



## Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 02:12 PM JST

PDB ID : 8Z3K / pdb\_00008z3k  
EMDB ID : EMD-39746  
Title : The structure of type III CRISPR-associated deaminase in complex 2cA6-2ATP  
Authors : Chen, M.R.; Li, Z.X.; Xiao, Y.B.  
Deposited on : 2024-04-15  
Resolution : 3.19 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

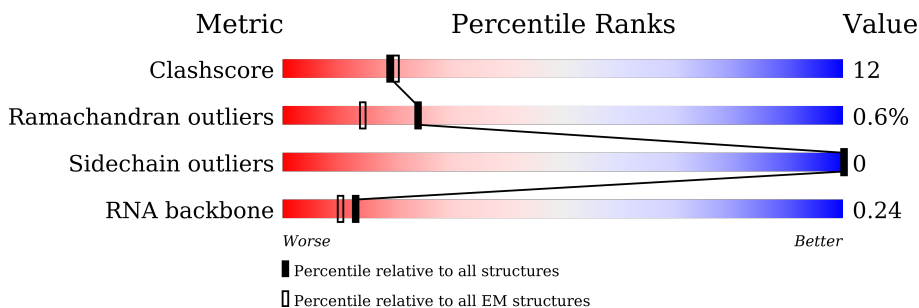
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.19 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	635	72% 24% .
1	B	635	70% 26% ..
1	C	635	69% 27% ..
1	D	635	69% 27% .
1	E	635	44% 18% 38%
1	F	635	43% 19% 38%
2	H	6	33% 50% 17%
2	I	6	33% 33% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	B	702	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25475 atoms, of which 24 are hydrogens and 0 are deuteriums.

In the tables below, 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 Adenosine deaminase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	613	Total	C	N	O	S	0	0
			4741	2992	884	843	22		
1	B	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
1	C	613	Total	C	N	O	S	0	0
			4810	3039	893	856	22		
1	D	614	Total	C	N	O	S	0	0
			4759	3003	885	849	22		
1	E	395	Total	C	N	O	S	0	0
			3014	1888	566	545	15		
1	F	394	Total	C	N	O	S	0	0
			2979	1870	559	536	14		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	630	HIS	-	expression tag	UNP A0A6M1RED6
A	631	HIS	-	expression tag	UNP A0A6M1RED6
A	632	HIS	-	expression tag	UNP A0A6M1RED6
A	633	HIS	-	expression tag	UNP A0A6M1RED6
A	634	HIS	-	expression tag	UNP A0A6M1RED6
A	635	HIS	-	expression tag	UNP A0A6M1RED6
B	630	HIS	-	expression tag	UNP A0A6M1RED6
B	631	HIS	-	expression tag	UNP A0A6M1RED6
B	632	HIS	-	expression tag	UNP A0A6M1RED6
B	633	HIS	-	expression tag	UNP A0A6M1RED6
B	634	HIS	-	expression tag	UNP A0A6M1RED6
B	635	HIS	-	expression tag	UNP A0A6M1RED6
C	630	HIS	-	expression tag	UNP A0A6M1RED6
C	631	HIS	-	expression tag	UNP A0A6M1RED6
C	632	HIS	-	expression tag	UNP A0A6M1RED6
C	633	HIS	-	expression tag	UNP A0A6M1RED6
C	634	HIS	-	expression tag	UNP A0A6M1RED6
C	635	HIS	-	expression tag	UNP A0A6M1RED6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	630	HIS	-	expression tag	UNP A0A6M1RED6
D	631	HIS	-	expression tag	UNP A0A6M1RED6
D	632	HIS	-	expression tag	UNP A0A6M1RED6
D	633	HIS	-	expression tag	UNP A0A6M1RED6
D	634	HIS	-	expression tag	UNP A0A6M1RED6
D	635	HIS	-	expression tag	UNP A0A6M1RED6
E	630	HIS	-	expression tag	UNP A0A6M1RED6
E	631	HIS	-	expression tag	UNP A0A6M1RED6
E	632	HIS	-	expression tag	UNP A0A6M1RED6
E	633	HIS	-	expression tag	UNP A0A6M1RED6
E	634	HIS	-	expression tag	UNP A0A6M1RED6
E	635	HIS	-	expression tag	UNP A0A6M1RED6
F	630	HIS	-	expression tag	UNP A0A6M1RED6
F	631	HIS	-	expression tag	UNP A0A6M1RED6
F	632	HIS	-	expression tag	UNP A0A6M1RED6
F	633	HIS	-	expression tag	UNP A0A6M1RED6
F	634	HIS	-	expression tag	UNP A0A6M1RED6
F	635	HIS	-	expression tag	UNP A0A6M1RED6

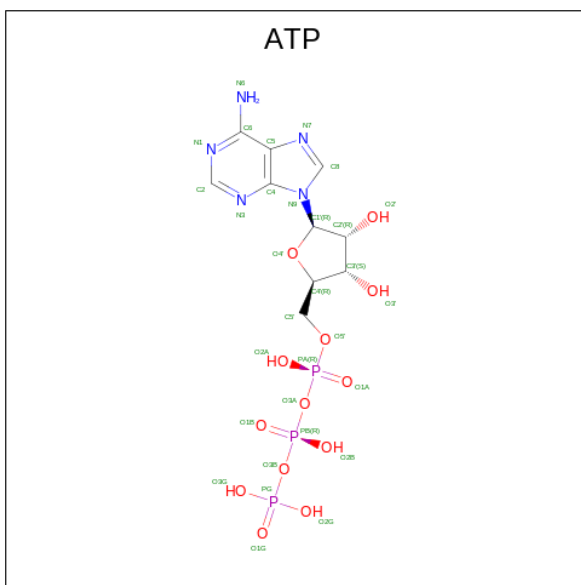
- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	6	Total	C	N	O	P	
			132	60	30	36	6	0
2	I	6	Total	C	N	O	P	
			132	60	30	36	6	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

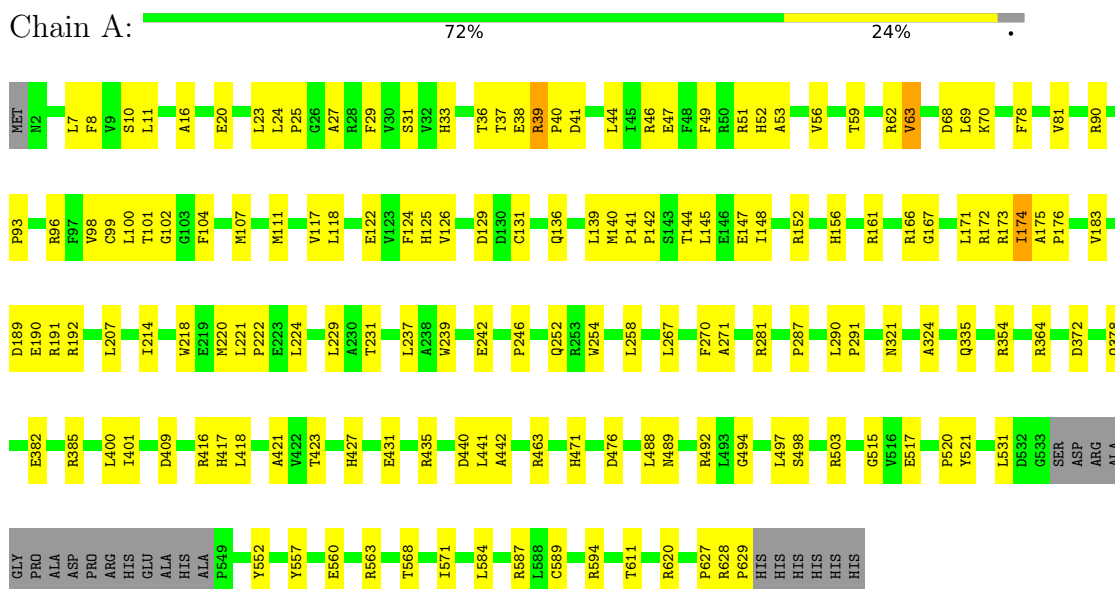


Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

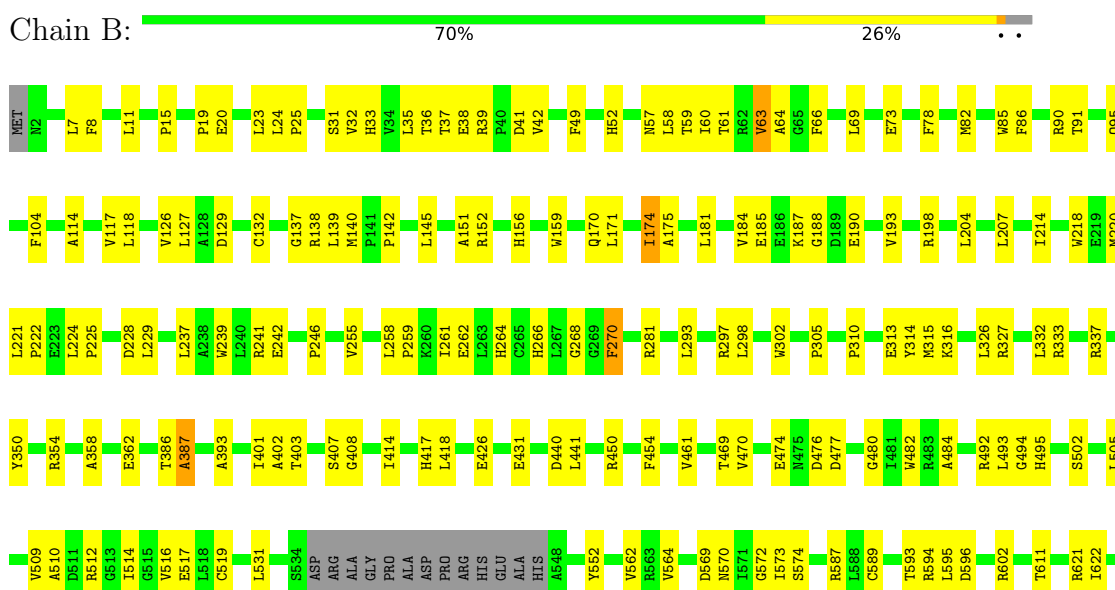
### 3 Residue-property plots

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



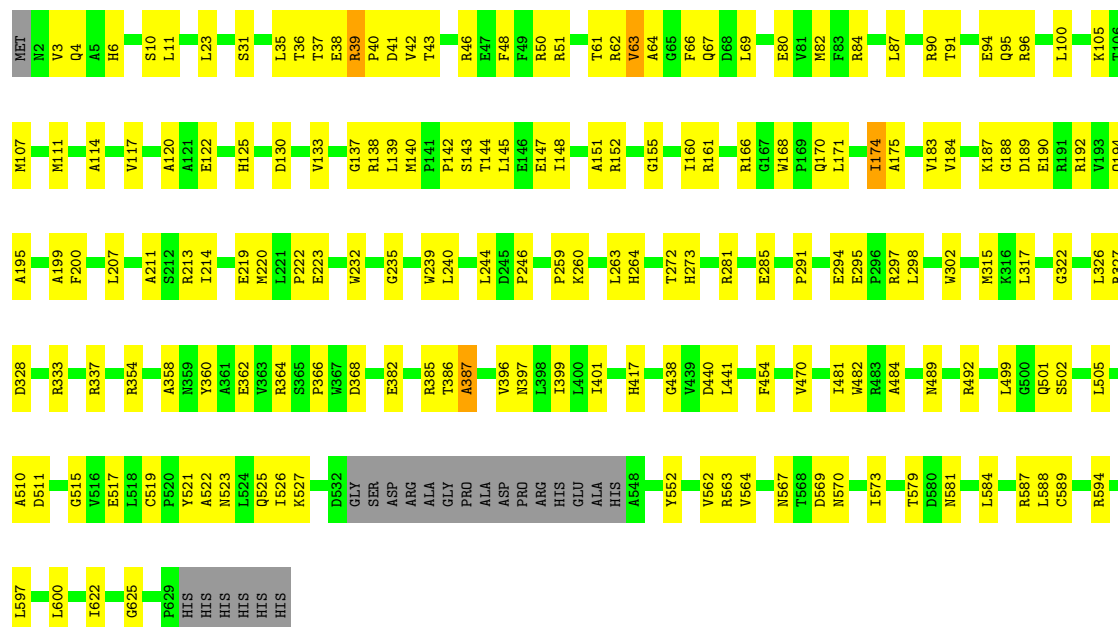
- Molecule 1: Adenosine deaminase domain-containing protein



