wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2024 – 07:06 PM EST

PDB ID	:	4QQZ
Title	:	Crystal structure of T. fusca Cas3-AMPPNP
Authors	:	Ke, A.; Huo, Y.; Nam, K.H.
Deposited on	:	2014-06-30
Resolution	:	2.93 Å(reported)

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

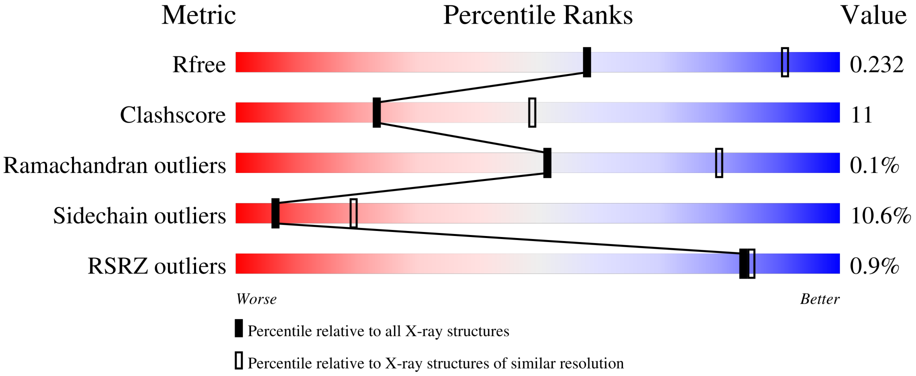
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

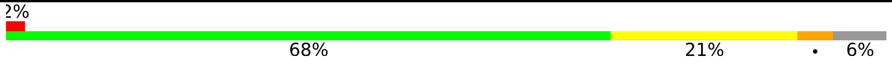
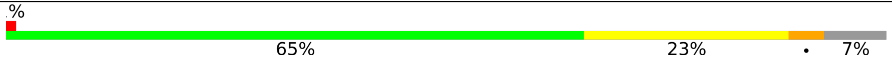
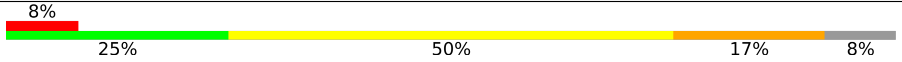
The reported resolution of this entry is 2.93 Å.

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.



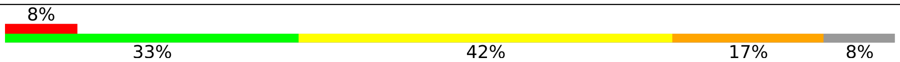
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	964	
1	C	964	
1	E	964	
1	G	964	
2	B	12	

Continued on next page...

Continued from previous page...

Mol	**Chain**	**Length**	**Quality of chain**
2	D	12	
2	F	12	
2	H	12	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 28851 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 CRISPR-associated helicase, Cas3 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total 7022	C 4460	N 1250	O 1285	S 27	0	0	0
1	C	902	Total 7001	C 4441	N 1243	O 1290	S 27	0	0	0
1	E	899	Total 6985	C 4434	N 1243	O 1281	S 27	0	0	0
1	G	892	Total 6923	C 4398	N 1230	O 1268	S 27	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q47PJ0
A	-18	GLY	-	expression tag	UNP Q47PJ0
A	-17	SER	-	expression tag	UNP Q47PJ0
A	-16	SER	-	expression tag	UNP Q47PJ0
A	-15	HIS	-	expression tag	UNP Q47PJ0
A	-14	HIS	-	expression tag	UNP Q47PJ0
A	-13	HIS	-	expression tag	UNP Q47PJ0
A	-12	HIS	-	expression tag	UNP Q47PJ0
A	-11	HIS	-	expression tag	UNP Q47PJ0
A	-10	HIS	-	expression tag	UNP Q47PJ0
A	-9	SER	-	expression tag	UNP Q47PJ0
A	-8	SER	-	expression tag	UNP Q47PJ0
A	-7	GLY	-	expression tag	UNP Q47PJ0
A	-6	LEU	-	expression tag	UNP Q47PJ0
A	-5	VAL	-	expression tag	UNP Q47PJ0
A	-4	PRO	-	expression tag	UNP Q47PJ0
A	-3	ARG	-	expression tag	UNP Q47PJ0
A	-2	GLY	-	expression tag	UNP Q47PJ0
A	-1	SER	-	expression tag	UNP Q47PJ0
A	0	HIS	-	expression tag	UNP Q47PJ0
C	-19	MET	-	initiating methionine	UNP Q47PJ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	expression tag	UNP Q47PJ0
C	-17	SER	-	expression tag	UNP Q47PJ0
C	-16	SER	-	expression tag	UNP Q47PJ0
C	-15	HIS	-	expression tag	UNP Q47PJ0
C	-14	HIS	-	expression tag	UNP Q47PJ0
C	-13	HIS	-	expression tag	UNP Q47PJ0
C	-12	HIS	-	expression tag	UNP Q47PJ0
C	-11	HIS	-	expression tag	UNP Q47PJ0
C	-10	HIS	-	expression tag	UNP Q47PJ0
C	-9	SER	-	expression tag	UNP Q47PJ0
C	-8	SER	-	expression tag	UNP Q47PJ0
C	-7	GLY	-	expression tag	UNP Q47PJ0
C	-6	LEU	-	expression tag	UNP Q47PJ0
C	-5	VAL	-	expression tag	UNP Q47PJ0
C	-4	PRO	-	expression tag	UNP Q47PJ0
C	-3	ARG	-	expression tag	UNP Q47PJ0
C	-2	GLY	-	expression tag	UNP Q47PJ0
C	-1	SER	-	expression tag	UNP Q47PJ0
C	0	HIS	-	expression tag	UNP Q47PJ0
E	-19	MET	-	initiating methionine	UNP Q47PJ0
E	-18	GLY	-	expression tag	UNP Q47PJ0
E	-17	SER	-	expression tag	UNP Q47PJ0
E	-16	SER	-	expression tag	UNP Q47PJ0
E	-15	HIS	-	expression tag	UNP Q47PJ0
E	-14	HIS	-	expression tag	UNP Q47PJ0
E	-13	HIS	-	expression tag	UNP Q47PJ0
E	-12	HIS	-	expression tag	UNP Q47PJ0
E	-11	HIS	-	expression tag	UNP Q47PJ0
E	-10	HIS	-	expression tag	UNP Q47PJ0
E	-9	SER	-	expression tag	UNP Q47PJ0
E	-8	SER	-	expression tag	UNP Q47PJ0
E	-7	GLY	-	expression tag	UNP Q47PJ0
E	-6	LEU	-	expression tag	UNP Q47PJ0
E	-5	VAL	-	expression tag	UNP Q47PJ0
E	-4	PRO	-	expression tag	UNP Q47PJ0
E	-3	ARG	-	expression tag	UNP Q47PJ0
E	-2	GLY	-	expression tag	UNP Q47PJ0
E	-1	SER	-	expression tag	UNP Q47PJ0
E	0	HIS	-	expression tag	UNP Q47PJ0
G	-19	MET	-	initiating methionine	UNP Q47PJ0
G	-18	GLY	-	expression tag	UNP Q47PJ0
G	-17	SER	-	expression tag	UNP Q47PJ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	SER	-	expression tag	UNP Q47PJ0
G	-15	HIS	-	expression tag	UNP Q47PJ0
G	-14	HIS	-	expression tag	UNP Q47PJ0
G	-13	HIS	-	expression tag	UNP Q47PJ0
G	-12	HIS	-	expression tag	UNP Q47PJ0
G	-11	HIS	-	expression tag	UNP Q47PJ0
G	-10	HIS	-	expression tag	UNP Q47PJ0
G	-9	SER	-	expression tag	UNP Q47PJ0
G	-8	SER	-	expression tag	UNP Q47PJ0
G	-7	GLY	-	expression tag	UNP Q47PJ0
G	-6	LEU	-	expression tag	UNP Q47PJ0
G	-5	VAL	-	expression tag	UNP Q47PJ0
G	-4	PRO	-	expression tag	UNP Q47PJ0
G	-3	ARG	-	expression tag	UNP Q47PJ0
G	-2	GLY	-	expression tag	UNP Q47PJ0
G	-1	SER	-	expression tag	UNP Q47PJ0
G	0	HIS	-	expression tag	UNP Q47PJ0

