Full wwPDB X-ray Structure Validation 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)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

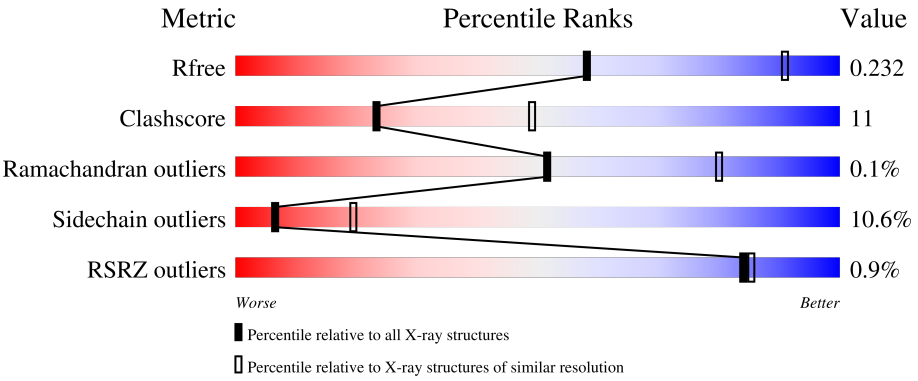
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.93 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	2% 68% 21% • 6%
1	C	964	70% 20% • 6%
1	E	964	70% 20% • 7%
1	G	964	% 65% 23% • 7%
2	B	12	8% 25% 50% 17% 8%

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Mol	Chain	Length	Quality of chain
2	D	12	25% 42% 25% 8%
2	F	12	8% 33% 42% 17% 8%
2	H	12	33% 25% 33% 8%

2 Entry composition (i)

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	C	N	O	S	0	0	0
			7022	4460	1250	1285	27			
1	C	902	Total	C	N	O	S	0	0	0
			7001	4441	1243	1290	27			
1	E	899	Total	C	N	O	S	0	0	0
			6985	4434	1243	1281	27			
1	G	892	Total	C	N	O	S	0	0	0
			6923	4398	1230	1268	27			

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

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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

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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

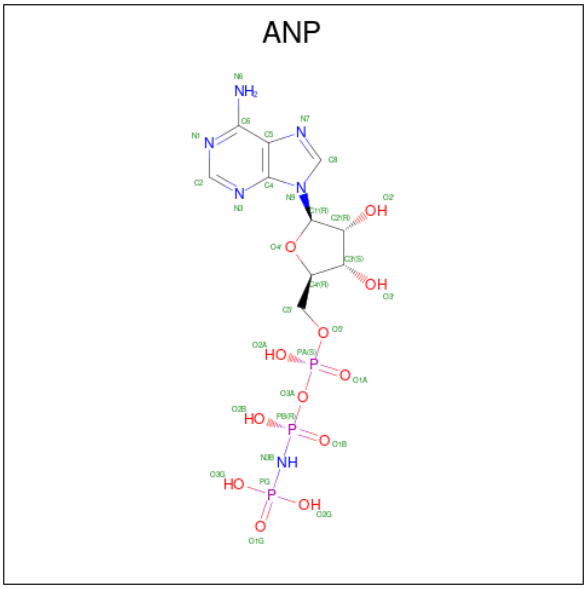
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

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

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

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

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



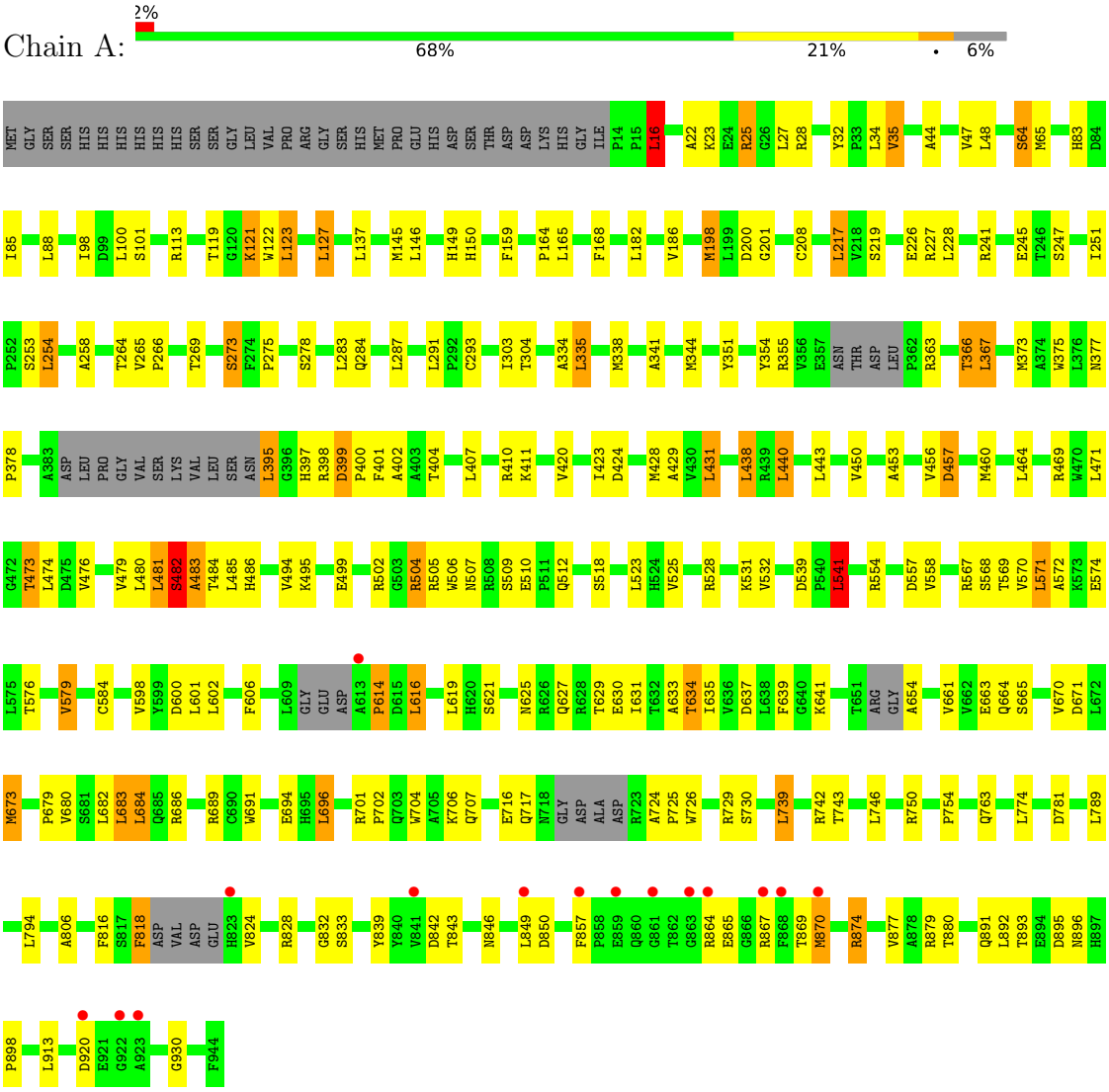
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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.

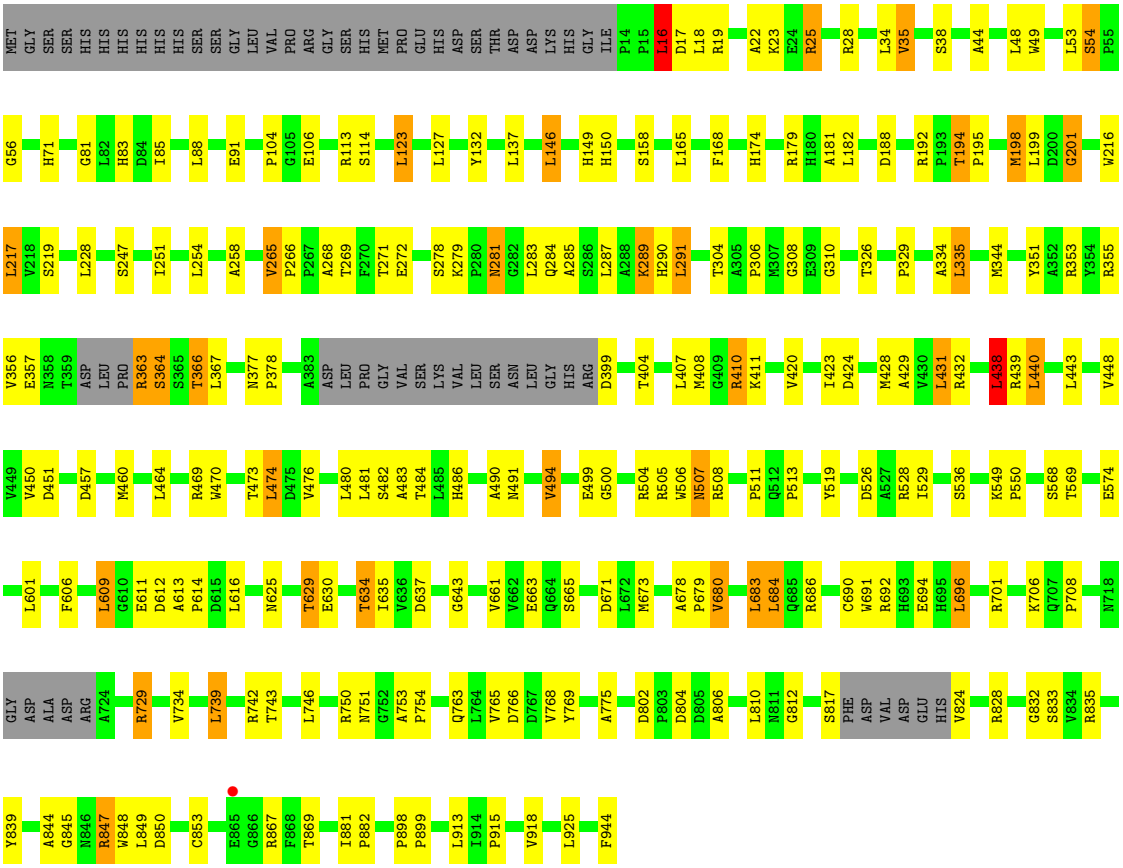
• Molecule 1: CRISPR-associated helicase, Cas3 family

Chain A:



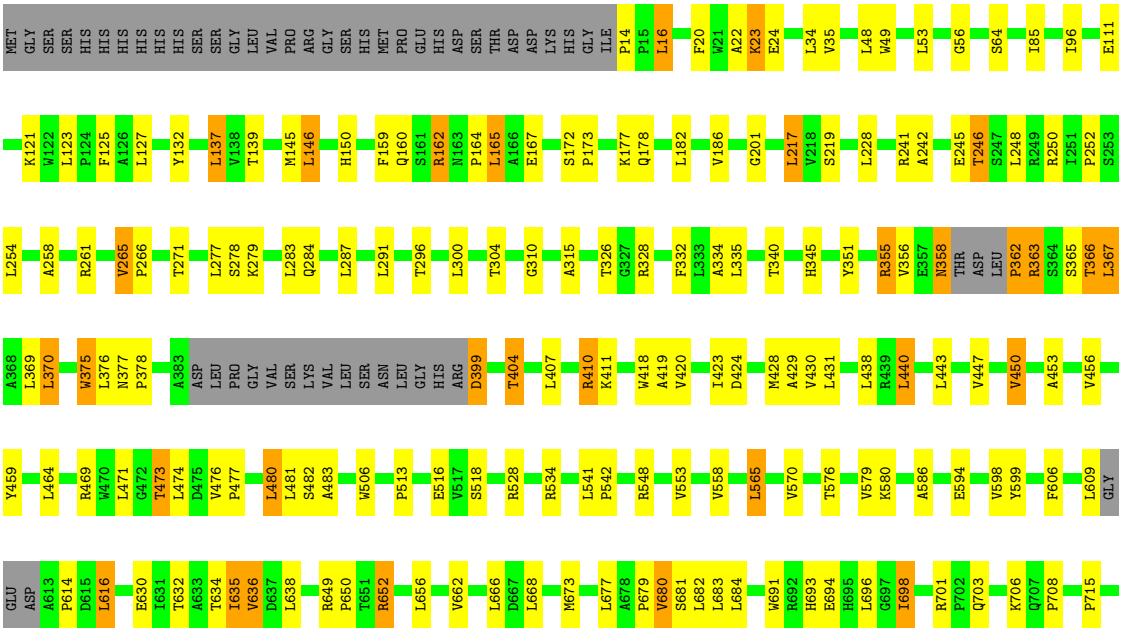
• Molecule 1: CRISPR-associated helicase, Cas3 family

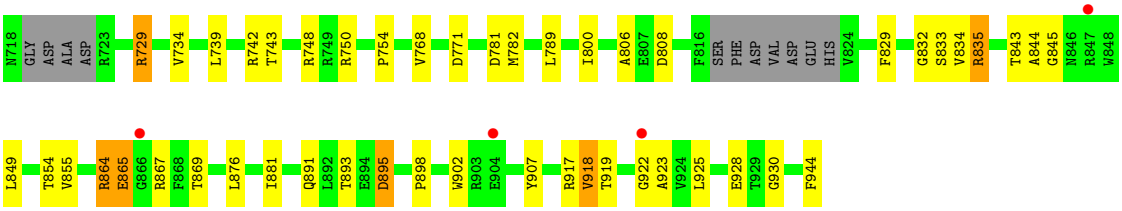
Chain C:



