



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 12:20 am BST

PDB ID : 3GLF
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

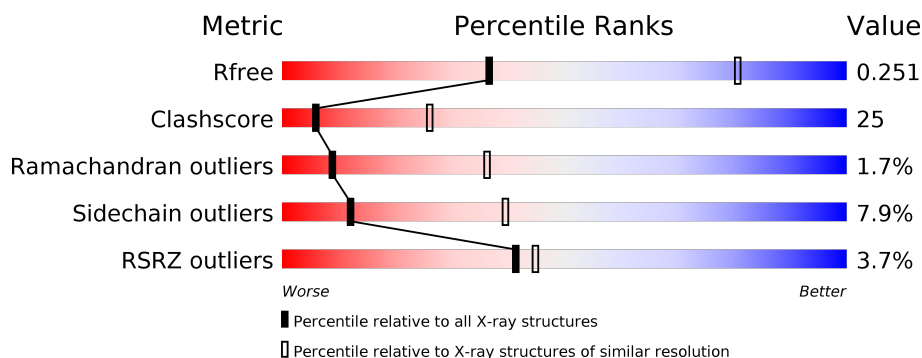
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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}	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>15%</div> <div> <div>48%</div> <div>44%</div> <div>5%</div> </div> </div>
1	F	343	<div> <div>7%</div> <div> <div>50%</div> <div>42%</div> <div>5%</div> </div> </div>
2	B	395	<div> <div>4%</div> <div> <div>54%</div> <div>35%</div> <div>8%</div> </div> </div>
2	C	395	<div> <div>3%</div> <div> <div>52%</div> <div>33%</div> <div>7%</div> <div>8%</div> </div> </div>
2	D	395	<div> <div>3%</div> <div> <div>50%</div> <div>37%</div> <div>8%</div> </div> </div>
2	G	395	<div> <div>2%</div> <div> <div>59%</div> <div>34%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	395	<div><div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>50%36%6%8%</div></div></div>
2	I	395	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>49%38%. . 8%</div></div>
3	E	334	<div><div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>63%34%. </div></div></div>
3	J	334	<div><div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>66%30%. </div></div></div>
4	K	15	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>13%80%7%</div></div>
4	M	15	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%13%73%7%</div></div>
5	L	10	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>40%60%</div></div>
5	N	10	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>60%40%</div></div>

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			

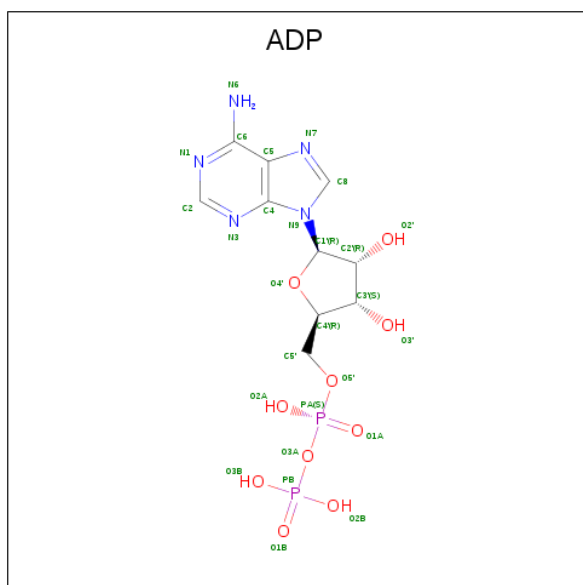
- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3').

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').

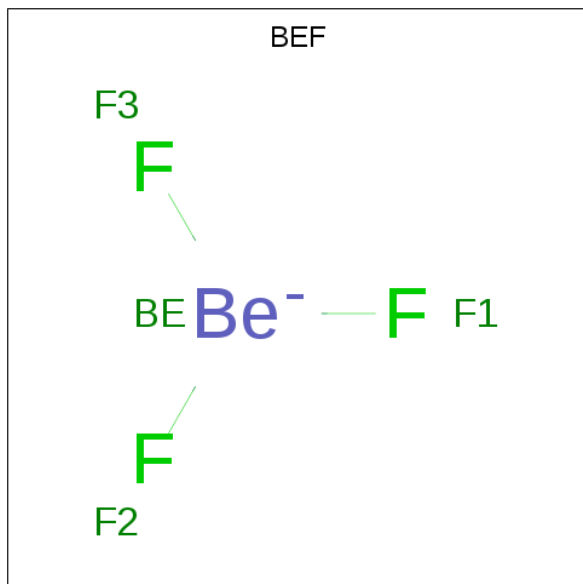
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			
5	N	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			

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



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

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

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

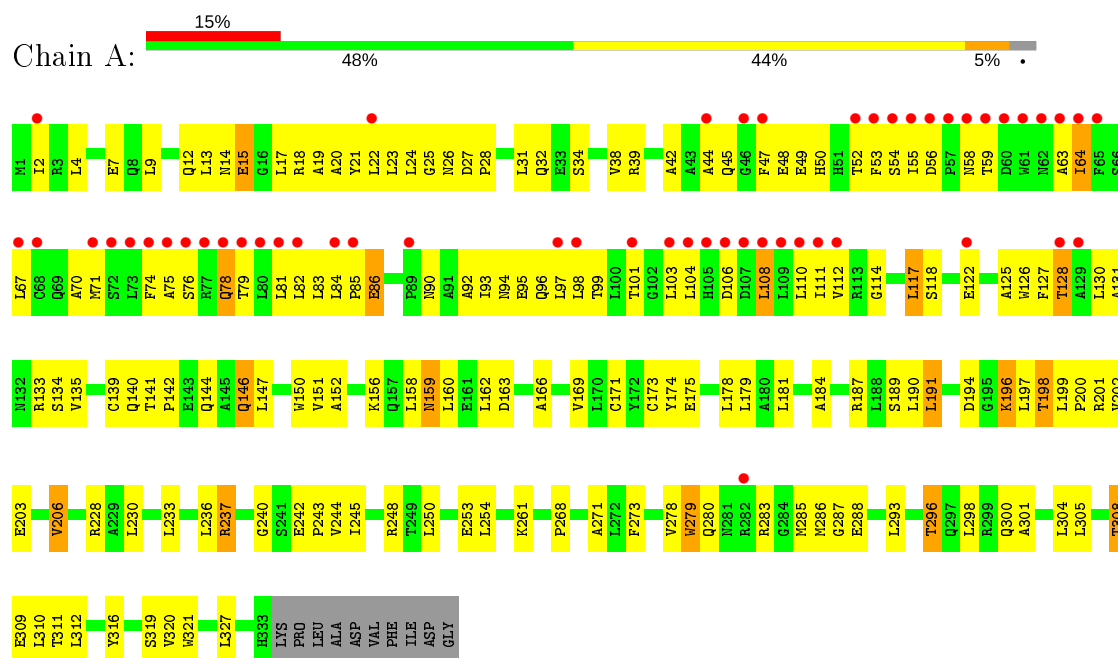
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

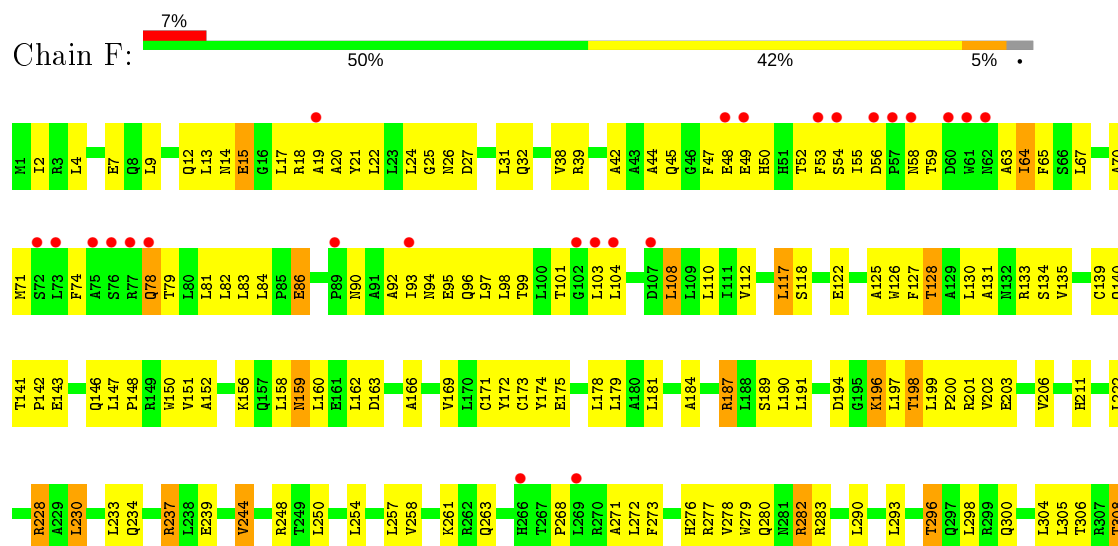
3 Residue-property plots

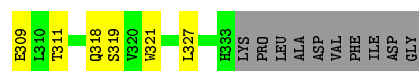
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

