



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:44 am BST

PDB ID : 4PJ1
Title : Crystal structure of the human mitochondrial chaperonin symmetrical 'foot-ball' complex
Authors : Frolow, F.; Azem, A.; Nisemblat, S.
Deposited on : 2014-05-10
Resolution : 3.15 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:

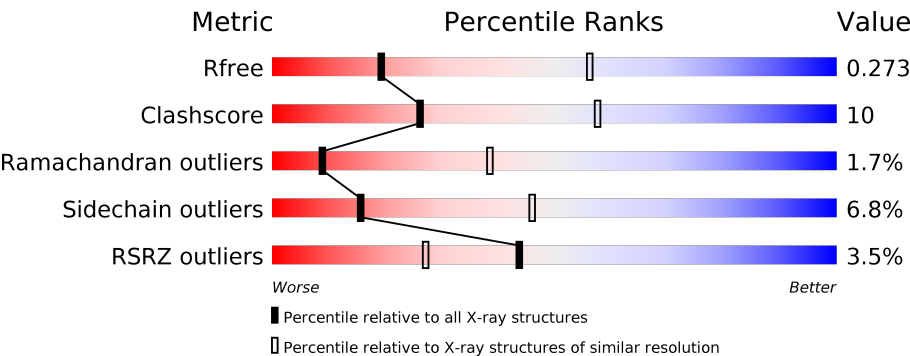
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	558	<div><div>5%</div><div><div></div><div>65%</div><div>27%</div><div>• 6%</div></div></div>
1	B	558	<div><div>8%</div><div><div></div><div>62%</div><div>27%</div><div>5% • 6%</div></div></div>
1	C	558	<div><div>2%</div><div><div></div><div>69%</div><div>23%</div><div>• 6%</div></div></div>
1	D	558	<div><div>4%</div><div><div></div><div>65%</div><div>25%</div><div>• 6%</div></div></div>
1	E	558	<div><div>2%</div><div><div></div><div>69%</div><div>22%</div><div>• 6%</div></div></div>
1	F	558	<div><div>3%</div><div><div></div><div>71%</div><div>20%</div><div>• 6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	558	
1	H	558	
1	I	558	
1	J	558	
1	K	558	
1	L	558	
1	M	558	
1	N	558	
2	1	114	
2	2	114	
2	O	114	
2	P	114	
2	Q	114	
2	R	114	
2	S	114	
2	T	114	
2	U	114	
2	V	114	
2	W	114	
2	X	114	
2	Y	114	
2	Z	114	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 65963 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 60 kDa heat shock protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	B	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	C	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	D	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	E	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	F	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	G	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	H	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	I	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	J	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	K	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	L	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	M	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	N	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			

There are 406 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	GLY	-	expression tag	UNP P10809
A	-23	SER	-	expression tag	UNP P10809
A	-22	HIS	-	expression tag	UNP P10809
A	-21	HIS	-	expression tag	UNP P10809
A	-20	HIS	-	expression tag	UNP P10809
A	-19	HIS	-	expression tag	UNP P10809
A	-18	HIS	-	expression tag	UNP P10809
A	-17	HIS	-	expression tag	UNP P10809
A	-16	HIS	-	expression tag	UNP P10809
A	-15	HIS	-	expression tag	UNP P10809
A	-14	GLY	-	expression tag	UNP P10809
A	-13	SER	-	expression tag	UNP P10809
A	-12	ASP	-	expression tag	UNP P10809
A	-11	TYR	-	expression tag	UNP P10809
A	-10	ASP	-	expression tag	UNP P10809
A	-9	ILE	-	expression tag	UNP P10809
A	-8	PRO	-	expression tag	UNP P10809
A	-7	THR	-	expression tag	UNP P10809
A	-6	THR	-	expression tag	UNP P10809
A	-5	GLU	-	expression tag	UNP P10809
A	-4	ASN	-	expression tag	UNP P10809
A	-3	LEU	-	expression tag	UNP P10809
A	-2	TYR	-	expression tag	UNP P10809
A	-1	PHE	-	expression tag	UNP P10809
A	0	GLN	-	expression tag	UNP P10809
A	1	GLY	-	expression tag	UNP P10809
A	2	SER	-	expression tag	UNP P10809
A	323	LYS	GLU	engineered mutation	UNP P10809
B	-25	MET	-	expression tag	UNP P10809
B	-24	GLY	-	expression tag	UNP P10809
B	-23	SER	-	expression tag	UNP P10809
B	-22	HIS	-	expression tag	UNP P10809
B	-21	HIS	-	expression tag	UNP P10809
B	-20	HIS	-	expression tag	UNP P10809
B	-19	HIS	-	expression tag	UNP P10809
B	-18	HIS	-	expression tag	UNP P10809
B	-17	HIS	-	expression tag	UNP P10809
B	-16	HIS	-	expression tag	UNP P10809
B	-15	HIS	-	expression tag	UNP P10809
B	-14	GLY	-	expression tag	UNP P10809
B	-13	SER	-	expression tag	UNP P10809
B	-12	ASP	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	TYR	-	expression tag	UNP P10809
B	-10	ASP	-	expression tag	UNP P10809
B	-9	ILE	-	expression tag	UNP P10809
B	-8	PRO	-	expression tag	UNP P10809
B	-7	THR	-	expression tag	UNP P10809
B	-6	THR	-	expression tag	UNP P10809
B	-5	GLU	-	expression tag	UNP P10809
B	-4	ASN	-	expression tag	UNP P10809
B	-3	LEU	-	expression tag	UNP P10809
B	-2	TYR	-	expression tag	UNP P10809
B	-1	PHE	-	expression tag	UNP P10809
B	0	GLN	-	expression tag	UNP P10809
B	1	GLY	-	expression tag	UNP P10809
B	2	SER	-	expression tag	UNP P10809
B	323	LYS	GLU	engineered mutation	UNP P10809
C	-25	MET	-	expression tag	UNP P10809
C	-24	GLY	-	expression tag	UNP P10809
C	-23	SER	-	expression tag	UNP P10809
C	-22	HIS	-	expression tag	UNP P10809
C	-21	HIS	-	expression tag	UNP P10809
C	-20	HIS	-	expression tag	UNP P10809
C	-19	HIS	-	expression tag	UNP P10809
C	-18	HIS	-	expression tag	UNP P10809
C	-17	HIS	-	expression tag	UNP P10809
C	-16	HIS	-	expression tag	UNP P10809
C	-15	HIS	-	expression tag	UNP P10809
C	-14	GLY	-	expression tag	UNP P10809
C	-13	SER	-	expression tag	UNP P10809
C	-12	ASP	-	expression tag	UNP P10809
C	-11	TYR	-	expression tag	UNP P10809
C	-10	ASP	-	expression tag	UNP P10809
C	-9	ILE	-	expression tag	UNP P10809
C	-8	PRO	-	expression tag	UNP P10809
C	-7	THR	-	expression tag	UNP P10809
C	-6	THR	-	expression tag	UNP P10809
C	-5	GLU	-	expression tag	UNP P10809
C	-4	ASN	-	expression tag	UNP P10809
C	-3	LEU	-	expression tag	UNP P10809
C	-2	TYR	-	expression tag	UNP P10809
C	-1	PHE	-	expression tag	UNP P10809
C	0	GLN	-	expression tag	UNP P10809
C	1	GLY	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	SER	-	expression tag	UNP P10809
C	323	LYS	GLU	engineered mutation	UNP P10809
D	-25	MET	-	expression tag	UNP P10809
D	-24	GLY	-	expression tag	UNP P10809
D	-23	SER	-	expression tag	UNP P10809
D	-22	HIS	-	expression tag	UNP P10809
D	-21	HIS	-	expression tag	UNP P10809
D	-20	HIS	-	expression tag	UNP P10809
D	-19	HIS	-	expression tag	UNP P10809
D	-18	HIS	-	expression tag	UNP P10809
D	-17	HIS	-	expression tag	UNP P10809
D	-16	HIS	-	expression tag	UNP P10809
D	-15	HIS	-	expression tag	UNP P10809
D	-14	GLY	-	expression tag	UNP P10809
D	-13	SER	-	expression tag	UNP P10809
D	-12	ASP	-	expression tag	UNP P10809
D	-11	TYR	-	expression tag	UNP P10809
D	-10	ASP	-	expression tag	UNP P10809
D	-9	ILE	-	expression tag	UNP P10809
D	-8	PRO	-	expression tag	UNP P10809
D	-7	THR	-	expression tag	UNP P10809
D	-6	THR	-	expression tag	UNP P10809
D	-5	GLU	-	expression tag	UNP P10809
D	-4	ASN	-	expression tag	UNP P10809
D	-3	LEU	-	expression tag	UNP P10809
D	-2	TYR	-	expression tag	UNP P10809
D	-1	PHE	-	expression tag	UNP P10809
D	0	GLN	-	expression tag	UNP P10809
D	1	GLY	-	expression tag	UNP P10809
D	2	SER	-	expression tag	UNP P10809
D	323	LYS	GLU	engineered mutation	UNP P10809
E	-25	MET	-	expression tag	UNP P10809
E	-24	GLY	-	expression tag	UNP P10809
E	-23	SER	-	expression tag	UNP P10809
E	-22	HIS	-	expression tag	UNP P10809
E	-21	HIS	-	expression tag	UNP P10809
E	-20	HIS	-	expression tag	UNP P10809
E	-19	HIS	-	expression tag	UNP P10809
E	-18	HIS	-	expression tag	UNP P10809
E	-17	HIS	-	expression tag	UNP P10809
E	-16	HIS	-	expression tag	UNP P10809
E	-15	HIS	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	GLY	-	expression tag	UNP P10809
E	-13	SER	-	expression tag	UNP P10809
E	-12	ASP	-	expression tag	UNP P10809
E	-11	TYR	-	expression tag	UNP P10809
E	-10	ASP	-	expression tag	UNP P10809
E	-9	ILE	-	expression tag	UNP P10809
E	-8	PRO	-	expression tag	UNP P10809
E	-7	THR	-	expression tag	UNP P10809
E	-6	THR	-	expression tag	UNP P10809
E	-5	GLU	-	expression tag	UNP P10809
E	-4	ASN	-	expression tag	UNP P10809
E	-3	LEU	-	expression tag	UNP P10809
E	-2	TYR	-	expression tag	UNP P10809
E	-1	PHE	-	expression tag	UNP P10809
E	0	GLN	-	expression tag	UNP P10809
E	1	GLY	-	expression tag	UNP P10809
E	2	SER	-	expression tag	UNP P10809
E	323	LYS	GLU	engineered mutation	UNP P10809
F	-25	MET	-	expression tag	UNP P10809
F	-24	GLY	-	expression tag	UNP P10809
F	-23	SER	-	expression tag	UNP P10809
F	-22	HIS	-	expression tag	UNP P10809
F	-21	HIS	-	expression tag	UNP P10809
F	-20	HIS	-	expression tag	UNP P10809
F	-19	HIS	-	expression tag	UNP P10809
F	-18	HIS	-	expression tag	UNP P10809
F	-17	HIS	-	expression tag	UNP P10809
F	-16	HIS	-	expression tag	UNP P10809
F	-15	HIS	-	expression tag	UNP P10809
F	-14	GLY	-	expression tag	UNP P10809
F	-13	SER	-	expression tag	UNP P10809
F	-12	ASP	-	expression tag	UNP P10809
F	-11	TYR	-	expression tag	UNP P10809
F	-10	ASP	-	expression tag	UNP P10809
F	-9	ILE	-	expression tag	UNP P10809
F	-8	PRO	-	expression tag	UNP P10809
F	-7	THR	-	expression tag	UNP P10809
F	-6	THR	-	expression tag	UNP P10809
F	-5	GLU	-	expression tag	UNP P10809
F	-4	ASN	-	expression tag	UNP P10809
F	-3	LEU	-	expression tag	UNP P10809
F	-2	TYR	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	PHE	-	expression tag	UNP P10809
F	0	GLN	-	expression tag	UNP P10809
F	1	GLY	-	expression tag	UNP P10809
F	2	SER	-	expression tag	UNP P10809
F	323	LYS	GLU	engineered mutation	UNP P10809
G	-25	MET	-	expression tag	UNP P10809
G	-24	GLY	-	expression tag	UNP P10809
G	-23	SER	-	expression tag	UNP P10809
G	-22	HIS	-	expression tag	UNP P10809
G	-21	HIS	-	expression tag	UNP P10809
G	-20	HIS	-	expression tag	UNP P10809
G	-19	HIS	-	expression tag	UNP P10809
G	-18	HIS	-	expression tag	UNP P10809
G	-17	HIS	-	expression tag	UNP P10809
G	-16	HIS	-	expression tag	UNP P10809
G	-15	HIS	-	expression tag	UNP P10809
G	-14	GLY	-	expression tag	UNP P10809
G	-13	SER	-	expression tag	UNP P10809
G	-12	ASP	-	expression tag	UNP P10809
G	-11	TYR	-	expression tag	UNP P10809
G	-10	ASP	-	expression tag	UNP P10809
G	-9	ILE	-	expression tag	UNP P10809
G	-8	PRO	-	expression tag	UNP P10809
G	-7	THR	-	expression tag	UNP P10809
G	-6	THR	-	expression tag	UNP P10809
G	-5	GLU	-	expression tag	UNP P10809
G	-4	ASN	-	expression tag	UNP P10809
G	-3	LEU	-	expression tag	UNP P10809
G	-2	TYR	-	expression tag	UNP P10809
G	-1	PHE	-	expression tag	UNP P10809
G	0	GLN	-	expression tag	UNP P10809
G	1	GLY	-	expression tag	UNP P10809
G	2	SER	-	expression tag	UNP P10809
G	323	LYS	GLU	engineered mutation	UNP P10809
H	-25	MET	-	expression tag	UNP P10809
H	-24	GLY	-	expression tag	UNP P10809
H	-23	SER	-	expression tag	UNP P10809
H	-22	HIS	-	expression tag	UNP P10809
H	-21	HIS	-	expression tag	UNP P10809
H	-20	HIS	-	expression tag	UNP P10809
H	-19	HIS	-	expression tag	UNP P10809
H	-18	HIS	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	HIS	-	expression tag	UNP P10809
H	-16	HIS	-	expression tag	UNP P10809
H	-15	HIS	-	expression tag	UNP P10809
H	-14	GLY	-	expression tag	UNP P10809
H	-13	SER	-	expression tag	UNP P10809
H	-12	ASP	-	expression tag	UNP P10809
H	-11	TYR	-	expression tag	UNP P10809
H	-10	ASP	-	expression tag	UNP P10809
H	-9	ILE	-	expression tag	UNP P10809
H	-8	PRO	-	expression tag	UNP P10809
H	-7	THR	-	expression tag	UNP P10809
H	-6	THR	-	expression tag	UNP P10809
H	-5	GLU	-	expression tag	UNP P10809
H	-4	ASN	-	expression tag	UNP P10809
H	-3	LEU	-	expression tag	UNP P10809
H	-2	TYR	-	expression tag	UNP P10809
H	-1	PHE	-	expression tag	UNP P10809
H	0	GLN	-	expression tag	UNP P10809
H	1	GLY	-	expression tag	UNP P10809
H	2	SER	-	expression tag	UNP P10809
H	323	LYS	GLU	engineered mutation	UNP P10809
I	-25	MET	-	expression tag	UNP P10809
I	-24	GLY	-	expression tag	UNP P10809
I	-23	SER	-	expression tag	UNP P10809
I	-22	HIS	-	expression tag	UNP P10809
I	-21	HIS	-	expression tag	UNP P10809
I	-20	HIS	-	expression tag	UNP P10809
I	-19	HIS	-	expression tag	UNP P10809
I	-18	HIS	-	expression tag	UNP P10809
I	-17	HIS	-	expression tag	UNP P10809
I	-16	HIS	-	expression tag	UNP P10809
I	-15	HIS	-	expression tag	UNP P10809
I	-14	GLY	-	expression tag	UNP P10809
I	-13	SER	-	expression tag	UNP P10809
I	-12	ASP	-	expression tag	UNP P10809
I	-11	TYR	-	expression tag	UNP P10809
I	-10	ASP	-	expression tag	UNP P10809
I	-9	ILE	-	expression tag	UNP P10809
I	-8	PRO	-	expression tag	UNP P10809
I	-7	THR	-	expression tag	UNP P10809
I	-6	THR	-	expression tag	UNP P10809
I	-5	GLU	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	ASN	-	expression tag	UNP P10809
I	-3	LEU	-	expression tag	UNP P10809
I	-2	TYR	-	expression tag	UNP P10809
I	-1	PHE	-	expression tag	UNP P10809
I	0	GLN	-	expression tag	UNP P10809
I	1	GLY	-	expression tag	UNP P10809
I	2	SER	-	expression tag	UNP P10809
I	323	LYS	GLU	engineered mutation	UNP P10809
J	-25	MET	-	expression tag	UNP P10809
J	-24	GLY	-	expression tag	UNP P10809
J	-23	SER	-	expression tag	UNP P10809
J	-22	HIS	-	expression tag	UNP P10809
J	-21	HIS	-	expression tag	UNP P10809
J	-20	HIS	-	expression tag	UNP P10809
J	-19	HIS	-	expression tag	UNP P10809
J	-18	HIS	-	expression tag	UNP P10809
J	-17	HIS	-	expression tag	UNP P10809
J	-16	HIS	-	expression tag	UNP P10809
J	-15	HIS	-	expression tag	UNP P10809
J	-14	GLY	-	expression tag	UNP P10809
J	-13	SER	-	expression tag	UNP P10809
J	-12	ASP	-	expression tag	UNP P10809
J	-11	TYR	-	expression tag	UNP P10809
J	-10	ASP	-	expression tag	UNP P10809
J	-9	ILE	-	expression tag	UNP P10809
J	-8	PRO	-	expression tag	UNP P10809
J	-7	THR	-	expression tag	UNP P10809
J	-6	THR	-	expression tag	UNP P10809
J	-5	GLU	-	expression tag	UNP P10809
J	-4	ASN	-	expression tag	UNP P10809
J	-3	LEU	-	expression tag	UNP P10809
J	-2	TYR	-	expression tag	UNP P10809
J	-1	PHE	-	expression tag	UNP P10809
J	0	GLN	-	expression tag	UNP P10809
J	1	GLY	-	expression tag	UNP P10809
J	2	SER	-	expression tag	UNP P10809
J	323	LYS	GLU	engineered mutation	UNP P10809
K	-25	MET	-	expression tag	UNP P10809
K	-24	GLY	-	expression tag	UNP P10809
K	-23	SER	-	expression tag	UNP P10809
K	-22	HIS	-	expression tag	UNP P10809
K	-21	HIS	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-20	HIS	-	expression tag	UNP P10809
K	-19	HIS	-	expression tag	UNP P10809
K	-18	HIS	-	expression tag	UNP P10809
K	-17	HIS	-	expression tag	UNP P10809
K	-16	HIS	-	expression tag	UNP P10809
K	-15	HIS	-	expression tag	UNP P10809
K	-14	GLY	-	expression tag	UNP P10809
K	-13	SER	-	expression tag	UNP P10809
K	-12	ASP	-	expression tag	UNP P10809
K	-11	TYR	-	expression tag	UNP P10809
K	-10	ASP	-	expression tag	UNP P10809
K	-9	ILE	-	expression tag	UNP P10809
K	-8	PRO	-	expression tag	UNP P10809
K	-7	THR	-	expression tag	UNP P10809
K	-6	THR	-	expression tag	UNP P10809
K	-5	GLU	-	expression tag	UNP P10809
K	-4	ASN	-	expression tag	UNP P10809
K	-3	LEU	-	expression tag	UNP P10809
K	-2	TYR	-	expression tag	UNP P10809
K	-1	PHE	-	expression tag	UNP P10809
K	0	GLN	-	expression tag	UNP P10809
K	1	GLY	-	expression tag	UNP P10809
K	2	SER	-	expression tag	UNP P10809
K	323	LYS	GLU	engineered mutation	UNP P10809
L	-25	MET	-	expression tag	UNP P10809
L	-24	GLY	-	expression tag	UNP P10809
L	-23	SER	-	expression tag	UNP P10809
L	-22	HIS	-	expression tag	UNP P10809
L	-21	HIS	-	expression tag	UNP P10809
L	-20	HIS	-	expression tag	UNP P10809
L	-19	HIS	-	expression tag	UNP P10809
L	-18	HIS	-	expression tag	UNP P10809
L	-17	HIS	-	expression tag	UNP P10809
L	-16	HIS	-	expression tag	UNP P10809
L	-15	HIS	-	expression tag	UNP P10809
L	-14	GLY	-	expression tag	UNP P10809
L	-13	SER	-	expression tag	UNP P10809
L	-12	ASP	-	expression tag	UNP P10809
L	-11	TYR	-	expression tag	UNP P10809
L	-10	ASP	-	expression tag	UNP P10809
L	-9	ILE	-	expression tag	UNP P10809
L	-8	PRO	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	THR	-	expression tag	UNP P10809
L	-6	THR	-	expression tag	UNP P10809
L	-5	GLU	-	expression tag	UNP P10809
L	-4	ASN	-	expression tag	UNP P10809
L	-3	LEU	-	expression tag	UNP P10809
L	-2	TYR	-	expression tag	UNP P10809
L	-1	PHE	-	expression tag	UNP P10809
L	0	GLN	-	expression tag	UNP P10809
L	1	GLY	-	expression tag	UNP P10809
L	2	SER	-	expression tag	UNP P10809
L	323	LYS	GLU	engineered mutation	UNP P10809
M	-25	MET	-	expression tag	UNP P10809
M	-24	GLY	-	expression tag	UNP P10809
M	-23	SER	-	expression tag	UNP P10809
M	-22	HIS	-	expression tag	UNP P10809
M	-21	HIS	-	expression tag	UNP P10809
M	-20	HIS	-	expression tag	UNP P10809
M	-19	HIS	-	expression tag	UNP P10809
M	-18	HIS	-	expression tag	UNP P10809
M	-17	HIS	-	expression tag	UNP P10809
M	-16	HIS	-	expression tag	UNP P10809
M	-15	HIS	-	expression tag	UNP P10809
M	-14	GLY	-	expression tag	UNP P10809
M	-13	SER	-	expression tag	UNP P10809
M	-12	ASP	-	expression tag	UNP P10809
M	-11	TYR	-	expression tag	UNP P10809
M	-10	ASP	-	expression tag	UNP P10809
M	-9	ILE	-	expression tag	UNP P10809
M	-8	PRO	-	expression tag	UNP P10809
M	-7	THR	-	expression tag	UNP P10809
M	-6	THR	-	expression tag	UNP P10809
M	-5	GLU	-	expression tag	UNP P10809
M	-4	ASN	-	expression tag	UNP P10809
M	-3	LEU	-	expression tag	UNP P10809
M	-2	TYR	-	expression tag	UNP P10809
M	-1	PHE	-	expression tag	UNP P10809
M	0	GLN	-	expression tag	UNP P10809
M	1	GLY	-	expression tag	UNP P10809
M	2	SER	-	expression tag	UNP P10809
M	323	LYS	GLU	engineered mutation	UNP P10809
N	-25	MET	-	expression tag	UNP P10809
N	-24	GLY	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-23	SER	-	expression tag	UNP P10809
N	-22	HIS	-	expression tag	UNP P10809
N	-21	HIS	-	expression tag	UNP P10809
N	-20	HIS	-	expression tag	UNP P10809
N	-19	HIS	-	expression tag	UNP P10809
N	-18	HIS	-	expression tag	UNP P10809
N	-17	HIS	-	expression tag	UNP P10809
N	-16	HIS	-	expression tag	UNP P10809
N	-15	HIS	-	expression tag	UNP P10809
N	-14	GLY	-	expression tag	UNP P10809
N	-13	SER	-	expression tag	UNP P10809
N	-12	ASP	-	expression tag	UNP P10809
N	-11	TYR	-	expression tag	UNP P10809
N	-10	ASP	-	expression tag	UNP P10809
N	-9	ILE	-	expression tag	UNP P10809
N	-8	PRO	-	expression tag	UNP P10809
N	-7	THR	-	expression tag	UNP P10809
N	-6	THR	-	expression tag	UNP P10809
N	-5	GLU	-	expression tag	UNP P10809
N	-4	ASN	-	expression tag	UNP P10809
N	-3	LEU	-	expression tag	UNP P10809
N	-2	TYR	-	expression tag	UNP P10809
N	-1	PHE	-	expression tag	UNP P10809
N	0	GLN	-	expression tag	UNP P10809
N	1	GLY	-	expression tag	UNP P10809
N	2	SER	-	expression tag	UNP P10809
N	323	LYS	GLU	engineered mutation	UNP P10809

- Molecule 2 is a protein called 10 kDa heat shock protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	P	105	Total	C	N	O	S	0	0	0
			788	507	133	147	1			
2	Q	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	R	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	S	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	T	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	102	Total	C	N	O	S	0	0	0
			773	498	130	144	1			
2	V	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	W	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	X	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	Y	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	Z	108	Total	C	N	O	S	0	0	0
			815	524	138	152	1			
2	1	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	2	104	Total	C	N	O	S	0	0	0
			783	504	132	146	1			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	103	LYS	-	expression tag	UNP P61604
O	104	LEU	-	expression tag	UNP P61604
O	105	ALA	-	expression tag	UNP P61604
O	106	ALA	-	expression tag	UNP P61604
O	107	ALA	-	expression tag	UNP P61604
O	108	LEU	-	expression tag	UNP P61604
O	109	GLU	-	expression tag	UNP P61604
O	110	HIS	-	expression tag	UNP P61604
O	111	HIS	-	expression tag	UNP P61604
O	112	HIS	-	expression tag	UNP P61604
O	113	HIS	-	expression tag	UNP P61604
O	114	HIS	-	expression tag	UNP P61604
P	103	LYS	-	expression tag	UNP P61604
P	104	LEU	-	expression tag	UNP P61604
P	105	ALA	-	expression tag	UNP P61604
P	106	ALA	-	expression tag	UNP P61604
P	107	ALA	-	expression tag	UNP P61604
P	108	LEU	-	expression tag	UNP P61604
P	109	GLU	-	expression tag	UNP P61604
P	110	HIS	-	expression tag	UNP P61604
P	111	HIS	-	expression tag	UNP P61604
P	112	HIS	-	expression tag	UNP P61604
P	113	HIS	-	expression tag	UNP P61604

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Chain	Residue	Modelled	Actual	Comment	Reference
P	114	HIS	-	expression tag	UNP P61604
Q	103	LYS	-	expression tag	UNP P61604
Q	104	LEU	-	expression tag	UNP P61604
Q	105	ALA	-	expression tag	UNP P61604
Q	106	ALA	-	expression tag	UNP P61604
Q	107	ALA	-	expression tag	UNP P61604
Q	108	LEU	-	expression tag	UNP P61604
Q	109	GLU	-	expression tag	UNP P61604
Q	110	HIS	-	expression tag	UNP P61604
Q	111	HIS	-	expression tag	UNP P61604
Q	112	HIS	-	expression tag	UNP P61604
Q	113	HIS	-	expression tag	UNP P61604
Q	114	HIS	-	expression tag	UNP P61604
R	103	LYS	-	expression tag	UNP P61604
R	104	LEU	-	expression tag	UNP P61604
R	105	ALA	-	expression tag	UNP P61604
R	106	ALA	-	expression tag	UNP P61604
R	107	ALA	-	expression tag	UNP P61604
R	108	LEU	-	expression tag	UNP P61604
R	109	GLU	-	expression tag	UNP P61604
R	110	HIS	-	expression tag	UNP P61604
R	111	HIS	-	expression tag	UNP P61604
R	112	HIS	-	expression tag	UNP P61604
R	113	HIS	-	expression tag	UNP P61604
R	114	HIS	-	expression tag	UNP P61604
S	103	LYS	-	expression tag	UNP P61604
S	104	LEU	-	expression tag	UNP P61604
S	105	ALA	-	expression tag	UNP P61604
S	106	ALA	-	expression tag	UNP P61604
S	107	ALA	-	expression tag	UNP P61604
S	108	LEU	-	expression tag	UNP P61604
S	109	GLU	-	expression tag	UNP P61604
S	110	HIS	-	expression tag	UNP P61604
S	111	HIS	-	expression tag	UNP P61604
S	112	HIS	-	expression tag	UNP P61604
S	113	HIS	-	expression tag	UNP P61604
S	114	HIS	-	expression tag	UNP P61604
T	103	LYS	-	expression tag	UNP P61604
T	104	LEU	-	expression tag	UNP P61604
T	105	ALA	-	expression tag	UNP P61604
T	106	ALA	-	expression tag	UNP P61604
T	107	ALA	-	expression tag	UNP P61604

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Chain	Residue	Modelled	Actual	Comment	Reference
T	108	LEU	-	expression tag	UNP P61604
T	109	GLU	-	expression tag	UNP P61604
T	110	HIS	-	expression tag	UNP P61604
T	111	HIS	-	expression tag	UNP P61604
T	112	HIS	-	expression tag	UNP P61604
T	113	HIS	-	expression tag	UNP P61604
T	114	HIS	-	expression tag	UNP P61604
U	103	LYS	-	expression tag	UNP P61604
U	104	LEU	-	expression tag	UNP P61604
U	105	ALA	-	expression tag	UNP P61604
U	106	ALA	-	expression tag	UNP P61604
U	107	ALA	-	expression tag	UNP P61604
U	108	LEU	-	expression tag	UNP P61604
U	109	GLU	-	expression tag	UNP P61604
U	110	HIS	-	expression tag	UNP P61604
U	111	HIS	-	expression tag	UNP P61604
U	112	HIS	-	expression tag	UNP P61604
U	113	HIS	-	expression tag	UNP P61604
U	114	HIS	-	expression tag	UNP P61604
V	103	LYS	-	expression tag	UNP P61604
V	104	LEU	-	expression tag	UNP P61604
V	105	ALA	-	expression tag	UNP P61604
V	106	ALA	-	expression tag	UNP P61604
V	107	ALA	-	expression tag	UNP P61604
V	108	LEU	-	expression tag	UNP P61604
V	109	GLU	-	expression tag	UNP P61604
V	110	HIS	-	expression tag	UNP P61604
V	111	HIS	-	expression tag	UNP P61604
V	112	HIS	-	expression tag	UNP P61604
V	113	HIS	-	expression tag	UNP P61604
V	114	HIS	-	expression tag	UNP P61604
W	103	LYS	-	expression tag	UNP P61604
W	104	LEU	-	expression tag	UNP P61604
W	105	ALA	-	expression tag	UNP P61604
W	106	ALA	-	expression tag	UNP P61604
W	107	ALA	-	expression tag	UNP P61604
W	108	LEU	-	expression tag	UNP P61604
W	109	GLU	-	expression tag	UNP P61604
W	110	HIS	-	expression tag	UNP P61604
W	111	HIS	-	expression tag	UNP P61604
W	112	HIS	-	expression tag	UNP P61604
W	113	HIS	-	expression tag	UNP P61604

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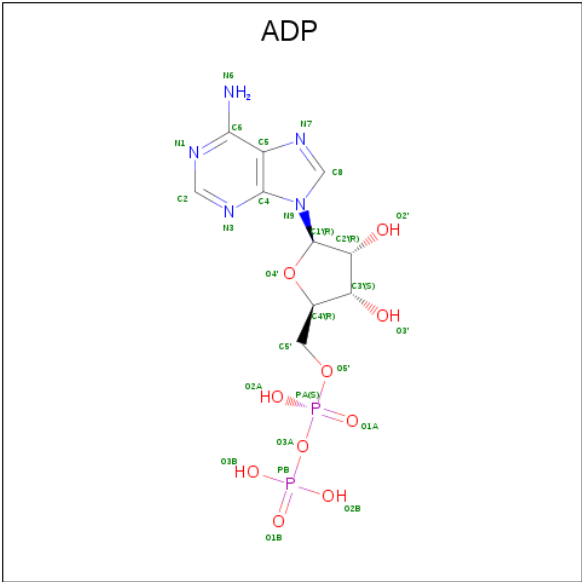
Chain	Residue	Modelled	Actual	Comment	Reference
W	114	HIS	-	expression tag	UNP P61604
X	103	LYS	-	expression tag	UNP P61604
X	104	LEU	-	expression tag	UNP P61604
X	105	ALA	-	expression tag	UNP P61604
X	106	ALA	-	expression tag	UNP P61604
X	107	ALA	-	expression tag	UNP P61604
X	108	LEU	-	expression tag	UNP P61604
X	109	GLU	-	expression tag	UNP P61604
X	110	HIS	-	expression tag	UNP P61604
X	111	HIS	-	expression tag	UNP P61604
X	112	HIS	-	expression tag	UNP P61604
X	113	HIS	-	expression tag	UNP P61604
X	114	HIS	-	expression tag	UNP P61604
Y	103	LYS	-	expression tag	UNP P61604
Y	104	LEU	-	expression tag	UNP P61604
Y	105	ALA	-	expression tag	UNP P61604
Y	106	ALA	-	expression tag	UNP P61604
Y	107	ALA	-	expression tag	UNP P61604
Y	108	LEU	-	expression tag	UNP P61604
Y	109	GLU	-	expression tag	UNP P61604
Y	110	HIS	-	expression tag	UNP P61604
Y	111	HIS	-	expression tag	UNP P61604
Y	112	HIS	-	expression tag	UNP P61604
Y	113	HIS	-	expression tag	UNP P61604
Y	114	HIS	-	expression tag	UNP P61604
Z	103	LYS	-	expression tag	UNP P61604
Z	104	LEU	-	expression tag	UNP P61604
Z	105	ALA	-	expression tag	UNP P61604
Z	106	ALA	-	expression tag	UNP P61604
Z	107	ALA	-	expression tag	UNP P61604
Z	108	LEU	-	expression tag	UNP P61604
Z	109	GLU	-	expression tag	UNP P61604
Z	110	HIS	-	expression tag	UNP P61604
Z	111	HIS	-	expression tag	UNP P61604
Z	112	HIS	-	expression tag	UNP P61604
Z	113	HIS	-	expression tag	UNP P61604
Z	114	HIS	-	expression tag	UNP P61604
1	103	LYS	-	expression tag	UNP P61604
1	104	LEU	-	expression tag	UNP P61604
1	105	ALA	-	expression tag	UNP P61604
1	106	ALA	-	expression tag	UNP P61604
1	107	ALA	-	expression tag	UNP P61604

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Chain	Residue	Modelled	Actual	Comment	Reference
1	108	LEU	-	expression tag	UNP P61604
1	109	GLU	-	expression tag	UNP P61604
1	110	HIS	-	expression tag	UNP P61604
1	111	HIS	-	expression tag	UNP P61604
1	112	HIS	-	expression tag	UNP P61604
1	113	HIS	-	expression tag	UNP P61604
1	114	HIS	-	expression tag	UNP P61604
2	103	LYS	-	expression tag	UNP P61604
2	104	LEU	-	expression tag	UNP P61604
2	105	ALA	-	expression tag	UNP P61604
2	106	ALA	-	expression tag	UNP P61604
2	107	ALA	-	expression tag	UNP P61604
2	108	LEU	-	expression tag	UNP P61604
2	109	GLU	-	expression tag	UNP P61604
2	110	HIS	-	expression tag	UNP P61604
2	111	HIS	-	expression tag	UNP P61604
2	112	HIS	-	expression tag	UNP P61604
2	113	HIS	-	expression tag	UNP P61604
2	114	HIS	-	expression tag	UNP P61604

