



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:01 am BST

PDB ID : 5LBA
Title : Crystal structure of human RECQL5 helicase in complex with DSPL fragment(1-cyclohexyl-3-(oxolan-2-ylmethyl)urea, SGC - Diamond XChem I04-1 fragment screening.
Authors : Newman, J.A.; Aitkenhead, H.; Talon, R.; Savitsky, P.; Krojer, T.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on : 2016-06-15
Resolution : 2.50 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	:	2.11
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)	:	2.11

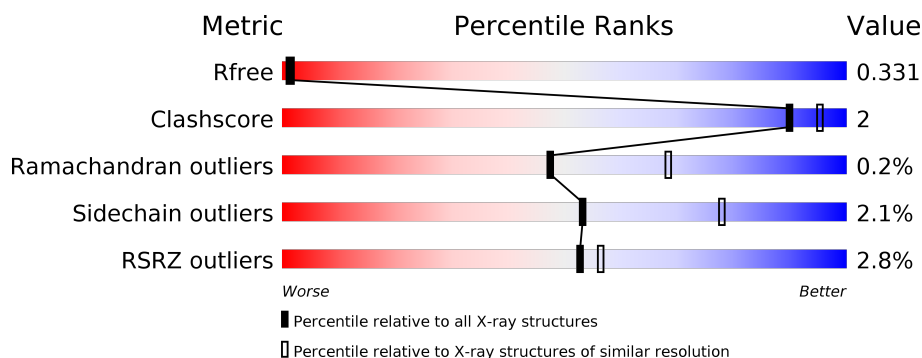
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	445	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>
1	B	445	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	445	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>• •</div> </div> </div>
1	D	445	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13954 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 ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	434	Total	C	N	O	S	0	3	0
			3383	2137	604	618	24			
1	A	430	Total	C	N	O	S	0	1	0
			3352	2120	599	611	22			
1	C	432	Total	C	N	O	S	0	0	0
			3343	2113	595	613	22			
1	D	437	Total	C	N	O	S	0	1	0
			3394	2147	604	620	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	SER	-	expression tag	UNP O94762
B	10	MET	-	expression tag	UNP O94762
A	9	SER	-	expression tag	UNP O94762
A	10	MET	-	expression tag	UNP O94762
C	9	SER	-	expression tag	UNP O94762
C	10	MET	-	expression tag	UNP O94762
D	9	SER	-	expression tag	UNP O94762
D	10	MET	-	expression tag	UNP O94762

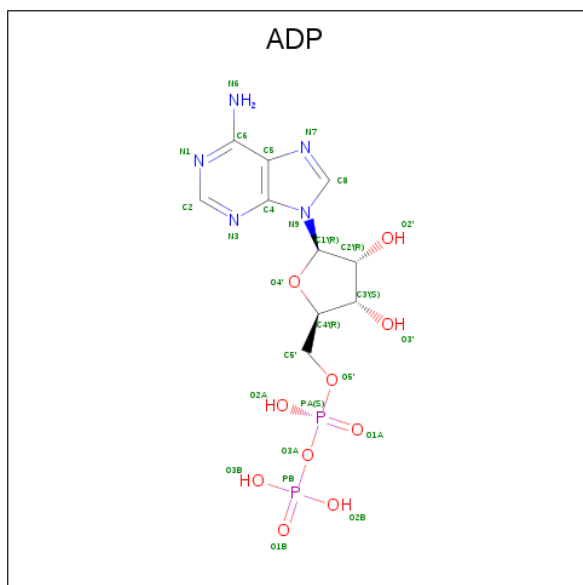
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



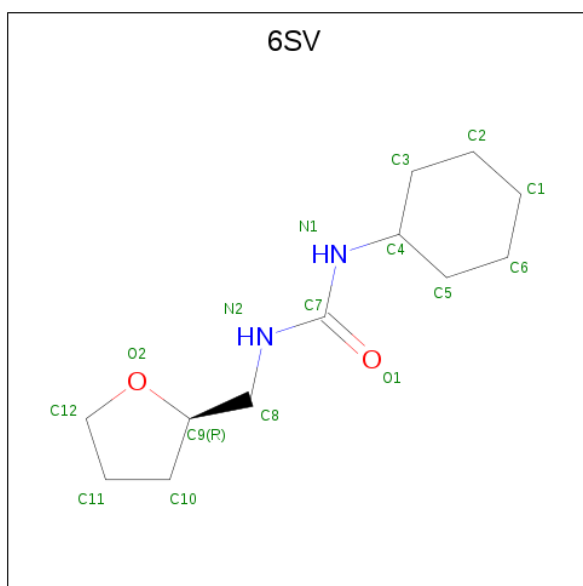
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 1-cyclohexyl-3-[[[(2 {R})-oxolan-2-yl]methyl]urea (three-letter code: 6SV) (formula: C₁₂H₂₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			16	12	2	2		