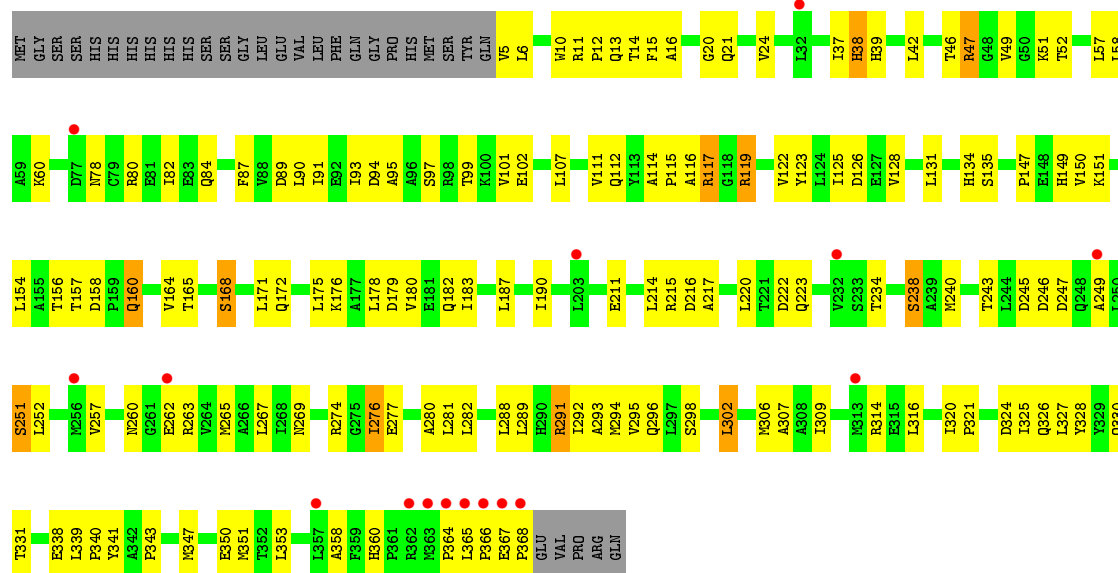


• Molecule 1: DNA polymerase III subunit delta

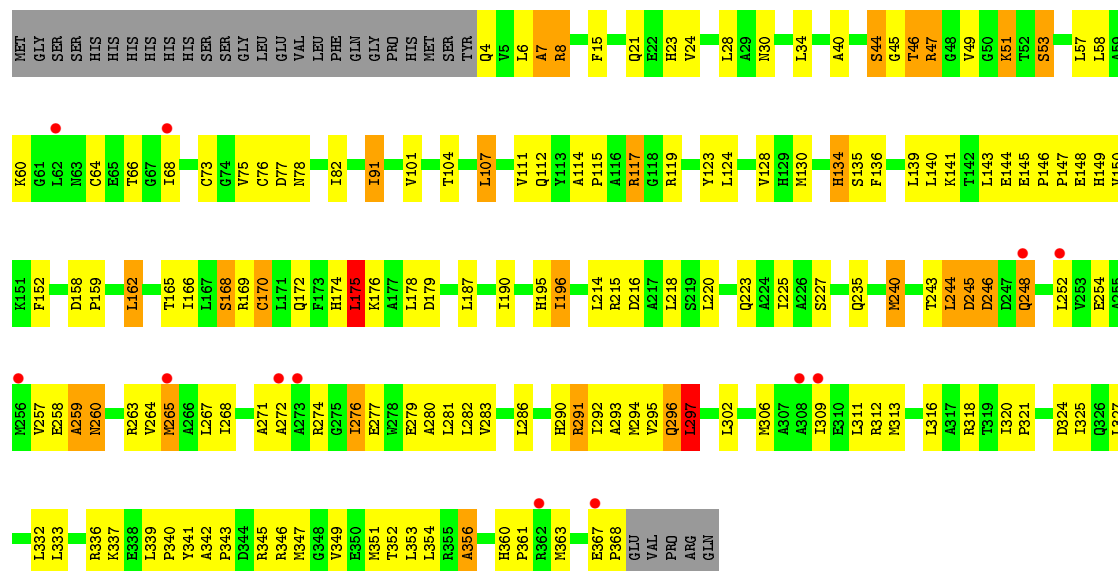




• Molecule 2: DNA polymerase III subunit tau

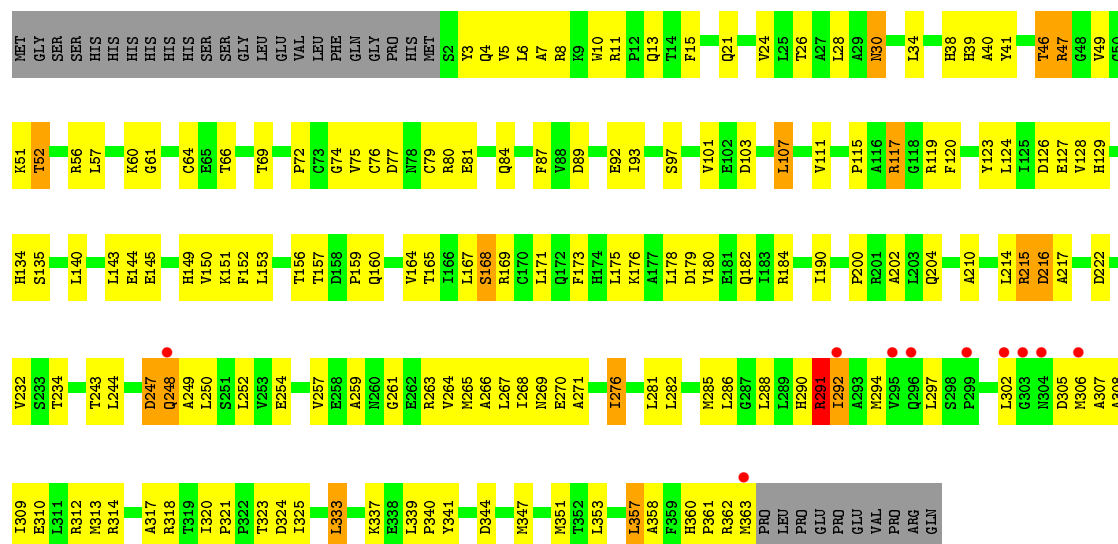


• Molecule 2: DNA polymerase III subunit tau

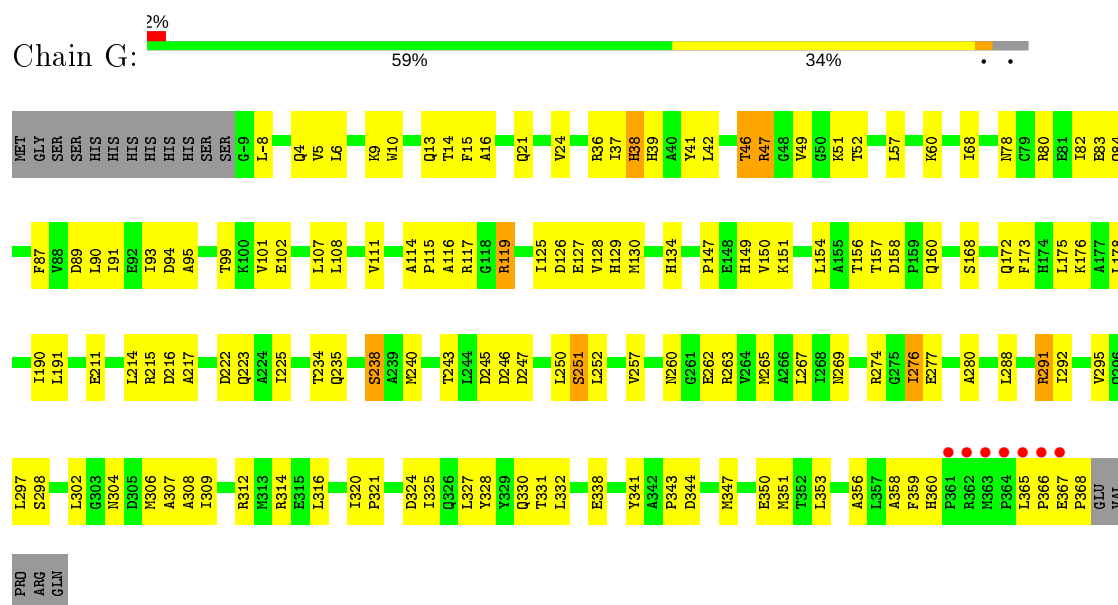


• Molecule 2: DNA polymerase III subunit tau

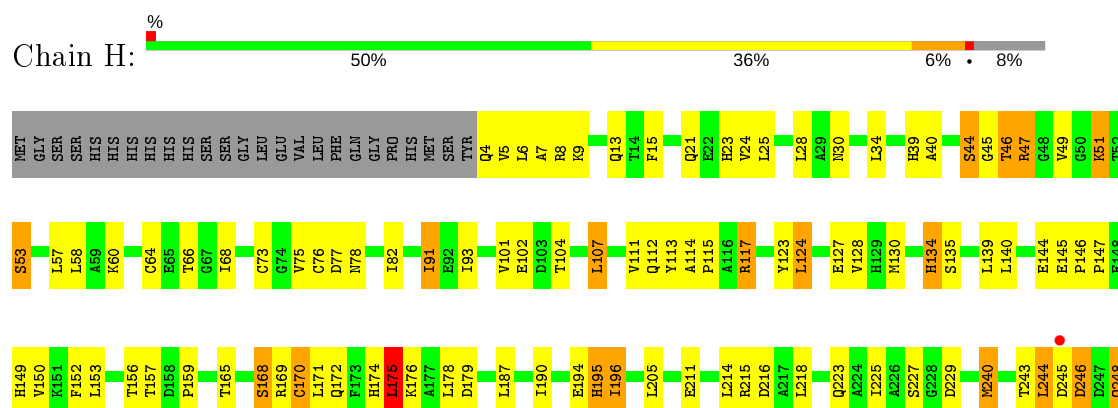


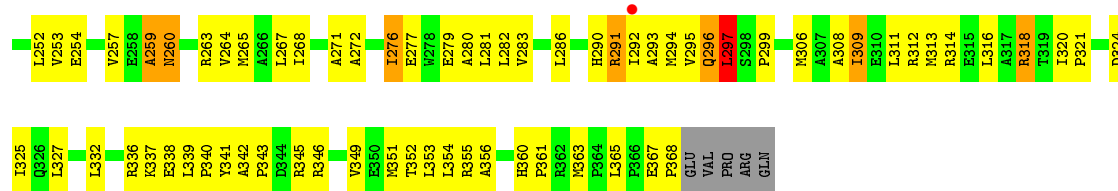


- Molecule 2: DNA polymerase III subunit tau



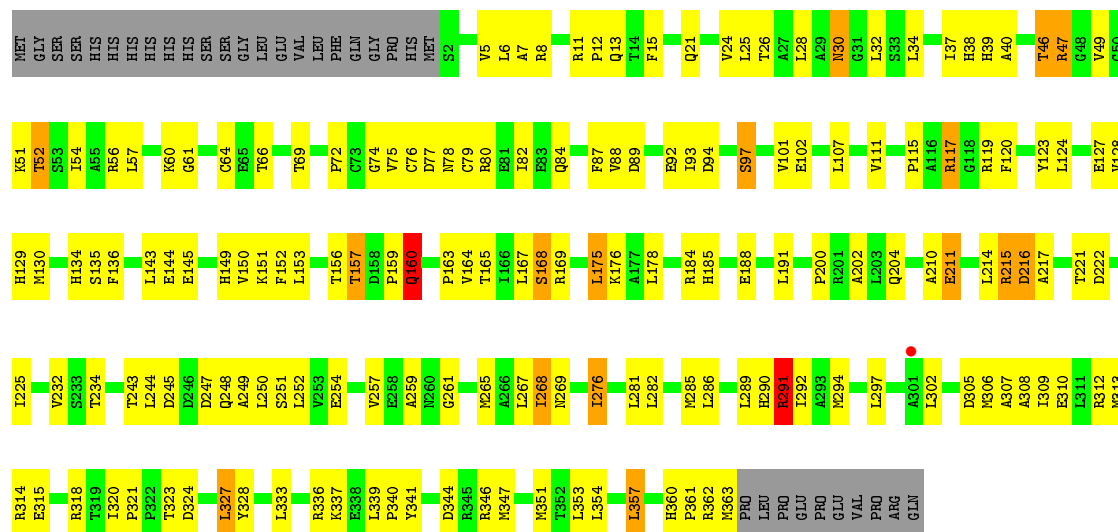
- Molecule 2: DNA polymerase III subunit tau





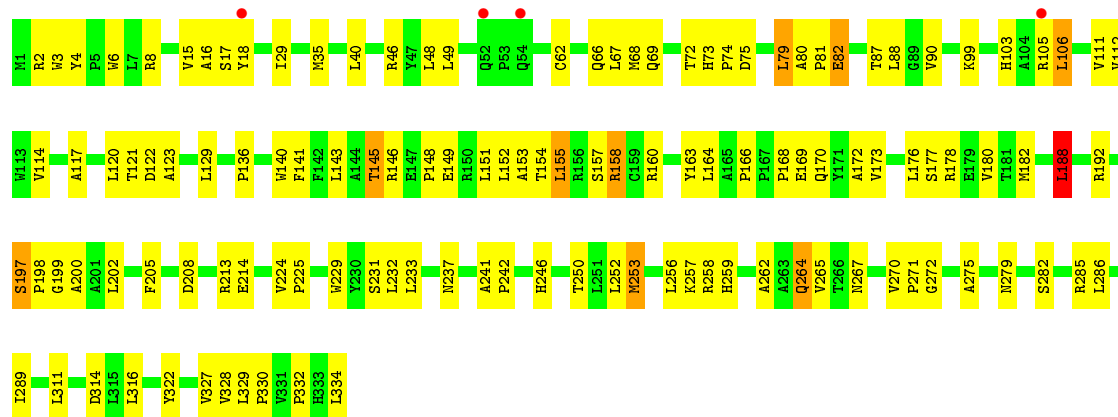
• Molecule 2: DNA polymerase III subunit tau

Chain I: 49% 38% 8%



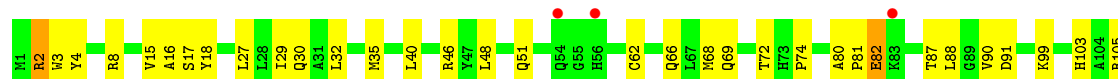
• Molecule 3: DNA polymerase III subunit delta'

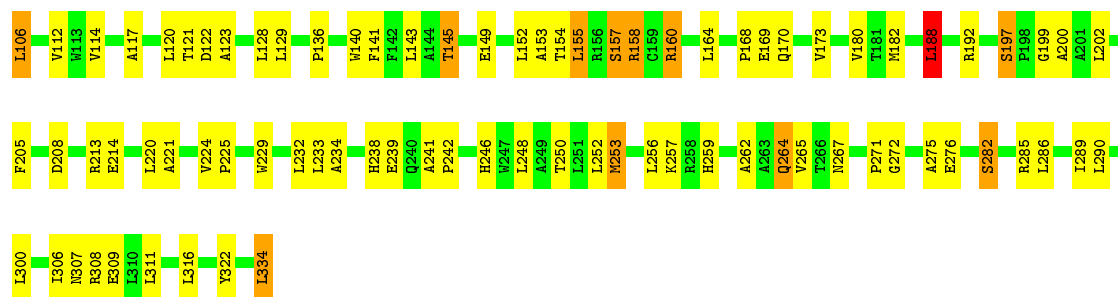
Chain E: 63% 34%



• Molecule 3: DNA polymerase III subunit delta'

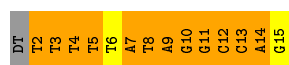
Chain J: 66% 30%





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

Chain K: 13% 80% 7%



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

Chain M: 7% 13% 73% 7%



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

Chain L: 40% 60%



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

Chain N: 60% 40%



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 0.209 , 0.251	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)	0.30 , 47.5	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, BEF, MG, ADP

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	0.72	0/2697	0.78	3/3664 (0.1%)
1	F	0.73	0/2697	0.78	3/3664 (0.1%)
2	B	0.72	0/2876	0.81	0/3900
2	C	0.72	1/2885 (0.0%)	0.86	6/3912 (0.2%)
2	D	0.77	1/2863 (0.0%)	0.89	0/3879
2	G	0.75	2/2992 (0.1%)	0.83	1/4057 (0.0%)
2	H	0.86	4/2885 (0.1%)	0.92	4/3912 (0.1%)
2	I	0.92	4/2863 (0.1%)	0.96	2/3879 (0.1%)
3	E	0.89	2/2666 (0.1%)	0.91	5/3639 (0.1%)
3	J	0.89	1/2666 (0.0%)	0.91	2/3639 (0.1%)
4	K	1.97	6/320 (1.9%)	2.68	32/492 (6.5%)
4	M	1.96	5/320 (1.6%)	2.58	27/492 (5.5%)
5	L	1.76	3/223 (1.3%)	2.80	28/342 (8.2%)
5	N	1.76	2/223 (0.9%)	2.75	25/342 (7.3%)
All	All	0.87	31/29176 (0.1%)	1.01	138/39813 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	C	0	1
2	G	0	1
2	H	0	1
2	I	0	1
All	All	0	5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	11	DG	C3'-O3'	-8.40	1.33	1.44
2	H	127	GLU	CG-CD	8.31	1.64	1.51
4	M	9	DA	C3'-O3'	-8.17	1.33	1.44
5	N	6	DC	C3'-O3'	-7.52	1.34	1.44
2	G	127	GLU	CG-CD	7.35	1.62	1.51
4	K	14	DA	C3'-O3'	-7.10	1.34	1.44
2	I	211	GLU	CG-CD	7.05	1.62	1.51
2	I	127	GLU	CG-CD	6.73	1.62	1.51
4	K	9	DA	C3'-O3'	-6.68	1.35	1.44
4	M	5	DT	N1-C2	6.65	1.43	1.38
4	K	11	DG	C3'-O3'	-6.33	1.35	1.44
2	C	148	GLU	CG-CD	6.17	1.61	1.51
2	H	102	GLU	CG-CD	6.16	1.61	1.51
5	L	5	DC	C3'-O3'	-6.14	1.35	1.44
4	M	11	DG	O3'-P	-6.03	1.53	1.61
2	H	338	GLU	CG-CD	5.96	1.60	1.51
5	L	6	DC	C3'-O3'	-5.89	1.36	1.44
2	I	160	GLN	CG-CD	5.88	1.64	1.51
3	E	214	GLU	CG-CD	5.77	1.60	1.51
3	E	149	GLU	CG-CD	5.66	1.60	1.51
4	K	13	DC	C3'-O3'	-5.62	1.36	1.44
2	H	338	GLU	CD-OE1	5.55	1.31	1.25
4	K	6	DT	C3'-O3'	-5.49	1.36	1.44
5	N	1	DC	N1-C6	-5.44	1.33	1.37
3	J	149	GLU	CD-OE2	5.43	1.31	1.25
4	M	10	DG	C3'-O3'	-5.39	1.36	1.44
5	L	1	DC	N1-C6	-5.33	1.33	1.37
2	D	127	GLU	CG-CD	5.31	1.59	1.51
4	K	10	DG	C3'-O3'	-5.26	1.37	1.44
2	G	338	GLU	CG-CD	5.21	1.59	1.51
2	I	315	GLU	CG-CD	5.08	1.59	1.51

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	5	DT	O4'-C1'-N1	-11.71	99.80	108.00
4	K	5	DT	O4'-C1'-N1	-11.64	99.85	108.00
5	L	5	DC	O4'-C4'-C3'	-11.36	99.19	106.00
5	N	2	DT	N3-C4-O4	10.52	126.21	119.90
5	N	5	DC	O4'-C4'-C3'	-10.37	99.78	106.00
4	K	2	DT	C4-C5-C7	10.10	125.06	119.00
4	K	14	DA	O4'-C1'-N9	-9.90	101.07	108.00
5	L	7	DT	N3-C4-O4	9.72	125.73	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	11	DG	N1-C6-O6	9.64	125.68	119.90
5	N	7	DT	C5-C4-O4	-9.61	118.18	124.90
4	K	6	DT	O5'-P-OP2	-9.36	97.28	105.70
4	M	14	DA	O4'-C1'-N9	-9.24	101.53	108.00
5	L	9	DT	O4'-C1'-C2'	-9.08	98.63	105.90
5	L	7	DT	C5-C4-O4	-9.06	118.56	124.90
5	N	1	DC	C4'-C3'-C2'	-8.73	95.24	103.10
4	M	2	DT	C4-C5-C7	8.60	124.16	119.00
2	C	107	LEU	CA-CB-CG	-8.60	95.53	115.30
5	L	6	DC	O4'-C4'-C3'	-8.55	100.87	106.00
5	N	7	DT	N3-C4-O4	8.52	125.01	119.90
4	M	5	DT	N3-C2-O2	-8.45	117.23	122.30
5	L	9	DT	C5-C4-O4	-8.35	119.05	124.90
5	N	2	DT	C5-C4-O4	-8.31	119.08	124.90
5	N	1	DC	C5-C6-N1	-8.17	116.91	121.00
5	N	1	DC	C6-N1-C2	8.13	123.55	120.30
4	K	13	DC	O4'-C1'-C2'	-8.12	99.40	105.90
4	K	12	DC	O4'-C1'-N1	-8.10	102.33	108.00
5	L	1	DC	C4'-C3'-C2'	-8.09	95.81	103.10
4	K	12	DC	O4'-C4'-C3'	-7.99	101.21	106.00