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		

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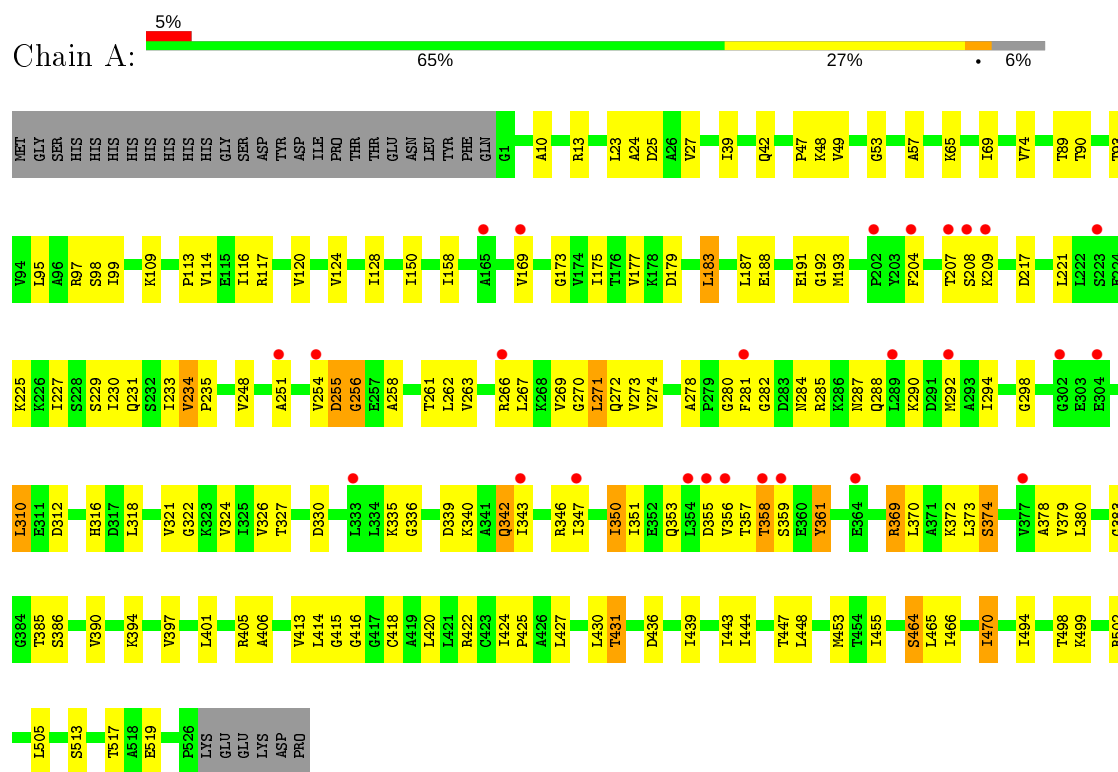
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0

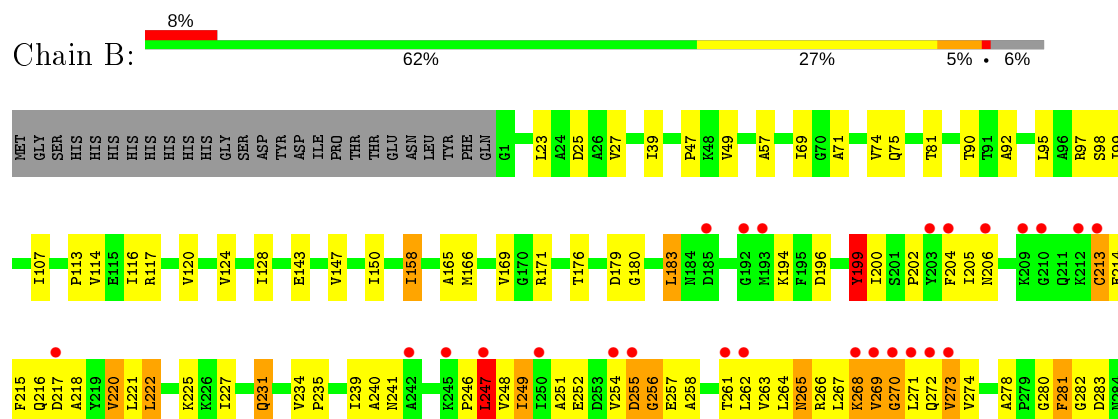
3 Residue-property plots [i](#)

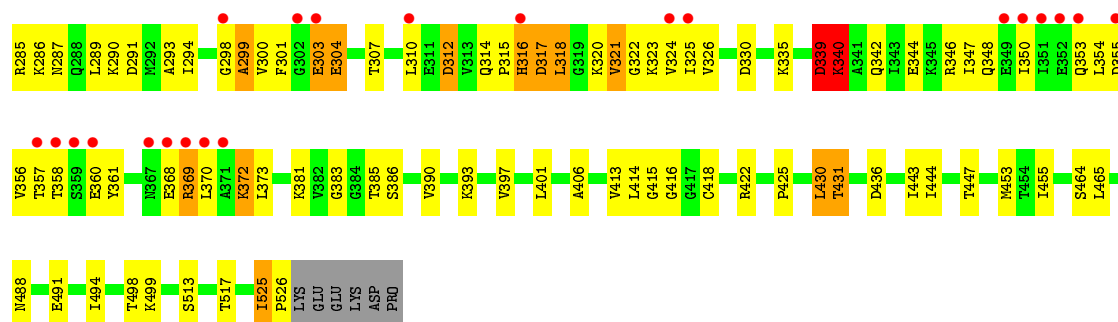
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 60 kDa heat shock protein, mitochondrial

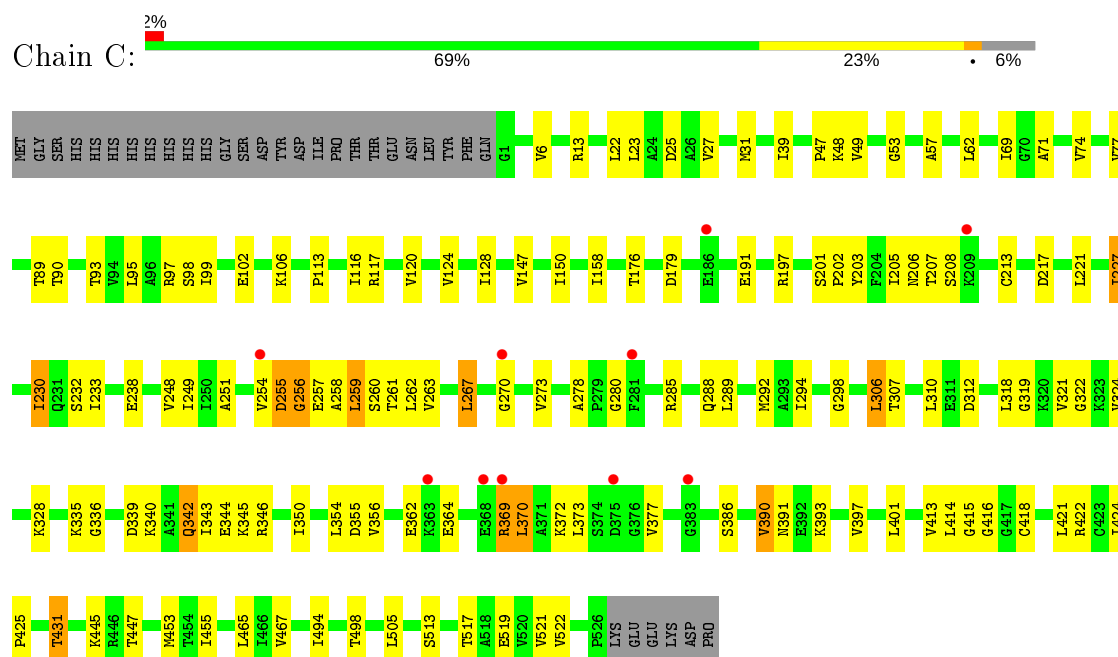


- Molecule 1: 60 kDa heat shock protein, mitochondrial

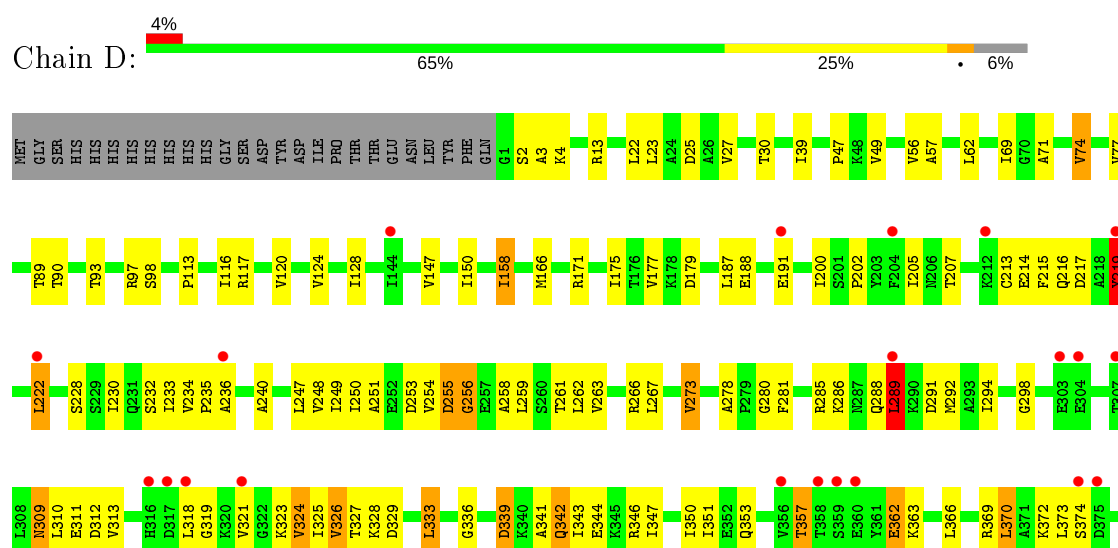


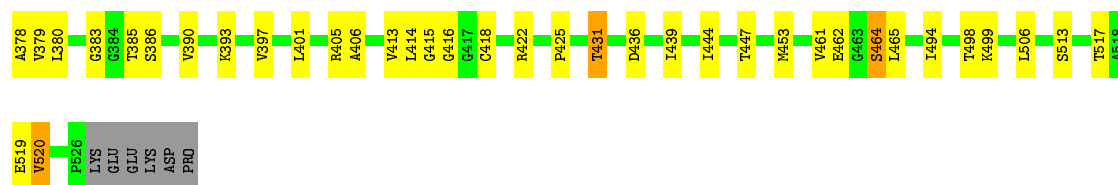


- Molecule 1: 60 kDa heat shock protein, mitochondrial

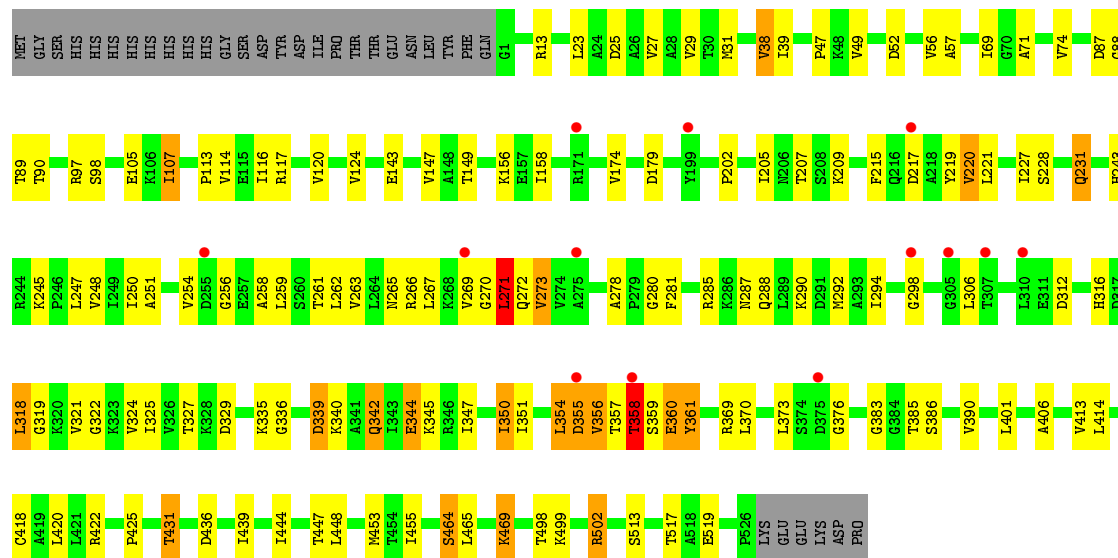


- Molecule 1: 60 kDa heat shock protein, mitochondrial

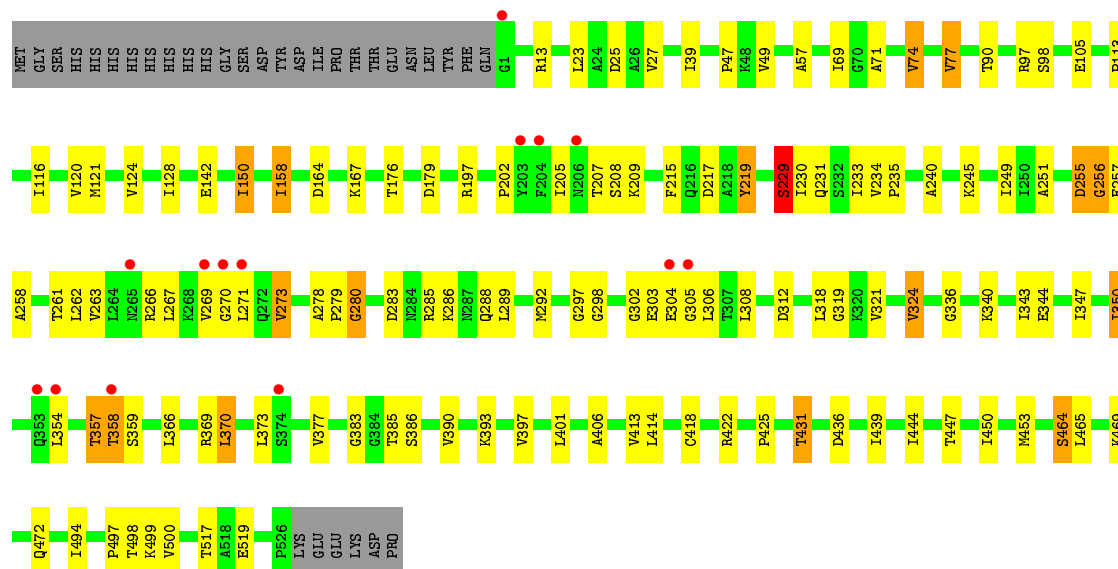




- Molecule 1: 60 kDa heat shock protein, mitochondrial



- Molecule 1: 60 kDa heat shock protein, mitochondrial

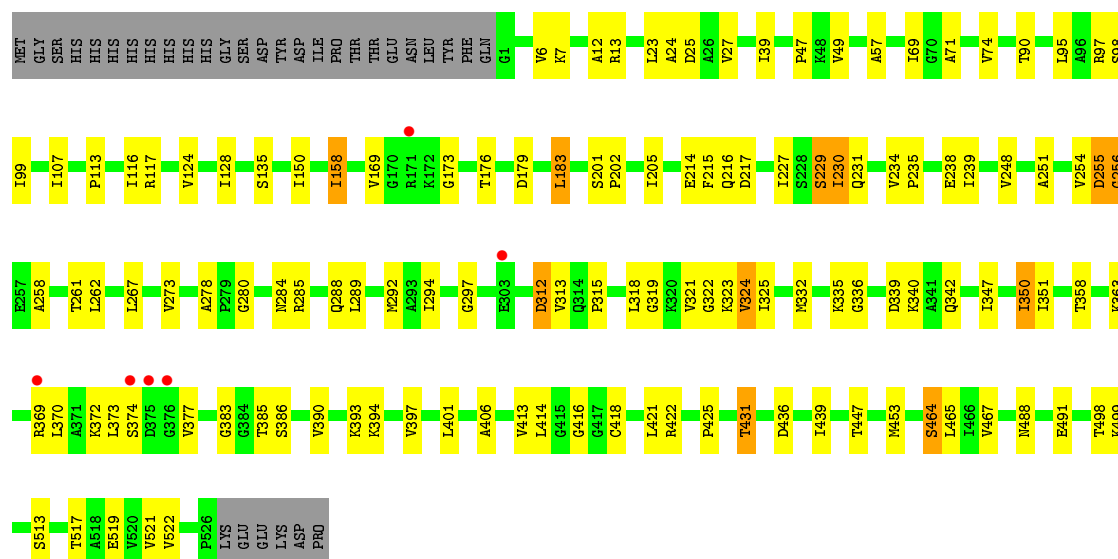


- Molecule 1: 60 kDa heat shock protein, mitochondrial

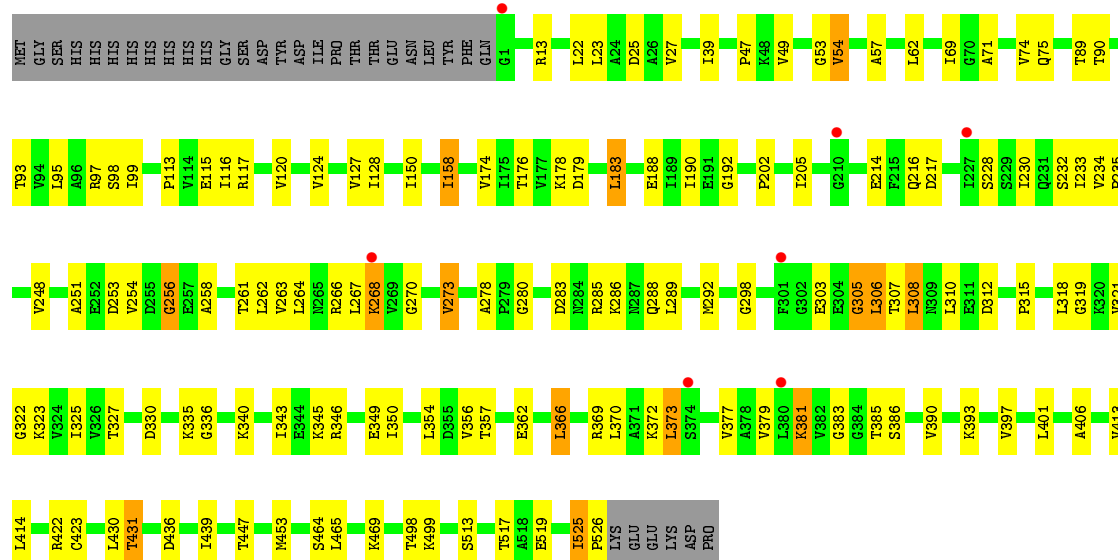




- Molecule 1: 60 kDa heat shock protein, mitochondrial

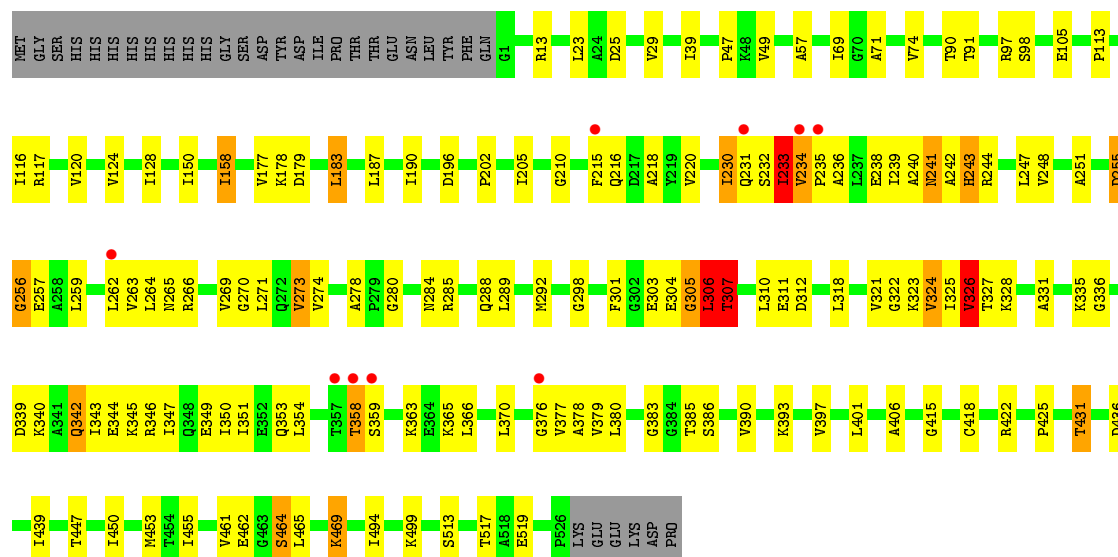


- Molecule 1: 60 kDa heat shock protein, mitochondrial

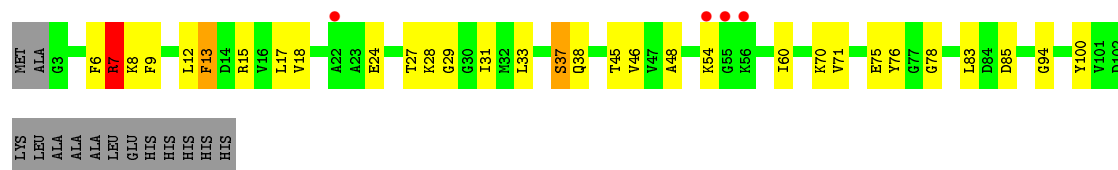


- Molecule 1: 60 kDa heat shock protein, mitochondrial





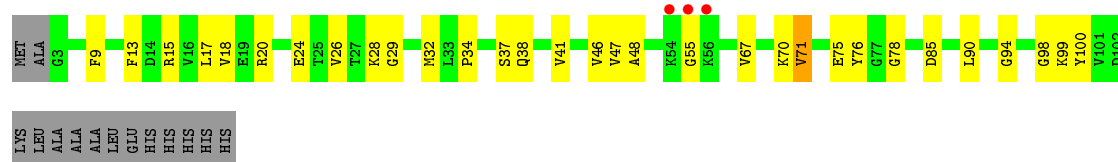
- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial

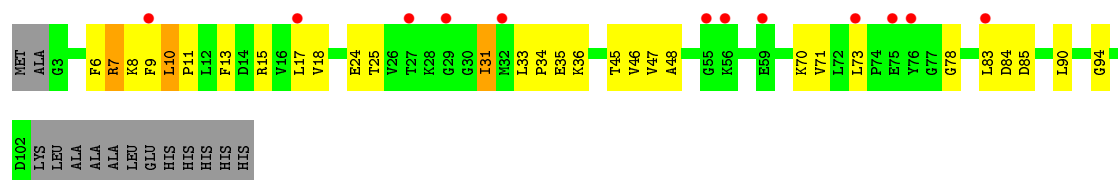


- Molecule 2: 10 kDa heat shock protein, mitochondrial

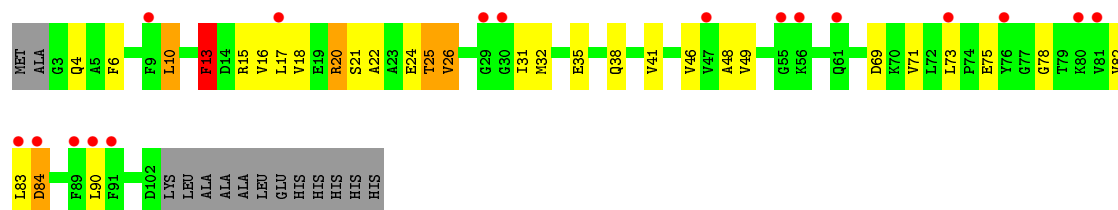


- Molecule 2: 10 kDa heat shock protein, mitochondrial

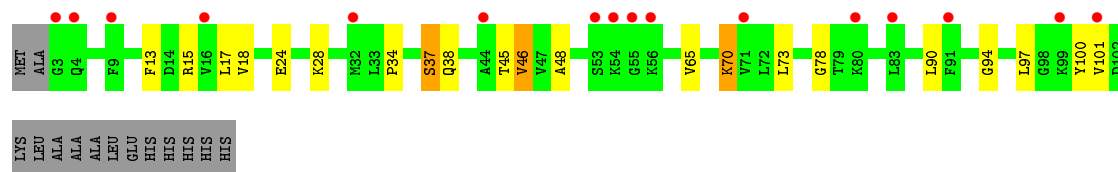




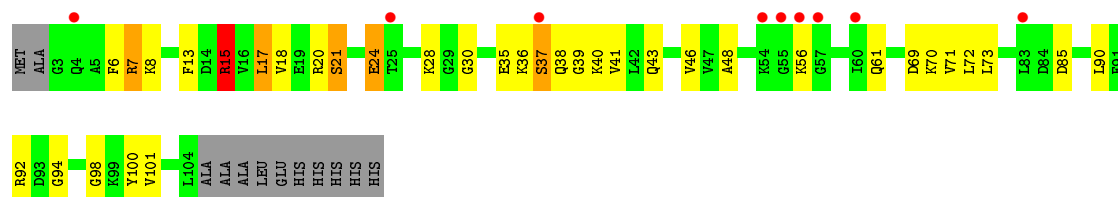
- Molecule 2: 10 kDa heat shock protein, mitochondrial



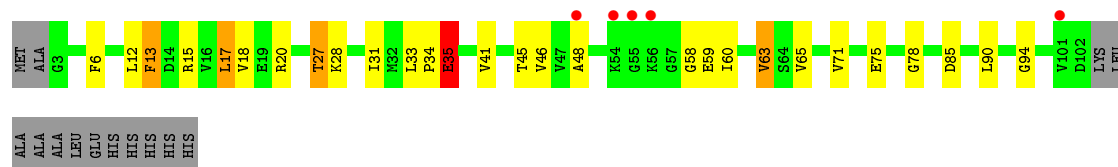
- Molecule 2: 10 kDa heat shock protein, mitochondrial



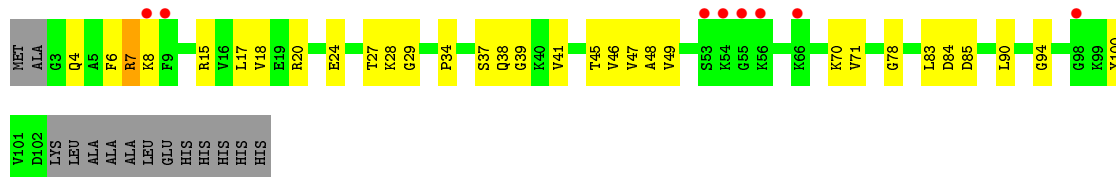
- Molecule 2: 10 kDa heat shock protein, mitochondrial



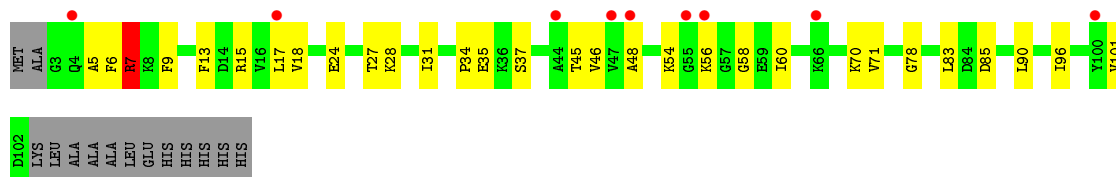
- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial



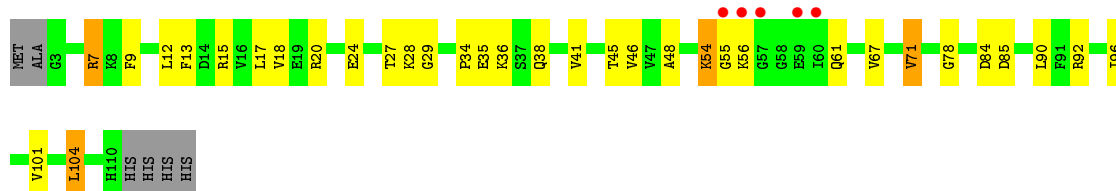
- Molecule 2: 10 kDa heat shock protein, mitochondrial



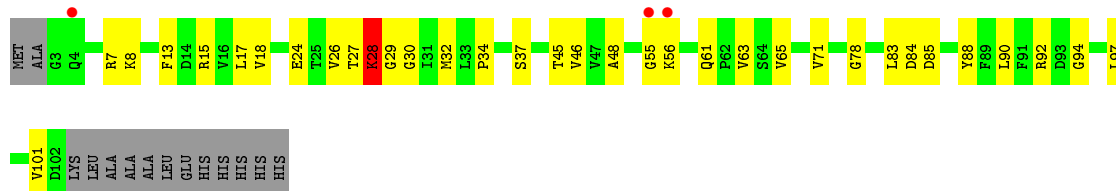
- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial

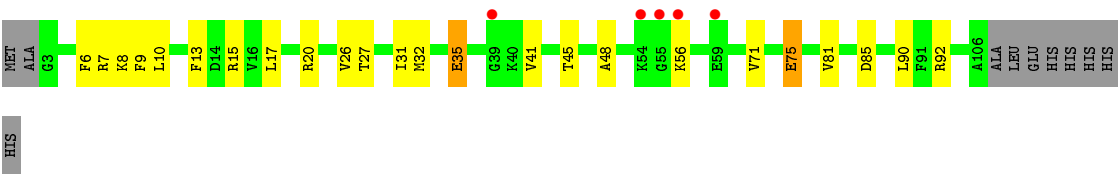


- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	199.10Å 199.10Å 627.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.77 – 3.15 49.77 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.77-3.15) 99.4 (49.77-3.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.241 , 0.270 0.247 , 0.273	Depositor DCC
R_{free} test set	10852 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	102.6	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	65963	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: 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	0.26	0/3950	0.53	0/5328
1	B	0.27	0/3950	0.60	2/5328 (0.0%)
1	C	0.26	0/3950	0.51	1/5328 (0.0%)
1	D	0.25	0/3950	0.54	4/5328 (0.1%)
1	E	0.25	0/3950	0.52	1/5328 (0.0%)
1	F	0.25	0/3950	0.51	0/5328
1	G	0.26	0/3950	0.55	1/5328 (0.0%)
1	H	0.25	0/3950	0.51	0/5328
1	I	0.24	0/3950	0.49	0/5328
1	J	0.25	0/3950	0.51	0/5328
1	K	0.25	0/3950	0.51	0/5328
1	L	0.26	0/3950	0.52	0/5328
1	M	0.26	0/3950	0.51	0/5328
1	N	0.26	0/3950	0.55	2/5328 (0.0%)
2	1	0.25	0/767	0.61	1/1030 (0.1%)
2	2	0.27	0/794	0.63	0/1066
2	O	0.25	0/767	0.59	0/1030
2	P	0.26	0/799	0.61	0/1073
2	Q	0.25	0/767	0.59	0/1030
2	R	0.26	0/767	0.63	0/1030
2	S	0.29	0/767	0.71	1/1030 (0.1%)
2	T	0.24	0/767	0.62	0/1030
2	U	0.27	0/784	0.72	1/1052 (0.1%)
2	V	0.24	0/767	0.57	0/1030
2	W	0.26	0/767	0.59	0/1030
2	X	0.25	0/767	0.54	0/1030
2	Y	0.25	0/767	0.55	0/1030
2	Z	0.26	0/827	0.64	2/1111 (0.2%)
All	All	0.26	0/66174	0.54	16/89194 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	D	0	1
1	G	0	3
1	K	0	1
1	N	0	5
2	S	0	1
2	U	0	2
2	V	0	1
2	Z	0	1
All	All	0	19

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	LEU	CA-CB-CG	8.52	134.88	115.30
1	B	247	LEU	CA-CB-CG	6.66	130.61	115.30
2	U	15	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	D	333	LEU	CA-CB-CG	6.37	129.94	115.30
1	N	210	GLY	N-CA-C	-5.92	98.31	113.10
1	G	259	LEU	CA-CB-CG	5.77	128.57	115.30
1	N	306	LEU	CA-CB-CG	5.68	128.38	115.30
2	Z	55	GLY	N-CA-C	5.62	127.16	113.10
1	D	222	LEU	CA-CB-CG	5.59	128.15	115.30
1	D	219	TYR	CA-CB-CG	5.45	123.75	113.40
2	Z	104	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	270	GLY	N-CA-C	5.23	126.17	113.10
1	C	259	LEU	CA-CB-CG	5.04	126.89	115.30
2	S	10	LEU	CA-CB-CG	5.04	126.88	115.30
1	E	271	LEU	CA-CB-CG	5.03	126.87	115.30
2	1	55	GLY	N-CA-C	5.01	125.62	113.10