• Molecule 1: CRISPR-associated helicase, Cas3 family

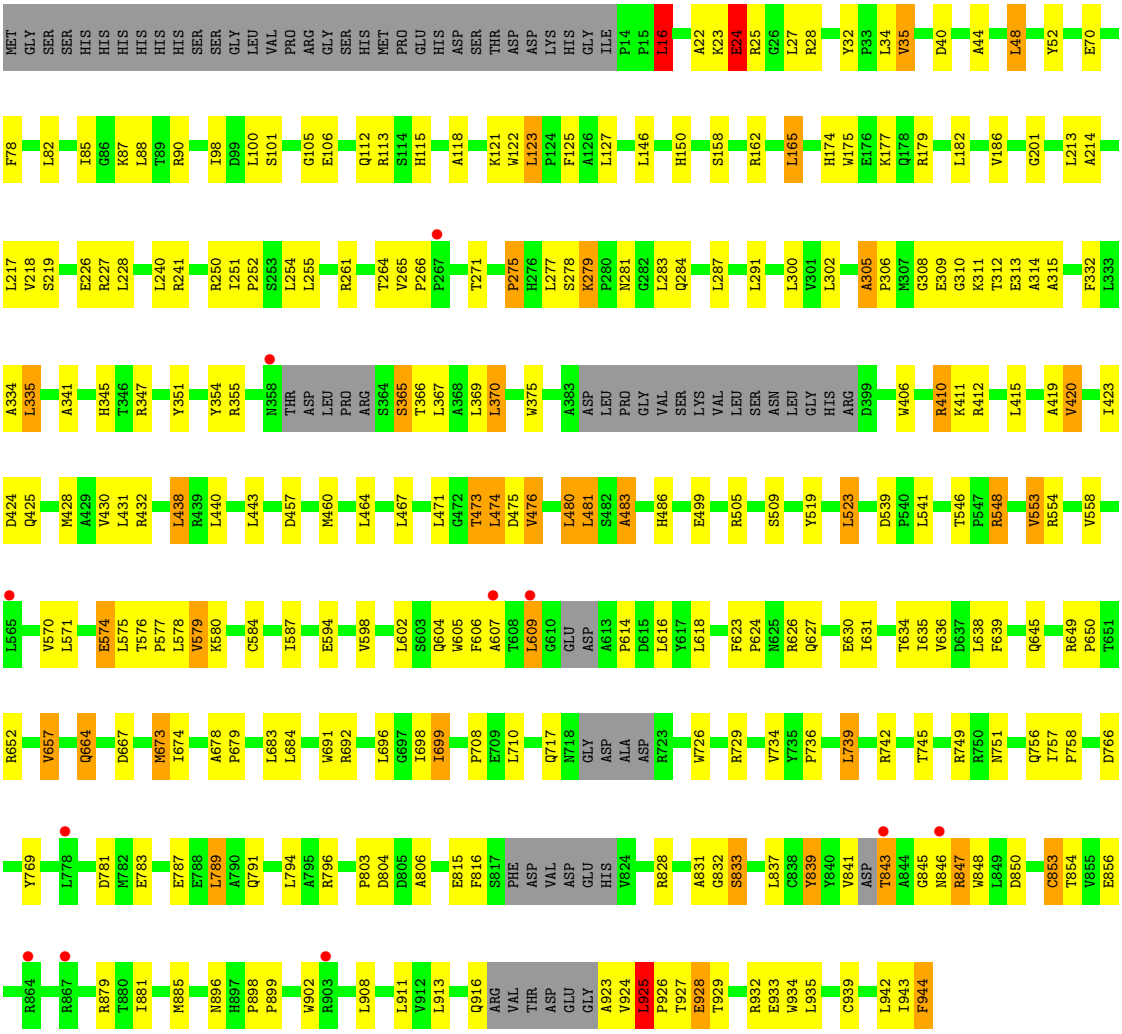
Chain E:





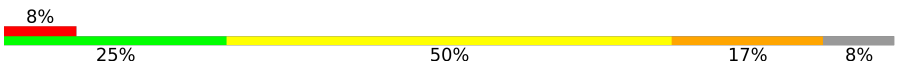
• Molecule 1: CRISPR-associated helicase, Cas3 family

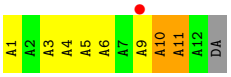
Chain G:



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

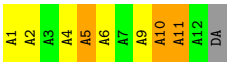
Chain B:





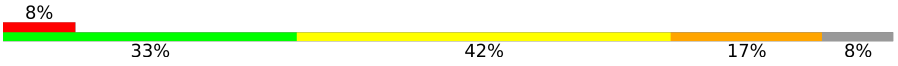
• Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

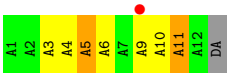
Chain D:



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

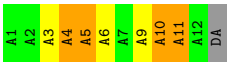
Chain F:





• 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 (i)

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 (i)

5.1 Standard geometry (i)

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

All (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
2	D	11	DA	O4'-C4'-C3'	10.68	112.41	106.00
2	B	4	DA	O4'-C4'-C3'	-10.04	99.98	106.00
2	H	10	DA	N7-C8-N9	9.78	118.69	113.80
1	A	482	SER	O-C-N	-9.75	107.11	122.70
2	H	11	DA	O4'-C4'-C3'	9.74	111.84	106.00
2	D	10	DA	C1'-O4'-C4'	-9.25	100.85	110.10
2	B	11	DA	O4'-C4'-C3'	8.93	111.36	106.00
1	A	874	ARG	NE-CZ-NH2	-8.89	115.86	120.30
2	D	1	DA	O4'-C4'-C3'	-8.52	100.89	106.00
1	G	483	ALA	CB-CA-C	-8.50	97.35	110.10
2	H	11	DA	O4'-C1'-N9	8.49	113.94	108.00
2	D	11	DA	C4'-C3'-C2'	-8.46	95.48	103.10
2	D	10	DA	O4'-C4'-C3'	8.44	111.06	106.00
2	H	10	DA	O4'-C1'-N9	8.42	113.89	108.00
2	F	9	DA	O4'-C1'-N9	8.38	113.87	108.00
2	B	10	DA	O4'-C1'-C2'	-8.35	99.22	105.90
2	B	11	DA	O4'-C1'-N9	8.35	113.84	108.00
2	H	10	DA	C8-N9-C4	-8.20	102.52	105.80
2	F	11	DA	C4'-C3'-C2'	-8.13	95.78	103.10
2	B	10	DA	C8-N9-C4	-8.05	102.58	105.80
2	B	10	DA	N7-C8-N9	8.04	117.82	113.80
2	D	9	DA	O4'-C1'-N9	7.98	113.59	108.00
2	F	10	DA	O4'-C1'-N9	7.95	113.56	108.00
2	F	4	DA	O4'-C4'-C3'	-7.81	101.31	106.00
2	B	10	DA	C4'-C3'-O3'	-7.76	90.31	109.70
2	H	11	DA	C4'-C3'-C2'	-7.66	96.21	103.10
2	F	10	DA	C1'-O4'-C4'	-7.48	102.62	110.10
2	H	10	DA	C5-N7-C8	-7.43	100.19	103.90
2	D	4	DA	O4'-C4'-C3'	-7.37	101.55	104.50
2	F	10	DA	O4'-C1'-C2'	-7.16	100.17	105.90
2	H	10	DA	P-O5'-C5'	-7.11	109.52	120.90
2	B	4	DA	C4'-C3'-C2'	-7.02	96.78	103.10
1	G	16	LEU	CA-CB-CG	6.98	131.35	115.30
1	E	895	ASP	CB-CG-OD1	-6.96	112.03	118.30
2	H	9	DA	O4'-C1'-N9	6.81	112.77	108.00
1	A	483	ALA	N-CA-C	-6.78	92.71	111.00
2	H	10	DA	C5'-C4'-O4'	6.55	121.75	109.30
2	H	5	DA	O5'-P-OP2	-6.44	99.90	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	9	DA	O4'-C1'-C2'	-6.34	100.83	105.90
2	F	5	DA	N1-C6-N6	6.32	122.39	118.60
1	A	16	LEU	CA-CB-CG	6.18	129.50	115.30
2	B	1	DA	C5-C6-N1	-5.97	114.71	117.70
1	G	623	PHE	C-N-CD	5.96	140.92	128.40
2	B	10	DA	O4'-C1'-N9	5.95	112.17	108.00
1	C	279	LYS	C-N-CD	5.91	140.82	128.40
1	G	305	ALA	C-N-CD	5.89	140.77	128.40
2	D	11	DA	O4'-C1'-C2'	-5.89	101.19	105.90
2	B	11	DA	C4'-C3'-C2'	-5.85	97.83	103.10
1	E	895	ASP	CB-CG-OD2	5.84	123.56	118.30
2	B	9	DA	C4'-C3'-C2'	-5.73	97.94	103.10
1	C	201	GLY	C-N-CD	5.70	140.36	128.40
1	G	24	GLU	CB-CA-C	5.64	121.69	110.40
2	B	11	DA	O4'-C1'-C2'	-5.64	101.39	105.90
2	H	11	DA	C1'-O4'-C4'	-5.61	104.49	110.10
2	F	4	DA	C1'-O4'-C4'	-5.56	104.54	110.10
2	F	11	DA	OP1-P-O3'	5.52	117.35	105.20
1	A	541	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	523	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	606	PHE	CG-CD2-CE2	5.50	126.85	120.80
2	D	2	DA	N1-C6-N6	5.49	121.90	118.60
1	C	438	LEU	CB-CG-CD1	-5.49	101.67	111.00
2	B	4	DA	N1-C6-N6	5.48	121.89	118.60
2	F	11	DA	C1'-O4'-C4'	-5.47	104.62	110.10
1	G	279	LYS	C-N-CD	5.47	139.90	128.40
1	A	606	PHE	CZ-CE2-CD2	-5.36	113.67	120.10
2	D	5	DA	O4'-C1'-N9	-5.36	104.25	108.00
1	C	16	LEU	CA-CB-CG	5.33	127.55	115.30
2	B	10	DA	O4'-C4'-C3'	-5.32	102.37	104.50
2	D	10	DA	C8-N9-C4	5.32	107.93	105.80
2	F	10	DA	C4'-C3'-C2'	-5.29	98.34	103.10
1	E	362	PRO	N-CA-CB	-5.26	96.81	102.60
1	G	696	LEU	CA-CB-CG	5.23	127.33	115.30
2	D	11	DA	C1'-O4'-C4'	-5.22	104.88	110.10
2	H	4	DA	C1'-O4'-C4'	-5.21	104.89	110.10
2	D	10	DA	C4'-C3'-C2'	-5.21	98.41	103.10
1	E	16	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	870	MET	CG-SD-CE	-5.19	91.90	100.20
2	B	11	DA	O5'-P-OP2	-5.15	101.06	105.70
2	F	3	DA	N1-C6-N6	5.13	121.68	118.60
1	E	483	ALA	N-CA-C	-5.11	97.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	395	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	482	SER	C-N-CA	5.02	134.24	121.70

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 (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	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.

