Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 10:19 am BST

PDB ID	:	7QDX
Title	:	bacterial IMPDH chimera
Authors	:	Labesse, G.; Gelin, M.; Munier-Lehmann, H.; Gedeon, A.; Haouz, A.
Deposited on	:	2021-11-30
Resolution	:	2.90 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:

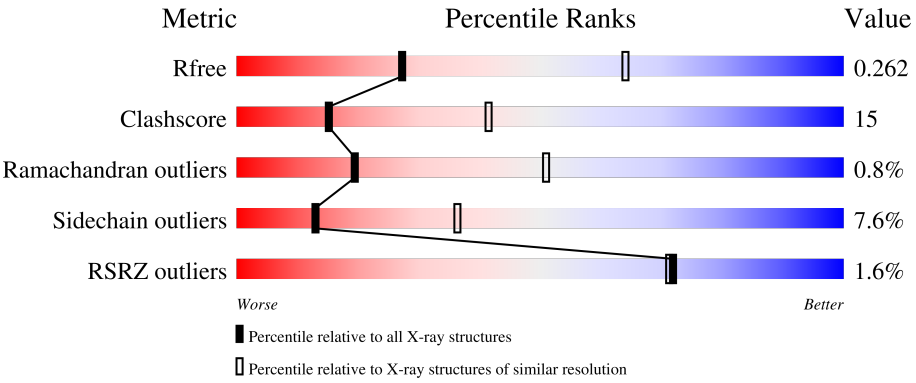
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	507	2% 51% 26% . 21%
1	B	507	% 55% 22% . 21%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6131 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			2973	1853	531	573	16			
1	B	403	Total	C	N	O	S	1	1	0
			2985	1861	536	572	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0ADG7
A	2	GLY	-	expression tag	UNP P0ADG7
A	3	SER	-	expression tag	UNP P0ADG7
A	4	SER	-	expression tag	UNP P0ADG7
A	5	HIS	-	expression tag	UNP P0ADG7
A	6	HIS	-	expression tag	UNP P0ADG7
A	7	HIS	-	expression tag	UNP P0ADG7
A	8	HIS	-	expression tag	UNP P0ADG7
A	9	HIS	-	expression tag	UNP P0ADG7
A	10	HIS	-	expression tag	UNP P0ADG7
A	11	SER	-	expression tag	UNP P0ADG7
A	12	SER	-	expression tag	UNP P0ADG7
A	13	GLY	-	expression tag	UNP P0ADG7
A	14	LEU	-	expression tag	UNP P0ADG7
A	15	VAL	-	expression tag	UNP P0ADG7
A	16	PRO	-	expression tag	UNP P0ADG7
A	17	ARG	-	expression tag	UNP P0ADG7
A	18	GLY	-	expression tag	UNP P0ADG7
A	19	SER	-	expression tag	UNP P0ADG7
A	20	HIS	-	expression tag	UNP P0ADG7
B	1	MET	-	initiating methionine	UNP P0ADG7
B	2	GLY	-	expression tag	UNP P0ADG7
B	3	SER	-	expression tag	UNP P0ADG7
B	4	SER	-	expression tag	UNP P0ADG7
B	5	HIS	-	expression tag	UNP P0ADG7

Continued on next page...

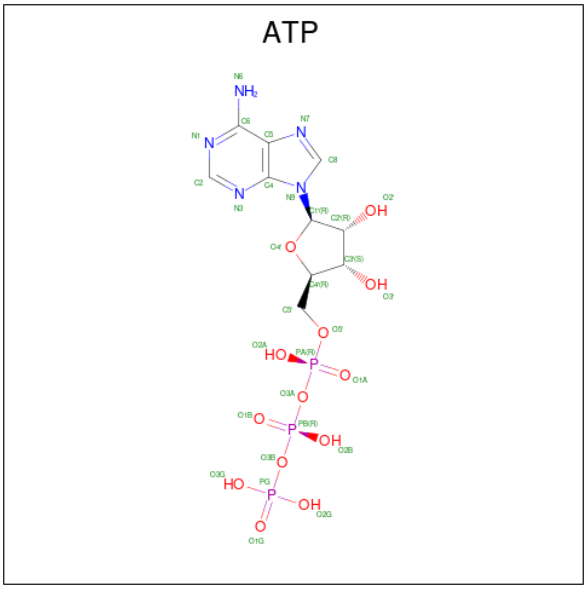
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP P0ADG7
B	7	HIS	-	expression tag	UNP P0ADG7
B	8	HIS	-	expression tag	UNP P0ADG7
B	9	HIS	-	expression tag	UNP P0ADG7
B	10	HIS	-	expression tag	UNP P0ADG7
B	11	SER	-	expression tag	UNP P0ADG7
B	12	SER	-	expression tag	UNP P0ADG7
B	13	GLY	-	expression tag	UNP P0ADG7
B	14	LEU	-	expression tag	UNP P0ADG7
B	15	VAL	-	expression tag	UNP P0ADG7
B	16	PRO	-	expression tag	UNP P0ADG7
B	17	ARG	-	expression tag	UNP P0ADG7
B	18	GLY	-	expression tag	UNP P0ADG7
B	19	SER	-	expression tag	UNP P0ADG7
B	20	HIS	-	expression tag	UNP P0ADG7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

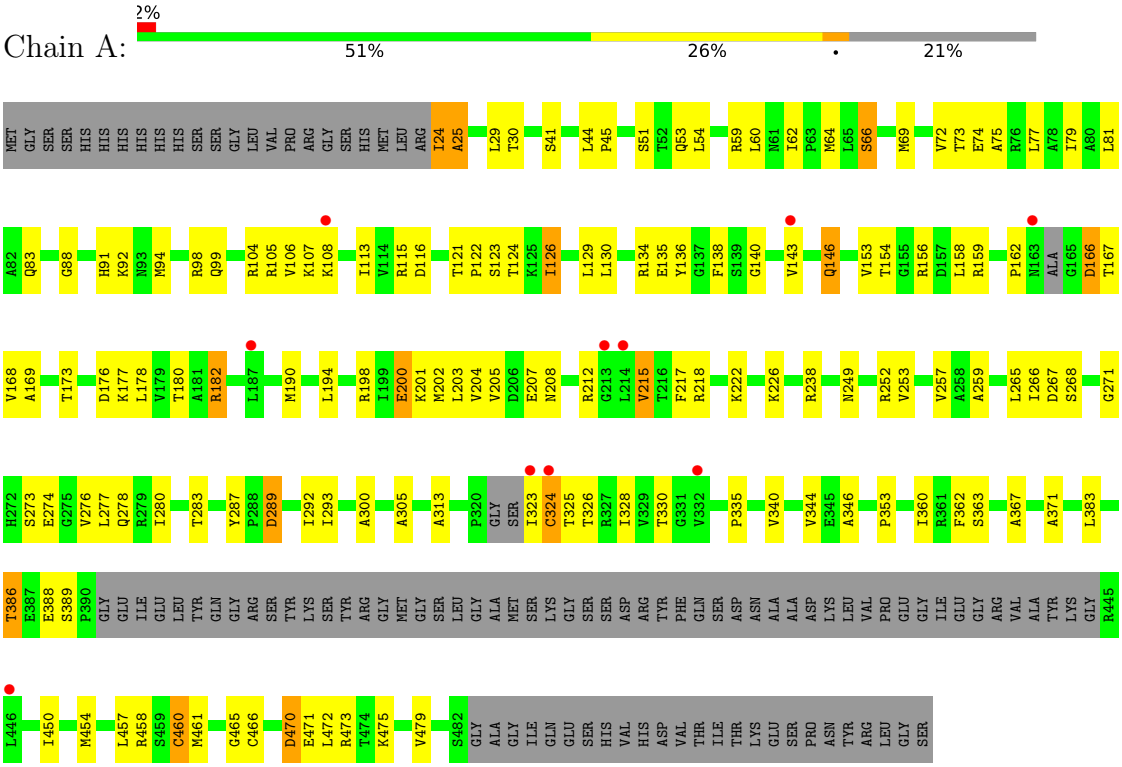
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	24	Total	O	0	0
			24	24		

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.

