



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 PM UTC

PDB ID : 3GLF / pdb_00003glf
Title : Crystal Structure of the Ecoli Clamp Loader Bound to Primer-Template DNA
Authors : Simonetta, K.R.; Kuriyan, J.
Deposited on : 2009-03-12
Resolution : 3.39 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

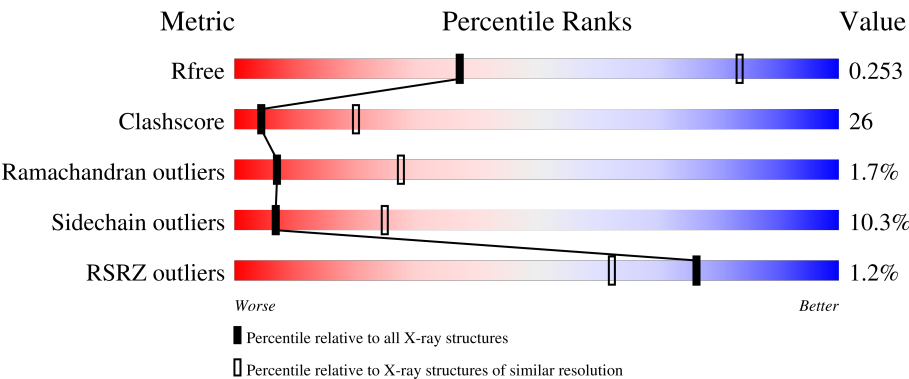
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.39 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}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	5% 44% 46% 7%
1	F	343	% 48% 42% 7%
2	B	395	% 50% 35% 7% 8%
2	C	395	% 48% 34% 10% 8%
2	D	395	% 45% 40% 7% 8%

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Mol	Chain	Length	Quality of chain
2	G	395	% 56% 34% 6%
2	H	395	% 47% 35% 9%
2	I	395	% 44% 40% 6%
3	E	334	59% 35% 5%
3	J	334	62% 30% 7%
4	K	15	13% 53% 27%
4	M	15	13% 47% 33%
5	L	10	10% 80% 10%
5	N	10	30% 50% 20%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28758 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
			2829	1779	511	523	16			
2	C	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
2	D	362	Total	C	N	O	S	0	0	0
			2818	1770	510	522	16			
2	G	378	Total	C	N	O	S	0	0	0
			2941	1852	529	543	17			
2	H	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
2	I	362	Total	C	N	O	S	0	0	0
			2818	1770	510	522	16			

There are 132 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
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
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
D	-17	HIS	-	expression tag	UNP P06710
D	-16	HIS	-	expression tag	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
I	-2	GLY	-	expression tag	UNP P06710
I	-1	PRO	-	expression tag	UNP P06710
I	0	HIS	-	expression tag	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			

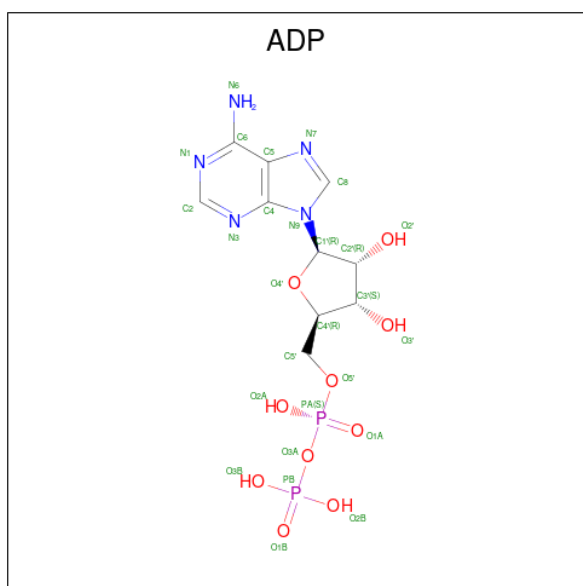
- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3').

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').

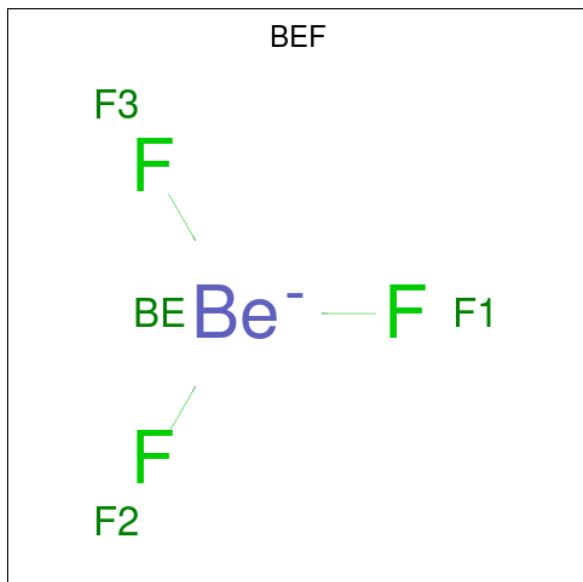
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			
5	N	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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 (CCD ID: BEF) (formula: BeF₃).



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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

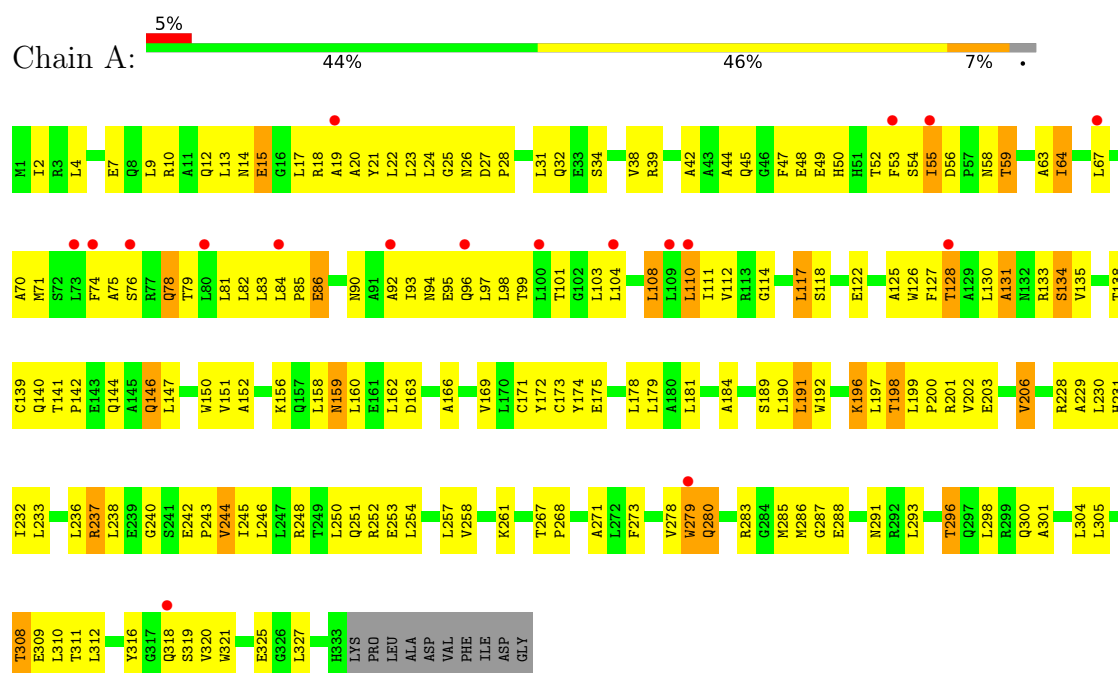
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

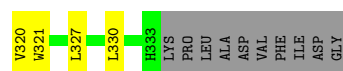
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA polymerase III subunit delta

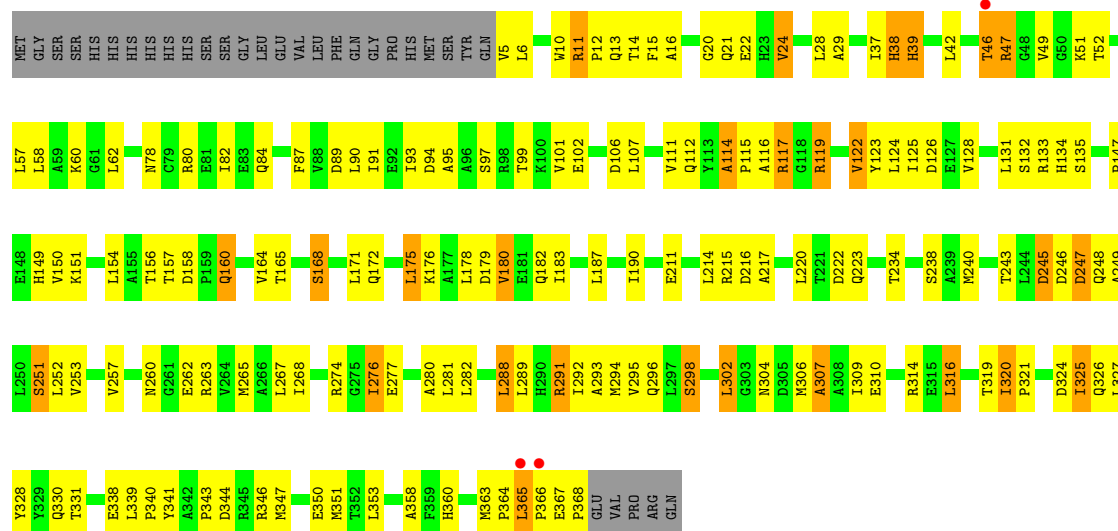


• Molecule 1: DNA polymerase III subunit delta

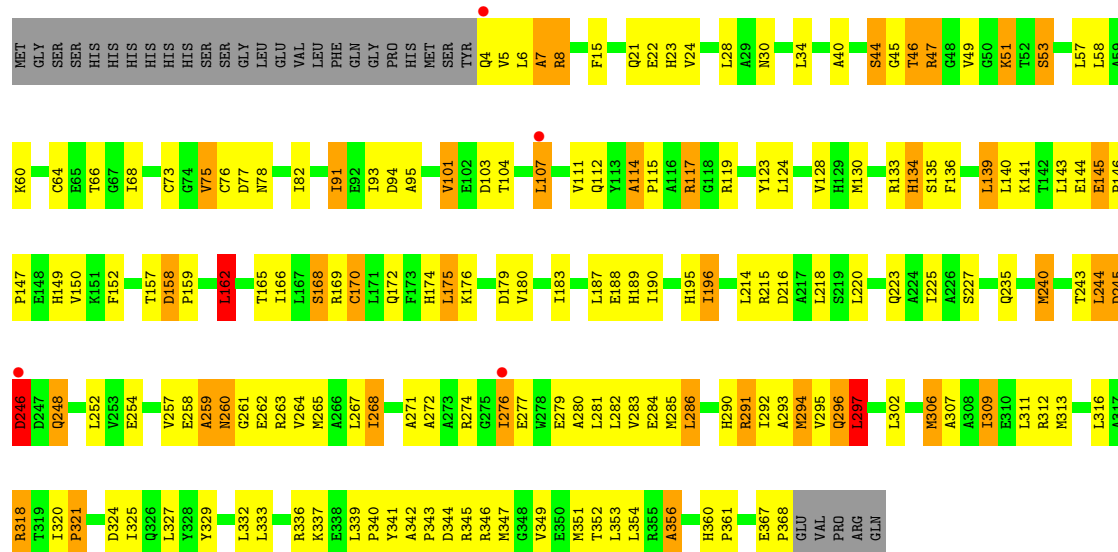




• Molecule 2: DNA polymerase III subunit tau

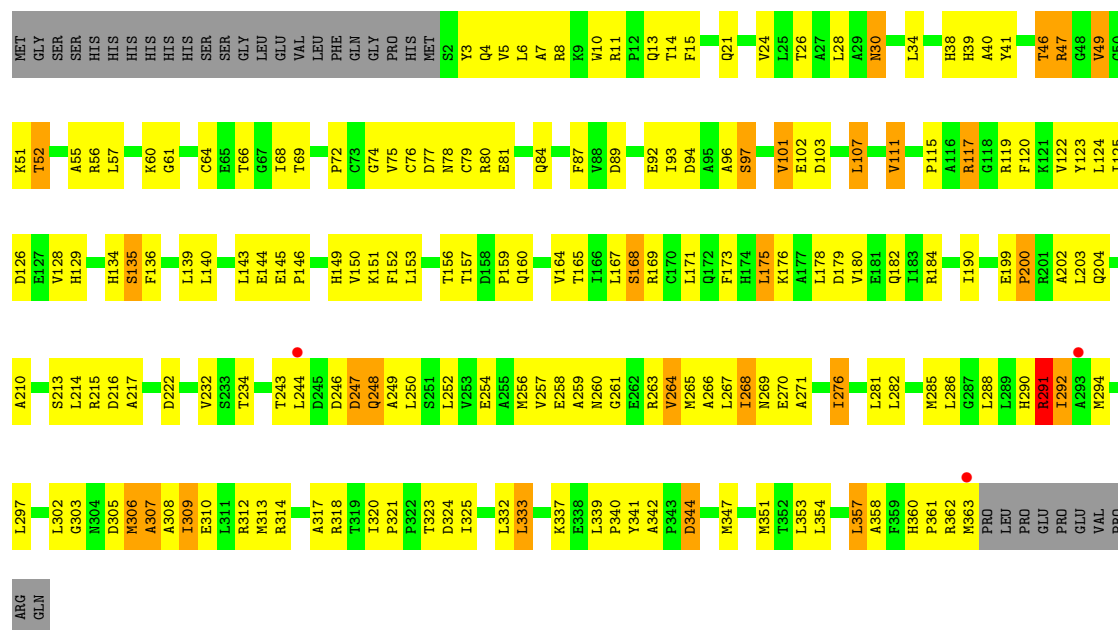


• Molecule 2: DNA polymerase III subunit tau

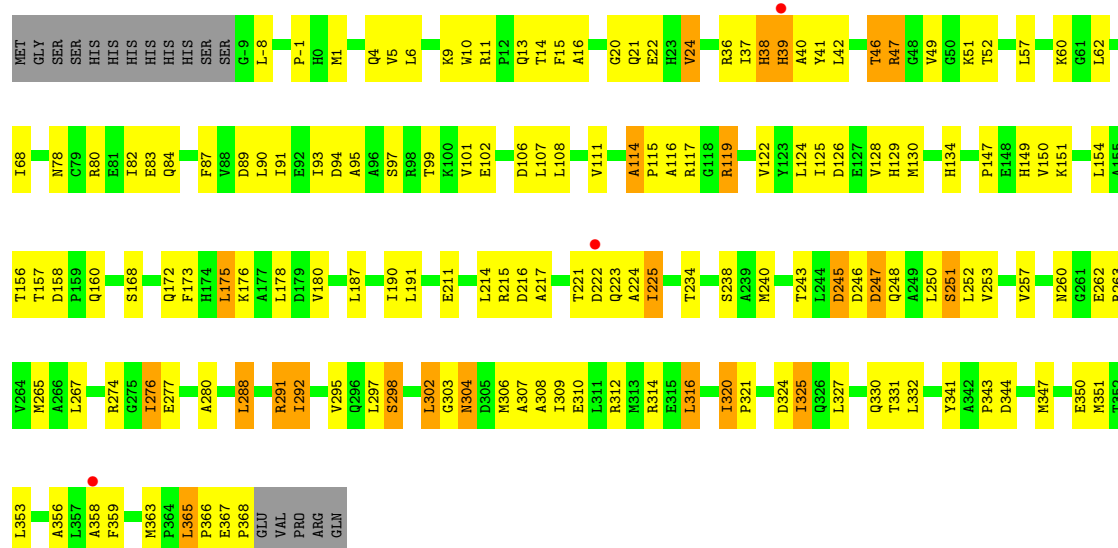


• Molecule 2: DNA polymerase III subunit tau

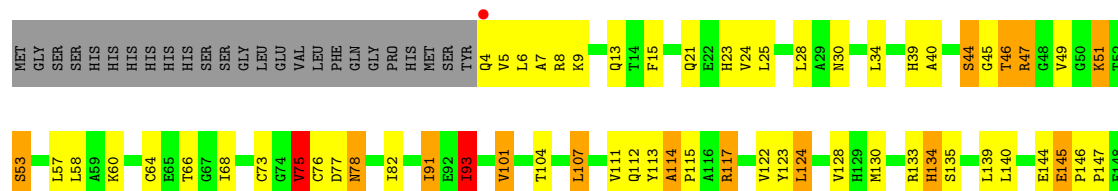


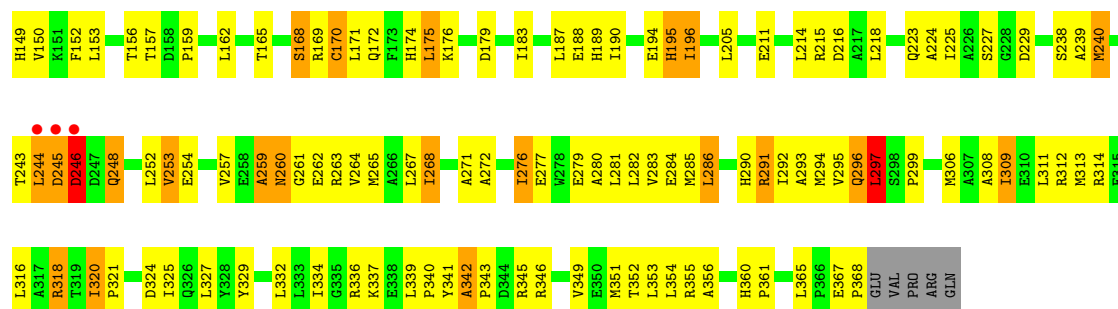


- Molecule 2: DNA polymerase III subunit tau

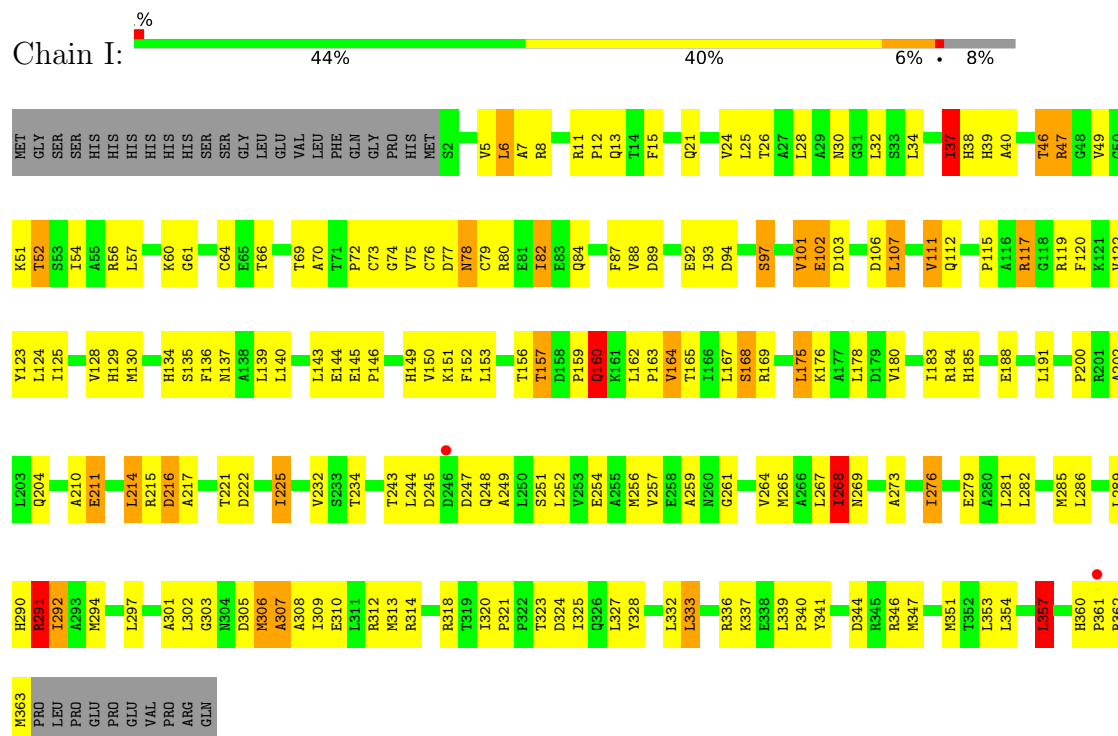


- Molecule 2: DNA polymerase III subunit tau

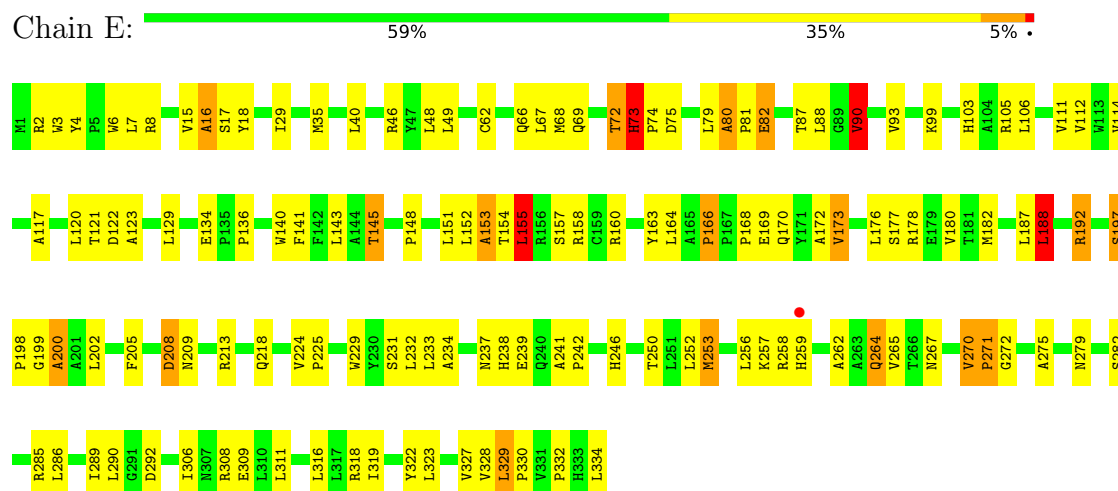




- Molecule 2: DNA polymerase III subunit tau

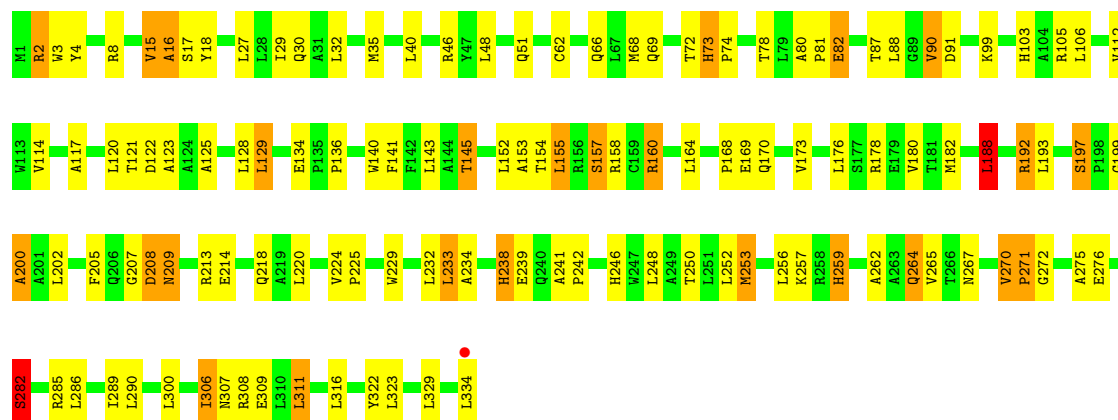


- Molecule 3: DNA polymerase III subunit delta'



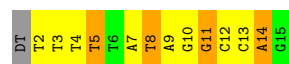
- Molecule 3: DNA polymerase III subunit delta'

Chain J: 

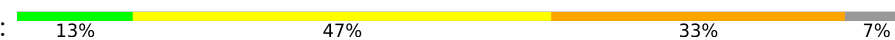


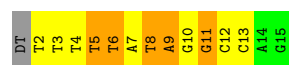
- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')

Chain K: 

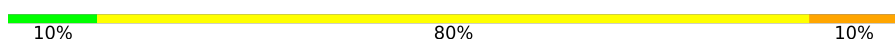


- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')

Chain M: 



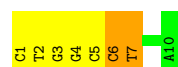
- Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.26Å 219.95Å 273.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.39 49.97 – 3.39	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.97-3.39) 97.5 (49.97-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.221 , 0.260 0.213 , 0.253	Depositor DCC
R_{free} test set	4166 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	92.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28758	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, 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	0.92	0/2697	1.12	14/3664 (0.4%)
1	F	0.90	1/2697 (0.0%)	1.11	9/3664 (0.2%)
2	B	0.90	1/2876 (0.0%)	1.19	18/3900 (0.5%)
2	C	0.87	0/2885	1.21	19/3912 (0.5%)
2	D	0.96	3/2863 (0.1%)	1.23	16/3879 (0.4%)
2	G	0.91	0/2992	1.21	22/4057 (0.5%)
2	H	1.06	1/2885 (0.0%)	1.29	22/3912 (0.6%)
2	I	1.15	6/2863 (0.2%)	1.31	15/3879 (0.4%)
3	E	1.14	2/2666 (0.1%)	1.30	21/3639 (0.6%)
3	J	1.12	5/2666 (0.2%)	1.25	13/3639 (0.4%)
4	K	0.98	0/320	1.69	4/492 (0.8%)
4	M	0.99	0/320	1.62	6/492 (1.2%)
5	L	0.80	0/223	1.73	2/342 (0.6%)
5	N	0.83	0/223	1.71	4/342 (1.2%)
All	All	0.99	19/29176 (0.1%)	1.25	185/39813 (0.5%)

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	B	0	1
2	C	0	1
2	G	0	1
2	H	0	1
2	I	0	1
All	All	0	5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	306	ILE	CA-CB	-8.75	1.45	1.54
3	J	306	ILE	CA-CB	-7.00	1.47	1.54
2	I	164	VAL	CA-CB	-6.57	1.46	1.54
2	I	101	VAL	CA-CB	-6.50	1.46	1.54
1	F	244	VAL	CA-CB	-6.00	1.47	1.54
2	I	37	ILE	CA-CB	-5.92	1.47	1.54
2	I	273	ALA	CA-CB	-5.83	1.44	1.53
3	E	173	VAL	CA-CB	-5.59	1.46	1.54
2	D	49	VAL	CA-CB	-5.48	1.48	1.54
2	I	183	ILE	CA-CB	-5.48	1.47	1.54
3	J	125	ALA	CA-CB	-5.42	1.45	1.53
3	J	282	SER	CA-C	-5.34	1.46	1.53
2	H	93	ILE	CA-CB	-5.30	1.47	1.54
3	J	259	HIS	CA-C	-5.28	1.45	1.52
3	J	200	ALA	CA-CB	-5.25	1.45	1.53
2	B	319	THR	CA-CB	5.18	1.59	1.52
2	D	111	VAL	CA-C	-5.14	1.47	1.52
2	D	96	ALA	CA-CB	-5.01	1.44	1.53
2	I	160	GLN	CG-CD	5.01	1.64	1.52