All (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
1:G:609:LEU:HD12	1:G:609:LEU:H	1.23	1.04
1:A:598:VAL:HA	1:A:601:LEU:HD21	1.40	1.02
1:G:587:ILE:HD11	1:G:657:VAL:HG22	1.03	1.01
1:A:266:PRO:HD2	1:A:355:ARG:NH1	1.77	1.00
1:C:25:ARG:HG2	1:C:25:ARG:HH11	1.23	0.99
1:A:266:PRO:HD2	1:A:355:ARG:HH12	1.24	0.98
1:C:410:ARG:HE	1:C:410:ARG:HA	1.30	0.96
1:G:923:ALA:N	1:G:925:LEU:HD22	1.81	0.94
1:A:601:LEU:HD12	1:A:602:LEU:N	1.82	0.93
1:E:865:GLU:OE1	1:E:865:GLU:N	2.04	0.91
1:G:308:GLY:HA2	4:G:1003:ANP:O3A	1.69	0.91
1:E:832:GLY:HA2	2:F:5:DA:H61	1.35	0.90
1:G:618:LEU:HD13	1:G:657:VAL:CG1	2.03	0.89
1:G:618:LEU:CD1	1:G:657:VAL:CG1	2.49	0.89
1:G:483:ALA:O	1:G:519:TYR:CE1	2.26	0.89
1:G:410:ARG:HG3	1:G:410:ARG:HH11	1.36	0.89
1:G:618:LEU:HD13	1:G:657:VAL:HG12	1.53	0.88
1:G:281:ASN:HD22	1:G:284:GLN:CD	1.77	0.86
1:A:832:GLY:HA2	2:B:5:DA:H61	1.41	0.86
1:G:896:ASN:HD21	1:G:929:THR:HG21	1.39	0.85
1:A:303:ILE:HB	1:A:481:LEU:HD13	1.57	0.85
1:A:865:GLU:HB3	1:A:867:ARG:HH21	1.42	0.83
1:C:410:ARG:CZ	1:C:411:LYS:H	1.92	0.82
1:A:150:HIS:CE1	2:B:11:DA:H5'	2.15	0.82
1:E:284:GLN:OE1	4:E:1003:ANP:H2	1.80	0.82
1:G:924:VAL:O	1:G:925:LEU:HD13	1.80	0.82
1:C:198:MET:HG3	1:C:199:LEU:N	1.94	0.81
1:E:404:THR:HG22	1:E:407:LEU:H	1.44	0.81
1:A:598:VAL:HA	1:A:601:LEU:CD2	2.12	0.80
1:E:363:ARG:CD	1:E:363:ARG:H	1.91	0.80
1:G:841:VAL:C	1:G:843:THR:HG23	2.01	0.80
1:C:506:TRP:HH2	1:C:511:PRO:O	1.63	0.80
1:G:310:GLY:CA	4:G:1003:ANP:O1A	2.30	0.79
1:G:896:ASN:ND2	1:G:929:THR:HG21	1.97	0.79
1:C:410:ARG:HA	1:C:410:ARG:NE	1.97	0.78
1:G:717:GLN:HE22	1:G:726:TRP:H	1.30	0.78
1:G:311:LYS:O	1:G:312:THR:C	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:HIS:CE1	2:H:11:DA:H5'	2.21	0.76
1:C:308:GLY:N	4:C:1003:ANP:O3G	2.16	0.75
1:C:198:MET:HG3	1:C:199:LEU:H	1.52	0.75
1:A:284:GLN:HE22	4:A:1003:ANP:H2	1.52	0.74
1:G:664:GLN:HE22	2:H:4:DA:H5'	1.53	0.74
1:A:694:GLU:HG2	1:A:701:ARG:HH21	1.53	0.74
1:G:281:ASN:ND2	1:G:284:GLN:CD	2.40	0.74
1:C:363:ARG:HB2	1:C:364:SER:HA	1.68	0.73
1:G:899:PRO:HG2	1:G:902:TRP:CD1	2.22	0.73
1:C:833:SER:H	2:D:6:DA:H61	1.34	0.73
1:G:308:GLY:HA2	4:G:1003:ANP:PA	2.28	0.73
1:C:25:ARG:HG2	1:C:25:ARG:NH1	1.97	0.73
1:C:680:VAL:HG13	1:C:743:THR:HG23	1.71	0.73
1:C:150:HIS:CE1	2:D:11:DA:H5'	2.23	0.73
1:A:571:LEU:HD23	1:A:602:LEU:HD21	1.71	0.72
1:G:841:VAL:HG13	1:G:846:ASN:O	1.90	0.71
1:C:216:TRP:HZ3	1:C:438:LEU:HD11	1.56	0.71
1:C:506:TRP:CH2	1:C:511:PRO:O	2.44	0.71
1:C:832:GLY:HA2	2:D:5:DA:H61	1.56	0.71
1:C:266:PRO:O	1:C:355:ARG:NH2	2.22	0.70
1:C:410:ARG:NE	1:C:411:LYS:H	1.88	0.70
1:E:150:HIS:CE1	2:F:11:DA:H5'	2.25	0.70
1:A:23:LYS:NZ	1:A:219:SER:OG	2.24	0.70
1:A:671:ASP:OD1	1:A:701:ARG:NH1	2.24	0.70
1:C:25:ARG:HH11	1:C:25:ARG:CG	2.03	0.70
1:G:841:VAL:O	1:G:843:THR:HG23	1.92	0.69
1:G:609:LEU:HD12	1:G:609:LEU:N	2.01	0.69
1:G:841:VAL:HG22	1:G:846:ASN:O	1.91	0.69
1:G:850:ASP:OD1	1:G:850:ASP:N	2.25	0.69
1:E:363:ARG:H	1:E:363:ARG:HD2	1.58	0.69
1:A:482:SER:OG	1:A:483:ALA:O	2.04	0.69
1:A:410:ARG:O	1:A:411:LYS:HB2	1.94	0.68
1:E:358:ASN:H	1:E:358:ASN:ND2	1.90	0.68
1:E:694:GLU:HG2	1:E:701:ARG:HH21	1.59	0.68
1:G:310:GLY:HA2	4:G:1003:ANP:O1A	1.91	0.68
1:G:313:GLU:OE2	1:G:347:ARG:NH2	2.27	0.68
1:A:303:ILE:HB	1:A:481:LEU:CD1	2.24	0.68
1:G:896:ASN:HD21	1:G:929:THR:CG2	2.06	0.68
1:G:281:ASN:ND2	1:G:284:GLN:OE1	2.27	0.67
1:A:818:PHE:HE2	1:C:114:SER:HG	1.43	0.67
1:A:479:VAL:HG12	1:A:481:LEU:CD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PRO:O	1:A:355:ARG:NH2	2.22	0.67
1:G:925:LEU:HB3	1:G:926:PRO:HD3	1.77	0.67
1:G:935:LEU:HD23	1:G:943:ILE:HD12	1.76	0.67
1:E:85:ILE:HG13	1:E:182:LEU:HD23	1.76	0.66
1:E:919:THR:O	1:E:922:GLY:N	2.26	0.66
1:G:266:PRO:O	1:G:355:ARG:NH2	2.28	0.66
1:G:539:ASP:OD1	1:G:541:LEU:HG	1.96	0.65
1:G:916:GLN:C	1:G:924:VAL:CG1	2.64	0.65
1:G:833:SER:H	2:H:6:DA:H61	1.45	0.65
1:C:113:ARG:NH2	1:C:168:PHE:O	2.29	0.65
1:G:370:LEU:HB3	1:G:425:GLN:HG3	1.79	0.65
1:C:310:GLY:HA2	4:C:1003:ANP:O1A	1.96	0.65
1:G:607:ALA:O	1:G:609:LEU:HG	1.97	0.65
1:G:927:THR:HG22	1:G:928:GLU:H	1.62	0.64
1:G:309:GLU:HA	1:G:309:GLU:OE1	1.96	0.64
1:G:832:GLY:HA2	2:H:5:DA:H61	1.61	0.64
1:A:742:ARG:NH1	1:A:781:ASP:OD1	2.31	0.64
1:A:663:GLU:OE2	1:A:686:ARG:NH1	2.30	0.64
1:A:266:PRO:CD	1:A:355:ARG:HH12	2.05	0.63
1:E:742:ARG:NH1	1:E:781:ASP:OD1	2.31	0.63
1:A:85:ILE:HG13	1:A:182:LEU:HD23	1.79	0.63
1:G:471:LEU:HD22	1:G:476:VAL:HG21	1.80	0.63
1:G:833:SER:N	2:H:6:DA:H61	1.96	0.63
1:A:865:GLU:HB3	1:A:867:ARG:NH2	2.12	0.63
1:G:618:LEU:HD13	1:G:657:VAL:HG11	1.80	0.63
1:G:717:GLN:NE2	1:G:726:TRP:H	1.96	0.63
1:A:429:ALA:HB1	1:A:440:LEU:HD13	1.81	0.63
1:A:502:ARG:NH2	1:A:505:ARG:O	2.28	0.62
1:A:633:ALA:O	1:A:637:ASP:HB2	1.99	0.62
1:C:568:SER:HA	1:C:601:LEU:HD21	1.81	0.62
1:A:265:VAL:HG13	1:A:355:ARG:NH2	2.15	0.62
1:A:864:ARG:HG3	1:A:865:GLU:OE2	1.99	0.62
1:C:281:ASN:HB2	1:C:284:GLN:OE1	2.00	0.62
1:C:363:ARG:HB2	1:C:364:SER:CA	2.29	0.62
1:C:150:HIS:ND1	2:D:11:DA:H5'	2.14	0.62
1:C:23:LYS:HA	1:C:25:ARG:HH12	1.65	0.62
1:C:22:ALA:HB2	1:C:34:LEU:HA	1.81	0.61
1:C:216:TRP:CZ3	1:C:438:LEU:HD11	2.35	0.61
1:E:679:PRO:HG2	1:E:682:LEU:HD12	1.80	0.61
1:G:106:GLU:OE2	1:G:179:ARG:NH2	2.32	0.61
1:G:334:ALA:HB1	1:G:423:ILE:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:652:ARG:HH21	1:E:652:ARG:HB3	1.66	0.61
1:A:680:VAL:HG13	1:A:743:THR:HG23	1.81	0.61
1:E:150:HIS:ND1	2:F:11:DA:H5'	2.16	0.61
1:E:23:LYS:NZ	1:E:219:SER:OG	2.33	0.60
1:G:925:LEU:HB3	1:G:926:PRO:CD	2.31	0.60
1:G:226:GLU:OE2	1:G:250:ARG:NH1	2.33	0.60
1:G:604:GLN:C	1:G:606:PHE:H	2.04	0.60
1:E:160:GLN:NE2	1:G:796:ARG:HD2	2.16	0.60
1:E:729:ARG:NH2	1:G:101:SER:O	2.34	0.60
4:E:1003:ANP:N3B	4:E:1003:ANP:O1A	2.32	0.60
1:G:308:GLY:CA	4:G:1003:ANP:O3A	2.49	0.60
1:E:22:ALA:HB2	1:E:34:LEU:HA	1.82	0.60
1:E:429:ALA:HB1	1:E:440:LEU:HD13	1.84	0.60
1:A:507:ASN:HB2	1:A:510:GLU:HB2	1.84	0.60
1:C:429:ALA:HB1	1:C:440:LEU:HD13	1.83	0.60
1:C:366:THR:HG21	1:C:404:THR:HG22	1.84	0.60
1:G:579:VAL:HG13	1:G:614:PRO:HG3	1.84	0.60
1:E:450:VAL:HG13	1:E:480:LEU:HD12	1.83	0.59
1:C:750:ARG:NH2	1:C:754:PRO:O	2.34	0.59
1:G:673:MET:HE2	1:G:710:LEU:HD13	1.84	0.59
1:C:216:TRP:CD1	2:D:11:DA:H8	2.20	0.59
1:A:378:PRO:HA	1:A:874:ARG:HH22	1.67	0.59
1:C:310:GLY:N	4:C:1003:ANP:O1A	2.35	0.59
2:H:10:DA:H2"	2:H:11:DA:O4'	2.02	0.59
1:E:125:PHE:HB2	1:E:165:LEU:HD13	1.84	0.59
1:E:242:ALA:O	1:E:246:THR:OG1	2.21	0.59
1:G:645:GLN:HG2	1:G:698:ILE:HD13	1.83	0.59
1:E:376:LEU:HD13	1:E:907:TYR:CZ	2.38	0.59
1:G:261:ARG:O	1:G:365:SER:HB3	2.03	0.59
1:G:410:ARG:HH11	1:G:410:ARG:CG	2.10	0.59
1:C:404:THR:HG23	1:C:407:LEU:H	1.68	0.58
1:C:484:THR:HG23	1:C:484:THR:O	2.03	0.58
1:C:867:ARG:HH22	1:C:869:THR:HA	1.67	0.58
1:G:351:TYR:CZ	1:G:355:ARG:HD3	2.39	0.58
1:A:706:LYS:O	1:A:707:GLN:NE2	2.19	0.58
1:G:742:ARG:NH2	1:G:769:TYR:O	2.37	0.57
1:A:334:ALA:HB1	1:A:423:ILE:HA	1.86	0.57
1:E:24:GLU:HG2	1:E:96:ILE:HG21	1.86	0.57
1:E:506:TRP:CH2	1:E:513:PRO:HD3	2.40	0.57
1:C:49:TRP:HA	1:C:53:LEU:HD13	1.85	0.57
1:C:506:TRP:CH2	1:C:513:PRO:HD3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:856:GLU:OE1	1:G:856:GLU:N	2.26	0.57
1:E:696:LEU:HD23	1:E:698:ILE:HD11	1.85	0.56
1:E:893:THR:HG23	1:E:895:ASP:OD1	2.04	0.56
1:A:150:HIS:ND1	2:B:11:DA:H5'	2.20	0.56
1:G:927:THR:HG22	1:G:928:GLU:N	2.19	0.56
1:C:310:GLY:CA	4:C:1003:ANP:O1A	2.54	0.56
1:C:673:MET:HE1	1:C:686:ARG:HB3	1.86	0.56
1:E:20:PHE:CE2	1:E:178:GLN:HG3	2.41	0.56
1:E:334:ALA:HB1	1:E:423:ILE:HA	1.88	0.56
1:E:366:THR:HG21	1:E:404:THR:HB	1.87	0.56
1:E:666:LEU:HG	1:E:668:LEU:HG	1.87	0.56
1:E:20:PHE:HE2	1:E:178:GLN:HG3	1.71	0.56
1:G:305:ALA:O	1:G:311:LYS:CE	2.54	0.56
1:A:567:ARG:O	1:A:570:VAL:HG12	2.05	0.56
1:G:483:ALA:O	1:G:519:TYR:HE1	1.80	0.56
1:E:453:ALA:O	1:E:456:VAL:HG13	2.06	0.56
1:G:916:GLN:C	1:G:924:VAL:HG11	2.26	0.56
1:A:258:ALA:O	1:A:404:THR:HG21	2.05	0.56
1:C:54:SER:OG	1:C:329:PRO:HD2	2.06	0.56
1:C:106:GLU:OE2	1:C:179:ARG:NH2	2.33	0.56
1:A:479:VAL:HG12	1:A:481:LEU:HD22	1.88	0.56
1:C:410:ARG:NH1	1:C:411:LYS:H	2.04	0.56
1:E:586:ALA:HB3	1:E:673:MET:HG3	1.88	0.56
1:G:558:VAL:HG22	1:G:570:VAL:HG21	1.87	0.55
1:G:125:PHE:HB2	1:G:165:LEU:HD13	1.87	0.55
1:G:587:ILE:CD1	1:G:657:VAL:CG2	2.64	0.55
1:C:17:ASP:OD2	1:C:19:ARG:NE	2.35	0.55
1:G:213:LEU:HD13	1:G:415:LEU:HD13	1.88	0.55
1:A:457:ASP:H	1:A:460:MET:HE3	1.71	0.55
1:A:664:GLN:O	1:A:689:ARG:NH2	2.41	0.54
1:E:447:VAL:HG22	1:E:477:PRO:HG2	1.89	0.54
1:G:908:LEU:HA	1:G:911:LEU:HD12	1.88	0.54
1:C:606:PHE:CE2	1:C:614:PRO:HG2	2.43	0.54
1:E:469:ARG:O	1:E:473:THR:HG22	2.08	0.54
1:E:680:VAL:HG13	1:E:743:THR:HG23	1.88	0.54
1:A:539:ASP:OD1	1:A:541:LEU:HG	2.07	0.54
1:G:201:GLY:HA3	1:G:806:ALA:O	2.06	0.54
1:G:745:THR:O	1:G:749:ARG:HG2	2.07	0.54
1:A:702:PRO:HB2	1:A:704:TRP:CD1	2.42	0.54
1:C:844:ALA:N	1:C:845:GLY:HA2	2.21	0.54
1:G:311:LYS:O	1:G:314:ALA:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:O	1:A:473:THR:HG22	2.07	0.54
1:C:363:ARG:NH2	1:C:364:SER:OG	2.40	0.54
1:G:841:VAL:O	1:G:924:VAL:HG23	2.07	0.54
1:A:201:GLY:HA3	1:A:806:ALA:O	2.08	0.54
1:C:18:LEU:HD23	1:C:35:VAL:HG21	1.89	0.54
1:C:505:ARG:HD3	1:C:802:ASP:OD2	2.08	0.54
1:E:558:VAL:HB	1:E:565:LEU:HD13	1.89	0.54
1:A:570:VAL:HG13	1:A:571:LEU:N	2.23	0.53
1:C:351:TYR:CZ	1:C:355:ARG:HD3	2.42	0.53
1:A:399:ASP:OD1	1:A:400:PRO:HD2	2.08	0.53
1:G:499:GLU:HG2	1:G:505:ARG:HA	1.91	0.53
