



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:51 AM UTC

PDB ID : 4Z9M / pdb_00004z9m
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 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:

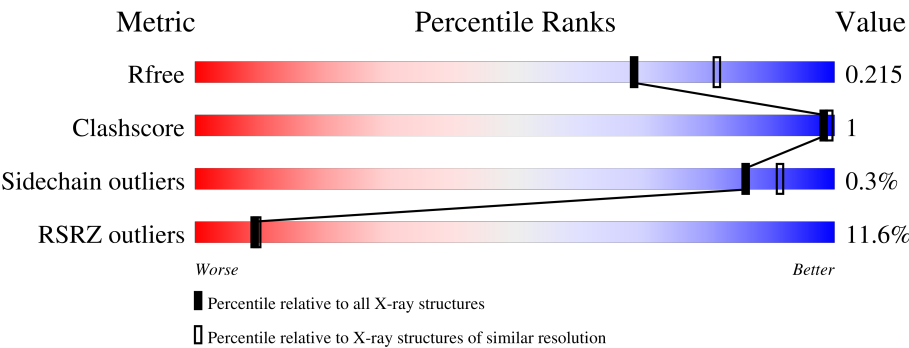
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	392	22% 88% 10%
1	B	392	17% 75% 23%
1	C	392	8% 92%
1	D	392	6% 93%
1	E	392	2% 93% 6%

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Mol	Chain	Length	Quality of chain
1	F	392	
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	G	503	-	-	-	X
3	UNX	H	503	-	-	-	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:

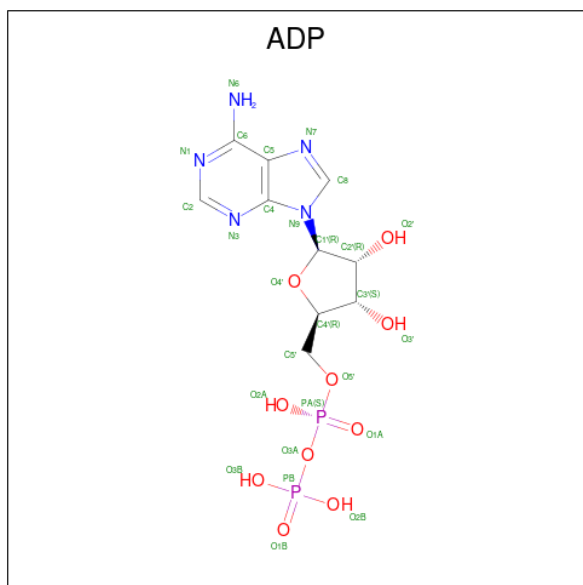
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP P17540
A	26	SER	-	expression tag	UNP P17540
B	25	GLY	-	expression tag	UNP P17540
B	26	SER	-	expression tag	UNP P17540
C	25	GLY	-	expression tag	UNP P17540
C	26	SER	-	expression tag	UNP P17540
D	25	GLY	-	expression tag	UNP P17540
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 (CCD ID: 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 (CCD ID: UNX) (formula: X).

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

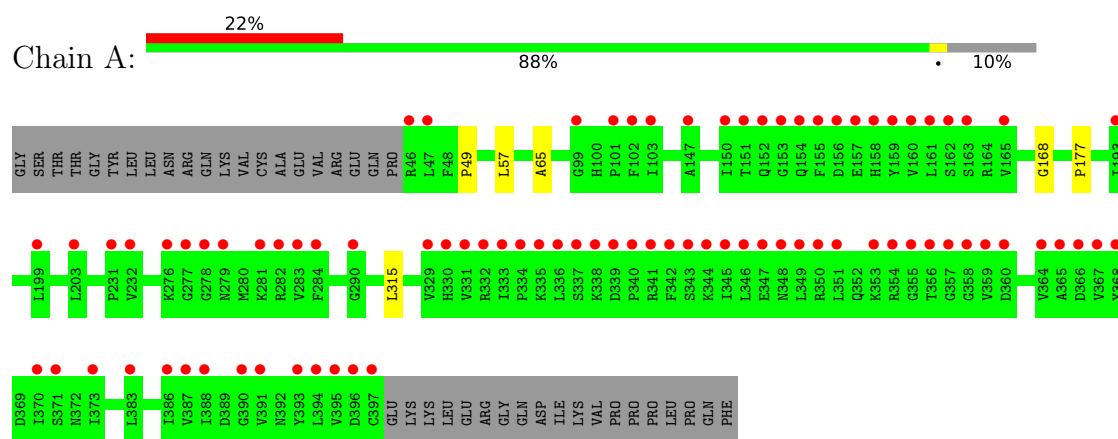
- Molecule 4 is water.

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

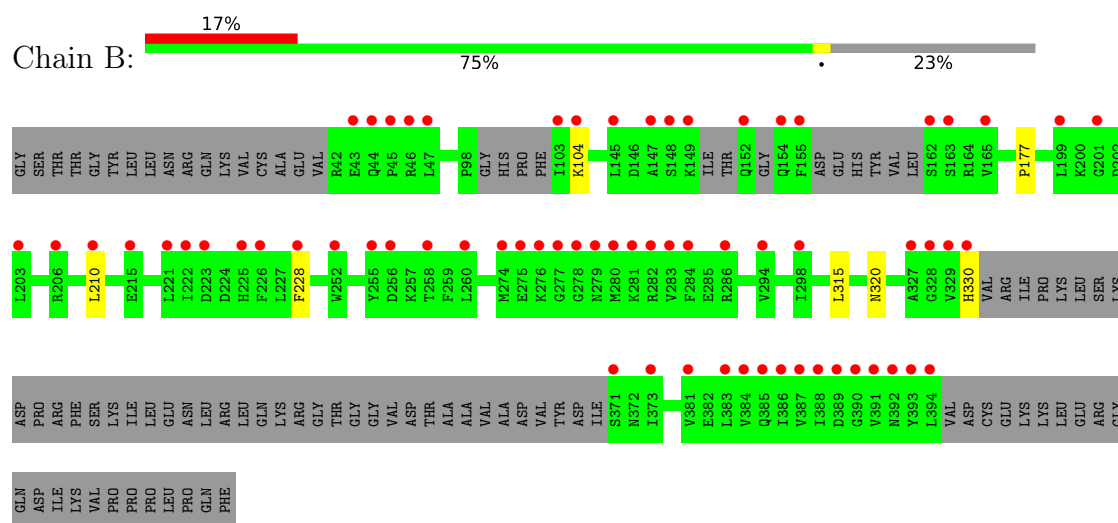
3 Residue-property plots

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.

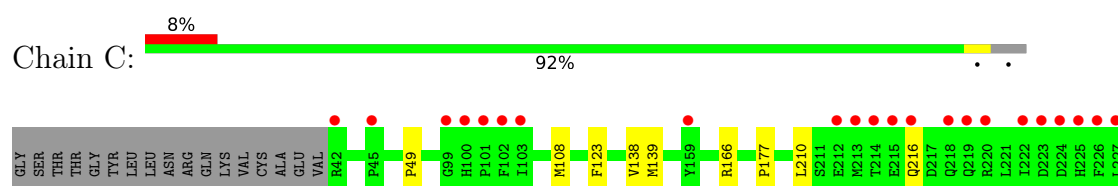
- Molecule 1: Creatine kinase S-type, mitochondrial

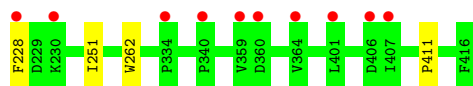


- Molecule 1: Creatine kinase S-type, mitochondrial

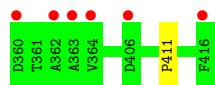
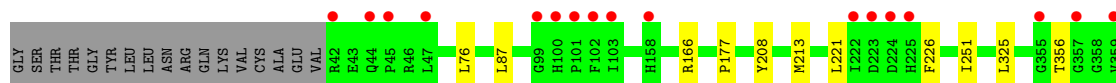
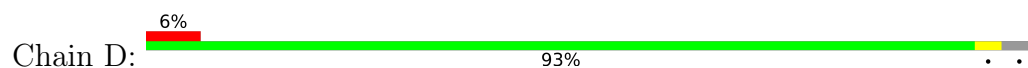


- Molecule 1: Creatine kinase S-type, mitochondrial

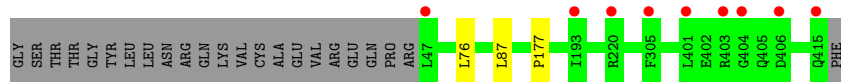




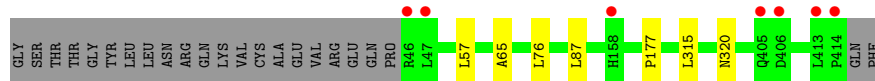
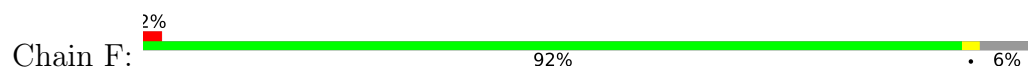
- Molecule 1: Creatine kinase S-type, mitochondrial



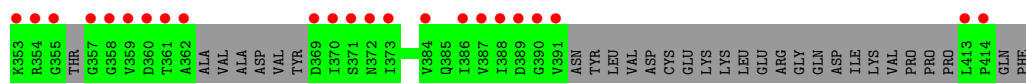
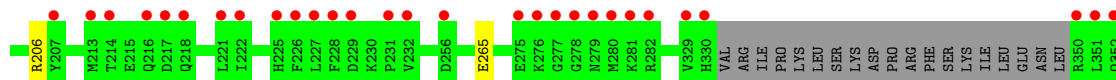
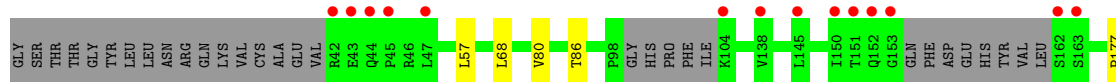
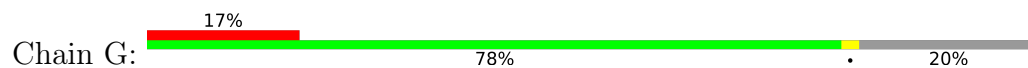
- Molecule 1: Creatine kinase S-type, mitochondrial



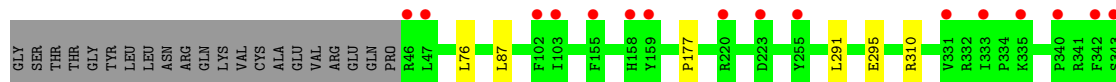
- Molecule 1: Creatine kinase S-type, mitochondrial

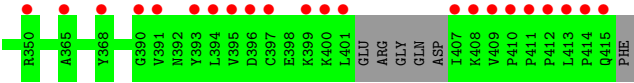


- Molecule 1: Creatine kinase S-type, mitochondrial



- 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 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.4 (40.00-2.10) 95.4 (40.00-2.10)	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 (Not available) , 0.215	Depositor DCC
R_{free} test set	4570 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 , 39.3	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 [i](#)

5.1 Standard geometry [i](#)

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	1.00	1/2705 (0.0%)	0.82	1/3682 (0.0%)
1	B	0.92	0/2385	0.77	1/3236 (0.0%)
1	C	1.01	3/3030 (0.1%)	0.81	1/4107 (0.0%)
1	D	1.00	1/3045 (0.0%)	0.78	1/4126 (0.0%)
1	E	0.93	0/3029	0.78	1/4104 (0.0%)
1	F	0.95	0/3052	0.77	1/4130 (0.0%)
1	G	0.98	0/2455	0.79	1/3325 (0.0%)
1	H	0.98	0/2974	0.78	1/4034 (0.0%)
All	All	0.97	5/22675 (0.0%)	0.79	8/30744 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	PRO	CA-C	7.79	1.56	1.51
1	D	411	PRO	CA-C	6.34	1.55	1.51
1	C	177	PRO	CA-C	6.06	1.57	1.52
1	C	411	PRO	CA-C	6.06	1.56	1.52
1	C	49	PRO	CA-C	5.04	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	PRO	N-CA-C	7.10	119.36	110.70
1	A	177	PRO	N-CA-C	7.07	119.32	110.70
1	G	177	PRO	N-CA-C	7.02	119.26	110.70
1	F	177	PRO	N-CA-C	6.74	118.92	110.70
1	E	177	PRO	N-CA-C	6.73	118.91	110.70
1	D	177	PRO	N-CA-C	6.66	118.82	110.70
1	H	177	PRO	N-CA-C	6.33	118.42	110.70
1	B	177	PRO	N-CA-C	6.07	118.11	110.70

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	2	0
1	B	2323	0	2159	2	0
1	C	2952	0	2852	6	0
1	D	2965	0	2885	6	0
1	E	2948	0	2896	1	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	0	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	25	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 1.

