



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:41 PM UTC

PDB ID : 4PJ1 / pdb_00004pj1
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 types of validation reports are described at

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

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

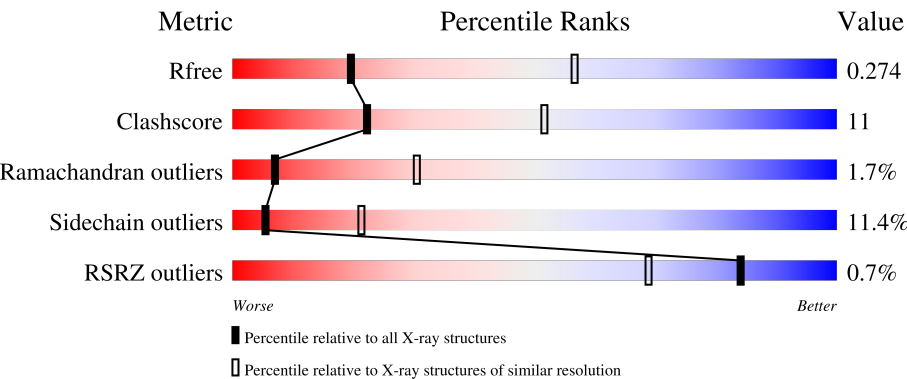
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.15 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.



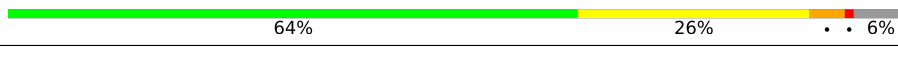
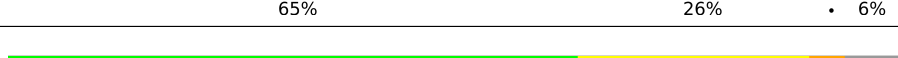
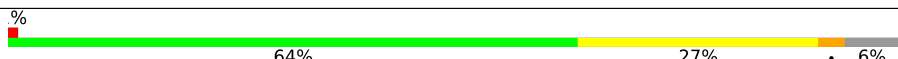
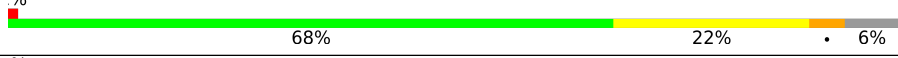
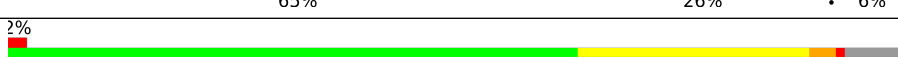
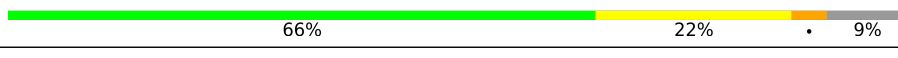
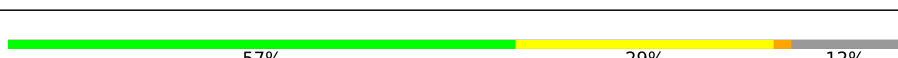
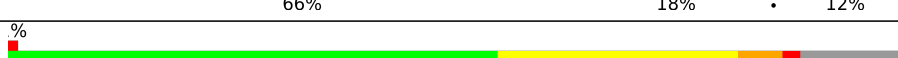
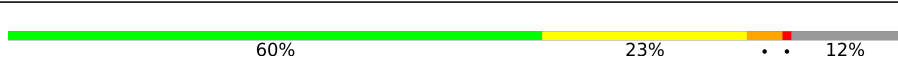
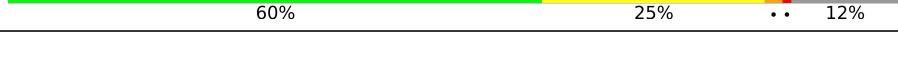
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	558	
1	B	558	
1	C	558	
1	D	558	
1	E	558	

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Mol	Chain	Length	Quality of chain
1	F	558	
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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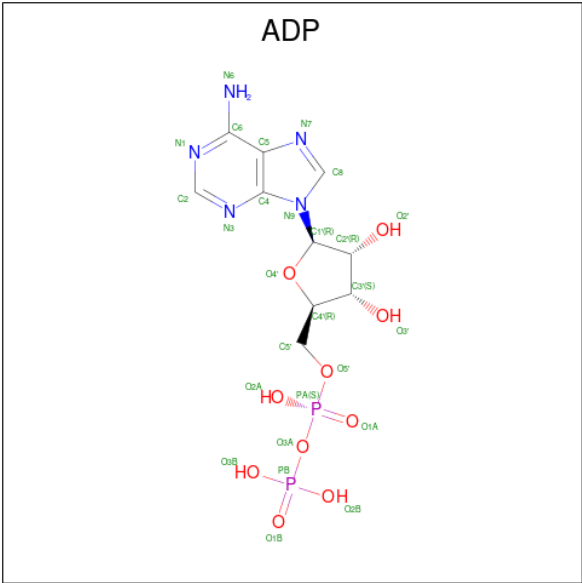
Chain	Residue	Modelled	Actual	Comment	Reference
W	114	HIS	-	expression tag	UNP P61604
X	103	LYS	-	expression tag	UNP P61604
X	104	LEU	-	expression tag	UNP P61604
X	105	ALA	-	expression tag	UNP P61604
X	106	ALA	-	expression tag	UNP P61604
X	107	ALA	-	expression tag	UNP P61604
X	108	LEU	-	expression tag	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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		

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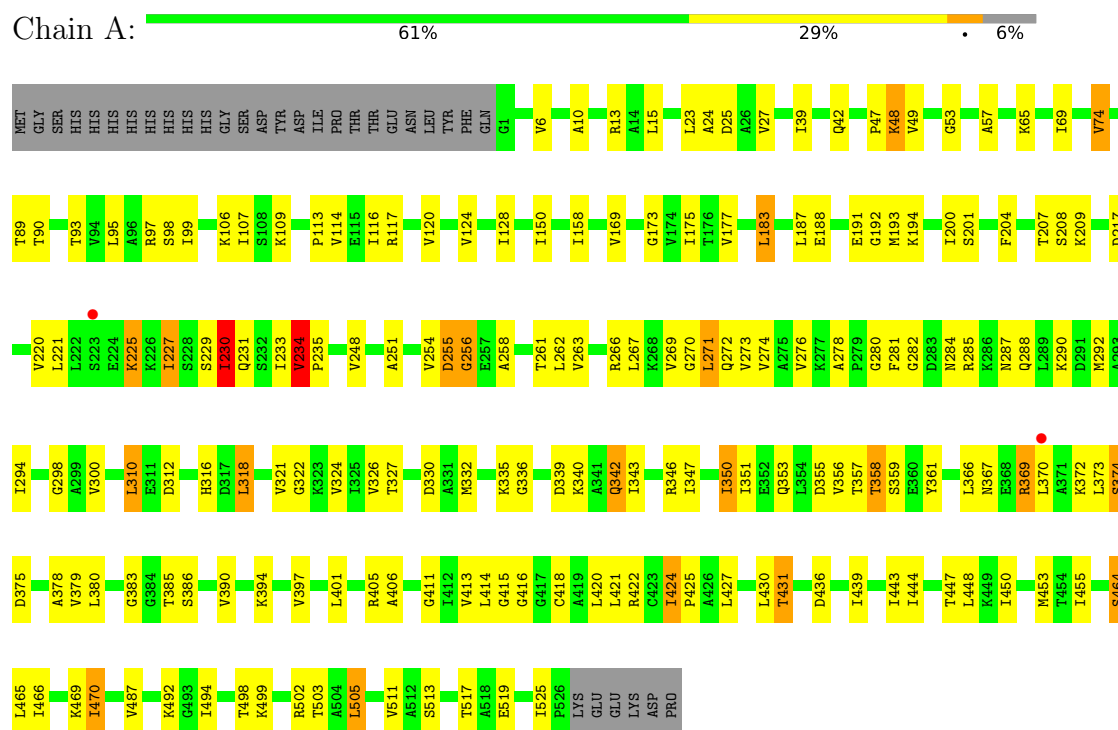
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0

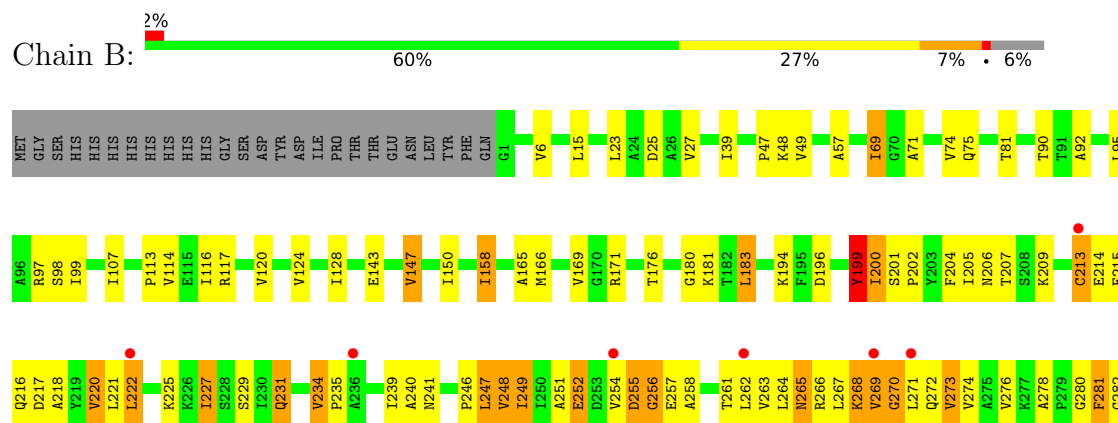
3 Residue-property plots

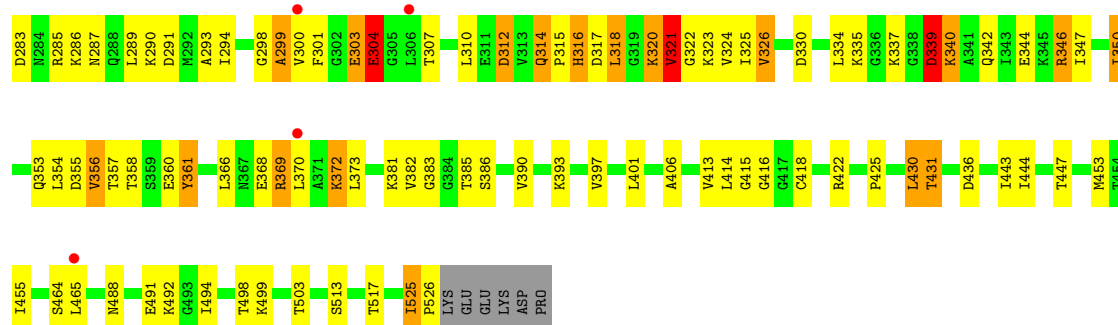
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 60 kDa heat shock protein, mitochondrial



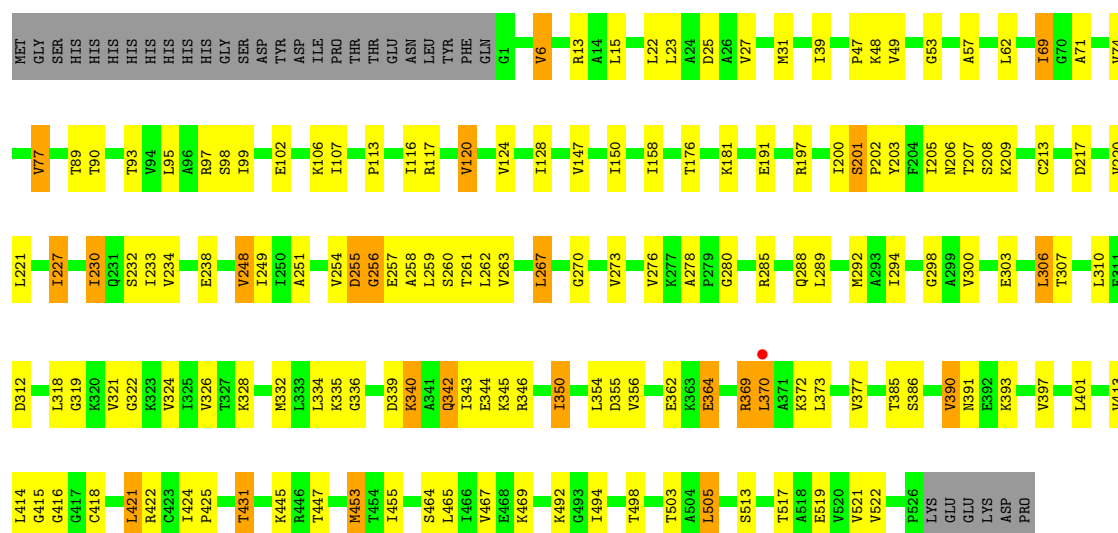
- Molecule 1: 60 kDa heat shock protein, mitochondrial





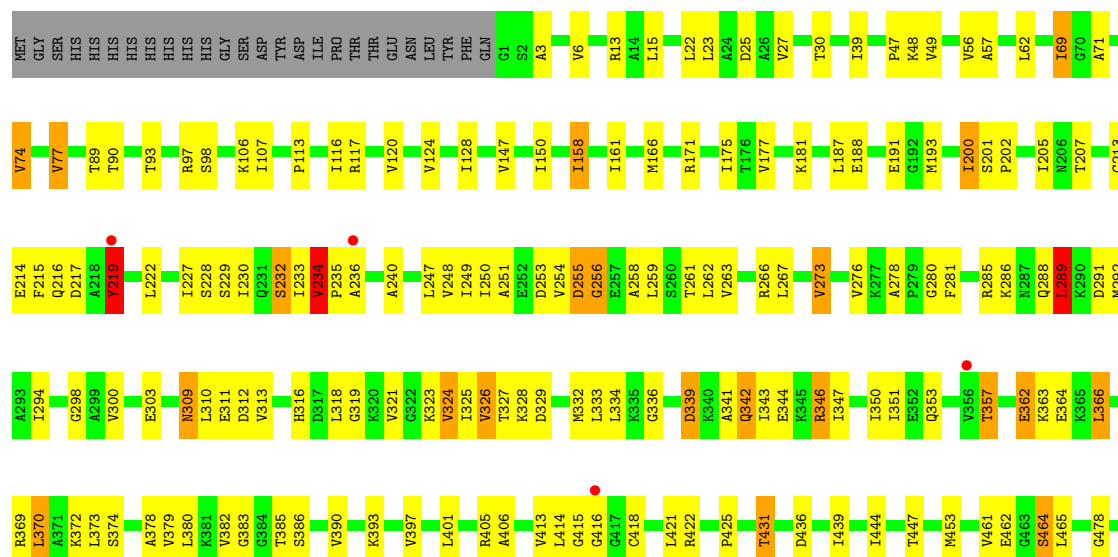
- Molecule 1: 60 kDa heat shock protein, mitochondrial