1:E:399:ASP:OD1	1:E:399:ASP:N	2.40	0.53
1:E:300:LEU:HD21	1:E:480:LEU:HD22	1.91	0.53
1:E:594:GLU:O	1:E:598:VAL:HG23	2.08	0.53
1:E:854:THR:OG1	1:E:855:VAL:N	2.41	0.53
1:G:275:PRO:HG2	1:G:354:TYR:OH	2.09	0.53
1:A:22:ALA:HB2	1:A:34:LEU:HA	1.89	0.53
1:A:598:VAL:O	1:A:601:LEU:HG	2.09	0.53
1:C:625:ASN:O	1:C:629:THR:HG23	2.09	0.53
1:C:289:LYS:HB3	1:C:290:HIS:CD2	2.44	0.52
1:G:932:ARG:NH1	1:G:944:PHE:CD2	2.77	0.52
1:A:378:PRO:HA	1:A:874:ARG:NH2	2.24	0.52
1:A:833:SER:H	2:B:6:DA:H61	1.56	0.52
1:G:410:ARG:HG3	1:G:410:ARG:NH1	2.15	0.52
1:G:554:ARG:NH1	1:G:574:GLU:OE2	2.42	0.52
1:C:410:ARG:NE	1:C:410:ARG:CA	2.71	0.52
1:C:473:THR:HG22	1:C:500:GLY:O	2.10	0.52
1:G:354:TYR:HD2	1:G:355:ARG:HG2	1.75	0.52
1:C:247:SER:O	1:C:251:ILE:HD13	2.08	0.52
1:G:678:ALA:HB3	1:G:683:LEU:HD13	1.92	0.52
1:E:895:ASP:OD1	1:E:895:ASP:N	2.25	0.52
1:E:258:ALA:O	1:E:404:THR:HG21	2.09	0.52
1:G:627:GLN:O	1:G:631:ILE:HG13	2.10	0.52
1:G:457:ASP:H	1:G:460:MET:HE3	1.75	0.52
1:A:679:PRO:HD2	1:A:682:LEU:HD12	1.92	0.52
1:A:614:PRO:HB3	1:A:654:ALA:N	2.25	0.52
1:A:619:LEU:HG	1:A:661:VAL:HG21	1.92	0.52
1:C:404:THR:O	1:C:408:MET:HG2	2.10	0.52
1:E:351:TYR:O	1:E:355:ARG:HB2	2.10	0.52
1:E:864:ARG:O	1:E:867:ARG:HG2	2.10	0.52
1:E:310:GLY:HA2	4:E:1003:ANP:O2A	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:679:PRO:HB3	1:E:739:LEU:HD21	1.92	0.51
1:A:602:LEU:HB2	1:A:616:LEU:HD11	1.93	0.51
1:C:630:GLU:O	1:C:634:THR:HG23	2.11	0.51
1:G:113:ARG:HD3	1:G:118:ALA:HB2	1.92	0.51
1:G:634:THR:O	1:G:638:LEU:HG	2.10	0.51
1:G:664:GLN:NE2	2:H:4:DA:H5'	2.22	0.51
1:A:424:ASP:O	1:A:428:MET:HG3	2.09	0.51
1:C:268:ALA:HB1	1:C:272:GLU:HB2	1.93	0.51
1:A:453:ALA:O	1:A:456:VAL:HG13	2.11	0.51
1:A:598:VAL:O	1:A:601:LEU:CD1	2.58	0.51
1:A:601:LEU:HD12	1:A:601:LEU:C	2.30	0.51
1:G:85:ILE:HG13	1:G:182:LEU:HD23	1.92	0.51
1:C:188:ASP:OD1	1:C:192:ARG:NE	2.43	0.51
1:C:486:HIS:CD2	1:C:766:ASP:HA	2.46	0.51
1:E:345:HIS:CD2	1:E:369:LEU:HB2	2.46	0.51
1:A:572:ALA:O	1:A:576:THR:OG1	2.25	0.51
1:C:428:MET:HA	1:C:431:LEU:HD22	1.93	0.50
1:G:925:LEU:O	1:G:926:PRO:C	2.48	0.50
1:E:370:LEU:HD22	1:E:419:ALA:HB1	1.93	0.50
1:G:219:SER:CB	2:H:11:DA:H2"	2.41	0.50
1:A:471:LEU:HD22	1:A:476:VAL:HG21	1.93	0.50
1:A:159:PHE:CE2	1:A:164:PRO:HG3	2.46	0.50
1:G:219:SER:OG	2:H:11:DA:H2"	2.11	0.50
1:A:145:MET:HG3	1:A:208:CYS:HB2	1.94	0.50
1:A:363:ARG:O	1:A:398:ARG:NH2	2.45	0.50
1:C:281:ASN:HB2	1:C:284:GLN:CD	2.31	0.50
1:C:363:ARG:CB	1:C:364:SER:HA	2.38	0.50
1:G:150:HIS:ND1	2:H:11:DA:H5'	2.26	0.50
1:A:865:GLU:CB	1:A:867:ARG:HH21	2.20	0.50
1:C:742:ARG:NH1	1:C:775:ALA:HB2	2.26	0.50
1:G:22:ALA:C	1:G:23:LYS:HG2	2.31	0.50
1:G:847:ARG:C	1:G:848:TRP:CD1	2.85	0.50
1:C:304:THR:HG22	1:C:482:SER:HB3	1.93	0.50
1:C:457:ASP:H	1:C:460:MET:HE3	1.76	0.50
1:C:750:ARG:NH2	1:C:753:ALA:O	2.40	0.50
1:G:837:LEU:HB3	1:G:913:LEU:HD23	1.92	0.50
1:A:576:THR:O	1:A:579:VAL:HG13	2.12	0.50
1:G:90:ARG:NH2	1:G:105:GLY:O	2.33	0.50
1:A:64:SER:HB3	1:A:200:ASP:OD1	2.11	0.49
1:E:201:GLY:HA3	1:E:806:ALA:O	2.12	0.49
1:G:649:ARG:NE	1:G:699:ILE:HD13	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LEU:CD1	1:A:602:LEU:HG	2.42	0.49
1:C:353:ARG:HH22	1:C:399:ASP:CG	2.16	0.49
1:E:261:ARG:O	1:E:365:SER:HB3	2.13	0.49
1:E:430:VAL:HA	1:E:800:ILE:HD13	1.94	0.49
1:G:16:LEU:HD11	1:G:35:VAL:HG21	1.93	0.49
1:G:898:PRO:HB2	1:G:902:TRP:HB2	1.93	0.49
1:G:742:ARG:NH1	1:G:781:ASP:OD2	2.46	0.49
1:A:366:THR:HB	1:A:402:ALA:O	2.12	0.49
1:C:663:GLU:OE2	1:C:686:ARG:NH1	2.42	0.49
1:E:332:PHE:HA	1:E:419:ALA:O	2.13	0.49
1:E:606:PHE:CD2	1:E:614:PRO:HD2	2.48	0.49
1:G:311:LYS:O	1:G:313:GLU:N	2.44	0.49
1:G:553:VAL:HG12	1:G:710:LEU:HD23	1.95	0.49
1:G:691:TRP:CE3	1:G:708:PRO:HD3	2.46	0.49
1:A:665:SER:O	1:A:665:SER:OG	2.29	0.49
1:C:216:TRP:HD1	2:D:11:DA:H2'	1.78	0.49
1:G:604:GLN:C	1:G:606:PHE:N	2.65	0.49
1:A:251:ILE:O	1:A:254:LEU:HB2	2.13	0.49
1:E:844:ALA:N	1:E:845:GLY:HA2	2.26	0.49
1:G:305:ALA:O	1:G:311:LYS:NZ	2.46	0.49
1:A:121:LYS:HE2	1:A:168:PHE:CE1	2.48	0.48
1:A:525:VAL:HG22	1:A:532:VAL:HG22	1.94	0.48
1:C:410:ARG:HH22	1:C:439:ARG:HH22	1.61	0.48
1:G:22:ALA:HB2	1:G:34:LEU:HA	1.95	0.48
1:G:474:LEU:O	1:G:475:ASP:HB2	2.12	0.48
1:A:65:MET:HA	1:A:198:MET:O	2.14	0.48
1:A:625:ASN:O	1:A:629:THR:HG23	2.13	0.48
1:C:637:ASP:O	1:C:643:GLY:HA3	2.12	0.48
1:A:584:CYS:HB3	1:A:639:PHE:CE2	2.47	0.48
1:C:216:TRP:CD1	2:D:11:DA:C8	3.00	0.48
1:C:469:ARG:O	1:C:473:THR:HG23	2.14	0.48
1:E:287:LEU:O	1:E:291:LEU:HB2	2.13	0.48
1:G:604:GLN:O	1:G:606:PHE:N	2.46	0.48
1:E:111:GLU:HB2	1:G:794:LEU:HD11	1.94	0.48
1:G:624:PRO:HB3	1:G:879:ARG:O	2.14	0.48
1:G:23:LYS:NZ	1:G:219:SER:OG	2.46	0.48
1:E:918:VAL:HA	1:E:923:ALA:O	2.13	0.48
1:G:783:GLU:O	1:G:787:GLU:HG3	2.14	0.48
1:A:101:SER:O	1:C:729:ARG:NH2	2.46	0.48
1:C:507:ASN:ND2	1:E:771:ASP:OD1	2.47	0.48
1:C:44:ALA:HA	1:C:251:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:516:GLU:HG3	1:E:534:ARG:NH2	2.29	0.47
1:G:828:ARG:HB2	2:H:5:DA:C2	2.49	0.47
1:A:746:LEU:HD13	1:A:774:LEU:HD11	1.95	0.47
1:C:611:GLU:HA	1:C:612:ASP:HA	1.53	0.47
1:E:132:TYR:HB3	1:E:139:THR:OG1	2.14	0.47
1:G:227:ARG:HD2	1:G:250:ARG:HH11	1.78	0.47
1:A:25:ARG:O	1:A:27:LEU:HG	2.15	0.47
1:A:119:THR:HG23	1:A:123:LEU:HD22	1.97	0.47
1:A:877:VAL:O	1:A:880:THR:OG1	2.28	0.47
1:C:38:SER:HB3	1:C:81:GLY:O	2.14	0.47
1:C:691:TRP:CG	1:C:708:PRO:HB3	2.49	0.47
1:C:742:ARG:NH2	1:C:769:TYR:O	2.47	0.47
1:E:410:ARG:O	1:E:411:LYS:HB2	2.15	0.47
1:E:679:PRO:HG3	1:E:739:LEU:HD21	1.96	0.47
1:E:691:TRP:CG	1:E:708:PRO:HB3	2.49	0.47
1:E:750:ARG:NH2	1:E:754:PRO:O	2.47	0.47
1:G:306:PRO:HG3	1:G:519:TYR:CZ	2.50	0.47
1:G:839:TYR:OH	1:G:847:ARG:NH1	2.48	0.47
1:A:287:LEU:O	1:A:291:LEU:HB2	2.15	0.47
1:A:750:ARG:NH2	1:A:754:PRO:O	2.47	0.47
1:C:410:ARG:O	1:C:411:LYS:HB2	2.14	0.47
1:G:345:HIS:HA	1:G:420:VAL:HG11	1.97	0.47
1:G:554:ARG:NH2	1:G:574:GLU:OE2	2.44	0.47
1:A:706:LYS:HG3	1:A:707:GLN:HG2	1.97	0.47
1:A:828:ARG:HB2	2:B:5:DA:C2	2.49	0.47
4:A:1003:ANP:H2'	4:A:1003:ANP:N3	2.30	0.47
1:C:499:GLU:HG2	1:C:505:ARG:HA	1.97	0.47
1:C:508:ARG:HG2	1:C:508:ARG:HH11	1.79	0.47
1:C:609:LEU:HB2	1:C:613:ALA:HB2	1.96	0.47
1:G:410:ARG:CG	1:G:410:ARG:NH1	2.73	0.47
1:A:338:MET:SD	1:A:373:MET:HG3	2.55	0.47
1:E:367:LEU:HD13	1:E:418:TRP:HB2	1.96	0.47
1:G:252:PRO:HB3	1:G:261:ARG:HH22	1.79	0.47
1:A:601:LEU:HD12	1:A:602:LEU:HG	1.96	0.47
1:E:864:ARG:C	1:E:865:GLU:HG2	2.36	0.47
1:A:679:PRO:HB3	1:A:739:LEU:HD13	1.96	0.47
1:C:306:PRO:HG3	1:C:519:TYR:CZ	2.49	0.47
1:E:541:LEU:HD13	1:E:542:PRO:HD2	1.95	0.47
1:A:16:LEU:HD11	1:A:35:VAL:HG21	1.97	0.46
1:A:696:LEU:HD12	1:A:696:LEU:HA	1.73	0.46
1:G:345:HIS:CD2	1:G:369:LEU:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLN:HE22	4:A:1003:ANP:C2	2.24	0.46
1:A:404:THR:CG2	1:A:407:LEU:H	2.29	0.46
1:E:471:LEU:HB3	1:E:476:VAL:HG22	1.96	0.46
1:G:287:LEU:O	1:G:291:LEU:HB2	2.14	0.46
1:G:300:LEU:HD11	1:G:480:LEU:HD22	1.97	0.46
1:E:694:GLU:HG2	1:E:701:ARG:NH2	2.27	0.46
1:G:24:GLU:O	1:G:27:LEU:HG	2.15	0.46
1:G:44:ALA:HA	1:G:251:ILE:HD13	1.97	0.46
1:G:471:LEU:HB3	1:G:476:VAL:HG22	1.97	0.46
1:A:32:TYR:HD1	1:A:228:LEU:HD13	1.80	0.46
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.78	0.46
1:C:149:HIS:CD2	1:C:150:HIS:CD2	3.04	0.46
1:E:424:ASP:O	1:E:428:MET:HG3	2.15	0.46
1:G:214:ALA:O	1:G:218:VAL:HG22	2.15	0.46
1:G:571:LEU:HD11	1:G:598:VAL:HG13	1.98	0.46
1:C:694:GLU:HG2	1:C:701:ARG:HH21	1.80	0.46
1:A:247:SER:O	1:A:251:ILE:HD12	2.15	0.46
1:A:351:TYR:O	1:A:355:ARG:HB2	2.15	0.46
1:A:479:VAL:HG12	1:A:481:LEU:HD21	1.96	0.46
1:C:844:ALA:H	1:C:845:GLY:HA2	1.81	0.46
1:A:410:ARG:CZ	2:B:10:DA:OP2	2.63	0.46
1:C:470:TRP:O	1:C:474:LEU:HD22	2.14	0.46
1:E:49:TRP:HA	1:E:53:LEU:HD13	1.98	0.46
1:G:916:GLN:O	1:G:924:VAL:HG11	2.16	0.46
1:G:432:ARG:HD3	1:G:815:GLU:O	2.16	0.46
1:E:898:PRO:HB2	1:E:902:TRP:HB2	1.98	0.46
1:G:594:GLU:O	1:G:598:VAL:HG23	2.16	0.46
1:A:16:LEU:HD21	1:A:35:VAL:HG11	1.98	0.45
1:A:98:ILE:HD13	1:A:100:LEU:HD21	1.97	0.45
1:G:789:LEU:HD23	1:G:789:LEU:HA	1.73	0.45
1:C:146:LEU:HD12	1:C:146:LEU:HA	1.86	0.45
1:C:217:LEU:HA	1:C:217:LEU:HD12	1.67	0.45
1:E:358:ASN:ND2	1:E:358:ASN:N	2.59	0.45
1:A:395:LEU:C	1:A:397:HIS:H	2.20	0.45
1:C:848:TRP:CG	1:C:853:CYS:HA	2.51	0.45
1:A:891:GLN:O	1:A:930:GLY:HA2	2.15	0.45
1:G:636:VAL:HG13	1:G:667:ASP:O	2.16	0.45
1:C:678:ALA:HB3	1:C:683:LEU:HD13	1.99	0.45
1:E:162:ARG:H	1:E:162:ARG:NE	2.14	0.45
1:E:558:VAL:HG22	1:E:570:VAL:HG21	1.99	0.45
1:G:332:PHE:HA	1:G:419:ALA:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:587:ILE:CG1	1:G:657:VAL:HG22	2.42	0.45
1:G:630:GLU:O	1:G:634:THR:HG23	2.16	0.45
1:A:602:LEU:HD23	1:A:602:LEU:HA	1.73	0.45
1:C:56:GLY:HA3	1:C:326:THR:O	2.16	0.45
1:C:104:PRO:HD2	1:C:174:HIS:ND1	2.32	0.45
1:E:56:GLY:HA3	1:E:326:THR:O	2.17	0.45
1:E:159:PHE:HB2	1:E:167:GLU:OE1	2.17	0.45
1:G:848:TRP:CE3	1:G:856:GLU:HA	2.52	0.45
1:A:113:ARG:NH2	1:A:168:PHE:O	2.32	0.45
1:A:630:GLU:O	1:A:634:THR:HG23	2.16	0.45
1:E:833:SER:H	2:F:6:DA:H61	1.65	0.45
1:C:83:HIS:HD2	1:C:149:HIS:CD2	2.34	0.45
1:C:198:MET:CG	1:C:199:LEU:N	2.73	0.45
1:C:609:LEU:HD13	1:C:609:LEU:HA	1.81	0.45
1:E:145:MET:CE	1:E:146:LEU:HD13	2.46	0.45
1:G:227:ARG:CD	1:G:250:ARG:HH11	2.30	0.45
1:G:406:TRP:CZ3	1:G:412:ARG:HD3	2.52	0.45
1:G:679:PRO:HG3	1:G:739:LEU:HD13	1.97	0.45
1:A:601:LEU:HD12	1:A:602:LEU:H	1.77	0.45
1:E:252:PRO:HB3	1:E:261:ARG:HH22	1.82	0.45
1:G:587:ILE:HA	1:G:674:ILE:O	2.17	0.44
