Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:57 pm BST

PDB ID	:	6I7E
Title	:	Plasmodium falciparum Myosin A, Pre-powerstroke
Authors	:	Robert-Paganin, J.; Auguin, D.; Moussaoui, D.; Jousset, G.; Baum, J.; Trybus, K.M.; Houdusse, A.
Deposited on	:	2018-11-16
Resolution	:	3.49 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 ⓘ symbol.

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

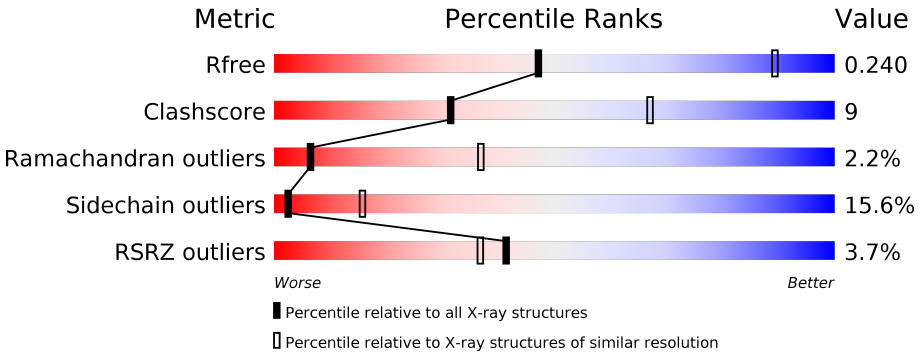
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	768	4% 67% 27% 5% •

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
4	VO4	A	803	-	-	X	-

2 Entry composition

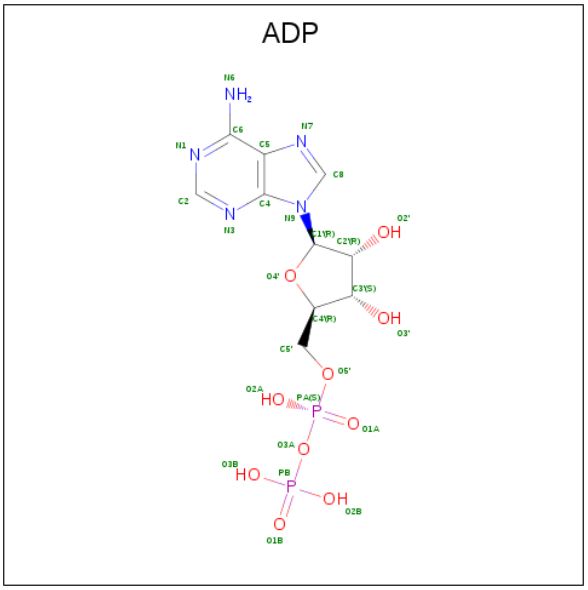
There are 4 unique types of molecules in this entry. The entry contains 6061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myosin-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	761	6028	3835	1014	1147	1	31	0	1	0