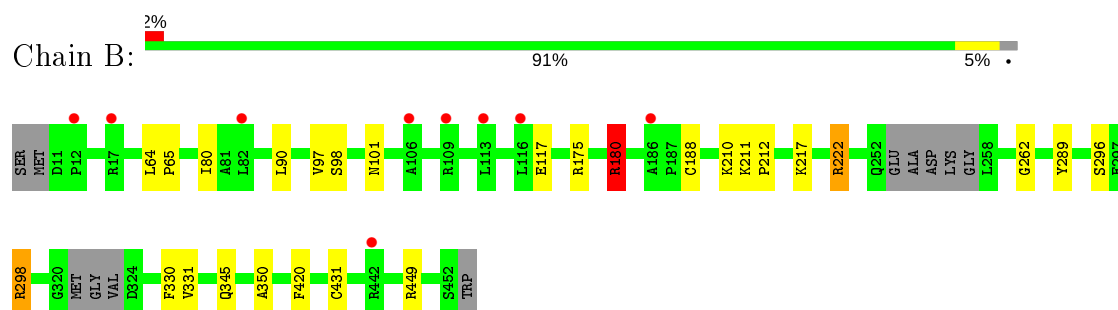
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	101	Total	O	0	0
			101	101		
7	A	88	Total	O	0	0
			88	88		
7	C	68	Total	O	0	0
			68	68		
7	D	81	Total	O	0	0
			81	81		

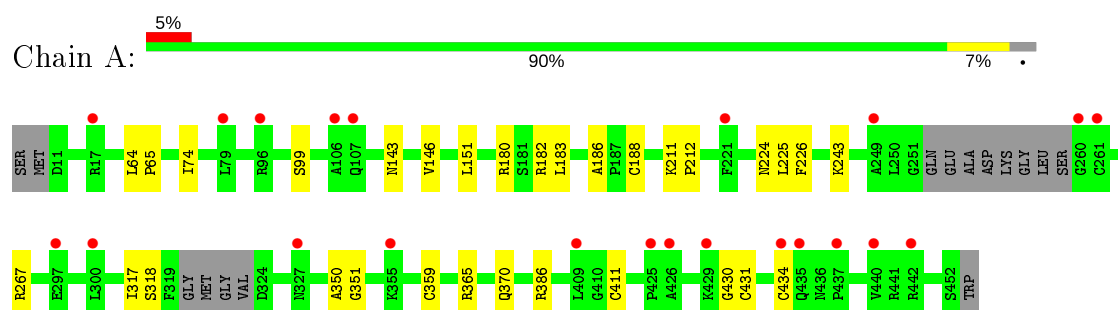
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

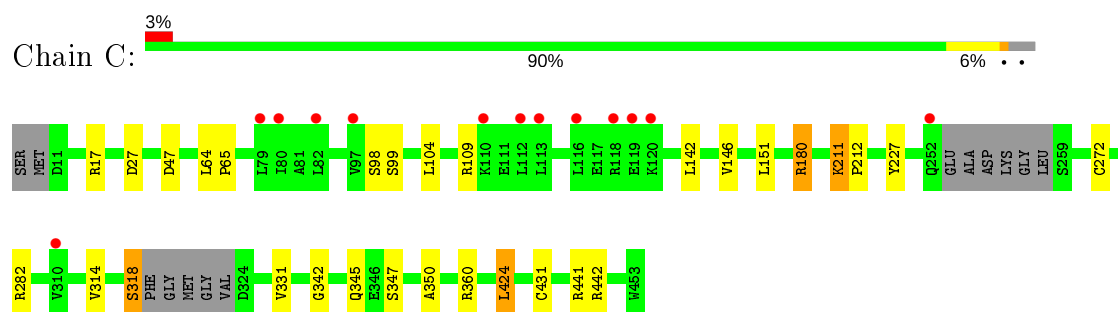
- Molecule 1: ATP-dependent DNA helicase Q5



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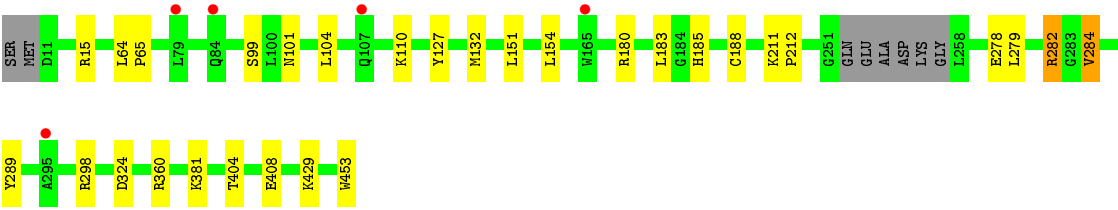


- Molecule 1: ATP-dependent DNA helicase Q5



- Molecule 1: ATP-dependent DNA helicase Q5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.93 Å 85.26 Å 105.92 Å 109.90° 90.02° 97.01°	Depositor
Resolution (Å)	79.49 – 2.50 76.13 – 2.47	Depositor EDS
% Data completeness (in resolution range)	92.3 (79.49-2.50) 80.8 (76.13-2.47)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.48 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.237 , 0.303 0.271 , 0.331	Depositor DCC
R_{free} test set	3041 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.6	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	0.88	EDS
Total number of atoms	13954	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9809e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, ZN, DMS, 6SV, 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	0.61	0/3416	0.74	1/4617 (0.0%)
1	B	0.64	0/3447	0.78	4/4660 (0.1%)
1	C	0.59	0/3408	0.74	4/4613 (0.1%)
1	D	0.60	0/3461	0.74	2/4683 (0.0%)
All	All	0.61	0/13732	0.75	11/18573 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	424	LEU	CA-CB-CG	6.58	130.43	115.30
1	D	360	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	386	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	222	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	298	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	449	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	180	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	15	ARG	NE-CZ-NH1	5.23	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	441	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	442	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	LYS	Peptide
1	B	211	LYS	Peptide
1	C	211	LYS	Peptide
1	D	211	LYS	Peptide

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	3352	0	3371	13	0
1	B	3383	0	3386	11	0
1	C	3343	0	3331	13	0
1	D	3394	0	3393	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	D	4	0	6	0	0
6	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	88	0	0	1	0
7	B	101	0	0	2	0
7	C	68	0	0	3	0
7	D	81	0	0	1	0
All	All	13954	0	13547	49	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 2.

