wwPDB X-ray Structure Validation Summary Report (i)

Nov 2, 2023 – 02:59 AM EDT

PDB ID	:	3Q8Y
Title	:	Crystal structure of Staphylococcus aureus nucleoside diphosphate kinase complexed with ADP and Vanadate
Authors	:	Srivastava, S.K.; Rajasree, K.; Gopal, B.
Deposited on	:	2011-01-07
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

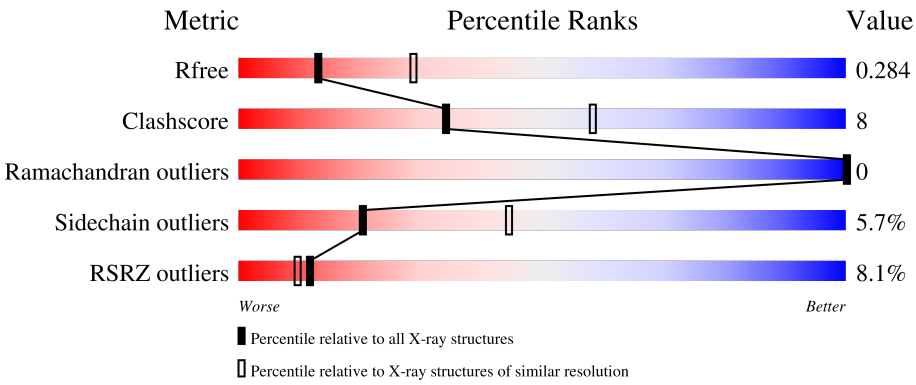
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	6% 75% 17% • 5%
1	B	157	4% 78% 16% • 5%
1	C	157	6% 80% 12% • 5%
1	D	157	6% 78% 14% • 5%
1	E	157	5% 79% 15% • 5%

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Mol	Chain	Length	Quality of chain
1	F	157	5% 82% 11% • 5%
1	G	157	6% 78% 14% • 5%
1	H	157	24% 76% 18% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	158	-	-	-	X
3	VO4	A	159	-	-	X	-
3	VO4	B	159	-	-	X	-
3	VO4	D	159	-	-	X	-
3	VO4	E	159	-	-	X	-
3	VO4	F	158	-	-	X	-
3	VO4	G	159	-	-	X	-
3	VO4	H	159	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9560 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	149	1156	728	202	221	5	0	0	0
1	B	149	1156	728	202	221	5	0	0	0
1	C	149	1152	726	202	219	5	0	0	0
1	D	149	1157	729	202	221	5	0	0	0
1	E	149	1144	721	201	217	5	0	0	0
1	F	149	1157	729	202	221	5	0	0	0
1	G	149	1153	727	202	219	5	0	0	0
1	H	149	1157	729	202	221	5	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	LEU	-	expression tag	UNP Q5HFV4
A	151	GLU	-	expression tag	UNP Q5HFV4
A	152	HIS	-	expression tag	UNP Q5HFV4
A	153	HIS	-	expression tag	UNP Q5HFV4
A	154	HIS	-	expression tag	UNP Q5HFV4
A	155	HIS	-	expression tag	UNP Q5HFV4
A	156	HIS	-	expression tag	UNP Q5HFV4
A	157	HIS	-	expression tag	UNP Q5HFV4
B	150	LEU	-	expression tag	UNP Q5HFV4
B	151	GLU	-	expression tag	UNP Q5HFV4
B	152	HIS	-	expression tag	UNP Q5HFV4
B	153	HIS	-	expression tag	UNP Q5HFV4
B	154	HIS	-	expression tag	UNP Q5HFV4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	155	HIS	-	expression tag	UNP Q5HFV4
B	156	HIS	-	expression tag	UNP Q5HFV4
B	157	HIS	-	expression tag	UNP Q5HFV4
C	150	LEU	-	expression tag	UNP Q5HFV4
C	151	GLU	-	expression tag	UNP Q5HFV4
C	152	HIS	-	expression tag	UNP Q5HFV4
C	153	HIS	-	expression tag	UNP Q5HFV4
C	154	HIS	-	expression tag	UNP Q5HFV4
C	155	HIS	-	expression tag	UNP Q5HFV4
C	156	HIS	-	expression tag	UNP Q5HFV4
C	157	HIS	-	expression tag	UNP Q5HFV4
D	150	LEU	-	expression tag	UNP Q5HFV4
D	151	GLU	-	expression tag	UNP Q5HFV4
D	152	HIS	-	expression tag	UNP Q5HFV4
D	153	HIS	-	expression tag	UNP Q5HFV4
D	154	HIS	-	expression tag	UNP Q5HFV4
D	155	HIS	-	expression tag	UNP Q5HFV4
D	156	HIS	-	expression tag	UNP Q5HFV4
D	157	HIS	-	expression tag	UNP Q5HFV4
E	150	LEU	-	expression tag	UNP Q5HFV4
E	151	GLU	-	expression tag	UNP Q5HFV4
E	152	HIS	-	expression tag	UNP Q5HFV4
E	153	HIS	-	expression tag	UNP Q5HFV4
E	154	HIS	-	expression tag	UNP Q5HFV4
E	155	HIS	-	expression tag	UNP Q5HFV4
E	156	HIS	-	expression tag	UNP Q5HFV4
E	157	HIS	-	expression tag	UNP Q5HFV4
F	150	LEU	-	expression tag	UNP Q5HFV4
F	151	GLU	-	expression tag	UNP Q5HFV4
F	152	HIS	-	expression tag	UNP Q5HFV4
F	153	HIS	-	expression tag	UNP Q5HFV4
F	154	HIS	-	expression tag	UNP Q5HFV4
F	155	HIS	-	expression tag	UNP Q5HFV4
F	156	HIS	-	expression tag	UNP Q5HFV4
F	157	HIS	-	expression tag	UNP Q5HFV4
G	150	LEU	-	expression tag	UNP Q5HFV4
G	151	GLU	-	expression tag	UNP Q5HFV4
G	152	HIS	-	expression tag	UNP Q5HFV4
G	153	HIS	-	expression tag	UNP Q5HFV4
G	154	HIS	-	expression tag	UNP Q5HFV4
G	155	HIS	-	expression tag	UNP Q5HFV4
G	156	HIS	-	expression tag	UNP Q5HFV4

