Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 07:10 PM EDT

PDB ID	:	3GLG
Title	:	Crystal Structure of a Mutant (gammaT157A) E. coli Clamp Loader Bound to Primer-Template DNA
Authors	:	Simonetta, K.R.; Seyedin, S.N.; Kuriyan, J.
Deposited on	:	2009-03-12
Resolution	:	3.25 Å(reported)

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

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

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

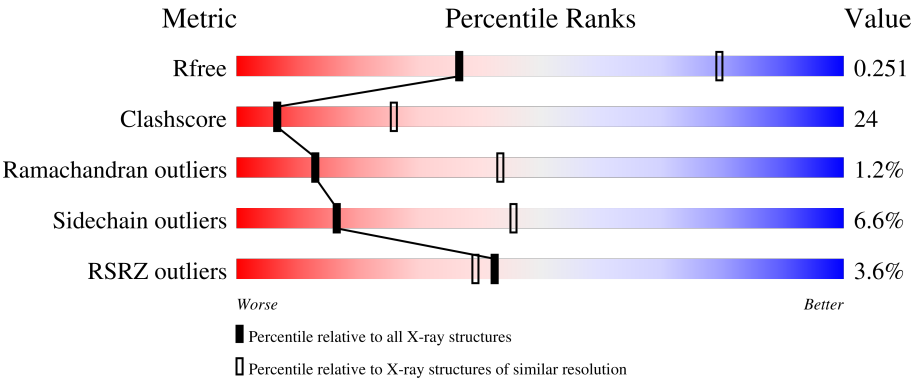
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	343	15% 50% 43% 5%
1	F	343	7% 54% 38% 5%
2	B	395	4% 54% 35% 8%
2	C	395	3% 53% 34% 8%
2	D	395	3% 55% 32% 8%

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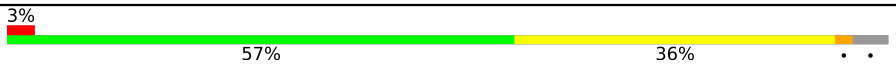
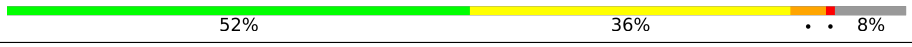
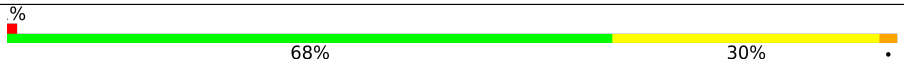
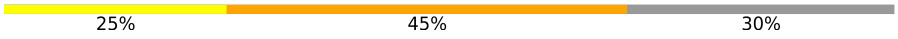
Mol	Chain	Length	Quality of chain
2	G	395	
2	H	395	
2	I	395	
3	E	334	
3	J	334	
4	K	20	
4	M	20	
5	L	10	
5	N	10	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 28746 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 DNA polymerase III subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2650	1678	482	480	10			
1	F	333	Total	C	N	O	S	0	0	0
			2650	1678	482	480	10			

- Molecule 2 is a protein called DNA polymerase III subunit tau.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	0	0
			2827	1778	511	522	16			
2	C	365	Total	C	N	O	S	0	0	0
			2836	1783	513	524	16			
2	D	362	Total	C	N	O	S	0	0	0
			2816	1769	510	521	16			
2	G	378	Total	C	N	O	S	0	0	0
			2939	1851	529	542	17			
2	H	365	Total	C	N	O	S	0	0	0
			2836	1783	513	524	16			
2	I	362	Total	C	N	O	S	0	0	0
			2816	1769	510	521	16			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	expression tag	UNP P06710
B	-20	GLY	-	expression tag	UNP P06710
B	-19	SER	-	expression tag	UNP P06710
B	-18	SER	-	expression tag	UNP P06710
B	-17	HIS	-	expression tag	UNP P06710
B	-16	HIS	-	expression tag	UNP P06710
B	-15	HIS	-	expression tag	UNP P06710
B	-14	HIS	-	expression tag	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P06710
B	-12	HIS	-	expression tag	UNP P06710
B	-11	SER	-	expression tag	UNP P06710
B	-10	SER	-	expression tag	UNP P06710
B	-9	GLY	-	expression tag	UNP P06710
B	-8	LEU	-	expression tag	UNP P06710
B	-7	GLU	-	expression tag	UNP P06710
B	-6	VAL	-	expression tag	UNP P06710
B	-5	LEU	-	expression tag	UNP P06710
B	-4	PHE	-	expression tag	UNP P06710
B	-3	GLN	-	expression tag	UNP P06710
B	-2	GLY	-	expression tag	UNP P06710
B	-1	PRO	-	expression tag	UNP P06710
B	0	HIS	-	expression tag	UNP P06710
B	157	ALA	THR	engineered mutation	UNP P06710
C	-21	MET	-	expression tag	UNP P06710
C	-20	GLY	-	expression tag	UNP P06710
C	-19	SER	-	expression tag	UNP P06710
C	-18	SER	-	expression tag	UNP P06710
C	-17	HIS	-	expression tag	UNP P06710
C	-16	HIS	-	expression tag	UNP P06710
C	-15	HIS	-	expression tag	UNP P06710
C	-14	HIS	-	expression tag	UNP P06710
C	-13	HIS	-	expression tag	UNP P06710
C	-12	HIS	-	expression tag	UNP P06710
C	-11	SER	-	expression tag	UNP P06710
C	-10	SER	-	expression tag	UNP P06710
C	-9	GLY	-	expression tag	UNP P06710
C	-8	LEU	-	expression tag	UNP P06710
C	-7	GLU	-	expression tag	UNP P06710
C	-6	VAL	-	expression tag	UNP P06710
C	-5	LEU	-	expression tag	UNP P06710
C	-4	PHE	-	expression tag	UNP P06710
C	-3	GLN	-	expression tag	UNP P06710
C	-2	GLY	-	expression tag	UNP P06710
C	-1	PRO	-	expression tag	UNP P06710
C	0	HIS	-	expression tag	UNP P06710
C	157	ALA	THR	engineered mutation	UNP P06710
D	-21	MET	-	expression tag	UNP P06710
D	-20	GLY	-	expression tag	UNP P06710
D	-19	SER	-	expression tag	UNP P06710
D	-18	SER	-	expression tag	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	HIS	-	expression tag	UNP P06710
D	-16	HIS	-	expression tag	UNP P06710
D	-15	HIS	-	expression tag	UNP P06710
D	-14	HIS	-	expression tag	UNP P06710
D	-13	HIS	-	expression tag	UNP P06710
D	-12	HIS	-	expression tag	UNP P06710
D	-11	SER	-	expression tag	UNP P06710
D	-10	SER	-	expression tag	UNP P06710
D	-9	GLY	-	expression tag	UNP P06710
D	-8	LEU	-	expression tag	UNP P06710
D	-7	GLU	-	expression tag	UNP P06710
D	-6	VAL	-	expression tag	UNP P06710
D	-5	LEU	-	expression tag	UNP P06710
D	-4	PHE	-	expression tag	UNP P06710
D	-3	GLN	-	expression tag	UNP P06710
D	-2	GLY	-	expression tag	UNP P06710
D	-1	PRO	-	expression tag	UNP P06710
D	0	HIS	-	expression tag	UNP P06710
D	157	ALA	THR	engineered mutation	UNP P06710
G	-21	MET	-	expression tag	UNP P06710
G	-20	GLY	-	expression tag	UNP P06710
G	-19	SER	-	expression tag	UNP P06710
G	-18	SER	-	expression tag	UNP P06710
G	-17	HIS	-	expression tag	UNP P06710
G	-16	HIS	-	expression tag	UNP P06710
G	-15	HIS	-	expression tag	UNP P06710
G	-14	HIS	-	expression tag	UNP P06710
G	-13	HIS	-	expression tag	UNP P06710
G	-12	HIS	-	expression tag	UNP P06710
G	-11	SER	-	expression tag	UNP P06710
G	-10	SER	-	expression tag	UNP P06710
G	-9	GLY	-	expression tag	UNP P06710
G	-8	LEU	-	expression tag	UNP P06710
G	-7	GLU	-	expression tag	UNP P06710
G	-6	VAL	-	expression tag	UNP P06710
G	-5	LEU	-	expression tag	UNP P06710
G	-4	PHE	-	expression tag	UNP P06710
G	-3	GLN	-	expression tag	UNP P06710
G	-2	GLY	-	expression tag	UNP P06710
G	-1	PRO	-	expression tag	UNP P06710
G	0	HIS	-	expression tag	UNP P06710
G	157	ALA	THR	engineered mutation	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-21	MET	-	expression tag	UNP P06710
H	-20	GLY	-	expression tag	UNP P06710
H	-19	SER	-	expression tag	UNP P06710
H	-18	SER	-	expression tag	UNP P06710
H	-17	HIS	-	expression tag	UNP P06710
H	-16	HIS	-	expression tag	UNP P06710
H	-15	HIS	-	expression tag	UNP P06710
H	-14	HIS	-	expression tag	UNP P06710
H	-13	HIS	-	expression tag	UNP P06710
H	-12	HIS	-	expression tag	UNP P06710
H	-11	SER	-	expression tag	UNP P06710
H	-10	SER	-	expression tag	UNP P06710
H	-9	GLY	-	expression tag	UNP P06710
H	-8	LEU	-	expression tag	UNP P06710
H	-7	GLU	-	expression tag	UNP P06710
H	-6	VAL	-	expression tag	UNP P06710
H	-5	LEU	-	expression tag	UNP P06710
H	-4	PHE	-	expression tag	UNP P06710
H	-3	GLN	-	expression tag	UNP P06710
H	-2	GLY	-	expression tag	UNP P06710
H	-1	PRO	-	expression tag	UNP P06710
H	0	HIS	-	expression tag	UNP P06710
H	157	ALA	THR	engineered mutation	UNP P06710
I	-21	MET	-	expression tag	UNP P06710
I	-20	GLY	-	expression tag	UNP P06710
I	-19	SER	-	expression tag	UNP P06710
I	-18	SER	-	expression tag	UNP P06710
I	-17	HIS	-	expression tag	UNP P06710
I	-16	HIS	-	expression tag	UNP P06710
I	-15	HIS	-	expression tag	UNP P06710
I	-14	HIS	-	expression tag	UNP P06710
I	-13	HIS	-	expression tag	UNP P06710
I	-12	HIS	-	expression tag	UNP P06710
I	-11	SER	-	expression tag	UNP P06710
I	-10	SER	-	expression tag	UNP P06710
I	-9	GLY	-	expression tag	UNP P06710
I	-8	LEU	-	expression tag	UNP P06710
I	-7	GLU	-	expression tag	UNP P06710
I	-6	VAL	-	expression tag	UNP P06710
I	-5	LEU	-	expression tag	UNP P06710
I	-4	PHE	-	expression tag	UNP P06710
I	-3	GLN	-	expression tag	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	expression tag	UNP P06710
I	-1	PRO	-	expression tag	UNP P06710
I	0	HIS	-	expression tag	UNP P06710
I	157	ALA	THR	engineered mutation	UNP P06710

- Molecule 3 is a protein called DNA polymerase III subunit delta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			
3	J	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

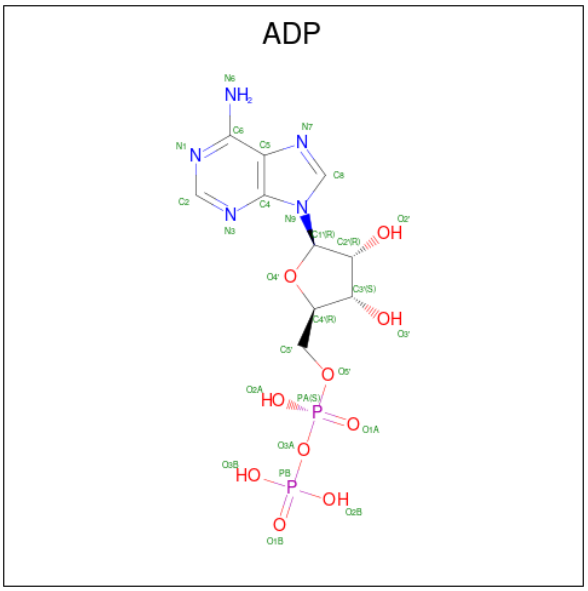
- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	14	Total	C	N	O	P	0	0	0
			287	138	48	87	14			
4	M	14	Total	C	N	O	P	0	0	0
			287	138	48	87	14			

- Molecule 5 is a DNA chain called DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3').

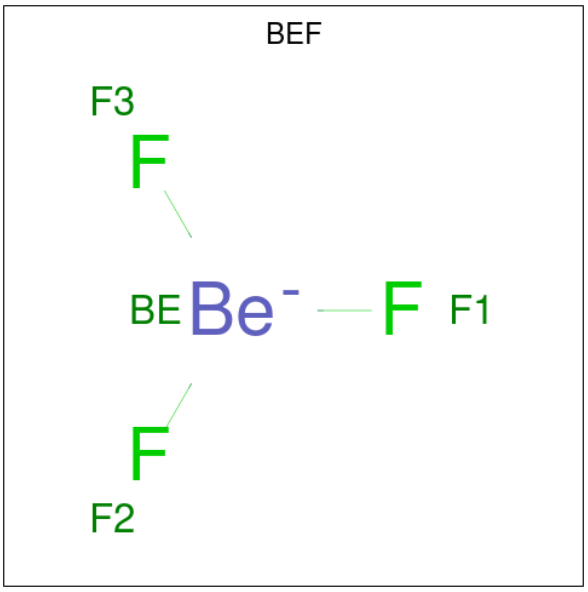
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			
5	N	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Be F 4 1 3	0	0
7	C	1	Total Be F 4 1 3	0	0
7	D	1	Total Be F 4 1 3	0	0
7	G	1	Total Be F 4 1 3	0	0
7	I	1	Total Be F 4 1 3	0	0
7	I	1	Total Be F 4 1 3	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	C	1	Total Mg 1 1	0	0
8	D	1	Total Mg 1 1	0	0
8	G	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0
8	I	1	Total Mg 1 1	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

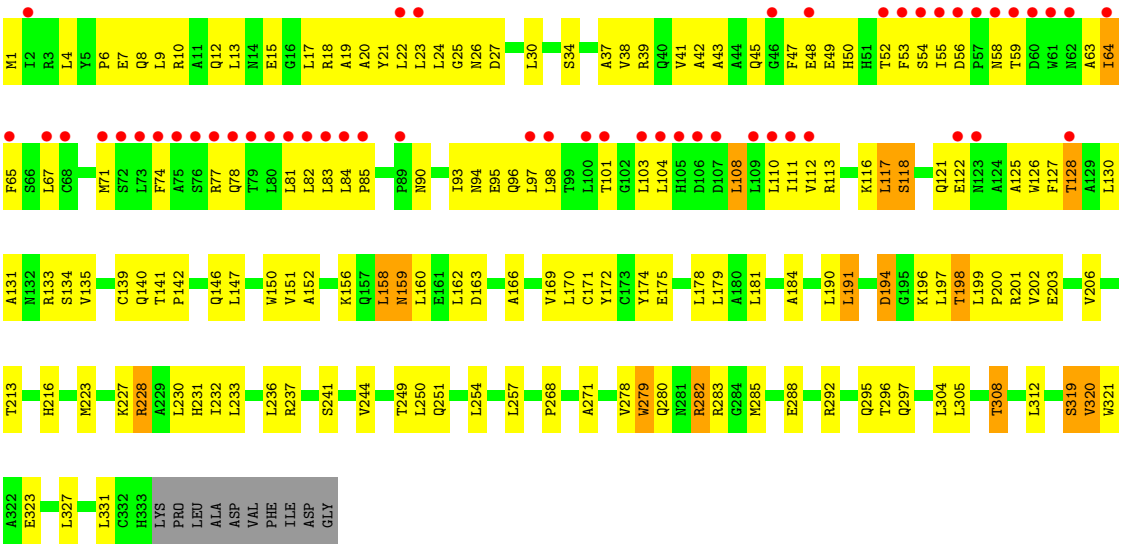
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Zn 1 1	0	0
9	C	1	Total Zn 1 1	0	0
9	D	1	Total Zn 1 1	0	0
9	E	1	Total Zn 1 1	0	0
9	G	1	Total Zn 1 1	0	0
9	H	1	Total Zn 1 1	0	0
9	I	1	Total Zn 1 1	0	0
9	J	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

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

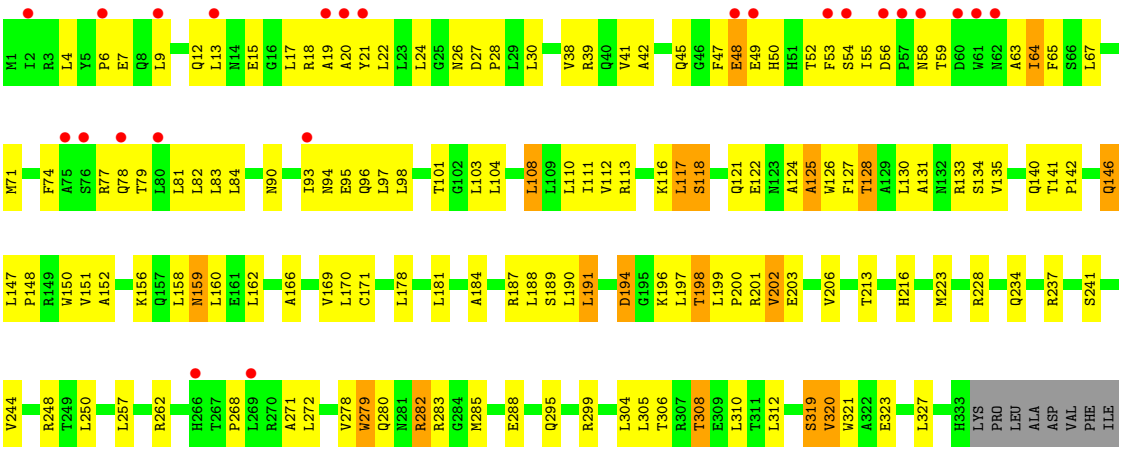
• Molecule 1: DNA polymerase III subunit delta

Chain A:



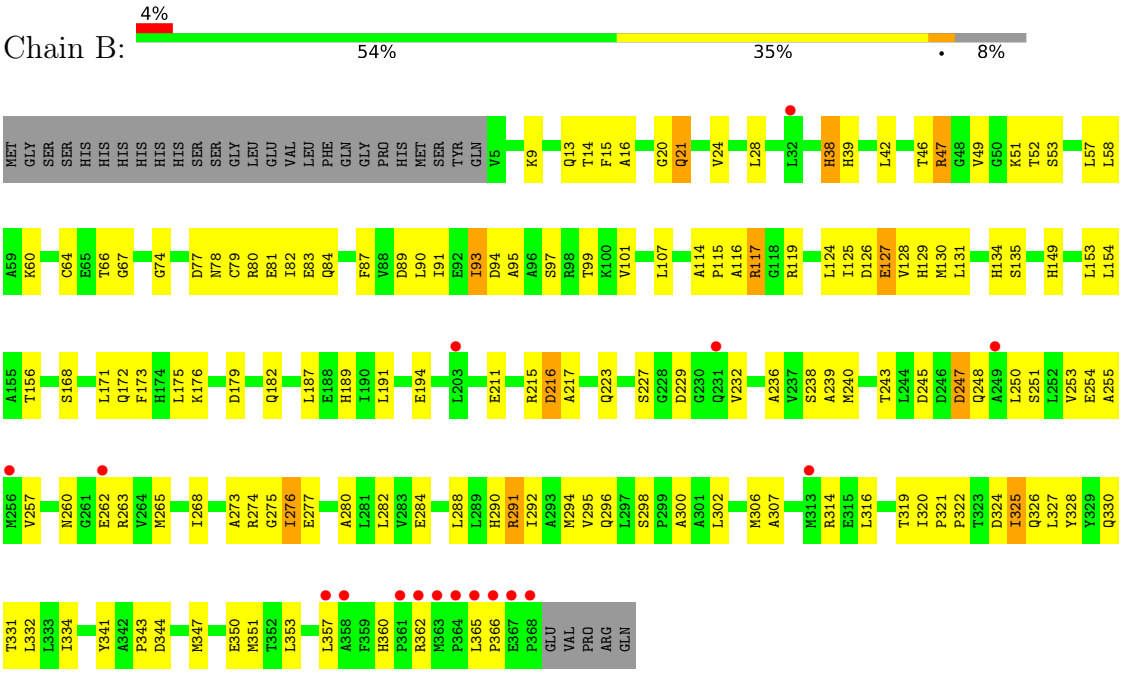
• Molecule 1: DNA polymerase III subunit delta

Chain F:



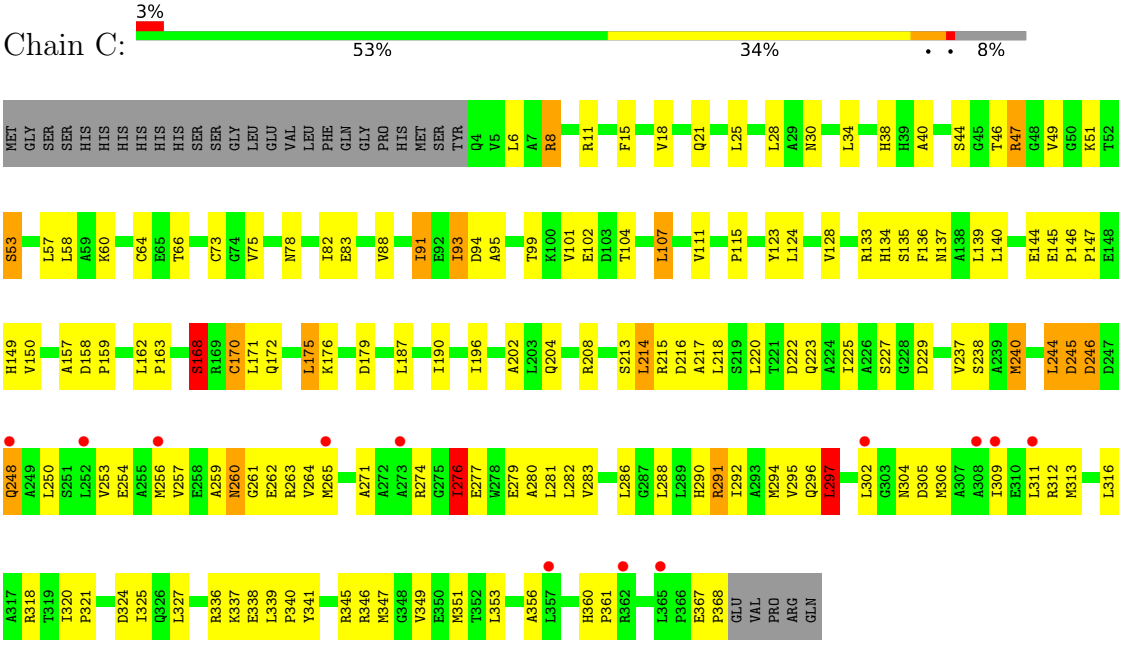
• Molecule 2: DNA polymerase III subunit tau

Chain B:



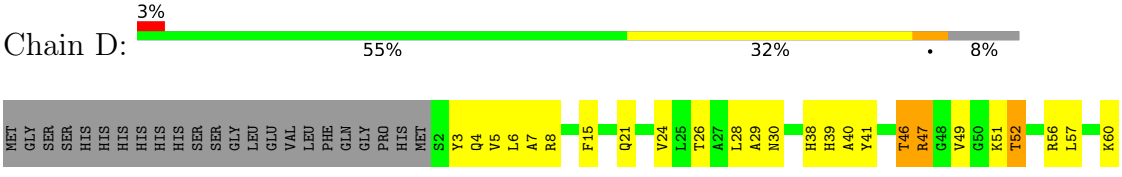
• Molecule 2: DNA polymerase III subunit tau

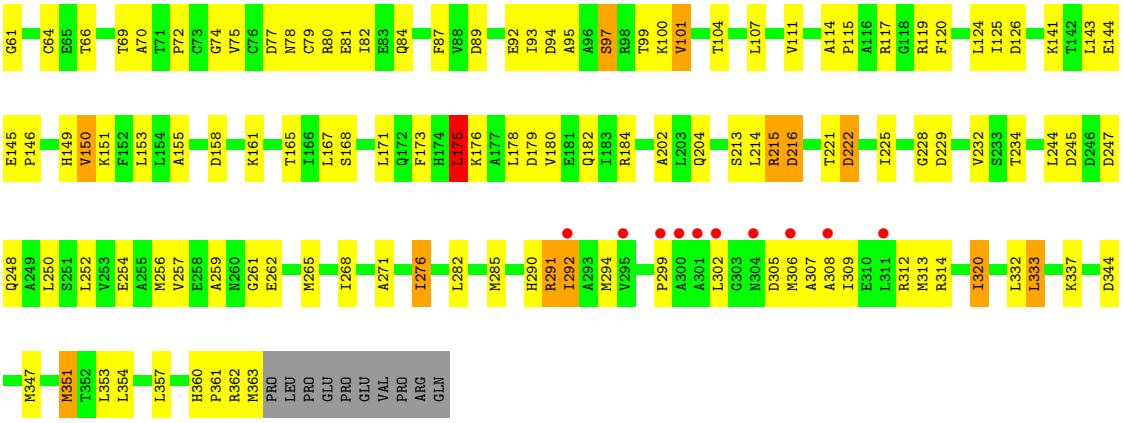
Chain C:



• Molecule 2: DNA polymerase III subunit tau

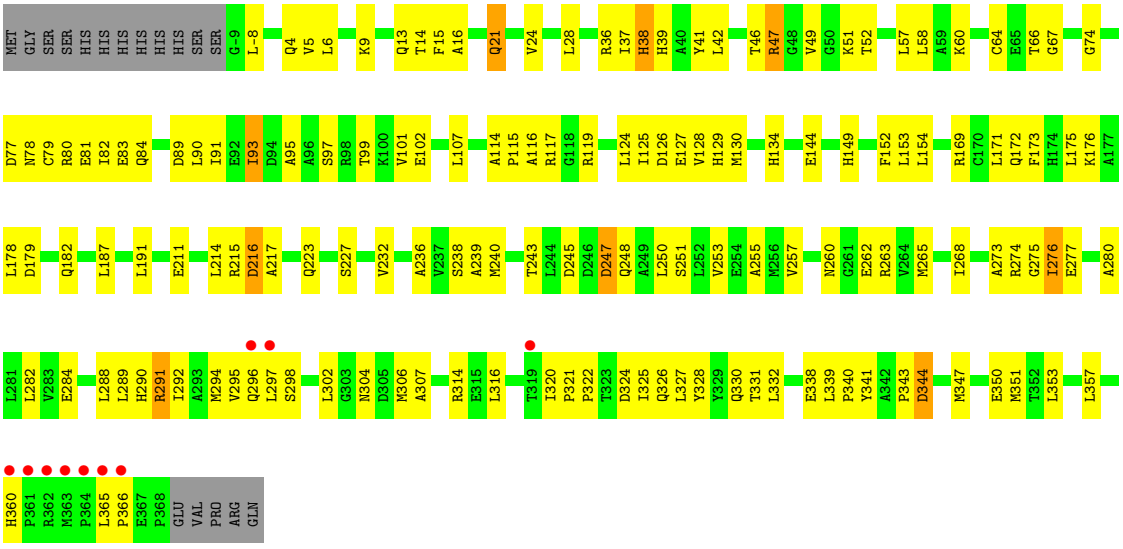
Chain D:





