



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 12:32 PM EDT

PDB ID : 4QQX  
Title : Crystal structure of *T. fusca* Cas3-ATP  
Authors : Ke, A.; Huo, Y.; Nam, K.H.  
Deposited on : 2014-06-30  
Resolution : 3.34 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](mailto: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>.

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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 : 2.35.1  
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) : 2.35.1

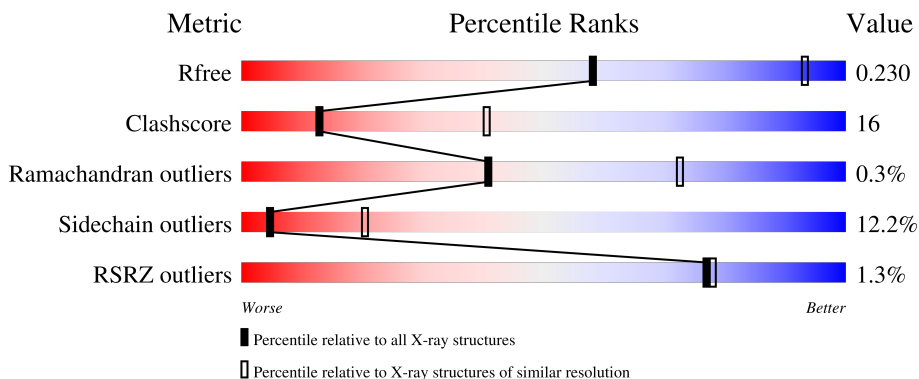
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.34 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.




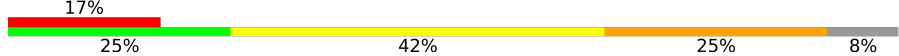

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	964	 2% 60% 28% 5% 6%
1	C	964	 % 58% 31% 5% 7%
1	E	964	 % 65% 25% 5% 7%
1	G	964	 % 54% 33% 5% 8%
2	B	12	 25% 42% 25% 8%

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

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 28826 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
			Total	C	N	O	S			
1	A	903	7028	4463	1251	1287	27	0	0	0
1	C	899	6977	4428	1237	1285	27	0	0	0
1	E	901	6995	4438	1242	1288	27	0	0	0
1	G	887	6906	4390	1224	1266	26	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

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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

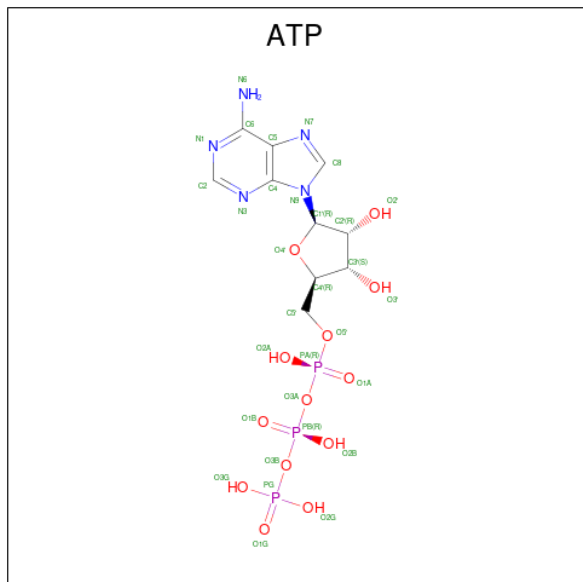
- Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3').

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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

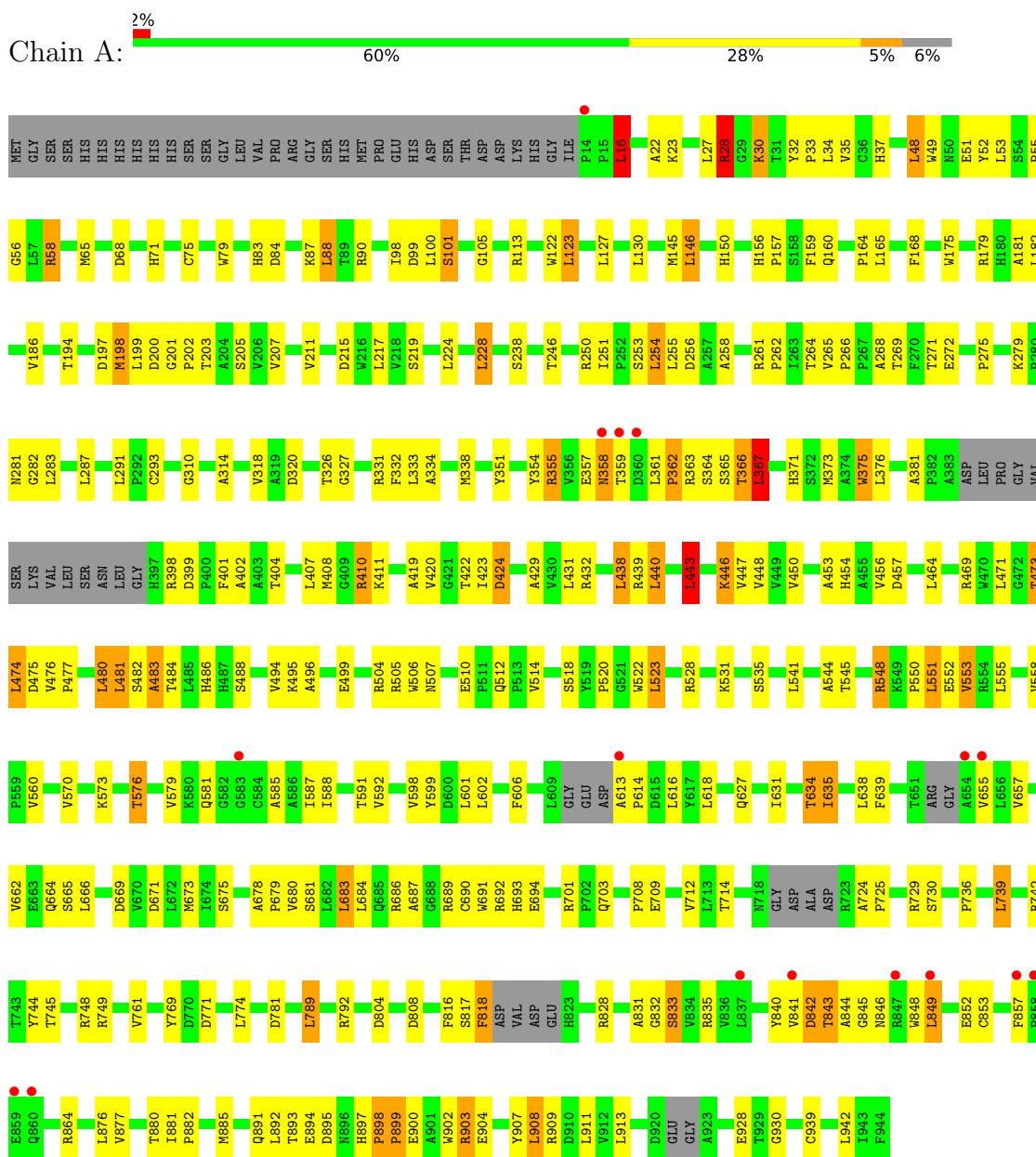


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots i

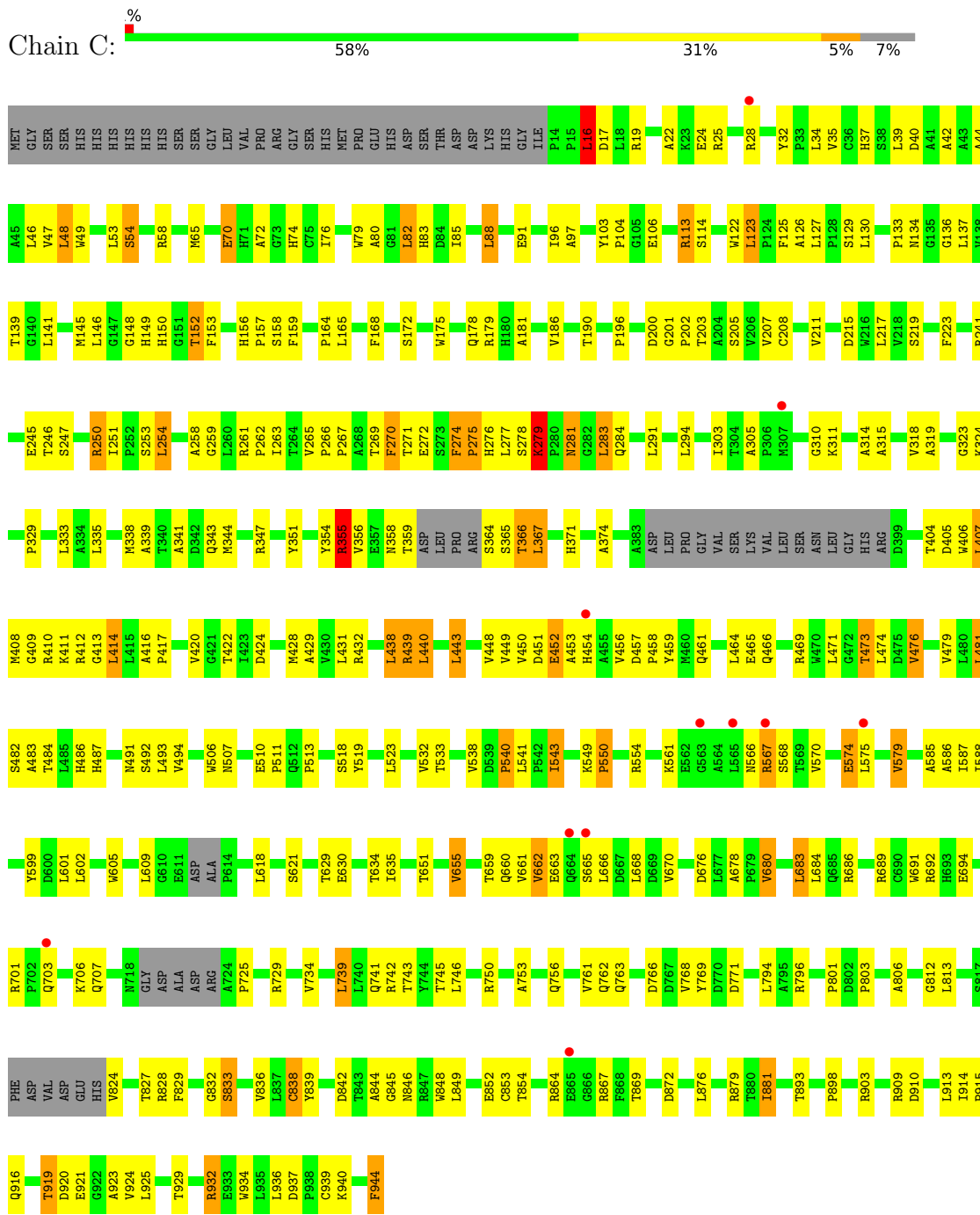
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

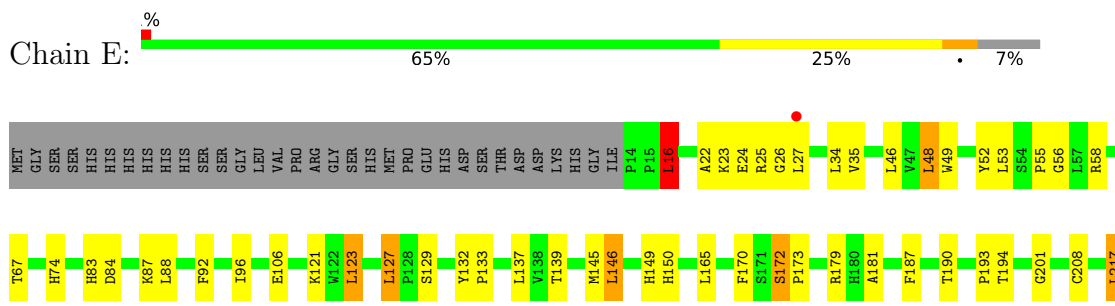


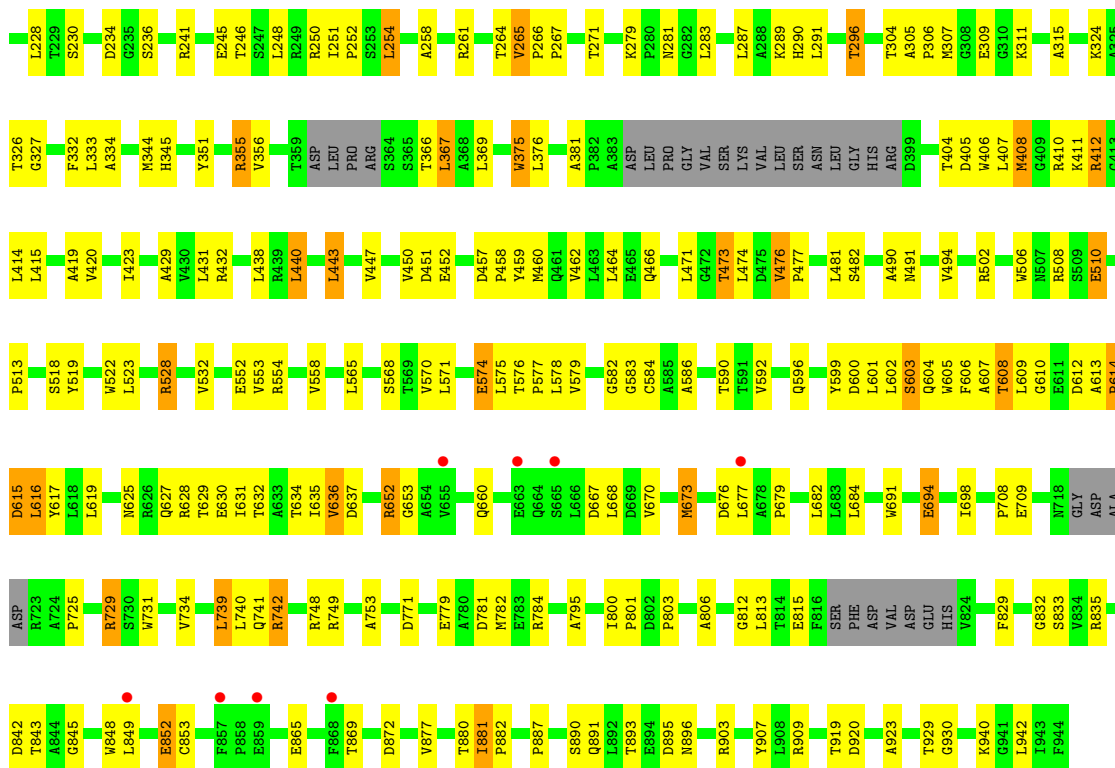
- Molecule 1: CRISPR-associated helicase, Cas3 family



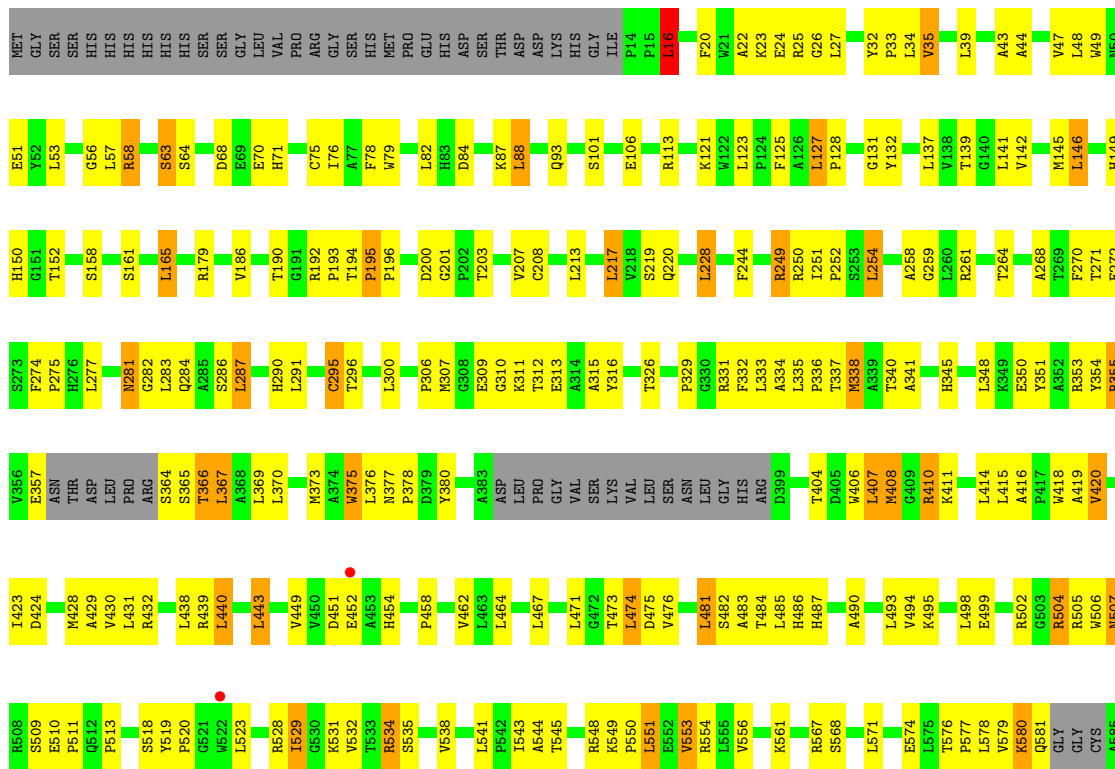


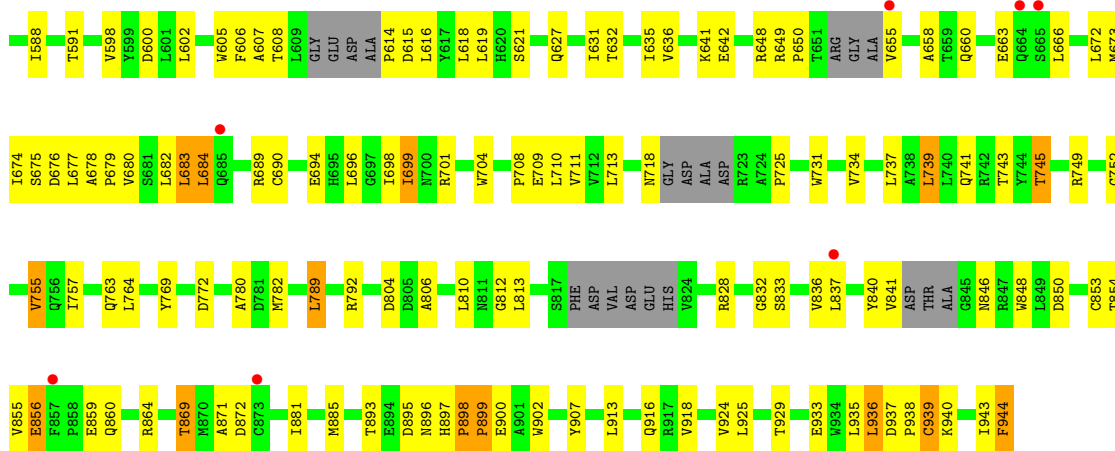
• Molecule 1: CRISPR-associated helicase, Cas3 family