All (49) 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:C:342:GLY:O	7:C:601:HOH:O	1.89	0.91
1:B:180:ARG:HD3	1:B:188:CYS:HB2	1.80	0.62
1:A:365:ARG:NH2	7:A:603:HOH:O	2.37	0.58
1:A:180:ARG:HD3	1:A:188:CYS:HB2	1.87	0.57
1:C:47:ASP:OD2	1:C:180:ARG:NH1	2.38	0.56
1:A:411:CYS:SG	1:A:434:CYS:SG	3.04	0.55
1:C:272:CYS:SG	1:C:314:VAL:O	2.64	0.55
1:A:226:PHE:HA	1:A:430:GLY:O	2.07	0.55
1:A:180:ARG:NH1	1:A:186:ALA:O	2.40	0.55
1:B:331:VAL:HG23	1:B:350:ALA:HB2	1.90	0.54
1:C:227:TYR:HH	1:C:347:SER:HG	1.55	0.52
1:C:109:ARG:HD3	1:D:453:TRP:CZ3	2.45	0.52
1:C:345:GLN:N	7:C:601:HOH:O	2.43	0.51
1:B:175:ARG:NH1	7:B:603:HOH:O	2.37	0.50
1:C:345:GLN:HB3	7:C:601:HOH:O	2.12	0.49
1:C:64:LEU:HB3	1:C:65:PRO:HD3	1.95	0.49
1:A:146:VAL:HG22	1:A:183:LEU:CD2	2.43	0.48
1:A:225:LEU:HD11	1:A:350:ALA:O	2.14	0.48
1:D:99:SER:HA	1:D:127:TYR:O	2.14	0.48
1:C:17:ARG:NH1	1:C:27:ASP:O	2.47	0.47
1:D:279:LEU:HD22	1:D:284:VAL:HG11	1.96	0.47
1:B:64:LEU:HB3	1:B:65:PRO:HD3	1.97	0.46
1:D:404:THR:O	1:D:408:GLU:HB2	2.17	0.45
1:D:154:LEU:HD22	1:D:183:LEU:HD12	1.98	0.45
1:A:74:ILE:HD12	1:A:151:LEU:HD21	1.99	0.44
1:C:331:VAL:HG23	1:C:350:ALA:HB2	1.98	0.44
1:D:279:LEU:HB3	1:D:284:VAL:HG13	2.00	0.44
1:A:267:ARG:NH2	1:A:370:GLN:HG2	2.32	0.44
1:A:143:ASN:OD1	1:A:182:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:ND2	1:A:351:GLY:O	2.51	0.43
1:B:289:TYR:CE1	1:B:298:ARG:HG3	2.53	0.43
1:B:262:GLY:HA3	1:B:330:PHE:CE2	2.54	0.43
1:B:298:ARG:NH1	7:B:614:HOH:O	2.52	0.43
1:B:217:LYS:NZ	1:B:420:PHE:O	2.50	0.42
1:A:64:LEU:HB3	1:A:65:PRO:HD3	2.02	0.42
1:B:90:LEU:HB2	1:B:97:VAL:HG11	2.02	0.42
1:D:101:ASN:HA	1:D:132:MET:HG3	2.01	0.42
1:C:142:LEU:O	1:C:146:VAL:HG23	2.19	0.41
1:C:318:SER:O	1:C:318:SER:OG	2.35	0.41
1:D:154:LEU:O	1:D:188:CYS:HA	2.20	0.41
1:D:64:LEU:HB3	1:D:65:PRO:HD3	2.03	0.41
1:B:180:ARG:NH2	1:B:210:LYS:HG3	2.35	0.41
1:A:226:PHE:O	1:A:359:CYS:N	2.49	0.41
1:D:289:TYR:CE1	1:D:298:ARG:HG2	2.56	0.41
1:B:80:ILE:HG23	1:B:101:ASN:ND2	2.36	0.41
1:D:381:LYS:NZ	7:D:603:HOH:O	2.46	0.41
1:C:211:LYS:HA	1:C:211:LYS:HD3	1.90	0.41
1:D:278:GLU:O	1:D:282:ARG:HD3	2.20	0.41
1:D:278:GLU:O	1:D:282:ARG:CD	2.70	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	425/445 (96%)	410 (96%)	14 (3%)	1 (0%)	47	68
1	B	431/445 (97%)	420 (97%)	10 (2%)	1 (0%)	47	68
1	C	426/445 (96%)	408 (96%)	17 (4%)	1 (0%)	47	68
1	D	434/445 (98%)	419 (96%)	14 (3%)	1 (0%)	47	68
All	All	1716/1780 (96%)	1657 (97%)	55 (3%)	4 (0%)	47	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	212	PRO
1	B	212	PRO
1	C	212	PRO
1	A	212	PRO

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	358/373 (96%)	353 (99%)	5 (1%)	67	86
1	B	361/373 (97%)	354 (98%)	7 (2%)	57	80
1	C	355/373 (95%)	346 (98%)	9 (2%)	47	73
1	D	361/373 (97%)	352 (98%)	9 (2%)	47	73
All	All	1435/1492 (96%)	1405 (98%)	30 (2%)	53	78