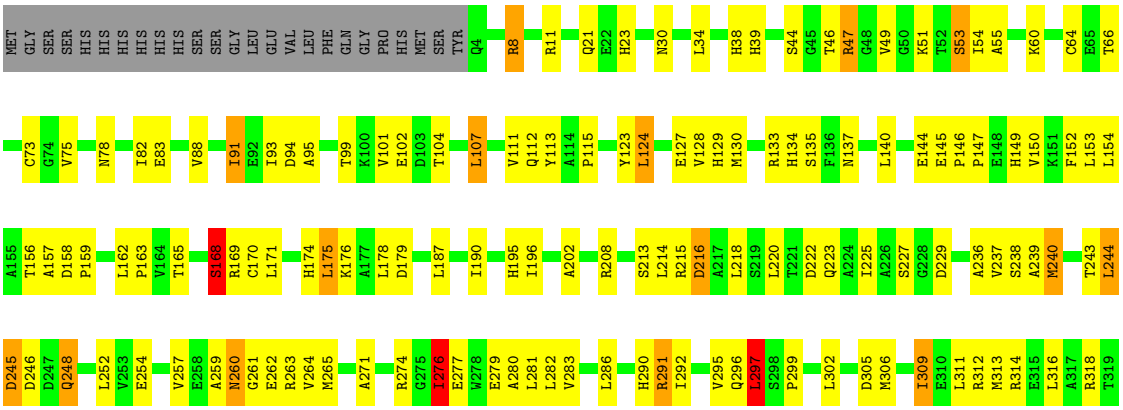
• Molecule 2: DNA polymerase III subunit tau

Chain G:



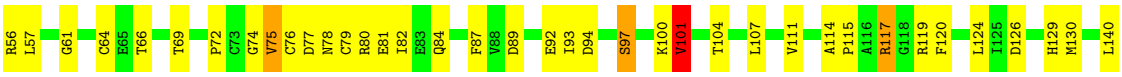
• Molecule 2: DNA polymerase III subunit tau

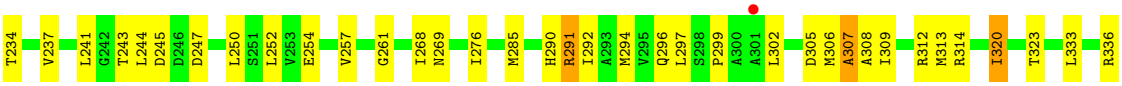
Chain H:



• Molecule 2: DNA polymerase III subunit tau

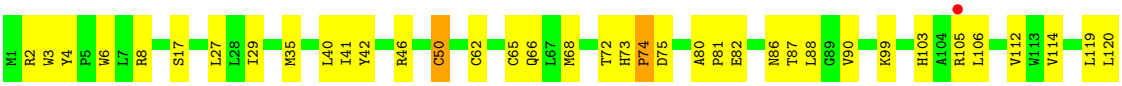
Chain I:

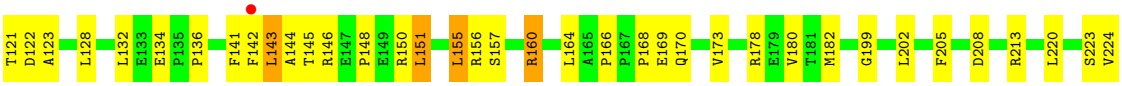


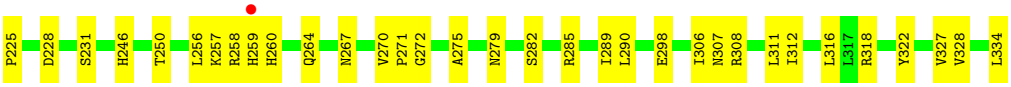


• Molecule 3: DNA polymerase III subunit delta'

Chain E:

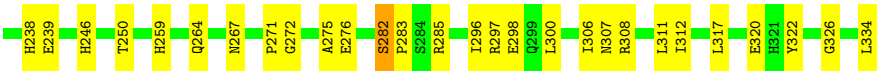






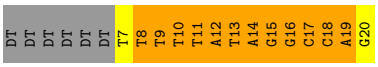
• Molecule 3: DNA polymerase III subunit delta'

Chain J:



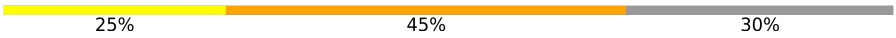
• Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')

Chain K:



• Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')

Chain M:



• Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')

Chain L:

• Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.10Å 219.10Å 274.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.25 49.24 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.24-3.25) 98.7 (49.24-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.224 , 0.263 0.211 , 0.251	Depositor DCC
R_{free} test set	4745 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	97.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28746	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.66	0/2697	0.73	0/3664
1	F	0.68	0/2697	0.73	0/3664
2	B	0.68	1/2874 (0.0%)	0.78	0/3897
2	C	0.66	1/2883 (0.0%)	0.82	2/3909 (0.1%)
2	D	0.68	0/2861	0.86	1/3876 (0.0%)
2	G	0.68	1/2990 (0.0%)	0.78	1/4054 (0.0%)
2	H	0.82	4/2883 (0.1%)	0.90	2/3909 (0.1%)
2	I	0.86	2/2861 (0.1%)	0.93	2/3876 (0.1%)
3	E	0.85	0/2666	0.89	1/3639 (0.0%)
3	J	0.84	1/2666 (0.0%)	0.88	0/3639
4	K	1.92	6/320 (1.9%)	2.63	39/492 (7.9%)
4	M	1.81	3/320 (0.9%)	2.51	21/492 (4.3%)
5	L	1.58	4/223 (1.8%)	2.69	24/342 (7.0%)
5	N	1.76	4/223 (1.8%)	2.58	25/342 (7.3%)
All	All	0.81	27/29164 (0.1%)	0.97	118/39795 (0.3%)

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
2	C	0	1
2	H	0	1
3	E	0	1
3	J	0	1
All	All	0	4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	14	DA	C3'-O3'	-8.93	1.32	1.44
2	B	127	GLU	CG-CD	7.35	1.62	1.51
2	H	127	GLU	CD-OE1	7.06	1.33	1.25
4	K	11	DT	C3'-O3'	-7.03	1.34	1.44
4	K	14	DA	C3'-O3'	-6.89	1.34	1.44
2	G	127	GLU	CG-CD	6.56	1.61	1.51
5	L	2	DT	C3'-O3'	-6.41	1.35	1.44
5	N	6	DC	C3'-O3'	-6.37	1.35	1.44
2	H	102	GLU	CG-CD	6.28	1.61	1.51
2	H	127	GLU	CG-CD	6.26	1.61	1.51
5	L	1	DC	N1-C6	-6.12	1.33	1.37
4	K	19	DA	N7-C5	-5.98	1.35	1.39
5	N	2	DT	C3'-O3'	-5.90	1.36	1.44
3	J	159	CYS	CB-SG	-5.89	1.72	1.81
5	N	5	DC	C3'-O3'	-5.72	1.36	1.44
4	M	16	DG	C3'-O3'	-5.55	1.36	1.44
5	L	6	DC	C3'-O3'	-5.27	1.37	1.44
5	L	5	DC	C3'-O3'	-5.24	1.37	1.44
2	I	75	VAL	CB-CG1	5.21	1.63	1.52
5	N	9	DT	P-O5'	5.20	1.65	1.59
4	K	15	DG	C3'-O3'	-5.19	1.37	1.44
4	M	13	DT	O3'-P	-5.18	1.54	1.61
2	I	161	LYS	CD-CE	5.09	1.64	1.51
4	K	18	DC	N1-C6	-5.06	1.34	1.37
2	H	338	GLU	CD-OE1	5.06	1.31	1.25
4	K	18	DC	C3'-O3'	-5.04	1.37	1.44
2	C	102	GLU	CG-CD	5.02	1.59	1.51

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	10	DT	O4'-C1'-N1	-13.46	98.58	108.00
4	M	10	DT	O4'-C1'-N1	-13.27	98.71	108.00
4	K	19	DA	O4'-C1'-N9	-11.97	99.62	108.00
4	M	11	DT	O5'-P-OP2	-10.33	96.40	105.70
5	L	7	DT	N3-C4-O4	10.13	125.98	119.90
4	M	19	DA	O4'-C1'-N9	-10.11	100.92	108.00
5	L	7	DT	C5-C4-O4	-9.56	118.21	124.90
5	L	1	DC	O4'-C4'-C3'	-9.37	100.38	106.00
4	K	17	DC	O4'-C1'-N1	-9.15	101.60	108.00
5	L	6	DC	O4'-C4'-C3'	-9.06	100.56	106.00
4	M	16	DG	N1-C6-O6	9.04	125.32	119.90
5	L	5	DC	O4'-C4'-C3'	-8.86	100.69	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	7	DT	N3-C2-O2	8.85	127.61	122.30
4	K	11	DT	O5'-P-OP2	-8.01	98.49	105.70
4	M	10	DT	N3-C2-O2	-7.96	117.53	122.30
5	L	10	DA	O4'-C1'-N9	7.79	113.46	108.00
4	K	11	DT	O4'-C1'-C2'	-7.73	99.71	105.90
5	L	9	DT	O4'-C1'-C2'	-7.72	99.72	105.90
5	N	7	DT	C5-C4-O4	-7.71	119.50	124.90
5	N	10	DA	O4'-C1'-C2'	-7.68	99.75	105.90
5	L	9	DT	C1'-O4'-C4'	-7.58	102.52	110.10
5	L	4	DG	O4'-C1'-N9	-7.58	102.70	108.00
5	N	10	DA	O4'-C1'-N9	7.45	113.22	108.00
5	N	7	DT	N3-C4-O4	7.31	124.29	119.90
4	M	16	DG	C5-C6-O6	-7.28	124.23	128.60
5	N	1	DC	C4'-C3'-C2'	-7.18	96.64	103.10
4	K	16	DG	O4'-C4'-C3'	-7.11	101.66	104.50
5	L	7	DT	P-O3'-C3'	7.01	128.12	119.70
2	H	107	LEU	CA-CB-CG	-7.01	99.17	115.30
4	M	18	DC	O4'-C1'-N1	7.01	112.91	108.00
4	M	12	DA	C8-N9-C4	-7.00	103.00	105.80
4	M	10	DT	N1-C2-O2	6.97	128.68	123.10
5	L	9	DT	C5-C4-O4	-6.96	120.03	124.90
2	C	107	LEU	CA-CB-CG	-6.94	99.34	115.30
5	N	6	DC	O4'-C4'-C3'	-6.92	101.73	104.50
2	H	216	ASP	CB-CG-OD1	6.89	124.50	118.30
5	N	5	DC	O4'-C4'-C3'	-6.89	101.74	104.50
5	L	6	DC	C6-N1-C2	6.81	123.02	120.30
5	L	1	DC	C4'-C3'-C2'	-6.73	97.05	103.10
5	N	9	DT	O4'-C1'-C2'	-6.64	100.59	105.90
4	K	13	DT	O4'-C4'-C3'	-6.61	101.86	104.50
5	L	9	DT	N3-C4-O4	6.55	123.83	119.90
5	N	9	DT	N3-C4-O4	6.51	123.81	119.90
4	M	13	DT	N3-C2-O2	-6.45	118.43	122.30
4	K	18	DC	N3-C4-N4	6.44	122.51	118.00
5	L	1	DC	O4'-C1'-N1	6.42	112.50	108.00
5	L	7	DT	OP1-P-OP2	6.38	129.18	119.60
5	N	5	DC	C1'-O4'-C4'	-6.33	103.77	110.10
4	M	16	DG	C6-C5-N7	-6.32	126.61	130.40
5	N	9	DT	C5-C4-O4	-6.32	120.48	124.90
4	K	16	DG	C4-C5-N7	6.30	113.32	110.80
4	K	11	DT	OP2-P-O3'	6.24	118.92	105.20
4	K	13	DT	N3-C4-O4	6.23	123.64	119.90
5	N	7	DT	N3-C2-O2	6.21	126.02	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	18	DC	C1'-O4'-C4'	-6.20	103.90	110.10
4	K	18	DC	O4'-C1'-C2'	-6.14	100.99	105.90
5	N	2	DT	N3-C4-O4	6.08	123.55	119.90
5	N	2	DT	O4'-C1'-C2'	-6.03	101.07	105.90
4	K	14	DA	N1-C6-N6	5.99	122.20	118.60
5	N	2	DT	C5-C4-O4	-5.94	120.74	124.90
4	K	19	DA	O4'-C1'-C2'	-5.93	101.16	105.90
4	K	19	DA	N1-C6-N6	5.91	122.15	118.60
5	L	6	DC	O3'-P-O5'	5.86	115.14	104.00
4	M	9	DT	C4-C5-C7	5.86	122.52	119.00
4	K	9	DT	C4'-C3'-C2'	-5.86	97.83	103.10
4	K	14	DA	OP2-P-O3'	5.81	117.98	105.20
5	L	7	DT	N1-C2-O2	-5.74	118.50	123.10
4	K	14	DA	C5-C6-N1	-5.74	114.83	117.70
5	N	9	DT	C1'-O4'-C4'	-5.71	104.39	110.10
4	K	12	DA	C8-N9-C4	-5.70	103.52	105.80
5	L	2	DT	O4'-C1'-C2'	-5.70	101.34	105.90
4	M	16	DG	C5-N7-C8	-5.68	101.46	104.30
3	E	146	ARG	NE-CZ-NH1	-5.67	117.46	120.30
2	D	175	LEU	CA-CB-CG	5.66	128.31	115.30
4	K	10	DT	N3-C2-O2	-5.62	118.93	122.30
5	N	1	DC	C3'-C2'-C1'	-5.62	95.76	102.50
5	N	1	DC	C4-C5-C6	5.60	120.20	117.40
4	K	10	DT	O4'-C1'-C2'	-5.59	101.42	105.90
4	K	14	DA	C4-C5-C6	5.59	119.80	117.00
5	N	1	DC	O4'-C4'-C3'	-5.59	102.26	104.50
4	K	10	DT	C4-C5-C7	5.59	122.35	119.00
4	K	13	DT	O4'-C1'-N1	5.57	111.90	108.00
4	K	16	DG	C5-C6-O6	-5.57	125.26	128.60
4	K	16	DG	C2-N3-C4	-5.56	109.12	111.90
4	K	9	DT	C4-C5-C7	5.55	122.33	119.00
4	M	9	DT	O4'-C1'-N1	5.52	111.87	108.00
5	N	6	DC	O3'-P-O5'	5.51	114.48	104.00
2	I	101	VAL	CB-CA-C	-5.49	100.97	111.40
2	I	175	LEU	CA-CB-CG	5.48	127.90	115.30
5	L	7	DT	OP2-P-O3'	5.44	117.17	105.20
4	K	20	DG	C1'-O4'-C4'	-5.44	104.66	110.10
5	N	7	DT	OP2-P-O3'	5.43	117.16	105.20
4	M	17	DC	O4'-C1'-N1	-5.43	104.20	108.00
5	N	7	DT	OP1-P-OP2	5.42	127.73	119.60
4	K	13	DT	P-O5'-C5'	-5.42	112.24	120.90
4	M	9	DT	C4'-C3'-C2'	-5.39	98.25	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	16	DG	N1-C6-O6	5.33	123.09	119.90
4	K	19	DA	C6-C5-N7	-5.32	128.58	132.30
4	K	19	DA	C4-C5-C6	5.31	119.66	117.00
4	K	8	DT	N3-C4-O4	5.31	123.08	119.90
4	M	20	DG	O4'-C1'-N9	5.30	111.71	108.00
5	L	4	DG	C5-N7-C8	-5.29	101.65	104.30
5	N	6	DC	N3-C2-O2	5.28	125.59	121.90
5	L	3	DG	OP1-P-OP2	5.25	127.48	119.60
4	M	9	DT	P-O5'-C5'	-5.22	112.56	120.90
5	N	4	DG	OP1-P-OP2	5.21	127.41	119.60
4	K	12	DA	P-O3'-C3'	5.20	125.94	119.70
2	C	107	LEU	CB-CG-CD1	5.19	119.82	111.00
2	G	344	ASP	N-CA-C	-5.17	97.06	111.00
4	K	9	DT	P-O5'-C5'	-5.16	112.64	120.90
4	K	10	DT	P-O5'-C5'	-5.15	112.66	120.90
4	M	10	DT	P-O5'-C5'	-5.11	112.72	120.90
4	M	13	DT	P-O5'-C5'	-5.08	112.76	120.90
4	K	16	DG	C1'-O4'-C4'	-5.08	105.02	110.10
5	N	1	DC	C5'-C4'-O4'	-5.04	99.72	109.30
4	K	12	DA	N7-C8-N9	5.04	116.32	113.80
5	L	6	DC	P-O3'-C3'	5.04	125.75	119.70
4	M	11	DT	O3'-P-O5'	-5.04	94.43	104.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	245	ASP	Peptide
3	E	264	GLN	Peptide
2	H	245	ASP	Peptide
3	J	264	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2650	0	2703	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2650	0	2703	162	0
2	B	2827	0	2877	152	1
2	C	2836	0	2884	169	0
2	D	2816	0	2861	146	0
2	G	2939	0	2985	153	0
2	H	2836	0	2884	175	1
2	I	2816	0	2861	138	1
3	E	2601	0	2603	87	1
3	J	2601	0	2603	94	0
4	K	287	0	161	20	0
4	M	287	0	161	17	0
5	L	200	0	115	5	0
5	N	200	0	115	6	0
6	B	27	0	12	4	0
6	C	27	0	12	3	0
6	D	27	0	12	3	0
6	G	27	0	12	4	0
6	H	27	0	12	2	0
6	I	27	0	12	3	0
7	B	4	0	0	1	0
7	C	4	0	0	0	0
7	D	4	0	0	1	0
7	G	4	0	0	1	0
7	I	8	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
All	All	28746	0	28588	1348	2

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 24.