All (25) 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: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:208:TYR:HB3	1:D:213:MET:HE2	1.92	0.51
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:108:MET:HE2	1:C:123:PHE:CE1	2.52	0.45
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:A:168:GLY:C	1:A:315:LEU:HD21	2.45	0.42
1:D:166:ARG:HD2	1:D:166:ARG:C	2.44	0.42
1:B:315:LEU:HD12	1:B:320:ASN:O	2.20	0.42
1:C:166:ARG:HD2	1:C:166:ARG:C	2.45	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:OE1	1:G:265[B]:GLU:HA	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 [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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%)	70	78
1	C	304/342 (89%)	303 (100%)	1 (0%)	86	91
1	D	309/342 (90%)	308 (100%)	1 (0%)	86	91
1	E	316/342 (92%)	316 (100%)	0	100	100
1	F	320/342 (94%)	320 (100%)	0	100	100
1	G	235/342 (69%)	234 (100%)	1 (0%)	84	89
1	H	301/342 (88%)	300 (100%)	1 (0%)	86	91
All	All	2273/2736 (83%)	2267 (100%)	6 (0%)	86	91

All (6) 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	G	206	ARG
1	H	310	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	B	299	GLN
1	C	78	ASN
1	C	218	GLN
1	D	78	ASN
1	D	225	HIS
1	F	158	HIS
1	G	83	ASN

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Mol	Chain	Res	Type
1	G	385	GLN

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 oligosaccharides 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	C	501	-	28,29,29	1.58	6 (21%)	43,45,45	1.78	9 (20%)
2	ADP	G	501[A]	-	28,29,29	1.38	4 (14%)	43,45,45	1.87	9 (20%)
2	ADP	B	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.87	9 (20%)
2	ADP	G	501[B]	-	28,29,29	1.38	4 (14%)	43,45,45	1.84	9 (20%)
2	ADP	F	501	-	28,29,29	1.69	6 (21%)	43,45,45	1.81	12 (27%)
2	ADP	H	501	-	28,29,29	1.39	3 (10%)	43,45,45	1.86	8 (18%)
2	ADP	E	501	-	28,29,29	1.65	6 (21%)	43,45,45	1.76	10 (23%)
2	ADP	D	501	-	28,29,29	1.51	5 (17%)	43,45,45	1.86	12 (27%)
2	ADP	A	501	-	28,29,29	1.51	4 (14%)	43,45,45	1.81	10 (23%)

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	C	501	-	-	2/16/32/32	0/3/3/3
2	ADP	G	501[A]	-	-	2/16/32/32	0/3/3/3
2	ADP	B	501	-	-	2/16/32/32	0/3/3/3
2	ADP	G	501[B]	-	-	5/16/32/32	0/3/3/3
2	ADP	F	501	-	-	2/16/32/32	0/3/3/3
2	ADP	H	501	-	-	1/16/32/32	0/3/3/3
2	ADP	E	501	-	-	2/16/32/32	0/3/3/3
2	ADP	D	501	-	-	4/16/32/32	0/3/3/3
2	ADP	A	501	-	-	2/16/32/32	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	ADP	PA-O3A	4.77	1.64	1.59
2	E	501	ADP	C5-C4	4.63	1.47	1.39
2	A	501	ADP	C5-C4	4.63	1.47	1.39
2	C	501	ADP	C5-C4	4.44	1.47	1.39
2	D	501	ADP	C5-C4	4.41	1.47	1.39
2	F	501	ADP	C5-C4	4.34	1.46	1.39
2	H	501	ADP	C5-C4	4.08	1.46	1.39
2	B	501	ADP	C5-C4	4.01	1.46	1.39
2	G	501[B]	ADP	C5-C4	3.92	1.46	1.39
2	G	501[A]	ADP	C5-C4	3.41	1.45	1.39
2	A	501	ADP	C8-N7	3.23	1.37	1.31
2	H	501	ADP	C8-N7	3.20	1.37	1.31
2	E	501	ADP	PA-O3A	3.16	1.62	1.59
2	D	501	ADP	C5-C6	3.15	1.49	1.41
2	G	501[B]	ADP	C5-N7	-3.10	1.33	1.39
2	E	501	ADP	C8-N7	3.00	1.37	1.31
2	F	501	ADP	C8-N7	2.92	1.37	1.31
2	C	501	ADP	C8-N7	2.89	1.37	1.31
2	B	501	ADP	C5-C6	2.86	1.49	1.41
2	H	501	ADP	C5-C6	2.84	1.48	1.41
2	G	501[A]	ADP	C8-N7	2.80	1.37	1.31
2	E	501	ADP	C4-N9	-2.77	1.31	1.37
2	A	501	ADP	C5-C6	2.71	1.48	1.41
2	G	501[A]	ADP	C5-N7	-2.58	1.34	1.39
2	C	501	ADP	C5-N7	-2.54	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	ADP	C5-C6	2.53	1.48	1.41
2	D	501	ADP	C8-N7	2.50	1.36	1.31
2	B	501	ADP	C8-N7	2.49	1.36	1.31
2	E	501	ADP	C5-N7	-2.47	1.34	1.39
2	D	501	ADP	PA-O3A	2.41	1.62	1.59
2	G	501[A]	ADP	C5-C6	2.38	1.47	1.41
2	A	501	ADP	C5-N7	-2.37	1.34	1.39
2	C	501	ADP	C2-N1	2.32	1.38	1.33
2	B	501	ADP	C5-N7	-2.30	1.34	1.39
2	C	501	ADP	C5-C6	2.25	1.47	1.41
2	F	501	ADP	C5-N7	-2.20	1.35	1.39
2	E	501	ADP	C5-C6	2.19	1.47	1.41
2	F	501	ADP	C4-N9	-2.19	1.33	1.37
2	G	501[B]	ADP	C8-N7	2.17	1.35	1.31
2	D	501	ADP	C4-N9	-2.15	1.33	1.37
2	G	501[B]	ADP	C5-C6	2.09	1.46	1.41
2	C	501	ADP	PA-O3A	2.08	1.61	1.59

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501[B]	ADP	C5-C4-N3	-6.10	118.32	126.72
2	H	501	ADP	C5-C4-N3	-5.81	118.72	126.72
2	G	501[A]	ADP	C5-C4-N3	-5.79	118.75	126.72
2	B	501	ADP	C5-C4-N3	-5.61	118.99	126.72
2	A	501	ADP	C5-C4-N3	-5.53	119.10	126.72
2	C	501	ADP	C5-C4-N3	-5.46	119.20	126.72
2	D	501	ADP	C5-C4-N3	-5.22	119.53	126.72
2	F	501	ADP	C5-C4-N3	-5.12	119.66	126.72
2	G	501[B]	ADP	N3-C4-N9	4.87	135.45	127.17
2	E	501	ADP	C5-C4-N3	-4.84	120.05	126.72
2	G	501[A]	ADP	N3-C4-N9	4.41	134.66	127.17
2	B	501	ADP	N3-C4-N9	4.38	134.62	127.17
2	H	501	ADP	N3-C2-N1	-4.33	122.03	128.58
2	H	501	ADP	N3-C4-N9	4.31	134.49	127.17
2	E	501	ADP	N3-C2-N1	-4.28	122.10	128.58
2	F	501	ADP	N3-C2-N1	-4.27	122.12	128.58
2	B	501	ADP	N3-C2-N1	-4.25	122.15	128.58
2	C	501	ADP	N3-C4-N9	4.23	134.37	127.17
2	A	501	ADP	N3-C4-N9	4.20	134.30	127.17
2	H	501	ADP	C2-N3-C4	4.19	122.08	111.83
2	A	501	ADP	N3-C2-N1	-4.16	122.28	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ADP	N3-C2-N1	-4.14	122.31	128.58
2	D	501	ADP	N3-C4-N9	4.10	134.13	127.17
2	D	501	ADP	N3-C2-N1	-4.01	122.50	128.58
2	B	501	ADP	C2-N3-C4	3.99	121.57	111.83
2	G	501[A]	ADP	N3-C2-N1	-3.95	122.61	128.58
2	E	501	ADP	N3-C4-N9	3.91	133.82	127.17
2	A	501	ADP	C2-N3-C4	3.91	121.37	111.83
2	F	501	ADP	N3-C4-N9	3.87	133.75	127.17
2	F	501	ADP	C2-N3-C4	3.85	121.23	111.83
2	G	501[A]	ADP	C2-N3-C4	3.84	121.20	111.83
2	G	501[B]	ADP	C2-N3-C4	3.79	121.08	111.83
2	G	501[B]	ADP	N3-C2-N1	-3.78	122.86	128.58
2	D	501	ADP	C2-N3-C4	3.70	120.87	111.83
2	E	501	ADP	C4-N9-C8	3.57	109.49	105.74
2	E	501	ADP	C2-N3-C4	3.45	120.25	111.83
2	C	501	ADP	C2-N3-C4	3.44	120.24	111.83
2	C	501	ADP	C4-C5-N7	-3.42	106.67	110.58
2	G	501[A]	ADP	C4-C5-N7	-3.40	106.69	110.58
2	B	501	ADP	C4-C5-N7	-3.37	106.73	110.58
2	D	501	ADP	C4-C5-N7	-3.31	106.80	110.58
2	A	501	ADP	C4-C5-N7	-3.26	106.86	110.58
2	F	501	ADP	C4-C5-N7	-3.25	106.86	110.58
2	D	501	ADP	C4-N9-C8	3.15	109.04	105.74
2	G	501[A]	ADP	C4-N9-C8	3.09	108.99	105.74
2	B	501	ADP	C4-N9-C8	3.04	108.93	105.74
2	H	501	ADP	C4-C5-N7	-3.01	107.14	110.58
2	E	501	ADP	C4-C5-N7	-2.99	107.16	110.58
2	F	501	ADP	C4-N9-C8	2.97	108.86	105.74
2	G	501[A]	ADP	N9-C8-N7	-2.93	109.77	113.94
2	C	501	ADP	C4-N9-C8	2.92	108.80	105.74
2	G	501[A]	ADP	C5-N7-C8	2.87	107.96	103.45
2	A	501	ADP	C4-N9-C8	2.78	108.65	105.74
2	D	501	ADP	O3B-PB-O2B	2.72	118.01	107.80
2	B	501	ADP	C5-N7-C8	2.70	107.69	103.45
2	G	501[B]	ADP	O4'-C1'-N9	2.69	113.25	108.09
2	G	501[B]	ADP	C4-C5-N7	-2.62	107.58	110.58
2	B	501	ADP	N9-C8-N7	-2.59	110.26	113.94
2	C	501	ADP	C5-N7-C8	2.59	107.51	103.45
2	D	501	ADP	C5-N7-C8	2.58	107.50	103.45
2	G	501[B]	ADP	C5-N7-C8	2.56	107.48	103.45
2	A	501	ADP	C5-N7-C8	2.55	107.46	103.45
2	D	501	ADP	N9-C8-N7	-2.55	110.31	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	ADP	C4-N9-C8	2.47	108.33	105.74
2	A	501	ADP	N9-C8-N7	-2.47	110.43	113.94
2	E	501	ADP	N9-C8-N7	-2.47	110.44	113.94
2	H	501	ADP	N9-C8-N7	-2.44	110.48	113.94
2	H	501	ADP	C5-N7-C8	2.42	107.26	103.45
2	F	501	ADP	N9-C8-N7	-2.39	110.55	113.94
2	E	501	ADP	C2-N1-C6	2.37	122.63	118.73
2	C	501	ADP	N9-C8-N7	-2.36	110.59	113.94
2	F	501	ADP	C5-N7-C8	2.35	107.14	103.45
2	A	501	ADP	O3A-PB-O1B	-2.32	98.85	111.04
2	G	501[B]	ADP	N9-C8-N7	-2.28	110.70	113.94
2	D	501	ADP	O2A-PA-O3A	2.28	113.43	107.27
2	G	501[A]	ADP	O4'-C1'-N9	2.21	112.33	108.09
2	F	501	ADP	O2A-PA-O3A	2.19	113.18	107.27
2	G	501[B]	ADP	C4-N9-C8	2.16	108.01	105.74
2	C	501	ADP	C2-N1-C6	2.16	122.27	118.73
2	F	501	ADP	C6-C5-N7	2.15	136.23	132.09
2	A	501	ADP	C6-C5-N7	2.15	136.23	132.09
2	D	501	ADP	C2-N1-C6	2.13	122.23	118.73
2	E	501	ADP	C5-N7-C8	2.12	106.78	103.45
2	F	501	ADP	O4'-C1'-N9	2.10	112.13	108.09
2	F	501	ADP	C2-N1-C6	2.10	122.18	118.73
2	D	501	ADP	C6-C5-N7	2.09	136.12	132.09
2	E	501	ADP	O4'-C1'-N9	2.07	112.06	108.09
2	B	501	ADP	C6-C5-N7	2.04	136.01	132.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

