



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2022 – 06:16 PM JST

PDB ID : 7WHG
Title : Lokiarchaeota gelsolin (2DGel) bound to two molecules of rabbit actin
Authors : Robinson, R.C.; Akil, C.
Deposited on : 2021-12-30
Resolution : 3.25 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.30
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) : 2.30

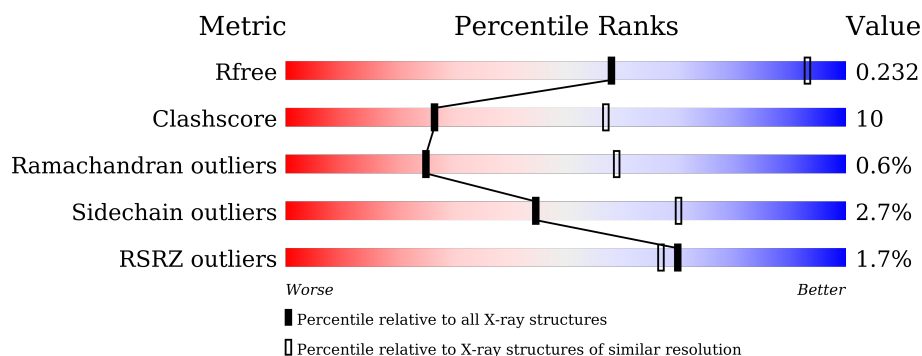
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 $\leq 5\%$. 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	377	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	B	377	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
2	G	335	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>24%</div> <div>34%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7607 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.

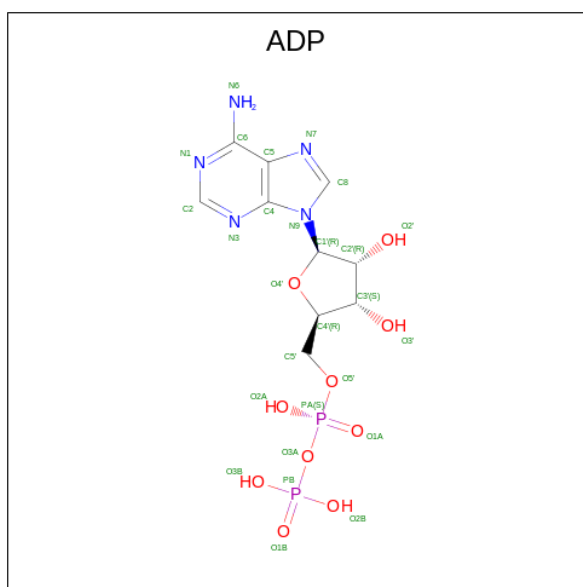
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2899	1833	488	558	20			
1	B	371	Total	C	N	O	S	0	0	0
			2900	1837	489	553	21			

- Molecule 2 is a protein called Lokiarchaeota gelsolin (2DGel).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	221	Total	C	N	O	S	0	0	0
			1745	1107	289	344	5			

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



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

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

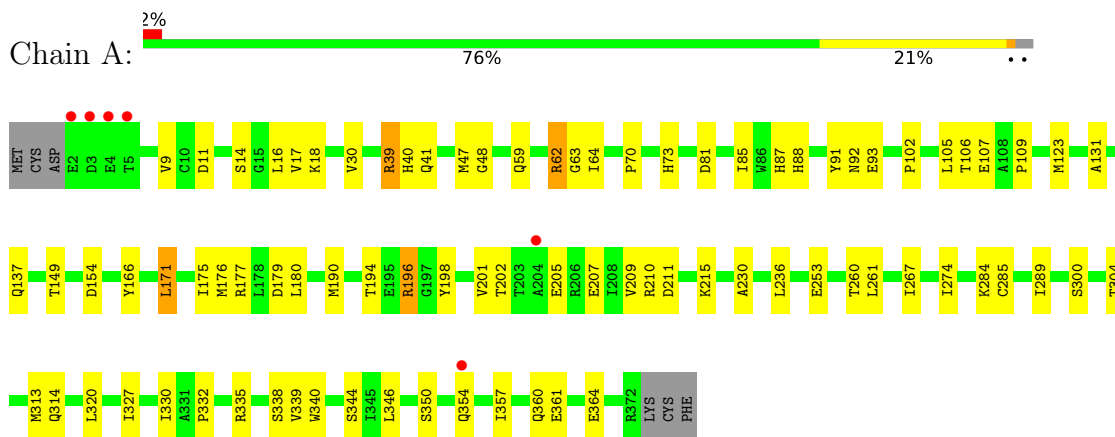
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	1	Total	Ca	0	0
			1	1		
4	G	6	Total	Ca	0	0
			6	6		

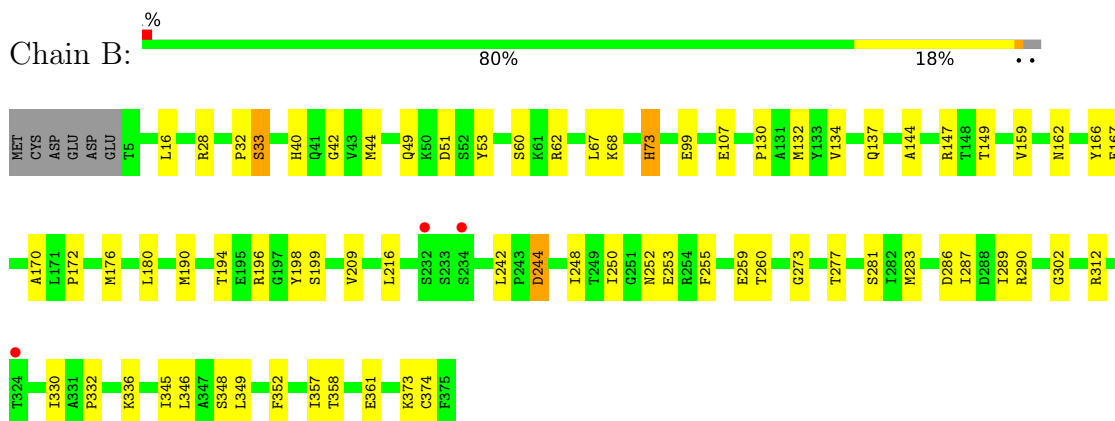
3 Residue-property plots

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.

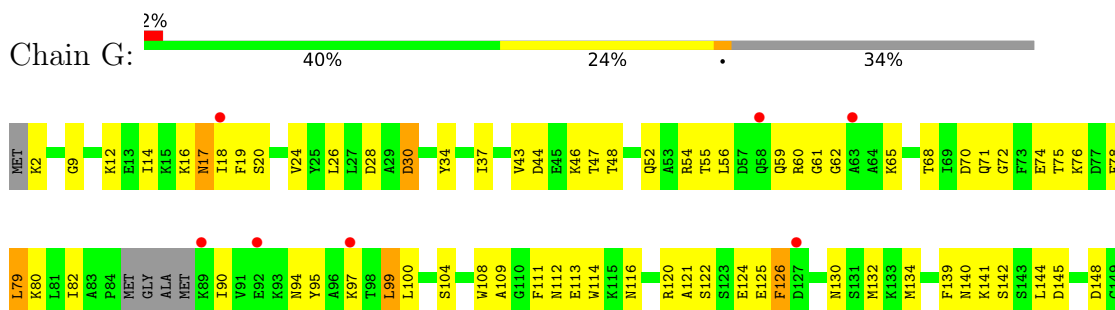
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Lokiarchaeota gelsolin (2DGeI)