All (1348) 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)
2:H:351:MET:HE1	2:I:290:HIS:HA	1.17	1.12
2:D:362:ARG:O	2:D:363:MET:HG2	1.50	1.09
1:F:118:SER:HB3	1:F:121:GLN:HG3	1.38	1.05
2:D:361:PRO:HB3	3:J:272:GLY:HA2	1.42	1.01
1:A:118:SER:HB3	1:A:121:GLN:HG3	1.42	1.01
2:D:361:PRO:CB	3:J:272:GLY:HA2	1.91	1.00
2:I:362:ARG:O	2:I:363:MET:HG2	1.61	1.00
2:G:101:VAL:HG21	2:G:134:HIS:HB3	1.42	1.00
1:F:95:GLU:HA	1:F:98:LEU:HD12	1.48	0.96
2:H:318:ARG:HH11	2:H:318:ARG:HB2	1.28	0.96
3:J:2:ARG:HD3	3:J:4:TYR:CE1	2.01	0.96
2:B:101:VAL:HG21	2:B:134:HIS:HB3	1.46	0.95
2:G:216:ASP:OD1	2:H:168:SER:HB2	1.65	0.95
1:A:95:GLU:HA	1:A:98:LEU:HD12	1.48	0.94
2:I:216:ASP:OD1	3:J:157:SER:HB3	1.69	0.93
2:I:302:LEU:HD11	2:I:306:MET:HG3	1.48	0.93
2:I:26:THR:O	2:I:30:ASN:HB2	1.67	0.92
3:E:106:LEU:HD23	3:E:106:LEU:O	1.69	0.92
2:H:351:MET:CE	2:I:290:HIS:HA	2.00	0.92
2:G:351:MET:HG2	2:H:290:HIS:HD2	1.35	0.91
2:H:367:GLU:HG3	2:H:368:PRO:HD2	1.52	0.91
2:G:21:GLN:OE1	2:G:175:LEU:HB3	1.68	0.91
2:D:115:PRO:HD3	2:D:149:HIS:HD2	1.37	0.90
2:I:51:LYS:HB2	6:I:410:ADP:O2B	1.73	0.89
2:D:26:THR:O	2:D:30:ASN:HB2	1.73	0.89
2:I:52:THR:HG23	6:I:410:ADP:O1B	1.72	0.89
1:F:18:ARG:HB3	1:F:133:ARG:O	1.73	0.88
2:B:216:ASP:OD1	2:C:168:SER:HB2	1.74	0.88
2:C:318:ARG:HH11	2:C:318:ARG:HB2	1.38	0.88
2:G:49:VAL:HG11	2:G:176:LYS:O	1.74	0.87
3:E:2:ARG:HD3	3:E:4:TYR:CE1	2.09	0.87
2:D:51:LYS:HB2	6:D:404:ADP:O2B	1.74	0.87
2:I:38:HIS:HD2	2:I:40:ALA:H	1.22	0.87
3:J:106:LEU:HD23	3:J:106:LEU:O	1.75	0.86
2:H:351:MET:HE1	2:I:290:HIS:CA	2.03	0.86
2:B:51:LYS:HB2	6:B:400:ADP:O2B	1.74	0.86
2:B:49:VAL:HG11	2:B:176:LYS:O	1.75	0.86
3:J:170:GLN:HA	3:J:170:GLN:OE1	1.75	0.86
2:H:21:GLN:NE2	2:H:49:VAL:HG12	1.91	0.85
1:F:20:ALA:HB3	1:F:134:SER:HB3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LEU:HD22	2:B:306:MET:HG3	1.57	0.85
2:G:51:LYS:HB2	6:G:406:ADP:O2B	1.76	0.85
1:A:18:ARG:HB3	1:A:133:ARG:O	1.75	0.84
2:D:38:HIS:HD2	2:D:40:ALA:H	1.20	0.84
1:A:39:ARG:CZ	1:A:50:HIS:HB3	2.07	0.84
2:H:318:ARG:HB2	2:H:318:ARG:NH1	1.93	0.84
2:D:302:LEU:HD11	2:D:306:MET:HG3	1.57	0.84
2:C:367:GLU:HG3	2:C:368:PRO:HD2	1.58	0.84
1:A:20:ALA:HB3	1:A:134:SER:HB3	1.60	0.83
2:G:302:LEU:HD22	2:G:306:MET:HG3	1.59	0.83
2:D:268:ILE:HD11	2:D:353:LEU:HD12	1.61	0.82
1:F:117:LEU:HD12	1:F:122:GLU:HG2	1.59	0.82
2:C:341:TYR:HB2	2:D:333:LEU:HD11	1.62	0.82
1:F:39:ARG:CZ	1:F:50:HIS:HB3	2.10	0.82
1:F:53:PHE:CD1	1:F:67:LEU:HD21	2.16	0.81
1:A:117:LEU:HD12	1:A:122:GLU:HG2	1.62	0.81
2:B:292:ILE:HD13	2:B:316:LEU:HD23	1.62	0.81
2:H:78:ASN:O	2:H:82:ILE:HG13	1.80	0.81
2:H:341:TYR:HB2	2:I:333:LEU:HD11	1.62	0.81
2:D:361:PRO:HG2	3:J:275:ALA:CB	2.10	0.81
2:H:91:ILE:HD12	2:H:123:TYR:CE2	2.17	0.80
2:D:115:PRO:HD3	2:D:149:HIS:CD2	2.16	0.80
2:G:365:LEU:CD1	2:H:297:LEU:HD23	2.10	0.80
1:A:53:PHE:CD1	1:A:67:LEU:HD21	2.16	0.80
3:J:3:TRP:HH2	3:J:8:ARG:HG3	1.46	0.80
2:C:21:GLN:NE2	2:C:49:VAL:HG12	1.97	0.80
2:C:318:ARG:HB2	2:C:318:ARG:NH1	1.97	0.79
2:I:47:ARG:HG2	2:I:47:ARG:O	1.81	0.79
2:D:361:PRO:HG2	3:J:275:ALA:HB2	1.65	0.79
2:H:244:LEU:H	2:H:244:LEU:HD12	1.47	0.79
1:F:59:THR:HG23	1:F:63:ALA:HB3	1.65	0.78
1:A:59:THR:HG23	1:A:63:ALA:HB3	1.64	0.78
3:E:3:TRP:HH2	3:E:8:ARG:HG3	1.47	0.78
1:F:98:LEU:HD23	1:F:126:TRP:HB3	1.65	0.78
2:D:216:ASP:OD1	3:E:157:SER:HB3	1.83	0.78
2:I:24:VAL:HG21	2:I:175:LEU:HD22	1.66	0.78
2:I:115:PRO:HD3	2:I:149:HIS:HD2	1.49	0.77
2:G:15:PHE:HE2	2:G:57:LEU:HB3	1.50	0.77
2:G:215:ARG:HH11	6:G:406:ADP:H5'1	1.50	0.77
2:H:259:ALA:HB2	2:H:360:HIS:CE1	2.20	0.77
2:B:15:PHE:HE2	2:B:57:LEU:HB3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:THR:OG1	2:C:135:SER:HB2	1.85	0.77
2:I:302:LEU:CD1	2:I:306:MET:HG3	2.15	0.77
2:B:215:ARG:HH11	6:B:400:ADP:H5'1	1.51	0.76
2:G:115:PRO:HD3	2:G:149:HIS:HD2	1.49	0.76
1:A:98:LEU:HD23	1:A:126:TRP:HB3	1.67	0.76
2:C:246:ASP:HB3	2:C:309:ILE:HD12	1.68	0.76
2:B:115:PRO:HD3	2:B:149:HIS:HD2	1.49	0.76
2:H:104:THR:OG1	2:H:135:SER:HB2	1.85	0.76
1:F:244:VAL:HG21	4:M:10:DT:H71	1.68	0.76
2:C:78:ASN:O	2:C:82:ILE:HG13	1.84	0.76
2:C:259:ALA:HB2	2:C:360:HIS:CE1	2.21	0.76
2:B:21:GLN:OE1	2:B:175:LEU:HB3	1.85	0.76
4:M:13:DT:H2"	4:M:14:DA:O5'	1.85	0.76
2:I:268:ILE:HD11	2:I:353:LEU:HD12	1.68	0.75
3:E:170:GLN:HA	3:E:170:GLN:OE1	1.84	0.75
2:G:95:ALA:O	2:G:99:THR:HG22	1.85	0.75
1:A:71:MET:HB2	1:A:108:LEU:HG	1.66	0.75
2:C:341:TYR:CB	2:D:333:LEU:HD11	2.17	0.75
3:J:46:ARG:HD2	3:J:68:MET:HG2	1.68	0.75
2:D:361:PRO:HB2	3:J:272:GLY:HA2	1.67	0.75
2:G:64:CYS:SG	2:G:66:THR:HG23	2.26	0.75
1:A:304:LEU:O	1:A:308:THR:HG23	1.87	0.75
2:I:115:PRO:HD3	2:I:149:HIS:CD2	2.21	0.75
2:I:291:ARG:O	2:I:294:MET:HB2	1.86	0.74
3:J:285:ARG:HD3	3:J:322:TYR:O	1.87	0.74
2:C:244:LEU:H	2:C:244:LEU:HD12	1.52	0.74
1:F:71:MET:HB2	1:F:108:LEU:HG	1.70	0.74
4:K:13:DT:H2"	4:K:14:DA:O5'	1.87	0.74
2:B:179:ASP:HB3	2:B:182:GLN:HG3	1.69	0.74
2:D:344:ASP:HB2	2:D:347:MET:H	1.53	0.74
2:I:216:ASP:OD1	3:J:157:SER:CB	2.34	0.74
1:A:54:SER:HB3	1:A:83:LEU:HD12	1.69	0.74
2:D:302:LEU:CD1	2:D:306:MET:HG3	2.18	0.74
2:B:21:GLN:HE21	2:B:21:GLN:HA	1.53	0.74
2:B:351:MET:HG2	2:C:290:HIS:HD2	1.52	0.74
2:G:291:ARG:HG2	2:G:306:MET:CE	2.18	0.73
1:A:280:GLN:HA	1:A:283:ARG:HG3	1.71	0.73
2:B:291:ARG:HG2	2:B:306:MET:CE	2.18	0.73
2:D:202:ALA:HB2	2:D:234:THR:HA	1.71	0.73
2:G:179:ASP:HB3	2:G:182:GLN:HG3	1.71	0.73
1:F:237:ARG:HG3	1:F:321:TRP:CE2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:21:GLN:HA	2:G:21:GLN:HE21	1.52	0.73
3:J:41:ILE:HD13	3:J:142:PHE:HB3	1.70	0.72
2:D:291:ARG:O	2:D:294:MET:HB2	1.89	0.72
1:F:308:THR:HB	1:F:323:GLU:OE1	1.89	0.72
2:G:365:LEU:HD11	2:H:297:LEU:HD23	1.71	0.72
2:H:49:VAL:HG11	2:H:176:LYS:O	1.89	0.72
1:F:280:GLN:HA	1:F:283:ARG:HG3	1.72	0.72
2:H:246:ASP:HB3	2:H:309:ILE:HD12	1.70	0.72
3:J:199:GLY:HA2	3:J:202:LEU:HB3	1.71	0.72
2:I:362:ARG:O	2:I:363:MET:CG	2.36	0.72
1:F:54:SER:HB3	1:F:83:LEU:HD12	1.70	0.72
3:E:46:ARG:HD2	3:E:68:MET:HG2	1.70	0.72
2:G:101:VAL:CG2	2:G:134:HIS:HB3	2.20	0.72
2:G:292:ILE:HD13	2:G:316:LEU:HD23	1.71	0.72
2:C:196:ILE:HD12	2:C:225:ILE:HD13	1.72	0.72
1:A:312:LEU:HD13	1:A:320:VAL:HG21	1.72	0.71
2:D:77:ASP:O	2:D:81:GLU:HG3	1.90	0.71
1:F:304:LEU:O	1:F:308:THR:HG23	1.90	0.71
4:K:17:DC:H2"	4:K:18:DC:O5'	1.89	0.71
2:B:64:CYS:SG	2:B:66:THR:HG23	2.30	0.71
2:B:347:MET:HG2	2:C:290:HIS:CE1	2.25	0.71
2:B:343:PRO:HG3	2:C:286:LEU:HB2	1.73	0.71
2:H:51:LYS:HG2	6:H:408:ADP:O2B	1.90	0.71
1:A:17:LEU:CD1	1:A:45:GLN:HE21	2.04	0.71
2:B:21:GLN:HE22	2:B:176:LYS:H	1.38	0.70
2:D:362:ARG:O	2:D:363:MET:CG	2.35	0.70
2:C:21:GLN:NE2	2:C:175:LEU:HB3	2.06	0.70
1:F:237:ARG:HG3	1:F:321:TRP:CD2	2.26	0.70
2:H:196:ILE:HD12	2:H:225:ILE:HD13	1.74	0.70
1:A:244:VAL:HG21	4:K:10:DT:H71	1.72	0.70
4:M:17:DC:H2"	4:M:18:DC:O5'	1.92	0.70
2:D:24:VAL:HG21	2:D:175:LEU:HD22	1.74	0.70
3:J:224:VAL:HB	3:J:225:PRO:HD3	1.73	0.70
2:C:91:ILE:HD12	2:C:123:TYR:CE2	2.27	0.69
1:A:93:ILE:O	1:A:97:LEU:HG	1.92	0.69
2:H:30:ASN:O	2:H:34:LEU:HB2	1.92	0.69
2:H:21:GLN:HE22	2:H:49:VAL:HG12	1.57	0.69
1:F:52:THR:HG22	1:F:81:LEU:HD23	1.73	0.69
2:I:252:LEU:HD13	2:I:285:MET:CE	2.23	0.69
2:D:111:VAL:HG13	2:D:150:VAL:HG21	1.74	0.69
2:H:21:GLN:NE2	2:H:175:LEU:HB3	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:111:VAL:HG13	2:I:150:VAL:HG21	1.75	0.69
3:J:213:ARG:HH21	3:J:267:ASN:HD22	1.38	0.68
2:H:196:ILE:CD1	2:H:225:ILE:HD13	2.24	0.68
2:B:101:VAL:CG2	2:B:134:HIS:HB3	2.22	0.68
1:F:118:SER:CB	1:F:121:GLN:HG3	2.22	0.68
1:A:244:VAL:HG21	4:K:10:DT:C7	2.23	0.68
2:I:64:CYS:SG	2:I:66:THR:HG23	2.32	0.68
2:C:351:MET:HE1	2:D:290:HIS:HA	1.74	0.68
2:G:15:PHE:CE2	2:G:57:LEU:HB3	2.28	0.68
1:A:250:LEU:HD23	1:A:305:LEU:HD13	1.76	0.68
3:E:29:ILE:HD13	3:E:40:LEU:HD23	1.76	0.68
2:G:351:MET:HE1	2:H:290:HIS:HA	1.76	0.68
3:E:224:VAL:HB	3:E:225:PRO:HD3	1.76	0.68
2:B:257:VAL:HG21	2:B:320:ILE:HD11	1.76	0.68
2:C:283:VAL:HA	2:C:286:LEU:HD12	1.76	0.67
2:G:21:GLN:HE22	2:G:176:LYS:H	1.40	0.67
2:H:47:ARG:HG3	2:I:168:SER:HB2	1.76	0.67
2:G:240:MET:O	2:G:243:THR:HB	1.94	0.67
2:I:77:ASP:O	2:I:81:GLU:HG3	1.94	0.67
2:G:39:HIS:CD2	2:G:39:HIS:H	2.10	0.67
2:B:77:ASP:O	2:B:81:GLU:HB2	1.95	0.67
2:D:360:HIS:HB3	2:D:361:PRO:HD3	1.76	0.67
2:B:223:GLN:HG2	2:B:240:MET:SD	2.34	0.67
3:E:213:ARG:HH21	3:E:267:ASN:HD22	1.42	0.67
2:D:38:HIS:CD2	2:D:40:ALA:H	2.09	0.67
2:G:365:LEU:HD12	2:G:366:PRO:HD2	1.75	0.67
1:F:74:PHE:CD1	1:F:74:PHE:O	2.48	0.66
2:I:184:ARG:HD3	2:I:204:GLN:NE2	2.09	0.66
3:J:199:GLY:HA2	3:J:202:LEU:CB	2.26	0.66
4:M:14:DA:H2"	4:M:15:DG:O5'	1.94	0.66
1:F:213:THR:H	1:F:216:HIS:CD2	2.14	0.66
2:I:21:GLN:NE2	2:I:49:VAL:HG12	2.10	0.66
2:B:260:ASN:HD22	2:B:263:ARG:CB	2.09	0.66
1:A:127:PHE:HA	1:A:130:LEU:HD12	1.78	0.66
2:C:147:PRO:HB2	2:C:149:HIS:CE1	2.31	0.66
2:G:223:GLN:HB2	2:H:171:LEU:HD22	1.76	0.66
1:F:17:LEU:CD1	1:F:45:GLN:HE21	2.08	0.66
2:H:144:GLU:HG2	2:H:145:GLU:HG3	1.77	0.66
2:I:344:ASP:HB2	2:I:347:MET:H	1.61	0.66
4:K:15:DG:H2"	4:K:16:DG:O5'	1.95	0.66
3:E:285:ARG:HD3	3:E:322:TYR:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:21:GLN:HA	2:G:21:GLN:NE2	2.11	0.66
2:B:15:PHE:CE2	2:B:57:LEU:HB3	2.30	0.66
1:F:22:LEU:HD23	1:F:112:VAL:HB	1.78	0.66
1:A:38:VAL:CG1	1:A:111:ILE:HD11	2.26	0.66
2:C:282:LEU:O	2:C:286:LEU:HD12	1.96	0.66
1:F:118:SER:HB3	1:F:121:GLN:CG	2.23	0.66
1:F:312:LEU:HD13	1:F:320:VAL:HG21	1.78	0.66
2:B:265:MET:HE1	2:B:350:GLU:HG2	1.78	0.66
2:D:184:ARG:HD3	2:D:204:GLN:NE2	2.10	0.66
2:H:64:CYS:SG	2:H:66:THR:HG23	2.36	0.65
2:D:93:ILE:HD11	2:D:107:LEU:HD23	1.76	0.65
1:F:56:ASP:HB2	1:F:58:ASN:HB2	1.78	0.65
2:C:341:TYR:CE1	2:D:337:LYS:HD2	2.32	0.65
2:B:21:GLN:HA	2:B:21:GLN:NE2	2.11	0.65
2:D:347:MET:O	2:D:351:MET:HG3	1.97	0.65
3:E:41:ILE:HD13	3:E:142:PHE:HB3	1.78	0.65
1:F:93:ILE:O	1:F:97:LEU:HG	1.96	0.65
1:A:22:LEU:HD23	1:A:112:VAL:HB	1.79	0.65
2:B:260:ASN:HD22	2:B:263:ARG:HB2	1.60	0.65
1:A:39:ARG:NH2	1:A:50:HIS:HB3	2.11	0.65
1:A:56:ASP:HB2	1:A:58:ASN:HB2	1.77	0.65
2:B:265:MET:CE	2:B:350:GLU:HG2	2.27	0.65
2:C:49:VAL:HG11	2:C:176:LYS:O	1.96	0.64
1:F:147:LEU:HD23	1:F:171:CYS:SG	2.37	0.64
2:I:202:ALA:HB2	2:I:234:THR:HA	1.78	0.64
2:B:91:ILE:HG22	2:B:93:ILE:HD13	1.78	0.64
2:C:30:ASN:O	2:C:34:LEU:HB2	1.97	0.64
2:C:196:ILE:CD1	2:C:225:ILE:HD13	2.28	0.64
2:H:318:ARG:HH11	2:H:318:ARG:CB	2.07	0.64
1:A:39:ARG:NH1	1:A:50:HIS:HB3	2.12	0.64
2:C:292:ILE:O	2:C:296:GLN:HG3	1.98	0.64
2:H:341:TYR:O	2:I:336:ARG:NH1	2.30	0.64
5:N:2:DT:H2"	5:N:3:DG:C8	2.32	0.64
1:A:97:LEU:HD13	1:A:126:TRP:CH2	2.33	0.64
2:G:115:PRO:HD3	2:G:149:HIS:CD2	2.33	0.64
2:B:39:HIS:H	2:B:39:HIS:CD2	2.16	0.64
1:F:198:THR:HG23	1:F:201:ARG:HD2	1.79	0.64
2:G:47:ARG:O	2:G:47:ARG:HG2	1.98	0.64
1:A:118:SER:CB	1:A:121:GLN:HG3	2.23	0.64
2:B:257:VAL:HG21	2:B:320:ILE:CD1	2.27	0.64
2:C:277:GLU:O	2:C:280:ALA:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:PRO:CD	2:C:149:HIS:HD2	2.10	0.63
3:J:114:VAL:HB	3:J:143:LEU:HD23	1.80	0.63
2:B:255:ALA:HB2	2:B:263:ARG:NH1	2.14	0.63
2:H:53:SER:OG	6:H:408:ADP:O1A	2.16	0.63
1:A:198:THR:HG23	1:A:201:ARG:HD2	1.80	0.63
3:J:99:LYS:HD3	3:J:105:ARG:HH22	1.62	0.63
2:H:147:PRO:HB2	2:H:149:HIS:CE1	2.33	0.63
2:C:51:LYS:HG2	6:C:402:ADP:O2B	1.97	0.63
2:C:353:LEU:O	2:C:356:ALA:HB3	1.99	0.63
1:A:74:PHE:O	1:A:74:PHE:CD1	2.52	0.63
1:A:237:ARG:HG3	1:A:321:TRP:CD2	2.33	0.63
1:F:39:ARG:NH2	1:F:50:HIS:HB3	2.14	0.63
2:H:367:GLU:HG3	2:H:368:PRO:CD	2.28	0.63
2:I:309:ILE:CG2	2:I:313:MET:HG2	2.28	0.63
3:J:82:GLU:HA	3:J:82:GLU:OE1	1.98	0.63
2:I:93:ILE:HD11	2:I:107:LEU:HD23	1.80	0.63
2:D:124:LEU:HD12	2:D:153:LEU:O	1.99	0.63
3:E:72:THR:HG23	3:E:72:THR:O	1.98	0.62
2:I:302:LEU:HD11	2:I:306:MET:CG	2.26	0.62
1:A:237:ARG:HG3	1:A:321:TRP:CE2	2.34	0.62
2:B:215:ARG:NH2	7:B:401:BEF:F2	2.20	0.62
2:H:265:MET:HE3	2:I:294:MET:SD	2.39	0.62
2:H:292:ILE:HG13	2:H:313:MET:HE1	1.80	0.62
1:A:41:VAL:O	1:A:45:GLN:HG2	1.98	0.62
2:B:365:LEU:HD12	2:B:366:PRO:HD2	1.78	0.62
3:E:182:MET:HG3	3:E:205:PHE:CE1	2.34	0.62
2:C:337:LYS:CE	3:E:334:LEU:HD22	2.29	0.62
2:B:115:PRO:HD3	2:B:149:HIS:CD2	2.32	0.62
2:G:351:MET:HG2	2:H:290:HIS:CD2	2.25	0.62
2:H:292:ILE:O	2:H:296:GLN:HG3	2.00	0.62
1:F:64:ILE:HG13	1:F:96:GLN:HB3	1.82	0.62
2:I:184:ARG:HD3	2:I:204:GLN:HE22	1.64	0.62
2:B:296:GLN:NE2	2:B:322:PRO:HG3	2.15	0.62
2:C:367:GLU:OE2	2:D:362:ARG:NH1	2.33	0.62
2:D:179:ASP:HB3	2:D:182:GLN:HG3	1.82	0.62
2:H:115:PRO:CD	2:H:149:HIS:HD2	2.12	0.62
3:J:182:MET:HG3	3:J:205:PHE:CE1	2.35	0.62
3:J:62:CYS:O	3:J:66:GLN:HG3	2.00	0.61
2:C:21:GLN:HE22	2:C:49:VAL:HG12	1.63	0.61
2:H:265:MET:CE	2:I:294:MET:SD	2.88	0.61
2:D:21:GLN:NE2	2:D:49:VAL:HG12	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:O	1:A:50:HIS:HD2	1.82	0.61
1:A:64:ILE:HG13	1:A:96:GLN:HB3	1.82	0.61
2:C:137:ASN:HD22	2:C:137:ASN:H	1.46	0.61
2:D:309:ILE:CG2	2:D:313:MET:HG2	2.31	0.61
1:F:128:THR:O	1:F:131:ALA:HB3	2.00	0.61
2:H:101:VAL:HG23	4:M:17:DC:OP1	2.00	0.61
2:D:47:ARG:O	2:D:47:ARG:HG2	2.01	0.61
1:F:250:LEU:HD23	1:F:305:LEU:HD13	1.83	0.61
2:I:360:HIS:HB3	2:I:361:PRO:HD3	1.82	0.61
2:C:53:SER:OG	6:C:402:ADP:O1A	2.18	0.61
1:A:181:LEU:O	1:A:184:ALA:HB3	2.00	0.61
2:B:128:VAL:O	2:B:128:VAL:HG22	2.00	0.61
2:C:115:PRO:HD3	2:C:149:HIS:HD2	1.65	0.61
3:E:199:GLY:HA2	3:E:202:LEU:HB3	1.83	0.61
2:G:257:VAL:HG21	2:G:320:ILE:HD11	1.82	0.61
2:H:223:GLN:HG3	2:H:240:MET:HE1	1.83	0.61
2:B:240:MET:O	2:B:243:THR:HB	2.00	0.61
1:F:117:LEU:HB2	1:F:122:GLU:HG3	1.82	0.61
1:F:190:LEU:CD2	2:G:36:ARG:HD2	2.30	0.61
2:I:49:VAL:HG11	2:I:176:LYS:O	2.00	0.61
2:B:95:ALA:O	2:B:99:THR:HG22	2.01	0.60
2:C:318:ARG:HH11	2:C:318:ARG:CB	2.13	0.60
3:J:99:LYS:HD3	3:J:105:ARG:NH2	2.16	0.60
1:A:282:ARG:HD3	1:A:285:MET:HE2	1.83	0.60
3:E:121:THR:HG22	3:E:122:ASP:N	2.15	0.60
1:F:304:LEU:HD23	1:F:327:LEU:HD13	1.83	0.60
2:H:283:VAL:HA	2:H:286:LEU:HD12	1.83	0.60
2:B:343:PRO:HG3	2:C:286:LEU:CB	2.31	0.60
2:C:101:VAL:HG22	2:C:134:HIS:HB3	1.82	0.60
2:C:137:ASN:HA	2:C:140:LEU:HG	1.83	0.60
2:C:223:GLN:HB3	2:D:171:LEU:HD22	1.83	0.60
2:G:351:MET:CE	2:H:290:HIS:HA	2.31	0.60
2:D:61:GLY:HA2	2:D:72:PRO:HG3	1.84	0.60
2:G:257:VAL:HG21	2:G:320:ILE:CD1	2.31	0.60
3:J:202:LEU:HD23	3:J:202:LEU:O	2.02	0.60
2:D:184:ARG:HD3	2:D:204:GLN:HE22	1.65	0.60
1:F:101:THR:HG21	1:F:126:TRP:HB2	1.83	0.60
1:A:78:GLN:HG3	1:A:108:LEU:HD22	1.82	0.60
1:F:12:GLN:O	1:F:12:GLN:HG3	2.02	0.60
2:B:295:VAL:HA	2:B:298:SER:O	2.01	0.60
2:G:260:ASN:HD22	2:G:263:ARG:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HB2	1:A:122:GLU:HG3	1.83	0.60
2:B:257:VAL:HG22	2:B:328:TYR:CE2	2.37	0.60
2:C:292:ILE:HG13	2:C:313:MET:HE1	1.82	0.60
2:I:309:ILE:HG22	2:I:313:MET:HG2	1.84	0.60
1:A:308:THR:HB	1:A:323:GLU:OE1	2.02	0.60
2:C:341:TYR:CZ	2:D:337:LYS:HD2	2.36	0.60
1:F:127:PHE:HA	1:F:130:LEU:HD12	1.84	0.60
2:H:47:ARG:O	2:H:47:ARG:HG2	2.01	0.60
2:H:60:LYS:NZ	2:H:83:GLU:HG3	2.17	0.60
2:H:128:VAL:HG22	2:H:128:VAL:O	2.01	0.60
1:A:162:LEU:HD22	1:A:166:ALA:HB3	1.83	0.59
2:B:341:TYR:CE1	2:C:337:LYS:HE3	2.37	0.59
2:C:202:ALA:HB1	2:C:237:VAL:HG21	1.83	0.59
1:F:181:LEU:O	1:F:184:ALA:HB3	2.02	0.59
1:F:97:LEU:HD13	1:F:126:TRP:CH2	2.37	0.59
1:F:268:PRO:HD2	1:F:271:ALA:HB3	1.84	0.59
2:C:246:ASP:HB3	2:C:309:ILE:CD1	2.32	0.59
1:A:64:ILE:HD12	1:A:96:GLN:HG2	1.84	0.59
1:F:78:GLN:HG3	1:F:108:LEU:HD22	1.82	0.59
2:H:246:ASP:HB3	2:H:309:ILE:CD1	2.32	0.59
2:C:282:LEU:O	2:C:286:LEU:CD1	2.50	0.59
1:F:39:ARG:NH1	1:F:50:HIS:HB3	2.17	0.59
2:H:44:SER:CB	2:H:159:PRO:HG3	2.32	0.59
1:A:52:THR:HG22	1:A:81:LEU:HD23	1.82	0.59
1:A:147:LEU:HD23	1:A:171:CYS:SG	2.42	0.59
2:C:60:LYS:NZ	2:C:83:GLU:HG3	2.17	0.59
2:D:6:LEU:H	2:D:6:LEU:HD12	1.66	0.59
2:D:49:VAL:HG11	2:D:176:LYS:O	2.02	0.59
2:H:93:ILE:HD13	2:H:107:LEU:HD13	1.83	0.59
1:A:38:VAL:HG11	1:A:111:ILE:HD11	1.83	0.59
2:C:88:VAL:HG12	2:C:88:VAL:O	2.02	0.59
1:F:90:ASN:O	1:F:94:ASN:HB2	2.02	0.59
2:G:77:ASP:O	2:G:81:GLU:HB2	2.01	0.59
2:H:229:ASP:HB2	2:I:30:ASN:HD21	1.67	0.59
3:J:112:VAL:HB	3:J:141:PHE:CD1	2.37	0.59
2:B:253:VAL:CG1	2:B:316:LEU:HD21	2.33	0.59
2:G:341:TYR:O	2:H:336:ARG:NH1	2.32	0.59
2:H:365:LEU:HD11	2:I:297:LEU:HD12	1.85	0.59
4:K:12:DA:H2"	4:K:13:DT:O5'	2.03	0.59
5:L:2:DT:H2"	5:L:3:DG:C8	2.38	0.59
1:A:94:ASN:OD1	1:A:126:TRP:NE1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:7:DT:H2"	5:L:8:DA:O5'	2.03	0.59
2:C:260:ASN:O	2:C:264:VAL:HG23	2.01	0.59
2:C:351:MET:CE	2:D:290:HIS:HA	2.33	0.59
2:D:309:ILE:HG22	2:D:313:MET:HG2	1.84	0.59
2:B:296:GLN:CD	2:B:322:PRO:HG3	2.23	0.58
2:D:232:VAL:O	2:D:232:VAL:HG12	2.03	0.58
1:F:41:VAL:O	1:F:45:GLN:HG2	2.03	0.58
3:J:29:ILE:HD13	3:J:40:LEU:HD23	1.84	0.58
1:A:12:GLN:O	1:A:12:GLN:HG3	2.02	0.58
2:B:328:TYR:HH	2:B:360:HIS:CD2	2.21	0.58
1:F:13:LEU:HD11	1:F:38:VAL:HG22	1.85	0.58
2:G:215:ARG:NH2	7:G:407:BEF:F2	2.25	0.58
2:G:291:ARG:O	2:G:295:VAL:HG23	2.03	0.58
1:A:27:ASP:HB2	1:A:141:THR:OG1	2.03	0.58
4:M:15:DG:H2"	4:M:16:DG:O5'	2.02	0.58
1:A:90:ASN:O	1:A:94:ASN:HB2	2.02	0.58
2:B:91:ILE:HG22	2:B:93:ILE:CD1	2.33	0.58
2:G:67:GLY:HA2	2:G:119:ARG:NH2	2.19	0.58
4:M:12:DA:H2"	4:M:13:DT:O5'	2.02	0.58
1:A:126:TRP:O	1:A:130:LEU:HG	2.04	0.58
2:D:15:PHE:HE2	2:D:57:LEU:HB3	1.69	0.58
3:E:82:GLU:HA	3:E:82:GLU:OE1	2.03	0.58
2:G:91:ILE:HG22	2:G:93:ILE:HD13	1.86	0.58
2:I:347:MET:O	2:I:351:MET:HG3	2.03	0.58
2:H:341:TYR:CE1	2:I:337:LYS:HD2	2.39	0.58
1:F:156:LYS:O	1:F:159:ASN:N	2.37	0.57
2:G:125:ILE:HB	2:G:154:LEU:HD22	1.86	0.57
5:N:7:DT:H2"	5:N:8:DA:O5'	2.04	0.57
1:A:56:ASP:HB2	1:A:58:ASN:H	1.69	0.57
1:A:101:THR:HG21	1:A:126:TRP:HB2	1.85	0.57
2:B:292:ILE:CD1	2:B:316:LEU:HD23	2.33	0.57
3:E:202:LEU:HD23	3:E:202:LEU:O	2.04	0.57
1:F:190:LEU:HD21	2:G:36:ARG:HD2	1.87	0.57
1:F:244:VAL:HG21	4:M:10:DT:C7	2.33	0.57
2:G:327:LEU:HD12	2:G:330:GLN:OE1	2.04	0.57
1:A:118:SER:HB3	1:A:121:GLN:CG	2.26	0.57
2:B:47:ARG:HG2	2:B:47:ARG:O	2.03	0.57
1:F:64:ILE:HD12	1:F:96:GLN:HG2	1.85	0.57
2:G:295:VAL:HA	2:G:298:SER:O	2.02	0.57
4:K:14:DA:H2"	4:K:15:DG:O5'	2.04	0.57
1:A:10:ARG:NH1	1:A:37:ALA:HB2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:H	1:A:216:HIS:CD2	2.23	0.57
2:C:291:ARG:HD2	2:C:306:MET:SD	2.44	0.57
2:G:250:LEU:HA	2:G:288:LEU:HD12	1.87	0.57
2:H:115:PRO:HD3	2:H:149:HIS:HD2	1.68	0.57
2:I:80:ARG:O	2:I:84:GLN:HG3	2.05	0.57
2:D:184:ARG:CD	2:D:204:GLN:NE2	2.68	0.57
1:F:126:TRP:O	1:F:130:LEU:HG	2.04	0.57
2:I:69:THR:HG21	2:I:72:PRO:HA	1.86	0.57
2:I:232:VAL:HG12	2:I:232:VAL:O	2.02	0.57
2:I:245:ASP:OD1	2:I:245:ASP:O	2.23	0.57
2:C:260:ASN:O	2:C:260:ASN:OD1	2.23	0.57
2:G:260:ASN:HD22	2:G:263:ARG:CB	2.17	0.57
1:F:74:PHE:O	1:F:74:PHE:CG	2.58	0.57
2:G:21:GLN:HE21	2:G:21:GLN:CA	2.17	0.57
2:B:124:LEU:HD13	2:B:153:LEU:HB2	1.87	0.57
1:F:38:VAL:CG1	1:F:111:ILE:HD11	2.35	0.57
1:F:190:LEU:HD11	2:G:38:HIS:HE1	1.70	0.57
2:G:276:ILE:CG2	2:G:277:GLU:N	2.67	0.57
2:H:282:LEU:O	2:H:286:LEU:HD12	2.04	0.57
1:F:13:LEU:CD1	1:F:38:VAL:HG22	2.35	0.56
2:G:4:GLN:NE2	2:G:9:LYS:HG3	2.19	0.56
2:G:129:HIS:CD2	2:G:130:MET:SD	2.98	0.56
2:G:343:PRO:HG3	2:H:286:LEU:HB2	1.86	0.56
2:B:171:LEU:HD23	2:B:173:PHE:CE2	2.41	0.56
2:G:28:LEU:HD13	2:G:58:LEU:HD13	1.85	0.56
2:H:101:VAL:HG22	2:H:134:HIS:HB3	1.85	0.56
2:H:324:ASP:O	2:H:327:LEU:HB3	2.05	0.56
2:I:184:ARG:CD	2:I:204:GLN:NE2	2.68	0.56
1:A:179:LEU:HD11	2:B:168:SER:HA	1.86	0.56
2:C:254:GLU:HG2	2:C:316:LEU:HD11	1.86	0.56
2:C:339:LEU:HD11	2:C:345:ARG:O	2.06	0.56
2:D:15:PHE:CE2	2:D:57:LEU:HB3	2.40	0.56
2:G:82:ILE:HG23	2:G:90:LEU:HD23	1.87	0.56
2:G:223:GLN:HG2	2:G:240:MET:SD	2.45	0.56
2:G:265:MET:HE1	2:G:350:GLU:HG2	1.88	0.56
1:A:128:THR:O	1:A:131:ALA:HB3	2.05	0.56
2:B:125:ILE:HB	2:B:154:LEU:HD22	1.88	0.56
2:C:190:ILE:HD12	2:C:218:LEU:HD21	1.87	0.56
2:C:292:ILE:HG13	2:C:313:MET:CE	2.35	0.56