Chain C: 66% 24% 6%

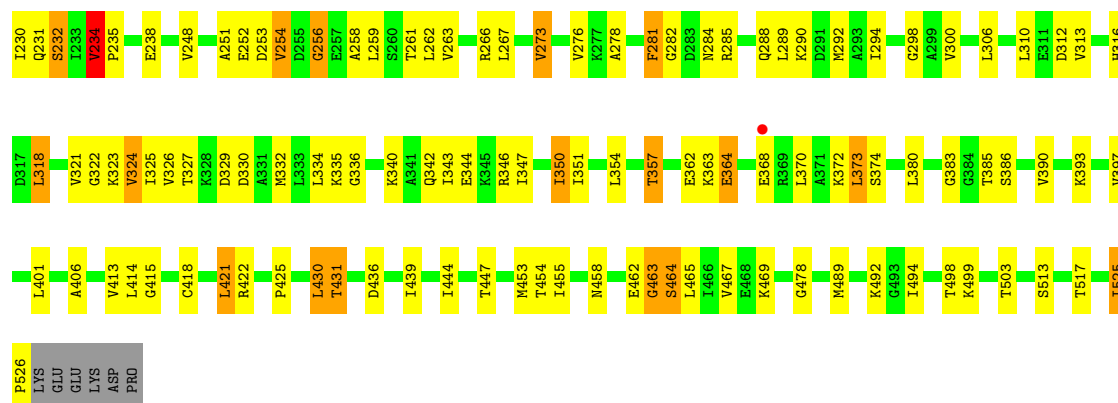


- Molecule 1: 60 kDa heat shock protein, mitochondrial

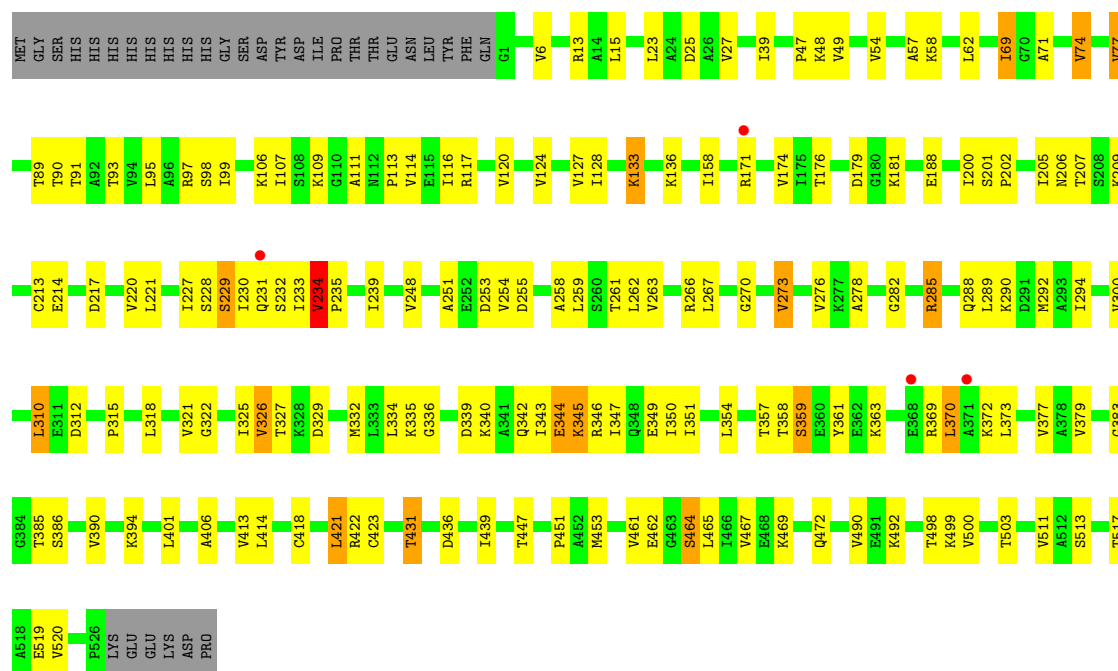
Chain D: 61% 29% 6%



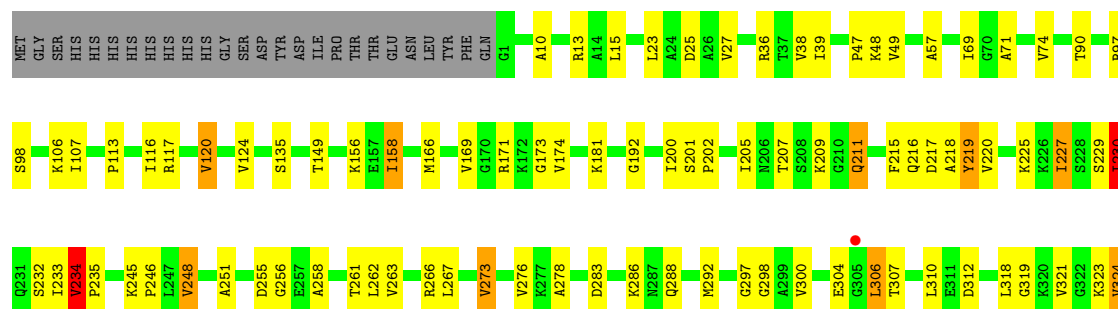


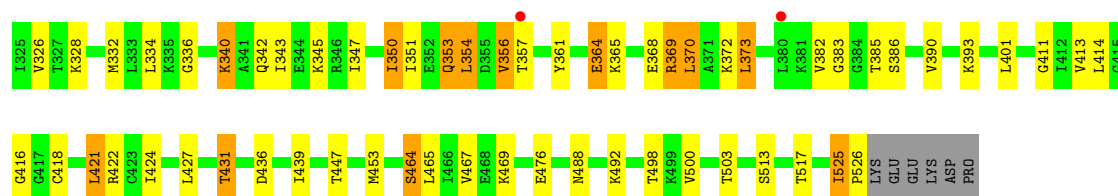


- Molecule 1: 60 kDa heat shock protein, mitochondrial

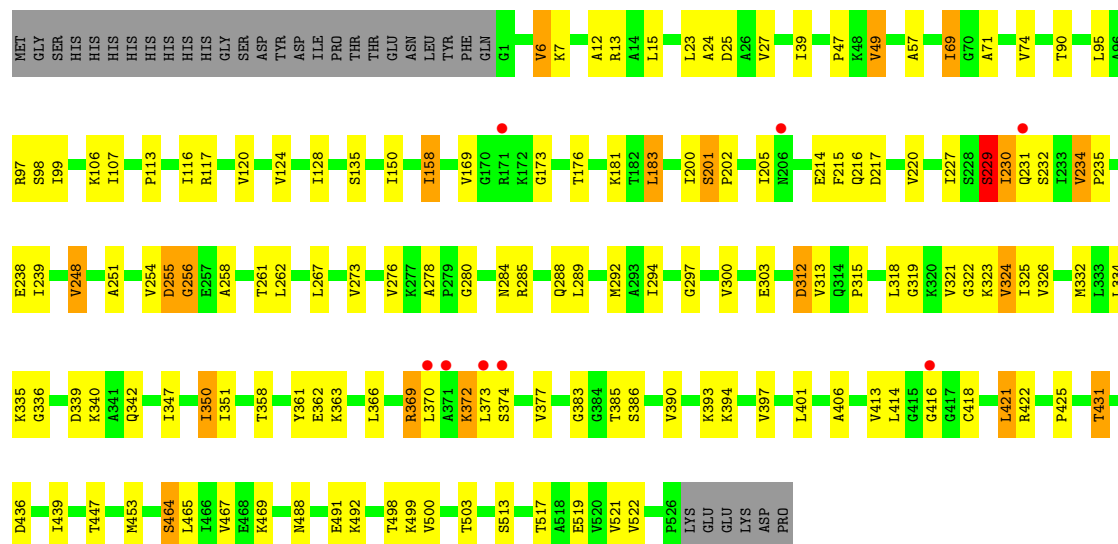


- Molecule 1: 60 kDa heat shock protein, mitochondrial

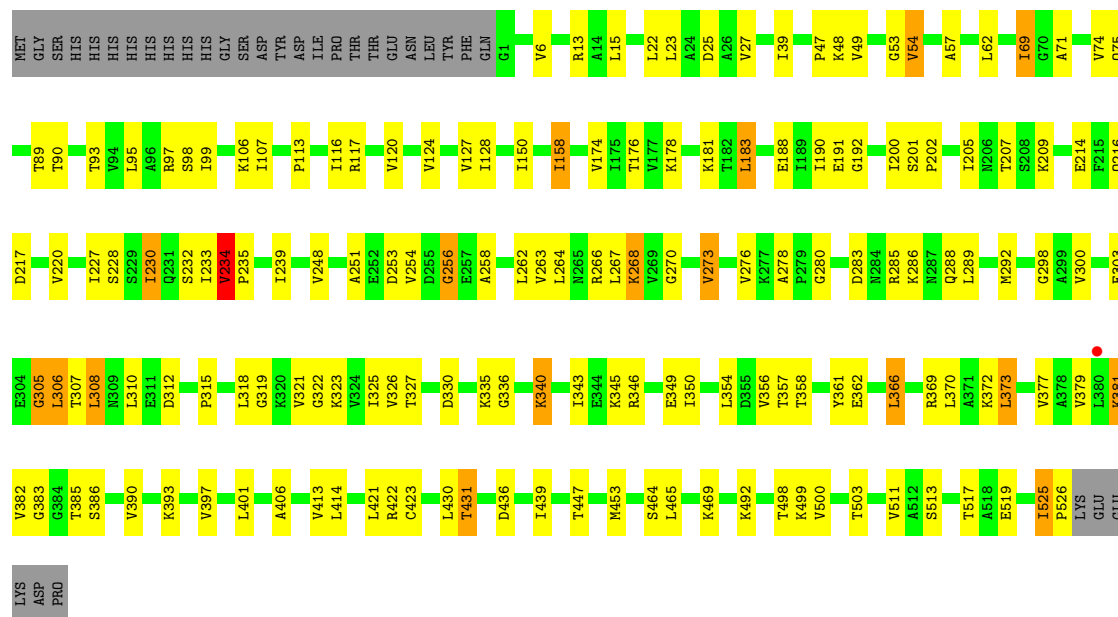




- Molecule 1: 60 kDa heat shock protein, mitochondrial

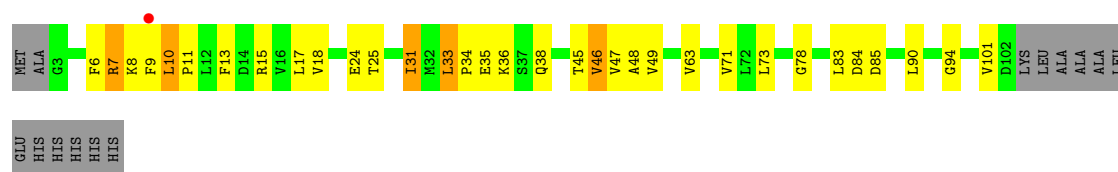


- Molecule 1: 60 kDa heat shock protein, mitochondrial

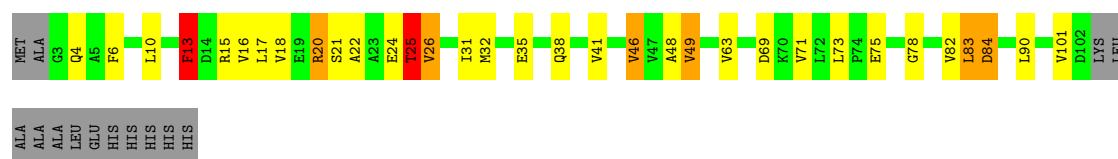


- Molecule 1: 60 kDa heat shock protein, mitochondrial

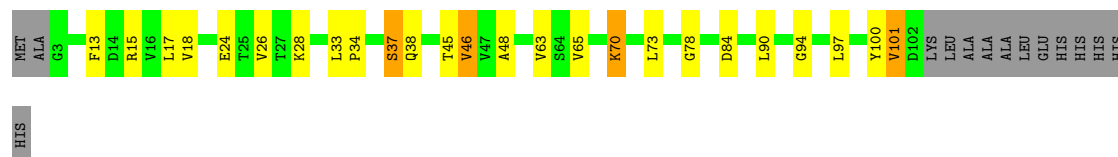
- Molecule 2: 10 kDa heat shock protein, mitochondrial



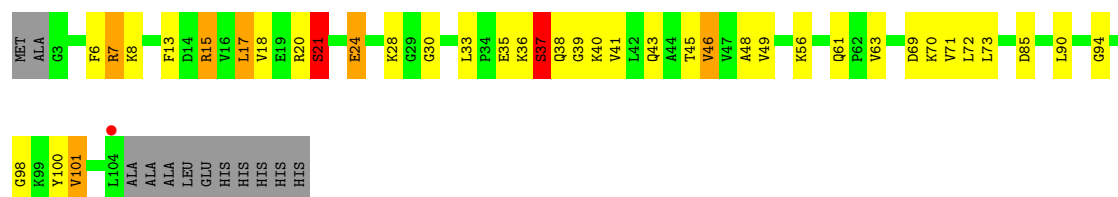
- Molecule 2: 10 kDa heat shock protein, mitochondrial



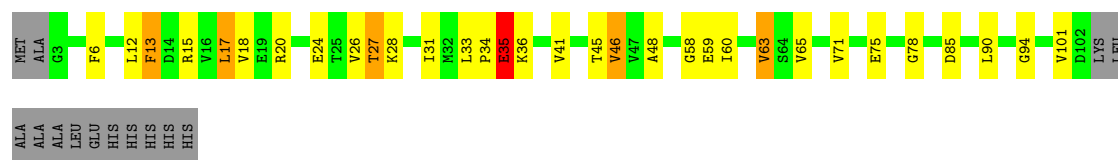
- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial

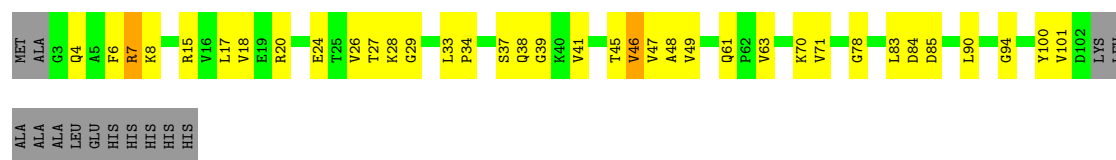


- Molecule 2: 10 kDa heat shock protein, mitochondrial

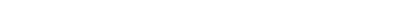


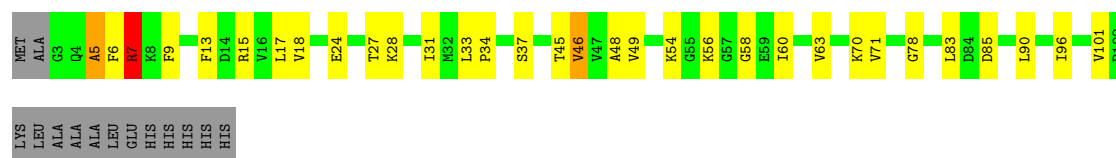
- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain W: 56% 30% 12%