F150		VAL
D153		LYS
L154		ALA
G155		ASP
W177		ILE
		THR
		GLU
S180		ALA
I181		ARG
		SER
R185		SER
		ALA
L188		ALA
		PRO
E191		GLY
		ILE
D199		PRO
I200		GLY
E201		ARG
		ILE
A204		ASP
A205		THR
L206		ALA
D207		ILE
R208		LEU
		THR
K213		ILE
		GLN
A217		LYS
		THR
L226		GLU
		GLY
		GLU
		ARG
		ARG
		ARG
		CYS
		PRO
		GLU
		CYS
		ASN
		ILE
		ILE
		ASP
		LYS
		PRO
		GLN
		MET
		ILE
		ILE
		HIS
		GLU
		THR
		VAL
		ASP
		LYS
		LYS
		SER
		ASN
		ILE
		ILE
		LEU
		ASP

TYR
PRO
ARG
VAL
TYR
GLY
LYS
LYS
PHE
LYS
CYS
GLY
SER
CYS
GLY
VAL
GLU
TRP
ARG
GLU
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.66Å 72.06Å 100.39Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 19.91 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.25) 87.9 (19.91-3.25)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.29Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.175 , 0.232 0.172 , 0.232	Depositor DCC
R_{free} test set	845 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CA, ADP, HIC

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	0.60	0/2948	0.76	2/3994 (0.1%)
1	B	0.49	0/2950	0.66	0/3994
2	G	0.57	1/1771 (0.1%)	0.68	1/2380 (0.0%)
All	All	0.55	1/7669 (0.0%)	0.70	3/10368 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	191	GLU	CB-CG	5.06	1.61	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	226	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	171	LEU	CA-CB-CG	-5.31	103.09	115.30
1	A	320	LEU	CB-CG-CD2	-5.14	102.27	111.00

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	2899	0	2861	51	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2900	0	2872	47	1
2	G	1745	0	1731	68	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	G	6	0	0	0	0
All	All	7607	0	7488	155	1

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 10.