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

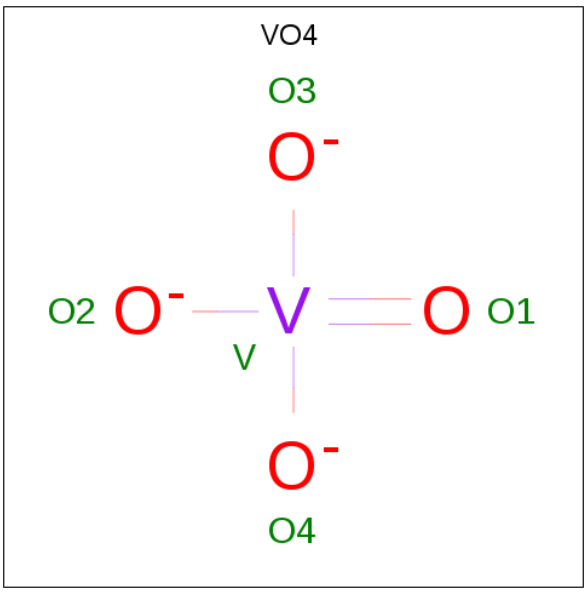


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



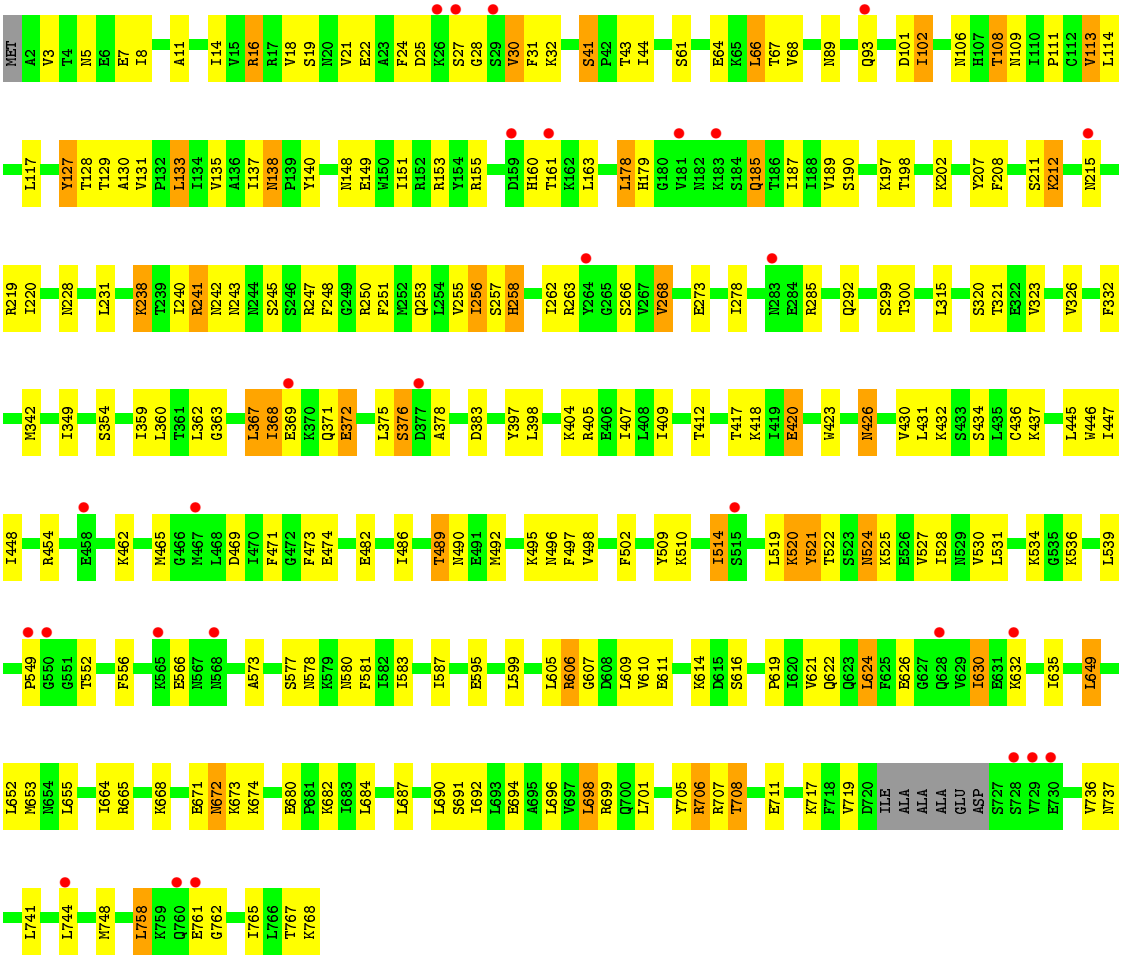
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O V 5 4 1	0	0

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: Myosin-A

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	197.46Å 197.46Å 178.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.17 – 3.49 25.17 – 3.49	Depositor EDS
% Data completeness (in resolution range)	58.7 (25.17-3.49) 58.8 (25.17-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 3.46Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.193 , 0.233 0.211 , 0.240	Depositor DCC
R_{free} test set	774 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	139.9	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 159.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6061	wwPDB-VP
Average B, all atoms (Å^2)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, MG, ADP, SEP

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	0.48	0/6122	0.74	0/8255

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

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	6028	0	6095	106	0
2	A	27	0	12	0	0
3	A	1	0	0	0	0
4	A	5	0	0	4	0
All	All	6061	0	6107	110	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 9.