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	329	LEU	CA-C-N	14.53	134.72	119.89
3	E	329	LEU	C-N-CA	14.53	134.72	119.89
3	J	329	LEU	CA-C-N	10.68	130.79	119.89
3	J	329	LEU	C-N-CA	10.68	130.79	119.89
3	J	73	HIS	CA-C-N	10.68	133.19	119.84
3	J	73	HIS	C-N-CA	10.68	133.19	119.84
3	E	73	HIS	CA-C-N	9.76	132.04	119.84
3	E	73	HIS	C-N-CA	9.76	132.04	119.84
2	I	146	PRO	CA-C-N	9.75	129.83	119.89
2	I	146	PRO	C-N-CA	9.75	129.83	119.89
2	I	303	GLY	N-CA-C	9.57	122.94	111.93
3	J	208	ASP	N-CA-C	-9.49	101.40	113.16
2	B	304	ASN	N-CA-C	-8.78	101.71	111.28
2	H	162	LEU	CA-C-N	8.41	130.35	119.84
2	H	162	LEU	C-N-CA	8.41	130.35	119.84
2	C	133	ARG	N-CA-C	-8.22	102.32	111.28
2	D	146	PRO	CA-C-N	8.17	128.19	119.78
2	D	146	PRO	C-N-CA	8.17	128.19	119.78
2	C	114	ALA	CA-C-N	8.00	127.75	119.76
2	C	114	ALA	C-N-CA	8.00	127.75	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	270	VAL	CA-C-N	-7.81	111.78	120.45
3	J	270	VAL	C-N-CA	-7.81	111.78	120.45
2	G	245	ASP	N-CA-C	7.76	120.69	108.67
3	J	271	PRO	N-CA-C	-7.73	104.69	114.35
2	G	304	ASN	N-CA-C	-7.67	102.92	111.28
3	J	209	ASN	N-CA-C	7.56	119.21	110.97
3	E	208	ASP	N-CA-C	-7.41	104.24	113.28
3	J	238	HIS	N-CA-C	-7.37	98.57	108.74
2	I	101	VAL	CB-CA-C	-7.36	102.38	112.02
1	F	131	ALA	N-CA-C	7.32	119.95	111.02
1	A	231	HIS	N-CA-C	-7.24	103.32	111.14
2	G	344	ASP	N-CA-C	-7.12	96.65	108.32
2	G	248	GLN	N-CA-C	7.04	120.76	111.75
1	A	192	TRP	CA-C-N	7.03	127.18	119.87
1	A	192	TRP	C-N-CA	7.03	127.18	119.87
2	H	145	GLU	CA-C-N	7.00	127.59	120.38
2	H	145	GLU	C-N-CA	7.00	127.59	120.38
2	C	5	VAL	N-CA-C	6.91	117.82	107.80
2	D	111	VAL	N-CA-C	-6.83	105.94	111.81
2	B	310	GLU	N-CA-C	6.78	119.25	111.11
2	H	101	VAL	CB-CA-C	-6.78	103.15	112.24
2	B	248	GLN	N-CA-C	6.78	120.42	111.75
3	J	15	VAL	CB-CA-C	-6.77	103.35	111.81
2	G	310	GLU	N-CA-C	6.75	119.26	111.02
2	I	211	GLU	N-CA-C	-6.73	102.38	111.54
1	A	131	ALA	N-CA-C	6.65	119.14	111.02
3	E	80	ALA	CA-C-N	-6.65	113.41	120.66
3	E	80	ALA	C-N-CA	-6.65	113.41	120.66
2	C	162	LEU	CA-C-N	6.65	128.15	119.84
2	C	162	LEU	C-N-CA	6.65	128.15	119.84
2	D	246	ASP	N-CA-C	6.64	118.52	111.28
2	G	247	ASP	N-CA-C	6.55	119.42	111.82
2	G	114	ALA	CA-C-N	6.50	127.01	119.99
2	G	114	ALA	C-N-CA	6.50	127.01	119.99
2	B	122	VAL	N-CA-C	6.49	116.98	107.37
2	H	342	ALA	CA-C-N	6.48	126.41	119.28
2	H	342	ALA	C-N-CA	6.48	126.41	119.28
2	H	75	VAL	N-CA-C	6.44	116.71	111.62
1	F	192	TRP	CA-C-N	6.40	126.53	119.87
1	F	192	TRP	C-N-CA	6.40	126.53	119.87
2	C	286	LEU	N-CA-C	-6.34	104.45	111.36
1	A	267	THR	CA-C-N	-6.31	114.15	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	THR	C-N-CA	-6.31	114.15	120.21
3	E	238	HIS	N-CA-C	-6.28	100.07	108.74
2	B	247	ASP	N-CA-C	6.24	119.06	111.82
2	C	145	GLU	CA-C-N	6.20	126.77	120.38
2	C	145	GLU	C-N-CA	6.20	126.77	120.38
2	G	365	LEU	N-CA-C	6.20	117.47	109.72
2	D	122	VAL	CB-CA-C	-6.18	102.60	111.19
2	C	68	ILE	CB-CA-C	-6.17	101.16	111.29
2	D	101	VAL	CB-CA-C	-6.14	103.97	112.02
2	H	114	ALA	CA-C-N	6.12	126.60	119.99
2	H	114	ALA	C-N-CA	6.12	126.60	119.99
4	M	11	DG	C4'-C3'-O3'	-6.11	100.83	110.00
2	H	5	VAL	N-CA-C	6.10	116.64	107.80
2	B	114	ALA	CA-C-N	6.04	126.52	119.99
2	B	114	ALA	C-N-CA	6.04	126.52	119.99
2	B	344	ASP	N-CA-C	-6.03	97.62	108.48
2	I	122	VAL	CB-CA-C	-6.03	102.82	111.19
2	D	303	GLY	N-CA-C	6.02	120.25	112.54
3	J	129	LEU	N-CA-C	6.00	117.62	111.14
2	H	245	ASP	N-CA-C	5.99	119.28	109.76
2	H	68	ILE	CB-CA-C	-5.99	101.47	111.29
2	C	107	LEU	CA-CB-CG	-5.93	95.53	116.30
1	F	56	ASP	CA-C-N	-5.89	114.04	119.82
1	F	56	ASP	C-N-CA	-5.89	114.04	119.82
2	B	245	ASP	N-CA-C	5.86	117.75	108.67
2	I	357	LEU	N-CA-C	-5.83	104.62	110.97
3	E	271	PRO	N-CA-C	-5.78	106.46	114.27
1	A	318	GLN	N-CA-C	-5.78	106.36	113.41
2	H	224	ALA	N-CA-C	-5.77	104.91	111.14
4	K	14	DA	P-O3'-C3'	-5.77	111.55	120.20
3	E	129	LEU	N-CA-C	5.76	117.37	111.14
2	H	286	LEU	N-CA-C	-5.74	105.03	111.28
4	K	11	DG	C4'-C3'-O3'	-5.73	101.40	110.00
4	M	5	DT	O4'-C1'-N1	-5.73	99.80	108.40
2	C	246	ASP	N-CA-C	5.72	119.73	112.87
2	C	101	VAL	CB-CA-C	-5.71	104.56	112.04
4	K	5	DT	O4'-C1'-N1	-5.70	99.85	108.40
2	I	78	ASN	N-CA-C	5.68	118.41	111.82
2	H	320	ILE	N-CA-C	5.68	114.36	107.61
2	H	122	VAL	N-CA-C	5.66	115.74	107.37
2	D	55	ALA	N-CA-C	-5.66	104.81	110.97
2	I	268	ILE	CB-CA-C	-5.64	104.53	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	155	LEU	N-CA-C	-5.62	104.78	111.69
2	G	363	MET	CA-C-N	5.59	125.58	120.21
2	G	363	MET	C-N-CA	5.59	125.58	120.21
4	M	9	DA	C4'-C3'-O3'	-5.59	101.62	110.00
2	G	11	ARG	CA-C-N	5.59	125.51	119.76
2	G	11	ARG	C-N-CA	5.59	125.51	119.76
2	C	101	VAL	N-CA-C	-5.58	105.40	110.82
1	A	246	LEU	N-CA-C	-5.57	105.12	111.14
2	B	11	ARG	CA-C-N	5.56	125.84	119.83
2	B	11	ARG	C-N-CA	5.56	125.84	119.83
2	H	133	ARG	N-CA-C	-5.56	105.22	111.28
2	B	298	SER	CA-C-N	5.54	125.20	119.05
2	B	298	SER	C-N-CA	5.54	125.20	119.05
2	D	309	ILE	CB-CA-C	-5.53	103.14	112.16
1	A	291	ASN	N-CA-C	5.52	117.38	111.36
3	J	193	LEU	N-CA-C	-5.51	105.43	111.82
2	H	107	LEU	CA-CB-CG	-5.51	97.02	116.30
2	H	246	ASP	N-CA-C	5.50	119.47	112.87
3	E	200	ALA	N-CA-C	-5.49	105.38	111.36
2	C	158	ASP	CA-C-N	5.48	125.00	119.19
2	C	158	ASP	C-N-CA	5.48	125.00	119.19
1	A	55	ILE	N-CA-C	5.47	115.20	106.88
2	B	365	LEU	N-CA-C	5.46	116.54	109.72
4	M	8	DT	P-O5'-C5'	-5.46	111.82	120.00
2	G	298	SER	CA-C-N	5.45	124.64	118.97
2	G	298	SER	C-N-CA	5.45	124.64	118.97
3	E	319	ILE	N-CA-C	-5.45	105.41	110.53
2	G	24	VAL	N-CA-C	-5.45	106.50	111.67
1	A	325	GLU	N-CA-C	-5.44	105.35	111.28
4	M	6	DT	O3'-P-O5'	-5.43	95.85	104.00
2	G	122	VAL	N-CA-C	5.40	115.56	107.51
1	F	317	GLY	N-CA-C	5.40	119.92	112.37
3	E	166	PRO	CA-C-N	5.39	123.54	119.66
3	E	166	PRO	C-N-CA	5.39	123.54	119.66
4	K	8	DT	P-O3'-C3'	-5.39	112.12	120.20
2	I	162	LEU	CA-C-N	5.39	125.39	119.90
2	I	162	LEU	C-N-CA	5.39	125.39	119.90
2	G	292	ILE	CB-CA-C	-5.37	105.00	112.04
2	I	279	GLU	N-CA-C	-5.36	105.55	111.71
2	D	213	SER	N-CA-C	5.33	117.10	108.41
2	B	307	ALA	N-CA-C	5.31	122.12	110.80
3	E	90	VAL	CB-CA-C	-5.31	105.12	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	5	DC	C4'-C3'-O3'	-5.28	102.08	110.00
2	G	245	ASP	CA-C-N	5.28	129.04	120.60
2	G	245	ASP	C-N-CA	5.28	129.04	120.60
2	D	344	ASP	N-CA-C	-5.27	101.40	109.41
5	N	6	DC	O5'-C5'-C4'	-5.25	102.93	110.80
2	I	73	CYS	N-CA-C	5.24	116.80	111.14
2	B	363	MET	CA-C-N	5.24	125.98	120.11
2	B	363	MET	C-N-CA	5.24	125.98	120.11
2	C	245	ASP	N-CA-C	5.24	118.08	109.76
5	N	7	DT	C5'-C4'-O4'	-5.23	101.56	109.40
1	A	280	GLN	N-CA-C	5.22	117.65	111.33
2	D	68	ILE	CB-CA-C	-5.21	105.67	111.35
1	F	279	TRP	CA-CB-CG	5.20	123.49	113.60
2	G	303	GLY	N-CA-C	5.19	118.84	112.14
2	D	78	ASN	N-CA-C	5.19	117.84	111.82
5	L	9	DT	O4'-C1'-C2'	-5.18	98.63	106.40
1	F	84	LEU	CA-C-N	5.17	125.15	120.03
1	F	84	LEU	C-N-CA	5.17	125.15	120.03
2	B	24	VAL	N-CA-C	-5.17	106.76	111.67
1	A	279	TRP	CA-CB-CG	5.15	123.39	113.60
3	E	93	VAL	CB-CA-C	-5.15	105.12	112.22
4	M	8	DT	P-O3'-C3'	-5.14	112.48	120.20
1	A	134	SER	N-CA-C	5.14	118.44	110.17
2	H	145	GLU	CB-CA-C	-5.12	104.80	111.15
2	H	78	ASN	N-CA-C	5.12	117.52	111.33
2	D	203	LEU	N-CA-C	-5.11	105.89	111.82
5	N	1	DC	C5'-C4'-O4'	-5.10	101.75	109.40
2	I	111	VAL	CB-CA-C	-5.09	105.79	111.80
5	N	7	DT	C4'-C3'-O3'	-5.06	102.41	110.00
2	C	321	PRO	CA-C-N	5.05	125.08	119.32
2	C	321	PRO	C-N-CA	5.05	125.08	119.32
3	E	209	ASN	N-CA-C	5.04	116.46	110.97
3	E	270	VAL	CA-C-N	-5.04	114.60	120.04
3	E	270	VAL	C-N-CA	-5.04	114.60	120.04
2	G	40	ALA	N-CA-C	5.04	116.24	107.93
2	D	342	ALA	CA-C-N	5.03	125.30	119.47
2	D	342	ALA	C-N-CA	5.03	125.30	119.47
2	I	70	ALA	N-CA-C	-5.03	107.18	113.72
3	E	72	THR	N-CA-C	5.02	116.49	108.41

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	246	ASP	Peptide
2	C	245	ASP	Peptide
2	G	246	ASP	Peptide
2	H	245	ASP	Peptide
2	I	157	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2650	0	2703	175	0
1	F	2650	0	2703	165	0
2	B	2829	0	2879	163	1
2	C	2838	0	2886	175	1
2	D	2818	0	2863	182	0
2	G	2941	0	2987	148	0
2	H	2838	0	2886	172	2
2	I	2818	0	2863	180	1
3	E	2601	0	2603	120	1
3	J	2601	0	2603	126	0
4	K	287	0	161	17	0
4	M	287	0	161	14	0
5	L	200	0	115	5	0
5	N	200	0	115	4	0
6	B	27	0	12	3	0
6	C	27	0	12	3	0
6	D	27	0	12	3	0
6	G	27	0	12	2	0
6	H	27	0	12	4	0
6	I	27	0	12	2	0
7	B	4	0	0	1	0
7	C	4	0	0	0	0
7	D	4	0	0	0	0
7	G	4	0	0	1	0
7	H	4	0	0	0	0
7	I	4	0	0	1	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	28758	0	28600	1517	3

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 26.