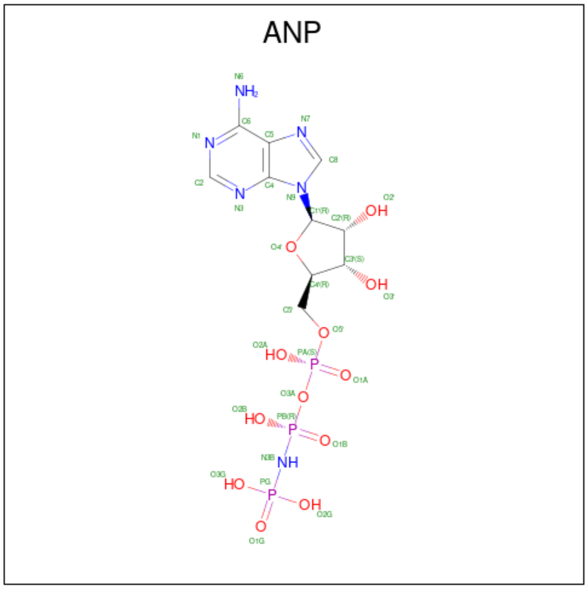
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP *AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total 197	C 90	N 45	O 51	P 11	0	0	0
2	D	11	Total 197	C 90	N 45	O 51	P 11	0	0	0
2	F	11	Total 197	C 90	N 45	O 51	P 11	0	0	0
2	H	11	Total 197	C 90	N 45	O 51	P 11	0	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Fe 2	0	0
3	C	2	Total 2	Fe 2	0	0
3	E	2	Total 2	Fe 2	0	0
3	G	2	Total 2	Fe 2	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



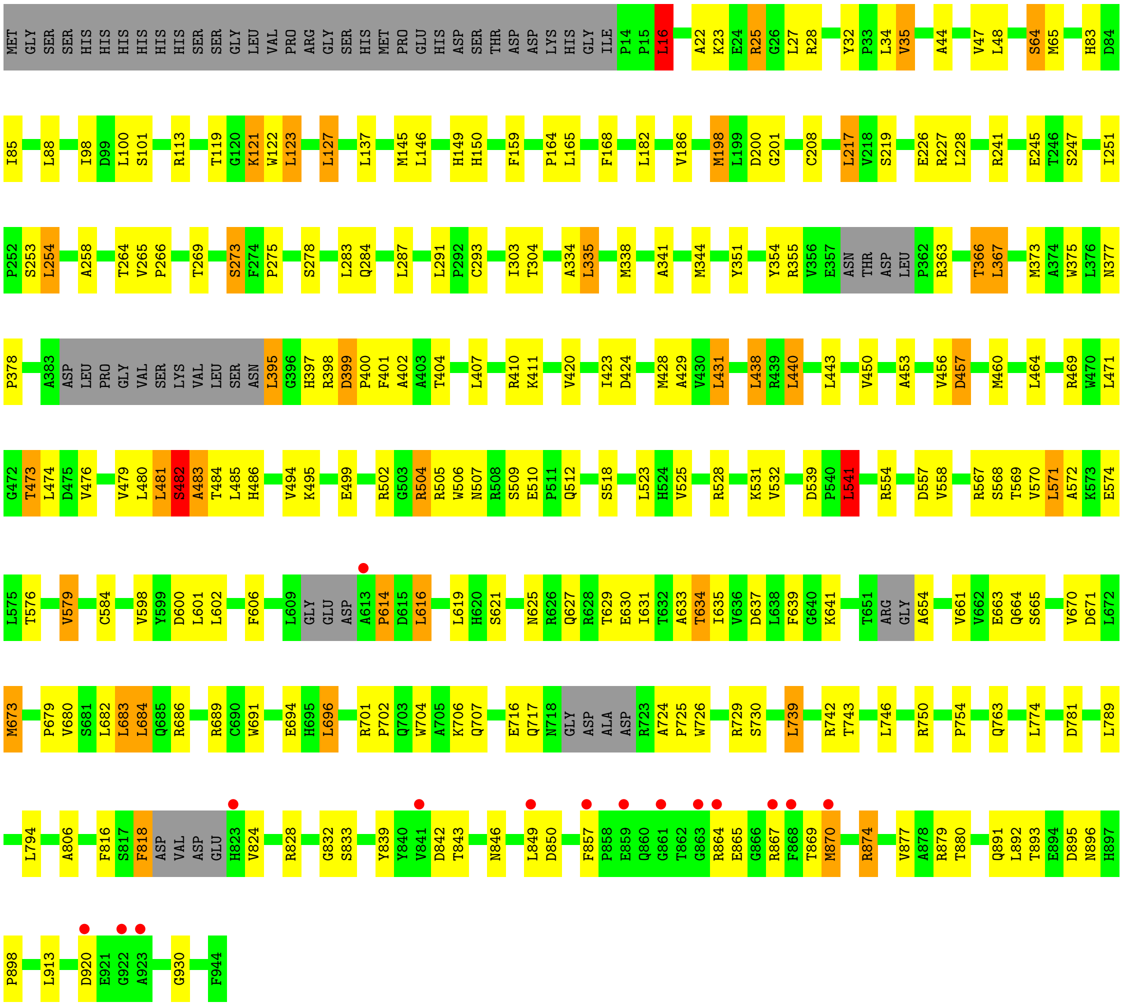
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
4	C	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
4	E	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
4	G	1	31	10	6	12	3	0	0

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.