P629  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

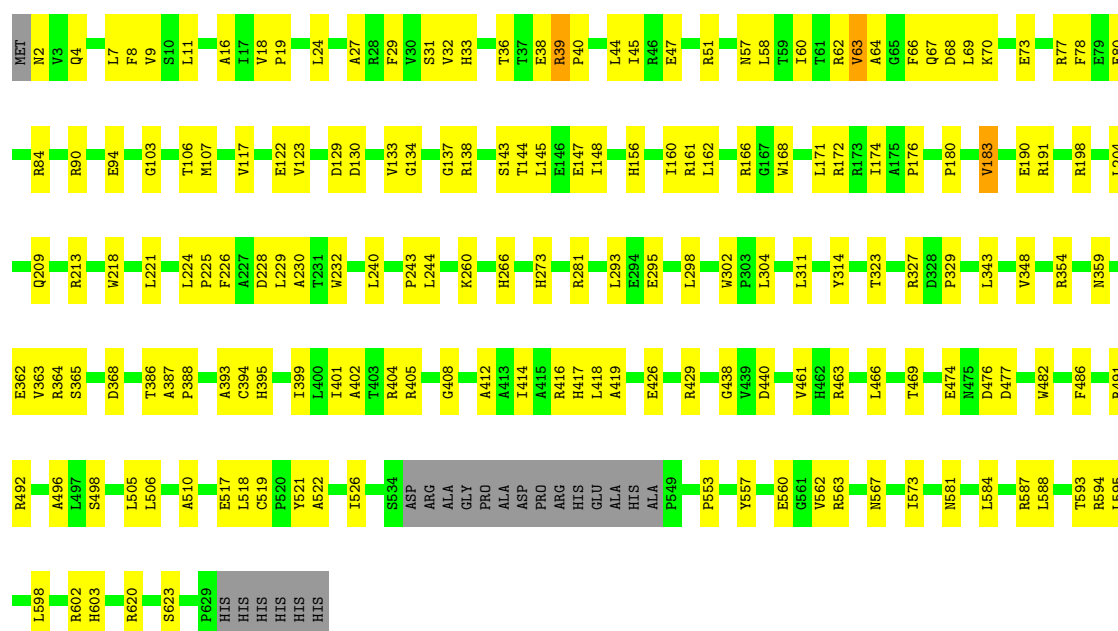
• Molecule 1: Adenosine deaminase domain-containing protein

Chain C:  69% 27% ..



• Molecule 1: Adenosine deaminase domain-containing protein

Chain D:  69% 27% .



• Molecule 1: Adenosine deaminase domain-containing protein



Chain E:  44% 18% 38%

MET	THR	ALA	LEU	P243	S365	R492	Q614
ASN	ARG	GLU	GLN	L244	D388	L493	R615
VAL	VAL	VAL	VAL	D245	D388	G494	L618
GLN	ALA	PHE	GLU	R246	R374	S498	L626
ALA	GLY	HIS	GLU	R247	F377	R503	P627
HIS	PHE	LEU	LYS	D251	M381	R507	P628
LEU	GLN	ASP	GLY	W254	T386	V516	HIS
PHE	ASP	LEU	ASP	I261	T386	E517	HIS
VAL	LYS	ASP	ASP	E270	L391	L518	HIS
GLY	GLU	CYS	VAL	A271	P392	Y521	HIS
THR	ASP	VAL	GLN	T272	N397	A522	
ALA	ASP	GLY	ALA	G274	L400	N523	
PRO	PHE	GLN	ALA	R281	I401	R530	
ALA	GLU	VAL	PHE	E285	A402	L531	
PRO	VAL	PRO	GLY	R286	T403	G532	
GLU	VAL	PRO	THR	P287	R404	G533	
ALA	MET	PRO	PHE	G288	R405	ASP	
ALA	PHE	LEU	LEU	L289	A406	ASP	
ARG	THR	THR	GLN	L290	S407	ALA	
THR	PHE	GLU	ASP	P291	H417	GLY	
GLY	LEU	LEU	LEU	E296	L418	PRO	
ALA	ALA	ILE	LEU	L298	A419	ALA	
ARG	THR	GLY	GLN	W302	A420	ASP	
VAL	THR	ALA	ALA	N321	D430	PRO	
THR	ARG	HIS	ALA	T323	A433	ARG	
GLU	VAL	THR	TRP	L325	C434	HIS	
ARG	CYS	TRP	GLU	R326	D440	ALA	
PRO	THR	LEU	ILE	R327	V461	Y552	
ASP	GLY	ARG	ARG	D328	C464	V564	
VAL	THR	GLY	TRP	P329	V468	N567	
THR	PHE	PRO	GLU	G330	T469	L584	
ILE	LYS	ARG	ARG	C331	V470	R587	
ARG	THR	TRP	ARG	L332	H471	T593	
PHE	ALA	PRO	GLN	C336	D476	R594	
ARG	ALA	LEU	ARG	L339	W482	H599	
ARG	GLN	ARG	ARG	V348	R483	R602	
HIS	LYS	ARG	ILE	S356	A484	E606	
ALA	ALA	ILE	ALA	Y360	D487	C610	
PRO	ALA	PRO	GLU	A361	E362		
GLY	THR	GLN	W239				
ASN	VAL	THR	LEU				
THR	GLY	ALA	PHE				
ILE	ALA	PRO	ILE				

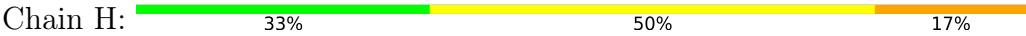
- Molecule 1: Adenosine deaminase domain-containing protein

Chain F:  43% 19% 38%

MET	THR	ALA	LEU	C286	D372	E504
ASN	ARG	GLU	GLN	H266	F377	L505
VAL	VAL	VAL	VAL	L267	Q378	L506
GLN	GLY	PHE	VAL	G268	C269	I514
ALA	ALA	GLU	GLU	C269	F270	E517
HIS	PHE	VAL	LYS	A271	T272	L518
LEU	GLN	LEU	GLY	R278	R278	C519
PHE	ASP	ASP	ASP	E285	E285	P520
VAL	LYS	ASP	ASP	P287	P287	Y521
VAL	ASP	ASP	ASP	L290	L290	K527
GLY	GLU	CYS	VAL	E295	E295	G528
THR	GLU	GLY	GLN	L298	L298	L531
ALA	ASP	ALA	ALA	W302	W302	P532
PRO	HIS	PRO	ALA	P308	P308	G533
ALA	ALA	PRO	GLY	G318	G318	ASP
PRO	VAL	PRO	THR	N321	N321	ASP
ALA	PHE	PRO	PHE	G322	G322	ALA
ALA	MET	THR	THR	L326	L326	GLY
GLU	GLU	LEU	LEU	R327	R327	PRO
GLY	PHE	GLU	ASP	L332	L332	ALA
ALA	THR	ALA	ALA	E334	E334	ALA
VAL	GLY	ARG	ARG	Q336	Q336	HIS
VAL	THR	VAL	THR	R337	R337	ALA
GLU	VAL	TRP	TRP	C349	C349	ASP
ARG	CYS	ILE	ILE	Y350	Y350	PRO
ASP	THR	ARG	ARG	A351	A351	ALA
PRO	GLY	GLY	GLY	E352	E352	ASP
PRO	THR	LEU	LEU	V353	V353	ASP
ASP	VAL	VAL	VAL	R354	R354	ALA
THR	GLY	THR	THR	C355	C355	ALA
LEU	PHE	PRO	PRO	S356	S356	ALA
ILE	LYS	LEU	LEU	A361	A361	ALA
ARG	THR	ARG	ARG	V254	V254	ALA
GLU	THR	GLN	GLN	V255	V255	ALA
ARG	MET	LYS	LYS	L240	L240	ALA
PHE	SER	ALA	ALA	L244	L244	ALA
PHE	ALA	MET	ALA	W254	W254	ALA
ARG	ALA	ARG	ARG	V255	V255	ALA
ARG	ALA	ILE	ILE	V363	V363	ALA
ARG	ALA	ALA	ALA	R364	R364	ALA
ARG	ALA	PRO	PRO	S365	S365	ALA
ARG	ALA	GLU	GLU	D368	D368	ALA
ARG	ALA	VAL	VAL	V369	V369	ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
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ARG	ALA	LEU	LEU			ALA
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ARG	ALA	GLY	GLY			ALA
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ARG	ALA	ASN	ASN			ALA
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ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
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ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
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ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
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ARG	ALA	GLY	GLY			ALA
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ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
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ARG	ALA	GLY	GLY			ALA
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ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
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ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
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ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	GLY	GLY			ALA
ARG	ALA	THR	THR			ALA
ARG	ALA	VAL	VAL			ALA
ARG	ALA	ASN	ASN			ALA
ARG	ALA	LEU	LEU			ALA
ARG	ALA	THR	THR			ALA



- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*A)-3')



- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*A)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 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, ZN

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	0.19	0/4852	0.32	0/6603
1	B	0.19	0/4936	0.34	0/6712
1	C	0.17	0/4926	0.36	0/6699
1	D	0.16	0/4871	0.32	0/6628
1	E	0.16	0/3079	0.36	0/4196
1	F	0.16	0/3044	0.35	0/4152
2	H	0.21	0/149	0.16	0/230
2	I	0.15	0/149	0.19	0/230
All	All	0.17	0/26006	0.34	0/35450

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4741	0	4688	108	0
1	B	4820	0	4786	133	0
1	C	4810	0	4778	131	0
1	D	4759	0	4701	124	0
1	E	3014	0	2983	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2979	0	2932	81	0
2	H	132	0	67	3	0
2	I	132	0	67	3	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	B	31	12	11	11	0
4	C	31	12	12	7	0
All	All	25451	24	25025	630	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 12.