All (1517) 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:CE	2:I:290:HIS:HA	1.75	1.15
2:H:351:MET:HE1	2:I:290:HIS:HA	1.16	1.12
1:F:95:GLU:HA	1:F:98:LEU:HD12	1.33	1.08
1:A:95:GLU:HA	1:A:98:LEU:HD12	1.35	1.07
2:I:216:ASP:OD1	3:J:157:SER:HB2	1.57	1.03
2:G:101:VAL:HG21	2:G:134:HIS:HB3	1.42	1.01
2:D:361:PRO:HB3	3:J:272:GLY:HA2	1.44	1.00
1:A:244:VAL:HG21	4:K:5:DT:H71	1.42	0.99
2:G:351:MET:HE2	2:H:290:HIS:HA	1.43	0.99
2:I:362:ARG:O	2:I:363:MET:HG2	1.63	0.98
2:D:362:ARG:O	2:D:363:MET:HG2	1.64	0.97
2:B:101:VAL:HG21	2:B:134:HIS:HB3	1.42	0.97
2:B:351:MET:HE2	2:C:290:HIS:HA	1.46	0.97
1:A:117:LEU:HD12	1:A:122:GLU:HG2	1.47	0.97
2:D:361:PRO:HG2	3:J:275:ALA:CB	1.96	0.96
1:F:18:ARG:HB3	1:F:133:ARG:O	1.64	0.96
2:B:115:PRO:HD3	2:B:149:HIS:HD2	1.29	0.94
1:F:117:LEU:HD12	1:F:122:GLU:HG2	1.48	0.94
2:H:292:ILE:HG13	2:H:313:MET:HE1	1.49	0.94
2:I:52:THR:HG23	6:I:410:ADP:O1B	1.70	0.92
3:J:2:ARG:HD3	3:J:4:TYR:CE1	2.04	0.92
1:A:18:ARG:HB3	1:A:133:ARG:O	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:115:PRO:HD3	2:G:149:HIS:HD2	1.31	0.92
3:E:106:LEU:HD23	3:E:106:LEU:O	1.69	0.92
2:D:52:THR:HG23	6:D:404:ADP:O1B	1.70	0.91
2:C:292:ILE:HG13	2:C:313:MET:HE1	1.52	0.91
2:G:302:LEU:HD22	2:G:306:MET:HG3	1.52	0.90
2:I:184:ARG:HD3	2:I:204:GLN:NE2	1.86	0.90
2:B:302:LEU:HD22	2:B:306:MET:HG3	1.49	0.89
2:B:265:MET:HE1	2:B:350:GLU:HG2	1.54	0.88
2:D:184:ARG:HD3	2:D:204:GLN:NE2	1.88	0.88
1:F:20:ALA:HB3	1:F:134:SER:HB3	1.53	0.88
2:H:30:ASN:O	2:H:34:LEU:HB2	1.74	0.87
3:J:106:LEU:HD23	3:J:106:LEU:O	1.74	0.87
3:J:82:GLU:HA	3:J:82:GLU:OE1	1.70	0.87
2:I:252:LEU:HD13	2:I:285:MET:CE	2.05	0.87
3:J:46:ARG:HD2	3:J:68:MET:HG2	1.56	0.87
1:A:20:ALA:HB3	1:A:134:SER:HB3	1.55	0.87
2:D:38:HIS:HD2	2:D:40:ALA:H	1.19	0.87
2:G:21:GLN:OE1	2:G:175:LEU:HB3	1.75	0.87
2:I:38:HIS:HD2	2:I:40:ALA:H	1.23	0.87
3:E:82:GLU:HA	3:E:82:GLU:OE1	1.73	0.86
2:D:129:HIS:HD1	2:D:156:THR:HG1	1.19	0.85
2:D:21:GLN:NE2	2:D:49:VAL:HG12	1.91	0.85
3:E:46:ARG:HD2	3:E:68:MET:HG2	1.56	0.85
2:G:39:HIS:CD2	2:G:39:HIS:H	1.95	0.84
2:C:30:ASN:O	2:C:34:LEU:HB2	1.78	0.84
2:C:351:MET:HE1	2:D:290:HIS:HA	1.58	0.84
2:G:15:PHE:HE2	2:G:57:LEU:HB3	1.41	0.84
2:G:95:ALA:O	2:G:99:THR:HG22	1.76	0.84
2:H:144:GLU:HG2	2:H:145:GLU:HG3	1.60	0.84
2:H:265:MET:HE3	2:I:294:MET:SD	2.18	0.84
2:B:291:ARG:HG2	2:B:306:MET:HE3	1.58	0.84
2:G:4:GLN:NE2	2:G:9:LYS:HG3	1.93	0.84
2:C:265:MET:HE2	2:C:354:LEU:HD21	1.58	0.83
2:I:47:ARG:HG2	2:I:47:ARG:O	1.75	0.83
2:D:361:PRO:CB	3:J:272:GLY:HA2	2.08	0.83
2:G:216:ASP:OD1	2:H:168:SER:HB2	1.78	0.83
2:G:351:MET:HE2	2:H:290:HIS:CA	2.07	0.83
2:D:51:LYS:HB2	6:D:404:ADP:O2B	1.77	0.82
2:I:21:GLN:NE2	2:I:49:VAL:HG12	1.94	0.82
3:J:224:VAL:HB	3:J:225:PRO:HD3	1.60	0.82
2:C:351:MET:CE	2:D:290:HIS:HA	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:268:ILE:HD11	2:D:353:LEU:HD12	1.60	0.82
2:D:115:PRO:HD3	2:D:149:HIS:HD2	1.44	0.82
4:M:7:DA:H2''	4:M:8:DT:O5'	1.80	0.82
3:E:2:ARG:HD3	3:E:4:TYR:CE1	2.14	0.81
2:I:216:ASP:OD1	3:J:157:SER:CB	2.27	0.81
2:B:15:PHE:HE2	2:B:57:LEU:HB3	1.44	0.81
2:B:260:ASN:HD22	2:B:263:ARG:HB2	1.43	0.81
3:J:99:LYS:HD3	3:J:105:ARG:HH22	1.44	0.81
2:G:260:ASN:HD22	2:G:263:ARG:HB2	1.45	0.81
2:I:51:LYS:HB2	6:I:410:ADP:O2B	1.79	0.81
1:F:244:VAL:HG21	4:M:5:DT:H71	1.61	0.81
2:I:339:LEU:HB3	2:I:340:PRO:HD3	1.63	0.81
3:J:285:ARG:HD3	3:J:322:TYR:O	1.80	0.81
2:D:361:PRO:HG2	3:J:275:ALA:HB3	1.61	0.80
2:G:291:ARG:HG2	2:G:306:MET:HE3	1.64	0.80
2:D:144:GLU:HG2	2:D:145:GLU:HG3	1.64	0.80
3:J:99:LYS:HD3	3:J:105:ARG:NH2	1.96	0.80
2:B:115:PRO:HD3	2:B:149:HIS:CD2	2.16	0.79
2:I:101:VAL:HG23	4:M:10:DG:OP1	1.81	0.79
3:J:202:LEU:HD23	3:J:202:LEU:O	1.83	0.79
2:G:115:PRO:HD3	2:G:149:HIS:CD2	2.18	0.79
3:J:170:GLN:HA	3:J:170:GLN:OE1	1.83	0.79
2:H:351:MET:CE	2:I:290:HIS:CA	2.60	0.78
4:M:9:DA:H2''	4:M:10:DG:O5'	1.82	0.78
3:E:224:VAL:HB	3:E:225:PRO:HD3	1.65	0.78
2:D:363:MET:HE2	3:J:276:GLU:OE1	1.84	0.78
1:A:59:THR:HG23	1:A:63:ALA:HB3	1.64	0.78
3:J:199:GLY:HA2	3:J:202:LEU:HB3	1.65	0.78
2:H:265:MET:HE2	2:H:354:LEU:HD21	1.63	0.78
3:E:99:LYS:HD3	3:E:105:ARG:HH22	1.49	0.78
2:I:144:GLU:HG2	2:I:145:GLU:HG3	1.63	0.78
2:I:291:ARG:O	2:I:294:MET:HB2	1.84	0.78
1:A:49:GLU:HB2	1:A:78:GLN:HB3	1.67	0.77
4:K:7:DA:H2''	4:K:8:DT:O5'	1.82	0.77
3:E:202:LEU:HD23	3:E:202:LEU:O	1.85	0.77
2:C:115:PRO:HD3	2:C:149:HIS:HD2	1.49	0.77
2:H:367:GLU:HG3	2:H:368:PRO:HD2	1.65	0.77
1:A:53:PHE:CD1	1:A:67:LEU:HD21	2.20	0.76
1:F:53:PHE:CD1	1:F:67:LEU:HD21	2.20	0.76
2:I:265:MET:HE2	3:J:257:LYS:HD3	1.68	0.75
1:A:19:ALA:HB1	1:A:104:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:CZ	1:A:50:HIS:HB3	2.16	0.75
2:B:39:HIS:H	2:B:39:HIS:CD2	2.02	0.75
2:B:347:MET:HG2	2:C:290:HIS:CE1	2.22	0.75
2:H:292:ILE:HG13	2:H:313:MET:CE	2.16	0.75
2:D:347:MET:O	2:D:351:MET:HG3	1.86	0.75
1:F:22:LEU:HD23	1:F:112:VAL:HB	1.67	0.75
1:F:59:THR:HG23	1:F:63:ALA:HB3	1.68	0.75
2:D:339:LEU:HB3	2:D:340:PRO:HD3	1.69	0.75
2:I:115:PRO:HD3	2:I:149:HIS:HD2	1.51	0.75
2:C:367:GLU:HG3	2:C:368:PRO:HD2	1.69	0.74
1:F:49:GLU:HB2	1:F:78:GLN:HB3	1.69	0.74
3:J:114:VAL:HB	3:J:143:LEU:HD23	1.69	0.74
2:B:257:VAL:HG21	2:B:320:ILE:HD11	1.70	0.73
2:G:15:PHE:CE2	2:G:57:LEU:HB3	2.21	0.73
2:G:265:MET:HE1	2:G:350:GLU:HG2	1.70	0.73
1:F:39:ARG:CZ	1:F:50:HIS:HB3	2.19	0.73
2:G:49:VAL:HG11	2:G:176:LYS:O	1.88	0.73
2:H:318:ARG:HH11	2:H:318:ARG:HB3	1.52	0.73
2:I:268:ILE:HD11	2:I:353:LEU:HD12	1.71	0.73
2:I:49:VAL:HG11	2:I:176:LYS:O	1.88	0.72
2:I:26:THR:O	2:I:30:ASN:HB2	1.89	0.72
1:A:22:LEU:HD23	1:A:112:VAL:HB	1.70	0.72
2:B:21:GLN:OE1	2:B:175:LEU:HB3	1.88	0.72
2:B:351:MET:HE2	2:C:290:HIS:CA	2.19	0.72
2:H:318:ARG:HH11	2:H:318:ARG:CB	2.03	0.72
2:B:15:PHE:CE2	2:B:57:LEU:HB3	2.25	0.71
4:K:9:DA:H2''	4:K:10:DG:O5'	1.90	0.71
2:H:4:GLN:HA	2:H:4:GLN:OE1	1.90	0.71
3:J:3:TRP:HH2	3:J:8:ARG:HG3	1.56	0.71
2:D:184:ARG:HD3	2:D:204:GLN:HE22	1.56	0.71
2:G:101:VAL:CG2	2:G:134:HIS:HB3	2.20	0.71
2:G:351:MET:HG2	2:H:290:HIS:HD2	1.55	0.71
2:H:78:ASN:O	2:H:82:ILE:HG13	1.89	0.71
3:J:88:LEU:HD23	3:J:120:LEU:CD2	2.21	0.71
2:B:215:ARG:HH11	6:B:400:ADP:H5'1	1.54	0.71
2:G:47:ARG:O	2:G:47:ARG:HG2	1.90	0.71
3:E:99:LYS:HD3	3:E:105:ARG:NH2	2.05	0.71
2:I:243:THR:HG22	2:I:244:LEU:N	2.05	0.71
2:H:115:PRO:HD3	2:H:149:HIS:HD2	1.55	0.71
1:A:244:VAL:HG21	4:K:5:DT:C7	2.18	0.71
3:E:29:ILE:HD13	3:E:40:LEU:HD23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:VAL:HG12	2:D:156:THR:HB	1.73	0.70
1:A:25:GLY:HA3	1:A:139:CYS:HB2	1.73	0.70
2:B:252:LEU:HD23	2:B:267:LEU:HD12	1.73	0.70
3:J:202:LEU:HD23	3:J:202:LEU:C	2.16	0.70
2:C:292:ILE:HG13	2:C:313:MET:CE	2.22	0.70
1:F:19:ALA:HB1	1:F:104:LEU:HD22	1.73	0.70
2:I:184:ARG:HD3	2:I:204:GLN:HE22	1.52	0.70
2:C:144:GLU:HG2	2:C:145:GLU:HG3	1.71	0.70
2:G:215:ARG:HH11	6:G:406:ADP:H5'1	1.56	0.70
2:I:347:MET:O	2:I:351:MET:HG3	1.91	0.70
1:F:74:PHE:CD1	1:F:74:PHE:O	2.45	0.69
2:B:95:ALA:O	2:B:99:THR:HG22	1.93	0.69
2:D:252:LEU:HD13	2:D:285:MET:CE	2.22	0.69
2:G:257:VAL:HG21	2:G:320:ILE:HD11	1.74	0.69
2:I:252:LEU:HD13	2:I:285:MET:HE2	1.73	0.69
2:I:252:LEU:HD13	2:I:285:MET:HE1	1.74	0.69
2:C:4:GLN:HA	2:C:4:GLN:OE1	1.91	0.69
2:D:256:MET:HE1	2:D:332:LEU:HD11	1.74	0.69
1:F:179:LEU:HG	1:F:179:LEU:O	1.93	0.69
2:C:318:ARG:HH11	2:C:318:ARG:HB3	1.58	0.69
1:A:64:ILE:HD12	1:A:96:GLN:HG2	1.75	0.68
3:E:246:HIS:O	3:E:250:THR:HG23	1.93	0.68
2:B:49:VAL:HG11	2:B:176:LYS:O	1.93	0.68
2:H:101:VAL:HG23	4:M:12:DC:OP1	1.92	0.68
2:C:291:ARG:HD2	2:C:306:MET:SD	2.33	0.68
2:C:51:LYS:HG3	6:C:402:ADP:O2B	1.92	0.68
2:B:51:LYS:HB2	6:B:400:ADP:O2B	1.94	0.68
1:A:147:LEU:HD23	1:A:171:CYS:SG	2.34	0.68
2:C:318:ARG:HH11	2:C:318:ARG:CB	2.07	0.68
1:F:147:LEU:HD23	1:F:171:CYS:SG	2.34	0.68
2:D:38:HIS:CD2	2:D:39:HIS:H	2.12	0.68
2:B:216:ASP:OD1	2:C:168:SER:HB2	1.94	0.67
2:D:26:THR:O	2:D:30:ASN:HB2	1.94	0.67
2:D:47:ARG:O	2:D:47:ARG:HG2	1.93	0.67
2:D:291:ARG:O	2:D:294:MET:HB2	1.94	0.67
1:F:268:PRO:HD2	1:F:271:ALA:HB3	1.76	0.67
3:E:253:MET:HG3	3:E:253:MET:O	1.94	0.67
2:H:21:GLN:NE2	2:H:49:VAL:HG12	2.09	0.67
2:C:101:VAL:CG2	2:C:134:HIS:HB3	2.24	0.67
3:E:90:VAL:HG12	4:K:8:DT:H5''	1.77	0.67
3:J:121:THR:HG22	3:J:122:ASP:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:253:MET:HG3	3:J:253:MET:O	1.94	0.67
2:I:360:HIS:HB3	2:I:361:PRO:HD3	1.75	0.67
3:E:202:LEU:HD23	3:E:202:LEU:C	2.20	0.67
2:B:291:ARG:HG2	2:B:306:MET:CE	2.25	0.67
2:H:318:ARG:HB2	2:H:318:ARG:NH1	2.10	0.67
2:I:64:CYS:SG	2:I:66:THR:HG23	2.35	0.67
1:F:64:ILE:HD12	1:F:96:GLN:HG2	1.76	0.67
1:F:304:LEU:O	1:F:308:THR:HG23	1.94	0.67
2:C:282:LEU:HD11	2:C:349:VAL:HG22	1.77	0.67
1:A:93:ILE:O	1:A:97:LEU:HG	1.94	0.67
2:D:115:PRO:HD3	2:D:149:HIS:CD2	2.29	0.67
2:D:254:GLU:OE2	2:D:312:ARG:HD2	1.94	0.67
3:E:182:MET:HG3	3:E:205:PHE:CE1	2.30	0.67
3:E:199:GLY:HA2	3:E:202:LEU:HB3	1.76	0.66
1:F:126:TRP:O	1:F:130:LEU:HG	1.96	0.66
2:G:125:ILE:HB	2:G:154:LEU:HD22	1.77	0.66
2:B:101:VAL:CG2	2:B:134:HIS:HB3	2.20	0.66
3:E:121:THR:HG22	3:E:122:ASP:N	2.09	0.66
2:H:244:LEU:H	2:H:244:LEU:HD12	1.59	0.66
2:H:337:LYS:NZ	3:J:334:LEU:HD22	2.10	0.66
2:I:24:VAL:HG21	2:I:175:LEU:HD22	1.77	0.66
2:I:38:HIS:CD2	2:I:39:HIS:H	2.14	0.66
3:J:246:HIS:O	3:J:250:THR:HG23	1.94	0.66
2:B:21:GLN:HA	2:B:21:GLN:NE2	2.10	0.66
2:D:101:VAL:HG23	4:K:10:DG:OP1	1.95	0.66
2:D:309:ILE:HG22	2:D:313:MET:HG2	1.77	0.66
1:F:78:GLN:HG3	1:F:108:LEU:CD2	2.26	0.66
3:J:46:ARG:CD	3:J:68:MET:HG2	2.26	0.66
2:C:283:VAL:HA	2:C:286:LEU:HD12	1.77	0.66
2:G:252:LEU:HD23	2:G:267:LEU:HD12	1.76	0.66
1:A:126:TRP:O	1:A:130:LEU:HG	1.96	0.66
2:B:125:ILE:HB	2:B:154:LEU:HD22	1.78	0.66
2:C:147:PRO:HD2	2:C:150:VAL:HB	1.77	0.66
2:C:78:ASN:O	2:C:82:ILE:HG13	1.95	0.66
2:D:360:HIS:HB3	2:D:361:PRO:HD3	1.77	0.66
2:I:184:ARG:CD	2:I:204:GLN:NE2	2.59	0.66
3:E:46:ARG:CD	3:E:68:MET:HG2	2.24	0.66
1:F:52:THR:HG22	1:F:81:LEU:HD23	1.77	0.66
1:A:74:PHE:O	1:A:74:PHE:CD1	2.50	0.65
2:D:117:ARG:CZ	2:D:117:ARG:HB3	2.27	0.65
2:G:291:ARG:HG2	2:G:306:MET:CE	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:88:LEU:HD23	3:J:120:LEU:HD23	1.78	0.65
2:B:47:ARG:HG2	2:B:47:ARG:O	1.96	0.65
2:D:265:MET:HE2	3:E:257:LYS:HD3	1.78	0.65
2:I:80:ARG:O	2:I:84:GLN:HG3	1.97	0.65
2:C:367:GLU:OE2	2:D:362:ARG:NH1	2.28	0.65
2:C:15:PHE:HE1	2:C:57:LEU:HB3	1.61	0.65
2:D:216:ASP:OD1	3:E:157:SER:HB2	1.96	0.65
1:F:13:LEU:CD1	1:F:38:VAL:HG22	2.27	0.65
2:B:223:GLN:HG2	2:B:240:MET:SD	2.37	0.65
2:I:115:PRO:HD3	2:I:149:HIS:CD2	2.32	0.65
2:C:21:GLN:NE2	2:C:175:LEU:HB3	2.11	0.64
2:D:49:VAL:HG12	2:D:49:VAL:O	1.97	0.64
2:D:244:LEU:HD21	2:D:276:ILE:HG12	1.78	0.64
1:A:97:LEU:HD13	1:A:126:TRP:CH2	2.31	0.64
2:I:254:GLU:OE2	2:I:312:ARG:HD2	1.97	0.64
3:E:285:ARG:HD3	3:E:322:TYR:O	1.97	0.64
2:I:309:ILE:HG22	2:I:313:MET:HG2	1.80	0.64
2:C:91:ILE:HD12	2:C:123:TYR:CE2	2.33	0.64
2:H:147:PRO:HD2	2:H:150:VAL:HB	1.79	0.64
2:D:184:ARG:CD	2:D:204:GLN:NE2	2.61	0.64
3:J:29:ILE:HD13	3:J:40:LEU:HD23	1.79	0.64
2:C:318:ARG:NH1	2:C:318:ARG:HB2	2.13	0.64
2:D:61:GLY:HA2	2:D:72:PRO:HG3	1.80	0.64
2:D:202:ALA:HB2	2:D:234:THR:HA	1.80	0.64
3:E:155:LEU:HD12	3:E:155:LEU:C	2.23	0.63
1:A:78:GLN:HG3	1:A:108:LEU:CD2	2.27	0.63
3:E:259:HIS:ND1	3:J:259:HIS:CE1	2.67	0.63
1:A:27:ASP:HB2	1:A:141:THR:OG1	1.97	0.63
1:A:117:LEU:CD1	1:A:122:GLU:HG2	2.25	0.63
1:A:280:GLN:HA	1:A:283:ARG:HG3	1.80	0.63
2:B:314:ARG:HH11	2:B:314:ARG:HG2	1.63	0.63
2:C:347:MET:HG2	2:D:290:HIS:CD2	2.33	0.63
2:G:314:ARG:HH11	2:G:314:ARG:HG2	1.63	0.63
2:G:365:LEU:CD1	2:H:297:LEU:HD23	2.27	0.63
2:G:51:LYS:HB2	6:G:406:ADP:O2B	1.99	0.63
2:H:318:ARG:CB	2:H:318:ARG:NH1	2.62	0.63
2:I:128:VAL:HG12	2:I:156:THR:HB	1.81	0.63
2:C:15:PHE:CE1	2:C:57:LEU:HB3	2.34	0.63
2:I:232:VAL:HG12	2:I:232:VAL:O	1.97	0.63
2:D:309:ILE:CG2	2:D:313:MET:HG2	2.28	0.63
1:F:13:LEU:HD13	1:F:38:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:256:MET:HE1	2:I:332:LEU:HD11	1.81	0.63
2:D:257:VAL:HG21	2:D:320:ILE:HD11	1.79	0.63
3:E:112:VAL:HB	3:E:141:PHE:CD1	2.34	0.63
1:F:296:THR:O	1:F:300:GLN:HG3	1.98	0.63
2:C:44:SER:HB3	2:C:159:PRO:HG3	1.81	0.63
2:C:337:LYS:CE	3:E:334:LEU:HD22	2.29	0.63
1:F:152:ALA:O	1:F:156:LYS:HD2	1.99	0.63
3:E:3:TRP:HH2	3:E:8:ARG:HG3	1.62	0.62
2:I:309:ILE:CG2	2:I:313:MET:HG2	2.29	0.62
2:C:114:ALA:HB1	2:C:115:PRO:HD2	1.80	0.62
2:H:44:SER:HB3	2:H:159:PRO:HG3	1.81	0.62
1:A:162:LEU:HD22	1:A:166:ALA:HB3	1.81	0.62
2:D:302:LEU:HD21	2:D:310:GLU:HB2	1.81	0.62
2:G:343:PRO:HB3	2:H:283:VAL:HG13	1.80	0.62
1:A:2:ILE:HG13	1:A:18:ARG:HH12	1.64	0.62
2:C:342:ALA:HB1	2:C:343:PRO:HD2	1.81	0.62
2:D:21:GLN:NE2	2:D:49:VAL:CG1	2.63	0.62
1:F:93:ILE:O	1:F:97:LEU:HG	1.99	0.62
2:H:342:ALA:HB1	2:H:343:PRO:HD2	1.80	0.62
1:A:152:ALA:O	1:A:156:LYS:HD2	2.00	0.62
1:F:56:ASP:HB2	1:F:58:ASN:HB2	1.81	0.62
1:F:117:LEU:CD1	1:F:122:GLU:HG2	2.27	0.62
2:H:23:HIS:CE1	2:H:24:VAL:HG23	2.35	0.62
2:D:243:THR:HG22	2:D:244:LEU:N	2.14	0.62
2:H:91:ILE:HD12	2:H:123:TYR:CE2	2.35	0.62
1:A:71:MET:HB2	1:A:108:LEU:HG	1.81	0.62
2:B:15:PHE:HE2	2:B:57:LEU:CB	2.13	0.62
2:B:128:VAL:O	2:B:128:VAL:HG22	2.00	0.62
2:G:21:GLN:HA	2:G:21:GLN:NE2	2.14	0.62
3:J:182:MET:HG3	3:J:205:PHE:CE1	2.35	0.62
2:G:119:ARG:NH1	2:G:119:ARG:HG2	2.15	0.61
2:H:47:ARG:NH1	2:H:216:ASP:OD2	2.32	0.61
2:H:21:GLN:NE2	2:H:175:LEU:HB3	2.15	0.61
4:M:2:DT:H2''	4:M:3:DT:OP1	1.99	0.61
2:C:47:ARG:O	2:C:47:ARG:HG2	1.98	0.61
3:E:259:HIS:CE1	3:J:259:HIS:CE1	2.88	0.61
1:F:27:ASP:HB2	1:F:141:THR:OG1	1.99	0.61
3:E:103:HIS:CD2	3:E:103:HIS:H	2.17	0.61
1:F:128:THR:O	1:F:131:ALA:HB3	2.00	0.61
1:F:160:LEU:HD11	1:F:189:SER:HB3	1.82	0.61
1:F:2:ILE:HG13	1:F:18:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:GLN:NE2	2:C:49:VAL:HG12	2.13	0.61
3:J:224:VAL:CB	3:J:225:PRO:HD3	2.29	0.61
2:C:23:HIS:CE1	2:C:24:VAL:HG23	2.36	0.61
2:H:101:VAL:CG2	2:H:134:HIS:HB3	2.30	0.61
2:I:69:THR:HG21	2:I:72:PRO:HA	1.82	0.61
2:D:49:VAL:HG11	2:D:176:LYS:O	2.00	0.61
3:E:72:THR:HG23	3:E:72:THR:O	1.99	0.61
3:E:114:VAL:HB	3:E:143:LEU:HD23	1.83	0.61
2:D:38:HIS:CD2	2:D:40:ALA:H	2.11	0.61
2:D:252:LEU:HD13	2:D:285:MET:HE2	1.82	0.61
3:E:170:GLN:HA	3:E:170:GLN:OE1	1.99	0.61
2:B:52:THR:HG21	2:B:126:ASP:OD2	2.00	0.60
2:B:277:GLU:O	2:B:280:ALA:HB3	2.01	0.60
3:E:80:ALA:HB1	3:E:81:PRO:CD	2.31	0.60
1:F:25:GLY:HA3	1:F:139:CYS:HB2	1.81	0.60
2:G:351:MET:HE3	2:H:329:TYR:CD1	2.35	0.60
2:I:117:ARG:CZ	2:I:117:ARG:HB3	2.28	0.60
2:H:114:ALA:HB1	2:H:115:PRO:HD2	1.82	0.60
2:H:341:TYR:O	2:I:336:ARG:NH1	2.34	0.60
2:H:64:CYS:SG	2:H:66:THR:HG23	2.41	0.60
1:A:196:LYS:C	1:A:197:LEU:HD23	2.27	0.60
1:F:12:GLN:O	1:F:12:GLN:HG3	2.00	0.60
2:H:341:TYR:HB2	2:I:333:LEU:HD11	1.83	0.60
2:C:341:TYR:CE1	2:D:337:LYS:HD2	2.37	0.60
3:E:68:MET:HE3	3:E:68:MET:HA	1.82	0.60
1:F:71:MET:HB2	1:F:108:LEU:HG	1.84	0.60
2:G:178:LEU:HD12	2:G:214:LEU:HB2	1.84	0.60
2:I:178:LEU:HD13	2:I:214:LEU:HD12	1.84	0.60
2:I:261:GLY:HA2	2:I:357:LEU:HD21	1.83	0.60
1:A:304:LEU:O	1:A:308:THR:HG23	2.01	0.60
2:B:265:MET:CE	2:B:350:GLU:HG2	2.30	0.60
2:H:49:VAL:HG11	2:H:176:LYS:O	2.02	0.60
2:H:282:LEU:HD11	2:H:349:VAL:HG22	1.83	0.60
2:C:246:ASP:HB3	2:C:309:ILE:HD12	1.84	0.59
2:C:318:ARG:CB	2:C:318:ARG:NH1	2.64	0.59
2:D:30:ASN:O	2:D:34:LEU:HG	2.02	0.59
2:D:361:PRO:HG2	3:J:275:ALA:HB2	1.82	0.59
1:F:196:LYS:C	1:F:197:LEU:HD23	2.27	0.59
3:J:68:MET:HE3	3:J:68:MET:HA	1.84	0.59
3:J:155:LEU:HD12	3:J:155:LEU:C	2.27	0.59
1:F:282:ARG:HG2	1:F:282:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:223:GLN:HG2	2:G:240:MET:SD	2.42	0.59
2:G:351:MET:CE	2:H:290:HIS:HA	2.27	0.59
2:D:6:LEU:H	2:D:6:LEU:HD12	1.66	0.59
1:F:97:LEU:HD13	1:F:126:TRP:CH2	2.37	0.59
2:H:47:ARG:O	2:H:47:ARG:HG2	2.03	0.59
2:C:47:ARG:NH1	2:C:216:ASP:OD2	2.35	0.59
2:C:353:LEU:O	2:C:356:ALA:HB3	2.02	0.59
2:G:314:ARG:HG2	2:G:314:ARG:NH1	2.18	0.59
1:F:175:GLU:OE2	1:F:228:ARG:NH2	2.36	0.59
2:C:53:SER:OG	6:C:402:ADP:O1A	2.20	0.59
2:D:5:VAL:HG13	2:D:222:ASP:OD2	2.02	0.59
3:E:46:ARG:HH22	3:E:69:GLN:HE21	1.51	0.59
2:H:259:ALA:HB2	2:H:360:HIS:CE1	2.38	0.59
2:H:367:GLU:HG3	2:H:368:PRO:CD	2.31	0.59
3:J:197:SER:OG	3:J:200:ALA:HB3	2.02	0.59
1:A:296:THR:O	1:A:300:GLN:HG3	2.03	0.58
2:B:257:VAL:HG21	2:B:320:ILE:CD1	2.33	0.58
2:B:314:ARG:HG2	2:B:314:ARG:NH1	2.18	0.58
1:F:304:LEU:HD23	1:F:327:LEU:HD13	1.85	0.58
2:G:252:LEU:HD13	2:G:353:LEU:HD11	1.85	0.58
2:I:61:GLY:HA2	2:I:72:PRO:HG3	1.85	0.58
2:B:341:TYR:CE1	2:C:337:LYS:HG3	2.38	0.58
2:D:75:VAL:HG12	2:D:75:VAL:O	2.01	0.58
3:E:90:VAL:CG1	4:K:8:DT:H5"	2.33	0.58
3:E:224:VAL:CB	3:E:225:PRO:HD3	2.32	0.58
3:J:112:VAL:HB	3:J:141:PHE:CD1	2.38	0.58
1:A:39:ARG:NH2	1:A:50:HIS:HB3	2.17	0.58
2:H:53:SER:OG	6:H:408:ADP:O1A	2.21	0.58
2:I:24:VAL:HG21	2:I:175:LEU:CD2	2.32	0.58
2:C:254:GLU:O	2:C:257:VAL:HG22	2.03	0.58
2:D:80:ARG:O	2:D:84:GLN:HG3	2.03	0.58
3:J:213:ARG:HH21	3:J:267:ASN:HD22	1.49	0.58
3:E:197:SER:OG	3:E:200:ALA:HB3	2.03	0.58
2:C:40:ALA:CB	2:C:170:CYS:HB3	2.34	0.58
2:D:232:VAL:O	2:D:232:VAL:HG12	2.01	0.58
3:E:88:LEU:HD23	3:E:120:LEU:HD23	1.86	0.58
3:E:224:VAL:HG12	3:E:225:PRO:N	2.17	0.58
1:F:198:THR:HG23	1:F:201:ARG:HD2	1.84	0.58
1:A:17:LEU:CD1	1:A:45:GLN:HE21	2.17	0.58
2:C:347:MET:HG2	2:D:290:HIS:CG	2.38	0.58
2:G:365:LEU:HD12	2:G:366:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:246:ASP:HB3	2:H:309:ILE:HD12	1.84	0.58
2:C:28:LEU:HD22	2:C:58:LEU:HD22	1.85	0.58
2:H:248:GLN:O	2:H:248:GLN:HG3	2.02	0.58
1:A:28:PRO:HB3	2:B:164:VAL:HG21	1.86	0.57
2:H:283:VAL:HA	2:H:286:LEU:HD12	1.84	0.57
2:I:257:VAL:HG21	2:I:320:ILE:HD11	1.85	0.57
1:F:237:ARG:HG3	1:F:321:TRP:CE2	2.39	0.57
2:I:75:VAL:O	2:I:75:VAL:HG12	2.04	0.57
2:C:6:LEU:O	2:C:7:ALA:C	2.47	0.57
2:D:216:ASP:OD1	3:E:157:SER:CB	2.52	0.57
2:D:354:LEU:HD12	3:E:253:MET:HE2	1.87	0.57
1:A:56:ASP:HB2	1:A:58:ASN:HB2	1.84	0.57
2:B:343:PRO:HG3	2:C:286:LEU:HB2	1.86	0.57
3:E:80:ALA:HB1	3:E:81:PRO:HD3	1.86	0.57
3:J:2:ARG:HD3	3:J:4:TYR:HE1	1.66	0.57
3:J:103:HIS:CD2	3:J:103:HIS:H	2.21	0.57
4:M:9:DA:C2'	4:M:10:DG:O5'	2.51	0.57
1:A:52:THR:HG22	1:A:81:LEU:HD23	1.86	0.57
3:E:88:LEU:HD23	3:E:120:LEU:CD2	2.34	0.57
1:F:128:THR:O	1:F:131:ALA:CB	2.53	0.57
2:H:279:GLU:OE2	2:H:336:ARG:NE	2.37	0.57
3:J:80:ALA:HB1	3:J:81:PRO:CD	2.35	0.57
1:A:198:THR:HG23	1:A:201:ARG:HD2	1.85	0.57
2:C:60:LYS:HA	2:C:82:ILE:HD12	1.85	0.57
3:E:169:GLU:O	3:E:173:VAL:HG23	2.04	0.57
1:F:13:LEU:HD22	1:F:21:TYR:CZ	2.39	0.57
2:D:178:LEU:HD13	2:D:214:LEU:HD12	1.87	0.57
2:I:30:ASN:O	2:I:34:LEU:HG	2.05	0.57
2:C:271:ALA:O	2:C:276:ILE:HG23	2.04	0.57
2:G:341:TYR:O	2:H:336:ARG:NH1	2.37	0.57
2:I:215:ARG:NH1	3:J:157:SER:OG	2.38	0.57
1:A:12:GLN:O	1:A:12:GLN:HG3	2.03	0.56
2:C:277:GLU:O	2:C:280:ALA:HB3	2.04	0.56
2:C:339:LEU:N	2:C:340:PRO:HD2	2.20	0.56
3:E:259:HIS:ND1	3:J:259:HIS:ND1	2.52	0.56
2:G:341:TYR:CE1	2:H:337:LYS:HG3	2.40	0.56
1:F:17:LEU:CD1	1:F:45:GLN:HE21	2.18	0.56
2:G:240:MET:O	2:G:243:THR:HB	2.05	0.56
3:J:3:TRP:CH2	3:J:8:ARG:HG3	2.40	0.56
1:F:21:TYR:CE1	1:F:135:VAL:HB	2.41	0.56
1:F:318:GLN:CD	1:F:318:GLN:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:114:ALA:HA	2:G:149:HIS:CD2	2.41	0.56
3:J:121:THR:HG22	3:J:123:ALA:H	1.70	0.56
2:C:244:LEU:H	2:C:244:LEU:HD12	1.70	0.56
3:E:48:LEU:HD13	3:E:140:TRP:CD1	2.40	0.56
3:E:213:ARG:HH21	3:E:267:ASN:HD22	1.54	0.56
3:J:46:ARG:HH22	3:J:69:GLN:HE21	1.54	0.56
1:F:101:THR:HG21	1:F:126:TRP:HB2	1.87	0.56
1:F:280:GLN:HA	1:F:283:ARG:HG3	1.87	0.56
2:H:216:ASP:OD1	2:I:168:SER:HA	2.05	0.56
2:H:260:ASN:O	2:H:264:VAL:HG23	2.05	0.56
1:A:13:LEU:HD22	1:A:21:TYR:CZ	2.41	0.56
2:B:351:MET:HG2	2:C:290:HIS:HD2	1.71	0.56
2:C:104:THR:OG1	2:C:135:SER:HB2	2.06	0.56
2:D:344:ASP:HB2	2:D:347:MET:H	1.71	0.56
3:E:35:MET:HE1	3:E:166:PRO:HA	1.87	0.56
2:H:15:PHE:CE1	2:H:57:LEU:HB3	2.41	0.56
1:A:128:THR:O	1:A:131:ALA:HB3	2.06	0.56
2:G:93:ILE:HG12	2:G:107:LEU:HD22	1.88	0.56
2:I:128:VAL:HG22	2:I:128:VAL:O	2.05	0.56
2:H:44:SER:CB	2:H:159:PRO:HG3	2.35	0.55
2:I:6:LEU:H	2:I:6:LEU:HD12	1.71	0.55
2:I:21:GLN:NE2	2:I:49:VAL:CG1	2.67	0.55
5:N:4:DG:H2''	5:N:5:DC:O5'	2.07	0.55
2:C:49:VAL:HG11	2:C:176:LYS:O	2.06	0.55
1:A:71:MET:CB	1:A:108:LEU:HG	2.36	0.55
2:C:341:TYR:CB	2:D:333:LEU:HD11	2.37	0.55
2:D:24:VAL:HG21	2:D:175:LEU:CD2	2.36	0.55
3:E:117:ALA:HB3	3:E:145:THR:HG23	1.88	0.55
2:H:47:ARG:HD2	2:I:164:VAL:HG22	1.89	0.55
2:I:184:ARG:CD	2:I:204:GLN:HE21	2.19	0.55
2:C:260:ASN:O	2:C:264:VAL:HG23	2.06	0.55
1:A:81:LEU:HD12	1:A:82:LEU:H	1.71	0.55
2:B:265:MET:HE1	2:B:350:GLU:CG	2.31	0.55
4:K:2:DT:H2''	4:K:3:DT:OP1	2.06	0.55
1:A:175:GLU:OE2	1:A:228:ARG:NH2	2.39	0.55
2:B:128:VAL:HG12	2:B:156:THR:HB	1.88	0.55
2:I:243:THR:CG2	2:I:244:LEU:N	2.70	0.55
3:J:169:GLU:O	3:J:173:VAL:HG23	2.06	0.55
2:C:259:ALA:HB2	2:C:360:HIS:CE1	2.41	0.55
1:F:39:ARG:NH2	1:F:50:HIS:HB3	2.21	0.55
1:F:71:MET:CB	1:F:108:LEU:HG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:362:ARG:O	2:I:363:MET:CG	2.47	0.55
2:D:119:ARG:HG2	2:D:120:PHE:CD2	2.41	0.55
1:A:127:PHE:HA	1:A:130:LEU:HD12	1.87	0.55
1:A:250:LEU:HD23	1:A:305:LEU:HD13	1.89	0.55
2:C:215:ARG:HD2	2:D:168:SER:OG	2.06	0.55
2:G:128:VAL:O	2:G:128:VAL:HG22	2.05	0.55
3:J:264:GLN:HG3	3:J:265:VAL:N	2.20	0.55
2:I:164:VAL:HG22	2:I:164:VAL:O	2.05	0.55
1:A:101:THR:HG21	1:A:126:TRP:HB2	1.88	0.54
2:I:202:ALA:HB2	2:I:234:THR:HA	1.89	0.54
2:I:309:ILE:HG22	2:I:309:ILE:O	2.06	0.54
2:B:292:ILE:HD13	2:B:316:LEU:HD23	1.89	0.54
1:A:160:LEU:HD11	1:A:189:SER:HB3	1.89	0.54
1:A:179:LEU:HG	1:A:179:LEU:O	2.07	0.54
2:B:147:PRO:HB2	2:B:150:VAL:HG23	1.89	0.54
2:B:365:LEU:HD12	2:B:366:PRO:HD2	1.88	0.54
1:F:190:LEU:CD2	2:G:36:ARG:HD2	2.37	0.54
4:K:10:DG:H2''	4:K:11:DG:O5'	2.08	0.54
2:I:244:LEU:HD21	2:I:276:ILE:HG12	1.88	0.54
3:J:199:GLY:HA2	3:J:202:LEU:CB	2.35	0.54
2:B:20:GLY:O	2:B:21:GLN:HB2	2.06	0.54
3:J:80:ALA:HB1	3:J:81:PRO:HD3	1.89	0.54
1:A:26:ASN:ND2	1:A:140:GLN:OE1	2.40	0.54
1:A:48:GLU:O	1:A:50:HIS:HD2	1.90	0.54
3:E:35:MET:CE	3:E:166:PRO:HA	2.38	0.54
2:G:175:LEU:HD23	2:G:175:LEU:N	2.23	0.54
2:H:327:LEU:HD23	2:H:361:PRO:HG3	1.90	0.54
1:A:268:PRO:HD2	1:A:271:ALA:HB3	1.88	0.54
1:F:248:ARG:HG3	4:M:4:DT:H4'	1.89	0.54
2:D:210:ALA:HB2	2:D:217:ALA:HB2	1.89	0.54
2:D:159:PRO:HD2	2:D:160:GLN:H	1.70	0.54
2:D:321:PRO:HD2	2:D:324:ASP:HB2	1.90	0.54
3:J:35:MET:HG2	3:J:197:SER:HB2	1.90	0.54
3:J:271:PRO:HD2	3:J:272:GLY:H	1.72	0.54
1:A:90:ASN:O	1:A:94:ASN:HB2	2.07	0.53
1:A:278:VAL:HG12	1:A:283:ARG:HG2	1.90	0.53
1:A:237:ARG:HG3	1:A:321:TRP:CD2	2.43	0.53
2:B:240:MET:O	2:B:243:THR:HB	2.08	0.53
2:B:288:LEU:HD23	2:B:288:LEU:N	2.21	0.53
2:D:124:LEU:HD12	2:D:153:LEU:O	2.08	0.53
2:G:351:MET:HG2	2:H:290:HIS:CD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ILE:HG12	2:B:107:LEU:HD22	1.90	0.53
2:D:265:MET:HE2	3:E:257:LYS:CD	2.38	0.53
2:G:-1:PRO:O	2:G:1:MET:HE2	2.09	0.53
2:I:6:LEU:HD13	2:I:222:ASP:OD2	2.08	0.53
1:A:13:LEU:CD1	1:A:38:VAL:HG22	2.37	0.53
2:H:111:VAL:HG13	2:H:150:VAL:HG21	1.91	0.53
2:H:276:ILE:HD11	2:H:281:LEU:HD22	1.89	0.53
2:B:38:HIS:ND1	2:B:38:HIS:N	2.57	0.53
2:B:114:ALA:HA	2:B:149:HIS:CD2	2.43	0.53
2:C:51:LYS:CG	6:C:402:ADP:O2B	2.57	0.53
2:C:215:ARG:O	2:C:216:ASP:C	2.51	0.53
1:F:282:ARG:HG2	1:F:282:ARG:NH1	2.24	0.53
2:G:52:THR:HG21	2:G:126:ASP:OD2	2.08	0.53
2:H:324:ASP:O	2:H:327:LEU:HB3	2.07	0.53
2:I:40:ALA:HA	2:I:152:PHE:O	2.08	0.53
2:I:252:LEU:CD1	2:I:285:MET:HE2	2.38	0.53
7:I:411:BEF:F2	3:J:158:ARG:NH1	2.27	0.53
2:D:123:TYR:HB2	2:D:152:PHE:CD2	2.44	0.53
3:E:264:GLN:HG3	3:E:265:VAL:N	2.21	0.53
2:C:101:VAL:HG23	4:K:12:DC:OP1	2.09	0.53
2:C:147:PRO:HB2	2:C:149:HIS:CE1	2.43	0.53
2:C:268:ILE:HD11	2:C:353:LEU:HD12	1.90	0.53
1:A:86:GLU:OE2	1:A:86:GLU:HA	2.09	0.53
3:E:2:ARG:CG	3:E:3:TRP:N	2.71	0.53
1:F:17:LEU:HD11	1:F:45:GLN:HE21	1.74	0.53
1:F:55:ILE:HG22	1:F:93:ILE:HD13	1.91	0.53
1:F:237:ARG:HG3	1:F:321:TRP:CD2	2.44	0.53
2:G:49:VAL:HG12	2:G:49:VAL:O	2.09	0.53
2:G:327:LEU:HD12	2:G:330:GLN:OE1	2.09	0.53
2:H:60:LYS:HA	2:H:82:ILE:HD12	1.90	0.53
2:B:49:VAL:HG12	2:B:49:VAL:O	2.07	0.53
2:G:80:ARG:O	2:G:84:GLN:HG2	2.08	0.53
2:H:339:LEU:N	2:H:340:PRO:HD2	2.24	0.53
3:J:15:VAL:O	3:J:18:TYR:N	2.42	0.53
1:A:42:ALA:O	1:A:47:PHE:HD1	1.92	0.53
2:B:21:GLN:HE22	2:B:176:LYS:H	1.57	0.53
2:B:260:ASN:HD22	2:B:263:ARG:CB	2.17	0.53
2:D:362:ARG:O	2:D:363:MET:CG	2.49	0.53
2:G:158:ASP:OD1	2:G:160:GLN:HB3	2.09	0.53
2:H:140:LEU:HD22	2:H:169:ARG:CZ	2.39	0.53
4:K:12:DC:H2''	4:K:13:DC:O5'	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:LEU:HD12	2:D:6:LEU:N	2.24	0.52
2:D:24:VAL:HG21	2:D:175:LEU:HD22	1.91	0.52
3:E:15:VAL:O	3:E:18:TYR:N	2.42	0.52
3:J:155:LEU:HD12	3:J:155:LEU:O	2.08	0.52
2:C:111:VAL:HG13	2:C:150:VAL:HG21	1.90	0.52
2:I:354:LEU:HD12	3:J:253:MET:HE2	1.90	0.52
3:J:81:PRO:HB3	3:J:87:THR:O	2.09	0.52
1:F:74:PHE:O	1:F:74:PHE:CG	2.62	0.52
2:H:15:PHE:HE1	2:H:57:LEU:HB3	1.72	0.52
2:I:323:THR:HB	2:I:362:ARG:NH2	2.25	0.52
1:A:14:ASN:O	1:A:15:GLU:C	2.53	0.52
1:A:128:THR:O	1:A:131:ALA:CB	2.58	0.52
1:A:304:LEU:HD23	1:A:327:LEU:HD13	1.91	0.52
2:D:252:LEU:HG	2:D:267:LEU:HD23	1.91	0.52
2:D:291:ARG:O	2:D:292:ILE:C	2.53	0.52
1:F:90:ASN:O	1:F:94:ASN:HB2	2.09	0.52
1:F:162:LEU:HD22	1:F:166:ALA:HB3	1.91	0.52
2:G:38:HIS:ND1	2:G:38:HIS:N	2.57	0.52
2:G:39:HIS:H	2:G:39:HIS:HD2	1.55	0.52
2:H:291:ARG:HD2	2:H:306:MET:SD	2.49	0.52
2:D:21:GLN:HE22	2:D:49:VAL:CG1	2.22	0.52
1:F:42:ALA:O	1:F:47:PHE:HD1	1.93	0.52
1:F:122:GLU:O	1:F:127:PHE:CD2	2.63	0.52
2:I:46:THR:HB	2:I:47:ARG:HE	1.74	0.52
1:A:179:LEU:HD11	2:B:168:SER:HA	1.91	0.52
2:B:80:ARG:O	2:B:84:GLN:HG2	2.10	0.52
2:D:184:ARG:CD	2:D:204:GLN:HE21	2.23	0.52
2:G:42:LEU:HG	2:G:172:GLN:HG3	1.91	0.52
3:J:72:THR:HG23	3:J:72:THR:O	2.10	0.52
2:C:44:SER:CB	2:C:159:PRO:HG3	2.40	0.52
2:H:243:THR:HG22	2:H:244:LEU:O	2.10	0.52
3:J:2:ARG:CG	3:J:3:TRP:N	2.72	0.52
2:B:295:VAL:HA	2:B:298:SER:O	2.10	0.52
2:C:254:GLU:OE2	2:C:312:ARG:CD	2.58	0.52
2:H:47:ARG:HD3	2:H:47:ARG:H	1.75	0.52
1:A:84:LEU:HD11	1:A:112:VAL:HG13	1.91	0.52
2:B:150:VAL:O	2:B:151:LYS:HD3	2.10	0.52
2:B:215:ARG:NH2	7:B:401:BEF:F2	2.30	0.52
2:G:245:ASP:C	2:G:247:ASP:H	2.16	0.52
1:A:26:ASN:OD1	1:A:27:ASP:N	2.43	0.51
1:A:142:PRO:HB2	1:A:147:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:260:ASN:HD22	2:G:263:ARG:CB	2.21	0.51
1:A:13:LEU:HD13	1:A:38:VAL:HG22	1.91	0.51
2:D:111:VAL:HG13	2:D:150:VAL:HG21	1.91	0.51
3:E:154:THR:O	3:E:158:ARG:HD2	2.09	0.51
1:F:24:LEU:HD11	1:F:117:LEU:HD11	1.92	0.51
2:H:6:LEU:O	2:H:7:ALA:C	2.53	0.51
2:I:94:ASP:CG	2:I:97:SER:HB2	2.35	0.51
2:I:111:VAL:HG13	2:I:150:VAL:HG21	1.93	0.51
2:C:347:MET:HG3	2:D:290:HIS:CE1	2.45	0.51
2:D:261:GLY:HA2	2:D:357:LEU:HD21	1.92	0.51
2:G:21:GLN:HE22	2:G:176:LYS:H	1.59	0.51
2:H:28:LEU:HD22	2:H:58:LEU:HD22	1.92	0.51
2:H:254:GLU:O	2:H:257:VAL:HG22	2.11	0.51
2:I:302:LEU:CD1	2:I:306:MET:HG3	2.40	0.51
4:M:10:DG:H2''	4:M:11:DG:O5'	2.10	0.51
1:A:56:ASP:HB2	1:A:58:ASN:H	1.75	0.51
1:A:261:LYS:HE2	1:A:293:LEU:O	2.11	0.51
2:C:316:LEU:HD23	2:C:320:ILE:HD11	1.92	0.51
2:D:259:ALA:HB2	2:D:360:HIS:HB2	1.92	0.51
1:F:21:TYR:CD1	1:F:135:VAL:HB	2.45	0.51
2:H:104:THR:OG1	2:H:135:SER:HB2	2.11	0.51
2:C:248:GLN:O	2:C:248:GLN:HG3	2.09	0.51
1:F:42:ALA:O	1:F:47:PHE:CD1	2.64	0.51
1:F:261:LYS:HE2	1:F:293:LEU:O	2.08	0.51
2:G:320:ILE:HG23	2:G:321:PRO:HD2	1.92	0.51
2:I:302:LEU:HD21	2:I:310:GLU:HB2	1.92	0.51
2:C:337:LYS:NZ	3:E:334:LEU:HD22	2.26	0.51
2:C:339:LEU:HD11	2:C:345:ARG:O	2.10	0.51
2:G:128:VAL:HG12	2:G:156:THR:HB	1.92	0.51
3:J:241:ALA:N	3:J:242:PRO:CD	2.73	0.51
1:A:17:LEU:HD11	1:A:45:GLN:HE21	1.75	0.51
3:E:121:THR:CG2	3:E:122:ASP:N	2.74	0.51
1:F:50:HIS:ND1	1:F:79:THR:HB	2.25	0.51
1:A:55:ILE:HG22	1:A:93:ILE:HD13	1.91	0.51
1:A:181:LEU:O	1:A:184:ALA:HB3	2.11	0.51
2:B:215:ARG:HD3	6:B:400:ADP:H5'1	1.93	0.51
2:D:93:ILE:HD11	2:D:107:LEU:HD21	1.92	0.51
2:H:73:CYS:O	2:H:75:VAL:HG13	2.11	0.51
2:I:344:ASP:HB2	2:I:347:MET:H	1.76	0.51
3:J:285:ARG:O	3:J:289:ILE:HG13	2.11	0.51
2:C:360:HIS:CD2	2:C:361:PRO:HD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:224:VAL:HG12	3:J:225:PRO:N	2.24	0.50
2:B:215:ARG:O	2:B:216:ASP:C	2.54	0.50
2:C:367:GLU:CD	2:D:362:ARG:HH12	2.19	0.50
1:F:59:THR:HG23	1:F:63:ALA:CB	2.39	0.50
1:F:81:LEU:HD12	1:F:82:LEU:H	1.76	0.50
1:A:142:PRO:CD	1:A:178:LEU:HD11	2.41	0.50
2:B:178:LEU:HD12	2:B:214:LEU:HB2	1.92	0.50
1:F:90:ASN:OD1	1:F:92:ALA:HB3	2.11	0.50
2:G:178:LEU:CD1	2:G:214:LEU:HD22	2.42	0.50
2:H:365:LEU:HD11	2:I:297:LEU:HD12	1.92	0.50
5:N:6:DC:H2''	5:N:7:DT:O5'	2.10	0.50
1:A:21:TYR:CD1	1:A:135:VAL:HB	2.47	0.50
2:B:252:LEU:HD13	2:B:353:LEU:HD11	1.94	0.50
2:C:216:ASP:OD1	2:D:168:SER:HA	2.11	0.50
2:C:341:TYR:HB2	2:D:333:LEU:HD11	1.92	0.50
3:E:279:ASN:O	3:J:282:SER:HB2	2.11	0.50
1:F:4:LEU:HD12	1:F:135:VAL:CG1	2.42	0.50
2:G:147:PRO:HB2	2:G:150:VAL:HG23	1.94	0.50
2:G:257:VAL:HG21	2:G:320:ILE:CD1	2.40	0.50
2:G:347:MET:HG2	2:H:290:HIS:CE1	2.46	0.50
2:H:147:PRO:HB2	2:H:149:HIS:CE1	2.46	0.50
2:I:123:TYR:HB2	2:I:152:PHE:CD2	2.47	0.50
3:J:62:CYS:O	3:J:66:GLN:HG3	2.11	0.50
3:J:121:THR:CG2	3:J:122:ASP:N	2.74	0.50
1:A:74:PHE:O	1:A:74:PHE:CG	2.64	0.50
1:F:22:LEU:HD13	1:F:127:PHE:HE1	1.76	0.50
1:A:97:LEU:HD13	1:A:126:TRP:CZ3	2.47	0.50
2:C:190:ILE:HD12	2:C:218:LEU:HD21	1.94	0.50
2:H:51:LYS:CG	6:H:408:ADP:O2B	2.60	0.50
2:H:355:ARG:O	2:H:356:ALA:C	2.53	0.50
2:I:129:HIS:CD2	2:I:130:MET:HG2	2.46	0.50
2:C:367:GLU:HG3	2:C:368:PRO:CD	2.39	0.50
2:D:64:CYS:SG	2:D:66:THR:HG23	2.52	0.50
1:F:64:ILE:HG13	1:F:96:GLN:HB3	1.94	0.50
1:A:42:ALA:O	1:A:47:PHE:CD1	2.65	0.50
1:A:59:THR:HG23	1:A:63:ALA:CB	2.38	0.50
2:B:14:THR:HG22	2:B:16:ALA:H	1.77	0.50
2:B:158:ASP:OD1	2:B:160:GLN:HB3	2.12	0.50
2:C:64:CYS:SG	2:C:66:THR:HG23	2.51	0.50
2:C:316:LEU:CD2	2:C:320:ILE:HD11	2.42	0.50
1:F:26:ASN:ND2	1:F:140:GLN:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:365:LEU:HD11	2:H:297:LEU:HD23	1.94	0.50
1:A:21:TYR:CE1	1:A:135:VAL:HB	2.46	0.50
1:A:104:LEU:HD13	1:A:133:ARG:CD	2.42	0.50
2:D:179:ASP:HB3	2:D:182:GLN:HG3	1.93	0.50
2:H:360:HIS:CD2	2:H:361:PRO:HD2	2.47	0.50
2:I:210:ALA:HB2	2:I:217:ALA:HB2	1.93	0.50
2:I:243:THR:HG22	2:I:244:LEU:H	1.76	0.50
2:B:78:ASN:O	2:B:82:ILE:HG13	2.12	0.49
2:B:94:ASP:OD1	2:B:94:ASP:C	2.54	0.49
2:B:119:ARG:HG2	2:B:119:ARG:NH1	2.26	0.49
2:B:327:LEU:HD12	2:B:330:GLN:OE1	2.11	0.49
3:E:271:PRO:HD2	3:E:272:GLY:H	1.77	0.49
2:I:56:ARG:HD3	2:I:92:GLU:OE1	2.12	0.49
1:A:58:ASN:O	1:A:59:THR:C	2.54	0.49
2:C:321:PRO:O	2:C:324:ASP:HB2	2.12	0.49
2:G:129:HIS:CD2	2:G:130:MET:SD	3.05	0.49
2:I:150:VAL:O	2:I:151:LYS:HD3	2.13	0.49
1:A:31:LEU:O	1:A:32:GLN:C	2.55	0.49
2:B:257:VAL:HG22	2:B:328:TYR:CE2	2.47	0.49
2:B:341:TYR:CZ	2:C:337:LYS:HG3	2.47	0.49
2:I:159:PRO:HD2	2:I:160:GLN:H	1.77	0.49
2:C:136:PHE:O	2:C:139:LEU:HB2	2.12	0.49
1:F:2:ILE:HG13	1:F:18:ARG:NH1	2.27	0.49
1:F:67:LEU:O	1:F:70:ALA:HB3	2.12	0.49
1:F:250:LEU:HG	1:F:250:LEU:O	2.09	0.49
2:G:13:GLN:HG3	2:G:83:GLU:OE2	2.12	0.49
2:H:124:LEU:HA	2:H:153:LEU:O	2.13	0.49
2:H:337:LYS:HZ1	3:J:334:LEU:HD22	1.77	0.49
3:J:271:PRO:CD	3:J:272:GLY:H	2.24	0.49
2:B:125:ILE:HB	2:B:154:LEU:CD2	2.43	0.49
3:E:35:MET:HG2	3:E:197:SER:HB2	1.93	0.49
2:H:145:GLU:N	2:H:146:PRO:HD3	2.27	0.49
2:I:6:LEU:HD12	2:I:6:LEU:N	2.27	0.49
1:A:278:VAL:O	1:A:279:TRP:C	2.55	0.49
2:B:234:THR:O	2:B:238:SER:HB3	2.12	0.49
2:D:243:THR:CG2	2:D:244:LEU:N	2.76	0.49
2:I:21:GLN:HE22	2:I:49:VAL:CG1	2.26	0.49
1:A:48:GLU:O	1:A:50:HIS:CD2	2.66	0.49
1:A:55:ILE:O	1:A:85:PRO:HG3	2.13	0.49
2:C:324:ASP:O	2:C:327:LEU:HB3	2.12	0.49
2:D:61:GLY:CA	2:D:72:PRO:HG3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:VAL:CG1	2:D:156:THR:HB	2.43	0.49
3:E:3:TRP:CH2	3:E:8:ARG:HG3	2.45	0.49
3:E:155:LEU:HD12	3:E:155:LEU:O	2.13	0.49
1:F:13:LEU:HD22	1:F:21:TYR:CE1	2.47	0.49
2:H:215:ARG:HD2	2:I:168:SER:OG	2.13	0.49
3:J:232:LEU:O	3:J:233:LEU:C	2.55	0.49
1:A:2:ILE:HG13	1:A:18:ARG:NH1	2.27	0.49
2:C:140:LEU:HD22	2:C:169:ARG:CZ	2.43	0.49
1:F:48:GLU:O	1:F:50:HIS:HD2	1.95	0.49
2:G:367:GLU:HG3	2:G:368:PRO:HD2	1.95	0.49
3:J:188:LEU:HD12	3:J:192:ARG:HD2	1.93	0.49
3:J:213:ARG:NH1	3:J:213:ARG:HG2	2.28	0.49
2:C:327:LEU:HD23	2:C:361:PRO:HG3	1.94	0.49
3:E:73:HIS:ND1	3:E:73:HIS:C	2.70	0.49
2:H:268:ILE:HD11	2:H:353:LEU:HD12	1.95	0.49
1:A:24:LEU:HD11	1:A:117:LEU:HD11	1.94	0.49
2:C:265:MET:HG2	2:D:297:LEU:CD2	2.43	0.49
2:D:87:PHE:CE2	2:D:89:ASP:HB2	2.48	0.49
3:E:232:LEU:O	3:E:233:LEU:C	2.55	0.49
1:F:142:PRO:CD	1:F:178:LEU:HD11	2.43	0.49
2:H:51:LYS:HG3	6:H:408:ADP:O2B	2.13	0.49
2:H:196:ILE:HD12	2:H:225:ILE:CD1	2.43	0.49
2:H:276:ILE:O	2:H:276:ILE:HG13	2.13	0.49
2:H:295:VAL:O	2:H:296:GLN:C	2.56	0.49
2:H:351:MET:HE2	2:I:290:HIS:CB	2.43	0.49
1:A:237:ARG:HG3	1:A:321:TRP:CE2	2.47	0.48
2:B:101:VAL:HG21	2:B:134:HIS:CB	2.30	0.48
2:C:101:VAL:HA	2:C:135:SER:HB3	1.94	0.48
2:D:40:ALA:HA	2:D:152:PHE:O	2.12	0.48
2:D:69:THR:HG21	2:D:72:PRO:HA	1.95	0.48
3:E:106:LEU:O	3:E:106:LEU:CD2	2.53	0.48
3:E:188:LEU:HD12	3:E:192:ARG:HD2	1.95	0.48
2:G:13:GLN:OE1	2:G:83:GLU:HG3	2.13	0.48
2:H:271:ALA:O	2:H:276:ILE:HG23	2.13	0.48
2:I:252:LEU:HG	2:I:267:LEU:HD23	1.94	0.48