All (110) 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:315:LEU:HD11	1:A:363:GLY:HA3	1.60	0.82
1:A:16:ARG:HH12	1:A:109:ASN:HA	1.47	0.79
1:A:489:THR:HA	1:A:649:LEU:HD11	1.66	0.76
1:A:581:PHE:HE2	1:A:583:ILE:HD11	1.53	0.74
1:A:109:ASN:HD22	1:A:111:PRO:HD2	1.58	0.67
1:A:492:MET:HG2	1:A:528:ILE:HD11	1.76	0.67
1:A:250:ARG:HB3	1:A:469:ASP:HB3	1.78	0.66
1:A:256:ILE:HG23	1:A:262:ILE:HG13	1.77	0.66
1:A:630:ILE:H	1:A:630:ILE:HD13	1.61	0.65
1:A:198:THR:HG22	1:A:202:LYS:HD2	1.78	0.64
4:A:803:VO4:V	4:A:803:VO4:O4	1.54	0.64
1:A:397:TYR:HB2	1:A:621:VAL:HG21	1.79	0.64
4:A:803:VO4:V	4:A:803:VO4:O3	1.56	0.63
1:A:253:GLN:HB2	1:A:266:SER:HB3	1.82	0.62
4:A:803:VO4:O1	4:A:803:VO4:V	1.56	0.62
1:A:16:ARG:NH1	1:A:109:ASN:HA	2.15	0.62
4:A:803:VO4:O2	4:A:803:VO4:V	1.56	0.62
1:A:495:LYS:HD2	1:A:524:ASN:HB3	1.82	0.61
1:A:292:GLN:HB3	1:A:332:PHE:HB2	1.81	0.61
1:A:179:HIS:CE1	1:A:258:HIS:H	2.19	0.60
1:A:376:SER:C	1:A:378:ALA:H	2.05	0.59
1:A:368:ILE:HD13	1:A:369:GLU:H	1.68	0.59
1:A:605:LEU:HD23	1:A:610:VAL:HG22	1.85	0.59
1:A:502:PHE:HB3	1:A:520:LYS:HB3	1.85	0.58
1:A:606:ARG:HH21	1:A:635:ILE:HA	1.68	0.58
1:A:434:SER:HA	1:A:437:LYS:HD2	1.85	0.58
1:A:278:ILE:HG13	1:A:437:LYS:HE2	1.85	0.58
1:A:519:LEU:HA	1:A:698:LEU:HD22	1.84	0.58
1:A:24:PHE:HE2	1:A:61:SER:O	1.86	0.58
1:A:581:PHE:CE2	1:A:583:ILE:HD11	2.37	0.58
1:A:323:VAL:HB	1:A:326:VAL:HB	1.86	0.56
1:A:737:ASN:O	1:A:741:LEU:HG	2.06	0.56
1:A:256:ILE:HD11	1:A:465:MET:HB2	1.89	0.54
1:A:510:LYS:HG3	1:A:514:ILE:HD13	1.89	0.54
1:A:525:LYS:HA	1:A:528:ILE:HG22	1.90	0.54
1:A:495:LYS:HB2	1:A:524:ASN:ND2	2.24	0.53
1:A:208:PHE:HB3	1:A:256:ILE:HG21	1.89	0.53
1:A:502:PHE:HB3	1:A:520:LYS:HD3	1.91	0.53
1:A:521:TYR:OH	1:A:691:SER:HA	2.08	0.53
1:A:238:LYS:HB3	1:A:285:ARG:HB2	1.91	0.52
1:A:273:GLU:HG3	1:A:482:GLU:HG2	1.93	0.51
1:A:61:SER:HB3	1:A:66:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:HB3	1:A:133:LEU:HB2	1.92	0.50
1:A:178:LEU:HD12	1:A:185:GLN:H	1.76	0.50
1:A:671:GLU:HB2	1:A:682:LYS:HE3	1.92	0.50
1:A:744:LEU:HD23	1:A:748:MET:HB3	1.93	0.50
1:A:509:TYR:HB3	1:A:514:ILE:HA	1.93	0.50
1:A:531:LEU:HD21	1:A:583:ILE:HG21	1.95	0.49
1:A:187:ILE:HG23	1:A:664:ILE:HD13	1.93	0.49
1:A:114:LEU:HD22	1:A:680:GLU:HG2	1.94	0.49
1:A:133:LEU:HD12	1:A:133:LEU:H	1.78	0.49
1:A:138:ASN:HD22	1:A:140:TYR:H	1.60	0.48
1:A:238:LYS:HG2	1:A:243:ASN:HA	1.95	0.48
1:A:521:TYR:CZ	1:A:694:GLU:HB2	2.48	0.48
1:A:426:ASN:HD22	1:A:426:ASN:H	1.61	0.48