All (155) 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:B:147:ARG:NH2	2:G:70:ASP:OD1	2.10	0.85
2:G:17:ASN:HD22	2:G:82:ILE:HG23	1.47	0.79
2:G:95:TYR:HE2	2:G:226:LEU:HB3	1.48	0.79
1:A:314:GLN:NE2	1:A:327:ILE:O	2.20	0.75
2:G:44:ASP:HB2	2:G:99:LEU:HD21	1.70	0.74
1:B:287:ILE:HD12	1:B:290:ARG:HH21	1.52	0.74
1:B:180:LEU:HD11	1:B:260:THR:HG22	1.69	0.73
1:A:39:ARG:NH1	1:A:40:HIS:HB2	2.04	0.72
2:G:24:VAL:HG22	2:G:37:ILE:HA	1.72	0.71
1:B:357:ILE:HD11	1:B:373:LYS:HG3	1.77	0.66
1:B:162:ASN:HB2	1:B:176:MET:HB2	1.78	0.66
1:A:335:ARG:HA	1:A:338:SER:HB3	1.77	0.64
1:B:149:THR:HG23	1:B:166:TYR:HA	1.78	0.64
1:A:107:GLU:O	1:A:137:GLN:HG3	1.97	0.64
1:B:190:MET:HG3	1:B:209:VAL:HG21	1.78	0.64
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.80	0.64
2:G:43:VAL:O	2:G:47:THR:HG22	1.97	0.63
2:G:124:GLU:HG3	2:G:125:GLU:OE1	1.98	0.63
2:G:120:ARG:NH1	2:G:148:ASP:OD2	2.31	0.63
2:G:60:ARG:O	2:G:62:GLY:N	2.29	0.62
1:B:62:ARG:HB2	1:B:67:LEU:HD11	1.82	0.62
1:B:302:GLY:HA2	1:B:336:LYS:HG3	1.81	0.62
2:G:104:SER:O	2:G:112:ASN:HB3	2.01	0.61
1:A:62:ARG:HG2	1:A:63:GLY:N	2.16	0.60
1:A:39:ARG:N	1:A:64:ILE:O	2.35	0.60
1:B:107:GLU:O	1:B:137:GLN:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HG3	1:A:40:HIS:H	1.66	0.60
1:A:11:ASP:HA	1:A:106:THR:OG1	2.01	0.59
1:A:47:MET:N	1:A:48:GLY:HA3	2.17	0.59
1:A:39:ARG:HH12	1:A:40:HIS:HB2	1.66	0.59
1:A:361:GLU:HA	1:A:364:GLU:HG2	1.85	0.58
1:B:196:ARG:HD2	1:B:253:GLU:OE2	2.03	0.58
1:A:190:MET:HG3	1:A:209:VAL:HG21	1.86	0.57
1:B:345:ILE:HG21	2:G:47:THR:HG23	1.88	0.56
1:B:287:ILE:HD12	1:B:290:ARG:NH2	2.20	0.56
2:G:121:ALA:HB2	2:G:134:MET:CE	2.37	0.55
2:G:14:ILE:HG22	2:G:16:LYS:H	1.72	0.54
1:B:345:ILE:HD13	2:G:100:LEU:HD21	1.89	0.54
1:A:62:ARG:HG2	1:A:63:GLY:H	1.73	0.53
1:A:16:LEU:HB2	1:A:18:LYS:HZ2	1.74	0.53
2:G:114:TRP:NE1	2:G:116:ASN:OD1	2.42	0.53
1:A:106:THR:HB	1:A:137:GLN:HG2	1.91	0.53
2:G:20:SER:OG	2:G:94:ASN:O	2.27	0.53
2:G:126:PHE:CD2	2:G:132:MET:HA	2.44	0.53
2:G:141:LYS:HD2	2:G:207:ASP:OD1	2.08	0.52
1:B:357:ILE:HG12	1:B:373:LYS:HE3	1.90	0.52
2:G:44:ASP:HB2	2:G:99:LEU:CD2	2.38	0.52
1:A:194:THR:HA	1:A:198:TYR:O	2.09	0.52
1:B:244:ASP:OD1	1:B:244:ASP:N	2.40	0.52
2:G:17:ASN:ND2	2:G:82:ILE:HG23	2.21	0.52
1:B:176:MET:HG3	1:B:281:SER:HB2	1.93	0.51
1:B:144:ALA:HA	2:G:47:THR:HB	1.93	0.50
1:A:88:HIS:CD2	1:A:92:ASN:HD22	2.30	0.50
1:A:205:GLU:O	1:A:209:VAL:HG23	2.12	0.50
1:B:242:LEU:HD21	1:B:248:ILE:HD12	1.94	0.50
2:G:43:VAL:HA	2:G:46:LYS:HD3	1.93	0.50
1:B:167:GLU:OE2	2:G:65:LYS:HA	2.12	0.50
2:G:201:GLU:OE2	2:G:208:ARG:NH2	2.41	0.50
2:G:44:ASP:OD2	2:G:99:LEU:HD23	2.12	0.49
2:G:9:GLY:HA2	2:G:48:THR:HG21	1.93	0.49
2:G:122:SER:HB3	2:G:124:GLU:CG	2.43	0.49
1:B:345:ILE:HG21	2:G:47:THR:CG2	2.41	0.49
2:G:139:PHE:CE2	2:G:206:LEU:HA	2.48	0.49
1:A:131:ALA:HA	1:A:357:ILE:O	2.13	0.49
2:G:153:ASP:OD2	2:G:181:ILE:HD13	2.12	0.49
1:B:33:SER:O	1:B:33:SER:OG	2.30	0.49
2:G:155:GLY:HA2	2:G:185:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:34:TYR:CE1	2:G:78:PHE:HB2	2.48	0.48
1:A:88:HIS:CE1	1:A:93:GLU:HG2	2.49	0.48
1:B:44:MET:CE	1:B:51:ASP:HA	2.44	0.48
1:B:283:MET:SD	1:B:290:ARG:NH1	2.86	0.48
1:B:170:ALA:O	1:B:172:PRO:HD3	2.14	0.48
2:G:144:LEU:HD22	2:G:150:PHE:CD2	2.49	0.48
1:A:230:ALA:HB2	1:A:236:LEU:HD12	1.94	0.48
1:B:16:LEU:HD23	1:B:32:PRO:HA	1.96	0.48
2:G:2:LYS:HB2	2:G:28:ASP:HB3	1.96	0.47
2:G:199:ASP:OD1	2:G:199:ASP:N	2.40	0.47
1:A:16:LEU:HB2	1:A:18:LYS:NZ	2.29	0.47
1:A:70:PRO:HG3	1:A:81:ASP:HB3	1.97	0.47
2:G:74:GLU:HB3	2:G:78:PHE:HD2	1.80	0.47
1:A:180:LEU:HD11	1:A:260:THR:HG22	1.97	0.47
1:A:202:THR:OG1	1:A:205:GLU:HG3	2.14	0.47
1:B:286:ASP:HB3	1:B:289:ILE:HG12	1.97	0.47
2:G:60:ARG:C	2:G:62:GLY:H	2.15	0.47
2:G:120:ARG:NH1	2:G:122:SER:HG	2.13	0.47
1:A:346:LEU:HA	1:A:346:LEU:HD12	1.48	0.46
1:B:287:ILE:CD1	1:B:290:ARG:HH21	2.26	0.46
1:A:14:SER:OG	3:A:401:ADP:O1B	2.29	0.46
2:G:95:TYR:CE2	2:G:226:LEU:HB3	2.38	0.46
1:A:109:PRO:HB3	1:A:175:ILE:HD13	1.97	0.46
1:A:180:LEU:HD12	1:A:267:ILE:HD11	1.98	0.46
1:B:68:LYS:HB2	1:B:68:LYS:HE2	1.76	0.46
1:B:49:GLN:HG3	1:B:53:TYR:OH	2.16	0.45
2:G:204:ALA:O	2:G:208:ARG:HG3	2.16	0.45
1:A:149:THR:HG23	1:A:166:TYR:HA	1.97	0.45
1:B:345:ILE:CD1	2:G:100:LEU:HD21	2.46	0.45
2:G:75:THR:HG23	2:G:78:PHE:H	1.81	0.45
2:G:124:GLU:H	2:G:124:GLU:HG2	1.27	0.45
2:G:26:LEU:HD12	2:G:34:TYR:O	2.17	0.44
1:B:330:ILE:HG22	1:B:332:PRO:HD3	1.98	0.44
1:A:177:ARG:NH1	1:A:179:ASP:OD2	2.51	0.44
1:A:207:GLU:OE1	1:A:210:ARG:NH2	2.51	0.44
1:B:147:ARG:HG2	2:G:68:THR:HG21	1.99	0.44
1:A:350:SER:N	2:G:130:ASN:OD1	2.46	0.44
1:B:73:HIC:HA	1:B:159:VAL:HB	1.99	0.44
1:A:9:VAL:HG21	1:A:344:SER:HA	1.99	0.44
2:G:44:ASP:N	2:G:44:ASP:OD1	2.51	0.43
1:B:40:HIS:O	1:B:42:GLY:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:71:GLN:HG3	2:G:72:GLY:N	2.32	0.43
2:G:121:ALA:HB2	2:G:134:MET:HE3	1.99	0.43
2:G:134:MET:SD	2:G:177:TRP:CG	3.12	0.43
1:B:194:THR:HA	1:B:198:TYR:O	2.18	0.43
2:G:79:LEU:HD23	2:G:79:LEU:HA	1.80	0.43
1:A:154:ASP:HA	1:A:300:SER:O	2.18	0.43
1:B:346:LEU:HG	1:B:352:PHE:CD2	2.54	0.43
2:G:188:LEU:H	2:G:188:LEU:HD23	1.84	0.43
1:B:99:GLU:O	1:B:130:PRO:HG3	2.19	0.43
1:A:304:THR:OG1	1:A:335:ARG:HD2	2.18	0.42
1:B:273:GLY:O	1:B:277:THR:HG23	2.19	0.42
1:A:261:LEU:HB3	1:A:274:ILE:HD13	2.01	0.42
2:G:55:THR:O	2:G:59:GLN:HG3	2.20	0.42
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.75	0.42
2:G:113:GLU:H	2:G:113:GLU:HG2	1.40	0.42
1:A:102:PRO:HB3	1:A:131:ALA:HB3	2.00	0.42
2:G:140:ASN:ND2	2:G:142:SER:OG	2.53	0.42
2:G:30:ASP:O	2:G:60:ARG:NH1	2.52	0.42
2:G:108:TRP:HZ2	2:G:114:TRP:CG	2.38	0.42
1:A:340:TRP:CZ3	1:A:344:SER:HB2	2.55	0.42
1:A:105:LEU:HD11	1:A:123:MET:SD	2.59	0.41
1:A:330:ILE:HG22	1:A:332:PRO:HD3	2.02	0.41
1:B:349:LEU:HD21	2:G:48:THR:HG23	2.02	0.41
2:G:19:PHE:HB2	2:G:90:ILE:O	2.20	0.41
1:B:259:GLU:CD	1:B:312:ARG:HH12	2.24	0.41
2:G:122:SER:HB3	2:G:124:GLU:HG2	2.02	0.41
1:A:176:MET:CE	1:A:284:LYS:HD2	2.50	0.41
1:B:216:LEU:HB3	1:B:250:ILE:HD11	2.01	0.41
2:G:145:ASP:H	2:G:150:PHE:HZ	1.68	0.41
1:A:180:LEU:C	1:A:180:LEU:HD23	2.41	0.41
1:B:132:MET:CE	1:B:134:VAL:HG23	2.51	0.41
2:G:76:LYS:O	2:G:80:LYS:HG2	2.20	0.41
1:A:211:ASP:OD1	1:A:215:LYS:NZ	2.44	0.41
1:B:358:THR:OG1	1:B:361:GLU:HG3	2.20	0.41
2:G:16:LYS:HB3	2:G:18:ILE:HG13	2.02	0.41
1:B:252:ASN:HA	1:B:255:PHE:CE2	2.55	0.41
2:G:111:PHE:CZ	2:G:213:LYS:HD2	2.56	0.41
1:A:17:VAL:O	1:A:30:VAL:HA	2.21	0.41
1:A:81:ASP:O	1:A:85:ILE:HG12	2.20	0.41
2:G:52:GLN:O	2:G:56:LEU:HG	2.21	0.41
1:B:44:MET:HE3	1:B:51:ASP:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:PHE:CE2	2:G:213:LYS:HD2	2.56	0.40
2:G:120:ARG:HG3	2:G:150:PHE:CE1	2.57	0.40
1:A:87:HIS:CE1	1:A:91:TYR:CD2	3.10	0.40
1:A:196:ARG:HD2	1:A:253:GLU:OE2	2.22	0.40
1:A:300:SER:HB2	1:A:338:SER:OG	2.21	0.40
1:B:28:ARG:NH1	2:G:109:ALA:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:NE2	1:B:99:GLU:OE1[2_555]	2.16	0.04

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	368/377 (98%)	351 (95%)	14 (4%)	3 (1%)	19	52
1	B	368/377 (98%)	356 (97%)	11 (3%)	1 (0%)	41	72
2	G	217/335 (65%)	203 (94%)	12 (6%)	2 (1%)	17	50
All	All	953/1089 (88%)	910 (96%)	37 (4%)	6 (1%)	25	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	61	GLY
2	G	217	ALA
1	B	244	ASP
1	A	62	ARG
1	A	201	VAL
1	A	339	VAL