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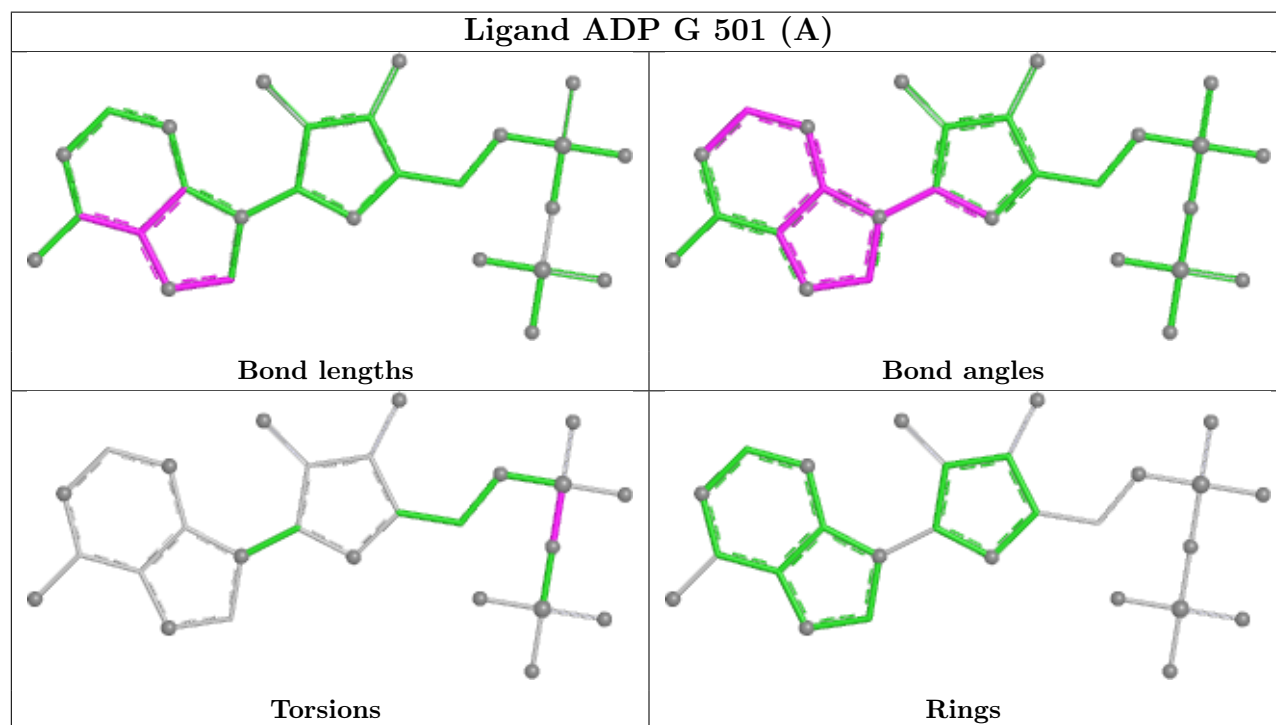
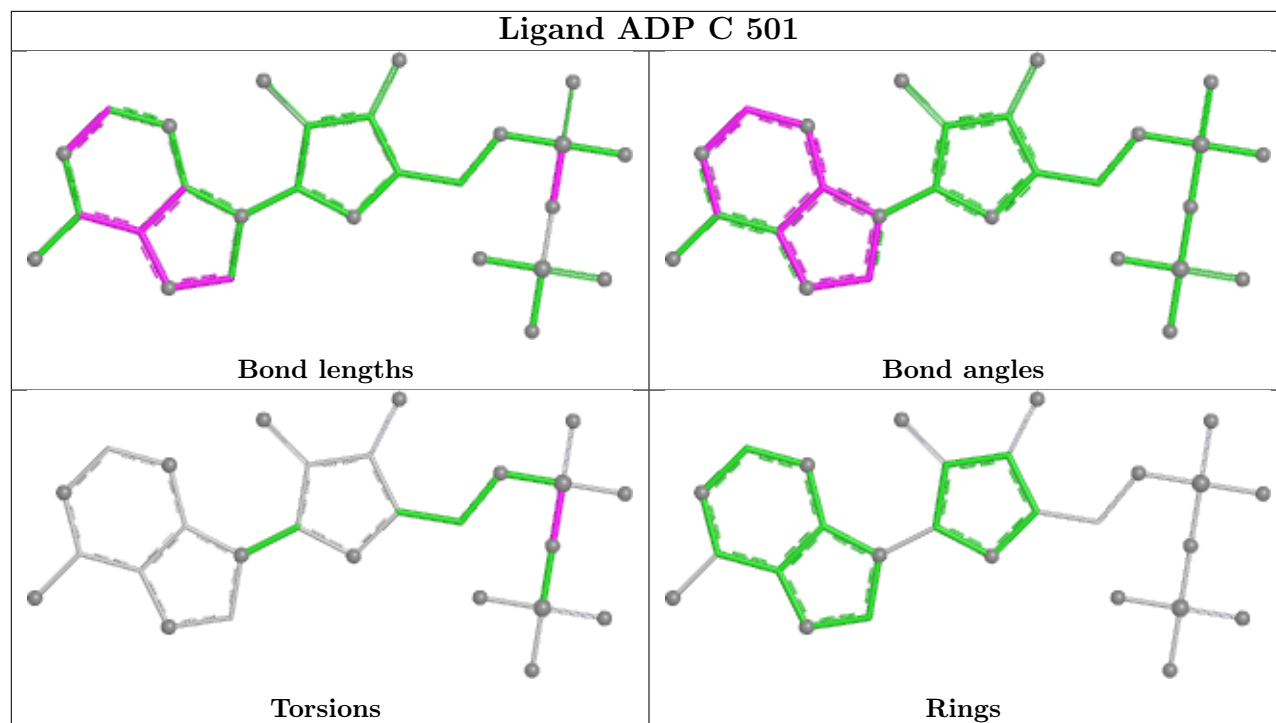
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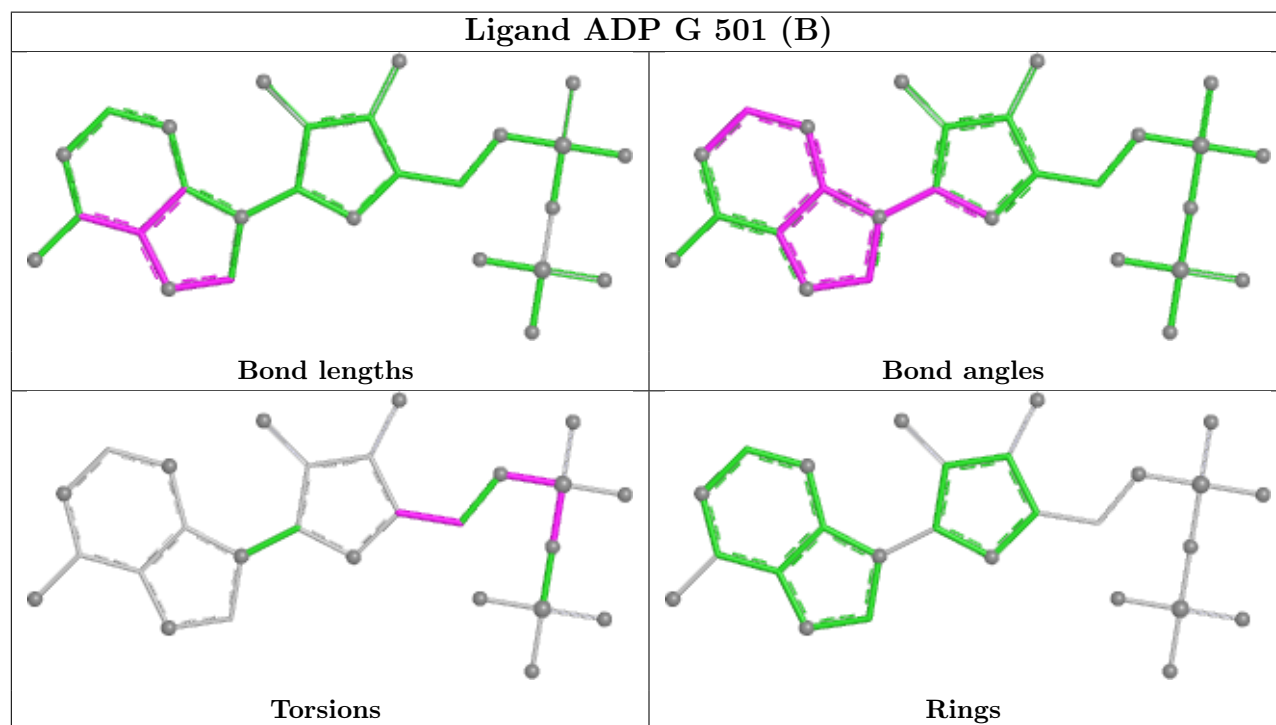
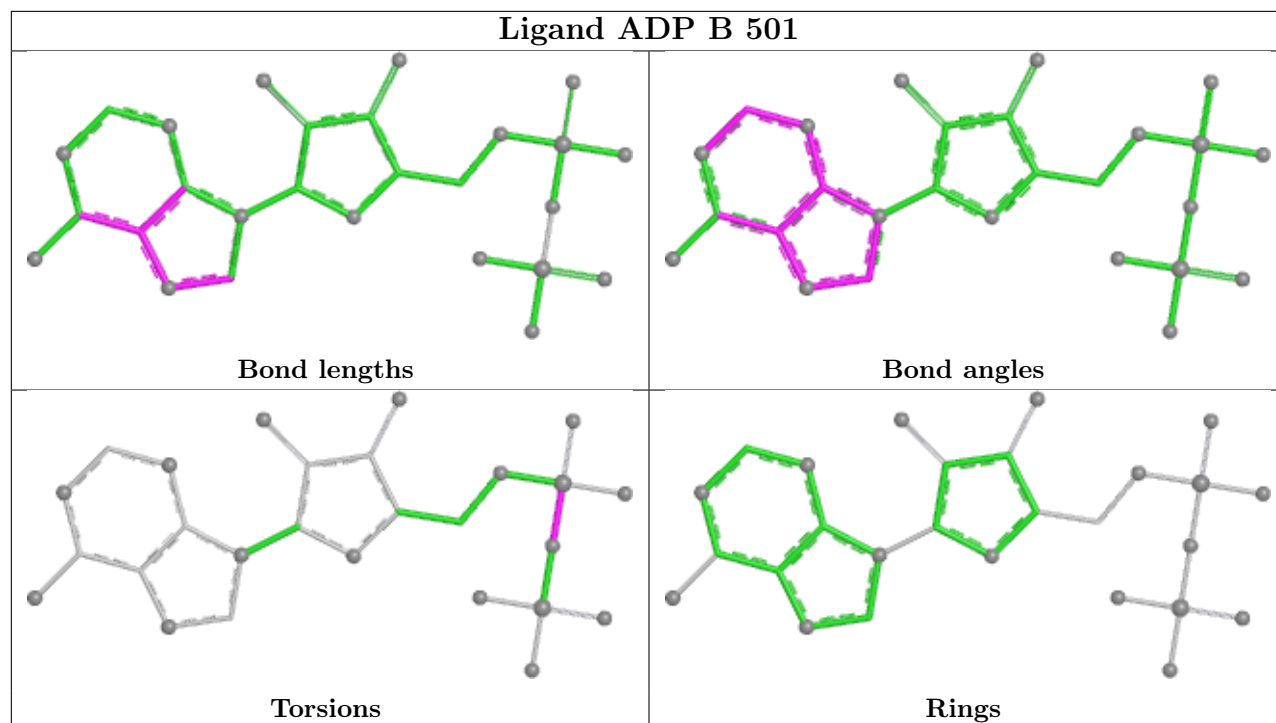
Mol	Chain	Res	Type	Atoms
2	D	501	ADP	PB-O3A-PA-O2A
2	F	501	ADP	PB-O3A-PA-O2A
2	A	501	ADP	PB-O3A-PA-O1A
2	B	501	ADP	PB-O3A-PA-O1A
2	E	501	ADP	PB-O3A-PA-O1A
2	F	501	ADP	PB-O3A-PA-O1A
2	A	501	ADP	PB-O3A-PA-O2A
2	C	501	ADP	PB-O3A-PA-O1A
2	G	501[A]	ADP	PB-O3A-PA-O2A
2	G	501[B]	ADP	PB-O3A-PA-O2A