1:A:665:ARG:HB3	1:A:690:LEU:HD22	1.95	0.48
1:A:473:PHE:CE2	1:A:490:ASN:HB3	2.49	0.48
1:A:25:ASP:HB3	1:A:28:GLY:O	2.14	0.48
1:A:611:GLU:HG2	1:A:630:ILE:HG21	1.95	0.48
1:A:155:ARG:HH12	1:A:212:LYS:N	2.12	0.47
1:A:474:GLU:HG3	1:A:486:ILE:HG21	1.96	0.47
1:A:672:ASN:HB3	1:A:674:LYS:HE2	1.96	0.46
1:A:367:LEU:HD12	1:A:432:LYS:HD3	1.96	0.46
1:A:228:ASN:HA	1:A:250:ARG:HH22	1.80	0.46
1:A:102:ILE:HG21	1:A:113:VAL:HG13	1.97	0.46
1:A:127:TYR:HA	1:A:135:VAL:O	2.15	0.46
1:A:160:HIS:HA	1:A:163:LEU:HD12	1.98	0.46
1:A:18:VAL:HG23	1:A:19:SEP:H	1.80	0.46
1:A:255:VAL:HG12	1:A:263:ARG:HB3	1.98	0.45
1:A:359:ILE:HG23	1:A:436:CYS:HB3	1.98	0.45
1:A:248:PHE:HE2	1:A:250:ARG:HB2	1.81	0.45
1:A:573:ALA:HB3	1:A:577:SER:HA	1.98	0.45
1:A:497:PHE:CE2	1:A:691:SER:HB2	2.50	0.45
1:A:248:PHE:CE2	1:A:250:ARG:HB2	2.52	0.45
1:A:502:PHE:CD2	1:A:520:LYS:HB3	2.52	0.45
1:A:140:TYR:CZ	1:A:673:LYS:HA	2.51	0.45
1:A:405:ARG:O	1:A:409:ILE:HB	2.16	0.45
1:A:495:LYS:HA	1:A:498:VAL:HG22	1.99	0.44
1:A:497:PHE:HE2	1:A:691:SER:HB2	1.82	0.44
1:A:619:PRO:HA	1:A:622:GLN:HE21	1.82	0.44
1:A:607:GLY:HA2	1:A:632:LYS:HA	1.99	0.44
1:A:11:ALA:HA	1:A:14:ILE:HD12	1.99	0.44
1:A:404:LYS:O	1:A:407:ILE:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:HG3	1:A:320:SER:O	2.17	0.44
1:A:240:ILE:HG22	1:A:241:ARG:HH12	1.82	0.44
1:A:684:LEU:HA	1:A:687:LEU:HD12	1.99	0.43
1:A:423:TRP:HA	1:A:423:TRP:CE3	2.53	0.43
1:A:151:ILE:HG23	1:A:207:TYR:CD1	2.54	0.43
1:A:251:PHE:HB3	1:A:268:VAL:HG23	2.00	0.43
1:A:611:GLU:HA	1:A:614:LYS:HB2	2.00	0.43
1:A:5:ASN:HA	1:A:8:ILE:HD12	2.01	0.42
1:A:717:LYS:H	1:A:717:LYS:HD2	1.84	0.42
1:A:117:LEU:HD22	1:A:137:ILE:HD11	2.02	0.42
1:A:495:LYS:CD	1:A:524:ASN:HB3	2.49	0.42
1:A:41:SER:HB3	1:A:44:ILE:HD12	2.02	0.42
1:A:748:MET:SD	1:A:762:GLY:CA	3.08	0.42
1:A:762:GLY:HA2	1:A:765:ILE:HD12	2.01	0.42
1:A:446:TRP:HE3	1:A:447:ILE:HG13	1.85	0.42
1:A:527:VAL:HA	1:A:530:VAL:HG12	2.01	0.42
1:A:708:THR:HG22	1:A:711:GLU:HG3	2.02	0.42
1:A:19:SEP:HB3	1:A:89:ASN:HD22	1.85	0.41
1:A:376:SER:C	1:A:378:ALA:N	2.73	0.41
1:A:108:THR:HB	1:A:696:LEU:HD13	2.02	0.41
1:A:707:ARG:HD3	1:A:711:GLU:OE1	2.21	0.41
1:A:315:LEU:HD13	1:A:360:LEU:HA	2.03	0.41
1:A:621:VAL:O	1:A:624:LEU:HB2	2.21	0.41
1:A:342:MET:HE3	1:A:342:MET:HB2	1.97	0.40
1:A:573:ALA:HB2	1:A:580:ASN:HB2	2.03	0.40
1:A:705:TYR:CB	1:A:758:LEU:HB2	2.51	0.40
1:A:148:ASN:HA	1:A:151:ILE:HD12	2.03	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	757/768 (99%)	652 (86%)	88 (12%)	17 (2%)	6 37