5	L	1	DC	C6-N1-C2	7.99	123.50	120.30
2	H	107	LEU	CA-CB-CG	-7.95	97.02	115.30
5	L	8	DA	O4'-C1'-N9	7.72	113.40	108.00
4	K	2	DT	C6-C5-C7	-7.67	118.30	122.90
5	L	2	DT	N3-C4-O4	7.58	124.45	119.90
5	N	10	DA	O4'-C1'-C2'	-7.51	99.89	105.90
4	M	4	DT	C4-C5-C7	7.48	123.49	119.00
4	K	8	DT	O4'-C1'-N1	7.39	113.18	108.00
4	K	5	DT	N3-C2-O2	-7.38	117.87	122.30
4	M	6	DT	O5'-P-OP2	-7.35	99.08	105.70
5	L	1	DC	O4'-C4'-C3'	-7.34	101.56	104.50
5	N	9	DT	O4'-C1'-C2'	-7.33	100.03	105.90
4	K	11	DG	N1-C6-O6	7.23	124.24	119.90
4	M	8	DT	O4'-C1'-N1	7.16	113.01	108.00
5	L	1	DC	O4'-C1'-N1	7.15	113.00	108.00
5	N	1	DC	N1-C2-O2	7.13	123.18	118.90
4	M	2	DT	C6-C5-C7	-7.09	118.64	122.90
5	L	7	DT	N3-C2-O2	6.92	126.45	122.30
4	K	14	DA	P-O3'-C3'	-6.79	111.55	119.70
4	M	11	DG	C5-C6-O6	-6.79	124.53	128.60
4	M	5	DT	N1-C2-O2	6.72	128.47	123.10
5	L	6	DC	N3-C2-O2	6.65	126.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	4	DT	C4-C5-C7	6.63	122.98	119.00
4	M	11	DG	C5-N7-C8	-6.62	100.99	104.30
5	N	9	DT	C1'-O4'-C4'	-6.61	103.49	110.10
4	M	11	DG	N3-C2-N2	-6.56	115.31	119.90
4	M	12	DC	O4'-C1'-N1	-6.54	103.42	108.00
1	A	187	ARG	NE-CZ-NH1	-6.52	117.04	120.30
5	L	10	DA	O4'-C1'-N9	6.49	112.54	108.00
4	M	11	DG	C8-N9-C4	-6.43	103.83	106.40
4	M	7	DA	O4'-C4'-C3'	6.43	109.86	106.00
5	N	9	DT	C5-C4-O4	-6.36	120.45	124.90
5	L	6	DC	C6-N1-C2	6.35	122.84	120.30
5	L	2	DT	C5-C4-O4	-6.34	120.46	124.90
4	K	8	DT	P-O3'-C3'	-6.32	112.12	119.70
4	M	11	DG	C2-N3-C4	-6.25	108.77	111.90
5	N	8	DA	O4'-C1'-N9	6.25	112.37	108.00
4	K	3	DT	N3-C4-O4	6.23	123.64	119.90
2	H	175	LEU	CA-CB-CG	6.20	129.55	115.30
4	K	6	DT	OP2-P-O3'	6.19	118.81	105.20
5	N	1	DC	C3'-C2'-C1'	-6.17	95.09	102.50
4	K	11	DG	C2-N3-C4	-6.14	108.83	111.90
4	K	6	DT	N3-C4-O4	6.10	123.56	119.90
1	F	187	ARG	NE-CZ-NH1	-6.09	117.26	120.30
5	L	9	DT	N3-C4-O4	6.05	123.53	119.90
5	L	9	DT	C1'-O4'-C4'	-6.04	104.06	110.10
4	M	11	DG	N7-C8-N9	6.02	116.11	113.10
4	M	8	DT	P-O3'-C3'	-6.01	112.48	119.70
3	E	79	LEU	CB-CG-CD2	-5.95	100.89	111.00
5	N	10	DA	O4'-C1'-N9	5.87	112.11	108.00
5	L	1	DC	C6-N1-C1'	-5.83	113.81	120.80
3	E	146	ARG	NE-CZ-NH1	-5.81	117.40	120.30
4	M	11	DG	C6-C5-N7	-5.79	126.93	130.40
5	N	9	DT	OP1-P-OP2	5.77	128.25	119.60
4	K	11	DG	N3-C4-C5	5.77	131.48	128.60
3	E	314	ASP	CB-CG-OD1	5.76	123.49	118.30
5	L	5	DC	N3-C2-O2	5.73	125.91	121.90
5	L	1	DC	C3'-C2'-C1'	-5.71	95.65	102.50
2	C	107	LEU	CB-CG-CD1	5.71	120.70	111.00
4	K	10	DG	O4'-C1'-N9	-5.70	104.01	108.00
4	M	8	DT	P-O5'-C5'	-5.68	111.82	120.90
5	N	9	DT	N3-C4-O4	5.67	123.30	119.90
5	L	1	DC	C5-C6-N1	-5.67	118.17	121.00
5	L	5	DC	N1-C2-O2	-5.65	115.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	178	LEU	CA-CB-CG	-5.65	102.31	115.30
4	M	9	DA	N1-C6-N6	5.64	121.98	118.60
5	L	1	DC	N1-C2-O2	5.60	122.26	118.90
4	K	11	DG	N3-C2-N2	-5.58	115.99	119.90
4	K	5	DT	N1-C2-O2	5.58	127.56	123.10
5	N	1	DC	N3-C2-O2	-5.57	118.00	121.90
2	C	162	LEU	CA-CB-CG	5.52	128.00	115.30
2	I	175	LEU	CA-CB-CG	5.49	127.93	115.30
3	J	334	LEU	CA-CB-CG	5.46	127.86	115.30
4	M	4	DT	N1-C2-O2	5.46	127.47	123.10
4	M	11	DG	N3-C4-N9	-5.44	122.73	126.00
2	I	327	LEU	CA-CB-CG	-5.44	102.79	115.30
2	C	175	LEU	CA-CB-CG	5.42	127.76	115.30
4	K	3	DT	C5-C4-O4	-5.42	121.11	124.90
5	N	6	DC	C5-C4-N4	-5.41	116.41	120.20
4	K	8	DT	C5-C4-O4	-5.40	121.12	124.90
4	K	9	DA	OP2-P-O3'	5.39	117.05	105.20
2	C	178	LEU	CA-CB-CG	-5.36	102.97	115.30
4	M	8	DT	C1'-O4'-C4'	-5.32	104.78	110.10
2	G	344	ASP	N-CA-C	-5.32	96.65	111.00
5	L	7	DT	P-O3'-C3'	5.28	126.04	119.70
5	N	1	DC	C6-N1-C1'	-5.28	114.47	120.80
5	N	7	DT	N3-C2-O2	5.27	125.46	122.30
4	K	6	DT	N3-C2-O2	5.26	125.46	122.30
5	N	6	DC	N3-C2-O2	5.26	125.58	121.90
4	K	11	DG	C4-C5-N7	5.25	112.90	110.80
5	N	1	DC	C2-N3-C4	-5.23	117.29	119.90
2	C	68	ILE	CB-CA-C	-5.22	101.16	111.60
5	L	5	DC	N3-C4-N4	5.21	121.64	118.00
4	M	13	DC	O4'-C1'-C2'	-5.20	101.74	105.90
4	K	15	DG	O4'-C1'-C2'	-5.18	101.75	105.90
4	K	7	DA	O4'-C4'-C3'	5.17	109.10	106.00
4	K	13	DC	C1'-O4'-C4'	-5.17	104.93	110.10
1	F	279	TRP	CA-CB-CG	5.15	123.49	113.70
3	J	106	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	228	ARG	NE-CZ-NH2	-5.13	117.74	120.30
4	K	11	DG	C5-C6-O6	-5.12	125.53	128.60
1	A	279	TRP	CA-CB-CG	5.10	123.39	113.70
2	H	68	ILE	CB-CA-C	-5.07	101.47	111.60
4	K	10	DG	O4'-C1'-C2'	-5.06	101.85	105.90
4	M	8	DT	C5-C4-O4	-5.06	121.36	124.90
3	E	106	LEU	CA-CB-CG	5.05	126.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	7	DT	C1'-O4'-C4'	-5.03	105.07	110.10
5	L	7	DT	OP2-P-O3'	5.02	116.24	105.20
1	A	187	ARG	NE-CZ-NH2	5.01	122.81	120.30
3	E	129	LEU	CB-CG-CD1	-5.01	102.49	111.00

