



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:48 PM BST

PDB ID : 4Z9M
Title : Crystal structure of human sarcomeric mitochondrial creatine kinase
Authors : Rabeh, W.M.; Tempel, W.; Nedyalkova, L.; Landry, R.; Arrowsmith, C.H.;
Edwards, A.M.; Bountra, C.; Bochkarev, A.; Park, H.; Structural Genomics
Consortium (SGC)
Deposited on : 2015-04-10
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

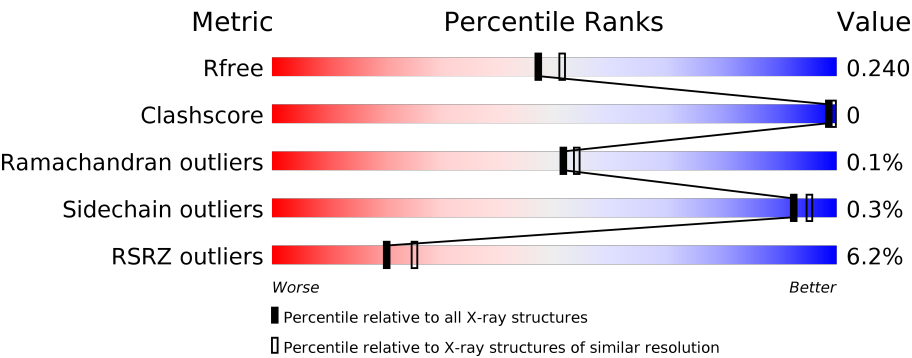
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	392	<div><div>12%</div><div><div></div><div>89%</div><div></div><div>10%</div></div></div>
1	B	392	<div><div>9%</div><div><div></div><div>75%</div><div></div><div>23%</div></div></div>
1	C	392	<div><div>5%</div><div><div></div><div>93%</div><div></div><div></div></div></div>
1	D	392	<div><div>5%</div><div><div></div><div>93%</div><div></div><div></div></div></div>
1	E	392	<div><div>%</div><div><div></div><div>93%</div><div></div><div>6%</div></div></div>
1	F	392	<div><div></div><div><div></div><div>92%</div><div></div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	392	
1	H	392	

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
3	UNX	A	503	-	-	-	X
3	UNX	B	502	-	-	-	X
3	UNX	C	502	-	-	-	X
3	UNX	C	503	-	-	-	X
3	UNX	E	503	-	-	-	X
3	UNX	E	504	-	-	-	X
3	UNX	E	505	-	-	X	-
3	UNX	F	509	-	-	-	X
3	UNX	G	503	-	-	-	X
3	UNX	H	503	-	-	-	X
3	UNX	H	504	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23253 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 Creatine kinase S-type, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2649	1657	472	505	15			
1	B	300	Total	C	N	O	S	0	7	0
			2323	1461	414	433	15			
1	C	375	Total	C	N	O	S	0	7	1
			2952	1870	524	542	16			
1	D	375	Total	C	N	O	S	0	5	0
			2965	1875	524	549	17			
1	E	369	Total	C	N	O	S	0	8	0
			2948	1861	525	546	16			
1	F	369	Total	C	N	O	S	0	7	0
			2968	1871	535	546	16			
1	G	313	Total	C	N	O	S	0	3	2
			2399	1507	437	440	15			
1	H	365	Total	C	N	O	S	0	10	0
			2894	1826	518	534	16			

There are 16 discrepancies between the modelled and reference sequences:

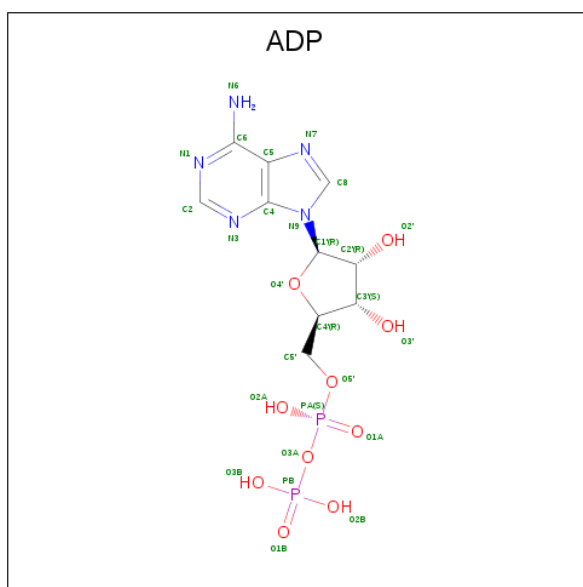
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP P17540
A	26	SER	-	expression tag	UNP P17540
B	25	GLY	-	expression tag	UNP P17540
B	26	SER	-	expression tag	UNP P17540
C	25	GLY	-	expression tag	UNP P17540
C	26	SER	-	expression tag	UNP P17540
D	25	GLY	-	expression tag	UNP P17540
D	26	SER	-	expression tag	UNP P17540
E	25	GLY	-	expression tag	UNP P17540
E	26	SER	-	expression tag	UNP P17540
F	25	GLY	-	expression tag	UNP P17540
F	26	SER	-	expression tag	UNP P17540
G	25	GLY	-	expression tag	UNP P17540

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Chain	Residue	Modelled	Actual	Comment	Reference
G	26	SER	-	expression tag	UNP P17540
H	25	GLY	-	expression tag	UNP P17540
H	26	SER	-	expression tag	UNP P17540

- 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		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	1
			46	20	10	14	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	5	Total X 5 5	0	0
3	D	8	Total X 8 8	0	0
3	E	15	Total X 15 15	0	0
3	H	13	Total X 13 13	0	0
3	B	6	Total X 6 6	0	0
3	C	6	Total X 6 6	0	0
3	A	7	Total X 7 7	0	0
3	F	11	Total X 11 11	0	0

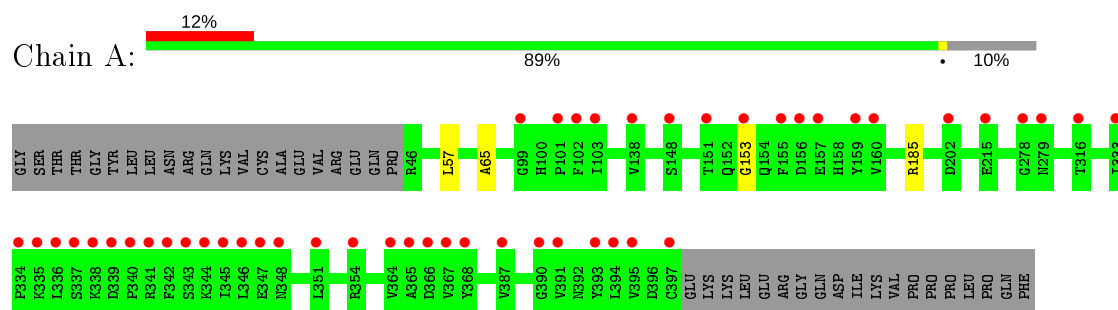
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 62 62	0	0
4	B	60	Total O 60 60	0	0
4	C	136	Total O 136 136	0	0
4	D	145	Total O 145 145	0	0
4	E	141	Total O 141 141	0	1
4	F	163	Total O 163 163	0	0
4	G	61	Total O 61 61	0	0
4	H	81	Total O 81 81	0	1

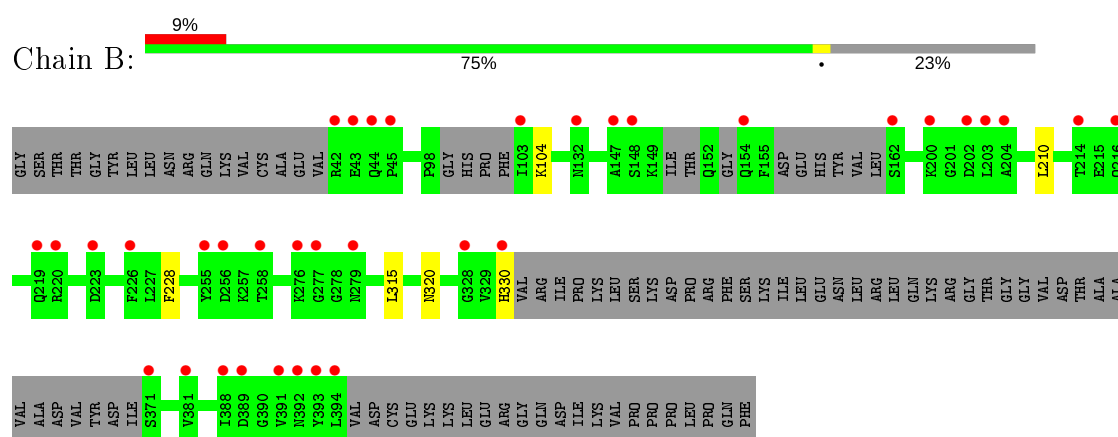
3 Residue-property plots [i](#)

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.

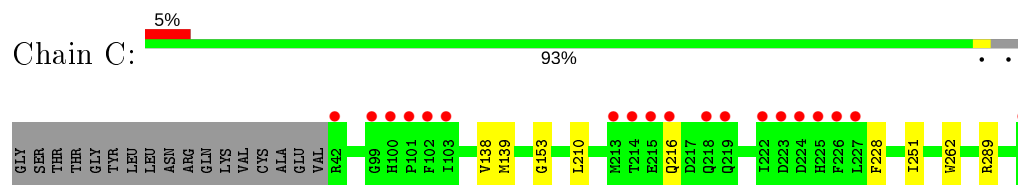
- Molecule 1: Creatine kinase S-type, mitochondrial



