Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2020 – 02:17 PM GMT

PDB ID	:	6YCX
Title	:	Plasmodium falciparum Myosin A full-length, pre-powerstroke state
Authors	:	Moussaoui, D.; Robblee, J.P.; Auguin, D.; Krementsova, E.B.; Robert-Paganin, J.; Trybus, K.M.; Houdusse, A.
Deposited on	:	2020-03-19
Resolution	:	3.99 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:

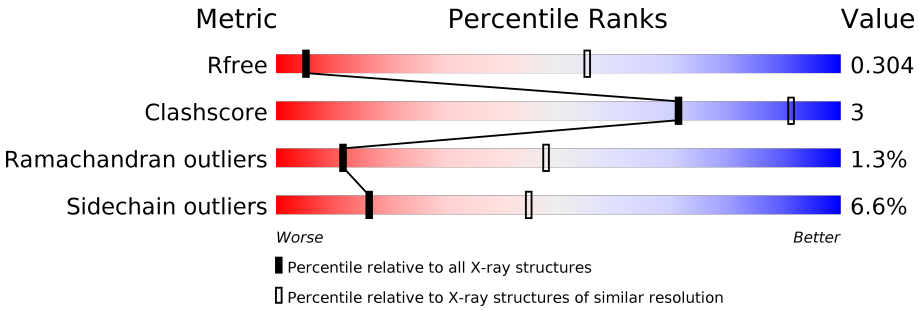
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 3.99 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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%

Mol	Chain	Length	Quality of chain
1	A	818	84% 14% •
1	B	818	85% 14% •
2	D	204	58% 7% 35%
2	H	204	52% 12% • 35%
3	F	134	81% 16% • •
4	G	134	69% 23% • 7%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	VO4	A	902	-	-	X	-
6	VO4	B	902	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17452 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
1	A	814	Total	C	N	O	P	S	0	11	0
			6541	4157	1110	1236	1	37			
1	B	817	Total	C	N	O	P	S	0	11	0
			6561	4169	1113	1241	1	37			

- Molecule 2 is a protein called Myosin A tail domain interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	133	Total	C	N	O	S	0	0	0
			1066	670	169	222	5			
2	H	133	Total	C	N	O	S	0	1	0
			1077	676	173	223	5			

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	133	Total	C	N	O	S	0	1	0
			1102	701	180	215	6			

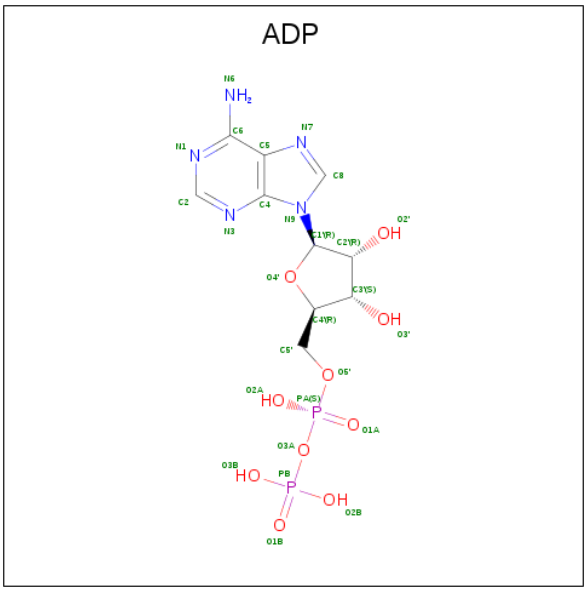
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	119	THR	SER	conflict	UNP A0A2I0BQX1

- Molecule 4 is a protein called Uncharacterized protein.

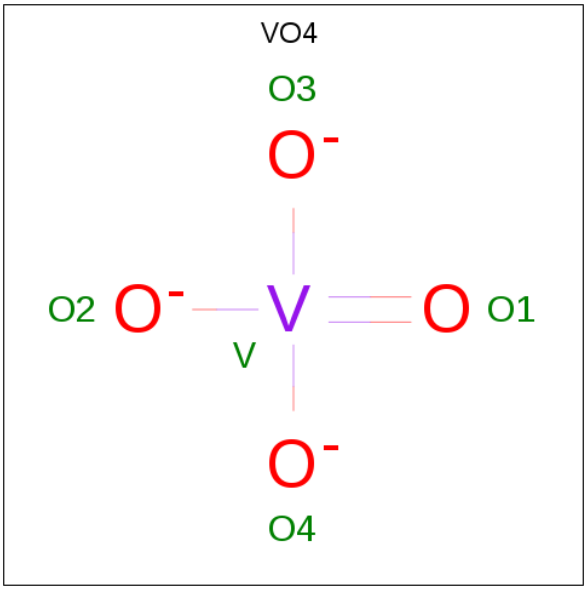
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	125	Total	C	N	O	S	0	1	0
			1039	665	167	201	6			