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	168	0
1	F	2650	0	2703	158	0
2	B	2829	0	2879	153	1
2	C	2838	0	2886	165	1
2	D	2818	0	2863	173	0
2	G	2941	0	2987	139	0
2	H	2838	0	2886	160	2
2	I	2818	0	2863	165	1
3	E	2601	0	2603	108	1
3	J	2601	0	2603	119	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1426	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 25.

All (1426) 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
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:H:351:MET:HE1	2:I:290:HIS:HA	1.13	1.06
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:O	3:J:106:LEU:HD23	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:I:252:LEU:HD13	2:I:285:MET:HE1	1.57	0.84
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: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:G:4:GLN:NE2	2:G:9:LYS:HG3	1.93	0.84
2:I:47:ARG:HG2	2:I:47:ARG:O	1.75	0.83
2:G:216:ASP:OD1	2:H:168:SER:HB2	1.78	0.83
2:D:361:PRO:CB	3:J:272:GLY:HA2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:G:351:MET:HE1	2:H:290:HIS:HA	1.62	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: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
3:J:202:LEU:HD23	3:J:202:LEU:O	1.83	0.79
2:I:101:VAL:HG23	4:M:10:DG:OP1	1.81	0.79
2:G:115:PRO:HD3	2:G:149:HIS:CD2	2.18	0.79
2:H:292:ILE:HG13	2:H:313:MET:HE1	1.65	0.79
3:J:170:GLN:OE1	3:J:170:GLN:HA	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
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
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
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:CD2	2:B:39:HIS:H	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
2:H:351:MET:HE1	2:I:290:HIS:CA	2.07	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
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:HB3	2:H:318:ARG:HH11	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:C:292:ILE:HG13	2:C:313:MET:HE1	1.72	0.72
2:B:21:GLN:OE1	2:B:175:LEU:HB3	1.88	0.72
2:H:318:ARG:CB	2:H:318:ARG:HH11	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
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:C:4:GLN:OE1	2:C:4:GLN:HA	1.91	0.69
2:C:351:MET:HE2	2:D:290:HIS:HA	1.73	0.69
1:F:179:LEU:O	1:F:179:LEU:HG	1.93	0.69
2:C:318:ARG:HB3	2:C:318:ARG:HH11	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:291:ARG:O	2:D:294:MET: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
1:F:268:PRO:HD2	1:F:271:ALA:HB3	1.76	0.67
3:E:253:MET:O	3:E:253:MET:HG3	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
3:J:253:MET:O	3:J:253:MET:HG3	1.94	0.67
2:I:360:HIS:HB3	2:I:361:PRO:HD3	1.75	0.67
2:B:21:GLN:HA	2:B:21:GLN:NE2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ARG:HG2	2:B:306:MET:CE	2.25	0.67
2:D:252:LEU:HD13	2:D:285:MET:HE1	1.77	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:304:LEU:O	1:F:308:THR:HG23	1.94	0.67
1:F:64:ILE:HD12	1:F:96:GLN:HG2	1.76	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
2:B:265:MET:HE1	2:B:350:GLU:HG2	1.76	0.66
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: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
3:J:202:LEU:HD23	3:J:202:LEU:C	2.16	0.66
1:A:74:PHE:CD1	1:A:74:PHE:O	2.50	0.65
2:D:117:ARG:HB3	2:D:117:ARG:CZ	2.27	0.65
2:G:291:ARG:HG2	2:G:306:MET:CE	2.26	0.65
3:J:88:LEU:HD23	3:J:120:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ARG:HG2	2:B:47:ARG:O	1.96	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:244:LEU:HD21	2:D:276:ILE:HG12	1.78	0.64
2:D:49:VAL:O	2:D:49:VAL:HG12	1.97	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:202:ALA:HB2	2:D:234:THR:HA	1.80	0.64
2:D:61:GLY:HA2	2:D:72:PRO:HG3	1.80	0.64
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:117:LEU:CD1	1:A:122:GLU:HG2	2.25	0.63
1:A:27:ASP:HB2	1:A:141:THR:OG1	1.97	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:G:351:MET:CE	2:H:290:HIS:HA	2.27	0.63
2:H:318:ARG:NH1	2:H:318:ARG:CB	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:O	2:I:232:VAL:HG12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:265:MET:HE2	3:E:257:LYS:HD3	1.79	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
3:E:202:LEU:HD23	3:E:202:LEU:C	2.20	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:117:LEU:CD1	1:F:122:GLU:HG2	2.27	0.62
1:F:56:ASP:HB2	1:F:58:ASN:HB2	1.81	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:128:VAL:O	2:B:128:VAL:HG22	2.00	0.62
2:B:15:PHE:HE2	2:B:57:LEU:CB	2.13	0.62
2:G:21:GLN:NE2	2:G:21:GLN:HA	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:HG2	2:C:47:ARG:O	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
2:G:265:MET:HE1	2:G:350:GLU:HG2	1.83	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:E:35:MET:HE1	3:E:166:PRO:HA	1.81	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:114:VAL:HB	3:E:143:LEU:HD23	1.83	0.61
3:E:72:THR:HG23	3:E:72:THR:O	1.99	0.61
2:D:38:HIS:CD2	2:D:40:ALA:H	2.11	0.61
3:E:170:GLN:HA	3:E:170:GLN:OE1	1.99	0.61
2:B:277:GLU:O	2:B:280:ALA:HB3	2.01	0.60
2:B:52:THR:HG21	2:B:126:ASP:OD2	2.00	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: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
2:B:265:MET:CE	2:B:350:GLU:HG2	2.30	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
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:D:75:VAL:O	2:D:75:VAL:HG12	2.01	0.60
2:H:282:LEU:HD11	2:H:349:VAL:HG22	1.83	0.60
2:H:49:VAL:HG11	2:H:176:LYS:O	2.02	0.60
2:C:246:ASP:HB3	2:C:309:ILE:HD12	1.84	0.59
2:C:318:ARG:NH1	2:C:318:ARG:CB	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
3:E:155:LEU:HD12	3:E:155:LEU:C	2.23	0.59
1:F:282:ARG:HG2	1:F:282:ARG:HH11	1.68	0.59
2:G:223:GLN:HG2	2:G:240:MET:SD	2.42	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:HG2	2:H:47:ARG:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:353:LEU:O	2:C:356:ALA:HB3	2.02	0.59
2:C:47:ARG:NH1	2:C:216:ASP:OD2	2.35	0.59
2:G:314:ARG:NH1	2:G:314:ARG:HG2	2.18	0.59
1:A:12:GLN:HG3	1:A:12:GLN:O	2.03	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:232:VAL:HG12	2:D:232:VAL:O	2.01	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:NH1	2:B:314:ARG:HG2	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
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
3:E:90:VAL:CG1	4:K:8:DT:H5"	2.33	0.58
1:A:39:ARG:NH2	1:A:50:HIS:HB3	2.17	0.58
2:D:363:MET:HE2	3:J:276:GLU:OE1	2.02	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
3:E:224:VAL:HG12	3:E:225:PRO:N	2.17	0.58
3:E:88:LEU:HD23	3:E:120:LEU:HD23	1.86	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
2:H:246:ASP:HB3	2:H:309:ILE:HD12	1.84	0.58
2:B:351:MET:HE1	2:C:290:HIS:HA	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:216:ASP:OD1	3:E:157:SER:CB	2.52	0.57
1:A:56:ASP:HB2	1:A:58:ASN:HB2	1.84	0.57
2:B:291:ARG:HG2	2:B:306:MET:HE1	1.87	0.57
2:B:343:PRO:HG3	2:C:286:LEU:HB2	1.86	0.57
2:C:351:MET:HE1	2:D:290:HIS:HA	1.86	0.57
3:E:80:ALA:HB1	3:E:81:PRO:HD3	1.86	0.57
3:J:103:HIS:H	3:J:103:HIS:CD2	2.21	0.57
3:J:2:ARG:HD3	3:J:4:TYR:HE1	1.66	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:B:351:MET:CE	2:C:290:HIS:HA	2.35	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:223:GLN:HG3	2:C:240:MET:HE1	1.86	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
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
2:B:291:ARG:HG2	2:B:306:MET:HE3	1.87	0.56
3:J:3:TRP:CH2	3:J:8:ARG:HG3	2.40	0.56
2:D:250:LEU:HD13	2:D:313:MET:HE1	1.87	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
1:F:21:TYR:CE1	1:F:135:VAL:HB	2.41	0.56
2:G:114:ALA:HA	2:G:149:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:121:THR:HG22	3:J:123:ALA:H	1.70	0.56
2:C:244:LEU:HD12	2:C:244:LEU:H	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:223:GLN:HG3	2:H:240:MET:HE1	1.88	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
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:21:GLN:NE2	2:I:49:VAL:CG1	2.67	0.55
2:I:6:LEU:HD12	2:I:6:LEU:H	1.71	0.55
5:N:4:DG:H2"	5:N:5:DC:O5'	2.07	0.55
1:A:196:LYS:C	1:A:197:LEU:HD23	2.27	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:D:24:VAL:HG21	2:D:175:LEU:CD2	2.36	0.55
2:C:341:TYR:CB	2:D:333:LEU:HD11	2.37	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
2:G:291:ARG:HG2	2:G:306:MET:HE3	1.87	0.55
1:A:81:LEU:HD12	1:A:82:LEU:H	1.71	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:196:LYS:C	1:F:197:LEU:HD23	2.27	0.55
1:F:39:ARG:NH2	1:F:50:HIS:HB3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:MET:CB	1:F:108:LEU:HG	2.37	0.55
2:G:291:ARG:HG2	2:G:306:MET:HE1	1.89	0.55
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
3:J:155:LEU:C	3:J:155:LEU:HD12	2.27	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:HG22	2:G:128:VAL:O	2.05	0.55
3:J:264:GLN:HG3	3:J:265:VAL:N	2.20	0.55
2:I:164:VAL:O	2:I:164:VAL:HG22	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:O	2:I:309:ILE:HG22	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
2:H:130:MET:HE1	2:I:134:HIS:HA	1.90	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
1:F:53:PHE:HE2	1:F:59:THR:HG1	1.56	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:278:VAL:HG12	1:A:283:ARG:HG2	1.90	0.53
1:A:90:ASN:O	1:A:94:ASN:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:93:ILE:HG12	2:B:107:LEU:HD22	1.90	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:114:ALA:HA	2:B:149:HIS:CD2	2.43	0.53
2:B:38:HIS:N	2:B:38:HIS:ND1	2.57	0.53
2:C:51:LYS:CG	6:C:402:ADP:O2B	2.57	0.53
1:F:282:ARG:NH1	1:F:282:ARG:HG2	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
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:HA	1:A:86:GLU:OE2	2.09	0.53
3:E:2:ARG:CG	3:E:3:TRP:N	2.71	0.53
1:F:237:ARG:HG3	1:F:321:TRP:CD2	2.44	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
2:G:327:LEU:HD12	2:G:330:GLN:OE1	2.09	0.53
2:G:49:VAL:HG12	2:G:49:VAL:O	2.09	0.53
2:H:60:LYS:HA	2:H:82:ILE:HD12	1.90	0.53
2:I:265:MET:HE2	3:J:257:LYS:HD3	1.90	0.53
2:B:49:VAL:O	2:B:49:VAL:HG12	2.07	0.53
2:C:6:LEU:O	2:C:7:ALA:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:24:VAL:HG21	2:D:175:LEU:HD22	1.91	0.52
2:D:6:LEU:N	2:D:6:LEU:HD12	2.24	0.52
3:E:15:VAL:O	3:E:18:TYR:N	2.42	0.52
3:J:155:LEU:O	3:J:155:LEU:HD12	2.08	0.52
2:C:111:VAL:HG13	2:C:150:VAL:HG21	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: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
1:F:162:LEU:HD22	1:F:166:ALA:HB3	1.91	0.52
1:F:90:ASN:O	1:F:94:ASN:HB2	2.09	0.52
2:G:38:HIS:ND1	2:G:38:HIS:N	2.57	0.52
2:G:39:HIS:HD2	2:G:39:HIS:H	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:122:GLU:O	1:F:127:PHE:CD2	2.63	0.52
1:F:42:ALA:O	1:F:47:PHE:HD1	1.93	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:O	3:J:72:THR:HG23	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:D:363:MET:HE3	3:J:221:ALA:HB1	1.91	0.52
1:A:142:PRO:HB2	1:A:147:LEU:HD12	1.91	0.51
1:A:26:ASN:OD1	1:A:27:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:GLN:CD	1:F:318:GLN:H	2.14	0.51
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: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:254:GLU:O	2:H:257:VAL:HG22	2.11	0.51
2:H:28:LEU:HD22	2:H:58:LEU:HD22	1.92	0.51
2:I:250:LEU:HD13	2:I:313:MET:HE3	1.93	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:261:LYS:HE2	1:A:293:LEU:O	2.11	0.51
1:A:56:ASP:HB2	1:A:58:ASN:H	1.75	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:HG3	2:C:248:GLN:O	2.09	0.51
2:I:347:MET:HE1	3:J:250:THR:HG22	1.91	0.51
1:F:261:LYS:HE2	1:F:293:LEU:O	2.08	0.51
1:F:42:ALA:O	1:F:47:PHE:CD1	2.64	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:339:LEU:HD11	2:C:345:ARG:O	2.10	0.51
2:C:337:LYS:NZ	3:E:334:LEU:HD22	2.26	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:181:LEU:O	1:A:184:ALA:HB3	2.11	0.51
1:A:55:ILE:HG22	1:A:93:ILE:HD13	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:360:HIS:CD2	2:C:361:PRO:HD2	2.46	0.50
3:J:224:VAL:HG12	3:J:225:PRO:N	2.24	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:H:147:PRO:HB2	2:H:149:HIS:CE1	2.46	0.50
2:G:347:MET:HG2	2:H:290:HIS:CE1	2.46	0.50
2:I:123:TYR:HB2	2:I:152:PHE:CD2	2.47	0.50
3:J:121:THR:CG2	3:J:122:ASP:N	2.74	0.50
3:J:62:CYS:O	3:J:66:GLN:HG3	2.11	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: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:158:ASP:OD1	2:B:160:GLN:HB3	2.12	0.50
2:B:14:THR:HG22	2:B:16:ALA:H	1.77	0.50
2:C:316:LEU:CD2	2:C:320:ILE:HD11	2.42	0.50
2:C:64:CYS:SG	2:C:66:THR:HG23	2.51	0.50
1:F:26:ASN:ND2	1:F:140:GLN:OE1	2.45	0.50
2:G:365:LEU:HD11	2:H:297:LEU:HD23	1.94	0.50
1:A:104:LEU:HD13	1:A:133:ARG:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TYR:CE1	1:A:135:VAL:HB	2.46	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:119:ARG:NH1	2:B:119:ARG:HG2	2.26	0.49
2:B:327:LEU:HD12	2:B:330:GLN:OE1	2.11	0.49
2:B:78:ASN:O	2:B:82:ILE:HG13	2.12	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
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
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
2:D:347:MET:HE1	3:E:250:THR:HG22	1.93	0.49
1:F:250:LEU:O	1:F:250:LEU:HG	2.09	0.49
1:F:254:LEU:HG	1:F:254:LEU:O	2.11	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
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
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
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:128:VAL:CG1	2:D:156:THR:HB	2.43	0.49
2:D:61:GLY:CA	2:D:72:PRO:HG3	2.43	0.49
3:E:155:LEU:O	3:E:155:LEU:HD12	2.13	0.49
3:E:3:TRP:CH2	3:E:8:ARG:HG3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	3:J:213:ARG:NH1	2.28	0.49
2:C:327:LEU:HD23	2:C:361:PRO:HG3	1.94	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
1:F:142:PRO:CD	1:F:178:LEU:HD11	2.43	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:51:LYS:HG3	6:H:408:ADP:O2B	2.13	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
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
2:C:215:ARG:O	2:C:216:ASP:C	2.51	0.48
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:321:PRO:O	2:H:324:ASP:HB2	2.14	0.48
2:H:293:ALA:HB2	2:H:325:ILE:HG21	1.96	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
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: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
2:I:252:LEU:HD13	2:I:285:MET:HE2	1.91	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:265:MET:HE3	2:I:294:MET:SD	2.53	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
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
3:E:81:PRO:HB3	3:E:87:THR:O	2.14	0.48
2:H:292:ILE:HG13	2:H:313:MET:HE3	1.96	0.48
2:B:47:ARG:NH2	2:B:211:GLU:O	2.47	0.47
2:C:291:ARG:O	2:C:294:MET:HB3	2.13	0.47
2:C:73:CYS:O	2:C:75:VAL:HG13	2.14	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
2:D:291:ARG:O	2:D:292:ILE:C	2.53	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
1:A:14:ASN:O	1:A:15:GLU:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:360:HIS:HD1	2:C:363:MET:H	1.62	0.47
3:E:2:ARG:HG2	3:E:3:TRP:N	2.28	0.47
2:G:15:PHE:HE2	2:G:57:LEU:CB	2.19	0.47
2:G:245:ASP:C	2:G:247:ASP:H	2.16	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: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:G:5:VAL:HG21	2:H:39:HIS:ND1	2.29	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
2:B:249:ALA:HB2	2:B:281:LEU:HD12	1.97	0.47
2:C:274:ARG:HB2	2:C:276:ILE:HG23	1.97	0.47
2:C:58:LEU:O	2:C:58:LEU:HD12	2.15	0.47
2:G:46:THR:HG22	2:G:47:ARG:HD3	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
2:C:139:LEU:HA	2:C:139:LEU:HD23	1.60	0.47
2:C:254:GLU:HG2	2:C:316:LEU:HD11	1.96	0.47
2:H:316:LEU:HD23	2:H:320:ILE:HD11	1.97	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:HD12	2:B:58:LEU:HA	1.58	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
3:J:30:GLN:HG3	3:J:30:GLN:O	2.15	0.47
1:A:162:LEU:HD23	1:A:197:LEU:HB2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:215:ARG:C	2:B:217:ALA:N	2.68	0.47
2:G:125:ILE:HB	2:G:154:LEU:CD2	2.44	0.47
2:G:328:TYR:HH	2:G:360:HIS:CD2	2.32	0.47
2:H:46:THR:O	2:H:49:VAL:HG23	2.15	0.47
2:H:6:LEU:O	2:H:7:ALA:C	2.53	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:HA	2:G:332:LEU:HD23	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
1:F:127:PHE:HA	1:F:130:LEU:HD12	1.97	0.46
1:F:52:THR:CG2	1:F:81:LEU:HD23	2.45	0.46
2:G:150:VAL:O	2:G:151:LYS:HD3	2.16	0.46
2:H:351:MET:HE2	2:I:290:HIS:HB2	1.97	0.46
3:J:224:VAL:CB	3:J:225:PRO:CD	2.92	0.46
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.75	0.46
1:A:81:LEU:HD12	1:A:82:LEU:N	2.30	0.46
2:C:341:TYR:CZ	2:D:337:LYS:HD2	2.50	0.46
3:E:152:LEU:HD12	3:E:152:LEU:HA	1.60	0.46
1:F:196:LYS:HE3	1:F:196:LYS:HB2	1.68	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:D:15:PHE:HE2	2:D:57:LEU:HB3	1.81	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
1:F:56:ASP:HB2	1:F:58:ASN:H	1.80	0.46
2:I:244:LEU:HA	2:I:244:LEU:HD23	1.61	0.46
1:A:254:LEU:HG	1:A:254:LEU:O	2.16	0.46
1:A:81:LEU:HD21	1:A:83:LEU:HD21	1.98	0.46
1:F:117:LEU:HB2	1:F:122:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:88:VAL:CG1	2:I:88:VAL:O	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
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:286:LEU:HD23	2:D:286:LEU:HA	1.80	0.46
2:D:52:THR:CG2	6:D:404:ADP:O1B	2.54	0.46
2:G:-8:LEU:HA	2:G:-8:LEU:HD12	1.73	0.46
2:I:353:LEU:HA	2:I:353:LEU:HD23	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:H:292:ILE:CG1	2:H:313:MET:HE3	2.46	0.46