- Molecule 1: Creatine kinase S-type, mitochondrial

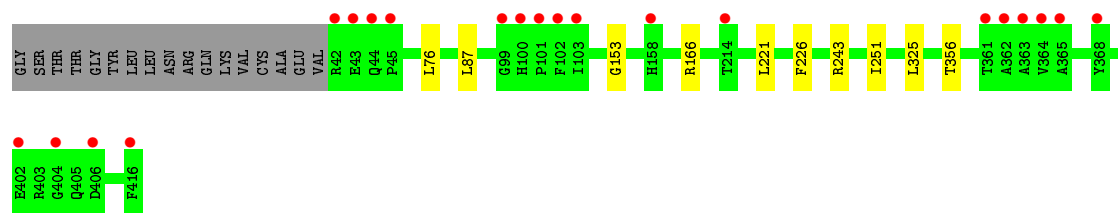


- Molecule 1: Creatine kinase S-type, mitochondrial

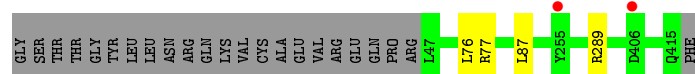


- Molecule 1: Creatine kinase S-type, mitochondrial

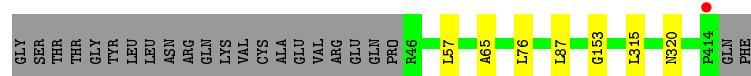




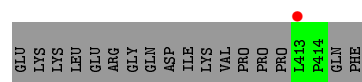
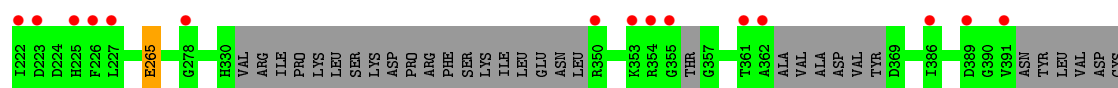
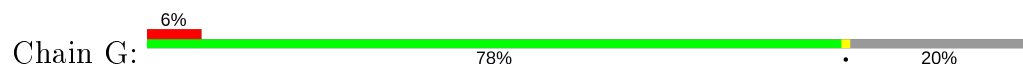
- Molecule 1: Creatine kinase S-type, mitochondrial



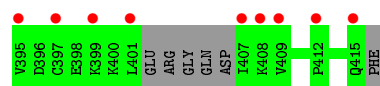
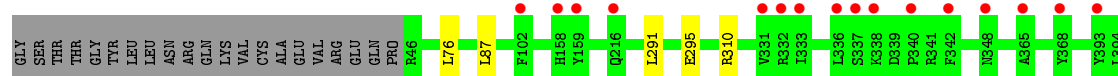
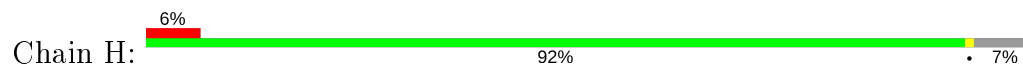
- Molecule 1: Creatine kinase S-type, mitochondrial



- Molecule 1: Creatine kinase S-type, mitochondrial



- Molecule 1: Creatine kinase S-type, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.06Å 106.06Å 114.93Å 70.12° 84.57° 68.61°	Depositor
Resolution (Å)	40.00 – 2.10 39.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.4 (40.00-2.10) 95.4 (39.94-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.236 0.209 , 0.240	Depositor DCC
R_{free} test set	4357 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23253	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: UNX, 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	0.71	0/2705	0.63	1/3682 (0.0%)
1	B	0.66	0/2385	0.63	0/3236
1	C	0.72	0/3030	0.66	1/4107 (0.0%)
1	D	0.72	0/3045	0.66	1/4126 (0.0%)
1	E	0.68	0/3029	0.64	0/4104
1	F	0.69	0/3052	0.65	0/4130
1	G	0.72	2/2455 (0.1%)	0.63	0/3325
1	H	0.70	0/2974	0.64	0/4034
All	All	0.70	2/22675 (0.0%)	0.64	3/30744 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	265[A]	GLU	CB-CG	6.25	1.64	1.52
1	G	265[B]	GLU	CB-CG	6.25	1.64	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	289	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	D	243	ARG	NE-CZ-NH2	5.04	122.82	120.30

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	2649	0	2421	1	0
1	B	2323	0	2159	2	0
1	C	2952	0	2852	4	0
1	D	2965	0	2885	4	0
1	E	2948	0	2896	3	0
1	F	2968	0	2932	3	0
1	G	2399	0	2246	3	0
1	H	2894	0	2777	2	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	46	0	24	0	0
2	H	27	0	12	0	0
3	A	7	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	8	0	0	0	0
3	E	15	0	0	2	0
3	F	11	0	0	0	0
3	G	5	0	0	0	0
3	H	13	0	0	0	0
4	A	62	0	0	0	0
4	B	60	0	0	0	0
4	C	136	0	0	0	0
4	D	145	0	0	0	0
4	E	141	0	0	0	0
4	F	163	0	0	0	0
4	G	61	0	0	0	0
4	H	81	0	0	0	0
All	All	23253	0	21276	22	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 0.

All (22) 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:E:289[A]:ARG:NH2	3:E:505:UNX:UNK	1.64	0.92
1:E:289[A]:ARG:HH22	3:E:505:UNX:UNK	1.31	0.71
1:D:226:PHE:HB3	1:D:251[B]:ILE:HD11	1.88	0.55
1:H:291:LEU:O	1:H:295[B]:GLU:HG3	2.09	0.52
1:D:76:LEU:HB2	1:D:87:LEU:HD22	1.92	0.50
1:D:221:LEU:HD22	1:D:251[B]:ILE:CD1	2.44	0.48
1:G:57:LEU:HD11	1:G:68:LEU:HD23	1.96	0.48
1:C:251:ILE:HD12	1:C:262[B]:TRP:CZ2	2.54	0.43
1:H:76:LEU:HB2	1:H:87:LEU:HD22	2.01	0.43
1:G:80:VAL:HG12	1:G:86:THR:HG22	2.00	0.43
1:B:315:LEU:HD12	1:B:320:ASN:O	2.20	0.42
1:E:76:LEU:HB2	1:E:87:LEU:HD22	2.02	0.42
1:F:315:LEU:HD12	1:F:320:ASN:O	2.19	0.42
1:B:210:LEU:HD11	1:B:228:PHE:CE1	2.55	0.42
1:G:265[B]:GLU:HA	1:G:265[B]:GLU:OE1	2.19	0.42
1:F:76:LEU:HB2	1:F:87:LEU:HD22	2.02	0.41
1:C:138:VAL:HG23	1:C:139:MET:HG3	2.01	0.41
1:C:210:LEU:HD11	1:C:228[A]:PHE:CE2	2.56	0.41
1:D:166:ARG:O	1:D:325:LEU:HA	2.21	0.40
1:A:57:LEU:HD13	1:A:65:ALA:HA	2.03	0.40
1:F:57:LEU:HD13	1:F:65:ALA:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	350/392 (89%)	344 (98%)	5 (1%)	1 (0%)	41	41
1	B	295/392 (75%)	284 (96%)	11 (4%)	0	100	100
1	C	376/392 (96%)	370 (98%)	5 (1%)	1 (0%)	41	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	378/392 (96%)	371 (98%)	6 (2%)	1 (0%)	41	41
1	E	373/392 (95%)	365 (98%)	8 (2%)	0	100	100
1	F	373/392 (95%)	367 (98%)	5 (1%)	1 (0%)	41	41
1	G	302/392 (77%)	292 (97%)	10 (3%)	0	100	100
1	H	367/392 (94%)	360 (98%)	7 (2%)	0	100	100
All	All	2814/3136 (90%)	2753 (98%)	57 (2%)	4 (0%)	51	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	153	GLY
1	D	153	GLY
1	F	153	GLY
1	A	153	GLY

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	257/342 (75%)	257 (100%)	0	100	100
1	B	231/342 (68%)	229 (99%)	2 (1%)	78	84
1	C	304/342 (89%)	303 (100%)	1 (0%)	92	95
1	D	309/342 (90%)	308 (100%)	1 (0%)	92	95
1	E	316/342 (92%)	315 (100%)	1 (0%)	92	95
1	F	320/342 (94%)	320 (100%)	0	100	100
1	G	235/342 (69%)	234 (100%)	1 (0%)	91	94
1	H	301/342 (88%)	300 (100%)	1 (0%)	92	95
All	All	2273/2736 (83%)	2266 (100%)	7 (0%)	92	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	LYS
1	B	330	HIS
1	C	216	GLN
1	D	356	THR
1	E	77	ARG
1	G	206	ARG
1	H	310	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

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 80 ligands modelled in this entry, 71 are unknown - leaving 9 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	D	501	-	24,29,29	1.20	3 (12%)	29,45,45	1.34	4 (13%)
2	ADP	F	501	-	24,29,29	1.05	2 (8%)	29,45,45	1.32	4 (13%)
2	ADP	H	501	-	24,29,29	1.14	2 (8%)	29,45,45	1.31	2 (6%)
2	ADP	G	501[B]	-	24,29,29	1.11	2 (8%)	29,45,45	1.27	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	501	-	24,29,29	1.14	2 (8%)	29,45,45	1.35	4 (13%)
2	ADP	C	501	-	24,29,29	1.22	3 (12%)	29,45,45	1.27	3 (10%)
2	ADP	E	501	-	24,29,29	1.18	3 (12%)	29,45,45	1.29	5 (17%)
2	ADP	G	501[A]	-	24,29,29	1.07	1 (4%)	29,45,45	1.32	3 (10%)
2	ADP	B	501	-	24,29,29	1.10	2 (8%)	29,45,45	1.35	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	D	501	-	-	5/12/32/32	0/3/3/3
2	ADP	F	501	-	-	2/12/32/32	0/3/3/3
2	ADP	H	501	-	-	1/12/32/32	0/3/3/3
2	ADP	G	501[B]	-	-	5/12/32/32	0/3/3/3
2	ADP	A	501	-	-	1/12/32/32	0/3/3/3
2	ADP	C	501	-	-	1/12/32/32	0/3/3/3
2	ADP	E	501	-	-	2/12/32/32	0/3/3/3
2	ADP	G	501[A]	-	-	2/12/32/32	0/3/3/3
2	ADP	B	501	-	-	2/12/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	ADP	C2-N3	3.11	1.37	1.32
2	C	501	ADP	C2-N3	2.88	1.36	1.32
2	B	501	ADP	C2-N3	2.79	1.36	1.32
2	A	501	ADP	C2-N3	2.74	1.36	1.32
2	G	501[B]	ADP	C2-N3	2.65	1.36	1.32
2	D	501	ADP	C2-N3	2.65	1.36	1.32
2	E	501	ADP	C2-N3	2.47	1.36	1.32
2	G	501[A]	ADP	C2-N3	2.43	1.36	1.32
2	E	501	ADP	C5-C4	2.43	1.47	1.40
2	A	501	ADP	C5-C4	2.42	1.47	1.40
2	F	501	ADP	C2-N3	2.35	1.35	1.32
2	D	501	ADP	O4'-C1'	2.32	1.44	1.41
2	C	501	ADP	C5-C4	2.30	1.47	1.40
2	D	501	ADP	C5-C4	2.28	1.47	1.40
2	E	501	ADP	C2'-C1'	-2.24	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	ADP	C2-N1	2.23	1.38	1.33
2	F	501	ADP	C5-C4	2.23	1.46	1.40
2	G	501[B]	ADP	O4'-C1'	2.20	1.44	1.41
2	H	501	ADP	C5-C4	2.05	1.46	1.40
2	B	501	ADP	C5-C4	2.01	1.46	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	ADP	N3-C2-N1	-4.25	122.03	128.68
2	E	501	ADP	N3-C2-N1	-4.21	122.10	128.68
2	F	501	ADP	N3-C2-N1	-4.20	122.12	128.68
2	B	501	ADP	N3-C2-N1	-4.18	122.15	128.68
2	A	501	ADP	N3-C2-N1	-4.09	122.28	128.68
2	C	501	ADP	N3-C2-N1	-4.07	122.31	128.68
2	D	501	ADP	N3-C2-N1	-3.95	122.50	128.68
2	G	501[A]	ADP	N3-C2-N1	-3.88	122.61	128.68
2	G	501[B]	ADP	N3-C2-N1	-3.72	122.86	128.68
2	G	501[B]	ADP	PA-O3A-PB	-2.81	123.18	132.83
2	G	501[A]	ADP	PA-O3A-PB	-2.81	123.18	132.83
2	B	501	ADP	PA-O3A-PB	-2.78	123.30	132.83
2	A	501	ADP	PA-O3A-PB	-2.74	123.44	132.83
2	D	501	ADP	O3B-PB-O2B	2.71	118.01	107.64
2	C	501	ADP	C4-C5-N7	-2.62	106.67	109.40
2	G	501[A]	ADP	C4-C5-N7	-2.60	106.69	109.40
2	B	501	ADP	C4-C5-N7	-2.56	106.73	109.40
2	D	501	ADP	C4-C5-N7	-2.49	106.80	109.40
2	A	501	ADP	C4-C5-N7	-2.44	106.86	109.40
2	F	501	ADP	C4-C5-N7	-2.43	106.86	109.40
2	F	501	ADP	O4'-C1'-C2'	-2.36	103.47	106.93
2	E	501	ADP	C2-N1-C6	2.26	122.63	118.75
2	E	501	ADP	PA-O3A-PB	-2.25	125.09	132.83
2	A	501	ADP	O3A-PB-O1B	-2.22	98.85	111.19
2	H	501	ADP	C4-C5-N7	-2.17	107.14	109.40
2	E	501	ADP	C4-C5-N7	-2.15	107.16	109.40
2	C	501	ADP	C2-N1-C6	2.06	122.27	118.75
2	D	501	ADP	C2-N1-C6	2.04	122.23	118.75
2	E	501	ADP	O4'-C1'-C2'	-2.02	103.97	106.93
2	F	501	ADP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