1:A:110:LEU:HD11	1:A:112:VAL:CG2	2.43	0.48
2:B:367:GLU:HG3	2:B:368:PRO:HD2	1.95	0.48
2:D:215:ARG:O	2:D:216:ASP:C	2.56	0.48
1:F:42:ALA:O	1:F:47:PHE:HB2	2.13	0.48
1:A:67:LEU:O	1:A:70:ALA:HB3	2.12	0.48
1:A:174:TYR:O	1:A:175:GLU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:282:LEU:O	2:C:286:LEU:HD12	2.13	0.48
3:E:271:PRO:CD	3:E:272:GLY:H	2.26	0.48
3:J:114:VAL:HB	3:J:143:LEU:CD2	2.42	0.48
1:A:144:GLN:NE2	1:A:228:ARG:NE	2.61	0.48
2:C:46:THR:HB	2:C:47:ARG:HE	1.78	0.48
2:D:15:PHE:CE2	2:D:57:LEU:HB3	2.49	0.48
2:I:215:ARG:O	2:I:216:ASP:C	2.57	0.48
4:K:9:DA:C2'	4:K:10:DG:O5'	2.59	0.48
1:A:199:LEU:N	1:A:200:PRO:HD2	2.28	0.48
2:D:38:HIS:CD2	2:D:39:HIS:N	2.82	0.48
3:E:176:LEU:O	3:E:178:ARG:N	2.46	0.48
1:F:84:LEU:HD11	1:F:112:VAL:HG13	1.96	0.48
2:C:260:ASN:C	2:C:260:ASN:OD1	2.55	0.48
2:D:269:ASN:ND2	3:E:264:GLN:HB3	2.28	0.48
1:F:101:THR:HG22	1:F:130:LEU:HD21	1.95	0.48
2:H:293:ALA:HB2	2:H:325:ILE:HG21	1.96	0.48
2:H:321:PRO:O	2:H:324:ASP:HB2	2.14	0.48
2:I:101:VAL:CG2	2:I:134:HIS:HB3	2.44	0.48
2:I:215:ARG:HG2	3:J:157:SER:O	2.14	0.48
2:I:314:ARG:O	2:I:318:ARG:HG3	2.13	0.48
3:J:202:LEU:C	3:J:202:LEU:CD2	2.86	0.48
1:A:48:GLU:HG3	1:A:49:GLU:HG3	1.95	0.48
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.61	0.48
2:G:13:GLN:CD	2:G:83:GLU:HG3	2.39	0.48
2:H:101:VAL:HG22	2:H:134:HIS:HB3	1.95	0.48
2:H:339:LEU:HD11	2:H:345:ARG:O	2.13	0.48
1:A:117:LEU:HB2	1:A:122:GLU:CG	2.44	0.48
1:A:117:LEU:HB2	1:A:122:GLU:HG3	1.95	0.48
1:A:144:GLN:HE22	1:A:228:ARG:NE	2.10	0.48
2:C:347:MET:CG	2:D:290:HIS:CD2	2.96	0.48
2:D:87:PHE:HE2	2:D:89:ASP:HB2	1.79	0.48
1:F:190:LEU:HD21	2:G:36:ARG:HD2	1.95	0.48
2:H:260:ASN:C	2:H:260:ASN:OD1	2.56	0.48
5:N:2:DT:H2''	5:N:3:DG:C8	2.48	0.48
2:B:47:ARG:HD3	2:B:47:ARG:N	2.29	0.48
2:G:101:VAL:O	2:G:102:GLU:C	2.57	0.48
2:I:76:CYS:O	2:I:77:ASP:C	2.54	0.48
3:J:90:VAL:HG12	4:M:8:DT:H5''	1.95	0.48
2:B:115:PRO:CD	2:B:149:HIS:HD2	2.14	0.48
2:B:215:ARG:C	2:B:217:ALA:N	2.68	0.48
3:E:81:PRO:HB3	3:E:87:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:ASN:O	1:F:59:THR:C	2.56	0.48
1:F:174:TYR:O	1:F:175:GLU:C	2.57	0.48
2:B:47:ARG:NH2	2:B:211:GLU:O	2.47	0.47
2:C:73:CYS:O	2:C:75:VAL:HG13	2.14	0.47
2:C:291:ARG:O	2:C:294:MET:HB3	2.13	0.47
2:D:354:LEU:CD1	3:E:253:MET:HE2	2.44	0.47
2:G:351:MET:HE2	2:H:290:HIS:CB	2.44	0.47
2:H:282:LEU:O	2:H:286:LEU:HD12	2.14	0.47
2:B:91:ILE:HD12	2:B:123:TYR:CZ	2.49	0.47
3:E:182:MET:HG3	3:E:205:PHE:CD1	2.49	0.47
2:I:38:HIS:CD2	2:I:39:HIS:N	2.81	0.47
3:J:117:ALA:HB3	3:J:145:THR:HG23	1.96	0.47
2:B:294:MET:C	2:B:296:GLN:H	2.23	0.47
2:D:167:LEU:O	2:D:169:ARG:N	2.47	0.47
2:D:215:ARG:NH1	3:E:157:SER:OG	2.47	0.47
2:D:302:LEU:CD1	2:D:306:MET:HG3	2.44	0.47
3:E:199:GLY:HA2	3:E:202:LEU:CB	2.43	0.47
1:F:56:ASP:HB2	1:F:58:ASN:CB	2.45	0.47
2:H:320:ILE:HG22	2:H:321:PRO:HD2	1.95	0.47
2:I:178:LEU:CD1	2:I:214:LEU:HD12	2.43	0.47
2:I:321:PRO:HD2	2:I:324:ASP:HB2	1.94	0.47
2:B:324:ASP:O	2:B:327:LEU:N	2.47	0.47
2:C:58:LEU:C	2:C:58:LEU:HD12	2.39	0.47
3:E:2:ARG:HG2	3:E:3:TRP:N	2.28	0.47
1:F:31:LEU:O	1:F:32:GLN:C	2.57	0.47
1:F:254:LEU:O	1:F:254:LEU:HG	2.11	0.47
2:G:15:PHE:HE2	2:G:57:LEU:CB	2.19	0.47
2:H:76:CYS:O	2:H:77:ASP:C	2.56	0.47
3:J:229:TRP:O	3:J:316:LEU:HD13	2.14	0.47
2:B:42:LEU:HG	2:B:172:GLN:HG3	1.96	0.47
2:C:47:ARG:HD3	2:C:47:ARG:H	1.79	0.47
2:D:21:GLN:HE21	2:D:49:VAL:HG12	1.72	0.47
2:D:52:THR:HG21	2:D:126:ASP:OD2	2.14	0.47
1:F:54:SER:HB3	1:F:83:LEU:HD12	1.96	0.47
2:G:5:VAL:HG21	2:H:39:HIS:ND1	2.29	0.47
2:G:274:ARG:NH2	2:G:276:ILE:CG1	2.77	0.47
2:G:291:ARG:O	2:G:295:VAL:HG23	2.15	0.47
2:C:254:GLU:OE2	2:C:312:ARG:HD3	2.14	0.47
1:F:13:LEU:CD2	1:F:21:TYR:CE1	2.98	0.47
2:G:215:ARG:NH2	2:H:169:ARG:NH1	2.63	0.47
2:B:183:ILE:HG12	2:B:214:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ALA:HB2	2:B:281:LEU:HD12	1.97	0.47
2:C:58:LEU:HD12	2:C:58:LEU:O	2.15	0.47
2:C:139:LEU:HD23	2:C:139:LEU:HA	1.60	0.47
2:C:254:GLU:HG2	2:C:316:LEU:HD11	1.96	0.47
2:C:274:ARG:HB2	2:C:276:ILE:HG23	1.97	0.47
1:F:14:ASN:O	1:F:15:GLU:C	2.58	0.47
2:G:46:THR:HG22	2:G:47:ARG:HD3	1.97	0.47
2:H:316:LEU:HD23	2:H:320:ILE:HD11	1.97	0.47
3:J:48:LEU:HD13	3:J:140:TRP:CD1	2.50	0.47
3:J:197:SER:OG	3:J:200:ALA:CB	2.63	0.47
1:A:82:LEU:HD12	1:A:110:LEU:HD11	1.97	0.47
1:A:298:LEU:O	1:A:301:ALA:HB3	2.15	0.47
2:B:58:LEU:HA	2:B:58:LEU:HD12	1.58	0.47
2:B:245:ASP:C	2:B:247:ASP:H	2.21	0.47
2:D:150:VAL:O	2:D:151:LYS:HD3	2.15	0.47
1:F:48:GLU:HG3	1:F:49:GLU:HG3	1.97	0.47
2:G:250:LEU:HA	2:G:288:LEU:HD12	1.97	0.47
2:H:291:ARG:O	2:H:294:MET:HB3	2.15	0.47
2:I:28:LEU:HD23	2:I:28:LEU:HA	1.63	0.47
1:A:162:LEU:HD23	1:A:197:LEU:HB2	1.96	0.47
2:D:76:CYS:O	2:D:77:ASP:C	2.58	0.47
1:F:181:LEU:O	1:F:184:ALA:HB3	2.14	0.47
2:G:277:GLU:O	2:G:280:ALA:HB3	2.15	0.47
2:H:13:GLN:C	2:H:57:LEU:HD21	2.40	0.47
2:I:259:ALA:HB2	2:I:360:HIS:HB2	1.96	0.47
1:A:56:ASP:HB2	1:A:58:ASN:CB	2.44	0.47
1:A:64:ILE:HG13	1:A:96:GLN:HB3	1.97	0.47
1:A:287:GLY:O	1:A:288:GLU:C	2.57	0.47
2:D:290:HIS:O	2:D:291:ARG:C	2.58	0.47
2:G:125:ILE:HB	2:G:154:LEU:CD2	2.44	0.47
2:H:46:THR:O	2:H:49:VAL:HG23	2.15	0.47
2:C:101:VAL:HG22	2:C:134:HIS:HB3	1.94	0.46
2:D:129:HIS:ND1	2:D:156:THR:OG1	2.25	0.46
2:D:159:PRO:CD	2:D:160:GLN:H	2.29	0.46
3:E:285:ARG:O	3:E:289:ILE:HG13	2.15	0.46
2:G:101:VAL:CG2	2:G:134:HIS:CB	2.92	0.46
2:G:332:LEU:HD23	2:G:332:LEU:HA	1.81	0.46
2:I:269:ASN:ND2	2:I:346:ARG:HH22	2.13	0.46
1:A:42:ALA:O	1:A:47:PHE:HB2	2.15	0.46
2:B:21:GLN:HA	2:B:21:GLN:HE21	1.79	0.46
2:C:40:ALA:HB1	2:C:170:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:THR:CG2	1:F:81:LEU:HD23	2.45	0.46
1:F:127:PHE:HA	1:F:130:LEU:HD12	1.97	0.46
2:G:150:VAL:O	2:G:151:LYS:HD3	2.16	0.46
3:J:224:VAL:CB	3:J:225:PRO:CD	2.92	0.46
1:A:81:LEU:HD12	1:A:82:LEU:N	2.30	0.46
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.75	0.46
2:C:341:TYR:CZ	2:D:337:LYS:HD2	2.50	0.46
3:E:152:LEU:HA	3:E:152:LEU:HD12	1.60	0.46
1:F:196:LYS:HB2	1:F:196:LYS:HE3	1.68	0.46
2:G:215:ARG:C	2:G:217:ALA:N	2.73	0.46
2:G:276:ILE:CG2	2:G:277:GLU:N	2.75	0.46
2:H:15:PHE:CD2	2:H:25:LEU:HD22	2.50	0.46
1:A:13:LEU:HD22	1:A:21:TYR:CE1	2.51	0.46
2:B:101:VAL:O	2:B:102:GLU:C	2.59	0.46
2:D:15:PHE:HE2	2:D:57:LEU:HB3	1.81	0.46
2:G:94:ASP:OD1	2:G:94:ASP:C	2.59	0.46
2:G:115:PRO:CD	2:G:149:HIS:HD2	2.15	0.46
2:B:276:ILE:CG2	2:B:277:GLU:N	2.79	0.46
2:B:291:ARG:HA	2:B:291:ARG:HD3	1.77	0.46
2:D:164:VAL:O	2:D:164:VAL:HG22	2.16	0.46
3:E:202:LEU:C	3:E:202:LEU:CD2	2.88	0.46
1:F:56:ASP:HB2	1:F:58:ASN:H	1.80	0.46
2:I:244:LEU:HD23	2:I:244:LEU:HA	1.61	0.46
3:J:30:GLN:O	3:J:30:GLN:HG3	2.15	0.46
3:J:233:LEU:O	3:J:234:ALA:C	2.59	0.46
1:A:81:LEU:HD21	1:A:83:LEU:HD21	1.98	0.46
1:A:254:LEU:O	1:A:254:LEU:HG	2.16	0.46
1:F:117:LEU:HB2	1:F:122:GLU:HG3	1.96	0.46
1:F:257:LEU:O	1:F:258:VAL:C	2.58	0.46
2:I:88:VAL:O	2:I:88:VAL:CG1	2.63	0.46
3:J:182:MET:HG3	3:J:205:PHE:CD1	2.51	0.46
5:L:4:DG:H2''	5:L:5:DC:O5'	2.15	0.46
1:A:190:LEU:HD11	2:B:38:HIS:HE1	1.80	0.46
1:A:253:GLU:OE1	1:A:286:MET:HE1	2.15	0.46
2:B:134:HIS:CG	4:K:14:DA:H5''	2.51	0.46
2:B:178:LEU:CD1	2:B:214:LEU:HD22	2.45	0.46
2:B:293:ALA:HB2	2:B:325:ILE:HG21	1.97	0.46
2:C:272:ALA:CB	2:C:346:ARG:NH1	2.78	0.46
2:C:282:LEU:O	2:C:286:LEU:CD1	2.64	0.46
2:D:52:THR:CG2	6:D:404:ADP:O1B	2.54	0.46
2:D:286:LEU:HD23	2:D:286:LEU:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:-8:LEU:HD12	2:G:-8:LEU:HA	1.73	0.46
2:I:313:MET:HE2	2:I:313:MET:HA	1.97	0.46
2:I:353:LEU:HD23	2:I:353:LEU:HA	1.69	0.46
3:J:300:LEU:HD23	3:J:300:LEU:HA	1.52	0.46
1:A:84:LEU:HD11	1:A:112:VAL:CG1	2.46	0.46
1:A:90:ASN:OD1	1:A:92:ALA:HB3	2.16	0.46
2:B:358:ALA:HA	2:B:365:LEU:HB3	1.98	0.46
2:C:282:LEU:CD1	2:C:349:VAL:HG22	2.45	0.46
2:G:191:LEU:HD23	2:G:191:LEU:HA	1.74	0.46
2:G:358:ALA:HA	2:G:365:LEU:HB3	1.98	0.46
2:I:15:PHE:CE2	2:I:57:LEU:HB3	2.50	0.46
2:I:101:VAL:HG21	2:I:134:HIS:HB3	1.97	0.46
2:B:360:HIS:O	2:B:364:PRO:HG3	2.16	0.46
2:B:365:LEU:CD1	2:C:297:LEU:HD23	2.45	0.46
1:F:81:LEU:HD12	1:F:82:LEU:N	2.31	0.46
2:H:279:GLU:O	2:H:283:VAL:HG23	2.16	0.46
2:H:291:ARG:HE	2:H:291:ARG:HB2	1.39	0.46
2:H:341:TYR:CB	2:I:333:LEU:HD11	2.45	0.46
4:K:10:DG:H2''	4:K:11:DG:C5'	2.45	0.46
1:A:316:TYR:CD1	5:L:10:DA:H2''	2.50	0.46
2:B:89:ASP:OD2	2:B:116:ALA:N	2.47	0.46
2:B:351:MET:HE3	2:C:329:TYR:CD1	2.51	0.46
2:C:21:GLN:OE1	2:C:21:GLN:HA	2.16	0.46
1:F:190:LEU:HD11	2:G:38:HIS:HE1	1.80	0.46
1:F:278:VAL:HG12	1:F:283:ARG:HG2	1.98	0.46
3:J:308:ARG:O	3:J:309:GLU:C	2.57	0.46
1:A:122:GLU:O	1:A:127:PHE:CD2	2.69	0.45
2:B:293:ALA:O	2:B:296:GLN:HB2	2.16	0.45
1:F:162:LEU:HD23	1:F:197:LEU:HB2	1.98	0.45
1:F:263:GLN:HB2	1:F:272:LEU:CD1	2.47	0.45
2:H:277:GLU:O	2:H:280:ALA:HB3	2.16	0.45
1:A:22:LEU:HD13	1:A:127:PHE:HE1	1.80	0.45
2:D:306:MET:O	2:D:308:ALA:N	2.48	0.45
3:E:4:TYR:HB3	3:E:6:TRP:CH2	2.52	0.45
3:E:229:TRP:O	3:E:316:LEU:HD13	2.17	0.45
2:H:353:LEU:O	2:H:356:ALA:HB3	2.15	0.45
2:I:167:LEU:O	2:I:169:ARG:N	2.50	0.45
1:A:146:GLN:H	1:A:146:GLN:HG3	1.58	0.45
2:C:196:ILE:HD12	2:C:225:ILE:CD1	2.46	0.45
2:C:281:LEU:HG	2:C:285:MET:HE3	1.98	0.45
1:F:268:PRO:HD2	1:F:271:ALA:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:276:ILE:HG23	2:G:277:GLU:N	2.31	0.45
3:J:2:ARG:HG2	3:J:3:TRP:N	2.31	0.45
2:B:94:ASP:OD2	2:C:141:LYS:HB2	2.17	0.45
2:B:358:ALA:HA	2:B:365:LEU:CB	2.46	0.45
2:D:56:ARG:HD3	2:D:92:GLU:OE1	2.16	0.45
2:D:244:LEU:HD23	2:D:244:LEU:HA	1.57	0.45
2:D:291:ARG:O	2:D:294:MET:N	2.50	0.45
2:B:320:ILE:HG23	2:B:321:PRO:HD2	1.97	0.45
2:C:260:ASN:O	2:C:260:ASN:OD1	2.35	0.45
2:D:306:MET:HB3	2:D:306:MET:HE3	1.69	0.45
1:F:55:ILE:CG2	1:F:93:ILE:HD13	2.45	0.45
1:F:261:LYS:CE	1:F:293:LEU:O	2.65	0.45
2:G:41:TYR:N	2:G:41:TYR:CD1	2.84	0.45
2:G:78:ASN:O	2:G:82:ILE:HG13	2.15	0.45
2:G:89:ASP:OD2	2:G:116:ALA:N	2.49	0.45
2:G:215:ARG:O	2:G:216:ASP:C	2.58	0.45
2:I:11:ARG:O	2:I:13:GLN:HG2	2.15	0.45
2:I:221:THR:O	2:I:225:ILE:HG13	2.17	0.45
1:A:71:MET:SD	1:A:103:LEU:HB3	2.57	0.45
2:C:76:CYS:O	2:C:77:ASP:C	2.60	0.45
2:D:6:LEU:C	2:D:8:ARG:H	2.24	0.45
2:D:101:VAL:CG2	2:D:134:HIS:HB3	2.46	0.45
2:D:264:VAL:HG12	2:D:265:MET:N	2.29	0.45
1:F:117:LEU:HB2	1:F:122:GLU:CG	2.45	0.45
2:G:215:ARG:NH2	7:G:407:BEF:F2	2.37	0.45
2:G:223:GLN:HB2	2:H:171:LEU:HD22	1.99	0.45
2:G:274:ARG:NH2	2:G:276:ILE:HG12	2.31	0.45
2:I:61:GLY:CA	2:I:72:PRO:HG3	2.46	0.45
1:A:23:LEU:HD21	1:A:34:SER:HB3	1.99	0.45
2:B:343:PRO:HB3	2:C:283:VAL:HG13	1.99	0.45
2:C:320:ILE:HG22	2:C:321:PRO:HD2	1.97	0.45
3:E:258:ARG:NH1	3:E:275:ALA:HA	2.31	0.45
1:F:4:LEU:HD12	1:F:135:VAL:HG13	1.99	0.45
1:F:55:ILE:HD11	1:F:82:LEU:HB3	1.98	0.45
1:F:172:TYR:CD2	1:F:172:TYR:C	2.95	0.45
2:H:215:ARG:O	2:H:216:ASP:C	2.60	0.45
2:H:351:MET:HE2	2:I:290:HIS:HA	1.84	0.45
2:I:15:PHE:HE2	2:I:57:LEU:HB3	1.81	0.45
2:I:210:ALA:O	2:I:211:GLU:C	2.59	0.45
2:I:276:ILE:HG21	2:I:281:LEU:HD13	1.98	0.45
3:J:253:MET:HE3	3:J:290:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:6:DC:H2''	5:L:7:DT:O5'	2.17	0.45
1:A:75:ALA:O	1:A:76:SER:C	2.60	0.45
1:A:150:TRP:CZ3	1:A:178:LEU:HD22	2.52	0.45
2:C:40:ALA:HB3	2:C:170:CYS:HB3	1.97	0.45
2:D:167:LEU:O	2:D:168:SER:C	2.58	0.45
2:D:259:ALA:HB2	2:D:360:HIS:CB	2.47	0.45
3:E:2:ARG:HD3	3:E:4:TYR:HE1	1.72	0.45
1:F:26:ASN:OD1	1:F:27:ASP:N	2.49	0.45
1:F:187:ARG:HG3	2:G:173:PHE:CE1	2.52	0.45
2:H:306:MET:HE2	2:H:306:MET:HB3	1.77	0.45
1:A:39:ARG:NH1	1:A:50:HIS:HB3	2.30	0.45
2:B:175:LEU:HD23	2:B:175:LEU:N	2.32	0.45
2:C:159:PRO:O	2:C:162:LEU:HG	2.17	0.45
2:D:361:PRO:HB2	3:J:272:GLY:HA2	1.95	0.45
2:I:6:LEU:H	2:I:6:LEU:CD1	2.29	0.45
3:J:154:THR:O	3:J:158:ARG:HD2	2.17	0.45
3:J:271:PRO:CD	3:J:272:GLY:N	2.78	0.45
1:A:53:PHE:HZ	1:A:63:ALA:HB1	1.81	0.45
2:C:344:ASP:OD2	2:C:347:MET:HE3	2.16	0.45
2:D:6:LEU:C	2:D:8:ARG:N	2.74	0.45
1:F:75:ALA:O	1:F:76:SER:C	2.60	0.45
1:F:82:LEU:HD12	1:F:110:LEU:HD11	1.99	0.45
2:G:250:LEU:HD23	2:G:312:ARG:CZ	2.47	0.45
2:G:320:ILE:HG21	2:G:325:ILE:HG13	1.97	0.45
2:G:359:PHE:CD1	2:G:359:PHE:N	2.84	0.45
2:H:40:ALA:CB	2:H:170:CYS:HB3	2.46	0.45
2:I:6:LEU:CD1	2:I:222:ASP:OD2	2.65	0.45
2:I:13:GLN:OE1	2:I:60:LYS:NZ	2.50	0.45
2:D:306:MET:O	2:D:309:ILE:N	2.49	0.44
2:D:323:THR:HB	2:D:362:ARG:NH2	2.32	0.44
2:G:106:ASP:O	2:G:107:LEU:C	2.59	0.44
2:I:56:ARG:NH1	2:I:92:GLU:OE2	2.50	0.44
1:A:81:LEU:HD12	1:A:111:ILE:O	2.17	0.44
1:A:163:ASP:OD2	1:A:198:THR:HA	2.17	0.44
2:C:107:LEU:HD23	2:C:107:LEU:HA	1.82	0.44
2:C:119:ARG:NH1	2:C:119:ARG:HG3	2.33	0.44
2:C:276:ILE:HD11	2:C:281:LEU:HD22	1.98	0.44
3:E:121:THR:HG22	3:E:123:ALA:H	1.83	0.44
2:G:288:LEU:HD23	2:G:288:LEU:N	2.32	0.44
2:G:292:ILE:HD13	2:G:316:LEU:HD23	1.99	0.44
2:G:324:ASP:O	2:G:327:LEU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:190:ILE:HD12	2:H:218:LEU:HD21	1.98	0.44
2:I:25:LEU:HD21	2:I:54:ILE:CD1	2.48	0.44
3:J:81:PRO:O	3:J:82:GLU:C	2.60	0.44
1:A:27:ASP:HA	1:A:28:PRO:HD3	1.82	0.44
1:A:48:GLU:HG3	1:A:49:GLU:N	2.32	0.44
1:A:81:LEU:HD13	1:A:111:ILE:HG22	2.00	0.44
2:B:346:ARG:O	2:B:347:MET:C	2.59	0.44
2:C:235:GLN:HA	2:C:235:GLN:OE1	2.18	0.44
3:E:15:VAL:O	3:E:18:TYR:HB2	2.17	0.44
3:E:176:LEU:C	3:E:178:ARG:N	2.75	0.44
1:F:257:LEU:HD23	1:F:257:LEU:HA	1.74	0.44
2:H:46:THR:HB	2:H:47:ARG:HE	1.82	0.44
2:I:119:ARG:HG2	2:I:120:PHE:CD2	2.52	0.44
3:J:152:LEU:HD12	3:J:152:LEU:HA	1.54	0.44
1:A:285:MET:O	1:A:288:GLU:HB3	2.18	0.44
2:B:20:GLY:C	2:B:22:GLU:HG3	2.42	0.44
2:C:21:GLN:O	2:C:22:GLU:C	2.60	0.44
2:C:279:GLU:OE2	2:C:336:ARG:NE	2.51	0.44
3:E:329:LEU:HA	3:E:330:PRO:HD3	1.82	0.44
1:F:156:LYS:O	1:F:159:ASN:N	2.47	0.44
2:G:47:ARG:NH2	2:G:211:GLU:O	2.50	0.44
2:G:351:MET:HE2	2:H:290:HIS:HB2	1.98	0.44
2:H:263:ARG:O	2:H:267:LEU:HB2	2.18	0.44
2:H:316:LEU:CD2	2:H:320:ILE:HD11	2.48	0.44
2:I:282:LEU:HA	2:I:282:LEU:HD23	1.57	0.44
3:J:252:LEU:HD23	3:J:252:LEU:HA	1.76	0.44
4:M:6:DT:H2"	4:M:7:DA:C8	2.53	0.44
2:C:115:PRO:HD3	2:C:149:HIS:CD2	2.39	0.44
2:D:139:LEU:O	2:D:140:LEU:C	2.61	0.44
1:F:162:LEU:HD23	1:F:162:LEU:HA	1.80	0.44
2:G:295:VAL:HA	2:G:298:SER:O	2.17	0.44
2:H:261:GLY:O	2:H:262:GLU:C	2.60	0.44
2:H:341:TYR:CE1	2:I:337:LYS:HD2	2.52	0.44
1:A:4:LEU:HD12	1:A:135:VAL:CG1	2.47	0.44
1:A:101:THR:HG22	1:A:130:LEU:HD21	2.00	0.44
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.81	0.44
2:B:164:VAL:HG13	2:B:165:THR:N	2.33	0.44
2:D:94:ASP:CG	2:D:97:SER:HB2	2.42	0.44
3:E:172:ALA:HB1	3:E:198:PRO:HG3	1.99	0.44
1:F:230:LEU:N	1:F:230:LEU:HD23	2.33	0.44
2:G:224:ALA:O	2:G:225:ILE:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:HG22	1:A:181:LEU:HD21	2.00	0.44
1:A:190:LEU:HD11	2:B:38:HIS:CE1	2.52	0.44
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.72	0.44
1:A:257:LEU:O	1:A:258:VAL:C	2.60	0.44
2:C:243:THR:HG22	2:C:244:LEU:O	2.18	0.44
2:D:199:GLU:O	2:D:200:PRO:C	2.60	0.44
3:E:176:LEU:HD23	3:E:176:LEU:HA	1.69	0.44
3:E:213:ARG:NH1	3:E:213:ARG:HG2	2.33	0.44
1:F:48:GLU:HG3	1:F:49:GLU:N	2.33	0.44
2:H:281:LEU:HG	2:H:285:MET:HE3	2.00	0.44
2:I:139:LEU:O	2:I:140:LEU:C	2.60	0.44
3:J:271:PRO:HD2	3:J:272:GLY:N	2.31	0.44
4:M:10:DG:H2''	4:M:11:DG:C5'	2.48	0.44
2:C:295:VAL:CG2	2:C:302:LEU:HB2	2.47	0.44
2:C:306:MET:HB3	2:C:306:MET:HE2	1.75	0.44
2:G:10:TRP:CE2	2:G:190:ILE:HG23	2.52	0.44
2:H:254:GLU:OE2	2:H:312:ARG:CD	2.66	0.44
2:I:184:ARG:HD2	2:I:204:GLN:HE21	1.82	0.44
3:J:207:GLY:C	3:J:209:ASN:H	2.25	0.44
1:A:55:ILE:CG2	1:A:93:ILE:HD13	2.47	0.44
2:B:42:LEU:HD12	2:B:154:LEU:O	2.18	0.44
2:B:101:VAL:HA	2:B:135:SER:OG	2.17	0.44
2:B:321:PRO:O	2:B:324:ASP:HB2	2.17	0.44
2:D:302:LEU:HD12	2:D:306:MET:HG3	2.00	0.44
2:G:21:GLN:NE2	2:G:21:GLN:CA	2.80	0.44
2:H:47:ARG:NH2	2:H:211:GLU:O	2.51	0.44
2:H:223:GLN:HG3	2:H:240:MET:HE1	2.00	0.44
6:H:408:ADP:H2'	6:H:408:ADP:N3	2.32	0.44
1:A:9:LEU:O	1:A:10:ARG:C	2.60	0.43
1:A:13:LEU:CD2	1:A:21:TYR:CE1	3.01	0.43
1:A:54:SER:HB3	1:A:83:LEU:HD12	2.00	0.43
1:A:273:PHE:HB3	1:A:283:ARG:HD2	2.00	0.43
2:B:128:VAL:O	2:B:128:VAL:CG2	2.65	0.43
2:D:101:VAL:HG21	2:D:134:HIS:HB3	2.00	0.43
2:D:333:LEU:C	2:D:333:LEU:HD12	2.42	0.43
1:F:39:ARG:NH1	1:F:50:HIS:HB3	2.32	0.43
2:G:306:MET:O	2:G:308:ALA:N	2.50	0.43
2:I:93:ILE:HD11	2:I:107:LEU:HD21	1.99	0.43
2:I:302:LEU:HD12	2:I:306:MET:HG3	1.98	0.43
2:I:354:LEU:HD23	2:I:354:LEU:HA	1.85	0.43
2:B:101:VAL:CG2	2:B:134:HIS:CB	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:HIS:O	2:C:291:ARG:C	2.61	0.43
3:E:176:LEU:C	3:E:178:ARG:H	2.26	0.43
3:E:241:ALA:N	3:E:242:PRO:CD	2.81	0.43
1:F:71:MET:SD	1:F:103:LEU:HB3	2.58	0.43
1:F:97:LEU:HD13	1:F:126:TRP:CZ3	2.53	0.43
1:F:273:PHE:HB3	1:F:283:ARG:HD2	1.99	0.43
2:G:20:GLY:C	2:G:22:GLU:HG3	2.44	0.43
2:I:257:VAL:HG12	2:I:328:TYR:CE2	2.53	0.43
3:J:15:VAL:O	3:J:16:ALA:C	2.60	0.43
3:J:306:ILE:CG1	3:J:307:ASN:N	2.81	0.43
1:A:9:LEU:HD11	1:A:13:LEU:HD21	2.00	0.43
1:A:156:LYS:O	1:A:159:ASN:N	2.51	0.43
1:A:172:TYR:CD2	1:A:172:TYR:C	2.96	0.43
2:D:28:LEU:HD23	2:D:28:LEU:HA	1.75	0.43
2:D:282:LEU:HD23	2:D:282:LEU:HA	1.63	0.43
2:D:306:MET:O	2:D:307:ALA:C	2.60	0.43
3:E:73:HIS:CE1	3:E:75:ASP:HB2	2.54	0.43
1:F:250:LEU:HD23	1:F:305:LEU:HD13	1.99	0.43
1:F:278:VAL:O	1:F:279:TRP:C	2.61	0.43
1:F:319:SER:O	1:F:320:VAL:C	2.61	0.43
2:G:42:LEU:HD12	2:G:154:LEU:O	2.18	0.43
2:G:91:ILE:HG22	2:G:93:ILE:CD1	2.49	0.43
2:I:6:LEU:C	2:I:8:ARG:H	2.26	0.43
1:A:82:LEU:HD12	1:A:112:VAL:HG22	2.00	0.43
2:C:223:GLN:HB3	2:D:171:LEU:HD22	1.99	0.43
1:F:71:MET:CG	1:F:103:LEU:HD13	2.47	0.43
2:H:292:ILE:HG22	2:H:325:ILE:CD1	2.48	0.43
2:H:299:PRO:O	2:H:314:ARG:NH2	2.52	0.43
2:I:306:MET:O	2:I:308:ALA:N	2.51	0.43
3:J:220:LEU:HD12	3:J:220:LEU:HA	1.59	0.43
1:A:251:GLN:O	1:A:252:ARG:C	2.60	0.43
2:B:6:LEU:HG	2:B:222:ASP:OD1	2.18	0.43
2:B:338:GLU:HB3	2:C:333:LEU:HD21	2.00	0.43
3:E:224:VAL:CB	3:E:225:PRO:CD	2.96	0.43
3:E:257:LYS:HB3	3:E:262:ALA:HB3	2.01	0.43
1:F:53:PHE:HZ	1:F:63:ALA:HB1	1.83	0.43
2:H:21:GLN:OE1	2:H:21:GLN:HA	2.18	0.43
2:H:229:ASP:CB	2:I:30:ASN:HD21	2.31	0.43
2:B:91:ILE:HG22	2:B:93:ILE:CD1	2.48	0.43
2:B:274:ARG:NH2	2:B:276:ILE:HG12	2.34	0.43
3:E:67:LEU:HD22	3:E:72:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:327:VAL:HG12	3:E:328:VAL:N	2.33	0.43
1:F:86:GLU:OE2	1:F:86:GLU:HA	2.16	0.43
1:F:110:LEU:HD11	1:F:112:VAL:CG2	2.49	0.43
1:F:173:CYS:SG	1:F:206:VAL:CG1	3.07	0.43
2:G:343:PRO:HG3	2:H:286:LEU:HB2	1.98	0.43
2:G:353:LEU:O	2:G:356:ALA:HB3	2.19	0.43
2:H:320:ILE:HA	2:H:321:PRO:HD3	1.79	0.43
2:I:136:PHE:HB3	2:I:163:PRO:HG2	2.00	0.43
2:I:245:ASP:OD1	2:I:245:ASP:O	2.36	0.43
1:A:38:VAL:CG1	1:A:111:ILE:HD11	2.48	0.43
1:A:71:MET:CG	1:A:103:LEU:HD13	2.48	0.43
1:A:245:ILE:O	1:A:245:ILE:HG22	2.18	0.43
2:B:28:LEU:O	2:B:29:ALA:C	2.61	0.43
2:B:124:LEU:HD12	2:B:124:LEU:C	2.44	0.43
2:C:254:GLU:O	2:C:258:GLU:HG3	2.18	0.43
2:G:82:ILE:HG23	2:G:90:LEU:HD23	1.99	0.43
2:H:93:ILE:HD11	2:H:107:LEU:HD22	1.99	0.43
2:I:38:HIS:CD2	2:I:40:ALA:H	2.15	0.43
2:B:90:LEU:HD12	2:B:122:VAL:O	2.18	0.43
2:B:215:ARG:NH2	2:C:169:ARG:NH1	2.66	0.43
2:D:6:LEU:H	2:D:6:LEU:CD1	2.29	0.43
2:D:41:TYR:HD2	2:D:173:PHE:HE2	1.64	0.43
3:E:62:CYS:O	3:E:66:GLN:HG3	2.19	0.43
3:E:152:LEU:O	3:E:153:ALA:C	2.62	0.43
2:G:4:GLN:HE22	2:G:9:LYS:HG3	1.76	0.43
2:G:291:ARG:HA	2:G:291:ARG:HD3	1.77	0.43
2:H:13:GLN:HA	2:H:13:GLN:OE1	2.19	0.43
2:H:44:SER:HA	2:H:156:THR:O	2.19	0.43
2:I:6:LEU:C	2:I:8:ARG:N	2.76	0.43
2:B:13:GLN:HB3	2:B:60:LYS:NZ	2.34	0.43
2:D:101:VAL:C	2:D:103:ASP:N	2.75	0.43
2:D:143:LEU:HA	2:D:143:LEU:HD12	1.74	0.43
1:F:150:TRP:CZ3	1:F:178:LEU:HD22	2.54	0.43
1:F:276:HIS:O	1:F:277:ARG:HB2	2.19	0.43
2:G:297:LEU:N	2:G:297:LEU:HD12	2.33	0.43
2:H:21:GLN:HE21	2:H:49:VAL:HG12	1.82	0.43
2:H:272:ALA:CB	2:H:346:ARG:NH1	2.81	0.43
2:I:143:LEU:HD12	2:I:143:LEU:HA	1.69	0.43
2:I:245:ASP:O	2:I:245:ASP:CG	2.62	0.43
3:J:51:GLN:HE21	3:J:51:GLN:HB2	1.66	0.43
5:L:1:DC:H1'	5:L:2:DT:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:OE1	1:A:286:MET:CE	2.67	0.43
2:C:23:HIS:HE1	2:C:174:HIS:O	2.00	0.43
2:C:101:VAL:HG21	2:C:134:HIS:HB3	2.00	0.43
2:C:145:GLU:N	2:C:146:PRO:HD3	2.34	0.43
2:D:77:ASP:O	2:D:81:GLU:HG3	2.19	0.43
2:D:341:TYR:N	2:D:341:TYR:CD1	2.87	0.43
3:E:197:SER:OG	3:E:200:ALA:CB	2.67	0.43
2:G:14:THR:HG22	2:G:16:ALA:H	1.84	0.43
3:J:27:LEU:CD1	3:J:160:ARG:HG2	2.49	0.43
3:J:286:LEU:HA	3:J:286:LEU:HD23	1.78	0.43
1:A:93:ILE:O	1:A:93:ILE:HG22	2.19	0.42
2:B:10:TRP:CE2	2:B:190:ILE:HG23	2.54	0.42
2:C:46:THR:O	2:C:49:VAL:HG23	2.18	0.42
1:F:82:LEU:HD12	1:F:112:VAL:HG22	2.01	0.42
1:F:298:LEU:HD23	1:F:298:LEU:HA	1.82	0.42
2:G:24:VAL:HG21	2:G:175:LEU:CD2	2.48	0.42
2:H:296:GLN:O	2:H:297:LEU:C	2.62	0.42
2:I:111:VAL:O	2:I:112:GLN:C	2.62	0.42
2:I:243:THR:CG2	2:I:244:LEU:H	2.30	0.42
2:I:265:MET:HE2	3:J:257:LYS:CD	2.45	0.42
2:I:320:ILE:HA	2:I:321:PRO:HD3	1.88	0.42
3:J:129:LEU:HD23	3:J:129:LEU:HA	1.76	0.42
3:J:238:HIS:O	3:J:308:ARG:HD3	2.19	0.42
1:A:56:ASP:C	1:A:58:ASN:H	2.25	0.42
2:B:82:ILE:HG12	2:B:87:PHE:CB	2.49	0.42
2:B:343:PRO:HG3	2:C:286:LEU:CB	2.49	0.42
2:D:14:THR:O	2:D:15:PHE:C	2.61	0.42
1:F:65:PHE:CD2	1:F:65:PHE:O	2.72	0.42
2:G:46:THR:O	2:G:47:ARG:C	2.61	0.42
2:H:47:ARG:HD2	2:I:164:VAL:CG2	2.47	0.42
2:H:152:PHE:O	2:H:153:LEU:HD23	2.19	0.42
2:I:87:PHE:CE2	2:I:89:ASP:HB2	2.53	0.42
1:A:142:PRO:HD2	1:A:178:LEU:HD11	2.01	0.42
1:A:196:LYS:O	1:A:197:LEU:HD23	2.20	0.42
2:B:320:ILE:HG21	2:B:325:ILE:HG13	2.01	0.42
2:B:339:LEU:N	2:B:340:PRO:CD	2.82	0.42
2:C:139:LEU:O	2:C:143:LEU:HB2	2.18	0.42
2:C:244:LEU:HD21	2:C:276:ILE:HD13	2.00	0.42
2:C:265:MET:HE2	2:C:354:LEU:CD2	2.39	0.42
2:G:124:LEU:HD12	2:G:124:LEU:C	2.43	0.42
1:A:50:HIS:ND1	1:A:79:THR:HB	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HD23	1:A:126:TRP:HB3	2.01	0.42
2:B:179:ASP:HB3	2:B:182:GLN:HG3	2.02	0.42
2:D:11:ARG:O	2:D:13:GLN:HG2	2.19	0.42
2:D:156:THR:O	2:D:156:THR:HG23	2.19	0.42
2:D:309:ILE:HG22	2:D:309:ILE:O	2.18	0.42
3:E:163:TYR:CD1	3:E:164:LEU:N	2.88	0.42
3:E:187:LEU:O	3:E:188:LEU:C	2.63	0.42
1:F:98:LEU:HD23	1:F:126:TRP:HB3	2.00	0.42
1:F:173:CYS:SG	1:F:206:VAL:HG11	2.59	0.42
2:G:358:ALA:HA	2:G:365:LEU:CB	2.49	0.42
2:H:23:HIS:HE1	2:H:174:HIS:O	2.02	0.42
2:H:253:VAL:O	2:H:254:GLU:C	2.62	0.42
2:H:281:LEU:C	2:H:283:VAL:N	2.77	0.42
3:J:128:LEU:HD12	3:J:128:LEU:HA	1.85	0.42
2:B:274:ARG:NH2	2:B:276:ILE:CG1	2.82	0.42
2:C:293:ALA:HB2	2:C:325:ILE:HG21	2.01	0.42
2:D:140:LEU:HD23	2:D:140:LEU:HA	1.82	0.42
1:F:147:LEU:HB3	1:F:148:PRO:HD3	2.02	0.42
1:F:233:LEU:HA	1:F:233:LEU:HD23	1.74	0.42
2:H:327:LEU:HD12	2:H:327:LEU:O	2.19	0.42
2:I:129:HIS:ND1	2:I:156:THR:OG1	2.34	0.42
2:I:167:LEU:O	2:I:168:SER:C	2.62	0.42
1:A:84:LEU:CD1	1:A:112:VAL:HG13	2.49	0.42
2:B:49:VAL:O	2:B:49:VAL:CG1	2.66	0.42
2:B:328:TYR:HH	2:B:360:HIS:CD2	2.38	0.42
3:J:27:LEU:HD12	3:J:160:ARG:HG2	2.02	0.42
3:J:316:LEU:HA	3:J:316:LEU:HD23	1.71	0.42
1:A:56:ASP:C	1:A:58:ASN:N	2.76	0.42
2:B:13:GLN:HB3	2:B:60:LYS:HZ2	1.84	0.42
2:B:46:THR:O	2:B:47:ARG:C	2.61	0.42
2:B:347:MET:CE	2:C:291:ARG:HH21	2.33	0.42
2:D:291:ARG:HD3	2:D:291:ARG:HA	1.84	0.42
3:E:15:VAL:O	3:E:16:ALA:C	2.62	0.42
3:E:73:HIS:HE1	3:E:75:ASP:HB2	1.85	0.42
3:E:148:PRO:O	3:E:151:LEU:HB2	2.19	0.42
2:G:13:GLN:HB3	2:G:60:LYS:NZ	2.35	0.42
1:A:237:ARG:O	1:A:240:GLY:N	2.44	0.42
1:A:312:LEU:HD12	1:A:312:LEU:O	2.19	0.42
2:B:107:LEU:HD12	2:B:107:LEU:HA	1.75	0.42
2:B:215:ARG:O	2:B:217:ALA:N	2.52	0.42
2:C:296:GLN:O	2:C:297:LEU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:GLN:NE2	2:D:271:ALA:HB2	2.34	0.42
2:G:216:ASP:CG	2:H:168:SER:HB2	2.43	0.42
2:H:367:GLU:HA	2:H:368:PRO:HD3	1.85	0.42
2:B:115:PRO:CD	2:B:149:HIS:CD2	2.96	0.42
2:C:223:GLN:HG3	2:C:240:MET:HE1	2.02	0.42
2:D:101:VAL:O	2:D:102:GLU:C	2.61	0.42
2:D:252:LEU:HD13	2:D:285:MET:HE1	2.00	0.42
2:G:119:ARG:CG	2:G:119:ARG:HH11	2.32	0.42
2:H:292:ILE:CG1	2:H:313:MET:CE	2.93	0.42
2:I:101:VAL:C	2:I:103:ASP:N	2.77	0.42
2:I:106:ASP:O	2:I:107:LEU:C	2.62	0.42
2:I:291:ARG:O	2:I:292:ILE:C	2.62	0.42
2:I:294:MET:HE3	2:I:301:ALA:HB1	2.02	0.42
2:I:306:MET:O	2:I:307:ALA:C	2.63	0.42
1:A:4:LEU:HD12	1:A:135:VAL:HG13	2.02	0.42
2:B:240:MET:O	2:B:240:MET:HG2	2.18	0.42
2:C:337:LYS:HE2	3:E:334:LEU:HD22	2.00	0.42
2:C:347:MET:CG	2:D:290:HIS:CG	3.03	0.42
2:D:13:GLN:OE1	2:D:60:LYS:NZ	2.53	0.42
1:F:261:LYS:HE2	1:F:290:LEU:O	2.19	0.42
2:G:265:MET:HE1	2:G:350:GLU:CG	2.46	0.42
2:H:205:LEU:HD23	2:H:205:LEU:HA	1.80	0.42
2:H:265:MET:HE2	2:H:354:LEU:CD2	2.43	0.42
3:J:48:LEU:HD23	3:J:48:LEU:HA	1.74	0.42
3:J:257:LYS:HB3	3:J:262:ALA:HB3	2.01	0.42
1:A:196:LYS:HB2	1:A:196:LYS:HE3	1.62	0.41
2:C:143:LEU:HD12	2:C:152:PHE:CD2	2.55	0.41
2:D:210:ALA:CB	2:D:217:ALA:HB2	2.48	0.41
2:D:314:ARG:O	2:D:318:ARG:HG3	2.19	0.41
2:H:130:MET:HE2	2:I:137:ASN:HB2	2.02	0.41
2:I:124:LEU:HD12	2:I:153:LEU:O	2.20	0.41
2:I:247:ASP:O	2:I:249:ALA:N	2.53	0.41
1:A:55:ILE:HD11	1:A:82:LEU:HB3	2.02	0.41
1:A:94:ASN:OD1	1:A:126:TRP:NE1	2.46	0.41
2:B:15:PHE:CE2	2:B:57:LEU:CB	2.96	0.41
2:B:94:ASP:OD1	2:B:94:ASP:O	2.38	0.41
2:C:158:ASP:HA	2:C:159:PRO:HD3	1.67	0.41
2:C:263:ARG:O	2:C:267:LEU:HB2	2.20	0.41
3:E:29:ILE:CD1	3:E:40:LEU:HD23	2.45	0.41
1:F:9:LEU:O	1:F:10:ARG:C	2.64	0.41
1:F:94:ASN:OD1	1:F:126:TRP:NE1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:114:ALA:CB	2:H:115:PRO:HD2	2.47	0.41
2:H:282:LEU:O	2:H:286:LEU:CD1	2.68	0.41
2:H:351:MET:CE	2:I:290:HIS:CB	2.98	0.41
2:I:64:CYS:O	2:I:119:ARG:NH2	2.52	0.41
2:I:185:HIS:O	2:I:188:GLU:HB3	2.20	0.41
1:A:248:ARG:HD2	4:K:5:DT:OP1	2.20	0.41
2:C:188:GLU:O	2:C:189:HIS:C	2.63	0.41
2:D:184:ARG:HD2	2:D:204:GLN:HE21	1.85	0.41
2:G:107:LEU:HD12	2:G:107:LEU:HA	1.72	0.41
2:G:108:LEU:O	2:G:111:VAL:HG12	2.20	0.41
2:G:221:THR:O	2:G:222:ASP:C	2.62	0.41
2:I:291:ARG:O	2:I:294:MET:N	2.49	0.41
3:J:106:LEU:O	3:J:106:LEU:CD2	2.57	0.41
3:J:213:ARG:HG2	3:J:213:ARG:HH11	1.84	0.41
2:B:111:VAL:HG13	2:B:112:GLN:N	2.35	0.41
2:C:114:ALA:CB	2:C:115:PRO:HD2	2.46	0.41
2:D:288:LEU:HD23	2:D:288:LEU:HA	1.84	0.41
1:F:211:HIS:HA	1:F:239:GLU:OE2	2.20	0.41
2:H:130:MET:HE1	2:I:134:HIS:HA	2.02	0.41
3:J:120:LEU:HD23	3:J:120:LEU:HA	1.86	0.41
1:A:228:ARG:O	1:A:229:ALA:C	2.61	0.41
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.85	0.41
2:B:106:ASP:O	2:B:107:LEU:C	2.64	0.41
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.76	0.41
2:C:45:GLY:O	2:C:51:LYS:HE3	2.20	0.41
2:C:261:GLY:O	2:C:262:GLU:C	2.61	0.41
2:C:276:ILE:O	2:C:276:ILE:HG13	2.15	0.41
3:E:286:LEU:HD23	3:E:286:LEU:HA	1.83	0.41
3:E:292:ASP:CG	3:E:318:ARG:HH21	2.29	0.41
3:E:308:ARG:O	3:E:309:GLU:C	2.63	0.41
1:F:42:ALA:C	1:F:47:PHE:HB2	2.46	0.41
1:F:104:LEU:HD13	1:F:133:ARG:CD	2.51	0.41
2:I:11:ARG:HA	2:I:12:PRO:HD3	1.87	0.41
2:I:32:LEU:HD23	2:I:37:ILE:CD1	2.50	0.41
3:J:164:LEU:HA	3:J:164:LEU:HD12	1.81	0.41
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.87	0.41
2:B:21:GLN:NE2	2:B:21:GLN:CA	2.78	0.41
2:B:302:LEU:HD23	2:B:302:LEU:HA	1.71	0.41
2:D:49:VAL:O	2:D:49:VAL:CG1	2.68	0.41
1:F:56:ASP:C	1:F:58:ASN:H	2.28	0.41
1:F:272:LEU:HD23	1:F:272:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:332:LEU:HD23	2:H:332:LEU:HA	1.53	0.41
2:I:6:LEU:O	2:I:8:ARG:N	2.53	0.41
2:I:215:ARG:HG2	2:I:215:ARG:HH11	1.85	0.41
2:I:291:ARG:HA	2:I:291:ARG:HD3	1.82	0.41
3:J:66:GLN:O	3:J:69:GLN:HB2	2.21	0.41
4:K:13:DC:H2''	4:K:14:DA:C8	2.56	0.41
4:M:12:DC:H2''	4:M:13:DC:O5'	2.21	0.41
1:A:104:LEU:HD13	1:A:133:ARG:HD2	2.03	0.41
2:B:245:ASP:O	2:B:274:ARG:HD2	2.21	0.41
2:B:251:SER:HB3	2:B:267:LEU:CD1	2.50	0.41
2:C:94:ASP:O	2:C:95:ALA:C	2.63	0.41
2:D:101:VAL:O	2:D:103:ASP:N	2.53	0.41
2:D:263:ARG:O	2:D:267:LEU:HB2	2.21	0.41
2:H:290:HIS:O	2:H:291:ARG:C	2.63	0.41
2:H:309:ILE:CG2	2:H:313:MET:HG2	2.50	0.41
2:I:101:VAL:O	2:I:102:GLU:C	2.64	0.41
2:I:128:VAL:O	2:I:128:VAL:CG2	2.67	0.41
2:I:191:LEU:HD23	2:I:191:LEU:HA	1.87	0.41
3:J:32:LEU:HD23	3:J:32:LEU:HA	1.85	0.41
3:J:103:HIS:H	3:J:103:HIS:HD2	1.68	0.41
3:J:311:LEU:HA	3:J:311:LEU:HD12	1.87	0.41
1:A:24:LEU:HA	1:A:114:GLY:O	2.20	0.41
2:C:166:ILE:O	2:C:169:ARG:HB2	2.21	0.41
2:D:10:TRP:CE2	2:D:190:ILE:HG23	2.56	0.41
3:E:233:LEU:HD12	3:E:237:ASN:HB2	2.02	0.41
3:E:327:VAL:CG1	3:E:328:VAL:N	2.83	0.41
1:F:81:LEU:HD21	1:F:83:LEU:HD21	2.01	0.41
1:F:234:GLN:OE1	2:G:304:ASN:HB2	2.20	0.41
2:H:4:GLN:OE1	2:H:4:GLN:CA	2.66	0.41
2:H:238:SER:O	2:H:239:ALA:C	2.64	0.41
2:I:286:LEU:HD23	2:I:286:LEU:HA	1.66	0.41
5:L:2:DT:H2''	5:L:3:DG:C8	2.55	0.41
1:A:97:LEU:CD1	1:A:126:TRP:CH2	3.03	0.41
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.58	0.41
2:B:5:VAL:HG12	2:B:6:LEU:N	2.35	0.41
2:C:292:ILE:HG22	2:C:325:ILE:CD1	2.51	0.41
2:C:339:LEU:N	2:C:340:PRO:CD	2.82	0.41
2:C:360:HIS:HA	2:C:361:PRO:HD3	1.88	0.41
2:D:3:TYR:CG	2:D:4:GLN:N	2.89	0.41
2:D:6:LEU:O	2:D:8:ARG:N	2.54	0.41
2:D:250:LEU:HD22	2:D:309:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:ILE:HG21	2:D:281:LEU:HD13	2.03	0.41
2:D:314:ARG:O	2:D:317:ALA:HB3	2.21	0.41
3:E:311:LEU:HD12	3:E:311:LEU:HA	1.81	0.41
3:E:316:LEU:HA	3:E:316:LEU:HD23	1.69	0.41
1:F:9:LEU:HD11	1:F:13:LEU:HD21	2.02	0.41
1:F:142:PRO:HD3	1:F:178:LEU:HD11	2.02	0.41
1:F:163:ASP:OD2	1:F:198:THR:HA	2.20	0.41
1:F:198:THR:CG2	1:F:201:ARG:HD2	2.50	0.41
1:F:222:LEU:HD23	1:F:222:LEU:HA	1.65	0.41
2:G:82:ILE:HG12	2:G:87:PHE:CB	2.51	0.41
2:G:251:SER:HB3	2:G:267:LEU:CD1	2.51	0.41
2:H:188:GLU:O	2:H:189:HIS:C	2.63	0.41
2:I:74:GLY:HA2	2:I:79:CYS:CB	2.51	0.41
2:I:289:LEU:HD23	2:I:289:LEU:HA	1.69	0.41
2:I:347:MET:HE1	3:J:246:HIS:HE1	1.85	0.41
3:J:46:ARG:CD	3:J:68:MET:CG	2.96	0.41
3:J:68:MET:HA	3:J:68:MET:CE	2.49	0.41
4:K:4:DT:O5'	4:K:4:DT:H2'	2.20	0.41
5:N:6:DC:C2'	5:N:7:DT:O5'	2.69	0.41
1:A:242:GLU:HA	1:A:243:PRO:HD3	1.99	0.41
2:B:249:ALA:HB2	2:B:281:LEU:CD1	2.51	0.41
2:B:260:ASN:ND2	2:B:263:ARG:HB2	2.23	0.41
2:C:220:LEU:HD23	2:C:220:LEU:HA	1.76	0.41
2:D:250:LEU:HD13	2:D:313:MET:CE	2.50	0.41
1:F:306:THR:HG23	3:J:311:LEU:HD12	2.03	0.41
2:G:6:LEU:HG	2:G:222:ASP:OD1	2.20	0.41
2:H:45:GLY:O	2:H:51:LYS:HE3	2.21	0.41
2:H:58:LEU:C	2:H:58:LEU:HD12	2.45	0.41
2:H:113:TYR:N	2:H:113:TYR:CD1	2.88	0.41
2:H:115:PRO:HD3	2:H:149:HIS:CD2	2.46	0.41
2:I:74:GLY:HA2	2:I:79:CYS:HB3	2.02	0.41
2:I:78:ASN:O	2:I:82:ILE:HG13	2.21	0.41
2:I:302:LEU:HD11	2:I:306:MET:HG3	2.03	0.41
2:I:341:TYR:CD1	2:I:341:TYR:N	2.89	0.41
1:A:142:PRO:HD3	1:A:178:LEU:HD11	2.03	0.40
1:A:144:GLN:NE2	1:A:228:ARG:HE	2.19	0.40
1:A:173:CYS:SG	1:A:206:VAL:HG11	2.61	0.40
2:B:353:LEU:HD23	2:B:353:LEU:HA	1.82	0.40
2:C:307:ALA:C	2:C:309:ILE:H	2.29	0.40
2:D:74:GLY:HA2	2:D:79:CYS:HB3	2.03	0.40
2:D:75:VAL:O	2:D:75:VAL:CG1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:111:VAL:HA	3:E:140:TRP:O	2.21	0.40
3:E:233:LEU:O	3:E:234:ALA:C	2.64	0.40
1:F:93:ILE:O	1:F:93:ILE:HG22	2.21	0.40
1:F:124:ALA:O	1:F:125:ALA:C	2.64	0.40
1:F:143:GLU:OE1	1:F:143:GLU:HA	2.21	0.40
1:F:278:VAL:O	1:F:283:ARG:HD3	2.20	0.40
2:H:139:LEU:HD23	2:H:139:LEU:HA	1.59	0.40
2:I:164:VAL:O	2:I:164:VAL:CG2	2.69	0.40
3:J:176:LEU:C	3:J:178:ARG:N	2.78	0.40
2:B:24:VAL:HG21	2:B:175:LEU:CD2	2.50	0.40
2:B:99:THR:HA	2:B:131:LEU:HD23	2.02	0.40
2:C:292:ILE:O	2:C:296:GLN:HG3	2.22	0.40
2:D:46:THR:HB	2:D:47:ARG:HE	1.86	0.40
2:D:135:SER:O	2:D:136:PHE:C	2.65	0.40
3:E:7:LEU:O	3:E:8:ARG:C	2.64	0.40
3:E:72:THR:O	3:E:72:THR:CG2	2.66	0.40
3:E:79:LEU:HD23	3:E:79:LEU:HA	1.72	0.40
3:E:252:LEU:HD23	3:E:252:LEU:HA	1.77	0.40
3:E:253:MET:HE3	3:E:290:LEU:HD21	2.04	0.40
1:F:199:LEU:N	1:F:200:PRO:HD2	2.36	0.40
2:G:47:ARG:HD3	2:G:47:ARG:N	2.36	0.40
2:G:128:VAL:O	2:G:128:VAL:CG2	2.69	0.40
2:I:5:VAL:HG13	2:I:222:ASP:OD2	2.21	0.40
2:I:327:LEU:HD23	2:I:327:LEU:HA	1.79	0.40
3:J:176:LEU:C	3:J:178:ARG:H	2.30	0.40
4:M:4:DT:O5'	4:M:4:DT:H2'	2.21	0.40
1:A:42:ALA:C	1:A:47:PHE:HB2	2.46	0.40
2:B:171:LEU:HA	2:B:171:LEU:HD12	1.87	0.40
2:B:276:ILE:HG23	2:B:277:GLU:N	2.36	0.40
2:B:347:MET:HE2	2:C:290:HIS:ND1	2.37	0.40
2:C:101:VAL:C	2:C:103:ASP:N	2.79	0.40
2:C:130:MET:HE1	2:D:134:HIS:HA	2.02	0.40
2:C:327:LEU:O	2:C:327:LEU:HD12	2.22	0.40
2:C:332:LEU:HA	2:C:332:LEU:HD23	1.55	0.40
2:D:247:ASP:O	2:D:249:ALA:N	2.54	0.40
1:F:56:ASP:C	1:F:58:ASN:N	2.79	0.40
2:G:24:VAL:HG22	2:G:173:PHE:HB3	2.03	0.40
2:G:320:ILE:HG23	2:G:321:PRO:CD	2.51	0.40
2:H:292:ILE:CG2	2:H:325:ILE:CD1	2.99	0.40
2:I:251:SER:HB3	2:I:267:LEU:HD21	2.02	0.40
2:I:259:ALA:HB2	2:I:360:HIS:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.94	0.40
2:B:132:SER:O	2:B:133:ARG:C	2.64	0.40
2:B:220:LEU:HA	2:B:220:LEU:HD23	1.90	0.40
2:D:266:ALA:O	2:D:270:GLU:HG3	2.22	0.40
1:F:151:VAL:HG22	1:F:181:LEU:HD21	2.03	0.40
2:G:6:LEU:HD23	2:G:6:LEU:HA	1.84	0.40
2:G:234:THR:O	2:G:238:SER:HB3	2.22	0.40
2:H:254:GLU:OE2	2:H:312:ARG:HD3	2.21	0.40
2:B:11:ARG:HA	2:B:12:PRO:HD3	1.79	0.40
2:B:294:MET:C	2:B:296:GLN:N	2.78	0.40
2:B:326:GLN:O	2:B:326:GLN:HG3	2.21	0.40
2:C:6:LEU:O	2:C:8:ARG:N	2.55	0.40
2:C:281:LEU:C	2:C:283:VAL:N	2.77	0.40
2:D:258:GLU:C	2:D:260:ASN:N	2.76	0.40
3:E:49:LEU:HD12	3:E:68:MET:SD	2.62	0.40
1:F:84:LEU:HD11	1:F:112:VAL:CG1	2.51	0.40
2:H:9:LYS:HD3	2:H:194:GLU:OE2	2.20	0.40
3:J:90:VAL:HG13	3:J:91:ASP:N	2.37	0.40
3:J:248:LEU:O	3:J:248:LEU:HD12	2.21	0.40