2:H:341:TYR:CB	2:I:333:LEU:HD11	2.34	0.56
2:I:38:HIS:CD2	2:I:40:ALA:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:MET:HE1	2:C:294:MET:SD	2.46	0.56
2:H:46:THR:O	2:H:49:VAL:HG23	2.06	0.56
2:I:124:LEU:HD12	2:I:153:LEU:O	2.05	0.56
2:B:47:ARG:H	2:B:47:ARG:HD3	1.70	0.56
2:D:52:THR:HG21	2:D:126:ASP:OD2	2.06	0.56
1:F:53:PHE:HE2	1:F:59:THR:HG1	1.53	0.56
2:H:129:HIS:CD2	2:H:130:MET:HG2	2.39	0.56
2:H:254:GLU:OE2	2:H:312:ARG:HD3	2.05	0.56
2:H:337:LYS:NZ	3:J:334:LEU:HD22	2.21	0.56
1:A:71:MET:CB	1:A:108:LEU:HG	2.35	0.56
2:C:147:PRO:HD2	2:C:150:VAL:HB	1.87	0.56
2:G:257:VAL:HG22	2:G:328:TYR:CE2	2.41	0.56
2:G:302:LEU:CD2	2:G:306:MET:HG3	2.34	0.56
3:J:223:SER:HB3	3:J:228:ASP:O	2.05	0.56
1:A:17:LEU:HD11	1:A:45:GLN:HE21	1.70	0.56
2:B:93:ILE:HG12	2:B:107:LEU:HD22	1.88	0.56
2:C:213:SER:HB3	2:C:216:ASP:HB2	1.88	0.56
1:F:152:ALA:O	1:F:156:LYS:HD2	2.05	0.56
2:H:339:LEU:HD11	2:H:345:ARG:O	2.06	0.56
1:F:162:LEU:HD22	1:F:166:ALA:HB3	1.88	0.56
1:A:104:LEU:HD13	1:A:133:ARG:HD2	1.88	0.56
1:F:194:ASP:HB3	1:F:196:LYS:HG2	1.87	0.56
1:F:278:VAL:HG12	1:F:283:ARG:HG2	1.89	0.56
2:H:47:ARG:HD2	2:I:164:VAL:HG22	1.88	0.56
1:A:9:LEU:HD11	1:A:13:LEU:HD21	1.87	0.55
2:B:14:THR:HG22	2:B:16:ALA:N	2.21	0.55
1:F:27:ASP:HB2	1:F:141:THR:OG1	2.05	0.55
3:J:72:THR:HG23	3:J:72:THR:O	2.06	0.55
2:C:64:CYS:SG	2:C:66:THR:HG23	2.46	0.55
3:E:112:VAL:HB	3:E:141:PHE:CD1	2.41	0.55
2:G:93:ILE:HG12	2:G:107:LEU:HD22	1.87	0.55
2:I:52:THR:HG21	2:I:126:ASP:OD2	2.06	0.55
1:A:42:ALA:O	1:A:47:PHE:HD1	1.89	0.55
1:A:55:ILE:HD11	1:A:82:LEU:HD22	1.89	0.55
1:A:278:VAL:HG12	1:A:283:ARG:HG2	1.88	0.55
1:F:48:GLU:HG3	1:F:49:GLU:N	2.21	0.55
2:D:361:PRO:HB3	3:J:272:GLY:CA	2.27	0.55
2:G:274:ARG:NH2	2:G:276:ILE:HG12	2.22	0.55
2:G:338:GLU:HG2	2:H:333:LEU:HD21	1.89	0.55
2:H:248:GLN:O	2:H:248:GLN:HG3	2.04	0.55
2:I:15:PHE:HE2	2:I:57:LEU:HB3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LEU:HD11	1:F:45:GLN:HE21	1.72	0.55
2:B:67:GLY:HA2	2:B:119:ARG:NH2	2.21	0.55
2:C:44:SER:CB	2:C:159:PRO:HG3	2.37	0.55
1:A:117:LEU:HB2	1:A:122:GLU:CG	2.37	0.55
2:C:47:ARG:O	2:C:47:ARG:HG2	2.05	0.55
1:F:42:ALA:O	1:F:47:PHE:HD1	1.90	0.55
1:F:48:GLU:O	1:F:50:HIS:HD2	1.89	0.55
2:C:260:ASN:OD1	2:C:263:ARG:HB3	2.07	0.55
2:I:213:SER:OG	2:I:216:ASP:HB2	2.07	0.55
4:M:9:DT:H2'	4:M:9:DT:O5'	2.07	0.55
2:D:158:ASP:OD2	2:D:161:LYS:HE3	2.05	0.54
2:H:260:ASN:OD1	2:H:260:ASN:O	2.26	0.54
2:B:274:ARG:NH2	2:B:276:ILE:HG12	2.22	0.54
2:C:254:GLU:OE2	2:C:312:ARG:CD	2.55	0.54
2:D:64:CYS:SG	2:D:66:THR:HG23	2.47	0.54
1:F:71:MET:CB	1:F:108:LEU:HG	2.37	0.54
2:G:91:ILE:HG22	2:G:93:ILE:CD1	2.36	0.54
2:G:128:VAL:O	2:G:128:VAL:HG22	2.07	0.54
2:H:213:SER:HB3	2:H:216:ASP:HB2	1.90	0.54
2:H:254:GLU:OE2	2:H:312:ARG:CD	2.55	0.54
2:H:279:GLU:OE2	2:H:336:ARG:NE	2.39	0.54
2:C:44:SER:HB3	2:C:159:PRO:HG3	1.89	0.54
3:E:62:CYS:O	3:E:66:GLN:HG3	2.07	0.54
3:E:224:VAL:HG12	3:E:225:PRO:N	2.21	0.54
2:G:296:GLN:NE2	2:G:322:PRO:HG3	2.22	0.54
2:H:215:ARG:HD2	2:I:168:SER:OG	2.08	0.54
3:J:121:THR:HG22	3:J:122:ASP:N	2.22	0.54
1:A:74:PHE:O	1:A:74:PHE:CG	2.60	0.54
1:A:194:ASP:HB3	1:A:196:LYS:HG2	1.88	0.54
2:C:93:ILE:HD13	2:C:107:LEU:HD13	1.90	0.54
1:F:104:LEU:HD13	1:F:133:ARG:HD2	1.90	0.54
2:H:147:PRO:HD2	2:H:150:VAL:HB	1.90	0.54
2:H:337:LYS:CE	3:J:334:LEU:HD22	2.38	0.54
2:B:82:ILE:HG23	2:B:90:LEU:HD23	1.89	0.54
2:D:46:THR:O	2:D:49:VAL:HG23	2.07	0.54
2:H:129:HIS:ND1	2:H:156:THR:OG1	2.40	0.54
2:B:302:LEU:CD2	2:B:306:MET:HG3	2.34	0.54
2:D:302:LEU:HD11	2:D:306:MET:CG	2.32	0.54
3:E:169:GLU:O	3:E:173:VAL:HG23	2.07	0.54
3:E:246:HIS:O	3:E:250:THR:HG23	2.08	0.54
3:E:259:HIS:CE1	3:J:259:HIS:CE1	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:277:GLU:O	2:H:280:ALA:HB3	2.07	0.54
2:C:196:ILE:HD12	2:C:225:ILE:CD1	2.38	0.54
2:D:87:PHE:CE2	2:D:89:ASP:HB2	2.43	0.54
2:D:261:GLY:HA3	3:E:260:HIS:ND1	2.23	0.54
3:E:199:GLY:HA2	3:E:202:LEU:CB	2.38	0.54
2:I:15:PHE:CE2	2:I:57:LEU:HB3	2.43	0.54
1:A:104:LEU:HD13	1:A:133:ARG:CD	2.36	0.54
2:C:40:ALA:CB	2:C:170:CYS:HB3	2.38	0.54
2:C:324:ASP:O	2:C:327:LEU:HB3	2.07	0.54
2:D:254:GLU:OE1	2:D:312:ARG:NH1	2.40	0.54
2:H:196:ILE:HD12	2:H:225:ILE:CD1	2.38	0.54
2:H:229:ASP:CB	2:I:30:ASN:HD21	2.21	0.54
2:D:93:ILE:HD11	2:D:107:LEU:CD2	2.38	0.54
2:G:291:ARG:HG2	2:G:306:MET:HE2	1.87	0.54
2:I:38:HIS:CD2	2:I:39:HIS:H	2.26	0.54
2:C:101:VAL:CG2	2:C:134:HIS:HB3	2.37	0.54
5:N:6:DC:H2"	5:N:7:DT:O5'	2.08	0.54
2:C:46:THR:O	2:C:49:VAL:HG23	2.08	0.53
2:C:254:GLU:OE2	2:C:312:ARG:HD3	2.09	0.53
2:D:252:LEU:HD13	2:D:285:MET:CE	2.38	0.53
2:H:44:SER:HB3	2:H:159:PRO:HG3	1.90	0.53
2:I:104:THR:O	2:I:107:LEU:HB3	2.08	0.53
1:A:56:ASP:HB2	1:A:58:ASN:CB	2.38	0.53
2:B:49:VAL:HG12	2:B:49:VAL:O	2.08	0.53
2:C:47:ARG:HG3	2:D:168:SER:HB2	1.90	0.53
2:G:14:THR:HG22	2:G:16:ALA:N	2.23	0.53
2:H:339:LEU:N	2:H:340:PRO:HD2	2.24	0.53
2:B:344:ASP:HB3	2:B:347:MET:HB2	1.89	0.53
2:C:137:ASN:H	2:C:137:ASN:ND2	2.05	0.53
4:K:9:DT:H2'	4:K:9:DT:O5'	2.08	0.53
2:C:128:VAL:HG22	2:C:128:VAL:O	2.08	0.53
2:G:47:ARG:NH2	2:G:211:GLU:O	2.41	0.53
2:H:145:GLU:N	2:H:146:PRO:HD3	2.23	0.53
3:E:114:VAL:CG2	3:E:143:LEU:HD23	2.39	0.53
2:G:4:GLN:HE21	2:G:9:LYS:HG3	1.72	0.53
2:I:129:HIS:CD2	2:I:130:MET:HG2	2.44	0.53
1:F:4:LEU:HD12	1:F:135:VAL:CG1	2.38	0.53
2:H:260:ASN:O	2:H:264:VAL:HG23	2.09	0.53
1:A:48:GLU:HG3	1:A:49:GLU:N	2.23	0.53
1:F:56:ASP:HB2	1:F:58:ASN:H	1.73	0.53
1:F:117:LEU:HB2	1:F:122:GLU:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:4:DG:H2"	5:N:5:DC:O5'	2.09	0.53
2:B:28:LEU:HD13	2:B:58:LEU:HD13	1.91	0.53
2:C:271:ALA:O	2:C:276:ILE:HG23	2.08	0.53
2:G:347:MET:HG2	2:H:290:HIS:CE1	2.45	0.53
2:I:61:GLY:HA2	2:I:72:PRO:HG3	1.89	0.53
2:I:221:THR:O	2:I:225:ILE:HG13	2.09	0.53
3:J:246:HIS:O	3:J:250:THR:HG23	2.09	0.53
1:A:84:LEU:HD11	1:A:112:VAL:HG13	1.91	0.52
2:B:236:ALA:O	2:B:239:ALA:HB3	2.09	0.52
2:D:80:ARG:O	2:D:84:GLN:HG3	2.09	0.52
2:G:5:VAL:HG21	2:H:39:HIS:ND1	2.23	0.52
2:H:137:ASN:HD22	2:H:137:ASN:H	1.55	0.52
1:F:55:ILE:HD11	1:F:82:LEU:HD22	1.91	0.52
1:F:282:ARG:HG2	1:F:282:ARG:HH11	1.73	0.52
2:C:347:MET:HG3	2:D:290:HIS:CE1	2.44	0.52
1:F:187:ARG:HG3	2:G:173:PHE:CE1	2.45	0.52
2:G:49:VAL:HG12	2:G:49:VAL:O	2.08	0.52
2:G:255:ALA:HB2	2:G:263:ARG:NH1	2.25	0.52
2:G:292:ILE:CD1	2:G:316:LEU:HD23	2.37	0.52
2:H:137:ASN:H	2:H:137:ASN:ND2	2.07	0.52
2:H:137:ASN:HA	2:H:140:LEU:HG	1.90	0.52
3:J:2:ARG:CG	3:J:3:TRP:N	2.72	0.52
3:J:81:PRO:HB3	3:J:87:THR:O	2.09	0.52
2:G:344:ASP:HB3	2:G:347:MET:HB2	1.92	0.52
2:G:365:LEU:HD13	2:H:297:LEU:HD23	1.88	0.52
2:B:21:GLN:HE21	2:B:21:GLN:CA	2.21	0.52
2:H:282:LEU:O	2:H:286:LEU:CD1	2.58	0.52
2:B:365:LEU:CD1	2:C:297:LEU:HD23	2.38	0.52
2:C:279:GLU:OE2	2:C:336:ARG:NE	2.40	0.52
2:C:295:VAL:CG2	2:C:302:LEU:HB2	2.38	0.52
3:E:114:VAL:HB	3:E:143:LEU:HD23	1.90	0.52
2:G:47:ARG:H	2:G:47:ARG:HD3	1.75	0.52
1:A:4:LEU:HD12	1:A:135:VAL:CG1	2.39	0.52
2:D:69:THR:HG21	2:D:72:PRO:HA	1.92	0.52
2:D:179:ASP:HB3	2:D:182:GLN:CG	2.40	0.52
1:F:104:LEU:HD13	1:F:133:ARG:CD	2.39	0.52
2:G:84:GLN:HE21	2:G:84:GLN:HA	1.74	0.52
2:H:47:ARG:NH1	2:H:216:ASP:OD2	2.42	0.52
2:I:24:VAL:HG21	2:I:175:LEU:CD2	2.38	0.52
2:C:248:GLN:O	2:C:248:GLN:HG3	2.09	0.52
2:C:367:GLU:HG3	2:C:368:PRO:CD	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:80:ALA:HB1	3:E:81:PRO:CD	2.40	0.52
2:D:184:ARG:HD2	2:D:204:GLN:HE21	1.74	0.52
2:D:333:LEU:C	2:D:333:LEU:HD12	2.30	0.52
1:A:48:GLU:O	1:A:50:HIS:CD2	2.62	0.51
2:C:215:ARG:NH2	2:D:144:GLU:OE1	2.40	0.51
1:F:262:ARG:NH2	3:J:320:GLU:OE1	2.43	0.51
1:A:152:ALA:O	1:A:156:LYS:HD2	2.11	0.51
2:B:47:ARG:NH2	2:B:211:GLU:O	2.43	0.51
2:B:253:VAL:HG12	2:B:316:LEU:HD21	1.92	0.51
2:B:291:ARG:O	2:B:295:VAL:HG23	2.11	0.51
2:H:292:ILE:HG13	2:H:313:MET:CE	2.39	0.51
1:A:162:LEU:HD23	1:A:197:LEU:HB2	1.93	0.51
2:B:49:VAL:CG1	2:B:176:LYS:O	2.54	0.51
2:C:144:GLU:HG2	2:C:145:GLU:HG3	1.91	0.51
3:E:90:VAL:HG12	4:K:13:DT:H5"	1.92	0.51
2:I:6:LEU:H	2:I:6:LEU:HD12	1.75	0.51
2:I:21:GLN:HE21	2:I:49:VAL:HG12	1.74	0.51
1:A:25:GLY:HA3	1:A:139:CYS:HB2	1.92	0.51
2:B:351:MET:CE	2:C:290:HIS:HA	2.41	0.51
1:F:56:ASP:HB2	1:F:58:ASN:CB	2.41	0.51
2:G:42:LEU:HG	2:G:172:GLN:HG3	1.91	0.51
2:I:78:ASN:O	2:I:82:ILE:HG13	2.11	0.51
2:I:309:ILE:HG22	2:I:309:ILE:O	2.10	0.51
2:B:276:ILE:CG2	2:B:277:GLU:N	2.74	0.51
2:C:223:GLN:HG3	2:C:240:MET:HE1	1.91	0.51
1:F:59:THR:HG23	1:F:63:ALA:CB	2.39	0.51
2:I:74:GLY:HA2	2:I:79:CYS:CB	2.41	0.51
1:A:26:ASN:ND2	1:A:140:GLN:OE1	2.43	0.51
2:D:21:GLN:HE21	2:D:49:VAL:HG12	1.74	0.51
2:C:101:VAL:HG23	4:K:17:DC:OP1	2.10	0.51
1:A:81:LEU:HD12	1:A:82:LEU:H	1.76	0.51
2:C:215:ARG:HD2	2:D:168:SER:OG	2.11	0.50
2:D:291:ARG:O	2:D:294:MET:N	2.44	0.50
4:K:10:DT:H2'	4:K:11:DT:H71	1.91	0.50
2:B:250:LEU:HA	2:B:288:LEU:HD12	1.92	0.50
2:C:254:GLU:O	2:C:257:VAL:HG22	2.11	0.50
1:F:81:LEU:HD13	1:F:111:ILE:HG22	1.93	0.50
1:F:279:TRP:O	1:F:283:ARG:HG2	2.10	0.50
2:G:13:GLN:HG3	2:G:83:GLU:OE2	2.11	0.50
2:H:339:LEU:N	2:H:340:PRO:CD	2.74	0.50
1:A:81:LEU:HD13	1:A:111:ILE:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:ASN:OD1	1:F:126:TRP:NE1	2.36	0.50
1:F:248:ARG:HG3	4:M:9:DT:H4'	1.92	0.50
2:I:250:LEU:HD13	2:I:313:MET:CE	2.41	0.50
1:A:156:LYS:O	1:A:159:ASN:N	2.45	0.50
1:F:22:LEU:HD13	1:F:127:PHE:HE1	1.77	0.50
2:G:124:LEU:HD13	2:G:153:LEU:HB2	1.93	0.50
2:G:296:GLN:CD	2:G:322:PRO:HG3	2.32	0.50
2:I:6:LEU:HD13	2:I:222:ASP:OD2	2.12	0.50
1:A:251:GLN:HE22	3:E:307:ASN:HD21	1.59	0.50
2:D:38:HIS:CD2	2:D:39:HIS:H	2.29	0.50
2:D:104:THR:O	2:D:107:LEU:HB3	2.10	0.50
1:A:304:LEU:HD23	1:A:327:LEU:HD13	1.94	0.50
2:C:339:LEU:N	2:C:340:PRO:HD2	2.27	0.50
2:D:101:VAL:HG22	4:K:15:DG:OP1	2.12	0.50
2:G:320:ILE:HG23	2:G:321:PRO:HD2	1.93	0.50
2:H:265:MET:HE2	2:I:294:MET:SD	2.52	0.50
4:M:14:DA:C2'	4:M:15:DG:O5'	2.59	0.50
2:B:67:GLY:HA2	2:B:119:ARG:HH21	1.77	0.50
2:C:208:ARG:HE	2:C:305:ASP:HB3	1.77	0.50
2:C:295:VAL:HG22	2:C:302:LEU:HB2	1.93	0.50
2:D:250:LEU:HD13	2:D:313:MET:CE	2.42	0.50
2:D:333:LEU:HD12	2:D:333:LEU:O	2.11	0.50
2:G:253:VAL:CG1	2:G:316:LEU:HD21	2.42	0.50
2:I:178:LEU:CD1	2:I:214:LEU:HD12	2.42	0.50
2:I:299:PRO:O	2:I:314:ARG:NH1	2.41	0.50
2:I:309:ILE:CG2	2:I:309:ILE:O	2.59	0.50
3:J:150:ARG:NH2	3:J:298:GLU:OE2	2.45	0.50
2:C:337:LYS:HE2	3:E:334:LEU:HD22	1.92	0.50
3:J:2:ARG:HD3	3:J:4:TYR:HE1	1.68	0.50
3:E:259:HIS:ND1	3:J:259:HIS:CE1	2.80	0.50
1:F:49:GLU:HB2	1:F:78:GLN:HB3	1.94	0.50
1:A:82:LEU:HD12	1:A:110:LEU:HD11	1.93	0.49
2:B:277:GLU:O	2:B:280:ALA:HB3	2.12	0.49
2:G:357:LEU:O	2:G:360:HIS:HB2	2.12	0.49
3:J:169:GLU:O	3:J:173:VAL:HG23	2.11	0.49
2:B:357:LEU:O	2:B:360:HIS:HB2	2.11	0.49
2:D:299:PRO:O	2:D:314:ARG:NH1	2.37	0.49
2:I:339:LEU:HB3	2:I:340:PRO:HD3	1.94	0.49
3:J:306:ILE:HD13	3:J:311:LEU:HD22	1.93	0.49
1:A:49:GLU:HB2	1:A:78:GLN:HB3	1.95	0.49
1:A:97:LEU:CD1	1:A:126:TRP:CH2	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:THR:HG21	2:B:126:ASP:OD2	2.11	0.49
2:G:321:PRO:O	2:G:324:ASP:HB2	2.11	0.49
4:M:15:DG:H2"	4:M:16:DG:C5'	2.42	0.49
2:B:284:GLU:O	2:B:288:LEU:HG	2.13	0.49
2:B:291:ARG:HG2	2:B:306:MET:HE2	1.94	0.49
3:E:103:HIS:CD2	3:E:103:HIS:H	2.30	0.49
3:J:80:ALA:HB1	3:J:81:PRO:CD	2.42	0.49
2:B:13:GLN:HG3	2:B:83:GLU:OE2	2.12	0.49
2:B:326:GLN:O	2:B:330:GLN:HG3	2.12	0.49
2:C:40:ALA:HB1	2:C:170:CYS:HB3	1.95	0.49
1:F:147:LEU:O	1:F:151:VAL:HG23	2.12	0.49
3:E:2:ARG:CG	3:E:3:TRP:N	2.75	0.49
1:F:278:VAL:O	1:F:283:ARG:HD3	2.13	0.49
2:H:178:LEU:CD1	2:H:214:LEU:HB2	2.42	0.49
3:J:30:GLN:O	3:J:30:GLN:HG3	2.13	0.49
2:C:274:ARG:HB2	2:C:276:ILE:HG23	1.95	0.49
2:H:190:ILE:HD12	2:H:218:LEU:HD21	1.94	0.49
3:J:239:GLU:O	3:J:239:GLU:HG2	2.12	0.49
4:K:15:DG:H2"	4:K:16:DG:C5'	2.42	0.49
4:M:13:DT:C2'	4:M:14:DA:O5'	2.57	0.49
2:D:114:ALA:HA	2:D:149:HIS:CD2	2.47	0.49
2:D:216:ASP:OD1	3:E:157:SER:CB	2.56	0.49
2:D:257:VAL:HG21	2:D:320:ILE:HD11	1.95	0.49
3:J:271:PRO:HD2	3:J:272:GLY:H	1.76	0.49
4:M:10:DT:H2'	4:M:11:DT:H71	1.94	0.49
1:A:53:PHE:HZ	1:A:63:ALA:HB1	1.76	0.49
1:A:59:THR:HG23	1:A:63:ALA:CB	2.40	0.49
1:A:268:PRO:HD2	1:A:271:ALA:HB3	1.94	0.49
2:B:321:PRO:O	2:B:324:ASP:HB2	2.13	0.49
2:B:351:MET:HG2	2:C:290:HIS:CD2	2.41	0.49
6:B:400:ADP:N3	6:B:400:ADP:H2'	2.28	0.49
2:C:254:GLU:OE1	2:C:312:ARG:HD3	2.12	0.49
3:E:46:ARG:CD	3:E:68:MET:HG2	2.42	0.49
1:F:52:THR:CG2	1:F:81:LEU:HD23	2.42	0.49
1:F:53:PHE:HZ	1:F:63:ALA:HB1	1.77	0.49
2:G:343:PRO:HB3	2:H:283:VAL:HG13	1.93	0.49
2:I:215:ARG:HG2	3:J:157:SER:O	2.13	0.49
5:L:6:DC:H2"	5:L:7:DT:O5'	2.13	0.49
2:D:5:VAL:HG13	2:D:222:ASP:OD2	2.13	0.48
2:G:276:ILE:HG23	2:G:277:GLU:N	2.28	0.48
1:A:170:LEU:HB3	1:A:181:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:PRO:HD2	2:C:149:HIS:HD2	1.77	0.48
2:C:339:LEU:N	2:C:340:PRO:CD	2.75	0.48
2:D:245:ASP:OD1	2:D:245:ASP:O	2.31	0.48
3:E:279:ASN:O	3:J:282:SER:HB2	2.13	0.48
2:G:284:GLU:O	2:G:288:LEU:HG	2.13	0.48
2:G:326:GLN:O	2:G:330:GLN:HG3	2.13	0.48
2:H:49:VAL:CG1	2:H:176:LYS:O	2.59	0.48
3:J:27:LEU:HD12	3:J:160:ARG:HG2	1.96	0.48
3:J:224:VAL:CB	3:J:225:PRO:HD3	2.41	0.48
1:A:1:MET:HE2	1:A:131:ALA:HA	1.95	0.48
2:H:101:VAL:CG2	2:H:134:HIS:HB3	2.42	0.48
2:H:279:GLU:O	2:H:283:VAL:HG23	2.13	0.48
2:D:6:LEU:O	2:D:8:ARG:N	2.46	0.48
3:E:35:MET:HE1	3:E:166:PRO:HA	1.95	0.48
3:J:114:VAL:CG2	3:J:143:LEU:HD23	2.43	0.48
3:J:128:LEU:O	3:J:132:LEU:HB2	2.13	0.48
5:N:6:DC:C2'	5:N:7:DT:O5'	2.62	0.48
3:E:150:ARG:NH2	3:E:298:GLU:OE2	2.46	0.48
2:G:74:GLY:HA2	2:G:79:CYS:HB3	1.95	0.48
2:G:215:ARG:NH2	2:H:169:ARG:NH1	2.61	0.48
2:H:46:THR:HB	2:H:47:ARG:HE	1.77	0.48
2:H:291:ARG:HD2	2:H:306:MET:SD	2.54	0.48
2:I:101:VAL:HG22	4:M:15:DG:OP1	2.13	0.48
1:A:17:LEU:HD13	1:A:45:GLN:HE21	1.78	0.48
2:B:15:PHE:HE2	2:B:57:LEU:CB	2.23	0.48
2:B:78:ASN:O	2:B:82:ILE:HG13	2.12	0.48
2:C:46:THR:HB	2:C:47:ARG:HE	1.77	0.48
1:F:9:LEU:HD11	1:F:13:LEU:HD21	1.95	0.48
1:F:24:LEU:CD1	1:F:117:LEU:HD11	2.44	0.48
1:F:162:LEU:HD23	1:F:197:LEU:HB2	1.94	0.48
1:F:262:ARG:HH22	3:J:320:GLU:CD	2.16	0.48
2:G:215:ARG:C	2:G:217:ALA:N	2.67	0.48
2:I:254:GLU:OE1	2:I:312:ARG:NH1	2.45	0.48
2:B:47:ARG:HD3	2:B:47:ARG:N	2.28	0.48
2:B:89:ASP:OD2	2:B:116:ALA:N	2.46	0.48
3:E:128:LEU:O	3:E:132:LEU:HB2	2.14	0.48
2:H:292:ILE:HG22	2:H:325:ILE:CD1	2.44	0.48
2:D:52:THR:O	2:D:56:ARG:HG3	2.14	0.48
2:D:265:MET:CE	3:E:257:LYS:HE2	2.43	0.48
3:E:90:VAL:CG1	4:K:13:DT:H5"	2.43	0.48
2:G:21:GLN:NE2	2:G:21:GLN:CA	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:114:ALA:HB1	2:G:115:PRO:HD2	1.95	0.48
2:H:260:ASN:OD1	2:H:263:ARG:HB3	2.14	0.48
2:I:158:ASP:OD2	2:I:161:LYS:HE3	2.13	0.48
2:C:15:PHE:HE1	2:C:57:LEU:HB3	1.79	0.48
2:H:165:THR:O	2:H:169:ARG:NH1	2.47	0.48
2:I:184:ARG:HD2	2:I:204:GLN:HE21	1.78	0.48
2:D:75:VAL:HG12	2:D:75:VAL:O	2.13	0.48
3:E:35:MET:CE	3:E:166:PRO:HA	2.44	0.48
2:G:13:GLN:HB3	2:G:60:LYS:NZ	2.29	0.48
2:H:202:ALA:HB1	2:H:237:VAL:HG21	1.95	0.48
1:A:251:GLN:HE22	3:E:307:ASN:ND2	2.11	0.47
2:B:24:VAL:HG21	2:B:175:LEU:HD22	1.96	0.47
2:B:74:GLY:HA2	2:B:79:CYS:HB3	1.95	0.47
2:C:254:GLU:CD	2:C:312:ARG:HD3	2.34	0.47
3:E:99:LYS:HD3	3:E:105:ARG:HH22	1.79	0.47
1:F:84:LEU:HD11	1:F:112:VAL:HG13	1.95	0.47
2:G:171:LEU:HD23	2:G:173:PHE:CE2	2.49	0.47
2:H:115:PRO:HD2	2:H:149:HIS:HD2	1.78	0.47
2:I:333:LEU:C	2:I:333:LEU:HD12	2.33	0.47
2:G:277:GLU:O	2:G:280:ALA:HB3	2.14	0.47
2:D:184:ARG:CD	2:D:204:GLN:HE21	2.27	0.47
2:G:215:ARG:NH1	6:G:406:ADP:H5'1	2.24	0.47
2:I:179:ASP:HB3	2:I:182:GLN:HG3	1.97	0.47
3:J:14:LEU:HD21	3:J:162:HIS:ND1	2.29	0.47
2:B:215:ARG:C	2:B:217:ALA:N	2.68	0.47
1:F:65:PHE:CD2	1:F:65:PHE:O	2.67	0.47
5:L:4:DG:H2"	5:L:5:DC:O5'	2.14	0.47
2:C:47:ARG:NH1	2:C:216:ASP:OD2	2.47	0.47
1:F:82:LEU:HD12	1:F:110:LEU:HD11	1.96	0.47
6:G:406:ADP:N3	6:G:406:ADP:H2'	2.27	0.47
2:H:73:CYS:O	2:H:75:VAL:HG13	2.15	0.47
1:A:55:ILE:O	1:A:85:PRO:HG3	2.15	0.47
1:A:156:LYS:O	1:A:159:ASN:HA	2.14	0.47
2:B:9:LYS:HD3	2:B:194:GLU:OE2	2.14	0.47
2:B:101:VAL:HA	2:B:135:SER:OG	2.14	0.47
2:B:326:GLN:O	2:B:326:GLN:HG3	2.14	0.47
2:H:44:SER:HB2	2:H:159:PRO:HG3	1.95	0.47
2:I:56:ARG:NH1	2:I:92:GLU:OE2	2.48	0.47
3:J:164:LEU:HA	3:J:164:LEU:HD12	1.52	0.47
1:A:19:ALA:HB1	1:A:104:LEU:HD22	1.95	0.47
2:B:191:LEU:HD11	2:B:232:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:ASP:HA	2:C:159:PRO:HD3	1.59	0.47
2:D:60:LYS:HE3	2:D:79:CYS:HB3	1.96	0.47
2:D:363:MET:HE2	3:J:276:GLU:OE1	2.14	0.47
3:E:50:CYS:HB2	3:E:65:CYS:SG	2.53	0.47
3:E:224:VAL:CB	3:E:225:PRO:HD3	2.43	0.47
1:F:13:LEU:HD22	1:F:21:TYR:CE1	2.50	0.47
1:F:48:GLU:HG3	1:F:49:GLU:H	1.80	0.47
1:F:304:LEU:O	1:F:308:THR:CG2	2.62	0.47
2:G:89:ASP:OD2	2:G:116:ALA:N	2.47	0.47
2:G:265:MET:CE	2:G:350:GLU:HG2	2.45	0.47
2:H:178:LEU:HD12	2:H:214:LEU:HB2	1.95	0.47
2:I:94:ASP:CG	2:I:97:SER:HB2	2.34	0.47
2:I:114:ALA:HA	2:I:149:HIS:CD2	2.49	0.47
2:I:247:ASP:OD1	2:I:312:ARG:NH2	2.47	0.47
1:A:24:LEU:CD1	1:A:117:LEU:HD11	2.45	0.47
2:H:38:HIS:CD2	2:H:171:LEU:HG	2.50	0.47
2:I:228:GLY:O	2:I:229:ASP:CB	2.62	0.47
2:I:347:MET:HE1	3:J:246:HIS:HE1	1.78	0.47
1:A:78:GLN:HG3	1:A:108:LEU:CD2	2.45	0.47
2:B:114:ALA:HB1	2:B:115:PRO:HD2	1.96	0.47
2:D:94:ASP:CG	2:D:97:SER:HB2	2.36	0.47
1:F:156:LYS:O	1:F:159:ASN:HA	2.14	0.47
2:G:67:GLY:HA2	2:G:119:ARG:HH21	1.78	0.47
2:G:84:GLN:HA	2:G:84:GLN:NE2	2.30	0.47
3:J:161:LEU:HD12	3:J:161:LEU:HA	1.74	0.47
3:E:259:HIS:ND1	3:J:259:HIS:ND1	2.63	0.47
1:F:128:THR:O	1:F:131:ALA:CB	2.63	0.47
2:G:125:ILE:HB	2:G:154:LEU:CD2	2.45	0.47
2:G:253:VAL:HG12	2:G:316:LEU:HD21	1.97	0.47
2:H:365:LEU:HD11	2:I:297:LEU:CD1	2.44	0.47
3:J:73:HIS:HA	3:J:74:PRO:HD2	1.38	0.47
3:J:121:THR:HG22	3:J:123:ALA:H	1.80	0.47
2:G:78:ASN:O	2:G:82:ILE:HG13	2.16	0.46
2:I:97:SER:O	3:J:94:ARG:NH1	2.49	0.46
1:A:13:LEU:HD11	1:A:38:VAL:HG22	1.95	0.46
1:A:42:ALA:O	1:A:47:PHE:CD1	2.67	0.46
1:A:97:LEU:HD12	1:A:126:TRP:CZ2	2.50	0.46
2:B:13:GLN:HB3	2:B:60:LYS:NZ	2.30	0.46
2:B:84:GLN:HA	2:B:84:GLN:HE21	1.80	0.46
1:F:81:LEU:HD12	1:F:82:LEU:H	1.80	0.46
1:F:122:GLU:O	1:F:127:PHE:CD2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:93:ILE:HD11	2:I:107:LEU:CD2	2.46	0.46
2:I:333:LEU:HD12	2:I:333:LEU:O	2.15	0.46
1:A:84:LEU:HD11	1:A:112:VAL:CG1	2.45	0.46
1:A:190:LEU:HD11	2:B:38:HIS:CE1	2.50	0.46
2:C:253:VAL:O	2:C:256:MET:HB3	2.16	0.46
2:D:56:ARG:NH1	2:D:92:GLU:OE2	2.48	0.46
3:E:2:ARG:HD3	3:E:4:TYR:HE1	1.70	0.46
2:G:84:GLN:HE21	2:G:84:GLN:CA	2.25	0.46
2:G:273:ALA:C	2:G:275:GLY:N	2.69	0.46
1:A:39:ARG:NH1	1:A:50:HIS:CB	2.76	0.46
1:A:56:ASP:C	1:A:58:ASN:H	2.17	0.46
1:A:190:LEU:HD11	2:B:38:HIS:HE1	1.80	0.46
3:E:220:LEU:HA	3:E:220:LEU:HD12	1.64	0.46
3:E:306:ILE:HD13	3:E:311:LEU:HD22	1.97	0.46
1:F:128:THR:HA	1:F:131:ALA:HB2	1.98	0.46
1:F:299:ARG:HG3	3:J:317:LEU:HB3	1.97	0.46
2:G:41:TYR:N	2:G:41:TYR:CD1	2.84	0.46
2:H:332:LEU:HA	2:H:332:LEU:HD23	1.60	0.46
3:J:114:VAL:CB	3:J:143:LEU:HD23	2.45	0.46
2:B:215:ARG:NH1	6:B:400:ADP:H5'1	2.25	0.46
2:C:18:VAL:HB	2:C:25:LEU:HD11	1.97	0.46
2:C:147:PRO:HB2	2:C:149:HIS:ND1	2.30	0.46
3:E:73:HIS:HA	3:E:74:PRO:HD2	1.40	0.46
2:B:257:VAL:HG22	2:B:328:TYR:HE2	1.77	0.46
2:C:28:LEU:HD22	2:C:58:LEU:HD22	1.97	0.46
2:C:279:GLU:O	2:C:283:VAL:HG23	2.15	0.46
2:D:256:MET:CE	2:D:332:LEU:HD11	2.46	0.46
3:E:86:ASN:O	3:E:119:LEU:HD22	2.16	0.46
1:F:26:ASN:ND2	1:F:140:GLN:OE1	2.47	0.46
2:G:-8:LEU:HD12	2:G:-8:LEU:HA	1.72	0.46
2:G:24:VAL:HG21	2:G:175:LEU:HD22	1.97	0.46
2:G:332:LEU:HD23	2:G:332:LEU:HA	1.79	0.46
2:H:11:ARG:HG3	2:H:53:SER:HB3	1.96	0.46
2:C:244:LEU:HD12	2:C:244:LEU:N	2.26	0.46
2:D:15:PHE:HD2	2:D:57:LEU:HD13	1.80	0.46
3:E:3:TRP:CH2	3:E:8:ARG:HG3	2.37	0.46
3:J:224:VAL:HG12	3:J:225:PRO:N	2.30	0.46
1:A:26:ASN:OD1	1:A:27:ASP:N	2.49	0.46
1:A:158:LEU:O	1:A:160:LEU:HG	2.16	0.46
2:C:60:LYS:HZ1	2:C:83:GLU:HG3	1.78	0.46