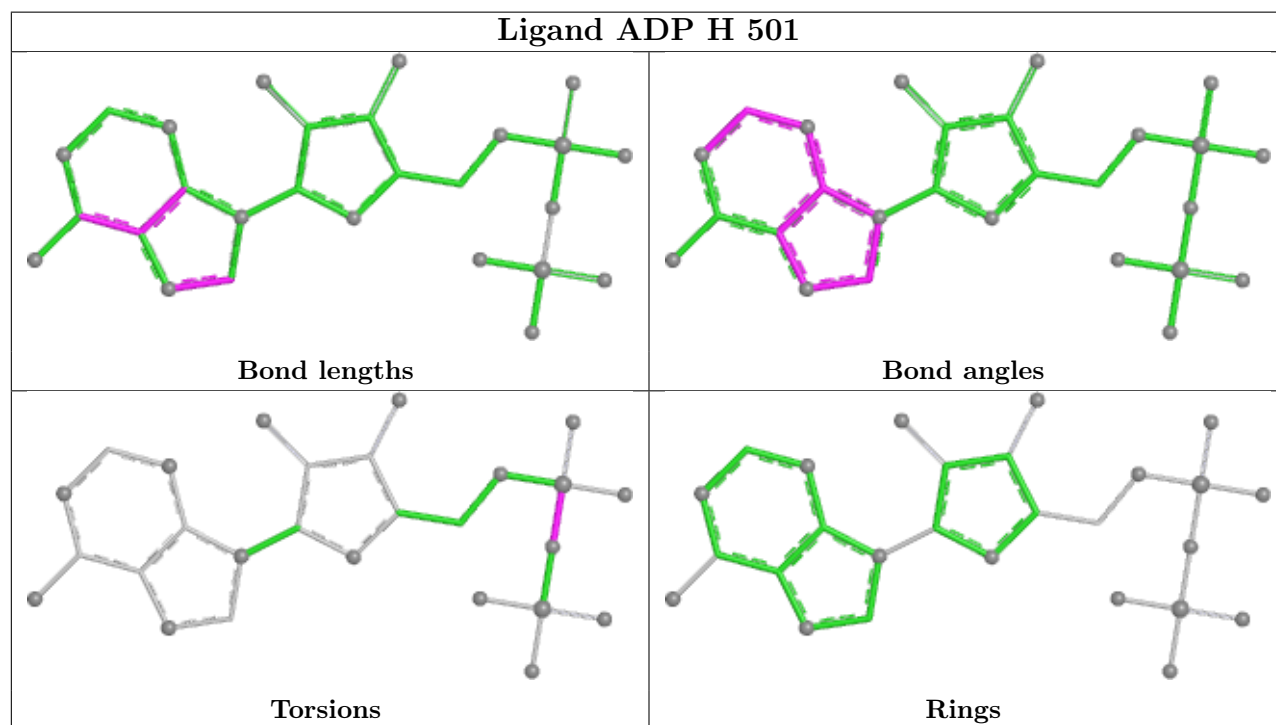
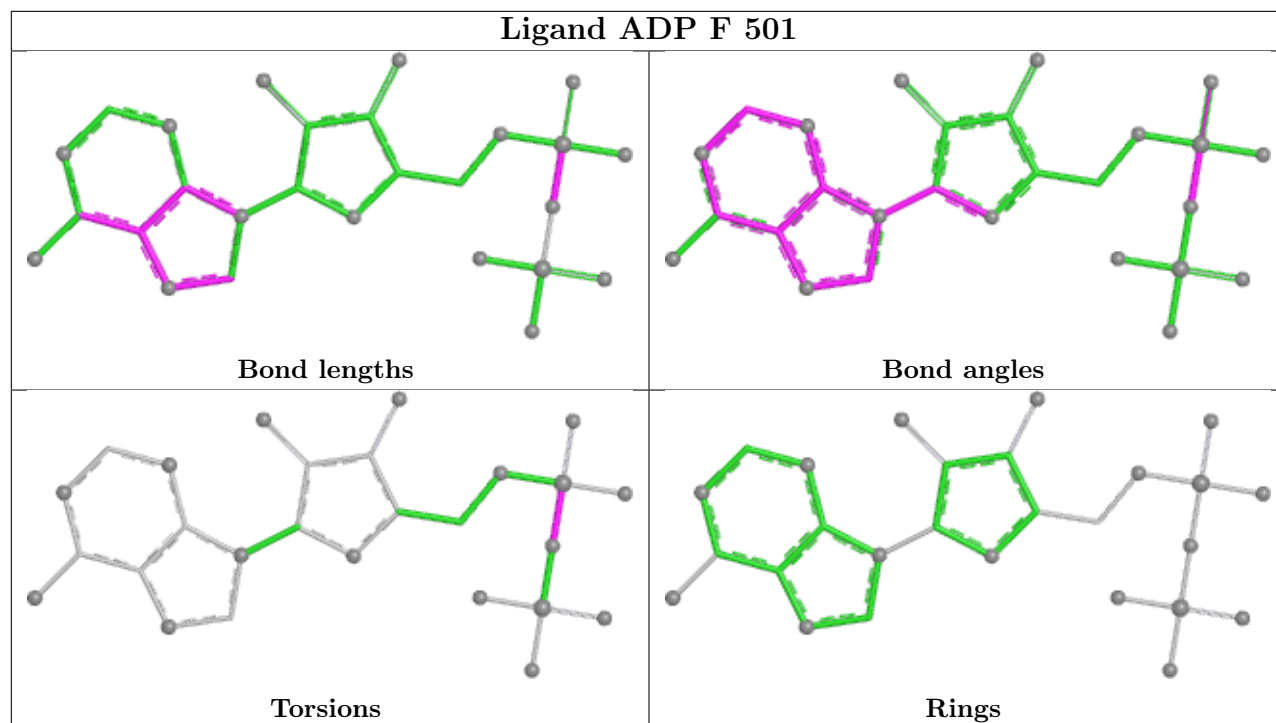
There are no ring outliers.