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	303	GLU	Peptide
1	B	304	GLU	Peptide
1	B	339	ASP	Peptide
1	D	280	GLY	Peptide
1	G	280	GLY	Peptide
1	G	359	SER	Peptide
1	G	374	SER	Peptide
1	K	304	GLU	Peptide
1	N	232	SER	Peptide
1	N	233	ILE	Peptide
1	N	243	HIS	Peptide
1	N	280	GLY	Peptide
1	N	305	GLY	Peptide
2	S	24	GLU	Peptide
2	U	21	SER	Peptide
2	U	36	LYS	Peptide
2	V	35	GLU	Peptide
2	Z	27	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	3918	0	4103	104	0
1	B	3918	0	4103	130	0
1	C	3918	0	4103	87	0
1	D	3918	0	4103	96	0
1	E	3918	0	4103	83	0
1	F	3918	0	4103	77	0
1	G	3918	0	4103	89	0
1	H	3918	0	4103	86	0
1	I	3918	0	4103	79	0
1	J	3918	0	4103	88	0
1	K	3918	0	4103	78	0
1	L	3918	0	4103	83	0
1	M	3918	0	4103	84	0
1	N	3918	0	4103	99	0
2	1	756	0	786	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	783	0	820	12	0
2	O	756	0	786	17	0
2	P	788	0	825	16	0
2	Q	756	0	786	16	0
2	R	756	0	786	14	0
2	S	756	0	786	20	0
2	T	756	0	786	10	0
2	U	773	0	810	26	0
2	V	756	0	786	12	0
2	W	756	0	786	16	0
2	X	756	0	786	14	0
2	Y	756	0	786	11	0
2	Z	815	0	849	16	0
3	A	27	0	12	2	0
3	B	27	0	12	2	0
3	C	27	0	12	2	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
3	I	27	0	12	1	0
3	J	27	0	12	0	0
3	K	27	0	12	1	0
3	L	27	0	12	1	0
3	M	27	0	12	0	0
3	N	27	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
All	All	65963	0	68774	1395	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1395) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLY:HA3	1:B:335:LYS:HB3	1.39	1.02
1:G:306:LEU:HA	1:G:307:THR:HB	1.52	0.91
1:G:206:ASN:ND2	1:G:213:CYS:SG	2.45	0.89
2:O:54:LYS:HA	2:O:60:ILE:HA	1.53	0.88
2:U:15:ARG:HG3	2:U:15:ARG:HH11	1.41	0.86
1:E:271:LEU:HD13	1:E:273:VAL:HG13	1.58	0.85
1:D:519:GLU:HG2	1:E:29:VAL:HG21	1.59	0.85
1:M:519:GLU:HG2	1:N:29:VAL:HG21	1.59	0.85
1:C:232:SER:HB2	1:C:310:LEU:HB2	1.59	0.83
1:G:304:GLU:HB2	1:G:305:GLY:HA3	1.61	0.82
1:K:232:SER:HB2	1:K:310:LEU:HB2	1.62	0.82
1:G:306:LEU:HG	1:G:307:THR:HG22	1.60	0.82
1:M:303:GLU:H	1:M:306:LEU:HD22	1.45	0.81
1:B:99:ILE:HG13	1:B:447:THR:HG21	1.64	0.79
1:B:213:CYS:HB3	1:B:326:VAL:HG22	1.64	0.79
1:G:232:SER:HB2	1:G:310:LEU:HB2	1.65	0.78
1:N:233:ILE:HG22	1:N:236:ALA:HB3	1.66	0.78
2:1:7:ARG:HB2	2:1:83:LEU:HD23	1.67	0.77
1:A:99:ILE:HG13	1:A:447:THR:HG21	1.65	0.77
1:K:23:LEU:HD21	1:K:57:ALA:HA	1.67	0.76
1:G:23:LEU:HD21	1:G:57:ALA:HA	1.67	0.76
1:B:321:VAL:HG13	1:B:322:GLY:H	1.49	0.76
1:E:23:LEU:HD21	1:E:57:ALA:HA	1.68	0.76
2:Y:56:LYS:NZ	2:Z:54:LYS:O	2.20	0.74
1:B:300:VAL:H	1:B:318:LEU:HD22	1.52	0.74
1:L:23:LEU:HD21	1:L:57:ALA:HA	1.69	0.74
1:I:290:LYS:HE2	1:I:346:ARG:HH22	1.52	0.73
2:R:33:LEU:HD12	2:R:34:PRO:HD2	1.70	0.73
1:C:255:ASP:HA	1:C:259:LEU:HD23	1.68	0.73
1:A:290:LYS:HE2	1:A:346:ARG:HH22	1.53	0.73
1:L:229:SER:HA	1:L:230:ILE:HB	1.71	0.73
1:H:99:ILE:HG13	1:H:447:THR:HG21	1.71	0.72
1:M:264:LEU:HG	1:M:268:LYS:HE3	1.71	0.72
1:M:190:ILE:HG22	1:M:373:LEU:HD21	1.69	0.72
1:L:215:PHE:HB2	1:L:324:VAL:HG13	1.72	0.72
1:D:215:PHE:HB2	1:D:324:VAL:HG13	1.71	0.72
1:M:23:LEU:HD21	1:M:57:ALA:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HD21	1:B:57:ALA:HA	1.71	0.72
2:S:83:LEU:HB2	2:S:84:ASP:HB2	1.70	0.71
1:C:23:LEU:HD21	1:C:57:ALA:HA	1.72	0.71
1:K:215:PHE:HB2	1:K:324:VAL:HG13	1.72	0.71
1:F:23:LEU:HD21	1:F:57:ALA:HA	1.73	0.71
1:D:520:VAL:HG13	1:E:38:VAL:HB	1.71	0.70
1:B:180:GLY:HA2	1:B:381:LYS:HG2	1.74	0.70
1:N:23:LEU:HD21	1:N:57:ALA:HA	1.72	0.70
2:U:17:LEU:HB3	2:U:48:ALA:HB3	1.74	0.70
1:M:303:GLU:HG2	1:M:305:GLY:H	1.57	0.69
1:I:23:LEU:HD21	1:I:57:ALA:HA	1.73	0.69
1:N:215:PHE:HB2	1:N:324:VAL:HG13	1.73	0.69
2:O:75:GLU:HG3	2:O:76:TYR:HD1	1.58	0.69
2:P:7:ARG:HB2	2:P:83:LEU:HD23	1.75	0.69
1:L:294:ILE:HG23	1:L:342:GLN:HG2	1.75	0.69
1:B:268:LYS:NZ	2:P:30:GLY:O	2.25	0.69
1:J:290:LYS:HE2	1:J:346:ARG:HH22	1.56	0.68
1:J:23:LEU:HD21	1:J:57:ALA:HA	1.74	0.68
2:Y:34:PRO:HG2	2:Y:37:SER:HB3	1.74	0.68
1:I:215:PHE:HB2	1:I:324:VAL:HG13	1.75	0.68
1:I:462:GLU:O	1:I:464:SER:N	2.26	0.68
1:J:229:SER:HB3	1:J:231:GLN:H	1.59	0.68
1:B:206:ASN:ND2	1:B:272:GLN:OE1	2.26	0.68
1:D:23:LEU:HD21	1:D:57:ALA:HA	1.74	0.68
1:H:203:TYR:OH	1:N:285:ARG:NH2	2.27	0.67
1:C:117:ARG:NH1	1:C:513:SER:OG	2.27	0.67
1:C:39:ILE:HG12	1:C:49:VAL:HG22	1.76	0.67
1:G:262:LEU:HD22	1:G:273:VAL:HG21	1.77	0.67
1:L:13:ARG:NH2	1:L:519:GLU:OE1	2.27	0.67
1:D:339:ASP:OD1	1:D:339:ASP:N	2.27	0.67
2:Q:75:GLU:HG3	2:Q:76:TYR:HD1	1.60	0.67
1:B:69:ILE:HG23	1:C:47:PRO:HG3	1.77	0.67
1:L:421:LEU:HD21	1:L:467:VAL:HG23	1.76	0.67
1:F:215:PHE:HB2	1:F:324:VAL:HG13	1.74	0.67
1:H:23:LEU:HD21	1:H:57:ALA:HA	1.76	0.67
1:N:326:VAL:HG21	1:N:331:ALA:HA	1.76	0.67
1:C:431:THR:O	1:C:431:THR:OG1	2.13	0.67
1:M:54:VAL:HG22	1:M:89:THR:HG21	1.77	0.67
1:E:13:ARG:NH2	1:E:519:GLU:OE1	2.28	0.66
1:K:431:THR:OG1	1:K:431:THR:O	2.13	0.66
1:L:229:SER:HB2	1:L:231:GLN:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:262:LEU:HD22	1:I:273:VAL:HG21	1.78	0.66
1:C:227:ILE:HG13	1:C:254:VAL:HG22	1.78	0.66
2:2:17:LEU:HB3	2:2:48:ALA:HB3	1.77	0.66
1:D:431:THR:O	1:D:431:THR:OG1	2.11	0.66
1:C:354:LEU:HD13	1:C:364:GLU:HG3	1.78	0.66
1:E:431:THR:OG1	1:E:431:THR:O	2.14	0.66
2:V:27:THR:HG22	2:V:33:LEU:HD11	1.77	0.65
2:1:94:GLY:O	2:2:15:ARG:NH2	2.29	0.65
2:X:34:PRO:HG2	2:X:37:SER:HB3	1.76	0.65
1:I:190:ILE:HG22	1:I:373:LEU:HD21	1.79	0.65
1:E:98:SER:HB3	1:E:447:THR:HG23	1.79	0.65
1:B:344:GLU:HA	1:B:347:ILE:HG12	1.79	0.65
1:E:294:ILE:HG23	1:E:342:GLN:HG2	1.79	0.65
1:J:221:LEU:HD21	1:J:310:LEU:HD21	1.79	0.65
1:M:13:ARG:NH2	1:M:519:GLU:OE1	2.29	0.65
1:D:13:ARG:NH2	1:D:519:GLU:OE1	2.29	0.65
1:M:268:LYS:NZ	2:1:32:MET:HB2	2.11	0.65
2:S:17:LEU:HB3	2:S:48:ALA:HB3	1.79	0.65
1:A:431:THR:O	1:A:431:THR:OG1	2.14	0.64
1:F:176:THR:HG21	1:F:369:ARG:HH21	1.61	0.64
1:M:431:THR:O	1:M:431:THR:OG1	2.13	0.64
1:L:117:ARG:NH1	1:L:513:SER:OG	2.30	0.64
1:G:117:ARG:NH1	1:G:513:SER:OG	2.31	0.64
1:F:304:GLU:H	1:F:305:GLY:HA3	1.62	0.64
1:G:234:VAL:HG21	2:U:28:LYS:HG2	1.79	0.64
1:M:192:GLY:O	1:M:373:LEU:HB3	1.97	0.64
2:Z:17:LEU:HB3	2:Z:48:ALA:HB3	1.80	0.64
1:E:358:THR:OG1	1:E:358:THR:O	2.13	0.64
2:W:28:LYS:N	2:W:29:GLY:HA3	2.13	0.64
2:Y:17:LEU:HB3	2:Y:48:ALA:HB3	1.79	0.64
1:B:291:ASP:OD1	1:B:346:ARG:NH1	2.31	0.64
1:J:262:LEU:HD22	1:J:273:VAL:HG21	1.80	0.64
2:Q:46:VAL:HG23	2:Q:71:VAL:HG11	1.80	0.64
1:B:268:LYS:HG2	1:B:269:VAL:HG12	1.80	0.63
1:D:251:ALA:O	1:D:278:ALA:N	2.30	0.63
1:A:23:LEU:HD21	1:A:57:ALA:HA	1.79	0.63
2:P:17:LEU:HB3	2:P:48:ALA:HB3	1.80	0.63
1:G:431:THR:OG1	1:G:431:THR:O	2.13	0.63
1:K:424:ILE:HA	1:K:427:LEU:HD23	1.80	0.63
2:X:17:LEU:HB3	2:X:48:ALA:HB3	1.79	0.63
2:V:17:LEU:HB3	2:V:48:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD21	1:B:289:LEU:HB2	1.81	0.63
1:B:117:ARG:NH1	1:B:513:SER:OG	2.32	0.63
1:D:69:ILE:HG23	1:E:47:PRO:HG3	1.80	0.63
2:T:17:LEU:HB3	2:T:48:ALA:HB3	1.80	0.63
1:A:23:LEU:HD13	1:A:74:VAL:HG13	1.81	0.63
1:J:95:LEU:HD11	1:J:451:PRO:HG3	1.81	0.62
1:M:232:SER:HB2	1:M:310:LEU:HB2	1.80	0.62
1:E:227:ILE:HB	1:E:254:VAL:HG22	1.81	0.62
1:G:301:PHE:HD1	1:G:308:LEU:HB3	1.63	0.62
1:H:251:ALA:O	1:H:278:ALA:N	2.33	0.62
1:K:306:LEU:HD21	1:L:202:PRO:HD2	1.81	0.62
2:1:17:LEU:HB3	2:1:48:ALA:HB3	1.81	0.62
1:C:98:SER:HB3	1:C:447:THR:HG23	1.81	0.62
1:A:221:LEU:HD21	1:A:310:LEU:HD21	1.80	0.62
2:W:38:GLN:HB2	2:W:39:GLY:HA2	1.82	0.62
1:B:246:PRO:HB3	1:B:272:GLN:HB2	1.80	0.62
1:A:47:PRO:HG3	1:G:69:ILE:HG23	1.80	0.62
1:H:431:THR:O	1:H:431:THR:OG1	2.13	0.62
1:M:39:ILE:HG12	1:M:49:VAL:HG22	1.82	0.62
1:B:234:VAL:HG23	2:P:31:ILE:HD11	1.80	0.61
1:B:194:LYS:H	1:B:373:LEU:HD13	1.65	0.61
1:J:431:THR:OG1	1:J:431:THR:O	2.14	0.61
2:Z:96:ILE:O	2:1:15:ARG:NH1	2.33	0.61
1:A:357:THR:O	1:A:359:SER:N	2.32	0.61
1:F:121:MET:HA	1:F:124:VAL:HG22	1.82	0.61
1:G:359:SER:O	1:G:361:TYR:N	2.33	0.61
1:K:192:GLY:O	1:K:373:LEU:HB3	1.99	0.61
2:R:17:LEU:HB3	2:R:48:ALA:HB3	1.82	0.61
1:G:230:ILE:HA	1:G:233:ILE:HG22	1.81	0.61
1:J:251:ALA:O	1:J:278:ALA:N	2.33	0.61
1:M:117:ARG:NH1	1:M:513:SER:OG	2.33	0.61
1:I:344:GLU:HA	1:I:347:ILE:HG12	1.83	0.61
1:M:98:SER:HB3	1:M:447:THR:HG23	1.83	0.61
1:C:251:ALA:O	1:C:278:ALA:N	2.34	0.61
1:E:262:LEU:HD22	1:E:273:VAL:HG21	1.82	0.61
1:K:39:ILE:HG12	1:K:49:VAL:HG22	1.81	0.61
1:D:219:TYR:CE1	1:D:247:LEU:HD13	2.35	0.61
1:M:69:ILE:HG23	1:N:47:PRO:HG3	1.83	0.61
1:A:262:LEU:HD22	1:A:273:VAL:HG21	1.82	0.61
1:E:220:VAL:HG13	1:E:319:GLY:HA3	1.82	0.61
1:H:327:THR:HG23	1:H:329:ASP:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:O	1:A:271:LEU:N	2.34	0.60
1:E:269:VAL:O	1:E:271:LEU:N	2.33	0.60
1:L:251:ALA:O	1:L:278:ALA:N	2.34	0.60
1:J:117:ARG:NH1	1:J:513:SER:OG	2.34	0.60
1:M:251:ALA:O	1:M:278:ALA:N	2.34	0.60
2:W:17:LEU:HB3	2:W:48:ALA:HB3	1.82	0.60
1:D:39:ILE:HG12	1:D:49:VAL:HG22	1.82	0.60
1:J:342:GLN:HA	1:J:345:LYS:HE2	1.83	0.60
1:M:354:LEU:HA	1:M:357:THR:HG22	1.83	0.60
1:N:233:ILE:HG23	1:N:311:GLU:HA	1.82	0.60
1:E:174:VAL:HG11	1:E:369:ARG:HG2	1.82	0.60
1:F:251:ALA:O	1:F:278:ALA:N	2.33	0.60
2:Z:46:VAL:HG23	2:Z:71:VAL:HG11	1.82	0.60
1:B:216:GLN:HG2	1:B:323:LYS:HG2	1.83	0.60
1:G:358:THR:OG1	1:G:358:THR:O	2.19	0.60
2:V:94:GLY:O	2:W:15:ARG:NH2	2.34	0.60
1:A:27:VAL:HG22	1:A:90:THR:HG23	1.83	0.60
1:E:306:LEU:HD22	1:F:263:VAL:HG21	1.83	0.60
1:I:69:ILE:HG23	1:J:47:PRO:HG3	1.84	0.60
2:1:26:VAL:HG12	2:1:32:MET:HG2	1.84	0.60
1:I:117:ARG:NH1	1:I:513:SER:OG	2.35	0.60
2:S:20:ARG:NH1	2:S:41:VAL:O	2.34	0.60
1:A:424:ILE:HA	1:A:427:LEU:HD23	1.84	0.60
1:C:13:ARG:NH2	1:C:519:GLU:OE1	2.33	0.60
1:H:210:GLY:O	1:H:211:GLN:HG2	2.02	0.60
1:M:264:LEU:O	1:M:268:LYS:HG3	2.02	0.60
1:B:262:LEU:HD22	1:B:273:VAL:HG21	1.83	0.59
1:I:251:ALA:O	1:I:278:ALA:N	2.35	0.59
1:M:322:GLY:HA3	1:M:335:LYS:HB2	1.84	0.59
1:F:164:ASP:HA	1:F:167:LYS:HE3	1.84	0.59
1:I:228:SER:HA	1:I:256:GLY:H	1.65	0.59
1:N:241:ASN:HD21	1:N:247:LEU:HB2	1.66	0.59
2:Q:17:LEU:HB3	2:Q:48:ALA:HB3	1.84	0.59
1:D:339:ASP:HB2	1:D:342:GLN:HB3	1.83	0.59
1:E:117:ARG:NH1	1:E:513:SER:OG	2.35	0.59
1:D:228:SER:O	1:D:230:ILE:HG13	2.02	0.59
1:K:421:LEU:HD21	1:K:467:VAL:HG13	1.84	0.59
1:N:117:ARG:NH1	1:N:513:SER:OG	2.35	0.59
1:I:192:GLY:O	1:I:373:LEU:HB3	2.02	0.59
1:K:98:SER:HB3	1:K:447:THR:HG23	1.85	0.59
1:M:283:ASP:HA	1:M:286:LYS:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:117:ARG:NH1	1:K:513:SER:OG	2.35	0.59
1:G:251:ALA:O	1:G:278:ALA:N	2.36	0.59
2:S:82:VAL:HG22	2:S:84:ASP:O	2.03	0.59
2:O:15:ARG:NH2	2:U:94:GLY:O	2.35	0.59
1:L:98:SER:HB3	1:L:447:THR:HG23	1.85	0.58
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.84	0.58
1:D:98:SER:HB3	1:D:447:THR:HG23	1.86	0.58
1:N:251:ALA:O	1:N:278:ALA:N	2.36	0.58
1:B:314:GLN:O	1:B:317:ASP:HB2	2.04	0.58
1:C:48:LYS:HE3	1:C:391:ASN:HB3	1.86	0.58
1:H:69:ILE:HG23	1:I:47:PRO:HG3	1.86	0.58
1:K:234:VAL:HG13	1:K:235:PRO:HD3	1.85	0.58
1:L:413:VAL:HB	1:L:498:THR:HG22	1.84	0.58
2:O:17:LEU:HB3	2:O:48:ALA:HB3	1.84	0.58
1:G:124:VAL:HA	1:G:127:VAL:HG12	1.85	0.58
1:C:306:LEU:HD23	1:D:263:VAL:HG21	1.86	0.58
1:B:266:ARG:HE	1:B:273:VAL:HG22	1.67	0.58
1:B:251:ALA:O	1:B:278:ALA:N	2.36	0.58
1:H:117:ARG:NH1	1:H:513:SER:OG	2.37	0.58
1:D:262:LEU:HD22	1:D:273:VAL:HG21	1.86	0.57
1:N:262:LEU:HD22	1:N:273:VAL:HG21	1.86	0.57
2:1:34:PRO:HG2	2:1:37:SER:HB2	1.86	0.57
1:F:278:ALA:HB1	1:F:289:LEU:HD11	1.86	0.57
1:J:39:ILE:HG12	1:J:49:VAL:HG22	1.86	0.57
2:W:34:PRO:HG2	2:W:37:SER:HB3	1.85	0.57
1:E:339:ASP:N	1:E:339:ASP:OD1	2.24	0.57
1:M:234:VAL:HG13	1:M:235:PRO:HD3	1.86	0.57
2:U:15:ARG:CG	2:U:15:ARG:HH11	2.16	0.57
1:A:117:ARG:NH1	1:A:513:SER:OG	2.37	0.57
1:A:271:LEU:HD22	1:A:272:GLN:H	1.69	0.57
1:A:383:GLY:O	1:A:390:VAL:HG22	2.04	0.57
1:I:284:ASN:ND2	1:I:363:LYS:HD2	2.19	0.57
1:A:347:ILE:HG21	1:A:372:LYS:HE2	1.86	0.57
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.87	0.57
1:K:262:LEU:HD22	1:K:273:VAL:HG21	1.87	0.57
1:N:431:THR:OG1	1:N:431:THR:O	2.13	0.57
1:D:117:ARG:NH1	1:D:513:SER:OG	2.38	0.57
1:K:251:ALA:O	1:K:278:ALA:N	2.36	0.57
1:N:233:ILE:HG21	1:N:310:LEU:O	2.04	0.57
1:M:124:VAL:HA	1:M:127:VAL:HG12	1.87	0.57
1:N:233:ILE:HG12	1:N:310:LEU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:HG13	1:C:505:LEU:HD22	1.87	0.57
1:G:120:VAL:O	1:G:124:VAL:HG23	2.04	0.57
1:J:383:GLY:O	1:J:390:VAL:HG22	2.04	0.57
1:K:113:PRO:HB2	1:K:517:THR:HA	1.87	0.57
1:M:27:VAL:HG22	1:M:90:THR:HG23	1.87	0.57
1:N:269:VAL:O	1:N:271:LEU:N	2.37	0.57
1:N:98:SER:HB3	1:N:447:THR:HG23	1.87	0.57
1:B:320:LYS:HA	1:B:321:VAL:HB	1.86	0.57
1:D:298:GLY:HA3	1:D:318:LEU:O	2.05	0.57
1:G:124:VAL:O	1:G:128:ILE:HG12	2.05	0.57
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.87	0.57
1:M:303:GLU:N	1:M:306:LEU:HD22	2.19	0.57
1:N:177:VAL:HG22	1:N:380:LEU:HD12	1.87	0.57
1:N:306:LEU:HA	1:N:307:THR:OG1	2.04	0.57
1:L:321:VAL:HA	1:L:336:GLY:HA2	1.87	0.56
1:L:25:ASP:OD1	1:L:97:ARG:NH1	2.37	0.56
1:B:39:ILE:HG12	1:B:49:VAL:HG22	1.86	0.56
1:G:13:ARG:NH2	1:G:519:GLU:OE1	2.37	0.56
1:J:327:THR:HG23	1:J:329:ASP:H	1.71	0.56
1:L:383:GLY:O	1:L:390:VAL:HG22	2.05	0.56
1:E:87:ASP:O	1:E:89:THR:N	2.35	0.56
1:G:306:LEU:HA	1:G:307:THR:CB	2.28	0.56
1:I:69:ILE:HD12	1:J:47:PRO:HB3	1.87	0.56
1:A:369:ARG:O	1:A:373:LEU:HG	2.05	0.56
1:B:218:ALA:O	1:B:321:VAL:HG11	2.05	0.56
1:C:230:ILE:HA	1:C:233:ILE:HG22	1.88	0.56
1:E:355:ASP:O	1:E:356:VAL:HG22	2.05	0.56
1:M:321:VAL:HA	1:M:336:GLY:HA2	1.88	0.56
1:C:280:GLY:HA2	1:C:285:ARG:HE	1.70	0.56
1:F:13:ARG:NH2	1:F:519:GLU:OE1	2.38	0.56
1:G:258:ALA:O	1:G:261:THR:OG1	2.22	0.56
1:I:98:SER:HB3	1:I:447:THR:HG23	1.88	0.56
1:J:98:SER:HB3	1:J:447:THR:HG23	1.88	0.56
1:M:113:PRO:HA	1:M:116:ILE:HD12	1.88	0.56
1:E:327:THR:HG23	1:E:329:ASP:H	1.71	0.56
1:G:95:LEU:HD11	1:G:451:PRO:HG3	1.86	0.56
1:I:177:VAL:HG22	1:I:380:LEU:HD12	1.88	0.56
1:L:229:SER:HA	1:L:230:ILE:CB	2.35	0.56
1:A:177:VAL:HG22	1:A:380:LEU:HD12	1.88	0.56
1:B:316:HIS:CG	1:B:316:HIS:O	2.58	0.56
1:F:158:ILE:HD11	1:F:393:LYS:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:GLY:O	1:L:319:GLY:HA2	2.05	0.56
1:N:383:GLY:O	1:N:390:VAL:HG22	2.05	0.56
1:C:120:VAL:O	1:C:124:VAL:HG23	2.06	0.56
1:J:124:VAL:HA	1:J:127:VAL:HG12	1.87	0.56
1:L:416:GLY:N	3:L:601:ADP:O2'	2.37	0.56
1:I:294:ILE:HG23	1:I:342:GLN:HG2	1.89	0.56
1:K:283:ASP:HA	1:K:286:LYS:HD3	1.88	0.56
1:H:298:GLY:HA3	1:H:318:LEU:O	2.05	0.55
1:J:263:VAL:HA	1:J:266:ARG:HB3	1.88	0.55
1:N:406:ALA:HB1	1:N:499:LYS:HB3	1.87	0.55
1:A:124:VAL:HG13	1:A:505:LEU:HD22	1.88	0.55
1:A:353:GLN:O	1:A:357:THR:OG1	2.24	0.55
1:G:301:PHE:CD1	1:G:308:LEU:HB3	2.41	0.55
1:G:327:THR:HG23	1:G:329:ASP:H	1.72	0.55
1:G:98:SER:HB3	1:G:447:THR:HG23	1.88	0.55
1:L:229:SER:HB2	1:L:231:GLN:H	1.71	0.55
1:M:262:LEU:HD22	1:M:273:VAL:HG21	1.87	0.55
1:H:47:PRO:HG3	1:N:69:ILE:HG23	1.87	0.55
1:A:120:VAL:O	1:A:124:VAL:HG23	2.07	0.55
1:E:251:ALA:O	1:E:278:ALA:N	2.39	0.55
1:L:39:ILE:HG12	1:L:49:VAL:HG12	1.88	0.55
1:N:304:GLU:HA	1:N:305:GLY:C	2.27	0.55
2:S:4:GLN:H	2:S:49:VAL:HG13	1.70	0.55
1:A:234:VAL:HG13	1:A:235:PRO:HD3	1.86	0.55
1:A:13:ARG:NH2	1:A:519:GLU:OE1	2.39	0.55
1:E:413:VAL:HB	1:E:498:THR:HG22	1.88	0.55
1:E:499:LYS:HG3	1:E:502:ARG:HH12	1.71	0.55
1:H:383:GLY:O	1:H:390:VAL:HG22	2.06	0.55
1:I:354:LEU:HD13	1:I:364:GLU:HG3	1.88	0.55
1:I:383:GLY:O	1:I:390:VAL:HG22	2.06	0.55
1:M:192:GLY:N	1:M:373:LEU:HD23	2.21	0.55
1:A:113:PRO:HB2	1:A:517:THR:HA	1.88	0.55
1:B:234:VAL:HG13	1:B:235:PRO:HD3	1.89	0.55
1:F:25:ASP:OD1	1:F:97:ARG:NH1	2.38	0.55
1:E:280:GLY:HA2	1:E:285:ARG:HG2	1.88	0.55
1:E:383:GLY:O	1:E:390:VAL:HG22	2.06	0.55
1:G:234:VAL:HG13	1:G:235:PRO:HD3	1.87	0.55
1:H:370:LEU:HA	1:H:373:LEU:HD12	1.89	0.55
1:L:234:VAL:HG13	1:L:235:PRO:HD3	1.89	0.55
1:B:262:LEU:O	1:B:265:ASN:ND2	2.39	0.55
1:F:219:TYR:OH	1:F:240:ALA:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:ILE:HG12	1:I:49:VAL:HG22	1.89	0.55
1:K:135:SER:OG	1:K:411:GLY:HA3	2.07	0.55
1:G:322:GLY:HA3	1:G:335:LYS:HB2	1.87	0.55
1:J:124:VAL:O	1:J:128:ILE:HG12	2.07	0.55
1:K:211:GLN:HA	1:K:211:GLN:HE21	1.71	0.55
2:U:15:ARG:NH1	2:U:15:ARG:HG3	2.17	0.55
1:C:113:PRO:HA	1:C:116:ILE:HD12	1.88	0.55
1:F:370:LEU:HA	1:F:373:LEU:HD12	1.89	0.55
1:G:39:ILE:HG12	1:G:49:VAL:HG22	1.88	0.55
1:K:298:GLY:HA3	1:K:318:LEU:O	2.07	0.55
1:K:525:ILE:HG13	1:K:526:PRO:HD2	1.89	0.55
2:W:7:ARG:HB3	2:W:83:LEU:HD23	1.87	0.55
2:1:7:ARG:NH1	2:1:88:TYR:OH	2.40	0.55
1:B:255:ASP:OD1	1:B:256:GLY:N	2.40	0.55
1:J:213:CYS:HB3	1:J:326:VAL:HG13	1.88	0.55
1:J:345:LYS:O	1:J:349:GLU:HG3	2.06	0.55
1:M:120:VAL:O	1:M:124:VAL:HG23	2.07	0.55
1:H:27:VAL:HG22	1:H:56:VAL:HG23	1.88	0.54
1:K:413:VAL:HB	1:K:498:THR:HG22	1.89	0.54
1:B:222:LEU:O	1:B:301:PHE:HB2	2.07	0.54
1:F:321:VAL:HA	1:F:336:GLY:HA2	1.89	0.54
1:F:383:GLY:O	1:F:390:VAL:HG22	2.07	0.54
1:F:98:SER:HB3	1:F:447:THR:HG23	1.89	0.54
1:D:383:GLY:O	1:D:390:VAL:HG22	2.07	0.54
1:E:25:ASP:OD1	1:E:97:ARG:NH1	2.37	0.54
1:H:25:ASP:OD1	1:H:97:ARG:NH1	2.39	0.54
1:J:120:VAL:O	1:J:124:VAL:HG23	2.06	0.54
1:L:113:PRO:HA	1:L:116:ILE:HD12	1.90	0.54
1:M:124:VAL:O	1:M:128:ILE:HG12	2.07	0.54
1:M:366:LEU:HD23	1:M:369:ARG:NH2	2.23	0.54
2:S:20:ARG:HB2	2:S:41:VAL:HG13	1.90	0.54
1:B:215:PHE:CZ	1:B:272:GLN:HB3	2.42	0.54
1:I:525:ILE:HG13	1:I:526:PRO:HD2	1.89	0.54
1:K:120:VAL:O	1:K:124:VAL:HG23	2.08	0.54
1:B:202:PRO:O	1:B:205:ILE:HG13	2.08	0.54
1:C:25:ASP:OD1	1:C:97:ARG:NH1	2.38	0.54
1:H:356:VAL:HG12	1:H:357:THR:HG23	1.90	0.54
1:H:39:ILE:HG12	1:H:49:VAL:HG22	1.89	0.54
1:J:113:PRO:HA	1:J:116:ILE:HD12	1.90	0.54
1:L:373:LEU:HB3	1:L:374:SER:C	2.27	0.54
2:T:97:LEU:HA	2:U:15:ARG:HE	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:369:ARG:O	1:L:372:LYS:HG3	2.08	0.54
1:L:488:ASN:HB3	1:L:491:GLU:HB3	1.89	0.54
1:E:39:ILE:HG12	1:E:49:VAL:HG22	1.89	0.54
1:H:113:PRO:HA	1:H:116:ILE:HD12	1.88	0.54
1:H:262:LEU:HD22	1:H:273:VAL:HG21	1.89	0.54
1:K:453:MET:HG3	1:K:467:VAL:HG21	1.89	0.54
1:M:268:LYS:HZ3	2:1:32:MET:HB2	1.72	0.54
1:I:113:PRO:HB2	1:I:517:THR:HA	1.90	0.54
1:J:91:THR:O	1:J:95:LEU:HD13	2.07	0.54
1:N:120:VAL:O	1:N:124:VAL:HG23	2.08	0.54
2:X:27:THR:HG23	2:X:31:ILE:O	2.07	0.54
1:G:124:VAL:HG13	1:G:505:LEU:HD22	1.89	0.54
1:G:383:GLY:O	1:G:390:VAL:HG22	2.08	0.54
1:K:416:GLY:N	3:K:601:ADP:O2'	2.36	0.54
1:K:25:ASP:OD1	1:K:97:ARG:NH1	2.38	0.53
1:K:383:GLY:O	1:K:390:VAL:HG22	2.07	0.53
1:B:113:PRO:HA	1:B:116:ILE:HD12	1.90	0.53
1:B:383:GLY:O	1:B:390:VAL:HG22	2.09	0.53
1:F:366:LEU:HA	1:F:369:ARG:HH11	1.73	0.53
1:I:120:VAL:O	1:I:124:VAL:HG23	2.08	0.53
1:A:248:VAL:HG21	1:A:324:VAL:HG21	1.89	0.53
1:B:320:LYS:HB2	1:B:321:VAL:HG12	1.89	0.53
1:C:413:VAL:HB	1:C:498:THR:HG22	1.90	0.53
1:H:176:THR:HG21	1:H:369:ARG:HH21	1.72	0.53
1:I:431:THR:O	1:I:431:THR:OG1	2.13	0.53
2:Z:7:ARG:NH1	2:Z:84:ASP:OD2	2.41	0.53
1:B:120:VAL:O	1:B:124:VAL:HG23	2.08	0.53
1:B:321:VAL:HG13	1:B:322:GLY:N	2.22	0.53
1:D:120:VAL:O	1:D:124:VAL:HG23	2.09	0.53
1:E:120:VAL:O	1:E:124:VAL:HG23	2.09	0.53
1:F:283:ASP:HA	1:F:286:LYS:HD3	1.89	0.53
1:N:326:VAL:HG21	1:N:331:ALA:CA	2.38	0.53
1:N:39:ILE:HG12	1:N:49:VAL:HG22	1.89	0.53
1:M:307:THR:H	1:N:269:VAL:HG11	1.74	0.53
2:S:13:PHE:HD1	2:S:13:PHE:H	1.55	0.53
1:B:301:PHE:CE2	1:B:318:LEU:HD21	2.43	0.53
1:E:243:HIS:O	1:E:245:LYS:HG2	2.09	0.53
1:F:39:ILE:HG12	1:F:49:VAL:HG22	1.90	0.53
1:L:464:SER:HA	1:L:467:VAL:HG12	1.89	0.53
1:A:288:GLN:O	1:A:292:MET:HG3	2.09	0.53
1:A:357:THR:HG22	1:A:359:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:GLY:N	3:D:601:ADP:O2'	2.36	0.53
1:G:386:SER:O	1:G:390:VAL:HG23	2.08	0.53
1:H:13:ARG:NH2	1:H:519:GLU:OE1	2.40	0.53
1:D:219:TYR:OH	1:D:236:ALA:O	2.27	0.53
1:D:286:LYS:O	1:D:289:LEU:HD22	2.08	0.53
1:F:305:GLY:O	1:F:306:LEU:HB3	2.09	0.53
1:L:394:LYS:HA	1:L:397:VAL:HG22	1.90	0.53
1:D:413:VAL:HB	1:D:498:THR:HG22	1.91	0.53
1:E:23:LEU:HD12	1:E:71:ALA:HB1	1.91	0.53
1:G:113:PRO:HA	1:G:116:ILE:HD12	1.91	0.53
1:B:113:PRO:HB2	1:B:517:THR:HA	1.89	0.53
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.91	0.53
1:L:284:ASN:ND2	1:L:363:LYS:HD3	2.24	0.53
1:L:431:THR:OG1	1:L:431:THR:O	2.13	0.53
1:A:192:GLY:N	1:A:373:LEU:HB3	2.25	0.52
1:B:227:ILE:HD12	1:B:249:ILE:HD11	1.91	0.52
1:C:339:ASP:HB3	1:C:342:GLN:HB3	1.90	0.52
1:F:357:THR:O	1:F:359:SER:N	2.42	0.52
1:G:25:ASP:OD1	1:G:97:ARG:NH1	2.37	0.52
1:N:322:GLY:HA3	1:N:335:LYS:HB2	1.91	0.52
2:2:41:VAL:HG12	2:2:75:GLU:HG2	1.92	0.52
1:C:113:PRO:HB2	1:C:517:THR:HA	1.90	0.52
1:D:309:ASN:OD1	1:D:311:GLU:N	2.42	0.52
1:I:329:ASP:N	1:I:329:ASP:OD1	2.42	0.52
1:N:25:ASP:OD1	1:N:97:ARG:NH1	2.39	0.52
1:D:23:LEU:HD12	1:D:71:ALA:HB1	1.91	0.52
1:E:263:VAL:HA	1:E:266:ARG:HB3	1.92	0.52
1:G:363:LYS:HA	1:G:366:LEU:HB2	1.91	0.52
1:H:120:VAL:O	1:H:124:VAL:HG23	2.09	0.52
1:J:288:GLN:O	1:J:292:MET:HG3	2.10	0.52
1:K:356:VAL:HG23	1:K:357:THR:H	1.74	0.52
1:N:113:PRO:HA	1:N:116:ILE:HD12	1.91	0.52
2:T:15:ARG:HB3	2:T:90:LEU:HD11	1.91	0.52
1:D:27:VAL:HG22	1:D:56:VAL:HG23	1.91	0.52
1:N:234:VAL:H	1:N:235:PRO:CD	2.22	0.52
1:D:288:GLN:O	1:D:292:MET:HG3	2.10	0.52
1:J:111:ALA:O	1:K:36:ARG:NH2	2.43	0.52
1:I:347:ILE:HA	1:I:350:ILE:HG22	1.92	0.52
1:G:113:PRO:HB2	1:G:517:THR:HA	1.91	0.52
1:I:234:VAL:HG13	1:I:235:PRO:HD3	1.92	0.52
1:A:113:PRO:HA	1:A:116:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:PRO:HB2	1:E:517:THR:HA	1.90	0.52
1:F:304:GLU:N	1:F:305:GLY:HA3	2.25	0.52
1:H:174:VAL:HG23	1:H:372:LYS:HG2	1.92	0.52
1:I:282:GLY:H	1:I:285:ARG:HH21	1.58	0.52
1:L:113:PRO:HB2	1:L:517:THR:HA	1.91	0.52
1:N:158:ILE:HD11	1:N:393:LYS:HE2	1.91	0.52
2:O:94:GLY:O	2:P:15:ARG:NH2	2.42	0.52
1:N:265:ASN:OD1	2:2:32:MET:HB2	2.09	0.52
1:A:258:ALA:O	1:A:261:THR:OG1	2.25	0.52
1:A:327:THR:OG1	1:A:330:ASP:OD1	2.26	0.52
1:E:298:GLY:HA3	1:E:318:LEU:O	2.10	0.52
1:F:23:LEU:HD12	1:F:71:ALA:HB1	1.92	0.52
2:O:27:THR:HG22	2:O:33:LEU:HD11	1.92	0.52
2:O:8:LYS:HA	2:U:101:VAL:HG22	1.92	0.52
1:B:369:ARG:O	1:B:373:LEU:HG	2.11	0.51
1:D:158:ILE:HD11	1:D:393:LYS:HE2	1.92	0.51
1:E:265:ASN:OD1	2:S:32:MET:N	2.31	0.51
1:E:347:ILE:HA	1:E:350:ILE:HG22	1.93	0.51
1:E:357:THR:O	1:E:359:SER:N	2.42	0.51
1:F:255:ASP:OD1	1:F:256:GLY:N	2.43	0.51
1:H:278:ALA:HB1	1:H:289:LEU:HD11	1.92	0.51
1:I:235:PRO:HA	1:I:238:GLU:HG2	1.92	0.51
1:J:386:SER:O	1:J:390:VAL:HG23	2.10	0.51
1:K:219:TYR:CZ	1:K:245:LYS:HB2	2.45	0.51
2:U:37:SER:HA	2:U:40:LYS:HG3	1.92	0.51
2:W:94:GLY:O	2:X:15:ARG:NH2	2.43	0.51
1:B:218:ALA:O	1:B:321:VAL:HG21	2.10	0.51
1:B:355:ASP:OD1	1:B:356:VAL:N	2.42	0.51
1:F:231:GLN:HA	1:F:233:ILE:HG22	1.92	0.51
1:G:91:THR:O	1:G:95:LEU:HD13	2.09	0.51
1:J:133:LYS:N	1:J:133:LYS:HD3	2.26	0.51
1:L:158:ILE:HD11	1:L:393:LYS:HE2	1.92	0.51
1:N:326:VAL:HG22	1:N:327:THR:H	1.74	0.51
1:A:192:GLY:O	1:A:373:LEU:HB2	2.10	0.51
1:D:369:ARG:O	1:D:373:LEU:HG	2.10	0.51
1:F:234:VAL:HG13	1:F:235:PRO:HD3	1.93	0.51
1:J:322:GLY:HA3	1:J:335:LYS:HB2	1.92	0.51
1:N:363:LYS:HA	1:N:366:LEU:HB2	1.93	0.51
1:A:255:ASP:OD1	1:A:256:GLY:N	2.43	0.51
1:B:23:LEU:HD12	1:B:71:ALA:HB1	1.92	0.51
1:D:113:PRO:HB2	1:D:517:THR:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:PRO:HA	1:D:116:ILE:HD12	1.91	0.51
1:G:10:ALA:HA	1:G:13:ARG:HB2	1.91	0.51
1:G:225:LYS:HE2	1:G:302:GLY:HA3	1.92	0.51
1:M:383:GLY:O	1:M:390:VAL:HG22	2.10	0.51
2:S:25:THR:O	2:S:26:VAL:HG22	2.11	0.51
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.93	0.51
1:B:386:SER:O	1:B:390:VAL:HG23	2.11	0.51
1:C:294:ILE:HG22	1:C:343:ILE:HG22	1.91	0.51
1:G:255:ASP:O	1:G:259:LEU:HB3	2.10	0.51
1:G:158:ILE:HD11	1:G:393:LYS:HE2	1.93	0.51
1:J:229:SER:OG	1:J:258:ALA:HB2	2.10	0.51
1:J:25:ASP:OD1	1:J:97:ARG:NH1	2.37	0.51
1:K:370:LEU:HA	1:K:373:LEU:HD12	1.92	0.51
1:N:202:PRO:O	1:N:205:ILE:HG13	2.11	0.51
2:1:15:ARG:HB3	2:1:90:LEU:HD11	1.93	0.51
1:B:525:ILE:HG13	1:B:526:PRO:HD2	1.91	0.51
1:D:347:ILE:O	1:D:351:ILE:HG12	2.10	0.51
1:F:302:GLY:O	1:F:303:GLU:HG2	2.11	0.51
1:H:269:VAL:O	1:H:271:LEU:N	2.43	0.51
1:M:525:ILE:HG13	1:M:526:PRO:HD2	1.91	0.51
2:Y:15:ARG:HB3	2:Y:90:LEU:HD11	1.93	0.51
1:B:316:HIS:O	1:B:316:HIS:ND1	2.44	0.51
1:B:418:CYS:O	1:B:422:ARG:HG2	2.11	0.51
1:A:339:ASP:HB3	1:A:342:GLN:HB3	1.93	0.51
1:K:413:VAL:HG22	1:K:414:LEU:H	1.76	0.51
1:M:280:GLY:HA2	1:M:285:ARG:HE	1.76	0.51
1:N:386:SER:O	1:N:390:VAL:HG23	2.11	0.51
2:Y:14:ASP:HB2	2:Y:92:ARG:HH11	1.75	0.51
2:1:63:VAL:HG12	2:1:65:VAL:H	1.76	0.51
1:E:113:PRO:HA	1:E:116:ILE:HD12	1.92	0.51
1:G:304:GLU:CB	1:G:305:GLY:HA3	2.37	0.51
1:G:413:VAL:HB	1:G:498:THR:HG22	1.91	0.51
1:K:386:SER:O	1:K:390:VAL:HG23	2.10	0.51
1:N:113:PRO:HB2	1:N:517:THR:HA	1.93	0.51
2:X:15:ARG:HB3	2:X:90:LEU:HD11	1.93	0.51
1:F:340:LYS:O	1:F:344:GLU:HG3	2.11	0.51
1:L:255:ASP:OD1	1:L:256:GLY:N	2.44	0.51
1:M:406:ALA:HB1	1:M:499:LYS:HB3	1.93	0.51
2:P:15:ARG:HB3	2:P:90:LEU:HD11	1.91	0.51
1:A:227:ILE:HB	1:A:254:VAL:HG22	1.92	0.50
1:B:231:GLN:HA	1:B:234:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ILE:HD11	1:F:494:ILE:HD13	1.93	0.50
1:G:406:ALA:HB1	1:G:499:LYS:HB3	1.93	0.50
1:H:461:VAL:HG12	1:H:462:GLU:H	1.75	0.50
1:J:461:VAL:HG12	1:J:462:GLU:H	1.76	0.50
1:L:386:SER:O	1:L:390:VAL:HG23	2.11	0.50
1:B:304:GLU:OE2	1:B:307:THR:HB	2.12	0.50
1:G:263:VAL:HA	1:G:266:ARG:HB3	1.93	0.50
1:G:298:GLY:HA3	1:G:318:LEU:O	2.11	0.50
1:N:278:ALA:HB1	1:N:289:LEU:HD11	1.93	0.50
1:A:294:ILE:HG23	1:A:342:GLN:NE2	2.26	0.50
1:A:394:LYS:HA	1:A:397:VAL:HG22	1.92	0.50
1:D:461:VAL:HG12	1:D:462:GLU:H	1.76	0.50
1:F:262:LEU:HD22	1:F:273:VAL:HG21	1.93	0.50
1:G:278:ALA:HB1	1:G:289:LEU:HD11	1.93	0.50
1:N:455:ILE:HD11	3:N:601:ADP:H4'	1.93	0.50
1:E:464:SER:HB2	1:K:464:SER:HB2	1.93	0.50
2:O:37:SER:OG	2:O:38:GLN:N	2.41	0.50
1:A:183:LEU:HD13	1:G:506:LEU:HD21	1.92	0.50
1:A:413:VAL:HB	1:A:498:THR:HG22	1.93	0.50
1:B:287:ASN:O	1:B:290:LYS:HG2	2.11	0.50
1:C:124:VAL:O	1:C:128:ILE:HG12	2.11	0.50
1:D:234:VAL:HG13	1:D:235:PRO:HD3	1.93	0.50
1:H:23:LEU:HD12	1:H:71:ALA:HB1	1.92	0.50
1:J:23:LEU:HD12	1:J:71:ALA:HB1	1.93	0.50
1:J:278:ALA:HB1	1:J:289:LEU:HD11	1.94	0.50
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.94	0.50
2:W:15:ARG:HB3	2:W:90:LEU:HD11	1.94	0.50
1:A:466:ILE:O	1:A:470:ILE:HG22	2.11	0.50
1:D:234:VAL:HG23	2:R:31:ILE:HG21	1.93	0.50
1:H:315:PRO:HA	1:H:318:LEU:HD13	1.93	0.50
1:K:476:GLU:O	1:K:488:ASN:ND2	2.45	0.50
2:O:18:VAL:HG12	2:O:46:VAL:HA	1.94	0.50
2:U:24:GLU:O	2:U:24:GLU:HG2	2.10	0.50
2:Z:7:ARG:HD3	2:Z:84:ASP:OD2	2.12	0.50
2:1:7:ARG:HD3	2:1:84:ASP:OD2	2.11	0.50
1:B:416:GLY:N	3:B:601:ADP:O2'	2.44	0.50
1:C:230:ILE:HD11	1:C:257:GLU:HB3	1.93	0.50
1:F:113:PRO:HA	1:F:116:ILE:HD12	1.93	0.50
1:C:421:LEU:HD21	1:C:467:VAL:HG13	1.93	0.50
1:D:255:ASP:OD1	1:D:256:GLY:N	2.45	0.50
1:D:327:THR:HG23	1:D:329:ASP:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:366:LEU:HA	1:H:369:ARG:HH11	1.76	0.50
1:H:386:SER:O	1:H:390:VAL:HG23	2.12	0.50
1:I:158:ILE:HD11	1:I:393:LYS:HE2	1.94	0.50
1:J:321:VAL:HA	1:J:336:GLY:HA2	1.92	0.50
1:B:258:ALA:O	1:B:261:THR:OG1	2.28	0.50
1:C:418:CYS:O	1:C:422:ARG:HG2	2.12	0.50
1:F:386:SER:O	1:F:390:VAL:HG23	2.12	0.50
1:A:280:GLY:HA2	1:A:285:ARG:HD3	1.92	0.49
1:D:386:SER:O	1:D:390:VAL:HG23	2.12	0.49
1:L:280:GLY:HA2	1:L:285:ARG:HE	1.77	0.49
1:F:116:ILE:HG13	1:F:436:ASP:HB3	1.94	0.49
1:H:239:ILE:HD11	1:H:315:PRO:CD	2.42	0.49
1:H:418:CYS:O	1:H:422:ARG:HG2	2.12	0.49
1:J:174:VAL:HG23	1:J:372:LYS:HG2	1.94	0.49
1:K:353:GLN:O	1:K:356:VAL:HG22	2.11	0.49
1:N:418:CYS:O	1:N:422:ARG:HG2	2.12	0.49
2:Q:46:VAL:HG12	2:Q:67:VAL:HA	1.93	0.49
2:Z:56:LYS:HB2	2:Z:61:GLN:OE1	2.12	0.49
2:Z:15:ARG:HB3	2:Z:90:LEU:HD11	1.95	0.49
1:E:228:SER:HA	1:E:256:GLY:H	1.78	0.49
1:E:406:ALA:HB1	1:E:499:LYS:HB3	1.94	0.49
1:H:322:GLY:HA3	1:H:335:LYS:HB2	1.94	0.49
1:I:386:SER:O	1:I:390:VAL:HG23	2.12	0.49
1:J:370:LEU:HA	1:J:373:LEU:HD12	1.94	0.49
1:C:258:ALA:O	1:C:262:LEU:HD13	2.12	0.49
1:D:191:GLU:N	1:D:191:GLU:OE1	2.46	0.49
1:I:25:ASP:OD1	1:I:97:ARG:NH1	2.42	0.49
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.94	0.49
1:M:386:SER:O	1:M:390:VAL:HG23	2.12	0.49
2:R:7:ARG:HB2	2:R:83:LEU:HD23	1.92	0.49
2:W:70:LYS:HG3	2:W:100:TYR:HD2	1.76	0.49
1:D:202:PRO:O	1:D:205:ILE:HG13	2.11	0.49
1:D:285:ARG:O	1:D:289:LEU:HD13	2.13	0.49
1:L:202:PRO:O	1:L:205:ILE:HG13	2.13	0.49
1:N:327:THR:OG1	1:N:328:LYS:N	2.43	0.49
1:A:418:CYS:O	1:A:422:ARG:HG2	2.13	0.49
1:B:368:GLU:O	1:B:372:LYS:HB2	2.13	0.49
1:C:203:TYR:CD1	1:C:267:LEU:HD11	2.47	0.49
1:G:203:TYR:CD1	1:G:267:LEU:HD11	2.47	0.49
1:H:113:PRO:HB2	1:H:517:THR:HA	1.95	0.49
1:N:326:VAL:HG13	1:N:327:THR:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:461:VAL:HG12	1:N:462:GLU:H	1.76	0.49
2:1:101:VAL:HG22	2:2:8:LYS:HA	1.94	0.49
1:B:406:ALA:HB1	1:B:499:LYS:HB3	1.93	0.49
1:G:375:ASP:HB2	1:G:376:GLY:HA2	1.94	0.49
1:K:113:PRO:HA	1:K:116:ILE:HD12	1.95	0.49
2:U:70:LYS:HB3	2:U:100:TYR:HD2	1.78	0.49
1:B:194:LYS:CE	1:B:330:ASP:HB3	2.43	0.49
1:E:287:ASN:O	1:E:290:LYS:HG2	2.13	0.49
1:F:219:TYR:CZ	1:F:245:LYS:HB2	2.47	0.49
1:H:102:GLU:O	1:H:106:LYS:HD3	2.13	0.49
1:N:436:ASP:HA	1:N:439:ILE:HD12	1.95	0.49
2:U:28:LYS:O	2:U:30:GLY:N	2.45	0.49
1:A:192:GLY:H	1:A:373:LEU:HB3	1.77	0.49
1:A:386:SER:O	1:A:390:VAL:HG23	2.12	0.49
1:A:39:ILE:HG12	1:A:49:VAL:HG22	1.95	0.49
1:B:266:ARG:HE	1:B:273:VAL:CG2	2.26	0.49
1:F:202:PRO:O	1:F:205:ILE:HG13	2.13	0.49
1:F:219:TYR:CE1	1:F:245:LYS:HB2	2.48	0.49
1:K:202:PRO:O	1:K:205:ILE:HG13	2.12	0.49
1:M:298:GLY:HA3	1:M:318:LEU:O	2.13	0.49
1:J:294:ILE:HG22	1:J:343:ILE:HD13	1.95	0.49
1:M:413:VAL:HB	1:M:498:THR:HG22	1.94	0.49
2:S:21:SER:HA	2:S:22:ALA:HA	1.64	0.49
2:2:6:PHE:O	2:2:8:LYS:N	2.46	0.48
1:C:369:ARG:O	1:C:373:LEU:HG	2.12	0.48
1:F:347:ILE:HA	1:F:350:ILE:HG22	1.95	0.48
1:I:113:PRO:HA	1:I:116:ILE:HD12	1.94	0.48
1:M:278:ALA:HB1	1:M:289:LEU:HD11	1.95	0.48
2:O:7:ARG:HB3	2:O:83:LEU:HD23	1.94	0.48
1:B:240:ALA:HB2	1:B:247:LEU:HD23	1.95	0.48
1:C:322:GLY:HA3	1:C:335:LYS:HB2	1.96	0.48
1:F:113:PRO:HB2	1:F:517:THR:HA	1.94	0.48
1:F:176:THR:HG21	1:F:369:ARG:NH2	2.26	0.48
1:K:69:ILE:HG23	1:L:47:PRO:HG3	1.95	0.48
2:P:35:GLU:HG2	2:P:35:GLU:O	2.13	0.48
1:B:248:VAL:HG11	1:B:324:VAL:HG11	1.95	0.48
1:L:239:ILE:HD11	1:L:315:PRO:CD	2.43	0.48
1:N:264:LEU:HD22	2:2:35:GLU:HA	1.95	0.48
2:V:18:VAL:HG12	2:V:46:VAL:HA	1.94	0.48
1:C:69:ILE:HG23	1:D:47:PRO:HG3	1.94	0.48
1:F:269:VAL:O	1:F:271:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:418:CYS:O	1:I:422:ARG:HG2	2.13	0.48
1:M:233:ILE:HD12	1:M:258:ALA:HB1	1.95	0.48
1:N:23:LEU:HD12	1:N:71:ALA:HB1	1.94	0.48
2:U:41:VAL:HG21	2:U:72:LEU:HD13	1.96	0.48
1:A:27:VAL:HG23	1:A:53:GLY:HA2	1.95	0.48
1:B:283:ASP:O	1:B:286:LYS:HG2	2.13	0.48
1:C:373:LEU:HD21	1:C:377:VAL:HG22	1.95	0.48
1:D:200:ILE:HG21	1:D:259:LEU:HD11	1.94	0.48
1:E:418:CYS:O	1:E:422:ARG:HG2	2.14	0.48
1:G:280:GLY:HA2	1:G:285:ARG:HE	1.79	0.48
1:L:69:ILE:HG23	1:M:47:PRO:HG3	1.95	0.48
1:C:259:LEU:HD12	1:C:260:SER:N	2.28	0.48
1:E:221:LEU:HD12	1:E:247:LEU:HD21	1.96	0.48
1:K:230:ILE:HA	1:K:233:ILE:HG22	1.95	0.48
1:L:23:LEU:HD12	1:L:71:ALA:HB1	1.95	0.48
1:M:288:GLN:O	1:M:292:MET:HG3	2.13	0.48
2:R:15:ARG:HB3	2:R:90:LEU:HD11	1.96	0.48
1:A:298:GLY:HA3	1:A:318:LEU:O	2.13	0.48
1:C:191:GLU:OE1	1:C:191:GLU:N	2.46	0.48
1:D:214:GLU:HG3	1:D:325:ILE:HG12	1.96	0.48
1:E:281:PHE:HD1	1:E:285:ARG:HH21	1.60	0.48
1:F:69:ILE:HG23	1:G:47:PRO:HG3	1.96	0.48
1:I:278:ALA:HB1	1:I:289:LEU:HD11	1.96	0.48
1:J:406:ALA:HB1	1:J:499:LYS:HB3	1.96	0.48
1:J:136:LYS:NZ	1:J:490:VAL:HG21	2.29	0.48
1:L:229:SER:OG	1:L:258:ALA:HB2	2.13	0.48
1:L:373:LEU:HA	1:L:374:SER:HB2	1.94	0.48
1:M:23:LEU:HD12	1:M:71:ALA:HB1	1.95	0.48
2:Q:98:GLY:HA3	2:R:9:PHE:CE1	2.49	0.48
1:A:290:LYS:HE3	1:A:346:ARG:HH12	1.78	0.48
1:A:464:SER:HB2	1:H:464:SER:HB2	1.95	0.48
1:C:74:VAL:HA	1:C:77:VAL:HG13	1.96	0.48
1:J:113:PRO:HB2	1:J:517:THR:HA	1.96	0.48
1:L:406:ALA:HB1	1:L:499:LYS:HB3	1.96	0.48
1:N:230:ILE:HG23	1:N:257:GLU:OE1	2.13	0.48
2:2:15:ARG:HB3	2:2:90:LEU:HD11	1.96	0.48
1:C:102:GLU:O	1:C:106:LYS:HD3	2.14	0.48
1:D:413:VAL:HG22	1:D:414:LEU:H	1.78	0.48
1:F:298:GLY:HA3	1:F:318:LEU:O	2.14	0.48
1:G:415:GLY:HA3	1:G:494:ILE:HG22	1.96	0.48
1:J:13:ARG:NH2	1:J:519:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:278:ALA:HB1	1:L:289:LEU:HD11	1.96	0.48