5.3.2 Protein sidechains ⓘ

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	313/319 (98%)	307 (98%)	6 (2%)	57	76
1	B	313/319 (98%)	308 (98%)	5 (2%)	62	79
2	G	186/283 (66%)	175 (94%)	11 (6%)	19	50
All	All	812/921 (88%)	790 (97%)	22 (3%)	44	70

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	59	GLN
1	A	196	ARG
1	A	313	MET
1	A	354	GLN
1	A	360	GLN
1	B	33	SER
1	B	60	SER
1	B	199	SER
1	B	348	SER
1	B	374	CYS
2	G	12	LYS
2	G	17	ASN
2	G	30	ASP
2	G	54	ARG
2	G	79	LEU
2	G	97	LYS
2	G	99	LEU
2	G	126	PHE
2	G	180	SER
2	G	188	LEU
2	G	226	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
2	G	140	ASN
2	G	162	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	HIC	B	73	1	8,11,12	1.83	2 (25%)	6,14,16	1.67	1 (16%)
1	HIC	A	73	1	8,11,12	2.07	2 (25%)	6,14,16	0.91	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
1	HIC	B	73	1	-	2/5/6/8	0/1/1/1
1	HIC	A	73	1	-	3/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-CG	4.78	1.43	1.36
1	B	73	HIC	CD2-CG	4.23	1.42	1.36
1	A	73	HIC	CD2-NE2	2.49	1.41	1.38
1	B	73	HIC	CD2-NE2	2.11	1.41	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIC	CB-CA-C	-3.51	104.89	111.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	O-C-CA-CB
1	A	73	HIC	CA-CB-CG-ND1
1	A	73	HIC	C-CA-CB-CG
1	B	73	HIC	CA-CB-CG-ND1
1	B	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	73	HIC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	B	401	4	24,29,29	1.09	1 (4%)	29,45,45	1.66	8 (27%)
3	ADP	A	401	4	24,29,29	0.93	1 (4%)	29,45,45	1.61	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	401	4	-	3/12/32/32	0/3/3/3
3	ADP	A	401	4	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ADP	C5-C4	2.90	1.48	1.40
3	A	401	ADP	C2'-C1'	-2.25	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ADP	C4-C5-N7	-4.13	105.10	109.40
3	A	401	ADP	N3-C2-N1	-3.59	123.07	128.68
3	B	401	ADP	C1'-N9-C4	-2.92	121.52	126.64
3	A	401	ADP	N6-C6-N1	2.87	124.53	118.57
3	B	401	ADP	C5-C6-N6	2.75	124.53	120.35
3	A	401	ADP	O3A-PB-O1B	-2.68	96.32	111.19
3	A	401	ADP	O2A-PA-O5'	2.58	119.74	107.75
3	B	401	ADP	O3B-PB-O2B	2.52	117.27	107.64
3	B	401	ADP	N3-C2-N1	-2.41	124.91	128.68
3	B	401	ADP	O5'-C5'-C4'	2.38	117.17	108.99
3	B	401	ADP	C2-N1-C6	2.37	122.80	118.75
3	B	401	ADP	PA-O3A-PB	-2.16	125.40	132.83
3	A	401	ADP	C2'-C3'-C4'	2.14	106.80	102.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

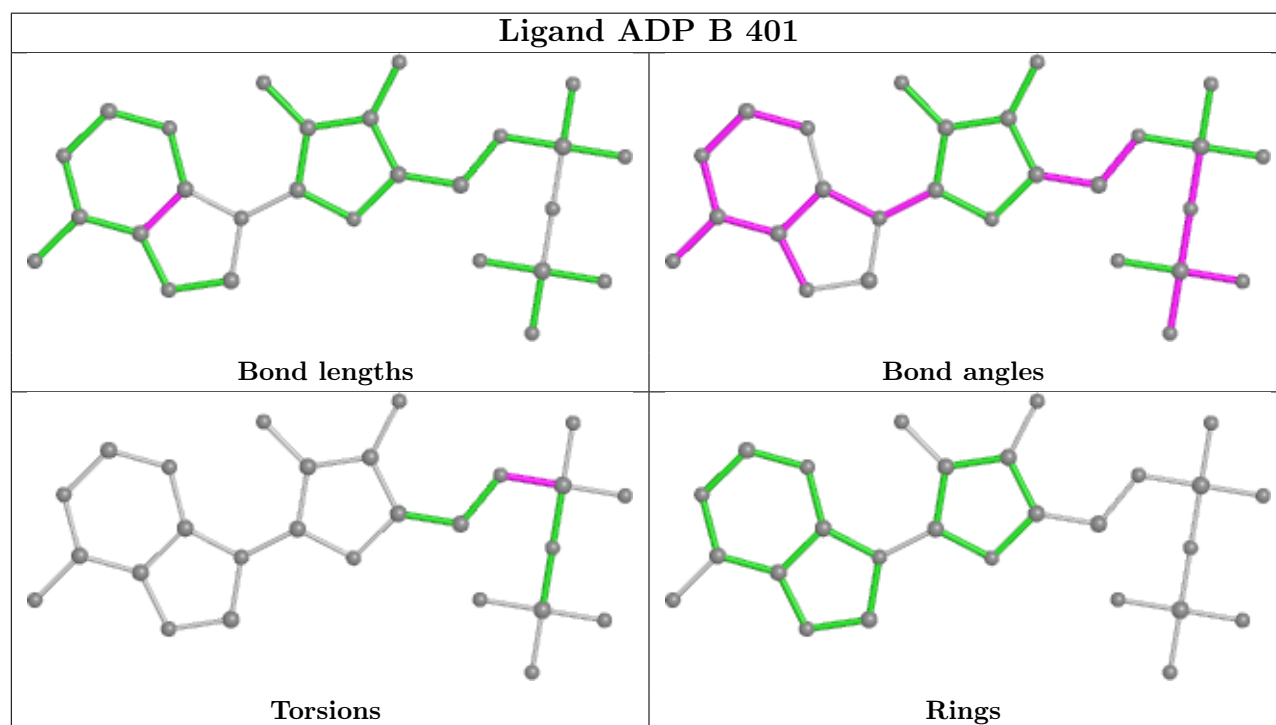
Mol	Chain	Res	Type	Atoms
3	B	401	ADP	C5'-O5'-PA-O1A
3	B	401	ADP	C5'-O5'-PA-O3A
3	B	401	ADP	C5'-O5'-PA-O2A