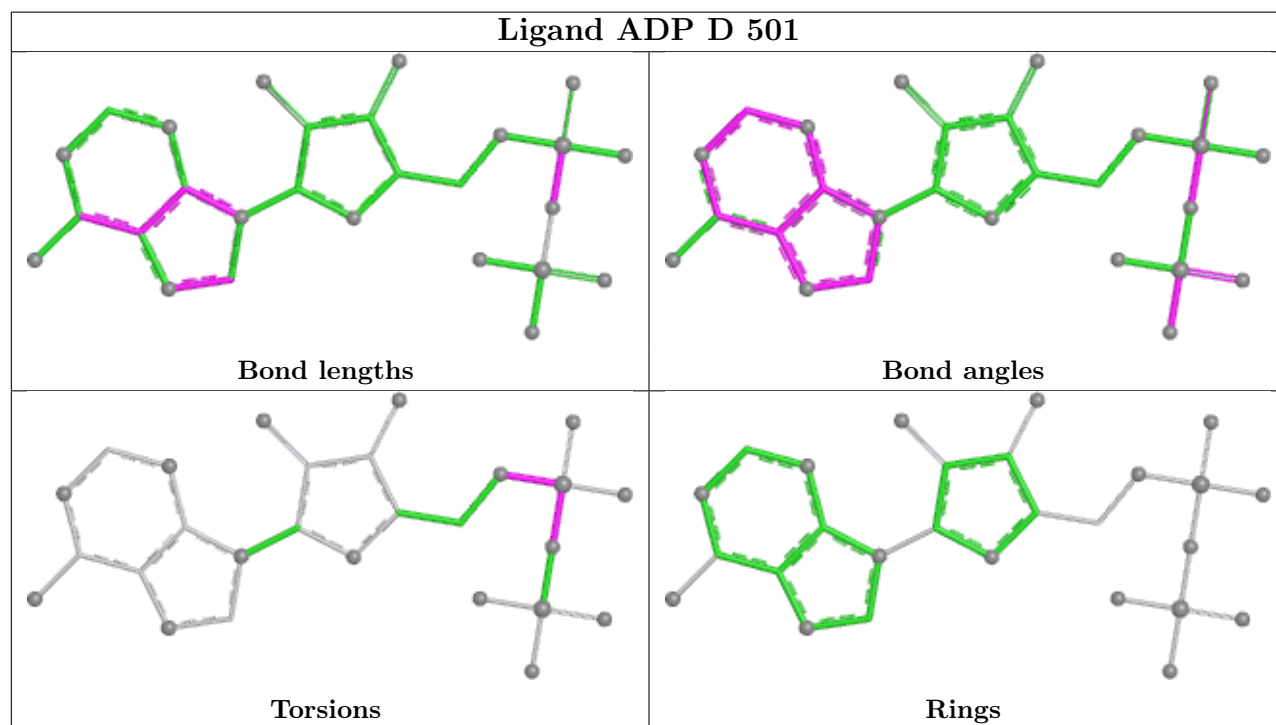
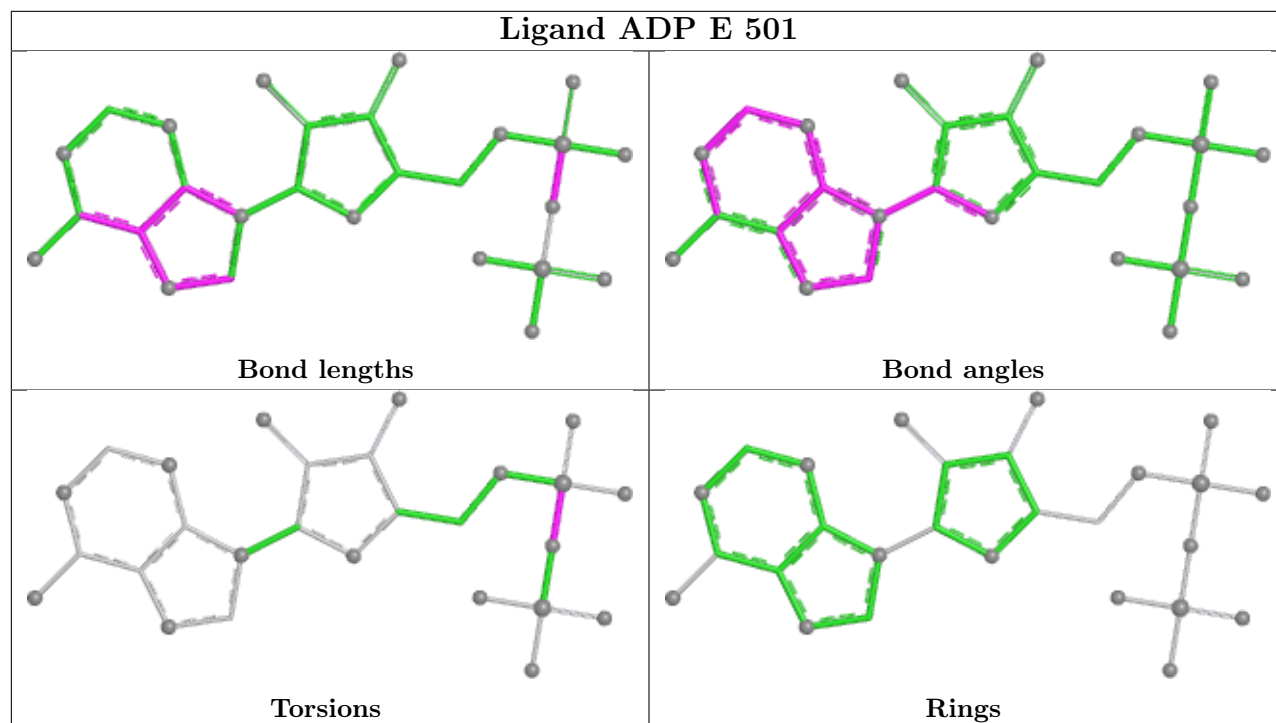
No monomer is involved in short contacts.

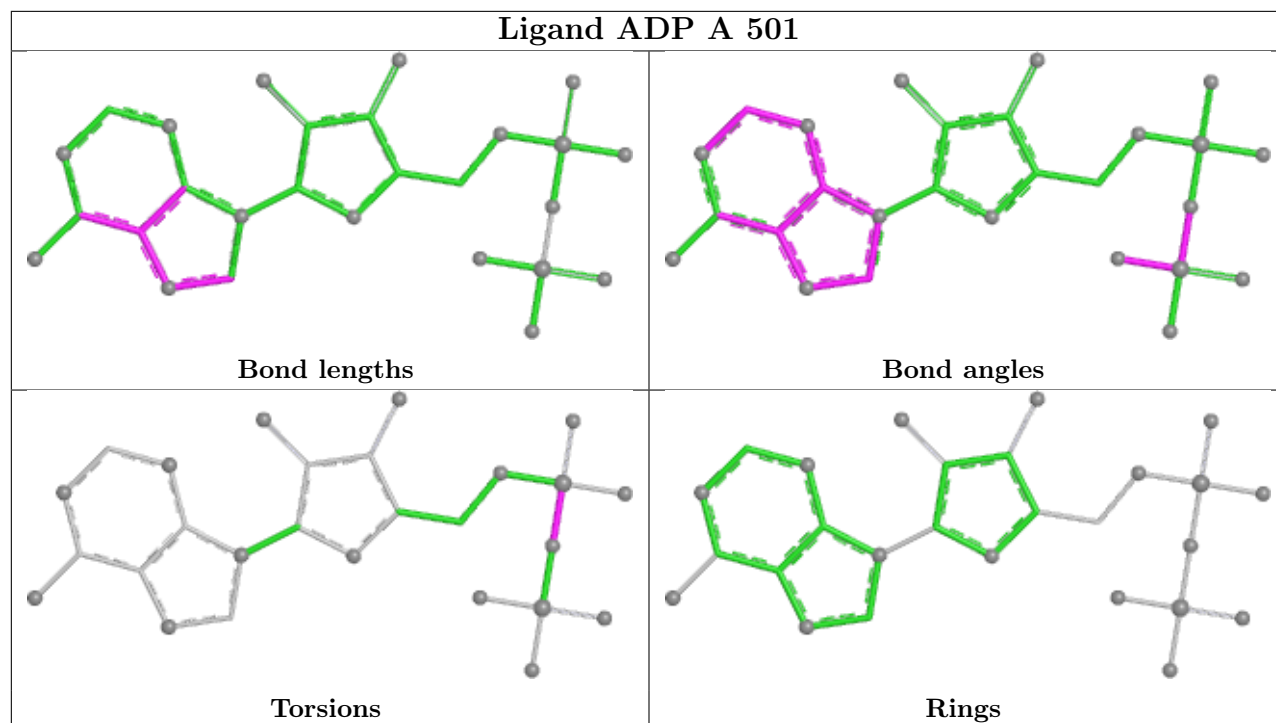
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	1.11	86 (24%) 2 2	22, 45, 89, 112	0
1	B	300/392 (76%)	1.00	67 (22%) 2 2	20, 44, 85, 98	7 (2%)
1	C	375/392 (95%)	0.24	32 (8%) 16 17	14, 30, 66, 90	7 (1%)
1	D	375/392 (95%)	0.19	23 (6%) 27 29	15, 30, 65, 97	5 (1%)
1	E	369/392 (94%)	0.03	9 (2%) 59 62	15, 32, 52, 72	8 (2%)
1	F	369/392 (94%)	-0.09	7 (1%) 66 69	18, 30, 48, 73	6 (1%)
1	G	313/392 (79%)	0.99	66 (21%) 2 2	13, 41, 81, 95	3 (0%)
1	H	365/392 (93%)	0.67	38 (10%) 11 12	20, 38, 75, 95	10 (2%)
All	All	2818/3136 (89%)	0.49	328 (11%) 9 10	13, 34, 77, 112	46 (1%)