All (3) 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]	1.99	0.21
3:E:178:ARG:NH2	2:H:195:HIS:O[4_545]	2.02	0.18
2:C:117:ARG:NE	2:H:117:ARG:NH2[2_555]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/343 (96%)	292 (88%)	34 (10%)	5 (2%)	8	29
1	F	331/343 (96%)	298 (90%)	29 (9%)	4 (1%)	10	34
2	B	362/395 (92%)	323 (89%)	36 (10%)	3 (1%)	16	44
2	C	363/395 (92%)	326 (90%)	31 (8%)	6 (2%)	7	27
2	D	360/395 (91%)	317 (88%)	34 (9%)	9 (2%)	4	21
2	G	376/395 (95%)	340 (90%)	33 (9%)	3 (1%)	16	44
2	H	363/395 (92%)	320 (88%)	37 (10%)	6 (2%)	7	27
2	I	360/395 (91%)	318 (88%)	33 (9%)	9 (2%)	4	21
3	E	332/334 (99%)	300 (90%)	24 (7%)	8 (2%)	4	22
3	J	332/334 (99%)	298 (90%)	28 (8%)	6 (2%)	6	26
All	All	3510/3724 (94%)	3132 (89%)	319 (9%)	59 (2%)	7	27

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
2	B	307	ALA
2	C	297	LEU
2	D	307	ALA
3	E	153	ALA
1	F	159	ASN
2	G	307	ALA
2	H	297	LEU
2	I	248	GLN
2	I	292	ILE
2	I	307	ALA
3	J	16	ALA
3	J	153	ALA
2	C	296	GLN
2	D	7	ALA
2	D	168	SER
2	D	248	GLN
2	D	292	ILE
3	E	16	ALA
3	E	177	SER
2	H	259	ALA
2	H	296	GLN
2	I	7	ALA
2	I	168	SER