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



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

- Molecule 6 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

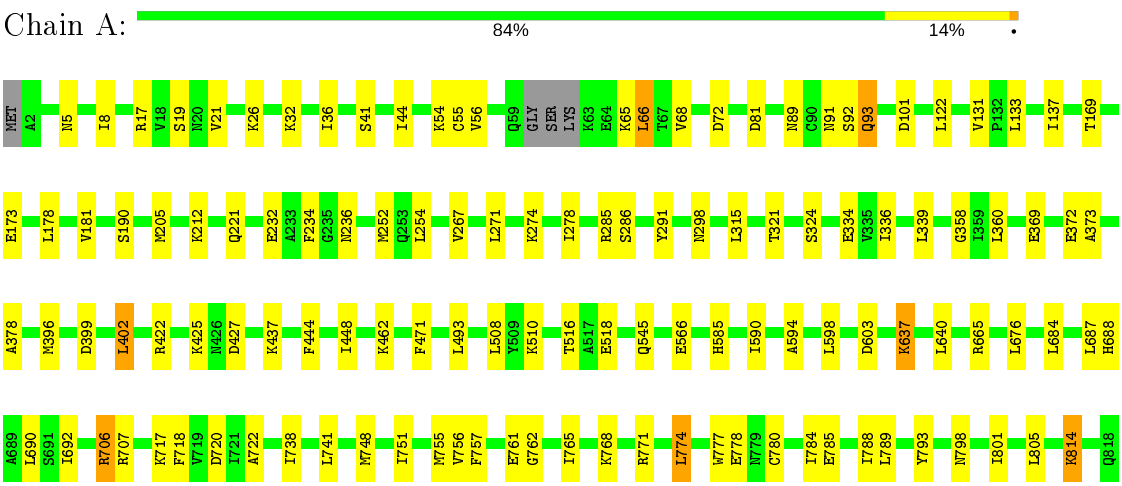
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	A	1	Total Mg 1 1	0	0

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. 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. 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.

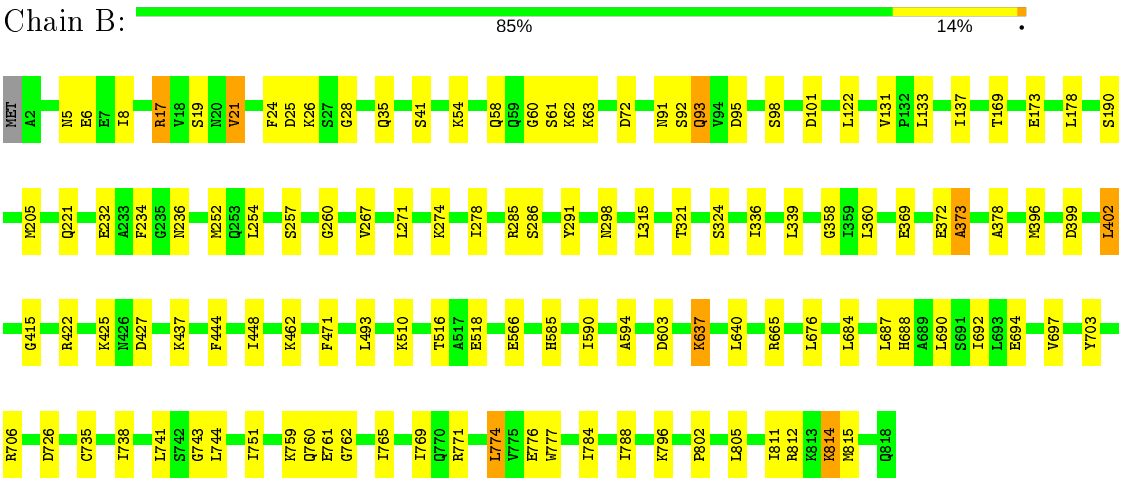
- Molecule 1: Myosin-A

Chain A:



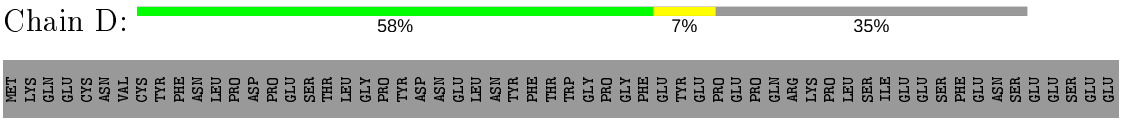
- Molecule 1: Myosin-A

Chain B:



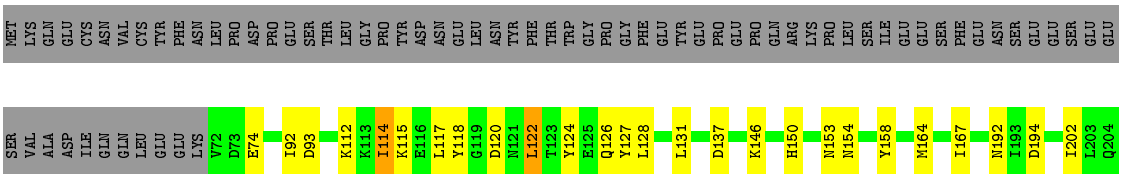
- Molecule 2: Myosin A tail domain interacting protein

Chain D:



- Molecule 2: Myosin A tail domain interacting protein

Chain H:

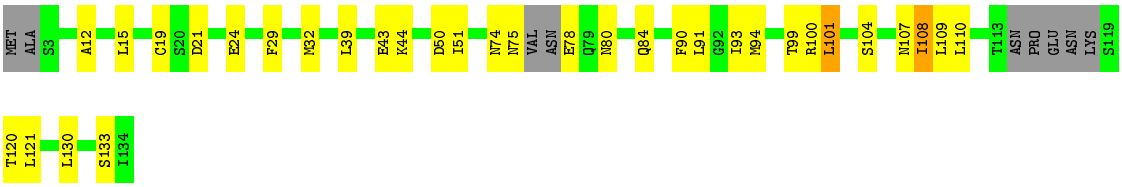


- Molecule 3: Uncharacterized protein

Chain F:

- Molecule 4: Uncharacterized protein

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	168.24Å 287.43Å 78.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 3.99 48.40 – 3.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.40-3.99) 99.6 (48.40-3.99)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 4.00Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.237 , 0.273 0.266 , 0.304	Depositor DCC
R_{free} test set	1663 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	154.1	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 139.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	17452	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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	0.41	0/6642	0.63	0/8952
1	B	0.39	0/6663	0.62	0/8981
2	D	0.39	0/1083	0.60	0/1461
2	H	0.39	0/1094	0.59	0/1475
3	F	0.43	0/1122	0.64	0/1514
4	G	0.43	0/1056	0.65	0/1420
All	All	0.40	0/17660	0.62	0/23803

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	6541	0	6628	45	0
1	B	6561	0	6654	41	0
2	D	1066	0	1018	4	0
2	H	1077	0	1030	10	0
3	F	1102	0	1080	11	0
4	G	1039	0	1021	17	0
5	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	27	0	12	0	0
6	A	5	0	0	4	0
6	B	5	0	0	4	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	17452	0	17455	122	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 (122) 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)
4:G:39:LEU:HB2	4:G:44:LYS:HG3	1.74	0.68
1:A:93:GLN:HA	1:B:93:GLN:HA	1.74	0.67
1:B:796:LYS:HB3	2:H:150:HIS:HE1	1.60	0.65
1:B:788:ILE:HG21	4:G:108:ILE:HG22	1.78	0.65
6:B:902:VO4:O2	6:B:902:VO4:V	1.56	0.63
6:A:902:VO4:V	6:A:902:VO4:O1	1.56	0.61
6:A:902:VO4:O4	6:A:902:VO4:V	1.57	0.61
6:B:902:VO4:V	6:B:902:VO4:O4	1.56	0.61
6:A:902:VO4:O2	6:A:902:VO4:V	1.57	0.61
6:B:902:VO4:V	6:B:902:VO4:O3	1.56	0.61
3:F:114:ASN:HB2	3:F:121:LEU:HD13	1.83	0.61
6:B:902:VO4:V	6:B:902:VO4:O1	1.56	0.60
2:H:128:LEU:HA	2:H:131:LEU:HD12	1.83	0.60
1:A:41:SER:HB3	1:A:44:ILE:HD12	1.84	0.60
6:A:902:VO4:V	6:A:902:VO4:O3	1.58	0.57
4:G:75:ASN:HA	4:G:80:ASN:HB2	1.86	0.57
3:F:84[B]:GLN:HE21	3:F:120:THR:HG23	1.71	0.56
1:A:793:TYR:HB3	3:F:15:LEU:HD22	1.88	0.56
1:B:17:ARG:HH12	1:B:21:VAL:HG22	1.71	0.54
1:A:798:ASN:HA	1:A:801:ILE:HD12	1.90	0.53
2:D:164:MET:HA	2:D:167:ILE:HD12	1.90	0.53
1:A:777:TRP:HA	1:A:780:CYS:HB3	1.91	0.53
1:A:508:LEU:HD21	1:A:755:MET:HE1	1.91	0.53
1:A:718:PHE:HE1	3:F:93:ILE:HG23	1.74	0.53
2:H:158:TYR:HB3	2:H:192:ASN:HB3	1.90	0.53
1:B:762:GLY:HA2	1:B:765:ILE:HD12	1.91	0.53
1:B:372:GLU:HB2	1:B:378:ALA:HB3	1.92	0.52
1:A:785:GLU:HA	3:F:101:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HE2	3:F:41:ASN:HD21	1.75	0.51
1:A:372:GLU:HB2	1:A:378:ALA:HB3	1.92	0.51
1:B:585:HIS:CD2	1:B:590:ILE:HD12	2.45	0.51
1:B:687:LEU:HA	1:B:692:ILE:HD12	1.92	0.51
1:A:585:HIS:CD2	1:A:590:ILE:HD12	2.45	0.51
4:G:91:LEU:HD21	4:G:109:LEU:HD11	1.93	0.51
4:G:90:PHE:HA	4:G:93:ILE:HD12	1.93	0.51
2:H:92:ILE:HD12	2:H:120:ASP:HA	1.93	0.51
4:G:101:LEU:HD23	4:G:104:SER:HB2	1.93	0.51
3:F:70:PHE:HB3	3:F:73:ILE:HD12	1.93	0.51
1:A:788:ILE:HG13	3:F:109:LEU:HB2	1.92	0.50
1:A:687:LEU:HA	1:A:692:ILE:HD12	1.93	0.50
1:B:133:LEU:HD23	1:B:665:ARG:HG3	1.94	0.50
1:B:777:TRP:HZ3	4:G:93:ILE:HG21	1.77	0.49
1:A:122:LEU:HA	1:A:676:LEU:HD22	1.94	0.49
1:B:122:LEU:HA	1:B:676:LEU:HD22	1.94	0.49
2:H:164:MET:HA	2:H:167:ILE:HD12	1.95	0.49
2:H:124:TYR:HA	2:H:127:TYR:HB3	1.94	0.49
1:B:637:LYS:HA	1:B:640:LEU:HD12	1.95	0.49
1:A:751:ILE:HD12	1:A:756:VAL:HG22	1.94	0.49
4:G:107:ASN:HA	4:G:110:LEU:HD12	1.95	0.48