1:A:367:LEU:HB2	1:A:401:PHE:HB3	2.00	0.44
1:C:285:ALA:O	1:C:289:LYS:HB2	2.18	0.44
1:E:22:ALA:C	1:E:23:LYS:HG2	2.37	0.44
1:E:864:ARG:C	1:E:865:GLU:CG	2.85	0.44
1:E:876:LEU:HD23	1:E:876:LEU:HA	1.82	0.44
1:A:683:LEU:HD12	1:A:683:LEU:HA	1.75	0.44
1:A:794:LEU:HD12	1:A:794:LEU:HA	1.84	0.44
1:A:269:THR:O	1:A:273:SER:OG	2.35	0.44
1:C:71:HIS:NE2	1:C:194:THR:O	2.49	0.44
1:C:132:TYR:CE2	1:C:195:PRO:HB3	2.52	0.44
1:E:241:ARG:HD2	1:E:245:GLU:OE2	2.17	0.44
1:G:174:HIS:HA	1:G:177:LYS:HE2	2.00	0.44
4:G:1003:ANP:O2B	4:G:1003:ANP:H5'2	2.17	0.44
1:C:258:ALA:O	1:C:404:THR:HG21	2.17	0.44
1:C:334:ALA:HB1	1:C:423:ILE:HA	1.98	0.44
1:C:490:ALA:O	1:C:494:VAL:HG13	2.17	0.44
1:G:736:PRO:HB2	1:G:739:LEU:HB2	2.00	0.44
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.84	0.44
1:C:828:ARG:HG3	2:D:5:DA:N3	2.33	0.44
1:G:548:ARG:NH2	1:G:692:ARG:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:LEU:HD12	1:C:123:LEU:HA	1.84	0.44
1:E:630:GLU:O	1:E:634:THR:HG23	2.18	0.44
1:A:627:GLN:O	1:A:631:ILE:HG13	2.17	0.44
1:E:459:TYR:CG	1:E:829:PHE:HB2	2.53	0.44
1:G:757:ILE:HA	1:G:758:PRO:HA	1.73	0.44
1:A:227:ARG:HH11	1:A:227:ARG:HA	1.83	0.43
1:E:335:LEU:HD22	1:E:340:THR:O	2.18	0.43
1:C:696:LEU:HD12	1:C:696:LEU:HA	1.84	0.43
1:G:831:ALA:HB1	1:G:885:MET:HB3	2.00	0.43
1:G:927:THR:O	1:G:933:GLU:HA	2.18	0.43
1:E:635:ILE:HD12	1:E:656:LEU:HD22	1.99	0.43
1:G:315:ALA:HB2	1:G:481:LEU:HD11	2.00	0.43
1:A:241:ARG:HD2	1:A:245:GLU:OE2	2.18	0.43
1:A:839:TYR:CE1	1:A:913:LEU:HB3	2.52	0.43
1:C:34:LEU:O	1:C:38:SER:OG	2.29	0.43
1:G:87:LYS:HE3	1:G:115:HIS:CD2	2.53	0.43
1:C:251:ILE:O	1:C:254:LEU:HB2	2.19	0.43
1:C:265:VAL:HA	1:C:266:PRO:HD3	1.81	0.43
1:C:410:ARG:NE	1:C:411:LYS:N	2.60	0.43
1:E:706:LYS:HB2	1:E:706:LYS:HE3	1.74	0.43
1:E:835:ARG:HE	1:E:835:ARG:HB3	1.43	0.43
1:E:917:ARG:O	1:E:925:LEU:N	2.40	0.43
1:G:410:ARG:HD3	1:G:410:ARG:HA	1.73	0.43
1:A:892:LEU:HD13	1:A:896:ASN:HB3	2.00	0.43
1:E:453:ALA:HB3	1:E:482:SER:HB2	1.99	0.43
1:E:891:GLN:O	1:E:930:GLY:HA2	2.18	0.43
1:G:430:VAL:HG11	1:G:467:LEU:HA	2.00	0.43
1:A:44:ALA:HA	1:A:251:ILE:HG21	2.00	0.43
1:A:83:HIS:HD2	1:A:149:HIS:CD2	2.36	0.43
1:C:671:ASP:OD1	1:C:701:ARG:NH1	2.50	0.43
1:E:284:GLN:OE1	4:E:1003:ANP:C2	2.60	0.43
1:G:78:PHE:CZ	1:G:82:LEU:HD11	2.53	0.43
1:G:486:HIS:CD2	1:G:766:ASP:HA	2.54	0.43
1:G:587:ILE:HD13	1:G:598:VAL:HG11	1.99	0.43
1:A:502:ARG:HG3	1:A:504:ARG:HG3	2.01	0.43
1:A:684:LEU:HD12	1:A:684:LEU:HA	1.90	0.43
1:E:165:LEU:HD12	1:E:165:LEU:HA	1.79	0.43
1:G:122:TRP:CE3	1:G:123:LEU:HD13	2.54	0.43
1:G:279:LYS:HB2	1:G:279:LYS:HE2	1.63	0.43
1:C:201:GLY:HA3	1:C:806:ALA:O	2.19	0.43
1:C:451:ASP:HA	1:C:481:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:438:LEU:HD23	1:G:438:LEU:HA	1.66	0.43
1:G:664:GLN:NE2	2:H:3:DA:O3'	2.52	0.43
1:G:896:ASN:ND2	1:G:929:THR:CG2	2.72	0.43
1:A:833:SER:N	2:B:6:DA:H61	2.17	0.43
1:E:265:VAL:HG22	1:E:355:ARG:HB3	2.01	0.43
1:E:632:THR:O	1:E:636:VAL:HG13	2.19	0.43
1:G:250:ARG:O	1:G:254:LEU:HD13	2.18	0.43
1:G:335:LEU:HD13	1:G:341:ALA:HA	2.00	0.43
1:G:415:LEU:HD21	1:G:438:LEU:HD22	2.01	0.43
1:C:16:LEU:HB3	1:C:181:ALA:HB1	2.00	0.42
1:E:217:LEU:HD12	1:E:217:LEU:HA	1.82	0.42
1:E:326:THR:OG1	1:E:328:ARG:HD2	2.19	0.42
1:G:302:LEU:HB3	1:G:523:LEU:HD22	1.99	0.42
1:G:587:ILE:O	1:G:587:ILE:HG13	2.19	0.42
1:G:847:ARG:C	1:G:848:TRP:CG	2.92	0.42
1:A:335:LEU:HD13	1:A:341:ALA:HA	2.01	0.42
1:C:692:ARG:NH1	4:C:1003:ANP:O2B	2.51	0.42
1:G:287:LEU:HD12	1:G:314:ALA:HB1	2.01	0.42
1:E:150:HIS:HD1	2:F:11:DA:H5'	1.80	0.42
1:E:375:TRP:HB2	1:E:907:TYR:OH	2.20	0.42
1:G:942:LEU:HD12	1:G:942:LEU:HA	1.86	0.42
1:A:621:SER:OG	2:B:3:DA:OP2	2.35	0.42
1:A:694:GLU:HG2	1:A:701:ARG:NH2	2.29	0.42
1:C:679:PRO:CG	1:C:739:LEU:HD13	2.49	0.42
2:D:10:DA:H2"	2:D:11:DA:O4'	2.19	0.42
1:E:864:ARG:HA	1:E:864:ARG:HD2	1.83	0.42
1:A:558:VAL:O	1:A:716:GLU:HG2	2.20	0.42
1:C:680:VAL:HG11	1:C:746:LEU:HD23	2.02	0.42
1:G:48:LEU:HD12	1:G:52:TYR:HB3	2.00	0.42
1:G:227:ARG:NH1	1:G:250:ARG:NH1	2.67	0.42
1:G:787:GLU:O	1:G:791:GLN:HG3	2.20	0.42
1:A:499:GLU:HG2	1:A:505:ARG:HA	2.01	0.42
1:A:849:LEU:HD13	1:A:857:PHE:HA	2.01	0.42
1:C:424:ASP:O	1:C:428:MET:HG3	2.19	0.42
1:E:376:LEU:HD13	1:E:907:TYR:CE2	2.54	0.42
1:E:599:TYR:CE1	1:E:616:LEU:HD13	2.54	0.42
1:G:424:ASP:O	1:G:428:MET:HG3	2.19	0.42
1:G:584:CYS:HB3	1:G:639:PHE:CE2	2.55	0.42
1:G:927:THR:O	1:G:934:TRP:N	2.42	0.42
1:C:228:LEU:HD12	1:C:228:LEU:HA	1.92	0.42
1:C:265:VAL:HG13	1:C:355:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:ARG:HD3	1:C:505:ARG:HH11	1.69	0.42
1:C:839:TYR:CE2	1:C:913:LEU:HB3	2.55	0.42
4:E:1003:ANP:PA	4:E:1003:ANP:O1G	2.77	0.42
1:A:864:ARG:O	1:A:865:GLU:HB2	2.18	0.42
2:B:5:DA:H2"	2:B:6:DA:O5'	2.19	0.42
1:C:201:GLY:O	1:C:810:LEU:HD21	2.20	0.42
1:C:432:ARG:NH1	1:C:812:GLY:O	2.53	0.42
1:G:32:TYR:OH	1:G:40:ASP:OD2	2.27	0.42
1:A:284:GLN:NE2	4:A:1003:ANP:H2	2.29	0.42
1:A:485:LEU:O	1:A:486:HIS:C	2.58	0.42
1:E:14:PRO:HG3	1:E:177:LYS:HD2	2.02	0.42
1:E:541:LEU:HD13	1:E:541:LEU:HA	1.93	0.42
1:E:565:LEU:HD21	1:E:715:PRO:HG3	2.01	0.42
1:E:683:LEU:HD12	1:E:683:LEU:HA	1.93	0.42
1:A:335:LEU:HD11	1:A:344:MET:HG2	2.01	0.41
1:A:404:THR:HG23	1:A:407:LEU:H	1.84	0.41
1:A:554:ARG:NH2	1:A:574:GLU:OE2	2.35	0.41
1:A:893:THR:OG1	1:A:895:ASP:OD1	2.21	0.41
1:C:765:VAL:O	1:C:768:VAL:HG12	2.20	0.41
1:C:835:ARG:NH2	1:C:882:PRO:HD3	2.35	0.41
1:C:839:TYR:CE1	1:C:847:ARG:HD2	2.54	0.41
1:C:850:ASP:N	1:C:850:ASP:OD1	2.52	0.41
1:E:146:LEU:HD12	1:E:146:LEU:HA	1.76	0.41
1:G:100:LEU:HD13	1:G:175:TRP:CZ2	2.55	0.41
1:A:47:VAL:HG11	1:A:251:ILE:HG22	2.02	0.41
1:E:159:PHE:CE2	1:E:164:PRO:HG3	2.55	0.41
1:G:24:GLU:O	1:G:27:LEU:HB2	2.18	0.41
1:G:255:LEU:HA	1:G:255:LEU:HD23	1.80	0.41
1:A:378:PRO:HG3	1:A:874:ARG:CZ	2.50	0.41
1:A:898:PRO:HA	1:A:913:LEU:HD11	2.02	0.41
1:C:287:LEU:O	1:C:291:LEU:HB2	2.20	0.41
1:C:691:TRP:CE2	1:C:701:ARG:HD2	2.55	0.41
1:C:839:TYR:CZ	1:C:915:PRO:HB3	2.54	0.41
1:C:898:PRO:HA	1:C:899:PRO:HD3	1.95	0.41
1:G:471:LEU:HD22	1:G:476:VAL:CG2	2.47	0.41
1:G:649:ARG:HG2	1:G:650:PRO:HD2	2.01	0.41
1:A:226:GLU:OE1	1:A:227:ARG:HD2	2.20	0.41
1:A:850:ASP:OD1	1:A:850:ASP:N	2.53	0.41
1:C:377:ASN:HA	1:C:378:PRO:HD3	1.87	0.41
1:C:491:ASN:OD1	1:C:513:PRO:HD2	2.21	0.41
1:E:377:ASN:HA	1:E:378:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:843:THR:OG1	1:G:845:GLY:O	2.36	0.41
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.88	0.41
1:A:495:LYS:NZ	1:A:512:GLN:OE1	2.52	0.41
1:A:679:PRO:CG	1:A:739:LEU:HD13	2.50	0.41
1:C:366:THR:HG23	1:C:407:LEU:HD12	2.03	0.41
1:E:691:TRP:HB3	1:E:694:GLU:HG3	2.01	0.41
1:A:395:LEU:HD13	1:A:398:ARG:NH1	2.36	0.41
1:A:670:VAL:HG21	1:A:673:MET:HG3	2.02	0.41
1:A:717:GLN:OE1	1:A:726:TRP:N	2.40	0.41
1:A:789:LEU:HD23	1:A:789:LEU:HA	1.70	0.41
1:G:848:TRP:HB3	1:G:853:CYS:HA	2.02	0.41
1:A:85:ILE:HD13	1:A:122:TRP:CZ3	2.56	0.41
1:A:265:VAL:HA	1:A:266:PRO:HD3	1.85	0.41
1:A:729:ARG:HA	1:A:729:ARG:HD3	1.81	0.41
1:C:410:ARG:CZ	1:C:411:LYS:N	2.73	0.41
1:C:549:LYS:HA	1:C:550:PRO:HD2	1.90	0.41
1:E:172:SER:HA	1:E:173:PRO:HD3	1.98	0.41
1:G:24:GLU:OE1	1:G:25:ARG:CA	2.69	0.41
1:G:649:ARG:CZ	1:G:699:ILE:HD13	2.50	0.41
1:A:275:PRO:HG3	1:A:354:TYR:CZ	2.55	0.41
1:A:481:LEU:HD22	1:A:481:LEU:N	2.35	0.41
1:A:691:TRP:HA	1:A:701:ARG:NH2	2.36	0.41
1:E:677:LEU:HD11	1:E:743:THR:HG22	2.03	0.41
1:E:748:ARG:HA	1:E:748:ARG:HD3	1.83	0.41
1:G:240:LEU:HD23	1:G:240:LEU:HA	1.91	0.41
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.97	0.41
1:A:479:VAL:CG1	1:A:481:LEU:HD21	2.51	0.41
1:A:601:LEU:HG	1:A:601:LEU:H	1.77	0.41
1:A:641:LYS:HE3	1:A:696:LEU:HD21	2.02	0.41
1:C:625:ASN:OD1	1:C:835:ARG:NH2	2.54	0.41
4:C:1003:ANP:PA	4:C:1003:ANP:O2G	2.79	0.41
1:E:355:ARG:HH11	1:E:355:ARG:HD2	1.73	0.41
1:G:227:ARG:HD2	1:G:250:ARG:NH1	2.36	0.41
1:G:575:LEU:HD23	1:G:575:LEU:HA	1.92	0.41
1:G:673:MET:HE2	1:G:710:LEU:CD1	2.50	0.41
1:G:935:LEU:O	1:G:942:LEU:HD12	2.20	0.41
4:G:1003:ANP:O2B	4:G:1003:ANP:C5'	2.69	0.41
1:A:395:LEU:HD13	1:A:398:ARG:HH12	1.86	0.41
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.90	0.41
1:C:85:ILE:HG13	1:C:182:LEU:HD23	2.03	0.41
1:C:219:SER:OG	2:D:11:DA:H2"	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:693:HIS:HB3	1:E:696:LEU:HD22	2.02	0.41
1:C:335:LEU:HD11	1:C:344:MET:HG2	2.02	0.40
1:E:265:VAL:HA	1:E:266:PRO:HD3	1.92	0.40
1:E:580:LYS:HD3	1:E:580:LYS:HA	1.89	0.40
1:E:698:ILE:H	1:E:698:ILE:HG13	1.33	0.40
1:G:848:TRP:CZ3	1:G:856:GLU:HA	2.56	0.40
1:A:557:ASP:HB3	1:A:716:GLU:HB3	2.03	0.40
1:C:526:ASP:OD2	1:C:529:ILE:HG12	2.21	0.40
1:E:137:LEU:HD21	1:E:808:ASP:HB3	2.03	0.40
1:E:315:ALA:CB	1:E:481:LEU:HD21	2.51	0.40
1:E:742:ARG:HH11	1:E:742:ARG:HD2	1.73	0.40
1:A:377:ASN:HA	1:A:378:PRO:HD3	1.89	0.40
1:C:269:THR:OG1	1:C:272:GLU:HG3	2.21	0.40
1:C:684:LEU:HD12	1:C:684:LEU:HA	1.95	0.40
1:E:367:LEU:HD13	1:E:418:TRP:CB	2.52	0.40
2:F:5:DA:H2"	2:F:6:DA:O5'	2.22	0.40
1:G:473:THR:HG21	1:G:803:PRO:HG2	2.03	0.40
1:C:679:PRO:HG3	1:C:739:LEU:HD13	2.03	0.40
1:E:599:TYR:CD1	1:E:616:LEU:HD13	2.57	0.40
1:E:638:LEU:HD22	1:E:650:PRO:HD3	2.03	0.40
1:A:724:ALA:HA	1:A:725:PRO:HD3	1.95	0.40
1:E:407:LEU:HD23	1:E:407:LEU:HA	1.83	0.40
1:E:649:ARG:HA	1:E:650:PRO:HD2	1.92	0.40
1:G:48:LEU:HD12	1:G:52:TYR:CB	2.51	0.40
1:G:98:ILE:HG23	1:G:100:LEU:HG	2.02	0.40
1:G:576:THR:HB	1:G:577:PRO:HD3	2.03	0.40
1:G:683:LEU:HD12	1:G:683:LEU:HA	1.95	0.40