1:N:346:ARG:O	1:N:350:ILE:HD12	2.14	0.48
2:Z:34:PRO:O	2:Z:36:LYS:N	2.45	0.48
1:C:370:LEU:HA	1:C:373:LEU:HD12	1.96	0.48
1:E:342:GLN:HA	1:E:345:LYS:HE2	1.95	0.48
1:J:234:VAL:HG13	1:J:235:PRO:HD3	1.95	0.48
1:K:263:VAL:HA	1:K:266:ARG:HB3	1.96	0.48
1:L:322:GLY:HA3	1:L:335:LYS:HB2	1.96	0.48
1:D:464:SER:HB2	1:L:464:SER:HB2	1.95	0.48
1:F:370:LEU:O	1:F:373:LEU:HB2	2.13	0.47
1:I:23:LEU:HD12	1:I:71:ALA:HB1	1.95	0.47
1:B:25:ASP:OD1	1:B:97:ARG:NH1	2.39	0.47
1:D:353:GLN:O	1:D:357:THR:OG1	2.31	0.47
1:I:91:THR:O	1:I:95:LEU:HD22	2.14	0.47
1:J:354:LEU:HA	1:J:357:THR:HG22	1.95	0.47
1:N:233:ILE:HG12	1:N:310:LEU:CB	2.45	0.47
1:N:190:ILE:HG13	1:N:377:VAL:HG22	1.95	0.47
2:Q:15:ARG:HB3	2:Q:90:LEU:HD11	1.96	0.47
1:B:293:ALA:CB	1:B:299:ALA:HB3	2.43	0.47
1:G:413:VAL:HG22	1:G:414:LEU:H	1.79	0.47
1:H:321:VAL:HA	1:H:336:GLY:HA2	1.96	0.47
1:F:464:SER:HB2	1:J:464:SER:HB2	1.95	0.47
1:M:158:ILE:HD11	1:M:393:LYS:HE2	1.96	0.47
1:M:263:VAL:HA	1:M:266:ARG:HB3	1.96	0.47
2:P:7:ARG:CB	2:P:83:LEU:HD23	2.41	0.47
2:T:70:LYS:HB2	2:T:100:TYR:HD2	1.78	0.47
2:W:100:TYR:CE1	2:X:9:PHE:HD1	2.32	0.47
1:F:413:VAL:HG22	1:F:414:LEU:H	1.79	0.47
1:J:290:LYS:HE3	1:J:346:ARG:HH12	1.79	0.47
1:L:124:VAL:O	1:L:128:ILE:HG12	2.14	0.47
1:N:288:GLN:O	1:N:292:MET:HG3	2.14	0.47
1:N:340:LYS:O	1:N:344:GLU:HG3	2.15	0.47
2:S:13:PHE:N	2:S:13:PHE:CD1	2.83	0.47
2:T:34:PRO:O	2:T:37:SER:OG	2.29	0.47
2:X:7:ARG:HB2	2:X:83:LEU:HD13	1.96	0.47
1:A:187:LEU:HD11	1:A:378:ALA:HB1	1.96	0.47
1:A:204:PHE:HB3	1:A:274:VAL:HG12	1.96	0.47
1:G:255:ASP:OD1	1:G:256:GLY:N	2.47	0.47
1:J:346:ARG:O	1:J:350:ILE:HD12	2.14	0.47
1:J:69:ILE:HG23	1:K:47:PRO:HG3	1.96	0.47
1:A:109:LYS:HB2	1:N:105:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:THR:HB	2:R:36:LYS:NZ	2.30	0.47
2:R:7:ARG:NH1	2:R:84:ASP:HB2	2.30	0.47
2:V:63:VAL:HG13	2:V:65:VAL:H	1.79	0.47
1:A:69:ILE:HG23	1:B:47:PRO:HG3	1.96	0.47
1:H:263:VAL:HA	1:H:266:ARG:HB3	1.97	0.47
1:H:280:GLY:HA2	1:H:285:ARG:HE	1.79	0.47
1:I:214:GLU:HG3	1:I:325:ILE:HG12	1.96	0.47
1:L:347:ILE:O	1:L:351:ILE:HG12	2.15	0.47
1:A:347:ILE:HA	1:A:350:ILE:HG22	1.96	0.47
1:D:25:ASP:OD1	1:D:97:ARG:NH1	2.40	0.47
1:G:288:GLN:O	1:G:292:MET:HG3	2.14	0.47
1:H:345:LYS:HD3	1:H:345:LYS:HA	1.75	0.47
1:K:347:ILE:HA	1:K:350:ILE:HG22	1.96	0.47
1:L:6:VAL:HG12	1:L:522:VAL:HG13	1.97	0.47
1:N:284:ASN:ND2	1:N:365:LYS:HD2	2.30	0.47
1:B:282:GLY:H	1:B:285:ARG:HH21	1.63	0.47
1:D:219:TYR:HE1	1:D:247:LEU:HD13	1.80	0.47
1:D:294:ILE:HG23	1:D:342:GLN:NE2	2.29	0.47
1:E:386:SER:O	1:E:390:VAL:HG23	2.14	0.47
1:L:173:GLY:HA2	1:L:373:LEU:CD2	2.45	0.47
1:N:233:ILE:O	1:N:233:ILE:HD12	2.15	0.47
2:Q:94:GLY:O	2:R:15:ARG:NH2	2.46	0.47
1:A:420:LEU:HB3	1:A:448:LEU:HD22	1.97	0.47
1:D:177:VAL:HG22	1:D:380:LEU:HD12	1.97	0.47
1:D:372:LYS:HG3	1:D:372:LYS:O	2.15	0.47
1:G:23:LEU:HD12	1:G:71:ALA:HB1	1.97	0.47
1:G:177:VAL:HG22	1:G:380:LEU:HD12	1.97	0.47
1:K:354:LEU:HD13	1:K:364:GLU:HG3	1.97	0.47
1:N:298:GLY:HA3	1:N:318:LEU:O	2.15	0.47
2:T:101:VAL:HG22	2:U:8:LYS:HA	1.97	0.47
1:B:124:VAL:O	1:B:128:ILE:HG12	2.14	0.47
1:C:89:THR:O	1:C:93:THR:HG23	2.15	0.47
1:F:340:LYS:O	1:F:343:ILE:HG13	2.14	0.47
1:F:406:ALA:HB1	1:F:499:LYS:HB3	1.97	0.47
1:H:255:ASP:HA	1:H:259:LEU:HD23	1.97	0.47
1:J:339:ASP:O	1:J:343:ILE:HG12	2.14	0.47
1:M:188:GLU:HB3	1:M:379:VAL:CG2	2.45	0.47
1:M:413:VAL:HG22	1:M:414:LEU:H	1.78	0.47
1:N:325:ILE:O	1:N:326:VAL:HB	2.14	0.47
1:N:190:ILE:O	1:N:376:GLY:HA2	2.14	0.47
2:R:6:PHE:HB2	2:R:47:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:O	1:A:128:ILE:HG12	2.14	0.47
1:H:124:VAL:O	1:H:128:ILE:HG12	2.15	0.47
2:X:18:VAL:HG12	2:X:46:VAL:HA	1.97	0.47
1:B:413:VAL:HG22	1:B:414:LEU:H	1.80	0.46
1:D:321:VAL:HA	1:D:336:GLY:HA2	1.96	0.46
1:E:436:ASP:HA	1:E:439:ILE:HD12	1.98	0.46
1:G:350:ILE:HG13	1:G:351:ILE:N	2.31	0.46
1:K:321:VAL:HA	1:K:336:GLY:HA2	1.96	0.46
1:A:191:GLU:HA	1:A:374:SER:H	1.80	0.46
1:J:369:ARG:O	1:J:373:LEU:HG	2.14	0.46
1:J:418:CYS:O	1:J:422:ARG:HG2	2.15	0.46
1:K:10:ALA:HA	1:K:13:ARG:HB2	1.97	0.46
1:K:347:ILE:O	1:K:351:ILE:HG12	2.15	0.46
1:A:89:THR:O	1:A:93:THR:HG23	2.16	0.46
1:H:363:LYS:HA	1:H:366:LEU:HD13	1.98	0.46
1:I:347:ILE:O	1:I:351:ILE:HG12	2.16	0.46
1:J:344:GLU:HA	1:J:347:ILE:HG12	1.98	0.46
1:L:418:CYS:O	1:L:422:ARG:HG2	2.14	0.46
1:C:416:GLY:N	3:C:601:ADP:O2'	2.48	0.46
1:F:418:CYS:O	1:F:422:ARG:HG2	2.14	0.46
1:I:192:GLY:N	1:I:373:LEU:HD23	2.30	0.46
1:J:127:VAL:HG23	1:J:423:CYS:CB	2.45	0.46
1:M:113:PRO:HB2	1:M:517:THR:HA	1.97	0.46
1:M:228:SER:HA	1:M:256:GLY:H	1.80	0.46
1:M:306:LEU:HG	1:M:308:LEU:N	2.31	0.46
1:A:281:PHE:HB3	1:A:284:ASN:HB3	1.98	0.46
1:A:322:GLY:HA3	1:A:335:LYS:HB2	1.97	0.46
1:B:299:ALA:HA	1:B:318:LEU:HB2	1.97	0.46
1:C:298:GLY:HA3	1:C:318:LEU:O	2.16	0.46
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.98	0.46
1:K:342:GLN:O	1:K:345:LYS:HB3	2.14	0.46
1:N:339:ASP:HB3	1:N:342:GLN:HB2	1.98	0.46
2:V:15:ARG:HB3	2:V:90:LEU:HD11	1.98	0.46
1:A:406:ALA:HB1	1:A:499:LYS:HB3	1.97	0.46
1:B:220:VAL:HG12	1:B:248:VAL:HG22	1.96	0.46
1:E:288:GLN:O	1:E:292:MET:HG3	2.16	0.46
1:F:373:LEU:HD21	1:F:377:VAL:HG22	1.98	0.46
1:H:288:GLN:O	1:H:292:MET:HG3	2.16	0.46
1:H:346:ARG:O	1:H:350:ILE:HD12	2.16	0.46
2:O:12:LEU:HB3	2:O:13:PHE:H	1.60	0.46
2:S:15:ARG:HB3	2:S:90:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:18:VAL:HG12	2:Y:46:VAL:HA	1.97	0.46
1:A:230:ILE:HD11	2:O:38:GLN:HB2	1.98	0.46
1:A:347:ILE:O	1:A:351:ILE:HG12	2.16	0.46
1:B:247:LEU:HD12	1:B:247:LEU:O	2.16	0.46
1:B:299:ALA:HA	1:B:318:LEU:CB	2.46	0.46
1:C:346:ARG:O	1:C:350:ILE:HD12	2.16	0.46
1:C:413:VAL:HG22	1:C:414:LEU:H	1.81	0.46
1:D:124:VAL:O	1:D:128:ILE:HG12	2.16	0.46
1:F:288:GLN:O	1:F:292:MET:HG3	2.16	0.46
1:H:89:THR:O	1:H:93:THR:HG23	2.15	0.46
1:K:149:THR:HG22	1:K:156:LYS:HA	1.98	0.46
2:O:70:LYS:HB2	2:O:100:TYR:HB2	1.98	0.46
2:Z:20:ARG:HB3	2:Z:41:VAL:HG13	1.98	0.46
1:A:207:THR:C	1:A:209:LYS:H	2.20	0.46
1:B:443:ILE:O	1:B:447:THR:HG23	2.16	0.46
1:E:325:ILE:HG13	1:E:325:ILE:O	2.16	0.46
1:F:258:ALA:O	1:F:261:THR:OG1	2.26	0.46
1:G:230:ILE:O	1:G:234:VAL:HG12	2.16	0.46
1:G:418:CYS:O	1:G:422:ARG:HG2	2.14	0.46
1:F:105:GLU:HB3	1:I:109:LYS:HB2	1.97	0.46
1:L:169:VAL:HG12	1:L:173:GLY:HA3	1.97	0.46
1:N:124:VAL:O	1:N:128:ILE:HG12	2.15	0.46
1:N:234:VAL:H	1:N:235:PRO:HD2	1.81	0.46
2:Y:7:ARG:NH1	2:Y:84:ASP:HB2	2.30	0.46
1:A:271:LEU:HD22	1:A:272:GLN:N	2.31	0.46
1:B:304:GLU:HG2	1:B:304:GLU:H	1.64	0.46
1:H:340:LYS:O	1:H:344:GLU:HG3	2.15	0.46
1:J:214:GLU:HG3	1:J:325:ILE:HG12	1.98	0.46
1:J:188:GLU:HB3	1:J:379:VAL:CG2	2.45	0.46
1:L:183:LEU:HD22	1:L:183:LEU:H	1.81	0.46
1:L:214:GLU:HG3	1:L:325:ILE:HG12	1.98	0.46
1:L:436:ASP:HA	1:L:439:ILE:HD12	1.98	0.46
1:M:327:THR:OG1	1:M:330:ASP:OD1	2.33	0.46
2:V:20:ARG:HB3	2:V:41:VAL:HG13	1.98	0.46
1:A:413:VAL:HG22	1:A:414:LEU:H	1.81	0.46
1:B:143:GLU:O	1:B:147:VAL:HG13	2.16	0.46
1:B:252:GLU:HG2	1:B:285:ARG:NH1	2.30	0.46
1:E:202:PRO:O	1:E:205:ILE:HG13	2.15	0.46
1:I:288:GLN:O	1:I:292:MET:HG3	2.15	0.46
1:I:298:GLY:HA3	1:I:318:LEU:O	2.16	0.46
1:I:372:LYS:O	1:I:372:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:ILE:HD11	1:J:315:PRO:CD	2.46	0.46
1:J:315:PRO:HA	1:J:318:LEU:HD13	1.98	0.46
1:K:23:LEU:HD12	1:K:71:ALA:HB1	1.97	0.46
1:M:127:VAL:HG23	1:M:423:CYS:CB	2.46	0.46
1:N:216:GLN:HA	1:N:323:LYS:HA	1.98	0.46
1:N:415:GLY:HA3	1:N:494:ILE:HG22	1.98	0.46
2:Z:101:VAL:HG22	2:1:8:LYS:HA	1.98	0.46
1:C:339:ASP:O	1:C:343:ILE:HG23	2.16	0.45
1:D:219:TYR:OH	1:D:240:ALA:HB2	2.16	0.45
1:D:213:CYS:HB3	1:D:326:VAL:HG13	1.98	0.45
1:E:347:ILE:O	1:E:351:ILE:HG12	2.15	0.45
1:F:369:ARG:O	1:F:373:LEU:HG	2.16	0.45
1:I:415:GLY:HA3	1:I:494:ILE:HG22	1.98	0.45
1:J:520:VAL:HB	1:K:38:VAL:HG22	1.98	0.45
1:L:315:PRO:HA	1:L:318:LEU:HD13	1.98	0.45
1:N:263:VAL:HA	1:N:266:ARG:HB3	1.98	0.45
1:B:263:VAL:HG12	1:B:266:ARG:HB2	1.97	0.45
1:B:350:ILE:HD13	1:B:368:GLU:HG2	1.97	0.45
1:B:71:ALA:O	1:B:75:GLN:HG3	2.17	0.45
1:D:258:ALA:O	1:D:261:THR:OG1	2.25	0.45
1:G:214:GLU:HG3	1:G:325:ILE:HG12	1.97	0.45
1:H:369:ARG:O	1:H:373:LEU:HG	2.16	0.45
1:I:306:LEU:HD22	1:J:263:VAL:HG21	1.98	0.45
1:M:346:ARG:O	1:M:350:ILE:HD12	2.16	0.45
1:N:230:ILE:HB	1:N:231:GLN:H	1.42	0.45
2:W:20:ARG:HB3	2:W:41:VAL:HG13	1.98	0.45
1:B:158:ILE:HD11	1:B:393:LYS:HE2	1.98	0.45
1:B:239:ILE:HD11	1:B:315:PRO:N	2.32	0.45
1:B:353:GLN:HE22	1:C:328:LYS:HB3	1.81	0.45
1:F:431:THR:O	1:F:431:THR:OG1	2.11	0.45
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.99	0.45
1:H:259:LEU:HD12	1:H:260:SER:N	2.32	0.45
1:H:306:LEU:HB2	1:I:259:LEU:HD22	1.99	0.45
1:J:232:SER:HB2	1:J:310:LEU:HB3	1.97	0.45
1:M:183:LEU:H	1:M:183:LEU:HD22	1.81	0.45
2:Q:18:VAL:HG12	2:Q:46:VAL:HG22	1.98	0.45
1:A:455:ILE:HD13	3:A:601:ADP:H1'	1.98	0.45
1:B:312:ASP:N	1:B:312:ASP:OD1	2.50	0.45
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.78	0.45
1:C:158:ILE:HD12	1:C:397:VAL:HG22	1.99	0.45
1:C:288:GLN:O	1:C:292:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:SER:O	1:C:390:VAL:HG13	2.16	0.45
1:D:89:THR:O	1:D:93:THR:HG23	2.16	0.45
1:M:71:ALA:O	1:M:75:GLN:HG3	2.17	0.45
2:1:56:LYS:HB2	2:1:61:GLN:OE1	2.17	0.45
1:A:361:TYR:CD1	1:A:361:TYR:O	2.69	0.45
1:B:213:CYS:SG	1:B:274:VAL:HG21	2.57	0.45
1:C:342:GLN:HE21	1:C:342:GLN:HB2	1.53	0.45
1:E:231:GLN:OE1	1:E:231:GLN:N	2.50	0.45
1:E:321:VAL:HA	1:E:336:GLY:HA2	1.98	0.45
1:G:71:ALA:O	1:G:75:GLN:HG3	2.16	0.45
1:I:258:ALA:O	1:I:261:THR:OG1	2.28	0.45
1:K:248:VAL:HG11	1:K:324:VAL:HG21	1.99	0.45
1:K:370:LEU:O	1:K:373:LEU:HB2	2.16	0.45
1:M:303:GLU:HG2	1:M:305:GLY:N	2.27	0.45
1:N:325:ILE:O	1:N:325:ILE:HG13	2.17	0.45
1:N:358:THR:HA	1:N:359:SER:HA	1.50	0.45
1:B:165:ALA:O	1:B:169:VAL:HG22	2.17	0.45
1:B:294:ILE:HD12	1:B:342:GLN:HG2	1.98	0.45
1:E:143:GLU:O	1:E:147:VAL:HG13	2.16	0.45
1:H:183:LEU:HD22	1:H:183:LEU:H	1.82	0.45
1:H:347:ILE:O	1:H:351:ILE:HG12	2.17	0.45
1:I:321:VAL:HA	1:I:336:GLY:HA2	1.99	0.45
1:J:436:ASP:HA	1:J:439:ILE:HD12	1.99	0.45
1:J:461:VAL:HG12	1:J:462:GLU:N	2.32	0.45
1:K:207:THR:C	1:K:209:LYS:H	2.20	0.45
1:K:230:ILE:O	1:K:234:VAL:HG12	2.17	0.45
1:N:196:ASP:OD1	1:N:196:ASP:N	2.45	0.45
1:C:176:THR:HG21	1:C:369:ARG:HD3	1.98	0.45
1:C:27:VAL:HG23	1:C:53:GLY:HA2	1.98	0.45
1:D:219:TYR:CE2	1:D:318:LEU:HD22	2.52	0.45
1:F:120:VAL:HG13	1:F:444:ILE:HD11	1.99	0.45
1:G:165:ALA:O	1:G:169:VAL:HG22	2.17	0.45
1:J:258:ALA:O	1:J:261:THR:OG1	2.33	0.45
1:A:415:GLY:HA3	1:A:494:ILE:HG22	1.99	0.45
1:B:431:THR:OG1	1:B:431:THR:O	2.15	0.45
1:E:258:ALA:O	1:E:261:THR:OG1	2.27	0.45
1:I:413:VAL:HG22	1:I:414:LEU:H	1.81	0.45
1:K:356:VAL:HG23	1:K:357:THR:N	2.32	0.45
1:L:413:VAL:HG22	1:L:414:LEU:H	1.81	0.45
1:N:353:GLN:HG2	1:N:366:LEU:HD11	1.99	0.45
1:C:238:GLU:HG2	2:Q:29:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:13:PHE:N	2:S:13:PHE:HD1	2.15	0.45
1:A:230:ILE:O	1:A:233:ILE:HG22	2.16	0.45
1:G:393:LYS:O	1:G:397:VAL:HG23	2.17	0.45
1:J:359:SER:O	1:J:361:TYR:N	2.41	0.45
1:L:116:ILE:HG13	1:L:436:ASP:HB3	1.99	0.45
1:M:174:VAL:HG23	1:M:372:LYS:HG2	1.98	0.45
1:D:263:VAL:HA	1:D:266:ARG:HB3	1.99	0.45
1:H:232:SER:HB2	1:H:310:LEU:HB2	1.98	0.45
1:H:413:VAL:HG22	1:H:414:LEU:H	1.81	0.45
1:I:393:LYS:O	1:I:397:VAL:HG23	2.17	0.45
1:L:227:ILE:HB	1:L:254:VAL:HG22	1.99	0.45
2:S:83:LEU:CB	2:S:84:ASP:HB2	2.43	0.45
2:Z:46:VAL:HG12	2:Z:67:VAL:HA	1.99	0.45
1:A:25:ASP:OD1	1:A:97:ARG:NH1	2.46	0.44
1:A:294:ILE:HG23	1:A:342:GLN:HE21	1.82	0.44
1:C:415:GLY:HA3	1:C:494:ILE:HG22	1.99	0.44
1:H:340:LYS:H	1:H:340:LYS:HG2	1.61	0.44
1:J:259:LEU:O	1:J:263:VAL:HG22	2.16	0.44
1:M:340:LYS:O	1:M:343:ILE:HG13	2.17	0.44
1:N:178:LYS:HE2	1:N:379:VAL:HG11	2.00	0.44
2:S:35:GLU:HG2	2:S:35:GLU:O	2.17	0.44
1:B:227:ILE:HB	1:B:254:VAL:HG22	1.99	0.44
1:D:362:GLU:HG2	1:D:362:GLU:O	2.17	0.44
1:I:406:ALA:HB1	1:I:499:LYS:HB3	1.98	0.44
1:J:202:PRO:O	1:J:205:ILE:HG13	2.17	0.44
1:J:344:GLU:HG2	1:J:345:LYS:N	2.32	0.44
1:M:174:VAL:HG11	1:M:369:ARG:HG2	1.98	0.44
1:N:13:ARG:NH2	1:N:519:GLU:OE1	2.49	0.44
2:Q:20:ARG:NH1	2:Q:41:VAL:O	2.47	0.44
1:B:199:TYR:CE1	1:B:204:PHE:CZ	3.05	0.44
1:C:206:ASN:OD1	1:C:207:THR:HG23	2.17	0.44
1:E:105:GLU:HB3	1:J:109:LYS:HB2	1.98	0.44
1:F:306:LEU:HD21	1:F:308:LEU:HD12	2.00	0.44
1:F:436:ASP:HA	1:F:439:ILE:HD12	1.99	0.44
1:G:109:LYS:HB2	1:H:105:GLU:HB3	2.00	0.44
1:I:430:LEU:HD12	1:I:430:LEU:HA	1.78	0.44
1:L:372:LYS:HG2	1:L:377:VAL:HG13	1.99	0.44
2:P:56:LYS:HD3	2:Q:55:GLY:HA2	1.98	0.44
2:T:70:LYS:HB2	2:T:100:TYR:HB2	2.00	0.44
2:U:20:ARG:HG2	2:U:21:SER:O	2.17	0.44
1:A:116:ILE:HG13	1:A:436:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG13	1:A:444:ILE:HD11	1.99	0.44
1:A:443:ILE:O	1:A:447:THR:HG23	2.17	0.44
1:B:322:GLY:O	1:B:323:LYS:HG3	2.18	0.44
1:B:346:ARG:O	1:B:350:ILE:HD12	2.18	0.44
1:D:255:ASP:HA	1:D:259:LEU:HD12	1.99	0.44
1:D:339:ASP:O	1:D:343:ILE:HG13	2.17	0.44
1:E:219:TYR:CD1	1:E:318:LEU:HD13	2.51	0.44
1:F:318:LEU:HB3	1:F:319:GLY:H	1.62	0.44
1:M:258:ALA:O	1:M:261:THR:OG1	2.32	0.44
1:M:393:LYS:O	1:M:397:VAL:HG23	2.18	0.44
1:N:183:LEU:HD22	1:N:183:LEU:H	1.82	0.44
1:B:357:THR:O	1:B:357:THR:HG23	2.18	0.44
1:B:422:ARG:O	1:B:425:PRO:HD2	2.17	0.44
1:C:355:ASP:OD1	1:C:356:VAL:HG13	2.17	0.44
1:D:461:VAL:HG12	1:D:462:GLU:N	2.33	0.44
1:L:422:ARG:O	1:L:425:PRO:HD2	2.18	0.44
2:U:15:ARG:HB3	2:U:90:LEU:HD11	1.99	0.44
1:L:238:GLU:HG2	2:Z:29:GLY:HA3	1.98	0.44
1:B:214:GLU:O	1:B:215:PHE:HD1	2.01	0.44
1:B:290:LYS:O	1:B:294:ILE:HG12	2.18	0.44
1:C:202:PRO:O	1:C:205:ILE:HG13	2.18	0.44
1:D:187:LEU:HD11	1:D:378:ALA:HB1	1.99	0.44
1:E:207:THR:C	1:E:209:LYS:H	2.21	0.44
1:K:297:GLY:O	1:K:319:GLY:HA2	2.18	0.44
1:L:239:ILE:HD11	1:L:315:PRO:HD3	1.99	0.44
1:L:373:LEU:HB3	1:L:374:SER:O	2.17	0.44
1:L:135:SER:HB2	1:L:498:THR:HG21	1.98	0.44
1:N:216:GLN:O	1:N:218:ALA:N	2.51	0.44
1:N:255:ASP:OD1	1:N:256:GLY:N	2.51	0.44
1:N:306:LEU:HA	1:N:307:THR:CB	2.47	0.44
2:Z:18:VAL:HG12	2:Z:46:VAL:HG22	1.98	0.44
1:C:318:LEU:HB3	1:C:319:GLY:H	1.60	0.44
1:D:233:ILE:HD11	1:D:249:ILE:HD13	2.00	0.44
1:D:188:GLU:HB3	1:D:379:VAL:CG2	2.48	0.44
1:D:418:CYS:O	1:D:422:ARG:HG2	2.17	0.44
1:F:229:SER:HB2	1:F:257:GLU:HB2	2.00	0.44
1:H:149:THR:CG2	1:H:156:LYS:HA	2.48	0.44
1:H:372:LYS:HG3	1:H:372:LYS:O	2.18	0.44
1:H:461:VAL:HG12	1:H:462:GLU:N	2.32	0.44
1:J:413:VAL:HG22	1:J:414:LEU:H	1.82	0.44
1:K:365:LYS:O	1:K:369:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:10:LEU:HA	2:R:11:PRO:HD2	1.89	0.44
2:R:94:GLY:O	2:S:15:ARG:NH2	2.50	0.44
2:S:18:VAL:HG23	2:S:46:VAL:HA	2.00	0.44
2:W:6:PHE:O	2:W:8:LYS:N	2.50	0.44
2:X:96:ILE:O	2:Y:15:ARG:NH1	2.51	0.44
1:A:229:SER:HB2	1:A:231:GLN:OE1	2.18	0.44
1:D:259:LEU:O	1:D:263:VAL:HG22	2.18	0.44
1:F:263:VAL:HA	1:F:266:ARG:HB3	2.00	0.44
1:G:464:SER:HB3	1:I:464:SER:HB2	2.00	0.44
1:I:7:LYS:HB3	1:I:12:ALA:HB2	2.00	0.44
2:W:4:GLN:H	2:W:49:VAL:HG23	1.82	0.44
2:Y:98:GLY:HA3	2:Z:9:PHE:CE1	2.53	0.44
1:B:183:LEU:HD22	1:B:183:LEU:H	1.82	0.44
1:B:81:THR:HG21	1:B:92:ALA:CB	2.48	0.44
1:C:321:VAL:HA	1:C:336:GLY:HA2	1.99	0.44
1:D:2:SER:HB3	1:D:4:LYS:HZ3	1.83	0.44
1:E:359:SER:HA	1:E:360:GLU:HA	1.74	0.44
1:F:124:VAL:O	1:F:128:ILE:HG12	2.18	0.44
1:J:207:THR:C	1:J:209:LYS:H	2.22	0.44
1:K:116:ILE:HG13	1:K:436:ASP:HB3	2.00	0.44
1:M:369:ARG:O	1:M:373:LEU:HB2	2.18	0.44
1:N:240:ALA:C	1:N:242:ALA:H	2.21	0.44
1:N:321:VAL:HA	1:N:336:GLY:HA2	1.99	0.44
2:O:6:PHE:O	2:O:8:LYS:N	2.51	0.44
2:Q:100:TYR:HD1	2:R:8:LYS:O	2.00	0.44
1:B:264:LEU:HD12	1:B:267:LEU:HD13	1.99	0.43
1:C:340:LYS:HG2	1:C:340:LYS:H	1.57	0.43
1:E:413:VAL:HG22	1:E:414:LEU:H	1.81	0.43
1:I:166:MET:HG2	1:I:171:ARG:HA	2.00	0.43
1:I:232:SER:HB2	1:I:310:LEU:HB2	2.00	0.43
1:F:472:GLN:NE2	1:J:472:GLN:OE1	2.51	0.43
1:K:218:ALA:HB2	1:K:246:PRO:HG2	2.00	0.43
2:R:18:VAL:HG12	2:R:46:VAL:HA	1.99	0.43
1:C:424:ILE:HG23	1:C:445:LYS:HG3	2.01	0.43
1:G:227:ILE:HG21	1:G:233:ILE:HD13	1.98	0.43
1:H:202:PRO:O	1:H:205:ILE:HG13	2.18	0.43
1:H:443:ILE:O	1:H:447:THR:HG23	2.19	0.43
1:I:281:PHE:HA	1:I:281:PHE:HD1	1.71	0.43
1:I:327:THR:OG1	1:I:330:ASP:OD1	2.34	0.43
1:J:228:SER:HA	1:J:255:ASP:O	2.18	0.43
1:N:235:PRO:O	1:N:239:ILE:N	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:24:GLU:O	2:P:33:LEU:HD11	2.18	0.43
1:B:393:LYS:O	1:B:397:VAL:HG23	2.18	0.43
1:E:248:VAL:HG11	1:E:324:VAL:HG11	2.00	0.43
1:E:420:LEU:HB3	1:E:448:LEU:HD22	2.01	0.43
1:F:393:LYS:O	1:F:397:VAL:HG23	2.17	0.43
1:G:420:LEU:HD23	1:G:505:LEU:HD12	2.00	0.43
1:H:176:THR:HG21	1:H:369:ARG:NH2	2.33	0.43
1:I:421:LEU:HD21	1:I:467:VAL:HG13	1.98	0.43
1:A:436:ASP:HA	1:A:439:ILE:HD12	2.01	0.43
1:C:340:LYS:O	1:C:343:ILE:HG13	2.17	0.43
1:C:422:ARG:O	1:C:425:PRO:HD2	2.18	0.43
1:D:116:ILE:HG13	1:D:436:ASP:HB3	2.01	0.43
1:D:436:ASP:HA	1:D:439:ILE:HD12	2.01	0.43
1:D:74:VAL:HA	1:D:77:VAL:HG13	2.00	0.43
1:H:203:TYR:CD1	1:H:267:LEU:HD11	2.53	0.43
1:H:436:ASP:HA	1:H:439:ILE:HD12	2.00	0.43
1:I:322:GLY:HA3	1:I:335:LYS:HB2	1.99	0.43
1:I:422:ARG:O	1:I:425:PRO:HD2	2.19	0.43
1:K:340:LYS:HG2	1:K:340:LYS:H	1.62	0.43
1:M:178:LYS:O	1:M:381:LYS:HA	2.18	0.43
1:B:166:MET:HG2	1:B:171:ARG:HA	1.99	0.43
1:D:166:MET:HG2	1:D:171:ARG:HA	2.00	0.43
1:D:341:ALA:O	1:D:344:GLU:HG3	2.18	0.43
1:H:239:ILE:HD11	1:H:315:PRO:HD3	2.00	0.43
1:H:373:LEU:HD21	1:H:377:VAL:HG22	2.01	0.43
1:I:340:LYS:O	1:I:343:ILE:HG13	2.17	0.43
1:J:116:ILE:HG13	1:J:436:ASP:HB3	2.01	0.43
1:M:216:GLN:HA	1:M:323:LYS:HA	2.00	0.43
1:M:315:PRO:HA	1:M:318:LEU:HD13	1.99	0.43
1:N:234:VAL:O	1:N:238:GLU:HG2	2.18	0.43
2:P:18:VAL:HG12	2:P:46:VAL:HA	2.00	0.43
2:Q:75:GLU:HG3	2:Q:76:TYR:CD1	2.47	0.43
1:A:263:VAL:HA	1:A:266:ARG:HB3	2.00	0.43
1:C:393:LYS:O	1:C:397:VAL:HG23	2.18	0.43
1:D:251:ALA:HB3	1:D:254:VAL:HG23	2.01	0.43
1:E:259:LEU:O	1:E:263:VAL:HG22	2.19	0.43
1:E:339:ASP:OD2	1:E:342:GLN:NE2	2.48	0.43
1:F:450:ILE:O	1:F:453:MET:HG2	2.18	0.43
2:Q:26:VAL:HG12	2:Q:32:MET:HG2	1.99	0.43
2:X:54:LYS:NZ	2:X:58:GLY:O	2.42	0.43
1:A:339:ASP:O	1:A:343:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLU:HG3	1:B:325:ILE:HG12	2.00	0.43
1:D:232:SER:HB2	1:D:310:LEU:HB2	2.00	0.43
1:E:27:VAL:HG12	1:E:90:THR:HG23	2.00	0.43
1:L:347:ILE:HA	1:L:350:ILE:HG22	1.99	0.43
1:M:202:PRO:O	1:M:205:ILE:HG13	2.19	0.43
1:N:461:VAL:HG12	1:N:462:GLU:N	2.32	0.43
2:W:7:ARG:HG2	2:W:84:ASP:OD2	2.18	0.43
2:2:17:LEU:HD11	2:2:81:VAL:HG21	1.99	0.43
1:A:207:THR:O	1:A:208:SER:OG	2.31	0.43
1:A:251:ALA:O	1:A:278:ALA:N	2.51	0.43
1:C:258:ALA:O	1:C:261:THR:OG1	2.31	0.43
1:K:258:ALA:O	1:K:261:THR:OG1	2.31	0.43
1:K:174:VAL:HG23	1:K:372:LYS:HG2	2.01	0.43
2:U:70:LYS:HB2	2:U:100:TYR:HB2	2.01	0.43
2:X:56:LYS:HD3	2:Y:55:GLY:HA2	2.00	0.43
1:A:98:SER:OG	1:A:447:THR:HG22	2.19	0.43
1:B:147:VAL:O	1:B:150:ILE:HG13	2.18	0.43
1:G:166:MET:HG2	1:G:171:ARG:HA	2.01	0.43
1:G:116:ILE:HG13	1:G:436:ASP:HB3	2.01	0.43
1:I:216:GLN:HA	1:I:323:LYS:HA	2.01	0.43
1:K:166:MET:HG2	1:K:171:ARG:HA	2.01	0.43
2:T:18:VAL:HG12	2:T:46:VAL:HA	2.00	0.43
2:Y:56:LYS:HD3	2:Z:54:LYS:HG3	2.01	0.43
1:B:353:GLN:O	1:B:354:LEU:HB3	2.18	0.43
1:C:6:VAL:HG12	1:C:522:VAL:HG13	1.99	0.43
1:H:120:VAL:HG13	1:H:444:ILE:HD11	2.01	0.43
1:H:149:THR:HG22	1:H:156:LYS:HA	2.00	0.43
1:H:206:ASN:OD1	1:H:207:THR:HG23	2.19	0.43
1:I:22:LEU:HD12	1:I:62:LEU:HD11	2.00	0.43
1:J:89:THR:O	1:J:93:THR:HG23	2.19	0.43
1:M:27:VAL:HG23	1:M:53:GLY:HA2	2.01	0.43
1:N:393:LYS:O	1:N:397:VAL:HG23	2.18	0.43
2:O:75:GLU:HG3	2:O:76:TYR:CD1	2.46	0.43
2:V:34:PRO:O	2:V:35:GLU:HG3	2.18	0.43
1:M:268:LYS:HZ2	2:1:32:MET:HB2	1.83	0.42
1:B:241:ASN:ND2	1:B:271:LEU:HD22	2.34	0.42
1:B:280:GLY:O	1:B:281:PHE:HB2	2.18	0.42
1:B:304:GLU:OE2	1:C:260:SER:HB3	2.19	0.42
1:B:120:VAL:HG13	1:B:444:ILE:HD11	2.01	0.42
1:C:255:ASP:OD1	1:C:256:GLY:N	2.52	0.42
1:D:22:LEU:HD23	1:D:62:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:ILE:HG13	1:E:436:ASP:HB3	2.01	0.42
1:F:207:THR:O	1:F:208:SER:OG	2.30	0.42
1:J:421:LEU:HD21	1:J:467:VAL:HG13	2.00	0.42
1:K:372:LYS:HG3	1:K:372:LYS:O	2.19	0.42
1:N:301:PHE:HB3	1:N:310:LEU:HG	2.01	0.42
1:N:347:ILE:O	1:N:351:ILE:HG12	2.19	0.42
2:U:18:VAL:HG23	2:U:46:VAL:HA	2.01	0.42
2:U:6:PHE:O	2:U:8:LYS:N	2.52	0.42
1:A:10:ALA:HA	1:A:13:ARG:HB2	2.01	0.42
1:A:114:VAL:O	1:A:117:ARG:HB3	2.18	0.42
1:A:175:ILE:HD12	1:A:405:ARG:HH21	1.82	0.42
1:D:363:LYS:HB3	1:D:366:LEU:HD23	2.01	0.42
1:E:149:THR:HG22	1:E:156:LYS:HA	2.01	0.42
1:G:202:PRO:O	1:G:205:ILE:HG13	2.19	0.42
1:G:365:LYS:O	1:G:368:GLU:HG2	2.19	0.42
1:I:263:VAL:HA	1:I:266:ARG:HB3	2.01	0.42
1:M:25:ASP:OD1	1:M:97:ARG:NH1	2.46	0.42
2:T:97:LEU:HD23	2:U:15:ARG:HE	1.83	0.42
2:U:56:LYS:HB2	2:U:61:GLN:OE1	2.19	0.42
2:W:18:VAL:HG12	2:W:46:VAL:HA	2.00	0.42
1:H:401:LEU:O	1:H:405:ARG:HG2	2.19	0.42
1:H:469:LYS:HD3	1:H:469:LYS:HA	1.84	0.42
1:K:225:LYS:HA	1:K:225:LYS:HD2	1.89	0.42
1:K:340:LYS:HA	1:K:343:ILE:HG12	2.01	0.42
2:1:27:THR:OG1	2:1:28:LYS:HD2	2.20	0.42
1:A:422:ARG:O	1:A:425:PRO:HD2	2.19	0.42
1:E:322:GLY:HA3	1:E:335:LYS:HB2	2.00	0.42
1:G:436:ASP:HA	1:G:439:ILE:HD12	2.02	0.42
1:H:259:LEU:O	1:H:263:VAL:HG22	2.19	0.42
1:I:147:VAL:O	1:I:150:ILE:HG13	2.19	0.42
1:I:252:GLU:HG3	1:I:285:ARG:NH1	2.35	0.42
1:I:290:LYS:HE3	1:I:346:ARG:HH12	1.85	0.42
1:J:74:VAL:HA	1:J:77:VAL:HG13	2.01	0.42
1:K:158:ILE:HD11	1:K:393:LYS:HE2	2.01	0.42
1:A:69:ILE:HD12	1:B:47:PRO:HB3	2.01	0.42
1:D:120:VAL:HG13	1:D:444:ILE:HD11	2.01	0.42
1:F:422:ARG:O	1:F:425:PRO:HD2	2.19	0.42
1:G:188:GLU:HB3	1:G:379:VAL:CG2	2.50	0.42
1:L:258:ALA:O	1:L:261:THR:OG1	2.29	0.42
1:M:174:VAL:HB	1:M:377:VAL:HG12	2.00	0.42
2:P:6:PHE:HB3	2:P:48:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:SER:OG	1:B:447:THR:HG22	2.20	0.42
1:E:469:LYS:HD3	1:E:469:LYS:HA	1.81	0.42
1:E:52:ASP:O	1:E:56:VAL:HG23	2.20	0.42
1:F:207:THR:C	1:F:209:LYS:H	2.22	0.42
1:H:253:ASP:OD1	1:H:254:VAL:N	2.53	0.42
1:J:114:VAL:O	1:J:117:ARG:HB3	2.19	0.42
1:L:7:LYS:HB3	1:L:12:ALA:HB2	2.01	0.42
1:B:356:VAL:O	1:B:357:THR:HG22	2.20	0.42
1:D:147:VAL:O	1:D:150:ILE:HG13	2.18	0.42
1:D:393:LYS:O	1:D:397:VAL:HG23	2.19	0.42
1:E:280:GLY:HA2	1:E:281:PHE:HA	1.76	0.42
1:G:95:LEU:O	1:G:99:ILE:HD12	2.20	0.42
1:L:173:GLY:HA2	1:L:373:LEU:HD22	2.01	0.42
1:L:201:SER:HA	1:L:202:PRO:HD2	1.85	0.42
1:L:176:THR:HG21	1:L:369:ARG:HD3	2.02	0.42
1:M:89:THR:O	1:M:93:THR:HG23	2.20	0.42
1:A:355:ASP:OD1	1:A:356:VAL:N	2.53	0.42
1:A:95:LEU:O	1:A:99:ILE:HD12	2.19	0.42
1:C:259:LEU:O	1:C:263:VAL:HG23	2.20	0.42
1:E:215:PHE:CE1	1:E:272:GLN:HB3	2.54	0.42
1:E:318:LEU:HB2	1:E:319:GLY:H	1.54	0.42
1:H:318:LEU:HB3	1:H:319:GLY:H	1.60	0.42
1:I:253:ASP:OD1	1:I:254:VAL:N	2.53	0.42
1:J:282:GLY:O	1:J:285:ARG:HG2	2.19	0.42
1:K:288:GLN:O	1:K:292:MET:HG3	2.20	0.42
1:N:248:VAL:HG13	1:N:274:VAL:HG13	2.02	0.42
1:A:287:ASN:HA	1:A:290:LYS:HG2	2.01	0.42
1:A:191:GLU:HB2	1:A:374:SER:HA	2.02	0.42
1:B:322:GLY:CA	1:B:335:LYS:HB3	2.29	0.42
1:C:455:ILE:HD13	3:C:601:ADP:H1'	2.02	0.42
1:E:120:VAL:HG13	1:E:444:ILE:HD11	2.02	0.42
1:F:197:ARG:HG3	1:F:279:PRO:HA	2.01	0.42
1:G:284:ASN:ND2	1:G:365:LYS:HD2	2.35	0.42
1:G:421:LEU:HD21	1:G:467:VAL:HG13	2.00	0.42
2:Q:34:PRO:HG2	2:Q:37:SER:HB3	2.01	0.42
1:A:255:ASP:CG	1:A:256:GLY:H	2.22	0.42
1:C:248:VAL:HG11	1:C:324:VAL:HG11	2.01	0.42
1:C:95:LEU:O	1:C:99:ILE:HD12	2.20	0.42
1:E:344:GLU:HG2	1:E:345:LYS:N	2.34	0.42
1:G:303:GLU:HG3	1:G:304:GLU:N	2.35	0.42
1:J:239:ILE:HD11	1:J:315:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:339:ASP:HB3	1:L:342:GLN:HB3	2.02	0.42
1:M:253:ASP:OD1	1:M:254:VAL:N	2.51	0.42
1:N:187:LEU:HD11	1:N:378:ALA:HB1	2.02	0.42
2:U:46:VAL:HG12	2:U:69:ASP:O	2.20	0.42
2:1:7:ARG:O	2:1:8:LYS:HG2	2.19	0.41
1:A:169:VAL:HG12	1:A:173:GLY:HA3	2.00	0.41
1:B:116:ILE:HG13	1:B:436:ASP:HB3	2.01	0.41
1:B:455:ILE:HD13	3:B:601:ADP:H1'	2.02	0.41
1:C:22:LEU:HD23	1:C:62:LEU:HD11	2.02	0.41
1:C:23:LEU:HD12	1:C:71:ALA:HB1	2.01	0.41
1:C:278:ALA:HB1	1:C:289:LEU:HD11	2.02	0.41
1:D:406:ALA:HB1	1:D:499:LYS:HB3	2.02	0.41
1:I:120:VAL:HG13	1:I:444:ILE:HD11	2.02	0.41
1:K:69:ILE:HD12	1:L:47:PRO:HB3	2.02	0.41
1:M:436:ASP:HA	1:M:439:ILE:HD12	2.02	0.41
2:2:6:PHE:O	2:2:9:PHE:N	2.29	0.41
1:C:158:ILE:HD11	1:C:393:LYS:HE2	2.02	0.41
1:E:354:LEU:O	1:E:356:VAL:N	2.53	0.41
1:G:199:TYR:OH	1:G:205:ILE:HD11	2.19	0.41
1:I:454:THR:O	1:I:458:ASN:ND2	2.36	0.41
1:J:54:VAL:O	1:J:58:LYS:HG3	2.20	0.41
1:L:255:ASP:CG	1:L:256:GLY:H	2.24	0.41
1:M:318:LEU:HB3	1:M:319:GLY:H	1.59	0.41
1:N:422:ARG:O	1:N:425:PRO:HD2	2.20	0.41
1:B:464:SER:HB2	1:N:464:SER:HB2	2.02	0.41
1:N:91:THR:OG1	3:N:601:ADP:O3B	2.35	0.41
2:S:83:LEU:N	2:S:84:ASP:O	2.53	0.41
2:1:18:VAL:HG12	2:1:46:VAL:HA	2.01	0.41
1:D:175:ILE:HD12	1:D:405:ARG:HH21	1.85	0.41
1:E:358:THR:HA	1:E:361:TYR:HB2	2.02	0.41
1:F:219:TYR:HA	1:F:319:GLY:O	2.21	0.41
1:H:149:THR:HG23	1:H:159:GLY:HA3	2.02	0.41
1:K:216:GLN:HA	1:K:323:LYS:HA	2.02	0.41
1:N:326:VAL:HG11	1:N:331:ALA:HA	2.02	0.41
1:N:116:ILE:HG13	1:N:436:ASP:HB3	2.01	0.41
2:S:6:PHE:HB3	2:S:48:ALA:HB2	2.02	0.41
2:U:35:GLU:HA	2:U:38:GLN:HB2	2.02	0.41
2:V:59:GLU:HG3	2:V:60:ILE:N	2.35	0.41
1:B:95:LEU:O	1:B:99:ILE:HD12	2.20	0.41
1:C:345:LYS:HE3	1:D:328:LYS:HE2	2.02	0.41
1:F:280:GLY:HA2	1:F:285:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:ASP:N	1:G:312:ASP:OD1	2.53	0.41
1:G:359:SER:O	1:G:362:GLU:N	2.48	0.41
1:H:219:TYR:HA	1:H:319:GLY:O	2.20	0.41
1:N:345:LYS:HE2	1:N:349:GLU:OE2	2.19	0.41
2:P:100:TYR:CE1	2:Q:9:PHE:HD1	2.39	0.41
2:U:43:GLN:HG2	2:U:72:LEU:HD21	2.01	0.41
1:A:321:VAL:HA	1:A:336:GLY:HA2	2.01	0.41
1:C:147:VAL:O	1:C:150:ILE:HG13	2.20	0.41
1:C:340:LYS:O	1:C:344:GLU:HG3	2.20	0.41
1:H:95:LEU:O	1:H:99:ILE:HD12	2.19	0.41
1:M:306:LEU:HG	1:M:308:LEU:H	1.84	0.41
1:N:235:PRO:HA	1:N:238:GLU:HB2	2.01	0.41
2:X:54:LYS:HA	2:X:60:ILE:HD13	2.02	0.41
1:F:297:GLY:O	1:F:319:GLY:HA2	2.20	0.41
1:E:69:ILE:HG23	1:F:47:PRO:HG3	2.02	0.41
1:J:347:ILE:O	1:J:351:ILE:HG12	2.20	0.41
1:L:216:GLN:HA	1:L:323:LYS:HA	2.03	0.41
1:N:339:ASP:O	1:N:343:ILE:HG13	2.20	0.41
2:P:7:ARG:O	2:P:8:LYS:HG2	2.20	0.41
1:A:225:LYS:HD2	1:A:225:LYS:HA	1.86	0.41
1:B:347:ILE:HG13	1:B:348:GLN:N	2.36	0.41
1:D:255:ASP:CG	1:D:256:GLY:H	2.24	0.41
1:E:422:ARG:O	1:E:425:PRO:HD2	2.20	0.41
1:G:188:GLU:HB3	1:G:379:VAL:HG23	2.03	0.41
1:L:288:GLN:O	1:L:292:MET:HG3	2.21	0.41
1:L:332:MET:HE2	1:L:332:MET:HB3	1.97	0.41
1:L:95:LEU:O	1:L:99:ILE:HD12	2.21	0.41
2:X:6:PHE:HZ	2:X:7:ARG:HH11	1.69	0.41
1:B:415:GLY:HA3	1:B:494:ILE:HG22	2.03	0.41
1:D:370:LEU:HA	1:D:373:LEU:HD12	2.03	0.41
1:F:74:VAL:HA	1:F:77:VAL:HG13	2.02	0.41
1:H:228:SER:O	1:H:256:GLY:HA3	2.21	0.41
1:H:214:GLU:HG3	1:H:325:ILE:HG12	2.02	0.41
1:H:422:ARG:O	1:H:425:PRO:HD2	2.20	0.41
1:I:455:ILE:HD11	3:I:601:ADP:H4'	2.02	0.41
1:J:95:LEU:O	1:J:99:ILE:HD12	2.20	0.41
1:K:418:CYS:O	1:K:422:ARG:HG2	2.19	0.41
1:L:312:ASP:N	1:L:312:ASP:OD1	2.52	0.41
1:M:95:LEU:O	1:M:99:ILE:HD12	2.20	0.41
2:S:46:VAL:HG12	2:S:69:ASP:O	2.21	0.41
1:B:488:ASN:HB3	1:B:491:GLU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:LEU:HD23	1:C:249:ILE:HG23	2.01	0.41
1:E:107:ILE:HG13	1:E:107:ILE:O	2.19	0.41
1:G:264:LEU:O	1:G:268:LYS:HB2	2.21	0.41
1:G:219:TYR:HA	1:G:319:GLY:O	2.21	0.41
1:G:469:LYS:HD3	1:G:469:LYS:HA	1.89	0.41
1:J:253:ASP:OD1	1:J:254:VAL:N	2.53	0.41
1:J:363:LYS:H	1:J:363:LYS:HG2	1.66	0.41
1:K:149:THR:CG2	1:K:156:LYS:HA	2.51	0.41
1:K:227:ILE:HG21	1:K:233:ILE:HD13	2.02	0.41
2:2:26:VAL:HG23	2:2:27:THR:HG22	2.03	0.41
1:A:188:GLU:HB3	1:A:379:VAL:CG2	2.51	0.41
1:A:280:GLY:HA2	1:A:285:ARG:CD	2.51	0.41
1:A:498:THR:O	1:A:502:ARG:HG2	2.21	0.41
1:B:264:LEU:HG	1:B:264:LEU:O	2.20	0.41
1:I:436:ASP:HA	1:I:439:ILE:HD12	2.03	0.41
1:J:206:ASN:OD1	1:J:207:THR:HG23	2.21	0.41
1:J:373:LEU:HD21	1:J:377:VAL:HG22	2.01	0.41
1:K:436:ASP:HA	1:K:439:ILE:HD12	2.03	0.41
1:L:393:LYS:O	1:L:397:VAL:HG13	2.21	0.41
1:N:259:LEU:O	1:N:263:VAL:HG22	2.21	0.41
1:N:450:ILE:O	1:N:453:MET:HG2	2.21	0.41
2:W:7:ARG:HA	2:W:7:ARG:HD2	1.74	0.41
2:V:58:GLY:HA2	2:2:56:LYS:HE2	2.03	0.41
1:A:281:PHE:H	1:A:285:ARG:CG	2.33	0.41
1:A:65:LYS:O	1:A:69:ILE:HG12	2.21	0.41
1:C:201:SER:HA	1:C:202:PRO:HD2	1.89	0.41
1:E:114:VAL:O	1:E:117:ARG:HB3	2.21	0.41
1:I:95:LEU:O	1:I:99:ILE:HD12	2.21	0.41
1:L:248:VAL:HG11	1:L:324:VAL:HG21	2.03	0.41
1:M:230:ILE:O	1:M:234:VAL:HG12	2.21	0.41
1:M:307:THR:H	1:N:269:VAL:CG1	2.33	0.41
2:V:6:PHE:HB3	2:V:48:ALA:HB2	2.03	0.41
1:A:192:GLY:O	1:A:193:MET:HG2	2.21	0.40
1:A:42:GLN:HE21	1:A:48:LYS:HG3	1.86	0.40
1:B:339:ASP:O	1:B:340:LYS:HB3	2.21	0.40
1:C:197:ARG:NH1	1:C:278:ALA:O	2.54	0.40
1:D:219:TYR:HB2	1:D:319:GLY:O	2.21	0.40
1:D:294:ILE:HG23	1:D:342:GLN:HG3	2.02	0.40
1:E:31:MET:HG2	1:E:455:ILE:CG1	2.52	0.40
1:F:497:PRO:HB2	1:F:500:VAL:HG23	2.02	0.40
1:K:169:VAL:HG12	1:K:173:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:232:SER:HB2	1:K:310:LEU:CB	2.42	0.40
2:O:6:PHE:CG	2:O:7:ARG:N	2.89	0.40
2:X:5:ALA:HB1	2:X:9:PHE:O	2.21	0.40
1:B:213:CYS:O	1:B:325:ILE:HA	2.21	0.40
1:D:291:ASP:OD1	1:D:346:ARG:HD3	2.20	0.40
1:D:232:SER:HA	1:D:311:GLU:HG3	2.03	0.40
1:G:6:VAL:HG22	1:G:522:VAL:HG22	2.03	0.40
1:H:297:GLY:O	1:H:319:GLY:HA2	2.21	0.40
1:I:114:VAL:O	1:I:117:ARG:HB3	2.20	0.40
1:L:24:ALA:HB3	1:L:97:ARG:HD3	2.03	0.40
1:N:190:ILE:CG1	1:N:377:VAL:HG22	2.52	0.40
2:P:102:ASP:OD1	2:P:102:ASP:N	2.54	0.40
2:O:9:PHE:CZ	2:U:98:GLY:HA3	2.56	0.40
1:A:416:GLY:N	3:A:601:ADP:O2'	2.54	0.40
1:B:340:LYS:O	1:B:344:GLU:HG3	2.21	0.40
1:C:31:MET:HG2	1:C:455:ILE:HG13	2.03	0.40
1:C:372:LYS:O	1:C:372:LYS:HG3	2.21	0.40
1:D:216:GLN:HA	1:D:323:LYS:HA	2.03	0.40
1:D:422:ARG:O	1:D:425:PRO:HD2	2.22	0.40
1:D:415:GLY:HA3	1:D:494:ILE:HG22	2.03	0.40
1:G:301:PHE:HE1	1:G:308:LEU:HD22	1.85	0.40
1:H:24:ALA:HB3	1:H:97:ARG:HD3	2.02	0.40
1:I:207:THR:HG22	1:I:212:LYS:O	2.21	0.40
1:M:214:GLU:HG3	1:M:325:ILE:HG12	2.02	0.40
1:M:22:LEU:HD23	1:M:62:LEU:HD11	2.02	0.40
1:N:469:LYS:HD3	1:N:469:LYS:HA	1.82	0.40
2:V:12:LEU:HB3	2:V:13:PHE:H	1.59	0.40
1:A:24:ALA:HB3	1:A:97:ARG:HD3	2.02	0.40
1:B:114:VAL:O	1:B:117:ARG:HB3	2.20	0.40
1:B:199:TYR:CZ	1:B:204:PHE:CZ	3.09	0.40
1:B:225:LYS:HD3	1:B:303:GLU:OE2	2.21	0.40
1:B:342:GLN:HG3	1:B:342:GLN:O	2.22	0.40
1:F:233:ILE:HD11	1:F:249:ILE:HD13	2.04	0.40
1:H:248:VAL:HG11	1:H:324:VAL:HG11	2.03	0.40
1:H:345:LYS:O	1:H:349:GLU:HG3	2.21	0.40
1:H:175:ILE:HG23	1:H:378:ALA:HB3	2.03	0.40
1:M:345:LYS:O	1:M:349:GLU:HG3	2.21	0.40
2:P:23:ALA:HB2	2:P:41:VAL:HB	2.02	0.40
2:T:94:GLY:O	2:U:15:ARG:NH2	2.55	0.40
1:B:196:ASP:OD1	1:B:196:ASP:N	2.44	0.40
1:B:353:GLN:C	1:B:355:ASP:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:OD1	1:C:213:CYS:HA	2.21	0.40
1:B:353:GLN:NE2	1:C:328:LYS:HB3	2.37	0.40
1:J:127:VAL:HG23	1:J:423:CYS:HB3	2.02	0.40
1:K:230:ILE:O	1:K:233:ILE:HG22	2.21	0.40
1:L:158:ILE:HG13	1:L:397:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/558 (94%)	494 (94%)	24 (5%)	6 (1%)	14	48
1	B	524/558 (94%)	487 (93%)	22 (4%)	15 (3%)	4	25
1	C	524/558 (94%)	492 (94%)	26 (5%)	6 (1%)	14	48
1	D	524/558 (94%)	494 (94%)	25 (5%)	5 (1%)	15	51
1	E	524/558 (94%)	489 (93%)	26 (5%)	9 (2%)	9	38
1	F	524/558 (94%)	490 (94%)	26 (5%)	8 (2%)	10	41
1	G	524/558 (94%)	489 (93%)	25 (5%)	10 (2%)	8	36
1	H	524/558 (94%)	493 (94%)	27 (5%)	4 (1%)	19	55
1	I	524/558 (94%)	493 (94%)	26 (5%)	5 (1%)	15	51
1	J	524/558 (94%)	497 (95%)	25 (5%)	2 (0%)	34	68
1	K	524/558 (94%)	496 (95%)	23 (4%)	5 (1%)	15	51
1	L	524/558 (94%)	494 (94%)	25 (5%)	5 (1%)	15	51
1	M	524/558 (94%)	489 (93%)	28 (5%)	7 (1%)	12	44
1	N	524/558 (94%)	486 (93%)	28 (5%)	10 (2%)	8	36
2	1	98/114 (86%)	88 (90%)	5 (5%)	5 (5%)	2	13
2	2	102/114 (90%)	94 (92%)	5 (5%)	3 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	98/114 (86%)	85 (87%)	7 (7%)	6 (6%)	1	10
2	P	103/114 (90%)	97 (94%)	3 (3%)	3 (3%)	4	25
2	Q	98/114 (86%)	91 (93%)	4 (4%)	3 (3%)	4	23
2	R	98/114 (86%)	88 (90%)	6 (6%)	4 (4%)	3	18
2	S	98/114 (86%)	86 (88%)	6 (6%)	6 (6%)	1	10
2	T	98/114 (86%)	92 (94%)	4 (4%)	2 (2%)	7	34
2	U	100/114 (88%)	91 (91%)	5 (5%)	4 (4%)	3	18
2	V	98/114 (86%)	92 (94%)	3 (3%)	3 (3%)	4	23
2	W	98/114 (86%)	91 (93%)	5 (5%)	2 (2%)	7	34
2	X	98/114 (86%)	91 (93%)	4 (4%)	3 (3%)	4	23
2	Y	98/114 (86%)	92 (94%)	2 (2%)	4 (4%)	3	18
2	Z	106/114 (93%)	91 (86%)	10 (9%)	5 (5%)	2	15
All	All	8727/9408 (93%)	8152 (93%)	425 (5%)	150 (2%)	9	38