● Molecule 1: CRISPR-associated helicase, Cas3 family





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

Chain B: 25% 42% 25% 8%



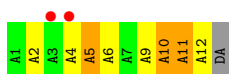
- Molecule 2: DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain D: 33% 42% 17% 8%



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

Chain F: 17% 25% 42% 25% 8%



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

Chain H: 25% 42% 25% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.25Å 222.81Å 125.09Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	46.98 – 3.34 46.98 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.98-3.34) 91.0 (46.98-3.11)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.172 , 0.227 0.176 , 0.230	Depositor DCC
$R_{free}$ test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.4	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.49	2/7205 (0.0%)	0.70	10/9828 (0.1%)
1	C	0.49	1/7151 (0.0%)	0.70	6/9754 (0.1%)
1	E	0.52	1/7170 (0.0%)	0.73	7/9782 (0.1%)
1	G	0.49	4/7077 (0.1%)	0.68	6/9649 (0.1%)
2	B	1.00	0/222	1.96	13/339 (3.8%)
2	D	1.06	0/222	1.98	11/339 (3.2%)
2	F	1.01	0/222	2.09	15/339 (4.4%)
2	H	0.93	0/222	1.71	5/339 (1.5%)
All	All	0.52	8/29491 (0.0%)	0.78	73/40369 (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	C	0	1
1	E	0	1
1	G	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	899	PRO	N-CD	5.46	1.55	1.47
1	G	898	PRO	N-CD	5.34	1.55	1.47
1	A	898	PRO	N-CD	5.25	1.55	1.47
1	C	275	PRO	N-CD	5.17	1.55	1.47
1	G	195	PRO	N-CD	5.16	1.55	1.47
1	G	196	PRO	N-CD	5.16	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	899	PRO	N-CD	5.04	1.54	1.47
1	E	614	PRO	N-CD	5.03	1.54	1.47

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	11	DA	O4'-C4'-C3'	10.51	112.31	106.00
2	B	5	DA	O4'-C1'-N9	-10.19	100.87	108.00
2	H	10	DA	C1'-O4'-C4'	-9.94	100.16	110.10
2	D	10	DA	C1'-O4'-C4'	-9.85	100.25	110.10
2	F	11	DA	O4'-C1'-N9	9.33	114.53	108.00
1	E	609	LEU	N-CA-C	-9.01	86.67	111.00
2	H	9	DA	O4'-C1'-N9	8.67	114.07	108.00
1	E	852	GLU	CB-CA-C	8.44	127.27	110.40
2	D	10	DA	O4'-C1'-C2'	-8.34	99.23	105.90
2	F	10	DA	O4'-C1'-C2'	-8.32	99.24	105.90
2	F	2	DA	O4'-C1'-N9	-8.17	102.28	108.00
1	G	608	THR	N-CA-C	8.16	133.03	111.00
2	B	10	DA	C1'-O4'-C4'	-8.12	101.98	110.10
2	D	11	DA	O4'-C1'-N9	8.07	113.65	108.00
1	A	523	LEU	CA-CB-CG	8.00	133.69	115.30
2	F	10	DA	O4'-C1'-N9	7.77	113.44	108.00
2	F	11	DA	C4'-C3'-C2'	-7.69	96.18	103.10
2	B	11	DA	O4'-C4'-C3'	7.67	110.60	106.00
2	D	4	DA	O4'-C1'-N9	7.51	113.26	108.00
2	B	9	DA	O4'-C1'-N9	7.51	113.25	108.00
2	H	10	DA	O4'-C1'-N9	7.48	113.24	108.00
2	D	11	DA	N1-C6-N6	7.46	123.07	118.60
2	D	5	DA	O4'-C1'-N9	-7.29	102.90	108.00
2	D	11	DA	O4'-C4'-C3'	7.21	110.33	106.00
1	E	852	GLU	C-N-CA	7.12	139.51	121.70
2	D	11	DA	C4'-C3'-C2'	-6.97	96.83	103.10
2	F	5	DA	O4'-C1'-N9	-6.77	103.26	108.00
2	F	10	DA	C1'-O4'-C4'	-6.76	103.34	110.10
1	G	16	LEU	CA-CB-CG	6.70	130.70	115.30
1	A	483	ALA	N-CA-C	-6.63	93.10	111.00
1	A	367	LEU	CA-CB-CG	6.61	130.50	115.30
1	C	16	LEU	CA-CB-CG	6.50	130.25	115.30
2	B	10	DA	O4'-C1'-C2'	-6.40	100.78	105.90
2	H	5	DA	O4'-C1'-N9	-6.39	103.53	108.00
2	B	4	DA	O4'-C4'-C3'	-6.33	101.97	104.50
2	D	11	DA	C5-C6-N6	-6.24	118.71	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	DA	O4'-C1'-N9	-6.18	103.67	108.00
1	C	540	PRO	N-CA-C	6.17	128.14	112.10
2	F	11	DA	C1'-O4'-C4'	-6.13	103.97	110.10
1	A	201	GLY	C-N-CD	5.99	140.99	128.40
1	C	279	LYS	C-N-CD	5.88	140.74	128.40
1	E	753	ALA	C-N-CD	5.84	140.66	128.40
2	B	11	DA	O4'-C1'-C2'	-5.80	101.26	105.90
1	C	274	PHE	C-N-CD	5.80	140.58	128.40
2	F	11	DA	OP1-P-O3'	5.79	117.93	105.20
1	A	898	PRO	C-N-CD	5.78	140.54	128.40
1	E	16	LEU	CA-CB-CG	5.78	128.59	115.30
1	G	195	PRO	C-N-CD	5.78	140.53	128.40
1	C	82	LEU	CB-CA-C	-5.76	99.26	110.20
2	F	11	DA	O4'-C1'-C2'	-5.73	101.31	105.90
1	A	443	LEU	CA-CB-CG	5.72	128.45	115.30
1	E	412	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	C	367	LEU	CA-CB-CG	5.61	128.21	115.30
1	G	194	THR	C-N-CD	5.60	140.17	128.40
1	A	897	HIS	C-N-CD	5.60	140.16	128.40
2	F	9	DA	O4'-C1'-N9	5.59	111.92	108.00
2	H	4	DA	O4'-C1'-N9	5.53	111.87	108.00
2	B	4	DA	C4'-C3'-C2'	-5.52	98.13	103.10
1	G	897	HIS	C-N-CD	5.49	139.92	128.40
2	F	4	DA	O4'-C4'-C3'	-5.48	102.31	104.50
2	D	10	DA	O4'-C1'-N9	5.48	111.84	108.00
1	A	28	ARG	N-CA-C	5.41	125.60	111.00
2	B	11	DA	C4'-C3'-C2'	-5.36	98.27	103.10
2	B	4	DA	C1'-O4'-C4'	-5.31	104.79	110.10
1	G	898	PRO	C-N-CD	5.31	139.55	128.40
1	A	362	PRO	N-CA-C	-5.26	98.43	112.10
2	F	5	DA	C5-N7-C8	-5.24	101.28	103.90
2	B	11	DA	N9-C1'-C2'	5.22	122.52	112.60
1	E	367	LEU	CA-CB-CG	5.20	127.26	115.30
2	D	1	DA	O4'-C4'-C3'	-5.13	102.45	104.50
2	F	5	DA	C4-C5-N7	5.10	113.25	110.70
1	A	16	LEU	CA-CB-CG	5.05	126.92	115.30
2	B	4	DA	N1-C6-N6	5.02	121.61	118.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	ARG	Sidechain
1	C	355	ARG	Sidechain
1	E	852	GLU	Peptide
1	G	355	ARG	Sidechain

## 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	7028	0	6975	227	0
1	C	6977	0	6922	233	0
1	E	6995	0	6939	184	0
1	G	6906	0	6862	297	0
2	B	197	0	99	12	0
2	D	197	0	99	8	0
2	F	197	0	99	7	0
2	H	197	0	99	15	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	12	1	0
4	C	31	0	12	6	0
4	E	31	0	12	2	0
4	G	31	0	12	7	0
All	All	28826	0	28142	939	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 16.