All (630) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:ASP:OD2	4:C:702:ATP:N6	1.94	1.00
1:D:63:VAL:HG12	1:D:64:ALA:H	1.35	0.90
1:C:63:VAL:HG12	1:C:64:ALA:H	1.36	0.89
1:B:268:GLY:HA3	4:B:702:ATP:PA	2.13	0.88
1:B:268:GLY:O	4:B:702:ATP:O1A	1.96	0.82
1:B:91:THR:HB	1:B:95:GLN:HG3	1.62	0.80
1:B:482:TRP:HB2	1:B:505:LEU:HD21	1.64	0.80
1:B:418:LEU:HD12	1:B:461:VAL:HG21	1.62	0.79
1:E:440:ASP:HB3	1:E:469:THR:HG23	1.64	0.78
1:D:60:ILE:HB	1:D:190:GLU:HA	1.66	0.78
1:A:62:ARG:NH2	1:A:190:GLU:OE2	2.17	0.78
1:B:327:ARG:NH1	1:B:362:GLU:OE2	2.19	0.76
1:E:298:LEU:HD12	1:E:302:TRP:HB3	1.67	0.75
1:F:582:LEU:HD12	1:F:597:LEU:HD11	1.69	0.75
1:C:80:GLU:OE2	1:C:84:ARG:NH1	2.19	0.73
1:D:144:THR:HB	1:D:147:GLU:HB2	1.69	0.73
1:A:423:THR:HG21	1:F:423:THR:HG21	1.68	0.73
1:C:315:MET:HE2	4:C:702:ATP:N3	2.04	0.73
1:C:521:TYR:HE1	1:C:584:LEU:HD13	1.52	0.73
1:F:308:PRO:HG3	1:F:528:GLY:HA3	1.72	0.71
1:D:84:ARG:NH1	1:D:180:PRO:O	2.23	0.71
1:A:140:MET:SD	1:A:140:MET:N	2.64	0.71
1:D:228:ASP:OD1	1:D:623:SER:OG	2.09	0.71
1:D:567:ASN:O	1:D:581:ASN:ND2	2.24	0.71
1:D:364:ARG:HH21	1:D:368:ASP:HB3	1.55	0.70
1:E:530:ARG:HH12	1:E:549:PRO:HD2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD12	1:C:111:MET:HE1	1.72	0.70
1:B:268:GLY:HA3	4:B:702:ATP:O1A	1.91	0.70
1:C:244:LEU:HB3	1:C:594:ARG:HG2	1.74	0.70
1:C:327:ARG:HH11	1:C:362:GLU:HG2	1.57	0.70
1:A:231:THR:O	1:A:628:ARG:NH2	2.24	0.70
1:B:474:GLU:OE1	1:B:495:HIS:ND1	2.20	0.70
1:E:281:ARG:NH1	1:E:291:PRO:O	2.24	0.69
1:A:38:GLU:HA	1:A:62:ARG:HD2	1.72	0.69
1:E:281:ARG:HG3	1:E:290:LEU:HD11	1.73	0.69
1:D:229:LEU:HD11	1:D:598:LEU:HD13	1.73	0.69
1:E:232:TRP:CD1	1:E:236:GLU:HG2	2.27	0.68
1:E:243:PRO:HA	1:E:593:THR:HA	1.74	0.68
1:A:122:GLU:OE2	1:A:161:ARG:NH1	2.26	0.68
1:C:567:ASN:O	1:C:581:ASN:ND2	2.26	0.68
1:E:251:ASP:OD1	1:E:594:ARG:NH1	2.27	0.67
1:B:11:LEU:HD11	1:B:15:PRO:HA	1.76	0.67
1:B:184:VAL:HG12	1:B:185:GLU:H	1.59	0.67
1:C:264:HIS:HD2	1:C:569:ASP:HA	1.60	0.67
1:B:268:GLY:C	4:B:702:ATP:O1A	2.38	0.67
1:C:160:ILE:HD13	1:D:69:LEU:HD21	1.76	0.67
1:D:225:PRO:O	1:D:602:ARG:NH1	2.28	0.66
1:F:364:ARG:HH21	1:F:368:ASP:HB3	1.61	0.66
1:D:144:THR:O	1:D:148:ILE:N	2.27	0.66
1:C:569:ASP:CG	4:C:702:ATP:N6	2.54	0.66
1:C:239:TRP:O	1:C:594:ARG:NH1	2.29	0.66
1:E:476:ASP:OD2	1:E:498:SER:OG	2.13	0.65
1:F:520:PRO:HD2	1:F:581:ASN:HD22	1.61	0.65
1:C:501:GLN:NE2	1:E:407:SER:O	2.29	0.65
1:D:168:TRP:HB2	1:D:171:LEU:HB2	1.79	0.65
1:E:270:PHE:O	1:E:321:ASN:ND2	2.31	0.64
1:F:351:ALA:HB3	1:F:396:VAL:HG12	1.80	0.64
1:B:403:THR:CG2	4:B:702:ATP:O3'	2.46	0.63
1:D:426:GLU:O	1:D:429:ARG:NH1	2.31	0.63
1:B:302:TRP:NE1	1:B:573:ILE:O	2.25	0.63
1:A:281:ARG:NH2	1:A:291:PRO:O	2.32	0.63
1:B:470:VAL:HG11	1:B:484:ALA:HB1	1.80	0.63
1:C:386:THR:HG23	1:C:387:ALA:H	1.63	0.63
1:F:554:LEU:HD23	1:F:592:LEU:HD21	1.81	0.63
1:C:46:ARG:O	1:C:50:ARG:N	2.28	0.63
1:C:354:ARG:NH2	1:C:517:GLU:OE1	2.32	0.63
1:D:354:ARG:NH1	1:D:440:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:HIS:HB2	1:F:570:ASN:HB3	1.81	0.62
1:C:51:ARG:HD2	1:C:145:LEU:HD21	1.82	0.61
1:C:354:ARG:NH1	1:C:440:ASP:OD2	2.32	0.61
1:E:386:THR:HA	1:E:391:LEU:HD12	1.81	0.61
1:A:27:ALA:HB1	1:A:29:PHE:CD2	2.35	0.61
1:B:354:ARG:NH1	1:B:440:ASP:OD2	2.33	0.61
1:F:258:LEU:HD12	1:F:259:PRO:HD2	1.82	0.61
1:B:268:GLY:CA	4:B:702:ATP:O1A	2.48	0.61
1:C:94:GLU:HG2	1:C:95:GLN:HG3	1.82	0.61
1:F:322:GLY:H	1:F:326:LEU:HD13	1.65	0.61
1:C:39:ARG:NH2	1:C:67:GLN:OE1	2.34	0.61
1:C:569:ASP:CG	4:C:702:ATP:HN61	2.07	0.61
1:F:349:CYS:SG	1:F:621:ARG:NH1	2.74	0.61
1:B:225:PRO:O	1:B:602:ARG:NH1	2.34	0.61
1:E:606:GLU:HA	1:E:615:ARG:HH21	1.65	0.61
1:B:132:CYS:O	1:B:139:LEU:N	2.34	0.60
1:C:526:ILE:HG23	1:C:527:LYS:HG2	1.81	0.60
1:C:10:SER:HB3	1:C:111:MET:HE3	1.82	0.60
1:F:266:HIS:O	1:F:268:GLY:N	2.34	0.60
1:A:62:ARG:HB3	1:A:192:ARG:HA	1.84	0.60
1:B:255:VAL:HA	1:B:258:LEU:HD23	1.83	0.60
1:E:220:MET:SD	1:E:220:MET:N	2.75	0.60
1:A:49:PHE:HA	1:A:53:ALA:HB3	1.84	0.59
1:C:213:ARG:HD3	1:C:232:TRP:C	2.28	0.59
1:E:516:VAL:HB	1:E:564:VAL:HG12	1.83	0.59
1:C:6:HIS:ND1	1:C:31:SER:OG	2.29	0.59
1:D:359:ASN:HD22	1:D:404:ARG:NH1	2.00	0.59
1:B:386:THR:HG23	1:B:387:ALA:H	1.67	0.59
1:C:48:PHE:HA	1:C:145:LEU:HD23	1.83	0.59
1:E:530:ARG:NH2	1:E:549:PRO:O	2.36	0.59
1:F:262:GLU:HB3	1:F:578:LEU:HD11	1.84	0.59
1:A:37:THR:HG21	2:H:4:A:C2	2.38	0.58
1:D:302:TRP:NE1	1:D:573:ILE:O	2.36	0.58
1:B:281:ARG:HH12	1:B:293:LEU:HA	1.68	0.58
1:B:495:HIS:NE2	1:B:519:CYS:SG	2.74	0.58
1:A:267:LEU:O	1:A:335:GLN:NE2	2.36	0.58
1:C:6:HIS:HD1	1:C:31:SER:HG	1.51	0.58
1:A:171:LEU:HA	1:A:174:ILE:HD11	1.85	0.58
1:B:516:VAL:HB	1:B:564:VAL:HG12	1.85	0.58
1:B:23:LEU:HD12	1:B:152:ARG:HG3	1.85	0.58
1:D:117:VAL:HG11	1:D:204:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:HIS:CE1	1:D:354:ARG:HD2	2.38	0.58
1:C:511:ASP:OD1	1:D:491:ARG:NH2	2.37	0.58
1:F:364:ARG:NH2	1:F:372:ASP:OD2	2.37	0.58
1:A:31:SER:HA	1:A:56:VAL:O	2.03	0.58
1:A:44:LEU:HD11	1:A:144:THR:HA	1.86	0.58
1:C:470:VAL:HG21	1:C:484:ALA:HB1	1.86	0.58
1:B:314:TYR:OH	1:B:574:SER:OG	2.20	0.57
1:C:46:ARG:NH2	1:C:189:ASP:OD1	2.33	0.57
1:D:38:GLU:OE2	1:D:66:PHE:N	2.30	0.57
1:D:402:ALA:HB1	1:D:414:ILE:HD12	1.86	0.57
1:D:416:ARG:NE	1:E:464:CYS:SG	2.73	0.57
1:E:482:TRP:HB3	1:F:463:ARG:HH21	1.70	0.57
1:B:242:GLU:HG3	1:B:594:ARG:HH12	1.69	0.57
1:D:243:PRO:HA	1:D:593:THR:HA	1.86	0.57
1:D:469:THR:HG22	1:D:492:ARG:HB2	1.86	0.57
1:B:315:MET:HE1	4:B:702:ATP:C8	2.40	0.57
1:A:46:ARG:NH1	1:A:189:ASP:OD1	2.38	0.57
1:D:133:VAL:HA	1:D:137:GLY:HA2	1.87	0.57
1:B:403:THR:HG23	4:B:702:ATP:O3'	2.05	0.57
1:B:7:LEU:HD22	1:B:32:VAL:HG13	1.87	0.56
1:C:62:ARG:NH2	1:C:190:GLU:HB3	2.20	0.56
1:B:333:ARG:HB3	1:B:337:ARG:HH11	1.70	0.56
1:A:11:LEU:HA	1:A:102:GLY:HA3	1.87	0.56
1:B:450:ARG:NH1	1:B:476:ASP:OD2	2.38	0.56
1:C:246:PRO:HG2	1:C:587:ARG:HB2	1.87	0.56
1:E:327:ARG:HD3	1:E:362:GLU:HG3	1.86	0.56
1:E:400:LEU:HB3	1:E:417:HIS:CE1	2.40	0.56
1:F:566:VAL:HB	1:F:600:LEU:HD21	1.87	0.56
1:A:354:ARG:HB3	1:A:401:ILE:HD11	1.87	0.56
1:A:171:LEU:HD21	1:A:207:LEU:HD13	1.88	0.56
1:A:431:GLU:OE1	1:A:435:ARG:NH1	2.38	0.56
1:B:401:ILE:O	1:B:417:HIS:ND1	2.38	0.56
1:D:506:LEU:HD21	1:D:560:GLU:HG3	1.87	0.56
1:A:409:ASP:HB2	1:F:463:ARG:HH22	1.70	0.56
1:C:521:TYR:CE1	1:C:584:LEU:HD13	2.38	0.56
1:A:220:MET:SD	1:A:220:MET:N	2.79	0.56
1:F:378:GLN:O	1:F:382:GLU:N	2.39	0.56
1:A:96:ARG:NH1	1:A:118:LEU:O	2.34	0.56
1:D:7:LEU:HB3	1:D:32:VAL:HG23	1.86	0.56
1:E:321:ASN:HD21	1:E:335:GLN:NE2	2.04	0.55
1:A:93:PRO:HG3	1:A:172:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ARG:HH21	1:B:222:PRO:HG2	1.71	0.55
1:B:313:GLU:O	1:B:316:LYS:HG3	2.05	0.55
1:D:365:SER:HB2	1:E:427:HIS:HA	1.88	0.55
1:C:219:GLU:OE1	1:C:219:GLU:N	2.35	0.55
1:D:73:GLU:OE2	1:D:77:ARG:NH2	2.39	0.55
1:B:431:GLU:OE2	1:B:611:THR:OG1	2.24	0.55
1:F:287:PRO:HA	1:F:290:LEU:HD13	1.88	0.55
1:E:239:TRP:CD1	1:E:629:PRO:HG3	2.42	0.55
1:C:502:SER:HB2	1:C:505:LEU:HB3	1.87	0.55
1:B:11:LEU:HB3	1:B:36:THR:HG22	1.88	0.55
4:C:702:ATP:H3'	4:C:702:ATP:O3A	2.07	0.55
1:D:311:LEU:HG	1:D:474:GLU:HG2	1.89	0.55
1:B:73:GLU:OE1	1:B:198:ARG:NH2	2.39	0.54
1:B:221:LEU:HA	1:B:224:LEU:HD13	1.88	0.54
1:C:151:ALA:O	1:C:155:GLY:N	2.40	0.54
1:F:495:HIS:NE2	1:F:519:CYS:SG	2.80	0.54
1:D:122:GLU:OE2	1:D:161:ARG:NE	2.41	0.54
1:B:140:MET:O	1:B:142:PRO:HD3	2.07	0.54
1:C:37:THR:OG1	1:C:66:PHE:O	2.24	0.54
1:E:226:PHE:HB3	1:E:602:ARG:NH2	2.22	0.54
1:C:482:TRP:CZ2	1:D:463:ARG:HD2	2.43	0.54
1:E:400:LEU:HD12	1:E:421:ALA:HB2	1.89	0.54
1:A:131:CYS:SG	1:A:156:HIS:NE2	2.77	0.54
1:C:382:GLU:OE1	1:C:385:ARG:NH1	2.40	0.54
1:D:63:VAL:CG1	1:D:64:ALA:H	2.15	0.54
1:C:63:VAL:HG12	1:C:64:ALA:N	2.15	0.54
1:C:259:PRO:HG2	1:C:622:ILE:HG23	1.89	0.54
1:D:47:GLU:OE2	1:D:51:ARG:NH2	2.40	0.54
1:D:78:PHE:CZ	1:D:107:MET:HG3	2.43	0.54
1:D:584:LEU:O	1:D:588:LEU:N	2.37	0.54
1:A:416:ARG:NE	1:F:426:GLU:OE2	2.40	0.54
1:D:45:ILE:HG22	1:D:58:LEU:HD21	1.89	0.53
1:D:240:LEU:HG	1:D:595:LEU:HB3	1.90	0.53
1:E:323:THR:O	1:E:327:ARG:NH2	2.41	0.53
1:E:418:LEU:HD12	1:E:461:VAL:HG11	1.88	0.53
1:F:336:CYS:HB2	1:F:377:PHE:CE1	2.44	0.53
1:C:69:LEU:HG	1:D:160:ILE:HG12	1.91	0.53
1:D:90:ARG:HD2	1:D:176:PRO:HG2	1.90	0.53
1:A:100:LEU:HD12	1:A:100:LEU:O	2.08	0.53
1:D:63:VAL:HG12	1:D:64:ALA:N	2.14	0.53
1:B:402:ALA:HB1	1:B:414:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:PRO:HG3	1:D:364:ARG:HH11	1.74	0.53
1:F:326:LEU:HB3	1:F:332:LEU:HD12	1.91	0.53
1:A:166:ARG:HD3	1:A:167:GLY:O	2.08	0.53
1:C:4:GLN:OE1	1:C:95:GLN:NE2	2.41	0.53
1:C:322:GLY:HA3	4:C:702:ATP:O3G	2.08	0.53
1:D:8:PHE:HD1	1:D:33:HIS:HB2	1.73	0.53
1:A:90:ARG:HE	1:A:176:PRO:HG3	1.74	0.53
1:F:244:LEU:HD21	1:F:594:ARG:HB2	1.91	0.53
1:A:497:LEU:O	1:A:557:TYR:OH	2.25	0.53
1:D:228:ASP:OD1	1:D:228:ASP:N	2.40	0.53
1:F:255:VAL:HG13	1:F:579:THR:HG23	1.90	0.53
1:A:10:SER:HB2	1:A:107:MET:HE2	1.91	0.52
1:C:401:ILE:HD13	4:C:702:ATP:H5'1	1.91	0.52
1:D:408:GLY:HA3	1:D:412:ALA:HB3	1.91	0.52
1:E:288:GLY:O	1:E:289:LYS:HE2	2.09	0.52
1:B:531:LEU:HD21	1:B:587:ARG:NE	2.24	0.52
1:C:240:LEU:O	1:C:240:LEU:HD23	2.09	0.52
1:D:221:LEU:HD12	1:D:230:ALA:HB3	1.91	0.52
1:D:129:ASP:OD1	1:D:156:HIS:HB3	2.10	0.52
1:F:492:ARG:NE	1:F:517:GLU:OE2	2.42	0.52
1:B:242:GLU:HG3	1:B:594:ARG:NH1	2.24	0.52
1:C:515:GLY:HA2	1:C:563:ARG:HB2	1.92	0.52
1:B:118:LEU:HD12	1:B:171:LEU:O	2.09	0.52