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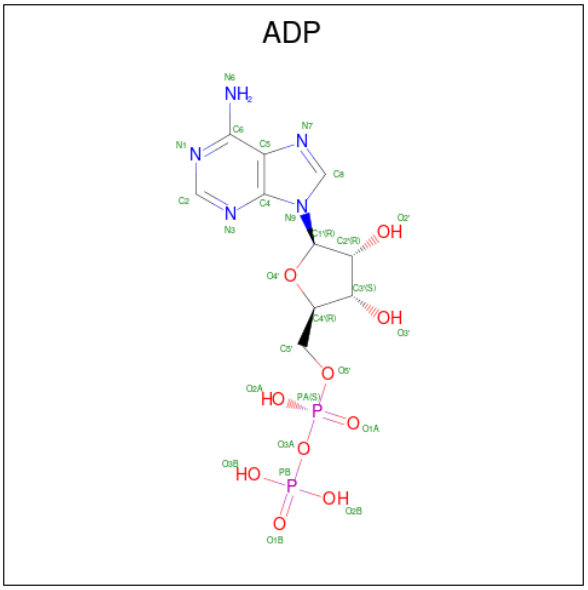
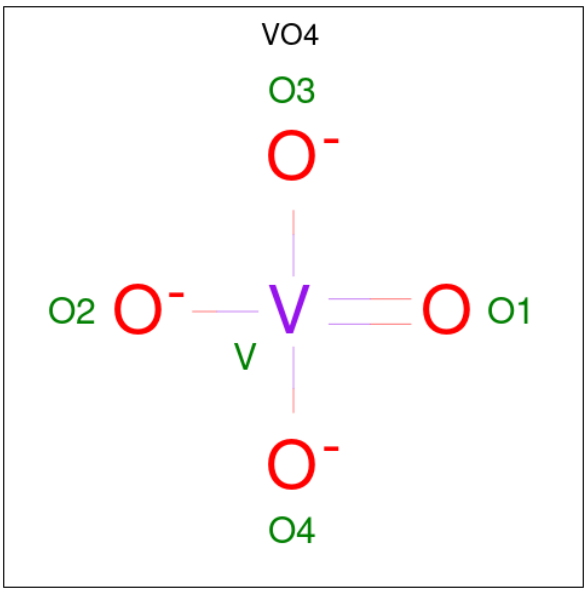
Chain	Residue	Modelled	Actual	Comment	Reference
G	157	HIS	-	expression tag	UNP Q5HFV4
H	150	LEU	-	expression tag	UNP Q5HFV4
H	151	GLU	-	expression tag	UNP Q5HFV4
H	152	HIS	-	expression tag	UNP Q5HFV4
H	153	HIS	-	expression tag	UNP Q5HFV4
H	154	HIS	-	expression tag	UNP Q5HFV4
H	155	HIS	-	expression tag	UNP Q5HFV4
H	156	HIS	-	expression tag	UNP Q5HFV4
H	157	HIS	-	expression tag	UNP Q5HFV4

- 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	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	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O V 5 4 1	0	0
3	B	1	Total O V 5 4 1	0	0
3	C	1	Total O V 5 4 1	0	0
3	D	1	Total O V 5 4 1	0	0
3	E	1	Total O V 5 4 1	0	0
3	F	1	Total O V 5 4 1	0	0
3	G	1	Total O V 5 4 1	0	0
3	H	1	Total O V 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	H	1	1	1	0	0

- Molecule 5 is water.

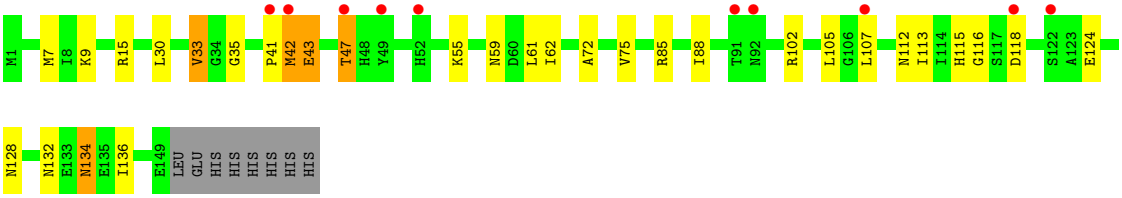
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	16	16	16	0	0
			Total	O		
5	B	22	22	22	0	0
			Total	O		
5	C	12	12	12	0	0
			Total	O		
5	D	10	10	10	0	0
			Total	O		
5	E	12	12	12	0	0
			Total	O		
5	F	12	12	12	0	0
			Total	O		
5	G	15	15	15	0	0
			Total	O		
5	H	23	23	23	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

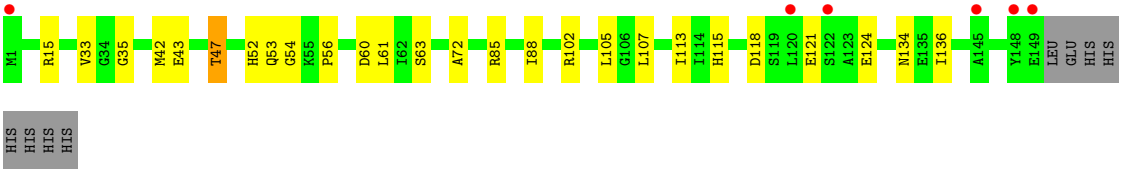
• Molecule 1: Nucleoside diphosphate kinase

Chain A:



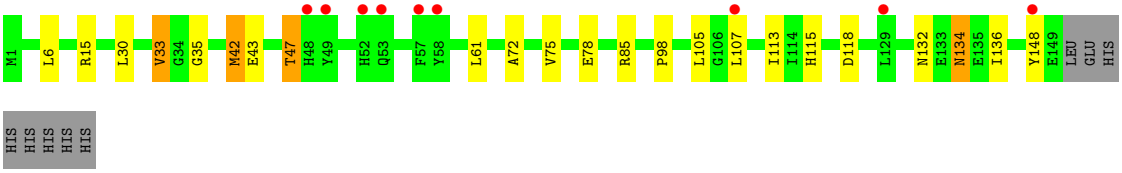
• Molecule 1: Nucleoside diphosphate kinase

Chain B:



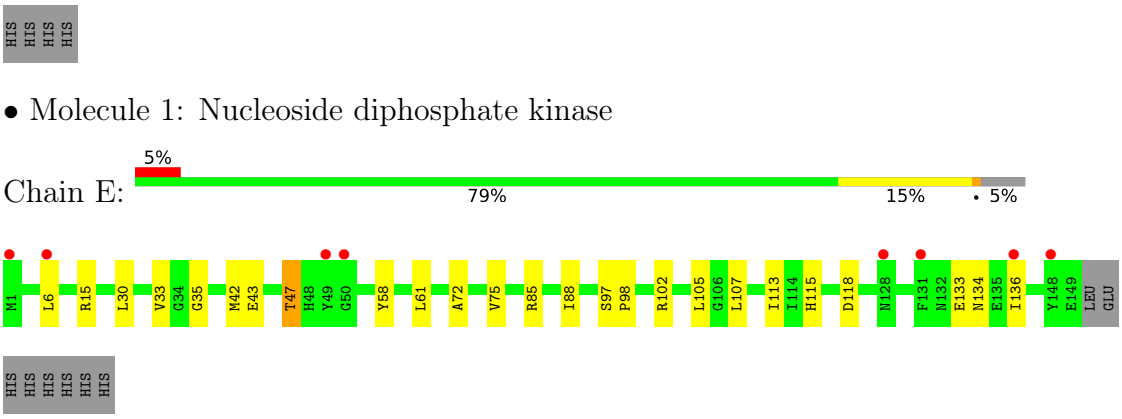
• Molecule 1: Nucleoside diphosphate kinase