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	102	PHE	9.0
1	A	345	ILE	7.6
1	G	357	GLY	7.4
1	B	103	ILE	6.8
1	H	255[A]	TYR	6.4
1	G	153	GLY	5.8
1	A	103	ILE	5.8
1	B	388	ILE	5.8
1	A	346	LEU	5.6
1	G	355	GLY	5.6
1	A	349	LEU	5.3
1	A	160	VAL	5.3
1	A	364	VAL	5.3
1	G	278	GLY	5.3
1	B	391	VAL	5.2
1	B	155	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	G	162	SER	5.2
1	C	214	THR	5.2
1	G	391	VAL	5.1
1	B	394	LEU	5.1
1	B	329	VAL	5.1
1	A	334	PRO	5.0
1	D	45	PRO	4.9
1	A	102	PHE	4.9
1	C	226	PHE	4.9
1	A	159	TYR	4.7
1	G	359	VAL	4.7
1	G	138	VAL	4.6
1	H	407	ILE	4.6
1	D	416	PHE	4.6
1	G	227	LEU	4.5
1	B	277	GLY	4.5
1	H	47	LEU	4.5
1	A	336	LEU	4.5
1	G	388	ILE	4.5
1	G	360	ASP	4.5
1	A	278	GLY	4.5
1	C	215	GLU	4.5
1	A	163	SER	4.4
1	A	333	ILE	4.4
1	B	328	GLY	4.4
1	G	226	PHE	4.4
1	A	331	VAL	4.4
1	D	102	PHE	4.3
1	B	162	SER	4.3
1	A	387	VAL	4.3
1	B	373	ILE	4.3
1	A	367	VAL	4.3
1	A	344	LYS	4.2
1	G	222	ILE	4.2
1	D	101	PRO	4.1
1	D	360	ASP	4.1
1	A	101	PRO	4.1
1	A	161	LEU	4.1
1	A	391	VAL	4.1
1	C	103	ILE	4.1
1	A	351	LEU	4.1
1	B	276	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	389	ASP	4.0
1	B	203	LEU	4.0
1	C	227[A]	LEU	4.0
1	H	413	LEU	3.9
1	A	277	GLY	3.9
1	B	278	GLY	3.9
1	D	355	GLY	3.9
1	D	363	ALA	3.9
1	B	147	ALA	3.9
1	G	362	ALA	3.9
1	E	47	LEU	3.9
1	G	151	THR	3.9
1	A	370	ILE	3.8
1	G	350	ARG	3.8
1	H	401	LEU	3.8
1	D	103	ILE	3.8
1	G	373	ILE	3.8
1	G	45	PRO	3.8
1	A	152	GLN	3.8
1	C	218	GLN	3.8
1	A	393	TYR	3.7
1	H	46	ARG	3.7
1	H	103	ILE	3.7
1	B	44	GLN	3.7
1	G	329	VAL	3.7
1	A	158	HIS	3.7
1	G	386	ILE	3.7
1	A	341	ARG	3.7
1	B	45	PRO	3.6
1	G	354	ARG	3.6
1	G	221	LEU	3.6
1	G	351	LEU	3.6
1	B	165	VAL	3.6
1	A	155	PHE	3.6
1	C	220	ARG	3.6
1	A	335	LYS	3.6
1	A	347	GLU	3.5
1	A	355	GLY	3.5
1	G	216	GLN	3.5
1	G	150	ILE	3.5
1	C	219	GLN	3.5
1	G	414	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	338	LYS	3.4
1	A	358	GLY	3.4
1	A	397	CYS	3.4
1	D	44	GLN	3.4
1	B	275	GLU	3.4
1	A	390	GLY	3.4
1	G	390	GLY	3.4
1	A	276	LYS	3.4
1	B	393	TYR	3.3
1	A	386	ILE	3.3
1	B	386	ILE	3.3
1	B	256	ASP	3.3
1	G	352	GLN	3.3
1	B	280	MET	3.3
1	G	217	ASP	3.3
1	B	255	TYR	3.3
1	A	388	ILE	3.3
1	G	276	LYS	3.3
1	H	415	GLN	3.3
1	H	414	PRO	3.2
1	A	150	ILE	3.2
1	B	163	SER	3.2
1	A	354	ARG	3.2
1	B	260	LEU	3.2
1	H	368	TYR	3.2
1	G	277	GLY	3.2
1	A	348	ASN	3.1
1	B	384	VAL	3.1
1	G	369	ASP	3.1
1	A	368	TYR	3.1
1	H	340	PRO	3.1
1	A	332	ARG	3.1
1	A	394	LEU	3.1
1	D	100	HIS	3.1
1	E	404	GLY	3.1
1	G	214	THR	3.1
1	D	42	ARG	3.1
1	A	365	ALA	3.1
1	A	359	VAL	3.1
1	H	400	LYS	3.1
1	H	155	PHE	3.0
1	B	149	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	47	LEU	3.0
1	C	359	VAL	3.0
1	B	215	GLU	3.0
1	F	414	PRO	3.0
1	C	100	HIS	3.0
1	B	252	TRP	3.0
1	B	284	PHE	3.0
1	H	158	HIS	3.0
1	C	213	MET	3.0
1	C	42	ARG	3.0
1	B	43	GLU	3.0
1	B	330	HIS	3.0
1	G	152	GLN	2.9
1	H	409	VAL	2.9
1	A	356	THR	2.9
1	D	224	ASP	2.9
1	B	327	ALA	2.9
1	D	364	VAL	2.9
1	H	411	PRO	2.9
1	H	399	LYS	2.9
1	C	223	ASP	2.9
1	B	152	GLN	2.9
1	A	350	ARG	2.9
1	G	282	ARG	2.9
1	H	412	PRO	2.9
1	A	342	PHE	2.9
1	F	47	LEU	2.8
1	A	232	VAL	2.8
1	B	222	ILE	2.8
1	H	159	TYR	2.8
1	G	229	ASP	2.8
1	A	283	VAL	2.8
1	H	410	PRO	2.8
1	D	47	LEU	2.8
1	B	283	VAL	2.8
1	E	406	ASP	2.8
1	C	222	ILE	2.8
1	B	298	ILE	2.7
1	B	392	ASN	2.7
1	B	371	SER	2.7
1	G	163	SER	2.7
1	A	153	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	390	GLY	2.7
1	A	151	THR	2.7
1	G	330	HIS	2.7
1	B	206	ARG	2.7
1	B	226	PHE	2.7
1	B	145	LEU	2.7
1	A	395	VAL	2.7
1	C	406	ASP	2.7
1	B	385	GLN	2.6
1	C	228[A]	PHE	2.6
1	H	102	PHE	2.6
1	G	225	HIS	2.6
1	A	329	VAL	2.6
1	G	353	LYS	2.6
1	F	46	ARG	2.6
1	G	358	GLY	2.6
1	C	225	HIS	2.6
1	D	158	HIS	2.6
1	A	156	ASP	2.6
1	A	366	ASP	2.6
1	D	406	ASP	2.6
1	G	207	TYR	2.6
1	C	364	VAL	2.6
1	C	216	GLN	2.6
1	B	279	ASN	2.6
1	A	337	SER	2.6
1	E	415	GLN	2.6
1	G	370	ILE	2.6
1	A	340	PRO	2.6
1	A	396	ASP	2.6
1	C	101	PRO	2.6
1	G	279	ASN	2.5
1	A	154	GLN	2.5
1	B	154	GLN	2.5
1	C	401	LEU	2.5
1	G	47	LEU	2.5
1	A	157	GLU	2.5
1	A	279	ASN	2.5
1	C	45	PRO	2.5
1	A	203	LEU	2.5
1	B	104	LYS	2.5
1	B	46	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	294	VAL	2.5
1	B	387	VAL	2.5
1	D	359	VAL	2.5
1	B	258	THR	2.5
1	E	220[A]	ARG	2.5
1	C	407	ILE	2.5
1	H	331	VAL	2.4
1	D	362	ALA	2.4
1	B	282	ARG	2.4
1	A	99	GLY	2.4
1	G	275	GLU	2.4
1	A	339	ASP	2.4
1	B	148	SER	2.4
1	B	274	MET	2.4
1	G	280	MET	2.4
1	G	104	LYS	2.4
1	H	408	LYS	2.4
1	G	413	LEU	2.4
1	F	406	ASP	2.4
1	A	373	ILE	2.4
1	A	353	LYS	2.4
1	G	231	PRO	2.4
1	B	383	LEU	2.4
1	D	99	GLY	2.4
1	H	390	GLY	2.4
1	A	193	ILE	2.4
1	B	381	VAL	2.4
1	G	384	VAL	2.4
1	F	158	HIS	2.4
1	B	201	GLY	2.3
1	G	387	VAL	2.3
1	C	159	TYR	2.3
1	H	396	ASP	2.3
1	H	342	PHE	2.3
1	A	162	SER	2.3
1	A	343	SER	2.3
1	H	333	ILE	2.3
1	G	42	ARG	2.3
1	G	389	ASP	2.3
1	A	330	HIS	2.2
1	B	225	HIS	2.2
1	C	212	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	360	ASP	2.2
1	E	403	ARG	2.2
1	A	281	LYS	2.2
1	D	225	HIS	2.2
1	H	393	TYR	2.2
1	B	281	LYS	2.2
1	C	224	ASP	2.2
1	E	193	ILE	2.2
1	G	43	GLU	2.2
1	G	218	GLN	2.2
1	A	383	LEU	2.2
1	H	394	LEU	2.2
1	B	286	ARG	2.2
1	G	371	SER	2.2
1	D	222	ILE	2.1
1	E	305	PHE	2.1
1	G	232	VAL	2.1
1	A	199	LEU	2.1
1	H	350[A]	ARG	2.1
1	A	231	PRO	2.1
1	C	334	PRO	2.1
1	C	340	PRO	2.1
1	C	99	GLY	2.1
1	H	365	ALA	2.1
1	B	199	LEU	2.1
1	G	372	ASN	2.1
1	C	360	ASP	2.1
1	A	282	ARG	2.1
1	A	357	GLY	2.1
1	G	228	PHE	2.1
1	H	395	VAL	2.1
1	A	371	SER	2.1
1	B	221	LEU	2.1
1	H	343	SER	2.1
1	A	46	ARG	2.1
1	C	230	LYS	2.1
1	H	335	LYS	2.1
1	B	228	PHE	2.1
1	A	147	ALA	2.1
1	B	47	LEU	2.0
1	E	401	LEU	2.0
1	F	413	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	223	ASP	2.0
1	F	405	GLN	2.0
1	G	44	GLN	2.0
1	G	361	THR	2.0
1	G	281	LYS	2.0
1	A	290	GLY	2.0
1	D	357	GLY	2.0
1	A	165	VAL	2.0
1	A	284	PHE	2.0
1	H	391	VAL	2.0
1	G	213	MET	2.0
1	B	210	LEU	2.0
1	G	145	LEU	2.0
1	D	223	ASP	2.0
1	G	256	ASP	2.0
1	H	223	ASP	2.0
1	H	220	ARG	2.0
1	H	397	CYS	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 oligosaccharides 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(Å ²)	Q<0.9
3	UNX	D	502	1/1	0.55	0.33	36,36,36,36	0
3	UNX	B	502	1/1	0.61	0.35	48,48,48,48	0
3	UNX	G	503	1/1	0.64	0.45	44,44,44,44	0
3	UNX	C	502	1/1	0.69	0.29	34,34,34,34	0
3	UNX	F	511	1/1	0.74	0.22	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UNX	E	512	1/1	0.75	0.22	36,36,36,36	0
3	UNX	H	504	1/1	0.75	0.40	42,42,42,42	0
3	UNX	H	503	1/1	0.77	0.40	43,43,43,43	0
3	UNX	E	509	1/1	0.78	0.16	21,21,21,21	0
3	UNX	A	502	1/1	0.81	0.39	37,37,37,37	0
3	UNX	E	503	1/1	0.81	0.29	33,33,33,33	0
3	UNX	E	505	1/1	0.81	0.36	17,17,17,17	1
3	UNX	H	508	1/1	0.81	0.17	36,36,36,36	0
3	UNX	C	507	1/1	0.83	0.18	39,39,39,39	0
3	UNX	H	506	1/1	0.84	0.20	41,41,41,41	0
3	UNX	B	503	1/1	0.85	0.40	44,44,44,44	0
3	UNX	G	502	1/1	0.85	0.29	33,33,33,33	0
3	UNX	H	505	1/1	0.85	0.34	42,42,42,42	0
3	UNX	D	508	1/1	0.85	0.14	28,28,28,28	0
3	UNX	G	506	1/1	0.85	0.14	36,36,36,36	0
3	UNX	H	513	1/1	0.85	0.26	36,36,36,36	0
3	UNX	A	503	1/1	0.86	0.37	40,40,40,40	0
3	UNX	B	507	1/1	0.86	0.24	42,42,42,42	0
3	UNX	D	505	1/1	0.87	0.15	27,27,27,27	0
3	UNX	C	503	1/1	0.87	0.32	39,39,39,39	0
3	UNX	A	508	1/1	0.88	0.14	27,27,27,27	0
3	UNX	G	505	1/1	0.88	0.13	31,31,31,31	0
3	UNX	E	502	1/1	0.88	0.23	25,25,25,25	0
2	ADP	B	501	27/27	0.89	0.14	48,77,96,97	0
3	UNX	A	504	1/1	0.89	0.26	28,28,28,28	0
3	UNX	H	502	1/1	0.89	0.13	31,31,31,31	0
2	ADP	G	501[B]	27/27	0.90	0.12	53,68,72,72	19
3	UNX	E	504	1/1	0.90	0.23	38,38,38,38	0
3	UNX	B	505	1/1	0.90	0.15	31,31,31,31	0
3	UNX	C	505	1/1	0.90	0.33	45,45,45,45	0
2	ADP	G	501[A]	27/27	0.90	0.12	41,48,57,64	19
3	UNX	F	510	1/1	0.90	0.14	26,26,26,26	0
3	UNX	G	504	1/1	0.91	0.35	34,34,34,34	0
3	UNX	D	509	1/1	0.91	0.15	28,28,28,28	0
3	UNX	E	506	1/1	0.91	0.35	42,42,42,42	0
3	UNX	F	505	1/1	0.91	0.32	20,20,20,20	0
3	UNX	H	509	1/1	0.91	0.26	37,37,37,37	0
3	UNX	F	508	1/1	0.91	0.29	47,47,47,47	0
3	UNX	F	512	1/1	0.92	0.23	31,31,31,31	0
3	UNX	E	516	1/1	0.92	0.10	32,32,32,32	0
3	UNX	F	503	1/1	0.92	0.08	17,17,17,17	0
3	UNX	E	507	1/1	0.92	0.14	34,34,34,34	0