1:D:24:LEU:HB3	1:D:27:ALA:HB2	1.91	0.52
1:D:171:LEU:HA	1:D:174:ILE:HD11	1.91	0.52
1:A:442:ALA:HB2	1:A:471:HIS:HB3	1.92	0.52
1:A:476:ASP:O	1:A:498:SER:OG	2.28	0.52
1:B:492:ARG:NE	1:B:517:GLU:OE2	2.41	0.52
1:F:470:VAL:O	1:F:494:GLY:N	2.40	0.52
1:A:24:LEU:HD12	1:A:25:PRO:HD2	1.92	0.52
1:E:374:ARG:NH1	1:E:434:CYS:O	2.43	0.52
1:B:33:HIS:ND1	1:B:59:THR:OG1	2.39	0.52
1:A:270:PHE:HB3	1:A:335:GLN:HE21	1.75	0.51
1:C:105:LYS:HG2	2:I:9:A:OP1	2.10	0.51
1:D:7:LEU:HD12	1:D:29:PHE:CE2	2.45	0.51
1:A:117:VAL:HG23	1:A:118:LEU:HD12	1.92	0.51
1:B:8:PHE:HE1	1:B:33:HIS:HD2	1.58	0.51
1:B:224:LEU:HD23	1:B:229:LEU:HB3	1.93	0.51
1:C:260:LYS:HE2	1:C:579:THR:HG22	1.92	0.51
1:E:323:THR:HA	1:E:360:TYR:HE1	1.76	0.51
1:B:174:ILE:HG22	1:B:175:ALA:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ASN:O	1:D:4:GLN:NE2	2.43	0.51
1:E:374:ARG:HE	1:E:428:TRP:NE1	2.08	0.51
1:F:272:THR:HG21	1:F:573:ILE:HD13	1.92	0.51
1:F:568:THR:HG21	1:F:578:LEU:HD22	1.92	0.51
1:A:63:VAL:HG22	1:A:81:VAL:HG11	1.91	0.51
1:D:80:GLU:HB2	1:D:198:ARG:HG3	1.93	0.51
1:F:438:GLY:HA2	1:F:467:ALA:O	2.09	0.51
1:F:459:THR:HA	1:F:462:HIS:CE1	2.45	0.51
1:F:278:ARG:NH1	1:F:295:GLU:OE2	2.44	0.51
1:C:62:ARG:HD2	1:C:192:ARG:HB2	1.93	0.51
1:C:144:THR:OG1	1:C:145:LEU:N	2.43	0.51
1:A:69:LEU:HD23	1:B:127:LEU:HD11	1.92	0.51
1:B:264:HIS:NE2	1:B:569:ASP:OD1	2.44	0.51
1:B:242:GLU:O	1:B:594:ARG:NH1	2.44	0.50
1:F:233:SER:OG	1:F:236:GLU:OE1	2.22	0.50
1:A:53:ALA:HB1	1:A:56:VAL:HG11	1.93	0.50
1:A:520:PRO:HB2	1:A:584:LEU:HD23	1.93	0.50
1:B:469:THR:HG22	1:B:492:ARG:HB2	1.93	0.50
1:F:271:ALA:O	1:F:321:ASN:ND2	2.45	0.50
1:B:450:ARG:HD3	1:B:480:GLY:HA2	1.93	0.50
1:C:482:TRP:CD1	1:C:505:LEU:HD13	2.46	0.50
1:B:137:GLY:O	1:B:138:ARG:HD3	2.11	0.50
1:B:426:GLU:OE1	1:C:366:PRO:HD2	2.11	0.50
1:E:324:ALA:HA	1:E:327:ARG:HH21	1.77	0.50
1:B:8:PHE:HE1	1:B:33:HIS:CD2	2.30	0.50
1:B:181:LEU:HD21	1:B:193:VAL:HG21	1.94	0.50
1:E:244:LEU:HD12	1:E:594:ARG:HD2	1.94	0.50
1:E:403:THR:O	1:E:405:ARG:N	2.44	0.50
1:A:52:HIS:HE1	1:A:145:LEU:HD22	1.77	0.50
1:B:37:THR:OG1	1:B:66:PHE:O	2.28	0.50
1:B:60:ILE:HB	1:B:190:GLU:HA	1.94	0.50
1:C:523:ASN:HA	1:C:526:ILE:HG22	1.92	0.50
1:A:492:ARG:NE	1:A:517:GLU:OE2	2.45	0.50
1:B:315:MET:HE1	4:B:702:ATP:N9	2.17	0.50
1:D:44:LEU:HG	1:D:145:LEU:HD21	1.94	0.50
1:F:497:LEU:HD21	1:F:527:LYS:HE3	1.92	0.50
1:D:440:ASP:OD1	1:D:440:ASP:N	2.42	0.50
1:F:302:TRP:NE1	1:F:573:ILE:O	2.42	0.50
1:B:220:MET:HE1	1:B:241:ARG:HH21	1.77	0.49
1:B:246:PRO:HG2	1:B:587:ARG:HB2	1.94	0.49
1:C:326:LEU:HB2	1:C:360:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:ASP:CG	1:E:231:THR:HA	2.37	0.49
1:E:521:TYR:CZ	1:E:584:LEU:HD13	2.47	0.49
1:A:291:PRO:HG3	1:A:324:ALA:HB1	1.93	0.49
1:B:259:PRO:HG2	1:B:622:ILE:HG23	1.95	0.49
1:C:298:LEU:HD13	1:C:302:TRP:HB2	1.95	0.49
1:E:483:ARG:NH1	1:E:487:ASP:OD2	2.45	0.49
1:D:80:GLU:HG3	1:D:198:ARG:HA	1.94	0.49
1:D:221:LEU:HA	1:D:224:LEU:HD12	1.93	0.49
1:D:260:LYS:HB2	1:D:348:VAL:HG12	1.92	0.49
1:A:7:LEU:HD12	1:A:29:PHE:CZ	2.48	0.49
1:A:39:ARG:H	1:A:40:PRO:HD2	1.77	0.49
1:B:298:LEU:HD13	1:B:302:TRP:HB2	1.94	0.49
1:A:427:HIS:HA	1:F:365:SER:HB2	1.93	0.49
1:B:262:GLU:OE2	1:B:264:HIS:N	2.37	0.49
1:C:584:LEU:HD12	1:C:587:ARG:HH21	1.77	0.49
1:D:510:ALA:HB2	1:D:562:VAL:HG22	1.94	0.49
1:A:129:ASP:OD1	1:A:129:ASP:N	2.41	0.49
1:B:117:VAL:HG21	1:B:204:LEU:HD11	1.94	0.49
1:B:171:LEU:HD13	1:B:174:ILE:HD11	1.94	0.49
1:C:166:ARG:NH1	1:D:209:GLN:OE1	2.35	0.49
1:E:427:HIS:HD2	1:E:428:TRP:CE2	2.30	0.49
1:A:418:LEU:HD21	1:A:441:LEU:HD21	1.94	0.49
1:E:336:CYS:HB2	1:E:377:PHE:CE1	2.48	0.49
1:A:354:ARG:NH2	1:A:440:ASP:OD2	2.33	0.49
1:B:354:ARG:NH2	1:B:517:GLU:OE1	2.46	0.49
1:B:476:ASP:OD1	1:B:477:ASP:N	2.40	0.49
1:C:584:LEU:O	1:C:588:LEU:N	2.35	0.49
1:C:100:LEU:HD12	1:C:100:LEU:O	2.13	0.49
1:F:471:HIS:HA	1:F:494:GLY:HA3	1.94	0.48
1:D:62:ARG:HH12	1:D:190:GLU:HB3	1.79	0.48
1:D:401:ILE:HA	1:D:440:ASP:OD1	2.12	0.48
1:B:129:ASP:HB2	1:B:156:HIS:HB2	1.96	0.48
1:C:133:VAL:HA	1:C:138:ARG:HE	1.79	0.48
1:C:386:THR:HG23	1:C:387:ALA:N	2.28	0.48
1:D:595:LEU:HA	1:D:598:LEU:HD12	1.96	0.48
1:A:463:ARG:HD3	1:F:411:ARG:HB3	1.95	0.48
1:C:440:ASP:OD1	1:C:441:LEU:N	2.47	0.48
1:D:31:SER:HA	1:D:57:ASN:HB2	1.94	0.48
1:C:223:GLU:OE1	1:C:223:GLU:N	2.43	0.48
1:F:477:ASP:OD1	1:F:479:GLU:N	2.45	0.48
1:A:214:ILE:HD11	1:B:218:TRP:CZ3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ALA:HB3	1:B:417:HIS:NE2	2.28	0.48
1:C:295:GLU:HG3	1:C:297:ARG:HH21	1.79	0.48
1:D:492:ARG:NE	1:D:517:GLU:OE2	2.46	0.48
1:C:160:ILE:HD11	1:D:106:THR:HG21	1.96	0.48
1:C:481:ILE:HG21	1:C:499:LEU:HD13	1.94	0.48
1:D:298:LEU:HB3	1:D:302:TRP:HB2	1.95	0.48
1:A:136:GLN:O	1:A:139:LEU:HD23	2.13	0.48
1:B:225:PRO:HD3	1:B:595:LEU:HD11	1.95	0.48
1:C:519:CYS:SG	1:C:522:ALA:HB3	2.54	0.48
1:D:476:ASP:O	1:D:498:SER:OG	2.32	0.48
1:F:502:SER:O	1:F:504:GLU:N	2.47	0.48
1:A:378:GLN:HE21	1:A:382:GLU:HG2	1.79	0.48
1:D:80:GLU:OE2	1:D:84:ARG:NE	2.46	0.48
1:D:304:LEU:HD13	1:D:587:ARG:HH22	1.79	0.47
1:E:285:GLU:HB2	1:E:330:GLY:HA3	1.95	0.47
1:A:224:LEU:HD23	1:A:229:LEU:HB2	1.97	0.47
1:C:489:ASN:ND2	1:D:486:PHE:O	2.35	0.47
1:D:226:PHE:HB2	1:D:229:LEU:HB2	1.95	0.47
1:F:232:TRP:HZ3	1:F:240:LEU:HD21	1.79	0.47
1:D:394:CYS:SG	1:D:395:HIS:N	2.87	0.47
1:F:232:TRP:CZ3	1:F:240:LEU:HD21	2.50	0.47
1:D:244:LEU:HD13	1:D:594:ARG:HG2	1.95	0.47
1:D:521:TYR:HE1	1:D:584:LEU:HD13	1.79	0.47
1:C:519:CYS:SG	1:C:569:ASP:HB2	2.55	0.47
1:D:133:VAL:HG23	1:D:137:GLY:HA2	1.95	0.47
1:B:297:ARG:HH21	1:B:298:LEU:HG	1.79	0.47
1:C:214:ILE:HD11	1:D:218:TRP:CD1	2.49	0.47
1:C:263:LEU:HD13	1:C:492:ARG:HH11	1.78	0.47
1:C:294:GLU:N	1:C:294:GLU:OE1	2.48	0.47
1:A:24:LEU:O	1:A:27:ALA:HB2	2.15	0.47
1:A:271:ALA:O	1:A:321:ASN:ND2	2.47	0.47
1:B:52:HIS:CD2	1:B:145:LEU:HD12	2.50	0.47
1:B:69:LEU:HB2	1:B:104:PHE:CE2	2.49	0.47
1:B:393:ALA:O	1:B:621:ARG:NH2	2.41	0.47
1:C:11:LEU:HB2	1:C:36:THR:HG22	1.97	0.47
1:D:405:ARG:O	1:D:405:ARG:HD3	2.14	0.47
1:E:223:GLU:HG2	1:E:224:LEU:N	2.30	0.47
1:E:336:CYS:HA	1:E:339:LEU:HD12	1.95	0.47
1:A:46:ARG:NH2	1:A:190:GLU:OE1	2.46	0.47
1:B:137:GLY:C	1:B:138:ARG:HD3	2.40	0.47
1:F:593:THR:HG23	1:F:596:ASP:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:THR:HG23	1:B:387:ALA:N	2.29	0.46
1:C:143:SER:OG	1:C:147:GLU:OE1	2.17	0.46
1:E:391:LEU:N	1:E:392:PRO:HD3	2.30	0.46
1:F:361:ALA:HB2	1:F:369:VAL:HG21	1.97	0.46
1:A:174:ILE:HG22	1:A:175:ALA:H	1.80	0.46
1:B:237:LEU:HB3	1:B:241:ARG:HH12	1.80	0.46
1:C:84:ARG:HH22	1:C:199:ALA:HB3	1.81	0.46
1:A:515:GLY:HA2	1:A:563:ARG:HB2	1.97	0.46
1:C:144:THR:O	1:C:148:ILE:HD13	2.15	0.46
1:C:222:PRO:HG2	1:D:620:ARG:HH21	1.80	0.46
1:C:364:ARG:HG2	1:C:368:ASP:HB2	1.97	0.46
1:A:242:GLU:HB2	1:A:594:ARG:HH12	1.80	0.46
1:B:151:ALA:HA	1:B:156:HIS:CE1	2.51	0.46
1:B:502:SER:OG	1:B:505:LEU:HD13	2.15	0.46
1:B:552:TYR:HB3	1:B:589:CYS:SG	2.55	0.46
1:E:274:GLY:N	1:E:295:GLU:OE2	2.47	0.46
1:F:499:LEU:HB3	1:F:506:LEU:HD12	1.98	0.46
1:B:41:ASP:OD1	1:B:42:VAL:N	2.49	0.46
1:C:358:ALA:HB3	1:C:417:HIS:CE1	2.51	0.46
1:D:166:ARG:HH22	1:D:172:ARG:HD3	1.80	0.46
1:E:503:ARG:NH2	1:E:507:ARG:HH21	2.13	0.46
1:F:430:ASP:OD1	1:F:430:ASP:N	2.48	0.46
1:E:531:LEU:HD12	1:E:587:ARG:HD2	1.98	0.46
1:F:425:ALA:HB2	1:F:466:LEU:HD21	1.97	0.46
1:A:568:THR:HG21	1:A:571:ILE:HG12	1.98	0.46
1:D:183:VAL:HG13	1:D:191:ARG:HD2	1.98	0.46
1:D:461:VAL:HG13	1:D:466:LEU:HB2	1.97	0.46
1:B:139:LEU:HD23	1:B:140:MET:N	2.31	0.46
1:B:261:ILE:HG23	1:B:350:TYR:HB3	1.98	0.46
1:D:122:GLU:CD	1:D:161:ARG:HE	2.24	0.46
1:E:365:SER:N	1:E:368:ASP:OD2	2.41	0.46
1:B:170:GLN:HE21	1:B:207:LEU:HD11	1.81	0.46
1:B:510:ALA:HB2	1:B:562:VAL:HG22	1.97	0.46
1:C:211:ALA:HA	1:C:214:ILE:HG22	1.97	0.46
1:C:441:LEU:HD21	1:C:454:PHE:HD2	1.81	0.46
1:C:552:TYR:HB3	1:C:589:CYS:SG	2.56	0.46
1:A:221:LEU:N	1:A:222:PRO:HD2	2.31	0.45
1:B:63:VAL:HG11	1:B:78:PHE:HD1	1.79	0.45
1:A:254:TRP:NE1	1:A:627:PRO:O	2.46	0.45
1:C:23:LEU:HD21	1:C:152:ARG:HD2	1.99	0.45
1:D:103:GLY:HA3	1:D:107:MET:SD	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ALA:HA	1:E:419:ALA:HB1	1.97	0.45
1:E:240:LEU:HA	1:E:594:ARG:HB2	1.98	0.45
1:E:518:LEU:O	1:E:567:ASN:N	2.46	0.45
1:B:310:PRO:HG2	1:B:313:GLU:OE1	2.17	0.45
1:C:96:ARG:HB2	1:C:120:ALA:HA	1.99	0.45
1:D:343:LEU:HD22	1:D:348:VAL:HG21	1.98	0.45
1:E:223:GLU:HB3	1:F:620:ARG:HD3	1.98	0.45
1:A:11:LEU:HD23	1:A:11:LEU:H	1.81	0.45
1:A:400:LEU:HD12	1:A:421:ALA:HB2	1.98	0.45
1:B:174:ILE:HG22	1:B:175:ALA:N	2.31	0.45
1:D:133:VAL:HG13	1:D:134:GLY:N	2.31	0.45
1:F:298:LEU:HD12	1:F:302:TRP:HB3	1.98	0.45
1:A:49:PHE:CD1	1:A:56:VAL:HG21	2.52	0.45
1:A:140:MET:O	1:A:142:PRO:HD3	2.17	0.45
1:B:8:PHE:HB3	1:B:85:TRP:HH2	1.82	0.45
1:D:477:ASP:N	1:D:477:ASP:OD1	2.48	0.45
1:D:519:CYS:SG	1:D:522:ALA:HB3	2.56	0.45
1:D:563:ARG:HG3	1:D:603:HIS:ND1	2.31	0.45
1:E:234:GLU:HA	1:E:237:LEU:HD12	1.99	0.45
1:B:313:GLU:OE1	1:B:313:GLU:N	2.50	0.45
1:B:407:SER:OG	1:B:408:GLY:N	2.49	0.45
1:D:7:LEU:HD21	1:D:9:VAL:HB	1.99	0.45
1:E:469:THR:OG1	1:E:492:ARG:HB3	2.17	0.45
1:B:138:ARG:O	1:B:138:ARG:HG2	2.16	0.45
1:D:273:HIS:HD2	1:D:295:GLU:HB3	1.82	0.45
1:D:387:ALA:HB1	1:D:388:PRO:HD2	1.99	0.45
1:E:229:LEU:HD22	1:E:626:ILE:HD11	1.98	0.45
1:B:270:PHE:O	1:B:572:GLY:HA3	2.17	0.45
1:F:356:SER:HB2	1:F:401:ILE:HG23	1.98	0.45
1:F:618:LEU:O	1:F:622:ILE:HG12	2.16	0.45