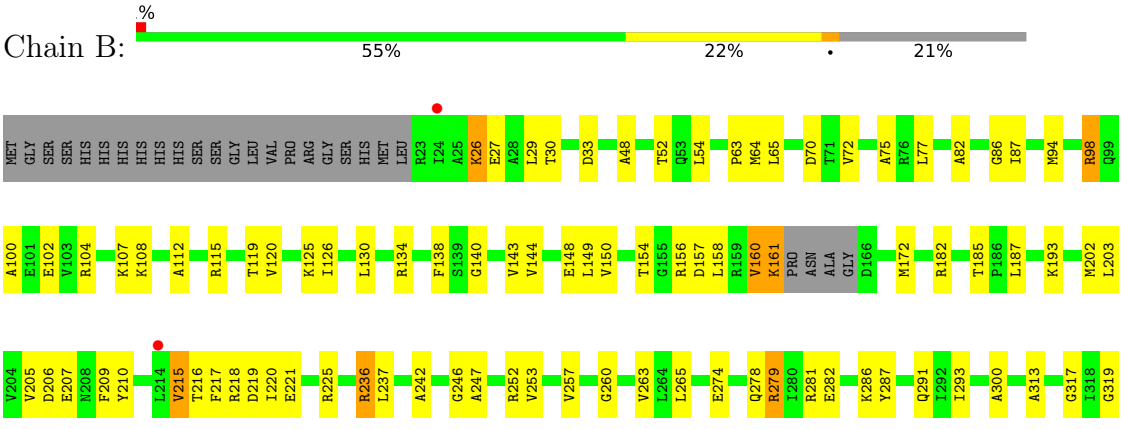
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

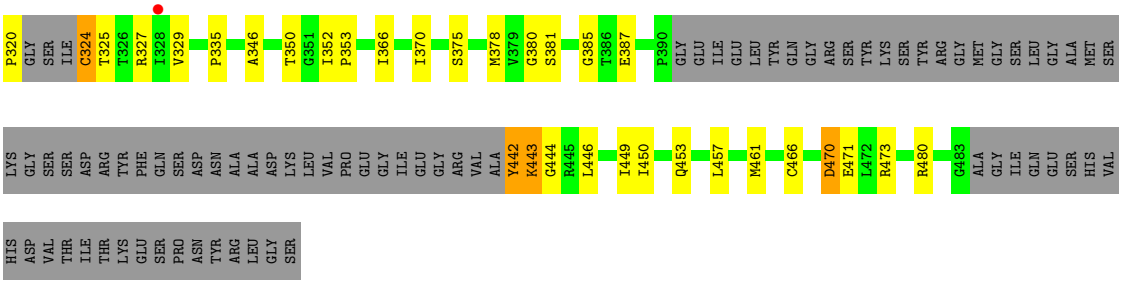
Chain A:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain B:




P320 GLY SER ILE C324 T325 T326 R327 I328 V329 P335 A346 T350 G351 I352 P353 I366 I370 S375 M378 V379 G380 S381 G385 T386 E387 P390 GLY GLU ILE GLU LEU TYR GLN GLY ARG SER TYR LYS SER TYR ARG GLY MET GLY SER LEU GLY ALA MET SER
LYS GLY SER SER ASP ARG TYR PHE GLN SER ASP ASN ALA ALA ASP LYS LEU VAL PRO GLU GLY ILE GLU GLY ARG VAL ALA Y442 K443 G444 R445 L446 I449 I450 Q453 L457 M461 C466 D470 E471 L472 R473 R480 G483 ALA GLY ILE GLN GLU SER HIS VAL
HIS ASP VAL THR ILE THR LYS GLU SER PRO ASN TYR ARG LEU GLY SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	109.27Å 109.27Å 176.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 2.90 47.09 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.05-2.90) 99.8 (47.09-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.201 , 0.267 0.197 , 0.262	Depositor DCC
R_{free} test set	1141 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	76.8	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6131	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: ATP, 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	0.46	0/3002	0.69	0/4055
1	B	0.50	0/3017	0.72	2/4071 (0.0%)
All	All	0.48	0/6019	0.70	2/8126 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	236[A]	ARG	CA-C-O	6.30	133.34	120.10
1	B	236[B]	ARG	CA-C-O	6.30	133.34	120.10

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	2973	0	3058	109	0
1	B	2985	0	3075	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	62	0	23	7	0
3	B	62	0	24	3	0
4	A	21	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	1	0
All	All	6131	0	6180	184	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 15.