All (939) 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:A:28:ARG:O	1:A:28:ARG:CD	1.95	1.14
1:A:28:ARG:HD2	1:A:30:LYS:HZ1	1.08	1.14
1:C:452:GLU:HG3	1:C:454:HIS:NE2	1.66	1.10
1:G:268:ALA:HB2	1:G:355:ARG:HH12	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:O	1:A:28:ARG:HD3	1.50	1.07
1:A:900:GLU:HG2	1:A:903:ARG:NH1	1.74	1.02
1:A:900:GLU:HG2	1:A:903:ARG:HH12	1.20	1.02
1:G:78:PHE:HB2	1:G:190:THR:HG21	1.01	1.01
1:A:265:VAL:CG1	1:A:355:ARG:NH2	2.25	0.99
1:G:268:ALA:CB	1:G:355:ARG:HH12	1.77	0.98
1:G:78:PHE:CB	1:G:190:THR:HG21	1.94	0.98
1:G:78:PHE:HB2	1:G:190:THR:CG2	1.95	0.97
1:G:268:ALA:CB	1:G:355:ARG:NH1	2.30	0.95
1:A:265:VAL:CG1	1:A:355:ARG:HH21	1.78	0.95
1:A:28:ARG:CD	1:A:30:LYS:HZ1	1.79	0.94
1:C:452:GLU:HG3	1:C:454:HIS:CD2	2.03	0.93
1:A:900:GLU:CG	1:A:903:ARG:HH12	1.83	0.92
1:E:578:LEU:HD11	1:E:583:GLY:O	1.70	0.91
1:G:506:TRP:HH2	1:G:511:PRO:O	1.53	0.91
1:E:606:PHE:CE2	1:E:614:PRO:HG2	2.06	0.90
1:G:606:PHE:CD2	1:G:614:PRO:HG2	2.07	0.90
1:G:268:ALA:HB2	1:G:355:ARG:NH1	1.87	0.89
1:E:613:ALA:O	1:E:652:ARG:HD3	1.73	0.89
1:A:832:GLY:HA2	2:B:5:DA:H61	1.39	0.88
1:A:28:ARG:O	1:A:28:ARG:NE	2.07	0.87
1:C:451:ASP:OD1	1:C:452:GLU:N	2.07	0.86
1:A:28:ARG:HD2	1:A:30:LYS:NZ	1.90	0.86
1:A:265:VAL:HG13	1:A:355:ARG:NH2	1.91	0.85
1:G:833:SER:H	2:H:6:DA:H61	1.25	0.85
1:C:452:GLU:CG	1:C:454:HIS:NE2	2.40	0.84
1:G:249:ARG:O	1:G:252:PRO:HD2	1.78	0.84
1:G:832:GLY:HA2	2:H:5:DA:H61	1.41	0.84
1:G:281:ASN:OD1	1:G:282:GLY:N	2.11	0.83
1:C:263:ILE:HD11	1:C:365:SER:OG	1.78	0.83
1:G:579:VAL:HG23	1:G:580:LYS:HD3	1.57	0.83
1:E:429:ALA:HB1	1:E:440:LEU:HD13	1.60	0.82
1:G:150:HIS:CE1	2:H:11:DA:H5'	2.15	0.82
1:C:358:ASN:O	1:C:359:THR:OG1	1.96	0.81
1:E:23:LYS:NZ	2:F:12:DA:OP2	2.12	0.81
1:A:28:ARG:CD	1:A:30:LYS:NZ	2.42	0.80
1:G:268:ALA:HB3	1:G:355:ARG:NH1	1.95	0.80
1:C:315:ALA:HB2	1:C:481:LEU:HD21	1.63	0.80
1:A:665:SER:O	1:A:666:LEU:HD12	1.81	0.79
1:G:518:SER:H	1:G:534:ARG:NH2	1.80	0.79
1:G:580:LYS:HB2	1:G:581:GLN:OE1	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:HD3	1:A:30:LYS:HE3	1.65	0.79
1:C:263:ILE:CD1	1:C:365:SER:OG	2.31	0.79
1:G:606:PHE:CE2	1:G:614:PRO:HG2	2.17	0.79
1:C:409:GLY:HA3	1:C:412:ARG:HD2	1.66	0.78
1:A:22:ALA:HB2	1:A:34:LEU:HA	1.65	0.78
1:C:125:PHE:HB2	1:C:165:LEU:HD13	1.63	0.78
1:C:159:PHE:CD2	1:C:164:PRO:HB3	2.20	0.77
1:E:578:LEU:HD12	1:E:582:GLY:C	2.05	0.77
1:E:150:HIS:CE1	2:F:11:DA:H5'	2.22	0.75
1:G:404:THR:CG2	1:G:407:LEU:HD23	2.16	0.75
1:G:506:TRP:CH2	1:G:511:PRO:O	2.40	0.75
1:C:246:THR:HG22	1:C:250:ARG:HH12	1.53	0.74
1:C:832:GLY:HA2	2:D:5:DA:H61	1.51	0.74
1:C:844:ALA:N	1:C:845:GLY:HA2	2.01	0.74
1:G:579:VAL:CG2	1:G:580:LYS:HE2	2.17	0.74
1:A:429:ALA:HB1	1:A:440:LEU:HD13	1.69	0.73
1:C:680:VAL:HG13	1:C:743:THR:HG23	1.70	0.73
1:A:150:HIS:CE1	2:B:11:DA:H5'	2.24	0.73
1:C:554:ARG:NH1	1:C:574:GLU:OE2	2.20	0.73
1:A:268:ALA:HB2	1:A:355:ARG:NH1	2.03	0.73
1:G:606:PHE:CE2	1:G:614:PRO:CG	2.72	0.73
1:G:580:LYS:HD3	1:G:580:LYS:N	2.02	0.72
1:A:908:LEU:HA	1:A:911:LEU:HD13	1.72	0.71
1:E:578:LEU:HD11	1:E:583:GLY:C	2.10	0.71
1:C:113:ARG:NH2	1:C:168:PHE:O	2.23	0.71
1:C:429:ALA:HB1	1:C:440:LEU:HD13	1.73	0.71
1:G:406:TRP:HE3	1:G:407:LEU:HD22	1.54	0.71
1:G:414:LEU:HD22	1:G:443:LEU:HD13	1.73	0.71
1:G:506:TRP:CZ3	1:G:510:GLU:HB3	2.25	0.71
1:E:881:ILE:HD11	1:E:942:LEU:HB2	1.72	0.71
1:C:833:SER:H	2:D:6:DA:H61	1.37	0.70
1:A:588:ILE:HG12	1:A:662:VAL:HG11	1.72	0.70
1:A:900:GLU:HA	1:A:903:ARG:NH1	2.06	0.70
1:G:602:LEU:HB3	1:G:616:LEU:HD11	1.73	0.70
1:A:903:ARG:HA	1:A:909:ARG:HG2	1.74	0.70
1:G:432:ARG:NH1	1:G:812:GLY:O	2.24	0.70
1:G:27:LEU:HD13	1:G:228:LEU:HD21	1.73	0.70
1:E:612:ASP:HB3	1:E:613:ALA:HA	1.72	0.70
1:G:579:VAL:HG23	1:G:580:LYS:HE2	1.71	0.70
1:C:432:ARG:NH1	1:C:812:GLY:O	2.25	0.70
1:G:414:LEU:HD22	1:G:443:LEU:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:PRO:O	1:C:355:ARG:NH2	2.25	0.70
1:C:279:LYS:O	1:C:279:LYS:HG3	1.90	0.70
1:G:579:VAL:HG23	1:G:580:LYS:CD	2.22	0.69
1:C:864:ARG:O	1:C:867:ARG:HG2	1.92	0.69
1:E:578:LEU:HD12	1:E:582:GLY:O	1.93	0.69
1:C:277:LEU:CD1	4:C:1003:ATP:N7	2.56	0.69
1:E:123:LEU:HG	1:E:127:LEU:HD22	1.73	0.69
1:G:258:ALA:O	1:G:407:LEU:HD21	1.92	0.69
1:C:869:THR:H	1:C:872:ASP:HB2	1.57	0.69
1:E:311:LYS:HE3	4:E:1003:ATP:O1B	1.91	0.69
1:A:551:LEU:HD23	1:A:553:VAL:HG12	1.75	0.69
1:A:742:ARG:NH1	1:A:781:ASP:OD1	2.26	0.69
1:A:376:LEU:HD21	1:A:907:TYR:CE1	2.27	0.69
1:G:333:LEU:HD22	1:G:449:VAL:HB	1.73	0.69
1:E:410:ARG:O	1:E:411:LYS:CG	2.40	0.68
1:E:410:ARG:O	1:E:411:LYS:HG3	1.93	0.68
1:G:869:THR:HG23	1:G:871:ALA:H	1.57	0.68
1:E:729:ARG:NH2	1:G:101:SER:O	2.26	0.68
1:A:268:ALA:CB	1:A:355:ARG:NH1	2.56	0.68
1:C:277:LEU:HD23	1:C:277:LEU:C	2.14	0.68
1:A:666:LEU:O	1:A:689:ARG:NH1	2.26	0.68
1:A:90:ARG:NH2	1:A:105:GLY:O	2.24	0.68
1:C:678:ALA:HB3	1:C:683:LEU:HD13	1.76	0.68
1:E:612:ASP:H	1:E:613:ALA:HB2	1.58	0.68
1:E:832:GLY:HA2	2:F:5:DA:H61	1.59	0.67
1:G:338:MET:HG3	2:H:5:DA:OP1	1.93	0.67
1:A:363:ARG:O	1:A:398:ARG:NH2	2.28	0.67
1:G:504:ARG:HG2	1:G:504:ARG:HH11	1.60	0.67
1:G:507:ASN:OD1	1:G:507:ASN:N	2.26	0.67
1:G:410:ARG:HH11	1:G:410:ARG:HG2	1.60	0.67
1:G:896:ASN:OD1	1:G:929:THR:HG23	1.95	0.67
1:A:899:PRO:HG2	1:A:902:TRP:CD1	2.30	0.67
1:A:265:VAL:HG11	1:A:355:ARG:HH21	1.60	0.66
1:A:771:ASP:HA	1:G:507:ASN:HD22	1.61	0.66
1:A:558:VAL:HG22	1:A:570:VAL:HG21	1.77	0.66
1:A:694:GLU:HG2	1:A:701:ARG:HH21	1.61	0.66
1:G:404:THR:HG23	1:G:407:LEU:H	1.61	0.66
1:C:429:ALA:HB2	1:C:439:ARG:HG2	1.78	0.66
1:G:429:ALA:HB1	1:G:440:LEU:HD13	1.78	0.66
1:A:65:MET:HA	1:A:198:MET:O	1.95	0.66
1:E:311:LYS:HB2	4:E:1003:ATP:O1B	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:SER:OG	1:A:686:ARG:NH2	2.29	0.66
1:A:898:PRO:HA	1:A:913:LEU:HD11	1.78	0.66
1:E:345:HIS:CD2	1:E:369:LEU:HB2	2.31	0.66
1:C:742:ARG:NH2	1:C:771:ASP:O	2.29	0.65
1:G:841:VAL:HA	1:G:846:ASN:O	1.97	0.65
1:A:585:ALA:HB3	1:A:655:VAL:HG22	1.78	0.65
1:G:673:MET:HE3	1:G:710:LEU:HD13	1.78	0.65
1:A:268:ALA:HB2	1:A:355:ARG:HH11	1.58	0.65
1:E:575:LEU:O	1:E:579:VAL:HG23	1.96	0.65
1:E:612:ASP:CB	1:E:613:ALA:HA	2.26	0.65
1:C:347:ARG:NH2	4:C:1003:ATP:O1A	2.28	0.65
1:A:447:VAL:HG22	1:A:477:PRO:HG2	1.78	0.65
1:E:578:LEU:O	1:E:582:GLY:N	2.30	0.65
1:C:471:LEU:HD22	1:C:476:VAL:HG21	1.80	0.64
1:G:600:ASP:OD2	1:G:940:LYS:NZ	2.27	0.64
1:C:449:VAL:HG13	1:C:479:VAL:HB	1.80	0.64
1:C:932:ARG:HE	1:C:944:PHE:C	2.00	0.64
1:A:200:ASP:OD1	1:A:203:THR:HB	1.97	0.64
1:G:106:GLU:OE2	1:G:179:ARG:NH2	2.26	0.64
1:G:145:MET:HG3	1:G:208:CYS:HB2	1.78	0.64
1:E:842:ASP:OD1	1:E:845:GLY:HA2	1.98	0.64
1:A:261:ARG:HD3	1:A:262:PRO:HD2	1.80	0.64
1:G:578:LEU:O	1:G:581:GLN:N	2.30	0.64
1:E:123:LEU:O	1:E:127:LEU:HB2	1.98	0.63
1:G:577:PRO:HB2	1:G:704:TRP:CG	2.33	0.63
1:G:896:ASN:OD1	1:G:929:THR:CG2	2.46	0.63
1:G:39:LEU:HD22	1:G:244:PHE:HB2	1.79	0.63
1:E:578:LEU:CD1	1:E:583:GLY:C	2.67	0.63
1:E:742:ARG:NH1	1:E:781:ASP:OD1	2.32	0.63
1:G:380:TYR:CE1	1:G:408:MET:HE3	2.33	0.63
1:C:246:THR:HG22	1:C:250:ARG:NH1	2.14	0.62
1:G:380:TYR:HE1	1:G:408:MET:HE3	1.63	0.62
1:E:558:VAL:HG22	1:E:570:VAL:HG21	1.81	0.62
1:G:261:ARG:O	1:G:365:SER:CB	2.47	0.62
1:G:261:ARG:O	1:G:365:SER:HB2	1.99	0.62
1:A:507:ASN:HB2	1:A:510:GLU:HB2	1.81	0.62
1:G:579:VAL:HG23	1:G:580:LYS:CE	2.29	0.62
1:G:833:SER:N	2:H:6:DA:H61	1.95	0.62
1:E:903:ARG:HA	1:E:909:ARG:HG3	1.81	0.62
1:C:725:PRO:O	1:C:741:GLN:NE2	2.25	0.62
1:G:310:GLY:HA2	4:G:1003:ATP:O2A	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:PRO:HB3	1:E:261:ARG:HH22	1.65	0.62
1:C:568:SER:HA	1:C:601:LEU:HD21	1.82	0.62
1:G:482:SER:OG	1:G:483:ALA:O	2.14	0.61
1:C:561:LYS:HG2	1:C:566:ASN:HB2	1.82	0.61
1:E:432:ARG:NH1	1:E:812:GLY:O	2.34	0.61
1:E:84:ASP:HB3	1:E:87:LYS:HD2	1.82	0.61
1:E:296:THR:O	1:E:296:THR:OG1	2.17	0.61
1:G:287:LEU:O	1:G:291:LEU:HB2	2.01	0.61
1:G:641:LYS:HE3	1:G:696:LEU:HD21	1.82	0.61
1:A:159:PHE:CE2	1:A:164:PRO:HG3	2.36	0.61
1:C:691:TRP:HB3	1:C:694:GLU:HB2	1.83	0.61
1:A:891:GLN:O	1:A:930:GLY:HA2	2.00	0.60
1:C:507:ASN:HB2	1:C:510:GLU:HB2	1.83	0.60
1:G:312:THR:HG22	1:G:316:TYR:CE2	2.37	0.60
1:G:518:SER:H	1:G:534:ARG:HH21	1.49	0.60
1:A:265:VAL:HG12	1:A:355:ARG:NH2	2.16	0.60
1:A:197:ASP:C	1:A:198:MET:HG3	2.22	0.60
1:A:469:ARG:O	1:A:473:THR:HG22	2.01	0.60
1:C:82:LEU:O	1:C:85:ILE:HG22	2.02	0.60
1:C:404:THR:O	1:C:408:MET:HG2	2.02	0.60
1:A:881:ILE:HD12	1:A:942:LEU:HD22	1.84	0.60
1:A:258:ALA:O	1:A:404:THR:HG21	2.02	0.60
1:A:358:ASN:N	1:A:358:ASN:OD1	2.32	0.60
1:G:149:HIS:CD2	1:G:150:HIS:CD2	2.90	0.60
1:G:523:LEU:HD12	1:G:534:ARG:HH11	1.67	0.60
1:G:615:ASP:O	1:G:655:VAL:N	2.35	0.60
1:G:899:PRO:HG2	1:G:902:TRP:CD1	2.36	0.60
1:C:261:ARG:O	1:C:365:SER:CB	2.50	0.60
1:C:277:LEU:HD21	1:C:279:LYS:O	2.02	0.60
1:G:380:TYR:HE1	1:G:408:MET:CE	2.14	0.60
1:A:665:SER:C	1:A:666:LEU:HD12	2.22	0.59
1:C:746:LEU:HD22	1:C:768:VAL:HB	1.84	0.59
1:C:630:GLU:O	1:C:634:THR:HG23	2.01	0.59
1:E:606:PHE:CD2	1:E:614:PRO:HG2	2.37	0.59
1:G:506:TRP:CE3	1:G:510:GLU:HB3	2.37	0.59
1:A:23:LYS:NZ	2:B:12:DA:OP2	2.35	0.59
1:A:818:PHE:HE2	1:C:114:SER:HG	1.50	0.59
1:A:548:ARG:NH2	1:A:692:ARG:O	2.36	0.59
1:C:666:LEU:HB3	1:C:668:LEU:HD13	1.85	0.59
1:E:600:ASP:OD1	1:E:940:LYS:NZ	2.34	0.59
1:G:745:THR:O	1:G:749:ARG:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:SER:O	1:C:251:ILE:HD12	2.01	0.59
1:C:344:MET:HA	1:C:347:ARG:HG3	1.83	0.59
1:E:432:ARG:HD3	1:E:815:GLU:O	2.02	0.59
1:G:520:PRO:HG3	1:G:545:THR:HG21	1.85	0.59
1:C:265:VAL:O	1:C:324:LYS:NZ	2.26	0.59
1:E:266:PRO:O	1:E:355:ARG:NH2	2.34	0.59
1:A:282:GLY:HA3	1:A:544:ALA:HB3	1.85	0.59
1:C:409:GLY:CA	1:C:412:ARG:HD2	2.32	0.59
1:C:471:LEU:HB3	1:C:476:VAL:HG22	1.85	0.59
1:E:832:GLY:HA2	2:F:5:DA:N6	2.17	0.59
1:G:333:LEU:HB2	1:G:420:VAL:HB	1.83	0.58
1:C:358:ASN:N	1:C:358:ASN:HD22	2.01	0.58
1:E:304:THR:HG22	1:E:482:SER:HB3	1.85	0.58
1:C:283:LEU:HA	1:C:543:ILE:HD12	1.85	0.58
1:C:404:THR:HG22	1:C:407:LEU:HB2	1.85	0.58
1:A:404:THR:HG23	1:A:407:LEU:H	1.68	0.58
1:A:484:THR:HG23	1:A:484:THR:O	2.03	0.58
1:C:585:ALA:HB3	1:C:655:VAL:HG23	1.85	0.58
1:C:662:VAL:O	1:C:689:ARG:NH2	2.24	0.58
1:E:351:TYR:CZ	1:E:355:ARG:HD3	2.38	0.58
1:G:275:PRO:HG3	1:G:354:TYR:OH	2.04	0.58
1:G:407:LEU:HD12	1:G:416:ALA:HB2	1.85	0.58
1:A:665:SER:HA	1:A:689:ARG:HH22	1.68	0.58
1:E:412:ARG:O	1:E:415:LEU:HB2	2.03	0.58
1:C:277:LEU:HD12	4:C:1003:ATP:N7	2.19	0.58
1:A:23:LYS:HD3	1:A:224:LEU:HD11	1.86	0.58
1:E:632:THR:O	1:E:636:VAL:HG13	2.03	0.58
1:A:37:HIS:CE1	1:A:215:ASP:OD1	2.56	0.58
1:A:410:ARG:HD3	1:A:410:ARG:N	2.19	0.58
1:G:22:ALA:C	1:G:23:LYS:HG2	2.24	0.58
1:A:587:ILE:HB	1:A:657:VAL:HG22	1.86	0.57
1:G:424:ASP:O	1:G:428:MET:HG3	2.04	0.57
1:C:79:TRP:O	1:C:146:LEU:HD21	2.03	0.57
1:C:750:ARG:NH1	1:C:753:ALA:O	2.37	0.57
1:C:849:LEU:HD23	1:C:879:ARG:NE	2.18	0.57
1:G:841:VAL:O	1:G:918:VAL:N	2.28	0.57
1:C:459:TYR:HE2	1:C:794:LEU:HD23	1.69	0.57
1:G:404:THR:HG21	1:G:407:LEU:HD23	1.87	0.57
1:G:642:GLU:O	1:G:648:ARG:NH2	2.37	0.57
1:C:305:ALA:O	1:C:483:ALA:HA	2.04	0.57
1:E:24:GLU:HG2	1:E:96:ILE:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ARG:O	1:C:365:SER:HB2	2.05	0.57
1:E:568:SER:HA	1:E:601:LEU:HD21	1.85	0.57
1:G:49:TRP:CH2	1:G:58:ARG:HG2	2.39	0.57
1:G:578:LEU:O	1:G:581:GLN:C	2.42	0.57
1:A:99:ASP:OD1	1:A:101:SER:OG	2.22	0.57
1:A:602:LEU:HB3	1:A:616:LEU:HD11	1.85	0.57
1:C:274:PHE:CE1	1:C:351:TYR:HE2	2.22	0.57
1:A:49:TRP:CZ2	1:A:58:ARG:HG2	2.40	0.57
1:C:267:PRO:HG3	1:C:324:LYS:HE2	1.86	0.57
1:G:192:ARG:N	1:G:193:PRO:CD	2.68	0.57
1:A:832:GLY:HA2	2:B:5:DA:N6	2.16	0.56
1:C:201:GLY:HA3	1:C:806:ALA:O	2.05	0.56
1:C:371:HIS:HB3	1:C:422:THR:HG23	1.86	0.56
1:G:679:PRO:HG2	1:G:682:LEU:HD12	1.86	0.56
1:C:588:ILE:HD12	1:C:662:VAL:HG11	1.86	0.56
1:E:506:TRP:CH2	1:E:513:PRO:HD3	2.39	0.56
1:A:113:ARG:NH2	1:A:168:PHE:O	2.38	0.56
1:A:606:PHE:CZ	1:A:614:PRO:HG2	2.41	0.56
1:E:490:ALA:O	1:E:494:VAL:HG13	2.04	0.56
1:G:332:PHE:HA	1:G:419:ALA:O	2.06	0.56
1:G:725:PRO:HG2	1:G:741:GLN:HG2	1.88	0.56
1:A:28:ARG:HD3	1:A:30:LYS:CE	2.34	0.56
1:E:145:MET:HG3	1:E:208:CYS:HB2	1.88	0.56
1:A:265:VAL:HG13	1:A:355:ARG:HH21	1.60	0.56
1:C:484:THR:HG23	1:C:484:THR:O	2.06	0.56
1:G:694:GLU:HG2	1:G:701:ARG:HH21	1.71	0.56
1:C:575:LEU:HD11	1:C:587:ILE:HD11	1.88	0.55
1:E:523:LEU:HD21	1:E:532:VAL:HG13	1.88	0.55
1:C:274:PHE:CE1	1:C:351:TYR:CE2	2.93	0.55
1:C:310:GLY:HA2	4:C:1003:ATP:O2A	2.06	0.55
1:C:335:LEU:HD13	1:C:341:ALA:HA	1.87	0.55
1:E:132:TYR:HB3	1:E:139:THR:OG1	2.06	0.55
1:G:410:ARG:NH1	2:H:9:DA:OP2	2.39	0.55
1:E:406:TRP:O	1:E:412:ARG:NH1	2.39	0.55
1:C:659:THR:O	1:C:662:VAL:HG12	2.07	0.55
1:E:251:ILE:HA	1:E:254:LEU:HD22	1.88	0.55
1:A:599:TYR:HB2	1:A:618:LEU:HD13	1.88	0.55
1:E:833:SER:H	2:F:6:DA:H61	1.55	0.55
1:E:607:ALA:O	1:E:610:GLY:HA3	2.07	0.55
1:E:612:ASP:CB	1:E:613:ALA:CA	2.85	0.55
1:G:268:ALA:HB3	1:G:355:ARG:CZ	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:282:GLY:HA3	1:G:544:ALA:HB3	1.89	0.55
1:C:203:THR:O	1:C:207:VAL:HG23	2.08	0.55
1:C:270:PHE:CE2	1:C:284:GLN:HB3	2.42	0.55
1:E:676:ASP:HB3	1:E:731:TRP:CH2	2.41	0.55
1:G:25:ARG:HD2	1:G:26:GLY:H	1.72	0.55
1:G:471:LEU:HD22	1:G:476:VAL:HG21	1.88	0.55
1:G:458:PRO:O	1:G:792:ARG:NH1	2.40	0.54
1:G:859:GLU:O	1:G:860:GLN:HG2	2.07	0.54
1:A:443:LEU:HA	1:A:446:LYS:HD3	1.90	0.54
1:E:315:ALA:HB2	1:E:481:LEU:HD11	1.89	0.54
1:E:877:VAL:HA	1:E:880:THR:HG23	1.89	0.54
1:G:899:PRO:CG	1:G:902:TRP:CD1	2.90	0.54
1:E:615:ASP:OD1	1:E:615:ASP:N	2.41	0.54
1:G:313:GLU:HA	1:G:316:TYR:HD2	1.72	0.54
1:G:937:ASP:OD1	1:G:939:CYS:N	2.38	0.54
1:A:831:ALA:HB1	1:A:885:MET:HB3	1.88	0.54
1:G:201:GLY:HA3	1:G:806:ALA:O	2.06	0.54
1:E:289:LYS:HD3	1:E:290:HIS:CE1	2.43	0.54
1:E:801:PRO:HD2	1:E:813:LEU:HD12	1.89	0.54
1:G:258:ALA:O	1:G:404:THR:HG21	2.08	0.54
1:A:877:VAL:O	1:A:880:THR:OG1	2.20	0.54
1:C:150:HIS:CE1	2:D:11:DA:H5'	2.42	0.54
1:G:149:HIS:NE2	1:G:150:HIS:CD2	2.76	0.54
1:G:329:PRO:O	1:G:331:ARG:NH1	2.41	0.54