2:D:126:ASP:OD1	2:D:155:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:223:SER:HB3	3:E:228:ASP:O	2.16	0.46
2:G:52:THR:HG21	2:G:126:ASP:OD2	2.16	0.46
3:J:46:ARG:CD	3:J:68:MET:HG2	2.43	0.46
3:J:220:LEU:HA	3:J:220:LEU:HD12	1.56	0.46
2:B:42:LEU:HG	2:B:172:GLN:HG3	1.97	0.46
2:B:125:ILE:HB	2:B:154:LEU:CD2	2.46	0.46
2:B:223:GLN:HB2	2:C:171:LEU:HD22	1.98	0.46
2:B:273:ALA:C	2:B:275:GLY:N	2.69	0.46
2:B:327:LEU:HD12	2:B:330:GLN:OE1	2.15	0.46
1:F:24:LEU:HD11	1:F:117:LEU:HD11	1.98	0.46
2:H:274:ARG:HB2	2:H:276:ILE:HG23	1.98	0.46
2:H:276:ILE:HD11	2:H:281:LEU:HD22	1.97	0.46
1:A:64:ILE:HG13	1:A:96:GLN:OE1	2.17	0.46
1:A:199:LEU:HB3	1:A:200:PRO:HD3	1.98	0.46
2:B:245:ASP:O	2:B:274:ARG:HD2	2.16	0.46
2:C:291:ARG:HE	2:C:291:ARG:HB2	1.36	0.46
2:D:143:LEU:HD12	2:D:143:LEU:HA	1.75	0.46
1:F:308:THR:CB	1:F:323:GLU:OE1	2.63	0.46
2:H:111:VAL:HG13	2:H:150:VAL:HG21	1.97	0.46
2:H:299:PRO:O	2:H:314:ARG:NH2	2.49	0.46
3:J:238:HIS:O	3:J:308:ARG:HD3	2.16	0.46
1:A:147:LEU:O	1:A:151:VAL:HG23	2.16	0.45
1:A:251:GLN:NE2	3:E:307:ASN:HD21	2.13	0.45
2:C:95:ALA:O	2:C:99:THR:HG22	2.16	0.45
1:F:78:GLN:HG3	1:F:108:LEU:CD2	2.46	0.45
1:F:160:LEU:HD11	1:F:189:SER:HB3	1.98	0.45
2:G:80:ARG:O	2:G:84:GLN:HG2	2.15	0.45
2:G:314:ARG:NH1	2:G:314:ARG:HG2	2.32	0.45
2:H:254:GLU:HG2	2:H:316:LEU:HD11	1.98	0.45
2:I:269:ASN:ND2	2:I:346:ARG:HH22	2.13	0.45
2:D:24:VAL:HG21	2:D:175:LEU:CD2	2.44	0.45
3:E:155:LEU:HD12	3:E:155:LEU:O	2.16	0.45
3:E:164:LEU:HA	3:E:164:LEU:HD12	1.48	0.45
2:G:302:LEU:HD23	2:G:302:LEU:HA	1.77	0.45
2:H:291:ARG:HE	2:H:291:ARG:HB2	1.33	0.45
1:A:13:LEU:CD1	1:A:38:VAL:HG22	2.46	0.45
1:A:304:LEU:O	1:A:308:THR:CG2	2.58	0.45
2:G:257:VAL:HG22	2:G:328:TYR:HE2	1.81	0.45
2:G:282:LEU:HA	2:G:282:LEU:HD23	1.52	0.45
2:G:320:ILE:HG21	2:G:325:ILE:HG13	1.98	0.45
1:A:223:MET:CG	1:A:285:MET:HG3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:THR:HA	2:B:131:LEU:HD23	1.97	0.45
2:C:38:HIS:CD2	2:C:171:LEU:HG	2.51	0.45
3:E:27:LEU:HD12	3:E:160:ARG:HG2	1.99	0.45
1:F:13:LEU:HD22	1:F:21:TYR:CZ	2.51	0.45
1:F:42:ALA:O	1:F:47:PHE:CD1	2.68	0.45
2:G:58:LEU:HD12	2:G:58:LEU:HA	1.81	0.45
2:I:150:VAL:O	2:I:151:LYS:HD3	2.15	0.45
3:J:29:ILE:O	3:J:144:ALA:HA	2.16	0.45
1:A:71:MET:SD	1:A:103:LEU:HB3	2.56	0.45
2:C:51:LYS:HE3	2:C:157:ALA:HA	1.99	0.45
2:C:320:ILE:HA	2:C:321:PRO:HD3	1.79	0.45
2:D:41:TYR:HD2	2:D:173:PHE:HE2	1.65	0.45
1:F:13:LEU:CD2	1:F:21:TYR:CE1	3.00	0.45
1:F:223:MET:CG	1:F:285:MET:HG3	2.46	0.45
1:F:310:LEU:HD21	3:J:306:ILE:HD12	1.98	0.45
2:H:244:LEU:HD12	2:H:244:LEU:N	2.23	0.45
1:A:48:GLU:HG3	1:A:49:GLU:H	1.82	0.45
2:B:365:LEU:HD11	2:C:297:LEU:HD23	1.99	0.45
1:F:101:THR:HA	1:F:130:LEU:HD21	1.97	0.45
1:F:116:LYS:HB3	1:F:140:GLN:NE2	2.32	0.45
1:F:170:LEU:HB3	1:F:181:LEU:HD11	1.99	0.45
1:F:282:ARG:HG2	1:F:282:ARG:NH1	2.32	0.45
1:F:306:THR:HG23	3:J:311:LEU:HD12	1.98	0.45
2:H:187:LEU:HD23	2:H:187:LEU:HA	1.79	0.45
2:H:208:ARG:HE	2:H:305:ASP:HB3	1.82	0.45
2:H:276:ILE:CD1	2:H:281:LEU:HB2	2.47	0.45
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.62	0.45
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.58	0.45
2:D:354:LEU:HA	2:D:354:LEU:HD23	1.72	0.45
3:E:29:ILE:CD1	3:E:40:LEU:HD23	2.44	0.45
2:I:87:PHE:CE2	2:I:89:ASP:HB2	2.52	0.45
1:A:13:LEU:HD22	1:A:21:TYR:CZ	2.52	0.45
1:A:150:TRP:CZ3	1:A:178:LEU:HD22	2.51	0.45
2:B:14:THR:HG22	2:B:16:ALA:H	1.82	0.45
2:D:3:TYR:CG	2:D:4:GLN:N	2.85	0.45
2:D:215:ARG:NE	6:D:404:ADP:H5'1	2.31	0.45
1:F:191:LEU:HA	1:F:191:LEU:HD23	1.70	0.45
2:I:184:ARG:CD	2:I:204:GLN:HE21	2.28	0.45
2:C:34:LEU:HD23	2:C:34:LEU:HA	1.67	0.45
2:C:94:ASP:OD1	2:C:94:ASP:C	2.54	0.45
1:F:22:LEU:HD13	1:F:127:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:VAL:HG11	1:F:111:ILE:HD11	1.99	0.45
1:F:64:ILE:HG13	1:F:96:GLN:OE1	2.17	0.45
1:A:47:PHE:CD2	1:A:77:ARG:HB3	2.52	0.44
2:C:136:PHE:O	2:C:139:LEU:HB2	2.17	0.44
2:D:215:ARG:HE	6:D:404:ADP:H5'1	1.82	0.44
2:D:363:MET:CE	3:J:276:GLU:OE1	2.65	0.44
2:H:88:VAL:HG12	2:H:88:VAL:O	2.17	0.44
3:J:103:HIS:CD2	3:J:103:HIS:H	2.34	0.44
2:H:254:GLU:O	2:H:257:VAL:HG22	2.17	0.44
5:L:6:DC:C2'	5:L:7:DT:O5'	2.66	0.44
1:A:13:LEU:HD22	1:A:21:TYR:CE1	2.52	0.44
2:B:171:LEU:HD12	2:B:171:LEU:HA	1.75	0.44
2:C:215:ARG:O	2:C:216:ASP:C	2.55	0.44
2:C:341:TYR:CB	2:D:333:LEU:CD1	2.94	0.44
2:D:262:GLU:HB2	3:E:260:HIS:O	2.18	0.44
1:F:142:PRO:HD3	1:F:178:LEU:HD11	2.00	0.44
2:G:215:ARG:NH1	2:H:144:GLU:OE1	2.50	0.44
2:H:271:ALA:O	2:H:276:ILE:HG23	2.17	0.44
3:J:306:ILE:HG12	3:J:307:ASN:N	2.32	0.44
2:B:134:HIS:CG	4:K:19:DA:H5"	2.51	0.44
2:C:8:ARG:NH2	2:D:146:PRO:O	2.50	0.44
2:C:137:ASN:ND2	2:C:137:ASN:N	2.66	0.44
2:D:247:ASP:OD1	2:D:312:ARG:NH2	2.50	0.44
2:I:18:VAL:HB	2:I:25:LEU:HD11	1.98	0.44
3:J:90:VAL:HG12	4:M:13:DT:H5"	1.99	0.44
3:J:308:ARG:HG2	3:J:312:ILE:HD12	1.99	0.44
1:A:142:PRO:HB2	1:A:147:LEU:HD12	2.00	0.44
1:A:172:TYR:HH	1:A:231:HIS:CE1	2.35	0.44
2:B:94:ASP:OD1	2:B:94:ASP:C	2.56	0.44
1:F:97:LEU:CD1	1:F:126:TRP:CH2	3.01	0.44
2:H:254:GLU:CD	2:H:312:ARG:HD3	2.37	0.44
2:H:95:ALA:O	2:H:99:THR:HG22	2.18	0.44
2:H:133:ARG:O	2:H:137:ASN:ND2	2.51	0.44
2:G:152:PHE:C	2:G:153:LEU:HD23	2.38	0.44
2:G:236:ALA:O	2:G:239:ALA:HB3	2.18	0.44
2:I:144:GLU:HB2	2:I:169:ARG:NE	2.33	0.44
1:A:278:VAL:O	1:A:283:ARG:HD3	2.18	0.44
2:B:320:ILE:HG23	2:B:321:PRO:HD2	1.99	0.44
2:C:337:LYS:HD3	3:E:334:LEU:HD22	1.99	0.44
2:C:360:HIS:HA	2:C:361:PRO:HD3	1.89	0.44
2:I:119:ARG:HG2	2:I:120:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD12	1:A:82:LEU:N	2.33	0.44
2:C:254:GLU:OE2	2:C:312:ARG:HG2	2.18	0.44
2:C:282:LEU:HD23	2:C:282:LEU:HA	1.79	0.44
2:D:120:PHE:CE1	2:D:151:LYS:HE2	2.53	0.44
2:D:306:MET:O	2:D:308:ALA:N	2.51	0.44
2:G:326:GLN:O	2:G:326:GLN:HG3	2.17	0.44
2:H:23:HIS:HE1	2:H:174:HIS:O	2.01	0.44
2:I:12:PRO:HG3	6:I:410:ADP:C2	2.53	0.44
2:I:178:LEU:HD13	2:I:214:LEU:HD12	1.99	0.44
1:A:56:ASP:C	1:A:58:ASN:N	2.71	0.43
2:D:228:GLY:O	2:D:229:ASP:CB	2.66	0.43
2:G:178:LEU:CD1	2:G:214:LEU:HD22	2.48	0.43
2:I:323:THR:HB	2:I:362:ARG:NH2	2.33	0.43
4:K:13:DT:C2'	4:K:14:DA:O5'	2.64	0.43
2:B:254:GLU:HG2	2:B:316:LEU:HD13	2.00	0.43
2:D:29:ALA:HA	2:D:70:ALA:HB1	1.99	0.43
1:F:50:HIS:ND1	1:F:79:THR:HB	2.34	0.43
1:F:188:LEU:CD1	1:F:202:VAL:HG22	2.48	0.43
2:I:100:LYS:O	2:I:104:THR:HG23	2.17	0.43
2:I:140:LEU:HD23	2:I:140:LEU:HA	1.86	0.43
2:B:288:LEU:N	2:B:288:LEU:HD23	2.33	0.43
2:C:111:VAL:HG13	2:C:150:VAL:HG21	1.99	0.43
2:D:95:ALA:O	2:D:99:THR:HG22	2.19	0.43
3:E:306:ILE:HG12	3:E:307:ASN:N	2.32	0.43
1:F:84:LEU:HD13	1:F:113:ARG:O	2.19	0.43
2:G:297:LEU:N	2:G:297:LEU:HD12	2.33	0.43
1:A:116:LYS:HB3	1:A:140:GLN:NE2	2.34	0.43
2:B:153:LEU:N	2:B:153:LEU:HD23	2.33	0.43
3:E:271:PRO:HD2	3:E:272:GLY:H	1.82	0.43
2:I:237:VAL:CG1	2:I:241:LEU:HD12	2.48	0.43
1:A:282:ARG:HD3	1:A:285:MET:CE	2.48	0.43
1:A:282:ARG:HG2	1:A:282:ARG:HH11	1.84	0.43
2:C:204:GLN:O	2:C:208:ARG:HG3	2.18	0.43
1:F:6:PRO:HG2	1:F:30:LEU:HD13	1.99	0.43
1:F:27:ASP:HA	1:F:28:PRO:HD3	1.79	0.43
1:F:71:MET:SD	1:F:103:LEU:HB3	2.58	0.43
1:F:198:THR:CG2	1:F:201:ARG:HD2	2.45	0.43
2:G:191:LEU:HD11	2:G:232:VAL:HG21	2.00	0.43
2:H:282:LEU:HA	2:H:282:LEU:HD23	1.74	0.43
2:I:257:VAL:HG21	2:I:320:ILE:HD11	1.99	0.43
2:I:261:GLY:HA2	2:I:357:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:7:DT:H2'	4:M:8:DT:H5'	1.99	0.43
1:A:23:LEU:HD21	1:A:34:SER:HB3	2.01	0.43
1:A:254:LEU:O	1:A:254:LEU:HG	2.18	0.43
2:B:127:GLU:HG3	2:C:140:LEU:HD12	2.00	0.43
2:B:260:ASN:HD22	2:B:263:ARG:HB3	1.80	0.43
2:C:260:ASN:OD1	2:C:260:ASN:C	2.56	0.43
2:D:119:ARG:HG2	2:D:120:PHE:CD2	2.53	0.43
2:D:347:MET:HE2	2:D:347:MET:HB2	1.76	0.43
1:F:19:ALA:HB1	1:F:104:LEU:HD22	2.01	0.43
1:F:48:GLU:O	1:F:50:HIS:CD2	2.69	0.43
2:G:215:ARG:O	2:G:217:ALA:N	2.52	0.43
2:G:268:ILE:HD11	2:G:353:LEU:HD12	1.99	0.43
2:H:94:ASP:C	2:H:94:ASP:OD1	2.55	0.43
2:H:260:ASN:OD1	2:H:260:ASN:C	2.57	0.43
2:I:3:TYR:CG	2:I:4:GLN:N	2.86	0.43
2:I:291:ARG:O	2:I:294:MET:N	2.50	0.43
2:B:314:ARG:NH1	2:B:314:ARG:HG2	2.34	0.43
2:C:214:LEU:O	2:C:217:ALA:HB3	2.19	0.43
2:D:74:GLY:HA2	2:D:79:CYS:CB	2.48	0.43
2:D:145:GLU:N	2:D:146:PRO:HD3	2.33	0.43
2:H:8:ARG:HH21	2:I:145:GLU:C	2.21	0.43
2:H:337:LYS:HE2	3:J:334:LEU:HD22	2.00	0.43
1:A:198:THR:OG1	1:A:200:PRO:HD2	2.19	0.43
2:B:80:ARG:O	2:B:84:GLN:HG2	2.19	0.43
2:D:178:LEU:HD23	2:D:178:LEU:HA	1.94	0.43
3:E:88:LEU:HD23	3:E:120:LEU:HD23	2.01	0.43
1:F:250:LEU:O	1:F:250:LEU:HG	2.19	0.43
2:H:295:VAL:HG22	2:H:302:LEU:HB2	2.01	0.43
3:J:296:ILE:O	3:J:297:ARG:C	2.55	0.43
1:A:43:ALA:HA	1:A:47:PHE:O	2.19	0.43
1:A:52:THR:CG2	1:A:81:LEU:HD23	2.48	0.43
2:B:129:HIS:CD2	2:B:130:MET:SD	3.12	0.43
2:B:319:THR:O	2:B:320:ILE:CG1	2.67	0.43
2:D:78:ASN:O	2:D:82:ILE:HG13	2.19	0.43
2:D:221:THR:O	2:D:225:ILE:HG13	2.19	0.43
2:D:347:MET:HE1	3:E:246:HIS:HE1	1.84	0.43
3:E:225:PRO:O	3:J:326:GLY:HA2	2.19	0.43
1:F:21:TYR:CD1	1:F:135:VAL:HB	2.54	0.43
1:F:310:LEU:CD2	3:J:306:ILE:HD12	2.49	0.43
2:G:101:VAL:O	2:G:102:GLU:C	2.57	0.43
2:G:191:LEU:HD23	2:G:191:LEU:HA	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:339:LEU:N	2:G:340:PRO:CD	2.82	0.43
2:H:8:ARG:NH2	2:I:146:PRO:O	2.51	0.43
2:H:21:GLN:HE22	2:H:49:VAL:CG1	2.27	0.43
2:H:243:THR:HG22	2:H:244:LEU:O	2.18	0.43
2:H:320:ILE:HA	2:H:321:PRO:HD3	1.79	0.43
2:I:144:GLU:HG2	2:I:145:GLU:HG3	2.00	0.43
1:A:65:PHE:CD2	1:A:65:PHE:O	2.72	0.43
1:A:228:ARG:O	1:A:232:ILE:HG13	2.19	0.43
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.85	0.43
2:B:265:MET:CE	2:C:294:MET:SD	3.06	0.43
2:C:316:LEU:HD23	2:C:320:ILE:HD11	2.00	0.43
1:F:124:ALA:O	1:F:125:ALA:C	2.57	0.43
1:F:234:GLN:OE1	2:G:304:ASN:HB2	2.18	0.43
2:H:115:PRO:HD2	2:H:149:HIS:CD2	2.53	0.43
2:H:259:ALA:HB2	2:H:360:HIS:ND1	2.31	0.43
2:H:295:VAL:CG2	2:H:302:LEU:HB2	2.49	0.43
2:I:145:GLU:N	2:I:146:PRO:HD3	2.34	0.43
2:I:243:THR:HG22	2:I:244:LEU:N	2.34	0.43
1:A:84:LEU:HD13	1:A:113:ARG:O	2.19	0.42
1:A:236:LEU:HA	1:A:236:LEU:HD23	1.79	0.42
1:A:285:MET:O	1:A:288:GLU:HB3	2.19	0.42
2:B:253:VAL:HG11	2:B:316:LEU:HD21	2.00	0.42
2:C:107:LEU:HD23	2:C:107:LEU:HA	1.96	0.42
2:D:47:ARG:HA	7:D:405:BEF:F3	2.09	0.42
3:E:99:LYS:HD3	3:E:105:ARG:NH2	2.33	0.42
2:G:274:ARG:NH2	2:G:276:ILE:CG1	2.82	0.42
2:H:60:LYS:HZ1	2:H:83:GLU:HG3	1.84	0.42
2:I:143:LEU:HA	2:I:143:LEU:HD12	1.67	0.42
4:K:7:DT:H2'	4:K:8:DT:H5'	2.00	0.42
1:A:279:TRP:O	1:A:283:ARG:HG2	2.19	0.42
2:B:320:ILE:HG21	2:B:325:ILE:HG13	2.00	0.42
2:C:115:PRO:HD2	2:C:149:HIS:CD2	2.53	0.42
2:H:124:LEU:HA	2:H:153:LEU:O	2.18	0.42
2:H:144:GLU:CG	2:H:145:GLU:HG3	2.47	0.42
2:I:51:LYS:HB2	2:I:51:LYS:HE2	1.64	0.42
2:I:126:ASP:OD1	2:I:155:ALA:HB3	2.19	0.42
1:A:47:PHE:CE2	1:A:77:ARG:HB3	2.55	0.42
2:B:128:VAL:HG12	2:B:156:THR:HB	2.01	0.42
2:C:73:CYS:O	2:C:75:VAL:HG13	2.19	0.42
3:E:258:ARG:NH1	3:E:275:ALA:HA	2.34	0.42
2:G:290:HIS:O	2:G:294:MET:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:3:TRP:CH2	3:J:8:ARG:HG3	2.37	0.42
1:A:24:LEU:HD11	1:A:117:LEU:HD11	2.01	0.42
2:B:53:SER:O	2:B:57:LEU:HG	2.19	0.42
2:D:361:PRO:HG2	3:J:275:ALA:HB3	1.95	0.42
1:F:146:GLN:H	1:F:146:GLN:HG3	1.59	0.42
2:H:223:GLN:HB3	2:I:171:LEU:HD22	2.01	0.42
3:J:151:LEU:HD12	3:J:151:LEU:HA	1.88	0.42
2:B:332:LEU:HD23	2:B:332:LEU:HA	1.81	0.42
2:C:229:ASP:CB	2:D:30:ASN:HD21	2.32	0.42
2:C:341:TYR:HB3	2:D:333:LEU:CD1	2.49	0.42
2:D:6:LEU:C	2:D:8:ARG:N	2.71	0.42
3:E:285:ARG:O	3:E:289:ILE:HG13	2.20	0.42
1:F:147:LEU:HB3	1:F:148:PRO:HD3	2.02	0.42
2:H:252:LEU:HD11	2:H:264:VAL:HG13	2.01	0.42
2:H:341:TYR:CZ	2:I:337:LYS:HD2	2.54	0.42
2:I:74:GLY:HA2	2:I:79:CYS:HB2	2.00	0.42
2:C:187:LEU:HA	2:C:187:LEU:HD23	1.70	0.42
2:D:6:LEU:C	2:D:8:ARG:H	2.22	0.42
1:F:54:SER:HA	1:F:83:LEU:HB2	2.02	0.42
2:H:215:ARG:NH2	2:I:144:GLU:OE1	2.46	0.42
2:H:261:GLY:O	2:H:262:GLU:C	2.58	0.42
2:I:347:MET:CE	3:J:246:HIS:HE1	2.32	0.42
3:J:99:LYS:CD	3:J:105:ARG:HH22	2.28	0.42
1:A:4:LEU:CD2	1:A:8:GLN:HB3	2.48	0.42
2:C:6:LEU:HD23	2:C:6:LEU:HA	1.78	0.42
2:C:229:ASP:HB2	2:D:30:ASN:HD21	1.84	0.42
2:C:321:PRO:O	2:C:324:ASP:HB2	2.19	0.42
2:D:167:LEU:O	2:D:168:SER:C	2.58	0.42
2:D:256:MET:HE1	2:D:332:LEU:HD11	2.00	0.42
2:D:347:MET:O	2:D:351:MET:CG	2.66	0.42
3:E:318:ARG:HH11	3:E:318:ARG:HD3	1.71	0.42
2:G:187:LEU:HD23	2:G:187:LEU:HA	1.80	0.42
2:H:54:ILE:O	2:H:55:ALA:C	2.58	0.42
1:A:13:LEU:CD2	1:A:21:TYR:CE1	3.03	0.42
1:A:21:TYR:CD1	1:A:135:VAL:HB	2.55	0.42
2:B:20:GLY:O	2:B:21:GLN:HB2	2.20	0.42
2:B:290:HIS:O	2:B:294:MET:HG3	2.19	0.42
2:C:220:LEU:HD23	2:C:220:LEU:HA	1.75	0.42
2:I:341:TYR:CD1	2:I:341:TYR:N	2.88	0.42
4:K:14:DA:C2'	4:K:15:DG:O5'	2.68	0.42
1:A:110:LEU:HD11	1:A:112:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:LYS:HA	2:C:82:ILE:CD1	2.50	0.42
2:D:150:VAL:O	2:D:151:LYS:HD3	2.20	0.42
2:D:259:ALA:HB2	2:D:360:HIS:HB2	2.02	0.42
2:D:291:ARG:O	2:D:292:ILE:C	2.59	0.42
3:E:81:PRO:HB3	3:E:87:THR:O	2.19	0.42
3:E:290:LEU:HA	3:E:290:LEU:HD12	1.80	0.42
1:F:190:LEU:HD11	2:G:38:HIS:CE1	2.53	0.42
1:F:199:LEU:HB3	1:F:200:PRO:HD3	2.02	0.42
2:I:306:MET:O	2:I:307:ALA:C	2.57	0.42
1:A:128:THR:HA	1:A:131:ALA:HB2	2.02	0.42
2:C:316:LEU:CD2	2:C:320:ILE:HD11	2.50	0.42
2:D:141:LYS:HA	2:D:141:LYS:HD2	1.87	0.42
1:F:81:LEU:HD12	1:F:82:LEU:N	2.34	0.42
1:F:257:LEU:HD23	1:F:257:LEU:HA	1.72	0.42
2:H:353:LEU:O	2:H:356:ALA:HB3	2.20	0.42
2:I:75:VAL:O	2:I:75:VAL:HG12	2.20	0.42
3:J:186:ALA:O	3:J:187:LEU:C	2.57	0.42
1:A:278:VAL:O	1:A:279:TRP:C	2.58	0.41
2:B:38:HIS:ND1	2:B:38:HIS:N	2.68	0.41
2:B:353:LEU:HD23	2:B:353:LEU:HA	1.83	0.41
2:D:244:LEU:HD21	2:D:276:ILE:HG12	2.02	0.41
3:E:73:HIS:CE1	3:E:75:ASP:HB2	2.55	0.41
3:E:327:VAL:CG1	3:E:328:VAL:N	2.83	0.41
1:F:162:LEU:HD23	1:F:162:LEU:HA	1.80	0.41
2:H:360:HIS:CD2	2:H:361:PRO:HD2	2.55	0.41
2:I:41:TYR:HD2	2:I:173:PHE:HE2	1.68	0.41
2:I:347:MET:HE1	3:J:246:HIS:CE1	2.55	0.41
1:A:6:PRO:HG2	1:A:30:LEU:HD13	2.01	0.41
2:B:360:HIS:CE1	2:B:362:ARG:HB2	2.55	0.41
1:F:39:ARG:NH1	1:F:50:HIS:CB	2.83	0.41
2:G:153:LEU:HD23	2:G:153:LEU:N	2.35	0.41
2:G:320:ILE:HA	2:G:321:PRO:HD3	1.80	0.41
3:J:271:PRO:CD	3:J:272:GLY:H	2.32	0.41
2:B:268:ILE:HD11	2:B:353:LEU:HD12	2.02	0.41
2:B:302:LEU:HD23	2:B:302:LEU:HA	1.81	0.41
2:C:304:ASN:OD1	2:C:304:ASN:O	2.38	0.41
2:G:13:GLN:CD	2:G:83:GLU:HG3	2.40	0.41
2:H:137:ASN:ND2	2:H:137:ASN:N	2.68	0.41
2:H:158:ASP:HA	2:H:159:PRO:HD3	1.64	0.41
2:I:201:ARG:CZ	2:I:205:LEU:HD21	2.50	0.41
1:A:56:ASP:CB	1:A:58:ASN:H	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:O	1:A:297:GLN:C	2.57	0.41
2:B:84:GLN:HA	2:B:84:GLN:NE2	2.35	0.41
2:B:330:GLN:O	2:B:334:ILE:HG13	2.20	0.41
2:B:344:ASP:HB3	2:B:347:MET:CB	2.50	0.41
1:F:84:LEU:HD11	1:F:112:VAL:CG1	2.50	0.41
1:F:184:ALA:O	1:F:188:LEU:HD12	2.20	0.41
2:H:51:LYS:HE3	2:H:157:ALA:HA	2.02	0.41
2:H:147:PRO:HB2	2:H:149:HIS:ND1	2.35	0.41
2:H:236:ALA:O	2:H:239:ALA:HB3	2.20	0.41
3:J:216:LEU:HA	3:J:216:LEU:HD12	1.70	0.41
2:B:229:ASP:HB2	2:C:30:ASN:ND2	2.36	0.41
2:C:51:LYS:CG	6:C:402:ADP:O2B	2.65	0.41
2:C:60:LYS:HA	2:C:82:ILE:HD12	2.03	0.41
2:C:346:ARG:O	2:C:349:VAL:N	2.53	0.41
2:C:367:GLU:CD	2:D:362:ARG:HH12	2.23	0.41
3:E:121:THR:HG22	3:E:123:ALA:H	1.86	0.41
2:G:6:LEU:HD23	2:G:6:LEU:HA	1.71	0.41
2:G:101:VAL:CG2	2:G:134:HIS:CB	2.96	0.41
2:I:74:GLY:HA2	2:I:79:CYS:HB3	2.02	0.41
2:I:94:ASP:OD2	2:I:97:SER:HB2	2.21	0.41
1:A:163:ASP:OD2	1:A:198:THR:HA	2.20	0.41
1:A:227:LYS:HG3	2:B:300:ALA:CB	2.50	0.41
2:B:187:LEU:HD23	2:B:187:LEU:HA	1.81	0.41
2:C:133:ARG:O	2:C:137:ASN:ND2	2.53	0.41
2:C:291:ARG:O	2:C:294:MET:HB3	2.20	0.41
1:F:26:ASN:OD1	1:F:27:ASP:N	2.52	0.41
1:F:56:ASP:C	1:F:58:ASN:H	2.24	0.41
1:F:150:TRP:CZ3	1:F:178:LEU:HD22	2.56	0.41
2:I:64:CYS:O	2:I:119:ARG:NH2	2.54	0.41
3:J:155:LEU:HD12	3:J:155:LEU:O	2.19	0.41
2:B:58:LEU:HD12	2:B:58:LEU:HA	1.74	0.41
2:B:320:ILE:HA	2:B:321:PRO:HD3	1.85	0.41
2:C:21:GLN:CD	2:C:175:LEU:HB3	2.41	0.41
2:D:51:LYS:HB2	2:D:51:LYS:HE2	1.70	0.41
2:D:178:LEU:HD13	2:D:214:LEU:HD12	2.03	0.41
3:E:29:ILE:O	3:E:144:ALA:HA	2.20	0.41
2:H:152:PHE:O	2:H:153:LEU:HD23	2.21	0.41
2:H:292:ILE:CG2	2:H:325:ILE:CD1	2.98	0.41
2:H:336:ARG:O	2:H:337:LYS:C	2.59	0.41
3:J:176:LEU:HD23	3:J:176:LEU:HA	1.82	0.41
1:A:128:THR:O	1:A:131:ALA:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:ARG:HG3	2:C:53:SER:HB3	2.02	0.41
2:C:338:GLU:C	2:C:340:PRO:HD2	2.41	0.41
2:D:125:ILE:HD13	2:D:125:ILE:HG21	1.80	0.41
2:D:178:LEU:CD1	2:D:214:LEU:HD12	2.50	0.41
2:D:309:ILE:HG22	2:D:309:ILE:O	2.19	0.41
3:E:148:PRO:O	3:E:151:LEU:HB2	2.21	0.41
1:F:101:THR:O	1:F:104:LEU:HD11	2.21	0.41
2:G:273:ALA:O	2:G:275:GLY:N	2.54	0.41
2:I:57:LEU:HD23	2:I:57:LEU:HA	1.90	0.41
1:A:53:PHE:CE1	1:A:67:LEU:HD21	2.54	0.41
1:A:292:ARG:NH1	1:A:331:LEU:O	2.53	0.41
2:B:82:ILE:HG12	2:B:87:PHE:CB	2.51	0.41
2:B:84:GLN:HE21	2:B:84:GLN:CA	2.31	0.41
2:B:191:LEU:HD23	2:B:191:LEU:HA	1.64	0.41
2:C:276:ILE:HD11	2:C:281:LEU:HB2	2.03	0.41
2:C:292:ILE:HG22	2:C:325:ILE:CD1	2.51	0.41
2:D:248:GLN:HE22	2:D:271:ALA:HA	1.86	0.41
3:E:41:ILE:O	3:E:42:TYR:C	2.59	0.41
3:E:151:LEU:HD12	3:E:151:LEU:HA	1.84	0.41
1:F:47:PHE:CD2	1:F:77:ARG:HB3	2.56	0.41
1:F:56:ASP:CB	1:F:58:ASN:H	2.33	0.41
1:F:98:LEU:CD2	1:F:126:TRP:HB3	2.42	0.41
1:F:237:ARG:CG	1:F:321:TRP:CE2	3.01	0.41
1:F:244:VAL:H	1:F:244:VAL:HG23	1.65	0.41
2:G:24:VAL:HG21	2:G:175:LEU:CD2	2.51	0.41
2:G:95:ALA:O	2:G:99:THR:CG2	2.63	0.41
2:G:178:LEU:HD12	2:G:214:LEU:HB2	2.03	0.41
2:G:245:ASP:O	2:G:274:ARG:HD2	2.21	0.41
2:H:321:PRO:O	2:H:324:ASP:HB2	2.21	0.41
3:J:300:LEU:HD23	3:J:300:LEU:HA	1.59	0.41
4:K:9:DT:O5'	4:K:9:DT:C2'	2.69	0.41
4:K:10:DT:C5	4:K:11:DT:H73	2.56	0.41
2:C:15:PHE:CE1	2:C:57:LEU:HB3	2.55	0.41
2:D:100:LYS:O	2:D:104:THR:HG23	2.20	0.41
2:D:250:LEU:HD13	2:D:313:MET:HE3	2.02	0.41
2:H:216:ASP:OD1	2:I:168:SER:HA	2.20	0.41
5:N:6:DC:H2"	5:N:7:DT:C5'	2.51	0.41
1:A:142:PRO:HD3	1:A:178:LEU:HD11	2.03	0.40
2:B:276:ILE:HG23	2:B:277:GLU:N	2.37	0.40
2:B:347:MET:CE	2:C:291:ARG:HH21	2.34	0.40
2:C:162:LEU:HA	2:C:163:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:GLU:HG2	2:D:145:GLU:HG3	2.02	0.40
2:D:254:GLU:OE2	2:D:312:ARG:HD2	2.21	0.40
3:E:308:ARG:HG2	3:E:312:ILE:HD12	2.02	0.40
2:I:306:MET:O	2:I:308:ALA:N	2.53	0.40
1:A:174:TYR:O	1:A:175:GLU:C	2.60	0.40
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.76	0.40
3:E:4:TYR:CB	3:E:6:TRP:CZ2	3.04	0.40
3:E:316:LEU:HA	3:E:316:LEU:HD23	1.68	0.40
2:G:353:LEU:HD23	2:G:353:LEU:HA	1.88	0.40
2:H:162:LEU:HA	2:H:163:PRO:HD3	1.93	0.40
2:H:276:ILE:HD11	2:H:281:LEU:HB2	2.02	0.40
2:I:124:LEU:HA	2:I:153:LEU:O	2.20	0.40
2:I:252:LEU:HD13	2:I:285:MET:HE1	2.02	0.40
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.87	0.40
2:C:261:GLY:O	2:C:262:GLU:C	2.59	0.40
3:E:256:LEU:HD23	3:E:256:LEU:HA	1.79	0.40
3:E:258:ARG:C	3:E:260:HIS:H	2.24	0.40
1:F:278:VAL:O	1:F:279:TRP:C	2.60	0.40
1:F:285:MET:O	1:F:288:GLU:HB3	2.21	0.40
2:G:24:VAL:HG22	2:G:173:PHE:HB3	2.03	0.40
2:G:328:TYR:OH	2:G:360:HIS:NE2	2.54	0.40
2:H:34:LEU:HD23	2:H:34:LEU:HA	1.64	0.40
2:H:112:GLN:HG3	2:H:113:TYR:N	2.37	0.40
2:H:220:LEU:HD23	2:H:220:LEU:HA	1.82	0.40
2:B:24:VAL:HG22	2:B:173:PHE:HB3	2.02	0.40
3:E:258:ARG:C	3:E:260:HIS:N	2.74	0.40
1:F:272:LEU:HA	1:F:272:LEU:HD23	1.66	0.40
3:J:223:SER:CB	3:J:228:ASP:O	2.69	0.40
1:A:142:PRO:HG2	1:A:147:LEU:HD12	2.03	0.40
2:C:145:GLU:N	2:C:146:PRO:HD3	2.37	0.40
2:C:250:LEU:HD13	2:C:288:LEU:HD13	2.03	0.40
2:D:282:LEU:HA	2:D:282:LEU:HD23	1.90	0.40
2:G:144:GLU:CG	2:G:169:ARG:HE	2.35	0.40
2:G:289:LEU:HD23	2:G:289:LEU:HA	1.79	0.40
2:H:154:LEU:N	2:H:154:LEU:CD1	2.84	0.40
2:H:154:LEU:N	2:H:154:LEU:HD12	2.34	0.40
2:I:76:CYS:O	2:I:77:ASP:C	2.60	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ARG:NH2	2:I:117:ARG:NE[2_555]	1.94	0.26
3:E:178:ARG:NH2	2:H:195:HIS:O[4_545]	2.06	0.14