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	98	SER
1	B	117	GLU
1	B	180	ARG
1	B	222	ARG
1	B	296	SER
1	B	345	GLN
1	B	431	CYS
1	A	99	SER
1	A	243	LYS
1	A	317	ILE
1	A	318	SER
1	A	431	CYS
1	C	98	SER
1	C	99	SER
1	C	104	LEU
1	C	151	LEU

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Mol	Chain	Res	Type
1	C	180	ARG
1	C	282	ARG
1	C	318	SER
1	C	424	LEU
1	C	431	CYS
1	D	104	LEU
1	D	110	LYS
1	D	151	LEU
1	D	180	ARG
1	D	185	HIS
1	D	282	ARG
1	D	284	VAL
1	D	324	ASP
1	D	429	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	GLN
1	A	345	GLN
1	C	86	GLN
1	C	345	GLN
1	D	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
5	DMS	A	504	-	3,3,3	0.54	0	3,3,3	0.74	0
5	DMS	D	504	-	3,3,3	0.48	0	3,3,3	0.84	0
4	ADP	D	503	2	24,29,29	1.18	3 (12%)	29,45,45	1.50	3 (10%)
4	ADP	B	503	2	24,29,29	1.14	3 (12%)	29,45,45	1.32	2 (6%)
5	DMS	B	504	-	3,3,3	0.45	0	3,3,3	0.82	0
4	ADP	A	502	2	24,29,29	1.02	2 (8%)	29,45,45	1.49	4 (13%)
6	6SV	B	505	-	17,17,17	0.37	0	21,21,21	1.01	1 (4%)
4	ADP	C	503	2	24,29,29	0.93	1 (4%)	29,45,45	1.51	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
4	ADP	B	503	2	-	3/12/32/32	0/3/3/3
4	ADP	A	502	2	-	1/12/32/32	0/3/3/3
4	ADP	C	503	2	-	1/12/32/32	0/3/3/3
4	ADP	D	503	2	-	5/12/32/32	0/3/3/3
6	6SV	B	505	-	-	5/9/24/24	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	ADP	O4'-C1'	2.57	1.44	1.41
4	A	502	ADP	C5-C4	2.57	1.47	1.40
4	B	503	ADP	C5-C4	2.48	1.47	1.40
4	D	503	ADP	C2'-C1'	-2.46	1.50	1.53
4	C	503	ADP	C5-C4	2.44	1.47	1.40
4	D	503	ADP	C5-C4	2.43	1.47	1.40
4	D	503	ADP	C2-N3	2.33	1.35	1.32
4	B	503	ADP	C2-N3	2.12	1.35	1.32
4	A	502	ADP	C2-N3	2.02	1.35	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	ADP	N3-C2-N1	-4.20	122.12	128.68
4	D	503	ADP	N3-C2-N1	-4.00	122.43	128.68
4	B	503	ADP	N3-C2-N1	-3.73	122.85	128.68
4	A	502	ADP	N3-C2-N1	-3.64	122.99	128.68
4	A	502	ADP	C4-C5-N7	-3.50	105.75	109.40
4	D	503	ADP	C4-C5-N7	-3.33	105.93	109.40
4	D	503	ADP	PA-O3A-PB	-3.24	121.69	132.83
4	B	503	ADP	C4-C5-N7	-3.10	106.17	109.40
4	A	502	ADP	PA-O3A-PB	-2.87	122.99	132.83
4	C	503	ADP	PA-O3A-PB	-2.73	123.47	132.83
4	A	502	ADP	C3'-C2'-C1'	2.67	104.99	100.98
4	C	503	ADP	C3'-C2'-C1'	2.59	104.87	100.98
6	B	505	6SV	O1-C7-N2	-2.52	118.12	122.50
4	C	503	ADP	C2-N1-C6	2.28	122.65	118.75
4	C	503	ADP	O3A-PB-O1B	-2.04	99.86	111.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