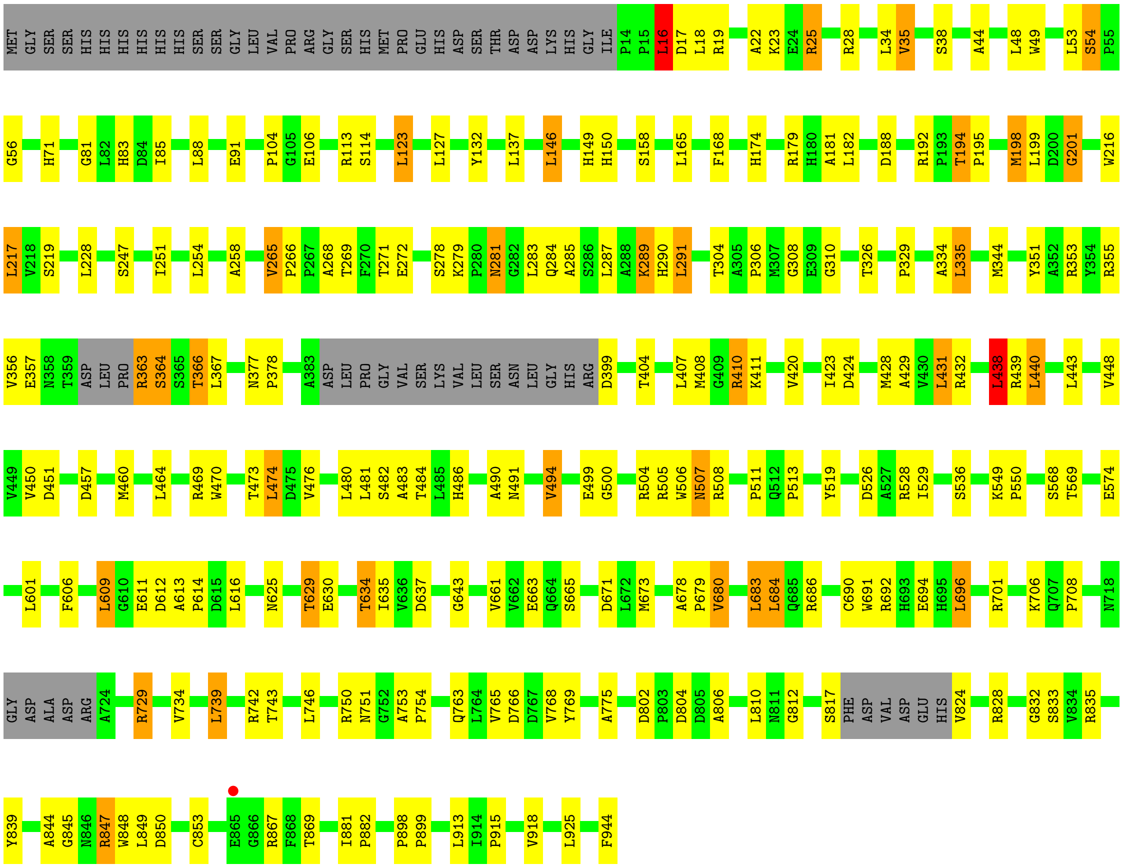
- Molecule 1: CRISPR-associated helicase, Cas3 family

Chain A:



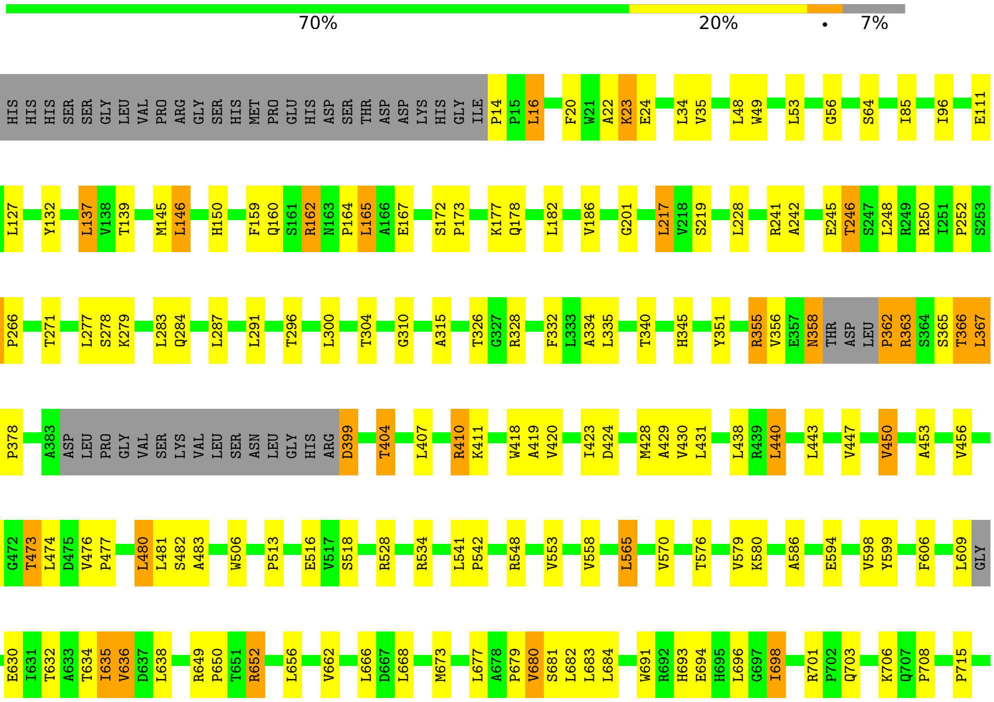
- Molecule 1: CRISPR-associated helicase, Cas3 family

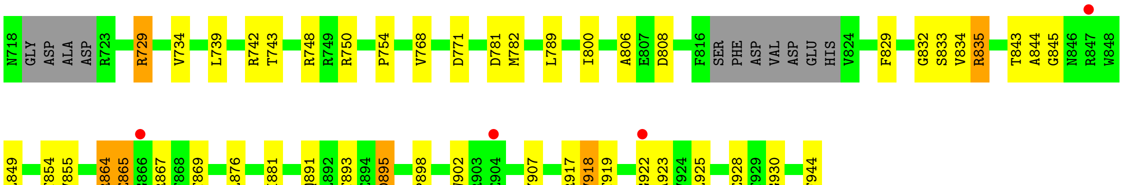
Chain C:



- Molecule 1: CRISPR-associated helicase, Cas3 family

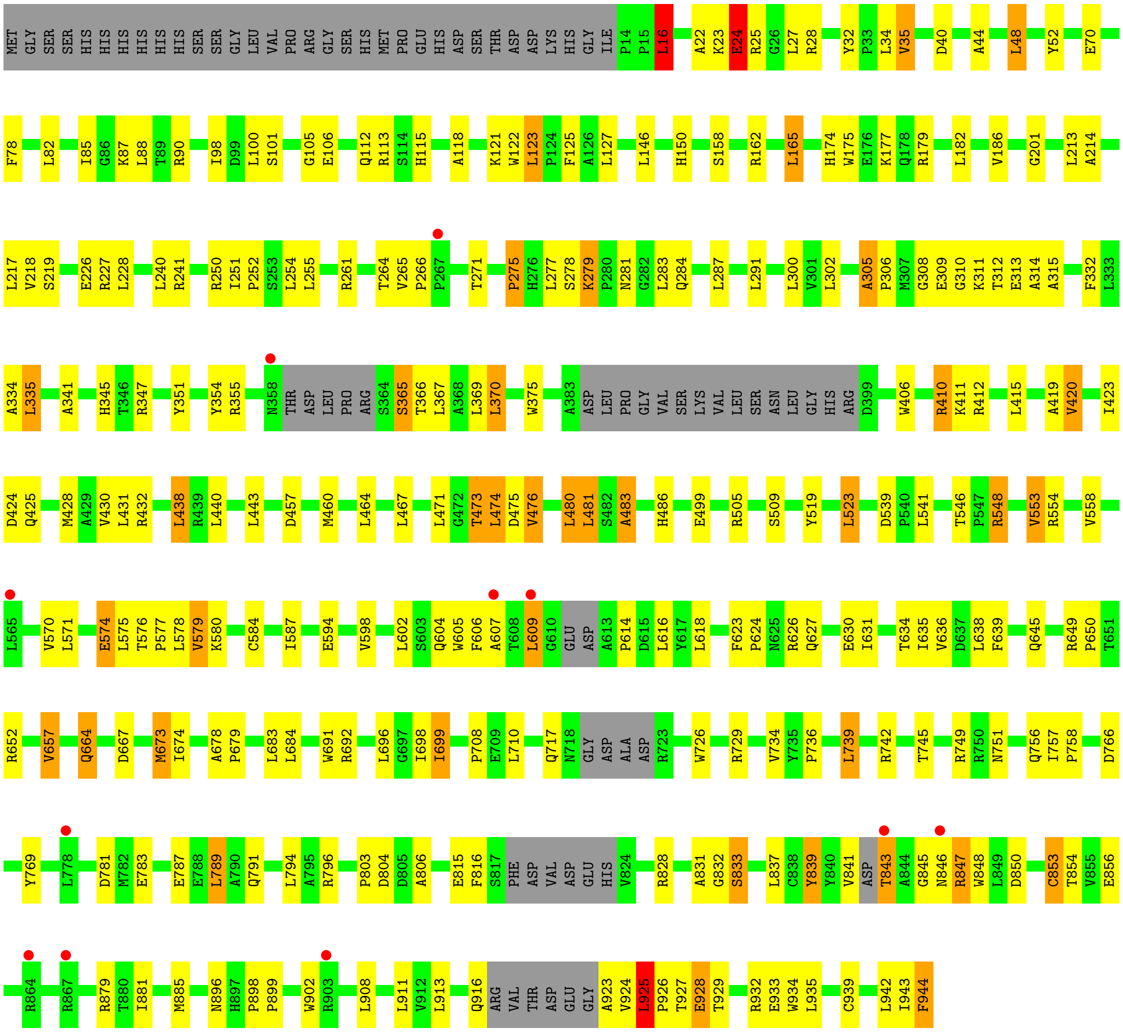
Chain E:





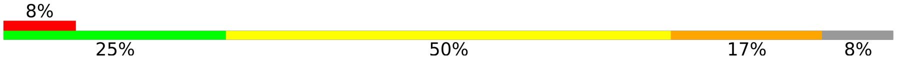
- Molecule 1: CRISPR-associated helicase, Cas3 family

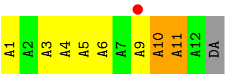
Chain G:



- Molecule 2: DNA (5’-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3’)

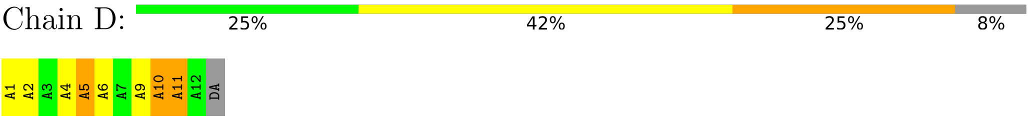
Chain B:





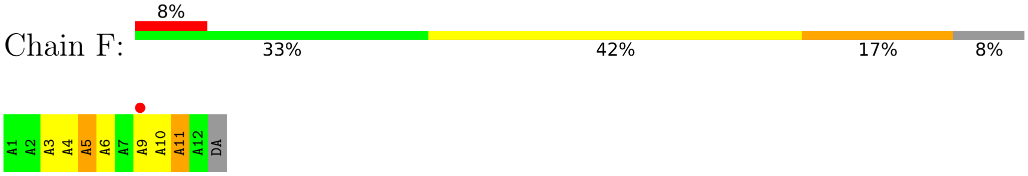
- Molecule 2: DNA (5’-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3’)

Chain D:



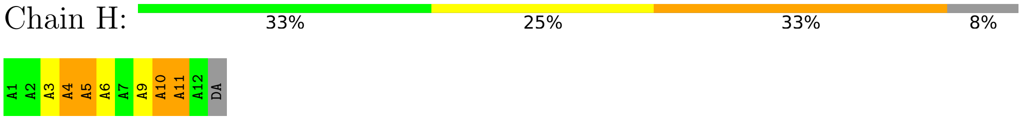
- Molecule 2: DNA (5’-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3’)

Chain F:



- Molecule 2: DNA (5’-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3’)

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.92Å 222.06Å 124.90Å 90.00° 104.29° 90.00°	Depositor
Resolution (Å)	50.11 – 2.93 50.11 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.11-2.93) 88.9 (50.11-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.182 , 0.234 0.184 , 0.232	Depositor DCC
R_{free} test set	2000 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.7	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	0.94	EDS
Total number of atoms	28851	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, FE

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	0.56	4/7199 (0.1%)	0.67	11/9817 (0.1%)
1	C	0.51	0/7176	0.64	4/9790 (0.0%)
1	E	0.49	0/7160	0.63	5/9766 (0.1%)
1	G	0.52	1/7095 (0.0%)	0.66	7/9675 (0.1%)
2	B	1.13	0/222	2.38	18/339 (5.3%)
2	D	1.09	0/222	2.36	14/339 (4.1%)
2	F	1.11	0/222	2.26	14/339 (4.1%)
2	H	0.93	0/222	2.13	14/339 (4.1%)
All	All	0.55	5/29518 (0.0%)	0.77	87/40404 (0.2%)

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	G	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	LEU	C-N	-15.87	0.97	1.34
1	A	614	PRO	N-CD	10.18	1.62	1.47
1	A	606	PHE	CE1-CZ	8.85	1.54	1.37
1	G	275	PRO	N-CD	8.81	1.60	1.47
1	A	484	THR	CB-CG2	-5.30	1.34	1.52

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	11	DA	O4'-C1'-N9	13.99	117.79	108.00
2	H	10	DA	O4'-C1'-C2'	-12.55	95.86	105.90
2	D	11	DA	O4'-C1'-N9	12.37	116.66	108.00
2	F	11	DA	O4'-C4'-C3'	12.25	113.35	106.00
2	B	9	DA	O4'-C1'-N9	11.96	116.37	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	482	SER	Mainchain
1	G	925	LEU	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	7022	0	6970	161	0
1	C	7001	0	6944	148	0
1	E	6985	0	6939	131	0
1	G	6923	0	6878	199	0
2	B	197	0	99	9	0
2	D	197	0	99	10	0
2	F	197	0	99	6	0
2	H	197	0	99	12	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	A	31	0	13	4	0
4	C	31	0	13	6	0
4	E	31	0	13	5	0
4	G	31	0	13	8	0
All	All	28851	0	28179	643	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 11.