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	331/343 (96%)	292 (88%)	33 (10%)	6 (2%)	8	35
1	F	331/343 (96%)	291 (88%)	34 (10%)	6 (2%)	8	35
2	B	362/395 (92%)	330 (91%)	28 (8%)	4 (1%)	14	46
2	C	363/395 (92%)	337 (93%)	22 (6%)	4 (1%)	14	46
2	D	360/395 (91%)	328 (91%)	28 (8%)	4 (1%)	14	46
2	G	376/395 (95%)	343 (91%)	30 (8%)	3 (1%)	19	52
2	H	363/395 (92%)	331 (91%)	29 (8%)	3 (1%)	19	52
2	I	360/395 (91%)	326 (91%)	28 (8%)	6 (2%)	9	36
3	E	332/334 (99%)	305 (92%)	24 (7%)	3 (1%)	17	50
3	J	332/334 (99%)	303 (91%)	26 (8%)	3 (1%)	17	50
All	All	3510/3724 (94%)	3186 (91%)	282 (8%)	42 (1%)	13	43

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	159	ASN
1	A	319	SER
2	D	307	ALA
3	E	74	PRO
1	F	15	GLU
1	F	159	ASN
1	F	319	SER

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Mol	Chain	Res	Type
2	G	307	ALA
2	I	307	ALA
3	J	74	PRO
1	A	125	ALA
1	A	320	VAL
2	B	247	ASP
2	B	248	GLN
2	B	307	ALA
2	C	168	SER
2	C	276	ILE
2	C	297	LEU
2	D	7	ALA
1	F	125	ALA
1	F	320	VAL
2	G	247	ASP
2	G	248	GLN
2	H	297	LEU
2	I	7	ALA
1	F	279	TRP
2	I	296	GLN
2	D	291	ARG
2	H	168	SER
2	I	16	ALA
2	I	292	ILE
3	J	16	ALA
1	A	279	TRP
2	C	246	ASP
2	I	291	ARG
2	B	189	HIS
2	H	276	ILE
2	D	292	ILE
3	J	168	PRO
3	E	168	PRO
3	E	136	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	283/291 (97%)	261 (92%)	22 (8%)	12	38
1	F	283/291 (97%)	261 (92%)	22 (8%)	12	38
2	B	300/328 (92%)	283 (94%)	17 (6%)	20	51
2	C	301/328 (92%)	276 (92%)	25 (8%)	11	36
2	D	298/328 (91%)	277 (93%)	21 (7%)	15	43
2	G	312/328 (95%)	295 (95%)	17 (5%)	22	53
2	H	301/328 (92%)	278 (92%)	23 (8%)	13	39
2	I	298/328 (91%)	279 (94%)	19 (6%)	17	47
3	E	270/270 (100%)	256 (95%)	14 (5%)	23	53
3	J	270/270 (100%)	259 (96%)	11 (4%)	30	60
All	All	2916/3090 (94%)	2725 (93%)	191 (7%)	16	45