1:A:637:LYS:HA	1:A:640:LEU:HD12	1.95	0.48
1:B:252:MET:HG2	1:B:267:VAL:HG22	1.96	0.48
1:A:36:ILE:HD11	1:A:68:VAL:HG11	1.95	0.47
1:B:54:LYS:HB3	1:B:72:ASP:HB3	1.97	0.47
1:A:5:ASN:HA	1:A:8:ILE:HD12	1.96	0.47
1:A:684:LEU:HA	1:A:687:LEU:HD12	1.96	0.47
1:A:133:LEU:HD23	1:A:665:ARG:HG3	1.96	0.47
1:B:95:ASP:HB3	1:B:98:SER:HB2	1.96	0.47
1:B:684:LEU:HA	1:B:687:LEU:HD12	1.96	0.47
1:A:278:ILE:HG13	1:A:437:LYS:HE2	1.97	0.47
1:A:54:LYS:HB3	1:A:72:ASP:HB3	1.97	0.47
1:B:5:ASN:HA	1:B:8:ILE:HD12	1.95	0.47
4:G:12:ALA:HA	4:G:15:LEU:HD12	1.97	0.47
1:A:252:MET:HG2	1:A:267:VAL:HG22	1.97	0.46
1:A:373:ALA:HB2	1:A:422:ARG:HB2	1.97	0.46
2:H:112:LYS:HG2	2:H:115:LYS:HD2	1.96	0.46
1:B:788:ILE:HG13	4:G:108:ILE:HB	1.96	0.46
1:B:802:PRO:HA	1:B:805:LEU:HD12	1.98	0.46
1:A:66:LEU:O	1:A:81:ASP:HA	2.16	0.46
1:B:278:ILE:HG13	1:B:437:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:LYS:HG2	1:B:516:THR:HA	1.98	0.46
1:B:771:ARG:HA	1:B:774:LEU:HB3	1.99	0.45
1:A:510:LYS:HG2	1:A:516:THR:HA	1.98	0.45
1:B:373:ALA:HB2	1:B:422:ARG:HB2	1.97	0.45
1:B:777:TRP:CZ3	4:G:93:ILE:HG21	2.52	0.45
1:A:55:CYS:HB3	1:A:68:VAL:HB	1.98	0.45
3:F:114:ASN:HD21	3:F:118:LYS:H	1.66	0.44
4:G:39:LEU:HB3	4:G:43:GLU:HB3	1.99	0.44
1:B:784:ILE:HG23	4:G:130:LEU:HD11	1.99	0.43
2:H:114:ILE:HA	2:H:117:LEU:HD12	1.99	0.43
1:A:181:VAL:HG21	1:A:707:ARG:NH1	2.34	0.43
1:B:285:ARG:HG2	1:B:291:TYR:CZ	2.53	0.43
1:B:358:GLY:HA3	1:B:396:MET:HG3	2.01	0.43
2:D:128:LEU:HA	2:D:131:LEU:HD12	1.99	0.43
1:A:232:GLU:O	1:A:236:ASN:HB2	2.19	0.43
1:A:358:GLY:HA3	1:A:396:MET:HG3	2.01	0.43
1:B:703:TYR:HA	1:B:759:LYS:HA	2.00	0.43
4:G:39:LEU:H	4:G:44:LYS:HE3	1.83	0.43
1:A:285:ARG:HG2	1:A:291:TYR:CZ	2.54	0.43
1:A:706:ARG:HB2	1:A:757:PHE:CD2	2.54	0.43
1:A:774:LEU:O	1:A:778:GLU:HB2	2.18	0.43
1:B:232:GLU:O	1:B:236:ASN:HB2	2.19	0.43
1:B:814:LYS:HD2	2:H:202:ILE:HA	2.01	0.42
4:G:84:GLN:HB3	4:G:120:THR:HB	2.00	0.42
1:B:399:ASP:HB3	1:B:402:LEU:HB2	2.00	0.42
1:A:286:SER:HB3	1:A:291:TYR:HE2	1.84	0.42
1:A:399:ASP:HB3	1:A:402:LEU:HB2	2.00	0.42
1:A:762:GLY:HA2	1:A:765:ILE:HD12	2.00	0.42
1:B:234:PHE:HB3	1:B:444:PHE:CD1	2.55	0.42
1:B:665:ARG:HE	1:B:690:LEU:HB3	1.85	0.42
1:A:369:GLU:HG3	1:A:425:LYS:HB2	2.02	0.41
1:A:234:PHE:HB3	1:A:444:PHE:CD1	2.55	0.41
4:G:29:PHE:HA	4:G:32:MET:HG2	2.01	0.41
1:A:56:VAL:O	1:A:68:VAL:HA	2.20	0.41
1:B:286:SER:HB3	1:B:291:TYR:HE2	1.85	0.41
1:B:694:GLU:O	1:B:697:VAL:HG22	2.19	0.41
1:B:735:CYS:HA	1:B:738:ILE:HD12	2.02	0.41
2:H:122:LEU:HB2	2:H:126:GLN:HB2	2.01	0.41
1:A:336:ILE:HA	1:A:339:LEU:HD12	2.02	0.41
1:A:665:ARG:HE	1:A:690:LEU:HB3	1.85	0.41
1:B:369:GLU:HG3	1:B:425:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:HA	1:B:339:LEU:HD12	2.02	0.41
2:D:98:ASN:HA	2:D:101:LYS:HD3	2.03	0.41
1:A:545[A]:GLN:HB3	1:A:598:LEU:HD21	2.03	0.41
1:B:811:ILE:O	1:B:815:MET:HG2	2.21	0.41
3:F:95:LYS:HA	3:F:99:THR:HG22	2.03	0.41
3:F:130:LEU:HA	3:F:133:SER:HB3	2.03	0.40
4:G:104:SER:HA	4:G:107:ASN:HD22	1.85	0.40
1:A:21:VAL:HA	1:A:89:ASN:HD21	1.86	0.40
1:A:814:LYS:HD2	2:D:202:ILE:HA	2.02	0.40
1:A:315:LEU:HD12	1:A:360:LEU:HA	2.03	0.40
1:B:257:SER:HB3	1:B:260:GLY:O	2.22	0.40
1:B:315:LEU:HD12	1:B:360:LEU:HA	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	820/818 (100%)	757 (92%)	56 (7%)	7 (1%)	17 55
1	B	825/818 (101%)	759 (92%)	52 (6%)	14 (2%)	9 43
2	D	131/204 (64%)	122 (93%)	8 (6%)	1 (1%)	19 58
2	H	132/204 (65%)	120 (91%)	12 (9%)	0	100 100
3	F	132/134 (98%)	116 (88%)	13 (10%)	3 (2%)	6 37
4	G	120/134 (90%)	109 (91%)	9 (8%)	2 (2%)	9 43
All	All	2160/2312 (93%)	1983 (92%)	150 (7%)	27 (1%)	12 48