1:C:333:ARG:HG2	1:C:337:ARG:HH21	1.81	0.45
1:E:261:ILE:HA	1:E:348:VAL:HG23	1.98	0.45
1:C:10:SER:HB2	1:C:107:MET:HE2	1.98	0.44
1:F:265:CYS:HB2	1:F:353:VAL:HA	1.99	0.44
1:A:47:GLU:OE2	1:A:51:ARG:NE	2.50	0.44
1:A:503:ARG:NH1	1:A:560:GLU:OE2	2.50	0.44
1:B:38:GLU:O	1:B:38:GLU:HG2	2.17	0.44
1:C:482:TRP:HD1	1:C:505:LEU:HD22	1.81	0.44
1:C:521:TYR:O	1:C:525:GLN:HG2	2.18	0.44
1:D:11:LEU:HB2	1:D:36:THR:HB	2.00	0.44
1:E:503:ARG:HH12	1:E:507:ARG:HE	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TRP:CH2	1:B:228:ASP:HA	2.53	0.44
1:A:435:ARG:HH22	1:A:611:THR:HG23	1.83	0.44
1:A:552:TYR:HB3	1:A:589:CYS:SG	2.58	0.44
1:C:41:ASP:OD1	1:C:42:VAL:N	2.50	0.44
1:D:39:ARG:HD3	1:D:67:GLN:HB2	1.99	0.44
1:F:265:CYS:HA	1:F:569:ASP:O	2.17	0.44
1:F:400:LEU:HB3	1:F:417:HIS:NE2	2.33	0.44
1:C:48:PHE:HD1	1:C:145:LEU:HB3	1.83	0.44
1:C:63:VAL:CG1	1:C:64:ALA:H	2.18	0.44
1:D:362:GLU:OE1	1:D:363:VAL:N	2.51	0.44
1:E:286:ASN:ND2	1:E:289:LYS:HG3	2.33	0.44
1:E:377:PHE:O	1:E:381:MET:N	2.40	0.44
1:E:599:HIS:HA	1:E:602:ARG:HB3	2.00	0.44
1:A:78:PHE:CZ	1:A:107:MET:HG3	2.53	0.44
1:C:80:GLU:OE1	1:C:195:ALA:HB2	2.18	0.44
1:D:7:LEU:HD12	1:D:29:PHE:HE2	1.82	0.44
1:C:37:THR:HG21	2:I:10:A:N1	2.32	0.44
1:A:37:THR:HG21	2:H:4:A:N1	2.33	0.44
1:A:258:LEU:HD23	1:A:627:PRO:HD2	2.00	0.44
1:B:31:SER:HA	1:B:57:ASN:O	2.17	0.44
1:B:33:HIS:HB3	1:B:85:TRP:HZ2	1.82	0.44
1:A:8:PHE:HE1	1:A:33:HIS:CD2	2.36	0.44
1:B:20:GLU:HB3	1:B:126:VAL:HG11	1.98	0.44
1:B:90:ARG:O	1:B:91:THR:OG1	2.31	0.44
1:E:468:VAL:HG12	1:E:470:VAL:HG23	2.00	0.44
1:F:477:ASP:OD1	1:F:478:ALA:N	2.51	0.44
1:A:98:VAL:HG13	1:A:111:MET:HE3	2.00	0.43
1:A:287:PRO:HA	1:A:290:LEU:HD23	2.00	0.43
1:B:24:LEU:HD12	1:B:25:PRO:HD2	2.00	0.43
1:B:333:ARG:HB3	1:B:337:ARG:NH1	2.32	0.43
1:A:11:LEU:HD21	1:A:36:THR:HG22	1.99	0.43
1:A:172:ARG:NH1	1:A:173:ARG:HG2	2.33	0.43
1:A:364:ARG:NH1	1:A:372:ASP:OD2	2.34	0.43
1:A:33:HIS:ND1	1:A:59:THR:OG1	2.47	0.43
1:A:531:LEU:HD21	1:A:587:ARG:CZ	2.47	0.43
1:B:187:LYS:HG2	1:B:188:GLY:H	1.83	0.43
1:F:610:CYS:HB2	1:F:614:GLN:HB3	2.01	0.43
1:D:440:ASP:HB3	1:D:469:THR:OG1	2.18	0.43
1:E:272:THR:O	1:E:273:HIS:ND1	2.50	0.43
1:A:183:VAL:HG23	1:A:191:ARG:HG3	2.01	0.43
1:A:218:TRP:CD1	1:B:214:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TRP:CZ3	1:B:221:LEU:HD22	2.53	0.43
1:C:3:VAL:HB	1:C:95:GLN:HG2	2.00	0.43
1:F:240:LEU:HD12	1:F:595:LEU:HD22	2.00	0.43
1:D:130:ASP:OD1	1:D:130:ASP:N	2.50	0.43
1:E:254:TRP:CD1	1:E:627:PRO:HG2	2.53	0.43
1:A:141:PRO:HB3	1:A:147:GLU:HG3	1.99	0.43
1:D:553:PRO:HB2	1:D:557:TYR:CZ	2.54	0.43
1:E:328:ASP:OD1	1:E:329:PRO:HD2	2.19	0.43
1:E:523:ASN:HD22	1:E:552:TYR:HE1	1.67	0.43
1:A:417:HIS:HE1	1:A:440:ASP:O	2.01	0.43
1:B:35:LEU:HD13	1:B:61:THR:HG23	2.00	0.43
1:B:302:TRP:O	1:B:305:PRO:HD3	2.19	0.43
1:C:219:GLU:C	1:C:220:MET:HG3	2.44	0.43
1:E:484:ALA:O	1:E:488:LEU:HB2	2.19	0.43
1:F:354:ARG:HG2	1:F:399:ILE:HB	1.99	0.43
1:A:23:LEU:HD13	1:A:152:ARG:HG3	2.00	0.43
1:C:140:MET:O	1:C:142:PRO:HD3	2.18	0.43
1:A:20:GLU:HB3	1:A:126:VAL:HG21	2.00	0.43
1:A:41:ASP:OD1	1:A:41:ASP:N	2.51	0.43
1:A:69:LEU:HD22	1:A:104:PHE:CD2	2.54	0.43
1:C:187:LYS:HA	1:C:187:LYS:HD3	1.76	0.43
1:D:417:HIS:ND1	1:D:418:LEU:HD12	2.34	0.43
1:D:440:ASP:HA	1:D:469:THR:O	2.19	0.43
1:E:232:TRP:HE1	1:E:237:LEU:HA	1.84	0.43
1:B:49:PHE:HD2	1:B:58:LEU:HB2	1.84	0.42
1:D:323:THR:O	1:D:327:ARG:HG3	2.18	0.42
1:F:362:GLU:HG2	1:F:363:VAL:N	2.34	0.42
1:F:611:THR:HG23	1:F:614:GLN:H	1.83	0.42
1:A:52:HIS:CE1	1:A:145:LEU:HD22	2.54	0.42
1:B:593:THR:OG1	1:B:596:ASP:OD2	2.30	0.42
1:C:143:SER:OG	1:C:143:SER:O	2.36	0.42
1:C:174:ILE:HG22	1:C:175:ALA:H	1.84	0.42
1:D:16:ALA:C	1:D:19:PRO:HD2	2.45	0.42
1:E:226:PHE:HB3	1:E:602:ARG:HH21	1.82	0.42
1:F:334:GLU:HA	1:F:337:ARG:HG2	2.02	0.42
1:C:38:GLU:HG2	1:C:192:ARG:HH21	1.84	0.42
1:E:430:ASP:OD2	1:E:433:ALA:HB3	2.19	0.42
1:E:471:HIS:HB2	1:E:494:GLY:HA3	2.00	0.42
1:A:382:GLU:OE1	1:A:385:ARG:NH2	2.52	0.42
1:B:64:ALA:N	1:B:193:VAL:O	2.50	0.42
1:D:94:GLU:OE1	1:D:94:GLU:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:VAL:HG23	1:D:162:LEU:HB2	2.01	0.42
1:D:314:TYR:CD2	1:D:526:ILE:HD11	2.54	0.42
1:D:354:ARG:HA	1:D:399:ILE:O	2.20	0.42
1:C:510:ALA:HB2	1:C:562:VAL:HG22	2.00	0.42
2:I:8:A:O2'	2:I:9:A:H5'	2.19	0.42
1:C:87:LEU:HD11	1:C:200:PHE:CE2	2.55	0.42
1:D:18:VAL:HB	1:D:19:PRO:HD3	2.01	0.42
1:F:531:LEU:HD12	1:F:587:ARG:HG3	2.01	0.42
1:A:99:CYS:HB2	1:A:124:PHE:CZ	2.55	0.42
1:B:441:LEU:HD21	1:B:454:PHE:HD2	1.84	0.42
1:B:470:VAL:O	1:B:494:GLY:N	2.52	0.42
1:B:509:VAL:HG13	1:B:514:ILE:HB	2.01	0.42
1:D:39:ARG:H	1:D:40:PRO:CD	2.32	0.42
1:A:101:THR:OG1	1:A:125:HIS:ND1	2.50	0.42
1:C:122:GLU:HG2	1:C:161:ARG:HE	1.84	0.42
1:F:364:ARG:NH2	1:F:368:ASP:HB3	2.31	0.42
1:F:531:LEU:HB2	1:F:587:ARG:O	2.20	0.42
1:A:36:THR:OG1	1:A:62:ARG:HA	2.19	0.42
1:A:246:PRO:O	1:A:252:GLN:NE2	2.51	0.42
1:B:82:MET:HE3	1:B:114:ALA:HB2	2.02	0.42
1:B:281:ARG:HH12	1:B:293:LEU:CA	2.32	0.42
1:C:281:ARG:NH2	1:C:291:PRO:O	2.51	0.42
1:D:386:THR:HG22	1:D:393:ALA:HB2	2.02	0.42
1:E:231:THR:O	1:E:628:ARG:NH2	2.53	0.42
1:E:246:PRO:HG2	1:E:247:ARG:NH1	2.35	0.42
1:C:90:ARG:O	1:C:91:THR:OG1	2.27	0.42
1:C:272:THR:HG23	1:C:273:HIS:ND1	2.35	0.42
1:D:68:ASP:O	1:D:70:LYS:HG2	2.20	0.42
1:E:326:LEU:HB3	1:E:332:LEU:HD13	2.02	0.42
1:E:356:SER:OG	1:E:401:ILE:HG23	2.20	0.42
1:A:16:ALA:HB1	1:A:148:ILE:HD11	2.02	0.41
1:A:218:TRP:CZ2	1:B:228:ASP:HA	2.55	0.41
1:B:86:PHE:HB3	1:B:118:LEU:HD21	2.01	0.41
1:B:129:ASP:OD1	2:H:3:A:N6	2.51	0.41
1:B:239:TRP:CZ3	1:B:629:PRO:HG3	2.54	0.41
1:D:476:ASP:OD1	1:D:496:ALA:HA	2.20	0.41
1:C:171:LEU:O	1:C:171:LEU:HD23	2.20	0.41
1:D:44:LEU:HD11	1:D:143:SER:HA	2.01	0.41
1:D:482:TRP:HD1	1:D:505:LEU:HD13	1.85	0.41
1:F:318:GLY:HA3	1:F:573:ILE:CD1	2.50	0.41
1:C:562:VAL:O	1:C:564:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:GLN:N	1:D:67:GLN:OE1	2.54	0.41
1:E:397:ASN:HD22	1:E:397:ASN:HA	1.70	0.41
1:A:239:TRP:CZ3	1:A:629:PRO:HG3	2.56	0.41
1:B:326:LEU:HD22	1:B:332:LEU:HA	2.02	0.41
1:B:493:LEU:HG	1:B:514:ILE:HG21	2.00	0.41
1:D:39:ARG:HB2	1:D:40:PRO:HD3	2.03	0.41
1:D:518:LEU:HD23	1:D:518:LEU:HA	1.89	0.41
1:C:43:THR:HA	1:C:46:ARG:HB2	2.02	0.41
1:C:62:ARG:HH21	1:C:190:GLU:HB3	1.85	0.41
1:C:396:VAL:C	1:C:397:ASN:HD22	2.29	0.41
1:D:399:ILE:HG13	1:D:438:GLY:O	2.21	0.41
1:E:614:GLN:HG2	1:E:618:LEU:HD23	2.01	0.41
1:A:494:GLY:HA2	1:A:517:GLU:HB2	2.03	0.41
1:C:100:LEU:O	1:C:125:HIS:ND1	2.50	0.41
1:C:187:LYS:HG3	1:C:188:GLY:H	1.85	0.41
1:C:597:LEU:HA	1:C:600:LEU:HD12	2.03	0.41
1:A:68:ASP:HB2	1:A:70:LYS:NZ	2.35	0.41
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.88	0.41
1:B:441:LEU:HD12	1:B:441:LEU:HA	1.94	0.41
1:C:39:ARG:H	1:C:40:PRO:CD	2.34	0.41
1:C:117:VAL:HG12	1:C:168:TRP:HE1	1.86	0.41
1:C:235:GLY:O	1:C:239:TRP:N	2.39	0.41
1:C:570:ASN:CG	1:C:573:ILE:HB	2.45	0.41
1:F:519:CYS:SG	1:F:569:ASP:HB2	2.60	0.41
1:F:594:ARG:HH11	1:F:597:LEU:HD23	1.85	0.41
1:A:7:LEU:HB2	1:A:29:PHE:CE1	2.56	0.41
1:F:254:TRP:HZ3	1:F:258:LEU:HD22	1.85	0.41
1:F:260:LYS:H	1:F:260:LYS:HG2	1.69	0.41
1:F:521:TYR:CZ	1:F:584:LEU:HD22	2.55	0.41
1:B:266:HIS:HB2	1:B:570:ASN:OD1	2.21	0.41
1:B:268:GLY:HA3	4:B:702:ATP:O2A	2.21	0.41
1:C:170:GLN:NE2	1:C:207:LEU:HD21	2.36	0.41
1:C:184:VAL:HG13	1:C:194:GLN:OE1	2.20	0.41
1:C:259:PRO:HG3	1:C:625:GLY:HA3	2.03	0.41
1:C:285:GLU:N	1:C:328:ASP:OD2	2.44	0.41
1:D:213:ARG:HD3	1:D:232:TRP:C	2.46	0.41
1:D:281:ARG:CZ	1:D:293:LEU:HB3	2.51	0.41
1:D:281:ARG:NH1	1:D:293:LEU:HB3	2.36	0.41
1:F:269:GLY:HA3	1:F:570:ASN:HB2	2.03	0.41
1:F:325:LEU:HD12	1:F:326:LEU:HD12	2.03	0.41
1:F:401:ILE:HA	1:F:440:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:ALA:HB1	1:F:476:ASP:HB3	2.03	0.41
1:C:41:ASP:OD1	1:C:43:THR:HG22	2.21	0.41
1:C:137:GLY:O	1:C:139:LEU:HD12	2.21	0.41
1:C:317:LEU:HD23	1:C:573:ILE:HG23	2.03	0.41
1:C:399:ILE:HG13	1:C:438:GLY:C	2.46	0.41
1:D:130:ASP:HB2	1:D:138:ARG:C	2.46	0.41
1:D:130:ASP:HB2	1:D:138:ARG:O	2.21	0.41
1:E:298:LEU:HD23	1:E:298:LEU:H	1.85	0.41
1:E:610:CYS:SG	1:E:614:GLN:HB3	2.61	0.41
1:B:19:PRO:O	1:B:23:LEU:HD23	2.22	0.40
1:B:126:VAL:HG22	1:B:159:TRP:CD1	2.56	0.40
1:B:570:ASN:ND2	1:B:573:ILE:HD12	2.36	0.40
1:C:35:LEU:HD23	1:C:61:THR:HB	2.03	0.40
1:F:240:LEU:HB3	1:F:595:LEU:CD2	2.52	0.40
1:F:554:LEU:HA	1:F:554:LEU:HD12	1.87	0.40
1:A:488:LEU:HD23	1:A:488:LEU:H	1.86	0.40
1:B:37:THR:HG23	1:B:37:THR:O	2.22	0.40
1:C:82:MET:HE3	1:C:114:ALA:HB2	2.03	0.40
1:C:130:ASP:O	1:C:138:ARG:HB3	2.21	0.40
1:D:595:LEU:HD23	1:D:595:LEU:H	1.87	0.40
1:F:285:GLU:HG2	1:F:328:ASP:OD1	2.21	0.40
1:F:482:TRP:CE2	1:F:505:LEU:HD13	2.56	0.40
1:A:489:ASN:HB3	1:B:512:ARG:HH12	1.86	0.40
1:E:232:TRP:HD1	1:E:233:SER:O	2.04	0.40
1:E:323:THR:HA	1:E:360:TYR:CE1	2.54	0.40
1:F:485:VAL:HG23	1:F:514:ILE:HG13	2.03	0.40
1:A:521:TYR:CE1	1:A:584:LEU:HD22	2.57	0.40
1:B:171:LEU:HD23	1:B:207:LEU:HD22	2.04	0.40
1:B:403:THR:HG21	4:B:702:ATP:O3'	2.21	0.40
1:F:298:LEU:HD12	1:F:302:TRP:CB	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	609/635 (96%)	560 (92%)	46 (8%)	3 (0%)	25	60
1	B	611/635 (96%)	562 (92%)	44 (7%)	5 (1%)	16	51
1	C	609/635 (96%)	544 (89%)	60 (10%)	5 (1%)	16	51
1	D	610/635 (96%)	560 (92%)	47 (8%)	3 (0%)	25	60
1	E	391/635 (62%)	349 (89%)	40 (10%)	2 (0%)	25	60
1	F	390/635 (61%)	349 (90%)	39 (10%)	2 (0%)	25	60
All	All	3220/3810 (84%)	2924 (91%)	276 (9%)	20 (1%)	24	57