The worst 5 of 643 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:G:618:LEU:CD1	1:G:657:VAL:HG12	1.71	1.21
1:G:587:ILE:HD11	1:G:657:VAL:CG2	1.76	1.14
1:G:310:GLY:N	4:G:1003:ANP:O1A	1.86	1.08
1:G:587:ILE:CD1	1:G:657:VAL:HG22	1.85	1.06
1:G:618:LEU:HD12	1:G:657:VAL:HG12	1.36	1.05

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	889/964 (92%)	853 (96%)	36 (4%)	0	100	100
1	C	892/964 (92%)	862 (97%)	29 (3%)	1 (0%)	51	80
1	E	887/964 (92%)	852 (96%)	35 (4%)	0	100	100
1	G	876/964 (91%)	830 (95%)	44 (5%)	2 (0%)	47	76
All	All	3544/3856 (92%)	3397 (96%)	144 (4%)	3 (0%)	51	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	605	TRP
1	C	483	ALA
1	G	853	CYS

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	744/796 (94%)	671 (90%)	73 (10%)	8	23
1	C	742/796 (93%)	665 (90%)	77 (10%)	7	20
1	E	740/796 (93%)	657 (89%)	83 (11%)	6	17
1	G	733/796 (92%)	651 (89%)	82 (11%)	6	17
All	All	2959/3184 (93%)	2644 (89%)	315 (11%)	6	19

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	928	GLU
1	G	602	LEU
1	G	70	GLU
1	G	366	THR
1	G	751	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	664	GLN
1	G	717	GLN
1	G	811	ASN
1	E	358	ASN
1	C	290	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	ANP	A	1003	-	29,33,33	1.22	4 (13%)	31,52,52	1.02	2 (6%)
4	ANP	C	1003	-	29,33,33	2.14	11 (37%)	31,52,52	2.53	13 (41%)
4	ANP	G	1003	-	29,33,33	1.84	10 (34%)	31,52,52	3.28	14 (45%)
4	ANP	E	1003	-	29,33,33	2.12	11 (37%)	31,52,52	2.75	10 (32%)

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	ANP	A	1003	-	-	6/14/38/38	0/3/3/3
4	ANP	C	1003	-	-	8/14/38/38	0/3/3/3
4	ANP	G	1003	-	-	7/14/38/38	0/3/3/3
4	ANP	E	1003	-	-	6/14/38/38	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	ANP	C2'-C1'	-5.15	1.45	1.53
4	E	1003	ANP	PB-O2B	-4.90	1.43	1.56
4	E	1003	ANP	C4-N3	-3.88	1.30	1.35
4	G	1003	ANP	PB-O2B	-3.71	1.46	1.56
4	E	1003	ANP	C2'-C1'	-3.56	1.48	1.53

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1003	ANP	O1G-PG-N3B	-9.97	97.09	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1003	ANP	O2B-PB-O1B	7.91	126.50	109.92
4	C	1003	ANP	O2B-PB-O1B	6.61	123.78	109.92
4	G	1003	ANP	O3'-C3'-C2'	-6.32	91.37	111.82
4	E	1003	ANP	O1G-PG-N3B	-6.22	102.62	111.77

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	ANP	PB-N3B-PG-O1G
4	C	1003	ANP	PG-N3B-PB-O1B
4	C	1003	ANP	PG-N3B-PB-O3A
4	C	1003	ANP	C5'-O5'-PA-O2A
4	C	1003	ANP	O4'-C4'-C5'-O5'

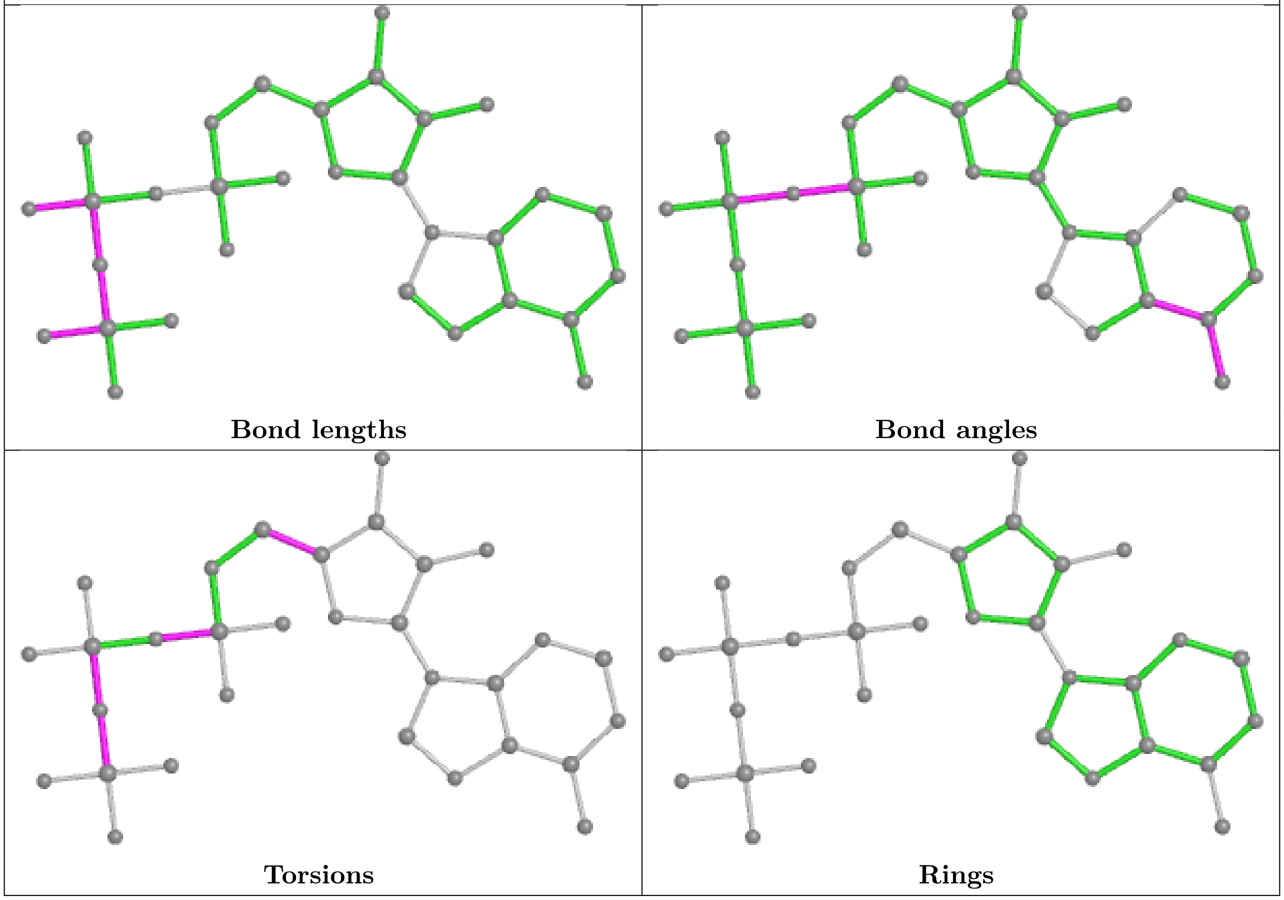
There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	ANP	4	0
4	C	1003	ANP	6	0
4	G	1003	ANP	8	0
4	E	1003	ANP	5	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 ANP A 1003