Chain C:



• Molecule 1: Nucleoside diphosphate kinase

Chain D:


HIS HIS HIS HIS
• Molecule 1: Nucleoside diphosphate kinase
Chain E:
5%
79%
15%
• 5%
M1 L6 R15 L30 V33 G34 G35 M42 E43 T47 H48 Y49 G50 Y58 L61 A72 V75 R85 I88 S97 P98 R102 L105 G106 L107 I113 I114 H115 D118 M128 F131 N132 E133 N134 E135 I136 Y148 E149 LEU GLU
HIS HIS HIS HIS HIS HIS
• Molecule 1: Nucleoside diphosphate kinase
Chain F:
5%
82%
11%
• 5%
M1 L6 K9 R15 L30 V33 M42 E43 T47 H52 Q53 G54 K55 P56 F57 L61 V75 R85 I88 R102 L107 I113 I114 H115 D118 E124 N134 E135 I136 E149 LEU GLU HIS HIS HIS HIS HIS HIS
• Molecule 1: Nucleoside diphosphate kinase
Chain G:
6%
78%
14%
• 5%
M1 L6 R15 L30 V33 G34 G35 M42 E43 T47 H52 Q53 G54 K55 P56 F57 Y58 N59 D60 L61 I62 S63 F64 A72 V75 R85 L105 G106 L107 G110 I113 I114 H115 D118 S122 A123 E124 I127 N132 E133 N134 E135 I136
E149 LEU GLU HIS HIS HIS HIS HIS HIS
• Molecule 1: Nucleoside diphosphate kinase
Chain H:
24%
76%
18%
• 5%
M1 E2 R3 T4 F5 L6 R15 I25 E26 R27 K28 G29 L30 V33 G34 G35 M42 E43 E46 T47 H48 Y49 D60 L61 I65 A72 M73 V74 V75 E76 N82 V83 S84 R85 I88 T91 I101 R102 L105 G106 L107 I113 I114 H115 D118
S122 A123 E126 I127 W130 F131 N132 E133 M134 E135 I136 T137 S138 Y139 R143 D144 A145 W146 L147 Y148 E149 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.91Å 71.37Å 160.08Å 90.00° 108.04° 90.00°	Depositor
Resolution (Å)	51.67 – 2.70 51.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (51.67-2.70) 99.6 (51.67-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.251 , 0.271 0.256 , 0.284	Depositor DCC
R_{free} test set	1777 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9560	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, VO4, MG

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	0.57	0/1179	0.64	0/1595
1	B	0.65	0/1179	0.71	0/1595
1	C	0.57	0/1175	0.66	0/1590
1	D	0.66	0/1180	0.70	1/1597 (0.1%)
1	E	0.58	0/1167	0.63	0/1581
1	F	0.62	0/1180	0.68	0/1597
1	G	0.59	0/1176	0.65	0/1592
1	H	0.47	0/1180	0.60	0/1597
All	All	0.59	0/9416	0.66	1/12744 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	102	ARG	NE-CZ-NH2	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1156	0	1140	25	0
1	B	1156	0	1140	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1152	0	1136	16	0
1	D	1157	0	1141	15	0
1	E	1144	0	1121	16	0
1	F	1157	0	1141	13	0
1	G	1153	0	1137	22	0
1	H	1157	0	1141	24	0
2	A	27	0	12	6	0
2	B	27	0	12	3	0
2	D	27	0	12	1	0
2	E	27	0	12	3	0
2	G	27	0	12	4	0
2	H	27	0	12	4	0
3	A	5	0	0	4	0
3	B	5	0	0	4	0
3	C	5	0	0	1	0
3	D	5	0	0	5	0
3	E	5	0	0	3	0
3	F	5	0	0	2	0
3	G	5	0	0	3	0
3	H	5	0	0	4	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
5	A	16	0	0	1	0
5	B	22	0	0	2	0
5	C	12	0	0	3	0
5	D	10	0	0	1	0
5	E	12	0	0	3	0
5	F	12	0	0	2	0
5	G	15	0	0	6	0
5	H	23	0	0	7	0
All	All	9560	0	9169	157	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 8.

The worst 5 of 157 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:H:76:GLU:HA	5:H:178:HOH:O	1.47	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASP:HB3	5:B:171:HOH:O	1.52	1.06
1:A:42:MET:HE1	1:B:54:GLY:O	1.58	1.04
1:H:2:GLU:O	5:H:178:HOH:O	1.82	0.97
2:A:158:ADP:H5'2	3:A:159:VO4:O3	1.64	0.97

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
1	B	147/157 (94%)	144 (98%)	3 (2%)	0	100	100
1	C	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
1	D	147/157 (94%)	143 (97%)	4 (3%)	0	100	100
1	E	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
1	F	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
1	G	147/157 (94%)	143 (97%)	4 (3%)	0	100	100
1	H	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
All	All	1176/1256 (94%)	1133 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/135 (93%)	116 (93%)	9 (7%)	14	34
1	B	125/135 (93%)	117 (94%)	8 (6%)	17	39
1	C	124/135 (92%)	118 (95%)	6 (5%)	25	53
1	D	125/135 (93%)	116 (93%)	9 (7%)	14	34
1	E	122/135 (90%)	117 (96%)	5 (4%)	30	59
1	F	125/135 (93%)	118 (94%)	7 (6%)	21	45
1	G	124/135 (92%)	116 (94%)	8 (6%)	17	38
1	H	125/135 (93%)	120 (96%)	5 (4%)	31	60
All	All	995/1080 (92%)	938 (94%)	57 (6%)	20	44