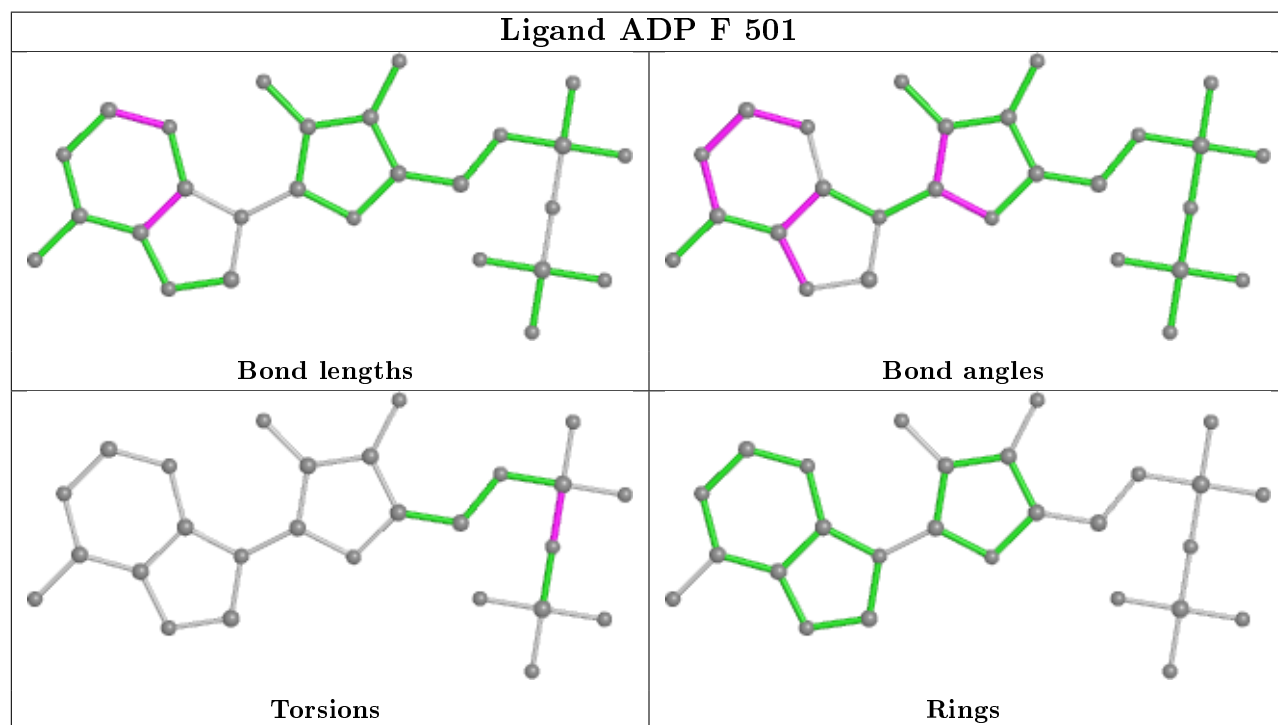
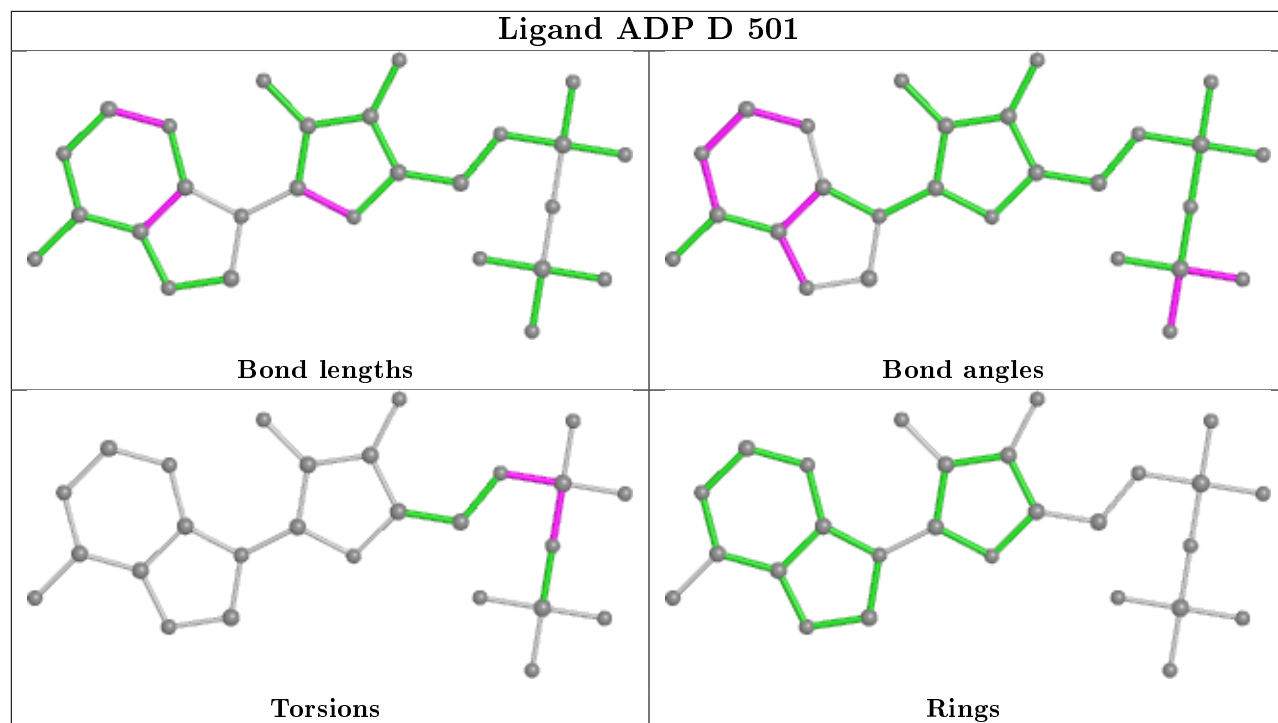
All (21) torsion outliers are listed below:

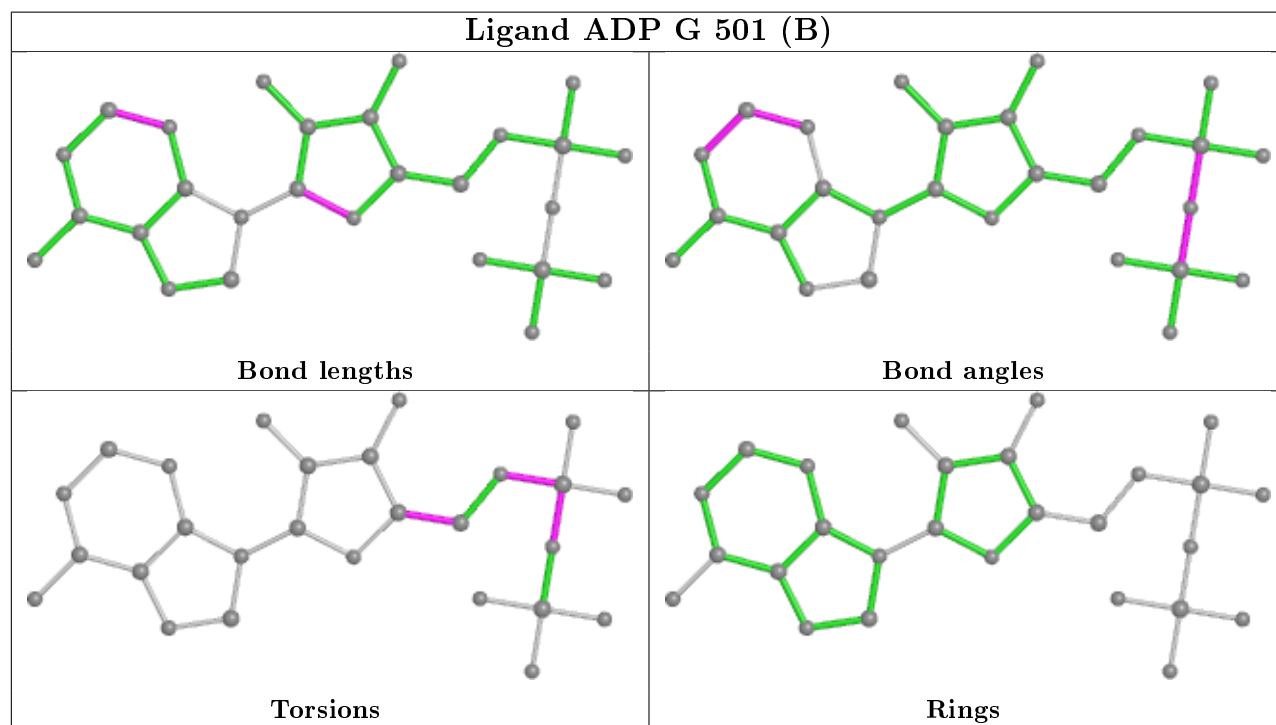
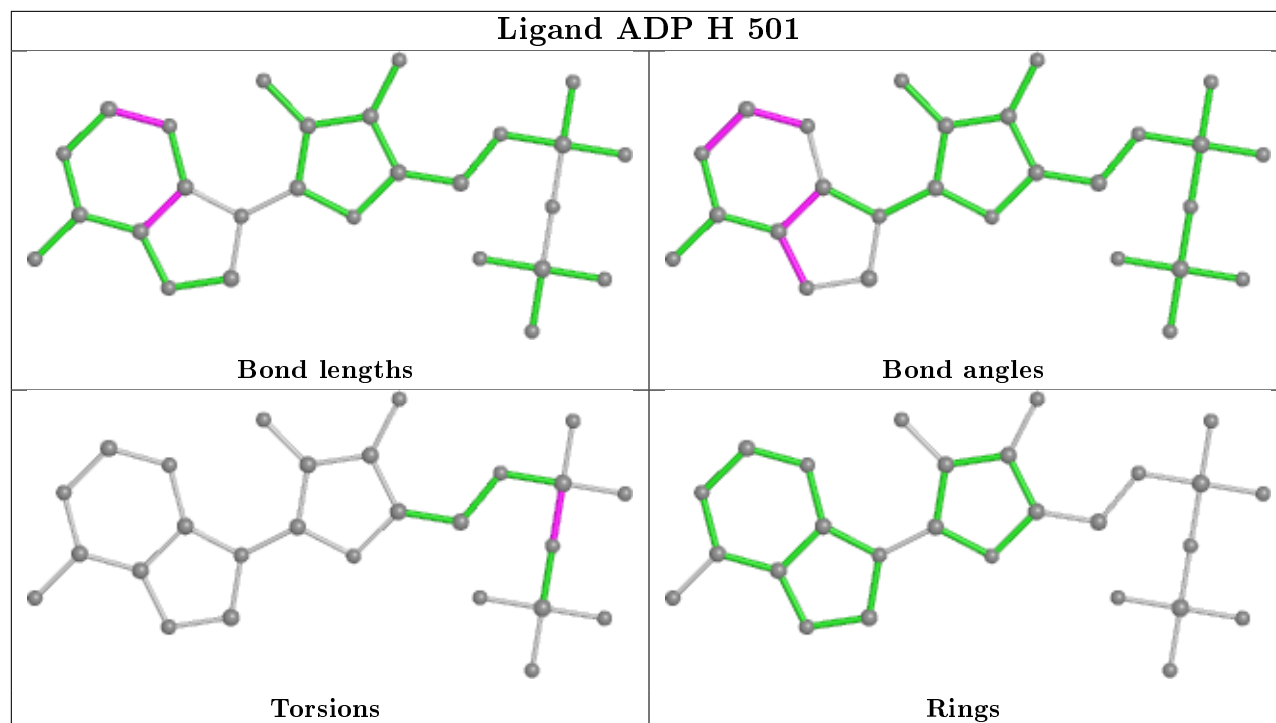
Mol	Chain	Res	Type	Atoms
2	G	501[B]	ADP	C5'-O5'-PA-O1A
2	G	501[B]	ADP	O4'-C4'-C5'-O5'
2	D	501	ADP	C5'-O5'-PA-O2A
2	G	501[B]	ADP	C3'-C4'-C5'-O5'
2	D	501	ADP	PB-O3A-PA-O1A
2	D	501	ADP	C5'-O5'-PA-O3A
2	H	501	ADP	PB-O3A-PA-O1A
2	G	501[B]	ADP	PB-O3A-PA-O1A
2	G	501[A]	ADP	PB-O3A-PA-O1A
2	C	501	ADP	PB-O3A-PA-O2A
2	E	501	ADP	PB-O3A-PA-O2A
2	B	501	ADP	PB-O3A-PA-O2A
2	F	501	ADP	PB-O3A-PA-O2A
2	D	501	ADP	PB-O3A-PA-O2A
2	G	501[B]	ADP	C5'-O5'-PA-O3A
2	G	501[A]	ADP	C5'-O5'-PA-O3A
2	F	501	ADP	PB-O3A-PA-O1A
2	A	501	ADP	PB-O3A-PA-O1A
2	E	501	ADP	PB-O3A-PA-O1A
2	B	501	ADP	PB-O3A-PA-O1A
2	D	501	ADP	C5'-O5'-PA-O1A

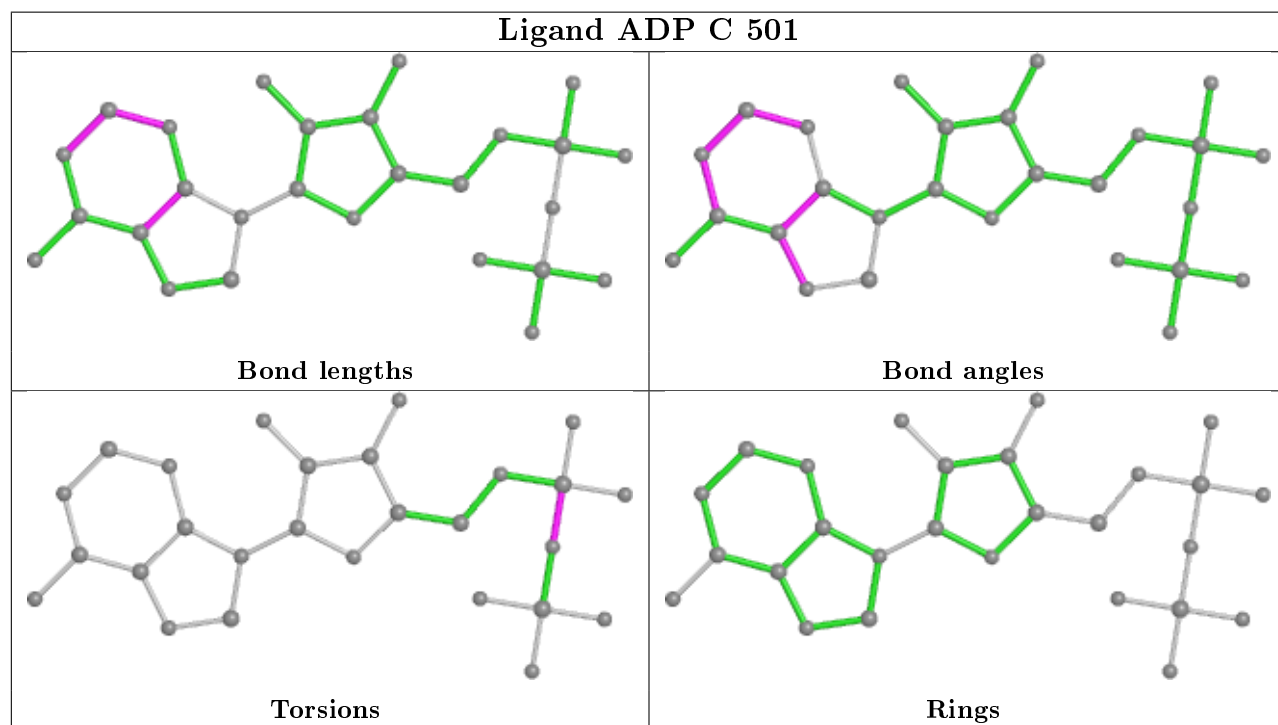
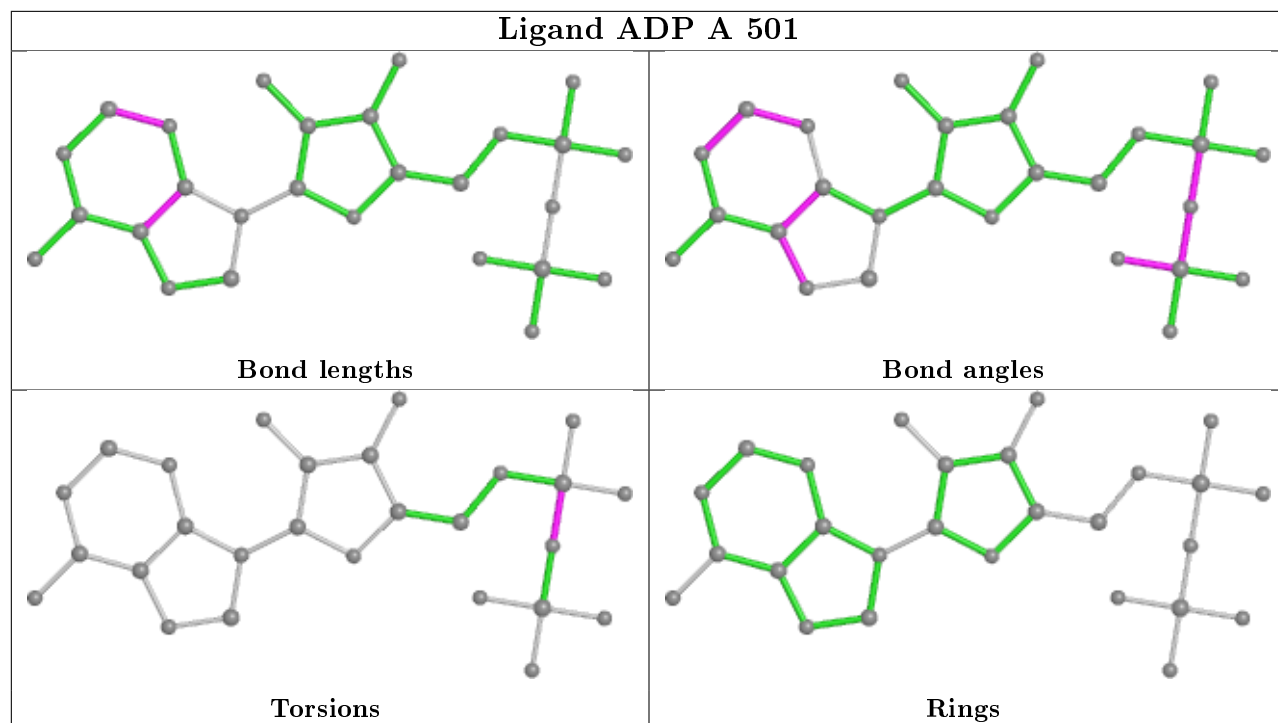
There are no ring outliers.