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	258	HIS
1	A	595	GLU
1	A	219	ARG
1	A	719	VAL
1	A	93	GLN
1	A	299	SER
1	A	420	GLU
1	A	520	LYS
1	A	626	GLU
1	A	672	ASN
1	A	131	VAL
1	A	376	SER
1	A	372	GLU
1	A	549	PRO
1	A	706	ARG
1	A	41	SER

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	675/679 (99%)	570 (84%)	105 (16%)	2 16

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	GLU
1	A	16	ARG
1	A	21	VAL

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Mol	Chain	Res	Type
1	A	22	GLU
1	A	27	SER
1	A	30	VAL
1	A	31	PHE
1	A	32	LYS
1	A	43	THR
1	A	64	GLU
1	A	66	LEU
1	A	67	THR
1	A	68	VAL
1	A	101	ASP
1	A	102	ILE
1	A	106	ASN
1	A	108	THR
1	A	113	VAL
1	A	127	TYR
1	A	128	THR
1	A	129	THR
1	A	133	LEU
1	A	138	ASN
1	A	149	GLU
1	A	153	ARG
1	A	161	THR
1	A	178	LEU
1	A	185	GLN
1	A	189	VAL
1	A	190	SER
1	A	197	LYS
1	A	211	SER
1	A	212	LYS
1	A	215	ASN
1	A	220	ILE
1	A	231	LEU
1	A	238	LYS
1	A	241	ARG
1	A	242	ASN
1	A	245	SER
1	A	247	ARG
1	A	256	ILE
1	A	257	SER
1	A	268	VAL
1	A	300	THR

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Mol	Chain	Res	Type
1	A	321	THR
1	A	349	ILE
1	A	354	SER
1	A	362	LEU
1	A	367	LEU
1	A	368	ILE
1	A	371	GLN
1	A	372	GLU
1	A	375	LEU
1	A	383	ASP
1	A	398	LEU
1	A	412	THR
1	A	417	THR
1	A	418	LYS
1	A	420	GLU
1	A	426	ASN
1	A	430	VAL
1	A	431	LEU
1	A	445	LEU
1	A	448	ILE
1	A	454	ARG
1	A	462	LYS
1	A	471	PHE
1	A	489	THR
1	A	496	ASN
1	A	514	ILE
1	A	521	TYR
1	A	522	THR
1	A	524	ASN
1	A	534	LYS
1	A	536	LYS
1	A	539	LEU
1	A	552	THR
1	A	556	PHE
1	A	566	GLU
1	A	578	ASN
1	A	587	ILE
1	A	599	LEU
1	A	606	ARG
1	A	609	LEU
1	A	616	SER
1	A	624	LEU

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Mol	Chain	Res	Type
1	A	630	ILE
1	A	649	LEU
1	A	652	LEU
1	A	653	MET
1	A	655	LEU
1	A	668	LYS
1	A	692	ILE
1	A	698	LEU
1	A	699	ARG
1	A	701	LEU
1	A	706	ARG
1	A	708	THR
1	A	736	VAL
1	A	758	LEU
1	A	761	GLU
1	A	767	THR
1	A	768	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	59	GLN
1	A	109	ASN
1	A	138	ASN
1	A	177	ASN
1	A	215	ASN
1	A	258	HIS
1	A	426	ASN
1	A	496	ASN
1	A	524	ASN
1	A	578	ASN
1	A	622	GLN
1	A	657	ASN
1	A	700	GLN
1	A	732	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	SEP	A	19	1	8,9,10	1.03	1 (12%)	8,12,14	2.37	1 (12%)

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
1	SEP	A	19	1	-	2/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	SEP	P-OG	-2.39	1.52	1.60