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	751	ILE

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Mol	Chain	Res	Type
3	F	3	SER
1	A	32	LYS
1	A	271	LEU
1	A	321	THR
1	A	603	ASP
1	B	62	LYS
1	B	271	LEU
1	B	321	THR
1	B	603	ASP
1	B	726	ASP
3	F	64	TYR
3	F	77	ASN
1	A	594	ALA
1	A	722	ALA
1	B	28	GLY
1	B	61	SER
1	B	594	ALA
2	D	174	ALA
4	G	101	LEU
1	B	373	ALA
4	G	74	ASN
1	B	60	GLY
1	A	131	VAL
1	B	131	VAL
1	B	743	GLY
1	B	415	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	732/725 (101%)	688 (94%)	44 (6%)	19 47
1	B	735/725 (101%)	690 (94%)	45 (6%)	18 47
2	D	119/186 (64%)	112 (94%)	7 (6%)	19 48
2	H	120/186 (64%)	110 (92%)	10 (8%)	11 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	126/126 (100%)	115 (91%)	11 (9%)	10 35
4	G	119/126 (94%)	106 (89%)	13 (11%)	6 26
All	All	1951/2074 (94%)	1821 (93%)	130 (7%)	16 44

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	26	LYS
1	A	65	LYS
1	A	66	LEU
1	A	91	ASN
1	A	92	SER
1	A	93	GLN
1	A	101	ASP
1	A	137	ILE
1	A	169	THR
1	A	173	GLU
1	A	178	LEU
1	A	190	SER
1	A	205	MET
1	A	221	GLN
1	A	254	LEU
1	A	274	LYS
1	A	298	ASN
1	A	324	SER
1	A	334	GLU
1	A	402	LEU
1	A	427	ASP
1	A	448	ILE
1	A	462	LYS
1	A	471	PHE
1	A	493	LEU
1	A	518	GLU
1	A	566	GLU
1	A	637	LYS
1	A	688	HIS
1	A	706	ARG
1	A	717	LYS
1	A	720	ASP
1	A	738	ILE

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Mol	Chain	Res	Type
1	A	741	LEU
1	A	748	MET
1	A	761	GLU
1	A	768	LYS
1	A	771	ARG
1	A	774	LEU
1	A	784	ILE
1	A	789	LEU
1	A	805	LEU
1	A	814	LYS
1	B	6	GLU
1	B	17	ARG
1	B	21	VAL
1	B	24	PHE
1	B	25	ASP
1	B	26	LYS
1	B	35	GLN
1	B	41	SER
1	B	58	GLN
1	B	63	LYS
1	B	91	ASN
1	B	92	SER
1	B	93	GLN
1	B	101	ASP
1	B	137	ILE
1	B	169	THR
1	B	173	GLU
1	B	178	LEU
1	B	190	SER
1	B	205	MET
1	B	221	GLN
1	B	254	LEU
1	B	274	LYS
1	B	298	ASN
1	B	324	SER
1	B	402	LEU
1	B	427	ASP
1	B	448	ILE
1	B	462	LYS
1	B	471	PHE
1	B	493	LEU
1	B	518	GLU