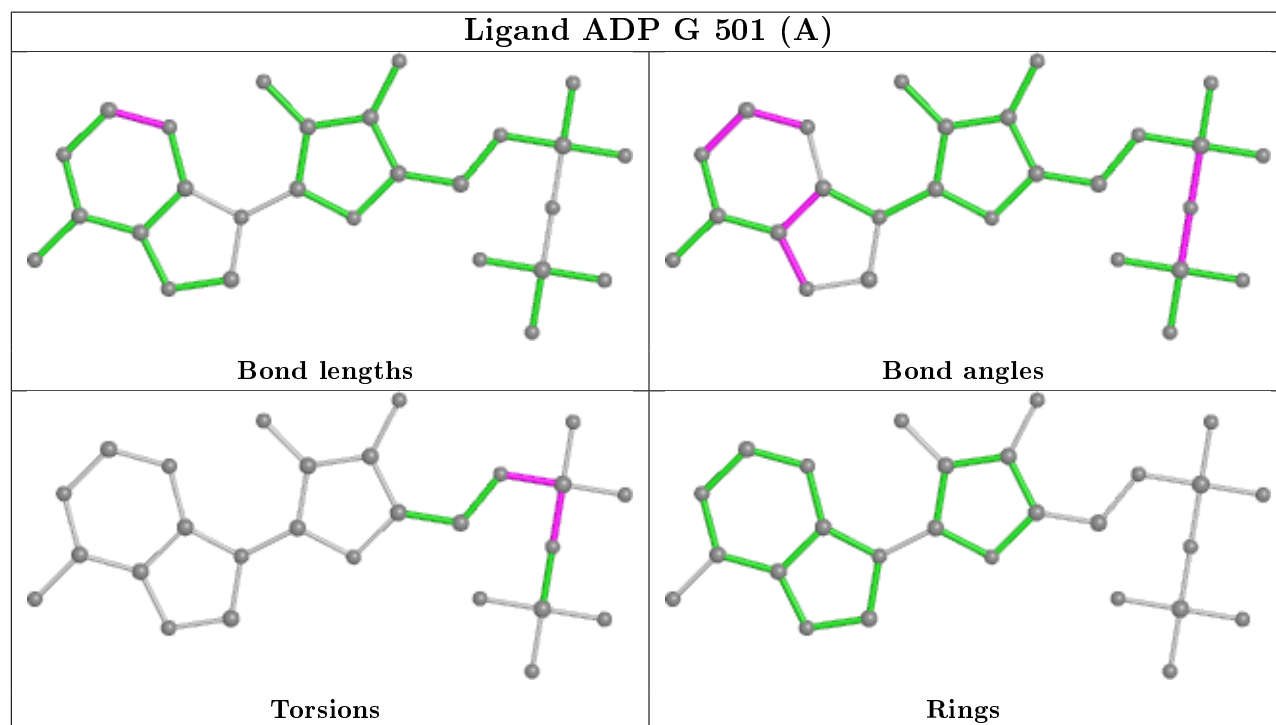
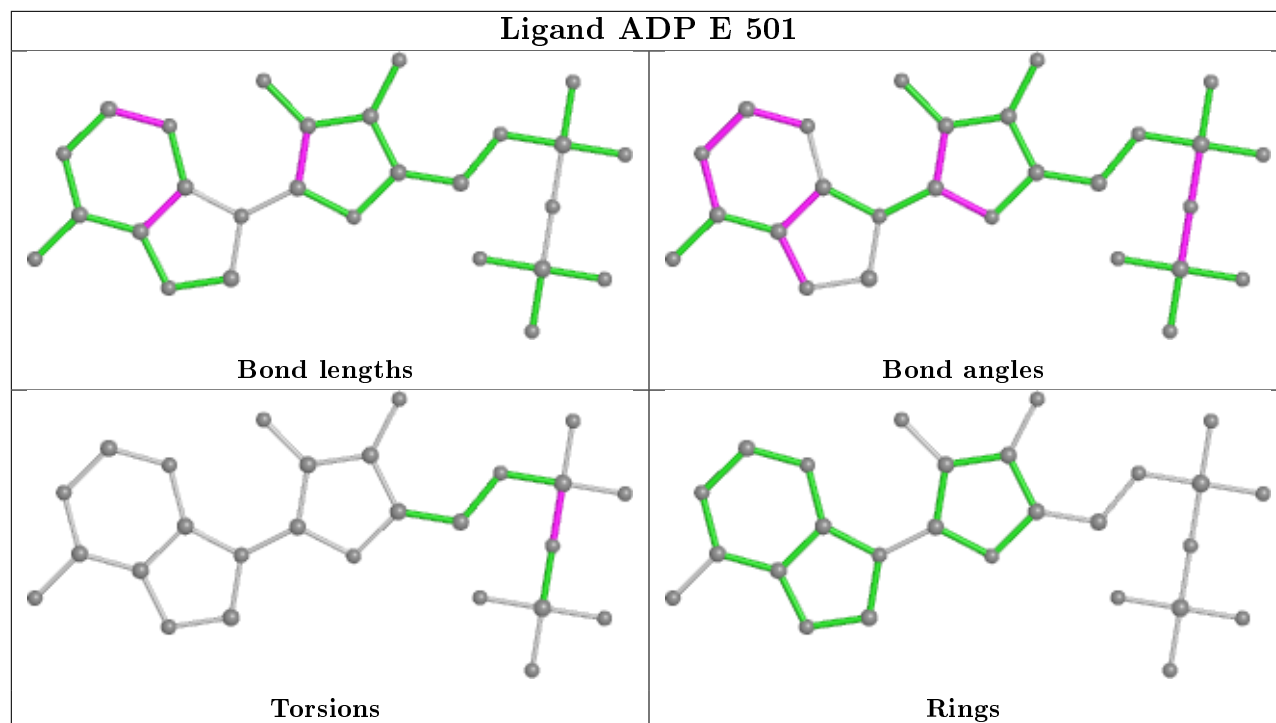
No monomer is involved in short contacts.