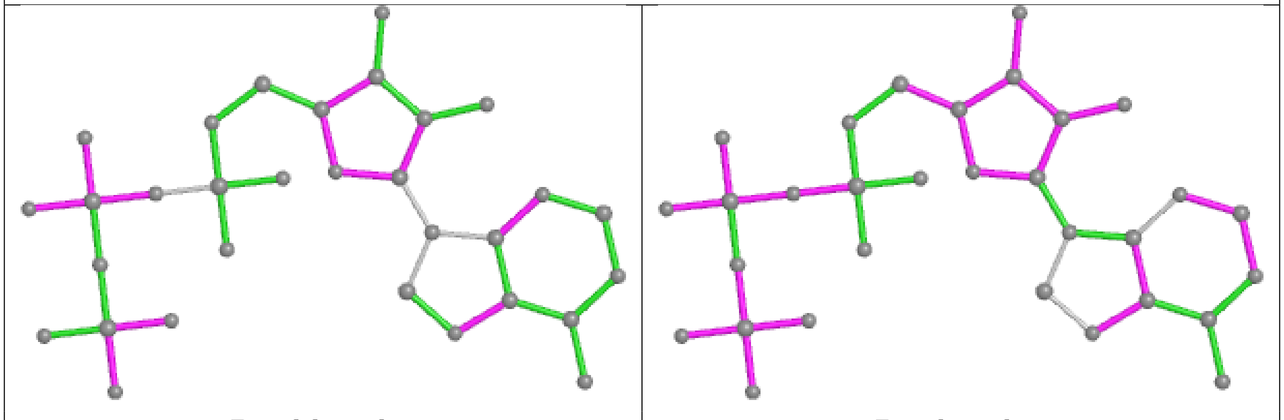
Bond lengths

Bond angles

Torsions

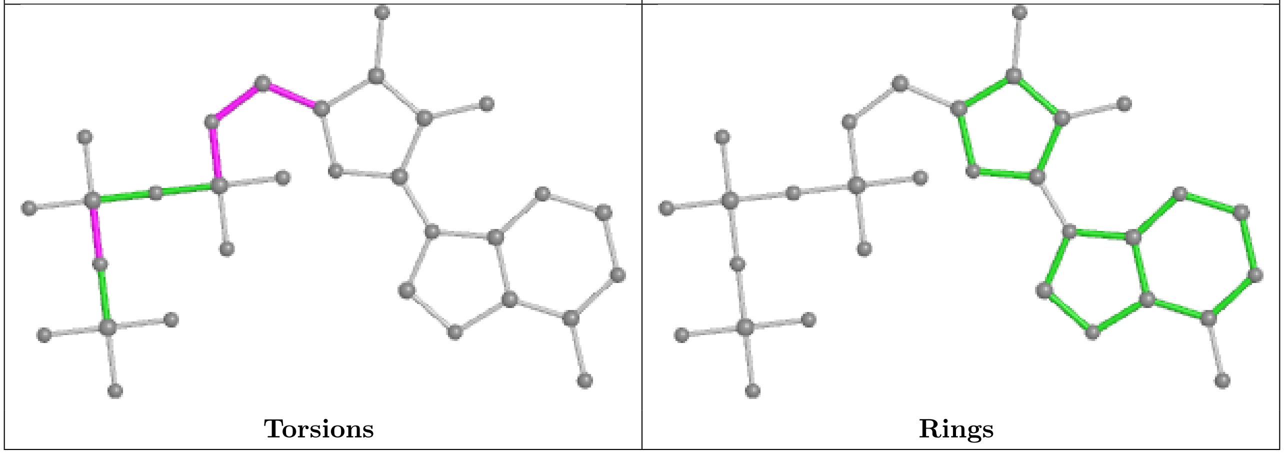
Rings

Ligand ANP C 1003



Bond lengths

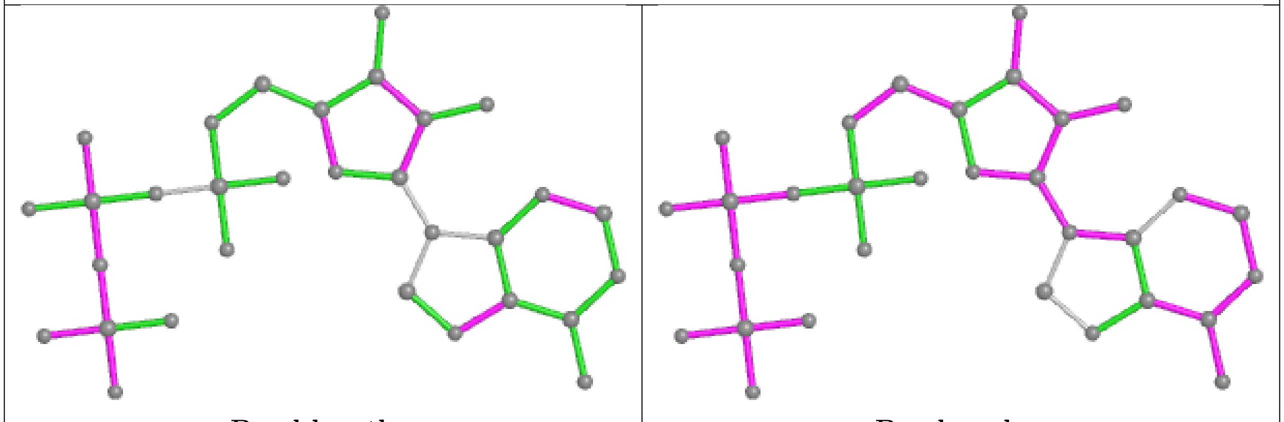
Bond angles



Torsions

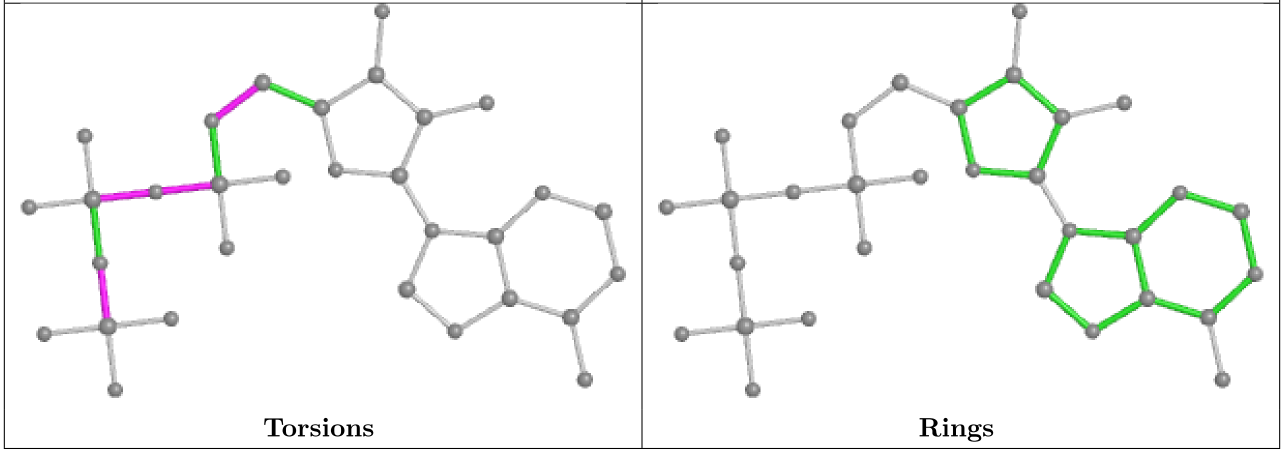
Rings

Ligand ANP G 1003



Bond lengths

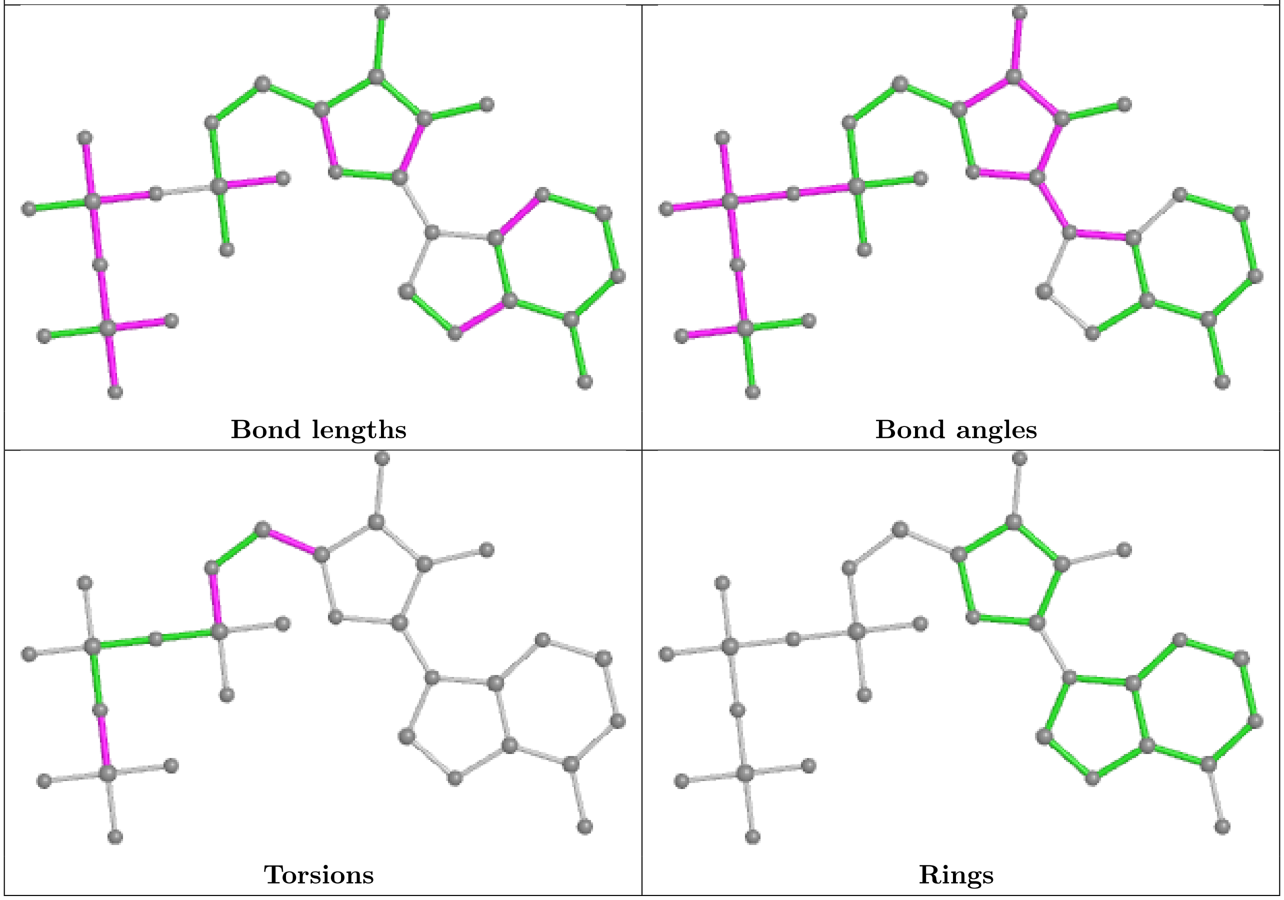
Bond angles



Torsions

Rings

Ligand ANP E 1003



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	481:LEU	C	482:SER	N	0.97

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	903/964 (93%)	-0.36	15 (1%)	70	71	18, 41, 83, 116	0
1	C	902/964 (93%)	-0.51	1 (0%)	95	96	22, 41, 66, 99	0
1	E	899/964 (93%)	-0.46	4 (0%)	92	93	16, 37, 70, 97	0
1	G	892/964 (92%)	-0.28	11 (1%)	79	80	23, 52, 89, 108	0
2	B	11/12 (91%)	0.22	1 (9%)	9	7	33, 44, 86, 103	0
2	D	11/12 (91%)	-0.09	0	100	100	35, 42, 83, 90	0
2	F	11/12 (91%)	0.34	1 (9%)	9	7	28, 39, 92, 94	0
2	H	11/12 (91%)	0.31	0	100	100	40, 56, 99, 101	0