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Mol	Chain	Res	Type
1	B	566	GLU
1	B	637	LYS
1	B	688	HIS
1	B	706	ARG
1	B	741	LEU
1	B	744	LEU
1	B	760	GLN
1	B	761	GLU
1	B	769	ILE
1	B	774	LEU
1	B	776	GLU
1	B	812	ARG
1	B	814	LYS
2	D	75	SER
2	D	118	TYR
2	D	120	ASP
2	D	122	LEU
2	D	133	ILE
2	D	153	ASN
2	D	162	SER
3	F	4	ASP
3	F	42	ASP
3	F	51	ILE
3	F	75	ASN
3	F	77	ASN
3	F	78	GLU
3	F	84[A]	GLN
3	F	84[B]	GLN
3	F	109	LEU
3	F	133	SER
3	F	134	ILE
4	G	19	CYS
4	G	21	ASP
4	G	24	GLU
4	G	50	ASP
4	G	51[A]	ILE
4	G	51[B]	ILE
4	G	78	GLU
4	G	94	MET
4	G	99	THR
4	G	100	ARG
4	G	108	ILE

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Mol	Chain	Res	Type
4	G	121	LEU
4	G	133	SER
2	H	74	GLU
2	H	93	ASP
2	H	114	ILE
2	H	118	TYR
2	H	122	LEU
2	H	137	ASP
2	H	146	LYS
2	H	153	ASN
2	H	154	ASN
2	H	194	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	371	GLN
1	A	672	ASN
1	B	35	GLN
1	B	49	ASN
1	B	91	ASN
1	B	107	HIS
1	B	371	GLN
1	B	800	ASN
2	D	94	ASN
3	F	33	ASN
3	F	68	GLN
3	F	75	ASN
3	F	77	ASN
3	F	89	ASN
3	F	114	ASN
4	G	52	ASN
4	G	107	ASN
2	H	150	HIS
2	H	154	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SEP	A	19	1	8,9,10	0.92	0	8,12,14	1.78	2 (25%)
1	SEP	B	19	1	8,9,10	0.89	0	8,12,14	2.99	2 (25%)

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	-	1/5/8/10	-
1	SEP	B	19	1	-	4/5/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	19	SEP	OG-CB-CA	7.84	115.77	108.14
1	A	19	SEP	O2P-P-OG	3.11	115.01	106.73
1	A	19	SEP	OG-CB-CA	3.04	111.10	108.14
1	B	19	SEP	O3P-P-OG	2.57	113.57	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	SEP	N-CA-CB-OG
1	B	19	SEP	N-CA-CB-OG
1	B	19	SEP	CB-OG-P-O1P
1	B	19	SEP	CA-CB-OG-P

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Mol	Chain	Res	Type	Atoms
1	B	19	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	B	901	7	24,29,29	0.73	0	29,45,45	0.91	2 (6%)
6	VO4	A	902	7	1,4,4	1.12	0	-		
5	ADP	A	901	7	24,29,29	0.61	0	29,45,45	0.72	1 (3%)
6	VO4	B	902	-	1,4,4	1.08	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
5	ADP	B	901	7	-	2/12/32/32	0/3/3/3
5	ADP	A	901	7	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	901	ADP	C5-C6-N6	2.34	123.91	120.35
5	B	901	ADP	C5-C6-N6	2.30	123.84	120.35
5	B	901	ADP	O3B-PB-O3A	2.19	111.97	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	ADP	PA-O3A-PB-O1B
5	B	901	ADP	C5'-O5'-PA-O1A

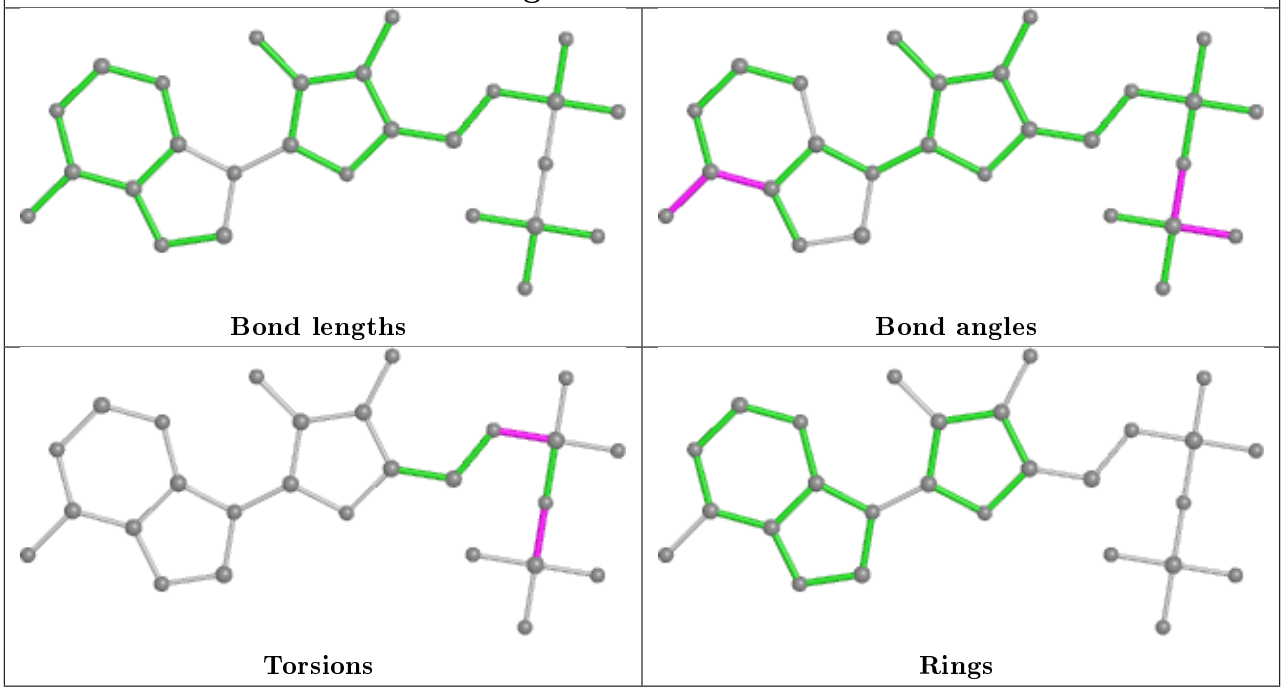
There are no ring outliers.