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	61	LEU
1	H	107	LEU
1	E	107	LEU
1	H	61	LEU
1	G	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	134	ASN
1	H	134	ASN
1	D	134	ASN
1	E	16	ASN
1	E	39	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	VO4	F	158	-	1,4,4	4.90	1 (100%)	-		
2	ADP	E	158	3,4	24,29,29	0.99	1 (4%)	29,45,45	1.43	5 (17%)
2	ADP	H	158	3,4	24,29,29	1.06	2 (8%)	29,45,45	1.33	4 (13%)
3	VO4	B	159	1	1,4,4	4.89	1 (100%)	-		
2	ADP	G	158	-	24,29,29	1.04	2 (8%)	29,45,45	1.55	5 (17%)
3	VO4	A	159	1	1,4,4	4.82	1 (100%)	-		
3	VO4	G	159	1	1,4,4	4.90	1 (100%)	-		
2	ADP	D	158	3,4	24,29,29	1.08	2 (8%)	29,45,45	1.28	2 (6%)
2	ADP	A	158	-	24,29,29	1.02	1 (4%)	29,45,45	1.30	3 (10%)
3	VO4	D	159	1,2	1,4,4	4.91	1 (100%)	-		
3	VO4	C	158	-	1,4,4	5.00	1 (100%)	-		
3	VO4	E	159	1,2	1,4,4	5.02	1 (100%)	-		
3	VO4	H	159	1,2	1,4,4	4.94	1 (100%)	-		
2	ADP	B	158	4	24,29,29	1.11	2 (8%)	29,45,45	1.19	4 (13%)

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	E	158	3,4	-	2/12/32/32	0/3/3/3
2	ADP	H	158	3,4	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	G	158	-	-	3/12/32/32	0/3/3/3
2	ADP	D	158	3,4	-	5/12/32/32	0/3/3/3
2	ADP	A	158	-	-	5/12/32/32	0/3/3/3
2	ADP	B	158	4	-	4/12/32/32	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	159	VO4	O1-V	5.02	1.92	1.63
3	C	158	VO4	O1-V	5.00	1.92	1.63
3	H	159	VO4	O1-V	4.94	1.91	1.63
3	D	159	VO4	O1-V	4.91	1.91	1.63
3	G	159	VO4	O1-V	4.90	1.91	1.63

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	158	ADP	N3-C2-N1	-4.07	122.32	128.68
2	G	158	ADP	N3-C2-N1	-3.97	122.48	128.68
2	H	158	ADP	N3-C2-N1	-3.81	122.72	128.68
2	G	158	ADP	C3'-C2'-C1'	3.69	106.53	100.98
2	E	158	ADP	N3-C2-N1	-3.64	123.00	128.68

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	158	ADP	C5'-O5'-PA-O2A
2	B	158	ADP	C3'-C4'-C5'-O5'
2	G	158	ADP	C4'-C5'-O5'-PA
2	H	158	ADP	PA-O3A-PB-O2B
2	E	158	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	158	VO4	2	0
2	E	158	ADP	3	0
2	H	158	ADP	4	0

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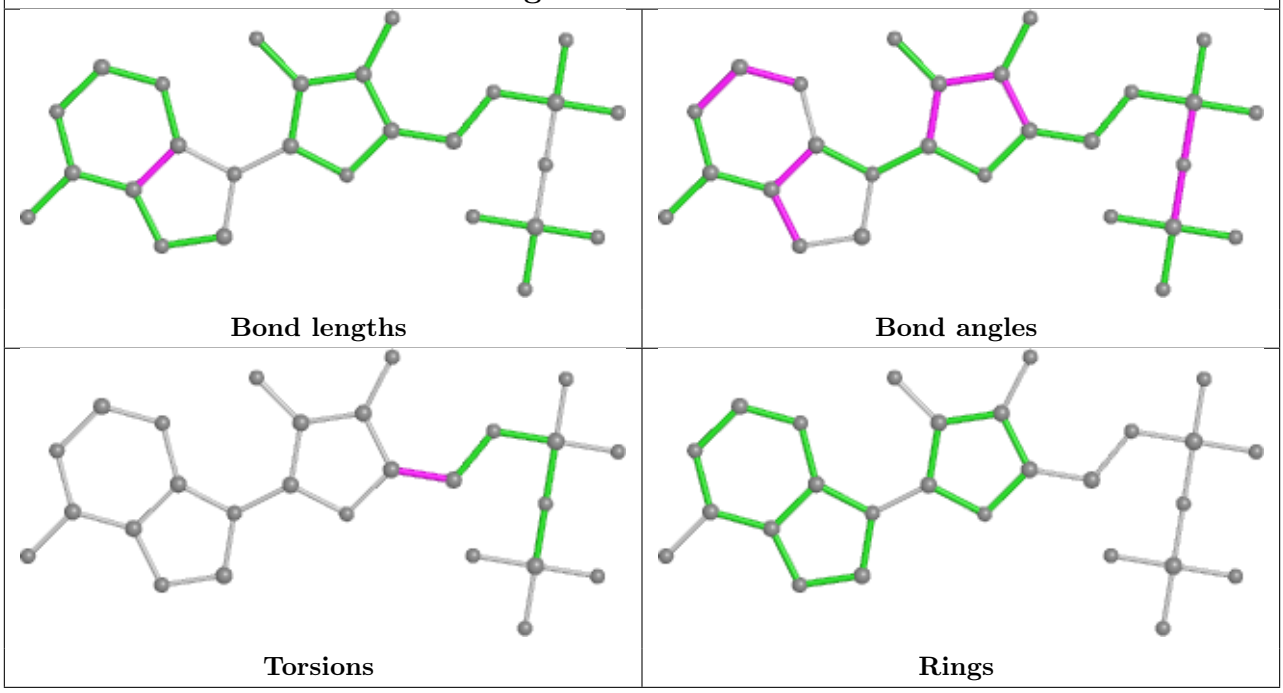
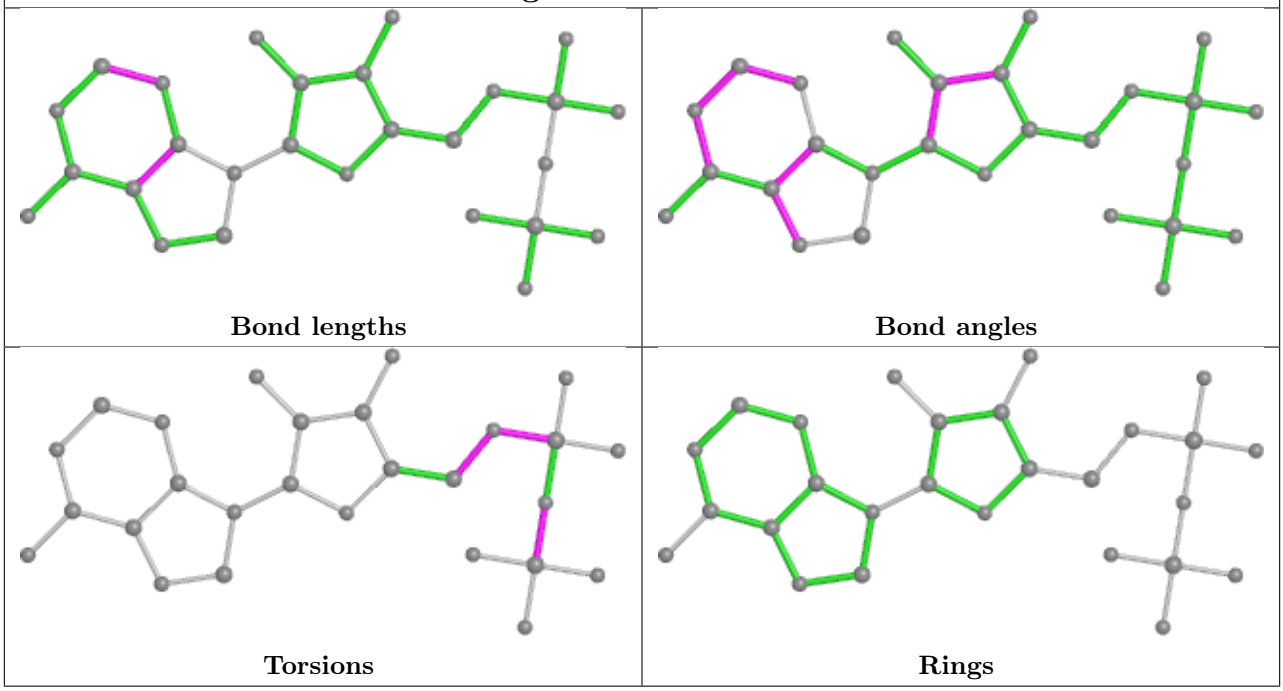
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	159	VO4	4	0
2	G	158	ADP	4	0
3	A	159	VO4	4	0
3	G	159	VO4	3	0
2	D	158	ADP	1	0
2	A	158	ADP	6	0
3	D	159	VO4	5	0
3	C	158	VO4	1	0
3	E	159	VO4	3	0
3	H	159	VO4	4	0
2	B	158	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