All (184) 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:159:ARG:NH2	1:B:221:GLU:OE1	1.58	1.33
1:A:159:ARG:NH2	1:B:221:GLU:CD	1.92	1.21
1:A:159:ARG:NH2	1:B:221:GLU:OE2	1.89	1.05
1:A:124:THR:O	1:A:167:THR:OG1	1.73	1.04
1:A:126:ILE:HD12	1:A:158:LEU:CD2	1.95	0.96
1:A:123:SER:O	1:A:167:THR:OG1	1.83	0.96
1:A:126:ILE:HD12	1:A:158:LEU:HD22	1.54	0.87
1:A:94:MET:HG2	1:A:98:ARG:HE	1.43	0.81
1:A:273:SER:HB2	1:A:276:VAL:HG22	1.66	0.78
1:B:75:ALA:HB2	1:B:102:GLU:OE1	1.85	0.76
1:A:340:VAL:O	1:A:344:VAL:HG23	1.86	0.75
1:A:94:MET:HG2	1:A:98:ARG:NE	2.02	0.74
1:A:94:MET:CG	1:A:98:ARG:HE	2.04	0.71
1:A:121:THR:HG22	1:A:123:SER:H	1.56	0.70
1:A:182:ARG:H	1:A:182:ARG:CZ	2.05	0.70
1:B:29:LEU:HD22	1:B:33:ASP:HB3	1.74	0.70
1:A:104:ARG:O	1:A:108:LYS:HG3	1.92	0.69
1:A:30:THR:HG22	1:A:335:PRO:HB3	1.75	0.68
1:A:64:MET:HE1	1:A:450:ILE:HD12	1.76	0.68
1:A:323:ILE:HG22	1:A:325:THR:HG23	1.76	0.67
1:A:457:LEU:O	1:A:461:MET:HG3	1.95	0.67
1:A:44:LEU:HD12	1:A:45:PRO:HD2	1.77	0.67
1:A:129:LEU:HD23	1:A:158:LEU:HD21	1.76	0.67
1:A:218:ARG:NH2	3:A:603:ATP:O2A	2.27	0.67
1:A:51:SER:OG	1:A:59:ARG:NH2	2.25	0.66
1:A:182:ARG:NH1	4:A:702:HOH:O	2.28	0.66
1:A:293:ILE:HG12	1:A:313:ALA:HB3	1.78	0.65
1:A:53:GLN:NE2	1:A:59:ARG:HD2	2.12	0.64
1:A:249:ASN:O	1:A:253:VAL:HG23	1.98	0.64
1:A:94:MET:O	1:A:252:ARG:NH2	2.27	0.63
1:A:113:ILE:HD12	1:A:113:ILE:H	1.62	0.63
1:A:156:ARG:HG3	3:A:604:ATP:H5'1	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ALA:HB1	1:B:219:ASP:HB3	1.80	0.62
1:A:200:GLU:OE1	3:A:603:ATP:O1G	2.17	0.62
1:A:200:GLU:HB2	3:A:604:ATP:PA	2.40	0.62
1:A:129:LEU:HD22	1:A:168:VAL:HG22	1.82	0.62
1:A:66:SER:HB2	1:A:88:GLY:HA2	1.81	0.61
1:B:75:ALA:CB	1:B:102:GLU:OE1	2.48	0.61
1:A:135:GLU:N	1:A:135:GLU:OE1	2.34	0.61
1:B:108:LYS:HD2	1:B:236[B]:ARG:NH2	2.16	0.61
1:B:108:LYS:CD	1:B:236[B]:ARG:NH2	2.64	0.60
1:A:79:ILE:HG13	1:A:106:VAL:HG13	1.82	0.60
1:B:160:VAL:HG23	1:B:161:LYS:H	1.67	0.60
1:A:72:VAL:HG12	1:A:73:THR:OG1	2.02	0.59
1:A:94:MET:HE3	1:A:99:GLN:HB2	1.84	0.59
1:B:319:GLY:O	1:B:327:ARG:NH1	2.35	0.59
1:B:350:THR:HB	1:B:352:ILE:HG12	1.85	0.58
1:A:126:ILE:O	1:A:130:LEU:HG	2.03	0.58
1:A:54:LEU:HD13	1:A:60:LEU:HD11	1.84	0.58
1:A:176:ASP:OD1	1:A:177:LYS:HG2	2.04	0.58
1:B:457:LEU:O	1:B:461:MET:HG3	2.04	0.58
1:A:266:ILE:HD12	1:A:280:ILE:HG13	1.84	0.57
1:A:75:ALA:HB1	1:A:105:ARG:HD3	1.87	0.57
1:B:138:PHE:HB3	3:B:604:ATP:H5'1	1.85	0.57
1:A:200:GLU:CD	3:A:603:ATP:O1G	2.42	0.57
1:B:108:LYS:CD	1:B:236[B]:ARG:HH21	2.18	0.57
1:A:66:SER:HB3	1:A:73:THR:OG1	2.05	0.57
1:A:79:ILE:O	1:A:83:GLN:HG3	2.04	0.56
1:A:383:LEU:O	1:A:386:THR:OG1	2.23	0.56
1:B:216:THR:O	1:B:220:ILE:HG13	2.06	0.56
1:B:387:GLU:N	1:B:444:GLY:O	2.39	0.56
1:B:461:MET:HB3	1:B:466:CYS:O	2.06	0.55
1:B:246:GLY:H	1:B:279:ARG:HE	1.55	0.55
1:A:83:GLN:HB3	1:A:226:LYS:HE3	1.90	0.54
1:A:129:LEU:HD21	1:A:153:VAL:HG11	1.89	0.54
1:B:278:GLN:O	1:B:282:GLU:HG3	2.07	0.54
1:A:277:LEU:HD11	1:A:305:ALA:HB1	1.90	0.54
1:A:69:MET:HB2	1:A:72:VAL:HB	1.90	0.53
1:B:115:ARG:HD2	1:B:236[B]:ARG:NH1	2.23	0.53
1:A:64:MET:CE	1:A:450:ILE:HD12	2.38	0.53
1:B:442:TYR:O	1:B:442:TYR:HD1	1.91	0.53
1:B:150:VAL:HG13	4:B:719:HOH:O	2.08	0.53
1:A:324:CYS:O	1:A:328:ILE:HG12	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLU:HG3	1:B:210:TYR:CE1	2.43	0.53
1:B:100:ALA:O	1:B:104:ARG:HG3	2.09	0.52
1:B:156:ARG:HD2	3:B:603:ATP:H5'2	1.91	0.52
1:A:470:ASP:HA	1:A:473:ARG:HD3	1.92	0.52
1:B:108:LYS:HD3	1:B:236[B]:ARG:HH21	1.74	0.52
1:A:92:LYS:NZ	4:A:701:HOH:O	2.22	0.52
1:B:72:VAL:O	1:B:77:LEU:HD13	2.11	0.51
1:B:94:MET:O	1:B:252:ARG:NH2	2.43	0.51
1:A:461:MET:HB3	1:A:466:CYS:O	2.11	0.51
1:A:470:ASP:N	1:A:470:ASP:OD1	2.44	0.51
1:B:205:VAL:HG13	1:B:209:PHE:HA	1.92	0.51
1:A:54:LEU:O	1:A:353:PRO:HG2	2.11	0.50
1:A:74:GLU:OE2	1:A:91:HIS:NE2	2.36	0.50
1:A:167:THR:HG1	1:A:168:VAL:H	1.57	0.50
1:A:190:MET:SD	1:A:215:VAL:HG11	2.51	0.49
1:A:271:GLY:HA2	1:A:276:VAL:HG21	1.94	0.49
1:A:135:GLU:OE2	1:A:136:TYR:HD1	1.95	0.49
1:A:180:THR:HG22	1:A:203:LEU:HB2	1.94	0.49
1:A:274:GLU:O	1:A:278:GLN:HB2	2.13	0.49
1:B:70:ASP:N	1:B:70:ASP:OD1	2.45	0.49
1:A:466:CYS:HB3	1:A:471:GLU:HB3	1.95	0.49
1:B:202:MET:HB3	1:B:215:VAL:HG13	1.93	0.49
1:B:263:VAL:HA	1:B:291:GLN:O	2.13	0.49
1:A:276:VAL:HG23	1:A:277:LEU:H	1.76	0.49
1:B:119:THR:HB	1:B:144:VAL:HG22	1.94	0.48
1:B:126:ILE:O	1:B:130:LEU:HD13	2.13	0.48
1:A:162:PRO:HG2	1:A:166:ASP:OD1	2.13	0.48
1:B:247:ALA:H	1:B:279:ARG:NE	2.11	0.48
1:A:194:LEU:HD21	1:A:202:MET:HB2	1.96	0.48
1:B:470:ASP:N	1:B:470:ASP:OD1	2.47	0.48
1:B:98:ARG:O	1:B:102:GLU:HG2	2.15	0.47
1:B:443:LYS:HE3	1:B:444:GLY:N	2.29	0.47
1:A:371:ALA:HA	1:A:472:LEU:O	2.14	0.47
1:B:30:THR:HB	1:B:335:PRO:HB3	1.97	0.47
1:B:221:GLU:HB3	1:B:225:ARG:NH2	2.29	0.47
1:B:274:GLU:OE2	1:B:281:ARG:NH2	2.48	0.47
1:B:257:VAL:HG11	1:B:287:TYR:CE1	2.49	0.47
1:A:104:ARG:HG3	1:A:259:ALA:HB1	1.95	0.47
1:B:319:GLY:N	1:B:320:PRO:HD3	2.30	0.47
1:A:123:SER:C	1:A:167:THR:OG1	2.52	0.46
1:A:465:GLY:O	1:A:475:LYS:NZ	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HA	1:A:129:LEU:HB3	1.96	0.46
1:A:173:THR:HG21	3:A:604:ATP:N3	2.31	0.46
1:B:65:LEU:HB2	1:B:378:MET:HG3	1.97	0.46
1:A:124:THR:C	1:A:167:THR:HG1	2.01	0.46
1:A:326:THR:O	1:A:330:THR:OG1	2.16	0.46
1:B:82:ALA:HA	1:B:86:GLY:O	2.16	0.46
1:B:140:GLY:HA2	1:B:154:THR:HA	1.96	0.46
1:A:123:SER:O	1:A:167:THR:CB	2.62	0.46
1:B:65:LEU:HD23	1:B:87:ILE:HG22	1.98	0.46
1:A:62:ILE:HD12	1:A:64:MET:HE2	1.99	0.45
1:A:257:VAL:HG11	1:A:287:TYR:CE1	2.52	0.45
1:B:443:LYS:HE3	1:B:444:GLY:H	1.81	0.45
1:A:124:THR:C	1:A:167:THR:OG1	2.50	0.45
1:B:182:ARG:O	1:B:185:THR:HG23	2.17	0.45
1:B:29:LEU:O	1:B:335:PRO:HB2	2.16	0.45
1:A:454:MET:O	1:A:458:ARG:HG3	2.17	0.45
1:B:242:ALA:HA	1:B:265:LEU:HB3	1.98	0.44
1:A:218:ARG:O	1:A:222:LYS:HG2	2.17	0.44
1:B:253:VAL:O	1:B:257:VAL:HG23	2.18	0.44
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.82	0.44
1:A:265:LEU:HG	1:A:267:ASP:HB2	1.99	0.44
1:A:154:THR:OG1	3:A:604:ATP:H5'2	2.18	0.43
1:B:156:ARG:N	3:B:603:ATP:O2B	2.47	0.43
1:A:202:MET:HB3	1:A:215:VAL:HG13	1.99	0.43
1:B:54:LEU:O	1:B:353:PRO:HG2	2.18	0.43
1:B:366:ILE:O	1:B:370:ILE:HG13	2.18	0.43
1:A:283:THR:HG22	1:A:292:ILE:HD11	1.99	0.43
1:A:287:TYR:C	1:A:289:ASP:H	2.22	0.43
1:B:107:LYS:HG3	1:B:260:GLY:O	2.19	0.43
1:B:149:LEU:HD21	1:B:203:LEU:HD13	2.01	0.43
1:B:375:SER:HA	1:B:473:ARG:HD2	2.00	0.43
1:B:442:TYR:O	1:B:442:TYR:CD1	2.72	0.42
1:B:300:ALA:HB1	1:B:346:ALA:HB2	2.01	0.42
1:B:466:CYS:HA	1:B:471:GLU:HG2	2.01	0.42
1:B:107:LYS:HA	1:B:107:LYS:HD2	1.70	0.42
1:A:167:THR:HG23	1:A:169:ALA:H	1.84	0.42
1:B:319:GLY:HA2	1:B:324:CYS:SG	2.60	0.42
1:B:385:GLY:O	1:B:443:LYS:HA	2.19	0.42
1:B:446:LEU:O	1:B:450:ILE:HG12	2.19	0.42
1:A:167:THR:OG1	1:A:168:VAL:N	2.52	0.42
1:A:386:THR:O	1:A:389:SER:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLY:HA3	1:A:201:LYS:HE2	2.02	0.42
1:B:64:MET:HE1	1:B:450:ILE:HD12	2.02	0.42
1:B:449:ILE:O	1:B:453:GLN:HG2	2.20	0.41
1:B:286:LYS:HB3	1:B:286:LYS:HE2	1.94	0.41
1:B:325:THR:O	1:B:329:VAL:HG23	2.20	0.41
1:A:122:PRO:HD3	1:A:143:VAL:HG12	2.02	0.41
1:B:29:LEU:HD22	1:B:33:ASP:CB	2.47	0.41
1:B:480:ARG:HE	1:B:480:ARG:HB2	1.69	0.41
1:A:198:ARG:HD2	1:B:157:ASP:OD1	2.21	0.41
1:A:388:GLU:OE1	1:A:388:GLU:N	2.42	0.41
1:B:120:VAL:HG23	1:B:143:VAL:HG22	2.01	0.41
1:A:24:ILE:HG22	1:A:25:ALA:H	1.86	0.41
1:A:107:LYS:NZ	1:A:238:ARG:HA	2.35	0.41
1:A:153:VAL:HG21	1:A:168:VAL:HG13	2.03	0.41
1:A:198:ARG:NH1	1:B:157:ASP:OD1	2.45	0.41
1:A:300:ALA:HB1	1:A:346:ALA:HB2	2.01	0.41
1:A:121:THR:HG23	1:A:122:PRO:HD2	2.03	0.41
1:A:207:GLU:HG3	1:A:208:ASN:OD1	2.21	0.41
1:B:48:ALA:HB1	1:B:461:MET:HE2	2.03	0.41
1:B:52:THR:HG21	1:B:63:PRO:HB3	2.03	0.40
1:A:94:MET:HE3	1:A:99:GLN:CB	2.50	0.40
1:A:204:VAL:HG12	1:A:212:ARG:HB2	2.04	0.40
1:B:293:ILE:HA	1:B:313:ALA:O	2.22	0.40
1:A:190:MET:O	1:A:194:LEU:HG	2.22	0.40
1:A:367:ALA:HB1	1:A:460:CYS:SG	2.62	0.40
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.83	0.40
1:A:146:GLN:OE1	1:A:146:GLN:HA	2.20	0.40
1:B:187:LEU:HD13	1:B:187:LEU:HA	1.85	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	394/507 (78%)	362 (92%)	31 (8%)	1 (0%)	41 71
1	B	396/507 (78%)	361 (91%)	30 (8%)	5 (1%)	12 37
All	All	790/1014 (78%)	723 (92%)	61 (8%)	6 (1%)	19 51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	LYS
1	B	160	VAL
1	B	27	GLU
1	A	25	ALA
1	B	380	GLY
1	B	317	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	312/397 (79%)	284 (91%)	28 (9%)	9 29
1	B	311/397 (78%)	292 (94%)	19 (6%)	18 48
All	All	623/794 (78%)	576 (92%)	47 (8%)	13 37