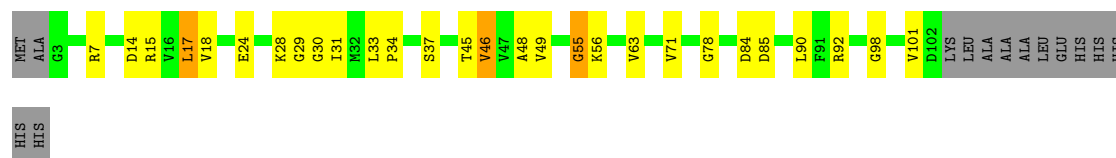
- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain X:  60% 25% .. 12%

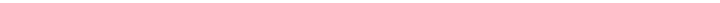


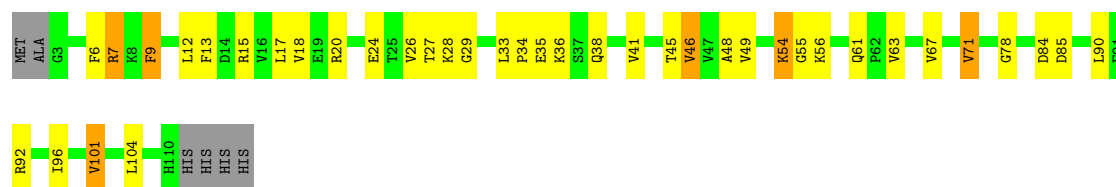
- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain Y: 63% 22% • 12%



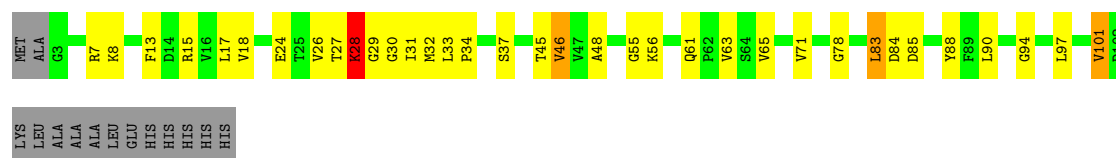
- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain Z:  61% 29% 5% 5%

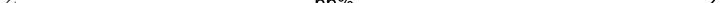


- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain 1: 57% 27% .. 12%



- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain 2:  66% 22% 9%



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) 99.3 (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 0.249 , 0.274	Depositor DCC
R_{free} test set	10852 reflections (4.99%)	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)	0.31 , 78.0	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	0.37	1/3950 (0.0%)	0.86	7/5328 (0.1%)
1	B	0.41	0/3950	0.92	14/5328 (0.3%)
1	C	0.37	0/3950	0.82	4/5328 (0.1%)
1	D	0.36	1/3950 (0.0%)	0.85	8/5328 (0.2%)
1	E	0.36	0/3950	0.83	8/5328 (0.2%)
1	F	0.37	1/3950 (0.0%)	0.83	3/5328 (0.1%)
1	G	0.38	1/3950 (0.0%)	0.88	10/5328 (0.2%)
1	H	0.34	0/3950	0.83	8/5328 (0.2%)
1	I	0.35	1/3950 (0.0%)	0.82	7/5328 (0.1%)
1	J	0.36	0/3950	0.83	7/5328 (0.1%)
1	K	0.36	1/3950 (0.0%)	0.84	5/5328 (0.1%)
1	L	0.36	0/3950	0.84	9/5328 (0.2%)
1	M	0.37	1/3950 (0.0%)	0.83	5/5328 (0.1%)
1	N	0.36	0/3950	0.87	8/5328 (0.2%)
2	1	0.36	0/767	0.94	3/1030 (0.3%)
2	2	0.38	0/794	1.09	6/1066 (0.6%)
2	O	0.34	0/767	0.92	1/1030 (0.1%)
2	P	0.34	0/799	0.98	3/1073 (0.3%)
2	Q	0.34	0/767	0.97	3/1030 (0.3%)
2	R	0.34	0/767	0.94	3/1030 (0.3%)
2	S	0.41	0/767	1.03	5/1030 (0.5%)
2	T	0.33	0/767	0.96	3/1030 (0.3%)
2	U	0.35	0/784	1.06	4/1052 (0.4%)
2	V	0.33	0/767	0.89	1/1030 (0.1%)
2	W	0.35	0/767	0.92	2/1030 (0.2%)
2	X	0.33	0/767	0.88	3/1030 (0.3%)
2	Y	0.34	0/767	0.93	3/1030 (0.3%)
2	Z	0.34	0/827	0.98	4/1111 (0.4%)
All	All	0.36	7/66174 (0.0%)	0.87	147/89194 (0.2%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	234	VAL	CA-CB	5.98	1.57	1.54
1	K	234	VAL	CA-CB	5.83	1.57	1.54
1	A	234	VAL	CA-CB	5.72	1.57	1.54
1	F	234	VAL	CA-CB	5.72	1.57	1.53
1	G	234	VAL	CA-CB	5.39	1.57	1.53
1	I	234	VAL	CA-CB	5.14	1.57	1.53
1	D	234	VAL	CA-CB	5.05	1.57	1.53

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	33	LEU	CA-C-N	10.64	131.07	119.90
2	2	33	LEU	C-N-CA	10.64	131.07	119.90
2	U	33	LEU	CA-C-N	9.81	130.20	119.90
2	U	33	LEU	C-N-CA	9.81	130.20	119.90
1	A	375	ASP	N-CA-C	-9.75	99.96	112.93
1	L	361	TYR	N-CA-C	-8.97	99.35	110.65
2	Z	55	GLY	N-CA-C	8.87	127.16	113.86
2	1	55	GLY	N-CA-C	8.84	125.62	114.66
1	A	230	ILE	N-CA-C	8.71	118.75	110.30
1	B	201	SER	CA-C-N	8.42	128.54	119.28
1	B	201	SER	C-N-CA	8.42	128.54	119.28
2	R	38	GLN	N-CA-C	-8.07	102.49	113.30
1	N	210	GLY	N-CA-C	-7.99	98.31	112.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	232	SER	N-CA-C	-7.90	103.64	113.20
2	Y	55	GLY	N-CA-C	7.81	124.34	114.66
1	B	304	GLU	N-CA-C	7.80	122.17	109.85
2	O	39	GLY	N-CA-C	7.63	122.08	110.18
1	N	232	SER	N-CA-C	-7.23	98.26	109.76
1	J	229	SER	N-CA-C	7.15	120.60	110.23
2	Q	33	LEU	CA-C-N	7.13	127.11	119.76
2	Q	33	LEU	C-N-CA	7.13	127.11	119.76
1	G	374	SER	N-CA-C	6.82	121.75	112.68
2	W	33	LEU	CA-C-N	6.79	126.75	119.76
2	W	33	LEU	C-N-CA	6.79	126.75	119.76
1	M	361	TYR	N-CA-C	-6.78	102.11	110.65
1	N	326	VAL	N-CA-C	6.74	123.36	109.34
1	E	201	SER	CA-C-N	6.68	126.62	119.28
1	E	201	SER	C-N-CA	6.68	126.62	119.28
2	S	83	LEU	N-CA-C	6.67	123.49	110.56
2	S	83	LEU	CA-C-N	6.53	133.45	121.70
2	S	83	LEU	C-N-CA	6.53	133.45	121.70
1	H	201	SER	CA-C-N	6.45	126.38	119.28
1	H	201	SER	C-N-CA	6.45	126.38	119.28
2	2	33	LEU	N-CA-C	6.42	117.89	109.93
2	X	33	LEU	CA-C-N	6.35	126.11	119.76
2	X	33	LEU	C-N-CA	6.35	126.11	119.76
1	F	201	SER	CA-C-N	6.35	126.26	119.28
1	F	201	SER	C-N-CA	6.35	126.26	119.28
1	C	181	LYS	N-CA-C	-6.31	105.89	113.97
2	Z	33	LEU	CA-C-N	6.24	126.19	119.76
2	Z	33	LEU	C-N-CA	6.24	126.19	119.76
1	C	201	SER	CA-C-N	6.22	126.13	119.28
1	C	201	SER	C-N-CA	6.22	126.13	119.28
1	J	201	SER	CA-C-N	6.20	126.10	119.28
1	J	201	SER	C-N-CA	6.20	126.10	119.28
1	G	201	SER	CA-C-N	6.20	126.10	119.28
1	G	201	SER	C-N-CA	6.20	126.10	119.28
1	L	201	SER	CA-C-N	6.19	126.09	119.28
1	L	201	SER	C-N-CA	6.19	126.09	119.28
1	M	201	SER	CA-C-N	6.19	126.08	119.28
1	M	201	SER	C-N-CA	6.19	126.08	119.28
1	B	181	LYS	N-CA-C	-6.18	106.06	113.97
2	2	100	TYR	N-CA-C	-6.18	99.20	109.46
1	D	181	LYS	N-CA-C	-6.17	106.07	113.97
1	M	230	ILE	N-CA-C	6.14	116.32	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	201	SER	CA-C-N	6.11	126.00	119.28
1	N	201	SER	C-N-CA	6.11	126.00	119.28
1	D	201	SER	CA-C-N	6.10	125.99	119.28
1	D	201	SER	C-N-CA	6.10	125.99	119.28
1	K	181	LYS	N-CA-C	-6.08	106.18	113.97
1	H	232	SER	N-CA-C	-6.06	105.87	113.20
2	T	84	ASP	N-CA-C	6.06	119.54	111.30
1	K	201	SER	CA-C-N	6.06	125.94	119.28
1	K	201	SER	C-N-CA	6.06	125.94	119.28
1	D	229	SER	CB-CA-C	-6.05	109.01	117.23
2	V	36	LYS	N-CA-C	-6.02	101.55	110.46
2	P	33	LEU	CA-C-N	5.98	125.92	119.76
2	P	33	LEU	C-N-CA	5.98	125.92	119.76
1	L	372	LYS	N-CA-C	5.98	119.82	110.32
2	Q	84	ASP	N-CA-C	5.97	119.43	111.30
1	E	181	LYS	N-CA-C	-5.94	106.36	113.97
1	A	201	SER	CA-C-N	5.93	125.81	119.28
1	A	201	SER	C-N-CA	5.93	125.81	119.28
1	G	361	TYR	N-CA-C	-5.93	105.04	112.93
1	N	233	ILE	N-CA-C	5.93	121.68	109.34
2	2	32	MET	N-CA-C	5.92	118.29	108.99
1	I	201	SER	CA-C-N	5.92	125.79	119.28
1	I	201	SER	C-N-CA	5.92	125.79	119.28
1	H	210	GLY	N-CA-C	-5.90	107.67	114.69
1	J	234	VAL	CA-C-N	-5.89	112.80	119.28
1	J	234	VAL	C-N-CA	-5.89	112.80	119.28
2	Y	33	LEU	CA-C-N	5.89	125.65	119.76
2	Y	33	LEU	C-N-CA	5.89	125.65	119.76
2	U	37	SER	N-CA-C	-5.88	98.28	110.80
1	E	232	SER	N-CA-C	-5.84	106.11	113.18
1	H	181	LYS	N-CA-C	-5.75	106.61	113.97
1	N	328	LYS	N-CA-C	5.72	118.29	111.71
1	E	228	SER	N-CA-C	-5.68	106.01	113.17
1	B	334	LEU	N-CA-C	5.65	119.75	111.34
2	1	33	LEU	CA-C-N	5.62	125.55	119.76
2	1	33	LEU	C-N-CA	5.62	125.55	119.76
1	B	320	LYS	CA-C-N	5.62	131.81	121.70
1	B	320	LYS	C-N-CA	5.62	131.81	121.70
1	I	181	LYS	N-CA-C	-5.59	106.82	113.97
1	J	181	LYS	N-CA-C	-5.55	106.86	113.97
2	T	33	LEU	CA-C-N	5.55	125.31	119.76
2	T	33	LEU	C-N-CA	5.55	125.31	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	181	LYS	N-CA-C	-5.55	106.87	113.97
2	X	5	ALA	N-CA-C	5.50	118.23	109.65
1	B	270	GLY	N-CA-C	5.48	126.17	113.18
1	D	219	TYR	CA-CB-CG	5.47	123.75	113.90
1	J	359	SER	N-CA-C	-5.47	100.48	109.40
2	U	21	SER	N-CA-C	-5.46	102.41	110.48
2	R	33	LEU	CA-C-N	5.43	125.61	119.90
2	R	33	LEU	C-N-CA	5.43	125.61	119.90
1	G	32	GLY	CA-C-N	5.40	125.05	119.05
1	G	32	GLY	C-N-CA	5.40	125.05	119.05
1	A	424	ILE	CB-CA-C	-5.37	108.60	113.70
1	D	232	SER	N-CA-C	-5.34	106.74	113.20
2	2	78	GLY	N-CA-C	5.33	118.06	111.93
1	B	229	SER	N-CA-C	5.31	118.38	110.52
1	D	289	LEU	CA-CB-CG	5.31	134.88	116.30
2	Z	9	PHE	N-CA-C	5.28	117.02	108.41
2	S	25	THR	CA-C-N	5.25	131.43	121.97
2	S	25	THR	C-N-CA	5.25	131.43	121.97
1	I	254	VAL	N-CA-C	-5.24	100.78	108.11
1	L	303	GLU	N-CA-C	5.23	116.83	108.41
1	E	32	GLY	CA-C-N	5.21	125.02	119.28
1	E	32	GLY	C-N-CA	5.21	125.02	119.28
1	D	303	GLU	N-CA-C	5.21	116.80	108.41
2	P	77	GLY	N-CA-C	5.21	123.13	113.76
1	B	229	SER	CA-C-N	5.20	127.47	120.50
1	B	229	SER	C-N-CA	5.20	127.47	120.50
1	K	230	ILE	N-CA-C	5.20	115.92	110.62
1	H	228	SER	N-CA-C	5.19	119.70	113.17
1	L	229	SER	CA-C-N	5.19	131.03	121.70
1	L	229	SER	C-N-CA	5.19	131.03	121.70
1	B	337	LYS	N-CA-C	5.18	118.12	110.46
1	B	361	TYR	N-CA-C	5.18	117.17	110.65
1	G	356	VAL	N-CA-C	5.17	115.22	107.51
1	I	463	GLY	N-CA-C	5.17	125.44	113.18
1	H	32	GLY	CA-C-N	5.15	124.95	119.28
1	H	32	GLY	C-N-CA	5.15	124.95	119.28
1	C	303	GLU	N-CA-C	5.14	116.69	108.41
1	E	303	GLU	N-CA-C	5.14	116.69	108.41
1	B	320	LYS	N-CA-C	5.13	116.73	108.32
1	A	318	LEU	CA-C-O	5.13	120.91	117.94
1	L	232	SER	N-CA-C	-5.12	107.00	113.20
1	L	181	LYS	N-CA-C	-5.12	107.41	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ILE	CB-CA-C	-5.09	107.33	114.00
1	G	318	LEU	CA-C-O	5.09	120.89	117.94
1	G	234	VAL	CB-CA-C	-5.08	108.97	114.35
1	N	361	TYR	N-CA-C	-5.07	106.78	113.12
1	I	232	SER	N-CA-C	-5.06	107.08	113.20
1	K	361	TYR	N-CA-C	-5.06	100.03	110.80
1	I	318	LEU	CA-C-O	5.05	120.87	117.94
1	G	181	LYS	N-CA-C	-5.02	107.55	113.97

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	SER	Peptide
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	106	0
1	B	3918	0	4103	133	0
1	C	3918	0	4103	91	0
1	D	3918	0	4103	98	0
1	E	3918	0	4103	83	0
1	F	3918	0	4103	79	0
1	G	3918	0	4103	92	0
1	H	3918	0	4103	89	0
1	I	3918	0	4103	81	0
1	J	3918	0	4103	94	0
1	K	3918	0	4103	81	0
1	L	3918	0	4103	83	0
1	M	3918	0	4103	85	0
1	N	3918	0	4103	100	0
2	1	756	0	786	18	0
2	2	783	0	820	13	0
2	O	756	0	786	18	0
2	P	788	0	825	17	0
2	Q	756	0	786	16	0
2	R	756	0	786	16	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	17	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	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1431	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 11.

