Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2023 – 01:20 pm BST

PDB ID	:	8CQX
Title	:	Ribokinase from T.sp mutant A92G
Authors	:	Timofeev, V.I.; Shevtsov, M.B.; Abramchik, Y.A.; Kostromina, M.A.; Zayats, E.A.; Kuranova, I.P.; Esipov, R.S.
Deposited on	:	2023-03-07
Resolution	:	2.27 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

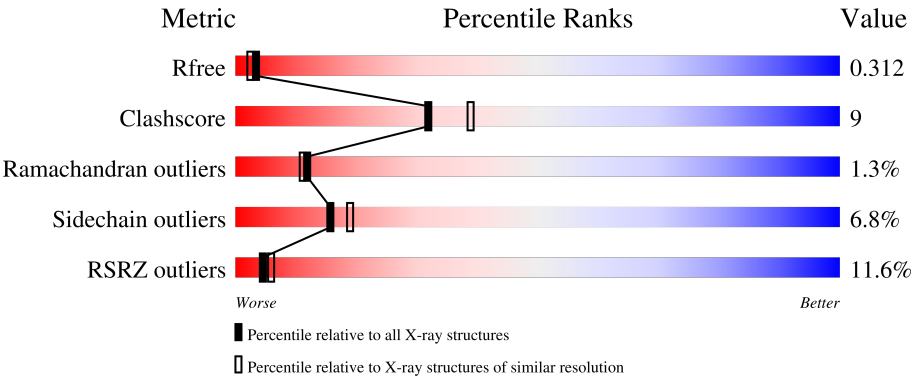
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	300	7% 80% 18% ·
1	B	300	2% 87% 11% ·
1	C	300	3% 84% 16%
1	D	300	34% 66% 30% ·

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
2	ADP	D	401	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9056 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.

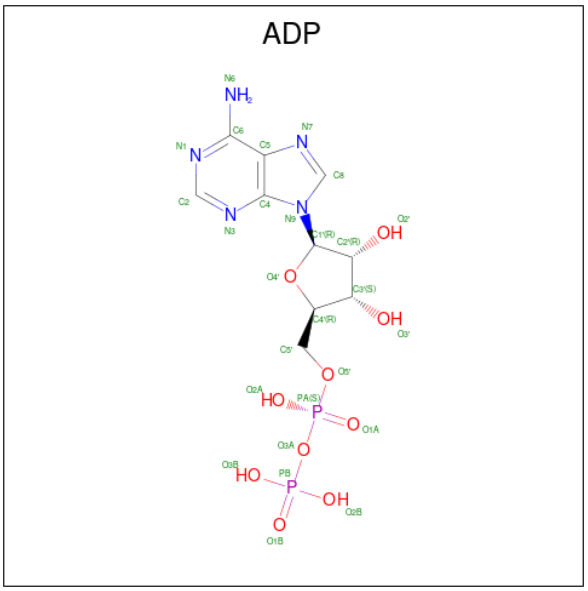
- Molecule 1 is a protein called Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	1	0
			2194	1383	398	409	4			
1	B	300	Total	C	N	O	S	0	0	0
			2183	1377	394	408	4			
1	C	300	Total	C	N	O	S	0	0	0
			2183	1377	394	408	4			
1	D	300	Total	C	N	O	S	0	0	0
			2183	1377	394	408	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLY	ALA	engineered mutation	UNP A0A0B0SD75
B	92	GLY	ALA	engineered mutation	UNP A0A0B0SD75
C	92	GLY	ALA	engineered mutation	UNP A0A0B0SD75
D	92	GLY	ALA	engineered mutation	UNP A0A0B0SD75

- 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
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	63	Total	O	0	0
			63	63		

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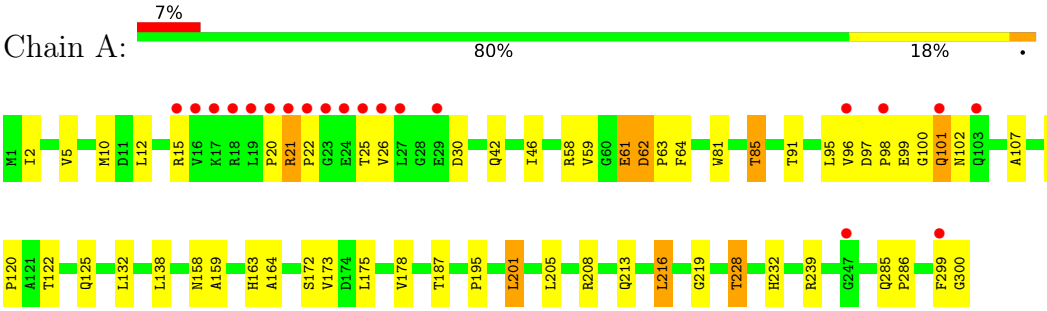
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	68	Total O 68 68	0	0
4	D	11	Total O 11 11	0	0

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.

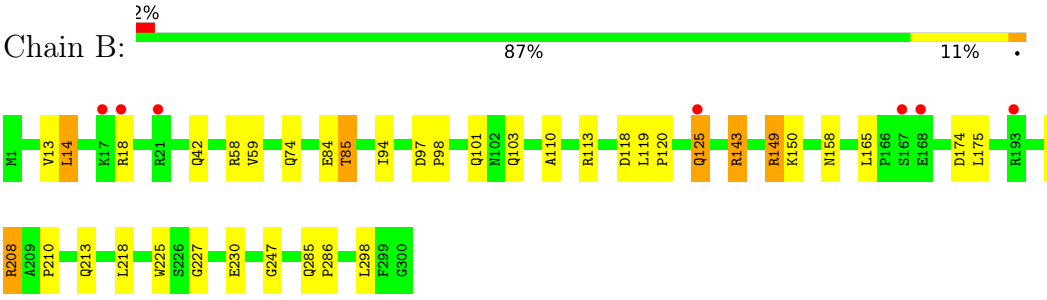
• Molecule 1: Ribokinase

Chain A:



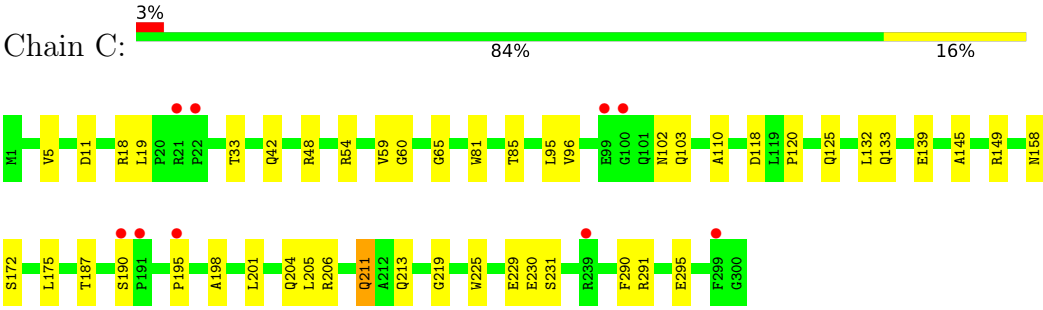
• Molecule 1: Ribokinase

Chain B:



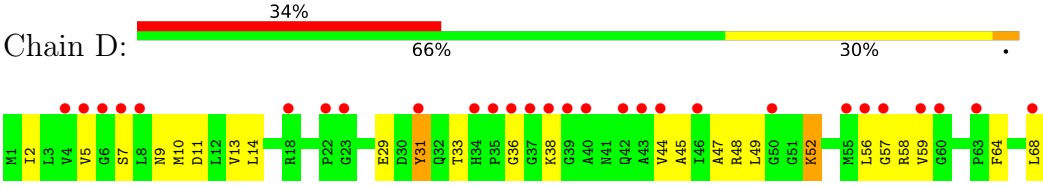
• Molecule 1: Ribokinase

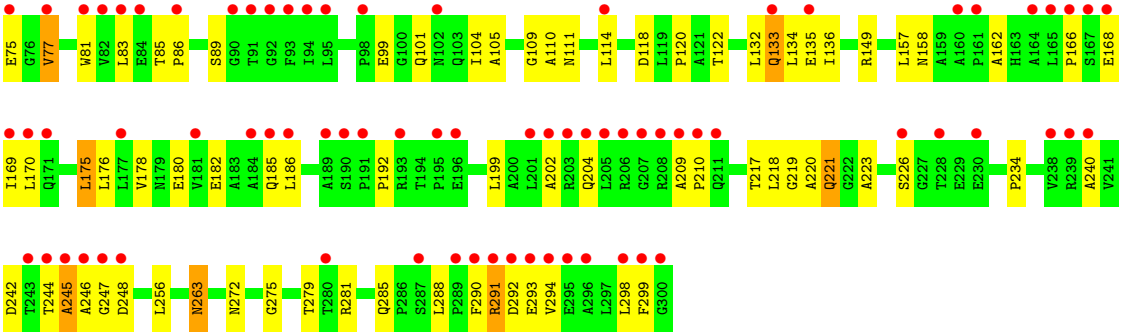
Chain C:



• Molecule 1: Ribokinase

Chain D:




E75 G76 V77 W81 V82 L83 E84 T85 P86 S89 G90 T91 G92 F93 I94 L95 P98 E99 G100 Q101 N102 Q103 I104 A105 G109 A110 N111 L114 D118 L119 P120 A121 T122 L132 Q133 L134 E135 I136 R149 L157 N158 A159 A160 P161 A162 H163 A164 L165 P166 S167 E168
I169 L170 Q171 L175 L176 L177 V178 N179 E180 V181 E182 A183 A184 Q185 L186 A189 S190 P191 P192 R193 T194 P195 E196 L199 A200 L201 A202 R203 Q204 L205 R206 G207 R208 A209 P210 Q211 T217 L218 G219 A220 Q221 G222 A223 S226 G227 T228 E229 E230 P234 V238 R239 A240 V241
D242 T243 T244 A245 A246 G247 D248 L256 N263 N272 G275 T279 T280 R281 Q285 P286 S287 L288 P289 F290 R291 D292 E293 V294 E295 A296 L297 L298 F299 G300

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.31Å 155.61Å 82.92Å 90.00° 96.37° 90.00°	Depositor
Resolution (Å)	29.52 – 2.27 29.52 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.52-2.27) 99.3 (29.52-2.27)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.229 , 0.311 0.233 , 0.312	Depositor DCC
R_{free} test set	2481 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9056	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.76	0/2232	0.95	2/3043 (0.1%)
1	B	0.74	0/2221	0.95	3/3029 (0.1%)
1	C	0.74	0/2221	0.91	0/3029
1	D	0.75	0/2221	0.91	0/3029
All	All	0.75	0/8895	0.93	5/12130 (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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	208	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	113	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	74	GLN	CB-CA-C	-5.39	99.61	110.40
1	B	143	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	247	GLY	Peptide