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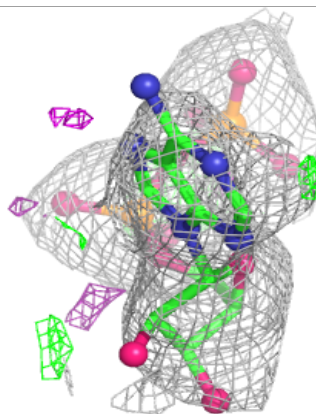
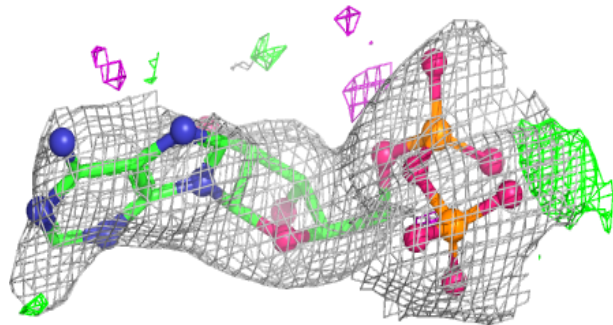
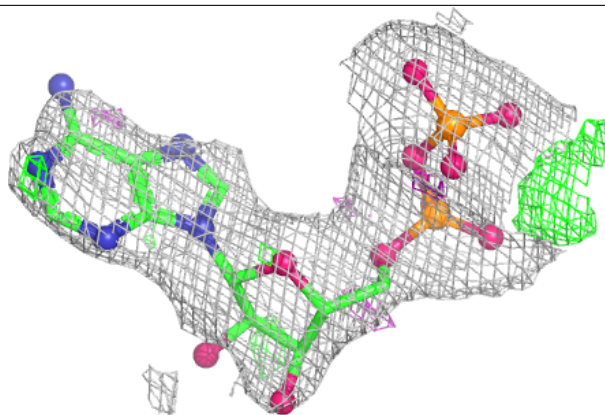
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UNX	B	504	1/1	0.92	0.11	28,28,28,28	0
3	UNX	D	503	1/1	0.92	0.14	36,36,36,36	0
3	UNX	E	513	1/1	0.92	0.12	36,36,36,36	0
3	UNX	B	506	1/1	0.93	0.20	24,24,24,24	0
3	UNX	F	504	1/1	0.93	0.14	36,36,36,36	0
3	UNX	E	508	1/1	0.93	0.09	27,27,27,27	0
3	UNX	D	504	1/1	0.93	0.20	28,28,28,28	0
3	UNX	E	510	1/1	0.94	0.08	25,25,25,25	0
2	ADP	A	501	27/27	0.94	0.09	37,50,65,66	0
3	UNX	H	507	1/1	0.94	0.24	30,30,30,30	0
3	UNX	A	506	1/1	0.94	0.09	36,36,36,36	0
2	ADP	H	501	27/27	0.94	0.09	35,40,43,43	0
3	UNX	F	502	1/1	0.94	0.28	21,21,21,21	0
3	UNX	H	514	1/1	0.94	0.18	35,35,35,35	0
3	UNX	F	507	1/1	0.95	0.13	23,23,23,23	0
3	UNX	D	506	1/1	0.95	0.24	28,28,28,28	0
3	UNX	C	506	1/1	0.95	0.12	15,15,15,15	0
3	UNX	H	510	1/1	0.95	0.11	27,27,27,27	0
3	UNX	H	511	1/1	0.95	0.14	27,27,27,27	0
3	UNX	E	515	1/1	0.95	0.07	23,23,23,23	0
3	UNX	A	507	1/1	0.95	0.18	31,31,31,31	0
3	UNX	F	509	1/1	0.96	0.29	35,35,35,35	0
3	UNX	C	504	1/1	0.96	0.09	27,27,27,27	0
2	ADP	D	501	27/27	0.96	0.07	30,41,44,47	0
3	UNX	A	505	1/1	0.97	0.08	21,21,21,21	0
3	UNX	D	507	1/1	0.97	0.17	7,7,7,7	0
3	UNX	F	506	1/1	0.98	0.14	13,13,13,13	0
3	UNX	E	511	1/1	0.98	0.16	20,20,20,20	0
2	ADP	C	501	27/27	0.98	0.05	25,29,31,35	0
2	ADP	E	501	27/27	0.98	0.05	24,28,30,33	0
3	UNX	E	514	1/1	0.98	0.06	20,20,20,20	0
2	ADP	F	501	27/27	0.98	0.05	22,27,29,30	0
3	UNX	H	512	1/1	0.99	0.03	26,26,26,26	0

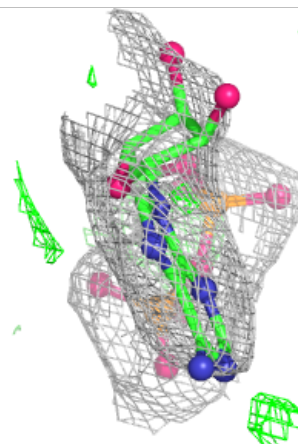
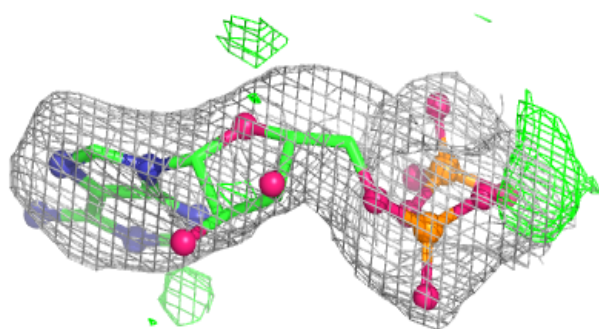
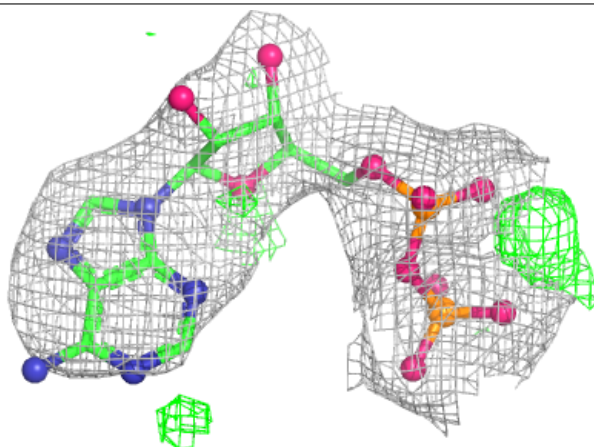
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP 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)

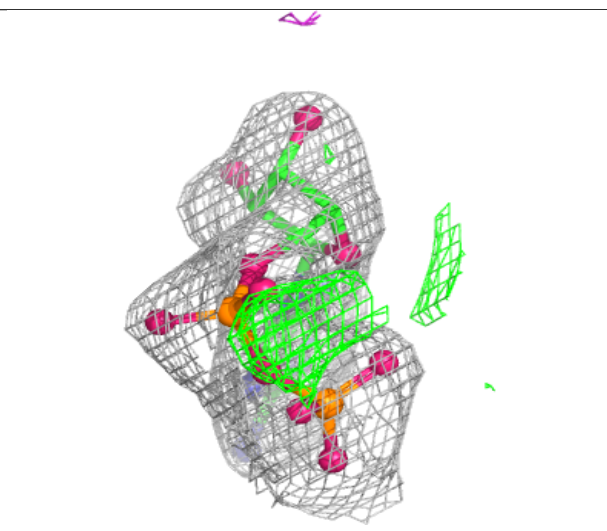
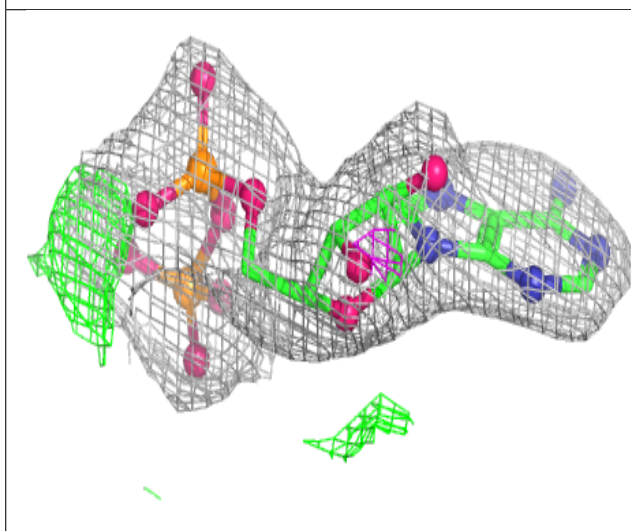
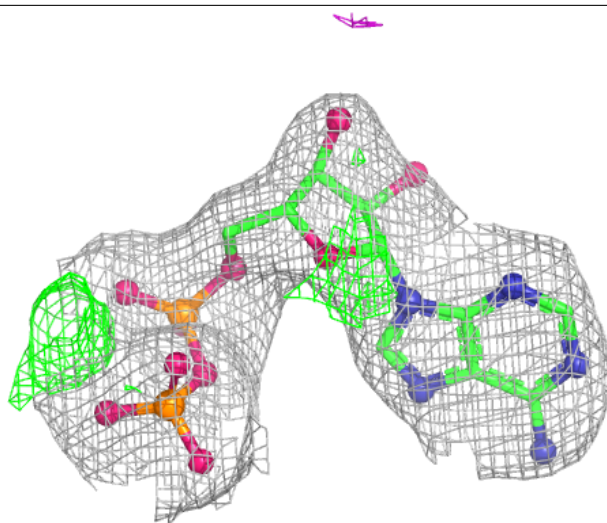
**Electron density around ADP G 501 (B):**

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



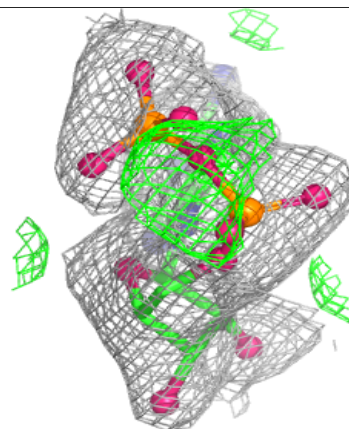
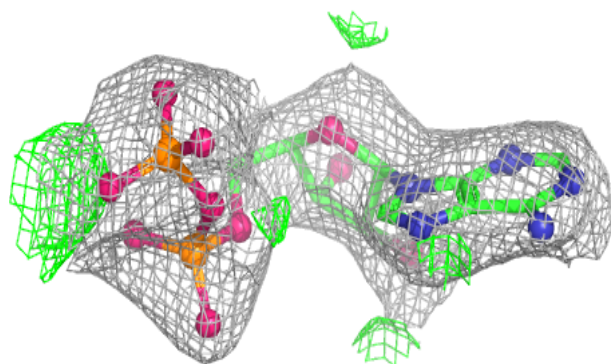
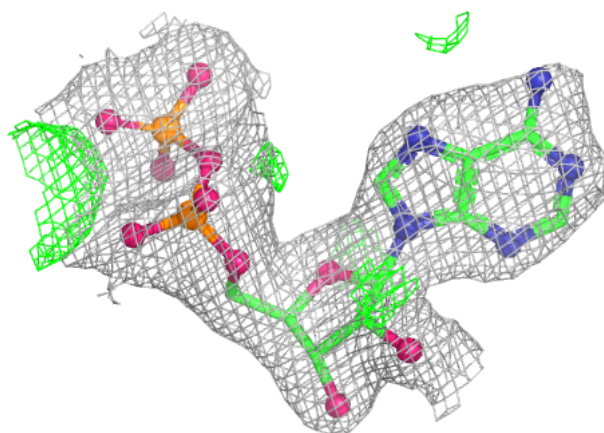
Electron density around ADP G 501 (A):