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Mol	Chain	Res	Type
2	I	291	ARG
3	J	74	PRO
1	A	15	GLU
1	A	44	ALA
2	B	160	GLN
2	D	291	ARG
3	E	74	PRO
1	F	44	ALA
1	F	125	ALA
1	A	125	ALA
2	C	7	ALA
2	C	195	HIS
1	F	15	GLU
2	H	195	HIS
2	I	160	GLN
3	J	188	LEU
2	C	259	ALA
2	C	356	ALA
2	D	200	PRO
2	D	358	ALA
3	E	188	LEU
2	I	102	GLU
2	D	247	ASP
3	E	136	PRO
2	H	308	ALA
2	I	200	PRO
3	J	136	PRO
1	A	320	VAL
3	J	168	PRO
2	G	68	ILE
2	B	180	VAL
3	E	168	PRO
2	G	225	ILE
3	E	332	PRO
2	H	253	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	252 (89%)	31 (11%)	6	22
1	F	283/291 (97%)	251 (89%)	32 (11%)	5	21
2	B	301/329 (92%)	274 (91%)	27 (9%)	9	30
2	C	302/329 (92%)	256 (85%)	46 (15%)	3	11
2	D	299/329 (91%)	277 (93%)	22 (7%)	13	38
2	G	313/329 (95%)	287 (92%)	26 (8%)	10	35
2	H	302/329 (92%)	260 (86%)	42 (14%)	3	14
2	I	299/329 (91%)	272 (91%)	27 (9%)	9	30
3	E	270/270 (100%)	248 (92%)	22 (8%)	11	36
3	J	270/270 (100%)	243 (90%)	27 (10%)	7	26
All	All	2922/3096 (94%)	2620 (90%)	302 (10%)	7	25