2:I:101:VAL:HG21	2:I:134:HIS:HB3	1.97	0.46
2:I:15:PHE:CE2	2:I:57:LEU:HB3	2.50	0.46
2:I:94:ASP:CG	2:I:97:SER:HB2	2.35	0.46
2:B:215:ARG:O	2:B:216:ASP:C	2.54	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
2:C:367:GLU:CD	2:D:362:ARG:HH12	2.19	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:HB2	2:H:291:ARG:HE	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
2:B:89:ASP:OD2	2:B:116:ALA:N	2.47	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
1:A:316:TYR:CD1	5:L:10:DA:H2"	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:TRP:O	3:E:316:LEU:HD13	2.17	0.45
3:E:4:TYR:HB3	3:E:6:TRP:CH2	2.52	0.45
2:G:276:ILE:HG23	2:G:277:GLU:N	2.31	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
1:F:268:PRO:HD2	1:F:271:ALA:CB	2.45	0.45
3:J:2:ARG:HG2	3:J:3:TRP:N	2.31	0.45
2:B:358:ALA:HA	2:B:365:LEU:CB	2.46	0.45
2:B:94:ASP:OD2	2:C:141:LYS:HB2	2.17	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:D:56:ARG:HD3	2:D:92:GLU:OE1	2.16	0.45
2:H:355:ARG:O	2:H:356:ALA:C	2.53	0.45
2:B:320:ILE:HG23	2:B:321:PRO:HD2	1.97	0.45
2:C:260:ASN:OD1	2:C:260:ASN:O	2.35	0.45
1:F:261:LYS:CE	1:F:293:LEU:O	2.65	0.45
1:F:55:ILE:CG2	1:F:93:ILE:HD13	2.45	0.45
2:G:89:ASP:OD2	2:G:116:ALA:N	2.49	0.45
2:G:41:TYR:CD1	2:G:41:TYR:N	2.84	0.45
2:G:78:ASN:O	2:G:82:ILE:HG13	2.15	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: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: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:G:215:ARG:NH2	7:G:407:BEF:F2	2.37	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:94:ASP:OD1	2:B:94:ASP:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:265:MET:CE	2:G:350:GLU:HG2	2.45	0.45
2:I:15:PHE:HE2	2:I:57:LEU:HB3	1.81	0.45
2:I:276:ILE:HG21	2:I:281:LEU:HD13	1.98	0.45
5:L:6:DC:H2''	5:L:7:DT:O5'	2.17	0.45
1:A:150:TRP:CZ3	1:A:178:LEU:HD22	2.52	0.45
1:A:58:ASN:O	1:A:59:THR:C	2.54	0.45
2:C:40:ALA:HB3	2:C:170:CYS:HB3	1.97	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:187:ARG:HG3	2:G:173:PHE:CE1	2.52	0.45
1:F:26:ASN:OD1	1:F:27:ASP:N	2.49	0.45
1:A:253:GLU:OE1	1:A:286:MET:HE1	2.16	0.45
1:A:31:LEU:O	1:A:32:GLN:C	2.55	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:I:6:LEU:CD1	2:I:6:LEU:H	2.29	0.45
3:J:154:THR:O	3:J:158:ARG:HD2	2.17	0.45
2:D:361:PRO:HB2	3:J:272:GLY:HA2	1.95	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
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:N	2:G:359:PHE:CD1	2.84	0.45
2:H:40:ALA:CB	2:H:170:CYS:HB3	2.46	0.45
2:I:13:GLN:OE1	2:I:60:LYS:NZ	2.50	0.45
2:I:6:LEU:CD1	2:I:222:ASP:OD2	2.65	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:I:56:ARG:NH1	2:I:92:GLU:OE2	2.50	0.44
1:A:163:ASP:OD2	1:A:198:THR:HA	2.17	0.44
1:A:278:VAL:O	1:A:279:TRP:C	2.55	0.44
1:A:81:LEU:HD12	1:A:111:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:190:ILE:HD12	2:H:218:LEU:HD21	1.98	0.44
2:H:93:ILE:HG22	2:H:93:ILE:O	2.17	0.44
2:I:25:LEU:HD21	2:I:54:ILE:CD1	2.48	0.44
1:A:81:LEU:HD13	1:A:111:ILE:HG22	2.00	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
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
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:HA	3:J:152:LEU:HD12	1.54	0.44
3:J:232:LEU:O	3:J:233:LEU:C	2.55	0.44
1:A:285:MET:O	1:A:288:GLU:HB3	2.18	0.44
2:C:279:GLU:OE2	2:C:336:ARG:NE	2.51	0.44
2:D:347:MET:HE2	2:D:347:MET:HB2	1.80	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: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:HD23	2:I:282:LEU:HA	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
1:A:53:PHE:HE2	1:A:59:THR:HG1	1.63	0.44
2:C:115:PRO:HD3	2:C:149:HIS:CD2	2.39	0.44
3:E:73:HIS:ND1	3:E:73:HIS:C	2.70	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:341:TYR:CE1	2:I:337:LYS:HD2	2.52	0.44
1:A:101:THR:HG22	1:A:130:LEU:HD21	2.00	0.44
1:A:4:LEU:HD12	1:A:135:VAL:CG1	2.47	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
3:E:172:ALA:HB1	3:E:198:PRO:HG3	1.99	0.44
3:E:232:LEU:O	3:E:233:LEU:C	2.55	0.44
1:F:230:LEU:N	1:F:230:LEU:HD23	2.33	0.44
2:H:295:VAL:O	2:H:296:GLN:C	2.56	0.44
1:A:151:VAL:HG22	1:A:181:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD11	2:B:38:HIS:CE1	2.52	0.44
1:A:236:LEU:HA	1:A:236:LEU:HD23	1.72	0.44
2:C:243:THR:HG22	2:C:244:LEU:O	2.18	0.44
3:E:176:LEU:HA	3:E:176:LEU:HD23	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
3:J:253:MET:HE3	3:J:290:LEU:HD21	1.99	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:B:265:MET:HE1	2:C:294:MET:SD	2.58	0.44
2:C:295:VAL:CG2	2:C:302:LEU:HB2	2.47	0.44
2:D:215:ARG:O	2:D:216:ASP:C	2.56	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
1:A:55:ILE:CG2	1:A:93:ILE:HD13	2.47	0.44
2:B:101:VAL:HA	2:B:135:SER:OG	2.17	0.44
2:B:42:LEU:HD12	2:B:154:LEU:O	2.18	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:CA	2:G:21:GLN:NE2	2.80	0.44
6:H:408:ADP:N3	6:H:408:ADP:H2'	2.32	0.44
2:H:47:ARG:NH2	2:H:211:GLU:O	2.51	0.44
1:A:13:LEU:CD2	1:A:21:TYR:CE1	3.01	0.43
1:A:174:TYR:O	1:A:175:GLU:C	2.56	0.43
1:A:273:PHE:HB3	1:A:283:ARG:HD2	2.00	0.43
1:A:54:SER:HB3	1:A:83:LEU:HD12	2.00	0.43
2:B:128:VAL:CG2	2:B:128:VAL:O	2.65	0.43
2:D:101:VAL:HG21	2:D:134:HIS:HB3	2.00	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:215:ARG:O	2:I:216:ASP:C	2.57	0.43
2:I:302:LEU:HD12	2:I:306:MET:HG3	1.98	0.43
2:I:354:LEU:HA	2:I:354:LEU:HD23	1.85	0.43
2:B:101:VAL:CG2	2:B:134:HIS:CB	2.92	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:I:306:MET:HE3	2:I:306:MET:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:257:VAL:HG12	2:I:328:TYR:CE2	2.53	0.43
3:J:202:LEU:CD2	3:J:202:LEU:C	2.86	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
2:C:260:ASN:OD1	2:C:260:ASN:C	2.55	0.43
2:C:265:MET:CE	2:C:354:LEU:HD21	2.48	0.43
2:D:282:LEU:HA	2:D:282:LEU:HD23	1.63	0.43
2:D:28:LEU:HA	2:D:28:LEU:HD23	1.75	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
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
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
2:C:292:ILE:CG1	2:C:313:MET:HE3	2.49	0.43
1:F:71:MET:CG	1:F:103:LEU:HD13	2.47	0.43
2:G:351:MET:HE2	2:H:290:HIS:HB2	1.99	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:HA	3:J:220:LEU:HD12	1.59	0.43
2:D:363:MET:CE	3:J:276:GLU:OE1	2.67	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:G:13:GLN:CD	2:G:83:GLU:HG3	2.39	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:274:ARG:NH2	2:B:276:ILE:HG12	2.34	0.43
2:B:91:ILE:HG22	2:B:93:ILE:CD1	2.48	0.43
3:E:327:VAL:HG12	3:E:328:VAL:N	2.33	0.43
3:E:67:LEU:HD22	3:E:72:THR:O	2.18	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
1:F:86:GLU:HA	1:F:86:GLU:OE2	2.16	0.43
2:G:101:VAL:O	2:G:102:GLU:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:260:ASN:OD1	2:H:260:ASN:C	2.56	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:245:ILE:HG22	1:A:245:ILE:O	2.18	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
2:C:254:GLU:O	2:C:258:GLU:HG3	2.18	0.43
2:C:58:LEU:C	2:C:58:LEU:HD12	2.39	0.43
1:F:58:ASN:O	1:F:59:THR:C	2.56	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:I:76:CYS:O	2:I:77:ASP:C	2.54	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:41:TYR:HD2	2:D:173:PHE:HE2	1.64	0.43
2:D:6:LEU:H	2:D:6:LEU:CD1	2.29	0.43
3:E:62:CYS:O	3:E:66:GLN:HG3	2.19	0.43
1:F:174:TYR:O	1:F:175:GLU:C	2.57	0.43
2:G:291:ARG:HD3	2:G:291:ARG:HA	1.77	0.43
2:G:4:GLN:HE22	2:G:9:LYS:HG3	1.76	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:B:13:GLN:HB3	2:B:60:LYS:NZ	2.34	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:HD12	2:G:297:LEU:N	2.33	0.43
2:H:272:ALA:CB	2:H:346:ARG:NH1	2.81	0.43
2:H:21:GLN:HE21	2:H:49:VAL:HG12	1.82	0.43
2:I:143:LEU:HD12	2:I:143:LEU:HA	1.69	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
1:A:253:GLU:OE1	1:A:286:MET:CE	2.67	0.43
2:B:294:MET:C	2:B:296:GLN:H	2.23	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:C:23:HIS:HE1	2:C:174:HIS:O	2.00	0.43
2:D:341:TYR:CD1	2:D:341:TYR:N	2.87	0.43
2:D:77:ASP:O	2:D:81:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:F:298:LEU:HD23	1.82	0.42
1:F:31:LEU:O	1:F:32:GLN:C	2.57	0.42
2:G:24:VAL:HG21	2:G:175:LEU:CD2	2.48	0.42
2:H:76:CYS:O	2:H:77:ASP:C	2.56	0.42
2:I:243:THR:CG2	2:I:244:LEU:H	2.30	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
3:J:68:MET:CE	3:J:68:MET:HA	2.49	0.42
2:B:343:PRO:HG3	2:C:286:LEU:CB	2.49	0.42
2:B:82:ILE:HG12	2:B:87:PHE:CB	2.49	0.42
1:F:65:PHE:O	1:F:65:PHE:CD2	2.72	0.42
2:H:152:PHE:O	2:H:153:LEU:HD23	2.19	0.42
2:H:47:ARG:HD2	2:I:164:VAL:CG2	2.47	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
1:A:98:LEU:HD23	1:A:126:TRP:HB3	2.01	0.42
1:A:50:HIS:ND1	1:A:79:THR:HB	2.34	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:HG23	2:D:156:THR:O	2.19	0.42
2:D:309:ILE:O	2:D:309:ILE:HG22	2.18	0.42
3:E:163:TYR:CD1	3:E:164:LEU:N	2.88	0.42
1:F:98:LEU:HD23	1:F:126:TRP:HB3	2.00	0.42
1:F:14:ASN:O	1:F:15:GLU:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:128:LEU:HD12	3:J:128:LEU:HA	1.85	0.42
2:B:245:ASP:C	2:B:247:ASP:H	2.21	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:HA	2:D:140:LEU:HD23	1.82	0.42
1:F:147:LEU:HB3	1:F:148:PRO:HD3	2.02	0.42
1:F:233:LEU:HD23	1:F:233:LEU:HA	1.74	0.42
2:H:327:LEU:O	2:H:327:LEU:HD12	2.19	0.42
2:I:129:HIS:ND1	2:I:156:THR:OG1	2.34	0.42
1:A:84:LEU:CD1	1:A:112:VAL:HG13	2.49	0.42
2:B:328:TYR:HH	2:B:360:HIS:CD2	2.38	0.42
2:B:49:VAL:O	2:B:49:VAL:CG1	2.66	0.42
3:J:27:LEU:HD12	3:J:160:ARG:HG2	2.02	0.42
3:J:316:LEU:HD23	3:J:316:LEU:HA	1.71	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
2:D:76:CYS:O	2:D:77:ASP:C	2.58	0.42
3:E:148:PRO:O	3:E:151:LEU:HB2	2.19	0.42
3:E:73:HIS:HE1	3:E:75:ASP:HB2	1.85	0.42
2:G:13:GLN:HB3	2:G:60:LYS:NZ	2.35	0.42
2:H:13:GLN:C	2:H:57:LEU:HD21	2.40	0.42
1:A:237:ARG:O	1:A:240:GLY:N	2.44	0.42
1:A:287:GLY:O	1:A:288:GLU:C	2.57	0.42
1:A:312:LEU:HD12	1:A:312:LEU:O	2.19	0.42
2:B:107:LEU:HA	2:B:107:LEU:HD12	1.75	0.42
2:B:215:ARG:O	2:B:217:ALA:N	2.52	0.42
2:D:248:GLN:NE2	2:D:271:ALA:HB2	2.34	0.42
2:D:290:HIS:O	2:D:291:ARG:C	2.58	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:G:119:ARG:CG	2:G:119:ARG:HH11	2.32	0.42
1:A:4:LEU:HD12	1:A:135:VAL:HG13	2.02	0.42
2:B:240:MET:HG2	2:B:240:MET:O	2.18	0.42
2:D:13:GLN:OE1	2:D:60:LYS:NZ	2.53	0.42
2:C:347:MET:CG	2:D:290:HIS:CG	3.03	0.42
2:C:337:LYS:HE2	3:E:334:LEU:HD22	2.00	0.42
1:F:261:LYS:HE2	1:F:290:LEU:O	2.19	0.42
2:H:205:LEU:HD23	2:H:205:LEU:HA	1.80	0.42
3:J:257:LYS:HB3	3:J:262:ALA:HB3	2.01	0.42
3:J:48:LEU:HD23	3:J:48:LEU:HA	1.74	0.42
1:A:196:LYS:HB2	1:A:196:LYS:HE3	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:LEU:HD12	2:C:152:PHE:CD2	2.55	0.41
2:D:167:LEU:O	2:D:168:SER:C	2.58	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:G:215:ARG:C	2:G:217:ALA:N	2.73	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:101:VAL:O	2:B:102:GLU:C	2.59	0.41
2:B:15:PHE:CE2	2:B:57:LEU:CB	2.96	0.41
2:B:94:ASP:O	2:B:94:ASP:OD1	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
2:D:6:LEU:C	2:D:8:ARG:H	2.24	0.41
3:E:29:ILE:CD1	3:E:40:LEU:HD23	2.45	0.41
1:F:94:ASN:OD1	1:F:126:TRP:NE1	2.47	0.41
2:G:94:ASP:OD1	2:G:94:ASP:C	2.59	0.41
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:H:5:VAL:O	2:H:5:VAL:HG12	2.18	0.41
2:I:185:HIS:O	2:I:188:GLU:HB3	2.20	0.41
2:I:64:CYS:O	2:I:119:ARG:NH2	2.52	0.41
2:D:184:ARG:HD2	2:D:204:GLN:HE21	1.85	0.41
2:D:6:LEU:C	2:D:8:ARG:N	2.74	0.41
3:E:202:LEU:C	3:E:202:LEU:CD2	2.88	0.41
2:G:107:LEU:HA	2:G:107:LEU:HD12	1.72	0.41
2:G:108:LEU:O	2:G:111:VAL:HG12	2.20	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
3:J:233:LEU:O	3:J:234:ALA:C	2.59	0.41
1:A:248:ARG:HD2	4:K:5:DT:OP1	2.20	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
1:F:257:LEU:O	1:F:258:VAL:C	2.58	0.41
3:J:120:LEU:HD23	3:J:120:LEU:HA	1.86	0.41
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.76	0.41
2:C:276:ILE:HG13	2:C:276:ILE:O	2.15	0.41
2:C:45:GLY:O	2:C:51:LYS:HE3	2.20	0.41
3:E:286:LEU:HA	3:E:286:LEU:HD23	1.83	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:HA	1:A:22:LEU:HD23	1.87	0.41
2:B:21:GLN:CA	2:B:21:GLN:NE2	2.78	0.41
2:B:302:LEU:HA	2:B:302:LEU:HD23	1.71	0.41
2:D:49:VAL:CG1	2:D:49:VAL:O	2.68	0.41
3:E:327:VAL:CG1	3:E:328:VAL:N	2.83	0.41
1:F:272:LEU:HD23	1:F:272:LEU:HA	1.82	0.41
2:H:332:LEU:HD23	2:H:332:LEU:HA	1.53	0.41
2:I:215:ARG:HG2	2:I:215:ARG:HH11	1.85	0.41
2:H:351:MET:HE2	2:I:290:HIS:CB	2.51	0.41
2:I:291:ARG:HA	2:I:291:ARG:HD3	1.82	0.41
2:I:6:LEU:O	2:I:8:ARG:N	2.53	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:251:SER:HB3	2:B:267:LEU:CD1	2.50	0.41
2:B:245:ASP:O	2:B:274:ARG:HD2	2.21	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:309:ILE:CG2	2:H:313:MET:HG2	2.50	0.41
2:I:128:VAL:O	2:I:128:VAL:CG2	2.67	0.41
2:I:191:LEU:HA	2:I:191:LEU:HD23	1.87	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
3:J:32:LEU:HA	3:J:32:LEU:HD23	1.85	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
1:F:234:GLN:OE1	2:G:304:ASN:HB2	2.20	0.41
1:F:81:LEU:HD21	1:F:83:LEU:HD21	2.01	0.41
2:H:4:GLN:CA	2:H:4:GLN:OE1	2.66	0.41
2:I:286:LEU:HD23	2:I:286:LEU:HA	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:308:ARG:O	3:J:309:GLU:C	2.57	0.41
5:L:2:DT:H2''	5:L:3:DG:C8	2.55	0.41
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.58	0.41
2:C:339:LEU:N	2:C:340:PRO:CD	2.82	0.41
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
2:D:3:TYR:CG	2:D:4:GLN:N	2.89	0.41
3:E:311:LEU:HA	3:E:311:LEU:HD12	1.81	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:222:LEU:HA	1:F:222:LEU:HD23	1.65	0.41
1:F:9:LEU:HD11	1:F:13:LEU:HD21	2.02	0.41
2:G:251:SER:HB3	2:G:267:LEU:CD1	2.51	0.41
2:H:265:MET:CE	2:H:354:LEU:HD21	2.51	0.41
2:I:289:LEU:HD23	2:I:289:LEU:HA	1.69	0.41
2:I:74:GLY:HA2	2:I:79:CYS:CB	2.51	0.41
3:J:46:ARG:CD	3:J:68:MET:CG	2.96	0.41
4:K:4:DT:O5'	4:K:4:DT:H2'	2.20	0.41
1:A:97:LEU:CD1	1:A:126:TRP:CH2	3.03	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:360:HIS:HA	2:C:361:PRO:HD3	1.88	0.41
2:D:250:LEU:HD22	2:D:309:ILE:HG23	2.02	0.41
2:D:6:LEU:O	2:D:8:ARG:N	2.54	0.41
3:E:316:LEU:HD23	3:E:316:LEU:HA	1.69	0.41
1:F:198:THR:CG2	1:F:201:ARG:HD2	2.50	0.41
2:G:82:ILE:HG12	2:G:87:PHE:CB	2.51	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:260:ASN:ND2	2:B:263:ARG:HB2	2.23	0.41
2:B:249:ALA:HB2	2:B:281:LEU:CD1	2.51	0.41
2:C:220:LEU:HA	2:C:220:LEU:HD23	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: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:H:45:GLY:O	2:H:51:LYS:HE3	2.21	0.41
2:I:302:LEU:HD11	2:I:306:MET:HG3	2.03	0.41
2:I:341:TYR:N	2:I:341:TYR:CD1	2.89	0.41
2:I:74:GLY:HA2	2:I:79:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:78:ASN:O	2:I:82:ILE:HG13	2.21	0.41
1:A:142:PRO:HD3	1:A:178:LEU:HD11	2.03	0.40
1:A:173:CYS:SG	1:A:206:VAL:HG11	2.61	0.40
1:A:144:GLN:NE2	1:A:228:ARG:HE	2.19	0.40
2:B:353:LEU:HD23	2:B:353:LEU:HA	1.82	0.40
2:D:75:VAL:CG1	2:D:75:VAL:O	2.69	0.40
2:D:74:GLY:HA2	2:D:79:CYS:HB3	2.03	0.40
3:E:111:VAL:HA	3:E:140:TRP:O	2.21	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
1:F:93:ILE:HG22	1:F:93:ILE:O	2.21	0.40
2:H:139:LEU:HA	2:H:139:LEU:HD23	1.59	0.40
2:I:164:VAL:CG2	2:I:164:VAL:O	2.69	0.40
2:B:99:THR:HA	2:B:131:LEU:HD23	2.02	0.40
2:B:24:VAL:HG21	2:B:175:LEU:CD2	2.50	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
3:E:252:LEU:HD23	3:E:252:LEU:HA	1.77	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
1:F:199:LEU:N	1:F:200:PRO:HD2	2.36	0.40
2:G:128:VAL:CG2	2:G:128:VAL:O	2.69	0.40
2:G:215:ARG:O	2:G:216:ASP:C	2.58	0.40
2:G:47:ARG:N	2:G:47:ARG:HD3	2.36	0.40
2:I:327:LEU:HD23	2:I:327:LEU:HA	1.79	0.40
2:I:5:VAL:HG13	2:I:222:ASP:OD2	2.21	0.40
4:M:4:DT:O5'	4:M:4:DT:H2'	2.21	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: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:C:76:CYS:O	2:C:77:ASP:C	2.60	0.40
2:C:130:MET:HE1	2:D:134:HIS:HA	2.02	0.40
2:D:247:ASP:O	2:D:249:ALA:N	2.54	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:259:ALA:HB2	2:I:360:HIS:CB	2.52	0.40
2:I:251:SER:HB3	2:I:267:LEU:HD21	2.02	0.40
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.94	0.40
2:B:220:LEU:HD23	2:B:220:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:265:MET:HE2	2:C:354:LEU:HD21	2.03	0.40
2:D:266:ALA:O	2:D:270:GLU:HG3	2.22	0.40
2:D:306:MET:HE3	2:D:309:ILE:HD12	2.02	0.40
3:E:271:PRO:CD	3:E:272:GLY:N	2.82	0.40
1:F:151:VAL:HG22	1:F:181:LEU:HD21	2.03	0.40
1:F:172:TYR:CD2	1:F:172:TYR:C	2.95	0.40
2:G:234:THR:O	2:G:238:SER:HB3	2.22	0.40
2:G:6:LEU:HA	2:G:6:LEU:HD23	1.84	0.40
2:H:215:ARG:O	2:H:216:ASP:C	2.60	0.40
2:H:254:GLU:OE2	2:H:312:ARG:HD3	2.21	0.40
2:H:360:HIS:HD1	2:H:363:MET:H	1.69	0.40
2:I:210:ALA:O	2:I:211:GLU:C	2.59	0.40
1:A:75:ALA:O	1:A:76:SER:C	2.60	0.40
2:B:11:ARG:HA	2:B:12:PRO:HD3	1.79	0.40
2:B:326:GLN:HG3	2:B:326:GLN:O	2.21	0.40
2:C:6:LEU:O	2:C:8:ARG:N	2.55	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:248:LEU:O	3:J:248:LEU:HD12	2.21	0.40
3:J:90:VAL:HG13	3:J:91:ASP:N	2.37	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%)	10	39
1	F	331/343 (96%)	298 (90%)	29 (9%)	4 (1%)	13	44
2	B	362/395 (92%)	323 (89%)	36 (10%)	3 (1%)	19	53
2	C	363/395 (92%)	326 (90%)	31 (8%)	6 (2%)	9	36
2	D	360/395 (91%)	317 (88%)	34 (9%)	9 (2%)	5	29
2	G	376/395 (95%)	340 (90%)	33 (9%)	3 (1%)	19	53
2	H	363/395 (92%)	320 (88%)	37 (10%)	6 (2%)	9	36
2	I	360/395 (91%)	318 (88%)	33 (9%)	9 (2%)	5	29
3	E	332/334 (99%)	300 (90%)	24 (7%)	8 (2%)	6	30
3	J	332/334 (99%)	298 (90%)	28 (8%)	6 (2%)	8	35
All	All	3510/3724 (94%)	3132 (89%)	319 (9%)	59 (2%)	9	36