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	64	ILE
1	A	108	LEU
1	A	117	LEU
1	A	118	SER
1	A	128	THR
1	A	146	GLN
1	A	158	LEU
1	A	169	VAL
1	A	191	LEU
1	A	194	ASP
1	A	198	THR
1	A	202	VAL
1	A	203	GLU
1	A	206	VAL
1	A	228	ARG
1	A	241	SER
1	A	249	THR
1	A	282	ARG
1	A	295	GLN
1	A	308	THR
1	A	319	SER
2	B	21	GLN
2	B	38	HIS

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Mol	Chain	Res	Type
2	B	46	THR
2	B	47	ARG
2	B	93	ILE
2	B	97	SER
2	B	117	ARG
2	B	216	ASP
2	B	227	SER
2	B	238	SER
2	B	247	ASP
2	B	251	SER
2	B	262	GLU
2	B	276	ILE
2	B	291	ARG
2	B	325	ILE
2	B	331	THR
2	C	8	ARG
2	C	47	ARG
2	C	53	SER
2	C	91	ILE
2	C	93	ILE
2	C	124	LEU
2	C	168	SER
2	C	170	CYS
2	C	172	GLN
2	C	175	LEU
2	C	179	ASP
2	C	214	LEU
2	C	222	ASP
2	C	227	SER
2	C	238	SER
2	C	240	MET
2	C	244	LEU
2	C	245	ASP
2	C	248	GLN
2	C	260	ASN
2	C	265	MET
2	C	276	ILE
2	C	291	ARG
2	C	297	LEU
2	C	311	LEU
2	D	28	LEU
2	D	46	THR

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Mol	Chain	Res	Type
2	D	47	ARG
2	D	52	THR
2	D	97	SER
2	D	101	VAL
2	D	117	ARG
2	D	150	VAL
2	D	165	THR
2	D	175	LEU
2	D	180	VAL
2	D	213	SER
2	D	215	ARG
2	D	216	ASP
2	D	222	ASP
2	D	276	ILE
2	D	305	ASP
2	D	320	ILE
2	D	333	LEU
2	D	351	MET
2	D	357	LEU
3	E	17	SER
3	E	50	CYS
3	E	134	GLU
3	E	143	LEU
3	E	145	THR
3	E	151	LEU
3	E	155	LEU
3	E	156	ARG
3	E	160	ARG
3	E	180	VAL
3	E	208	ASP
3	E	231	SER
3	E	270	VAL
3	E	282	SER
1	F	7	GLU
1	F	48	GLU
1	F	64	ILE
1	F	108	LEU
1	F	117	LEU
1	F	118	SER
1	F	128	THR
1	F	146	GLN
1	F	158	LEU

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Mol	Chain	Res	Type
1	F	169	VAL
1	F	191	LEU
1	F	194	ASP
1	F	198	THR
1	F	202	VAL
1	F	203	GLU
1	F	206	VAL
1	F	228	ARG
1	F	241	SER
1	F	282	ARG
1	F	295	GLN
1	F	308	THR
1	F	319	SER
2	G	21	GLN
2	G	37	ILE
2	G	38	HIS
2	G	46	THR
2	G	47	ARG
2	G	93	ILE
2	G	97	SER
2	G	117	ARG
2	G	216	ASP
2	G	227	SER
2	G	238	SER
2	G	247	ASP
2	G	251	SER
2	G	262	GLU
2	G	276	ILE
2	G	291	ARG
2	G	331	THR
2	H	8	ARG
2	H	47	ARG
2	H	53	SER
2	H	91	ILE
2	H	124	LEU
2	H	168	SER
2	H	170	CYS
2	H	175	LEU
2	H	179	ASP
2	H	222	ASP
2	H	227	SER
2	H	238	SER

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Mol	Chain	Res	Type
2	H	240	MET
2	H	244	LEU
2	H	245	ASP
2	H	248	GLN
2	H	260	ASN
2	H	276	ILE
2	H	291	ARG
2	H	297	LEU
2	H	309	ILE
2	H	311	LEU
2	H	334	ILE
2	I	28	LEU
2	I	46	THR
2	I	47	ARG
2	I	51	LYS
2	I	52	THR
2	I	97	SER
2	I	101	VAL
2	I	117	ARG
2	I	165	THR
2	I	175	LEU
2	I	180	VAL
2	I	213	SER
2	I	216	ASP
2	I	222	ASP
2	I	276	ILE
2	I	305	ASP
2	I	320	ILE
2	I	351	MET
2	I	357	LEU
3	J	17	SER
3	J	145	THR
3	J	155	LEU
3	J	156	ARG
3	J	160	ARG
3	J	180	VAL
3	J	188	LEU
3	J	208	ASP
3	J	231	SER
3	J	282	SER
3	J	283	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	45	GLN
1	A	50	HIS
1	A	144	GLN
1	A	216	HIS
1	A	303	GLN
2	B	21	GLN
2	B	39	HIS
2	B	84	GLN
2	B	248	GLN
2	B	260	ASN
2	C	23	HIS
2	C	149	HIS
2	C	290	HIS
2	C	304	ASN
2	D	30	ASN
2	D	38	HIS
2	D	149	HIS
2	D	172	GLN
2	D	204	GLN
2	D	269	ASN
3	E	30	GLN
3	E	51	GLN
3	E	52	GLN
3	E	54	GLN
3	E	56	HIS
3	E	103	HIS
3	E	246	HIS
3	E	267	ASN
3	E	287	GLN
3	E	307	ASN
1	F	35	GLN
1	F	45	GLN
1	F	50	HIS
1	F	216	HIS
2	G	4	GLN
2	G	21	GLN
2	G	39	HIS
2	G	84	GLN
2	G	248	GLN
2	G	260	ASN
2	G	269	ASN

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Mol	Chain	Res	Type
2	G	304	ASN
2	H	23	HIS
2	H	290	HIS
2	H	304	ASN
2	I	30	ASN
2	I	38	HIS
2	I	172	GLN
2	I	204	GLN
2	I	269	ASN
3	J	30	GLN
3	J	51	GLN
3	J	52	GLN
3	J	54	GLN
3	J	56	HIS
3	J	103	HIS
3	J	246	HIS
3	J	267	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 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	$\#\|Z\|>2$
6	ADP	H	408	8,7	24,29,29	1.15	2 (8%)	29,45,45	1.37	5 (17%)
6	ADP	B	400	8,7	24,29,29	1.19	2 (8%)	29,45,45	1.48	6 (20%)
6	ADP	C	402	8,7	24,29,29	1.15	2 (8%)	29,45,45	1.52	5 (17%)
6	ADP	G	406	8,7	24,29,29	1.20	3 (12%)	29,45,45	1.47	5 (17%)
6	ADP	D	404	8,7	24,29,29	1.18	2 (8%)	29,45,45	1.53	5 (17%)
6	ADP	I	410	8,7	24,29,29	1.41	3 (12%)	29,45,45	1.62	6 (20%)
7	BEF	I	409	6	0,3,3	-	-	-		
7	BEF	I	411	6	0,3,3	-	-	-		
7	BEF	B	401	6	0,3,3	-	-	-		
7	BEF	C	403	6	0,3,3	-	-	-		
7	BEF	G	407	6	0,3,3	-	-	-		
7	BEF	D	405	6	0,3,3	-	-	-		

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
6	ADP	H	408	8,7	-	0/12/32/32	0/3/3/3
6	ADP	B	400	8,7	-	3/12/32/32	0/3/3/3
6	ADP	C	402	8,7	-	1/12/32/32	0/3/3/3
6	ADP	G	406	8,7	-	3/12/32/32	0/3/3/3
6	ADP	D	404	8,7	-	5/12/32/32	0/3/3/3
6	ADP	I	410	8,7	-	2/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	410	ADP	C2'-C1'	-3.69	1.48	1.53
6	C	402	ADP	C2'-C1'	-3.01	1.49	1.53
6	D	404	ADP	C2'-C1'	-2.93	1.49	1.53
6	B	400	ADP	C5-C4	2.73	1.48	1.40
6	G	406	ADP	C5-C4	2.58	1.47	1.40
6	G	406	ADP	PB-O3B	2.57	1.64	1.54
6	H	408	ADP	PB-O3B	2.56	1.64	1.54
6	C	402	ADP	C5-C4	2.44	1.47	1.40
6	I	410	ADP	C4-N3	-2.37	1.32	1.35
6	G	406	ADP	C2'-C1'	-2.33	1.50	1.53
6	D	404	ADP	C5-C4	2.24	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	410	ADP	C5-C4	2.24	1.46	1.40
6	B	400	ADP	O4'-C1'	2.15	1.44	1.41
6	H	408	ADP	PB-O2B	-2.04	1.47	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	402	ADP	N3-C2-N1	-3.88	122.61	128.68
6	I	410	ADP	PA-O3A-PB	-3.54	120.69	132.83
6	I	410	ADP	O2B-PB-O1B	3.52	124.45	110.68
6	C	402	ADP	O2B-PB-O1B	3.35	123.80	110.68
6	H	408	ADP	C4-C5-N7	-3.35	105.91	109.40
6	G	406	ADP	C4-C5-N7	-3.11	106.16	109.40
6	D	404	ADP	PA-O3A-PB	-3.05	122.38	132.83
6	D	404	ADP	O2B-PB-O1B	2.93	122.15	110.68
6	H	408	ADP	O2B-PB-O1B	2.91	122.06	110.68
6	B	400	ADP	C3'-C2'-C1'	2.75	105.12	100.98
6	I	410	ADP	O2'-C2'-C1'	-2.70	100.88	110.85
6	H	408	ADP	N3-C2-N1	-2.65	124.53	128.68
6	G	406	ADP	O2B-PB-O1B	2.62	120.96	110.68
6	B	400	ADP	C4-C5-N7	-2.61	106.67	109.40
6	B	400	ADP	O2B-PB-O1B	2.59	120.84	110.68
6	G	406	ADP	C3'-C2'-C1'	2.47	104.70	100.98
6	D	404	ADP	C4-C5-N7	-2.47	106.83	109.40
6	B	400	ADP	N3-C2-N1	-2.42	124.89	128.68
6	I	410	ADP	O3B-PB-O2B	-2.39	98.49	107.64
6	G	406	ADP	PA-O3A-PB	-2.34	124.81	132.83
6	D	404	ADP	O3B-PB-O2B	-2.33	98.73	107.64
6	I	410	ADP	C4-C5-N7	-2.32	106.98	109.40
6	C	402	ADP	PA-O3A-PB	-2.30	124.92	132.83
6	H	408	ADP	PA-O3A-PB	-2.28	125.02	132.83
6	B	400	ADP	PA-O3A-PB	-2.27	125.02	132.83
6	C	402	ADP	C4-C5-N7	-2.25	107.05	109.40
6	D	404	ADP	O2'-C2'-C1'	-2.18	102.80	110.85
6	I	410	ADP	O2A-PA-O1A	2.16	122.90	112.24
6	G	406	ADP	N3-C2-N1	-2.15	125.31	128.68
6	C	402	ADP	O2A-PA-O1A	2.09	122.59	112.24
6	H	408	ADP	C2'-C3'-C4'	2.08	106.68	102.64
6	B	400	ADP	C2-N1-C6	2.04	122.23	118.75

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	400	ADP	C5'-O5'-PA-O2A
6	D	404	ADP	PA-O3A-PB-O3B
6	D	404	ADP	C5'-O5'-PA-O2A
6	G	406	ADP	C5'-O5'-PA-O2A
6	I	410	ADP	PA-O3A-PB-O3B
6	B	400	ADP	C5'-O5'-PA-O3A
6	D	404	ADP	C5'-O5'-PA-O3A
6	G	406	ADP	C5'-O5'-PA-O3A
6	B	400	ADP	C5'-O5'-PA-O1A
6	G	406	ADP	C5'-O5'-PA-O1A
6	D	404	ADP	PA-O3A-PB-O2B
6	I	410	ADP	PA-O3A-PB-O2B
6	C	402	ADP	C5'-O5'-PA-O3A
6	D	404	ADP	C5'-O5'-PA-O1A

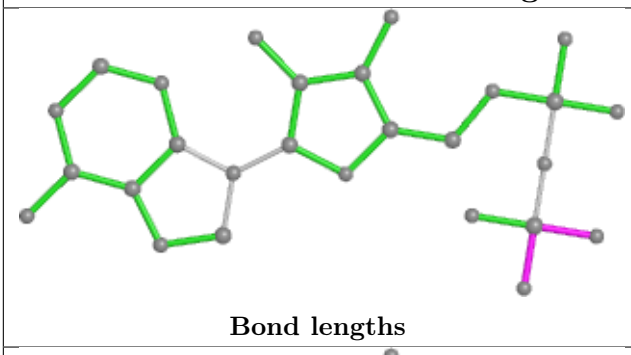
There are no ring outliers.

9 monomers are involved in 22 short contacts:

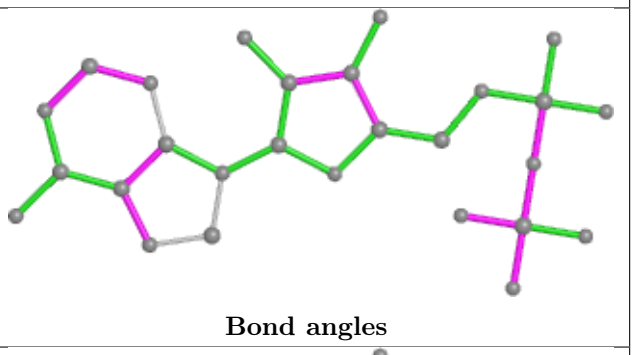
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	408	ADP	2	0
6	B	400	ADP	4	0
6	C	402	ADP	3	0
6	G	406	ADP	4	0
6	D	404	ADP	3	0
6	I	410	ADP	3	0
7	B	401	BEF	1	0
7	G	407	BEF	1	0
7	D	405	BEF	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