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	ALA
1	C	39	ARG
1	C	387	ALA
1	B	39	ARG
1	C	63	VAL
1	D	63	VAL
1	F	503	ARG
1	A	39	ARG
1	D	39	ARG
1	E	404	ARG
1	F	267	LEU
1	A	174	ILE
1	B	174	ILE
1	C	174	ILE
1	E	476	ASP
1	B	270	PHE
1	A	63	VAL
1	C	183	VAL
1	D	183	VAL
1	B	63	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	480/511 (94%)	480 (100%)	0	100	100
1	B	495/511 (97%)	495 (100%)	0	100	100
1	C	494/511 (97%)	494 (100%)	0	100	100
1	D	483/511 (94%)	483 (100%)	0	100	100
1	E	304/511 (60%)	304 (100%)	0	100	100
1	F	296/511 (58%)	296 (100%)	0	100	100
All	All	2552/3066 (83%)	2552 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	273	HIS
1	A	286	ASN
1	A	378	GLN
1	A	501	GLN
1	A	523	ASN
1	B	158	HIS
1	B	209	GLN
1	C	182	GLN
1	C	205	GLN
1	C	335	GLN
1	C	397	ASN
1	C	501	GLN
1	C	599	HIS
1	D	154	GLN
1	D	156	HIS
1	D	266	HIS
1	D	273	HIS
1	D	359	ASN
1	D	501	GLN
1	E	321	ASN
1	E	495	HIS
1	E	523	ASN
1	E	599	HIS
1	E	614	GLN