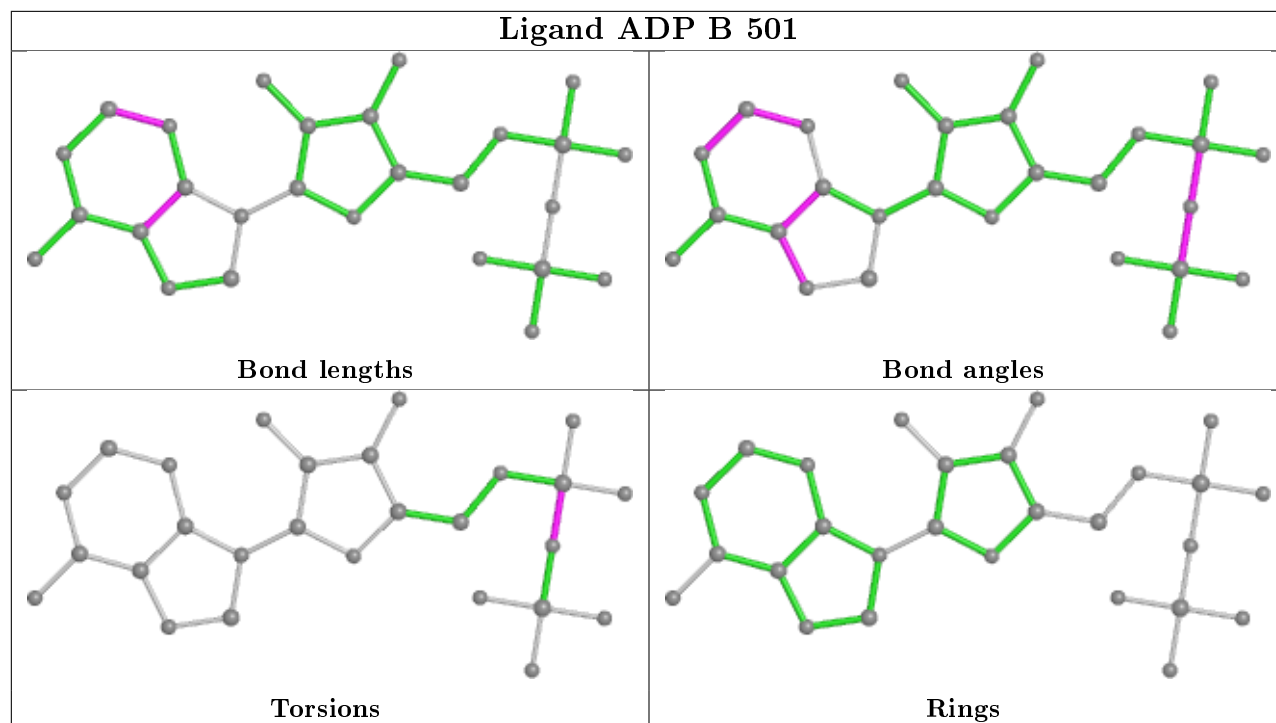
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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, 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	352/392 (89%)	0.63	48 (13%) 3 4	22, 45, 89, 112	0
1	B	300/392 (76%)	0.45	36 (12%) 4 5	21, 45, 85, 98	1 (0%)
1	C	375/392 (95%)	-0.01	20 (5%) 26 32	18, 31, 66, 90	2 (0%)
1	D	375/392 (95%)	-0.00	21 (5%) 24 29	19, 31, 65, 97	0
1	E	369/392 (94%)	-0.13	2 (0%) 91 92	20, 32, 52, 72	2 (0%)
1	F	369/392 (94%)	-0.25	1 (0%) 94 94	19, 30, 48, 73	0
1	G	313/392 (79%)	0.36	23 (7%) 15 19	21, 41, 81, 95	1 (0%)
1	H	365/392 (93%)	0.24	25 (6%) 17 21	21, 38, 75, 95	4 (1%)
All	All	2818/3136 (89%)	0.15	176 (6%) 20 25	18, 34, 77, 112	10 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	ILE	7.8
1	A	393	TYR	6.7
1	B	393	TYR	6.1
1	A	340	PRO	5.8
1	C	101	PRO	5.4
1	A	102	PHE	5.4
1	A	101	PRO	5.3
1	A	336	LEU	5.2
1	A	103	ILE	5.1
1	A	159	TYR	4.9
1	H	412	PRO	4.8
1	A	344	LYS	4.7
1	H	159	TYR	4.7
1	D	101	PRO	4.7
1	A	160	VAL	4.6
1	C	102	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	45	PRO	4.4
1	G	138	VAL	4.4
1	D	102	PHE	4.3
1	B	391	VAL	4.3
1	B	203	LEU	4.2
1	A	341	ARG	4.2
1	B	223	ASP	4.1
1	B	256	ASP	4.1
1	C	213	MET	4.1
1	A	397	CYS	4.1
1	D	45	PRO	4.1
1	A	391	VAL	4.0
1	A	346	LEU	4.0
1	A	343	SER	3.9
1	C	215	GLU	3.8
1	A	390	GLY	3.8
1	H	408	LYS	3.8
1	A	347	GLU	3.8
1	B	389	ASP	3.8
1	A	155	PHE	3.8
1	H	158	HIS	3.8
1	A	335	LYS	3.7
1	A	153	GLY	3.7
1	G	362	ALA	3.7
1	H	368	TYR	3.7
1	B	45	PRO	3.6
1	H	340	PRO	3.6
1	G	214	THR	3.6
1	A	342	PHE	3.5
1	D	103	ILE	3.5
1	D	404	GLY	3.5
1	A	337	SER	3.5
1	C	223	ASP	3.5
1	A	333	ILE	3.4
1	H	337	SER	3.4
1	B	162	SER	3.3
1	A	156	ASP	3.3
1	B	255	TYR	3.3
1	D	42	ARG	3.3
1	C	216	GLN	3.3
1	G	355	GLY	3.3
1	H	415	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	363	ALA	3.3
1	H	409	VAL	3.2
1	D	100	HIS	3.2
1	B	392	ASN	3.2
1	A	202	ASP	3.2
1	B	44	GLN	3.2
1	B	216	GLN	3.2
1	G	278	GLY	3.2
1	B	147	ALA	3.2
1	C	103	ILE	3.1
1	A	151	THR	3.1
1	A	366	ASP	3.1
1	G	354	ARG	3.1
1	B	148	SER	3.1
1	B	200	LYS	3.0
1	G	223	ASP	3.0
1	H	401	LEU	3.0
1	C	214	THR	3.0
1	G	353	LYS	3.0
1	A	394	LEU	3.0
1	H	333	ILE	3.0
1	H	395	VAL	3.0
1	A	278	GLY	2.9
1	H	399	LYS	2.9
1	C	42	ARG	2.9
1	B	276	LYS	2.9
1	C	219	GLN	2.9
1	H	407	ILE	2.8
1	D	362	ALA	2.8
1	A	365	ALA	2.8
1	A	367	VAL	2.8
1	G	222	ILE	2.8
1	A	387	VAL	2.8
1	B	388	ILE	2.8
1	H	102	PHE	2.8
1	A	368	TYR	2.8
1	H	336	LEU	2.8
1	H	332	ARG	2.7
1	A	157	GLU	2.7
1	G	151	THR	2.7
1	C	100	HIS	2.7
1	H	397	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	202	ASP	2.6
1	A	138	VAL	2.6
1	A	334	PRO	2.6
1	D	416	PHE	2.6
1	C	360	ASP	2.6
1	B	214	THR	2.6
1	G	386	ILE	2.6
1	D	158	HIS	2.6
1	B	226	PHE	2.6
1	C	226	PHE	2.6
1	C	225	HIS	2.5
1	D	368	TYR	2.5
1	B	277	GLY	2.5
1	H	393	TYR	2.5
1	A	148	SER	2.5
1	A	395	VAL	2.5
1	G	391	VAL	2.5
1	E	255	TYR	2.5
1	C	222	ILE	2.5
1	D	364	VAL	2.4
1	F	414	PRO	2.4
1	C	227[A]	LEU	2.4
1	G	413	LEU	2.4
1	E	406	ASP	2.4
1	B	328	GLY	2.4
1	G	216	GLN	2.4
1	A	364	VAL	2.4
1	G	218	GLN	2.3
1	A	351	LEU	2.3
1	B	42	ARG	2.3
1	D	214	THR	2.3
1	C	99	GLY	2.3
1	D	99	GLY	2.3
1	G	389	ASP	2.3
1	B	279	ASN	2.3
1	D	43	GLU	2.3
1	A	339	ASP	2.3
1	A	348	ASN	2.3
1	B	204	ALA	2.3
1	H	365	ALA	2.3
1	A	345	ILE	2.3
1	D	44	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	226	PHE	2.3
1	D	406	ASP	2.3
1	B	219	GLN	2.3
1	B	394	LEU	2.2
1	B	258	THR	2.2
1	A	99	GLY	2.2
1	B	154	GLN	2.2
1	G	225	HIS	2.2
1	G	361	THR	2.2
1	A	338	LYS	2.2
1	G	227	LEU	2.2
1	B	132[A]	ASN	2.2
1	H	338	LYS	2.2
1	A	215	GLU	2.2
1	A	316	THR	2.2
1	B	330	HIS	2.1
1	G	42	ARG	2.1
1	D	361	THR	2.1
1	D	365	ALA	2.1
1	H	348	ASN	2.1
1	C	224	ASP	2.1
1	H	342	PHE	2.1
1	A	279	ASN	2.1
1	A	354	ARG	2.1
1	C	363	ALA	2.1
1	G	350	ARG	2.1
1	H	216	GLN	2.1
1	B	43	GLU	2.0
1	C	218	GLN	2.0
1	D	402	GLU	2.0
1	B	381	VAL	2.0
1	B	220	ARG	2.0
1	B	371	SER	2.0
1	H	331	VAL	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 ⓘ

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(Å ²)	Q<0.9
3	UNX	E	506	1/1	0.54	0.21	42,42,42,42	0
3	UNX	H	503	1/1	0.55	0.93	43,43,43,43	0
3	UNX	F	511	1/1	0.58	0.27	42,42,42,42	0
3	UNX	E	503	1/1	0.59	0.82	33,33,33,33	0
3	UNX	H	504	1/1	0.61	0.84	42,42,42,42	0
3	UNX	B	502	1/1	0.70	0.65	48,48,48,48	0
3	UNX	E	504	1/1	0.70	0.62	38,38,38,38	0
3	UNX	B	505	1/1	0.72	0.29	31,31,31,31	0
3	UNX	G	503	1/1	0.74	0.43	44,44,44,44	0
3	UNX	F	509	1/1	0.75	0.47	35,35,35,35	0
3	UNX	C	503	1/1	0.76	0.47	39,39,39,39	0
3	UNX	A	503	1/1	0.76	0.52	40,40,40,40	0
3	UNX	C	502	1/1	0.79	0.46	34,34,34,34	0
3	UNX	H	513	1/1	0.83	0.16	36,36,36,36	0
3	UNX	F	508	1/1	0.84	0.42	47,47,47,47	0
3	UNX	A	502	1/1	0.85	0.80	37,37,37,37	0
3	UNX	H	508	1/1	0.86	0.11	36,36,36,36	0
3	UNX	A	508	1/1	0.86	0.28	27,27,27,27	0
3	UNX	B	507	1/1	0.87	0.65	42,42,42,42	0
3	UNX	G	504	1/1	0.87	0.50	34,34,34,34	0
3	UNX	B	503	1/1	0.88	0.47	44,44,44,44	0
3	UNX	D	509	1/1	0.88	0.35	28,28,28,28	0
3	UNX	A	504	1/1	0.88	0.45	28,28,28,28	0
3	UNX	F	505	1/1	0.89	0.60	20,20,20,20	0
3	UNX	C	505	1/1	0.89	0.34	45,45,45,45	0
3	UNX	C	507	1/1	0.89	0.13	39,39,39,39	0
3	UNX	D	508	1/1	0.89	0.14	28,28,28,28	0
3	UNX	G	506	1/1	0.90	0.16	36,36,36,36	0
3	UNX	C	504	1/1	0.90	0.23	27,27,27,27	0
3	UNX	D	502	1/1	0.91	0.50	36,36,36,36	0
3	UNX	F	504	1/1	0.91	0.15	36,36,36,36	0
3	UNX	G	505	1/1	0.91	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	A	507	1/1	0.91	0.45	31,31,31,31	0
3	UNX	E	512	1/1	0.92	0.25	36,36,36,36	0
3	UNX	E	502	1/1	0.92	0.43	25,25,25,25	0
3	UNX	F	510	1/1	0.92	0.13	26,26,26,26	0
3	UNX	E	515	1/1	0.92	0.18	23,23,23,23	0
3	UNX	H	506	1/1	0.92	0.11	41,41,41,41	0
3	UNX	E	510	1/1	0.92	0.15	25,25,25,25	0
3	UNX	E	508	1/1	0.92	0.14	27,27,27,27	0
3	UNX	H	509	1/1	0.93	0.32	37,37,37,37	0
3	UNX	H	505	1/1	0.93	0.49	42,42,42,42	0
3	UNX	H	511	1/1	0.93	0.41	27,27,27,27	0
3	UNX	G	502	1/1	0.93	0.61	33,33,33,33	0
3	UNX	F	503	1/1	0.93	0.12	17,17,17,17	0
2	ADP	G	501[B]	27/27	0.94	0.15	53,68,72,72	19
3	UNX	D	505	1/1	0.94	0.18	27,27,27,27	0
2	ADP	G	501[A]	27/27	0.94	0.15	41,48,57,64	19
3	UNX	E	513	1/1	0.94	0.12	36,36,36,36	0
3	UNX	B	504	1/1	0.94	0.20	28,28,28,28	0
3	UNX	H	507	1/1	0.94	0.28	30,30,30,30	0
3	UNX	E	505	1/1	0.94	0.35	17,17,17,17	1
3	UNX	D	506	1/1	0.94	0.37	28,28,28,28	0
3	UNX	A	506	1/1	0.94	0.10	36,36,36,36	0
2	ADP	B	501	27/27	0.94	0.14	48,77,96,97	0
3	UNX	F	502	1/1	0.95	0.48	21,21,21,21	0
3	UNX	B	506	1/1	0.95	0.25	24,24,24,24	0
3	UNX	D	503	1/1	0.95	0.09	36,36,36,36	0
3	UNX	H	514	1/1	0.95	0.15	35,35,35,35	0
3	UNX	H	502	1/1	0.95	0.14	31,31,31,31	0
3	UNX	H	510	1/1	0.95	0.24	27,27,27,27	0
2	ADP	A	501	27/27	0.95	0.12	37,50,65,66	0
2	ADP	H	501	27/27	0.96	0.11	35,40,43,43	0
3	UNX	E	507	1/1	0.96	0.07	34,34,34,34	0
3	UNX	D	504	1/1	0.96	0.36	28,28,28,28	0
3	UNX	F	507	1/1	0.97	0.22	23,23,23,23	0
3	UNX	A	505	1/1	0.97	0.34	21,21,21,21	0
3	UNX	E	516	1/1	0.97	0.11	32,32,32,32	0
3	UNX	H	512	1/1	0.97	0.07	26,26,26,26	0
3	UNX	F	512	1/1	0.98	0.34	31,31,31,31	0
2	ADP	C	501	27/27	0.98	0.09	25,29,31,35	0
2	ADP	D	501	27/27	0.98	0.08	30,41,44,47	0
2	ADP	F	501	27/27	0.99	0.08	22,27,29,30	0
3	UNX	E	514	1/1	0.99	0.15	20,20,20,20	0