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	GLY
1	A	358	THR
1	B	217	ASP
1	B	231	GLN
1	B	269	VAL
1	B	270	GLY
1	B	299	ALA
1	B	321	VAL
1	D	217	ASP
1	E	88	GLY
1	E	270	GLY
1	E	358	THR
1	F	217	ASP
1	F	270	GLY
1	F	358	THR
1	G	339	ASP
1	H	270	GLY
1	I	463	GLY
1	K	217	ASP
1	L	229	SER
1	L	230	ILE

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Mol	Chain	Res	Type
1	M	381	LYS
1	N	230	ILE
1	N	233	ILE
1	N	270	GLY
2	O	7	ARG
2	O	13	PHE
2	O	37	SER
2	P	13	PHE
2	Q	28	LYS
2	R	7	ARG
2	R	13	PHE
2	S	26	VAL
2	S	84	ASP
2	U	7	ARG
2	U	13	PHE
2	V	13	PHE
2	V	28	LYS
2	W	7	ARG
2	X	7	ARG
2	X	13	PHE
2	Y	28	LYS
2	Z	7	ARG
2	Z	13	PHE
2	Z	38	GLN
2	1	28	LYS
2	2	7	ARG
2	2	13	PHE
1	A	217	ASP
1	A	256	GLY
1	B	256	GLY
1	B	340	LYS
1	B	360	GLU
1	C	217	ASP
1	C	256	GLY
1	D	256	GLY
1	D	374	SER
1	E	217	ASP
1	E	354	LEU
1	E	356	VAL
1	F	256	GLY
1	G	217	ASP
1	G	256	GLY