All (1431) 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
1:A:99:ILE:HG13	1:A:447:THR:HG21	1.65	0.77
2:1:7:ARG:HB2	2:1:83:LEU:HD23	1.67	0.77
1:K:23:LEU:HD21	1:K:57:ALA:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:ILE:HG22	1:M:373:LEU:HD21	1.69	0.72
1:M:264:LEU:HG	1:M:268:LYS:HE3	1.71	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
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:23:LEU:HD21	1:J:57:ALA:HA	1.74	0.68
1:J:290:LYS:HE2	1:J:346:ARG:HH22	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:431:THR:O	1:F:431:THR:OG1	2.11	0.66
1:K:431:THR:O	1:K:431:THR:OG1	2.13	0.66
1:L:229:SER:HB2	1:L:231:GLN:N	2.09	0.66
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
1:D:431:THR:O	1:D:431:THR:OG1	2.11	0.66
2:2:17:LEU:HB3	2:2:48:ALA:HB3	1.77	0.66
1:C:354:LEU:HD13	1:C:364:GLU:HG3	1.78	0.66
1:E:431:THR:O	1:E:431:THR:OG1	2.14	0.66
2:V:27:THR:HG22	2:V:33:LEU:HD11	1.77	0.65
2:X:34:PRO:HG2	2:X:37:SER:HB3	1.76	0.65
2:1:94:GLY:O	2:2:15:ARG:NH2	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:G:431:THR:OG1	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
1:B:117:ARG:NH1	1:B:513:SER:OG	2.32	0.63
1:B:222:LEU:HD21	1:B:289:LEU:HB2	1.81	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
1:C:98:SER:HB3	1:C:447:THR:HG23	1.81	0.62
2:1:17:LEU:HB3	2:1:48:ALA:HB3	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:194:LYS:H	1:B:373:LEU:HD13	1.65	0.61
1:B:234:VAL:HG23	2:P:31:ILE:HD11	1.80	0.61
1:J:431:THR:O	1:J:431:THR:OG1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:431:THR:O	1:L:431:THR:OG1	2.13	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
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:F:332:MET:HE3	1:F:334:LEU:HD11	1.83	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
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:C:431:THR:O	1:C:431:THR:OG1	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:332:MET:HE3	1:K:334:LEU:HD11	1.84	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:N:304:GLU:HA	1:N:305:GLY:C	2.27	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:N:431:THR:O	1:N:431:THR:OG1	2.13	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
1:K:117:ARG:NH1	1:K:513:SER:OG	2.35	0.59
1:L:373:LEU:HB3	1:L:374:SER:C	2.27	0.59
1:G:251:ALA:O	1:G:278:ALA:N	2.36	0.59
1:L:332:MET:HE3	1:L:334:LEU:HD11	1.85	0.59
2:O:15:ARG:NH2	2:U:94:GLY:O	2.35	0.59
2:S:82:VAL:HG22	2:S:84:ASP:O	2.03	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:B:265:ASN:HA	2:P:32:MET:HE2	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:I:431:THR:O	1:I:431:THR:OG1	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ALA:O	1:B:278:ALA:N	2.36	0.58
1:B:266:ARG:HE	1:B:273:VAL:HG22	1.67	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
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
1:M:268:LYS:HZ3	2:1:32:MET:HB2	1.68	0.57
2:W:34:PRO:HG2	2:W:37:SER:HB3	1.85	0.57
2:1:34:PRO:HG2	2:1:37:SER:HB2	1.86	0.57
1:E:339:ASP:OD1	1:E:339:ASP:N	2.24	0.57
1:M:234:VAL:HG13	1:M:235:PRO:HD3	1.86	0.57
2:U:15:ARG:HH11	2:U:15:ARG:CG	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: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
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:H:332:MET:HE3	1:H:334:LEU:HD11	1.86	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:98:SER:HB3	1:N:447:THR:HG23	1.87	0.57
1:N:269:VAL:O	1:N:271:LEU:N	2.37	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:25:ASP:OD1	1:L:97:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:321:VAL:HA	1:L:336:GLY:HA2	1.87	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: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:J:327:THR:HG23	1:J:329:ASP:H	1.71	0.56
1:J:332:MET:HE3	1:J:334:LEU:HD11	1.86	0.56
1:L:383:GLY:O	1:L:390:VAL:HG22	2.05	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
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:98:SER:HB3	1:G:447:THR:HG23	1.88	0.55
1:G:301:PHE:CD1	1:G:308:LEU:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:THR:HG23	1:G:329:ASP:H	1.72	0.55
1:H:47:PRO:HG3	1:N:69:ILE:HG23	1.87	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: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
2:S:4:GLN:H	2:S:49:VAL:HG13	1.70	0.55
1:A:13:ARG:NH2	1:A:519:GLU:OE1	2.39	0.55
1:A:234:VAL:HG13	1:A:235:PRO:HD3	1.86	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
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:HE21	1:K:211:GLN:HA	1.71	0.55
2:U:15:ARG:HG3	2:U:15:ARG:NH1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:120:VAL:O	1:M:124:VAL:HG23	2.07	0.55
2:1:7:ARG:NH1	2:1:88:TYR:OH	2.40	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:98:SER:HB3	1:F:447:THR:HG23	1.89	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: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:39:ILE:HG12	1:H:49:VAL:HG22	1.89	0.54
1:H:356:VAL:HG12	1:H:357:THR:HG23	1.90	0.54
1:J:113:PRO:HA	1:J:116:ILE:HD12	1.90	0.54
2:T:97:LEU:HA	2:U:15:ARG:HE	1.72	0.54
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:39:ILE:HG12	1:N:49:VAL:HG22	1.89	0.53
1:N:326:VAL:HG21	1:N:331:ALA:CA	2.38	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
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:I:332:MET:HE3	1:I:334:LEU:HD11	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OD1	1:I:329:ASP:N	2.42	0.52
1:N:25:ASP:OD1	1:N:97:ARG:NH1	2.39	0.52
2:2:41:VAL:HG12	2:2:75:GLU:HG2	1.92	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
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: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
1:N:265:ASN:OD1	2:2:32:MET:HB2	2.09	0.52
2:O:8:LYS:HA	2:U:101:VAL:HG22	1.92	0.52
2:O:27:THR:HG22	2:O:33:LEU:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:J:133:LYS:N	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
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:158:ILE:HD11	1:G:393:LYS:HE2	1.93	0.51
1:G:255:ASP:O	1:G:259:LEU:HB3	2.10	0.51
1:J:25:ASP:OD1	1:J:97:ARG:NH1	2.37	0.51
1:J:229:SER:OG	1:J:258:ALA:HB2	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:1:15:ARG:HB3	2:1:90: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:E:332:MET:HE3	1:E:334:LEU:HD11	1.92	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
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
2:1:63:VAL:HG12	2:1:65:VAL:H	1.76	0.51
1:E:358:THR:O	1:E:358:THR:OG1	2.13	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:207:THR:C	1:A:209:LYS:H	2.20	0.50
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:MET:HE3	1:C:334:LEU:HD11	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
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
2:1:7:ARG:HD3	2:1:84:ASP:OD2	2.11	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
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:C:117:ARG:NH1	1:C:513:SER:HG	2.09	0.49
1:D:386:SER:O	1:D:390:VAL:HG23	2.12	0.49
1:K:207:THR:C	1:K:209:LYS:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:ARG:HB3	2:Z:90:LEU:HD11	1.95	0.49
2:Z:56:LYS:HB2	2:Z:61:GLN:OE1	2.12	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:OE1	1:D:191:GLU:N	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: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
1:N:461:VAL:HG12	1:N:462:GLU:H	1.76	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
2:1:101:VAL:HG22	2:2:8:LYS:HA	1.94	0.49
1:B:194:LYS:CE	1:B:330:ASP:HB3	2.43	0.49
1:D:332:MET:HE3	1:D:334:LEU:HD11	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HG12	1:A:49:VAL:HG22	1.95	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: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:E:207:THR:C	1:E:209:LYS:H	2.21	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
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
2:2:6:PHE:O	2:2:8:LYS:N	2.46	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:O	2:P:35:GLU:HG2	2.13	0.48
1:B:248:VAL:HG11	1:B:324:VAL:HG11	1.95	0.48
1:J:207:THR:C	1:J:209:LYS:H	2.22	0.48
1:L:239:ILE:HD11	1:L:315:PRO:CD	2.43	0.48
1:N:240:ALA:C	1:N:242:ALA:H	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:191:GLU:OE1	2.46	0.48
1:D:193:MET:HE1	1:D:292:MET:HG2	1.96	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:136:LYS:NZ	1:J:490:VAL:HG21	2.29	0.48
1:J:406:ALA:HB1	1:J:499:LYS:HB3	1.96	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
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:358:THR:O	1:G:358:THR:OG1	2.19	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
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
2:2:15:ARG:HB3	2:2:90:LEU:HD11	1.96	0.48
1:C:370:LEU:HA	1:C:373:LEU:HD12	1.96	0.48
1:D:464:SER:HB2	1:L:464:SER:HB2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:190:ILE:HG13	1:N:377:VAL:HG22	1.95	0.47
1:N:233:ILE:HG12	1:N:310:LEU:CB	2.45	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:F:464:SER:HB2	1:J:464:SER:HB2	1.95	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: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:109:LYS:HB2	1:N:105:GLU:HB3	1.97	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:C:307:THR:HB	2:R:36:LYS:NZ	2.30	0.47
1:G:255:ASP:OD1	1:G:256:GLY:N	2.47	0.47
1:J:69:ILE:HG23	1:K:47:PRO:HG3	1.96	0.47
1:J:346:ARG:O	1:J:350:ILE:HD12	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:282:GLY:H	1:B:285:ARG:HH21	1.63	0.47
1:D:25:ASP:OD1	1:D:97:ARG:NH1	2.40	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: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:I:478:GLY:C	1:I:489:MET:HE3	2.39	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:L:173:GLY:HA2	1:L:373:LEU:CD2	2.45	0.47
1:N:233:ILE:HD12	1:N:233:ILE:O	2.15	0.47
1:N:284:ASN:ND2	1:N:365:LYS:HD2	2.30	0.47
2:Q:94:GLY:O	2:R:15:ARG:NH2	2.46	0.47
1:A:255:ASP:CG	1:A:256:GLY:H	2.22	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:O	1:D:372:LYS:HG3	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:207:THR:C	1:F:209:LYS:H	2.22	0.47
1:F:255:ASP:CG	1:F:256:GLY:H	2.22	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:190:ILE:O	1:N:376:GLY:HA2	2.14	0.47
1:N:325:ILE:O	1:N:326:VAL:HB	2.14	0.47
2:R:6:PHE:HB2	2:R:47:VAL:O	2.15	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N:193:MET:HE1	1:N:292:MET:HG2	1.97	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:L:255:ASP:CG	1:L:256:GLY:H	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ILE:O	1:A:351:ILE:HG12	2.16	0.46
1:B:247:LEU:O	1:B:247:LEU:HD12	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:D:255:ASP:CG	1:D:256:GLY:H	2.24	0.46
1:F:288:GLN:O	1:F:292:MET:HG3	2.16	0.46
1:G:350:ILE:HG13	1:G:351:ILE:N	2.31	0.46
1:H:89:THR:O	1:H:93:THR:HG23	2.15	0.46
1:J:359:SER:C	1:J:361:TYR:H	2.23	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: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:105:GLU:HB3	1:I:109:LYS:HB2	1.97	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: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:H	1:B:304:GLU:HG2	1.64	0.46
1:H:340:LYS:O	1:H:344:GLU:HG3	2.15	0.46
1:J:188:GLU:HB3	1:J:379:VAL:CG2	2.45	0.46
1:J:214:GLU:HG3	1:J:325:ILE:HG12	1.98	0.46
1:L:183:LEU:H	1:L:183:LEU:HD22	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:J:239:ILE:HD11	1:J:315:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:213:CYS:HB3	1:D:326:VAL:HG13	1.98	0.45
1:D:219:TYR:OH	1:D:240:ALA:HB2	2.16	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:71:ALA:O	1:B:75:GLN:HG3	2.17	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: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: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:HD22	1:M:183:LEU:H	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:OD1	1:B:312:ASP:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:71:ALA:O	1:M:75:GLN:HG3	2.17	0.45
1:A:361:TYR:O	1:A:361:TYR:CD1	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:N	1:E:231:GLN:OE1	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
2:1:56:LYS:HB2	2:1:61:GLN:OE1	2.17	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:F:31:MET:HE2	1:F:91:THR:HG22	1.98	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: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:27:VAL:HG23	1:C:53:GLY:HA2	1.98	0.45
1:C:176:THR:HG21	1:C:369:ARG:HD3	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:353:GLN:C	1:B:355:ASP:H	2.25	0.45
1:B:431:THR:O	1:B:431:THR:OG1	2.15	0.45
1:C:238:GLU:HG2	2:Q:29:GLY:HA3	1.99	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
2:S:13:PHE:HD1	2:S:13:PHE:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:O	1:A:233:ILE:HG22	2.16	0.45
1:B:255:ASP:CG	1:B:256:GLY:H	2.25	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:O	2:S:35:GLU:HG2	2.17	0.44
1:B:227:ILE:HB	1:B:254:VAL:HG22	1.99	0.44
1:B:268:LYS:O	1:B:269:VAL:C	2.60	0.44
1:I:406:ALA:HB1	1:I:499:LYS:HB3	1.98	0.44
1:J:179:ASP:OD1	1:J:394:LYS:NZ	2.38	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:J:349:GLU:CD	1:K:328:LYS:HZ2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:393:LYS:O	1:M:397:VAL:HG23	2.18	0.44
1:N:183:LEU:H	1:N:183:LEU:HD22	1.82	0.44
1:B:357:THR:HG23	1:B:357:THR:O	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:362:GLU:O	1:D:362:GLU:HG2	2.17	0.44
1:D:461:VAL:HG12	1:D:462:GLU:N	2.33	0.44
1:I:372:LYS:O	1:I:372:LYS:HG3	2.16	0.44
1:L:238:GLU:HG2	2:Z:29:GLY:HA3	1.98	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: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:K:297:GLY:O	1:K:319:GLY:HA2	2.18	0.44
1:L:135:SER:HB2	1:L:498:THR:HG21	1.98	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: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:188:GLU:HB3	1:D:379:VAL:CG2	2.48	0.44
1:D:233:ILE:HD11	1:D:249:ILE:HD13	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:365:LYS:O	1:K:369:ARG:HG2	2.18	0.44
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:81:THR:HG21	1:B:92:ALA:CB	2.48	0.44
1:B:183:LEU:H	1:B:183:LEU:HD22	1.82	0.44
1:C:321:VAL:HA	1:C:336:GLY:HA2	1.99	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: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: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:H	1:C:340:LYS:HG2	1.57	0.43
1:E:413:VAL:HG22	1:E:414:LEU:H	1.81	0.43
1:F:472:GLN:NE2	1:J:472:GLN:OE1	2.51	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: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:HD1	1:I:281:PHE:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:MET:HE2	1:C:464:SER:HB3	2.00	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:74:VAL:HA	1:D:77:VAL:HG13	2.00	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: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:H	1:K:340:LYS:HG2	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:207:THR:C	1:M:209:LYS:H	2.26	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
1:G:255:ASP:CG	1:G:256:GLY:H	2.25	0.43
1:J:117:ARG:NH1	1:J:513:SER:HG	2.16	0.43
2:Q:26:VAL:HG12	2:Q:32:MET:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:174:VAL:HG23	1:K:372:LYS:HG2	2.01	0.43
1:K:258:ALA:O	1:K:261:THR:OG1	2.31	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
2:2:17:LEU:HD11	2:2:81:VAL:HG21	1.99	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:C:207:THR:C	1:C:209:LYS:H	2.27	0.43
1:G:116:ILE:HG13	1:G:436:ASP:HB3	2.01	0.43
1:G:166:MET:HG2	1:G:171:ARG:HA	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
1:K:411:GLY:C	1:K:498:THR:HG23	2.43	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:B:120:VAL:HG13	1:B:444:ILE:HD11	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLU:OE2	1:C:260:SER:HB3	2.19	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
1:E:116:ILE:HG13	1:E:436:ASP:HB3	2.01	0.42
1:J:421:LEU:HD21	1:J:467:VAL:HG13	2.00	0.42
1:K:372:LYS:O	1:K:372:LYS:HG3	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:6:PHE:O	2:U:8:LYS:N	2.52	0.42
2:U:18:VAL:HG23	2:U:46:VAL:HA	2.01	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:G:514:LEU:O	1:G:517:THR:OG1	2.34	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:HD2	1:K:225:LYS:HA	1.89	0.42
1:K:340:LYS:HA	1:K:343:ILE:HG12	2.01	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:230:ILE:C	1:H:232:SER:H	2.28	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
2:1:27:THR:OG1	2:1:28:LYS:HD2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:R:34:PRO:C	2:R:36:LYS:H	2.26	0.42
1:B:98:SER:OG	1:B:447:THR:HG22	2.20	0.42
1:B:207:THR:C	1:B:209:LYS:H	2.27	0.42
1:E:52:ASP:O	1:E:56:VAL:HG23	2.20	0.42
1:E:469:LYS:HD3	1:E:469:LYS:HA	1.81	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:N:326:VAL:HG21	1:N:330:ASP:C	2.45	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:176:THR:HG21	1:L:369:ARG:HD3	2.02	0.42
1:L:201:SER:HA	1:L:202:PRO:HD2	1.85	0.42
1:M:89:THR:O	1:M:93:THR:HG23	2.20	0.42
1:A:95:LEU:O	1:A:99:ILE:HD12	2.19	0.42
1:A:355:ASP:OD1	1:A:356:VAL:N	2.53	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
2:Z:6:PHE:O	2:Z:7:ARG:C	2.62	0.42
1:A:191:GLU:HB2	1:A:374:SER:HA	2.02	0.42
1:A:194:LYS:HD3	1:A:332:MET:HE2	2.02	0.42
1:A:287:ASN:HA	1:A:290:LYS:HG2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:95:LEU:O	1:C:99:ILE:HD12	2.20	0.42
1:C:248:VAL:HG11	1:C:324:VAL:HG11	2.01	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
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
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:H:372:LYS:HG3	1:H:372:LYS:O	2.18	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
2:1:7:ARG:O	2:1:8:LYS:HG2	2.19	0.41
1:B:464:SER:HB2	1:N:464:SER:HB2	2.02	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: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
2:S:83:LEU:N	2:S:84:ASP:O	2.53	0.41
2:2:6:PHE:O	2:2:9:PHE:N	2.29	0.41
1:D:175:ILE:HD12	1:D:405:ARG:HH21	1.85	0.41
1:D:478:GLY:HA3	1:D:489:MET:HE2	2.01	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:116:ILE:HG13	1:N:436:ASP:HB3	2.01	0.41
1:N:326:VAL:HG11	1:N:331:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:1:18:VAL:HG12	2:1:46:VAL:HA	2.01	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
1:G:312:ASP:OD1	1:G:312:ASP:N	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:E:69:ILE:HG23	1:F:47:PRO:HG3	2.02	0.41
1:F:297:GLY:O	1:F:319:GLY:HA2	2.20	0.41
1:H:207:THR:C	1:H:209:LYS:H	2.28	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:M:191:GLU:C	1:M:373:LEU:HD23	2.46	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: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:95:LEU:O	1:L:99:ILE:HD12	2.21	0.41
1:L:288:GLN:O	1:L:292:MET:HG3	2.21	0.41
2:O:14:ASP:CG	2:O:92:ARG:HH11	2.29	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:214:GLU:HG3	1:H:325:ILE:HG12	2.02	0.41
1:H:228:SER:O	1:H:256:GLY:HA3	2.21	0.41
1:H:422:ARG:O	1:H:425:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:L:312:ASP:N	2.52	0.41
1:M:95:LEU:O	1:M:99:ILE:HD12	2.20	0.41
1:M:358:THR:O	1:M:358:THR:OG1	2.35	0.41
2:S:46:VAL:HG12	2:S:69:ASP:O	2.21	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:411:GLY:C	1:A:498:THR:HG23	2.45	0.41
1:A:498:THR:O	1:A:502:ARG:HG2	2.21	0.41
1:B:264:LEU:O	1:B:264:LEU:HG	2.20	0.41
1:B:488:ASN:HB3	1:B:491:GLU:HB3	2.01	0.41
1:C:221:LEU:HD23	1:C:249:ILE:HG23	2.01	0.41
1:G:219:TYR:HA	1:G:319:GLY:O	2.21	0.41
1:G:264:LEU:O	1:G:268:LYS:HB2	2.21	0.41
1:G:469:LYS:HD3	1:G:469:LYS:HA	1.89	0.41
1:I:436:ASP:HA	1:I:439:ILE:HD12	2.03	0.41
1:J:136:LYS:HZ1	1:J:490:VAL:HG21	1.85	0.41
1:J:206:ASN:OD1	1:J:207:THR:HG23	2.21	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:J:373:LEU:HD21	1:J:377:VAL:HG22	2.01	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
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
2:2:6:PHE:O	2:2:7:ARG:C	2.64	0.41
2:2:26:VAL:HG23	2:2:27:THR:HG22	2.03	0.41
1:A:65:LYS:O	1:A:69:ILE:HG12	2.21	0.41
1:A:281:PHE:H	1:A:285:ARG:CG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:58:GLY:HA2	2:2:56:LYS:HE2	2.03	0.41
1:A:42:GLN:HE21	1:A:48:LYS:HG3	1.86	0.40
1:A:192:GLY:O	1:A:193:MET:HG2	2.21	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
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:232:SER:HA	1:D:311:GLU:HG3	2.03	0.40
1:D:291:ASP:OD1	1:D:346:ARG:HD3	2.20	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:O:9:PHE:CZ	2:U:98:GLY:HA3	2.56	0.40
2:P:102:ASP:OD1	2:P:102:ASP:N	2.54	0.40
2:R:6:PHE:O	2:R:7:ARG:C	2.64	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:HG3	1:C:372:LYS:O	2.21	0.40
1:D:216:GLN:HA	1:D:323:LYS:HA	2.03	0.40
1:D:415:GLY:HA3	1:D:494:ILE:HG22	2.03	0.40
1:D:422:ARG:O	1:D:425:PRO:HD2	2.22	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:22:LEU:HD23	1:M:62:LEU:HD11	2.02	0.40
1:M:214:GLU:HG3	1:M:325:ILE:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LYS:HD3	1:B:303:GLU:OE2	2.21	0.40
1:B:342:GLN:O	1:B:342:GLN:HG3	2.22	0.40
1:F:233:ILE:HD11	1:F:249:ILE:HD13	2.04	0.40
1:G:478:GLY:HA3	1:G:489:MET:HE2	2.04	0.40
1:H:175:ILE:HG23	1:H:378:ALA:HB3	2.03	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:M:345:LYS:O	1:M:349:GLU:HG3	2.21	0.40
1:N:327:THR:OG1	1:N:328:LYS:N	2.43	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:NE2	1:C:328:LYS:HB3	2.37	0.40
1:C:206:ASN:OD1	1:C:213:CYS:HA	2.21	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/558 (94%)	494 (94%)	24 (5%)	6 (1%)	11	39
1	B	524/558 (94%)	487 (93%)	22 (4%)	15 (3%)	3	20
1	C	524/558 (94%)	492 (94%)	26 (5%)	6 (1%)	11	39
1	D	524/558 (94%)	494 (94%)	25 (5%)	5 (1%)	12	41
1	E	524/558 (94%)	489 (93%)	26 (5%)	9 (2%)	7	30
1	F	524/558 (94%)	490 (94%)	26 (5%)	8 (2%)	8	33
1	G	524/558 (94%)	489 (93%)	25 (5%)	10 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	524/558 (94%)	493 (94%)	27 (5%)	4 (1%)	16	46
1	I	524/558 (94%)	493 (94%)	26 (5%)	5 (1%)	12	41
1	J	524/558 (94%)	497 (95%)	25 (5%)	2 (0%)	30	59
1	K	524/558 (94%)	496 (95%)	23 (4%)	5 (1%)	12	41
1	L	524/558 (94%)	494 (94%)	25 (5%)	5 (1%)	12	41
1	M	524/558 (94%)	489 (93%)	28 (5%)	7 (1%)	9	36
1	N	524/558 (94%)	486 (93%)	28 (5%)	10 (2%)	6	28
2	1	98/114 (86%)	88 (90%)	5 (5%)	5 (5%)	1	10
2	2	102/114 (90%)	94 (92%)	5 (5%)	3 (3%)	3	20
2	O	98/114 (86%)	85 (87%)	7 (7%)	6 (6%)	1	7
2	P	103/114 (90%)	97 (94%)	3 (3%)	3 (3%)	3	20
2	Q	98/114 (86%)	91 (93%)	4 (4%)	3 (3%)	3	18
2	R	98/114 (86%)	88 (90%)	6 (6%)	4 (4%)	2	14
2	S	98/114 (86%)	86 (88%)	6 (6%)	6 (6%)	1	7
2	T	98/114 (86%)	92 (94%)	4 (4%)	2 (2%)	6	27
2	U	100/114 (88%)	91 (91%)	5 (5%)	4 (4%)	2	14
2	V	98/114 (86%)	92 (94%)	3 (3%)	3 (3%)	3	18
2	W	98/114 (86%)	91 (93%)	5 (5%)	2 (2%)	6	27
2	X	98/114 (86%)	91 (93%)	4 (4%)	3 (3%)	3	18
2	Y	98/114 (86%)	92 (94%)	2 (2%)	4 (4%)	2	14
2	Z	106/114 (93%)	91 (86%)	10 (9%)	5 (5%)	2	11
All	All	8727/9408 (93%)	8152 (93%)	425 (5%)	150 (2%)	7	30