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	29	LEU
1	A	41	SER
1	A	66	SER
1	A	77	LEU
1	A	115	ARG
1	A	116	ASP
1	A	126	ILE
1	A	134	ARG
1	A	138	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	146	GLN
1	A	166	ASP
1	A	178	LEU
1	A	182	ARG
1	A	200	GLU
1	A	205	VAL
1	A	215	VAL
1	A	217	PHE
1	A	268	SER
1	A	289	ASP
1	A	324	CYS
1	A	360	ILE
1	A	362	PHE
1	A	363	SER
1	A	386	THR
1	A	460	CYS
1	A	470	ASP
1	A	479	VAL
1	B	26	LYS
1	B	98	ARG
1	B	125	LYS
1	B	134	ARG
1	B	158	LEU
1	B	161	LYS
1	B	172	MET
1	B	193	LYS
1	B	206	ASP
1	B	207	GLU
1	B	215	VAL
1	B	217	PHE
1	B	218	ARG
1	B	279	ARG
1	B	324	CYS
1	B	381	SER
1	B	442	TYR
1	B	443	LYS
1	B	470	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	272	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
3	ATP	A	603	2	26,33,33	3.13	9 (34%)	31,52,52	1.67	5 (16%)
3	ATP	A	604	1,2	26,33,33	0.76	1 (3%)	31,52,52	0.89	1 (3%)
3	ATP	B	604	2	26,33,33	0.62	0	31,52,52	0.84	1 (3%)
3	ATP	B	603	2	26,33,33	0.52	0	31,52,52	0.80	2 (6%)

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	ATP	A	603	2	-	6/18/38/38	0/3/3/3
3	ATP	A	604	1,2	-	5/18/38/38	0/3/3/3
3	ATP	B	604	2	-	5/18/38/38	0/3/3/3
3	ATP	B	603	2	-	4/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	ATP	O4'-C1'	-9.59	1.27	1.41
3	A	603	ATP	C2'-C3'	-8.03	1.31	1.53
3	A	603	ATP	C2'-C1'	4.73	1.60	1.53
3	A	603	ATP	O4'-C4'	3.63	1.53	1.45
3	A	603	ATP	C6-N6	3.31	1.46	1.34
3	A	603	ATP	C5'-C4'	-3.21	1.41	1.51
3	A	603	ATP	O3'-C3'	3.07	1.50	1.43
3	A	604	ATP	PA-O2A	2.41	1.66	1.55
3	A	603	ATP	C5-N7	-2.09	1.32	1.39
3	A	603	ATP	C4-N3	-2.04	1.32	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	ATP	C3'-C2'-C1'	5.39	109.09	100.98
3	A	603	ATP	N3-C2-N1	-4.31	121.95	128.68
3	A	603	ATP	PB-O3B-PG	-3.87	119.55	132.83
3	B	603	ATP	C5-C6-N6	2.54	124.22	120.35
3	A	603	ATP	C4-C5-N7	-2.33	106.97	109.40
3	B	603	ATP	PB-O3B-PG	2.31	140.75	132.83
3	A	604	ATP	C5-C6-N6	2.22	123.73	120.35
3	B	604	ATP	C5-C6-N6	2.22	123.72	120.35
3	A	603	ATP	C2'-C3'-C4'	2.05	106.63	102.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	ATP	C5'-O5'-PA-O1A
3	A	603	ATP	C5'-O5'-PA-O2A
3	A	603	ATP	C5'-O5'-PA-O3A
3	A	604	ATP	C3'-C4'-C5'-O5'
3	B	603	ATP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	603	ATP	C5'-O5'-PA-O3A
3	B	604	ATP	C5'-O5'-PA-O1A
3	A	604	ATP	O4'-C4'-C5'-O5'
3	B	604	ATP	O4'-C4'-C5'-O5'
3	B	604	ATP	C3'-C4'-C5'-O5'
3	A	603	ATP	PA-O3A-PB-O1B
3	B	604	ATP	PG-O3B-PB-O1B
3	A	603	ATP	PG-O3B-PB-O1B
3	B	604	ATP	C5'-O5'-PA-O3A
3	A	604	ATP	PG-O3B-PB-O1B
3	A	604	ATP	PG-O3B-PB-O2B
3	A	604	ATP	PB-O3A-PA-O2A
3	B	603	ATP	PB-O3A-PA-O2A
3	B	603	ATP	PB-O3B-PG-O1G
3	A	603	ATP	C3'-C4'-C5'-O5'

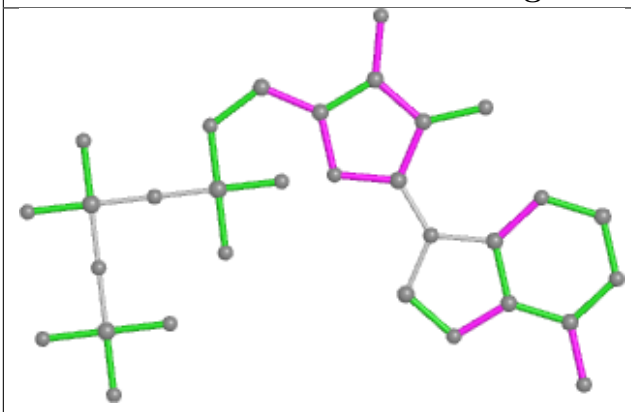
There are no ring outliers.

4 monomers are involved in 10 short contacts:

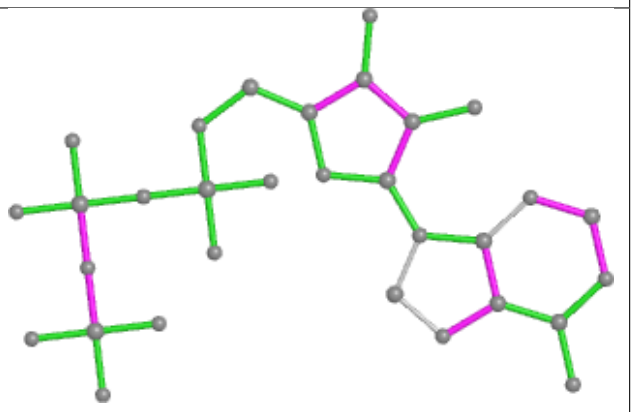
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	ATP	3	0
3	A	604	ATP	4	0
3	B	604	ATP	1	0
3	B	603	ATP	2	0