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	59	THR
1	A	64	ILE
1	A	78	GLN
1	A	86	GLU
1	A	99	THR
1	A	108	LEU
1	A	110	LEU
1	A	117	LEU
1	A	118	SER
1	A	128	THR
1	A	138	THR
1	A	146	GLN
1	A	158	LEU
1	A	169	VAL
1	A	191	LEU
1	A	196	LYS
1	A	198	THR
1	A	202	VAL
1	A	203	GLU
1	A	206	VAL
1	A	230	LEU
1	A	232	ILE

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Mol	Chain	Res	Type
1	A	237	ARG
1	A	238	LEU
1	A	244	VAL
1	A	296	THR
1	A	308	THR
1	A	309	GLU
1	A	311	THR
1	A	319	SER
2	B	37	ILE
2	B	38	HIS
2	B	39	HIS
2	B	46	THR
2	B	47	ARG
2	B	62	LEU
2	B	97	SER
2	B	117	ARG
2	B	119	ARG
2	B	157	THR
2	B	168	SER
2	B	175	LEU
2	B	180	VAL
2	B	187	LEU
2	B	251	SER
2	B	253	VAL
2	B	262	GLU
2	B	268	ILE
2	B	276	ILE
2	B	288	LEU
2	B	291	ARG
2	B	302	LEU
2	B	309	ILE
2	B	316	LEU
2	B	320	ILE
2	B	325	ILE
2	B	331	THR
2	C	8	ARG
2	C	44	SER
2	C	46	THR
2	C	47	ARG
2	C	51	LYS
2	C	53	SER
2	C	75	VAL

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Mol	Chain	Res	Type
2	C	91	ILE
2	C	93	ILE
2	C	112	GLN
2	C	117	ARG
2	C	124	LEU
2	C	128	VAL
2	C	134	HIS
2	C	139	LEU
2	C	157	THR
2	C	162	LEU
2	C	165	THR
2	C	168	SER
2	C	170	CYS
2	C	172	GLN
2	C	175	LEU
2	C	179	ASP
2	C	180	VAL
2	C	183	ILE
2	C	187	LEU
2	C	196	ILE
2	C	214	LEU
2	C	227	SER
2	C	240	MET
2	C	244	LEU
2	C	246	ASP
2	C	248	GLN
2	C	252	LEU
2	C	260	ASN
2	C	268	ILE
2	C	276	ILE
2	C	284	GLU
2	C	291	ARG
2	C	294	MET
2	C	297	LEU
2	C	306	MET
2	C	309	ILE
2	C	311	LEU
2	C	318	ARG
2	C	352	THR
2	D	30	ASN
2	D	46	THR
2	D	47	ARG

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Mol	Chain	Res	Type
2	D	52	THR
2	D	97	SER
2	D	107	LEU
2	D	117	ARG
2	D	125	ILE
2	D	135	SER
2	D	157	THR
2	D	165	THR
2	D	175	LEU
2	D	180	VAL
2	D	264	VAL
2	D	268	ILE
2	D	276	ILE
2	D	291	ARG
2	D	305	ASP
2	D	306	MET
2	D	325	ILE
2	D	333	LEU
2	D	357	LEU
3	E	17	SER
3	E	73	HIS
3	E	82	GLU
3	E	90	VAL
3	E	134	GLU
3	E	145	THR
3	E	155	LEU
3	E	160	ARG
3	E	180	VAL
3	E	188	LEU
3	E	192	ARG
3	E	197	SER
3	E	208	ASP
3	E	218	GLN
3	E	231	SER
3	E	239	GLU
3	E	253	MET
3	E	256	LEU
3	E	264	GLN
3	E	270	VAL
3	E	282	SER
3	E	323	LEU
1	F	7	GLU

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Mol	Chain	Res	Type
1	F	59	THR
1	F	64	ILE
1	F	78	GLN
1	F	86	GLU
1	F	99	THR
1	F	108	LEU
1	F	110	LEU
1	F	117	LEU
1	F	118	SER
1	F	128	THR
1	F	138	THR
1	F	146	GLN
1	F	158	LEU
1	F	169	VAL
1	F	191	LEU
1	F	196	LYS
1	F	198	THR
1	F	202	VAL
1	F	203	GLU
1	F	206	VAL
1	F	230	LEU
1	F	237	ARG
1	F	238	LEU
1	F	244	VAL
1	F	282	ARG
1	F	296	THR
1	F	308	THR
1	F	311	THR
1	F	318	GLN
1	F	319	SER
1	F	330	LEU
2	G	37	ILE
2	G	38	HIS
2	G	39	HIS
2	G	46	THR
2	G	47	ARG
2	G	62	LEU
2	G	97	SER
2	G	117	ARG
2	G	119	ARG
2	G	157	THR
2	G	168	SER

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Mol	Chain	Res	Type
2	G	175	LEU
2	G	180	VAL
2	G	187	LEU
2	G	251	SER
2	G	253	VAL
2	G	262	GLU
2	G	276	ILE
2	G	288	LEU
2	G	291	ARG
2	G	302	LEU
2	G	309	ILE
2	G	316	LEU
2	G	320	ILE
2	G	325	ILE
2	G	331	THR
2	H	8	ARG
2	H	44	SER
2	H	46	THR
2	H	47	ARG
2	H	51	LYS
2	H	53	SER
2	H	75	VAL
2	H	91	ILE
2	H	93	ILE
2	H	112	GLN
2	H	117	ARG
2	H	124	LEU
2	H	128	VAL
2	H	134	HIS
2	H	157	THR
2	H	165	THR
2	H	168	SER
2	H	170	CYS
2	H	172	GLN
2	H	175	LEU
2	H	179	ASP
2	H	183	ILE
2	H	187	LEU
2	H	196	ILE
2	H	214	LEU
2	H	227	SER
2	H	240	MET

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Mol	Chain	Res	Type
2	H	244	LEU
2	H	246	ASP
2	H	248	GLN
2	H	252	LEU
2	H	260	ASN
2	H	268	ILE
2	H	276	ILE
2	H	284	GLU
2	H	291	ARG
2	H	297	LEU
2	H	309	ILE
2	H	311	LEU
2	H	318	ARG
2	H	334	ILE
2	H	352	THR
2	I	6	LEU
2	I	37	ILE
2	I	46	THR
2	I	47	ARG
2	I	52	THR
2	I	82	ILE
2	I	97	SER
2	I	107	LEU
2	I	117	ARG
2	I	125	ILE
2	I	135	SER
2	I	157	THR
2	I	165	THR
2	I	175	LEU
2	I	180	VAL
2	I	214	LEU
2	I	216	ASP
2	I	225	ILE
2	I	264	VAL
2	I	268	ILE
2	I	276	ILE
2	I	291	ARG
2	I	305	ASP
2	I	306	MET
2	I	325	ILE
2	I	333	LEU
2	I	357	LEU

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Mol	Chain	Res	Type
3	J	2	ARG
3	J	17	SER
3	J	73	HIS
3	J	78	THR
3	J	82	GLU
3	J	90	VAL
3	J	134	GLU
3	J	145	THR
3	J	155	LEU
3	J	157	SER
3	J	160	ARG
3	J	180	VAL
3	J	188	LEU
3	J	192	ARG
3	J	197	SER
3	J	208	ASP
3	J	214	GLU
3	J	218	GLN
3	J	233	LEU
3	J	239	GLU
3	J	253	MET
3	J	256	LEU
3	J	264	GLN
3	J	270	VAL
3	J	282	SER
3	J	311	LEU
3	J	323	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	32	GLN
1	A	45	GLN
1	A	50	HIS
1	A	121	GLN
1	A	144	GLN
1	A	211	HIS
1	A	216	HIS
1	A	263	GLN
1	A	314	GLN
2	B	39	HIS

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Mol	Chain	Res	Type
2	B	84	GLN
2	B	149	HIS
2	B	182	GLN
2	B	235	GLN
2	B	260	ASN
2	C	23	HIS
2	C	112	GLN
2	C	134	HIS
2	C	149	HIS
2	C	290	HIS
2	C	326	GLN
2	C	330	GLN
2	D	38	HIS
2	D	84	GLN
2	D	134	HIS
2	D	149	HIS
2	D	172	GLN
2	D	174	HIS
2	D	204	GLN
2	D	269	ASN
2	D	330	GLN
2	D	360	HIS
3	E	25	HIS
3	E	51	GLN
3	E	52	GLN
3	E	54	GLN
3	E	69	GLN
3	E	101	ASN
3	E	103	HIS
3	E	264	GLN
3	E	267	ASN
3	E	287	GLN
1	F	12	GLN
1	F	32	GLN
1	F	40	GLN
1	F	45	GLN
1	F	50	HIS
1	F	51	HIS
1	F	78	GLN
1	F	121	GLN
1	F	144	GLN
1	F	216	HIS

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Mol	Chain	Res	Type
1	F	263	GLN
2	G	4	GLN
2	G	39	HIS
2	G	84	GLN
2	G	134	HIS
2	G	149	HIS
2	G	182	GLN
2	G	235	GLN
2	G	260	ASN
2	G	269	ASN
2	H	23	HIS
2	H	112	GLN
2	H	134	HIS
2	H	290	HIS
2	H	326	GLN
2	H	330	GLN
2	I	30	ASN
2	I	38	HIS
2	I	84	GLN
2	I	134	HIS
2	I	172	GLN
2	I	204	GLN
2	I	269	ASN
2	I	330	GLN
2	I	360	HIS
3	J	51	GLN
3	J	52	GLN
3	J	54	GLN
3	J	69	GLN
3	J	101	ASN
3	J	103	HIS
3	J	260	HIS
3	J	264	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	402	7,8	28,29,29	1.47	5 (17%)	43,45,45	1.88	10 (23%)
6	ADP	D	404	7,8	28,29,29	1.58	5 (17%)	43,45,45	1.70	12 (27%)
6	ADP	G	406	7,8	28,29,29	1.57	7 (25%)	43,45,45	1.77	12 (27%)
7	BEF	H	409	6	0,3,3	-	-	-		
7	BEF	G	407	6	0,3,3	-	-	-		
6	ADP	B	400	7,8	28,29,29	1.70	6 (21%)	43,45,45	1.75	13 (30%)
7	BEF	D	405	6	0,3,3	-	-	-		
7	BEF	B	401	6	0,3,3	-	-	-		
7	BEF	I	411	6	0,3,3	-	-	-		
7	BEF	C	403	6	0,3,3	-	-	-		
6	ADP	H	408	7,8	28,29,29	1.61	9 (32%)	43,45,45	1.82	11 (25%)
6	ADP	I	410	7,8	28,29,29	1.98	5 (17%)	43,45,45	1.63	11 (25%)

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	C	402	7,8	-	6/16/32/32	0/3/3/3
6	ADP	D	404	7,8	-	0/16/32/32	0/3/3/3
6	ADP	G	406	7,8	-	0/16/32/32	0/3/3/3
6	ADP	B	400	7,8	-	0/16/32/32	0/3/3/3
6	ADP	H	408	7,8	-	5/16/32/32	0/3/3/3
6	ADP	I	410	7,8	-	1/16/32/32	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	400	ADP	C5-C4	5.26	1.48	1.39
6	I	410	ADP	PA-O3A	5.11	1.65	1.59
6	C	402	ADP	C5-C4	4.90	1.47	1.39
6	I	410	ADP	C5-C4	4.54	1.47	1.39
6	G	406	ADP	C5-C4	4.47	1.47	1.39
6	D	404	ADP	C5-C4	4.19	1.46	1.39
6	I	410	ADP	C4-N9	-4.05	1.29	1.37
6	H	408	ADP	C5-C4	3.88	1.46	1.39
6	D	404	ADP	C5-N7	-3.39	1.32	1.39
6	B	400	ADP	PA-O3A	3.38	1.63	1.59
6	I	410	ADP	C5-N7	-3.35	1.33	1.39
6	D	404	ADP	C4-N9	-3.24	1.31	1.37
6	H	408	ADP	C5-N7	-3.06	1.33	1.39
6	H	408	ADP	C4-N9	-2.88	1.31	1.37
6	G	406	ADP	C4-N9	-2.70	1.32	1.37
6	H	408	ADP	PB-O1B	2.60	1.58	1.50
6	G	406	ADP	C5-C6	2.52	1.48	1.41
6	G	406	ADP	C5-N7	-2.51	1.34	1.39
6	B	400	ADP	C8-N7	2.46	1.36	1.31
6	B	400	ADP	C5-N7	-2.43	1.34	1.39
6	H	408	ADP	PA-O3A	2.39	1.62	1.59
6	C	402	ADP	C5-C6	2.35	1.47	1.41
6	C	402	ADP	C8-N7	2.34	1.36	1.31
6	B	400	ADP	C5-C6	2.33	1.47	1.41
6	I	410	ADP	PB-O2B	-2.22	1.46	1.54
6	G	406	ADP	PB-O3B	2.18	1.62	1.54
6	H	408	ADP	PB-O3B	2.17	1.62	1.54
6	G	406	ADP	PA-O3A	2.16	1.61	1.59
6	C	402	ADP	C4-N9	-2.12	1.33	1.37
6	B	400	ADP	C4-N9	-2.10	1.33	1.37
6	H	408	ADP	C8-N9	-2.09	1.34	1.37
6	D	404	ADP	PA-O3A	2.06	1.61	1.59
6	C	402	ADP	C5-N7	-2.03	1.35	1.39
6	H	408	ADP	C5-C6	2.03	1.46	1.41
6	D	404	ADP	C8-N9	-2.03	1.34	1.37
6	G	406	ADP	C8-N7	2.02	1.35	1.31
6	H	408	ADP	PB-O2B	-2.02	1.47	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	402	ADP	C5-C4-N3	-5.16	119.62	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	406	ADP	C5-C4-N3	-5.10	119.69	126.72
6	H	408	ADP	C5-C4-N3	-5.07	119.73	126.72
6	B	400	ADP	C5-C4-N3	-4.64	120.32	126.72
6	C	402	ADP	N3-C4-N9	4.41	134.67	127.17
6	I	410	ADP	C5-C4-N3	-4.23	120.90	126.72
6	H	408	ADP	N3-C4-N9	4.14	134.21	127.17
6	D	404	ADP	C5-C4-N3	-3.97	121.25	126.72
6	G	406	ADP	N3-C4-N9	3.82	133.67	127.17
6	B	400	ADP	N3-C4-N9	3.76	133.57	127.17
6	D	404	ADP	N3-C4-N9	3.70	133.47	127.17
6	H	408	ADP	C4-C5-N7	-3.54	106.54	110.58
6	C	402	ADP	O2B-PB-O1B	3.53	124.59	110.83
6	I	410	ADP	O2B-PB-O1B	3.50	124.48	110.83
6	H	408	ADP	C4-N9-C8	3.44	109.34	105.74
6	I	410	ADP	N3-C4-N9	3.35	132.87	127.17
6	C	402	ADP	C2-N3-C4	3.31	119.91	111.83
6	G	406	ADP	C4-C5-N7	-3.29	106.82	110.58
6	H	408	ADP	O2B-PB-O1B	3.24	123.47	110.83
6	C	402	ADP	N3-C2-N1	-3.21	123.72	128.58
6	D	404	ADP	C4-N9-C8	3.17	109.07	105.74
6	G	406	ADP	C2-N3-C4	2.94	119.01	111.83
6	H	408	ADP	C5-N7-C8	2.81	107.87	103.45
6	D	404	ADP	O2B-PB-O1B	2.81	121.79	110.83
6	B	400	ADP	C4-C5-N7	-2.81	107.37	110.58
6	C	402	ADP	C4-N9-C8	2.78	108.66	105.74
6	H	408	ADP	C2-N3-C4	2.74	118.53	111.83
6	C	402	ADP	C2'-C1'-N9	-2.68	106.64	113.30
6	B	400	ADP	O4'-C1'-N9	2.67	113.21	108.09
6	C	402	ADP	C2'-C3'-C4'	2.67	107.76	102.61
6	H	408	ADP	N9-C8-N7	-2.64	110.20	113.94
6	D	404	ADP	N3-C2-N1	-2.62	124.62	128.58
6	D	404	ADP	O3'-C3'-C4'	-2.58	103.68	111.08
6	B	400	ADP	C2-N3-C4	2.58	118.12	111.83
6	I	410	ADP	O2'-C2'-C1'	-2.57	101.24	110.10
6	D	404	ADP	C2-N1-C6	2.57	122.95	118.73
6	C	402	ADP	C4-C5-N7	-2.56	107.65	110.58
6	G	406	ADP	O2B-PB-O1B	2.55	120.78	110.83
6	I	410	ADP	O4'-C4'-C3'	-2.53	100.13	105.15
6	G	406	ADP	O3B-PB-O2B	-2.51	98.37	107.80
6	D	404	ADP	N6-C6-N1	2.51	123.97	118.38
6	D	404	ADP	O3B-PB-O2B	-2.51	98.39	107.80
6	G	406	ADP	O5'-PA-O1A	-2.44	99.27	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	400	ADP	O2B-PB-O1B	2.43	120.31	110.83
6	I	410	ADP	O3B-PB-O2B	-2.40	98.79	107.80
6	G	406	ADP	C2'-C1'-N9	-2.40	107.34	113.30
6	I	410	ADP	C2'-C3'-C4'	2.37	107.19	102.61
6	C	402	ADP	C2-N1-C6	2.35	122.60	118.73
6	I	410	ADP	C4-N9-C8	2.29	108.14	105.74
6	B	400	ADP	C4-N9-C8	2.29	108.14	105.74
6	G	406	ADP	C4-N9-C8	2.28	108.13	105.74
6	I	410	ADP	C4-C5-N7	-2.28	107.98	110.58
6	D	404	ADP	C2-N3-C4	2.27	117.37	111.83
6	D	404	ADP	O2'-C2'-C1'	-2.24	102.41	110.10
6	B	400	ADP	C2'-C1'-N9	-2.21	107.80	113.30
6	G	406	ADP	C5'-C4'-C3'	-2.20	107.28	115.21
6	I	410	ADP	O3A-PA-O1A	-2.19	104.12	110.70
6	B	400	ADP	O3B-PB-O2B	-2.19	99.60	107.80
6	B	400	ADP	O2'-C2'-C1'	-2.18	102.61	110.10
6	I	410	ADP	C4'-O4'-C1'	2.16	114.24	109.47
6	D	404	ADP	C4-C5-N7	-2.14	108.13	110.58
6	H	408	ADP	O3A-PA-O1A	-2.14	104.26	110.70
6	B	400	ADP	N3-C2-N1	-2.12	125.38	128.58
6	H	408	ADP	N3-C2-N1	-2.06	125.47	128.58
6	G	406	ADP	N3-C2-N1	-2.04	125.49	128.58
6	B	400	ADP	O5'-PA-O1A	-2.03	100.87	108.94
6	H	408	ADP	C2'-C3'-C4'	2.01	106.50	102.61
6	G	406	ADP	C6-C5-N7	2.01	135.96	132.09
6	B	400	ADP	C5-N7-C8	2.01	106.61	103.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	402	ADP	PA-O3A-PB-O3B
6	C	402	ADP	C5'-O5'-PA-O1A
6	C	402	ADP	C5'-O5'-PA-O2A
6	C	402	ADP	C5'-O5'-PA-O3A
6	H	408	ADP	PA-O3A-PB-O3B
6	H	408	ADP	C5'-O5'-PA-O2A
6	H	408	ADP	C5'-O5'-PA-O3A
6	H	408	ADP	C5'-O5'-PA-O1A
6	C	402	ADP	O4'-C4'-C5'-O5'
6	C	402	ADP	PA-O3A-PB-O2B
6	H	408	ADP	PA-O3A-PB-O2B

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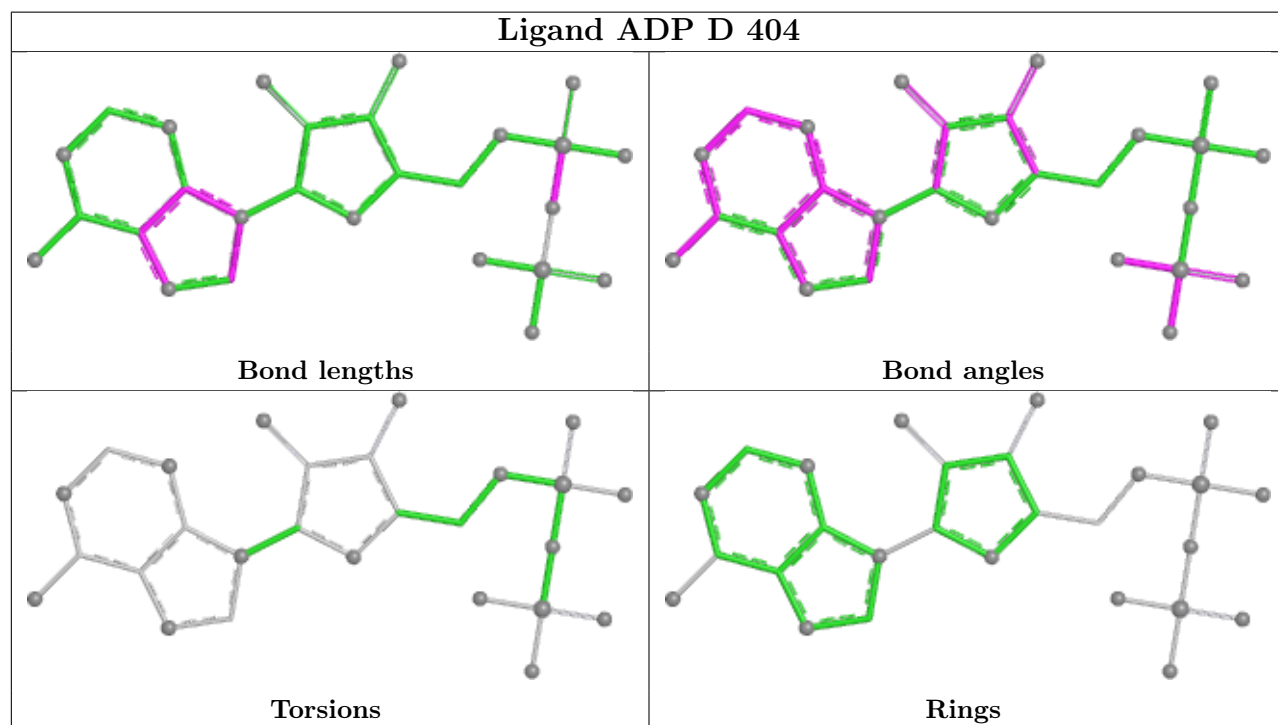
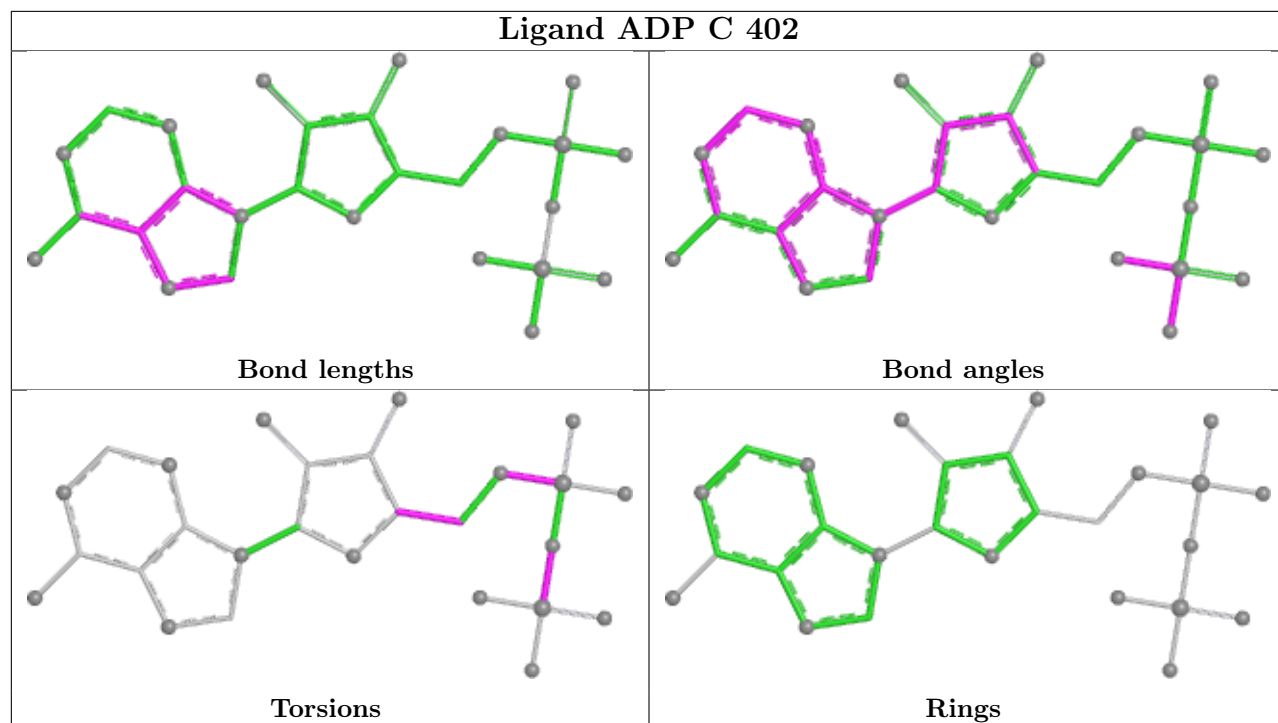
Mol	Chain	Res	Type	Atoms
6	I	410	ADP	PA-O3A-PB-O3B