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	425/455 (93%)	378 (89%)	47 (11%)	6	22
1	B	425/455 (93%)	371 (87%)	54 (13%)	4	18
1	C	425/455 (93%)	387 (91%)	38 (9%)	9	30
1	D	425/455 (93%)	368 (87%)	57 (13%)	4	16
1	E	425/455 (93%)	377 (89%)	48 (11%)	5	21
1	F	425/455 (93%)	385 (91%)	40 (9%)	8	29
1	G	425/455 (93%)	380 (89%)	45 (11%)	6	24
1	H	425/455 (93%)	379 (89%)	46 (11%)	6	23
1	I	425/455 (93%)	377 (89%)	48 (11%)	5	21
1	J	425/455 (93%)	379 (89%)	46 (11%)	6	23
1	K	425/455 (93%)	380 (89%)	45 (11%)	6	24
1	L	425/455 (93%)	382 (90%)	43 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	425/455 (93%)	378 (89%)	47 (11%)	6	22
1	N	425/455 (93%)	383 (90%)	42 (10%)	7	27
2	1	81/91 (89%)	71 (88%)	10 (12%)	4	19
2	2	83/91 (91%)	73 (88%)	10 (12%)	5	20
2	O	81/91 (89%)	71 (88%)	10 (12%)	4	19
2	P	83/91 (91%)	69 (83%)	14 (17%)	2	9
2	Q	81/91 (89%)	71 (88%)	10 (12%)	4	19
2	R	81/91 (89%)	69 (85%)	12 (15%)	3	13
2	S	81/91 (89%)	69 (85%)	12 (15%)	3	13
2	T	81/91 (89%)	69 (85%)	12 (15%)	3	13
2	U	83/91 (91%)	71 (86%)	12 (14%)	3	14
2	V	81/91 (89%)	68 (84%)	13 (16%)	2	11
2	W	81/91 (89%)	70 (86%)	11 (14%)	3	16
2	X	81/91 (89%)	70 (86%)	11 (14%)	3	16
2	Y	81/91 (89%)	71 (88%)	10 (12%)	4	19
2	Z	86/91 (94%)	72 (84%)	14 (16%)	2	10
All	All	7095/7644 (93%)	6288 (89%)	807 (11%)	5	21

All (807) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	15	LEU
1	A	48	LYS
1	A	74	VAL
1	A	106	LYS
1	A	107	ILE
1	A	150	ILE
1	A	158	ILE
1	A	183	LEU
1	A	200	ILE
1	A	220	VAL
1	A	225	LYS
1	A	227	ILE
1	A	230	ILE
1	A	234	VAL

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Mol	Chain	Res	Type
1	A	267	LEU
1	A	271	LEU
1	A	276	VAL
1	A	300	VAL
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	366	LEU
1	A	367	ASN
1	A	369	ARG
1	A	370	LEU
1	A	385	THR
1	A	401	LEU
1	A	421	LEU
1	A	430	LEU
1	A	431	THR
1	A	453	MET
1	A	464	SER
1	A	465	LEU
1	A	469	LYS
1	A	470	ILE
1	A	487	VAL
1	A	492	LYS
1	A	503	THR
1	A	505	LEU
1	A	511	VAL
1	A	525	ILE
1	B	6	VAL
1	B	15	LEU
1	B	48	LYS
1	B	69	ILE
1	B	74	VAL
1	B	107	ILE
1	B	147	VAL
1	B	158	ILE
1	B	176	THR
1	B	183	LEU