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	19	SEP	OG-CB-CA	6.06	114.04	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	SEP	N-CA-CB-OG
1	A	19	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	19	SEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	ADP	A	801	4	24,29,29	0.67	0	29,45,45	0.75	1 (3%)
4	VO4	A	803	3,2	1,4,4	1.16	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
2	ADP	A	801	4	-	7/12/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	ADP	C5-C6-N6	2.32	123.89	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O3B
2	A	801	ADP	C5'-O5'-PA-O2A
2	A	801	ADP	C5'-O5'-PA-O3A
2	A	801	ADP	C4'-C5'-O5'-PA
2	A	801	ADP	PA-O3A-PB-O2B
2	A	801	ADP	C5'-O5'-PA-O1A
2	A	801	ADP	PB-O3A-PA-O2A

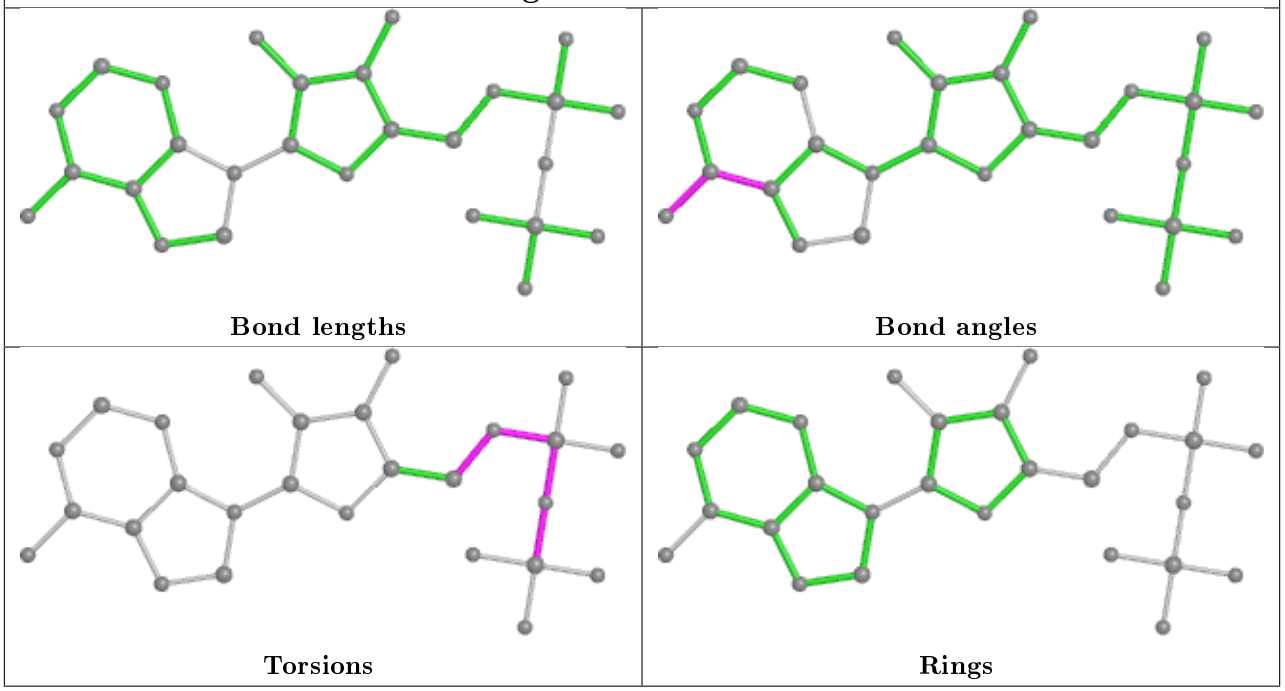
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	VO4	4	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.

Ligand ADP A 801



5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	760/768 (98%)	0.14	28 (3%) 41 37	105, 148, 194, 233	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	761	GLU	4.3
1	A	181	VAL	3.4
1	A	377	ASP	3.3
1	A	760	GLN	3.3
1	A	549	PRO	3.3
1	A	744	LEU	3.2
1	A	26	LYS	3.1
1	A	458	GLU	3.1
1	A	29	SER	3.0
1	A	369	GLU	3.0
1	A	183	LYS	3.0
1	A	283	ASN	2.8
1	A	27	SER	2.7
1	A	632	LYS	2.7
1	A	515	SER	2.7
1	A	161	THR	2.6
1	A	159	ASP	2.5
1	A	264	TYR	2.4
1	A	467	MET	2.4
1	A	215	ASN	2.4
1	A	628	GLN	2.3
1	A	729	VAL	2.2
1	A	565	LYS	2.2
1	A	730	GLU	2.2
1	A	93	GLN	2.1
1	A	550	GLY	2.1
1	A	728	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	568	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	A	19	10/11	0.90	0.15	162,164,174,174	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