2 monomers are involved in 8 short contacts:

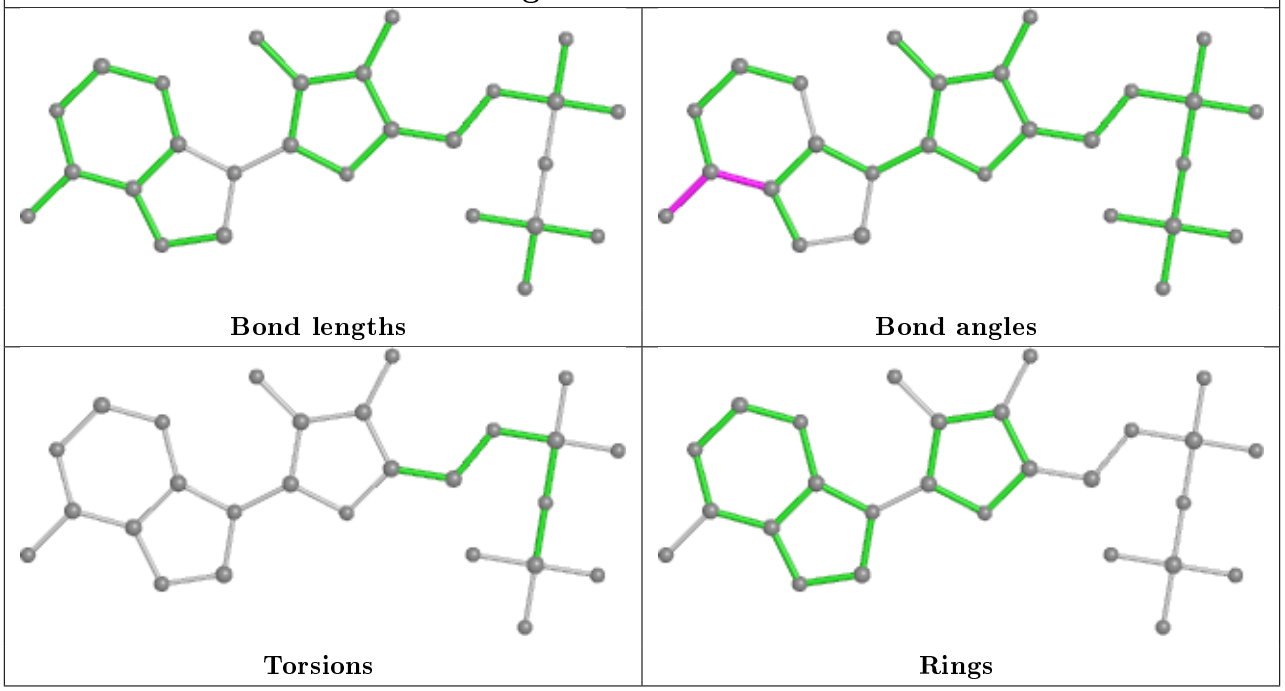
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	902	VO4	4	0
6	B	902	VO4	4	0

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 B 901



Ligand ADP A 901



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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

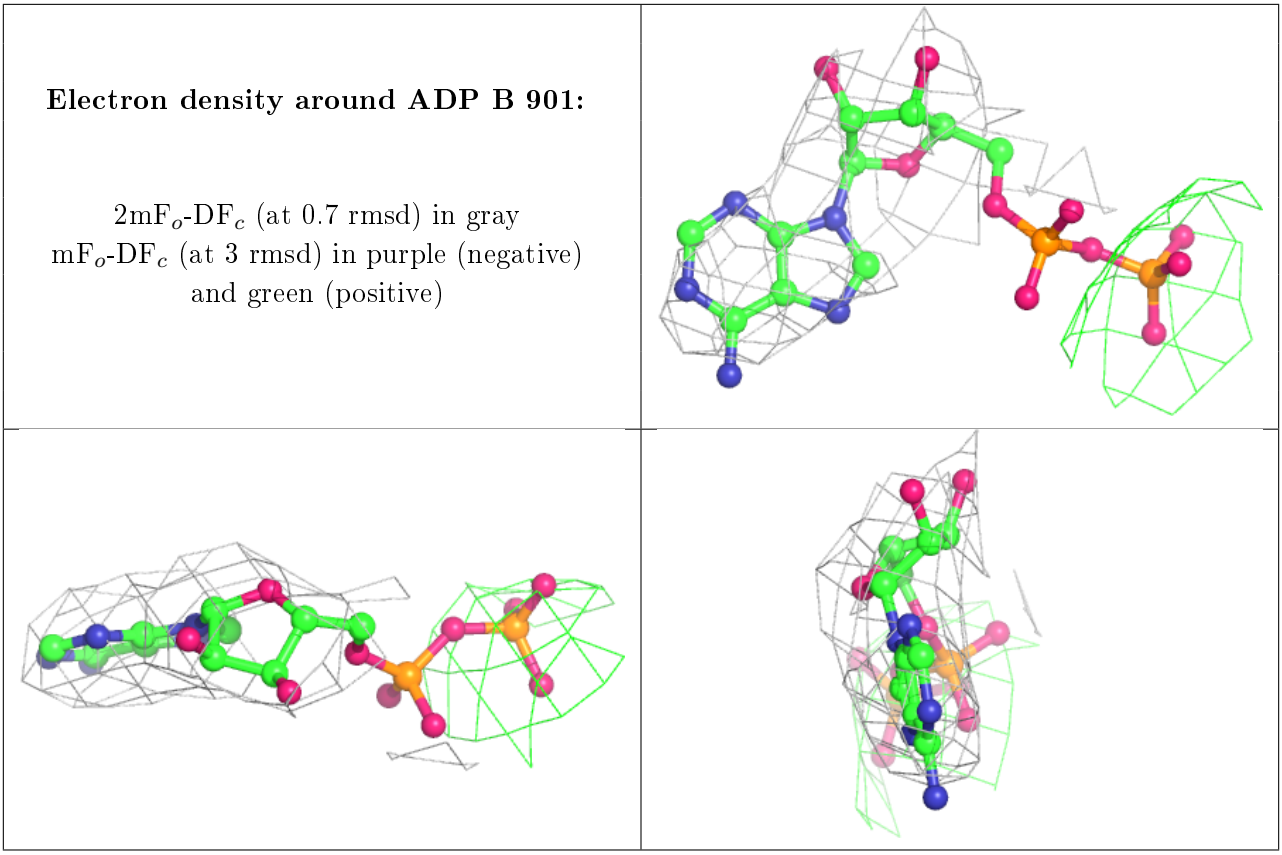
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