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Mol	Chain	Res	Type
1	B	199	TYR
1	B	200	ILE
1	B	213	CYS
1	B	220	VAL
1	B	221	LEU
1	B	222	LEU
1	B	227	ILE
1	B	234	VAL
1	B	247	LEU
1	B	248	VAL
1	B	249	ILE
1	B	252	GLU
1	B	257	GLU
1	B	265	ASN
1	B	268	LYS
1	B	273	VAL
1	B	276	VAL
1	B	310	LEU
1	B	312	ASP
1	B	314	GLN
1	B	316	HIS
1	B	318	LEU
1	B	321	VAL
1	B	326	VAL
1	B	346	ARG
1	B	350	ILE
1	B	356	VAL
1	B	358	THR
1	B	361	TYR
1	B	366	LEU
1	B	369	ARG
1	B	370	LEU
1	B	372	LYS
1	B	382	VAL
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	492	LYS
1	B	498	THR

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Mol	Chain	Res	Type
1	B	503	THR
1	B	525	ILE
1	C	6	VAL
1	C	15	LEU
1	C	69	ILE
1	C	77	VAL
1	C	90	THR
1	C	107	ILE
1	C	120	VAL
1	C	200	ILE
1	C	220	VAL
1	C	227	ILE
1	C	230	ILE
1	C	234	VAL
1	C	248	VAL
1	C	267	LEU
1	C	273	VAL
1	C	276	VAL
1	C	300	VAL
1	C	306	LEU
1	C	312	ASP
1	C	326	VAL
1	C	340	LYS
1	C	342	GLN
1	C	350	ILE
1	C	364	GLU
1	C	369	ARG
1	C	370	LEU
1	C	385	THR
1	C	390	VAL
1	C	401	LEU
1	C	421	LEU
1	C	431	THR
1	C	453	MET
1	C	465	LEU
1	C	469	LYS
1	C	492	LYS
1	C	503	THR
1	C	505	LEU
1	C	521	VAL
1	D	6	VAL
1	D	15	LEU

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Mol	Chain	Res	Type
1	D	30	THR
1	D	48	LYS
1	D	69	ILE
1	D	74	VAL
1	D	77	VAL
1	D	106	LYS
1	D	107	ILE
1	D	158	ILE
1	D	161	ILE
1	D	200	ILE
1	D	207	THR
1	D	219	TYR
1	D	222	LEU
1	D	227	ILE
1	D	234	VAL
1	D	248	VAL
1	D	250	ILE
1	D	253	ASP
1	D	267	LEU
1	D	273	VAL
1	D	276	VAL
1	D	281	PHE
1	D	289	LEU
1	D	300	VAL
1	D	309	ASN
1	D	312	ASP
1	D	313	VAL
1	D	316	HIS
1	D	324	VAL
1	D	326	VAL
1	D	333	LEU
1	D	339	ASP
1	D	342	GLN
1	D	346	ARG
1	D	350	ILE
1	D	357	THR
1	D	362	GLU
1	D	364	GLU
1	D	366	LEU
1	D	370	LEU
1	D	382	VAL
1	D	385	THR

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Mol	Chain	Res	Type
1	D	401	LEU
1	D	421	LEU
1	D	431	THR
1	D	453	MET
1	D	464	SER
1	D	465	LEU
1	D	492	LYS
1	D	500	VAL
1	D	503	THR
1	D	506	LEU
1	D	511	VAL
1	D	520	VAL
1	D	525	ILE
1	E	6	VAL
1	E	15	LEU
1	E	38	VAL
1	E	69	ILE
1	E	74	VAL
1	E	107	ILE
1	E	147	VAL
1	E	158	ILE
1	E	200	ILE
1	E	220	VAL
1	E	227	ILE
1	E	230	ILE
1	E	231	GLN
1	E	234	VAL
1	E	248	VAL
1	E	250	ILE
1	E	267	LEU
1	E	271	LEU
1	E	273	VAL
1	E	276	VAL
1	E	300	VAL
1	E	312	ASP
1	E	316	HIS
1	E	318	LEU
1	E	326	VAL
1	E	339	ASP
1	E	340	LYS
1	E	342	GLN
1	E	344	GLU

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Mol	Chain	Res	Type
1	E	350	ILE
1	E	358	THR
1	E	360	GLU
1	E	361	TYR
1	E	370	LEU
1	E	382	VAL
1	E	385	THR
1	E	401	LEU
1	E	421	LEU
1	E	431	THR
1	E	453	MET
1	E	464	SER
1	E	465	LEU
1	E	469	LYS
1	E	487	VAL
1	E	492	LYS
1	E	500	VAL
1	E	503	THR
1	E	525	ILE
1	F	6	VAL
1	F	15	LEU
1	F	48	LYS
1	F	69	ILE
1	F	74	VAL
1	F	77	VAL
1	F	107	ILE
1	F	150	ILE
1	F	158	ILE
1	F	200	ILE
1	F	219	TYR
1	F	220	VAL
1	F	227	ILE
1	F	229	SER
1	F	230	ILE
1	F	234	VAL
1	F	248	VAL
1	F	267	LEU
1	F	273	VAL
1	F	276	VAL
1	F	300	VAL
1	F	312	ASP
1	F	324	VAL

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Mol	Chain	Res	Type
1	F	326	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	421	LEU
1	F	431	THR
1	F	464	SER
1	F	465	LEU
1	F	469	LYS
1	F	492	LYS
1	F	498	THR
1	F	503	THR
1	F	511	VAL
1	F	525	ILE
1	G	15	LEU
1	G	48	LYS
1	G	69	ILE
1	G	74	VAL
1	G	106	LYS
1	G	107	ILE
1	G	120	VAL
1	G	150	ILE
1	G	158	ILE
1	G	161	ILE
1	G	200	ILE
1	G	206	ASN
1	G	209	LYS
1	G	220	VAL
1	G	227	ILE
1	G	234	VAL
1	G	248	VAL
1	G	259	LEU
1	G	267	LEU
1	G	273	VAL
1	G	276	VAL
1	G	281	PHE
1	G	300	VAL
1	G	308	LEU
1	G	312	ASP

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Mol	Chain	Res	Type
1	G	326	VAL
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	421	LEU
1	G	431	THR
1	G	453	MET
1	G	465	LEU
1	G	469	LYS
1	G	492	LYS
1	G	500	VAL
1	G	503	THR
1	G	505	LEU
1	G	511	VAL
1	G	525	ILE
1	H	6	VAL
1	H	15	LEU
1	H	22	LEU
1	H	48	LYS
1	H	69	ILE
1	H	74	VAL
1	H	150	ILE
1	H	158	ILE
1	H	171	ARG
1	H	183	LEU
1	H	200	ILE
1	H	208	SER
1	H	220	VAL
1	H	227	ILE
1	H	230	ILE
1	H	234	VAL
1	H	248	VAL
1	H	267	LEU
1	H	273	VAL
1	H	274	VAL
1	H	276	VAL
1	H	300	VAL

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Mol	Chain	Res	Type
1	H	304	GLU
1	H	306	LEU
1	H	312	ASP
1	H	326	VAL
1	H	340	LYS
1	H	350	ILE
1	H	356	VAL
1	H	358	THR
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	421	LEU
1	H	431	THR
1	H	464	SER
1	H	465	LEU
1	H	469	LYS
1	H	492	LYS
1	H	498	THR
1	H	500	VAL
1	H	503	THR
1	H	525	ILE
1	I	6	VAL
1	I	15	LEU
1	I	22	LEU
1	I	48	LYS
1	I	74	VAL
1	I	95	LEU
1	I	106	LYS
1	I	107	ILE
1	I	158	ILE
1	I	161	ILE
1	I	176	THR
1	I	200	ILE
1	I	220	VAL
1	I	227	ILE
1	I	230	ILE
1	I	231	GLN
1	I	234	VAL
1	I	248	VAL

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Mol	Chain	Res	Type
1	I	267	LEU
1	I	273	VAL
1	I	276	VAL
1	I	281	PHE
1	I	300	VAL
1	I	312	ASP
1	I	313	VAL
1	I	316	HIS
1	I	324	VAL
1	I	326	VAL
1	I	350	ILE
1	I	357	THR
1	I	364	GLU
1	I	368	GLU
1	I	370	LEU
1	I	373	LEU
1	I	374	SER
1	I	385	THR
1	I	401	LEU
1	I	421	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	492	LYS
1	I	498	THR
1	I	503	THR
1	I	525	ILE
1	J	6	VAL
1	J	15	LEU
1	J	48	LYS
1	J	62	LEU
1	J	69	ILE
1	J	74	VAL
1	J	77	VAL
1	J	106	LYS
1	J	107	ILE
1	J	133	LYS
1	J	158	ILE
1	J	171	ARG

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Mol	Chain	Res	Type
1	J	176	THR
1	J	200	ILE
1	J	220	VAL
1	J	227	ILE
1	J	230	ILE
1	J	233	ILE
1	J	234	VAL
1	J	248	VAL
1	J	267	LEU
1	J	273	VAL
1	J	276	VAL
1	J	285	ARG
1	J	300	VAL
1	J	310	LEU
1	J	312	ASP
1	J	326	VAL
1	J	340	LYS
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	421	LEU
1	J	431	THR
1	J	453	MET
1	J	464	SER
1	J	465	LEU
1	J	469	LYS
1	J	492	LYS
1	J	498	THR
1	J	500	VAL
1	J	503	THR
1	J	511	VAL
1	K	15	LEU
1	K	48	LYS
1	K	74	VAL
1	K	106	LYS
1	K	107	ILE
1	K	120	VAL
1	K	158	ILE
1	K	200	ILE

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Mol	Chain	Res	Type
1	K	211	GLN
1	K	219	TYR
1	K	220	VAL
1	K	227	ILE
1	K	229	SER
1	K	230	ILE
1	K	234	VAL
1	K	248	VAL
1	K	267	LEU
1	K	273	VAL
1	K	276	VAL
1	K	300	VAL
1	K	306	LEU
1	K	307	THR
1	K	312	ASP
1	K	324	VAL
1	K	326	VAL
1	K	340	LYS
1	K	350	ILE
1	K	353	GLN
1	K	364	GLU
1	K	368	GLU
1	K	369	ARG
1	K	370	LEU
1	K	373	LEU
1	K	382	VAL
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	492	LYS
1	K	500	VAL
1	K	503	THR
1	K	525	ILE
1	L	6	VAL
1	L	15	LEU
1	L	49	VAL
1	L	69	ILE
1	L	74	VAL

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Mol	Chain	Res	Type
1	L	106	LYS
1	L	107	ILE
1	L	120	VAL
1	L	150	ILE
1	L	158	ILE
1	L	183	LEU
1	L	200	ILE
1	L	220	VAL
1	L	234	VAL
1	L	248	VAL
1	L	262	LEU
1	L	267	LEU
1	L	273	VAL
1	L	276	VAL
1	L	300	VAL
1	L	312	ASP
1	L	313	VAL
1	L	324	VAL
1	L	326	VAL
1	L	340	LYS
1	L	350	ILE
1	L	358	THR
1	L	362	GLU
1	L	366	LEU
1	L	369	ARG
1	L	370	LEU
1	L	385	THR
1	L	401	LEU
1	L	421	LEU
1	L	431	THR
1	L	453	MET
1	L	464	SER
1	L	465	LEU
1	L	469	LYS
1	L	492	LYS
1	L	500	VAL
1	L	503	THR
1	L	521	VAL
1	M	6	VAL
1	M	15	LEU
1	M	48	LYS
1	M	54	VAL

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Mol	Chain	Res	Type
1	M	69	ILE
1	M	74	VAL
1	M	106	LYS
1	M	107	ILE
1	M	150	ILE
1	M	158	ILE
1	M	176	THR
1	M	183	LEU
1	M	200	ILE
1	M	220	VAL
1	M	227	ILE
1	M	234	VAL
1	M	239	ILE
1	M	248	VAL
1	M	267	LEU
1	M	268	LYS
1	M	273	VAL
1	M	276	VAL
1	M	300	VAL
1	M	308	LEU
1	M	312	ASP
1	M	326	VAL
1	M	340	LYS
1	M	356	VAL
1	M	366	LEU
1	M	370	LEU
1	M	373	LEU
1	M	382	VAL
1	M	385	THR
1	M	401	LEU
1	M	421	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	492	LYS
1	M	500	VAL
1	M	503	THR
1	M	511	VAL

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Mol	Chain	Res	Type
1	M	525	ILE
1	N	6	VAL
1	N	15	LEU
1	N	69	ILE
1	N	74	VAL
1	N	90	THR
1	N	106	LYS
1	N	107	ILE
1	N	150	ILE
1	N	158	ILE
1	N	161	ILE
1	N	183	LEU
1	N	200	ILE
1	N	220	VAL
1	N	225	LYS
1	N	227	ILE
1	N	230	ILE
1	N	234	VAL
1	N	243	HIS
1	N	244	ARG
1	N	273	VAL
1	N	276	VAL
1	N	303	GLU
1	N	306	LEU
1	N	307	THR
1	N	312	ASP
1	N	324	VAL
1	N	326	VAL
1	N	342	GLN
1	N	350	ILE
1	N	358	THR
1	N	370	LEU
1	N	385	THR
1	N	401	LEU
1	N	421	LEU
1	N	431	THR
1	N	464	SER
1	N	465	LEU
1	N	469	LYS
1	N	487	VAL
1	N	492	LYS
1	N	500	VAL

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Mol	Chain	Res	Type
1	N	503	THR
2	O	7	ARG
2	O	24	GLU
2	O	31	ILE
2	O	45	THR
2	O	46	VAL
2	O	63	VAL
2	O	71	VAL
2	O	83	LEU
2	O	85	ASP
2	O	101	VAL
2	P	12	LEU
2	P	24	GLU
2	P	26	VAL
2	P	27	THR
2	P	33	LEU
2	P	45	THR
2	P	46	VAL
2	P	47	VAL
2	P	49	VAL
2	P	63	VAL
2	P	71	VAL
2	P	83	LEU
2	P	85	ASP
2	P	101	VAL
2	Q	24	GLU
2	Q	38	GLN
2	Q	41	VAL
2	Q	47	VAL
2	Q	63	VAL
2	Q	71	VAL
2	Q	85	ASP
2	Q	86	LYS
2	Q	99	LYS
2	Q	101	VAL
2	R	10	LEU
2	R	24	GLU
2	R	25	THR
2	R	31	ILE
2	R	45	THR
2	R	46	VAL
2	R	49	VAL