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	2194	0	2244	41	0
1	B	2183	0	2232	27	0
1	C	2183	0	2232	25	0
1	D	2183	0	2232	68	0
2	A	27	0	12	0	0
2	B	27	0	12	2	0
2	C	27	0	12	0	0
2	D	27	0	12	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	60	0	0	1	0
4	B	63	0	0	0	0
4	C	68	0	0	0	0
4	D	11	0	0	2	0
All	All	9056	0	8988	158	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 (158) 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:D:217:THR:HG22	2:D:401:ADP:N3	1.61	1.15
1:C:85:THR:HG21	1:C:110:ALA:HB1	1.46	0.96
1:D:242:ASP:O	1:D:279:THR:HA	1.72	0.90
1:A:81:TRP:CZ3	1:A:120:PRO:HG2	2.07	0.90
1:C:85:THR:HG21	1:C:110:ALA:CB	2.02	0.89
1:D:9:ASN:OD1	1:D:111:ASN:ND2	2.10	0.85
1:D:219:GLY:O	1:D:221:GLN:N	2.15	0.78
1:C:59:VAL:O	1:C:85:THR:HG22	1.85	0.77
1:D:133:GLN:C	1:D:134:LEU:HD23	2.05	0.76
1:D:217:THR:CG2	2:D:401:ADP:N3	2.46	0.74
1:D:275:GLY:HA3	2:D:401:ADP:O2'	1.92	0.70
1:D:105:ALA:HB2	4:D:504:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:GLN:HE22	1:C:158:ASN:HD22	1.41	0.69
1:B:149:ARG:NH2	1:B:174:ASP:OD1	2.28	0.67
1:D:219:GLY:HA2	2:D:401:ADP:O5'	1.96	0.65
1:D:217:THR:HG22	2:D:401:ADP:C2	2.30	0.65
1:A:42:GLN:HE22	1:A:158:ASN:HD22	1.44	0.64
1:A:213:GLN:HE22	1:A:228:THR:CG2	2.11	0.64
1:D:2:ILE:HD11	1:D:256:LEU:HA	1.80	0.64
1:D:281:ARG:NH1	1:D:293:GLU:OE2	2.33	0.62
1:A:15:ARG:HA	1:A:96:VAL:O	2.00	0.62
1:D:263:ASN:HD22	1:D:263:ASN:H	1.49	0.61
1:C:54:ARG:HD3	1:C:81:TRP:CZ3	2.36	0.61
1:B:42:GLN:HE22	1:B:158:ASN:HD22	1.47	0.61
1:A:100:GLY:O	1:A:101:GLN:O	2.20	0.60
1:B:58:ARG:HB3	1:B:85:THR:HG21	1.83	0.60
1:D:52:LYS:N	1:D:52:LYS:HD2	2.16	0.59
1:D:134:LEU:HD23	1:D:134:LEU:N	2.18	0.59
1:B:118:ASP:O	1:B:120:PRO:HD3	2.03	0.59
1:D:133:GLN:HA	1:D:158:ASN:O	2.02	0.58
1:D:217:THR:HG22	2:D:401:ADP:C4	2.36	0.58
1:B:59:VAL:O	1:B:85:THR:HG23	2.03	0.58
1:C:85:THR:CG2	1:C:110:ALA:CB	2.81	0.58
1:D:48:ARG:NH1	1:D:285:GLN:O	2.37	0.58
1:D:57:GLY:HA2	1:D:114:LEU:HD22	1.86	0.58
1:D:245:ALA:CB	1:D:288:LEU:HD21	2.33	0.58
1:A:81:TRP:CE3	1:A:120:PRO:HG2	2.38	0.57
1:D:202:ALA:HB1	1:D:226:SER:HB3	1.85	0.57
1:A:59:VAL:O	1:A:85:THR:HG23	2.05	0.57
1:A:163:HIS:HD2	1:A:164:ALA:O	1.88	0.57
1:D:175:LEU:HD12	1:D:176:LEU:N	2.20	0.55
1:A:58:ARG:HB3	1:A:85:THR:HG21	1.89	0.55
1:D:217:THR:O	2:D:401:ADP:H2	1.90	0.55
1:C:95:LEU:O	1:C:102:ASN:HA	2.07	0.55
1:A:5:VAL:HB	1:A:132:LEU:CD2	2.37	0.55
1:A:213:GLN:HE22	1:A:228:THR:HG23	1.71	0.55
1:B:149:ARG:HH22	1:B:174:ASP:CG	2.11	0.54
1:D:9:ASN:O	1:D:36:GLY:N	2.37	0.54
1:A:25:THR:HG23	1:D:104:ILE:HG21	1.90	0.54
1:C:85:THR:CG2	1:C:110:ALA:HB1	2.30	0.54
1:C:206:ARG:NH1	1:C:230:GLU:OE1	2.37	0.54
1:D:71:GLY:O	1:D:75:GLU:HG2	2.08	0.54
1:C:171:GLN:HA	1:C:211:GLN:NE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LEU:O	1:D:291:ARG:NH1	2.41	0.52
1:D:219:GLY:C	1:D:221:GLN:H	2.10	0.52
1:B:175:LEU:HA	1:B:213:GLN:O	2.10	0.52
1:A:25:THR:HA	1:D:104:ILE:HB	1.92	0.52
1:D:118:ASP:O	1:D:120:PRO:HD3	2.09	0.52
2:D:401:ADP:H3'	2:D:401:ADP:O2A	2.10	0.51
1:D:13:VAL:O	1:D:31:TYR:HA	2.10	0.51
1:B:97:ASP:HB2	1:B:98:PRO:CD	2.40	0.51
1:D:38:LYS:HG3	1:D:135:GLU:OE2	2.11	0.51
1:D:169:ILE:O	1:D:170:LEU:HD23	2.10	0.51
1:A:118:ASP:O	1:A:120:PRO:HD3	2.11	0.50
1:D:59:VAL:O	1:D:85:THR:HG22	2.11	0.50
1:A:187:THR:HG21	1:A:201:LEU:HD23	1.94	0.50
1:D:56:LEU:HD23	1:D:56:LEU:C	2.31	0.50
1:D:81:TRP:CZ3	1:D:120:PRO:HG2	2.46	0.50
1:B:85:THR:CG2	1:B:110:ALA:HB1	2.42	0.50
1:C:133:GLN:HA	1:C:158:ASN:O	2.12	0.50
1:C:195:PRO:O	1:C:198:ALA:HB3	2.12	0.50
1:B:125:GLN:HE21	1:B:125:GLN:HA	1.76	0.50
1:C:149:ARG:NH1	1:C:172:SER:O	2.41	0.50
1:A:95:LEU:O	1:A:102:ASN:HA	2.12	0.49
1:B:208:ARG:HH11	1:B:208:ARG:HB3	1.77	0.49
1:D:134:LEU:HD21	1:D:157:LEU:HD11	1.93	0.49
1:C:60:GLY:HA2	1:C:85:THR:HG22	1.95	0.49
1:B:13:VAL:HG22	1:B:94:ILE:HB	1.95	0.49
1:B:59:VAL:O	1:B:85:THR:CG2	2.61	0.49
1:D:294:VAL:HG12	1:D:298:LEU:HD12	1.93	0.49
1:D:44:VAL:HG22	1:D:75:GLU:HG3	1.95	0.49
1:D:11:ASP:OD2	1:D:36:GLY:HA3	2.13	0.48
1:B:247:GLY:CA	2:B:401:ADP:O2B	2.62	0.48
1:D:132:LEU:O	1:D:158:ASN:N	2.46	0.48
1:A:187:THR:HG21	1:A:201:LEU:CD2	2.44	0.48
1:D:166:PRO:O	1:D:169:ILE:HG22	2.14	0.48
1:D:202:ALA:HB1	1:D:226:SER:CB	2.44	0.48
1:C:48:ARG:O	1:C:290:PHE:HA	2.14	0.47
1:A:2:ILE:HG21	1:A:46:ILE:HD13	1.96	0.47
1:D:11:ASP:O	1:D:33:THR:HA	2.15	0.47
1:D:58:ARG:HG3	1:D:83:LEU:O	2.15	0.47
1:C:19:LEU:HD13	1:C:103:GLN:HG3	1.95	0.46
1:A:26:VAL:O	1:D:105:ALA:HA	2.16	0.46
1:C:118:ASP:O	1:C:120:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:THR:HG21	1:B:110:ALA:HB1	1.97	0.46
1:D:64:PHE:O	1:D:68:LEU:HG	2.15	0.46
1:B:198:ALA:CB	1:B:218:LEU:HD11	2.46	0.45
1:D:170:LEU:HB3	1:D:209:ALA:HB2	1.98	0.45
1:A:21:ARG:HB3	1:A:22:PRO:CD	2.46	0.45
1:D:272:ASN:HA	2:D:401:ADP:O3'	2.16	0.45
1:B:206:ARG:O	1:B:210:PRO:HA	2.16	0.45
1:A:96:VAL:HA	1:A:101:GLN:O	2.16	0.45
1:A:62:ASP:HB2	1:A:63:PRO:CD	2.47	0.45
1:A:81:TRP:CZ2	1:A:122:THR:OG1	2.69	0.44
1:B:58:ARG:NH1	1:B:85:THR:HB	2.32	0.44
1:C:187:THR:HB	1:C:204:GLN:NE2	2.32	0.44
1:D:180:GLU:HG3	1:D:192:PRO:HG2	1.99	0.44
1:B:285:GLN:N	1:B:286:PRO:CD	2.80	0.44
1:D:10:MET:HB2	1:D:68:LEU:HD21	1.99	0.44
1:D:47:ALA:HB2	1:D:77:VAL:HG12	1.99	0.44
1:A:10:MET:HG2	1:A:64:PHE:CD1	2.53	0.44
1:B:14:LEU:HA	1:B:14:LEU:HD13	1.82	0.44
1:B:208:ARG:HH11	1:B:208:ARG:CB	2.30	0.44
1:A:58:ARG:NH1	1:A:85:THR:HB	2.32	0.44
1:A:61:GLU:O	1:A:62:ASP:O	2.35	0.44
1:D:132:LEU:O	1:D:157:LEU:HD12	2.16	0.44
1:D:290:PHE:HB2	1:D:292:ASP:OD1	2.17	0.44
1:C:145:ALA:O	1:C:149:ARG:HG3	2.18	0.44
1:D:14:LEU:CD1	1:D:29:GLU:O	2.66	0.44
1:A:81:TRP:CZ3	1:A:120:PRO:CG	2.90	0.44
1:D:132:LEU:HB2	1:D:157:LEU:HD13	1.99	0.43
1:A:20:PRO:HD3	4:D:504:HOH:O	2.18	0.43
1:C:5:VAL:HB	1:C:132:LEU:CD2	2.48	0.43
1:D:48:ARG:HD2	1:D:288:LEU:O	2.18	0.43
1:D:52:LYS:HD2	1:D:52:LYS:H	1.82	0.43
1:B:97:ASP:HB2	1:B:98:PRO:HD2	2.00	0.43
1:A:91:THR:OG1	1:A:107:ALA:HB3	2.19	0.43
1:D:45:ALA:O	1:D:49:LEU:HG	2.19	0.42
1:A:285:GLN:N	1:A:286:PRO:CD	2.83	0.42
1:B:119:LEU:HD12	1:B:143:ARG:HB3	2.01	0.42
1:D:178:VAL:HA	1:D:182:GLU:OE2	2.19	0.42
1:A:97:ASP:CB	1:A:98:PRO:CD	2.96	0.42
1:B:225:TRP:O	1:B:230:GLU:HA	2.20	0.42
1:C:171:GLN:HA	1:C:211:GLN:HE22	1.83	0.42
1:C:225:TRP:CZ3	1:C:229:GLU:CG	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:HG2	4:A:559:HOH:O	2.20	0.42
1:D:58:ARG:HA	1:D:83:LEU:O	2.20	0.42
1:D:68:LEU:O	1:D:72:LEU:HD12	2.19	0.42
1:D:85:THR:CG2	1:D:110:ALA:HB1	2.49	0.42
1:A:195:PRO:HB3	1:A:232:HIS:CD2	2.55	0.41
1:A:122:THR:HG22	1:A:125:GLN:NE2	2.34	0.41
1:C:59:VAL:HB	1:C:65:GLY:HA2	2.01	0.41
1:C:175:LEU:HA	1:C:213:GLN:O	2.19	0.41
1:A:81:TRP:CH2	1:A:122:THR:OG1	2.73	0.41
1:B:213:GLN:OE1	1:B:227:GLY:HA3	2.20	0.41
1:A:5:VAL:HB	1:A:132:LEU:HD23	2.01	0.41
1:A:85:THR:HG21	1:A:110:ALA:HB1	2.03	0.41
1:B:58:ARG:HH11	1:B:85:THR:HB	1.85	0.41
1:D:5:VAL:HB	1:D:132:LEU:HD23	2.03	0.41
1:D:162:ALA:HB1	1:D:186:LEU:HG	2.02	0.41
1:D:218:LEU:CD2	1:D:223:ALA:HA	2.51	0.41
1:A:159:ALA:HB3	1:A:178:VAL:HG12	2.04	0.40
1:D:7:SER:HB3	1:D:135:GLU:O	2.21	0.40
1:A:178:VAL:HG23	1:A:216:LEU:HG	2.03	0.40
1:A:299:PHE:O	1:A:300:GLY:C	2.60	0.40
1:A:25:THR:HG23	1:D:104:ILE:CG2	2.51	0.40
1:B:247:GLY:HA3	2:B:401:ADP:O2B	2.20	0.40
1:C:11:ASP:O	1:C:33:THR:HA	2.22	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	299/300 (100%)	278 (93%)	17 (6%)	4 (1%)	12 11
1	B	298/300 (99%)	288 (97%)	10 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	298/300 (99%)	282 (95%)	14 (5%)	2 (1%)	22 25
1	D	298/300 (99%)	256 (86%)	33 (11%)	9 (3%)	4 2
All	All	1193/1200 (99%)	1104 (92%)	74 (6%)	15 (1%)	12 11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	D	220	ALA
1	C	219	GLY
1	D	89	SER
1	D	240	ALA
1	D	210	PRO
1	D	246	ALA
1	A	30	ASP
1	A	62	ASP
1	C	168	GLU
1	D	245	ALA
1	A	219	GLY
1	D	234	PRO
1	D	109	GLY
1	D	86	PRO