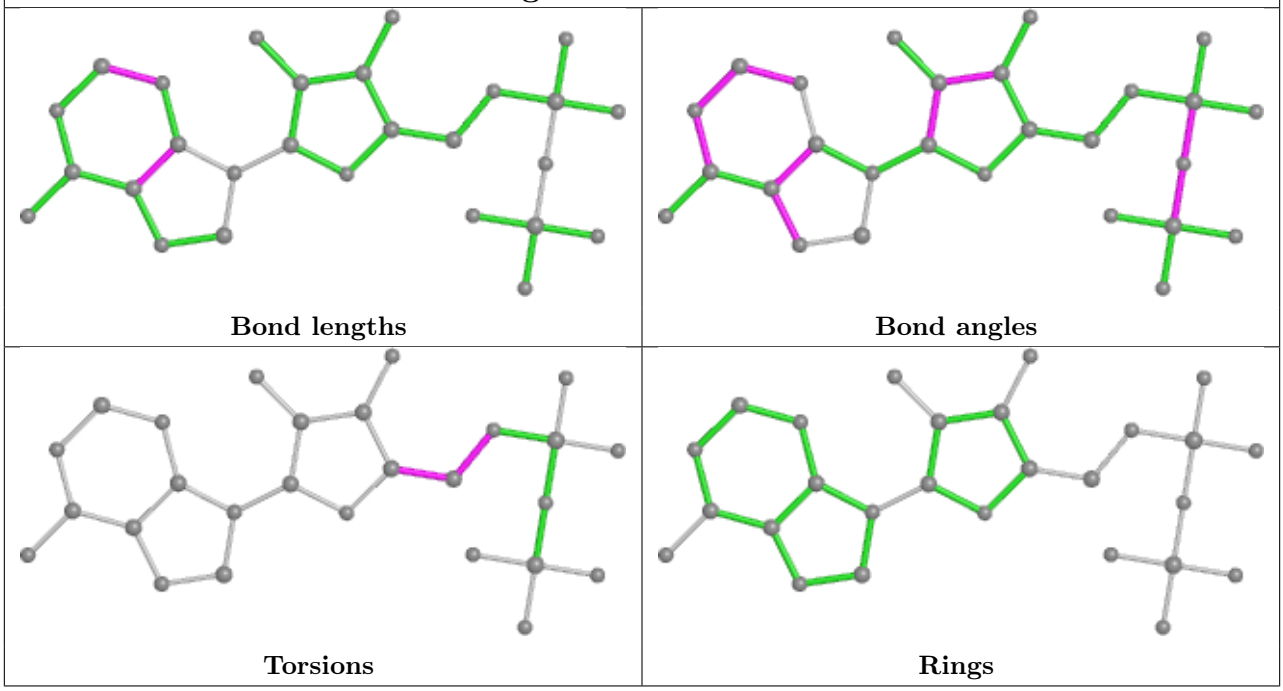
Ligand ADP E 158



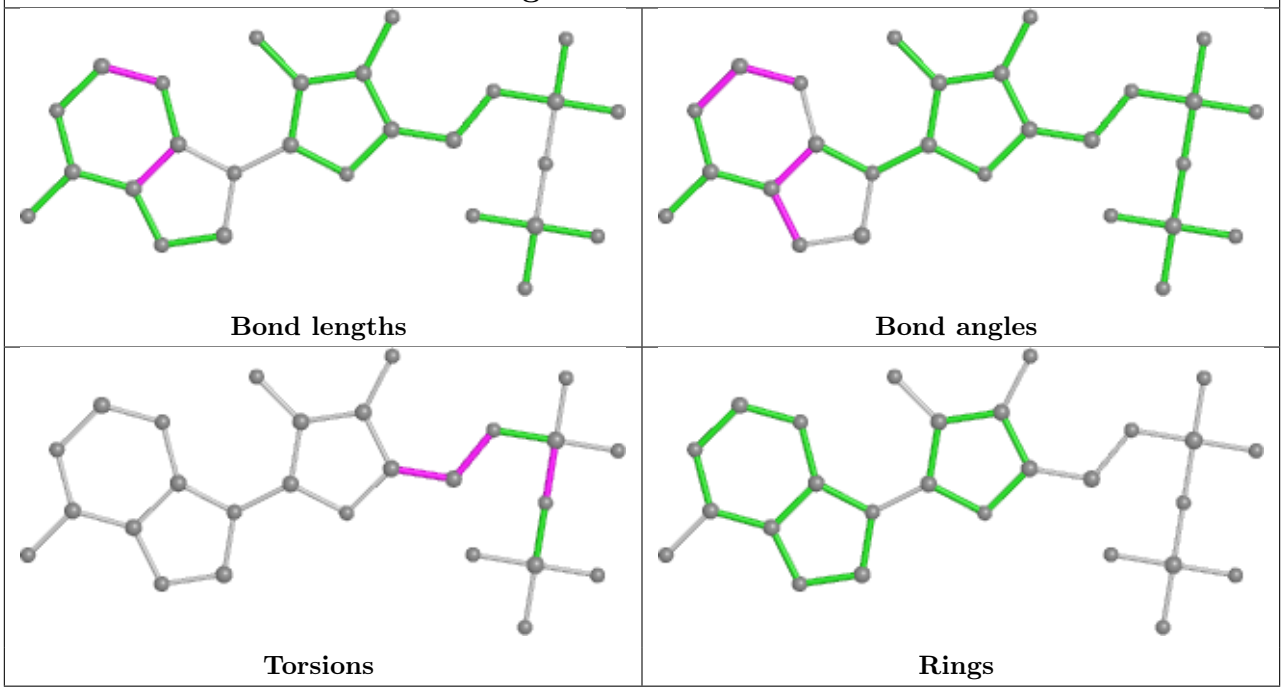
Ligand ADP H 158



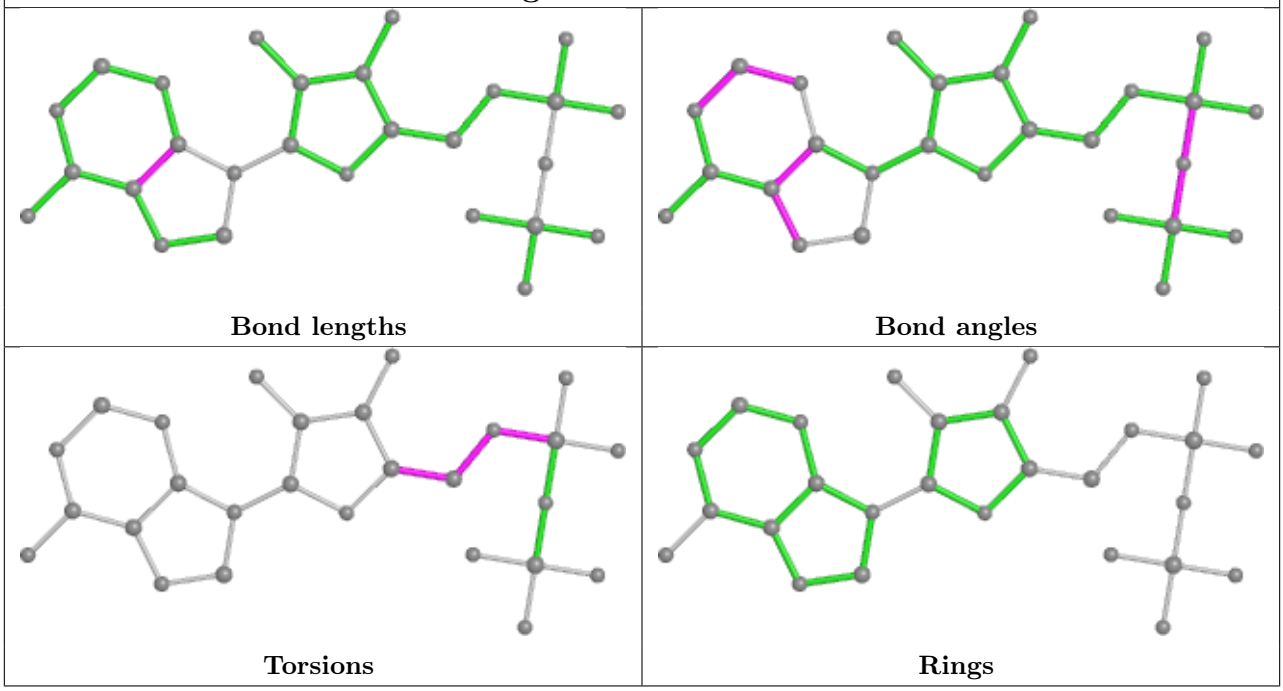
Ligand ADP G 158



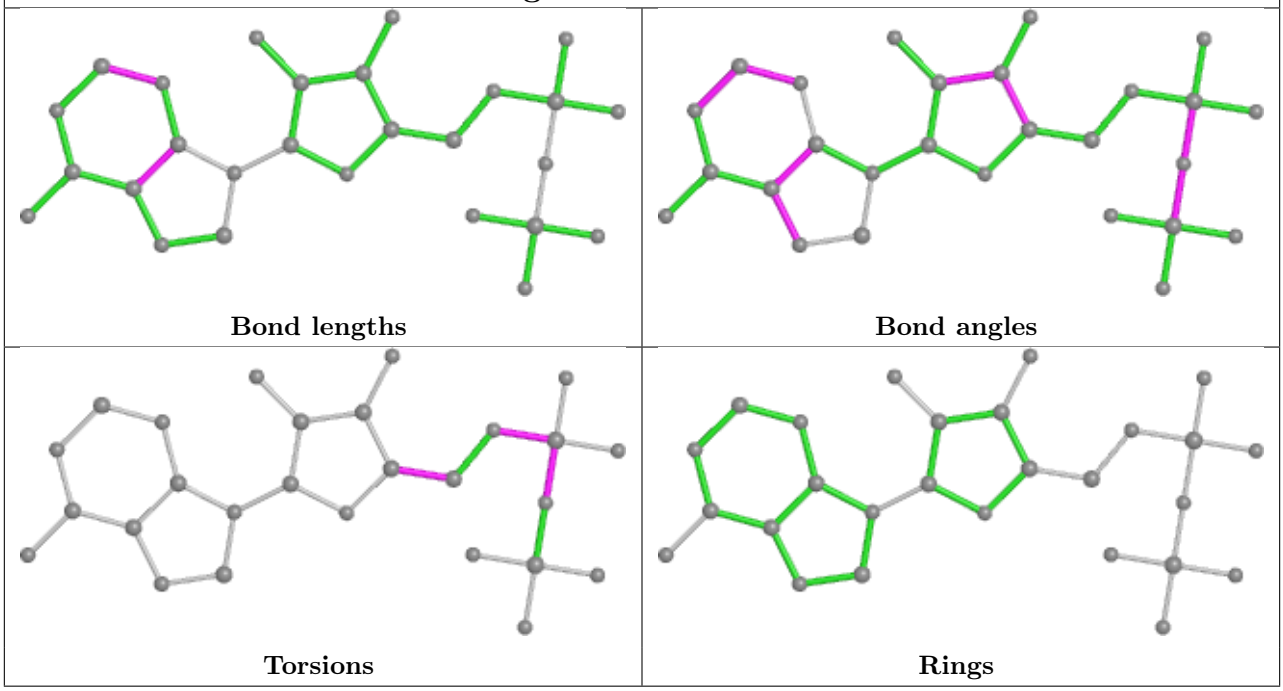
Ligand ADP D 158



Ligand ADP A 158



Ligand ADP B 158



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	149/157 (94%)	0.56	10 (6%)	17	16	45, 63, 91, 107	0
1	B	149/157 (94%)	0.22	6 (4%)	38	37	31, 50, 78, 86	0
1	C	149/157 (94%)	0.33	9 (6%)	21	20	35, 58, 100, 119	0
1	D	149/157 (94%)	0.31	9 (6%)	21	20	35, 55, 94, 109	0
1	E	149/157 (94%)	0.28	8 (5%)	25	24	37, 58, 88, 106	0
1	F	149/157 (94%)	0.35	8 (5%)	25	24	33, 56, 102, 119	0
1	G	149/157 (94%)	0.35	10 (6%)	17	16	37, 58, 90, 108	0
1	H	149/157 (94%)	1.16	37 (24%)	0	0	59, 86, 119, 132	0