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	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 (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	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

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	25	ARG
1	A	28	ARG
1	A	35	VAL
1	A	48	LEU
1	A	64	SER
1	A	88	LEU
1	A	121	LYS

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Mol	Chain	Res	Type
1	A	123	LEU
1	A	127	LEU
1	A	137	LEU
1	A	146	LEU
1	A	165	LEU
1	A	186	VAL
1	A	198	MET
1	A	217	LEU
1	A	253	SER
1	A	254	LEU
1	A	264	THR
1	A	273	SER
1	A	278	SER
1	A	283	LEU
1	A	293	CYS
1	A	304	THR
1	A	335	LEU
1	A	366	THR
1	A	367	LEU
1	A	375	TRP
1	A	399	ASP
1	A	420	VAL
1	A	431	LEU
1	A	438	LEU
1	A	440	LEU
1	A	443	LEU
1	A	450	VAL
1	A	457	ASP
1	A	464	LEU
1	A	473	THR
1	A	474	LEU
1	A	480	LEU
1	A	494	VAL
1	A	504	ARG
1	A	506	TRP
1	A	509	SER
1	A	518	SER
1	A	528	ARG
1	A	531	LYS
1	A	541	LEU
1	A	568	SER
1	A	569	THR

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Mol	Chain	Res	Type
1	A	571	LEU
1	A	579	VAL
1	A	600	ASP
1	A	616	LEU
1	A	634	THR
1	A	635	ILE
1	A	673	MET
1	A	683	LEU
1	A	684	LEU
1	A	696	LEU
1	A	730	SER
1	A	739	LEU
1	A	763	GLN
1	A	816	PHE
1	A	818	PHE
1	A	824	VAL
1	A	842	ASP
1	A	843	THR
1	A	846	ASN
1	A	869	THR
1	A	870	MET
1	A	879	ARG
1	A	920	ASP
1	C	16	LEU
1	C	25	ARG
1	C	28	ARG
1	C	35	VAL
1	C	48	LEU
1	C	54	SER
1	C	88	LEU
1	C	91	GLU
1	C	123	LEU
1	C	127	LEU
1	C	137	LEU
1	C	146	LEU
1	C	158	SER
1	C	165	LEU
1	C	194	THR
1	C	198	MET
1	C	217	LEU
1	C	265	VAL
1	C	271	THR

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Mol	Chain	Res	Type
1	C	278	SER
1	C	281	ASN
1	C	283	LEU
1	C	289	LYS
1	C	291	LEU
1	C	335	LEU
1	C	356	VAL
1	C	357	GLU
1	C	363	ARG
1	C	364	SER
1	C	366	THR
1	C	367	LEU
1	C	410	ARG
1	C	420	VAL
1	C	431	LEU
1	C	438	LEU
1	C	440	LEU
1	C	443	LEU
1	C	448	VAL
1	C	450	VAL
1	C	464	LEU
1	C	474	LEU
1	C	476	VAL
1	C	480	LEU
1	C	494	VAL
1	C	504	ARG
1	C	507	ASN
1	C	528	ARG
1	C	536	SER
1	C	569	THR
1	C	574	GLU
1	C	609	LEU
1	C	616	LEU
1	C	629	THR
1	C	634	THR
1	C	635	ILE
1	C	661	VAL
1	C	665	SER
1	C	680	VAL
1	C	683	LEU
1	C	684	LEU
1	C	690	CYS

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Mol	Chain	Res	Type
1	C	696	LEU
1	C	706	LYS
1	C	729	ARG
1	C	734	VAL
1	C	739	LEU
1	C	751	ASN
1	C	763	GLN
1	C	804	ASP
1	C	817	SER
1	C	824	VAL
1	C	847	ARG
1	C	849	LEU
1	C	881	ILE
1	C	918	VAL
1	C	925	LEU
1	C	944	PHE
1	E	16	LEU
1	E	23	LYS
1	E	35	VAL
1	E	48	LEU
1	E	64	SER
1	E	121	LYS
1	E	123	LEU
1	E	127	LEU
1	E	137	LEU
1	E	146	LEU
1	E	162	ARG
1	E	165	LEU
1	E	186	VAL
1	E	217	LEU
1	E	228	LEU
1	E	246	THR
1	E	248	LEU
1	E	250	ARG
1	E	254	LEU
1	E	265	VAL
1	E	271	THR
1	E	277	LEU
1	E	278	SER
1	E	279	LYS
1	E	283	LEU
1	E	296	THR

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Mol	Chain	Res	Type
1	E	304	THR
1	E	355	ARG
1	E	356	VAL
1	E	358	ASN
1	E	362	PRO
1	E	363	ARG
1	E	366	THR
1	E	367	LEU
1	E	370	LEU
1	E	375	TRP
1	E	399	ASP
1	E	404	THR
1	E	410	ARG
1	E	420	VAL
1	E	431	LEU
1	E	438	LEU
1	E	440	LEU
1	E	443	LEU
1	E	450	VAL
1	E	464	LEU
1	E	473	THR
1	E	474	LEU
1	E	480	LEU
1	E	518	SER
1	E	528	ARG
1	E	548	ARG
1	E	553	VAL
1	E	565	LEU
1	E	576	THR
1	E	579	VAL
1	E	609	LEU
1	E	616	LEU
1	E	635	ILE
1	E	636	VAL
1	E	652	ARG
1	E	662	VAL
1	E	680	VAL
1	E	681	SER
1	E	684	LEU
1	E	698	ILE
1	E	703	GLN
1	E	729	ARG

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Mol	Chain	Res	Type
1	E	734	VAL
1	E	768	VAL
1	E	782	MET
1	E	789	LEU
1	E	834	VAL
1	E	835	ARG
1	E	843	THR
1	E	849	LEU
1	E	864	ARG
1	E	865	GLU
1	E	869	THR
1	E	881	ILE
1	E	918	VAL
1	E	928	GLU
1	E	944	PHE
1	G	16	LEU
1	G	24	GLU
1	G	28	ARG
1	G	35	VAL
1	G	48	LEU
1	G	70	GLU
1	G	88	LEU
1	G	112	GLN
1	G	121	LYS
1	G	123	LEU
1	G	127	LEU
1	G	146	LEU
1	G	158	SER
1	G	162	ARG
1	G	165	LEU
1	G	186	VAL
1	G	217	LEU
1	G	228	LEU
1	G	241	ARG
1	G	264	THR
1	G	265	VAL
1	G	271	THR
1	G	277	LEU
1	G	278	SER
1	G	283	LEU
1	G	335	LEU
1	G	365	SER

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Mol	Chain	Res	Type
1	G	366	THR
1	G	367	LEU
1	G	370	LEU
1	G	375	TRP
1	G	410	ARG
1	G	411	LYS
1	G	420	VAL
1	G	431	LEU
1	G	438	LEU
1	G	440	LEU
1	G	443	LEU
1	G	464	LEU
1	G	473	THR
1	G	474	LEU
1	G	476	VAL
1	G	480	LEU
1	G	481	LEU
1	G	509	SER
1	G	523	LEU
1	G	546	THR
1	G	548	ARG
1	G	553	VAL
1	G	574	GLU
1	G	578	LEU
1	G	579	VAL
1	G	580	LYS
1	G	602	LEU
1	G	609	LEU
1	G	616	LEU
1	G	626	ARG
1	G	635	ILE
1	G	652	ARG
1	G	657	VAL
1	G	664	GLN
1	G	673	MET
1	G	684	LEU
1	G	699	ILE
1	G	729	ARG
1	G	734	VAL
1	G	739	LEU
1	G	751	ASN
1	G	756	GLN

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Mol	Chain	Res	Type
1	G	789	LEU
1	G	804	ASP
1	G	816	PHE
1	G	833	SER
1	G	839	TYR
1	G	843	THR
1	G	847	ARG
1	G	854	THR
1	G	881	ILE
1	G	925	LEU
1	G	928	GLU
1	G	939	CYS
1	G	944	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	290	HIS
1	E	358	ASN
1	G	281	ASN
1	G	664	GLN
1	G	717	GLN
1	G	811	ASN

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 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

All (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
4	E	1003	ANP	PG-O2G	-3.36	1.47	1.56
4	E	1003	ANP	PB-O3A	-3.20	1.55	1.59
4	C	1003	ANP	PB-O2B	-3.18	1.48	1.56
4	A	1003	ANP	PG-O1G	3.18	1.51	1.46
4	G	1003	ANP	PG-O2G	-3.15	1.48	1.56
4	A	1003	ANP	PB-O1B	3.11	1.51	1.46
4	G	1003	ANP	PG-N3B	3.11	1.71	1.63
4	E	1003	ANP	PG-N3B	3.06	1.71	1.63
4	G	1003	ANP	PG-O1G	3.01	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	ANP	O4'-C4'	-2.99	1.38	1.45
4	C	1003	ANP	PG-O2G	-2.96	1.48	1.56
4	G	1003	ANP	C2'-C3'	-2.94	1.45	1.53
4	A	1003	ANP	PG-N3B	2.92	1.71	1.63
4	G	1003	ANP	C5-N7	-2.91	1.29	1.39
4	E	1003	ANP	O4'-C4'	-2.82	1.38	1.45
4	C	1003	ANP	PG-O3G	-2.81	1.49	1.56
4	C	1003	ANP	C3'-C4'	-2.81	1.45	1.53
4	C	1003	ANP	O4'-C1'	-2.75	1.37	1.41
4	E	1003	ANP	PG-O3G	-2.75	1.49	1.56
4	C	1003	ANP	C5-N7	-2.59	1.30	1.39
4	C	1003	ANP	PB-O3A	-2.52	1.55	1.59
4	E	1003	ANP	PA-O2A	-2.49	1.43	1.55
4	G	1003	ANP	C2-N3	2.48	1.36	1.32
4	C	1003	ANP	PB-O1B	2.46	1.50	1.46
4	C	1003	ANP	C4-N3	-2.37	1.32	1.35
4	G	1003	ANP	PB-N3B	2.27	1.69	1.63
4	G	1003	ANP	C2'-C1'	-2.22	1.50	1.53
4	E	1003	ANP	C5-N7	-2.22	1.31	1.39
4	A	1003	ANP	PB-N3B	2.08	1.68	1.63
4	E	1003	ANP	PB-N3B	2.03	1.68	1.63
4	G	1003	ANP	O4'-C4'	-2.02	1.40	1.45

All (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
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
4	E	1003	ANP	PB-O3A-PA	-6.18	110.86	132.62
4	G	1003	ANP	C5-C6-N6	-6.03	111.18	120.35
4	G	1003	ANP	N6-C6-N1	5.79	130.60	118.57
4	C	1003	ANP	O1G-PG-N3B	-5.32	103.94	111.77
4	G	1003	ANP	O1B-PB-N3B	-4.54	105.09	111.77
4	C	1003	ANP	PB-O3A-PA	-4.28	117.55	132.62
4	C	1003	ANP	O2G-PG-O3G	4.17	118.75	107.64
4	G	1003	ANP	O2'-C2'-C3'	-4.12	98.50	111.82
4	G	1003	ANP	O5'-C5'-C4'	3.88	122.34	108.99
4	G	1003	ANP	N3-C2-N1	-3.86	122.65	128.68
4	C	1003	ANP	C4-C5-N7	-3.77	105.47	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1003	ANP	O3A-PB-N3B	-3.70	96.33	106.59
4	C	1003	ANP	O4'-C1'-C2'	-3.48	101.85	106.93
4	E	1003	ANP	O2B-PB-O3A	3.28	115.58	104.64
4	E	1003	ANP	C1'-N9-C4	3.25	132.35	126.64
4	E	1003	ANP	C2'-C3'-C4'	3.15	108.77	102.64
4	G	1003	ANP	O2B-PB-O3A	3.07	114.89	104.64
4	C	1003	ANP	O4'-C4'-C3'	-2.93	99.32	105.11
4	G	1003	ANP	O3G-PG-O1G	2.82	120.54	113.45
4	G	1003	ANP	O2G-PG-O3G	2.69	114.80	107.64
4	E	1003	ANP	C3'-C2'-C1'	-2.64	97.00	100.98
4	E	1003	ANP	O3'-C3'-C2'	-2.61	103.37	111.82
4	G	1003	ANP	C1'-N9-C4	2.46	130.97	126.64
4	C	1003	ANP	O3'-C3'-C4'	-2.40	104.10	111.05
4	C	1003	ANP	N3-C2-N1	-2.40	124.93	128.68
4	C	1003	ANP	O2'-C2'-C3'	-2.37	104.17	111.82
4	A	1003	ANP	C5-C6-N6	2.35	123.93	120.35
4	G	1003	ANP	O2B-PB-O1B	2.32	114.78	109.92
4	C	1003	ANP	C5'-C4'-C3'	-2.18	107.00	115.18
4	C	1003	ANP	C3'-C2'-C1'	2.12	104.17	100.98
4	E	1003	ANP	O4'-C1'-C2'	-2.10	103.85	106.93
4	C	1003	ANP	O3'-C3'-C2'	-2.10	105.03	111.82
4	A	1003	ANP	PB-O3A-PA	-2.05	125.39	132.62
4	G	1003	ANP	O4'-C1'-C2'	-2.04	103.94	106.93

There are no chirality outliers.