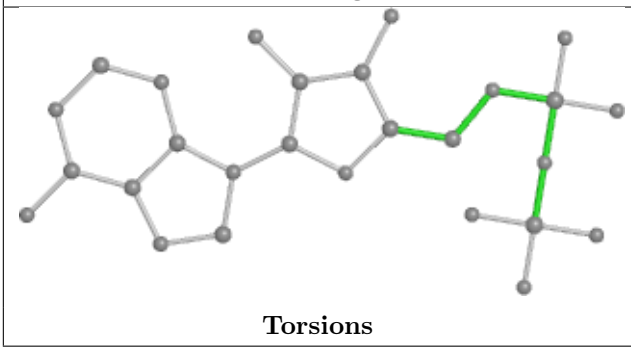
Ligand ADP H 408



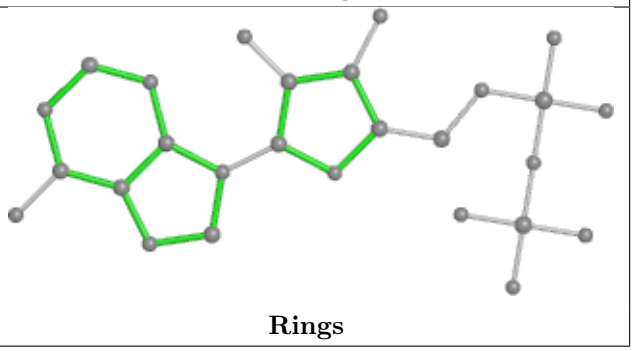
Bond lengths



Bond angles

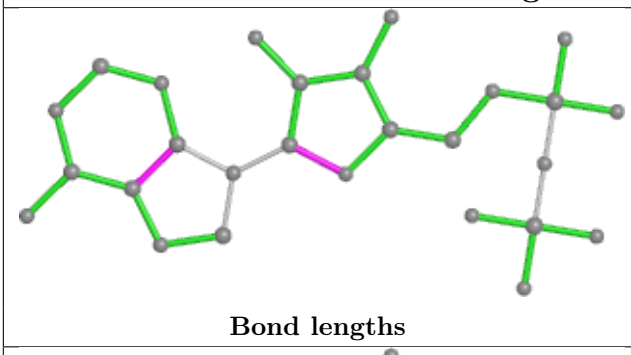


Torsions

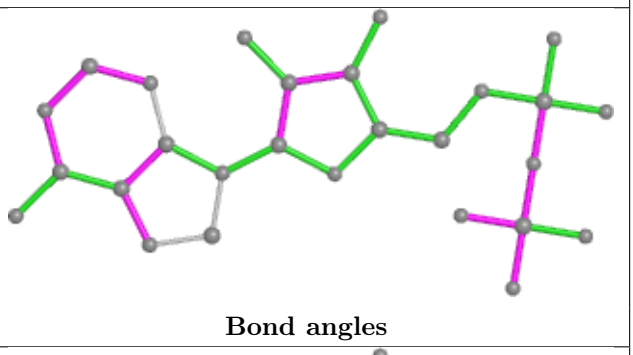


Rings

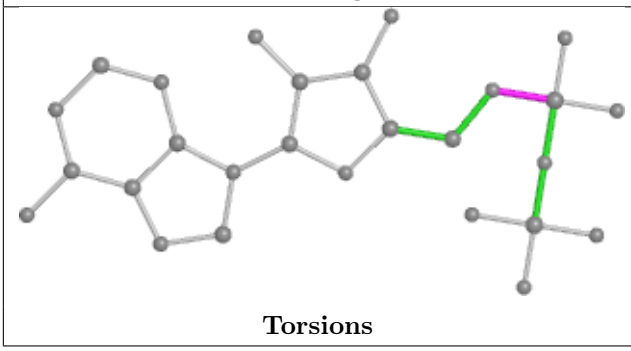
Ligand ADP B 400



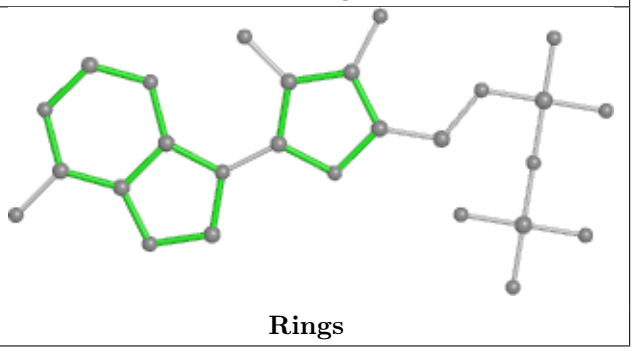
Bond lengths



Bond angles

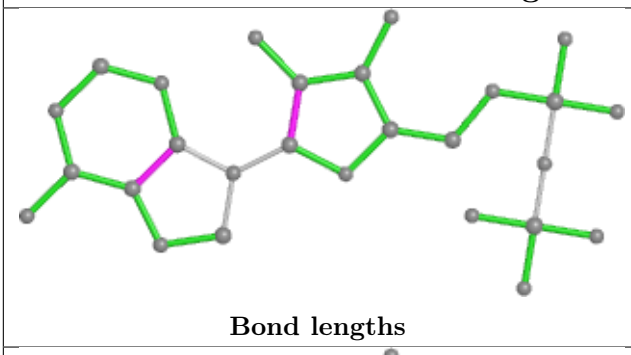


Torsions

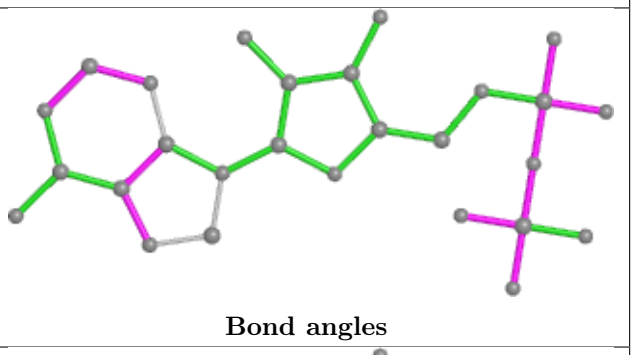


Rings

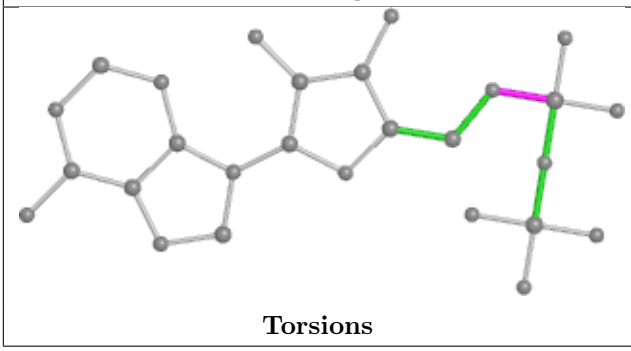
Ligand ADP C 402



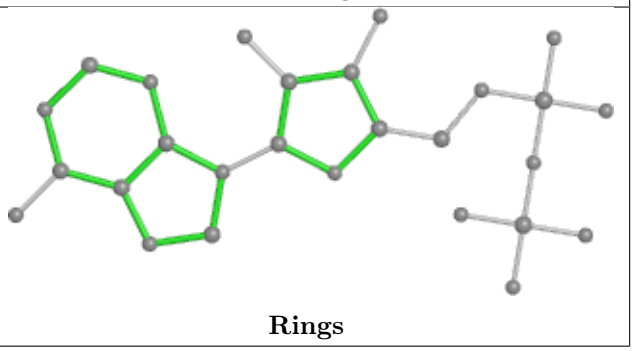
Bond lengths



Bond angles

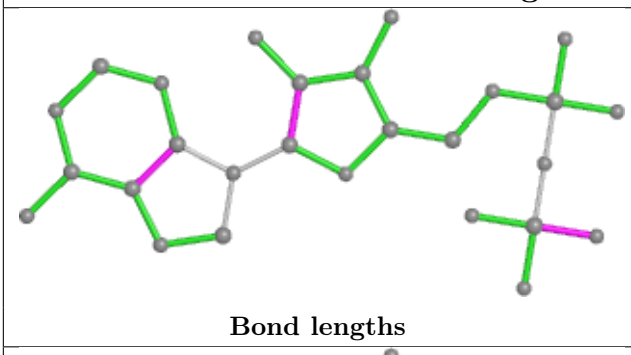


Torsions

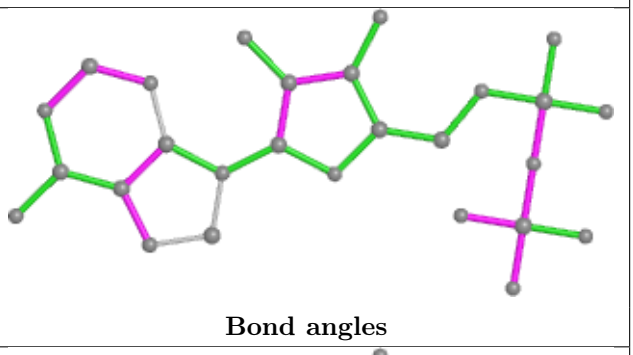


Rings

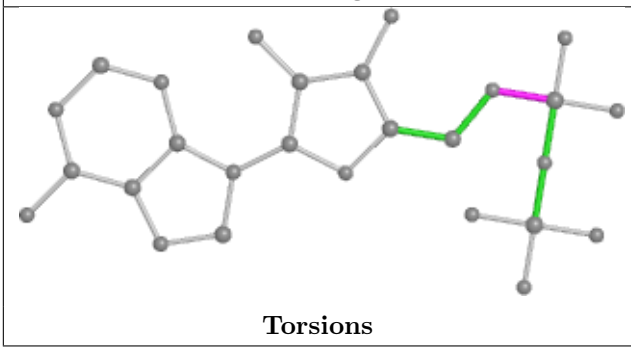
Ligand ADP G 406



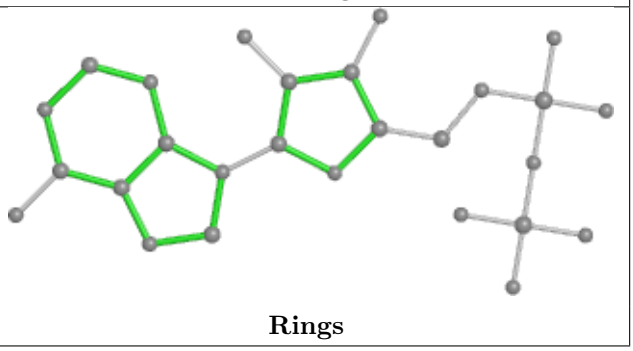
Bond lengths



Bond angles

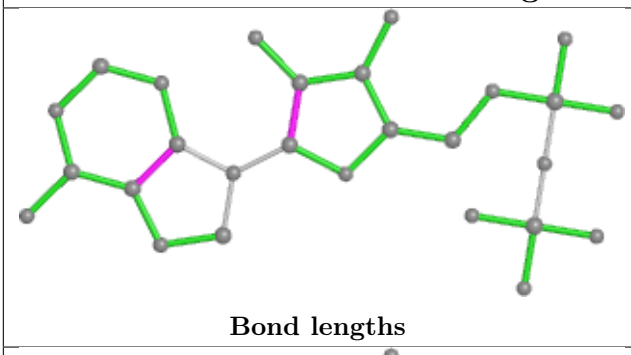


Torsions

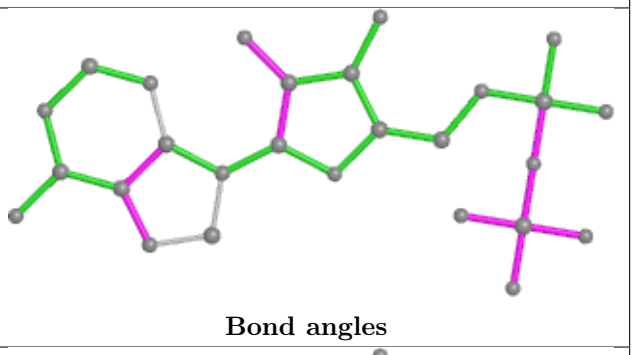


Rings

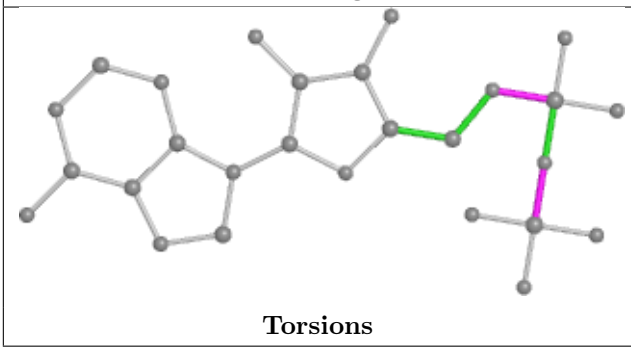
Ligand ADP D 404



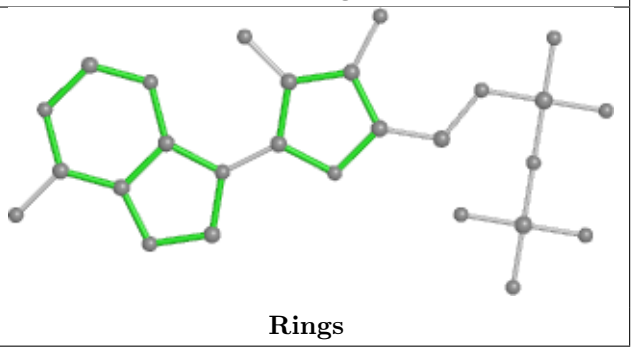
Bond lengths



Bond angles

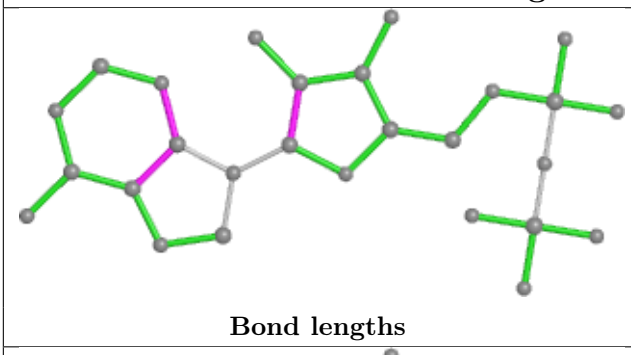


Torsions

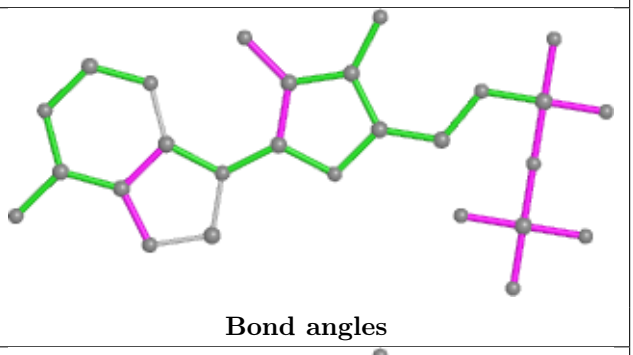


Rings

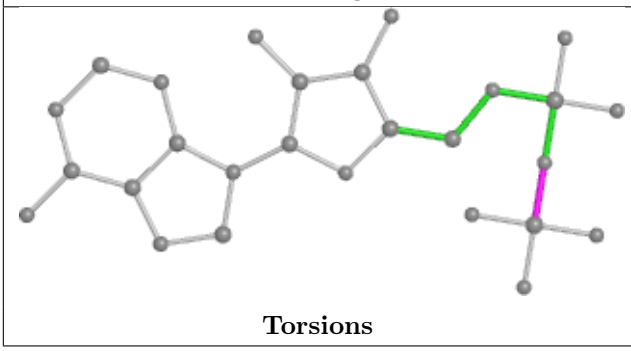
Ligand ADP I 410



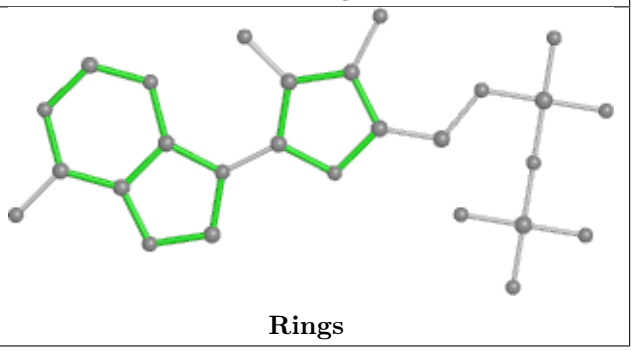
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	333/343 (97%)	0.69	52 (15%) 2 2	81, 139, 220, 252	0
1	F	333/343 (97%)	0.26	24 (7%) 15 15	76, 140, 204, 232	0
2	B	364/395 (92%)	0.17	17 (4%) 31 28	85, 134, 185, 215	0
2	C	365/395 (92%)	0.12	12 (3%) 46 43	76, 127, 196, 216	0
2	D	362/395 (91%)	0.12	10 (2%) 53 50	77, 117, 173, 206	0
2	G	378/395 (95%)	-0.03	10 (2%) 56 52	87, 118, 166, 207	0
2	H	365/395 (92%)	-0.17	0 100 100	68, 99, 141, 168	0
2	I	362/395 (91%)	-0.08	1 (0%) 94 94	63, 92, 135, 203	0
3	E	334/334 (100%)	-0.11	3 (0%) 84 84	74, 94, 145, 184	0
3	J	334/334 (100%)	-0.18	1 (0%) 94 94	71, 93, 140, 186	0
4	K	14/20 (70%)	-0.22	0 100 100	84, 95, 192, 198	0
4	M	14/20 (70%)	-0.24	0 100 100	82, 96, 193, 210	0
5	L	10/10 (100%)	-0.71	0 100 100	92, 95, 102, 105	0
5	N	10/10 (100%)	-0.71	0 100 100	83, 92, 107, 109	0
All	All	3578/3784 (94%)	0.07	130 (3%) 42 39	63, 112, 191, 252	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	PHE	12.6
1	A	55	ILE	11.0
1	A	61	TRP	8.5
1	A	128	THR	6.8
1	A	54	SER	6.6
1	A	57	PRO	6.6
1	A	75	ALA	6.6
1	A	76	SER	6.6

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Mol	Chain	Res	Type	RSRZ
2	D	302	LEU	6.6
1	A	89	PRO	5.8
1	F	57	PRO	5.7
1	A	80	LEU	5.7
2	B	365	LEU	5.6
1	F	61	TRP	5.6
1	A	104	LEU	5.5
1	A	56	ASP	5.5
1	F	62	ASN	5.5
1	F	53	PHE	5.5
1	A	73	LEU	5.3
1	A	62	ASN	5.3
1	A	60	ASP	5.2
1	A	68	CYS	5.2
2	B	366	PRO	5.0
2	G	362	ARG	4.4
2	B	367	GLU	4.3
1	F	19	ALA	4.3
1	A	110	LEU	4.1
1	A	72	SER	4.0
1	A	84	LEU	3.9
1	F	56	ASP	3.9
1	A	71	MET	3.9
1	A	82	LEU	3.9
1	A	67	LEU	3.8
1	F	60	ASP	3.8
2	B	368	PRO	3.8
1	A	101	THR	3.7
2	D	299	PRO	3.6
2	C	252	LEU	3.6
2	B	364	PRO	3.5
2	G	364	PRO	3.4
2	B	361	PRO	3.4
1	F	58	ASN	3.4
2	B	249	ALA	3.4
1	F	13	LEU	3.4
1	F	48	GLU	3.4
2	G	366	PRO	3.4
2	B	358	ALA	3.3
1	A	22	LEU	3.3
1	F	9	LEU	3.1
1	A	2	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	265	MET	3.1
1	A	58	ASN	3.0
2	B	256	MET	3.0
2	D	306	MET	3.0
2	C	273	ALA	3.0
1	A	81	LEU	2.9
1	A	112	VAL	2.9
1	A	59	THR	2.9
1	A	105	HIS	2.9
1	A	106	ASP	2.9
1	A	46	GLY	2.9
2	G	296	GLN	2.9
2	C	365	LEU	2.8
2	G	363	MET	2.8
2	C	308	ALA	2.8
1	A	85	PRO	2.8
1	A	64	ILE	2.8
2	C	302	LEU	2.8
2	D	292	ILE	2.8
2	B	362	ARG	2.7
1	A	109	LEU	2.7
1	F	2	ILE	2.7
2	D	300	ALA	2.7
2	G	365	LEU	2.7
2	B	32	LEU	2.7
2	C	248	GLN	2.7
1	A	74	PHE	2.6
2	G	360	HIS	2.6
2	B	357	LEU	2.6
1	F	76	SER	2.6
1	A	98	LEU	2.6
2	G	361	PRO	2.6
1	F	75	ALA	2.6
1	A	78	GLN	2.5
1	F	93	ILE	2.5
2	D	304	ASN	2.5
3	E	105	ARG	2.5
1	F	80	LEU	2.5
2	I	301	ALA	2.5
1	A	123	ASN	2.5
2	B	313	MET	2.5
1	A	65	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	262	GLU	2.5
2	C	309	ILE	2.4
1	F	266	HIS	2.4
1	F	54	SER	2.4
1	A	83	LEU	2.4
1	A	103	LEU	2.4
1	F	6	PRO	2.4
2	C	256	MET	2.4
1	A	122	GLU	2.4
2	C	362	ARG	2.3
1	F	78	GLN	2.3
1	A	111	ILE	2.3
1	F	21	TYR	2.3
2	D	295	VAL	2.3
2	D	308	ALA	2.3
1	A	107	ASP	2.3
1	F	49	GLU	2.2
1	A	100	LEU	2.2
1	A	79	THR	2.2
1	A	48	GLU	2.2
1	A	77	ARG	2.2
2	C	311	LEU	2.2
2	B	203	LEU	2.1
2	G	319	THR	2.1
2	B	363	MET	2.1
1	A	23	LEU	2.1
3	J	56	HIS	2.1
2	C	357	LEU	2.1
2	D	301	ALA	2.1
1	A	97	LEU	2.1
2	G	297	LEU	2.1
2	B	231	GLN	2.1
2	D	311	LEU	2.0
3	E	259	HIS	2.0
3	E	142	PHE	2.0
1	F	20	ALA	2.0
1	F	269	LEU	2.0
1	A	52	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

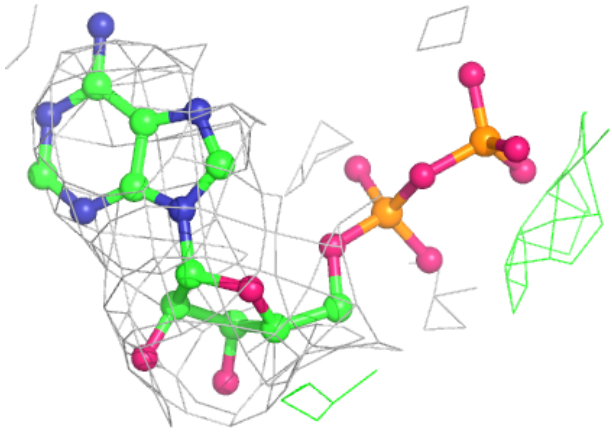
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

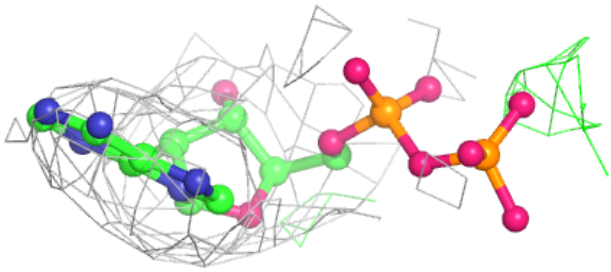
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	G	415	1/1	0.89	0.35	89,89,89,89	0
8	MG	D	414	1/1	0.92	0.41	85,85,85,85	0
6	ADP	B	400	27/27	0.93	0.26	100,109,115,117	0
7	BEF	I	411	4/4	0.94	0.33	76,76,77,78	0
8	MG	C	413	1/1	0.94	0.35	88,88,88,88	0
6	ADP	G	406	27/27	0.94	0.23	91,98,104,105	0
7	BEF	D	405	4/4	0.94	0.26	105,105,106,107	0
8	MG	I	417	1/1	0.94	0.36	67,67,67,67	0
9	ZN	E	421	1/1	0.95	0.12	146,146,146,146	0
9	ZN	J	425	1/1	0.95	0.13	143,143,143,143	0
7	BEF	C	403	4/4	0.96	0.24	95,96,96,97	0
8	MG	H	416	1/1	0.96	0.29	63,63,63,63	0
8	MG	B	412	1/1	0.96	0.46	89,89,89,89	0
6	ADP	C	402	27/27	0.96	0.18	90,99,104,106	0
7	BEF	G	407	4/4	0.96	0.28	96,96,97,97	0
7	BEF	I	409	4/4	0.97	0.22	72,72,72,72	0
7	BEF	B	401	4/4	0.97	0.36	94,95,95,95	0
6	ADP	D	404	27/27	0.97	0.19	92,103,109,111	0
9	ZN	D	420	1/1	0.97	0.10	157,157,157,157	0
6	ADP	H	408	27/27	0.97	0.19	74,76,81,82	0
9	ZN	I	424	1/1	0.97	0.13	117,117,117,117	0
6	ADP	I	410	27/27	0.97	0.23	67,74,78,79	0
9	ZN	B	418	1/1	0.98	0.09	163,163,163,163	0
9	ZN	G	422	1/1	0.98	0.12	198,198,198,198	0
9	ZN	C	419	1/1	0.99	0.06	149,149,149,149	0
9	ZN	H	423	1/1	0.99	0.11	121,121,121,121	0

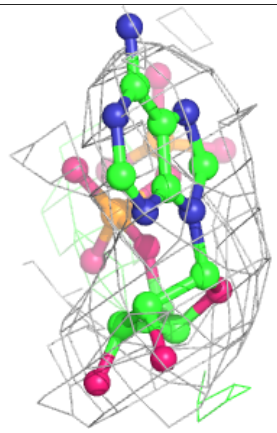
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 400:

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

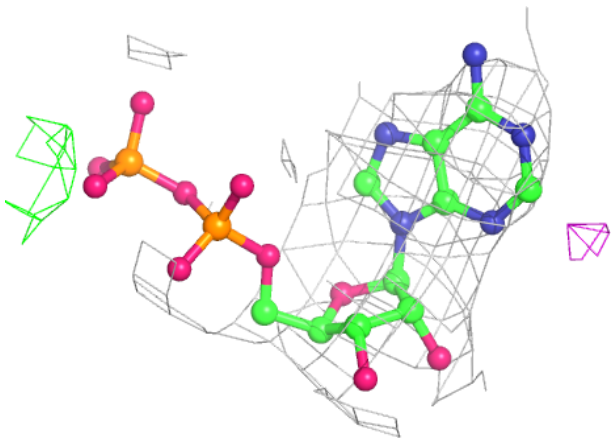


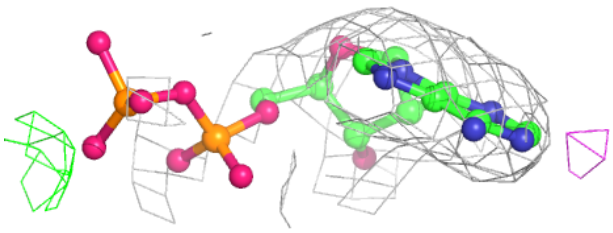


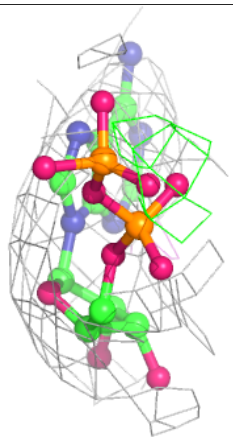


Electron density around ADP G 406:

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

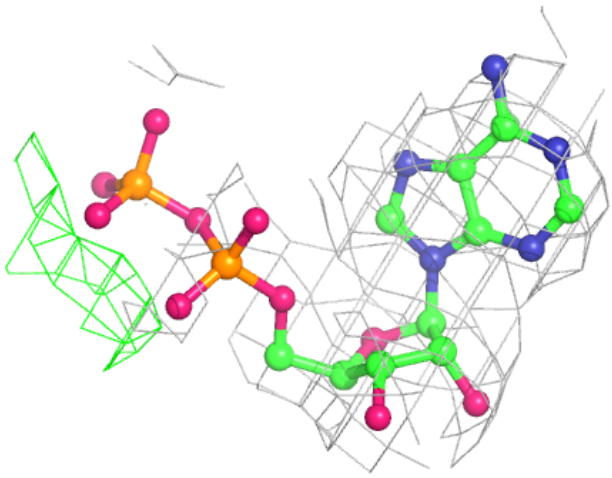


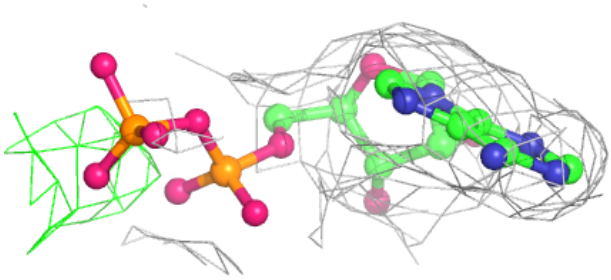


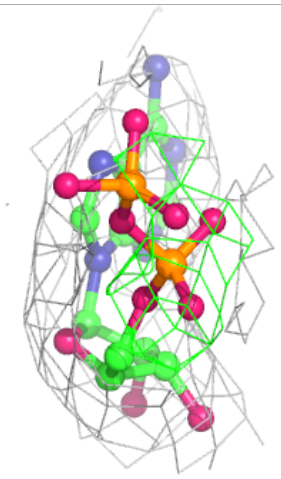


Electron density around ADP C 402:

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

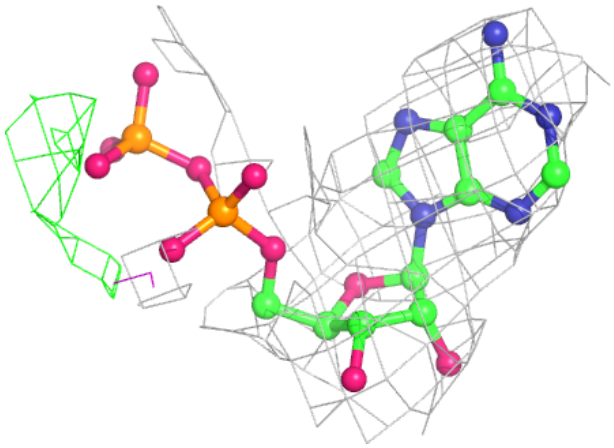


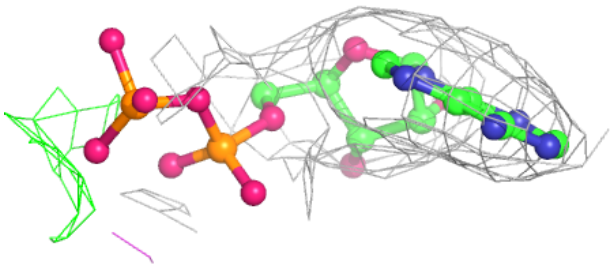


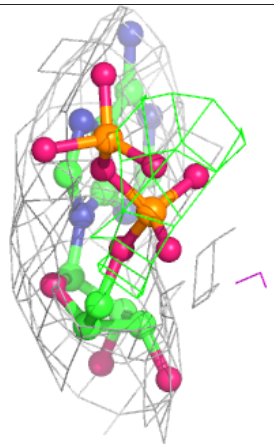


Electron density around ADP D 404:

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

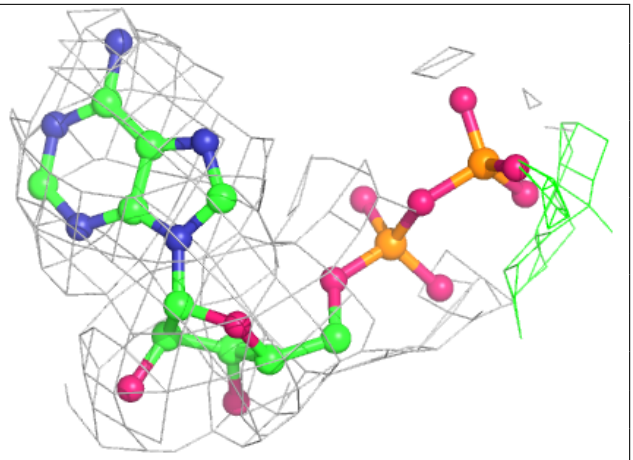


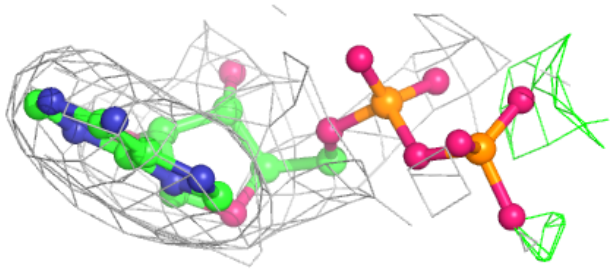


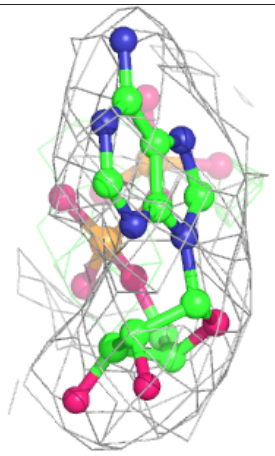


Electron density around ADP H 408:

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

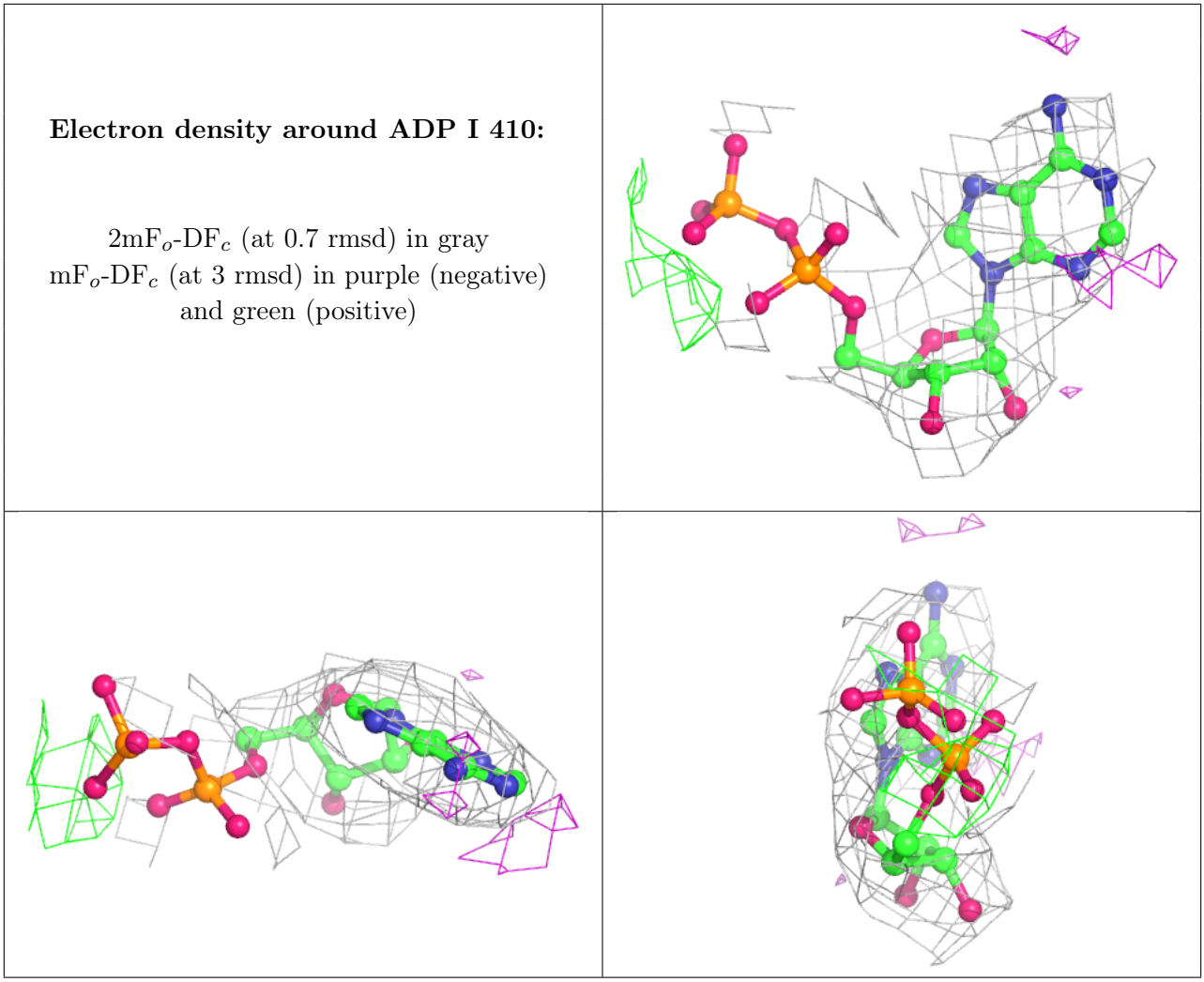






Electron density around ADP I 410:

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



6.5 Other polymers

There are no such residues in this entry.