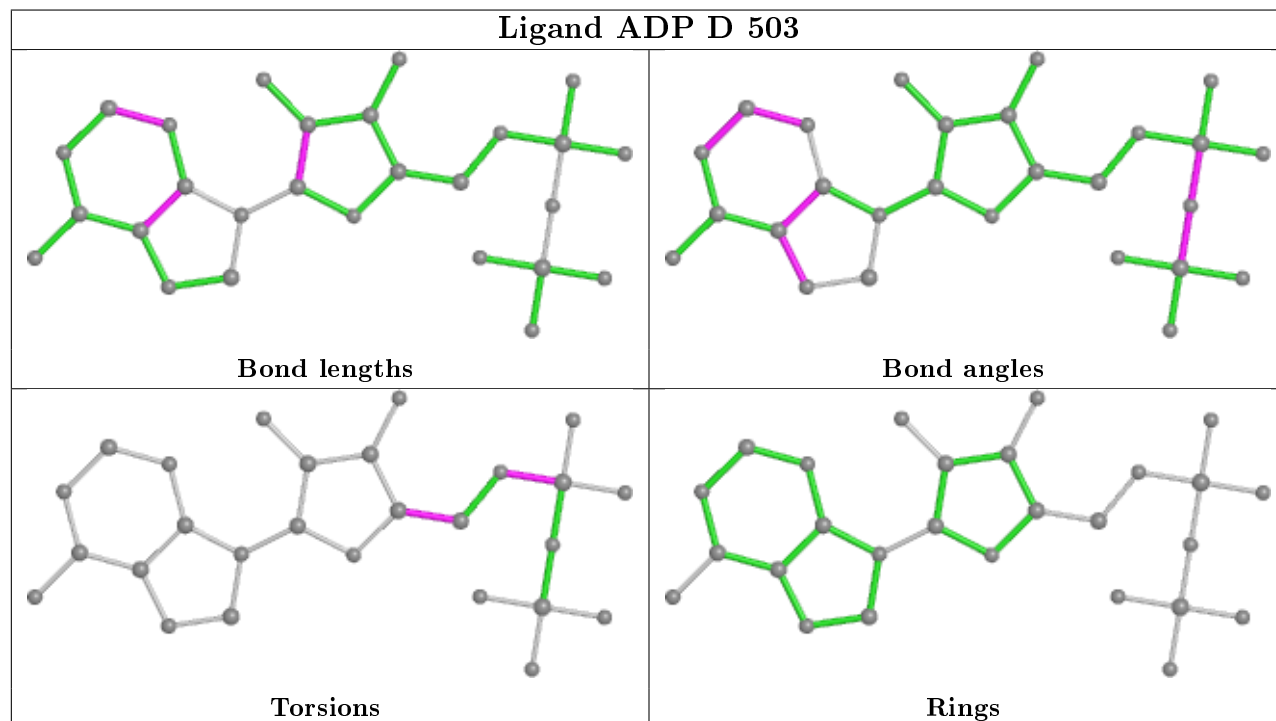
Mol	Chain	Res	Type	Atoms
4	D	503	ADP	C5'-O5'-PA-O1A
4	D	503	ADP	O4'-C4'-C5'-O5'
4	B	503	ADP	PA-O3A-PB-O3B
6	B	505	6SV	N1-C7-N2-C8
6	B	505	6SV	O1-C7-N2-C8
6	B	505	6SV	N2-C8-C9-C10
6	B	505	6SV	N2-C8-C9-O2
4	D	503	ADP	C3'-C4'-C5'-O5'
6	B	505	6SV	C3-C4-N1-C7
4	C	503	ADP	PA-O3A-PB-O1B
4	D	503	ADP	C5'-O5'-PA-O3A
4	D	503	ADP	C5'-O5'-PA-O2A
4	B	503	ADP	PA-O3A-PB-O1B
4	B	503	ADP	PA-O3A-PB-O2B
4	A	502	ADP	PA-O3A-PB-O3B

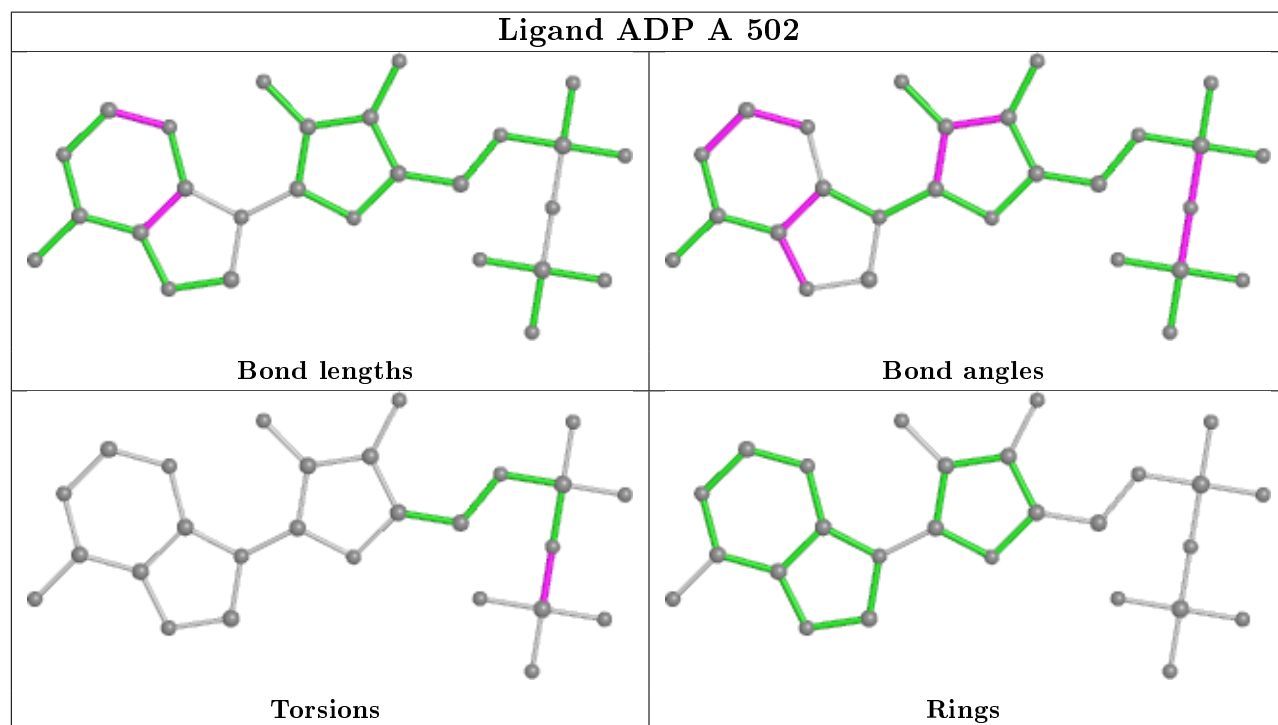
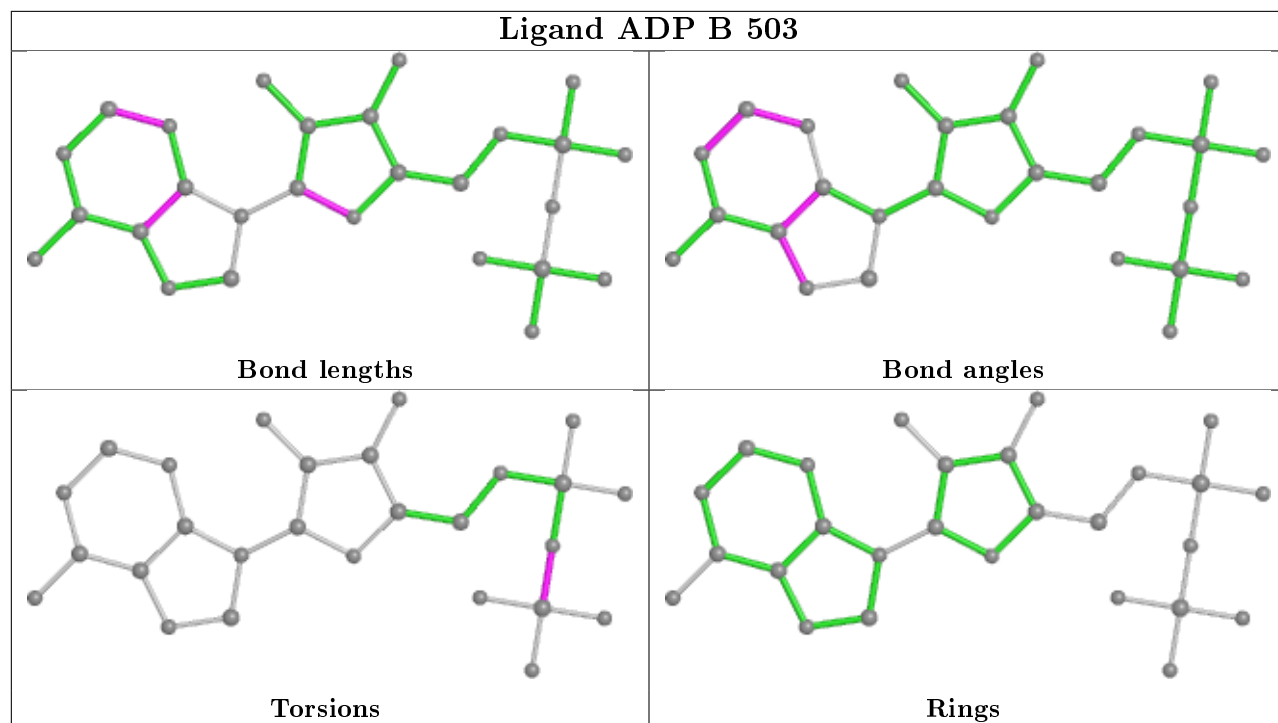
There are no ring outliers.