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Mol	Chain	Res	Type
1	G	270	GLY
1	G	308	LEU
1	H	217	ASP
1	H	359	SER
1	I	217	ASP
1	J	217	ASP
1	J	270	GLY
1	K	256	GLY
1	L	217	ASP
1	L	256	GLY
1	M	217	ASP
1	M	270	GLY
1	M	305	GLY
1	M	306	LEU
1	N	256	GLY
1	N	307	THR
2	O	28	LYS
2	O	29	GLY
2	P	27	THR
2	Q	13	PHE
2	R	35	GLU
2	S	13	PHE
2	S	25	THR
2	T	13	PHE
2	U	37	SER
2	Y	29	GLY
2	Z	35	GLU
2	1	13	PHE
2	1	29	GLY
1	B	339	ASP
1	C	270	GLY
1	E	355	ASP
1	E	373	LEU
1	G	360	GLU
1	H	229	SER
1	K	354	LEU
1	K	356	VAL
1	N	234	VAL
2	S	38	GLN
2	S	78	GLY
2	V	78	GLY
2	Y	30	GLY

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Mol	Chain	Res	Type
1	B	199	TYR
1	B	281	PHE
1	C	362	GLU
1	F	229	SER
1	G	307	THR
1	I	362	GLU
1	M	362	GLU
1	N	241	ASN
1	N	354	LEU
2	P	30	GLY
2	X	78	GLY
2	Z	78	GLY
2	1	30	GLY
2	1	78	GLY
2	2	35	GLU
1	A	255	ASP
1	B	200	ILE
1	B	255	ASP
1	C	255	ASP
1	D	3	ALA
1	F	255	ASP
1	G	255	ASP
1	G	338	GLY
1	I	357	THR
1	L	255	ASP
1	N	255	ASP
2	O	78	GLY
2	W	78	GLY
2	Y	78	GLY
1	A	282	GLY
1	B	298	GLY
1	C	208	SER
1	D	255	ASP
1	F	354	LEU
1	K	255	ASP
1	M	256	GLY
2	Q	78	GLY
2	T	78	GLY
1	N	326	VAL
2	R	78	GLY
1	E	376	GLY
1	I	256	GLY

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Mol	Chain	Res	Type
2	U	39	GLY
1	G	302	GLY
1	F	280	GLY

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	425/455 (93%)	399 (94%)	26 (6%)	18	50
1	B	425/455 (93%)	389 (92%)	36 (8%)	10	36
1	C	425/455 (93%)	408 (96%)	17 (4%)	31	64
1	D	425/455 (93%)	391 (92%)	34 (8%)	12	39
1	E	425/455 (93%)	394 (93%)	31 (7%)	14	43
1	F	425/455 (93%)	401 (94%)	24 (6%)	21	53
1	G	425/455 (93%)	402 (95%)	23 (5%)	22	55
1	H	425/455 (93%)	400 (94%)	25 (6%)	19	51
1	I	425/455 (93%)	394 (93%)	31 (7%)	14	43
1	J	425/455 (93%)	399 (94%)	26 (6%)	18	50
1	K	425/455 (93%)	398 (94%)	27 (6%)	17	49
1	L	425/455 (93%)	402 (95%)	23 (5%)	22	55
1	M	425/455 (93%)	397 (93%)	28 (7%)	16	47
1	N	425/455 (93%)	400 (94%)	25 (6%)	19	51
2	1	81/91 (89%)	74 (91%)	7 (9%)	10	35
2	2	83/91 (91%)	75 (90%)	8 (10%)	8	29
2	O	81/91 (89%)	75 (93%)	6 (7%)	13	43
2	P	83/91 (91%)	76 (92%)	7 (8%)	11	37
2	Q	81/91 (89%)	74 (91%)	7 (9%)	10	35
2	R	81/91 (89%)	72 (89%)	9 (11%)	6	24
2	S	81/91 (89%)	73 (90%)	8 (10%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	81/91 (89%)	72 (89%)	9 (11%)	6	24
2	U	83/91 (91%)	75 (90%)	8 (10%)	8	29
2	V	81/91 (89%)	72 (89%)	9 (11%)	6	24
2	W	81/91 (89%)	75 (93%)	6 (7%)	13	43
2	X	81/91 (89%)	72 (89%)	9 (11%)	6	24
2	Y	81/91 (89%)	74 (91%)	7 (9%)	10	35
2	Z	86/91 (94%)	77 (90%)	9 (10%)	7	26
All	All	7095/7644 (93%)	6610 (93%)	485 (7%)	16	46

All (485) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ILE
1	A	158	ILE
1	A	179	ASP
1	A	183	LEU
1	A	234	VAL
1	A	267	LEU
1	A	271	LEU
1	A	310	LEU
1	A	312	ASP
1	A	316	HIS
1	A	326	VAL
1	A	340	LYS
1	A	342	GLN
1	A	350	ILE
1	A	358	THR
1	A	361	TYR
1	A	369	ARG
1	A	370	LEU
1	A	385	THR
1	A	401	LEU
1	A	430	LEU
1	A	431	THR
1	A	453	MET
1	A	464	SER
1	A	465	LEU
1	A	470	ILE
1	B	74	VAL
1	B	107	ILE

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Mol	Chain	Res	Type
1	B	158	ILE
1	B	176	THR
1	B	179	ASP
1	B	183	LEU
1	B	199	TYR
1	B	213	CYS
1	B	220	VAL
1	B	221	LEU
1	B	222	LEU
1	B	247	LEU
1	B	249	ILE
1	B	257	GLU
1	B	265	ASN
1	B	268	LYS
1	B	273	VAL
1	B	310	LEU
1	B	312	ASP
1	B	316	HIS
1	B	317	ASP
1	B	318	LEU
1	B	340	LYS
1	B	358	THR
1	B	361	TYR
1	B	369	ARG
1	B	370	LEU
1	B	372	LYS
1	B	385	THR
1	B	401	LEU
1	B	430	LEU
1	B	431	THR
1	B	453	MET
1	B	465	LEU
1	B	498	THR
1	B	525	ILE
1	C	90	THR
1	C	179	ASP
1	C	227	ILE
1	C	230	ILE
1	C	267	LEU
1	C	273	VAL
1	C	306	LEU
1	C	312	ASP

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Mol	Chain	Res	Type
1	C	342	GLN
1	C	369	ARG
1	C	370	LEU
1	C	390	VAL
1	C	401	LEU
1	C	431	THR
1	C	453	MET
1	C	465	LEU
1	C	521	VAL
1	D	30	THR
1	D	74	VAL
1	D	158	ILE
1	D	179	ASP
1	D	207	THR
1	D	219	TYR
1	D	222	LEU
1	D	248	VAL
1	D	250	ILE
1	D	253	ASP
1	D	267	LEU
1	D	273	VAL
1	D	281	PHE
1	D	289	LEU
1	D	309	ASN
1	D	312	ASP
1	D	313	VAL
1	D	324	VAL
1	D	326	VAL
1	D	333	LEU
1	D	339	ASP
1	D	342	GLN
1	D	350	ILE
1	D	357	THR
1	D	362	GLU
1	D	370	LEU
1	D	385	THR
1	D	401	LEU
1	D	431	THR
1	D	453	MET
1	D	464	SER
1	D	465	LEU
1	D	506	LEU

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Mol	Chain	Res	Type
1	D	520	VAL
1	E	38	VAL
1	E	74	VAL
1	E	107	ILE
1	E	158	ILE
1	E	179	ASP
1	E	220	VAL
1	E	231	GLN
1	E	250	ILE
1	E	267	LEU
1	E	271	LEU
1	E	273	VAL
1	E	312	ASP
1	E	316	HIS
1	E	318	LEU
1	E	339	ASP
1	E	340	LYS
1	E	342	GLN
1	E	344	GLU
1	E	350	ILE
1	E	358	THR
1	E	360	GLU
1	E	361	TYR
1	E	370	LEU
1	E	385	THR
1	E	401	LEU
1	E	431	THR
1	E	453	MET
1	E	464	SER
1	E	465	LEU
1	E	469	LYS
1	E	502	ARG
1	F	74	VAL
1	F	77	VAL
1	F	142	GLU
1	F	150	ILE
1	F	158	ILE
1	F	179	ASP
1	F	219	TYR
1	F	229	SER
1	F	230	ILE
1	F	267	LEU

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Mol	Chain	Res	Type
1	F	273	VAL
1	F	312	ASP
1	F	324	VAL
1	F	350	ILE
1	F	357	THR
1	F	358	THR
1	F	370	LEU
1	F	385	THR
1	F	401	LEU
1	F	431	THR
1	F	464	SER
1	F	465	LEU
1	F	469	LYS
1	F	498	THR
1	G	74	VAL
1	G	150	ILE
1	G	158	ILE
1	G	179	ASP
1	G	206	ASN
1	G	259	LEU
1	G	267	LEU
1	G	273	VAL
1	G	281	PHE
1	G	308	LEU
1	G	312	ASP
1	G	340	LYS
1	G	350	ILE
1	G	358	THR
1	G	359	SER
1	G	370	LEU
1	G	373	LEU
1	G	385	THR
1	G	401	LEU
1	G	431	THR
1	G	465	LEU
1	G	469	LYS
1	G	525	ILE
1	H	74	VAL
1	H	150	ILE
1	H	158	ILE
1	H	171	ARG
1	H	179	ASP

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Mol	Chain	Res	Type
1	H	183	LEU
1	H	208	SER
1	H	267	LEU
1	H	273	VAL
1	H	274	VAL
1	H	304	GLU
1	H	312	ASP
1	H	358	THR
1	H	361	TYR
1	H	362	GLU
1	H	368	GLU
1	H	370	LEU
1	H	385	THR
1	H	401	LEU
1	H	405	ARG
1	H	431	THR
1	H	464	SER
1	H	465	LEU
1	H	469	LYS
1	H	498	THR
1	I	74	VAL
1	I	95	LEU
1	I	158	ILE
1	I	176	THR
1	I	179	ASP
1	I	231	GLN
1	I	248	VAL
1	I	267	LEU
1	I	273	VAL
1	I	281	PHE
1	I	312	ASP
1	I	313	VAL
1	I	316	HIS
1	I	324	VAL
1	I	350	ILE
1	I	357	THR
1	I	368	GLU
1	I	369	ARG
1	I	370	LEU
1	I	373	LEU
1	I	374	SER
1	I	385	THR

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Mol	Chain	Res	Type
1	I	401	LEU
1	I	430	LEU
1	I	431	THR
1	I	453	MET
1	I	464	SER
1	I	465	LEU
1	I	469	LYS
1	I	498	THR
1	I	525	ILE
1	J	15	LEU
1	J	62	LEU
1	J	74	VAL
1	J	133	LYS
1	J	158	ILE
1	J	171	ARG
1	J	176	THR
1	J	179	ASP
1	J	267	LEU
1	J	273	VAL
1	J	281	PHE
1	J	285	ARG
1	J	310	LEU
1	J	312	ASP
1	J	326	VAL
1	J	344	GLU
1	J	345	LYS
1	J	358	THR
1	J	370	LEU
1	J	385	THR
1	J	401	LEU
1	J	431	THR
1	J	453	MET
1	J	464	SER
1	J	465	LEU
1	J	498	THR
1	K	74	VAL
1	K	107	ILE
1	K	158	ILE
1	K	179	ASP
1	K	211	GLN
1	K	219	TYR
1	K	229	SER

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Mol	Chain	Res	Type
1	K	267	LEU
1	K	273	VAL
1	K	306	LEU
1	K	307	THR
1	K	312	ASP
1	K	324	VAL
1	K	350	ILE
1	K	353	GLN
1	K	368	GLU
1	K	369	ARG
1	K	370	LEU
1	K	373	LEU
1	K	385	THR
1	K	401	LEU
1	K	421	LEU
1	K	431	THR
1	K	464	SER
1	K	465	LEU
1	K	469	LYS
1	K	525	ILE
1	L	74	VAL
1	L	107	ILE
1	L	150	ILE
1	L	158	ILE
1	L	179	ASP
1	L	183	LEU
1	L	262	LEU
1	L	267	LEU
1	L	273	VAL
1	L	312	ASP
1	L	313	VAL
1	L	324	VAL
1	L	340	LYS
1	L	350	ILE
1	L	358	THR
1	L	370	LEU
1	L	385	THR
1	L	401	LEU
1	L	431	THR
1	L	453	MET
1	L	464	SER
1	L	465	LEU

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Mol	Chain	Res	Type
1	L	521	VAL
1	M	54	VAL
1	M	74	VAL
1	M	115	GLU
1	M	150	ILE
1	M	158	ILE
1	M	176	THR
1	M	179	ASP
1	M	183	LEU
1	M	248	VAL
1	M	267	LEU
1	M	268	LYS
1	M	273	VAL
1	M	308	LEU
1	M	312	ASP
1	M	356	VAL
1	M	366	LEU
1	M	370	LEU
1	M	373	LEU
1	M	385	THR
1	M	401	LEU
1	M	422	ARG
1	M	430	LEU
1	M	431	THR
1	M	453	MET
1	M	464	SER
1	M	465	LEU
1	M	469	LYS
1	M	525	ILE
1	N	74	VAL
1	N	90	THR
1	N	150	ILE
1	N	158	ILE
1	N	179	ASP
1	N	183	LEU
1	N	220	VAL
1	N	243	HIS
1	N	244	ARG
1	N	273	VAL
1	N	303	GLU
1	N	306	LEU
1	N	307	THR

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Mol	Chain	Res	Type
1	N	312	ASP
1	N	324	VAL
1	N	326	VAL
1	N	342	GLN
1	N	358	THR
1	N	370	LEU
1	N	385	THR
1	N	401	LEU
1	N	431	THR
1	N	464	SER
1	N	465	LEU
1	N	469	LYS
2	O	7	ARG
2	O	24	GLU
2	O	31	ILE
2	O	45	THR
2	O	71	VAL
2	O	85	ASP
2	P	12	LEU
2	P	24	GLU
2	P	27	THR
2	P	45	THR
2	P	47	VAL
2	P	71	VAL
2	P	85	ASP
2	Q	24	GLU
2	Q	38	GLN
2	Q	47	VAL
2	Q	70	LYS
2	Q	71	VAL
2	Q	85	ASP
2	Q	99	LYS
2	R	10	LEU
2	R	24	GLU
2	R	25	THR
2	R	31	ILE
2	R	45	THR
2	R	70	LYS
2	R	71	VAL
2	R	73	LEU
2	R	85	ASP
2	S	10	LEU

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Mol	Chain	Res	Type
2	S	13	PHE
2	S	16	VAL
2	S	20	ARG
2	S	31	ILE
2	S	71	VAL
2	S	73	LEU
2	S	75	GLU
2	T	24	GLU
2	T	28	LYS
2	T	37	SER
2	T	38	GLN
2	T	45	THR
2	T	46	VAL
2	T	65	VAL
2	T	70	LYS
2	T	73	LEU
2	U	7	ARG
2	U	15	ARG
2	U	17	LEU
2	U	24	GLU
2	U	71	VAL
2	U	73	LEU
2	U	85	ASP
2	U	92	ARG
2	V	17	LEU
2	V	27	THR
2	V	31	ILE
2	V	35	GLU
2	V	45	THR
2	V	63	VAL
2	V	71	VAL
2	V	75	GLU
2	V	85	ASP
2	W	24	GLU
2	W	27	THR
2	W	45	THR
2	W	47	VAL
2	W	71	VAL
2	W	85	ASP
2	X	7	ARG
2	X	24	GLU
2	X	28	LYS

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Mol	Chain	Res	Type
2	X	35	GLU
2	X	45	THR
2	X	70	LYS
2	X	71	VAL
2	X	85	ASP
2	X	101	VAL
2	Y	17	LEU
2	Y	24	GLU
2	Y	31	ILE
2	Y	45	THR
2	Y	71	VAL
2	Y	85	ASP
2	Y	92	ARG
2	Z	12	LEU
2	Z	24	GLU
2	Z	28	LYS
2	Z	45	THR
2	Z	54	LYS
2	Z	71	VAL
2	Z	85	ASP
2	Z	92	ARG
2	Z	104	LEU
2	1	24	GLU
2	1	28	LYS
2	1	45	THR
2	1	71	VAL
2	1	85	ASP
2	1	92	ARG
2	1	97	LEU
2	2	10	LEU
2	2	20	ARG
2	2	31	ILE
2	2	45	THR
2	2	71	VAL
2	2	75	GLU
2	2	85	ASP
2	2	92	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	265	ASN

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Mol	Chain	Res	Type
1	B	472	GLN
1	C	79	ASN
1	C	342	GLN
1	G	206	ASN
1	I	284	ASN
1	J	216	GLN
1	K	216	GLN
1	K	488	ASN
1	N	241	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 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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	$\# Z > 2$
3	ADP	D	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.35	3 (10%)
3	ADP	F	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	J	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.33	3 (10%)
3	ADP	L	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.39	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	N	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.37	3 (10%)
3	ADP	A	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.41	4 (13%)
3	ADP	C	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)
3	ADP	E	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.35	4 (13%)
3	ADP	H	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.37	3 (10%)
3	ADP	G	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	I	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.40	3 (10%)
3	ADP	K	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.38	3 (10%)
3	ADP	M	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
3	ADP	B	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.36	4 (13%)

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
3	ADP	D	601	-	-	7/12/32/32	0/3/3/3
3	ADP	F	601	-	-	5/12/32/32	0/3/3/3
3	ADP	J	601	-	-	5/12/32/32	0/3/3/3
3	ADP	L	601	-	-	4/12/32/32	0/3/3/3
3	ADP	N	601	-	-	4/12/32/32	0/3/3/3
3	ADP	A	601	-	-	4/12/32/32	0/3/3/3
3	ADP	C	601	-	-	6/12/32/32	0/3/3/3
3	ADP	E	601	-	-	7/12/32/32	0/3/3/3
3	ADP	H	601	-	-	2/12/32/32	0/3/3/3
3	ADP	G	601	-	-	4/12/32/32	0/3/3/3
3	ADP	I	601	-	-	7/12/32/32	0/3/3/3
3	ADP	K	601	-	-	5/12/32/32	0/3/3/3
3	ADP	M	601	-	-	4/12/32/32	0/3/3/3
3	ADP	B	601	-	-	5/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	ADP	C5-C4	2.49	1.47	1.40
3	B	601	ADP	C5-C4	2.49	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	601	ADP	C5-C4	2.48	1.47	1.40
3	E	601	ADP	C5-C4	2.47	1.47	1.40
3	N	601	ADP	C5-C4	2.45	1.47	1.40
3	K	601	ADP	C5-C4	2.43	1.47	1.40
3	H	601	ADP	C5-C4	2.43	1.47	1.40
3	D	601	ADP	C5-C4	2.42	1.47	1.40
3	J	601	ADP	C5-C4	2.42	1.47	1.40
3	G	601	ADP	C5-C4	2.42	1.47	1.40
3	A	601	ADP	C5-C4	2.42	1.47	1.40
3	C	601	ADP	C5-C4	2.41	1.47	1.40
3	L	601	ADP	C5-C4	2.41	1.47	1.40
3	I	601	ADP	C5-C4	2.37	1.47	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	601	ADP	N3-C2-N1	-3.31	123.50	128.68
3	H	601	ADP	N3-C2-N1	-3.31	123.51	128.68
3	A	601	ADP	N3-C2-N1	-3.31	123.51	128.68
3	D	601	ADP	N3-C2-N1	-3.30	123.53	128.68
3	C	601	ADP	N3-C2-N1	-3.29	123.53	128.68
3	N	601	ADP	N3-C2-N1	-3.29	123.53	128.68
3	J	601	ADP	N3-C2-N1	-3.29	123.54	128.68
3	K	601	ADP	N3-C2-N1	-3.28	123.55	128.68
3	L	601	ADP	N3-C2-N1	-3.26	123.59	128.68
3	B	601	ADP	N3-C2-N1	-3.25	123.60	128.68
3	E	601	ADP	N3-C2-N1	-3.23	123.63	128.68
3	F	601	ADP	N3-C2-N1	-3.22	123.64	128.68
3	C	601	ADP	PA-O3A-PB	-3.22	121.79	132.83
3	G	601	ADP	N3-C2-N1	-3.17	123.72	128.68
3	M	601	ADP	N3-C2-N1	-3.17	123.72	128.68
3	A	601	ADP	PA-O3A-PB	-3.16	121.98	132.83
3	G	601	ADP	PA-O3A-PB	-3.15	122.00	132.83
3	K	601	ADP	PA-O3A-PB	-3.05	122.35	132.83
3	I	601	ADP	PA-O3A-PB	-3.04	122.39	132.83
3	L	601	ADP	PA-O3A-PB	-3.01	122.48	132.83
3	N	601	ADP	C4-C5-N7	-2.97	106.30	109.40
3	F	601	ADP	PA-O3A-PB	-2.96	122.68	132.83
3	H	601	ADP	PA-O3A-PB	-2.95	122.71	132.83
3	I	601	ADP	C4-C5-N7	-2.93	106.35	109.40
3	M	601	ADP	PA-O3A-PB	-2.88	122.93	132.83
3	C	601	ADP	C4-C5-N7	-2.83	106.45	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	601	ADP	C4-C5-N7	-2.81	106.47	109.40
3	D	601	ADP	C4-C5-N7	-2.79	106.49	109.40
3	B	601	ADP	C4-C5-N7	-2.79	106.50	109.40
3	M	601	ADP	C3'-C2'-C1'	2.78	105.17	100.98
3	N	601	ADP	PA-O3A-PB	-2.78	123.29	132.83
3	K	601	ADP	C4-C5-N7	-2.77	106.51	109.40
3	L	601	ADP	C4-C5-N7	-2.76	106.52	109.40
3	A	601	ADP	C4-C5-N7	-2.74	106.54	109.40
3	H	601	ADP	C4-C5-N7	-2.74	106.55	109.40
3	D	601	ADP	PA-O3A-PB	-2.72	123.50	132.83
3	G	601	ADP	C4-C5-N7	-2.71	106.57	109.40
3	B	601	ADP	PA-O3A-PB	-2.71	123.53	132.83
3	E	601	ADP	C4-C5-N7	-2.70	106.58	109.40
3	F	601	ADP	C4-C5-N7	-2.69	106.59	109.40
3	M	601	ADP	C4-C5-N7	-2.68	106.61	109.40
3	E	601	ADP	PA-O3A-PB	-2.61	123.85	132.83
3	J	601	ADP	PA-O3A-PB	-2.53	124.15	132.83
3	E	601	ADP	C3'-C2'-C1'	2.45	104.66	100.98
3	B	601	ADP	C3'-C2'-C1'	2.29	104.43	100.98
3	F	601	ADP	C3'-C2'-C1'	2.27	104.40	100.98
3	C	601	ADP	C3'-C2'-C1'	2.20	104.29	100.98
3	G	601	ADP	C3'-C2'-C1'	2.19	104.28	100.98
3	A	601	ADP	C3'-C2'-C1'	2.02	104.02	100.98

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	ADP	PA-O3A-PB-O3B
3	D	601	ADP	C5'-O5'-PA-O1A
3	D	601	ADP	C5'-O5'-PA-O2A
3	E	601	ADP	C5'-O5'-PA-O3A
3	E	601	ADP	C3'-C4'-C5'-O5'
3	F	601	ADP	C5'-O5'-PA-O3A
3	F	601	ADP	C3'-C4'-C5'-O5'
3	L	601	ADP	C5'-O5'-PA-O2A
3	N	601	ADP	PB-O3A-PA-O5'
3	A	601	ADP	PB-O3A-PA-O5'
3	A	601	ADP	C5'-O5'-PA-O1A
3	A	601	ADP	C5'-O5'-PA-O2A
3	C	601	ADP	PB-O3A-PA-O5'
3	C	601	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	601	ADP	C5'-O5'-PA-O2A
3	I	601	ADP	C5'-O5'-PA-O2A
3	I	601	ADP	C5'-O5'-PA-O3A
3	J	601	ADP	C5'-O5'-PA-O2A
3	K	601	ADP	C5'-O5'-PA-O2A
3	B	601	ADP	PA-O3A-PB-O2B
3	B	601	ADP	C5'-O5'-PA-O1A
3	B	601	ADP	C5'-O5'-PA-O2A
3	M	601	ADP	PA-O3A-PB-O2B
3	G	601	ADP	O4'-C4'-C5'-O5'
3	G	601	ADP	C3'-C4'-C5'-O5'
3	M	601	ADP	O4'-C4'-C5'-O5'
3	M	601	ADP	C3'-C4'-C5'-O5'
3	E	601	ADP	O4'-C4'-C5'-O5'
3	F	601	ADP	O4'-C4'-C5'-O5'
3	I	601	ADP	O4'-C4'-C5'-O5'
3	I	601	ADP	C3'-C4'-C5'-O5'
3	C	601	ADP	C3'-C4'-C5'-O5'
3	I	601	ADP	PB-O3A-PA-O1A
3	J	601	ADP	PB-O3A-PA-O1A
3	N	601	ADP	PA-O3A-PB-O1B
3	L	601	ADP	C5'-O5'-PA-O3A
3	J	601	ADP	C5'-O5'-PA-O3A
3	K	601	ADP	C5'-O5'-PA-O3A
3	C	601	ADP	O4'-C4'-C5'-O5'
3	K	601	ADP	PB-O3A-PA-O2A
3	E	601	ADP	C5'-O5'-PA-O1A
3	F	601	ADP	C5'-O5'-PA-O1A
3	L	601	ADP	C5'-O5'-PA-O1A
3	I	601	ADP	C5'-O5'-PA-O1A
3	J	601	ADP	C5'-O5'-PA-O1A
3	K	601	ADP	C5'-O5'-PA-O1A
3	M	601	ADP	C5'-O5'-PA-O1A
3	D	601	ADP	C3'-C4'-C5'-O5'
3	B	601	ADP	C3'-C4'-C5'-O5'
3	I	601	ADP	PB-O3A-PA-O2A
3	J	601	ADP	PB-O3A-PA-O2A
3	H	601	ADP	PB-O3A-PA-O2A
3	E	601	ADP	PA-O3A-PB-O1B
3	L	601	ADP	PB-O3A-PA-O2A
3	G	601	ADP	PB-O3A-PA-O2A
3	D	601	ADP	PA-O3A-PB-O1B

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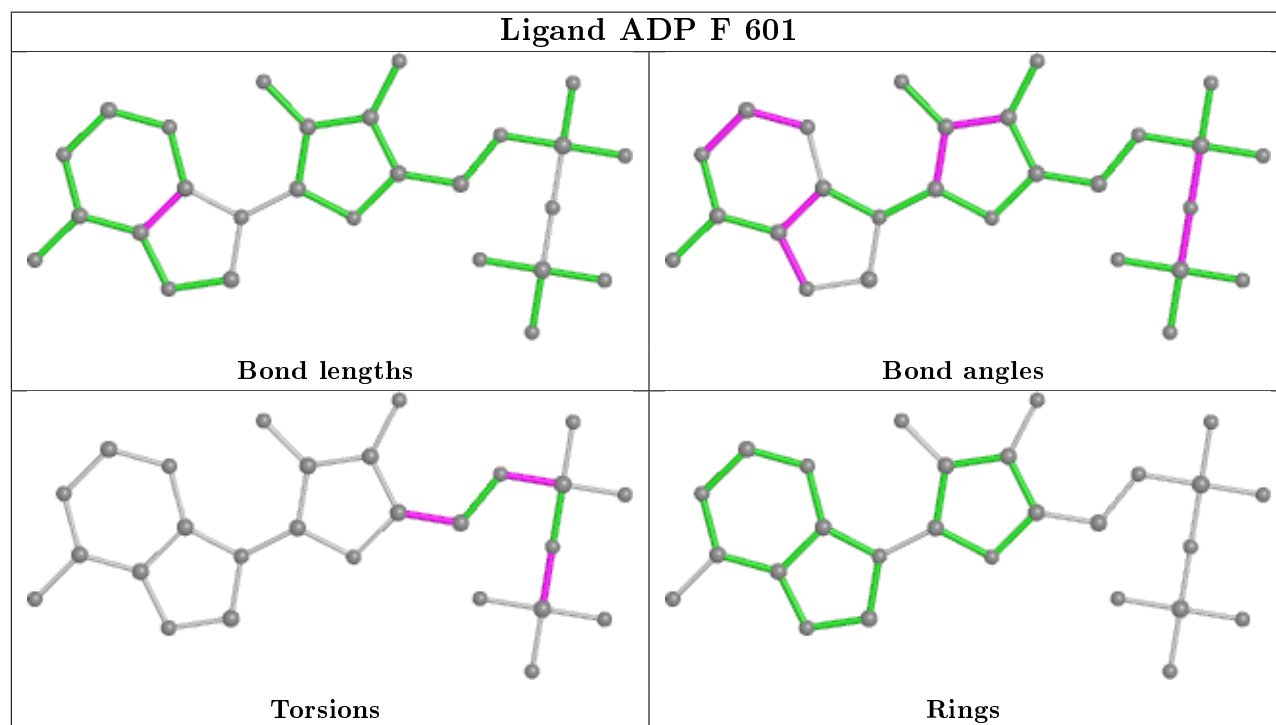
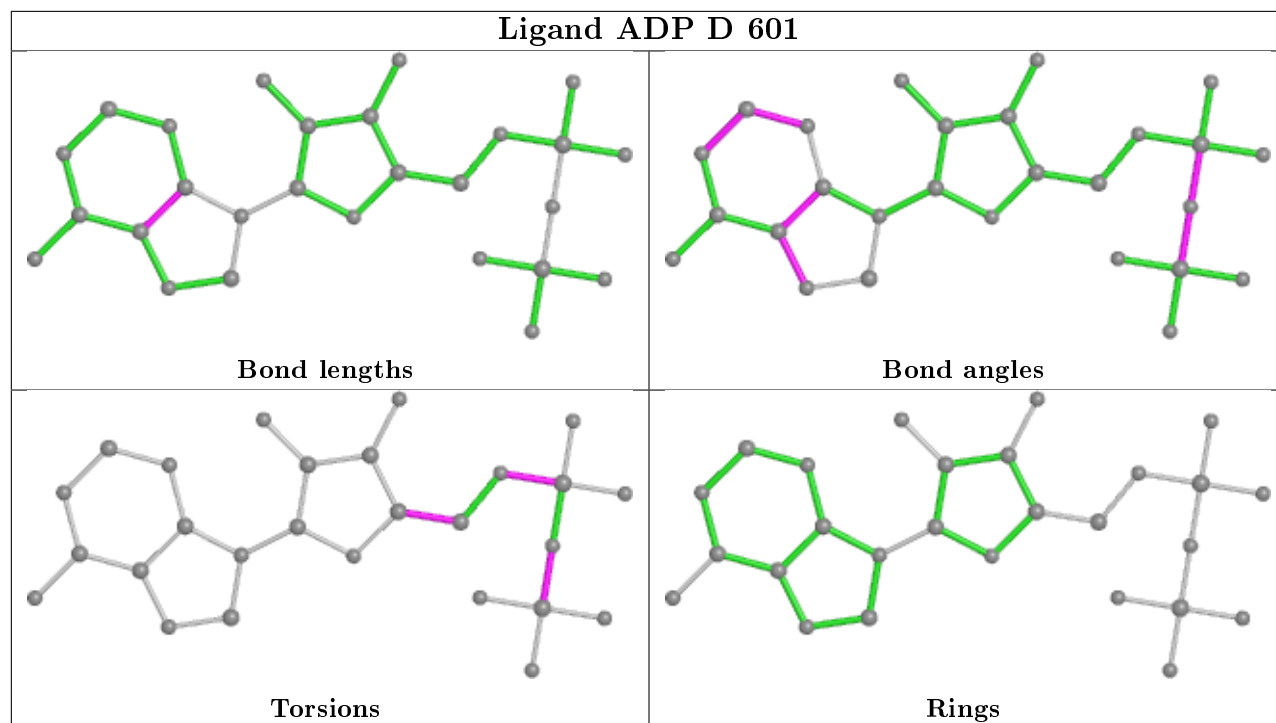
Mol	Chain	Res	Type	Atoms
3	D	601	ADP	PA-O3A-PB-O2B
3	E	601	ADP	PA-O3A-PB-O2B
3	E	601	ADP	PA-O3A-PB-O3B
3	F	601	ADP	PA-O3A-PB-O2B
3	N	601	ADP	PA-O3A-PB-O2B
3	N	601	ADP	PA-O3A-PB-O3B
3	D	601	ADP	C5'-O5'-PA-O3A
3	A	601	ADP	C5'-O5'-PA-O3A
3	C	601	ADP	C5'-O5'-PA-O3A
3	B	601	ADP	C5'-O5'-PA-O3A
3	H	601	ADP	PB-O3A-PA-O1A
3	K	601	ADP	PB-O3A-PA-O1A
3	G	601	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