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%)	256 (90%)	27 (10%)	8	30
1	F	283/291 (97%)	256 (90%)	27 (10%)	8	30
2	B	301/329 (92%)	282 (94%)	19 (6%)	18	49
2	C	302/329 (92%)	267 (88%)	35 (12%)	5	21
2	D	299/329 (91%)	280 (94%)	19 (6%)	17	48
2	G	313/329 (95%)	296 (95%)	17 (5%)	22	53
2	H	302/329 (92%)	266 (88%)	36 (12%)	5	20
2	I	299/329 (91%)	283 (95%)	16 (5%)	22	53
3	E	270/270 (100%)	254 (94%)	16 (6%)	19	51
3	J	270/270 (100%)	252 (93%)	18 (7%)	16	47
All	All	2922/3096 (94%)	2692 (92%)	230 (8%)	12	39

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	64	ILE
1	A	78	GLN
1	A	86	GLU
1	A	99	THR
1	A	106	ASP
1	A	108	LEU
1	A	117	LEU
1	A	118	SER
1	A	128	THR
1	A	146	GLN
1	A	158	LEU
1	A	169	VAL
1	A	191	LEU
1	A	194	ASP
1	A	196	LYS
1	A	198	THR
1	A	202	VAL
1	A	203	GLU
1	A	206	VAL
1	A	230	LEU
1	A	237	ARG
1	A	296	THR

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Mol	Chain	Res	Type
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	46	THR
2	B	47	ARG
2	B	97	SER
2	B	117	ARG
2	B	119	ARG
2	B	157	THR
2	B	168	SER
2	B	187	LEU
2	B	238	SER
2	B	251	SER
2	B	262	GLU
2	B	269	ASN
2	B	276	ILE
2	B	291	ARG
2	B	302	LEU
2	B	309	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	91	ILE
2	C	112	GLN
2	C	117	ARG
2	C	124	LEU
2	C	128	VAL
2	C	134	HIS
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	187	LEU

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Mol	Chain	Res	Type
2	C	196	ILE
2	C	214	LEU
2	C	227	SER
2	C	240	MET
2	C	244	LEU
2	C	245	ASP
2	C	246	ASP
2	C	248	GLN
2	C	252	LEU
2	C	260	ASN
2	C	265	MET
2	C	276	ILE
2	C	291	ARG
2	C	297	LEU
2	C	311	LEU
2	C	352	THR
2	D	30	ASN
2	D	46	THR
2	D	47	ARG
2	D	52	THR
2	D	97	SER
2	D	107	LEU
2	D	117	ARG
2	D	135	SER
2	D	157	THR
2	D	165	THR
2	D	180	VAL
2	D	215	ARG
2	D	216	ASP
2	D	276	ILE
2	D	291	ARG
2	D	305	ASP
2	D	325	ILE
2	D	333	LEU
2	D	357	LEU
3	E	17	SER
3	E	82	GLU
3	E	145	THR
3	E	155	LEU
3	E	158	ARG
3	E	160	ARG
3	E	180	VAL

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Mol	Chain	Res	Type
3	E	188	LEU
3	E	197	SER
3	E	208	ASP
3	E	231	SER
3	E	253	MET
3	E	256	LEU
3	E	264	GLN
3	E	270	VAL
3	E	282	SER
1	F	7	GLU
1	F	64	ILE
1	F	78	GLN
1	F	86	GLU
1	F	99	THR
1	F	108	LEU
1	F	117	LEU
1	F	118	SER
1	F	128	THR
1	F	146	GLN
1	F	158	LEU
1	F	169	VAL
1	F	191	LEU
1	F	194	ASP
1	F	196	LYS
1	F	198	THR
1	F	202	VAL
1	F	203	GLU
1	F	230	LEU
1	F	237	ARG
1	F	244	VAL
1	F	282	ARG
1	F	296	THR
1	F	308	THR
1	F	309	GLU
1	F	311	THR
1	F	319	SER
2	G	37	ILE
2	G	38	HIS
2	G	46	THR
2	G	47	ARG
2	G	117	ARG
2	G	119	ARG

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Mol	Chain	Res	Type
2	G	157	THR
2	G	168	SER
2	G	235	GLN
2	G	238	SER
2	G	251	SER
2	G	262	GLU
2	G	269	ASN
2	G	276	ILE
2	G	291	ARG
2	G	309	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	91	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	187	LEU
2	H	196	ILE
2	H	214	LEU
2	H	227	SER
2	H	240	MET
2	H	244	LEU
2	H	246	ASP
2	H	248	GLN
2	H	252	LEU
2	H	260	ASN
2	H	276	ILE
2	H	291	ARG

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Mol	Chain	Res	Type
2	H	297	LEU
2	H	309	ILE
2	H	311	LEU
2	H	318	ARG
2	H	352	THR
2	I	30	ASN
2	I	46	THR
2	I	47	ARG
2	I	52	THR
2	I	97	SER
2	I	117	ARG
2	I	135	SER
2	I	157	THR
2	I	165	THR
2	I	215	ARG
2	I	216	ASP
2	I	268	ILE
2	I	276	ILE
2	I	291	ARG
2	I	305	ASP
2	I	357	LEU
3	J	2	ARG
3	J	17	SER
3	J	82	GLU
3	J	145	THR
3	J	155	LEU
3	J	157	SER
3	J	158	ARG
3	J	160	ARG
3	J	180	VAL
3	J	188	LEU
3	J	197	SER
3	J	208	ASP
3	J	214	GLU
3	J	239	GLU
3	J	253	MET
3	J	256	LEU
3	J	264	GLN
3	J	282	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	50	HIS
1	A	144	GLN
1	A	216	HIS
2	B	39	HIS
2	B	84	GLN
2	B	260	ASN
2	C	23	HIS
2	C	112	GLN
2	C	134	HIS
2	C	290	HIS
2	C	304	ASN
2	D	30	ASN
2	D	38	HIS
2	D	134	HIS
2	D	149	HIS
2	D	172	GLN
2	D	204	GLN
2	D	269	ASN
2	D	360	HIS
3	E	51	GLN
3	E	52	GLN
3	E	54	GLN
3	E	69	GLN
3	E	103	HIS
3	E	246	HIS
3	E	267	ASN
3	E	287	GLN
1	F	45	GLN
1	F	50	HIS
1	F	144	GLN
1	F	216	HIS
2	G	4	GLN
2	G	39	HIS
2	G	84	GLN
2	G	260	ASN
2	H	23	HIS
2	H	112	GLN
2	H	134	HIS
2	H	290	HIS
2	H	304	ASN
2	I	30	ASN
2	I	38	HIS

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Mol	Chain	Res	Type
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	103	HIS
3	J	246	HIS
3	J	267	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
7	BEF	H	409	6	0,3,3	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	H	408	8,7	24,29,29	1.24	3 (12%)	29,45,45	1.45	4 (13%)
6	ADP	B	400	8,7	24,29,29	1.32	2 (8%)	29,45,45	1.54	6 (20%)
7	BEF	I	411	6	0,3,3	0.00	-	-		
7	BEF	D	405	6	0,3,3	0.00	-	-		
6	ADP	C	402	8,7	24,29,29	1.20	2 (8%)	29,45,45	1.65	5 (17%)
6	ADP	I	410	8,7	24,29,29	1.50	4 (16%)	29,45,45	1.57	6 (20%)
7	BEF	C	403	6	0,3,3	0.00	-	-		
7	BEF	B	401	6	0,3,3	0.00	-	-		
6	ADP	D	404	8,7	24,29,29	1.22	2 (8%)	29,45,45	1.66	9 (31%)
7	BEF	G	407	6	0,3,3	0.00	-	-		
6	ADP	G	406	8,7	24,29,29	1.21	3 (12%)	29,45,45	1.49	7 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	H	408	8,7	-	5/12/32/32	0/3/3/3
6	ADP	B	400	8,7	-	2/12/32/32	0/3/3/3
6	ADP	I	410	8,7	-	1/12/32/32	0/3/3/3
6	ADP	C	402	8,7	-	6/12/32/32	0/3/3/3
6	ADP	D	404	8,7	-	2/12/32/32	0/3/3/3
6	ADP	G	406	8,7	-	0/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	410	ADP	C2'-C1'	-3.87	1.47	1.53
6	C	402	ADP	C2'-C1'	-3.34	1.48	1.53
6	B	400	ADP	C2'-C1'	-3.08	1.49	1.53
6	D	404	ADP	C2'-C1'	-2.87	1.49	1.53
6	B	400	ADP	C5-C4	2.85	1.48	1.40
6	G	406	ADP	C2'-C1'	-2.81	1.49	1.53
6	C	402	ADP	C5-C4	2.61	1.47	1.40
6	H	408	ADP	PB-O1B	2.48	1.58	1.50
6	I	410	ADP	C4-N3	-2.44	1.32	1.35
6	I	410	ADP	C5-C4	2.36	1.47	1.40
6	G	406	ADP	C5-C4	2.32	1.47	1.40
6	I	410	ADP	PB-O2B	-2.15	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	404	ADP	C5-C4	2.13	1.46	1.40
6	G	406	ADP	PB-O3B	2.09	1.62	1.54
6	H	408	ADP	PB-O3B	2.08	1.62	1.54
6	H	408	ADP	O4'-C1'	2.04	1.43	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	402	ADP	PA-O3A-PB	-3.99	119.12	132.83
6	D	404	ADP	PA-O3A-PB	-3.59	120.50	132.83
6	C	402	ADP	O2B-PB-O1B	3.55	124.59	110.68
6	I	410	ADP	O2B-PB-O1B	3.52	124.48	110.68
6	H	408	ADP	PA-O3A-PB	-3.37	121.26	132.83
6	H	408	ADP	O2B-PB-O1B	3.27	123.47	110.68
6	I	410	ADP	PA-O3A-PB	-3.20	121.84	132.83
6	C	402	ADP	N3-C2-N1	-3.17	123.72	128.68
6	D	404	ADP	O2B-PB-O1B	2.84	121.79	110.68
6	B	400	ADP	PA-O3A-PB	-2.83	123.12	132.83
6	H	408	ADP	C4-C5-N7	-2.74	106.54	109.40
6	C	402	ADP	C2'-C3'-C4'	2.63	107.76	102.64
6	I	410	ADP	O2'-C2'-C1'	-2.60	101.24	110.85
6	D	404	ADP	N6-C6-N1	2.60	123.97	118.57
6	D	404	ADP	N3-C2-N1	-2.60	124.62	128.68
6	G	406	ADP	O2B-PB-O1B	2.58	120.78	110.68
6	G	406	ADP	PA-O3A-PB	-2.55	124.08	132.83
6	D	404	ADP	O3'-C3'-C4'	-2.55	103.68	111.05
6	I	410	ADP	O4'-C4'-C3'	-2.52	100.13	105.11
6	G	406	ADP	O5'-PA-O1A	-2.51	99.27	109.07
6	G	406	ADP	C4-C5-N7	-2.48	106.82	109.40
6	B	400	ADP	O2B-PB-O1B	2.46	120.31	110.68
6	D	404	ADP	C2-N1-C6	2.45	122.95	118.75
6	G	406	ADP	O3B-PB-O2B	-2.42	98.37	107.64
6	D	404	ADP	O3B-PB-O2B	-2.42	98.39	107.64
6	I	410	ADP	C2'-C3'-C4'	2.34	107.19	102.64
6	I	410	ADP	O3B-PB-O2B	-2.31	98.79	107.64
6	D	404	ADP	O2'-C2'-C1'	-2.29	102.41	110.85
6	C	402	ADP	C2-N1-C6	2.25	122.60	118.75
6	B	400	ADP	O2'-C2'-C1'	-2.23	102.61	110.85
6	B	400	ADP	N3-C2-N1	-2.11	125.38	128.68
6	G	406	ADP	C5'-C4'-C3'	-2.11	107.28	115.18
6	B	400	ADP	O3B-PB-O2B	-2.10	99.60	107.64
6	B	400	ADP	O5'-PA-O1A	-2.10	100.87	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	408	ADP	N3-C2-N1	-2.05	125.47	128.68
6	G	406	ADP	N3-C2-N1	-2.04	125.49	128.68
6	D	404	ADP	C5-C6-N1	-2.02	115.77	120.35

There are no chirality outliers.

All (16) 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	H	408	ADP	PA-O3A-PB-O3B
6	H	408	ADP	C5'-O5'-PA-O2A
6	D	404	ADP	C5'-O5'-PA-O3A
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	I	410	ADP	PA-O3A-PB-O3B
6	H	408	ADP	PA-O3A-PB-O2B
6	B	400	ADP	C5'-O5'-PA-O3A
6	C	402	ADP	C5'-O5'-PA-O3A
6	B	400	ADP	C5'-O5'-PA-O1A
6	D	404	ADP	C5'-O5'-PA-O1A

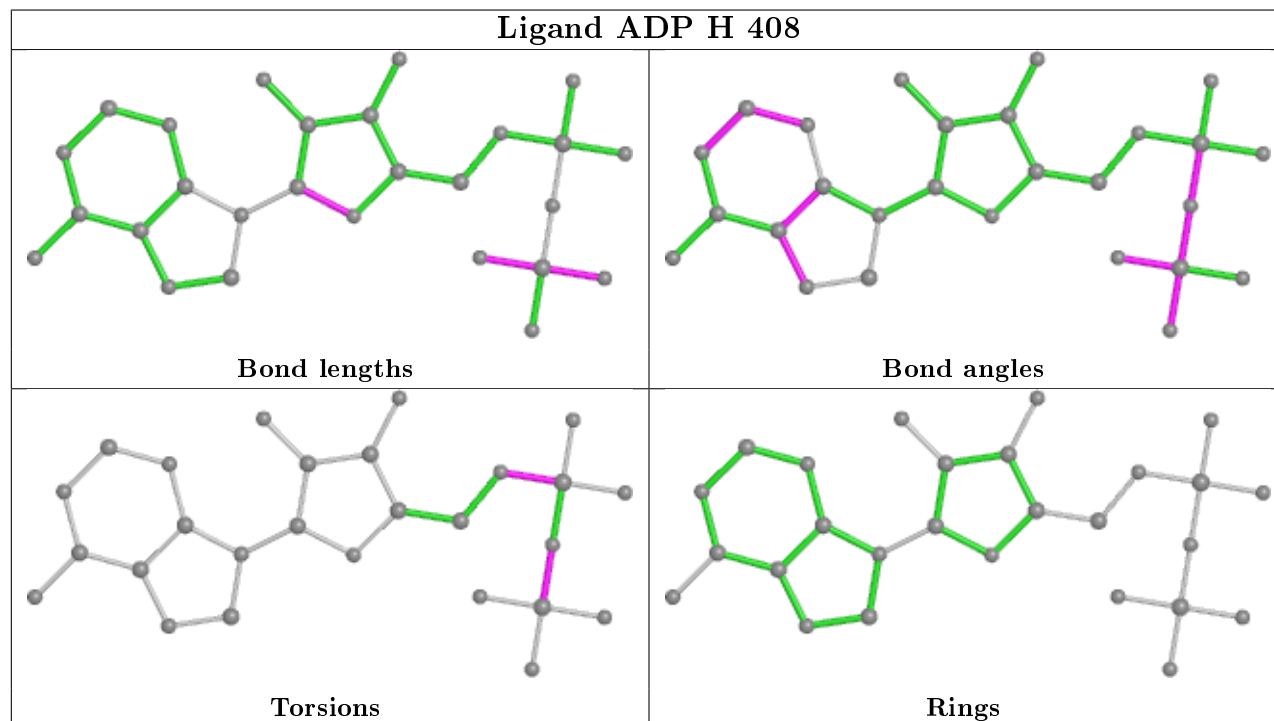
There are no ring outliers.