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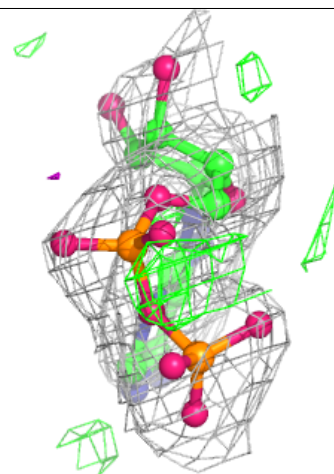
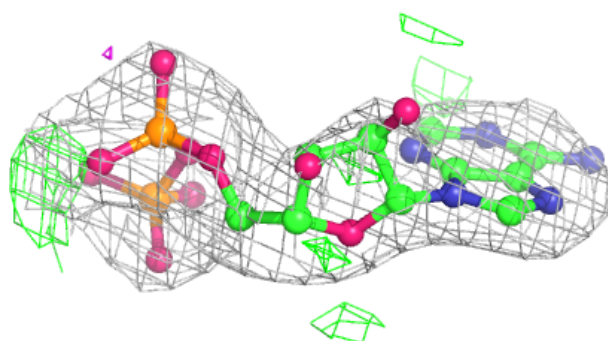
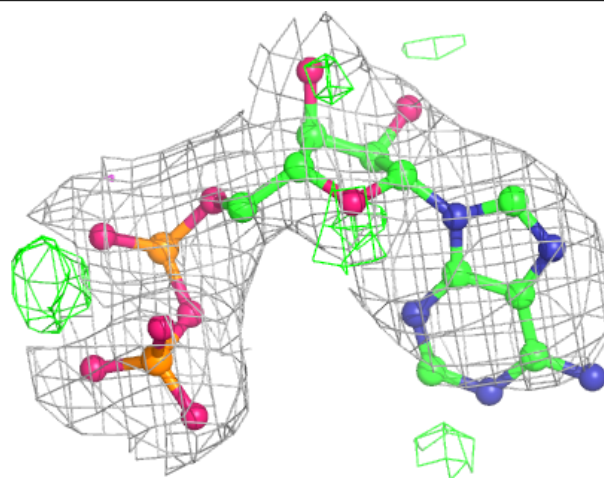
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	E	509	1/1	0.99	0.12	21,21,21,21	0
3	UNX	D	507	1/1	0.99	0.24	7,7,7,7	0
3	UNX	F	506	1/1	0.99	0.25	13,13,13,13	0
3	UNX	C	506	1/1	0.99	0.14	15,15,15,15	0
2	ADP	E	501	27/27	0.99	0.14	24,28,30,33	0
3	UNX	E	511	1/1	1.00	0.28	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.

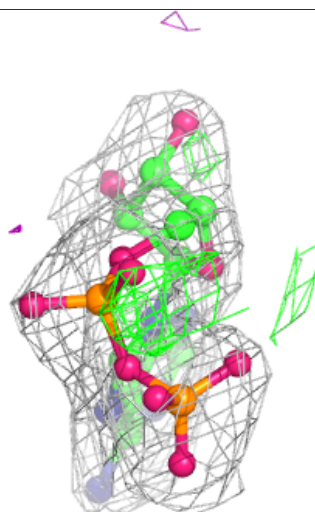
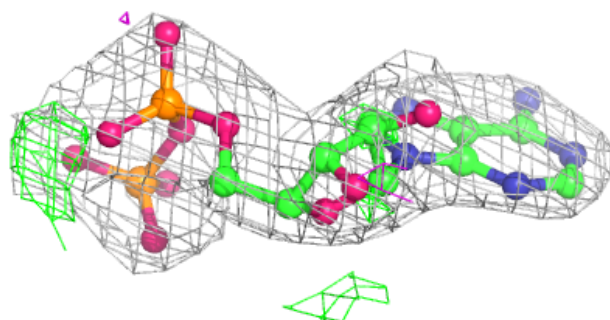
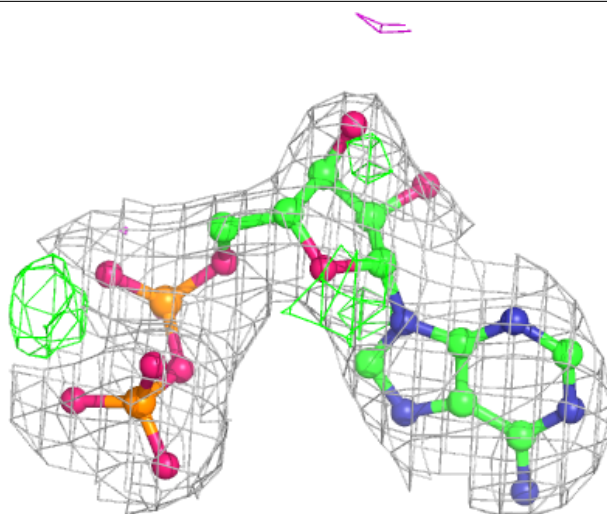
Electron density around ADP G 501 (B):

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



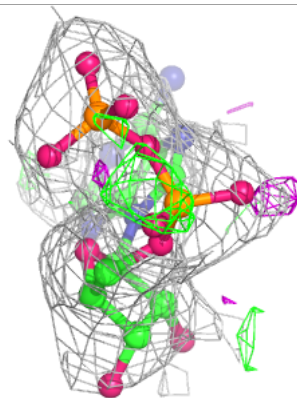
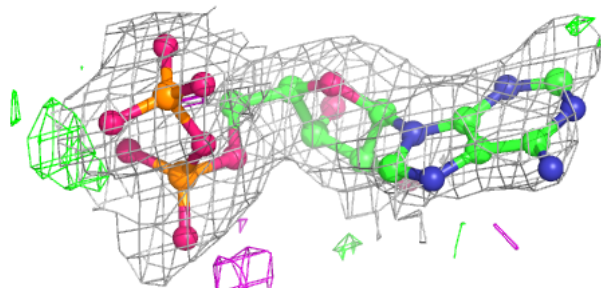
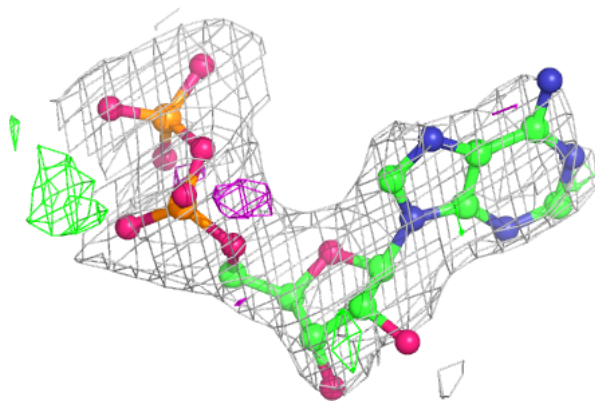
Electron density around ADP G 501 (A):

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

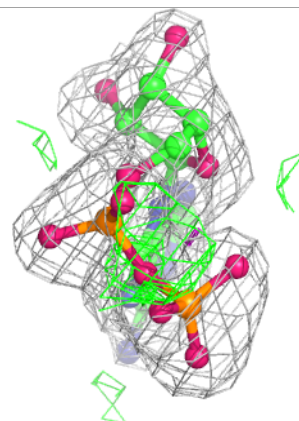
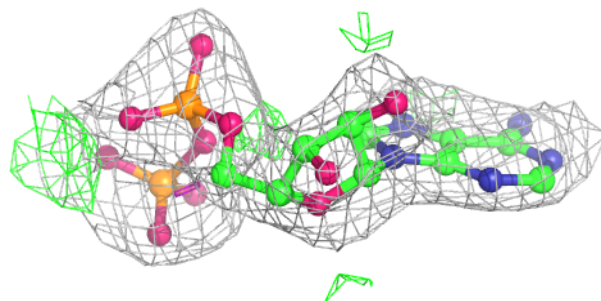
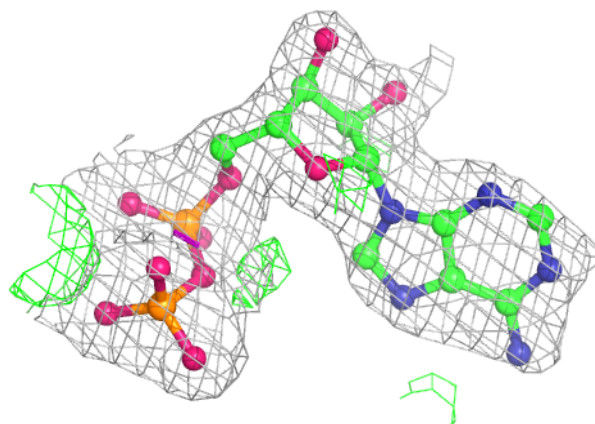


Electron density around ADP B 501:

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

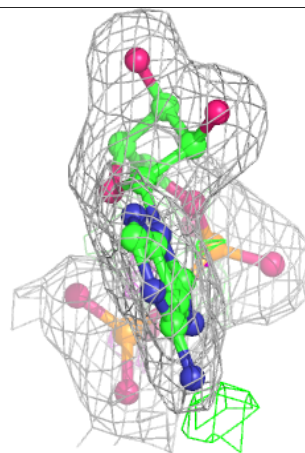
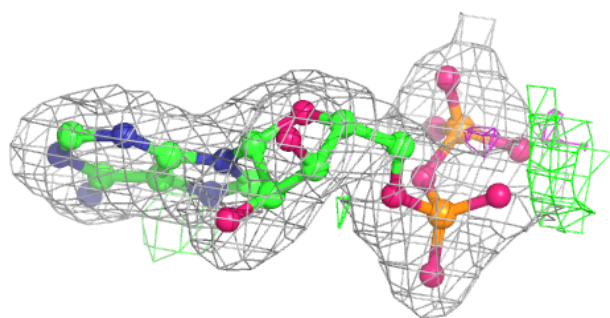
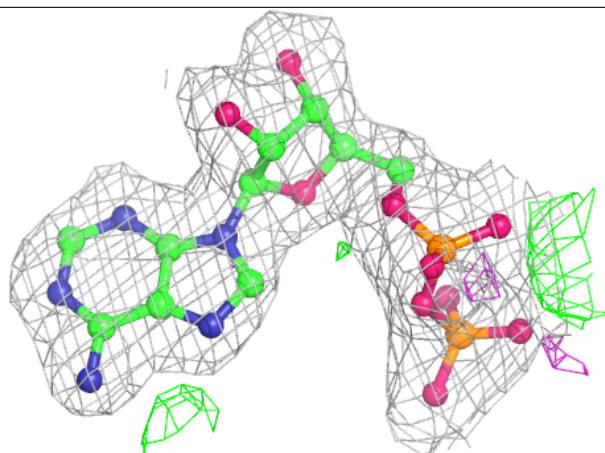
**Electron density around ADP A 501:**

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



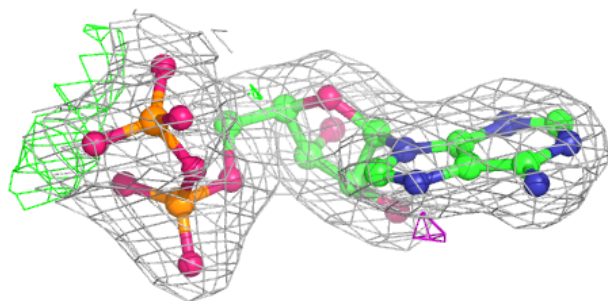
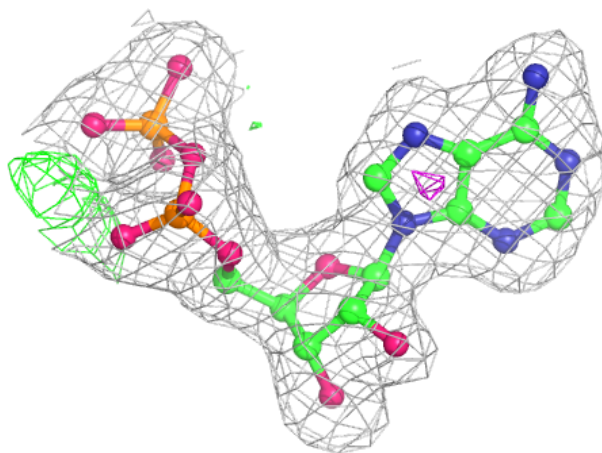
Electron density around ADP H 501:

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



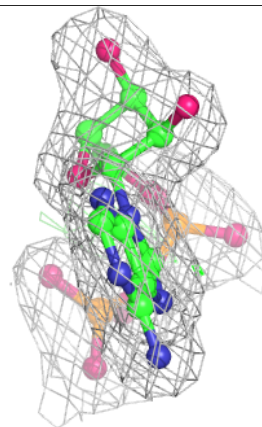
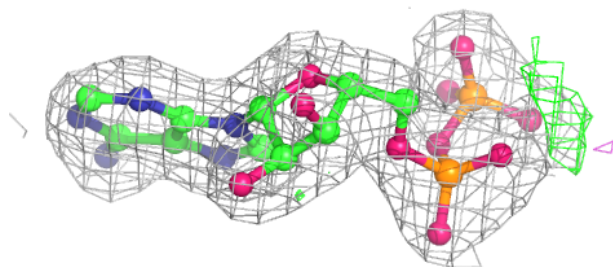
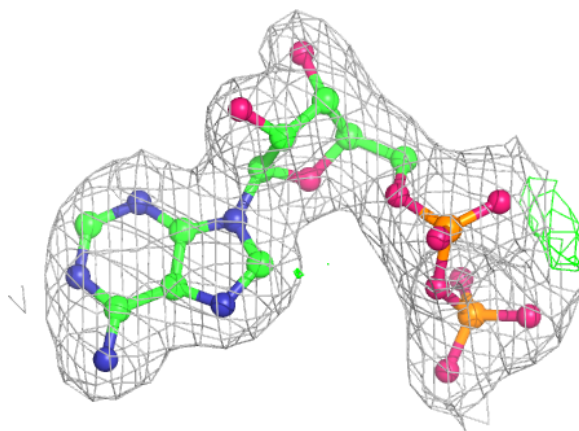
Electron density around ADP C 501:

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

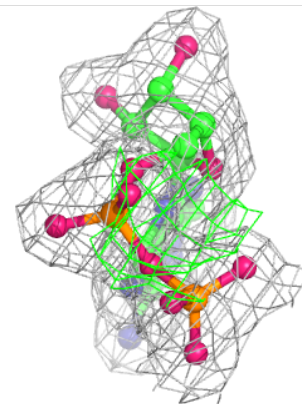
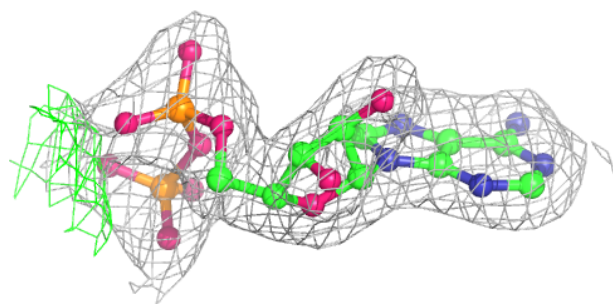
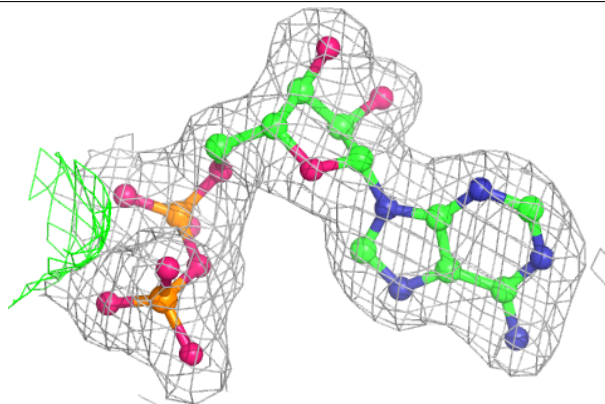


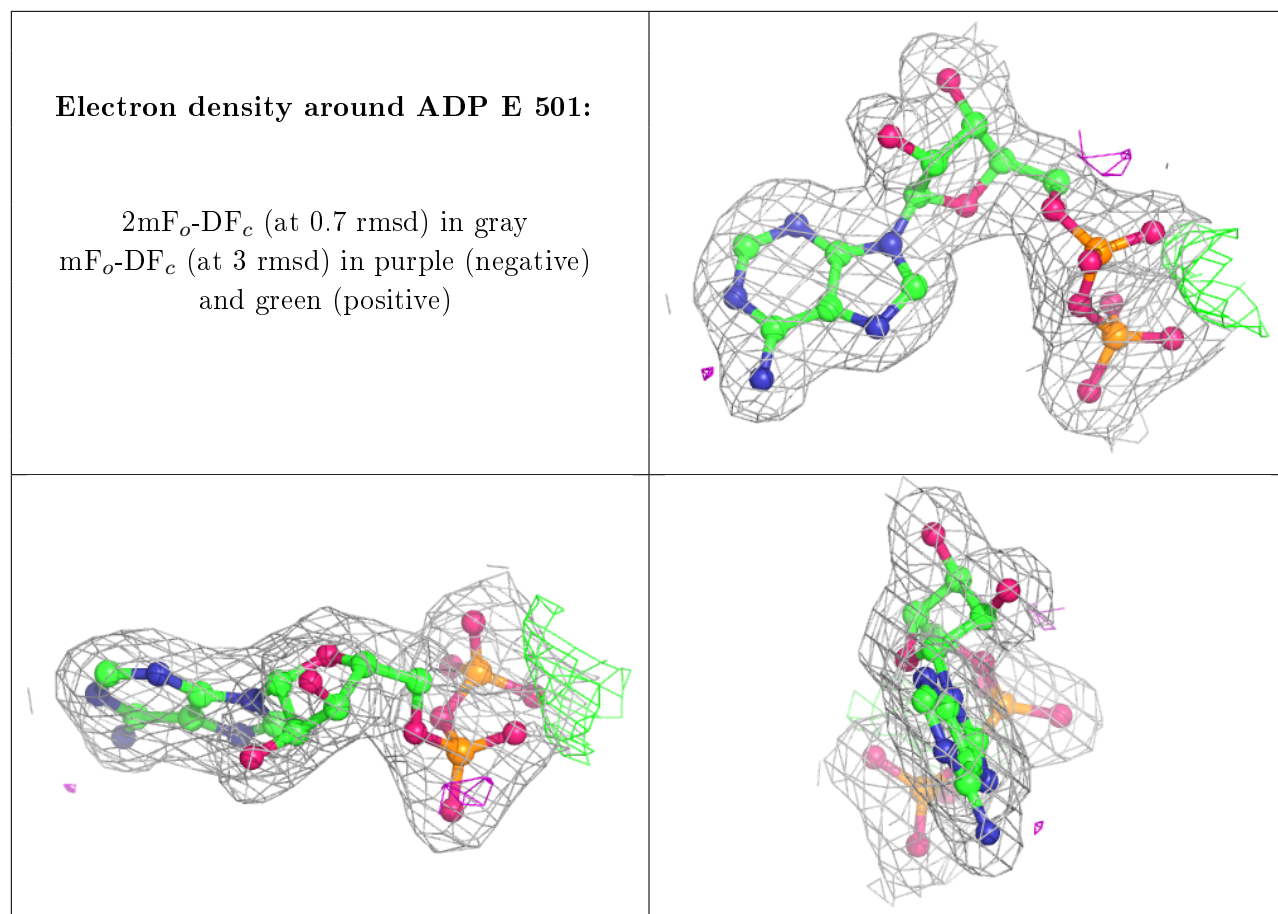
Electron density around ADP D 501:

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

**Electron density around ADP F 501:**

$2mF_o-DF_c$ (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.