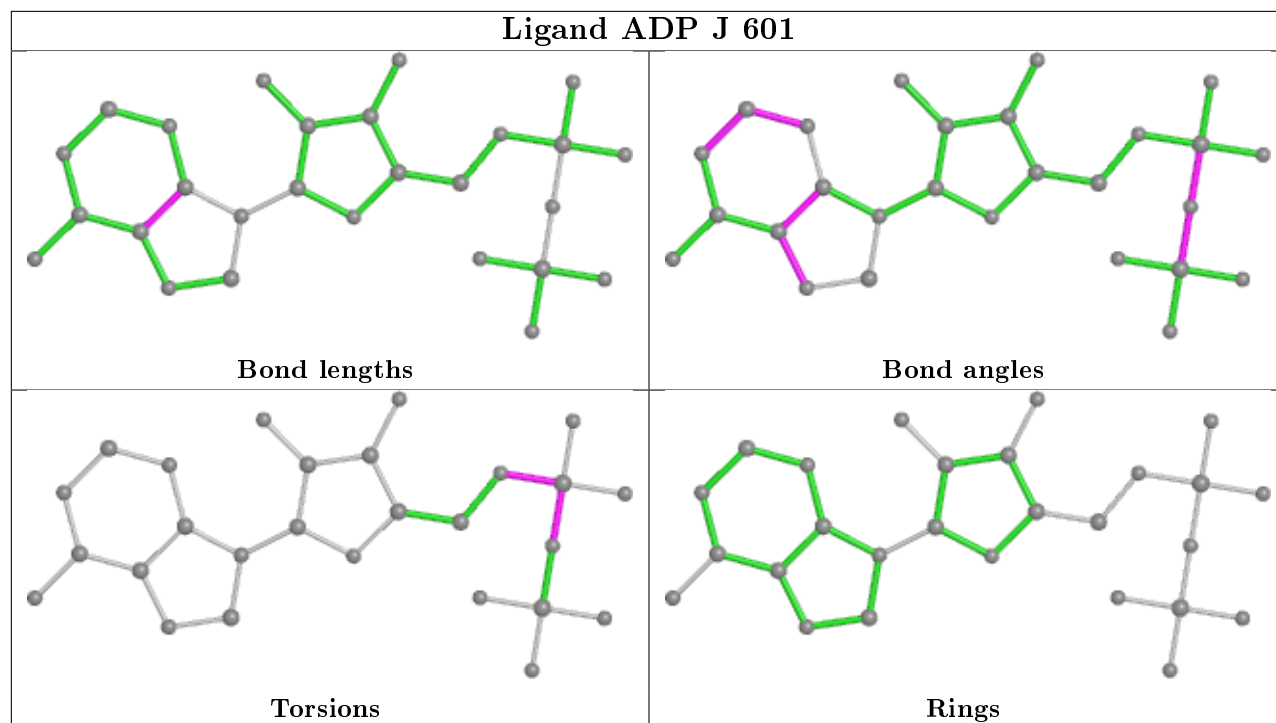
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	ADP	1	0
3	L	601	ADP	1	0
3	N	601	ADP	2	0
3	A	601	ADP	2	0
3	C	601	ADP	2	0
3	I	601	ADP	1	0
3	K	601	ADP	1	0
3	B	601	ADP	2	0

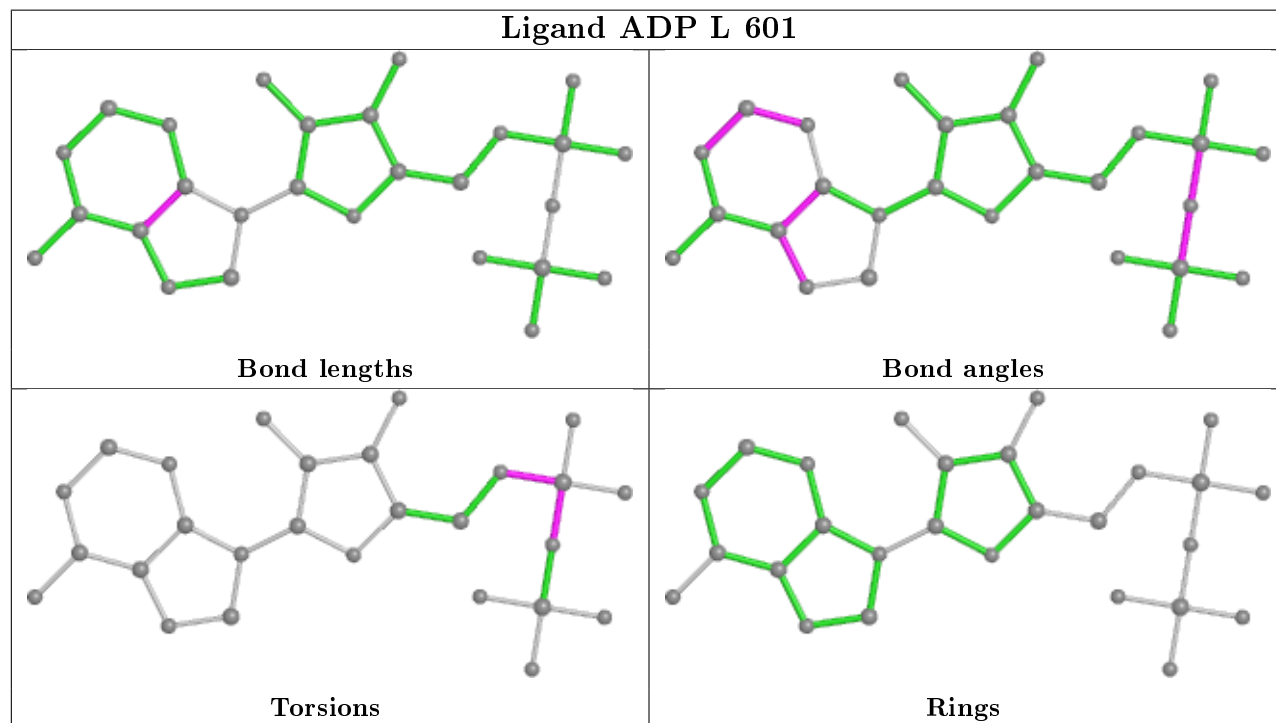
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

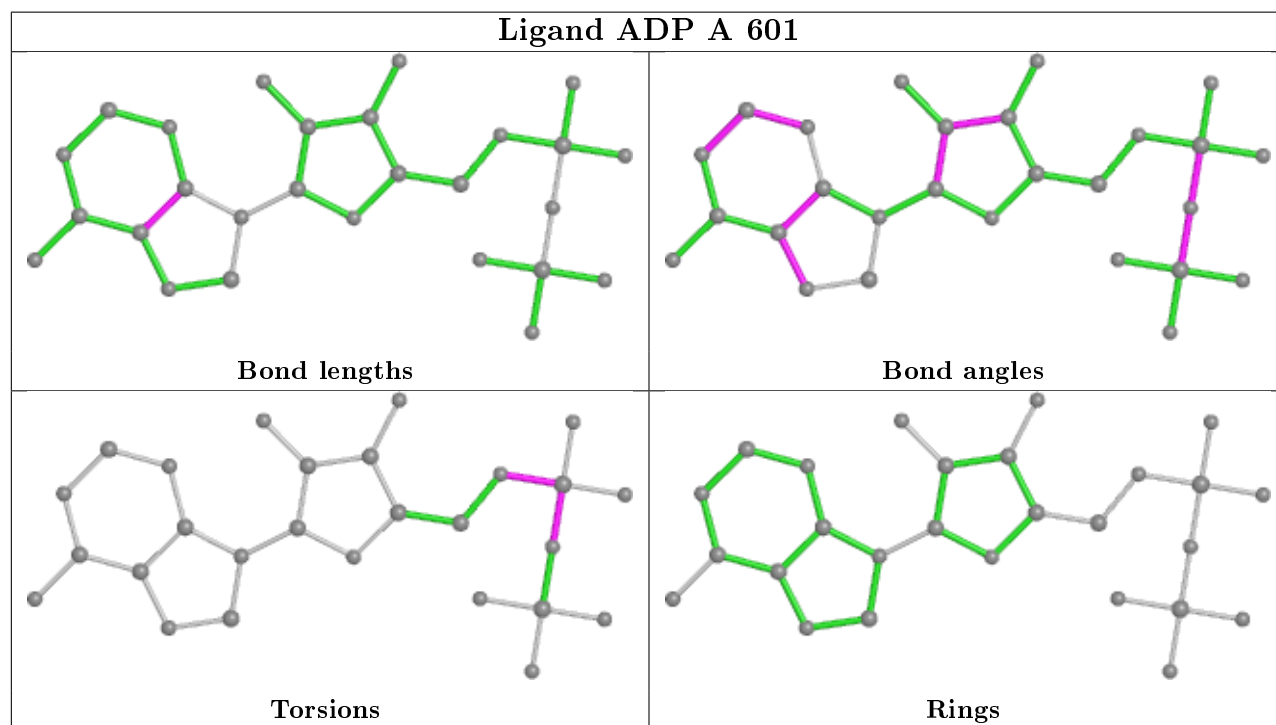
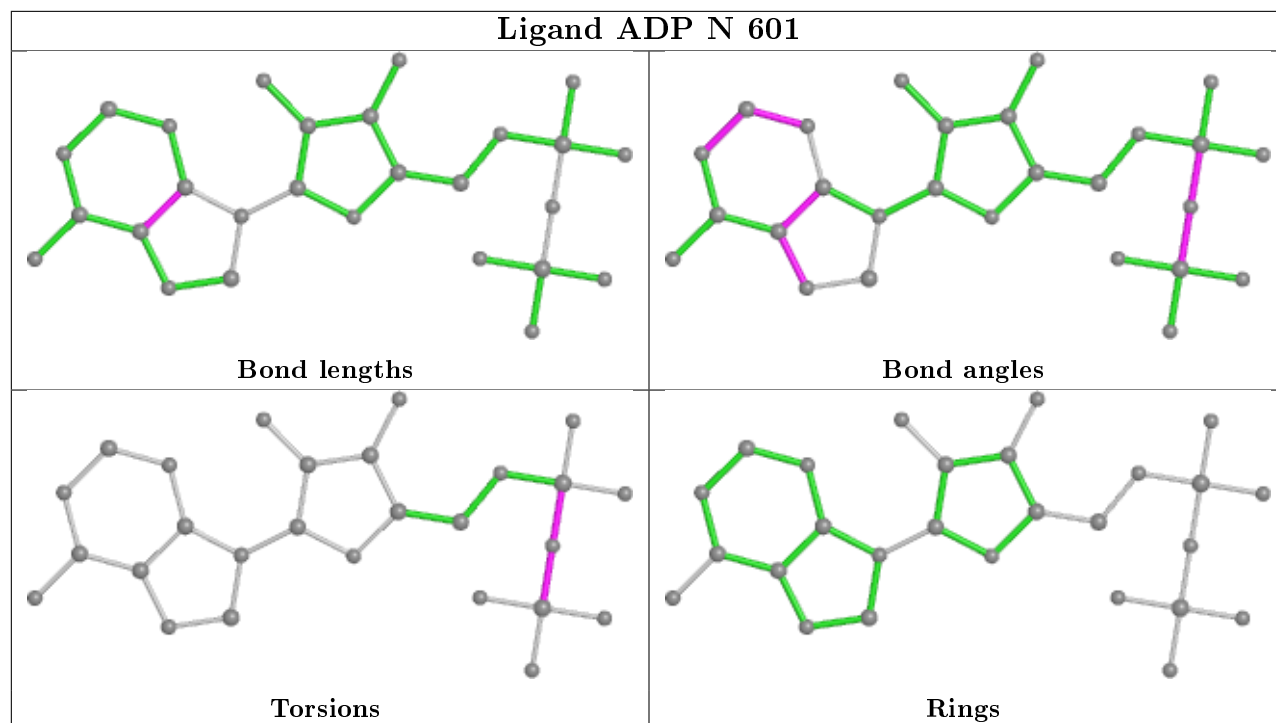


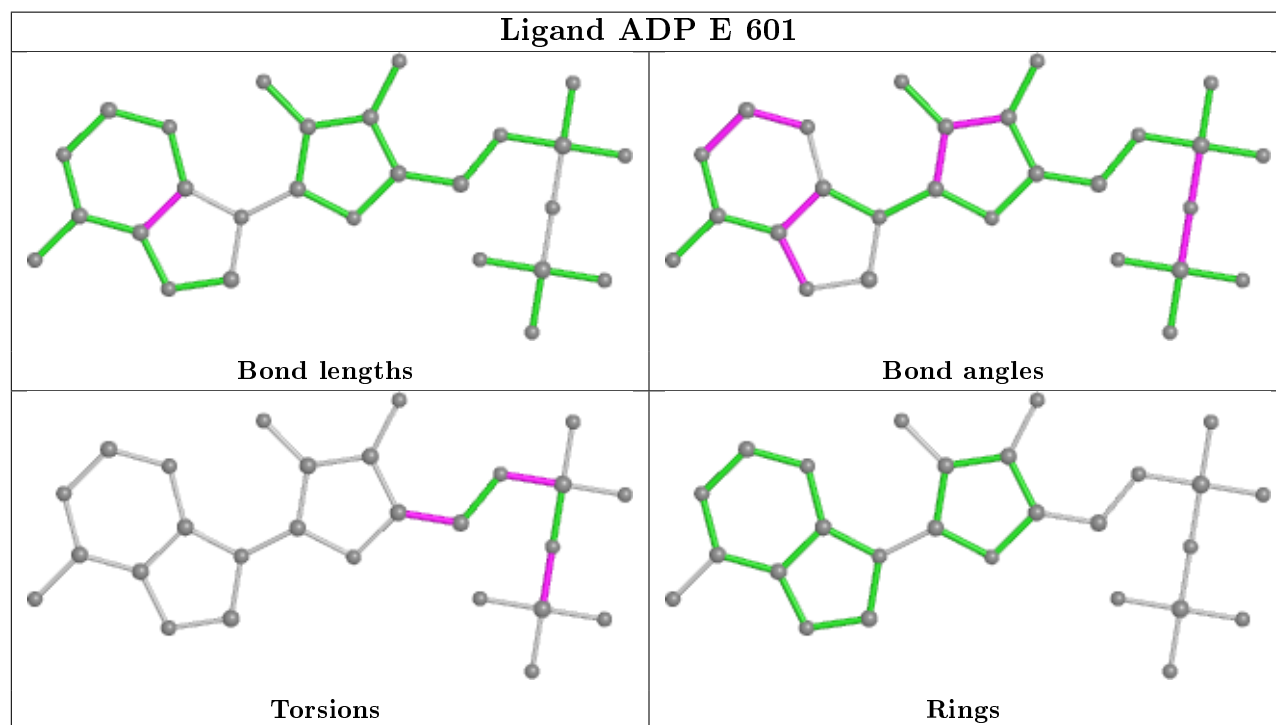
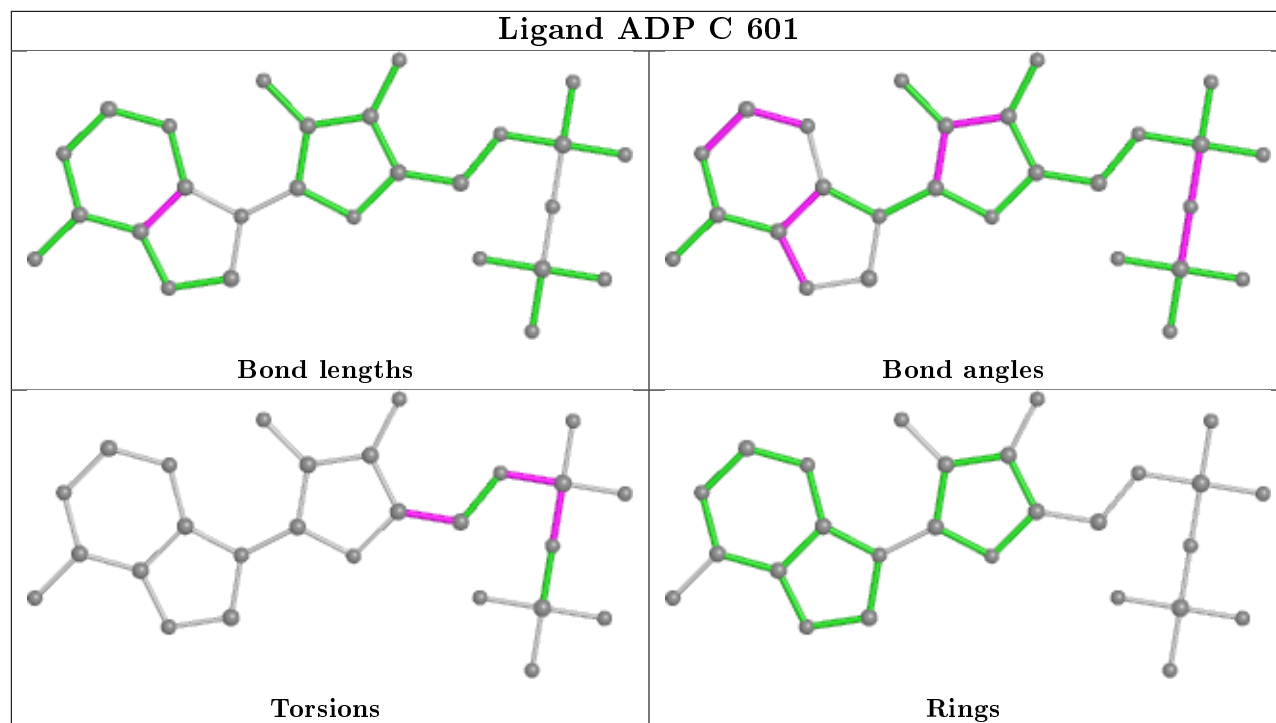
Ligand ADP J 601

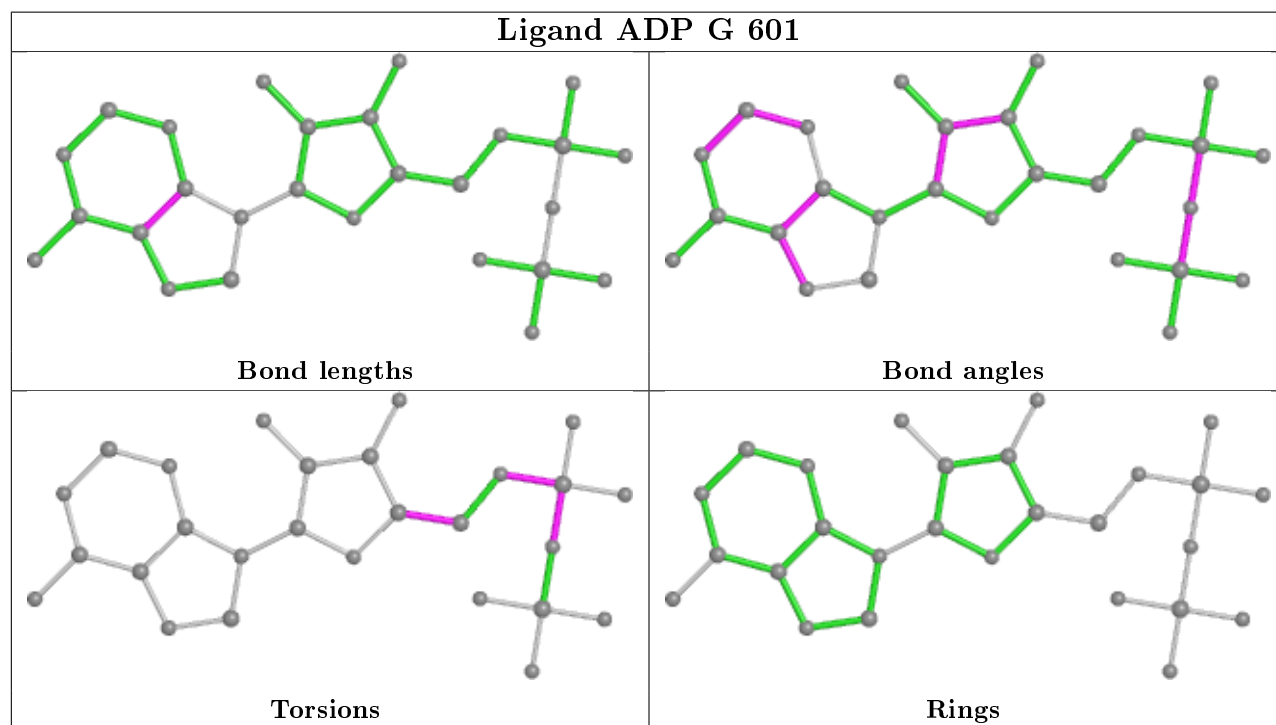
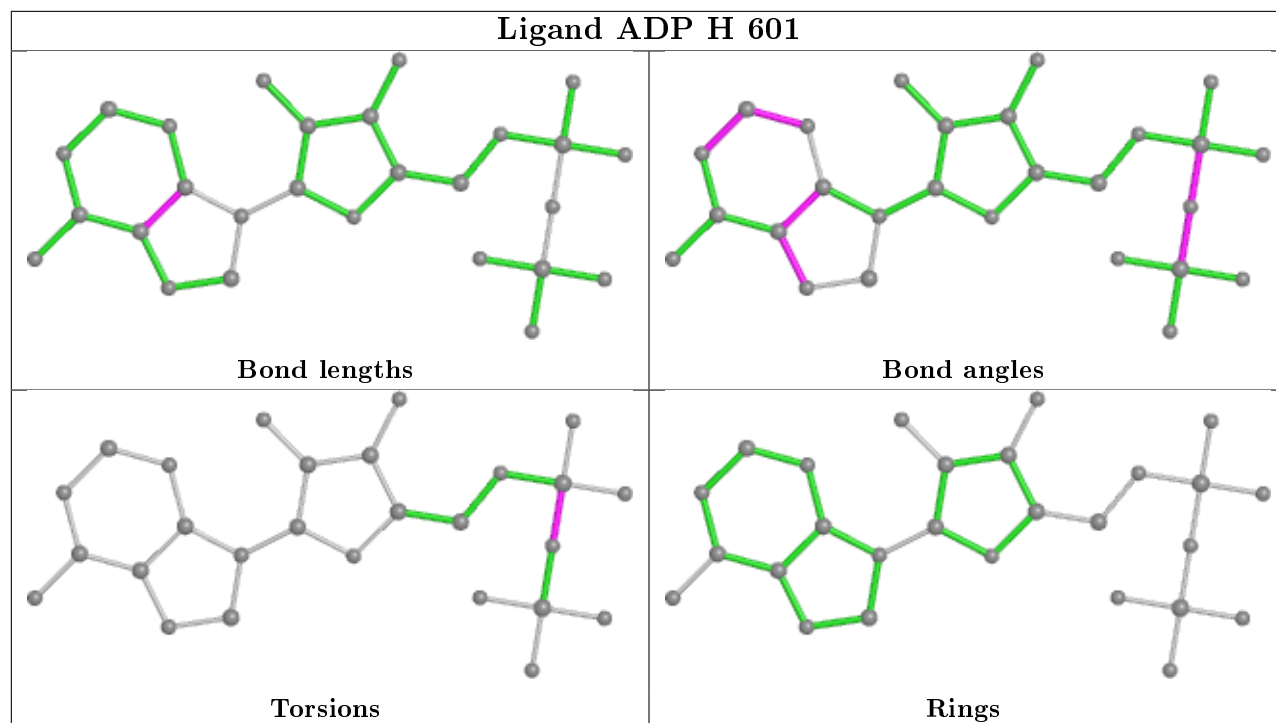