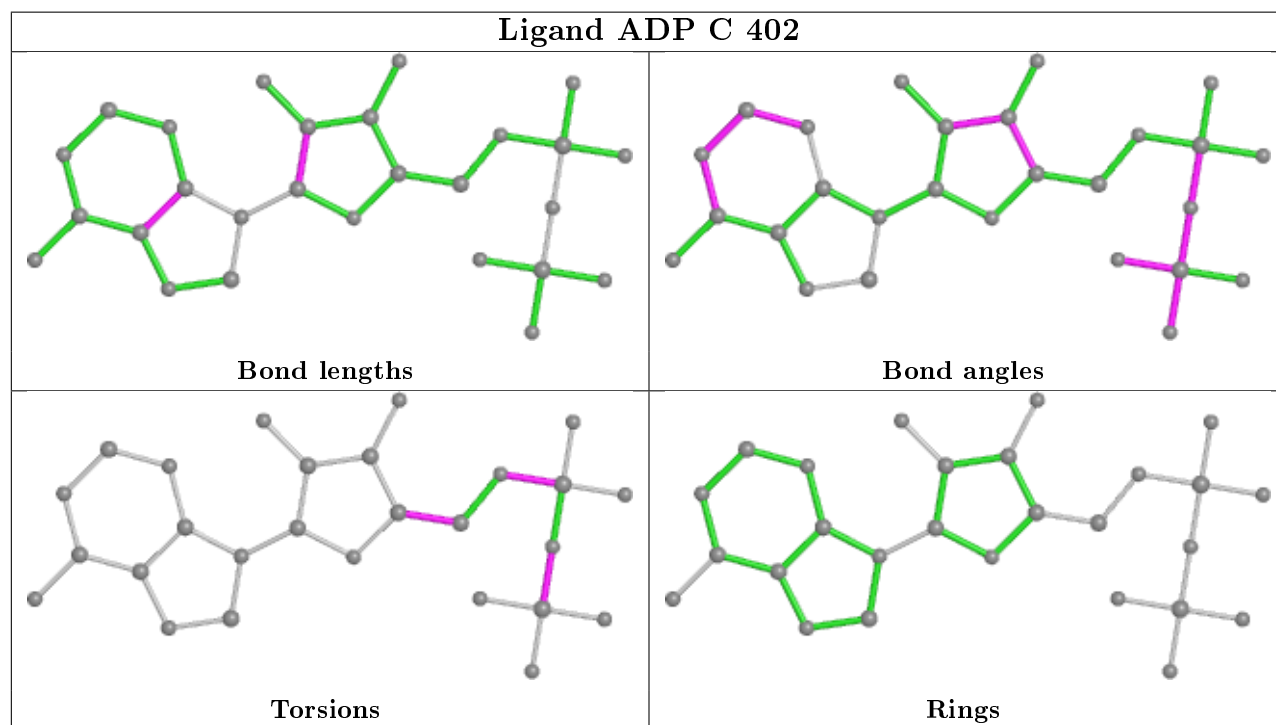
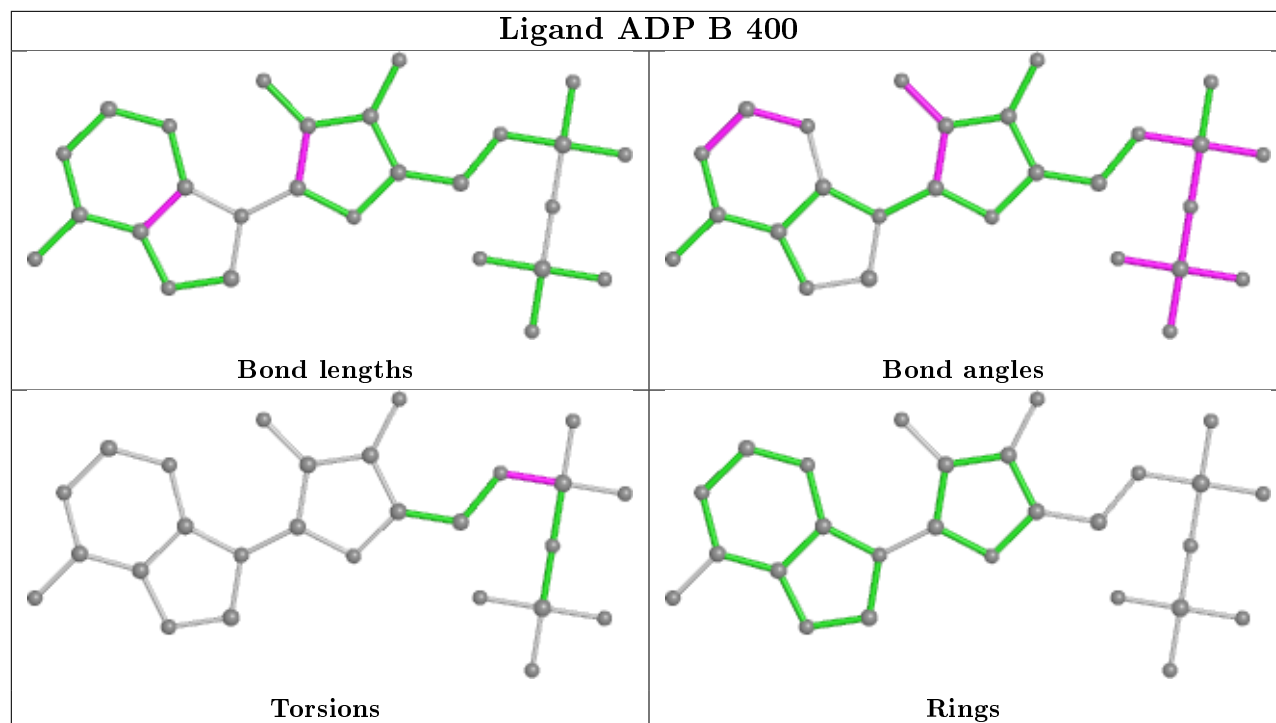
9 monomers are involved in 20 short contacts:

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

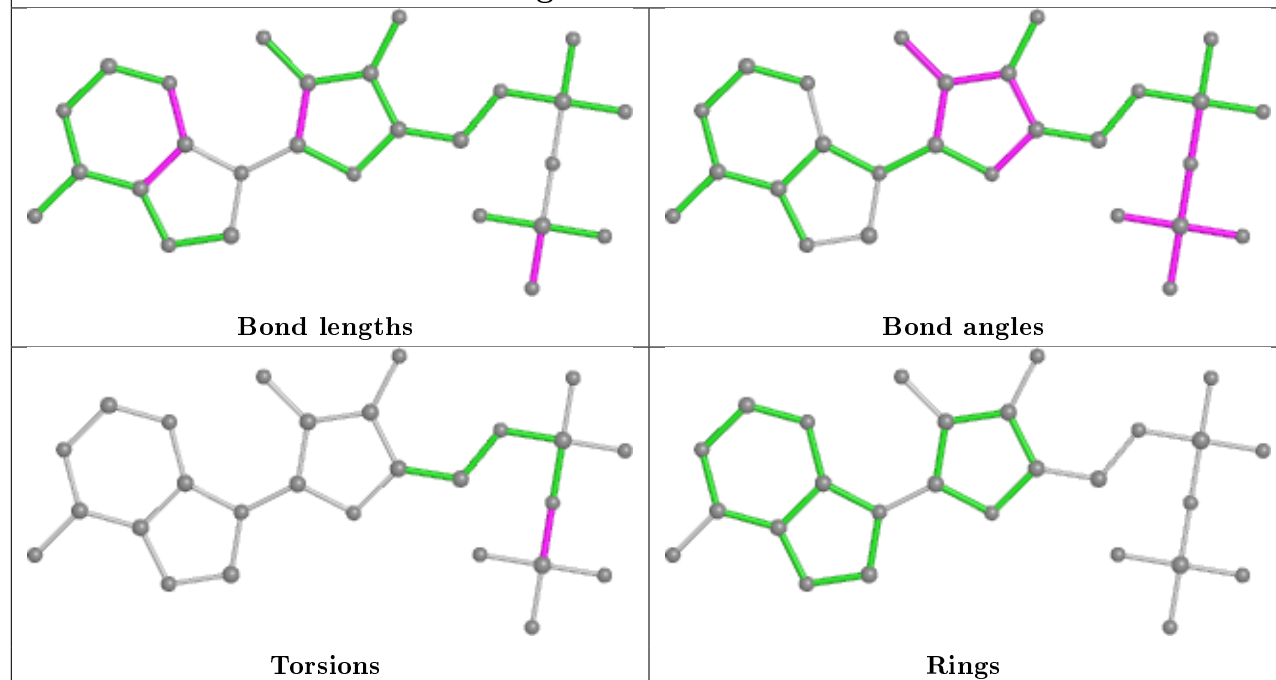
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

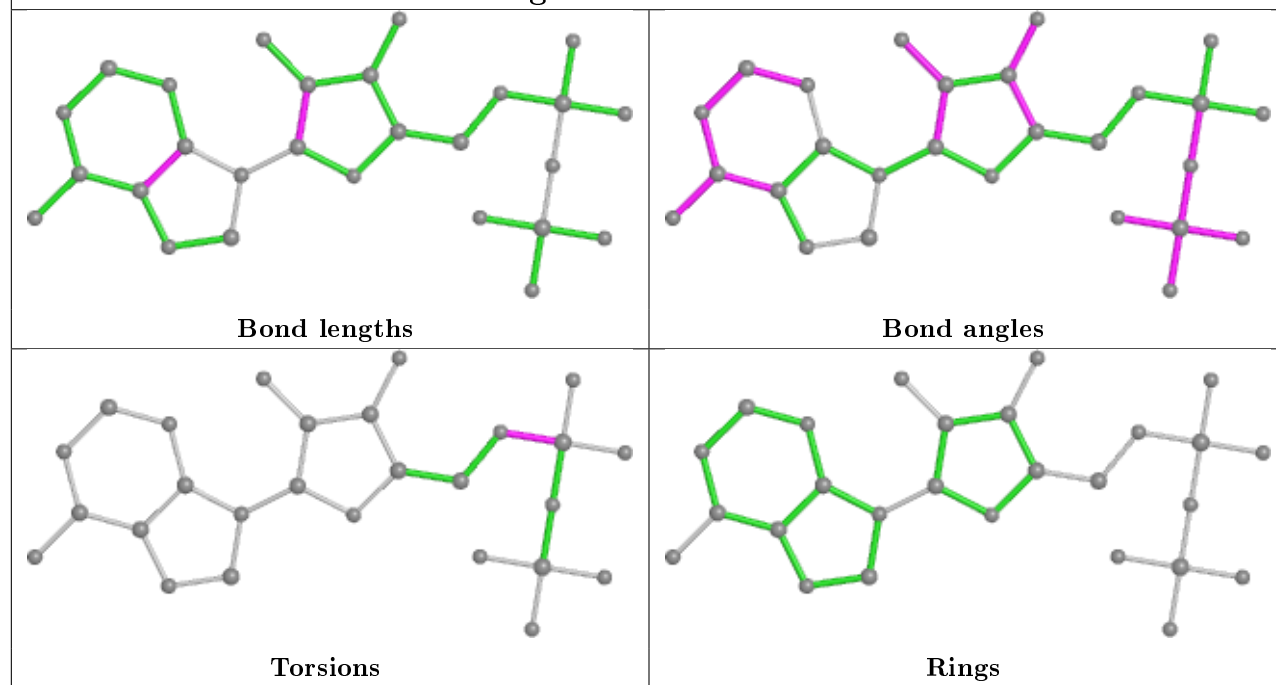


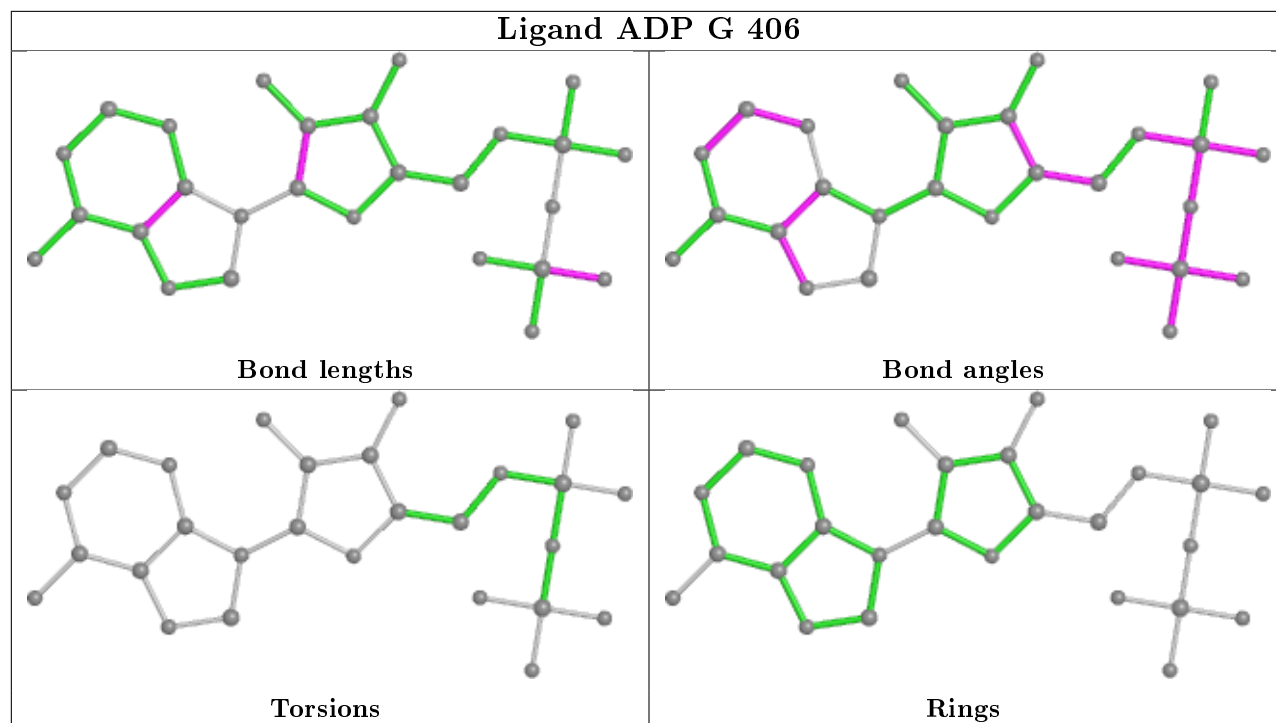


Ligand ADP I 410



Ligand ADP D 404





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.89	53 (15%) 1 2	73, 127, 209, 244	0
1	F	333/343 (97%)	0.40	25 (7%) 14 17	67, 127, 197, 222	0
2	B	364/395 (92%)	0.29	16 (4%) 34 38	76, 119, 164, 189	0
2	C	365/395 (92%)	0.23	12 (3%) 46 50	68, 114, 180, 208	0
2	D	362/395 (91%)	0.21	10 (2%) 53 57	69, 106, 156, 198	0
2	G	378/395 (95%)	0.08	7 (1%) 66 71	76, 101, 146, 182	0
2	H	365/395 (92%)	-0.05	2 (0%) 91 93	58, 88, 125, 165	0
2	I	362/395 (91%)	-0.02	1 (0%) 94 96	56, 80, 125, 184	0
3	E	334/334 (100%)	0.06	4 (1%) 79 83	67, 86, 134, 175	0
3	J	334/334 (100%)	0.02	3 (0%) 84 88	63, 84, 133, 172	0
4	K	14/15 (93%)	0.06	0 100 100	79, 87, 169, 171	0
4	M	14/15 (93%)	-0.16	0 100 100	76, 84, 174, 181	0
5	L	10/10 (100%)	-0.39	0 100 100	85, 88, 95, 105	0
5	N	10/10 (100%)	-0.40	0 100 100	81, 86, 98, 99	0
All	All	3578/3774 (94%)	0.20	133 (3%) 41 45	56, 101, 175, 244	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	PHE	10.9
1	A	55	ILE	9.4
1	A	61	TRP	8.7
1	F	61	TRP	8.3
1	A	62	ASN	7.1
1	A	73	LEU	6.9
1	A	89	PRO	6.7
1	A	68	CYS	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	75	ALA	6.4
1	A	128	THR	5.9
1	A	82	LEU	5.6
1	F	48	GLU	5.4
1	A	57	PRO	5.4
1	F	76	SER	5.4
1	A	110	LEU	5.3
1	A	76	SER	5.3
1	A	67	LEU	5.2
1	A	54	SER	5.1
1	F	53	PHE	5.1
1	F	60	ASP	5.1
1	A	72	SER	4.9
1	F	62	ASN	4.7
1	A	84	LEU	4.7
1	A	60	ASP	4.6
1	A	71	MET	4.6
1	A	80	LEU	4.6
1	A	85	PRO	4.6
2	B	367	GLU	4.6
1	A	104	LEU	4.5
2	D	302	LEU	4.4
1	A	101	THR	4.3
2	B	366	PRO	4.2
1	A	64	ILE	4.1
1	A	56	ASP	4.0
2	B	365	LEU	4.0
1	F	56	ASP	3.8
1	F	57	PRO	3.8
2	G	362	ARG	3.8
1	F	58	ASN	3.7
3	E	105	ARG	3.6
2	D	306	MET	3.5
1	A	79	THR	3.5
1	F	107	ASP	3.5
3	J	56	HIS	3.5
2	C	273	ALA	3.3
2	G	364	PRO	3.3
2	C	265	MET	3.3
1	A	107	ASP	3.2
2	B	363	MET	3.2
3	E	54	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	75	ALA	3.1
2	B	249	ALA	3.1
1	A	106	ASP	3.1
2	B	364	PRO	3.1
2	D	304	ASN	3.1
1	A	109	LEU	3.1
1	F	49	GLU	3.0
2	D	299	PRO	3.0
2	C	252	LEU	3.0
3	J	54	GLN	3.0
1	A	46	GLY	3.0
2	B	368	PRO	3.0
2	G	366	PRO	3.0
2	G	363	MET	3.0
2	B	232	VAL	3.0
3	E	52	GLN	3.0
1	F	78	GLN	3.0
2	B	362	ARG	3.0
1	A	22	LEU	2.9
1	F	266	HIS	2.9
1	A	111	ILE	2.9
2	C	367	GLU	2.9
2	B	256	MET	2.8
2	C	309	ILE	2.8
1	A	98	LEU	2.8
1	A	52	THR	2.8
1	A	112	VAL	2.8
2	H	245	ASP	2.8
1	F	77	ARG	2.8
2	B	313	MET	2.8
1	A	74	PHE	2.8
2	G	365	LEU	2.7
2	B	32	LEU	2.7
1	A	77	ARG	2.7
1	A	122	GLU	2.7
2	C	256	MET	2.6
1	A	2	ILE	2.6
1	F	103	LEU	2.6
1	F	19	ALA	2.6
1	F	89	PRO	2.6
1	A	103	LEU	2.5
2	C	308	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	59	THR	2.5
1	A	282	ARG	2.5
2	C	272	ALA	2.5
1	A	65	PHE	2.5
1	F	73	LEU	2.5
2	D	292	ILE	2.4
2	D	303	GLY	2.4
1	A	63	ALA	2.4
1	F	93	ILE	2.4
1	A	81	LEU	2.4
1	F	104	LEU	2.3
2	G	367	GLU	2.3
1	F	269	LEU	2.3
2	B	77	ASP	2.3
2	D	296	GLN	2.3
2	C	248	GLN	2.3
2	C	362	ARG	2.3
1	A	78	GLN	2.3
1	A	44	ALA	2.2
2	D	248	GLN	2.2
1	F	54	SER	2.2
1	F	72	SER	2.2
2	B	262	GLU	2.2
2	D	295	VAL	2.2
2	I	301	ALA	2.2
2	B	357	LEU	2.1
3	J	83	LYS	2.1
1	A	97	LEU	2.1
1	A	58	ASN	2.1
2	D	363	MET	2.1
1	A	108	LEU	2.1
2	H	292	ILE	2.1
1	F	102	GLY	2.1
3	E	18	TYR	2.1
1	A	129	ALA	2.1
2	C	68	ILE	2.1
2	B	203	LEU	2.1
1	A	105	HIS	2.1
2	G	361	PRO	2.0
1	A	47	PHE	2.0
2	C	62	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