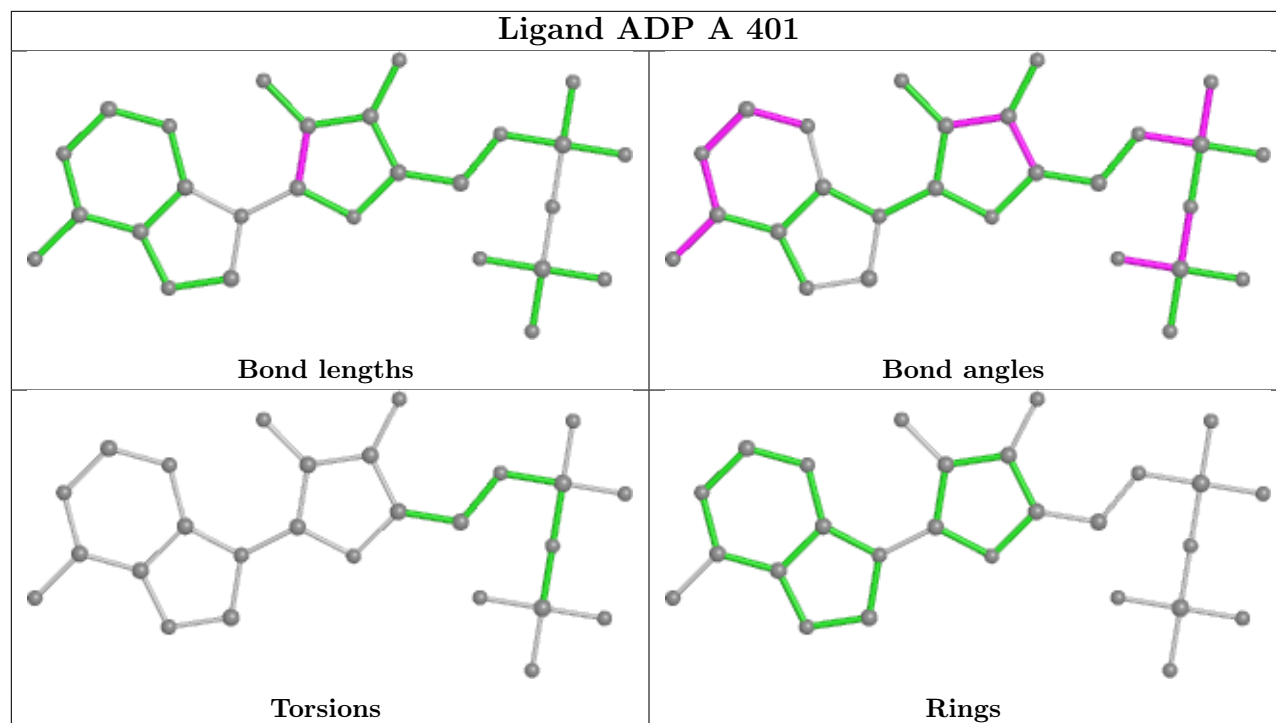
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	1	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 than 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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	370/377 (98%)	-0.50	6 (1%) 72 69	15, 45, 91, 154	0
1	B	370/377 (98%)	-0.32	3 (0%) 86 86	40, 74, 115, 144	0
2	G	221/335 (65%)	-0.02	7 (3%) 47 45	35, 77, 133, 152	0
All	All	961/1089 (88%)	-0.32	16 (1%) 70 67	15, 64, 118, 154	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	4.1
1	B	324	THR	3.5
1	A	4	GLU	3.4
2	G	18	ILE	3.2
1	A	204	ALA	2.9
1	A	2	GLU	2.6
2	G	89	LYS	2.5
2	G	92	GLU	2.4
1	B	234	SER	2.3
1	B	232	SER	2.3
2	G	63	ALA	2.2
1	A	354	GLN	2.2
1	A	5	THR	2.2
2	G	127	ASP	2.1
2	G	97	LYS	2.1
2	G	58	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	HIC	B	73	11/12	0.86	0.32	79,84,86,87	0
1	HIC	A	73	11/12	0.93	0.22	40,54,64,65	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

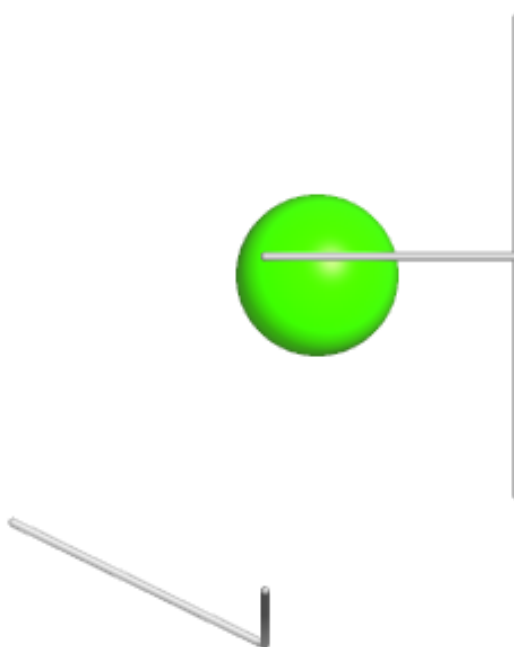
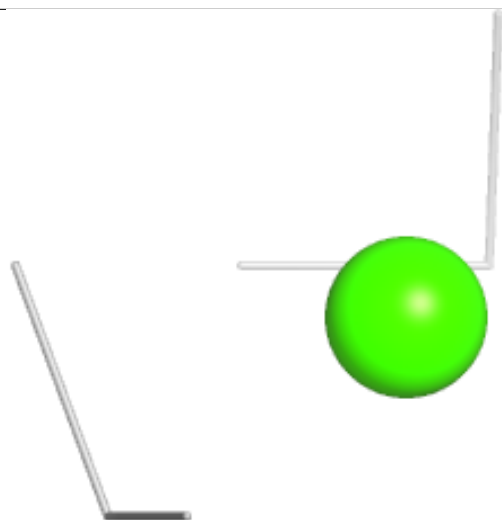
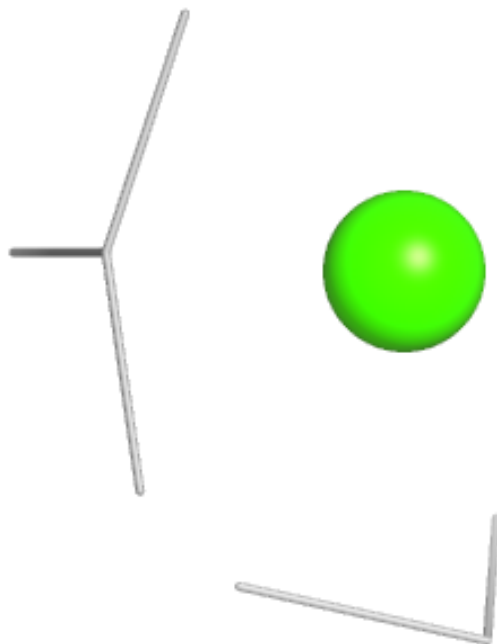
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	G	405	1/1	0.68	0.08	116,116,116,116	0
4	CA	B	402	1/1	0.89	0.30	55,55,55,55	0
4	CA	A	403	1/1	0.94	0.21	93,93,93,93	0
4	CA	G	406	1/1	0.94	0.20	78,78,78,78	0
4	CA	G	402	1/1	0.97	0.10	59,59,59,59	0
4	CA	G	403	1/1	0.97	0.06	64,64,64,64	0
3	ADP	B	401	27/27	0.97	0.15	41,48,54,56	0
4	CA	G	401	1/1	0.97	0.18	82,82,82,82	0
4	CA	G	404	1/1	0.98	0.04	35,35,35,35	0
4	CA	A	402	1/1	0.98	0.20	40,40,40,40	0
3	ADP	A	401	27/27	0.98	0.14	28,33,36,37	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.