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

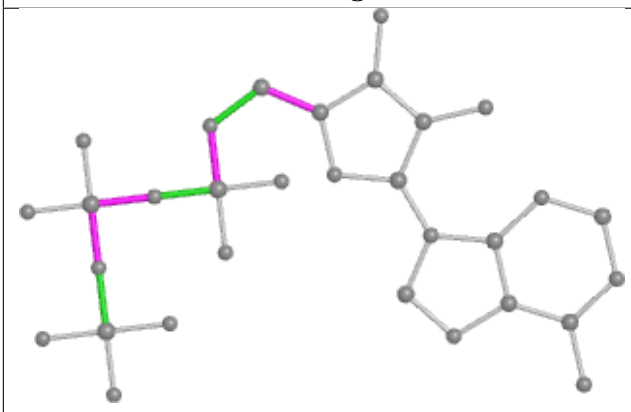
Ligand ATP A 603



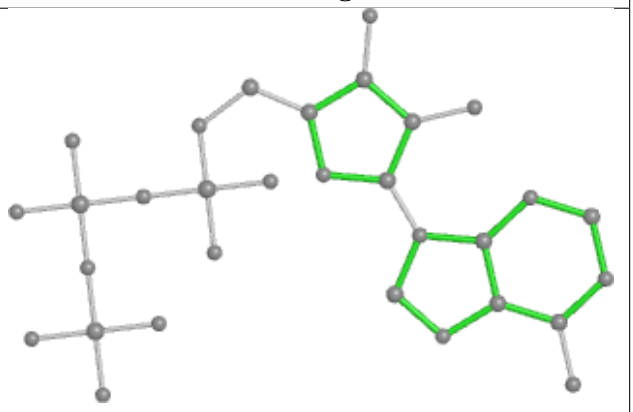
Bond lengths



Bond angles

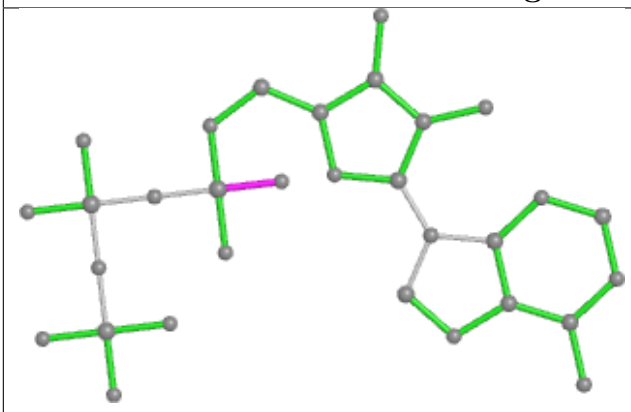


Torsions

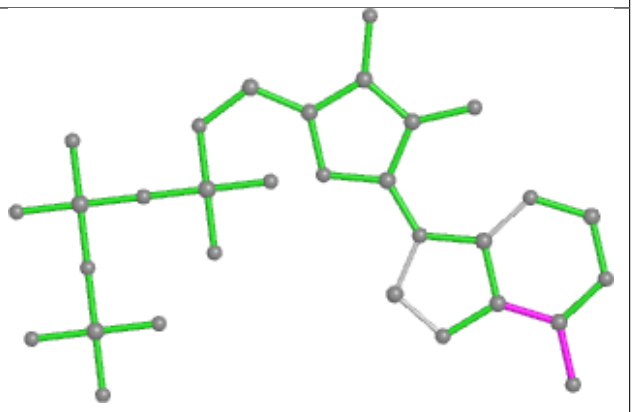


Rings

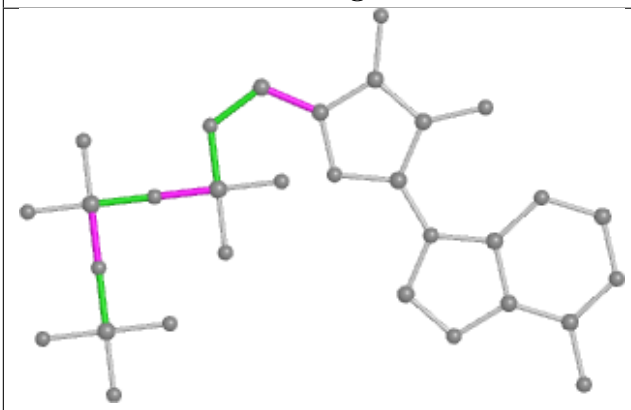
Ligand ATP A 604



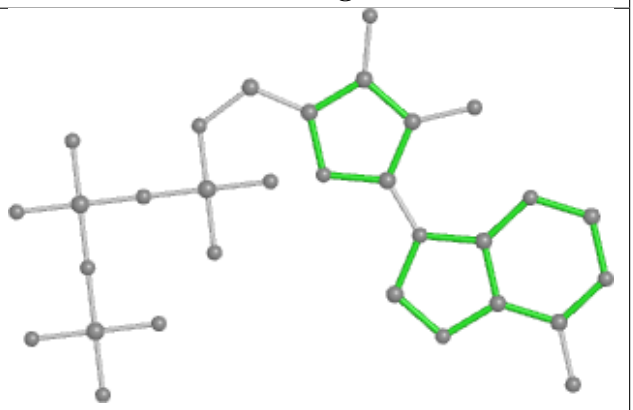
Bond lengths



Bond angles

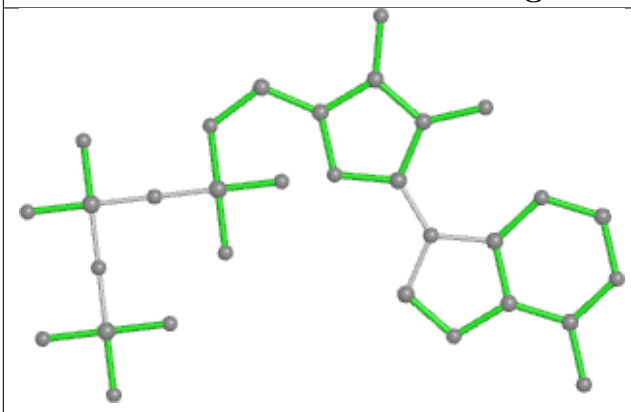


Torsions

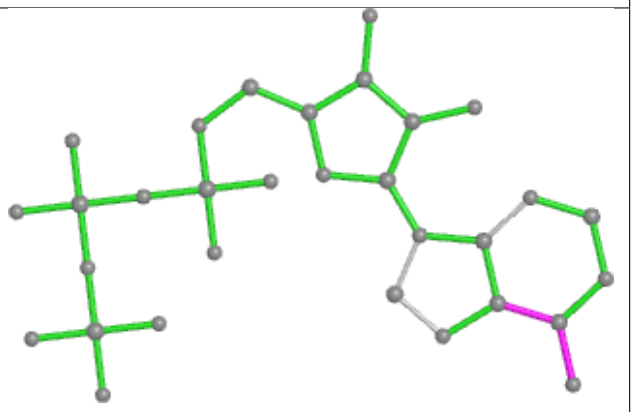


Rings

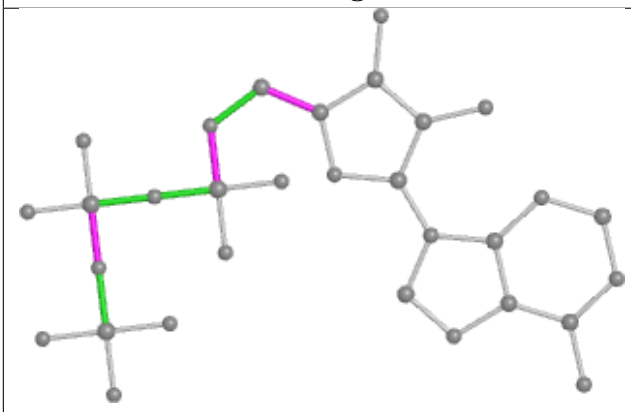
Ligand ATP B 604



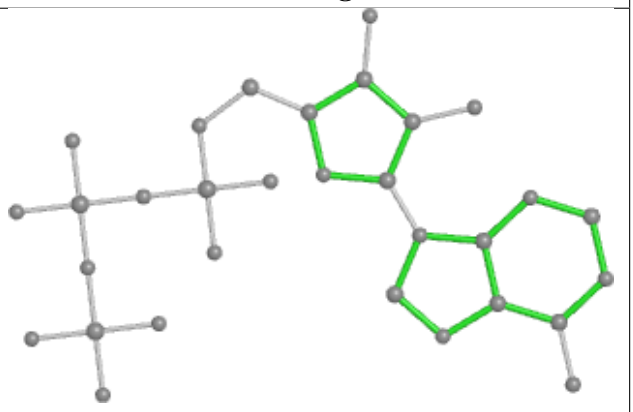
Bond lengths



Bond angles

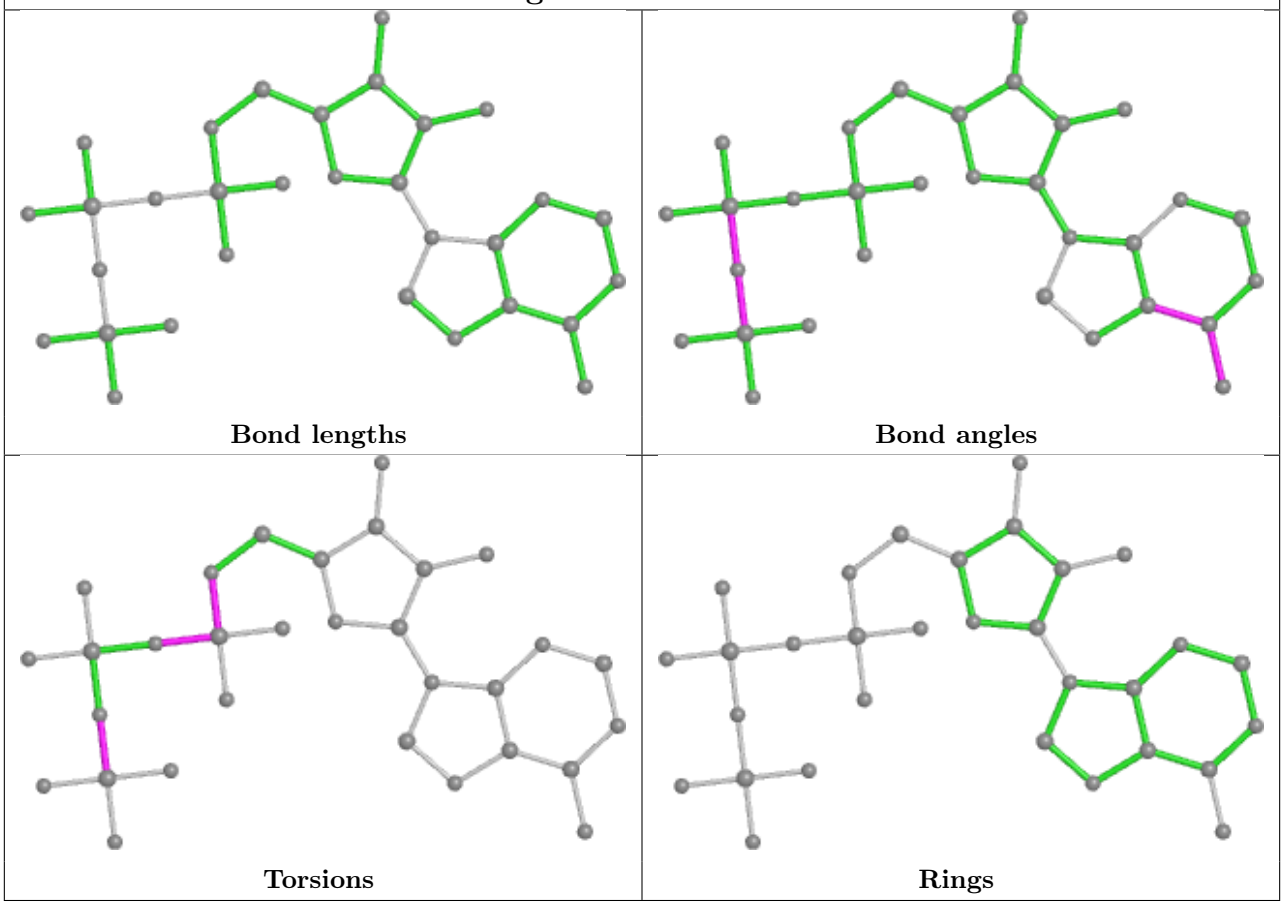


Torsions



Rings

Ligand ATP B 603



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

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	402/507 (79%)	0.17	10 (2%)	57	55	50, 74, 111, 141	13 (3%)
1	B	403/507 (79%)	0.11	3 (0%)	87	87	49, 65, 94, 137	19 (4%)
All	All	805/1014 (79%)	0.14	13 (1%)	72	71	49, 69, 104, 141	32 (3%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	CYS	3.4
1	B	24	ILE	3.3
1	A	323	ILE	2.9
1	A	214	LEU	2.8
1	B	328	ILE	2.6
1	A	213	GLY	2.6
1	A	446	LEU	2.4
1	A	332	VAL	2.3
1	A	163	ASN	2.3
1	B	214	LEU	2.2
1	A	143	VAL	2.1
1	A	187	LEU	2.1
1	A	108	LYS	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