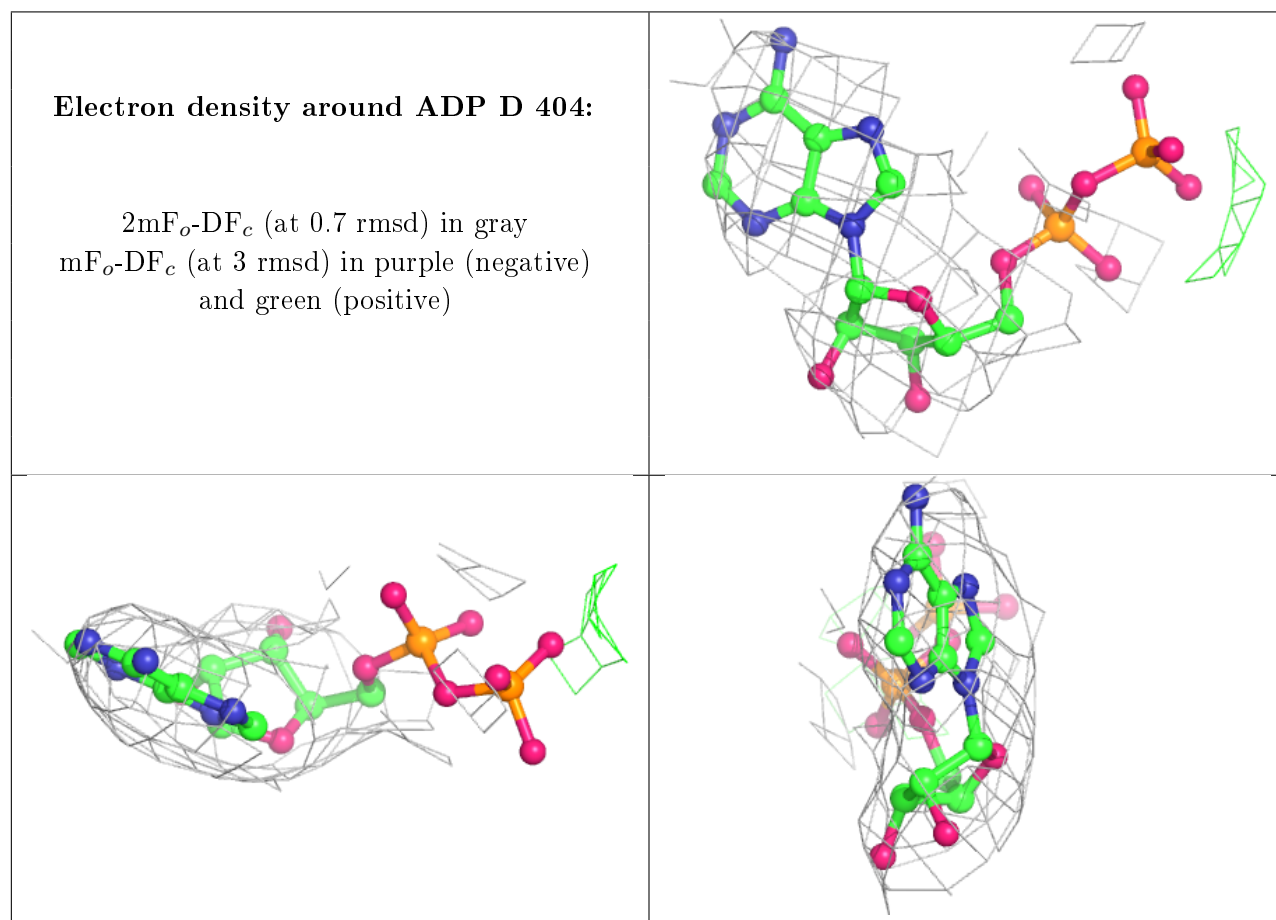
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

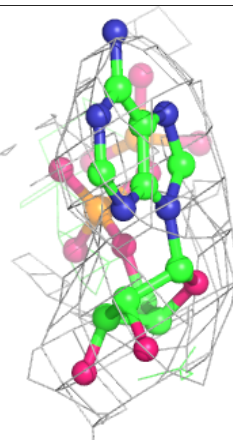
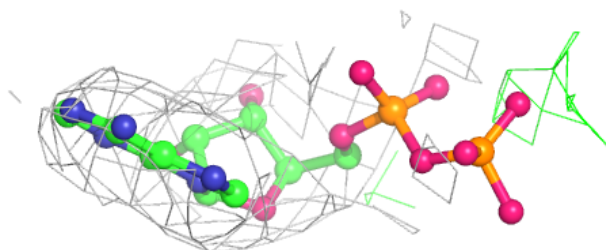
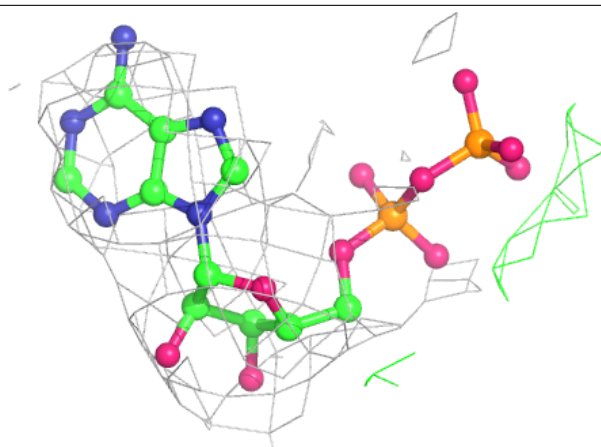
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MG	D	414	1/1	0.84	0.39	75,75,75,75	0
9	ZN	J	425	1/1	0.87	0.09	146,146,146,146	0
8	MG	B	412	1/1	0.92	0.38	79,79,79,79	0
8	MG	G	415	1/1	0.92	0.35	79,79,79,79	0
8	MG	H	416	1/1	0.93	0.26	57,57,57,57	0
8	MG	C	413	1/1	0.95	0.29	77,77,77,77	0
6	ADP	D	404	27/27	0.95	0.21	80,89,95,96	0
6	ADP	B	400	27/27	0.95	0.22	86,94,99,100	0
7	BEF	G	407	4/4	0.95	0.23	79,79,80,80	0
6	ADP	C	402	27/27	0.96	0.21	78,86,91,93	0
6	ADP	G	406	27/27	0.96	0.23	81,87,92,94	0
7	BEF	H	409	4/4	0.97	0.22	57,57,57,58	0
7	BEF	B	401	4/4	0.97	0.28	79,80,80,81	0
7	BEF	I	411	4/4	0.97	0.29	62,63,63,64	0
6	ADP	H	408	27/27	0.97	0.20	60,62,67,67	0
7	BEF	C	403	4/4	0.97	0.26	77,78,78,79	0
7	BEF	D	405	4/4	0.97	0.23	85,85,86,87	0
8	MG	I	417	1/1	0.97	0.39	58,58,58,58	0
9	ZN	D	420	1/1	0.97	0.07	133,133,133,133	0
9	ZN	E	421	1/1	0.98	0.06	161,161,161,161	0
9	ZN	B	418	1/1	0.98	0.07	144,144,144,144	0
9	ZN	H	423	1/1	0.98	0.10	112,112,112,112	0
6	ADP	I	410	27/27	0.98	0.23	62,68,72,73	0
9	ZN	G	422	1/1	0.99	0.12	160,160,160,160	0
9	ZN	C	419	1/1	0.99	0.06	130,130,130,130	0
9	ZN	I	424	1/1	0.99	0.10	99,99,99,99	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.



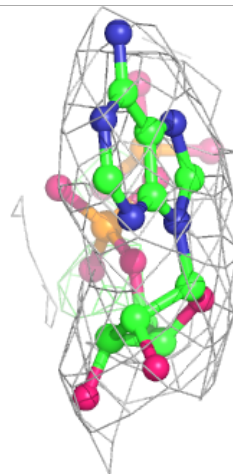
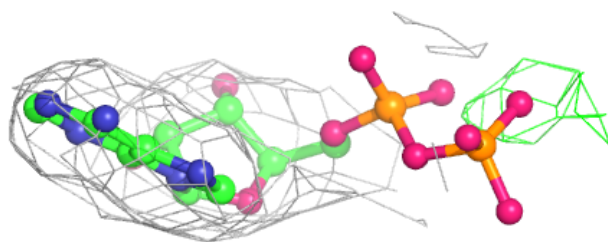
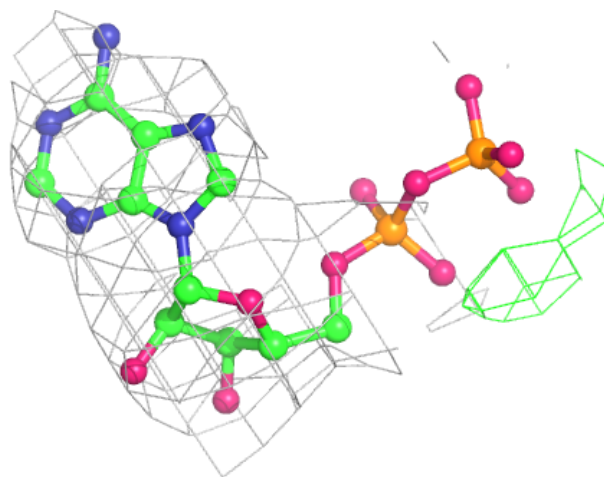
Electron density around ADP B 400:

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



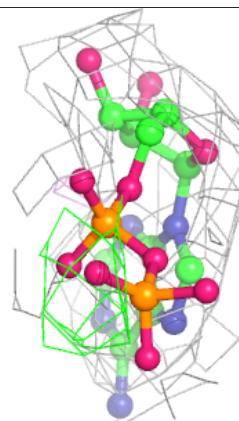
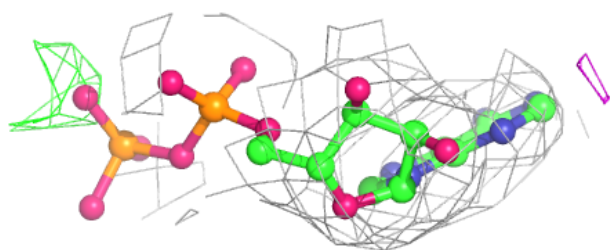
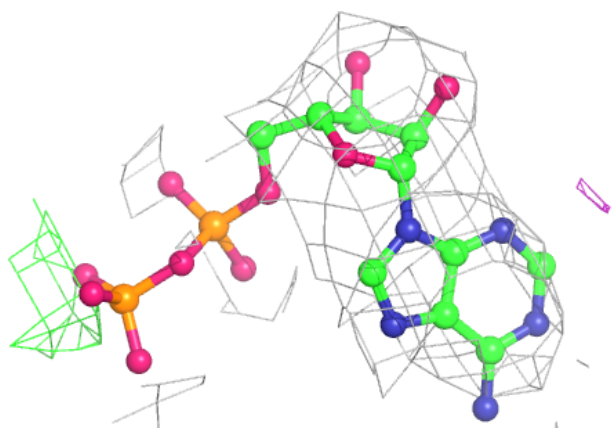
Electron density around ADP C 402:

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

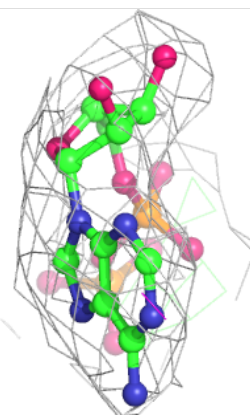
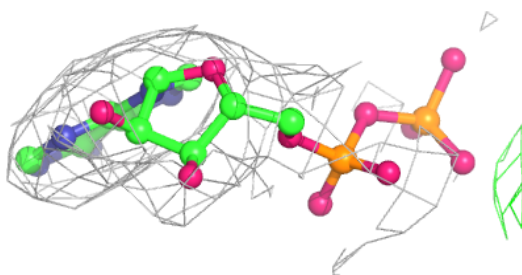
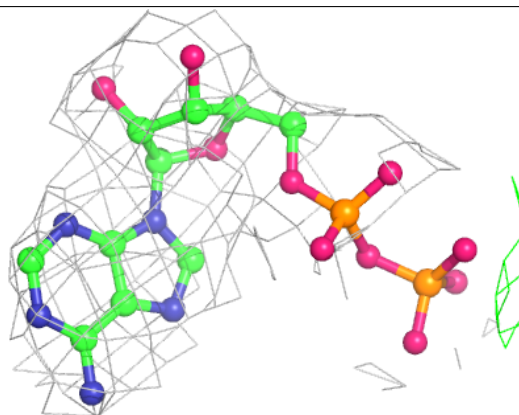


Electron density around ADP G 406:

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

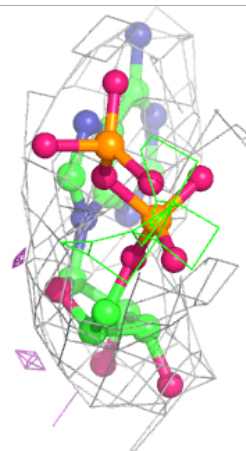
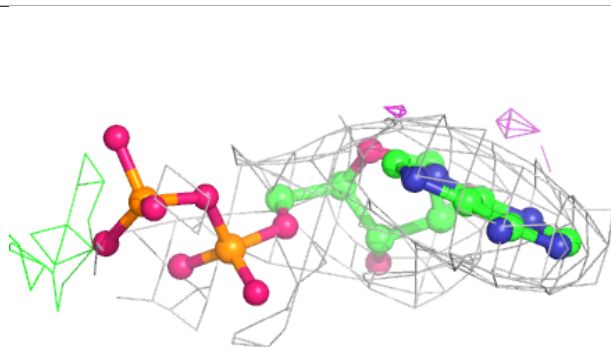
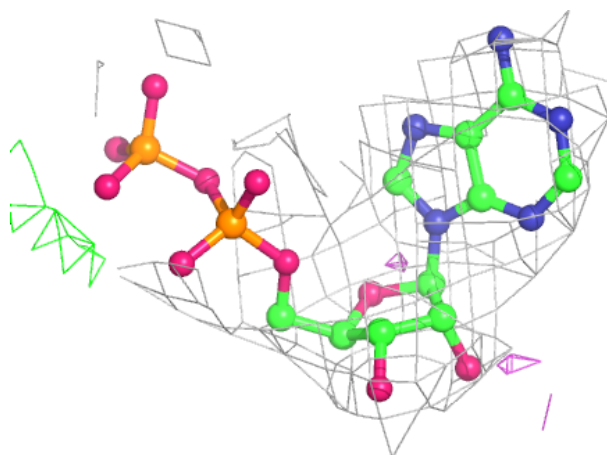
**Electron density around ADP H 408:**

$2mF_o-DF_c$ (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.