602	HIS	2.2
1	C	31	ILE	2.2
1	A	789	ILE	2.1
1	C	21	ILE	2.1
1	A	731	PRO	2.1
1	A	780	LEU	2.1
1	C	636	GLY	2.1
1	A	395	MET	2.1
1	A	48	VAL	2.1
1	A	784	VAL	2.1
1	A	518	ILE	2.1
1	C	149	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	335	LEU	2.1
1	C	558	SER	2.1
1	A	697	VAL	2.1
1	A	569	ARG	2.0
1	A	570	ASN	2.0
1	C	756	VAL	2.0
1	A	711	PHE	2.0
1	C	289	LYS	2.0
1	A	283	ALA	2.0
1	C	607	SER	2.0
1	C	551	HIS	2.0
1	A	462	TYR	2.0

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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

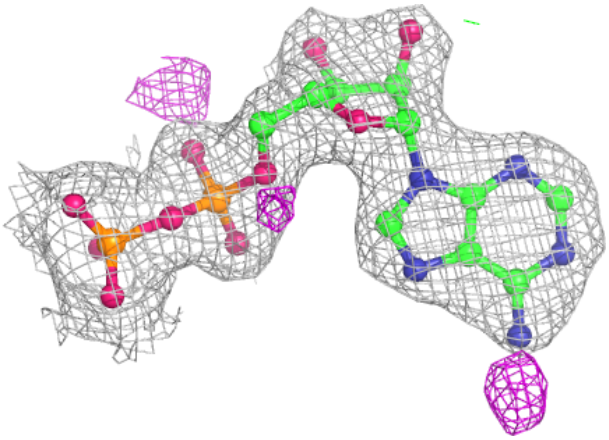
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGO	A	803	5/5	0.86	0.27	68,69,71,71	0
5	PO4	A	804	5/5	0.90	0.27	18,29,33,36	5
5	PO4	A	805	5/5	0.90	0.31	79,80,84,86	0
2	MG	C	803	1/1	0.97	0.15	31,31,31,31	0
2	MG	A	801	1/1	0.97	0.15	29,29,29,29	0
3	ADP	C	801	27/27	0.98	0.14	25,29,36,37	0
3	ADP	A	802	27/27	0.98	0.14	24,34,47,49	0
5	PO4	C	802	5/5	0.99	0.13	32,36,38,41	0

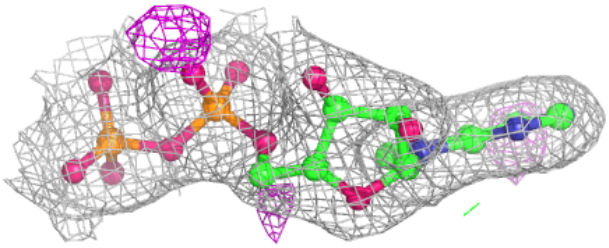
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

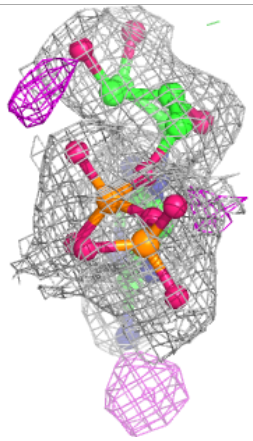
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP C 801:

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

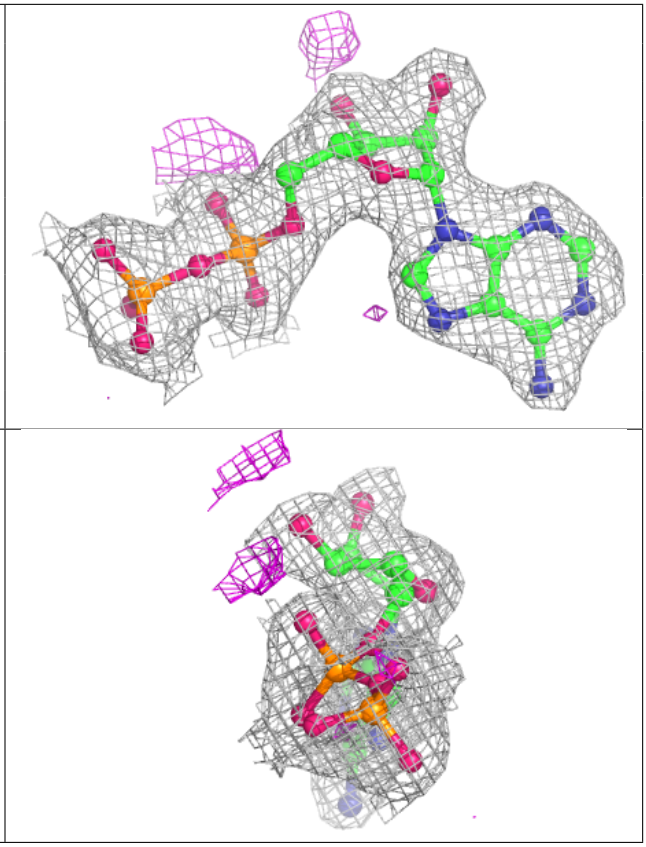






Electron density around ADP A 802:

$2mF_o$-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.