All	All	3640/3904 (93%)	-0.40	33 (0%)	84	85	16, 42, 81, 116	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	846	ASN	5.1
1	A	864	ARG	3.3
1	A	868	PHE	3.1
1	G	867	ARG	3.1
1	A	923	ALA	3.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

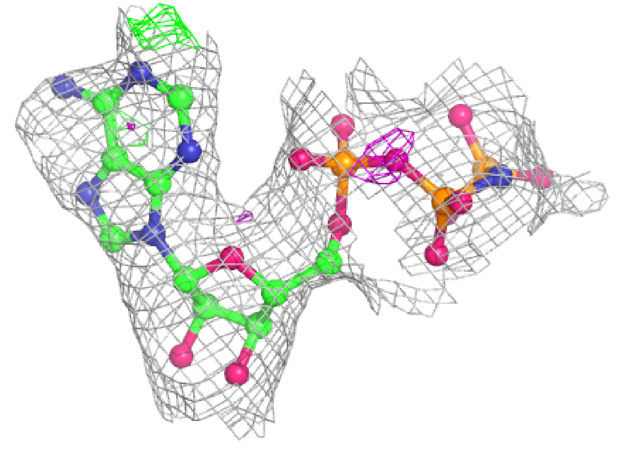
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

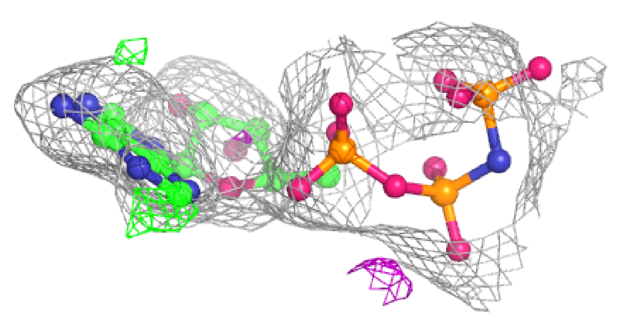
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	ANP	G	1003	31/31	0.79	0.18	70,94,121,141	0
4	ANP	E	1003	31/31	0.81	0.18	63,72,92,107	0
4	ANP	A	1003	31/31	0.90	0.15	51,67,83,115	0
4	ANP	C	1003	31/31	0.91	0.11	59,71,93,103	0
3	FE	E	1001	1/1	0.99	0.16	27,27,27,27	0
3	FE	E	1002	1/1	0.99	0.16	23,23,23,23	0
3	FE	G	1001	1/1	0.99	0.16	34,34,34,34	0
3	FE	G	1002	1/1	0.99	0.16	31,31,31,31	0
3	FE	A	1001	1/1	0.99	0.17	28,28,28,28	0
3	FE	A	1002	1/1	0.99	0.16	24,24,24,24	0
3	FE	C	1001	1/1	0.99	0.15	27,27,27,27	0
3	FE	C	1002	1/1	0.99	0.15	27,27,27,27	0