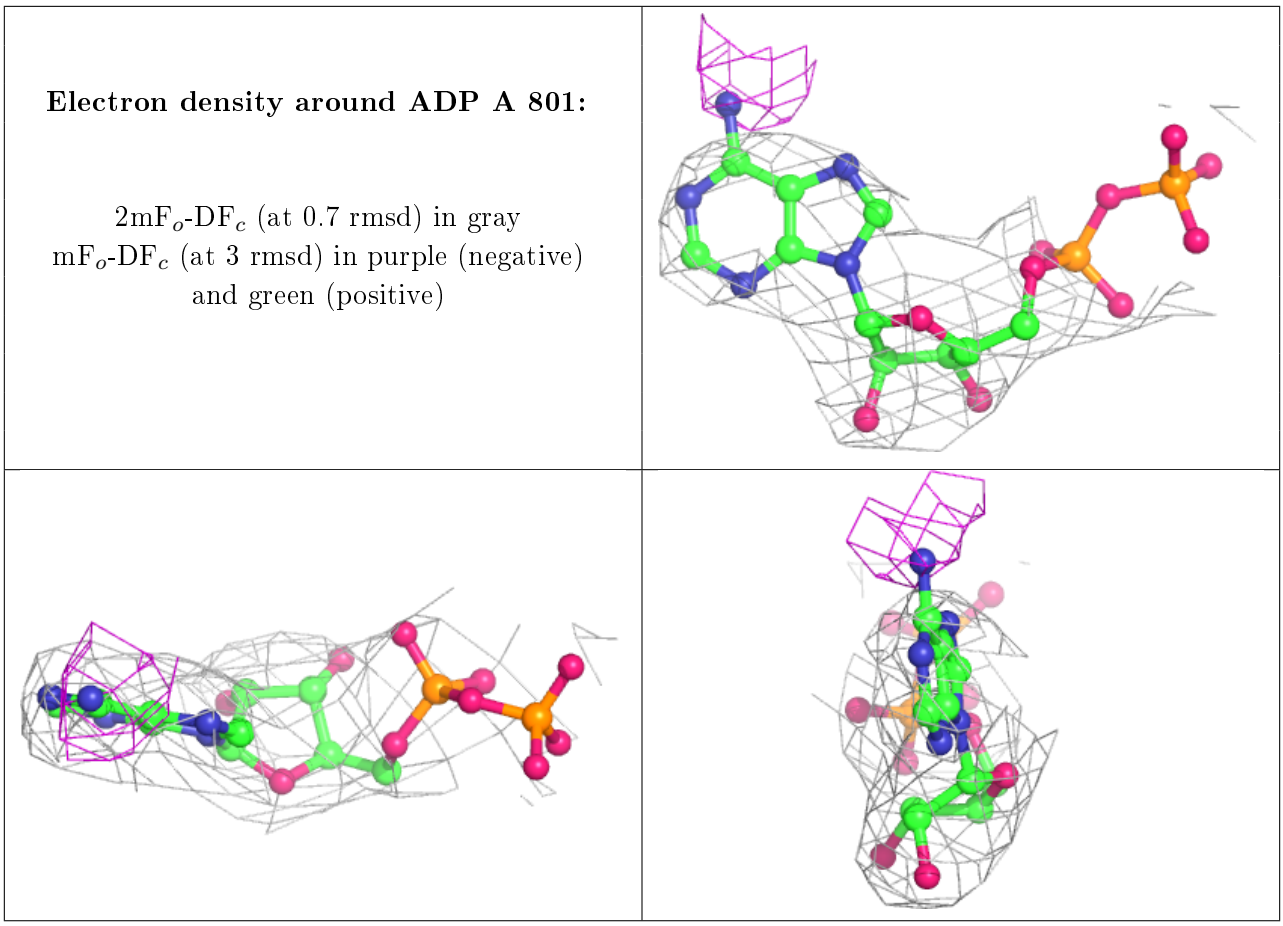
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	801	27/27	0.95	0.20	126,142,145,147	0
3	MG	A	802	1/1	0.98	0.15	109,109,109,109	0
4	VO4	A	803	5/5	0.99	0.20	144,144,145,145	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 801:

$2mF_o$-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.