1:G:404:THR:HG23	1:G:407:LEU:HD23	1.90	0.54
1:G:832:GLY:HA2	2:H:5:DA:N6	2.18	0.54
1:A:200:ASP:OD1	1:A:203:THR:CB	2.55	0.54
1:A:287:LEU:O	1:A:291:LEU:HB2	2.07	0.54
2:F:10:DA:H2''	2:F:11:DA:O4'	2.08	0.54
1:A:28:ARG:CD	1:A:30:LYS:CE	2.86	0.53
1:A:160:GLN:OE1	1:C:796:ARG:HD2	2.09	0.53
1:A:691:TRP:HE3	1:A:694:GLU:HG3	1.71	0.53
1:C:219:SER:OG	2:D:11:DA:H2''	2.08	0.53
1:C:659:THR:O	1:C:661:VAL:N	2.41	0.53
1:G:606:PHE:CD2	1:G:614:PRO:CG	2.86	0.53
1:A:552:GLU:HB2	1:A:709:GLU:HG3	1.90	0.53
1:G:23:LYS:NZ	1:G:219:SER:OG	2.40	0.53
1:G:380:TYR:CE1	1:G:408:MET:CE	2.91	0.53
1:C:842:ASP:OD1	1:C:846:ASN:N	2.41	0.53
1:E:725:PRO:HB2	1:E:741:GLN:HG2	1.89	0.53
1:G:551:LEU:HG	1:G:755:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:LEU:HD23	1:A:761:VAL:HG13	1.91	0.53
1:A:898:PRO:HA	1:A:913:LEU:CD1	2.38	0.53
1:E:287:LEU:O	1:E:291:LEU:HB2	2.08	0.53
1:G:335:LEU:HD13	1:G:341:ALA:HA	1.91	0.53
1:C:246:THR:CG2	1:C:250:ARG:HH12	2.20	0.53
1:A:592:VAL:HG12	2:B:2:DA:OP1	2.09	0.53
1:A:900:GLU:CG	1:A:903:ARG:NH1	2.53	0.53
1:C:279:LYS:O	4:C:1003:ATP:N6	2.42	0.53
1:G:410:ARG:H	1:G:410:ARG:HD2	1.72	0.53
1:G:678:ALA:HB3	1:G:683:LEU:HD13	1.91	0.53
1:C:133:PRO:HB2	1:C:136:GLY:HA3	1.90	0.52
1:E:106:GLU:HG3	1:E:172:SER:HB3	1.90	0.52
1:E:887:PRO:O	1:E:890:SER:OG	2.25	0.52
1:E:848:TRP:CE2	1:E:853:CYS:HB3	2.44	0.52
1:A:182:LEU:O	1:A:186:VAL:HG13	2.09	0.52
1:A:410:ARG:CD	1:A:410:ARG:H	2.21	0.52
1:C:270:PHE:CE1	1:C:274:PHE:HD2	2.27	0.52
1:G:44:ALA:HA	1:G:251:ILE:HD13	1.92	0.52
1:A:332:PHE:HA	1:A:419:ALA:O	2.09	0.52
1:A:357:GLU:OE1	1:A:357:GLU:N	2.34	0.52
1:A:835:ARG:NH2	1:A:882:PRO:HD3	2.24	0.52
1:C:275:PRO:HG3	1:C:354:TYR:CZ	2.45	0.52
1:C:725:PRO:HB2	1:C:741:GLN:HG2	1.90	0.52
1:E:25:ARG:O	1:E:27:LEU:HD13	2.10	0.52
1:G:430:VAL:HG11	1:G:467:LEU:HA	1.91	0.52
1:A:410:ARG:N	1:A:410:ARG:CD	2.73	0.52
1:C:37:HIS:ND1	1:C:37:HIS:O	2.42	0.52
1:C:506:TRP:HH2	1:C:511:PRO:O	1.93	0.52
1:G:484:THR:HG23	1:G:484:THR:O	2.10	0.52
1:C:663:GLU:OE2	1:C:686:ARG:NH1	2.29	0.52
1:G:404:THR:CG2	1:G:407:LEU:CD2	2.88	0.52
1:G:674:ILE:HG22	1:G:713:LEU:HD11	1.91	0.52
1:C:739:LEU:HD21	1:C:769:TYR:CE1	2.45	0.52
1:G:602:LEU:N	1:G:602:LEU:HD12	2.25	0.52
1:A:371:HIS:HB3	1:A:422:THR:HG23	1.92	0.51
1:A:669:ASP:OD2	1:A:693:HIS:N	2.28	0.51
1:C:47:VAL:HG11	1:C:251:ILE:HG22	1.92	0.51
1:C:473:THR:HG21	1:C:803:PRO:HG2	1.92	0.51
1:A:28:ARG:HB3	1:A:30:LYS:HZ2	1.74	0.51
1:A:49:TRP:CH2	1:A:58:ARG:HG2	2.45	0.51
1:C:739:LEU:HD11	1:C:769:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:567:ARG:NH2	1:G:676:ASP:OD2	2.44	0.51
1:G:598:VAL:O	1:G:602:LEU:HD13	2.10	0.51
1:C:801:PRO:HD2	1:C:813:LEU:HD12	1.91	0.51
1:C:459:TYR:CD2	1:C:829:PHE:HB2	2.45	0.51
1:C:684:LEU:HD13	1:C:761:VAL:HG13	1.91	0.51
1:A:729:ARG:CZ	1:C:104:PRO:HG3	2.40	0.51
1:E:149:HIS:NE2	1:E:150:HIS:CD2	2.78	0.51
1:E:451:ASP:OD1	1:E:452:GLU:N	2.43	0.51
1:G:84:ASP:HB3	1:G:87:LYS:HD2	1.93	0.51
1:A:691:TRP:CE3	1:A:694:GLU:HG3	2.45	0.51
1:G:49:TRP:CZ2	1:G:58:ARG:HG2	2.45	0.51
1:G:486:HIS:CD2	1:G:769:TYR:HD2	2.27	0.51
1:A:98:ILE:HD13	1:A:100:LEU:HD21	1.92	0.51
1:C:261:ARG:O	1:C:365:SER:HB3	2.11	0.51
1:C:414:LEU:HG	1:C:443:LEU:HD13	1.93	0.51
1:E:895:ASP:OD1	1:E:895:ASP:N	2.38	0.51
1:C:34:LEU:HD23	1:C:88:LEU:HD22	1.92	0.51
1:C:410:ARG:HD2	2:D:9:DA:H2'	1.93	0.51
1:C:519:TYR:HB3	1:C:762:GLN:HB2	1.93	0.51
1:E:625:ASN:O	1:E:629:THR:HG23	2.11	0.51
1:G:369:LEU:HB3	1:G:380:TYR:CE2	2.46	0.51
1:C:241:ARG:O	1:C:245:GLU:HG2	2.11	0.51
1:E:334:ALA:HB1	1:E:423:ILE:HA	1.93	0.50
1:E:691:TRP:HB3	1:E:694:GLU:HG2	1.91	0.50
1:G:63:SER:OG	1:G:64:SER:N	2.42	0.50
1:G:249:ARG:O	1:G:251:ILE:N	2.44	0.50
1:G:451:ASP:OD1	1:G:452:GLU:N	2.44	0.50
1:G:679:PRO:HB3	1:G:739:LEU:HD21	1.94	0.50
1:G:837:LEU:HB3	1:G:913:LEU:HD23	1.93	0.50
1:C:567:ARG:NH2	1:C:676:ASP:OD2	2.44	0.50
1:C:916:GLN:OE1	1:C:936:LEU:N	2.33	0.50
1:E:332:PHE:HA	1:E:419:ALA:O	2.12	0.50
1:G:131:GLY:O	1:G:195:PRO:HG2	2.12	0.50
1:C:335:LEU:HD11	1:C:344:MET:HG2	1.94	0.50
1:G:580:LYS:HD3	1:G:580:LYS:H	1.76	0.50
1:A:471:LEU:HD22	1:A:476:VAL:HG21	1.93	0.50
1:E:605:TRP:CD1	1:E:605:TRP:C	2.85	0.50
1:G:551:LEU:HD23	1:G:757:ILE:HD11	1.92	0.50
1:G:618:LEU:HD23	1:G:940:LYS:HA	1.92	0.50
1:C:281:ASN:HB2	1:C:284:GLN:OE1	2.10	0.50
1:E:605:TRP:HD1	1:E:605:TRP:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:848:TRP:CD2	1:E:853:CYS:HB3	2.46	0.50
1:G:282:GLY:O	1:G:543:ILE:HD11	2.11	0.50
1:A:362:PRO:HB2	1:A:365:SER:HB2	1.93	0.50
1:E:447:VAL:HG22	1:E:477:PRO:HG2	1.94	0.50
1:A:32:TYR:HD1	1:A:228:LEU:HD13	1.77	0.50
1:A:28:ARG:O	1:A:28:ARG:CG	2.58	0.50
1:A:482:SER:OG	1:A:483:ALA:O	2.20	0.50
1:G:312:THR:HG22	1:G:316:TYR:HE2	1.76	0.50
1:G:407:LEU:CD2	1:G:407:LEU:N	2.75	0.50
1:E:150:HIS:ND1	2:F:11:DA:H5'	2.27	0.49
1:E:576:THR:HB	1:E:577:PRO:HD3	1.94	0.49
1:G:345:HIS:HA	1:G:420:VAL:HG11	1.93	0.49
1:G:588:ILE:HB	1:G:675:SER:HB2	1.95	0.49
1:G:649:ARG:CG	1:G:650:PRO:HD2	2.42	0.49
1:C:351:TYR:CZ	1:C:355:ARG:HD3	2.46	0.49
1:G:277:LEU:HD21	4:G:1003:ATP:C4	2.47	0.49
1:G:632:THR:O	1:G:635:ILE:HG22	2.12	0.49
1:C:16:LEU:HB3	1:C:181:ALA:HB1	1.94	0.49
1:C:842:ASP:O	1:C:845:GLY:HA3	2.12	0.49
1:A:495:LYS:O	1:A:499:GLU:HG3	2.12	0.49
1:C:844:ALA:N	1:C:845:GLY:CA	2.73	0.49
1:E:599:TYR:CD1	1:E:616:LEU:HD22	2.48	0.49
1:G:486:HIS:HD2	1:G:769:TYR:HD2	1.61	0.49
1:G:606:PHE:CD1	1:G:606:PHE:N	2.81	0.49
1:A:404:THR:CG2	1:A:407:LEU:H	2.26	0.49
1:A:627:GLN:HG2	1:A:631:ILE:HD11	1.94	0.49
1:C:586:ALA:HB2	1:C:670:VAL:HG11	1.95	0.49
1:G:43:ALA:O	1:G:47:VAL:HG23	2.13	0.49
1:A:34:LEU:HD23	1:A:88:LEU:HD22	1.94	0.49
1:C:407:LEU:HD21	1:C:416:ALA:HB2	1.95	0.49
1:C:523:LEU:HD21	1:C:532:VAL:HG13	1.94	0.49
1:G:51:GLU:HB3	1:G:261:ARG:HH12	1.78	0.49
1:A:550:PRO:O	1:A:708:PRO:HG2	2.12	0.49
1:C:103:TYR:O	1:C:175:TRP:NE1	2.46	0.49
1:E:919:THR:HG22	1:E:923:ALA:H	1.77	0.49
1:G:56:GLY:HA3	1:G:326:THR:O	2.13	0.49
1:G:290:HIS:ND1	1:G:538:VAL:HB	2.28	0.49
1:C:663:GLU:OE2	1:C:686:ARG:HD2	2.13	0.49
1:E:305:ALA:HB3	1:E:311:LYS:HE2	1.94	0.49
1:G:284:GLN:NE2	1:G:309:GLU:O	2.46	0.49
1:G:404:THR:HG22	1:G:407:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ARG:O	1:G:365:SER:HB3	2.13	0.48
1:A:771:ASP:OD1	1:G:507:ASN:ND2	2.47	0.48
1:C:276:HIS:ND1	1:C:277:LEU:N	2.60	0.48
1:C:358:ASN:N	1:C:358:ASN:ND2	2.60	0.48
1:G:268:ALA:CB	1:G:355:ARG:CZ	2.89	0.48
1:G:407:LEU:HD23	1:G:407:LEU:N	2.28	0.48
1:A:471:LEU:HB3	1:A:476:VAL:HG22	1.95	0.48
1:A:366:THR:HB	1:A:402:ALA:O	2.12	0.48
1:A:555:LEU:HD23	1:A:712:VAL:HB	1.95	0.48
1:E:634:THR:O	1:E:637:ASP:HB3	2.13	0.48
1:A:678:ALA:HB3	1:A:683:LEU:HD13	1.96	0.48
1:C:404:THR:CG2	1:C:407:LEU:HB2	2.42	0.48
1:E:281:ASN:ND2	1:E:309:GLU:OE1	2.46	0.48
1:G:25:ARG:HD2	1:G:26:GLY:N	2.27	0.48
1:G:454:HIS:CD2	1:G:483:ALA:HB3	2.48	0.48
1:C:274:PHE:HE1	1:C:351:TYR:CD2	2.32	0.48
1:E:234:ASP:OD1	1:E:236:SER:OG	2.29	0.48
1:G:51:GLU:HB3	1:G:261:ARG:NH1	2.29	0.48
1:A:410:ARG:H	1:A:410:ARG:NE	2.12	0.48
1:A:679:PRO:HG3	1:A:739:LEU:HD13	1.96	0.48
1:E:406:TRP:CH2	1:E:412:ARG:HD3	2.49	0.48
1:G:217:LEU:O	1:G:220:GLN:HG3	2.13	0.48
1:G:474:LEU:O	1:G:475:ASP:HB2	2.14	0.48
1:A:736:PRO:HG2	1:A:739:LEU:HB2	1.95	0.48
1:A:744:TYR:OH	1:A:748:ARG:NH1	2.46	0.48
1:A:876:LEU:HA	1:A:876:LEU:HD23	1.70	0.48
1:C:466:GLN:OE1	1:C:469:ARG:HD2	2.14	0.48
1:G:259:GLY:HA2	1:G:364:SER:O	2.13	0.48
1:A:275:PRO:HG3	1:A:354:TYR:OH	2.14	0.48
1:E:26:GLY:C	1:E:27:LEU:HD12	2.35	0.48
1:E:56:GLY:HA3	1:E:326:THR:O	2.14	0.48
1:E:491:ASN:OD1	1:E:513:PRO:HD2	2.13	0.48
1:E:522:TRP:HE3	1:E:523:LEU:N	2.12	0.48
1:G:125:PHE:HB2	1:G:165:LEU:HD13	1.95	0.48
1:G:606:PHE:CE2	1:G:614:PRO:HG3	2.49	0.48
1:E:22:ALA:HB2	1:E:34:LEU:HA	1.96	0.47
1:E:375:TRP:CZ3	1:E:381:ALA:HB1	2.49	0.47
1:E:586:ALA:HB3	1:E:673:MET:HG2	1.95	0.47
1:G:486:HIS:CE1	1:G:487:HIS:CD2	3.01	0.47
1:G:627:GLN:O	1:G:631:ILE:HG13	2.14	0.47
1:E:596:GLN:O	1:E:599:TYR:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:549:LYS:HB3	1:G:708:PRO:HG2	1.96	0.47
1:A:28:ARG:CG	1:A:30:LYS:NZ	2.77	0.47
1:C:459:TYR:CE2	1:C:794:LEU:HD23	2.48	0.47
1:E:848:TRP:CD1	1:E:853:CYS:SG	3.07	0.47
1:G:471:LEU:HB3	1:G:476:VAL:HG22	1.96	0.47
1:A:268:ALA:HB3	1:A:355:ARG:NH1	2.29	0.47
1:A:833:SER:H	2:B:6:DA:H61	1.62	0.47
1:E:604:GLN:O	1:E:608:THR:HG23	2.14	0.47
1:G:274:PHE:CE2	1:G:313:GLU:HG3	2.48	0.47
1:A:739:LEU:HD23	1:A:739:LEU:HA	1.72	0.47
1:C:303:ILE:HB	1:C:481:LEU:HD13	1.96	0.47
1:C:456:VAL:HG23	1:C:456:VAL:O	2.15	0.47
1:E:267:PRO:HB3	1:E:324:LYS:HE2	1.97	0.47
1:A:375:TRP:HB2	1:A:907:TYR:OH	2.14	0.47
1:C:39:LEU:O	1:C:42:ALA:N	2.46	0.47
1:C:706:LYS:HG3	1:C:707:GLN:H	1.80	0.47
1:E:55:PRO:HD2	1:E:327:GLY:O	2.14	0.47
1:E:376:LEU:HG	1:E:907:TYR:CZ	2.50	0.47
1:E:893:THR:H	1:E:896:ASN:ND2	2.13	0.47
1:G:937:ASP:HB3	1:G:940:LYS:HB2	1.96	0.47
1:A:376:LEU:N	1:A:376:LEU:HD22	2.30	0.47
1:C:205:SER:O	1:C:208:CYS:HB3	2.15	0.47
1:E:473:THR:HG21	1:E:803:PRO:HG2	1.97	0.47
1:G:367:LEU:HD22	1:G:418:TRP:HB2	1.96	0.47
1:C:17:ASP:H	1:C:178:GLN:HE22	1.63	0.47
1:C:263:ILE:CD1	1:C:365:SER:CB	2.93	0.47
1:C:683:LEU:HD12	1:C:683:LEU:HA	1.73	0.47
1:C:691:TRP:CD1	1:C:691:TRP:N	2.83	0.47
1:E:46:LEU:HD12	1:E:46:LEU:HA	1.60	0.47
1:G:789:LEU:HD23	1:G:789:LEU:HA	1.73	0.47
1:E:627:GLN:O	1:E:631:ILE:HG13	2.15	0.46
1:G:213:LEU:HD22	1:G:415:LEU:HD13	1.97	0.46
1:A:84:ASP:HB3	1:A:87:LYS:HD2	1.96	0.46
1:A:310:GLY:HA2	4:A:1003:ATP:O2A	2.15	0.46
1:E:410:ARG:C	1:E:411:LYS:CG	2.84	0.46
1:E:552:GLU:HB2	1:E:709:GLU:HG3	1.97	0.46
1:G:307:MET:HA	4:G:1003:ATP:O1B	2.15	0.46
1:G:840:TYR:OH	1:G:936:LEU:HD11	2.16	0.46
1:A:275:PRO:HG3	1:A:354:TYR:CZ	2.51	0.46
1:C:106:GLU:HG3	1:C:172:SER:CB	2.44	0.46
1:C:338:MET:HG2	1:C:371:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:GLY:HA3	1:E:806:ALA:O	2.15	0.46
1:E:410:ARG:O	1:E:411:LYS:HG2	2.15	0.46
1:E:606:PHE:CE2	1:E:614:PRO:CG	2.88	0.46
1:A:88:LEU:HG	1:A:179:ARG:HG2	1.98	0.46
1:C:407:LEU:CD2	1:C:416:ALA:HB2	2.45	0.46
1:C:486:HIS:CD2	1:C:766:ASP:HA	2.50	0.46
1:E:617:TYR:CG	1:E:635:ILE:HD11	2.50	0.46
1:E:869:THR:O	1:E:872:ASP:N	2.48	0.46
1:G:848:TRP:HB3	1:G:853:CYS:HA	1.97	0.46
1:A:849:LEU:HD13	1:A:857:PHE:HA	1.96	0.46
1:C:339:ALA:O	1:C:343:GLN:HG3	2.15	0.46
1:C:440:LEU:HD12	1:C:440:LEU:HA	1.67	0.46
1:C:493:LEU:HD23	1:C:493:LEU:HA	1.78	0.46
1:A:486:HIS:HE2	1:A:769:TYR:HB2	1.80	0.46
1:A:694:GLU:OE1	1:A:701:ARG:NE	2.48	0.46
1:C:122:TRP:CE3	1:C:123:LEU:HD12	2.51	0.46
1:C:319:ALA:O	1:C:323:GLY:N	2.48	0.46
1:G:22:ALA:HB2	1:G:34:LEU:HA	1.98	0.46
1:G:850:ASP:OD1	1:G:850:ASP:N	2.43	0.46
1:A:840:TYR:O	1:A:848:TRP:N	2.44	0.46
1:C:22:ALA:HB2	1:C:34:LEU:HA	1.97	0.46
1:C:364:SER:O	1:C:364:SER:OG	2.27	0.46
1:E:83:HIS:HD2	1:E:149:HIS:CD2	2.34	0.46
1:G:68:ASP:OD1	1:G:71:HIS:HB2	2.15	0.46
1:A:207:VAL:O	1:A:211:VAL:HG23	2.16	0.46
1:C:32:TYR:OH	1:C:40:ASP:OD2	2.21	0.46
1:C:258:ALA:O	1:C:407:LEU:HD12	2.16	0.46
1:G:284:GLN:CD	1:G:284:GLN:H	2.19	0.46
1:C:263:ILE:HD13	1:C:417:PRO:HB2	1.97	0.46
1:C:575:LEU:O	1:C:579:VAL:HG12	2.16	0.46
1:C:839:TYR:CZ	1:C:915:PRO:HB3	2.51	0.46
1:E:241:ARG:HD2	1:E:245:GLU:OE2	2.15	0.46
1:E:893:THR:H	1:E:896:ASN:HD22	1.63	0.46
1:G:666:LEU:O	1:G:689:ARG:NH1	2.49	0.46
1:C:148:GLY:HA2	1:C:152:THR:O	2.15	0.46
1:G:79:TRP:CE2	1:G:142:VAL:HG21	2.51	0.46
1:G:348:LEU:HD23	1:G:367:LEU:HD11	1.98	0.46
1:A:494:VAL:HG21	1:A:514:VAL:HG23	1.97	0.45
1:A:505:ARG:HB3	1:A:506:TRP:H	1.61	0.45
1:C:150:HIS:ND1	2:D:11:DA:H5'	2.31	0.45
1:C:269:THR:OG1	1:C:272:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:ASP:O	1:C:452:GLU:C	2.54	0.45
1:E:258:ALA:O	1:E:404:THR:HG21	2.16	0.45
1:E:471:LEU:HD22	1:E:476:VAL:HG21	1.98	0.45
1:G:132:TYR:HB3	1:G:139:THR:OG1	2.16	0.45
1:G:150:HIS:ND1	2:H:11:DA:H5'	2.29	0.45
1:G:649:ARG:HG2	1:G:650:PRO:HD2	1.98	0.45
1:A:261:ARG:HB3	1:A:364:SER:O	2.16	0.45
1:A:338:MET:HG2	1:A:371:HIS:CG	2.51	0.45
1:A:522:TRP:O	1:A:535:SER:HB3	2.17	0.45
1:C:70:GLU:O	1:C:74:HIS:ND1	2.41	0.45
1:C:406:TRP:O	1:C:412:ARG:HD3	2.15	0.45
1:C:453:ALA:O	1:C:456:VAL:HG22	2.16	0.45
1:A:145:MET:CE	1:A:146:LEU:HD13	2.46	0.45
1:A:635:ILE:O	1:A:639:PHE:HD1	1.99	0.45
1:A:841:VAL:HA	1:A:846:ASN:O	2.17	0.45
1:C:261:ARG:HA	1:C:262:PRO:HD3	1.80	0.45
1:G:286:SER:HB2	1:G:543:ILE:CD1	2.46	0.45
1:G:454:HIS:HA	1:G:485:LEU:HD13	1.97	0.45
1:G:543:ILE:HD12	1:G:544:ALA:H	1.82	0.45
1:A:51:GLU:HB3	1:A:261:ARG:NH1	2.31	0.45
1:A:351:TYR:OH	1:A:355:ARG:HD3	2.17	0.45
1:C:76:ILE:HD13	1:C:207:VAL:HG13	1.99	0.45
1:E:630:GLU:O	1:E:634:THR:HG23	2.15	0.45
1:A:398:ARG:HG2	1:A:399:ASP:H	1.81	0.45
1:C:17:ASP:OD2	1:C:19:ARG:NE	2.43	0.45
1:C:443:LEU:HD12	1:C:443:LEU:HA	1.73	0.45
1:E:48:LEU:HD12	1:E:52:TYR:HB3	1.98	0.45
1:E:404:THR:HG23	1:E:407:LEU:H	1.81	0.45
1:E:891:GLN:O	1:E:930:GLY:HA2	2.16	0.45
1:G:334:ALA:HB1	1:G:423:ILE:HA	1.98	0.45
1:C:898:PRO:HA	1:C:913:LEU:HD11	1.99	0.45
1:C:903:ARG:HA	1:C:909:ARG:HG3	1.99	0.45
1:E:457:ASP:H	1:E:460:MET:HE3	1.81	0.45
1:G:127:LEU:HD12	1:G:127:LEU:HA	1.84	0.45
1:G:270:PHE:CE2	1:G:284:GLN:HB3	2.52	0.45
1:A:32:TYR:HA	1:A:33:PRO:HD3	1.76	0.45
1:A:483:ALA:O	1:A:484:THR:C	2.54	0.45
1:A:664:GLN:O	1:A:689:ARG:NH2	2.50	0.45
1:C:412:ARG:O	1:C:413:GLY:C	2.55	0.45
1:C:618:LEU:HD23	1:C:940:LYS:HA	1.99	0.45
1:G:332:PHE:CE2	1:G:334:ALA:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HD12	1:A:52:TYR:CB	2.47	0.45
1:E:217:LEU:HD12	1:E:217:LEU:HA	1.73	0.45
1:E:459:TYR:CD1	1:E:795:ALA:HB2	2.52	0.45
1:E:670:VAL:HG21	1:E:673:MET:HG3	1.99	0.45
1:E:835:ARG:NH2	1:E:882:PRO:HD3	2.32	0.45
1:G:251:ILE:O	1:G:254:LEU:HB2	2.17	0.45
1:G:451:ASP:OD2	1:G:481:LEU:HD23	2.17	0.45
1:A:56:GLY:HA3	1:A:326:THR:O	2.17	0.45
1:A:246:THR:HG23	1:A:250:ARG:NH1	2.32	0.45
1:C:506:TRP:CH2	1:C:513:PRO:HD3	2.52	0.45
1:G:410:ARG:HH11	1:G:410:ARG:CG	2.26	0.45
1:G:606:PHE:N	1:G:606:PHE:HD1	2.14	0.45
1:A:496:ALA:O	1:A:499:GLU:HB2	2.16	0.44
1:A:902:TRP:C	1:A:904:GLU:H	2.20	0.44
1:A:902:TRP:O	1:A:904:GLU:N	2.51	0.44