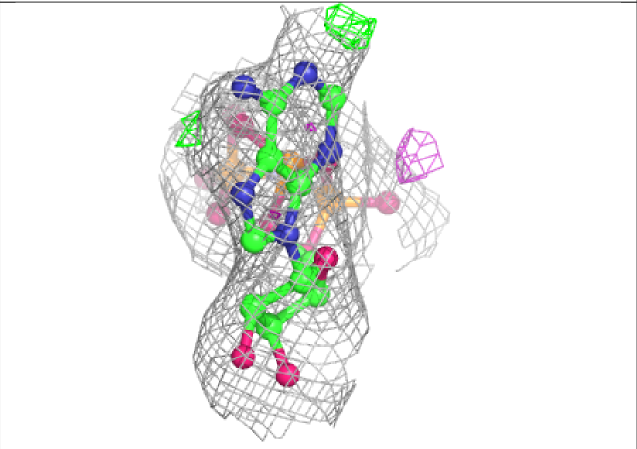
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP G 1003:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

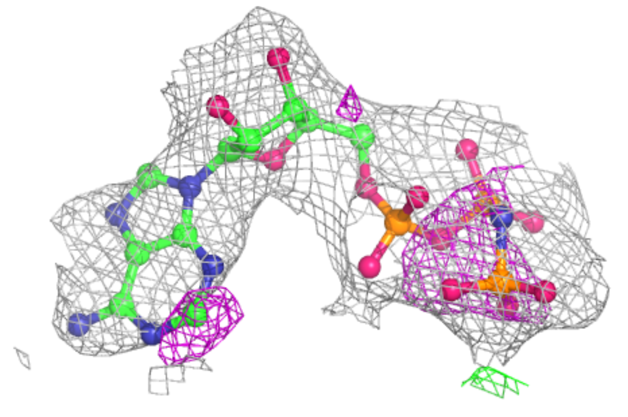


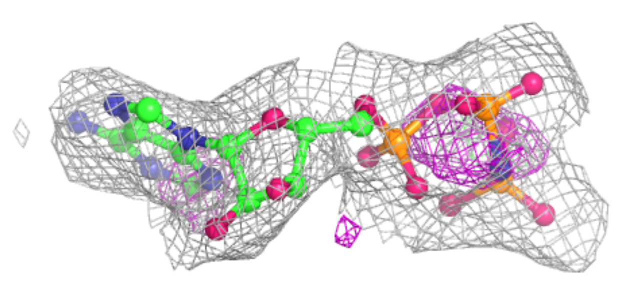


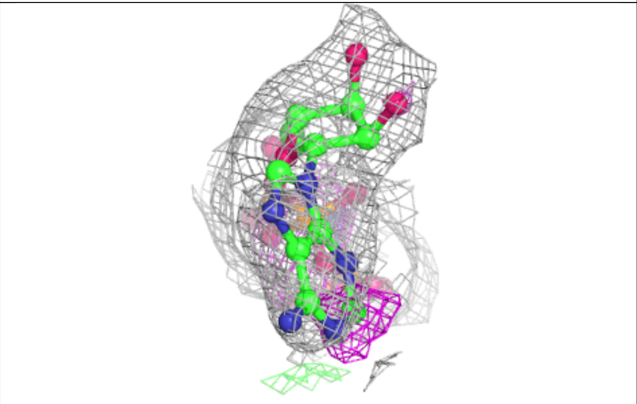


Electron density around ANP E 1003:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

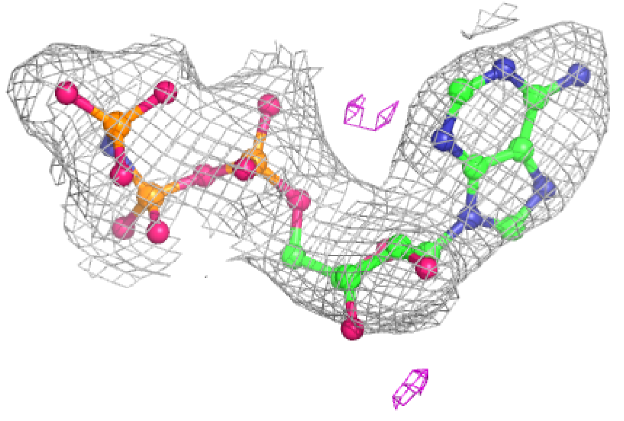


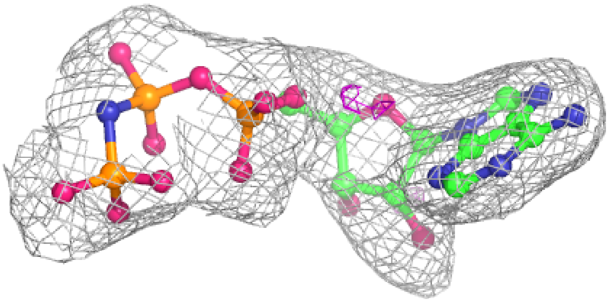


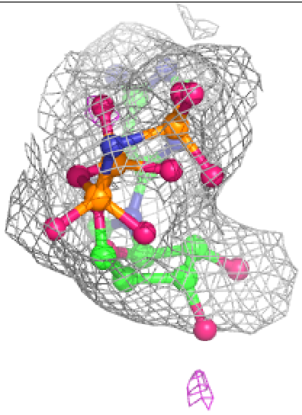


Electron density around ANP A 1003:

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

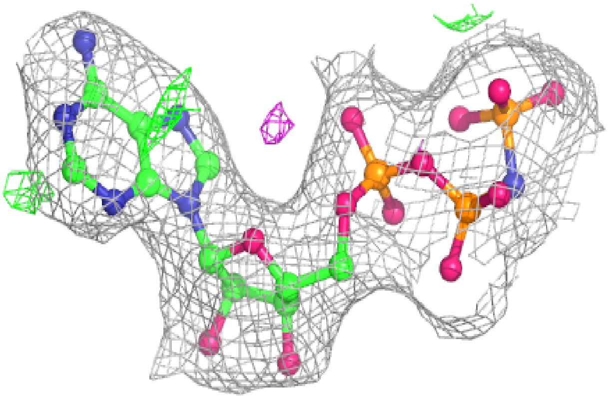


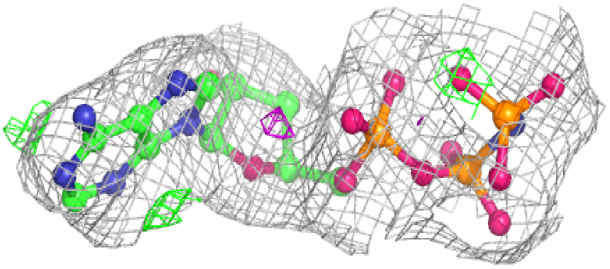


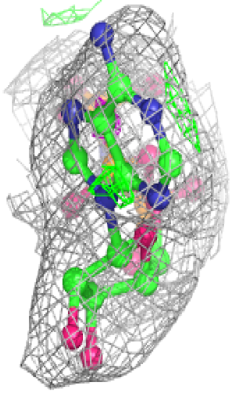


Electron density around ANP C 1003:

$2mF_o$-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.