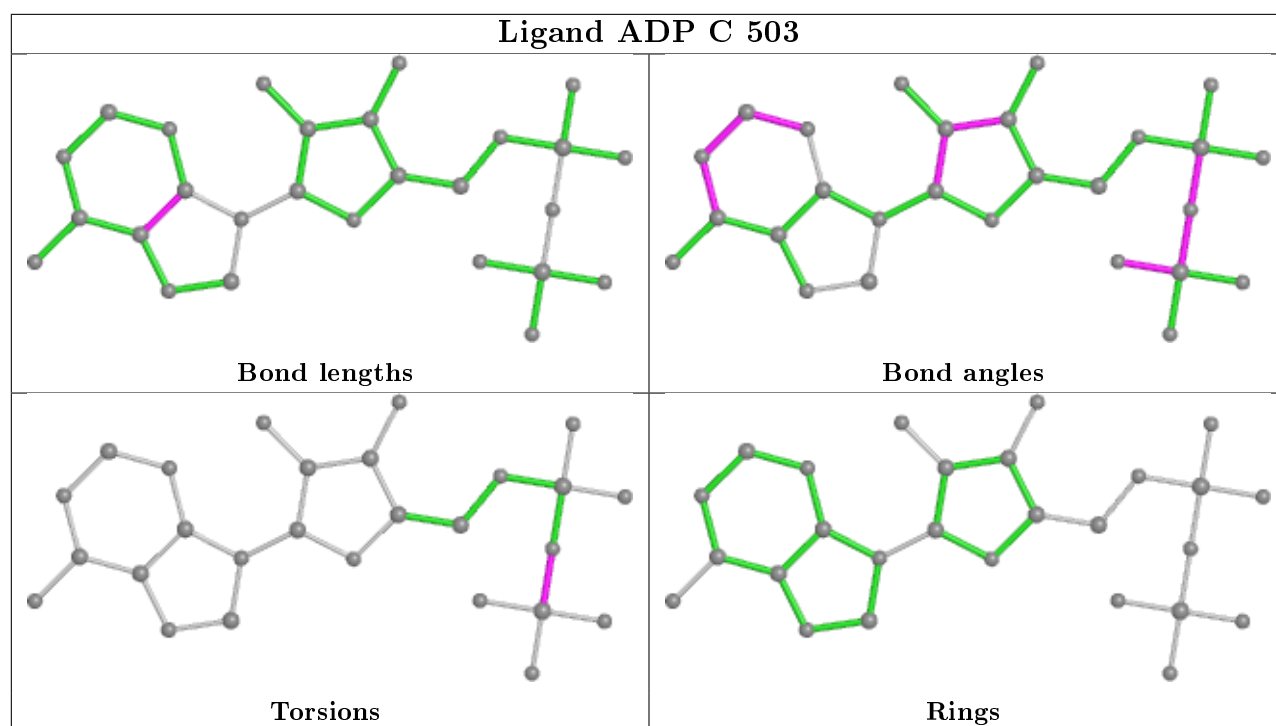
No monomer is involved in short contacts.