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Mol	Chain	Res	Type
1	F	264	HIS
1	F	395	HIS
1	F	581	ASN
1	F	601	GLN
1	F	614	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	5/6 (83%)	3 (60%)	0
2	I	5/6 (83%)	3 (60%)	0
All	All	10/12 (83%)	6 (60%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	2	A
2	H	3	A
2	H	5	A
2	I	8	A
2	I	9	A
2	I	11	A

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	C	702	-	26,33,33	0.90	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	B	702	-	26,33,33	0.61	0	31,52,52	1.04	2 (6%)

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	C	702	-	-	8/18/38/38	0/3/3/3
4	ATP	B	702	-	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	ATP	C5-C4	2.20	1.46	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	ATP	PB-O3B-PG	-4.57	117.15	132.83
4	C	702	ATP	N3-C2-N1	-3.53	123.16	128.68
4	C	702	ATP	C3'-C2'-C1'	3.20	105.79	100.98
4	C	702	ATP	PA-O3A-PB	-3.02	122.46	132.83
4	C	702	ATP	C4-C5-N7	-2.71	106.57	109.40
4	B	702	ATP	C5-C6-N6	2.33	123.89	120.35
4	B	702	ATP	PB-O3B-PG	2.05	139.85	132.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	702	ATP	C5'-O5'-PA-O2A
4	C	702	ATP	O4'-C4'-C5'-O5'
4	B	702	ATP	O4'-C4'-C5'-O5'