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	218/217 (100%)	204 (94%)	14 (6%)	17 21
1	B	217/217 (100%)	204 (94%)	13 (6%)	19 24
1	C	217/217 (100%)	206 (95%)	11 (5%)	24 31
1	D	217/217 (100%)	196 (90%)	21 (10%)	8 8
All	All	869/868 (100%)	810 (93%)	59 (7%)	16 19

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	21	ARG
1	A	61	GLU
1	A	85	THR
1	A	99	GLU
1	A	138	LEU
1	A	172	SER
1	A	173	VAL
1	A	175	LEU
1	A	201	LEU
1	A	205	LEU
1	A	216	LEU
1	A	228	THR
1	A	239	ARG
1	B	14	LEU
1	B	18	ARG
1	B	84	GLU
1	B	85	THR
1	B	101	GLN
1	B	103	GLN
1	B	125	GLN
1	B	149	ARG
1	B	150	LYS
1	B	165	LEU
1	B	206	ARG
1	B	208	ARG
1	B	298	LEU
1	C	18	ARG
1	C	96	VAL
1	C	125	GLN
1	C	139	GLU
1	C	190	SER
1	C	201	LEU
1	C	205	LEU
1	C	211	GLN
1	C	231	SER
1	C	291	ARG
1	C	295	GLU
1	D	31	TYR
1	D	52	LYS
1	D	72	LEU
1	D	77	VAL
1	D	99	GLU

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Mol	Chain	Res	Type
1	D	101	GLN
1	D	122	THR
1	D	133	GLN
1	D	136	ILE
1	D	149	ARG
1	D	168	GLU
1	D	175	LEU
1	D	185	GLN
1	D	199	LEU
1	D	204	GLN
1	D	221	GLN
1	D	244	THR
1	D	248	ASP
1	D	263	ASN
1	D	291	ARG
1	D	299	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	163	HIS
1	A	185	GLN
1	B	9	ASN
1	B	125	GLN
1	B	158	ASN
1	C	9	ASN
1	C	158	ASN
1	C	211	GLN
1	D	34	HIS
1	D	42	GLN
1	D	133	GLN
1	D	204	GLN
1	D	211	GLN
1	D	221	GLN
1	D	263	ASN

5.3.3 RNA

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 7 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
2	ADP	A	401	-	24,29,29	0.68	1 (4%)	29,45,45	0.83	0
2	ADP	B	401	-	24,29,29	0.78	1 (4%)	29,45,45	0.85	1 (3%)
2	ADP	C	401	-	24,29,29	0.66	1 (4%)	29,45,45	0.84	1 (3%)
2	ADP	D	401	-	24,29,29	0.66	0	29,45,45	1.05	3 (10%)

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	401	-	-	2/12/32/32	0/3/3/3
2	ADP	B	401	-	-	2/12/32/32	0/3/3/3
2	ADP	C	401	-	-	3/12/32/32	0/3/3/3
2	ADP	D	401	-	-	1/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ADP	C8-N7	-2.20	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ADP	C8-N7	-2.10	1.31	1.34
2	A	401	ADP	C8-N7	-2.01	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	ADP	C1'-N9-C4	2.45	130.94	126.64
2	B	401	ADP	C5-C6-N6	2.44	124.06	120.35
2	D	401	ADP	C5-C6-N6	2.34	123.91	120.35
2	D	401	ADP	C3'-C2'-C1'	2.32	104.47	100.98
2	C	401	ADP	O2A-PA-O1A	2.03	122.28	112.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	PA-O3A-PB-O2B
2	A	401	ADP	PA-O3A-PB-O3B
2	B	401	ADP	PA-O3A-PB-O2B
2	D	401	ADP	C4'-C5'-O5'-PA
2	C	401	ADP	PB-O3A-PA-O2A
2	B	401	ADP	PA-O3A-PB-O1B
2	C	401	ADP	PB-O3A-PA-O1A
2	C	401	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