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	430/445 (96%)	0.29	22 (5%) 28 29	21, 50, 86, 116	0
1	B	434/445 (97%)	0.04	9 (2%) 63 66	21, 43, 78, 101	0
1	C	432/445 (97%)	0.09	13 (3%) 50 53	22, 45, 83, 118	0
1	D	437/445 (98%)	-0.07	5 (1%) 80 82	20, 42, 77, 92	0
All	All	1733/1780 (97%)	0.09	49 (2%) 53 56	20, 45, 82, 118	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	79	LEU	7.8
1	A	107	GLN	5.2
1	A	442	ARG	4.6
1	A	426	ALA	4.3
1	C	252	GLN	4.3
1	C	110	LYS	4.1
1	A	261	CYS	3.6
1	A	106	ALA	3.5
1	C	82	LEU	3.4
1	C	118	ARG	3.3
1	C	119	GLU	3.1
1	B	442	ARG	3.1
1	A	300	LEU	3.1
1	A	327	ASN	2.8
1	C	112	LEU	2.7
1	D	295	ALA	2.7
1	A	260	GLY	2.6
1	A	249	ALA	2.6
1	A	440	VAL	2.5
1	B	82	LEU	2.5
1	A	79	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	409	LEU	2.5
1	D	79	LEU	2.5
1	C	80	ILE	2.5
1	C	310	VAL	2.4
1	B	116	LEU	2.4
1	C	116	LEU	2.4
1	A	434	CYS	2.4
1	A	17	ARG	2.4
1	A	435	GLN	2.3
1	A	429	LYS	2.3
1	C	97	VAL	2.3
1	B	109	ARG	2.2
1	A	425	PRO	2.2
1	B	17	ARG	2.2
1	B	106	ALA	2.2
1	D	84	GLN	2.2
1	C	120	LYS	2.2
1	A	355	LYS	2.2
1	C	113	LEU	2.2
1	B	113	LEU	2.1
1	D	107	GLN	2.1
1	A	297	GLU	2.1
1	D	165	TRP	2.1
1	B	186	ALA	2.0
1	A	221	PHE	2.0
1	A	437	PRO	2.0
1	A	96	ARG	2.0
1	B	12	PRO	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 carbohydrates 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,

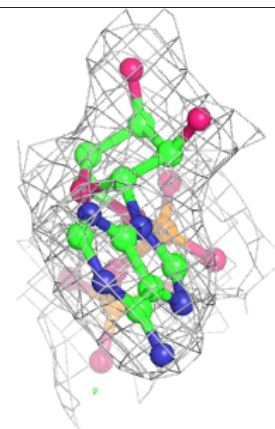
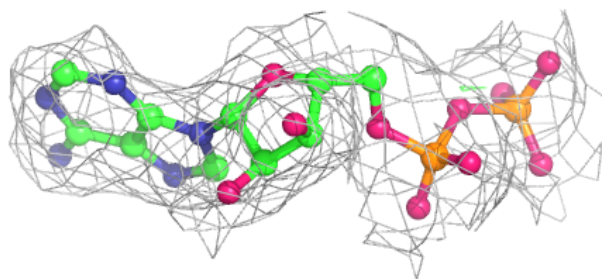
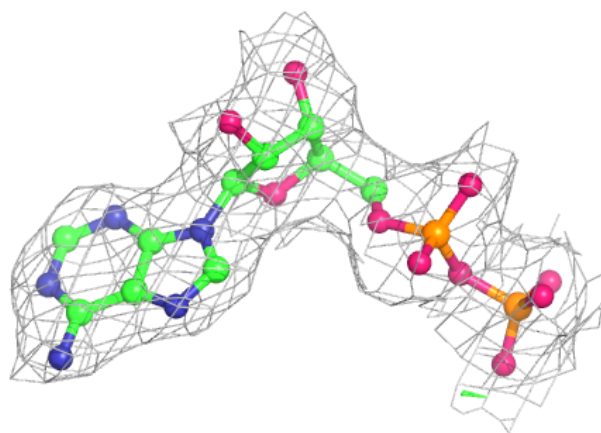
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	6SV	B	505	16/16	0.83	0.22	46,65,84,85	0
2	MG	A	501	1/1	0.93	0.06	43,43,43,43	0
2	MG	C	501	1/1	0.94	0.08	49,49,49,49	0
4	ADP	B	503	27/27	0.94	0.13	30,43,48,48	0
5	DMS	A	504	4/4	0.95	0.16	41,43,43,48	0
5	DMS	B	504	4/4	0.95	0.14	43,45,48,49	0
5	DMS	D	504	4/4	0.95	0.16	51,55,57,61	0
4	ADP	A	502	27/27	0.95	0.15	35,62,79,81	0
4	ADP	C	503	27/27	0.95	0.11	39,46,51,52	0
2	MG	B	501	1/1	0.96	0.07	35,35,35,35	0
4	ADP	D	503	27/27	0.96	0.11	35,50,57,60	0
3	ZN	B	502	1/1	0.98	0.07	35,35,35,35	0
3	ZN	A	503	1/1	0.98	0.11	53,53,53,53	0
2	MG	D	501	1/1	0.98	0.08	45,45,45,45	0
3	ZN	C	502	1/1	0.99	0.09	34,34,34,34	0
3	ZN	D	502	1/1	1.00	0.07	26,26,26,26	0