All	All	1192/1256 (94%)	0.44	97 (8%)	12	10	31, 61, 103, 132	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	148	TYR	8.9
1	G	56	PRO	8.7
1	H	74	VAL	6.0
1	H	145	ALA	5.3
1	C	58	TYR	5.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

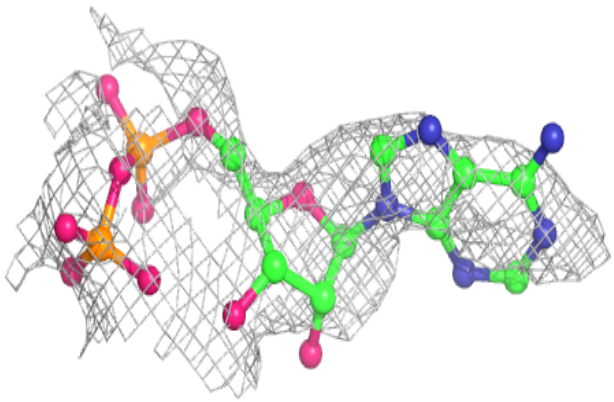
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

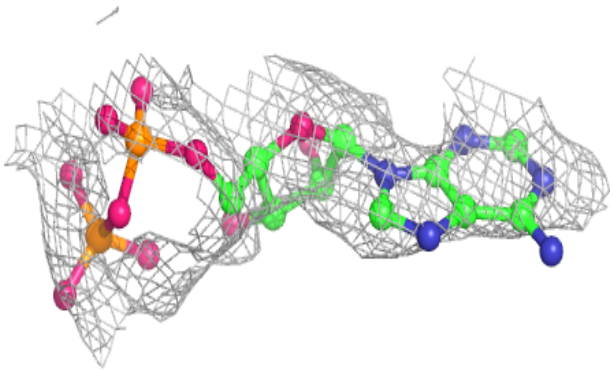
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	D	158	27/27	0.72	0.22	159,162,167,167	0
2	ADP	G	158	27/27	0.74	0.40	100,101,104,104	27
2	ADP	A	158	27/27	0.78	0.41	133,135,137,137	0
3	VO4	F	158	5/5	0.78	0.25	114,114,116,116	0
2	ADP	H	158	27/27	0.83	0.27	125,127,129,129	0
2	ADP	E	158	27/27	0.84	0.24	110,113,128,129	0
4	MG	B	160	1/1	0.86	0.08	53,53,53,53	0