Ligand ADP L 601

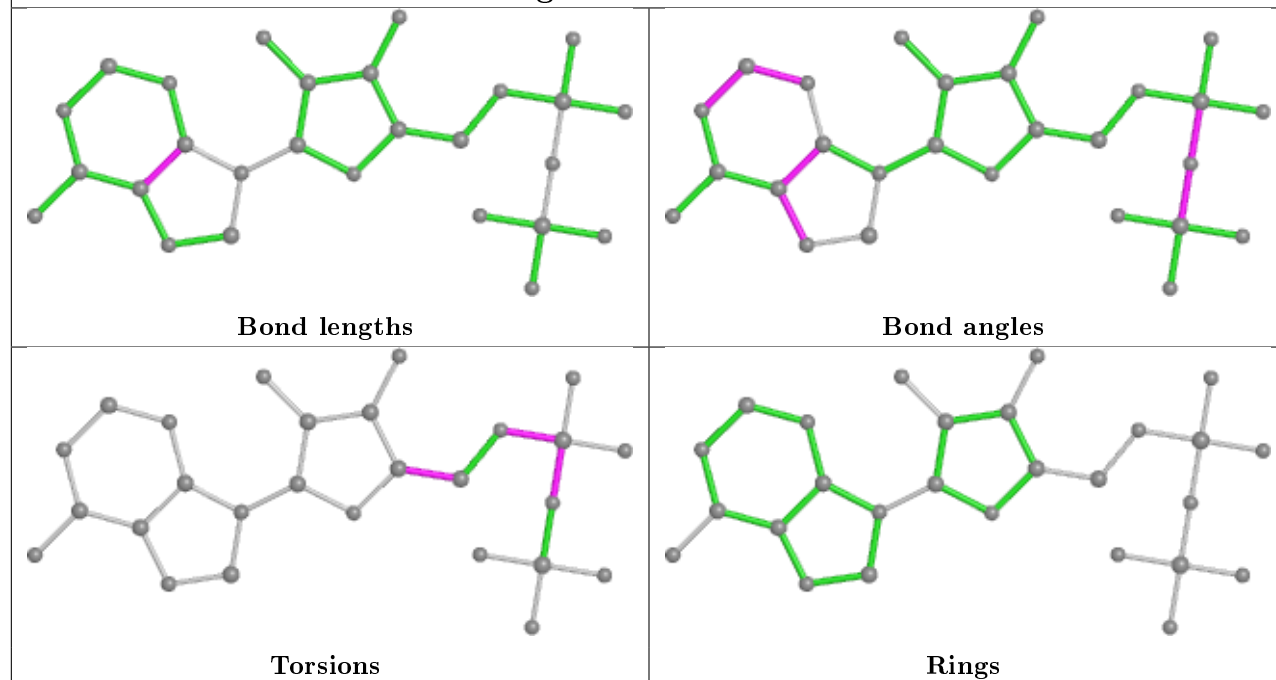




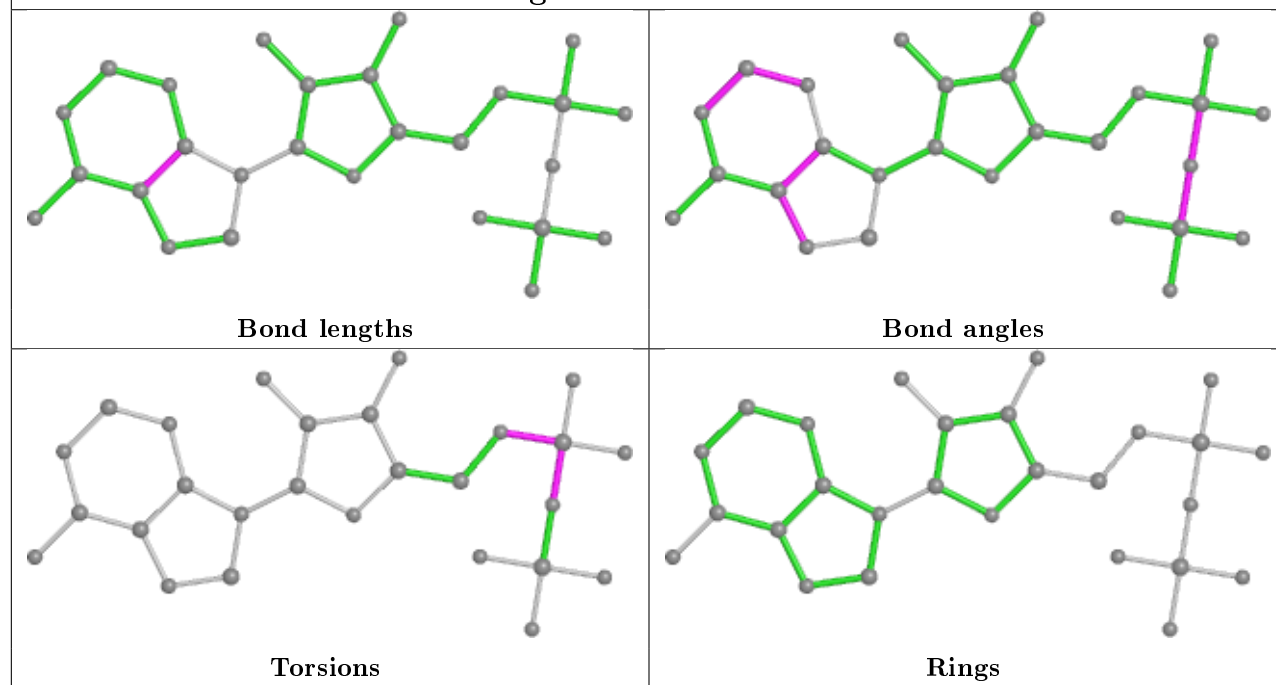


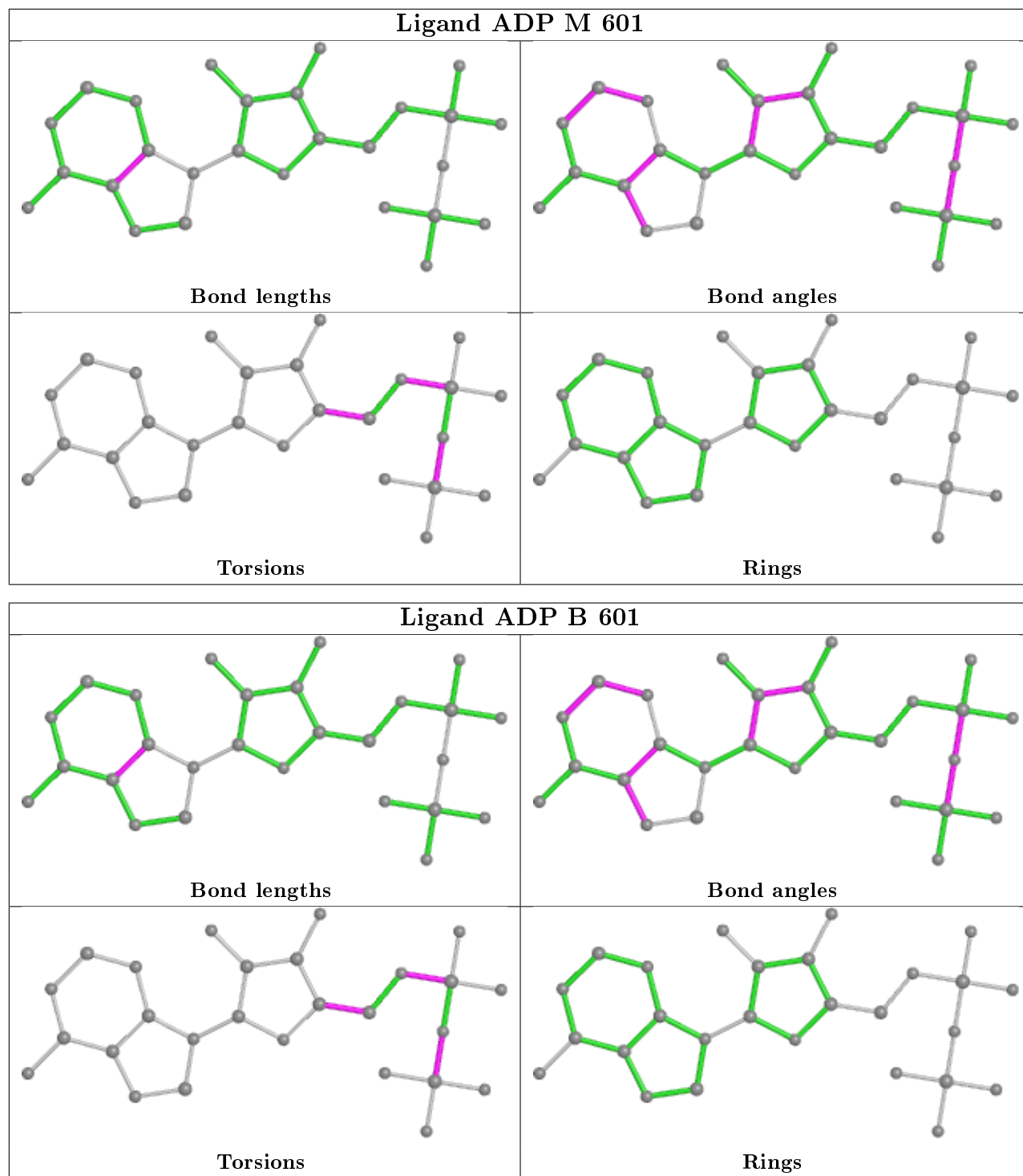


Ligand ADP I 601



Ligand ADP K 601





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	526/558 (94%)	0.22	26 (4%) 29 16	65, 112, 194, 225	0
1	B	526/558 (94%)	0.52	47 (8%) 9 5	66, 116, 232, 279	0
1	C	526/558 (94%)	0.03	10 (1%) 66 53	66, 109, 169, 217	0
1	D	526/558 (94%)	0.17	21 (3%) 38 23	61, 107, 195, 228	0
1	E	526/558 (94%)	0.15	13 (2%) 57 42	66, 106, 202, 226	0
1	F	526/558 (94%)	0.12	14 (2%) 54 38	67, 110, 166, 192	0
1	G	526/558 (94%)	0.04	5 (0%) 82 73	67, 102, 153, 196	0
1	H	526/558 (94%)	0.05	9 (1%) 70 57	66, 103, 160, 191	0
1	I	526/558 (94%)	0.14	11 (2%) 63 49	64, 103, 179, 203	0
1	J	526/558 (94%)	0.12	13 (2%) 57 42	65, 107, 164, 191	0
1	K	526/558 (94%)	0.12	15 (2%) 51 35	61, 106, 167, 207	0
1	L	526/558 (94%)	0.06	6 (1%) 80 70	66, 101, 151, 182	0
1	M	526/558 (94%)	0.12	7 (1%) 77 66	66, 112, 169, 207	0
1	N	526/558 (94%)	0.13	9 (1%) 70 57	70, 110, 165, 202	0
2	1	100/114 (87%)	0.17	3 (3%) 50 33	94, 117, 179, 210	0
2	2	104/114 (91%)	0.37	5 (4%) 30 17	101, 135, 185, 200	0
2	O	100/114 (87%)	0.45	4 (4%) 38 23	107, 139, 185, 194	0
2	P	105/114 (92%)	0.10	1 (0%) 82 73	93, 121, 199, 209	0
2	Q	100/114 (87%)	0.28	3 (3%) 50 33	84, 114, 179, 199	0
2	R	100/114 (87%)	0.69	12 (12%) 4 2	97, 136, 187, 201	0
2	S	100/114 (87%)	0.83	17 (17%) 1 1	127, 158, 194, 202	0
2	T	100/114 (87%)	0.87	16 (16%) 1 1	123, 157, 195, 224	0
2	U	102/114 (89%)	0.56	9 (8%) 10 5	121, 145, 193, 223	0
2	V	100/114 (87%)	0.45	5 (5%) 28 15	107, 134, 181, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	100/114 (87%)	0.35	8 (8%) 12 6	118, 145, 182, 197	0
2	X	100/114 (87%)	0.71	9 (9%) 9 5	118, 141, 201, 210	0
2	Y	100/114 (87%)	0.20	5 (5%) 28 15	97, 124, 181, 216	0
2	Z	108/114 (94%)	0.16	5 (4%) 32 18	91, 118, 170, 216	0
All	All	8783/9408 (93%)	0.19	308 (3%) 44 27	61, 113, 185, 279	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	305	GLY	10.5
1	L	374	SER	10.2
2	Y	55	GLY	9.6
1	B	358	THR	9.0
1	B	269	VAL	8.4
1	B	359	SER	8.3
2	U	56	LYS	8.2
1	B	210	GLY	8.0
1	B	270	GLY	7.8
1	K	358	THR	7.0
1	J	171	ARG	7.0
2	U	37	SER	6.8
2	X	56	LYS	6.4
1	E	305	GLY	6.3
1	B	302	GLY	6.2
2	T	56	LYS	6.0
1	A	223	SER	6.0
1	L	171	ARG	6.0
1	B	360	GLU	5.9
2	Q	56	LYS	5.8
2	U	55	GLY	5.8
1	B	357	THR	5.8
1	N	231	GLN	5.6
1	B	303	GLU	5.4
1	B	212	LYS	5.2
1	B	254	VAL	5.2
1	L	375	ASP	5.2
2	1	55	GLY	5.1
2	Q	55	GLY	5.1
2	T	55	GLY	4.8
1	B	367	ASN	4.8
2	Z	56	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	193	MET	4.7
2	U	54	LYS	4.7
2	R	56	LYS	4.7
1	J	375	ASP	4.6
1	K	357	THR	4.6
1	B	245	LYS	4.6
1	M	374	SER	4.6
2	W	54	LYS	4.5
1	F	304	GLU	4.5
1	N	235	PRO	4.5
1	K	306	LEU	4.4
2	2	56	LYS	4.4
2	T	4	GLN	4.4
1	N	358	THR	4.4
1	I	374	SER	4.4
1	B	352	GLU	4.4
1	G	357	THR	4.3
1	D	303	GLU	4.3
2	U	57	GLY	4.3
1	I	305	GLY	4.1
1	I	303	GLU	4.1
2	R	55	GLY	4.1
1	K	304	GLU	4.0
1	B	355	ASP	4.0
1	B	209	LYS	4.0
2	X	55	GLY	3.9
1	D	219	TYR	3.9
1	B	272	GLN	3.8
2	X	4	GLN	3.8
1	E	298	GLY	3.8
2	T	83	LEU	3.8
1	B	370	LEU	3.8
1	E	358	THR	3.7
2	P	56	LYS	3.7
2	T	53	SER	3.7
1	B	262	LEU	3.7
1	B	213	CYS	3.7
1	C	375	ASP	3.7
1	L	376	GLY	3.5
2	Q	54	LYS	3.5
2	V	54	LYS	3.5
1	D	317	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	353	GLN	3.5
2	S	55	GLY	3.5
1	D	359	SER	3.4
2	2	55	GLY	3.3
2	S	83	LEU	3.3
2	X	17	LEU	3.3
1	M	380	LEU	3.3
1	K	308	LEU	3.3
1	F	374	SER	3.3
1	A	359	SER	3.3
1	B	371	ALA	3.3
2	1	56	LYS	3.3
1	F	270	GLY	3.2
1	B	203	TYR	3.2
1	A	358	THR	3.2
1	G	375	ASP	3.2
1	H	356	VAL	3.2
1	B	271	LEU	3.2
2	O	56	LYS	3.2
1	A	302	GLY	3.1
1	L	303	GLU	3.1
2	R	27	THR	3.1
1	M	1	GLY	3.0
2	R	9	PHE	3.0
1	D	318	LEU	3.0
1	F	305	GLY	3.0
1	A	304	GLU	3.0
2	X	47	VAL	3.0
1	I	375	ASP	3.0
1	F	204	PHE	3.0
2	S	9	PHE	3.0
2	Y	56	LYS	3.0
1	A	207	THR	3.0
2	S	30	GLY	3.0
1	J	204	PHE	3.0
2	X	66	LYS	3.0
2	T	54	LYS	3.0
1	F	358	THR	3.0
2	Y	4	GLN	3.0
1	A	289	LEU	2.9
2	Z	57	GLY	2.9
1	B	217	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	Z	55	GLY	2.9
2	V	55	GLY	2.9
2	O	55	GLY	2.9
1	J	228	SER	2.9
1	F	353	GLN	2.8
1	I	212	LYS	2.8
2	Z	59	GLU	2.8
2	1	4	GLN	2.8
1	B	324	VAL	2.8
2	W	8	LYS	2.8
1	D	374	SER	2.8
1	A	208	SER	2.8
1	M	210	GLY	2.8
1	C	209	LYS	2.8
2	S	17	LEU	2.8
1	D	358	THR	2.8
2	2	54	LYS	2.7
1	K	307	THR	2.7
1	F	269	VAL	2.7
1	D	316	HIS	2.7
1	J	303	GLU	2.7
1	E	375	ASP	2.7
2	X	48	ALA	2.7
1	E	255	ASP	2.7
1	D	304	GLU	2.7
1	A	254	VAL	2.7
1	E	307	THR	2.7
1	E	355	ASP	2.7
1	A	209	LYS	2.7
1	F	271	LEU	2.7
1	G	303	GLU	2.7
1	B	250	ILE	2.7
1	B	261	THR	2.6
1	L	369	ARG	2.6
1	B	268	LYS	2.6
1	H	273	VAL	2.6
1	E	171	ARG	2.6
2	V	48	ALA	2.6
2	R	76	TYR	2.6
1	A	165	ALA	2.6
1	N	215	PHE	2.6
2	S	89	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	292	MET	2.6
1	B	368	GLU	2.6
1	B	298	GLY	2.5
1	C	369	ARG	2.5
1	J	376	GLY	2.5
1	F	206	ASN	2.5
2	W	9	PHE	2.5
1	F	203	TYR	2.5
1	I	306	LEU	2.5
1	B	185	ASP	2.5
1	B	242	ALA	2.5
2	R	29	GLY	2.5
1	C	363	LYS	2.5
2	R	17	LEU	2.5
2	S	73	LEU	2.5
1	E	217	ASP	2.5
2	S	56	LYS	2.5
1	A	354	LEU	2.5
2	T	71	VAL	2.5
1	D	375	ASP	2.5
1	G	304	GLU	2.4
1	J	382	VAL	2.4
2	R	73	LEU	2.4
1	J	203	TYR	2.4
1	A	343	ILE	2.4
1	A	355	ASP	2.4
1	H	374	SER	2.4
1	E	275	ALA	2.4
1	F	265	ASN	2.4
1	B	273	VAL	2.4
1	B	206	ASN	2.4
1	B	204	PHE	2.4
1	K	375	ASP	2.4
1	H	213	CYS	2.4
2	T	44	ALA	2.4
1	N	234	VAL	2.4
1	N	262	LEU	2.4
2	S	90	LEU	2.4
1	C	270	GLY	2.4
1	M	268	LYS	2.4
1	K	352	GLU	2.4
1	B	350	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	281	PHE	2.4
1	F	354	LEU	2.4
1	I	230	ILE	2.3
2	X	100	TYR	2.3
1	B	255	ASP	2.3
1	H	185	ASP	2.3
2	T	3	GLY	2.3
2	W	98	GLY	2.3
2	R	83	LEU	2.3
1	B	369	ARG	2.3
1	J	374	SER	2.3
2	O	22	ALA	2.3
1	D	307	THR	2.3
1	M	227	ILE	2.3
1	A	266	ARG	2.3
2	X	44	ALA	2.3
1	B	192	GLY	2.3
1	B	247	LEU	2.3
1	K	213	CYS	2.3
1	D	289	LEU	2.3
1	I	229	SER	2.3
1	D	212	LYS	2.3
1	D	236	ALA	2.3
1	C	383	GLY	2.3
1	K	374	SER	2.3
2	S	61	GLN	2.2
2	R	59	GLU	2.2
2	V	56	LYS	2.2
1	A	202	PRO	2.2
1	C	254	VAL	2.2
1	J	368	GLU	2.2
2	U	4	GLN	2.2
1	B	351	ILE	2.2
1	A	347	ILE	2.2
2	S	91	PHE	2.2
2	T	91	PHE	2.2
1	E	269	VAL	2.2
2	S	47	VAL	2.2
1	D	191	GLU	2.2
1	E	199	TYR	2.2
1	H	375	ASP	2.2
1	N	359	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	S	84	ASP	2.2
1	A	333	LEU	2.2
1	A	364	GLU	2.2
1	J	359	SER	2.2
2	U	25	THR	2.2
1	K	316	HIS	2.2
2	T	16	VAL	2.2
1	N	376	GLY	2.2
1	G	342	GLN	2.2
1	K	354	LEU	2.2
2	S	81	VAL	2.2
2	Y	49	VAL	2.2
2	W	55	GLY	2.2
2	V	101	VAL	2.2
1	K	209	LYS	2.2
1	K	334	LEU	2.2
1	A	281	PHE	2.2
1	B	349	GLU	2.2
2	Z	60	ILE	2.2
1	H	171	ARG	2.2
2	O	54	LYS	2.2
2	W	53	SER	2.1
2	R	75	GLU	2.1
2	T	80	LYS	2.1
2	T	99	LYS	2.1
2	S	76	TYR	2.1
2	T	9	PHE	2.1
1	I	270	GLY	2.1
1	B	316	HIS	2.1
1	B	325	ILE	2.1
1	D	144	ILE	2.1
1	A	356	VAL	2.1
1	A	377	VAL	2.1
1	J	227	ILE	2.1
1	A	204	PHE	2.1
1	A	169	VAL	2.1
1	C	368	GLU	2.1
1	D	360	GLU	2.1
2	W	66	LYS	2.1
1	H	274	VAL	2.1
2	S	29	GLY	2.1
2	U	83	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	307	THR	2.1
2	T	101	VAL	2.1
2	U	60	ILE	2.1
1	J	322	GLY	2.1
1	I	206	ASN	2.1
1	D	356	VAL	2.1
1	D	222	LEU	2.1
1	C	186	GLU	2.1
2	W	56	LYS	2.1
2	2	59	GLU	2.1
1	A	251	ALA	2.1
1	B	310	LEU	2.1
1	E	310	LEU	2.1
2	S	80	LYS	2.0
2	Y	54	LYS	2.0
1	M	301	PHE	2.0
2	T	32	MET	2.0
1	D	204	PHE	2.0
1	H	303	GLU	2.0
1	N	357	THR	2.0
2	2	39	GLY	2.0
1	D	321	VAL	2.0
1	F	1	GLY	2.0
2	R	32	MET	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](#)

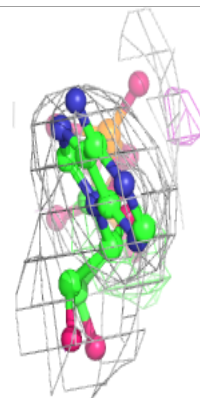
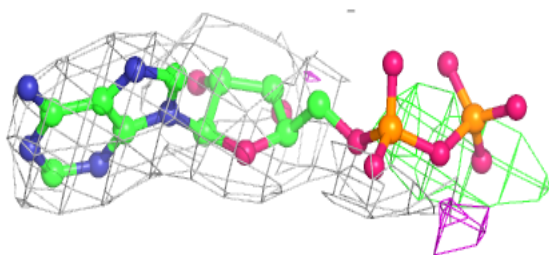
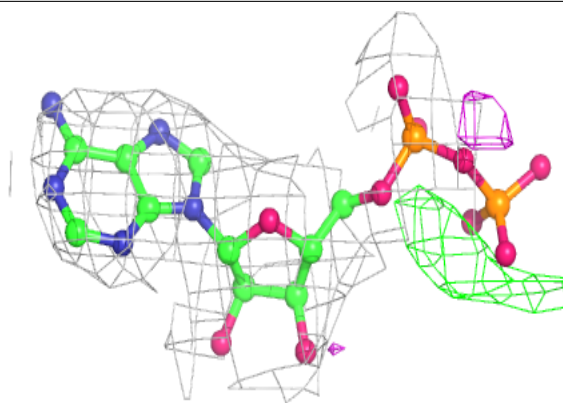
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	E	601	27/27	0.88	0.27	69,80,89,93	0
3	ADP	N	601	27/27	0.91	0.23	72,87,97,99	0
3	ADP	J	601	27/27	0.91	0.23	69,88,94,105	0
3	ADP	K	601	27/27	0.91	0.25	67,87,96,104	0
3	ADP	A	601	27/27	0.92	0.23	68,90,102,104	0
3	ADP	C	601	27/27	0.92	0.26	69,90,104,110	0
3	ADP	I	601	27/27	0.92	0.27	61,86,93,96	0
3	ADP	F	601	27/27	0.92	0.26	62,87,92,94	0
3	ADP	H	601	27/27	0.92	0.27	75,87,95,98	0
3	ADP	D	601	27/27	0.92	0.25	62,86,98,100	0
3	ADP	B	601	27/27	0.92	0.23	74,98,105,115	0
3	ADP	G	601	27/27	0.92	0.27	65,81,90,97	0
4	MG	B	602	1/1	0.94	0.28	74,74,74,74	0
4	MG	D	602	1/1	0.94	0.28	77,77,77,77	0
3	ADP	L	601	27/27	0.94	0.26	63,85,94,95	0
3	ADP	M	601	27/27	0.94	0.23	69,87,93,95	0
4	MG	H	602	1/1	0.95	0.34	73,73,73,73	0
4	MG	G	602	1/1	0.95	0.25	67,67,67,67	0
4	MG	J	602	1/1	0.95	0.29	66,66,66,66	0
4	MG	N	602	1/1	0.95	0.29	81,81,81,81	0
4	MG	I	602	1/1	0.96	0.29	60,60,60,60	0
4	MG	C	602	1/1	0.97	0.32	84,84,84,84	0
4	MG	K	602	1/1	0.98	0.27	61,61,61,61	0
4	MG	A	602	1/1	0.98	0.26	72,72,72,72	0
4	MG	E	602	1/1	0.98	0.30	62,62,62,62	0
4	MG	F	602	1/1	0.98	0.32	66,66,66,66	0
4	MG	L	602	1/1	0.98	0.32	72,72,72,72	0
4	MG	M	602	1/1	0.99	0.29	60,60,60,60	0

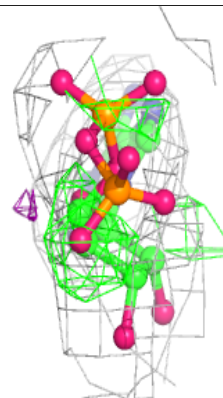
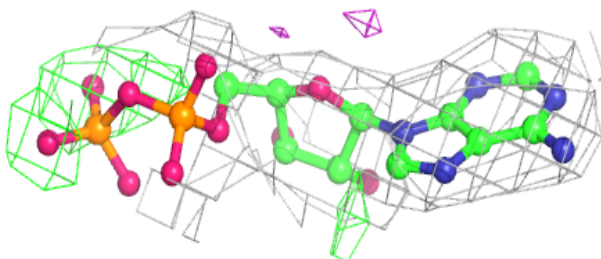
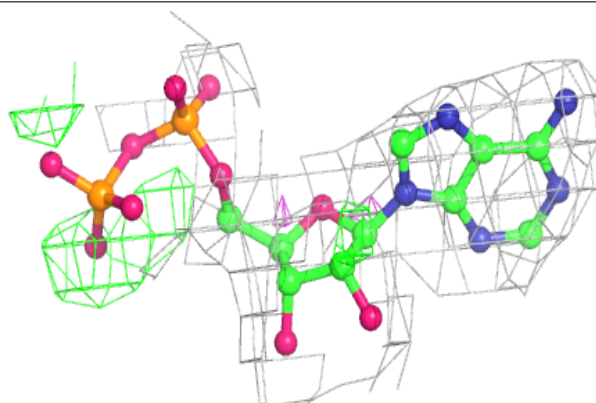
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP E 601:

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

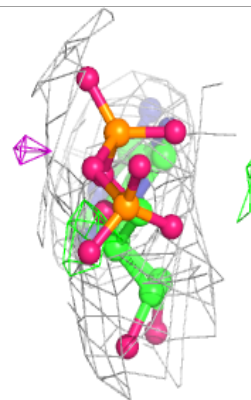
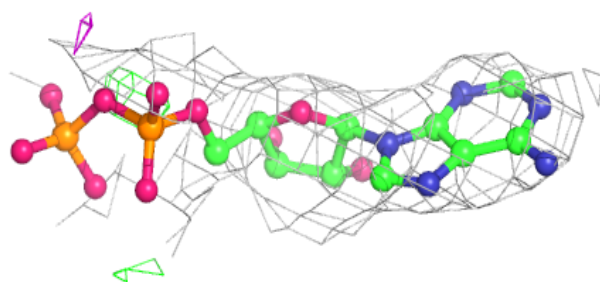
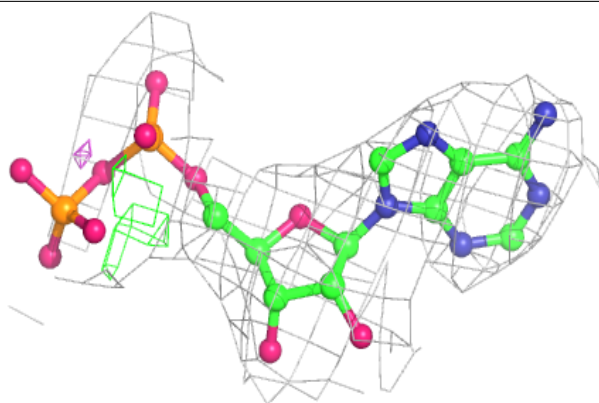
**Electron density around ADP N 601:**

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

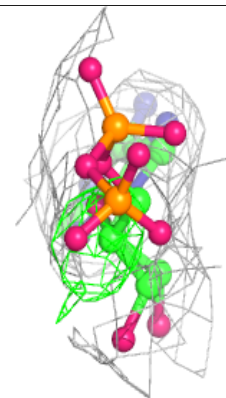
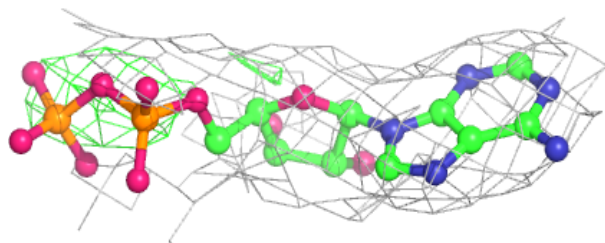
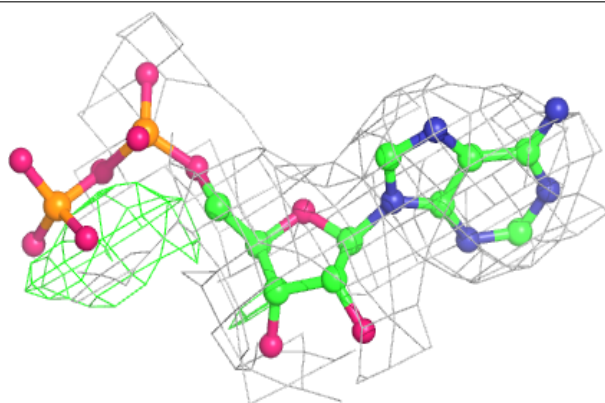


Electron density around ADP J 601:

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

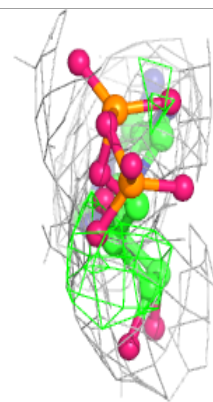
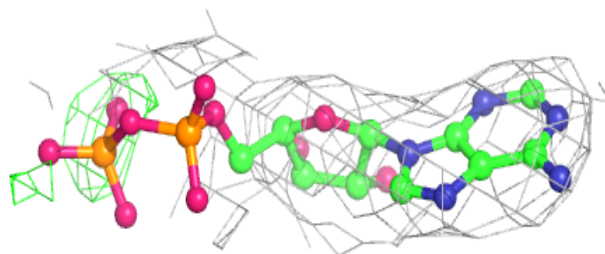
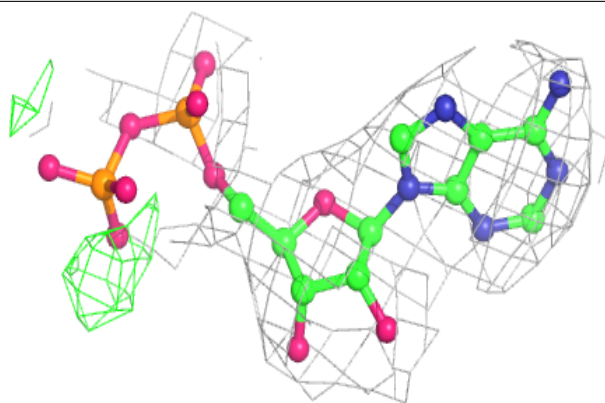
**Electron density around ADP K 601:**

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

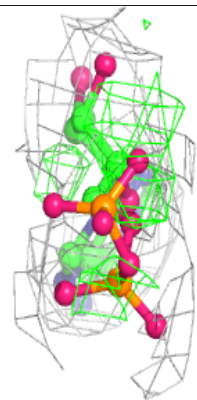
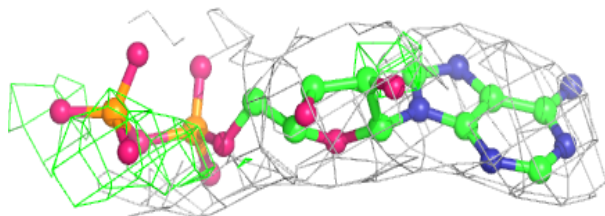
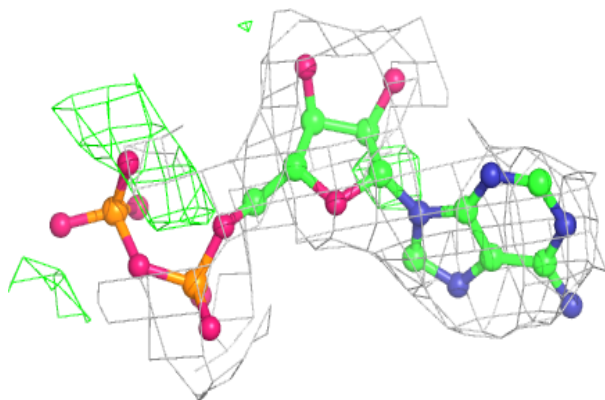


Electron density around ADP A 601:

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

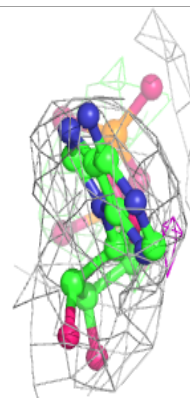
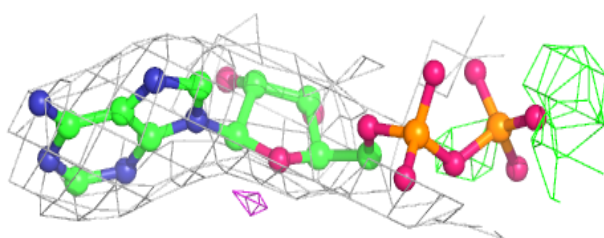
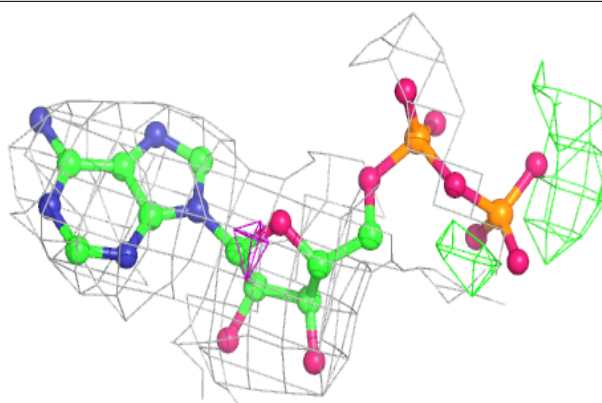
**Electron density around ADP C 601:**

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

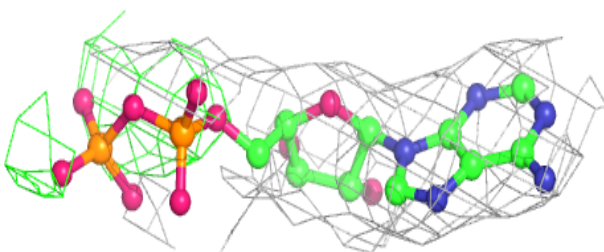
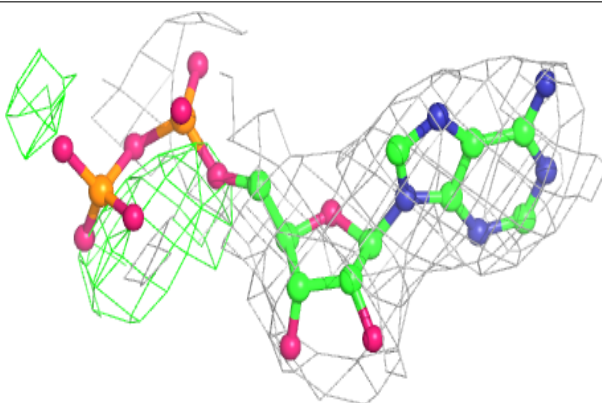


Electron density around ADP I 601:

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

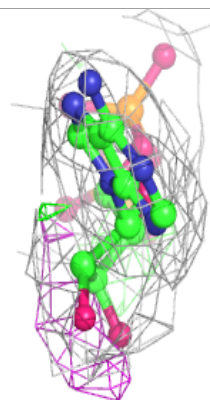
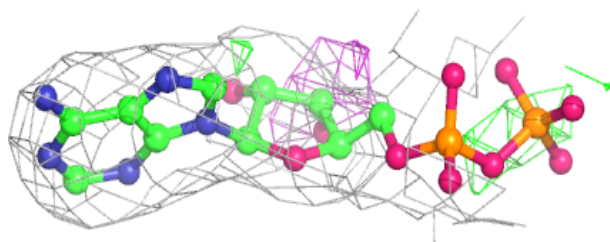
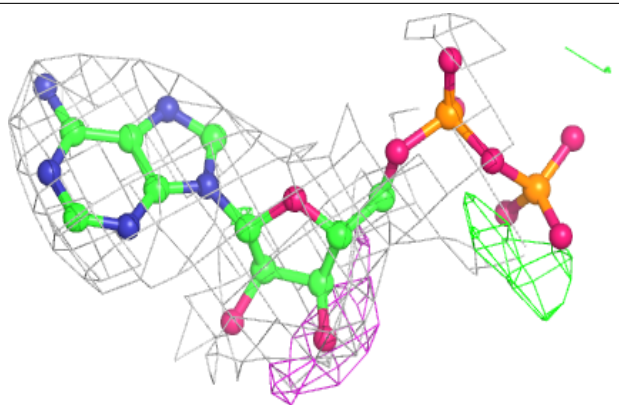
**Electron density around ADP F 601:**

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

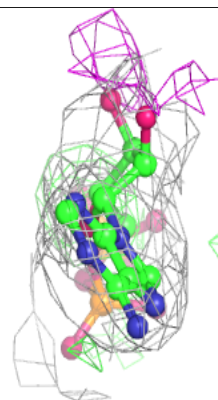
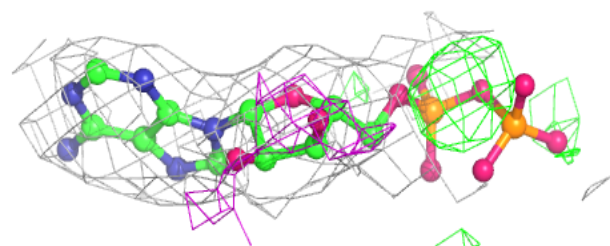
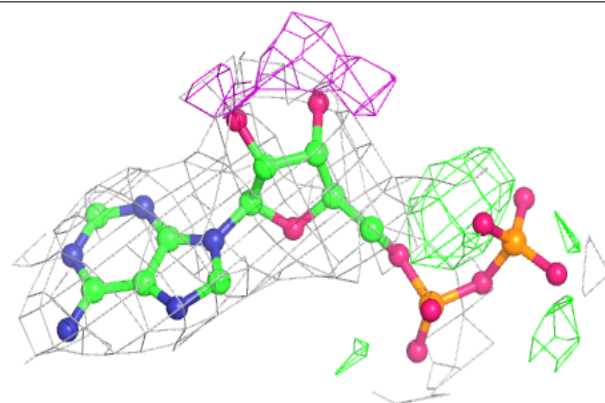


Electron density around ADP H 601:

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

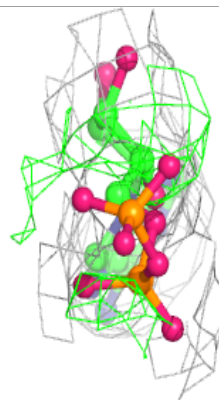
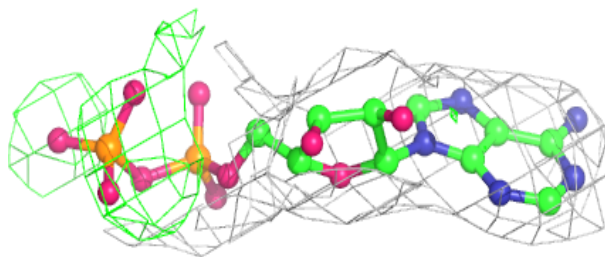
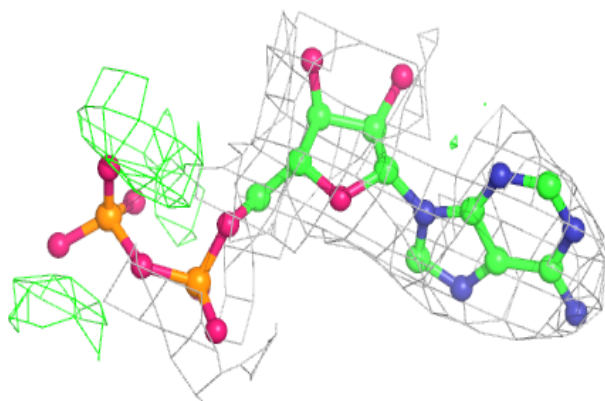
**Electron density around ADP D 601:**

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

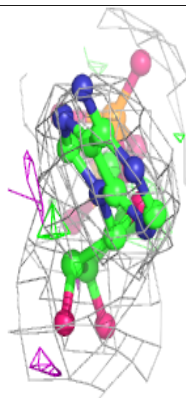
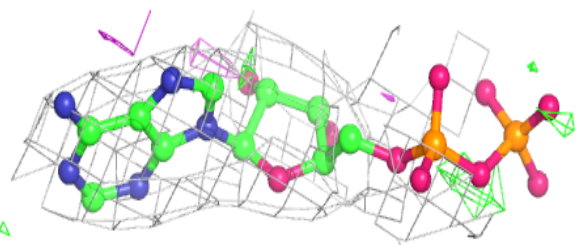
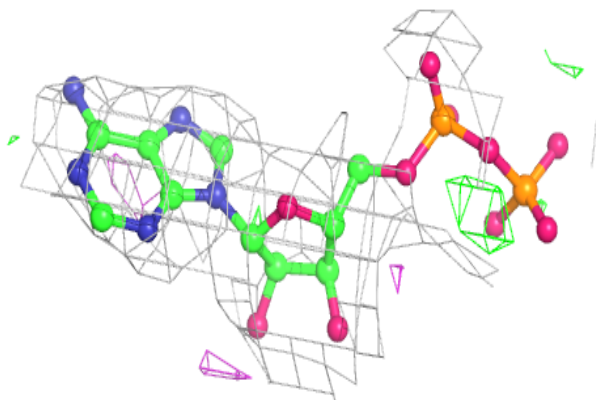


Electron density around ADP B 601:

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

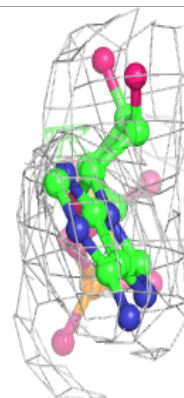
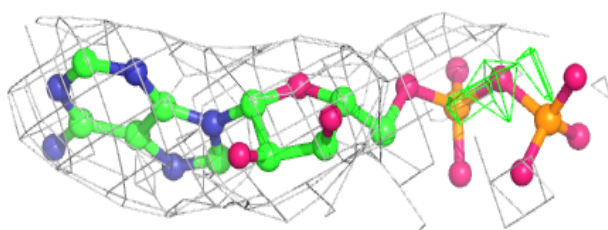
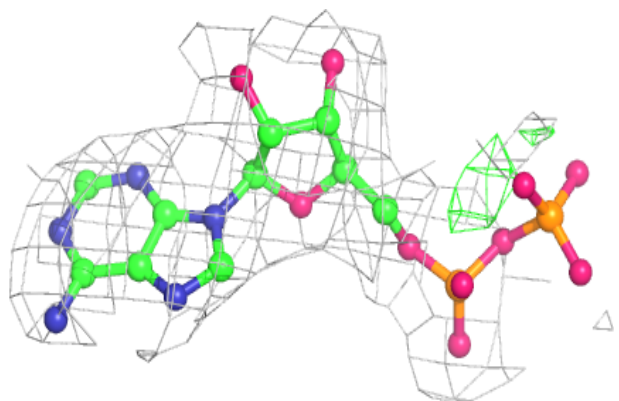
**Electron density around ADP G 601:**

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

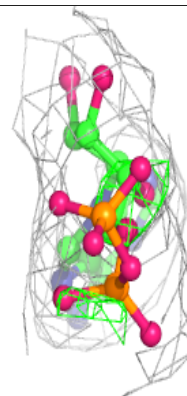
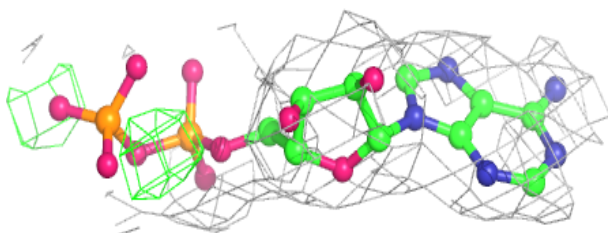
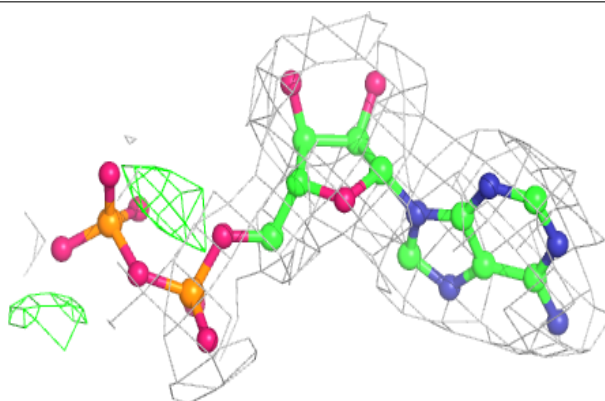


Electron density around ADP L 601:

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

**Electron density around ADP M 601:**

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



6.5 Other polymers

There are no such residues in this entry.