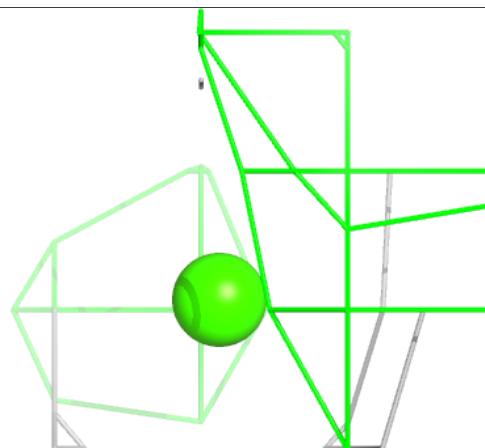
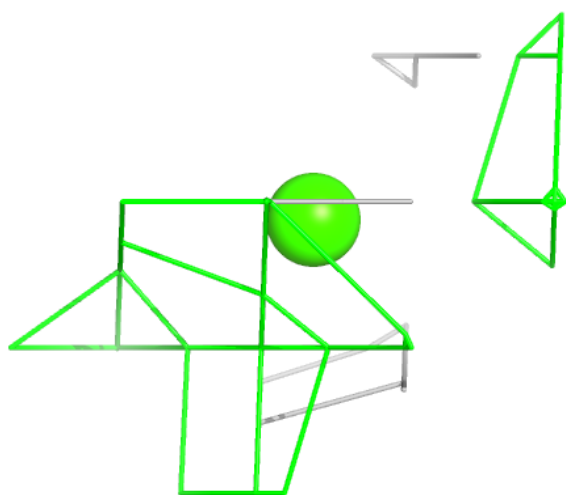
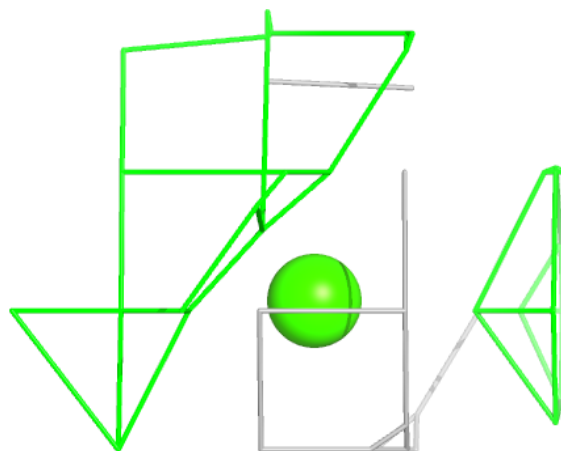
Electron density around CA G 405:

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



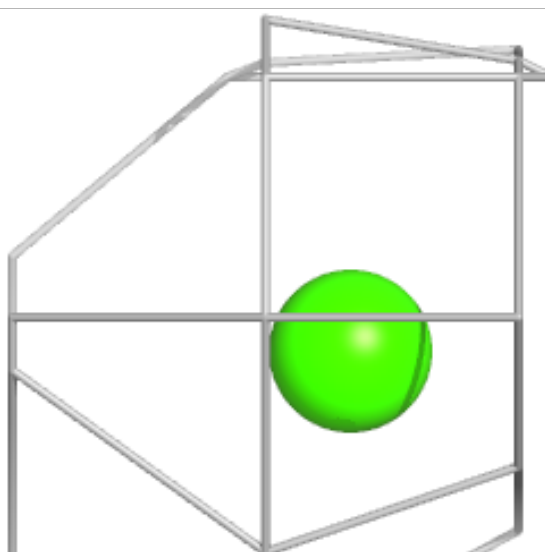
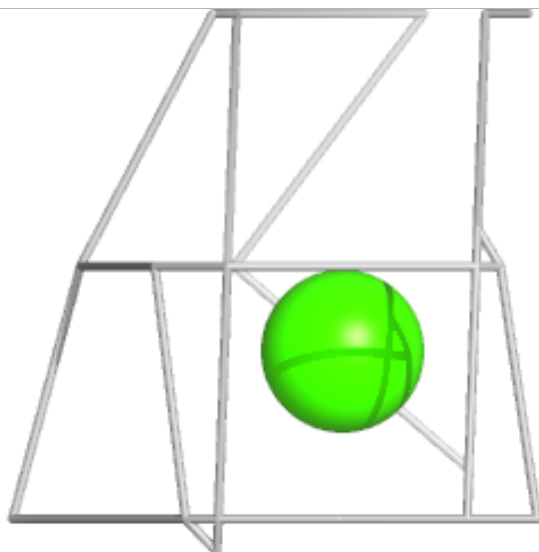
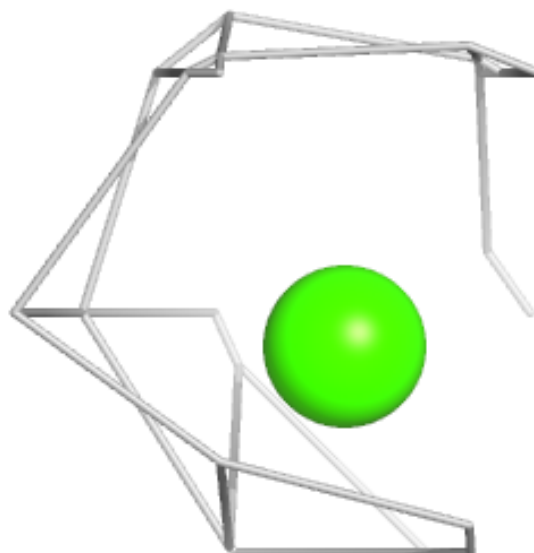
Electron density around CA B 402:

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and green (positive)



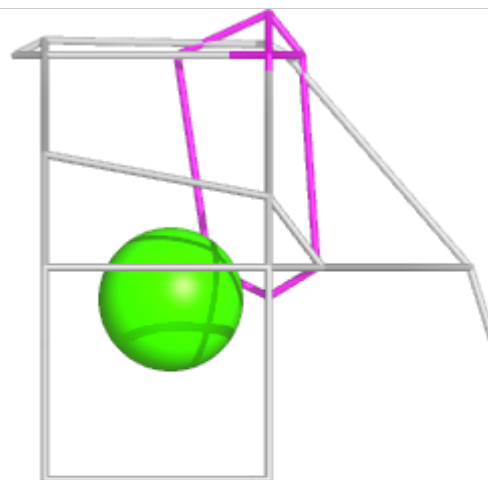
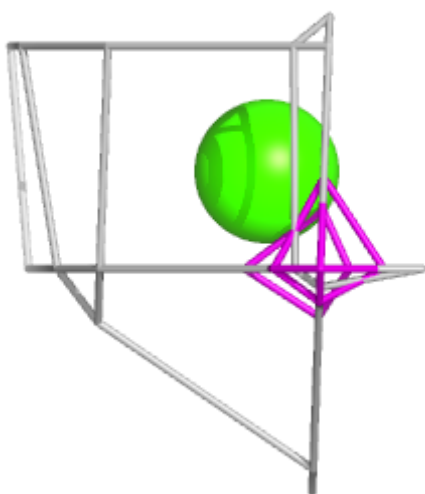
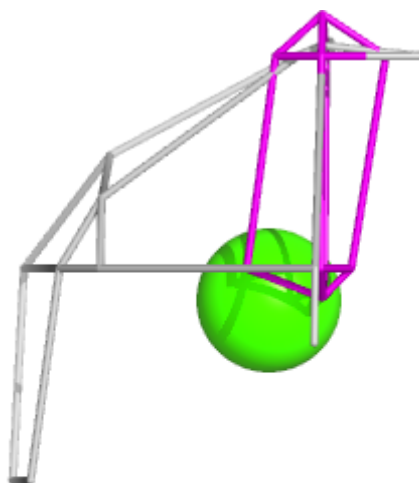
Electron density around CA A 403:

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and green (positive)