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



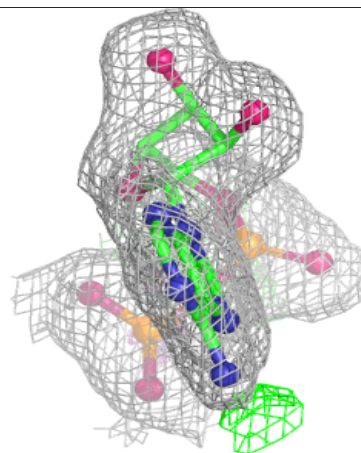
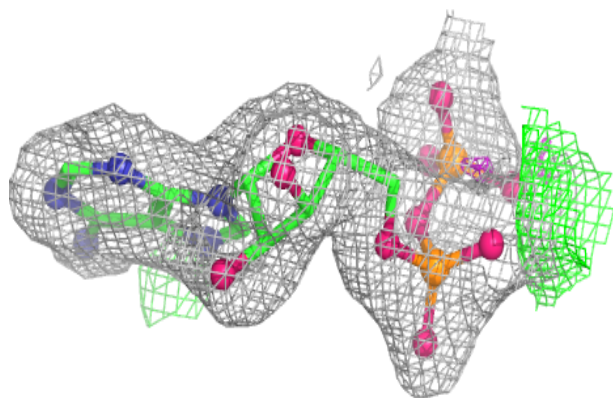
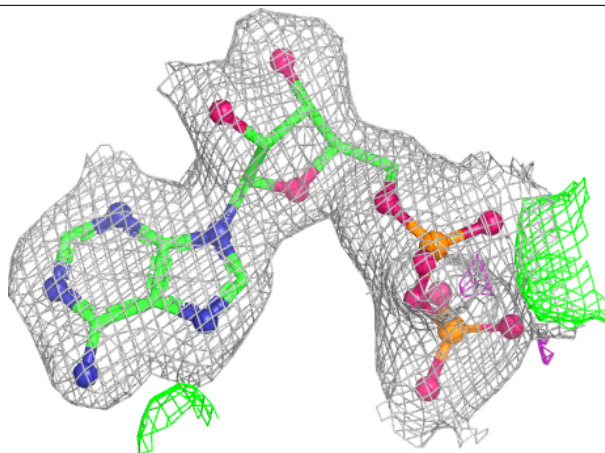
Electron density around ADP A 501:

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



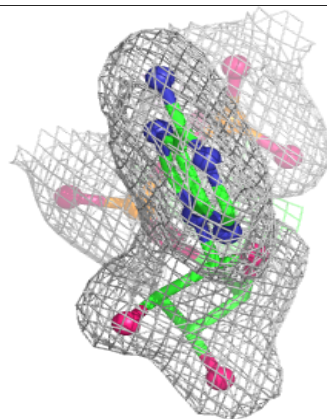
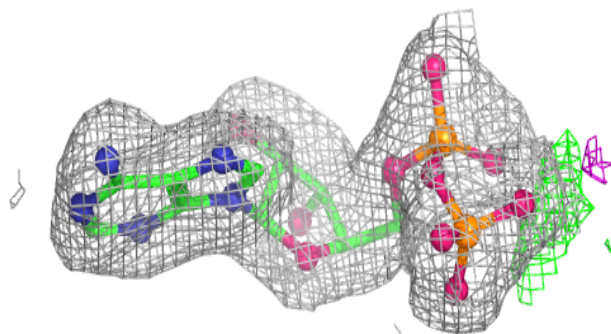
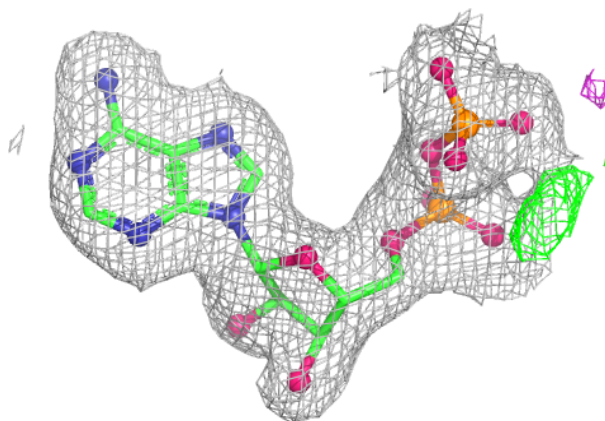
Electron density around ADP H 501:

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



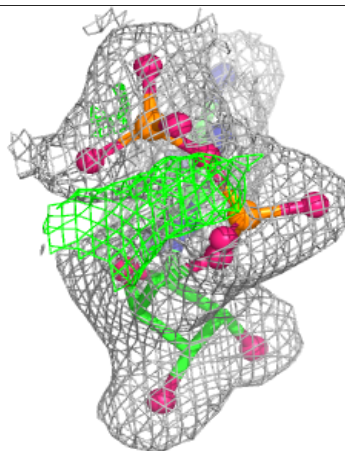
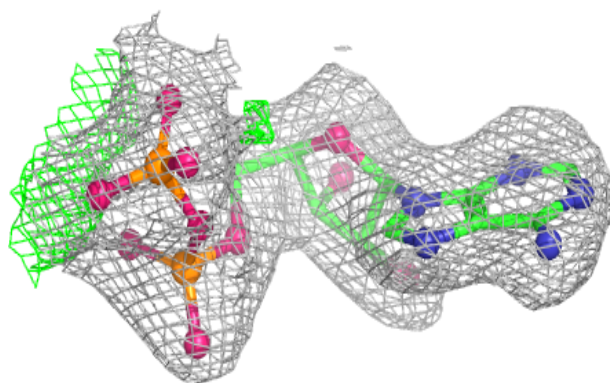
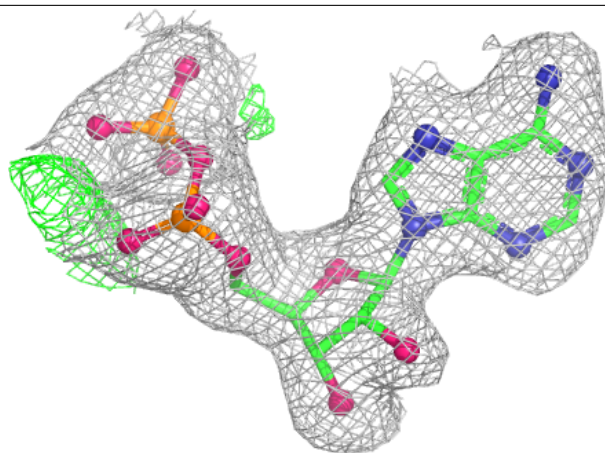
Electron density around ADP D 501:

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



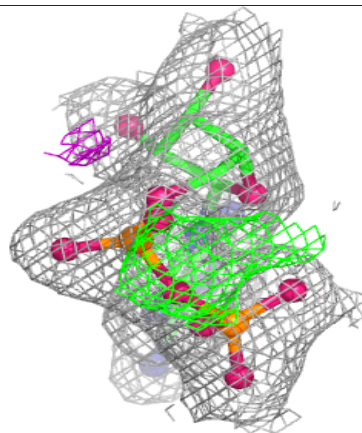
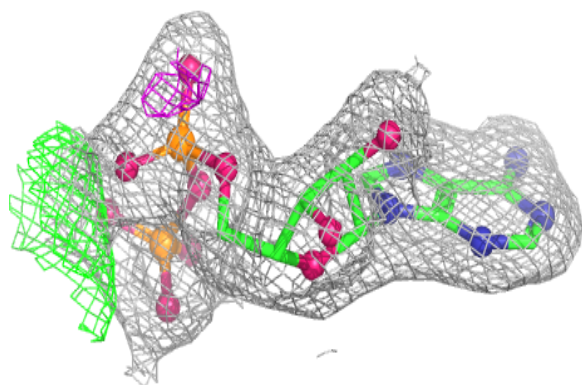
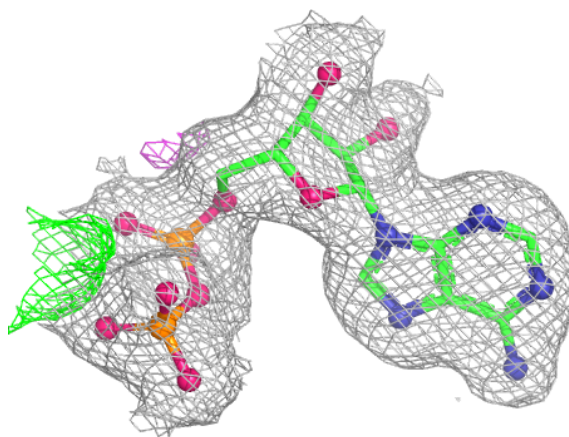
Electron density around ADP C 501:

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

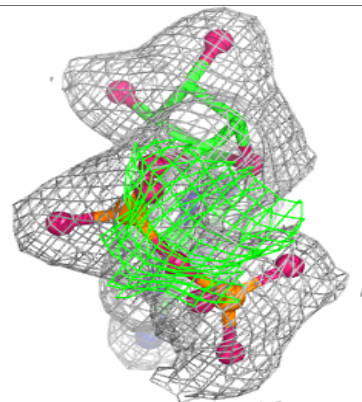
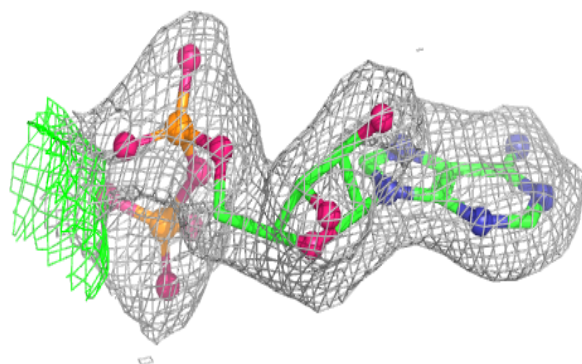
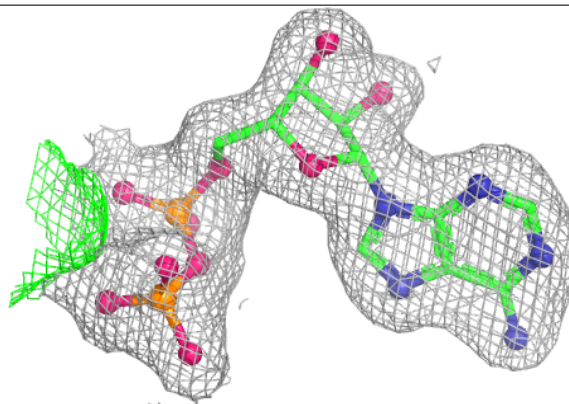


Electron density around ADP E 501:

$2mF_o - DF_c$ (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 ⓘ

There are no such residues in this entry.