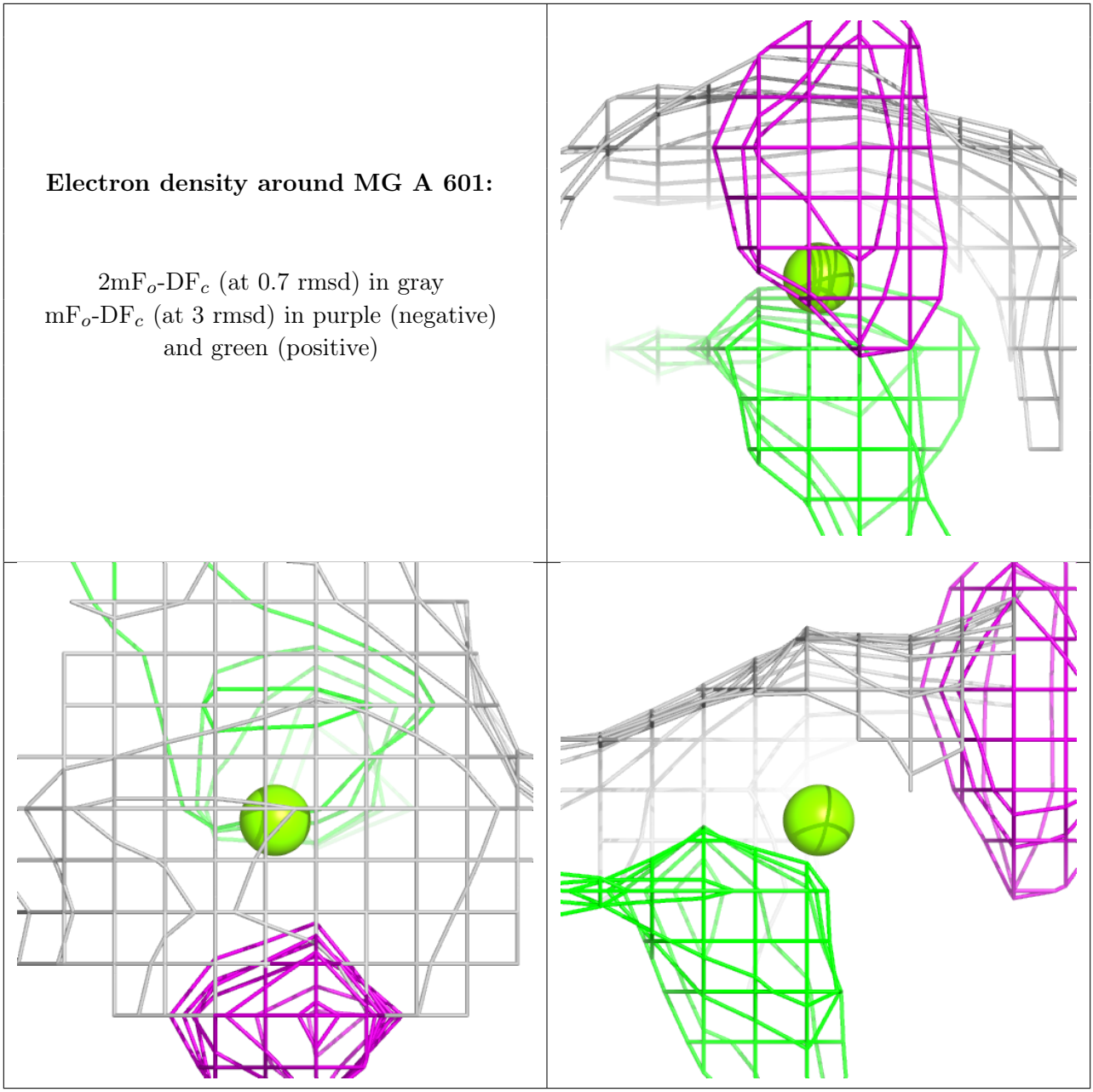
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MG	A	601	1/1	0.88	0.16	63,63,63,63	0
2	MG	B	601	1/1	0.94	0.12	55,55,55,55	0
2	MG	B	602	1/1	0.94	0.15	61,61,61,61	0
3	ATP	A	603	31/31	0.94	0.17	74,77,81,85	0
3	ATP	A	604	31/31	0.94	0.17	60,63,68,69	0
3	ATP	B	604	31/31	0.94	0.18	62,66,71,76	0
2	MG	A	602	1/1	0.97	0.17	65,65,65,65	0
3	ATP	B	603	31/31	0.98	0.15	48,56,64,68	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.

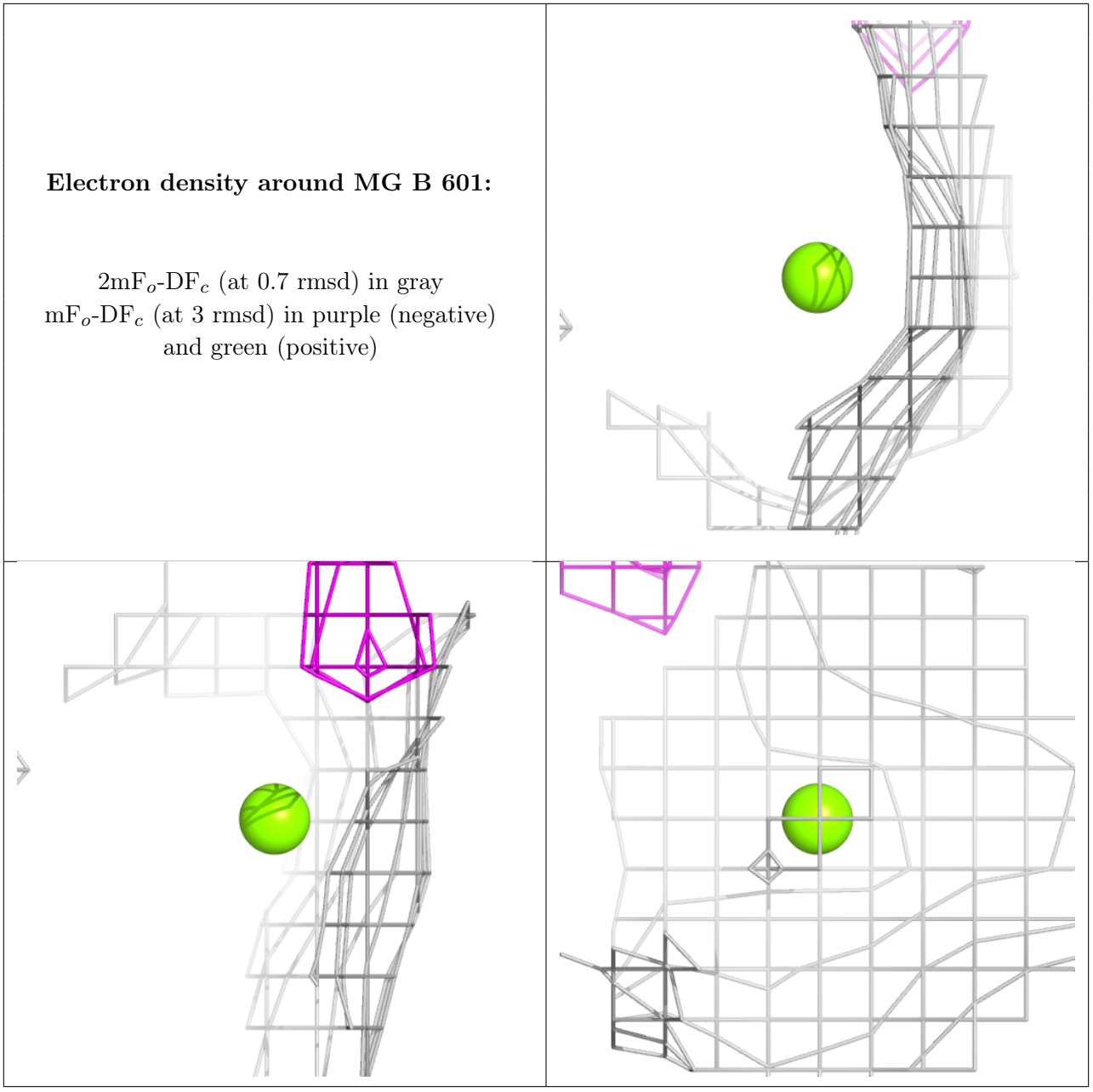
Electron density around MG A 601:

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



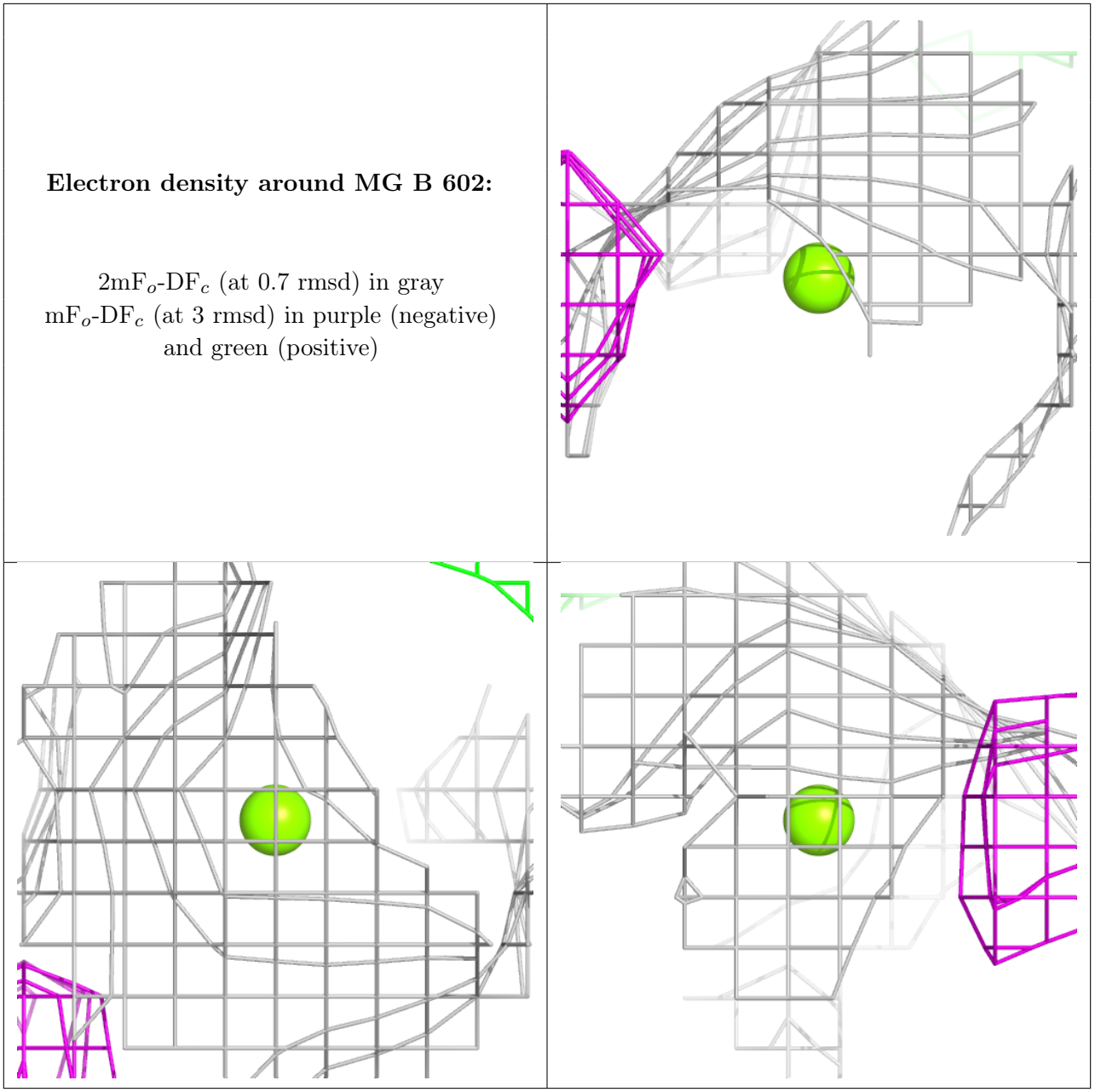
Electron density around MG B 601:

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



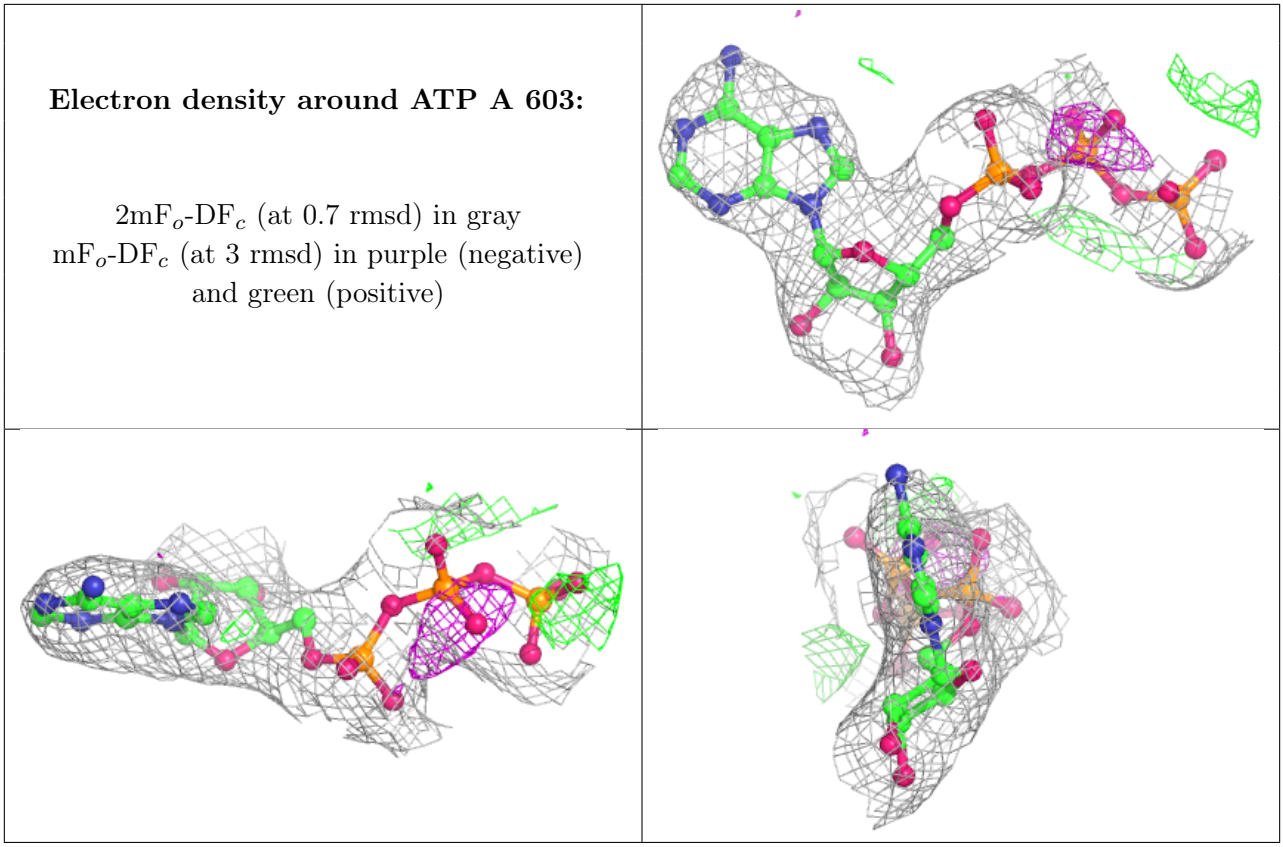
Electron density around MG B 602:

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



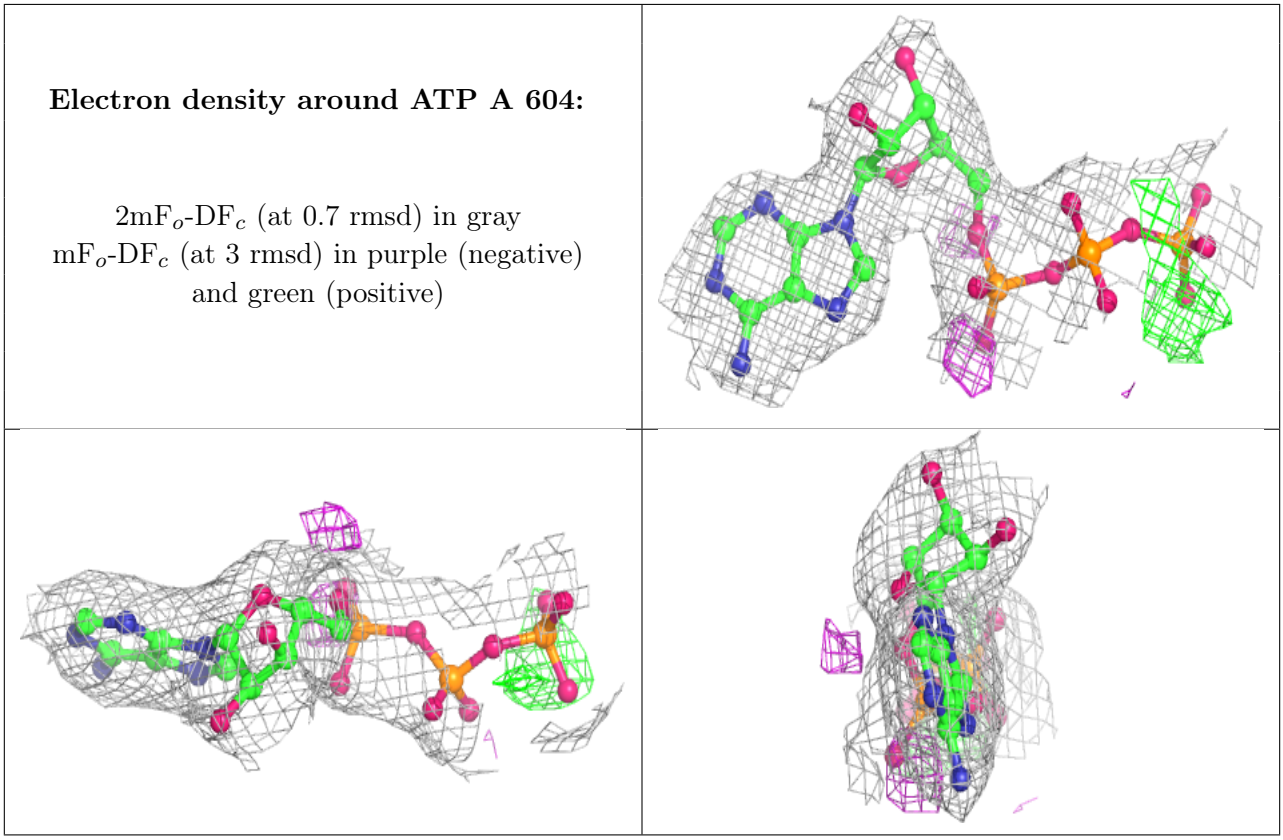
Electron density around ATP A 603:

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



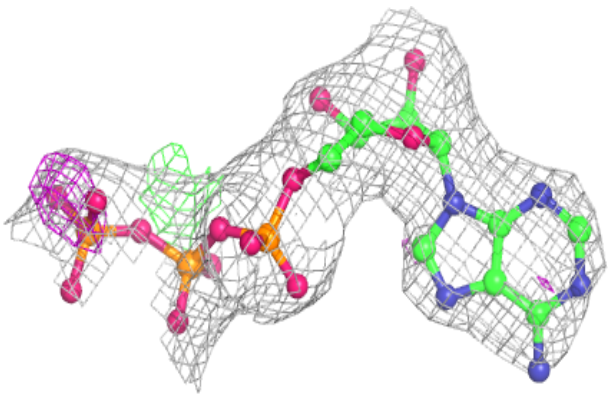
Electron density around ATP A 604:

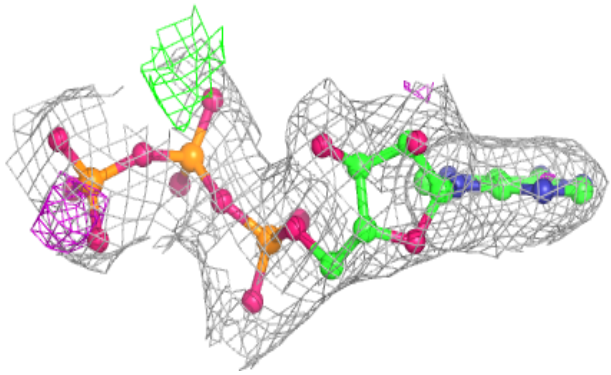
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

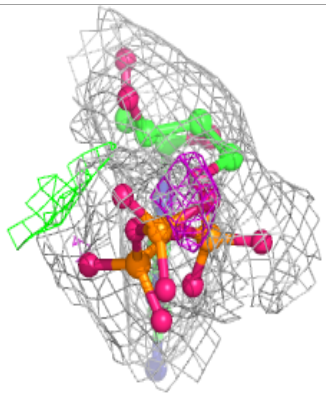


Electron density around ATP B 604:

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

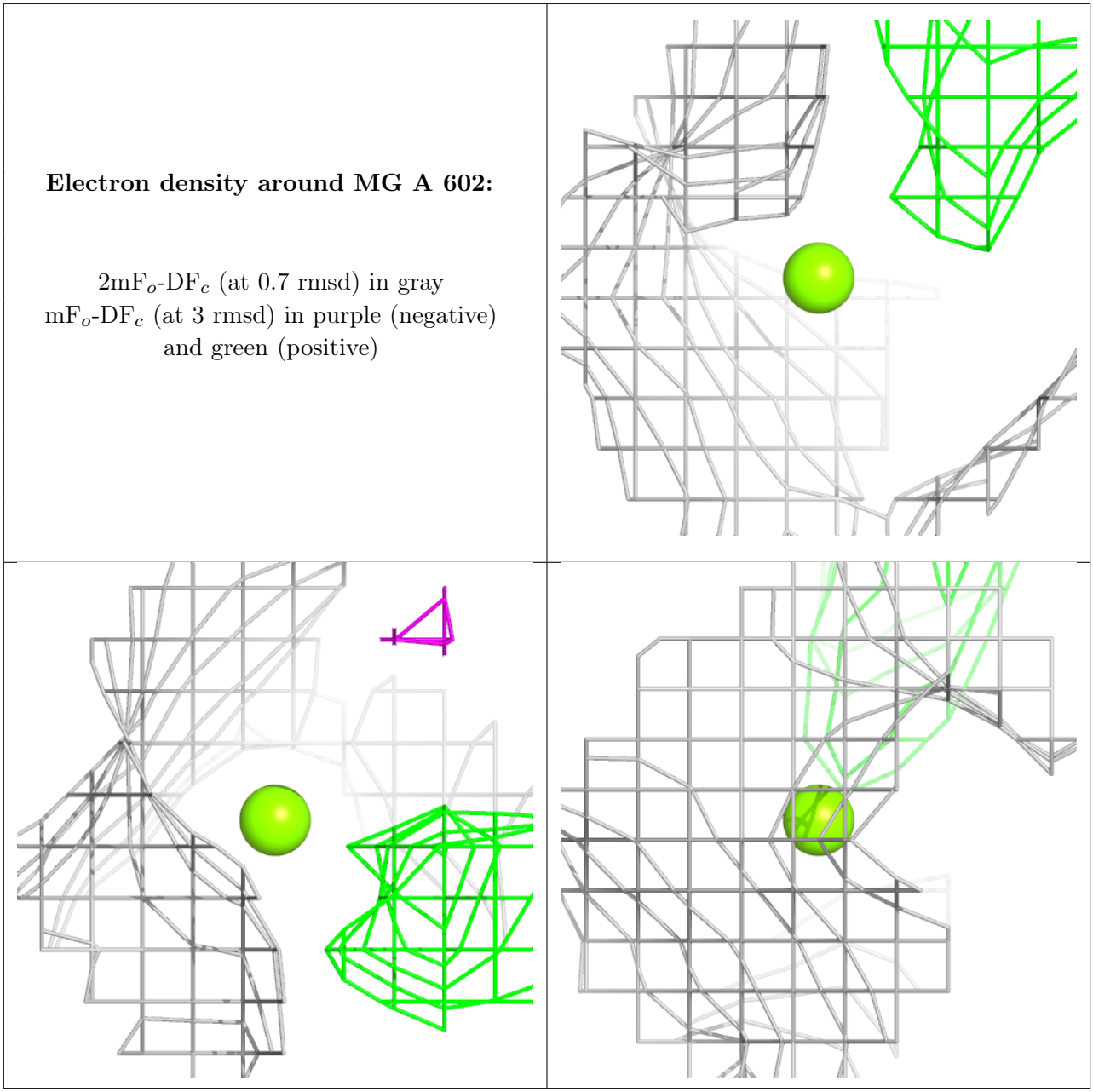






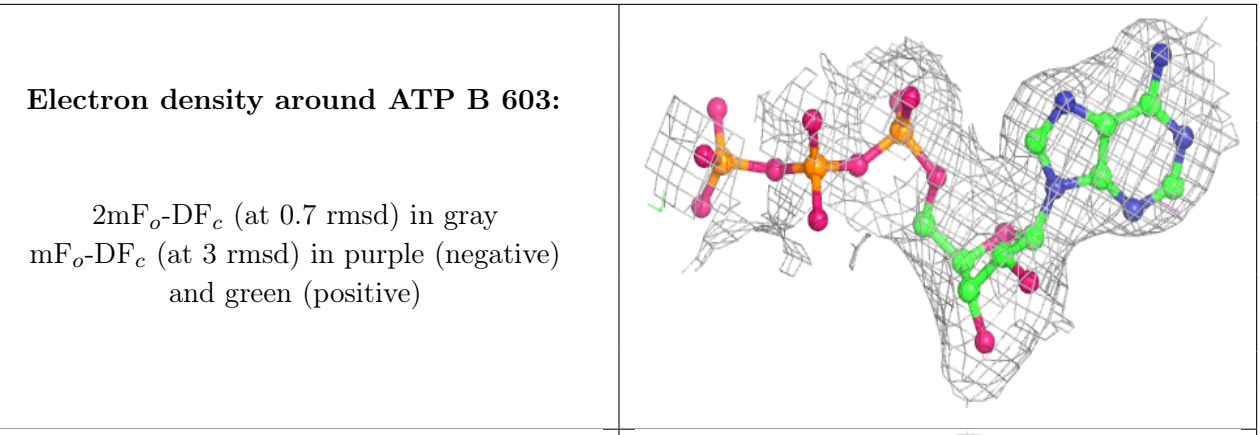
Electron density around MG A 602:

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



Electron density around ATP B 603:

$2mF_o$-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.