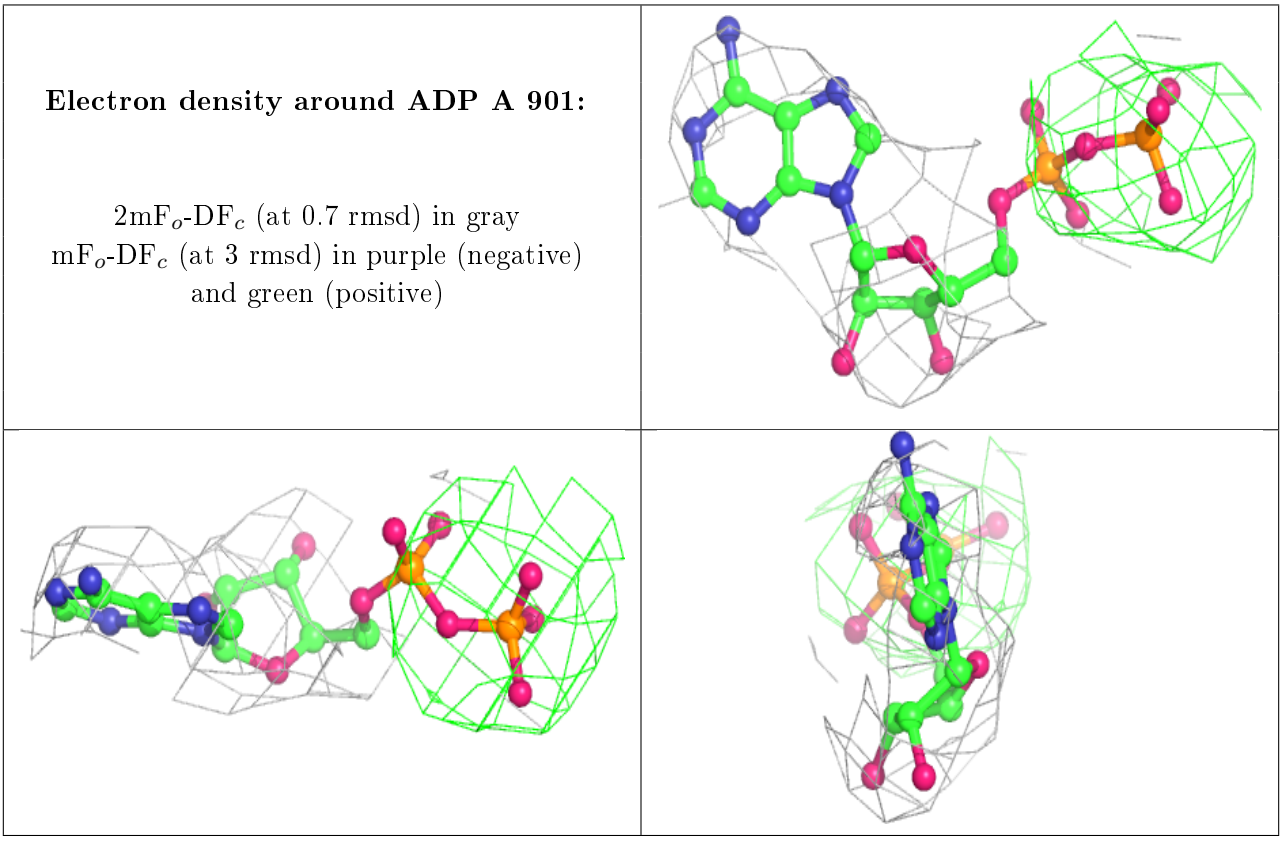
Electron density around ADP B 901:

$2mF_o$-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 901:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.