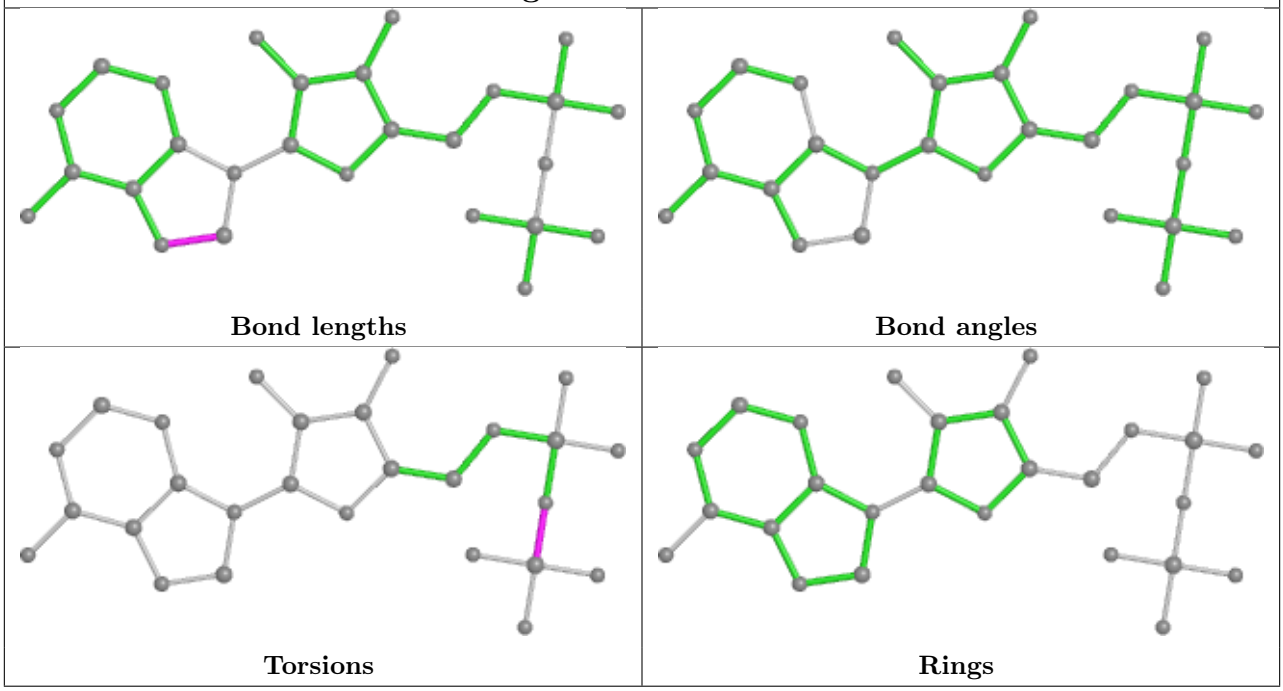
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ADP	2	0
2	D	401	ADP	9	0

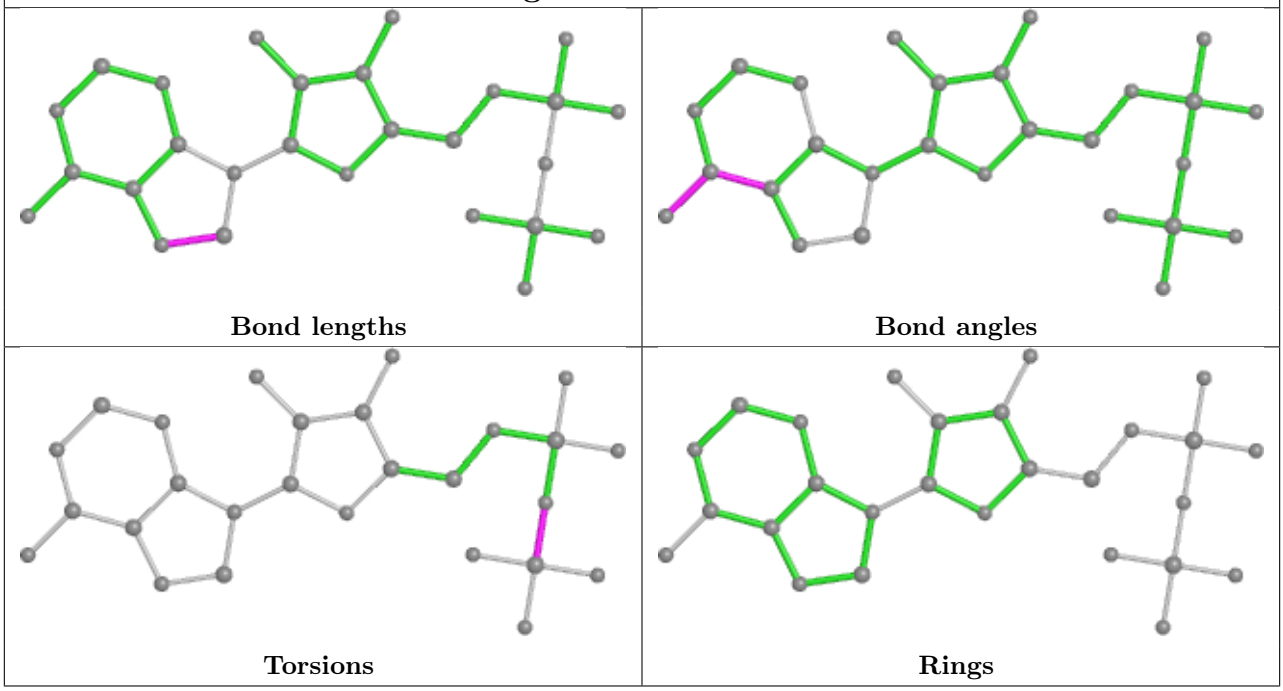
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