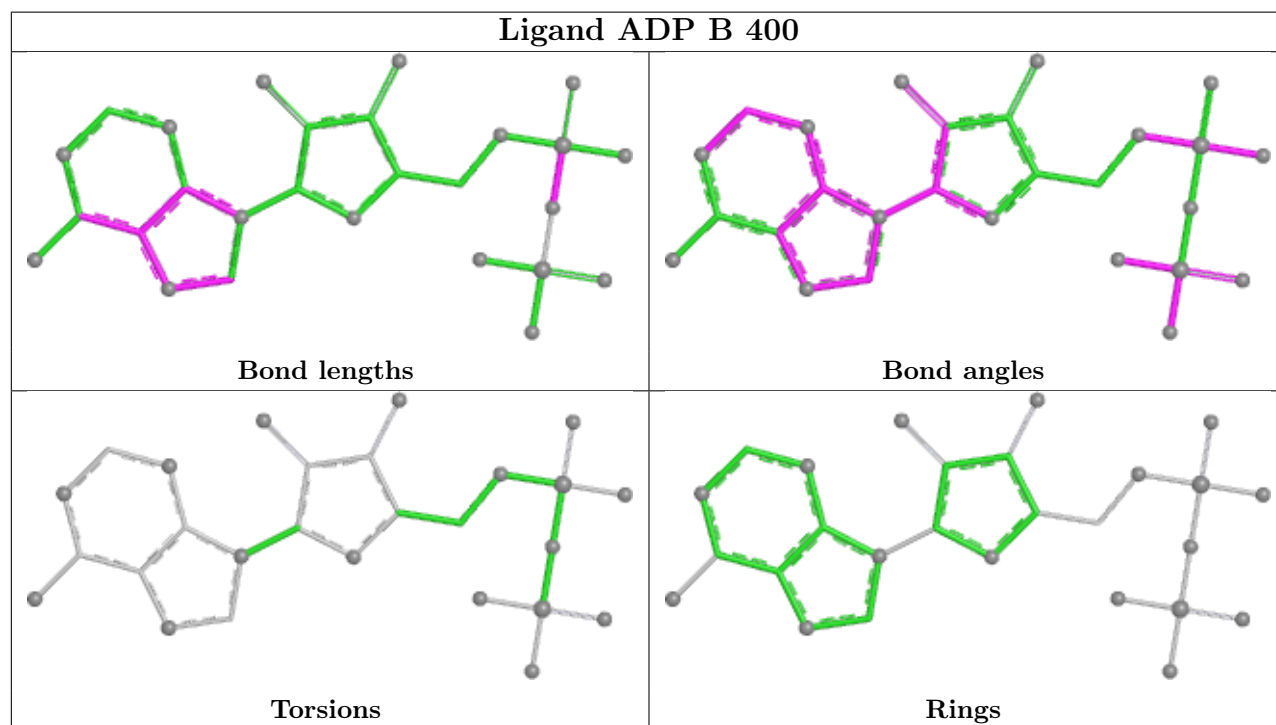
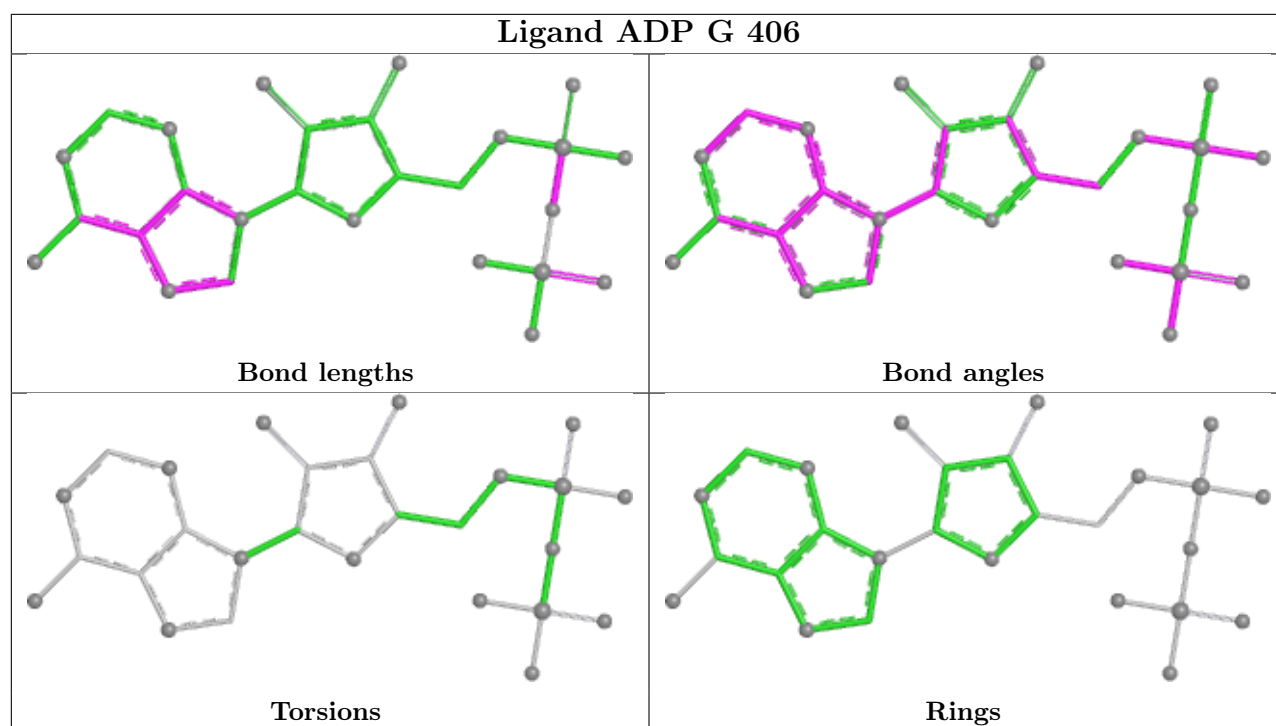
There are no ring outliers.

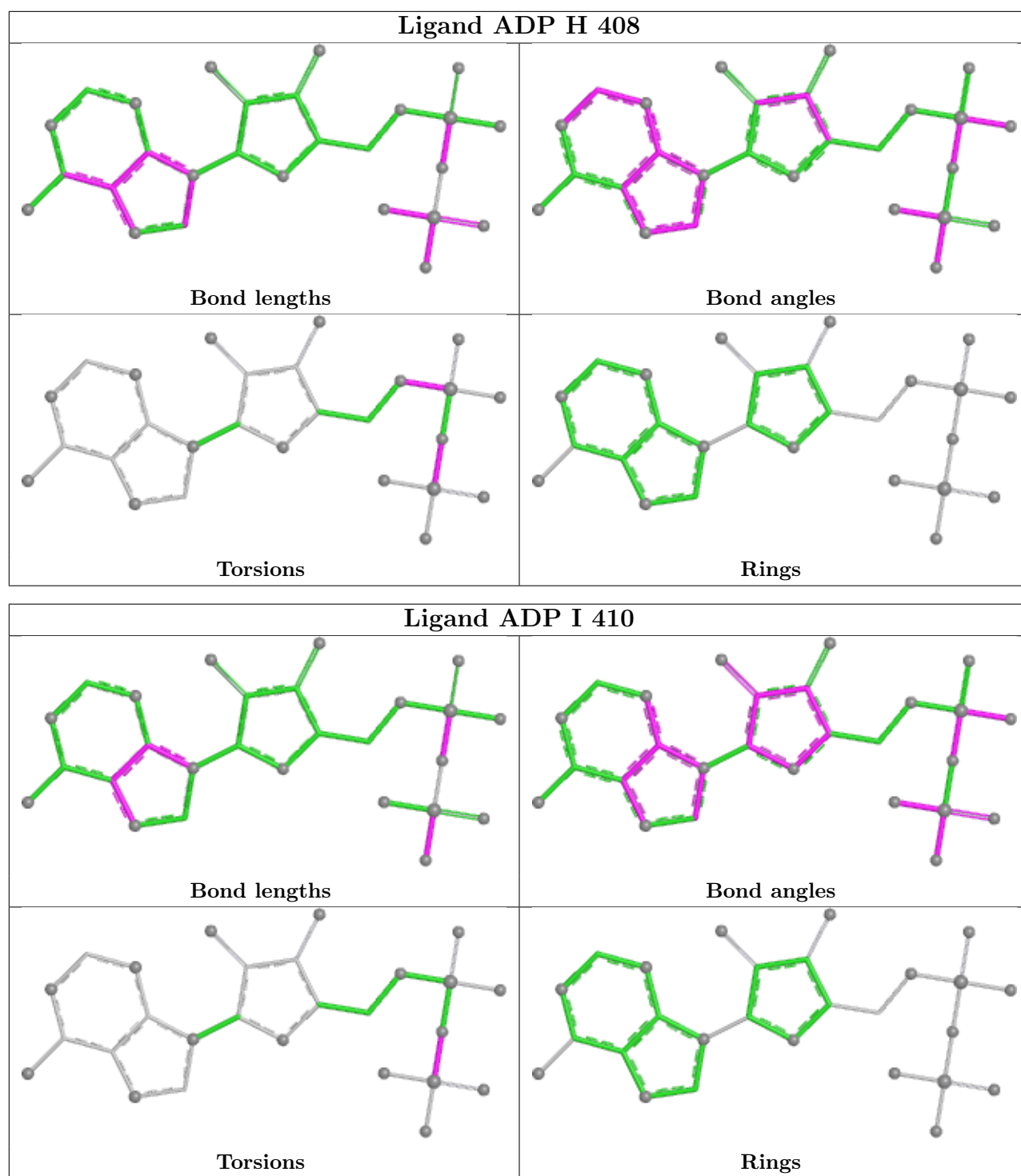
9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	402	ADP	3	0
6	D	404	ADP	3	0
6	G	406	ADP	2	0
7	G	407	BEF	1	0
6	B	400	ADP	3	0
7	B	401	BEF	1	0
7	I	411	BEF	1	0
6	H	408	ADP	4	0
6	I	410	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	333/343 (97%)	0.22	18 (5%) 31 23	73, 127, 209, 244	0
1	F	333/343 (97%)	0.06	5 (1%) 72 57	67, 127, 197, 222	0
2	B	364/395 (92%)	-0.01	3 (0%) 82 70	76, 119, 164, 189	0
2	C	365/395 (92%)	-0.03	4 (1%) 78 64	68, 114, 180, 208	0
2	D	362/395 (91%)	-0.03	3 (0%) 82 70	69, 106, 156, 198	0
2	G	378/395 (95%)	-0.13	3 (0%) 82 70	76, 101, 146, 182	0
2	H	365/395 (92%)	-0.24	4 (1%) 78 64	58, 88, 125, 165	0
2	I	362/395 (91%)	-0.22	2 (0%) 85 74	56, 80, 125, 184	0
3	E	334/334 (100%)	-0.26	1 (0%) 90 83	67, 86, 134, 175	0
3	J	334/334 (100%)	-0.27	1 (0%) 90 83	63, 84, 133, 172	0
4	K	14/15 (93%)	-0.24	0 100 100	79, 87, 169, 171	0
4	M	14/15 (93%)	-0.21	0 100 100	76, 84, 174, 181	0
5	L	10/10 (100%)	-0.66	0 100 100	85, 88, 95, 105	0
5	N	10/10 (100%)	-0.69	0 100 100	81, 86, 98, 99	0
All	All	3578/3774 (94%)	-0.10	44 (1%) 76 62	56, 101, 175, 244	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	365	LEU	4.9
1	A	55	ILE	4.3
1	F	96	GLN	3.5
1	A	53	PHE	3.3
2	G	358	ALA	3.2
2	D	363	MET	2.9
1	A	84	LEU	2.8
2	G	222	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	246	ASP	2.7
2	I	246	ASP	2.7
1	A	96	GLN	2.6
1	F	53	PHE	2.6
1	A	279	TRP	2.6
3	J	334	LEU	2.6
2	H	4	GLN	2.6
2	C	246	ASP	2.5
1	A	128	THR	2.5
1	A	74	PHE	2.5
2	D	244	LEU	2.4
2	I	361	PRO	2.4
1	A	80	LEU	2.3
1	A	100	LEU	2.3
2	B	46	THR	2.3
1	F	48	GLU	2.2
1	A	76	SER	2.2
1	A	318	GLN	2.2
1	A	109	LEU	2.2
2	C	107	LEU	2.2
2	B	366	PRO	2.2
1	A	67	LEU	2.2
1	A	73	LEU	2.2
2	G	39	HIS	2.1
1	A	110	LEU	2.1
2	C	4	GLN	2.1
2	D	293	ALA	2.1
1	A	104	LEU	2.1
2	C	276	ILE	2.1
1	A	92	ALA	2.1
1	F	55	ILE	2.1
2	H	245	ASP	2.1
1	A	19	ALA	2.0
2	H	244	LEU	2.0
3	E	259	HIS	2.0
1	F	67	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

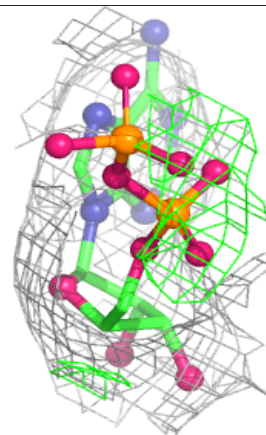
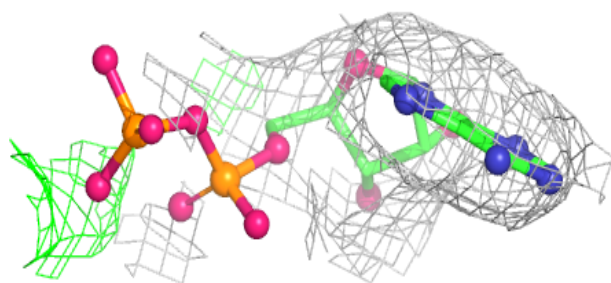
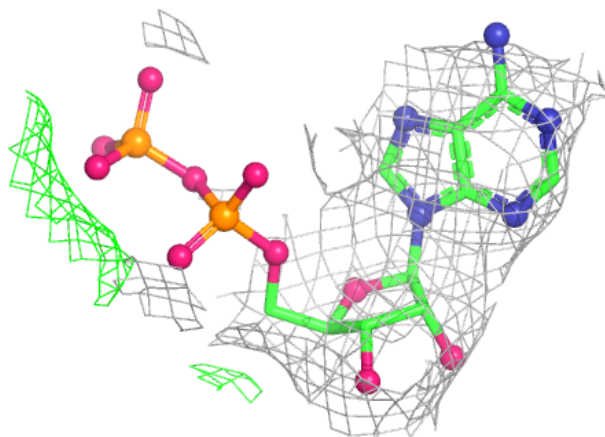
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	412	1/1	0.74	0.25	79,79,79,79	0
8	MG	D	414	1/1	0.77	0.29	75,75,75,75	0
8	MG	G	415	1/1	0.80	0.23	79,79,79,79	0
8	MG	C	413	1/1	0.85	0.20	77,77,77,77	0
8	MG	H	416	1/1	0.87	0.19	57,57,57,57	0
7	BEF	H	409	4/4	0.89	0.12	57,57,57,58	0
7	BEF	C	403	4/4	0.89	0.14	77,78,78,79	0
7	BEF	D	405	4/4	0.89	0.12	85,85,86,87	0
8	MG	I	417	1/1	0.90	0.21	58,58,58,58	0
7	BEF	G	407	4/4	0.91	0.12	79,79,80,80	0
7	BEF	B	401	4/4	0.91	0.14	79,80,80,81	0
7	BEF	I	411	4/4	0.91	0.12	62,63,63,64	0
6	ADP	B	400	27/27	0.97	0.06	86,94,99,100	0
6	ADP	C	402	27/27	0.97	0.07	78,86,91,93	0
6	ADP	D	404	27/27	0.97	0.07	80,89,95,96	0
6	ADP	G	406	27/27	0.97	0.08	81,87,92,94	0
6	ADP	H	408	27/27	0.97	0.06	60,62,67,67	0
6	ADP	I	410	27/27	0.97	0.07	62,68,72,73	0
9	ZN	J	425	1/1	0.98	0.04	146,146,146,146	0
9	ZN	G	422	1/1	0.99	0.05	160,160,160,160	0
9	ZN	D	420	1/1	0.99	0.03	133,133,133,133	0
9	ZN	E	421	1/1	1.00	0.02	161,161,161,161	0
9	ZN	C	419	1/1	1.00	0.02	130,130,130,130	0
9	ZN	H	423	1/1	1.00	0.02	112,112,112,112	0
9	ZN	I	424	1/1	1.00	0.01	99,99,99,99	0
9	ZN	B	418	1/1	1.00	0.03	144,144,144,144	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.

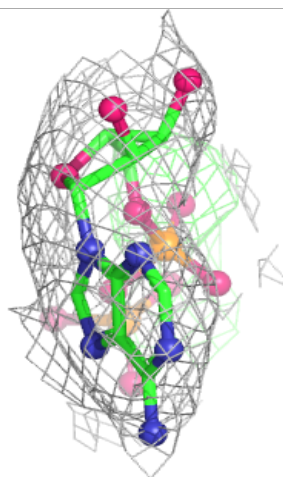
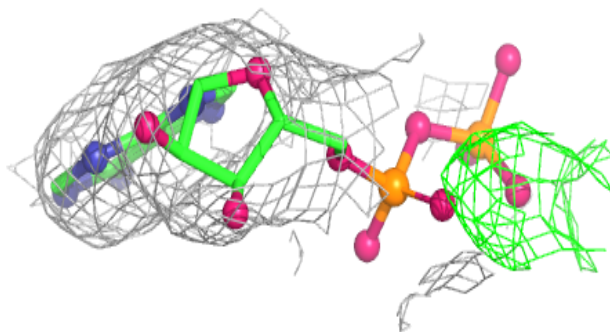
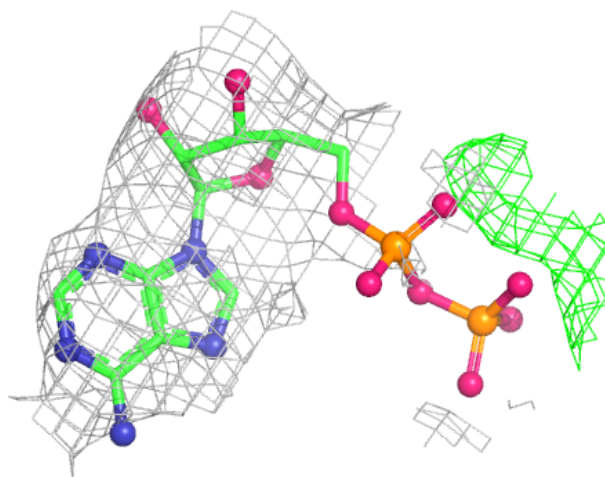
Electron density around ADP B 400:

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



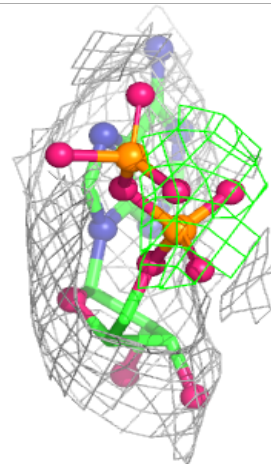
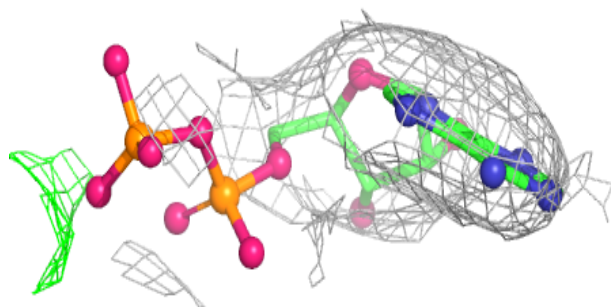
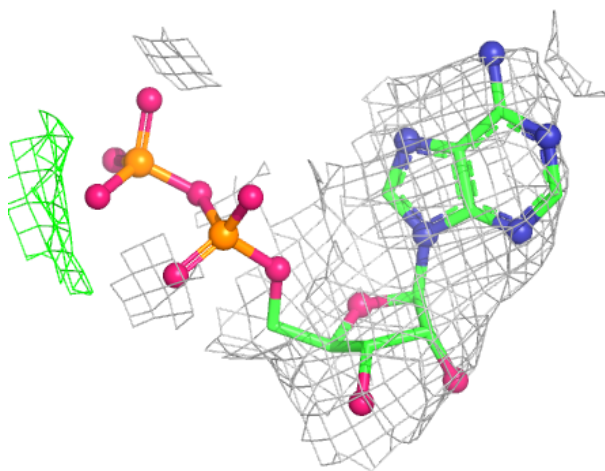
Electron density around ADP C 402:

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



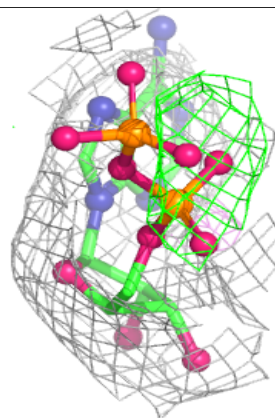
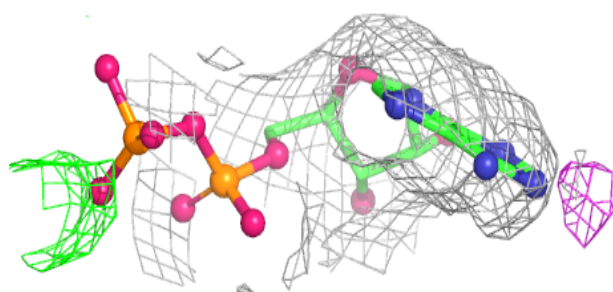
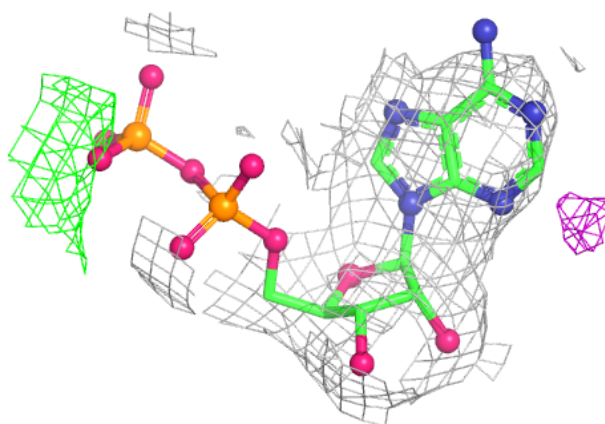
Electron density around ADP D 404:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

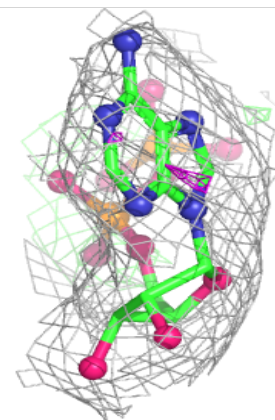
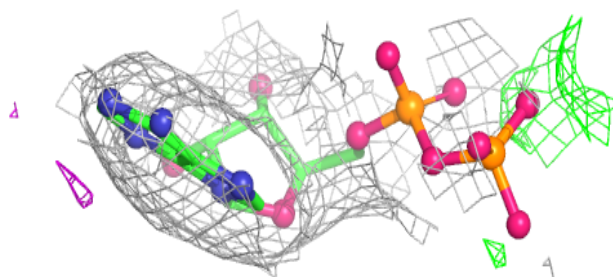
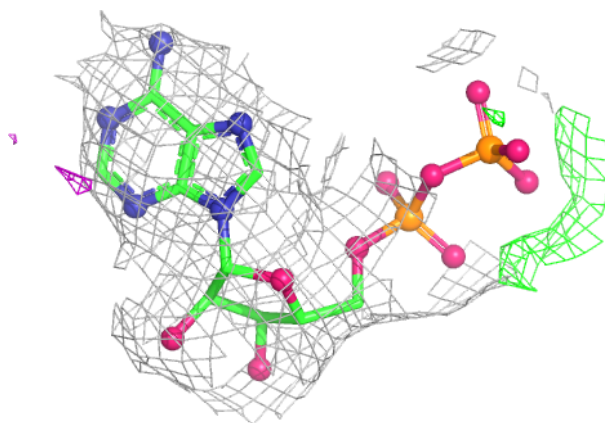


Electron density around ADP G 406:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

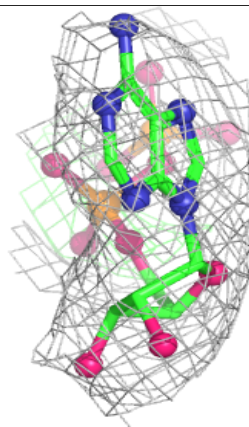
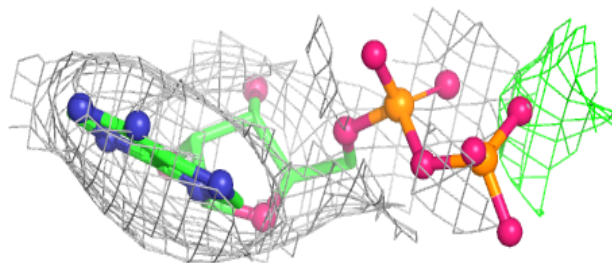
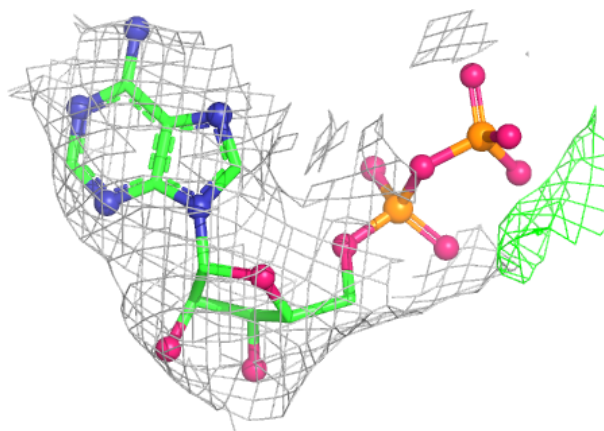
**Electron density around ADP H 408:**

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.