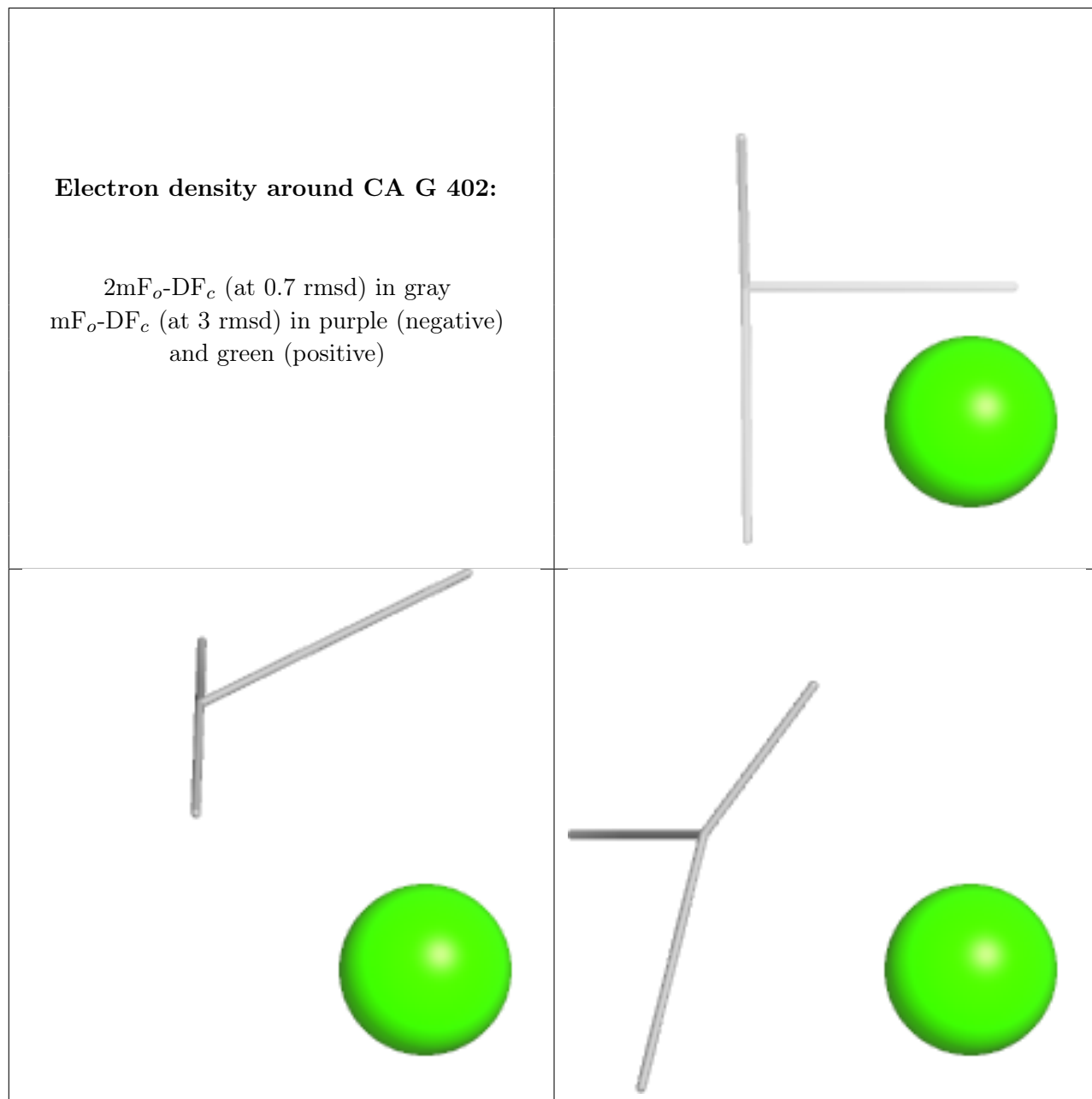
Electron density around CA G 406:

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and green (positive)



Electron density around CA G 402:

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



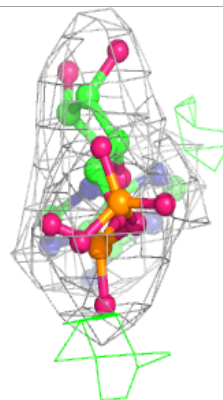
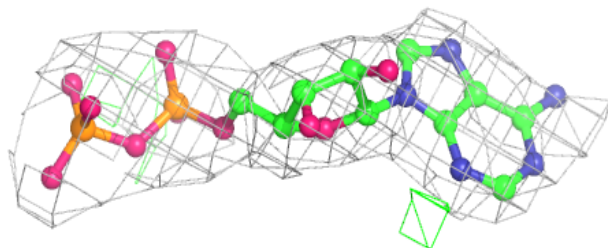
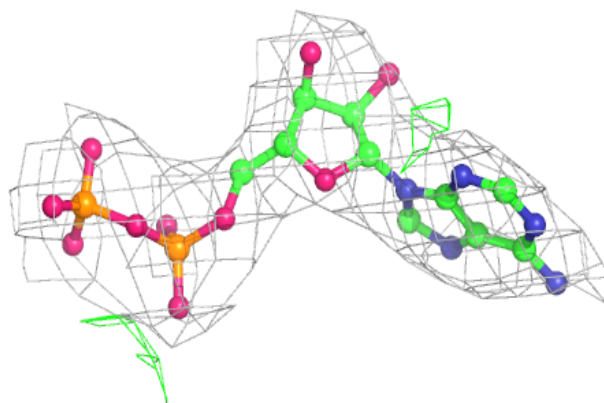
Electron density around CA G 403:

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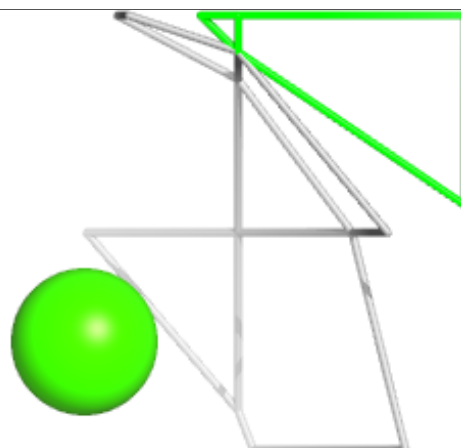
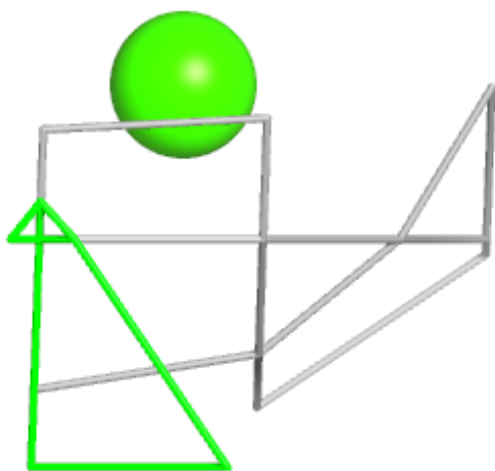
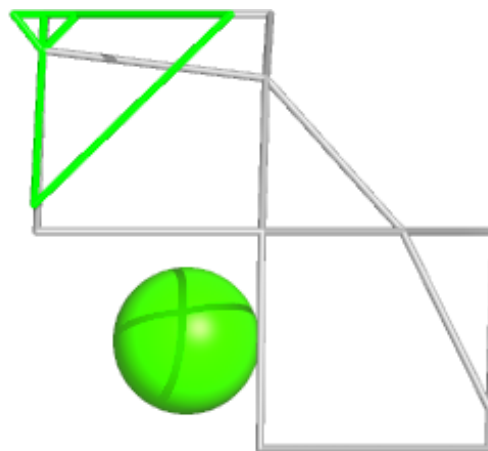
Electron density around ADP B 401:

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and green (positive)