1:C:96:ILE:HD12	1:C:97:ALA:H	1.81	0.44
1:C:294:LEU:HD21	1:C:533:THR:HG21	1.99	0.44
1:G:606:PHE:O	1:G:607:ALA:C	2.55	0.44
1:A:28:ARG:CD	1:A:30:LYS:HE3	2.39	0.44
1:G:451:ASP:HA	1:G:481:LEU:HB2	1.99	0.44
1:A:251:ILE:O	1:A:254:LEU:HB2	2.17	0.44
1:C:74:HIS:HD2	1:C:190:THR:O	2.00	0.44
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.74	0.44
1:E:74:HIS:HD2	1:E:190:THR:O	2.00	0.44
1:E:619:LEU:HA	1:E:619:LEU:HD12	1.80	0.44
1:G:87:LYS:HZ1	2:H:12:DA:P	2.40	0.44
1:G:350:GLU:HA	1:G:353:ARG:HB3	1.99	0.44
1:G:357:GLU:N	1:G:357:GLU:OE1	2.50	0.44
1:A:683:LEU:HD12	1:A:683:LEU:HA	1.71	0.44
1:A:902:TRP:CD1	1:A:902:TRP:N	2.85	0.44
1:C:49:TRP:CZ2	1:C:58:ARG:HG2	2.52	0.44
1:E:410:ARG:C	1:E:411:LYS:HG2	2.38	0.44
1:E:608:THR:C	1:E:610:GLY:H	2.20	0.44
1:G:84:ASP:OD2	1:G:87:LYS:NZ	2.49	0.44
1:G:504:ARG:HH11	1:G:504:ARG:CG	2.27	0.44
1:G:848:TRP:CE3	1:G:856:GLU:HA	2.52	0.44
1:G:893:THR:O	1:G:896:ASN:HB2	2.17	0.44
1:A:376:LEU:HD21	1:A:907:TYR:CD1	2.52	0.44
1:C:665:SER:O	1:C:665:SER:OG	2.29	0.44
1:E:599:TYR:HD1	1:E:616:LEU:HD22	1.82	0.44
1:A:613:ALA:HA	1:A:614:PRO:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ALA:N	1:A:845:GLY:HA2	2.33	0.44
1:C:80:ALA:HB2	1:C:211:VAL:HG22	2.00	0.44
1:G:605:TRP:O	1:G:605:TRP:CD1	2.70	0.44
4:G:1003:ATP:H5'1	4:G:1003:ATP:H8	1.83	0.44
1:A:65:MET:HG2	1:A:199:LEU:HD13	2.00	0.44
1:E:502:ARG:NH2	1:E:510:GLU:OE2	2.45	0.44
1:G:51:GLU:OE1	1:G:261:ARG:NH2	2.48	0.44
1:G:141:LEU:HA	1:G:141:LEU:HD23	1.71	0.44
1:G:561:LYS:HE3	1:G:561:LYS:HB2	1.82	0.44
1:A:265:VAL:HA	1:A:266:PRO:HD3	1.84	0.44
1:A:424:ASP:OD1	1:A:424:ASP:N	2.51	0.44
1:A:665:SER:C	1:A:666:LEU:CD1	2.85	0.44
1:E:146:LEU:HD12	1:E:146:LEU:HA	1.78	0.44
1:E:592:VAL:O	1:E:596:GLN:HG3	2.18	0.44
1:E:691:TRP:CZ3	1:E:708:PRO:HD3	2.53	0.44
1:A:808:ASP:OD1	1:A:808:ASP:N	2.51	0.44
1:C:16:LEU:O	1:C:16:LEU:HD12	2.17	0.44
1:C:44:ALA:O	1:C:48:LEU:HD22	2.17	0.44
1:E:459:TYR:CB	1:E:829:PHE:HB2	2.47	0.44
1:E:667:ASP:O	1:E:668:LEU:HD23	2.18	0.44
1:G:258:ALA:O	1:G:407:LEU:CD2	2.63	0.44
1:G:295:CYS:O	1:G:295:CYS:SG	2.75	0.44
1:G:462:VAL:HG23	1:G:792:ARG:HH11	1.82	0.44
1:G:490:ALA:O	1:G:494:VAL:HG13	2.17	0.44
1:G:520:PRO:HG3	1:G:545:THR:CG2	2.48	0.44
1:A:16:LEU:HB3	1:A:181:ALA:HB1	2.00	0.43
1:A:269:THR:OG1	1:A:272:GLU:HG3	2.17	0.43
1:G:315:ALA:HB2	1:G:481:LEU:HD11	1.99	0.43
1:G:677:LEU:HD11	1:G:743:THR:HG22	1.99	0.43
1:G:933:GLU:O	1:G:944:PHE:HA	2.18	0.43
1:A:156:HIS:HA	1:A:157:PRO:HD3	1.91	0.43
1:A:573:LYS:O	1:A:576:THR:OG1	2.35	0.43
1:C:549:LYS:HA	1:C:550:PRO:HD2	1.56	0.43
1:E:590:THR:HG21	1:E:731:TRP:HA	2.00	0.43
1:E:682:LEU:HD23	1:E:682:LEU:HA	1.69	0.43
1:E:691:TRP:HB3	1:E:694:GLU:CG	2.48	0.43
1:C:277:LEU:HD11	4:C:1003:ATP:N7	2.33	0.43
1:C:354:TYR:CD2	1:C:355:ARG:HG2	2.54	0.43
1:C:852:GLU:O	1:C:854:THR:HG23	2.18	0.43
1:E:87:LYS:HG2	1:E:92:PHE:CZ	2.53	0.43
1:A:410:ARG:C	1:A:411:LYS:CG	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:LEU:HB2	1:A:639:PHE:CD1	2.53	0.43
1:C:929:THR:HB	1:C:934:TRP:CD1	2.53	0.43
1:G:128:PRO:HA	1:G:132:TYR:O	2.19	0.43
1:G:375:TRP:CE2	1:G:408:MET:HG3	2.53	0.43
1:G:443:LEU:HA	1:G:443:LEU:HD12	1.72	0.43
1:E:306:PRO:HG3	1:E:519:TYR:CZ	2.53	0.43
1:E:554:ARG:NH1	1:E:574:GLU:OE2	2.48	0.43
1:E:599:TYR:O	1:E:603:SER:HB2	2.18	0.43
1:E:558:VAL:HG11	1:E:565:LEU:HB3	2.00	0.43
1:E:605:TRP:CD1	1:E:605:TRP:O	2.70	0.43
1:E:679:PRO:CG	1:E:739:LEU:HD13	2.48	0.43
1:G:506:TRP:CZ2	1:G:513:PRO:HD3	2.54	0.43
1:G:520:PRO:HG2	1:G:543:ILE:CG2	2.49	0.43
1:G:534:ARG:HG3	1:G:535:SER:N	2.34	0.43
1:A:200:ASP:OD2	1:A:202:PRO:HD2	2.18	0.43
1:A:320:ASP:HA	1:A:331:ARG:NH2	2.34	0.43
1:A:531:LYS:HD2	1:E:133:PRO:HB3	2.01	0.43
1:C:482:SER:OG	1:C:483:ALA:N	2.52	0.43
1:G:936:LEU:HG	1:G:936:LEU:O	2.19	0.43
1:A:634:THR:O	1:A:638:LEU:HG	2.18	0.43
1:C:72:ALA:O	1:C:76:ILE:HG13	2.18	0.43
1:C:405:ASP:O	1:C:408:MET:N	2.40	0.43
1:C:635:ILE:HD13	1:C:635:ILE:HA	1.93	0.43
1:G:506:TRP:CH2	1:G:511:PRO:C	2.91	0.43
1:A:373:MET:HA	1:A:373:MET:HE2	2.00	0.43
1:A:833:SER:N	2:B:6:DA:H61	2.17	0.43
1:A:842:ASP:HB2	1:A:843:THR:H	1.70	0.43
1:C:165:LEU:HD12	1:C:165:LEU:HA	1.67	0.43
1:E:440:LEU:HD12	1:E:440:LEU:HA	1.89	0.43
1:E:677:LEU:HD23	1:E:740:LEU:HD22	2.00	0.43
1:G:493:LEU:HD23	1:G:493:LEU:HA	1.89	0.43
1:G:694:GLU:HG2	1:G:701:ARG:NH2	2.33	0.43
1:G:869:THR:HG22	1:G:872:ASP:CG	2.39	0.43
1:G:916:GLN:OE1	1:G:935:LEU:HA	2.18	0.43
1:A:55:PRO:HD2	1:A:327:GLY:O	2.19	0.43
1:A:71:HIS:CE1	1:A:194:THR:HG1	2.37	0.43
1:A:202:PRO:O	1:A:205:SER:OG	2.27	0.43
1:A:367:LEU:HB3	1:A:401:PHE:HB3	2.01	0.43
1:A:908:LEU:O	1:A:911:LEU:HB2	2.19	0.43
1:C:223:PHE:CD1	1:C:254:LEU:HD21	2.54	0.43
1:C:263:ILE:HD11	1:C:365:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LEU:HD12	1:E:52:TYR:CB	2.48	0.43
1:E:333:LEU:HD12	1:E:344:MET:HG3	2.01	0.43
1:E:528:ARG:HH21	1:E:528:ARG:HB3	1.84	0.43
1:E:571:LEU:HD13	1:E:602:LEU:HD21	2.00	0.43
1:C:550:PRO:HG3	1:C:756:GLN:OE1	2.19	0.42
1:C:739:LEU:HD23	1:C:739:LEU:HA	1.77	0.42
1:C:842:ASP:OD1	1:C:845:GLY:HA2	2.19	0.42
1:E:458:PRO:O	1:E:462:VAL:HG23	2.19	0.42
1:G:495:LYS:O	1:G:499:GLU:HG3	2.18	0.42
1:G:571:LEU:HD11	1:G:598:VAL:HG22	2.01	0.42
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.80	0.42
1:A:456:VAL:HG23	1:A:456:VAL:O	2.20	0.42
1:C:49:TRP:HA	1:C:53:LEU:HD13	2.01	0.42
1:C:54:SER:HB3	1:C:329:PRO:HD2	2.00	0.42
1:C:126:ALA:O	1:C:129:SER:HB2	2.18	0.42
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.63	0.42
1:C:828:ARG:HG3	2:D:5:DA:N3	2.34	0.42
1:G:556:VAL:HG21	1:G:711:VAL:HG13	2.01	0.42
1:G:828:ARG:HB2	2:H:5:DA:C2	2.53	0.42
1:A:635:ILE:HD13	1:A:635:ILE:HA	1.91	0.42
1:E:170:PHE:HB3	1:E:179:ARG:NH2	2.34	0.42
1:E:466:GLN:NE2	1:E:800:ILE:O	2.46	0.42
1:G:32:TYR:HA	1:G:33:PRO:HD3	1.74	0.42
1:G:336:PRO:HG3	1:G:452:GLU:HG3	2.00	0.42
1:G:605:TRP:CE3	1:G:606:PHE:HE1	2.37	0.42
1:A:591:THR:HG22	2:B:2:DA:H5''	2.02	0.42
1:A:724:ALA:HA	1:A:725:PRO:HD3	1.82	0.42
1:A:789:LEU:HD23	1:A:789:LEU:HA	1.84	0.42
1:A:848:TRP:CD1	1:A:853:CYS:HB3	2.54	0.42
1:C:836:VAL:HB	1:C:914:ILE:HG12	2.01	0.42
1:C:919:THR:OG1	1:C:923:ALA:N	2.39	0.42
1:E:415:LEU:HA	1:E:415:LEU:HD23	1.79	0.42
1:E:502:ARG:HH22	1:E:510:GLU:CD	2.22	0.42
1:G:554:ARG:NH1	1:G:574:GLU:OE2	2.42	0.42
1:G:828:ARG:HG3	2:H:5:DA:N3	2.35	0.42
1:A:314:ALA:O	1:A:318:VAL:HG23	2.20	0.42
1:C:438:LEU:HD23	1:C:438:LEU:HA	1.86	0.42
1:E:311:LYS:HE3	1:E:311:LYS:HB2	1.86	0.42
1:G:588:ILE:HA	1:G:658:ALA:O	2.19	0.42
1:G:674:ILE:CG2	1:G:713:LEU:HD11	2.49	0.42
1:G:850:ASP:OD2	1:G:854:THR:OG1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:VAL:HG12	1:A:657:VAL:HG21	2.02	0.42
1:C:579:VAL:HG23	1:C:609:LEU:HD11	2.02	0.42
1:C:848:TRP:CG	1:C:853:CYS:HA	2.54	0.42
1:E:87:LYS:HE2	1:E:92:PHE:CZ	2.55	0.42
1:E:251:ILE:O	1:E:254:LEU:HB2	2.20	0.42
1:G:203:THR:O	1:G:207:VAL:HG23	2.20	0.42
1:G:439:ARG:NH1	1:G:439:ARG:HG3	2.35	0.42
1:G:676:ASP:HB3	1:G:731:TRP:CH2	2.54	0.42
1:A:256:ASP:HA	1:A:364:SER:HB2	2.02	0.42
1:A:398:ARG:HG2	1:A:399:ASP:N	2.35	0.42
1:A:828:ARG:HB2	2:B:5:DA:C2	2.54	0.42
1:A:840:TYR:N	1:A:848:TRP:O	2.46	0.42
1:C:46:LEU:O	1:C:49:TRP:HB3	2.19	0.42
1:E:691:TRP:CG	1:E:708:PRO:HB3	2.55	0.42
1:G:146:LEU:HD12	1:G:146:LEU:HA	1.93	0.42
1:A:453:ALA:O	1:A:456:VAL:HG13	2.20	0.42
1:A:627:GLN:O	1:A:631:ILE:HG13	2.19	0.42
1:C:881:ILE:HD13	1:C:881:ILE:HG21	1.86	0.42
1:E:49:TRP:HA	1:E:53:LEU:HD13	2.01	0.42
1:G:259:GLY:HA3	1:G:366:THR:HG23	2.02	0.42
1:G:313:GLU:OE2	4:G:1003:ATP:H2'	2.20	0.42
1:A:27:LEU:O	1:A:28:ARG:HB3	2.19	0.42
1:A:75:CYS:O	1:A:79:TRP:N	2.48	0.42
1:A:83:HIS:CG	1:A:84:ASP:N	2.88	0.42
1:A:893:THR:OG1	1:A:895:ASP:OD1	2.22	0.42
1:C:276:HIS:ND1	1:C:276:HIS:C	2.73	0.42
1:E:635:ILE:HG22	1:E:668:LEU:HD21	2.01	0.42
1:E:749:ARG:NH1	1:E:771:ASP:OD2	2.48	0.42
1:E:779:GLU:O	1:E:782:MET:N	2.53	0.42
1:C:200:ASP:N	1:C:200:ASP:OD1	2.53	0.42
1:E:842:ASP:OD1	1:E:845:GLY:CA	2.65	0.42
1:G:26:GLY:C	1:G:27:LEU:HD23	2.40	0.42
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.86	0.42
1:G:309:GLU:OE1	1:G:545:THR:HG22	2.20	0.42
1:G:523:LEU:HD21	1:G:532:VAL:HG13	2.01	0.42
1:G:529:ILE:HD11	1:G:531:LYS:HB2	2.02	0.42
1:G:810:LEU:O	1:G:813:LEU:HB2	2.19	0.42
1:A:219:SER:OG	2:B:11:DA:H2''	2.20	0.41
1:C:266:PRO:HA	1:C:267:PRO:HD3	1.95	0.41
1:E:49:TRP:CZ2	1:E:58:ARG:HG2	2.55	0.41
1:E:679:PRO:HG3	1:E:739:LEU:HD13	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:576:THR:O	1:G:579:VAL:HG22	2.20	0.41
1:G:621:SER:HG	2:H:3:DA:P	2.43	0.41
1:A:691:TRP:CZ2	1:A:701:ARG:HD2	2.54	0.41
1:C:65:MET:HE3	1:C:196:PRO:HG3	2.02	0.41
1:C:457:ASP:HB2	1:C:458:PRO:CD	2.50	0.41
1:C:666:LEU:HD23	1:C:666:LEU:HA	1.86	0.41
1:C:836:VAL:HG22	1:C:881:ILE:O	2.20	0.41
1:E:676:ASP:OD1	1:E:676:ASP:N	2.53	0.41
1:E:748:ARG:HA	1:E:748:ARG:HD3	1.84	0.41
1:G:310:GLY:HA3	4:G:1003:ATP:N7	2.35	0.41
1:G:376:LEU:HG	1:G:907:TYR:CZ	2.55	0.41
1:G:406:TRP:CE3	1:G:407:LEU:HD22	2.44	0.41
1:G:498:LEU:HD23	1:G:498:LEU:HA	1.95	0.41
1:G:576:THR:HB	1:G:577:PRO:HD3	2.02	0.41
1:A:100:LEU:HD13	1:A:175:TRP:CH2	2.56	0.41
1:A:745:THR:HG21	1:A:774:LEU:HA	2.03	0.41
1:C:270:PHE:C	1:C:270:PHE:CD1	2.93	0.41
1:G:337:THR:HG22	2:H:4:DA:O3'	2.20	0.41
1:G:410:ARG:C	1:G:411:LYS:CG	2.86	0.41
1:A:269:THR:HG23	1:A:272:GLU:OE1	2.20	0.41
1:A:671:ASP:OD1	1:A:701:ARG:HD3	2.21	0.41
1:C:83:HIS:HD2	1:C:149:HIS:CD2	2.38	0.41
1:C:461:GLN:O	1:C:465:GLU:HG3	2.20	0.41
1:E:16:LEU:HB2	1:E:181:ALA:HB1	2.03	0.41
1:G:549:LYS:HA	1:G:550:PRO:HD2	1.84	0.41
1:C:106:GLU:HG3	1:C:172:SER:HB2	2.01	0.41
1:C:148:GLY:HA3	1:C:153:PHE:CD1	2.55	0.41
1:C:491:ASN:OD1	1:C:513:PRO:HD2	2.21	0.41
1:G:407:LEU:HD23	1:G:407:LEU:H	1.85	0.41
1:G:551:LEU:HD11	1:G:553:VAL:HG13	2.02	0.41
1:G:676:ASP:HB3	1:G:731:TRP:CZ2	2.56	0.41
1:G:853:CYS:SG	1:G:918:VAL:HG11	2.60	0.41
1:A:48:LEU:HD12	1:A:52:TYR:HB2	2.02	0.41
1:C:39:LEU:HD23	1:C:39:LEU:HA	1.87	0.41
1:C:106:GLU:OE2	1:C:179:ARG:NH2	2.50	0.41
1:C:424:ASP:O	1:C:428:MET:HG3	2.20	0.41
1:C:937:ASP:OD2	1:C:940:LYS:N	2.54	0.41
1:G:410:ARG:NH1	2:H:9:DA:P	2.94	0.41
1:G:502:ARG:HG3	1:G:504:ARG:HG3	2.02	0.41
1:G:504:ARG:HG2	1:G:504:ARG:NH1	2.33	0.41
1:G:737:LEU:HD23	1:G:780:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:TRP:CZ3	1:A:381:ALA:HB1	2.56	0.41
1:A:474:LEU:O	1:A:475:ASP:HB2	2.20	0.41
2:B:5:DA:C6	2:B:6:DA:C6	3.09	0.41
1:C:832:GLY:HA2	2:D:5:DA:N6	2.28	0.41
1:E:414:LEU:HA	1:E:414:LEU:HD23	1.80	0.41
2:H:4:DA:H2''	2:H:5:DA:H5'	2.03	0.41
1:A:122:TRP:CE3	1:A:123:LEU:HD13	2.56	0.41
1:A:520:PRO:HG3	1:A:545:THR:HG23	2.03	0.41
1:C:270:PHE:HE2	1:C:284:GLN:HB3	1.85	0.41
1:G:34:LEU:HD23	1:G:88:LEU:HD22	2.02	0.41
1:G:272:GLU:O	1:G:275:PRO:HD3	2.21	0.41
1:G:836:VAL:HG23	1:G:881:ILE:HG23	2.02	0.41
1:A:375:TRP:CZ2	1:A:408:MET:HG2	2.56	0.41
1:A:450:VAL:HG22	1:A:480:LEU:HD12	2.03	0.41
1:C:263:ILE:HD12	1:C:365:SER:CB	2.51	0.41
1:C:314:ALA:O	1:C:318:VAL:HG23	2.20	0.41
1:G:20:PHE:HA	1:G:93:GLN:OE1	2.21	0.41
1:G:76:ILE:HA	1:G:79:TRP:CE3	2.55	0.41
1:G:471:LEU:HD22	1:G:476:VAL:CG2	2.51	0.41
1:G:519:TYR:HA	1:G:520:PRO:HA	1.86	0.41
1:G:534:ARG:HG3	1:G:535:SER:H	1.85	0.41
1:G:619:LEU:HA	1:G:619:LEU:HD12	1.83	0.41
4:G:1003:ATP:H5'1	4:G:1003:ATP:C8	2.56	0.41
1:A:495:LYS:NZ	1:A:512:GLN:OE1	2.49	0.41
1:C:156:HIS:HA	1:C:157:PRO:HD3	1.90	0.41
1:E:265:VAL:HA	1:E:266:PRO:HD3	1.76	0.41
1:G:16:LEU:HD21	1:G:35:VAL:HG11	2.03	0.41
1:G:78:PHE:CE1	1:G:82:LEU:HD11	2.56	0.41
1:G:632:THR:O	1:G:636:VAL:HG22	2.20	0.41
1:G:680:VAL:O	1:G:684:LEU:HD22	2.21	0.41
1:G:772:ASP:OD1	1:G:772:ASP:N	2.54	0.41
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.83	0.40
1:A:291:LEU:HD12	1:A:291:LEU:HA	1.91	0.40
1:A:334:ALA:HB1	1:A:423:ILE:HA	2.04	0.40
1:E:187:PHE:CE1	1:E:193:PRO:HD2	2.55	0.40
1:E:578:LEU:CD1	1:E:583:GLY:CA	2.99	0.40
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.78	0.40
1:G:345:HIS:CD2	1:G:367:LEU:HD12	2.57	0.40
1:G:899:PRO:O	1:G:900:GLU:C	2.60	0.40
1:A:454:HIS:HB3	1:A:482:SER:OG	2.22	0.40
1:C:838:CYS:HA	1:C:914:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:TYR:CG	1:E:829:PHE:HB2	2.55	0.40
1:E:742:ARG:HH11	1:E:742:ARG:HD2	1.71	0.40
1:G:407:LEU:CD1	1:G:416:ALA:HB2	2.50	0.40
1:A:150:HIS:ND1	2:B:11:DA:H5'	2.37	0.40
1:A:439:ARG:HG3	1:A:439:ARG:NH1	2.35	0.40
1:C:49:TRP:CH2	1:C:58:ARG:HG2	2.57	0.40
1:C:454:HIS:HB3	1:C:482:SER:OG	2.21	0.40
1:E:172:SER:HA	1:E:173:PRO:HD3	1.84	0.40
1:E:443:LEU:HD12	1:E:443:LEU:HA	1.90	0.40
1:E:583:GLY:O	1:E:653:GLY:HA2	2.21	0.40
1:G:351:TYR:O	1:G:355:ARG:HB3	2.20	0.40
1:G:660:GLN:HB3	1:G:663:GLU:OE1	2.21	0.40
1:G:699:ILE:O	1:G:699:ILE:HG13	2.21	0.40
1:A:480:LEU:C	1:A:481:LEU:HD13	2.41	0.40
1:C:428:MET:C	1:C:439:ARG:HD3	2.42	0.40
1:E:691:TRP:CE3	1:E:708:PRO:HD3	2.56	0.40
1:G:217:LEU:HA	1:G:217:LEU:HD12	1.83	0.40
1:G:580:LYS:N	1:G:580:LYS:CD	2.73	0.40
1:G:937:ASP:HA	1:G:938:PRO:HD2	1.91	0.40
1:A:439:ARG:HG3	1:A:439:ARG:HH11	1.87	0.40
1:C:37:HIS:CE1	1:C:215:ASP:OD1	2.74	0.40
1:C:259:GLY:HA3	1:C:366:THR:CG2	2.51	0.40
1:C:265:VAL:HA	1:C:266:PRO:HD3	1.86	0.40
1:C:275:PRO:CD	1:C:354:TYR:CZ	3.04	0.40
1:C:451:ASP:HA	1:C:481:LEU:HB2	2.03	0.40
1:C:842:ASP:O	1:C:845:GLY:CA	2.70	0.40
1:E:24:GLU:OE1	1:E:25:ARG:HG2	2.21	0.40
1:E:405:ASP:O	1:E:408:MET:HB2	2.21	0.40
1:E:742:ARG:NH1	1:E:784:ARG:HH11	2.19	0.40
1:G:306:PRO:HD2	1:G:309:GLU:HG3	2.02	0.40
1:G:377:ASN:HA	1:G:378:PRO:HD3	1.84	0.40
1:G:676:ASP:OD1	1:G:676:ASP:N	2.54	0.40
1:G:841:VAL:O	1:G:918:VAL:HG12	2.21	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%)	825 (93%)	60 (7%)	4 (0%)	34	68
1	C	887/964 (92%)	803 (90%)	79 (9%)	5 (1%)	25	60
1	E	891/964 (92%)	844 (95%)	46 (5%)	1 (0%)	51	82
1	G	869/964 (90%)	792 (91%)	75 (9%)	2 (0%)	47	78
All	All	3536/3856 (92%)	3264 (92%)	260 (7%)	12 (0%)	41	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	GLN
1	A	749	ARG
1	C	374	ALA
1	C	660	GLN
1	G	752	GLY
1	C	540	PRO
1	G	250	ARG
1	A	903	ARG
1	A	687	ALA
1	E	660	GLN
1	C	543	ILE
1	C	550	PRO