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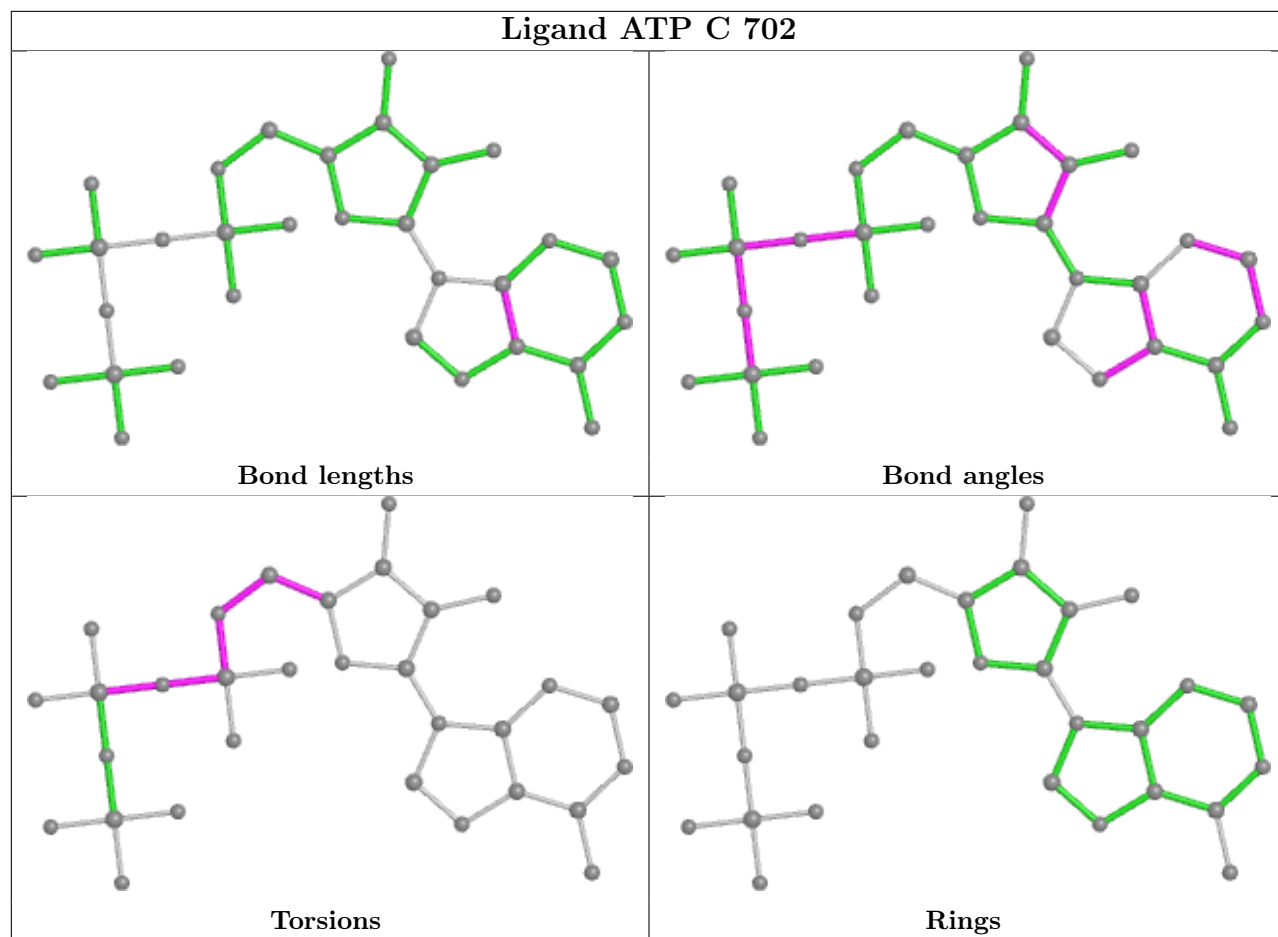
Mol	Chain	Res	Type	Atoms
4	B	702	ATP	C5'-O5'-PA-O3A
4	C	702	ATP	C5'-O5'-PA-O3A
4	C	702	ATP	C3'-C4'-C5'-O5'
4	B	702	ATP	C5'-O5'-PA-O2A
4	C	702	ATP	C5'-O5'-PA-O1A
4	C	702	ATP	C4'-C5'-O5'-PA
4	C	702	ATP	PA-O3A-PB-O1B
4	C	702	ATP	PB-O3A-PA-O1A

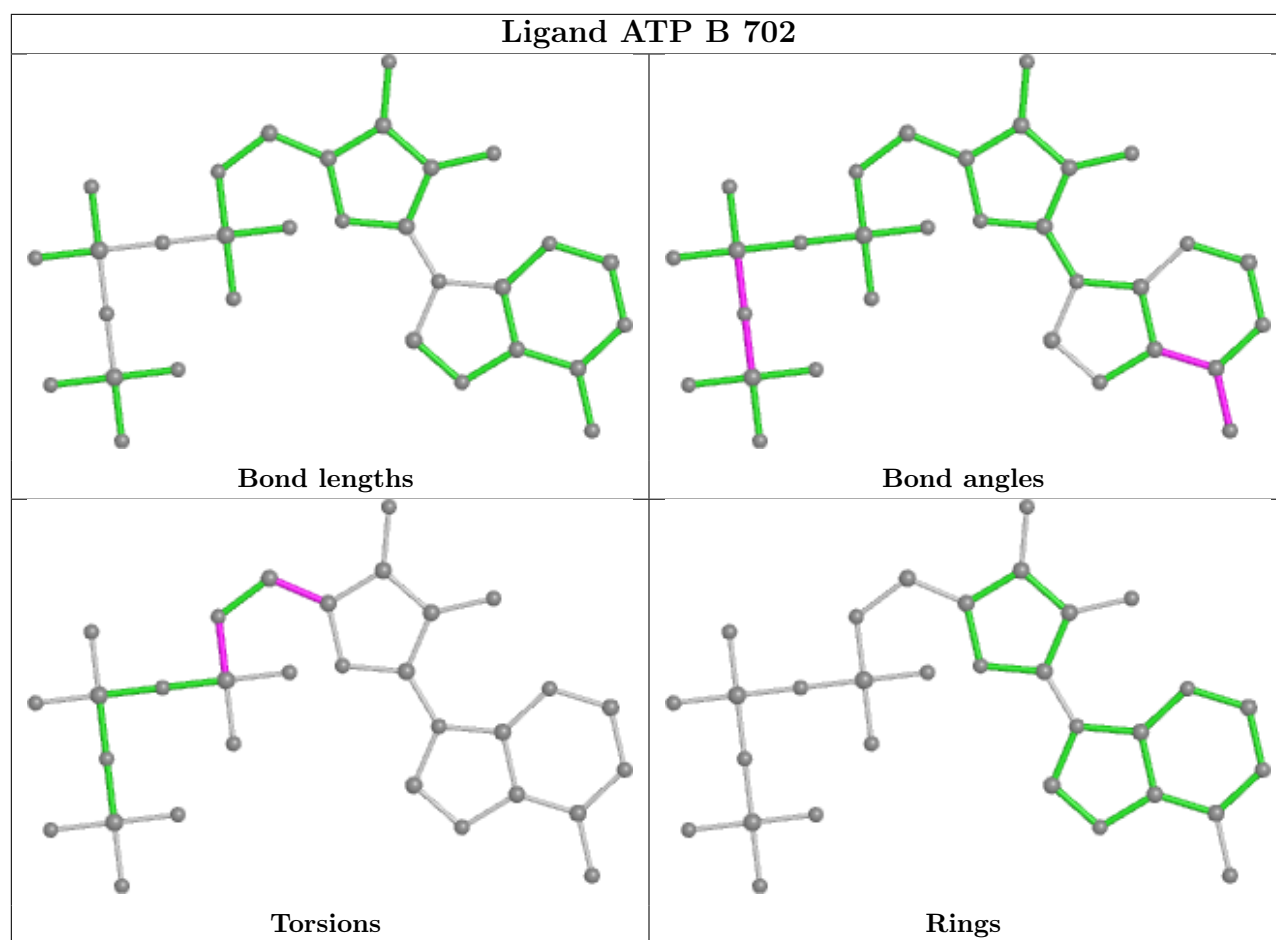
There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	702	ATP	7	0
4	B	702	ATP	11	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.