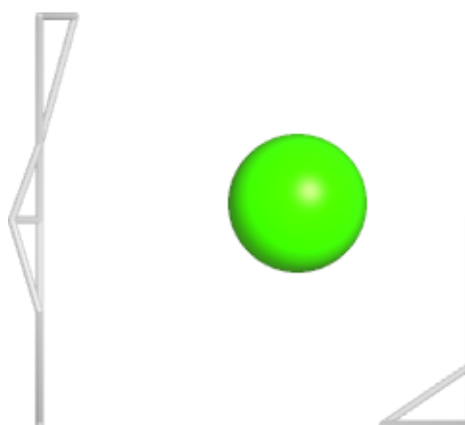
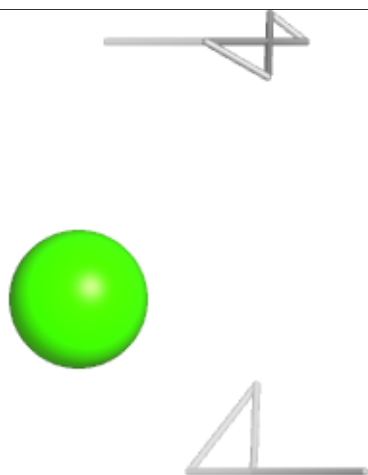
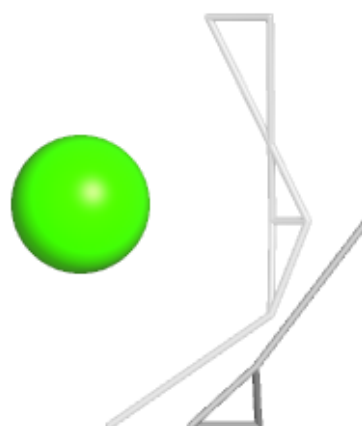
Electron density around CA G 401:

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



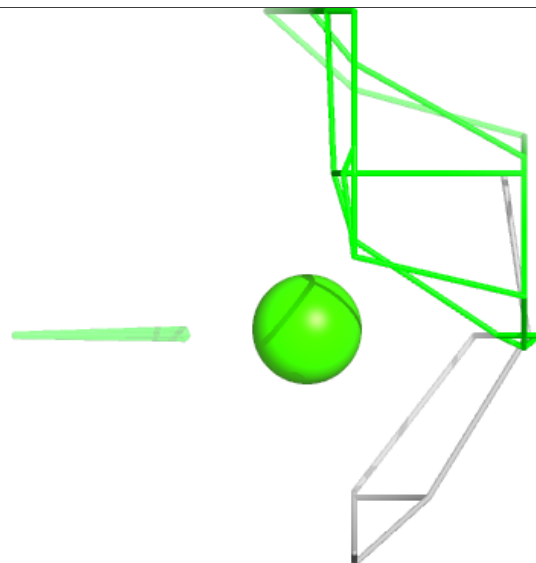
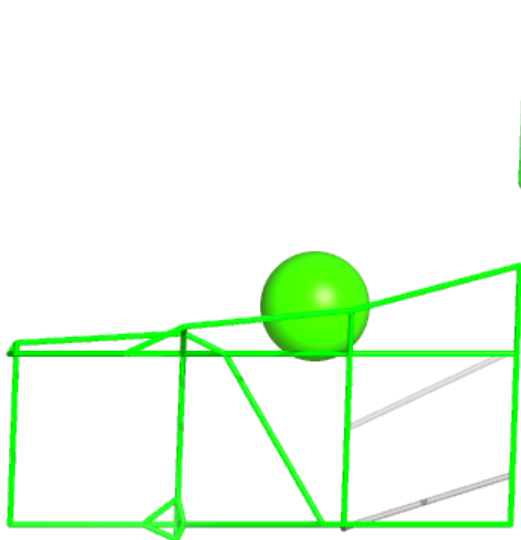
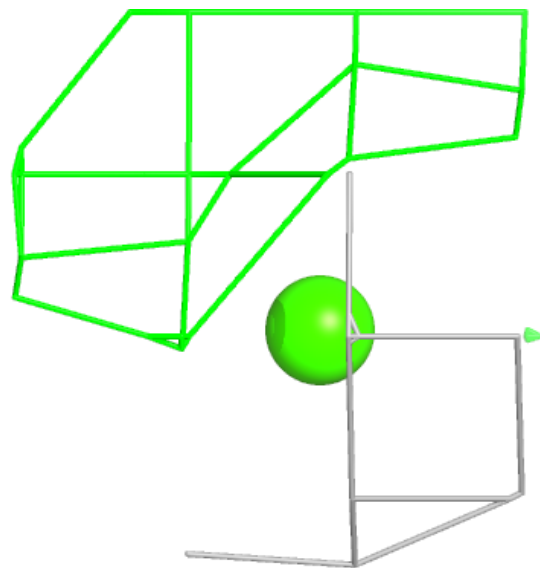
Electron density around CA G 404:

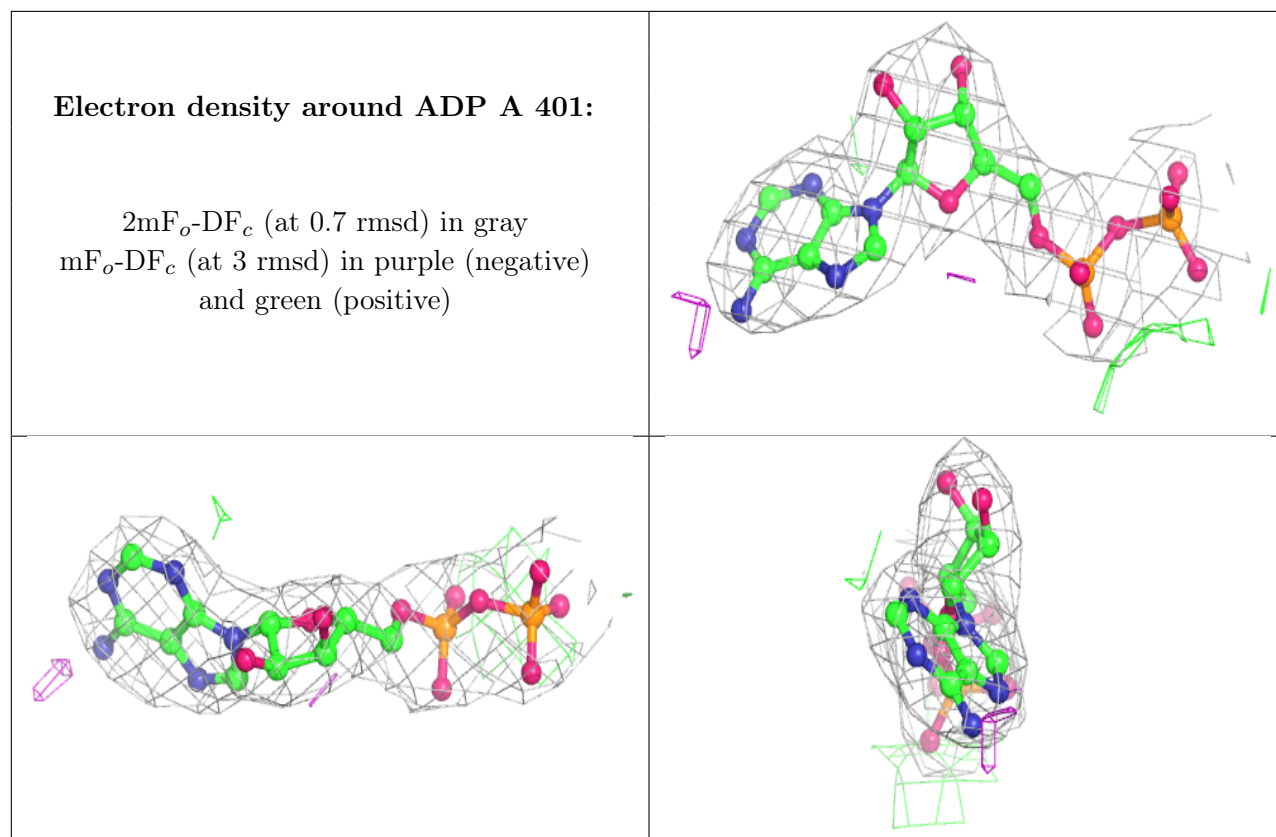
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA A 402:

$2mF_o-DF_c$ (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.