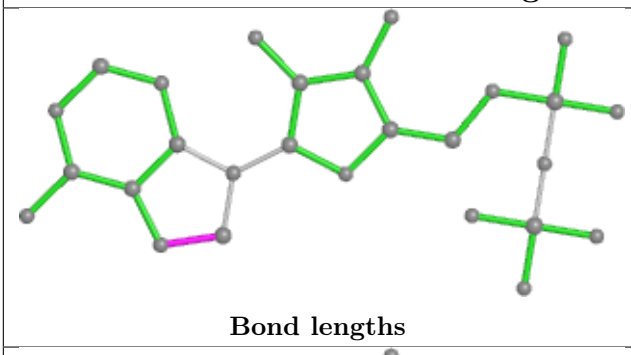
Ligand ADP A 401



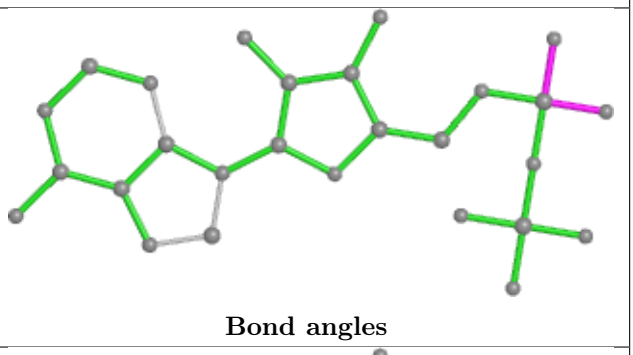
Ligand ADP B 401



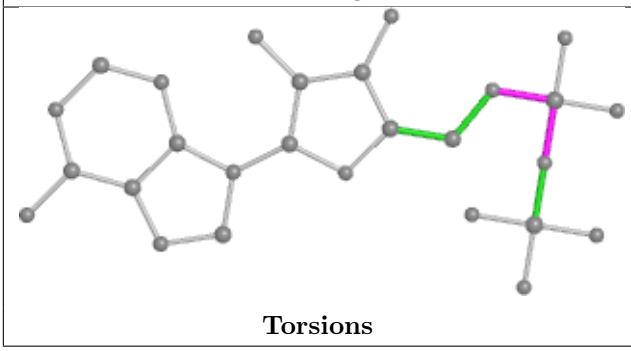
Ligand ADP C 401



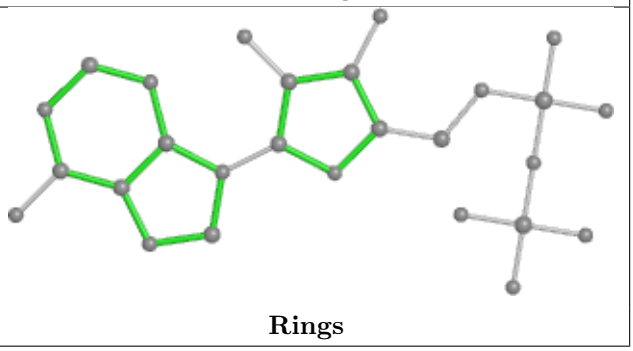
Bond lengths



Bond angles

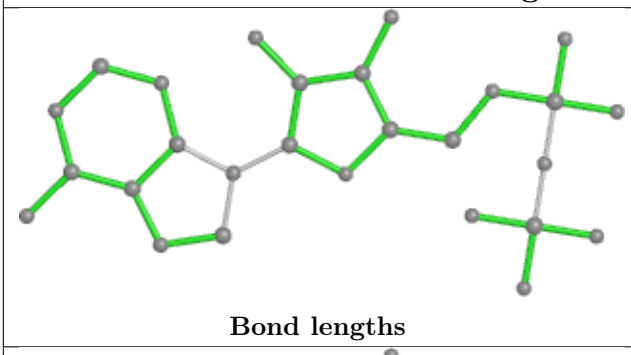


Torsions

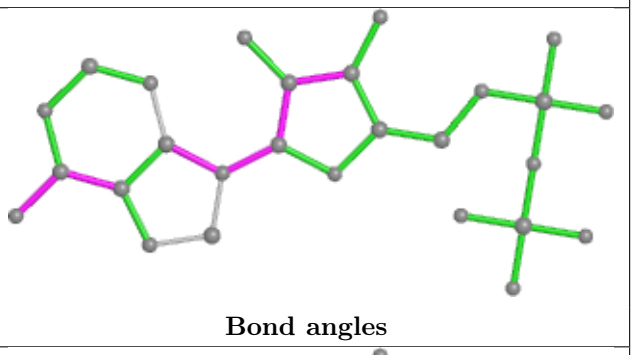


Rings

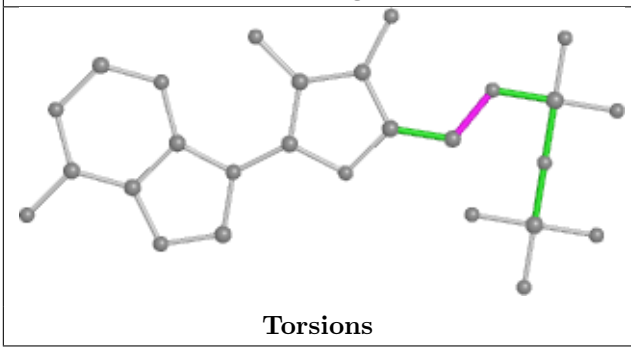
Ligand ADP D 401



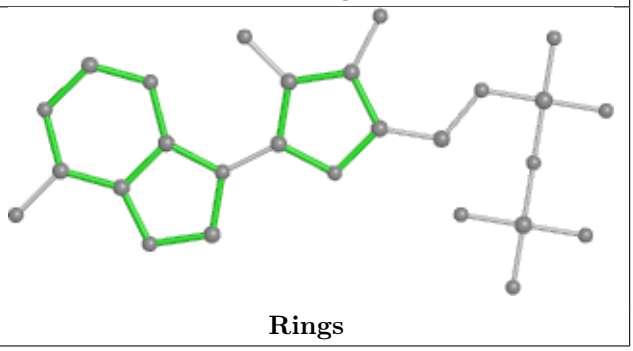
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	300/300 (100%)	0.39	20 (6%) 17 22	14, 27, 88, 164	0
1	B	300/300 (100%)	0.03	7 (2%) 60 66	16, 27, 56, 80	0
1	C	300/300 (100%)	0.07	9 (3%) 50 56	16, 28, 61, 96	0
1	D	300/300 (100%)	1.67	103 (34%) 0 0	27, 62, 98, 127	0
All	All	1200/1200 (100%)	0.54	139 (11%) 4 6	14, 32, 84, 164	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	GLU	10.6
1	A	23	GLY	9.9
1	D	207	GLY	8.8
1	A	22	PRO	8.7
1	D	245	ALA	8.1
1	A	19	LEU	6.7
1	D	246	ALA	6.2
1	A	18	ARG	6.2
1	D	299	PHE	6.1
1	A	26	VAL	6.0
1	A	17	LYS	5.4
1	D	185	GLN	5.4
1	A	20	PRO	5.3
1	A	25	THR	5.3
1	D	189	ALA	5.2
1	D	60	GLY	5.1
1	B	167	SER	4.7
1	D	191	PRO	4.6
1	D	167	SER	4.6
1	D	190	SER	4.5
1	D	8	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	205	LEU	4.3
1	D	77	VAL	4.3
1	D	168	GLU	4.3
1	A	29	GLU	4.2
1	D	86	PRO	4.2
1	C	100	GLY	4.1
1	D	206	ARG	4.1
1	D	203	ARG	4.1
1	D	300	GLY	4.0
1	A	103	GLN	4.0
1	A	27	LEU	3.9
1	D	196	GLU	3.8
1	D	83	LEU	3.8
1	D	290	PHE	3.8
1	D	5	VAL	3.7
1	D	160	ALA	3.7
1	D	39	GLY	3.6
1	D	181	VAL	3.6
1	D	164	ALA	3.6
1	D	59	VAL	3.6
1	A	299	PHE	3.5
1	C	239	ARG	3.5
1	D	239	ARG	3.5
1	A	16	VAL	3.5
1	D	202	ALA	3.4
1	D	280	THR	3.4
1	D	195	PRO	3.4
1	C	99	GLU	3.4
1	D	90	GLY	3.3
1	D	296	ALA	3.3
1	D	37	GLY	3.3
1	D	114	LEU	3.3
1	B	17	LYS	3.2
1	D	186	LEU	3.2
1	D	247	GLY	3.2
1	D	292	ASP	3.2
1	D	238	VAL	3.2
1	C	299	PHE	3.1
1	C	191	PRO	3.1
1	D	226	SER	3.1
1	D	31	TYR	3.1
1	A	101	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	81	TRP	3.0
1	D	210	PRO	3.0
1	D	94	ILE	2.9
1	D	38	LYS	2.9
1	D	209	ALA	2.9
1	B	18	ARG	2.9
1	D	102	ASN	2.9
1	D	40	ALA	2.9
1	D	22	PRO	2.9
1	D	204	GLN	2.8
1	A	21	ARG	2.8
1	D	240	ALA	2.8
1	D	23	GLY	2.8
1	D	289	PRO	2.7
1	D	133	GLN	2.7
1	D	63	PRO	2.7
1	D	91	THR	2.7
1	D	248	ASP	2.7
1	D	84	GLU	2.7
1	D	170	LEU	2.7
1	D	42	GLN	2.7
1	A	96	VAL	2.7
1	D	201	LEU	2.7
1	A	98	PRO	2.6
1	D	75	GLU	2.6
1	D	82	VAL	2.6
1	D	6	GLY	2.5
1	D	93	PHE	2.5
1	D	169	ILE	2.5
1	B	21	ARG	2.5
1	D	243	THR	2.5
1	D	56	LEU	2.5
1	D	211	GLN	2.5
1	D	34	HIS	2.5
1	D	171	GLN	2.5
1	D	7	SER	2.4
1	D	35	PRO	2.4
1	D	166	PRO	2.4
1	D	230	GLU	2.4
1	A	15	ARG	2.4
1	C	195	PRO	2.4
1	D	55	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	92	GLY	2.3
1	D	43	ALA	2.3
1	D	228	THR	2.3
1	D	4	VAL	2.3
1	D	50	GLY	2.3
1	D	184	ALA	2.3
1	D	208	ARG	2.3
1	D	98	PRO	2.3
1	D	291	ARG	2.3
1	B	168	GLU	2.2
1	C	190	SER	2.2
1	D	57	GLY	2.2
1	D	244	THR	2.2
1	D	68	LEU	2.2
1	D	165	LEU	2.2
1	D	177	LEU	2.2
1	D	293	GLU	2.2
1	B	125	GLN	2.2
1	D	95	LEU	2.2
1	D	298	LEU	2.2
1	D	135	GLU	2.2
1	B	193	ARG	2.1
1	D	18	ARG	2.1
1	D	193	ARG	2.1
1	D	161	PRO	2.1
1	D	46	ILE	2.1
1	D	44	VAL	2.1
1	D	287	SER	2.1
1	D	295	GLU	2.1
1	A	247	GLY	2.1
1	C	21	ARG	2.1
1	D	36	GLY	2.0
1	C	22	PRO	2.0
1	D	294	VAL	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)