### 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	746/796 (94%)	655 (88%)	91 (12%)	5	20
1	C	740/796 (93%)	641 (87%)	99 (13%)	4	17
1	E	741/796 (93%)	669 (90%)	72 (10%)	8	31
1	G	734/796 (92%)	635 (86%)	99 (14%)	4	17
All	All	2961/3184 (93%)	2600 (88%)	361 (12%)	5	20

All (361) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	28	ARG
1	A	30	LYS
1	A	35	VAL
1	A	48	LEU
1	A	53	LEU
1	A	58	ARG
1	A	68	ASP
1	A	88	LEU
1	A	101	SER
1	A	123	LEU
1	A	127	LEU
1	A	130	LEU
1	A	146	LEU
1	A	165	LEU
1	A	198	MET
1	A	217	LEU
1	A	228	LEU
1	A	238	SER
1	A	253	SER
1	A	254	LEU
1	A	264	THR
1	A	271	THR
1	A	279	LYS
1	A	281	ASN
1	A	283	LEU
1	A	293	CYS
1	A	333	LEU
1	A	358	ASN
1	A	359	THR
1	A	361	LEU
1	A	366	THR
1	A	367	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	375	TRP
1	A	410	ARG
1	A	420	VAL
1	A	424	ASP
1	A	431	LEU
1	A	432	ARG
1	A	438	LEU
1	A	440	LEU
1	A	443	LEU
1	A	446	LYS
1	A	448	VAL
1	A	457	ASP
1	A	464	LEU
1	A	473	THR
1	A	474	LEU
1	A	480	LEU
1	A	481	LEU
1	A	488	SER
1	A	504	ARG
1	A	518	SER
1	A	523	LEU
1	A	528	ARG
1	A	541	LEU
1	A	548	ARG
1	A	551	LEU
1	A	553	VAL
1	A	560	VAL
1	A	576	THR
1	A	579	VAL
1	A	581	GLN
1	A	601	LEU
1	A	634	THR
1	A	635	ILE
1	A	673	MET
1	A	680	VAL
1	A	681	SER
1	A	683	LEU
1	A	690	CYS
1	A	714	THR
1	A	730	SER
1	A	739	LEU
1	A	789	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	792	ARG
1	A	804	ASP
1	A	816	PHE
1	A	817	SER
1	A	818	PHE
1	A	833	SER
1	A	842	ASP
1	A	843	THR
1	A	849	LEU
1	A	852	GLU
1	A	864	ARG
1	A	892	LEU
1	A	894	GLU
1	A	908	LEU
1	A	928	GLU
1	A	939	CYS
1	C	16	LEU
1	C	24	GLU
1	C	25	ARG
1	C	28	ARG
1	C	35	VAL
1	C	48	LEU
1	C	54	SER
1	C	70	GLU
1	C	88	LEU
1	C	91	GLU
1	C	113	ARG
1	C	123	LEU
1	C	127	LEU
1	C	130	LEU
1	C	134	ASN
1	C	137	LEU
1	C	139	THR
1	C	145	MET
1	C	152	THR
1	C	158	SER
1	C	186	VAL
1	C	202	PRO
1	C	217	LEU
1	C	250	ARG
1	C	253	SER
1	C	254	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	270	PHE
1	C	271	THR
1	C	278	SER
1	C	279	LYS
1	C	281	ASN
1	C	283	LEU
1	C	311	LYS
1	C	333	LEU
1	C	355	ARG
1	C	356	VAL
1	C	366	THR
1	C	367	LEU
1	C	407	LEU
1	C	411	LYS
1	C	414	LEU
1	C	420	VAL
1	C	431	LEU
1	C	438	LEU
1	C	439	ARG
1	C	440	LEU
1	C	443	LEU
1	C	448	VAL
1	C	450	VAL
1	C	452	GLU
1	C	464	LEU
1	C	473	THR
1	C	474	LEU
1	C	476	VAL
1	C	481	LEU
1	C	487	HIS
1	C	492	SER
1	C	494	VAL
1	C	518	SER
1	C	538	VAL
1	C	541	LEU
1	C	567	ARG
1	C	570	VAL
1	C	574	GLU
1	C	579	VAL
1	C	599	TYR
1	C	602	LEU
1	C	605	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	621	SER
1	C	629	THR
1	C	651	THR
1	C	655	VAL
1	C	662	VAL
1	C	680	VAL
1	C	683	LEU
1	C	692	ARG
1	C	701	ARG
1	C	703	GLN
1	C	729	ARG
1	C	734	VAL
1	C	739	LEU
1	C	745	THR
1	C	763	GLN
1	C	824	VAL
1	C	827	THR
1	C	833	SER
1	C	838	CYS
1	C	876	LEU
1	C	881	ILE
1	C	893	THR
1	C	910	ASP
1	C	919	THR
1	C	920	ASP
1	C	921	GLU
1	C	924	VAL
1	C	925	LEU
1	C	932	ARG
1	C	939	CYS
1	C	944	PHE
1	E	16	LEU
1	E	35	VAL
1	E	48	LEU
1	E	67	THR
1	E	88	LEU
1	E	121	LYS
1	E	123	LEU
1	E	127	LEU
1	E	129	SER
1	E	137	LEU
1	E	146	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	165	LEU
1	E	172	SER
1	E	194	THR
1	E	217	LEU
1	E	228	LEU
1	E	230	SER
1	E	246	THR
1	E	248	LEU
1	E	250	ARG
1	E	254	LEU
1	E	264	THR
1	E	265	VAL
1	E	271	THR
1	E	279	LYS
1	E	283	LEU
1	E	296	THR
1	E	307	MET
1	E	355	ARG
1	E	356	VAL
1	E	366	THR
1	E	367	LEU
1	E	375	TRP
1	E	408	MET
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	476	VAL
1	E	508	ARG
1	E	510	GLU
1	E	518	SER
1	E	528	ARG
1	E	553	VAL
1	E	574	GLU
1	E	584	CYS
1	E	603	SER
1	E	608	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	615	ASP
1	E	616	LEU
1	E	628	ARG
1	E	636	VAL
1	E	652	ARG
1	E	673	MET
1	E	684	LEU
1	E	694	GLU
1	E	698	ILE
1	E	729	ARG
1	E	734	VAL
1	E	739	LEU
1	E	742	ARG
1	E	843	THR
1	E	849	LEU
1	E	865	GLU
1	E	881	ILE
1	E	920	ASP
1	E	929	THR
1	G	16	LEU
1	G	24	GLU
1	G	35	VAL
1	G	48	LEU
1	G	53	LEU
1	G	57	LEU
1	G	58	ARG
1	G	63	SER
1	G	70	GLU
1	G	75	CYS
1	G	88	LEU
1	G	113	ARG
1	G	121	LYS
1	G	123	LEU
1	G	127	LEU
1	G	137	LEU
1	G	146	LEU
1	G	152	THR
1	G	158	SER
1	G	161	SER
1	G	165	LEU
1	G	186	VAL
1	G	200	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	217	LEU
1	G	228	LEU
1	G	249	ARG
1	G	254	LEU
1	G	264	THR
1	G	271	THR
1	G	281	ASN
1	G	283	LEU
1	G	287	LEU
1	G	295	CYS
1	G	296	THR
1	G	300	LEU
1	G	311	LYS
1	G	338	MET
1	G	340	THR
1	G	366	THR
1	G	367	LEU
1	G	370	LEU
1	G	373	MET
1	G	375	TRP
1	G	407	LEU
1	G	408	MET
1	G	410	ARG
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	481	LEU
1	G	504	ARG
1	G	505	ARG
1	G	507	ASN
1	G	509	SER
1	G	528	ARG
1	G	529	ILE
1	G	534	ARG
1	G	541	LEU
1	G	548	ARG
1	G	551	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	553	VAL
1	G	568	SER
1	G	580	LYS
1	G	591	THR
1	G	672	LEU
1	G	683	LEU
1	G	684	LEU
1	G	690	CYS
1	G	698	ILE
1	G	699	ILE
1	G	709	GLU
1	G	718	ASN
1	G	734	VAL
1	G	739	LEU
1	G	745	THR
1	G	755	VAL
1	G	763	GLN
1	G	764	LEU
1	G	782	MET
1	G	789	LEU
1	G	804	ASP
1	G	855	VAL
1	G	856	GLU
1	G	864	ARG
1	G	869	THR
1	G	885	MET
1	G	895	ASP
1	G	898	PRO
1	G	924	VAL
1	G	925	LEU
1	G	936	LEU
1	G	939	CYS
1	G	943	ILE
1	G	944	PHE