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Mol	Chain	Res	Type
2	R	63	VAL
2	R	71	VAL
2	R	73	LEU
2	R	85	ASP
2	R	101	VAL
2	S	10	LEU
2	S	13	PHE
2	S	16	VAL
2	S	20	ARG
2	S	31	ILE
2	S	46	VAL
2	S	49	VAL
2	S	63	VAL
2	S	71	VAL
2	S	73	LEU
2	S	75	GLU
2	S	101	VAL
2	T	24	GLU
2	T	26	VAL
2	T	28	LYS
2	T	37	SER
2	T	38	GLN
2	T	45	THR
2	T	46	VAL
2	T	63	VAL
2	T	65	VAL
2	T	70	LYS
2	T	73	LEU
2	T	101	VAL
2	U	7	ARG
2	U	15	ARG
2	U	17	LEU
2	U	24	GLU
2	U	45	THR
2	U	46	VAL
2	U	49	VAL
2	U	63	VAL
2	U	71	VAL
2	U	73	LEU
2	U	85	ASP
2	U	101	VAL
2	V	17	LEU

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Mol	Chain	Res	Type
2	V	24	GLU
2	V	26	VAL
2	V	27	THR
2	V	31	ILE
2	V	35	GLU
2	V	45	THR
2	V	46	VAL
2	V	63	VAL
2	V	71	VAL
2	V	75	GLU
2	V	85	ASP
2	V	101	VAL
2	W	24	GLU
2	W	26	VAL
2	W	27	THR
2	W	45	THR
2	W	46	VAL
2	W	47	VAL
2	W	61	GLN
2	W	63	VAL
2	W	71	VAL
2	W	85	ASP
2	W	101	VAL
2	X	7	ARG
2	X	24	GLU
2	X	28	LYS
2	X	45	THR
2	X	46	VAL
2	X	49	VAL
2	X	63	VAL
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	46	VAL
2	Y	49	VAL
2	Y	63	VAL
2	Y	71	VAL

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Mol	Chain	Res	Type
2	Y	85	ASP
2	Y	101	VAL
2	Z	12	LEU
2	Z	24	GLU
2	Z	26	VAL
2	Z	28	LYS
2	Z	45	THR
2	Z	46	VAL
2	Z	49	VAL
2	Z	54	LYS
2	Z	63	VAL
2	Z	71	VAL
2	Z	85	ASP
2	Z	92	ARG
2	Z	101	VAL
2	Z	104	LEU
2	1	24	GLU
2	1	28	LYS
2	1	31	ILE
2	1	45	THR
2	1	46	VAL
2	1	71	VAL
2	1	83	LEU
2	1	85	ASP
2	1	97	LEU
2	1	101	VAL
2	2	10	LEU
2	2	20	ARG
2	2	31	ILE
2	2	45	THR
2	2	46	VAL
2	2	63	VAL
2	2	71	VAL
2	2	75	GLU
2	2	85	ASP
2	2	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	288	GLN

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Mol	Chain	Res	Type
1	B	79	ASN
1	B	265	ASN
1	B	287	ASN
1	B	288	GLN
1	B	353	GLN
1	C	342	GLN
1	D	18	GLN
1	D	79	ASN
1	D	146	GLN
1	E	18	GLN
1	E	79	ASN
1	E	342	GLN
1	F	18	GLN
1	F	42	GLN
1	F	134	GLN
1	F	206	ASN
1	F	231	GLN
1	F	288	GLN
1	F	402	ASN
1	F	472	GLN
1	G	75	GLN
1	G	79	ASN
1	G	284	ASN
1	G	288	GLN
1	G	353	GLN
1	G	402	ASN
1	H	79	ASN
1	H	211	GLN
1	H	402	ASN
1	I	79	ASN
1	I	146	GLN
1	I	284	ASN
1	I	402	ASN
1	J	18	GLN
1	J	211	GLN
1	J	216	GLN
1	J	231	GLN
1	K	18	GLN
1	K	79	ASN
1	K	216	GLN
1	K	342	GLN
1	K	402	ASN

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Mol	Chain	Res	Type
1	K	488	ASN
1	L	231	GLN
1	M	18	GLN
1	M	79	ASN
1	N	241	ASN
1	N	284	ASN
2	2	38	GLN

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 oligosaccharides 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	F	601	-	28,29,29	1.42	4 (14%)	43,45,45	1.81	9 (20%)
3	ADP	A	601	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	10 (23%)
3	ADP	G	601	-	28,29,29	1.40	5 (17%)	43,45,45	1.78	9 (20%)
3	ADP	K	601	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
3	ADP	M	601	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	601	-	28,29,29	1.43	5 (17%)	43,45,45	1.82	9 (20%)
3	ADP	C	601	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
3	ADP	H	601	-	28,29,29	1.41	4 (14%)	43,45,45	1.80	9 (20%)
3	ADP	J	601	-	28,29,29	1.42	5 (17%)	43,45,45	1.81	9 (20%)
3	ADP	L	601	-	28,29,29	1.41	4 (14%)	43,45,45	1.80	9 (20%)
3	ADP	I	601	-	28,29,29	1.41	4 (14%)	43,45,45	1.87	10 (23%)
3	ADP	N	601	-	28,29,29	1.44	5 (17%)	43,45,45	1.87	10 (23%)
3	ADP	E	601	-	28,29,29	1.42	4 (14%)	43,45,45	1.80	9 (20%)
3	ADP	D	601	-	28,29,29	1.42	4 (14%)	43,45,45	1.83	10 (23%)

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	F	601	-	-	5/16/32/32	0/3/3/3
3	ADP	A	601	-	-	4/16/32/32	0/3/3/3
3	ADP	G	601	-	-	4/16/32/32	0/3/3/3
3	ADP	K	601	-	-	5/16/32/32	0/3/3/3
3	ADP	M	601	-	-	4/16/32/32	0/3/3/3
3	ADP	B	601	-	-	5/16/32/32	0/3/3/3
3	ADP	C	601	-	-	6/16/32/32	0/3/3/3
3	ADP	H	601	-	-	2/16/32/32	0/3/3/3
3	ADP	J	601	-	-	5/16/32/32	0/3/3/3
3	ADP	L	601	-	-	4/16/32/32	0/3/3/3
3	ADP	I	601	-	-	7/16/32/32	0/3/3/3
3	ADP	N	601	-	-	4/16/32/32	0/3/3/3
3	ADP	E	601	-	-	7/16/32/32	0/3/3/3
3	ADP	D	601	-	-	7/16/32/32	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	ADP	C5-C4	4.73	1.47	1.39
3	B	601	ADP	C5-C4	4.72	1.47	1.39
3	M	601	ADP	C5-C4	4.71	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	ADP	C5-C4	4.70	1.47	1.39
3	N	601	ADP	C5-C4	4.67	1.47	1.39
3	K	601	ADP	C5-C4	4.64	1.47	1.39
3	H	601	ADP	C5-C4	4.64	1.47	1.39
3	D	601	ADP	C5-C4	4.62	1.47	1.39
3	J	601	ADP	C5-C4	4.62	1.47	1.39
3	G	601	ADP	C5-C4	4.62	1.47	1.39
3	A	601	ADP	C5-C4	4.62	1.47	1.39
3	C	601	ADP	C5-C4	4.61	1.47	1.39
3	L	601	ADP	C5-C4	4.60	1.47	1.39
3	I	601	ADP	C5-C4	4.55	1.47	1.39
3	I	601	ADP	C5-C6	2.83	1.48	1.41
3	N	601	ADP	C5-C6	2.79	1.48	1.41
3	K	601	ADP	C5-C6	2.78	1.48	1.41
3	C	601	ADP	C5-C6	2.78	1.48	1.41
3	D	601	ADP	C5-C6	2.77	1.48	1.41
3	B	601	ADP	C5-C6	2.76	1.48	1.41
3	F	601	ADP	C5-C6	2.76	1.48	1.41
3	L	601	ADP	C5-C6	2.76	1.48	1.41
3	E	601	ADP	C5-C6	2.75	1.48	1.41
3	M	601	ADP	C5-C6	2.75	1.48	1.41
3	J	601	ADP	C5-C6	2.74	1.48	1.41
3	H	601	ADP	C5-C6	2.74	1.48	1.41
3	A	601	ADP	C5-C6	2.73	1.48	1.41
3	G	601	ADP	C5-C6	2.71	1.48	1.41
3	N	601	ADP	C8-N7	2.51	1.36	1.31
3	I	601	ADP	C8-N7	2.50	1.36	1.31
3	J	601	ADP	C8-N7	2.49	1.36	1.31
3	K	601	ADP	C8-N7	2.44	1.36	1.31
3	C	601	ADP	C8-N7	2.44	1.36	1.31
3	B	601	ADP	C8-N7	2.44	1.36	1.31
3	D	601	ADP	C8-N7	2.43	1.36	1.31
3	L	601	ADP	C8-N7	2.43	1.36	1.31
3	A	601	ADP	C8-N7	2.42	1.36	1.31
3	H	601	ADP	C8-N7	2.42	1.36	1.31
3	F	601	ADP	C8-N7	2.41	1.36	1.31
3	E	601	ADP	C8-N7	2.39	1.36	1.31
3	G	601	ADP	C8-N7	2.36	1.36	1.31
3	M	601	ADP	C8-N7	2.35	1.36	1.31
3	M	601	ADP	C5-N7	-2.25	1.35	1.39
3	B	601	ADP	C5-N7	-2.23	1.35	1.39
3	F	601	ADP	C5-N7	-2.22	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	ADP	C5-N7	-2.21	1.35	1.39
3	G	601	ADP	C5-N7	-2.20	1.35	1.39
3	N	601	ADP	C5-N7	-2.19	1.35	1.39
3	E	601	ADP	C5-N7	-2.17	1.35	1.39
3	C	601	ADP	C5-N7	-2.17	1.35	1.39
3	J	601	ADP	C5-N7	-2.16	1.35	1.39
3	L	601	ADP	C5-N7	-2.16	1.35	1.39
3	H	601	ADP	C5-N7	-2.16	1.35	1.39
3	A	601	ADP	C5-N7	-2.14	1.35	1.39
3	K	601	ADP	C5-N7	-2.14	1.35	1.39
3	I	601	ADP	C5-N7	-2.11	1.35	1.39
3	B	601	ADP	PA-O3A	2.07	1.61	1.59
3	N	601	ADP	PA-O3A	2.07	1.61	1.59
3	J	601	ADP	PA-O3A	2.04	1.61	1.59
3	G	601	ADP	C4-N9	-2.01	1.33	1.37

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	601	ADP	C5-C4-N3	-5.75	118.80	126.72
3	C	601	ADP	C5-C4-N3	-5.73	118.83	126.72
3	B	601	ADP	C5-C4-N3	-5.70	118.87	126.72
3	M	601	ADP	C5-C4-N3	-5.67	118.90	126.72
3	F	601	ADP	C5-C4-N3	-5.66	118.92	126.72
3	A	601	ADP	C5-C4-N3	-5.66	118.93	126.72
3	D	601	ADP	C5-C4-N3	-5.63	118.97	126.72
3	J	601	ADP	C5-C4-N3	-5.60	119.01	126.72
3	E	601	ADP	C5-C4-N3	-5.57	119.04	126.72
3	I	601	ADP	C5-C4-N3	-5.57	119.05	126.72
3	K	601	ADP	C5-C4-N3	-5.55	119.07	126.72
3	L	601	ADP	C5-C4-N3	-5.52	119.12	126.72
3	H	601	ADP	C5-C4-N3	-5.49	119.16	126.72
3	G	601	ADP	C5-C4-N3	-5.43	119.24	126.72
3	F	601	ADP	N3-C4-N9	4.53	134.87	127.17
3	M	601	ADP	N3-C4-N9	4.51	134.83	127.17
3	B	601	ADP	N3-C4-N9	4.46	134.76	127.17
3	A	601	ADP	N3-C4-N9	4.40	134.65	127.17
3	C	601	ADP	N3-C4-N9	4.40	134.65	127.17
3	E	601	ADP	N3-C4-N9	4.40	134.65	127.17
3	N	601	ADP	N3-C4-N9	4.37	134.60	127.17
3	D	601	ADP	N3-C4-N9	4.37	134.60	127.17
3	J	601	ADP	N3-C4-N9	4.35	134.56	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	601	ADP	N3-C4-N9	4.34	134.54	127.17
3	G	601	ADP	N3-C4-N9	4.33	134.53	127.17
3	K	601	ADP	N3-C4-N9	4.31	134.50	127.17
3	L	601	ADP	N3-C4-N9	4.30	134.48	127.17
3	I	601	ADP	N3-C4-N9	4.24	134.37	127.17
3	N	601	ADP	C2-N3-C4	3.75	120.99	111.83
3	N	601	ADP	C4-C5-N7	-3.74	106.30	110.58
3	C	601	ADP	C2-N3-C4	3.74	120.97	111.83
3	I	601	ADP	C2-N3-C4	3.71	120.89	111.83
3	I	601	ADP	C4-C5-N7	-3.70	106.35	110.58
3	D	601	ADP	C2-N3-C4	3.69	120.85	111.83
3	J	601	ADP	C2-N3-C4	3.69	120.85	111.83
3	B	601	ADP	C2-N3-C4	3.69	120.84	111.83
3	A	601	ADP	C2-N3-C4	3.69	120.83	111.83
3	F	601	ADP	C2-N3-C4	3.68	120.81	111.83
3	K	601	ADP	C2-N3-C4	3.68	120.81	111.83
3	H	601	ADP	C2-N3-C4	3.65	120.74	111.83
3	L	601	ADP	C2-N3-C4	3.65	120.73	111.83
3	M	601	ADP	C2-N3-C4	3.64	120.73	111.83
3	E	601	ADP	C2-N3-C4	3.64	120.71	111.83
3	C	601	ADP	C4-C5-N7	-3.61	106.45	110.58
3	J	601	ADP	C4-C5-N7	-3.60	106.47	110.58
3	G	601	ADP	C2-N3-C4	3.58	120.58	111.83
3	D	601	ADP	C4-C5-N7	-3.58	106.49	110.58
3	B	601	ADP	C4-C5-N7	-3.57	106.50	110.58
3	K	601	ADP	C4-C5-N7	-3.56	106.51	110.58
3	L	601	ADP	C4-C5-N7	-3.55	106.52	110.58
3	A	601	ADP	C4-C5-N7	-3.54	106.54	110.58
3	H	601	ADP	C4-C5-N7	-3.53	106.55	110.58
3	G	601	ADP	C4-C5-N7	-3.51	106.57	110.58
3	E	601	ADP	C4-C5-N7	-3.50	106.58	110.58
3	F	601	ADP	C4-C5-N7	-3.49	106.59	110.58
3	M	601	ADP	C4-C5-N7	-3.48	106.61	110.58
3	I	601	ADP	N3-C2-N1	-3.36	123.50	128.58
3	H	601	ADP	N3-C2-N1	-3.35	123.51	128.58
3	A	601	ADP	N3-C2-N1	-3.35	123.51	128.58
3	D	601	ADP	N3-C2-N1	-3.34	123.53	128.58
3	C	601	ADP	N3-C2-N1	-3.34	123.53	128.58
3	N	601	ADP	N3-C2-N1	-3.34	123.53	128.58
3	J	601	ADP	N3-C2-N1	-3.33	123.54	128.58
3	K	601	ADP	N3-C2-N1	-3.32	123.55	128.58
3	L	601	ADP	N3-C2-N1	-3.30	123.59	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	ADP	N3-C2-N1	-3.29	123.60	128.58
3	E	601	ADP	N3-C2-N1	-3.27	123.63	128.58
3	F	601	ADP	N3-C2-N1	-3.26	123.64	128.58
3	G	601	ADP	N3-C2-N1	-3.21	123.72	128.58
3	M	601	ADP	N3-C2-N1	-3.21	123.72	128.58
3	I	601	ADP	O4'-C1'-N9	3.05	113.95	108.09
3	G	601	ADP	C4-N9-C8	2.99	108.88	105.74
3	N	601	ADP	O4'-C1'-N9	2.96	113.78	108.09
3	H	601	ADP	C4-N9-C8	2.96	108.84	105.74
3	F	601	ADP	C4-N9-C8	2.91	108.79	105.74
3	J	601	ADP	C4-N9-C8	2.87	108.75	105.74
3	L	601	ADP	C4-N9-C8	2.83	108.71	105.74
3	E	601	ADP	C4-N9-C8	2.82	108.69	105.74
3	I	601	ADP	C4-N9-C8	2.79	108.67	105.74
3	K	601	ADP	C4-N9-C8	2.79	108.67	105.74
3	B	601	ADP	C4-N9-C8	2.77	108.64	105.74
3	D	601	ADP	C4-N9-C8	2.75	108.63	105.74
3	M	601	ADP	C4-N9-C8	2.75	108.63	105.74
3	A	601	ADP	C4-N9-C8	2.75	108.62	105.74
3	N	601	ADP	C5-N7-C8	2.70	107.70	103.45
3	I	601	ADP	C5-N7-C8	2.68	107.67	103.45
3	C	601	ADP	C4-N9-C8	2.68	108.55	105.74
3	N	601	ADP	C4-N9-C8	2.64	108.51	105.74
3	B	601	ADP	C5-N7-C8	2.62	107.57	103.45
3	D	601	ADP	C5-N7-C8	2.61	107.55	103.45
3	H	601	ADP	C5-N7-C8	2.61	107.55	103.45
3	J	601	ADP	C5-N7-C8	2.60	107.54	103.45
3	C	601	ADP	C5-N7-C8	2.59	107.52	103.45
3	F	601	ADP	C5-N7-C8	2.59	107.52	103.45
3	G	601	ADP	C5-N7-C8	2.59	107.52	103.45
3	K	601	ADP	C5-N7-C8	2.58	107.51	103.45
3	L	601	ADP	C5-N7-C8	2.57	107.49	103.45
3	M	601	ADP	C5-N7-C8	2.57	107.49	103.45
3	A	601	ADP	C5-N7-C8	2.57	107.49	103.45
3	E	601	ADP	C5-N7-C8	2.54	107.45	103.45
3	I	601	ADP	C6-C5-N7	2.40	136.71	132.09
3	N	601	ADP	C6-C5-N7	2.34	136.59	132.09
3	J	601	ADP	C6-C5-N7	2.33	136.58	132.09
3	K	601	ADP	C6-C5-N7	2.31	136.54	132.09
3	H	601	ADP	C6-C5-N7	2.31	136.54	132.09
3	G	601	ADP	C6-C5-N7	2.30	136.52	132.09
3	L	601	ADP	C6-C5-N7	2.29	136.51	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	ADP	C6-C5-N7	2.27	136.47	132.09
3	C	601	ADP	C6-C5-N7	2.27	136.47	132.09
3	I	601	ADP	N9-C8-N7	-2.25	110.74	113.94
3	H	601	ADP	N9-C8-N7	-2.23	110.77	113.94
3	B	601	ADP	C6-C5-N7	2.22	136.37	132.09
3	E	601	ADP	C6-C5-N7	2.21	136.36	132.09
3	G	601	ADP	N9-C8-N7	-2.21	110.80	113.94
3	F	601	ADP	C6-C5-N7	2.21	136.35	132.09
3	A	601	ADP	C6-C5-N7	2.21	136.35	132.09
3	J	601	ADP	N9-C8-N7	-2.20	110.81	113.94
3	L	601	ADP	N9-C8-N7	-2.16	110.88	113.94
3	F	601	ADP	N9-C8-N7	-2.15	110.88	113.94
3	K	601	ADP	N9-C8-N7	-2.15	110.89	113.94
3	N	601	ADP	N9-C8-N7	-2.15	110.89	113.94
3	M	601	ADP	C6-C5-N7	2.14	136.21	132.09
3	D	601	ADP	N9-C8-N7	-2.14	110.90	113.94
3	B	601	ADP	N9-C8-N7	-2.13	110.92	113.94
3	A	601	ADP	N9-C8-N7	-2.12	110.93	113.94
3	C	601	ADP	N9-C8-N7	-2.10	110.96	113.94
3	E	601	ADP	N9-C8-N7	-2.09	110.97	113.94
3	M	601	ADP	N9-C8-N7	-2.06	111.01	113.94
3	D	601	ADP	O4'-C1'-N9	2.05	112.03	108.09
3	A	601	ADP	O4'-C1'-N9	2.03	111.99	108.09