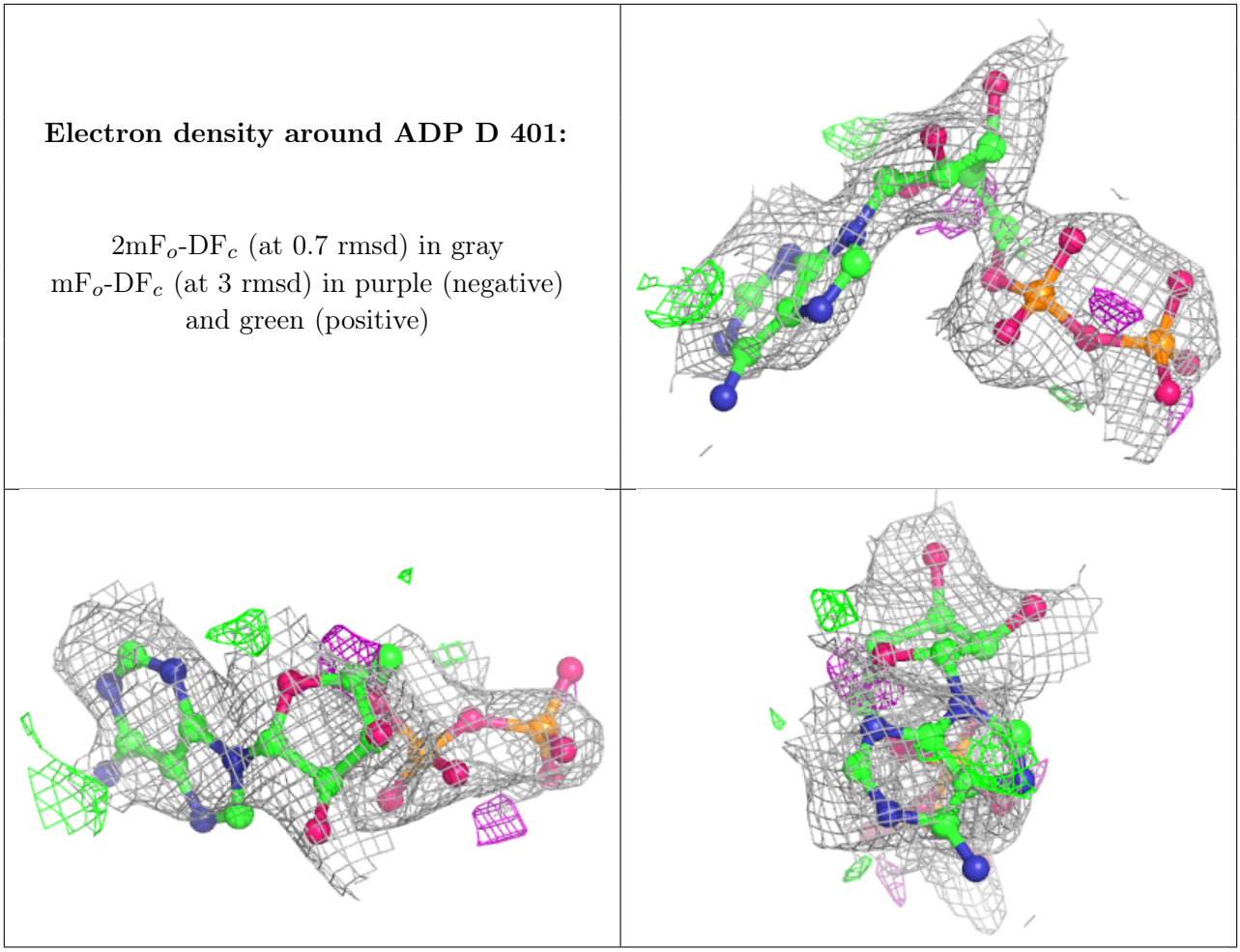
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	D	401	27/27	0.71	0.27	60,72,112,123	0
2	ADP	C	401	27/27	0.90	0.15	28,32,60,74	0
2	ADP	B	401	27/27	0.91	0.17	24,28,68,78	0
2	ADP	A	401	27/27	0.92	0.15	20,24,49,56	0
3	MG	A	402	1/1	0.99	0.16	23,23,23,23	0
3	MG	B	402	1/1	0.99	0.12	9,9,9,9	0
3	MG	C	402	1/1	0.99	0.12	20,20,20,20	0

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

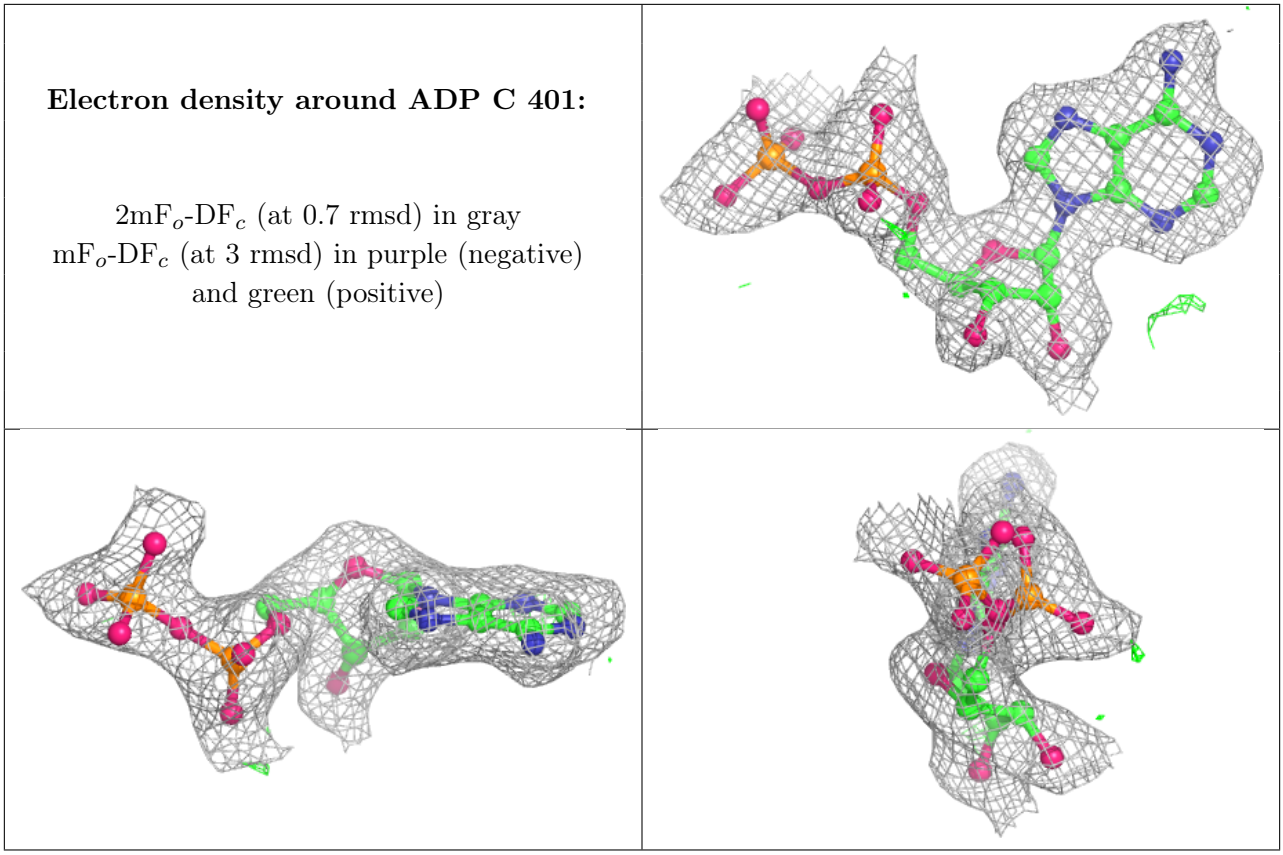
Electron density around ADP D 401:

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



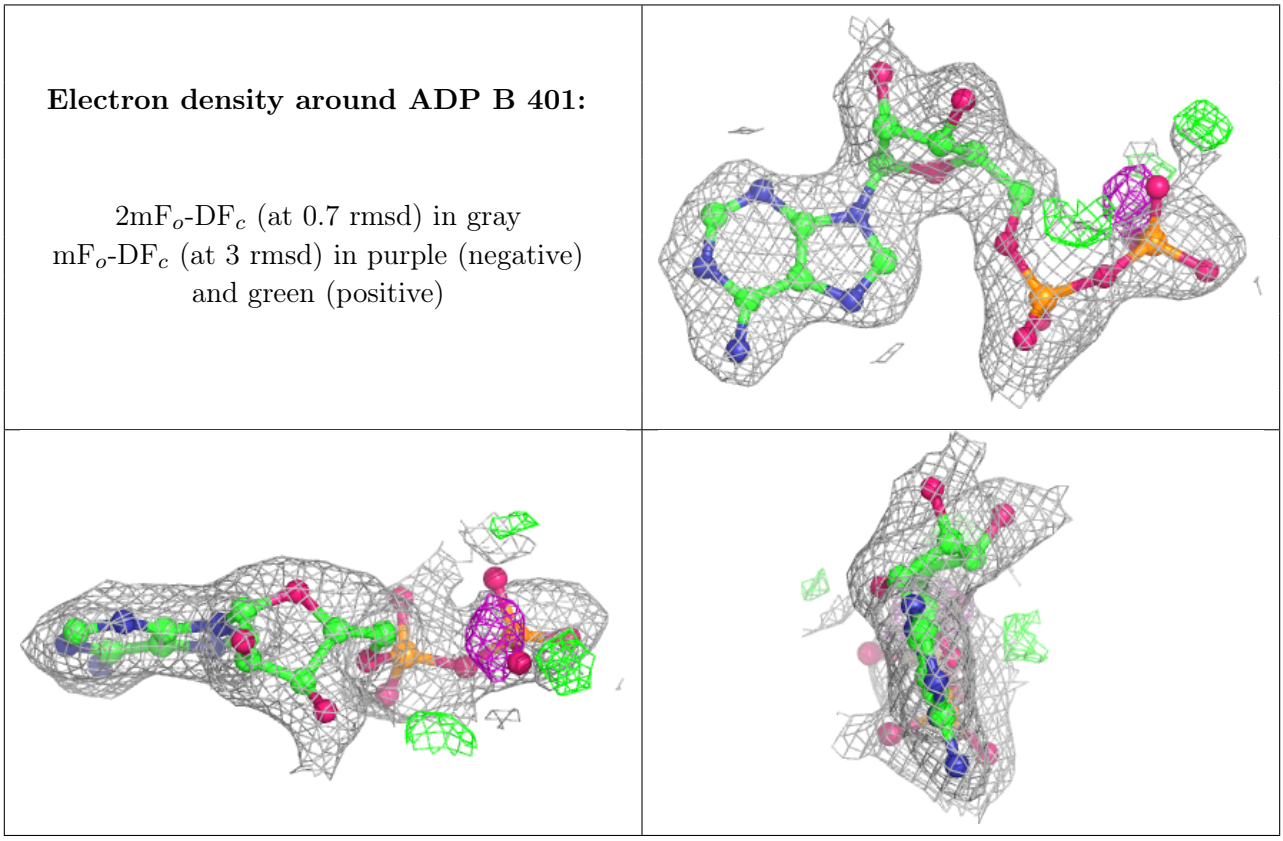
Electron density around ADP C 401:

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



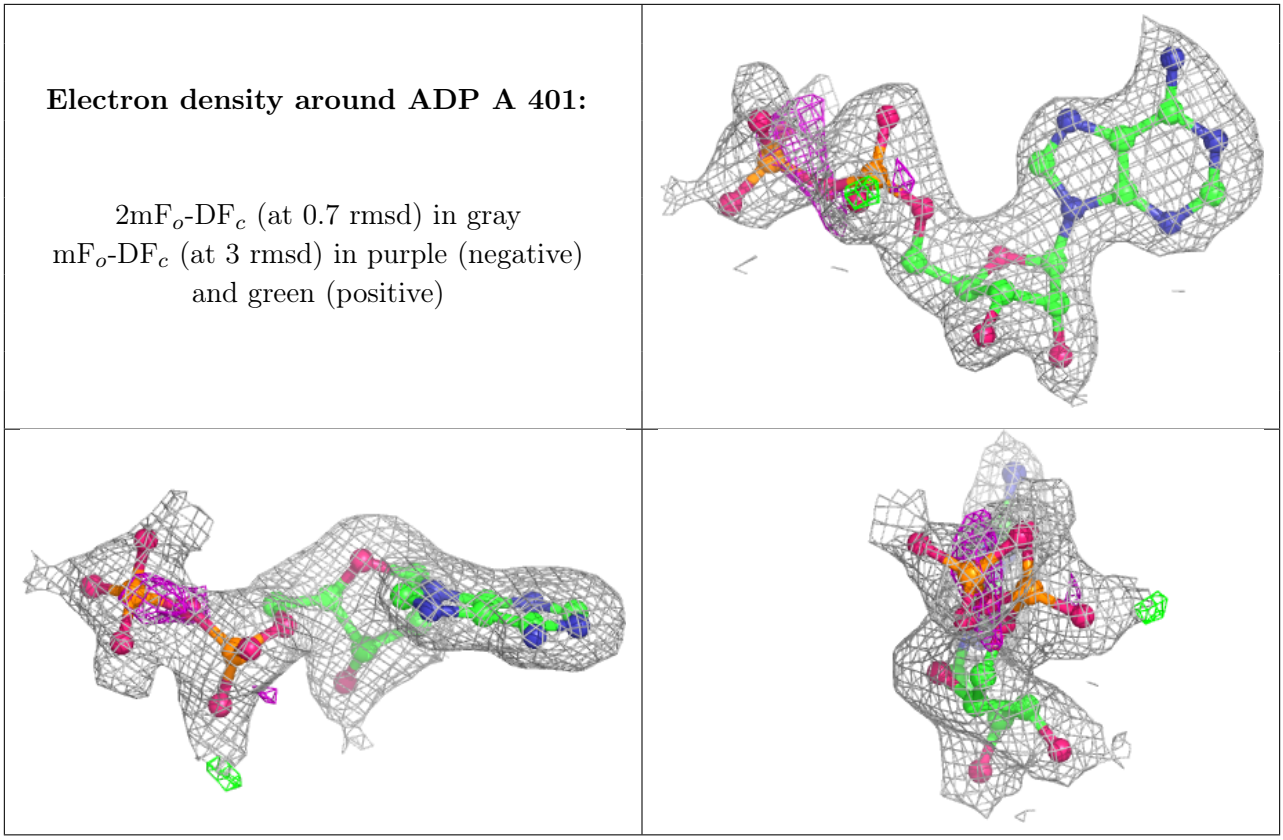
Electron density around ADP B 401:

$2mF_o$-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 401:

$2mF_o$-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.