4	MG	D	160	1/1	0.86	0.13	105,105,105,105	0
2	ADP	B	158	27/27	0.87	0.24	84,89,107,107	0
3	VO4	D	159	5/5	0.88	0.21	130,130,131,131	5
4	MG	H	160	1/1	0.88	0.09	74,74,74,74	0
3	VO4	C	158	5/5	0.89	0.17	100,100,101,102	0
3	VO4	A	159	5/5	0.89	0.20	94,95,96,97	0
3	VO4	G	159	5/5	0.91	0.15	86,86,87,88	5
4	MG	E	160	1/1	0.92	0.13	61,61,61,61	0
3	VO4	H	159	5/5	0.94	0.17	104,105,105,106	5
3	VO4	E	159	5/5	0.97	0.12	82,83,83,84	0
3	VO4	B	159	5/5	0.98	0.09	66,67,68,69	0

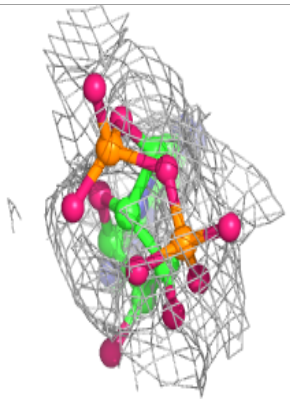
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 158:

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

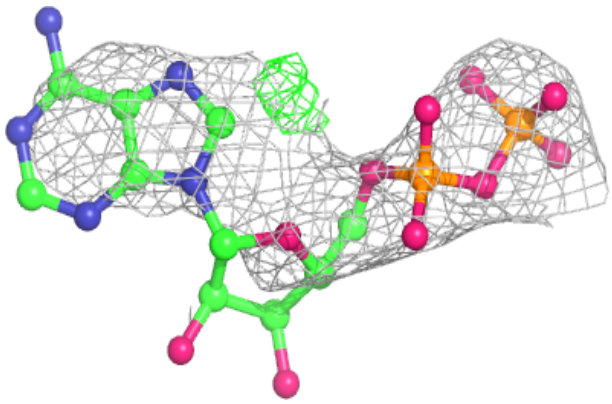


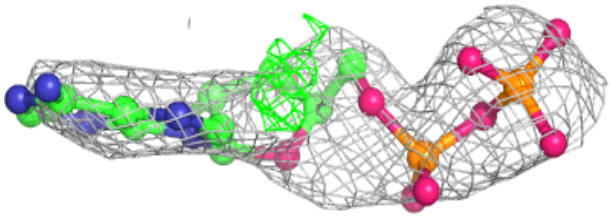


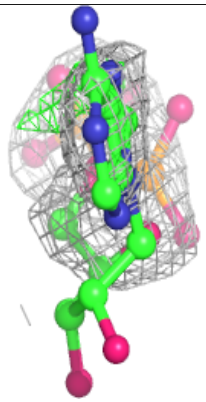


Electron density around ADP G 158:

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

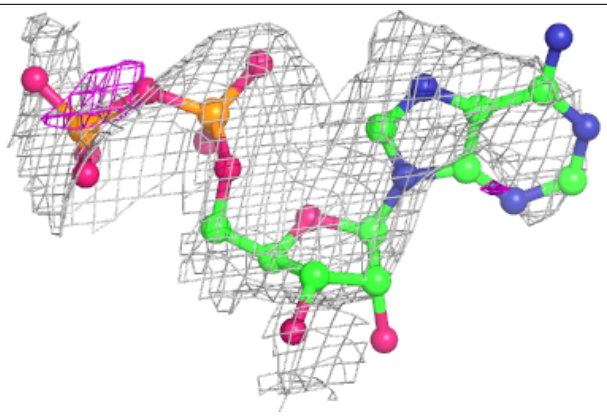


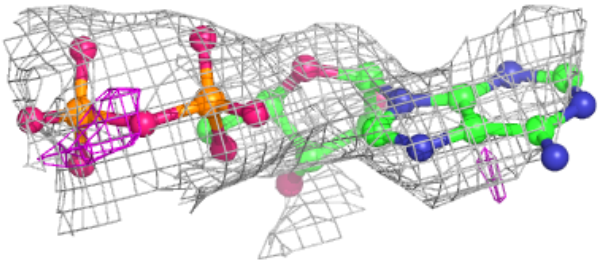


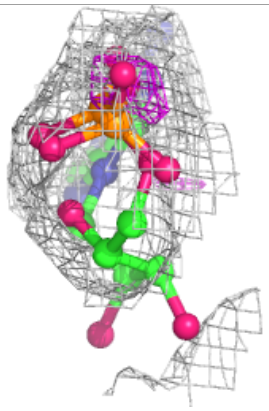


Electron density around ADP A 158:

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

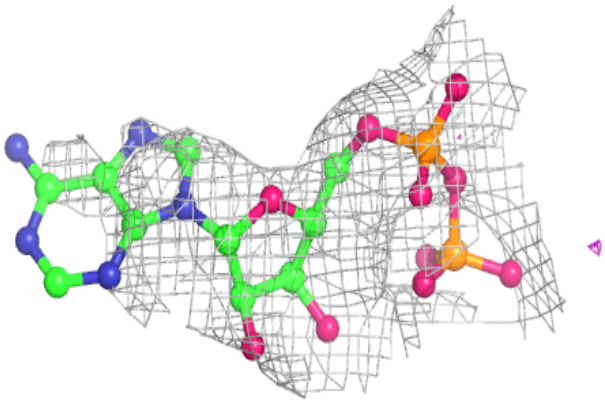


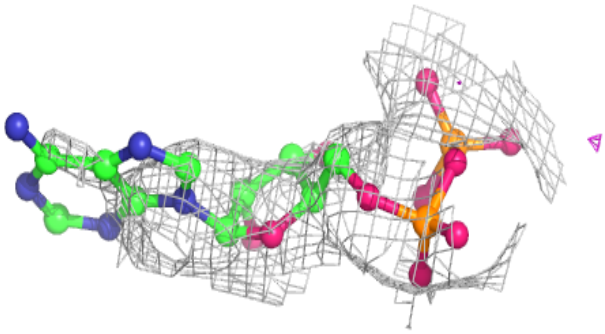




Electron density around ADP H 158:

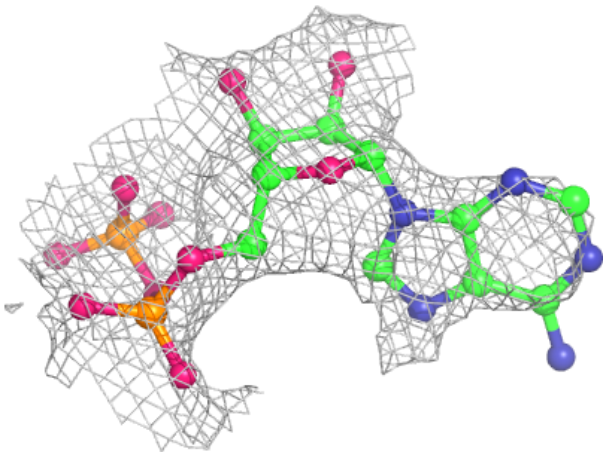
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

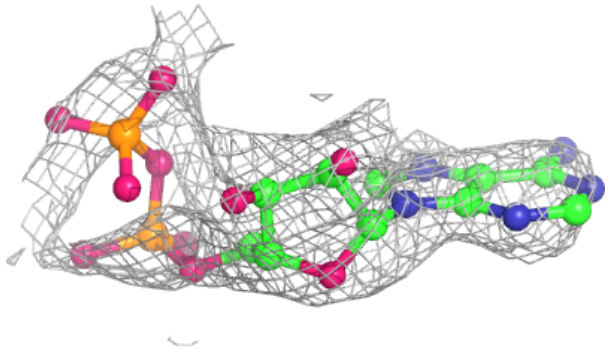


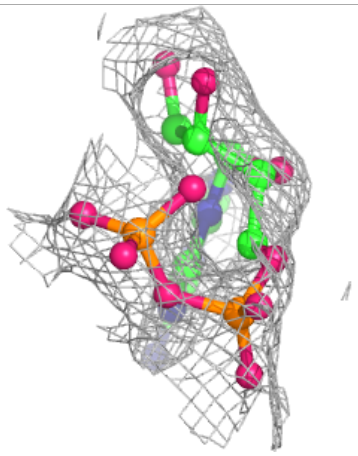


Electron density around ADP E 158:

$2mF_o$-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 158:

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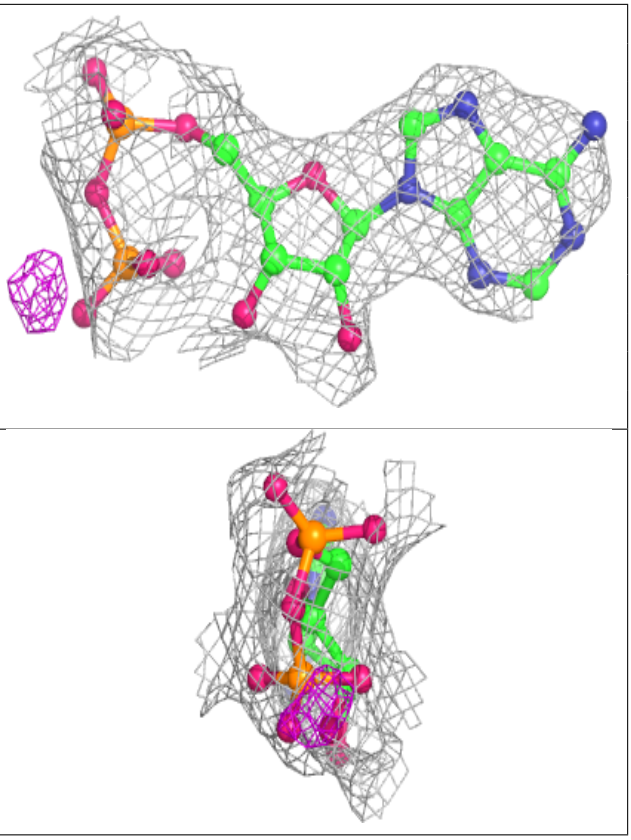
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.