All (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'
4	E	1003	ANP	PB-N3B-PG-O1G
4	E	1003	ANP	C5'-O5'-PA-O1A
4	E	1003	ANP	C5'-O5'-PA-O2A
4	E	1003	ANP	O4'-C4'-C5'-O5'
4	E	1003	ANP	C3'-C4'-C5'-O5'
4	G	1003	ANP	PB-N3B-PG-O1G
4	G	1003	ANP	PA-O3A-PB-O1B
4	G	1003	ANP	PA-O3A-PB-O2B
4	C	1003	ANP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	1003	ANP	O4'-C4'-C5'-O5'
4	A	1003	ANP	C3'-C4'-C5'-O5'
4	A	1003	ANP	PB-O3A-PA-O1A
4	G	1003	ANP	PB-O3A-PA-O5'
4	C	1003	ANP	C5'-O5'-PA-O3A
4	A	1003	ANP	PG-N3B-PB-O3A
4	G	1003	ANP	C4'-C5'-O5'-PA
4	C	1003	ANP	C4'-C5'-O5'-PA
4	A	1003	ANP	PB-O3A-PA-O2A
4	G	1003	ANP	PB-O3A-PA-O1A
4	G	1003	ANP	PB-O3A-PA-O2A
4	E	1003	ANP	C5'-O5'-PA-O3A
4	C	1003	ANP	C5'-O5'-PA-O1A

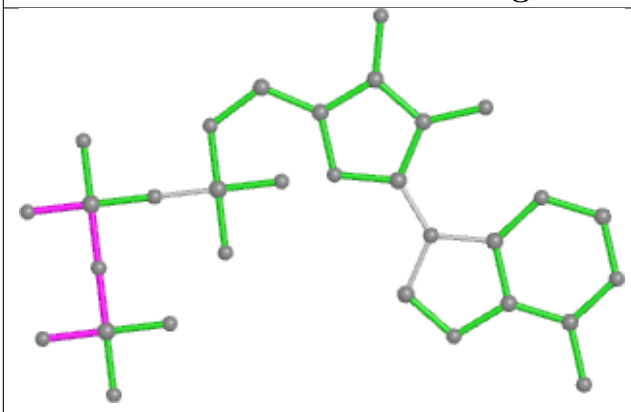
There are no ring outliers.

4 monomers are involved in 23 short contacts:

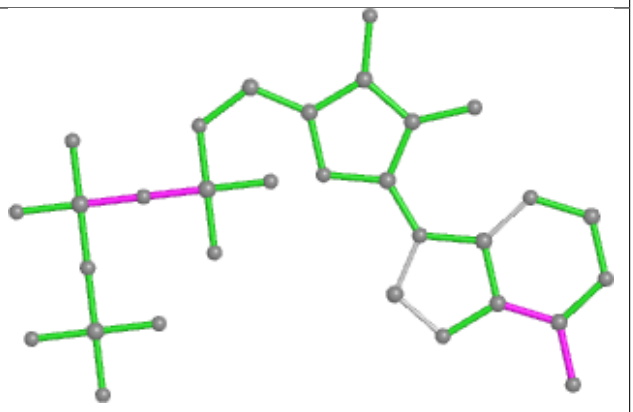
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	ANP	4	0
4	C	1003	ANP	6	0
4	G	1003	ANP	8	0
4	E	1003	ANP	5	0

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.

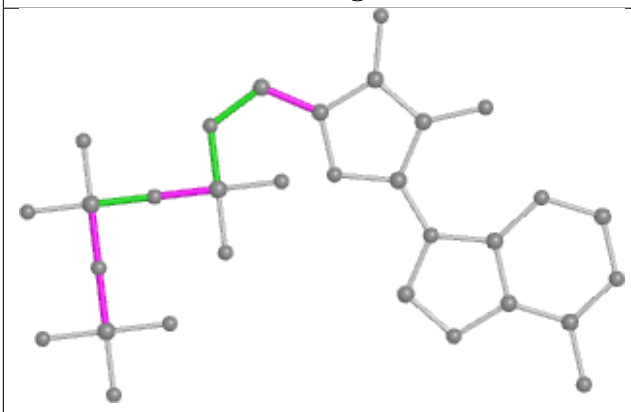
Ligand ANP A 1003



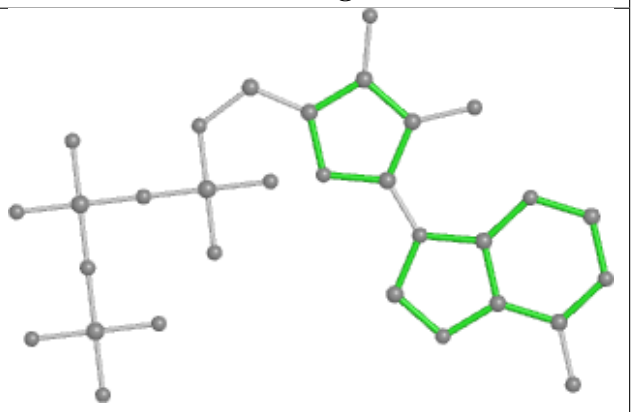
Bond lengths



Bond angles

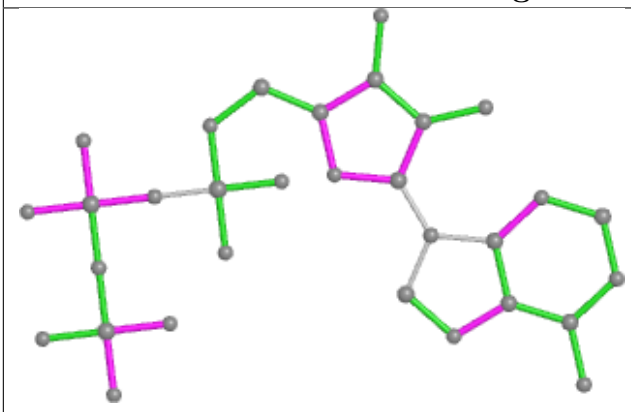


Torsions

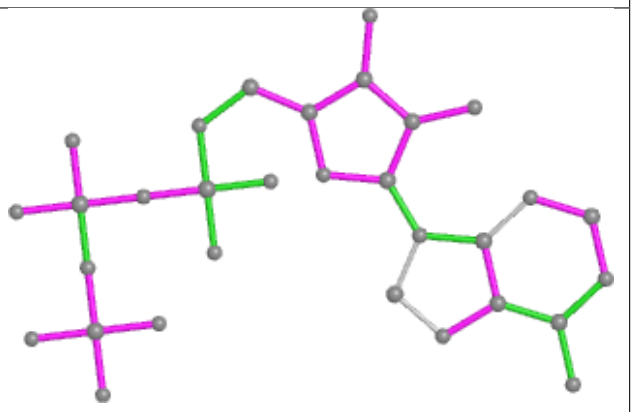


Rings

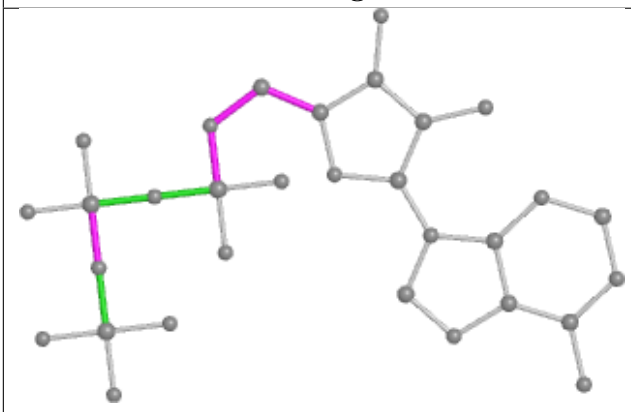
Ligand ANP C 1003



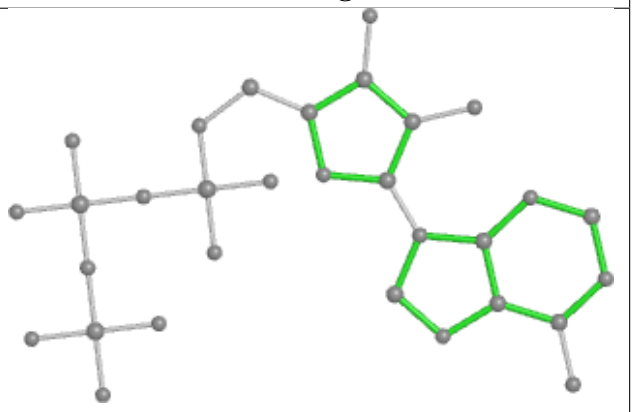
Bond lengths



Bond angles

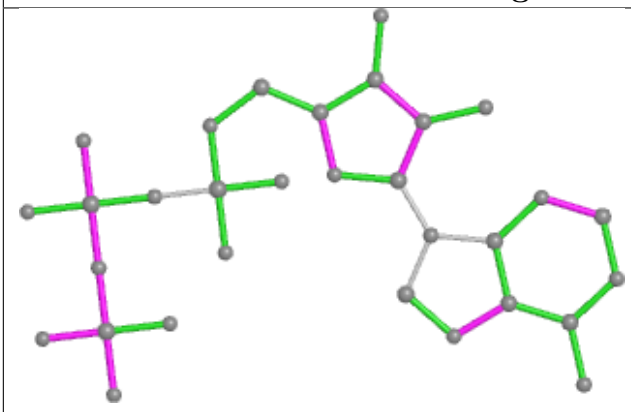


Torsions

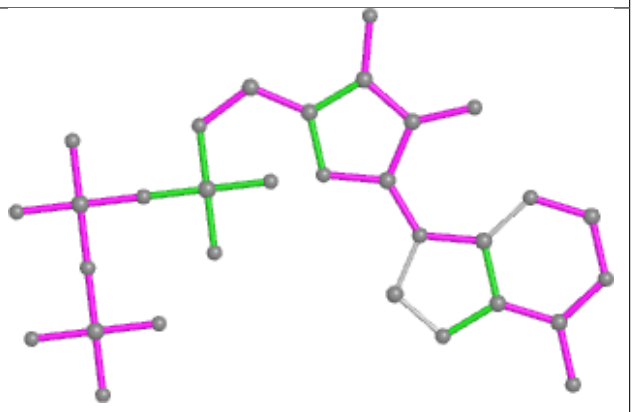


Rings

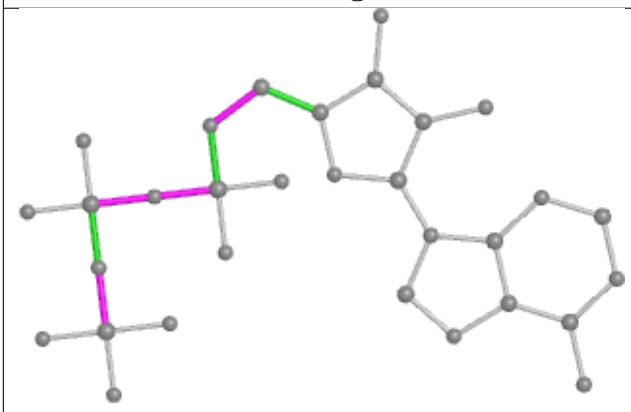
Ligand ANP G 1003



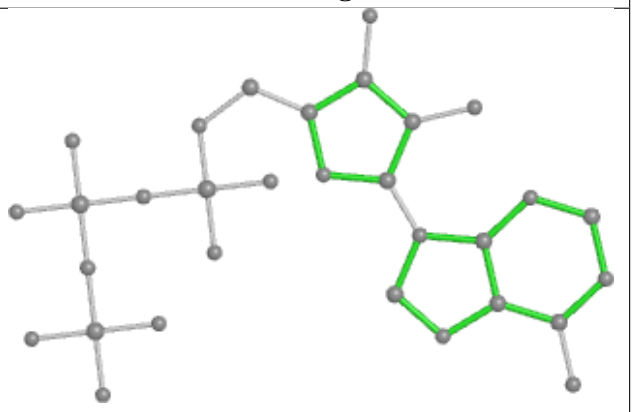
Bond lengths



Bond angles

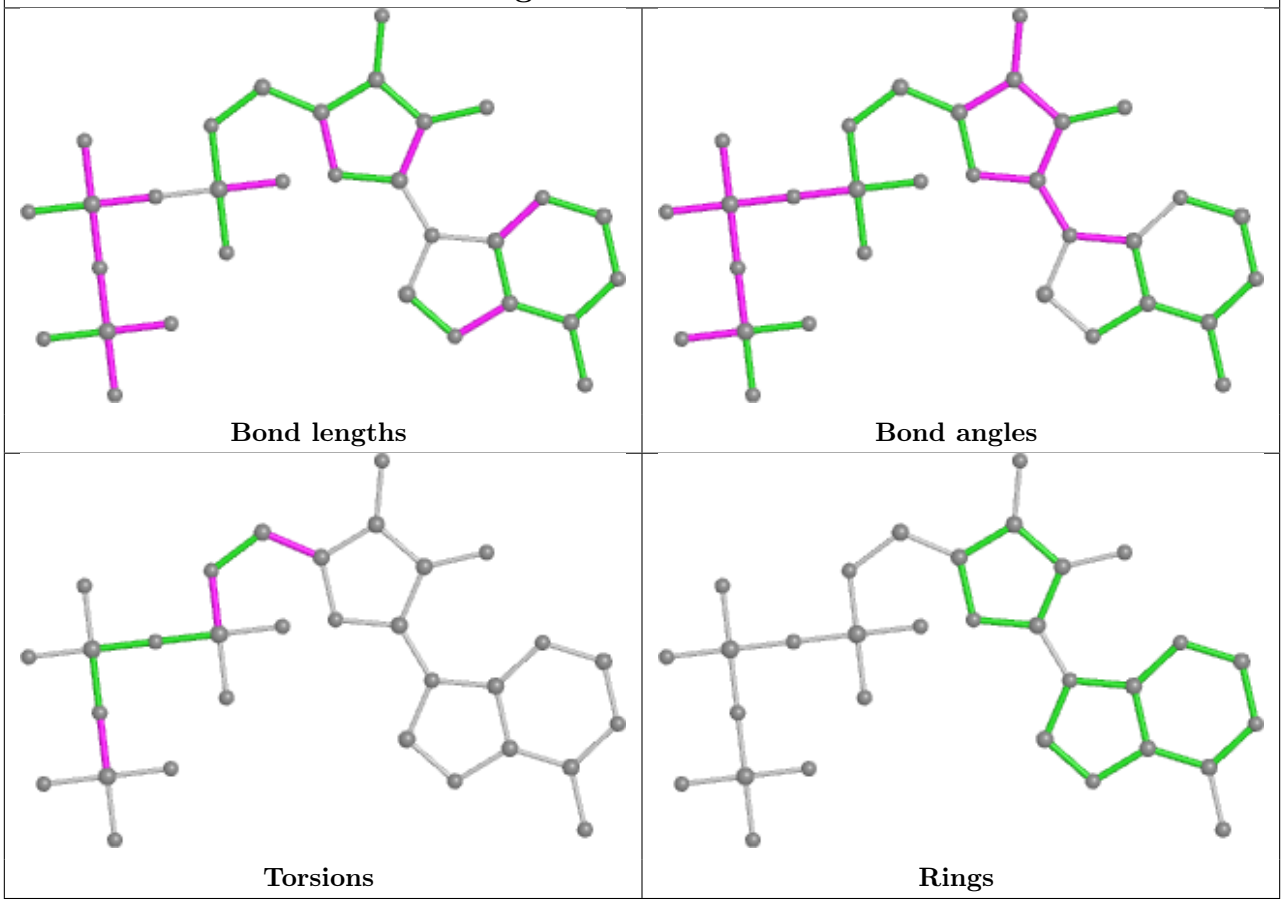


Torsions



Rings

Ligand ANP E 1003



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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