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	281	ASN
1	A	897	HIS
1	C	358	ASN
1	C	486	HIS

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Mol	Chain	Res	Type
1	C	645	GLN
1	E	94	GLN
1	E	290	HIS
1	E	707	GLN
1	E	896	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	ATP	E	1003	-	26,33,33	1.06	1 (3%)	31,52,52	1.57	7 (22%)
4	ATP	C	1003	-	26,33,33	1.00	1 (3%)	31,52,52	1.73	5 (16%)
4	ATP	G	1003	-	26,33,33	0.96	1 (3%)	31,52,52	1.51	5 (16%)
4	ATP	A	1003	-	26,33,33	1.06	1 (3%)	31,52,52	1.43	6 (19%)

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	ATP	E	1003	-	-	7/18/38/38	0/3/3/3
4	ATP	C	1003	-	-	3/18/38/38	0/3/3/3
4	ATP	G	1003	-	-	8/18/38/38	0/3/3/3
4	ATP	A	1003	-	-	4/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	ATP	C2'-C1'	-2.17	1.50	1.53
4	E	1003	ATP	C2'-C1'	-2.13	1.50	1.53
4	C	1003	ATP	C5-C4	2.10	1.46	1.40
4	G	1003	ATP	C5-C4	2.03	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1003	ATP	PA-O3A-PB	-4.34	117.95	132.83
4	C	1003	ATP	PB-O3B-PG	-4.14	118.61	132.83
4	A	1003	ATP	PA-O3A-PB	-4.07	118.86	132.83
4	C	1003	ATP	PA-O3A-PB	-4.01	119.06	132.83
4	C	1003	ATP	N3-C2-N1	-3.96	122.49	128.68
4	E	1003	ATP	PA-O3A-PB	-3.69	120.15	132.83
4	E	1003	ATP	N3-C2-N1	-3.49	123.22	128.68
4	G	1003	ATP	N3-C2-N1	-3.01	123.97	128.68
4	A	1003	ATP	N3-C2-N1	-2.90	124.15	128.68
4	A	1003	ATP	C4-C5-N7	-2.70	106.59	109.40
4	E	1003	ATP	PB-O3B-PG	-2.61	123.86	132.83
4	G	1003	ATP	C4-C5-N7	-2.56	106.73	109.40
4	E	1003	ATP	C4-C5-N7	-2.37	106.93	109.40
4	G	1003	ATP	PB-O3B-PG	-2.33	124.83	132.83
4	A	1003	ATP	O4'-C1'-C2'	-2.27	103.61	106.93
4	E	1003	ATP	O3G-PG-O2G	2.13	115.79	107.64
4	C	1003	ATP	O3'-C3'-C2'	-2.13	104.93	111.82
4	C	1003	ATP	C2-N1-C6	2.13	122.39	118.75
4	A	1003	ATP	PB-O3B-PG	-2.11	125.58	132.83
4	G	1003	ATP	O3'-C3'-C2'	-2.08	105.10	111.82
4	E	1003	ATP	C2-N1-C6	2.06	122.29	118.75
4	E	1003	ATP	O3'-C3'-C2'	-2.02	105.28	111.82
4	A	1003	ATP	O3G-PG-O2G	2.01	115.33	107.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	ATP	C5'-O5'-PA-O3A
4	C	1003	ATP	C5'-O5'-PA-O3A
4	E	1003	ATP	PB-O3B-PG-O2G
4	E	1003	ATP	C5'-O5'-PA-O1A
4	G	1003	ATP	C5'-O5'-PA-O2A
4	G	1003	ATP	O4'-C4'-C5'-O5'
4	G	1003	ATP	C3'-C4'-C5'-O5'
4	E	1003	ATP	C3'-C4'-C5'-O5'
4	E	1003	ATP	O4'-C4'-C5'-O5'
4	G	1003	ATP	C5'-O5'-PA-O3A
4	G	1003	ATP	PB-O3A-PA-O1A
4	A	1003	ATP	C5'-O5'-PA-O1A
4	A	1003	ATP	C5'-O5'-PA-O2A
4	C	1003	ATP	C5'-O5'-PA-O1A
4	E	1003	ATP	C5'-O5'-PA-O2A
4	G	1003	ATP	C5'-O5'-PA-O1A
4	E	1003	ATP	PB-O3B-PG-O3G
4	E	1003	ATP	C5'-O5'-PA-O3A
4	C	1003	ATP	O4'-C4'-C5'-O5'
4	A	1003	ATP	PB-O3A-PA-O1A
4	G	1003	ATP	PG-O3B-PB-O1B
4	G	1003	ATP	PB-O3A-PA-O2A

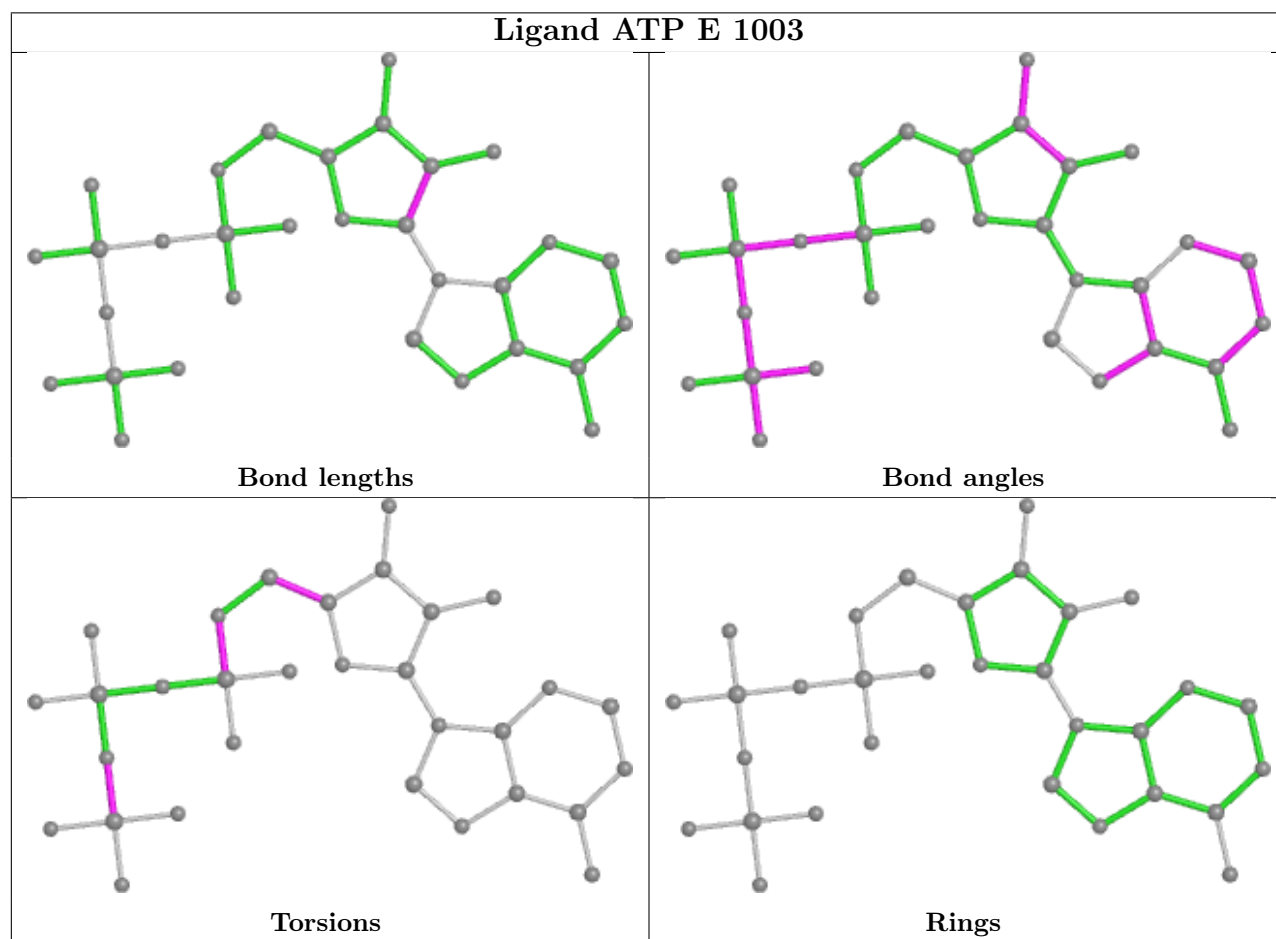
There are no ring outliers.

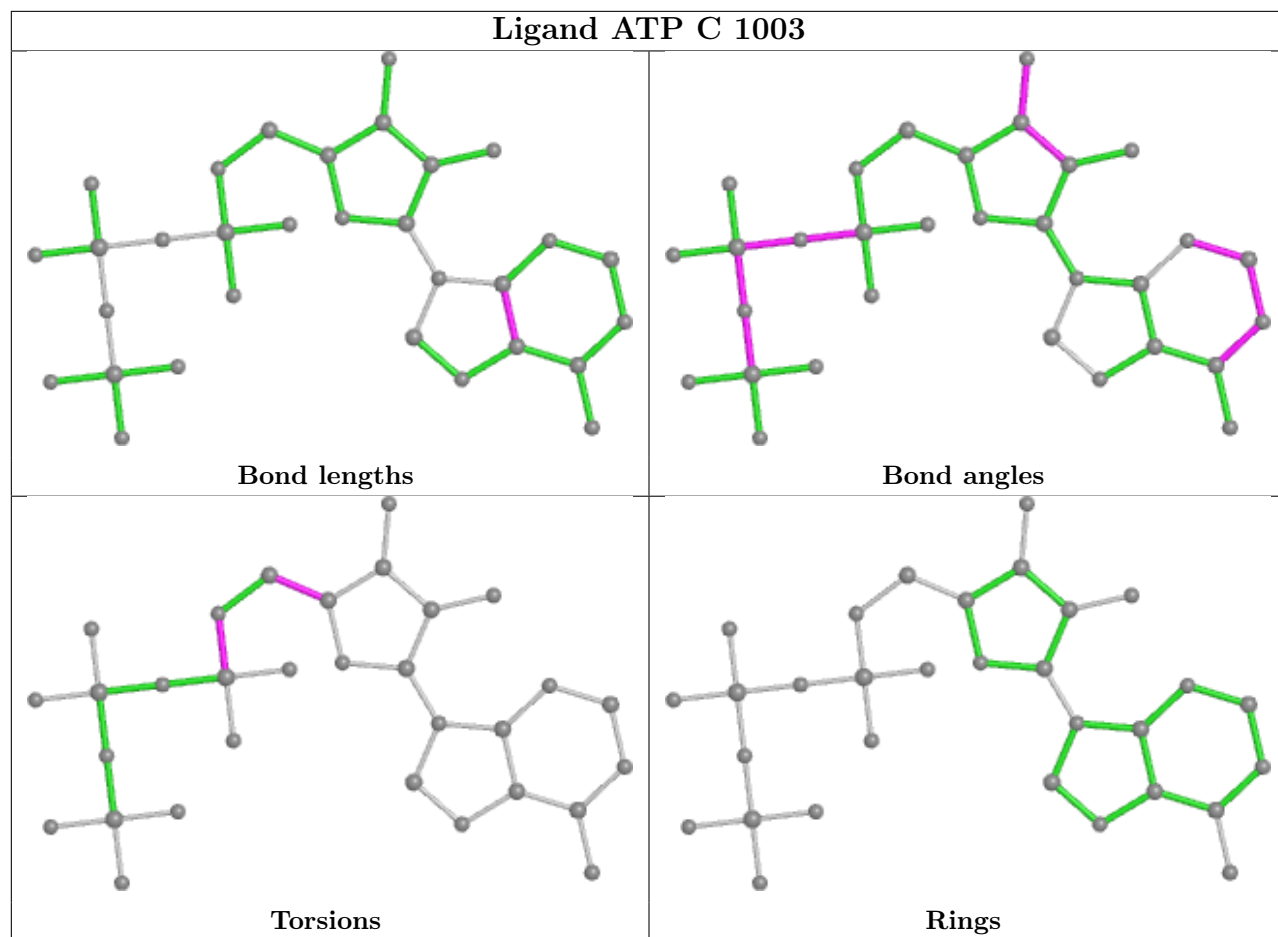
4 monomers are involved in 16 short contacts:

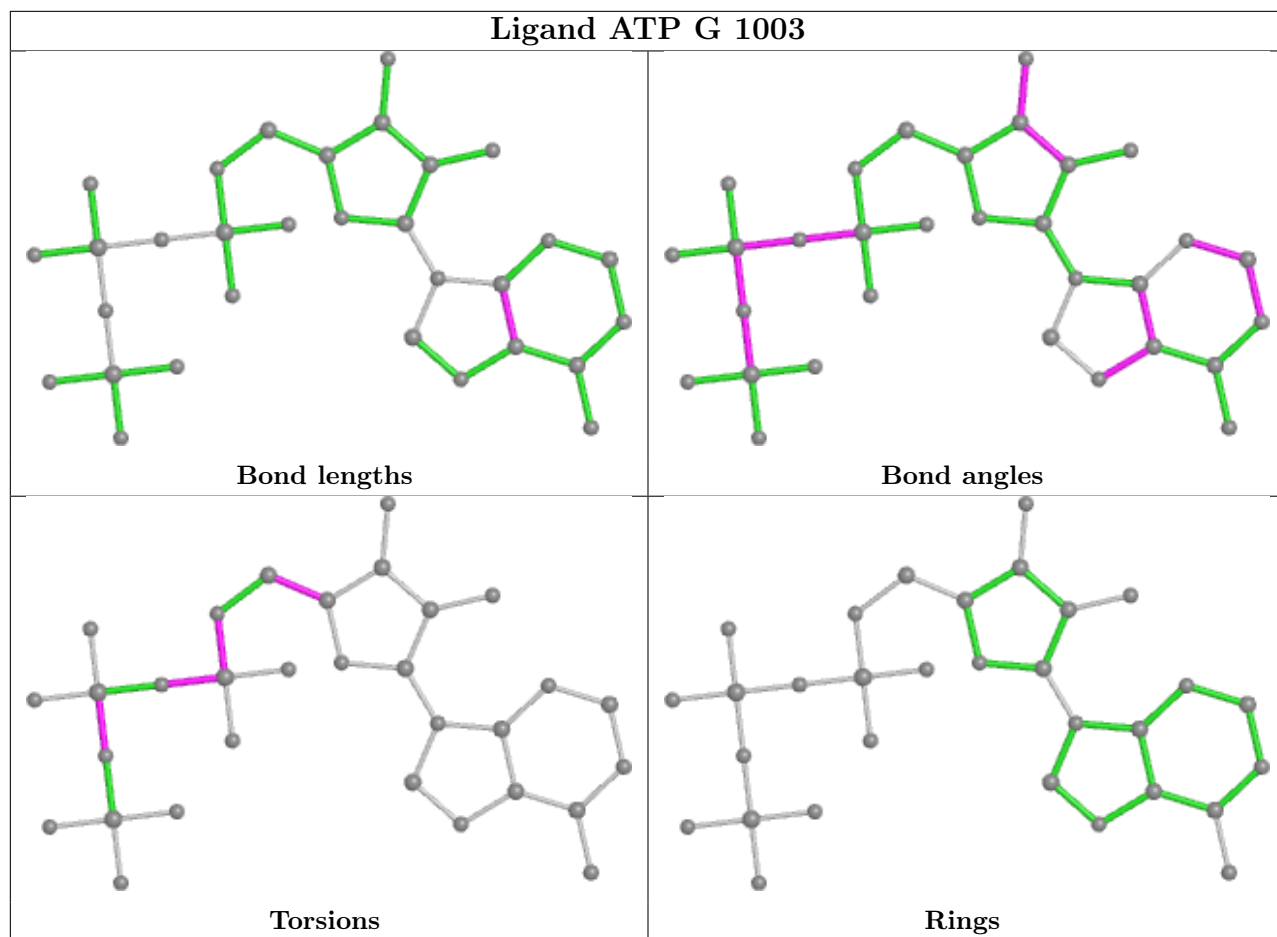
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1003	ATP	2	0
4	C	1003	ATP	6	0
4	G	1003	ATP	7	0
4	A	1003	ATP	1	0

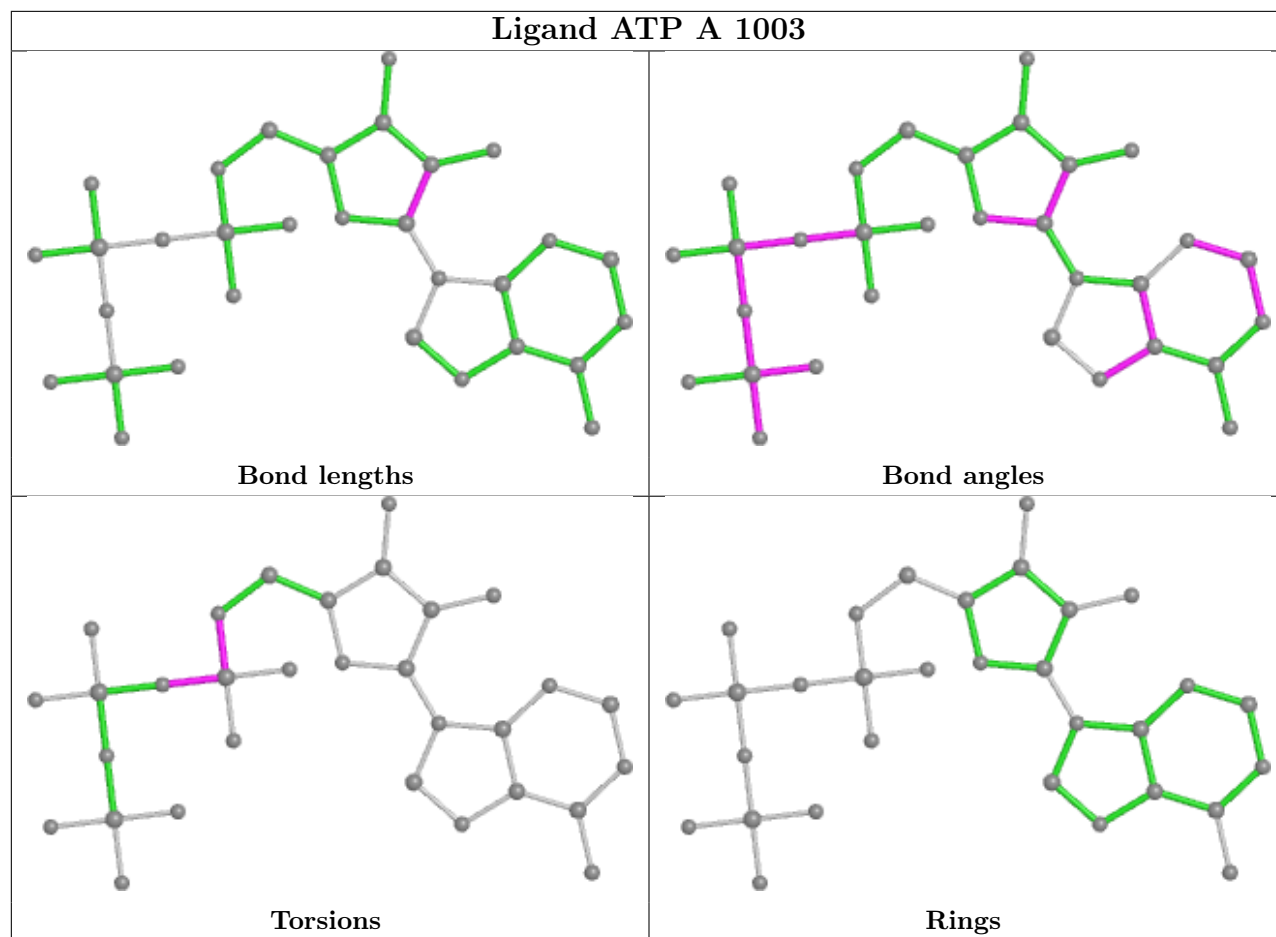
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	903/964 (93%)	-0.20	16 (1%) 68 67	61, 100, 153, 226	0
1	C	899/964 (93%)	-0.19	11 (1%) 79 79	65, 105, 153, 202	0
1	E	901/964 (93%)	-0.26	9 (0%) 82 83	57, 91, 141, 181	0
1	G	887/964 (92%)	-0.12	9 (1%) 82 83	66, 114, 170, 234	0
2	B	11/12 (91%)	0.75	0 100 100	95, 98, 170, 217	0
2	D	11/12 (91%)	0.46	0 100 100	91, 106, 184, 194	0
2	F	11/12 (91%)	0.96	2 (18%) 1 1	80, 95, 175, 217	0
2	H	11/12 (91%)	0.28	0 100 100	94, 113, 199, 208	0
All	All	3634/3904 (93%)	-0.18	47 (1%) 77 78	57, 103, 157, 234	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	849	LEU	4.3
1	A	654	ALA	3.6
1	G	857	PHE	3.5
1	A	359	THR	3.3
1	E	857	PHE	3.1
1	G	665	SER	3.0
1	A	360	ASP	2.9
1	A	655	VAL	2.8
1	C	563	GLY	2.7
1	E	663	GLU	2.7
1	C	865	GLU	2.7
1	A	857	PHE	2.7
1	C	565	LEU	2.6
1	A	613	ALA	2.6
2	F	3	DA	2.5
1	A	841	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	849	LEU	2.5
1	G	873	CYS	2.5
1	G	452	GLU	2.4
1	G	655	VAL	2.4
1	A	14	PRO	2.4
1	C	575	LEU	2.3
1	A	859	GLU	2.3
1	G	685	GLN	2.3
1	A	858	PRO	2.3
1	G	522	TRP	2.3
1	C	703	GLN	2.3
1	A	860	GLN	2.3
1	C	665	SER	2.2
1	C	664	GLN	2.2
1	E	27	LEU	2.2
1	E	868	PHE	2.2
1	A	583	GLY	2.2
1	E	677	LEU	2.2
1	C	28	ARG	2.2
1	C	567	ARG	2.2
1	G	664	GLN	2.2
1	E	859	GLU	2.1
1	G	837	LEU	2.1
1	E	665	SER	2.1
1	C	307	MET	2.1
1	A	847	ARG	2.0
1	A	837	LEU	2.0
1	C	454	HIS	2.0
1	A	358	ASN	2.0
2	F	4	DA	2.0
1	E	655	VAL	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

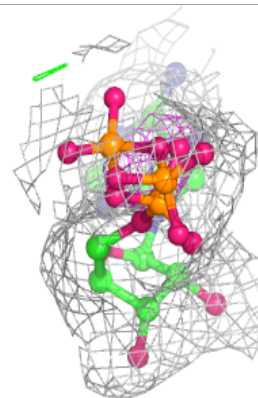
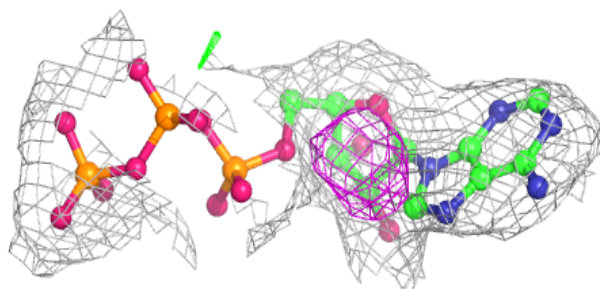
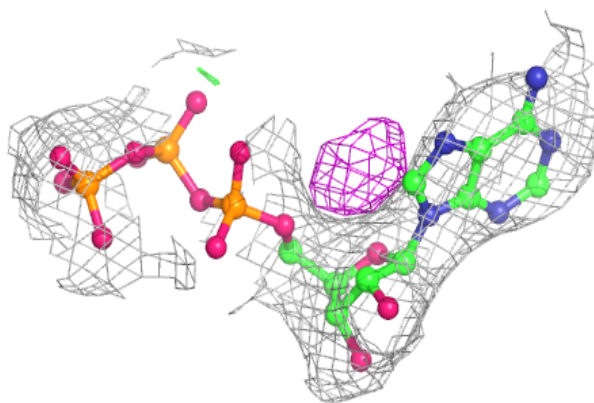
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ATP	A	1003	31/31	0.86	0.23	97,119,131,132	0
4	ATP	C	1003	31/31	0.86	0.22	124,143,160,164	0
4	ATP	G	1003	31/31	0.86	0.26	128,151,159,161	0
4	ATP	E	1003	31/31	0.93	0.21	91,111,120,128	0
3	FE	A	1001	1/1	0.95	0.20	79,79,79,79	0
3	FE	E	1001	1/1	0.95	0.18	80,80,80,80	0
3	FE	C	1002	1/1	0.96	0.17	82,82,82,82	0
3	FE	G	1002	1/1	0.98	0.16	79,79,79,79	0
3	FE	C	1001	1/1	0.99	0.17	77,77,77,77	0
3	FE	E	1002	1/1	0.99	0.15	70,70,70,70	0
3	FE	G	1001	1/1	0.99	0.15	77,77,77,77	0
3	FE	A	1002	1/1	0.99	0.17	73,73,73,73	0

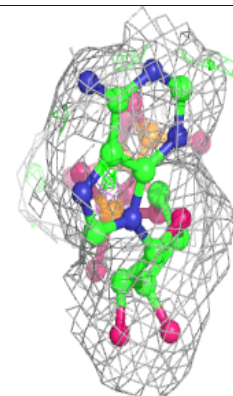
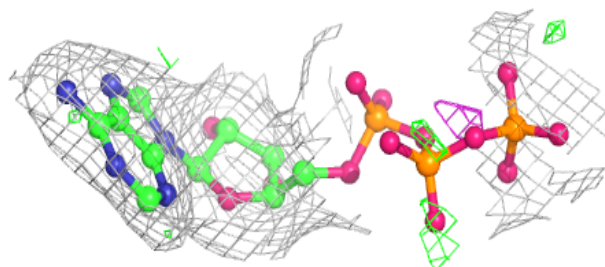
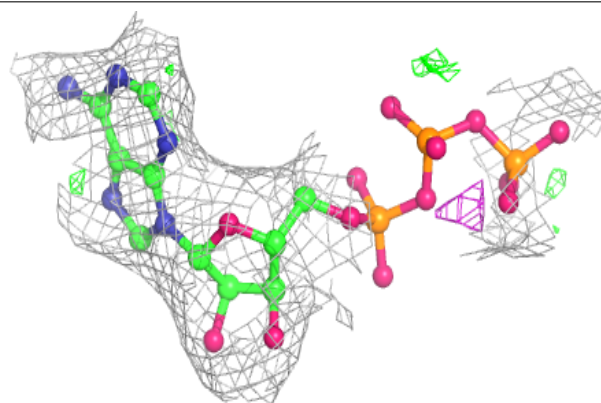
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP 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)

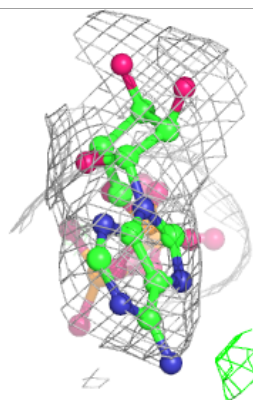
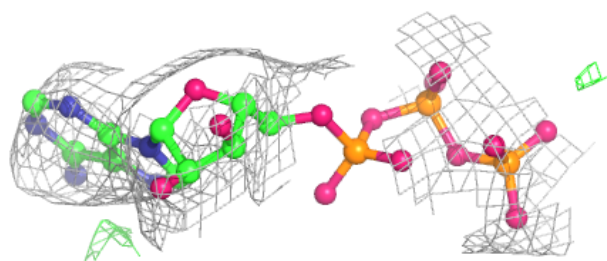
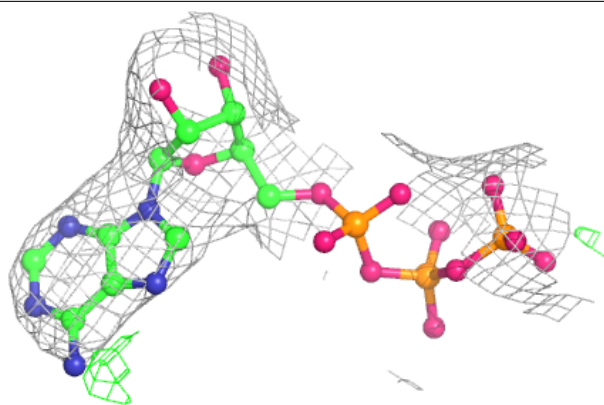
**Electron density around ATP C 1003:**

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

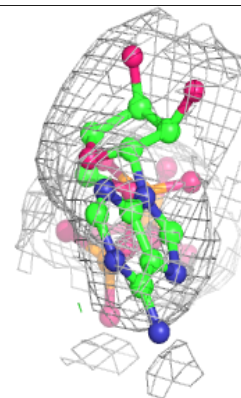
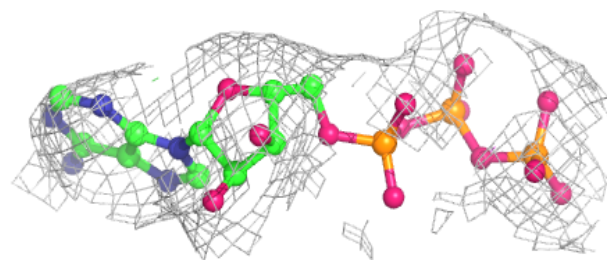
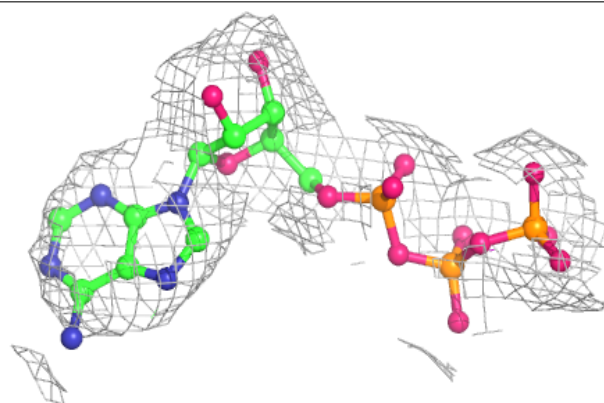


**Electron density around ATP G 1003:**

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

**Electron density around ATP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.