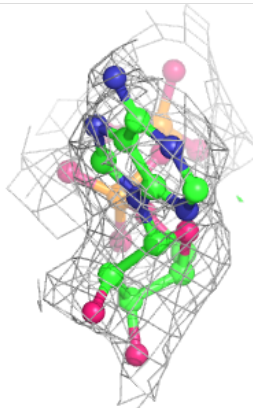
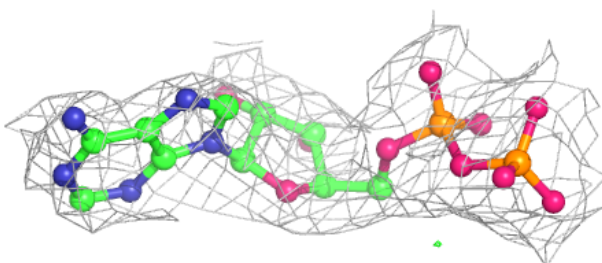
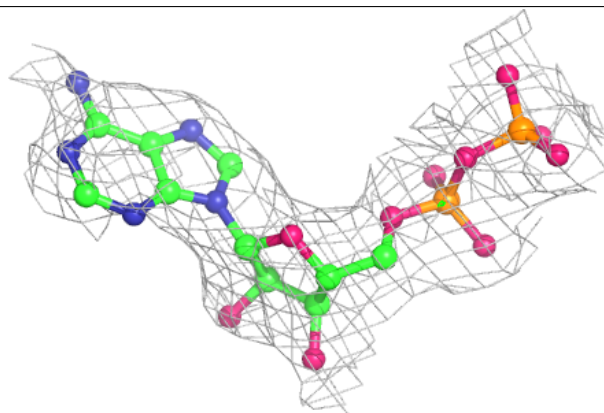
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 503:

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

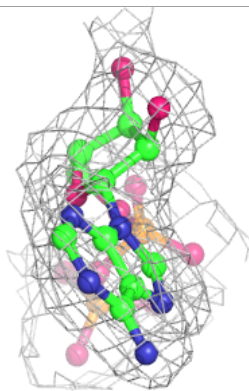
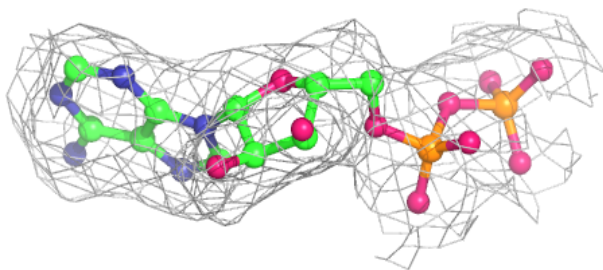
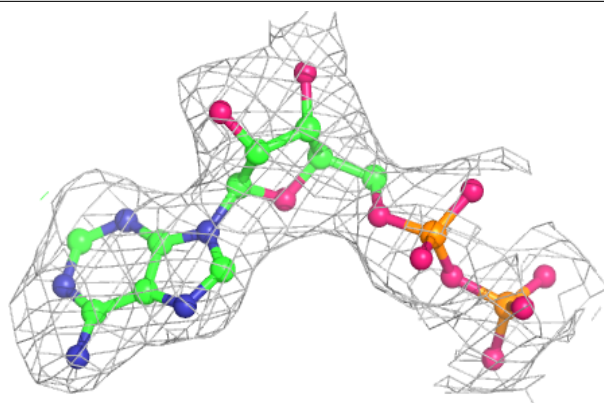
**Electron density around ADP A 502:**

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

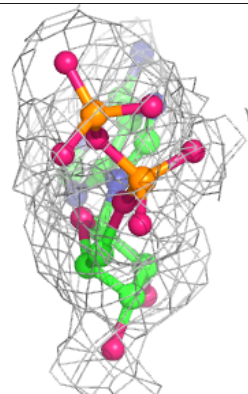
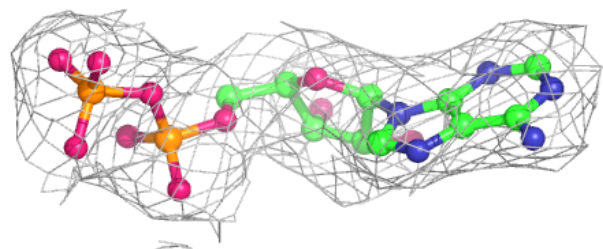
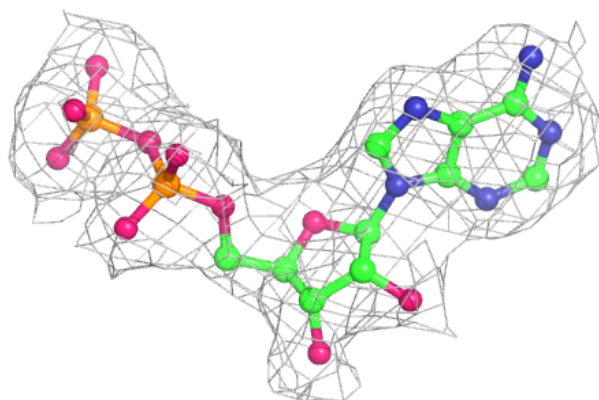


Electron density around ADP C 503:

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

**Electron density around ADP D 503:**

$2mF_o-DF_c$ (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.