All (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
1	G	903	ARG	2.9
1	E	847	ARG	2.9
1	A	857	PHE	2.8
1	G	843	THR	2.7
1	G	778	LEU	2.7
1	G	609	LEU	2.6
1	G	565	LEU	2.6
2	B	9	DA	2.5
1	G	607	ALA	2.5
2	F	9	DA	2.5
1	E	904	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	920	ASP	2.4
1	A	922	GLY	2.4
1	A	863	GLY	2.3
1	A	867	ARG	2.3
1	A	613	ALA	2.2
1	A	849	LEU	2.2
1	G	267	PRO	2.2
1	C	865	GLU	2.2
1	A	823	HIS	2.2
1	E	866	GLY	2.1
1	G	358	ASN	2.1
1	A	861	GLY	2.1
1	E	922	GLY	2.1
1	A	841	VAL	2.0
1	A	859	GLU	2.0
1	A	870	MET	2.0
1	G	864	ARG	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 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, 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

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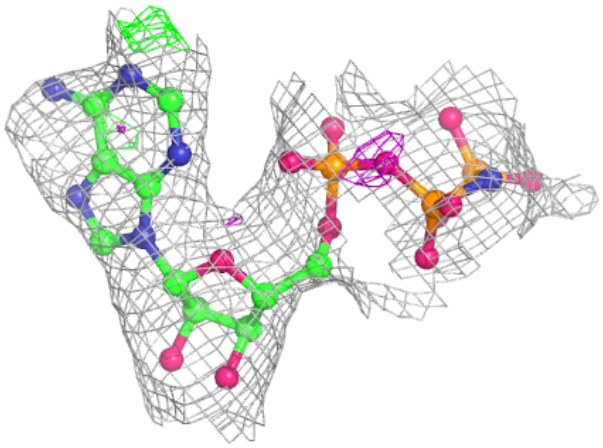
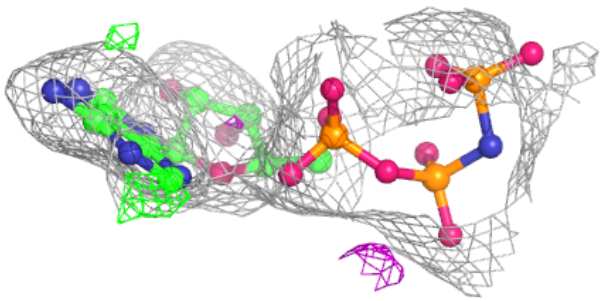
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE	G	1001	1/1	0.99	0.16	34,34,34,34	0
3	FE	G	1002	1/1	0.99	0.16	31,31,31,31	0
3	FE	A	1001	1/1	0.99	0.17	28,28,28,28	0
3	FE	A	1002	1/1	0.99	0.16	24,24,24,24	0
3	FE	C	1001	1/1	0.99	0.15	27,27,27,27	0
3	FE	C	1002	1/1	0.99	0.15	27,27,27,27	0

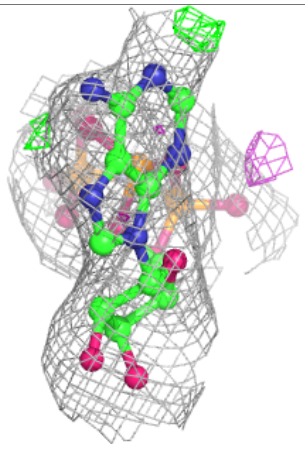
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

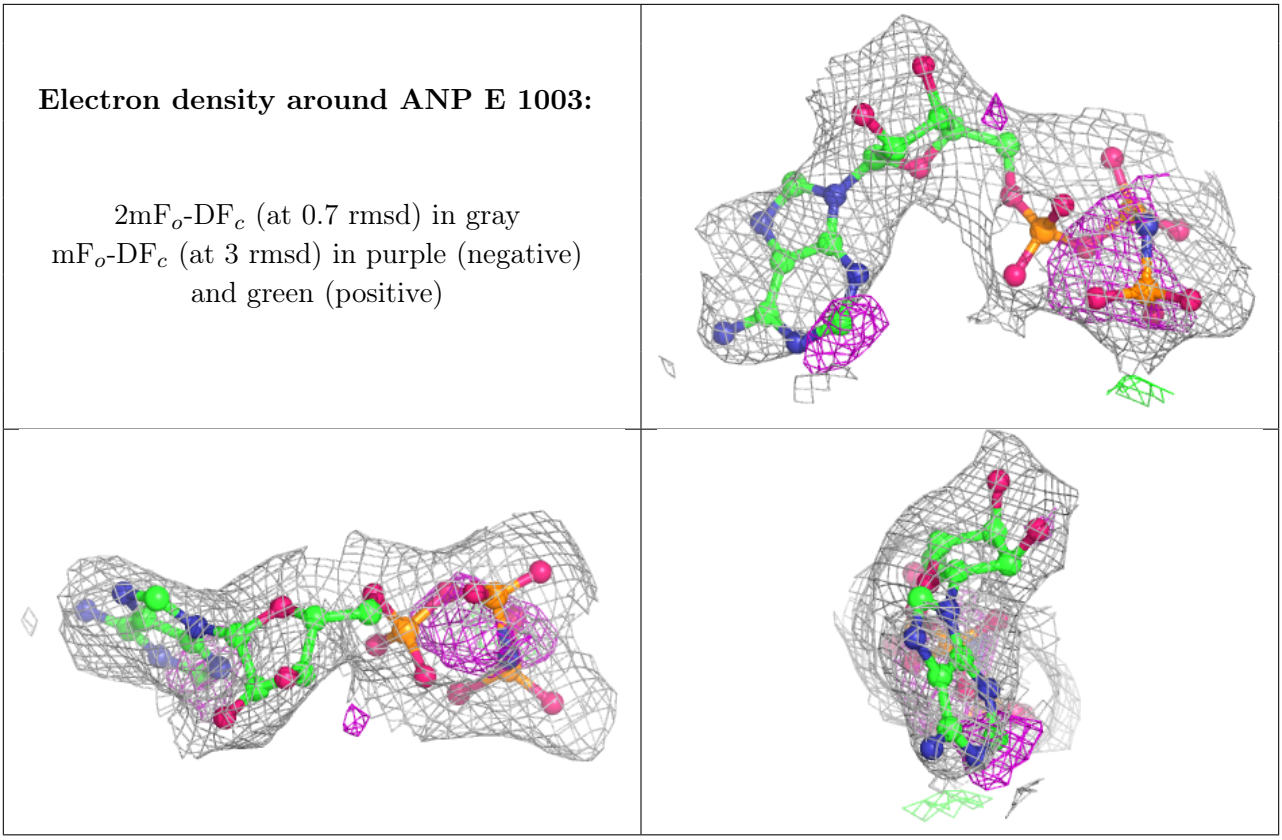






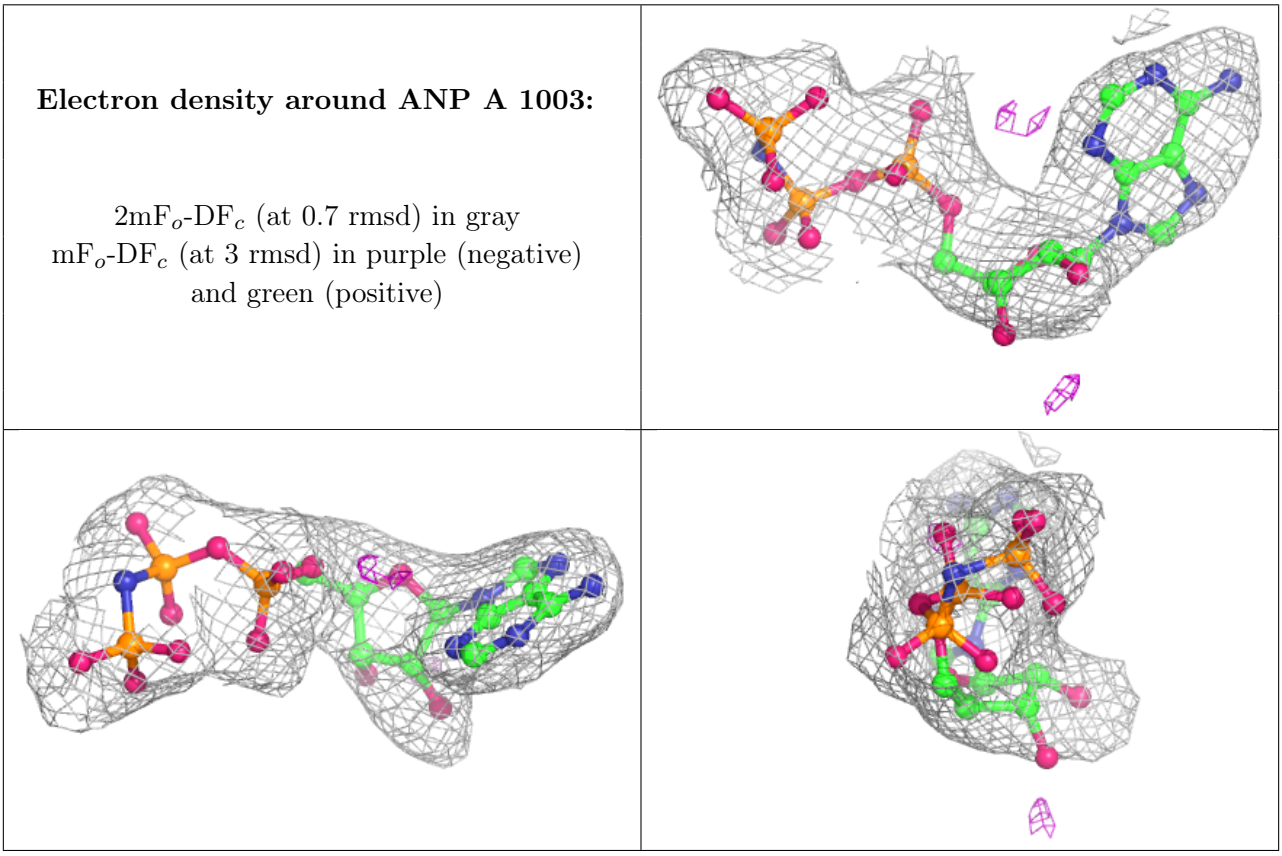
Electron density around ANP E 1003:

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



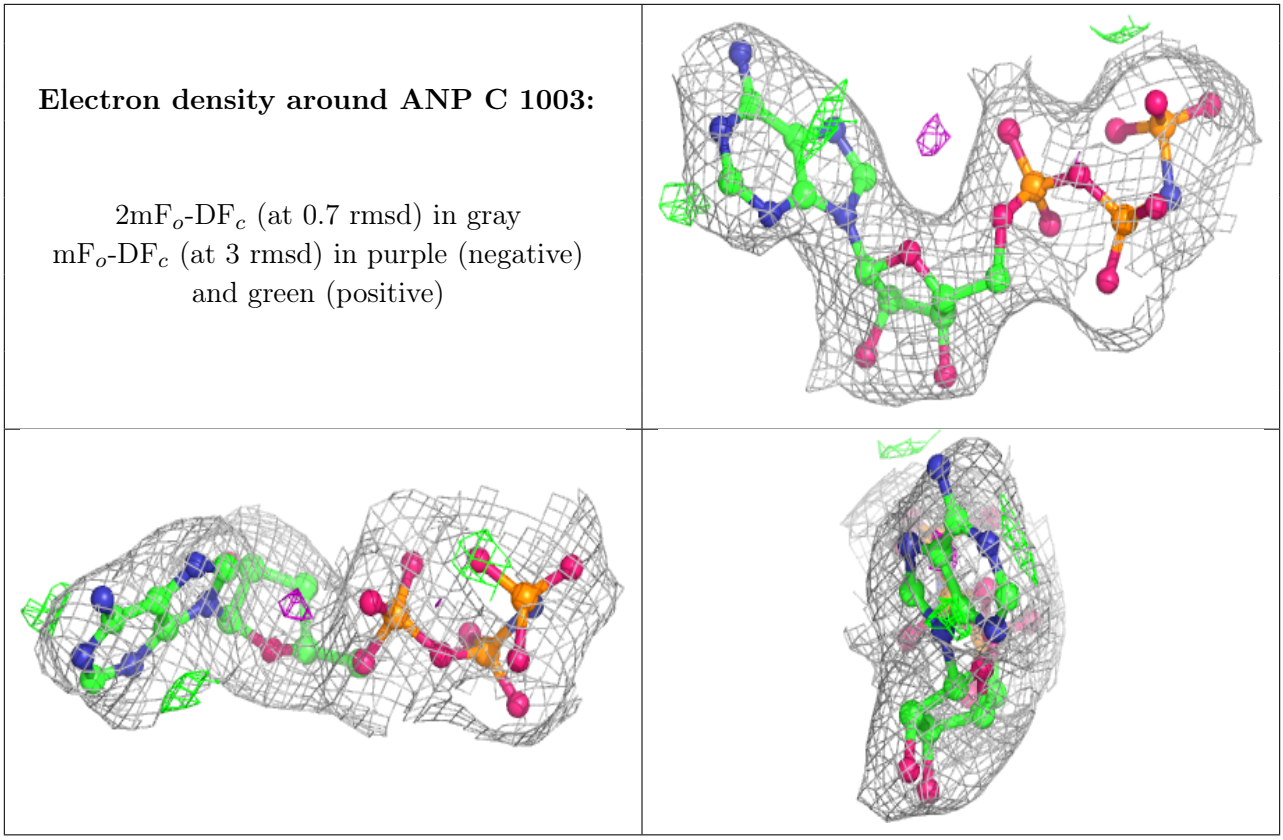
Electron density around ANP A 1003:

$2mF_o$-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 (i)

There are no such residues in this entry.