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	A	601	ADP	C5'-O5'-PA-O3A
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	B	601	ADP	C5'-O5'-PA-O3A
3	C	601	ADP	PB-O3A-PA-O5'
3	C	601	ADP	C5'-O5'-PA-O1A
3	C	601	ADP	C5'-O5'-PA-O2A
3	C	601	ADP	C5'-O5'-PA-O3A
3	D	601	ADP	PA-O3A-PB-O3B
3	D	601	ADP	C5'-O5'-PA-O1A

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

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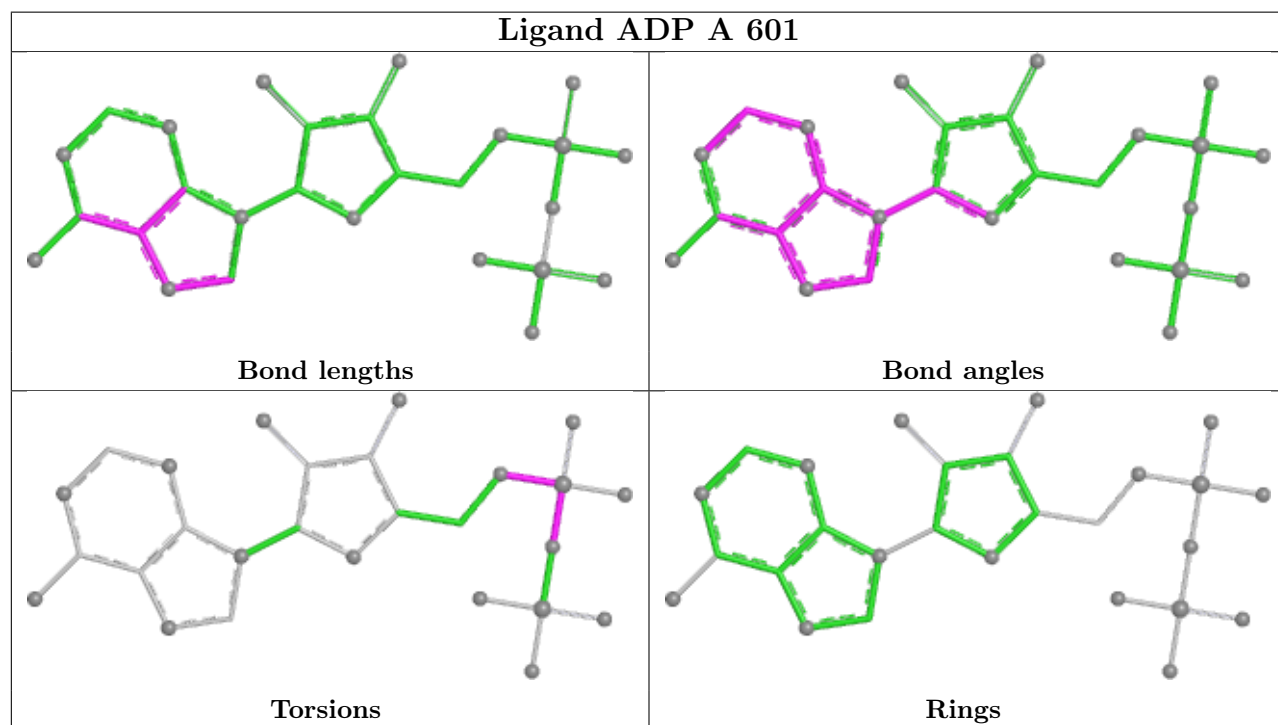
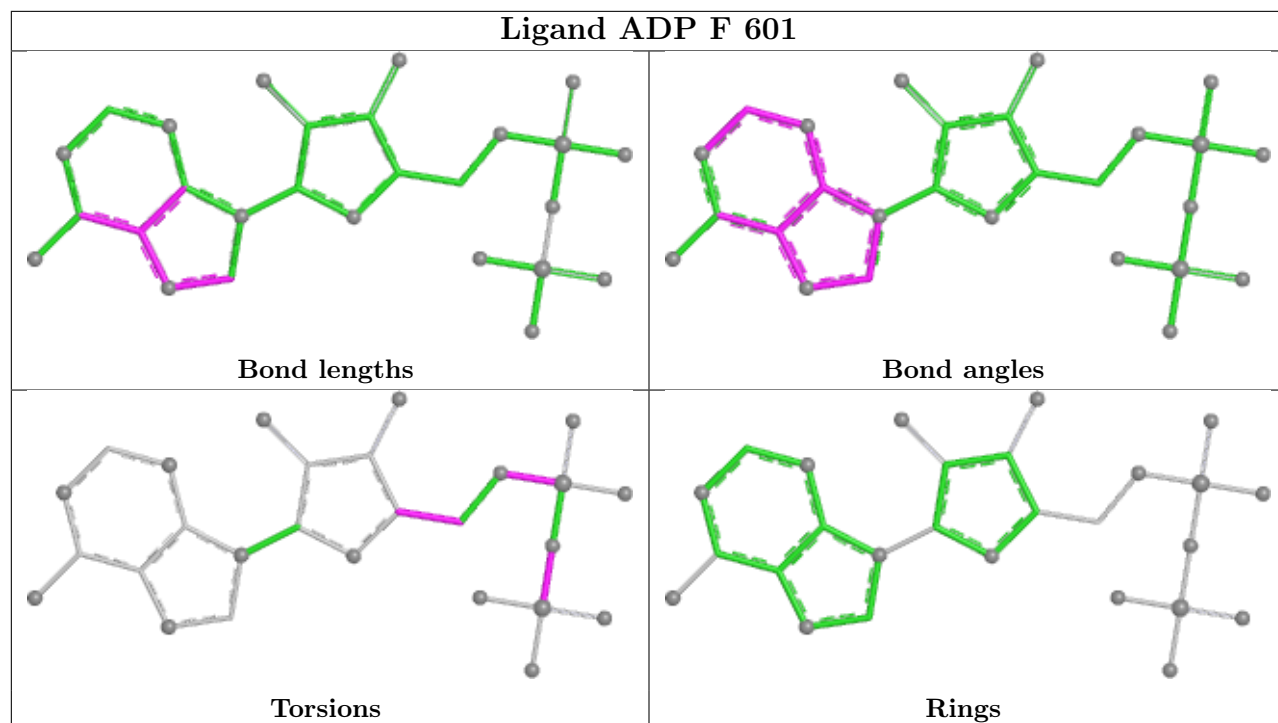
Mol	Chain	Res	Type	Atoms
3	J	601	ADP	PB-O3A-PA-O2A
3	E	601	ADP	PA-O3A-PB-O1B
3	G	601	ADP	PB-O3A-PA-O2A
3	L	601	ADP	PB-O3A-PA-O2A
3	D	601	ADP	PA-O3A-PB-O1B
3	D	601	ADP	PA-O3A-PB-O2B
3	E	601	ADP	PA-O3A-PB-O2B
3	E	601	ADP	PA-O3A-PB-O3B
3	F	601	ADP	PA-O3A-PB-O2B
3	N	601	ADP	PA-O3A-PB-O2B
3	N	601	ADP	PA-O3A-PB-O3B
3	H	601	ADP	PB-O3A-PA-O1A
3	K	601	ADP	PB-O3A-PA-O1A

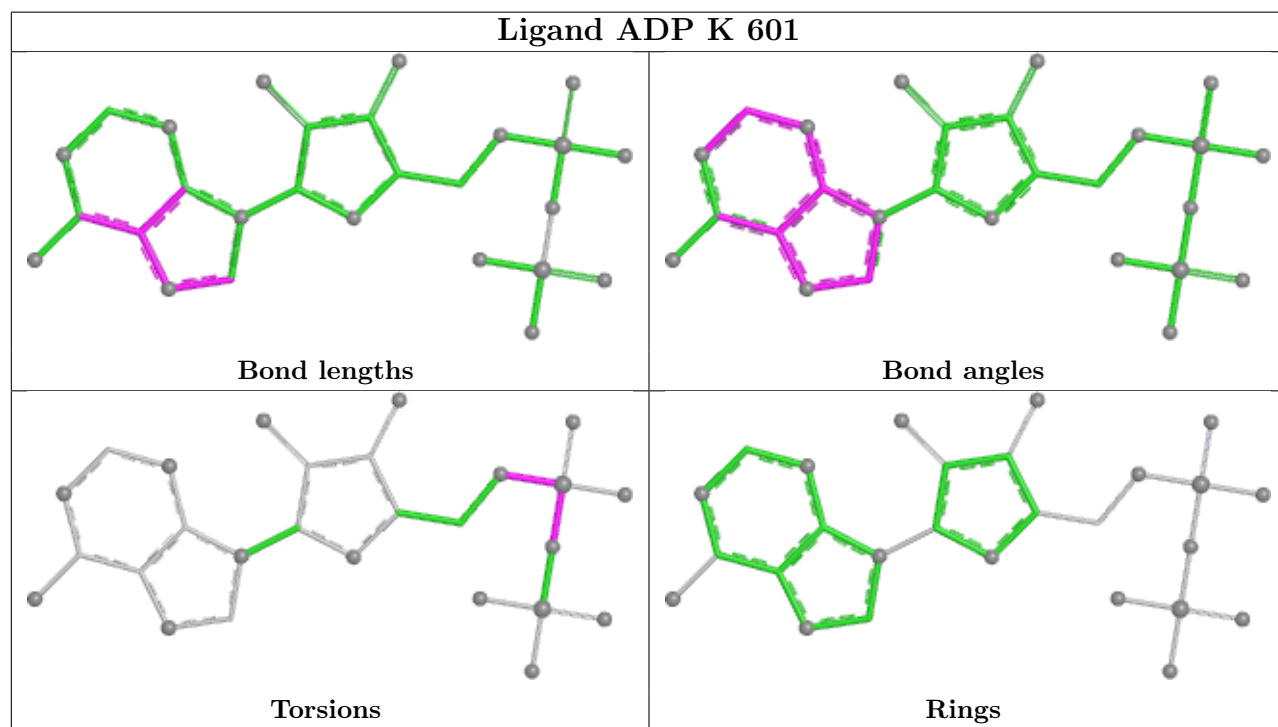
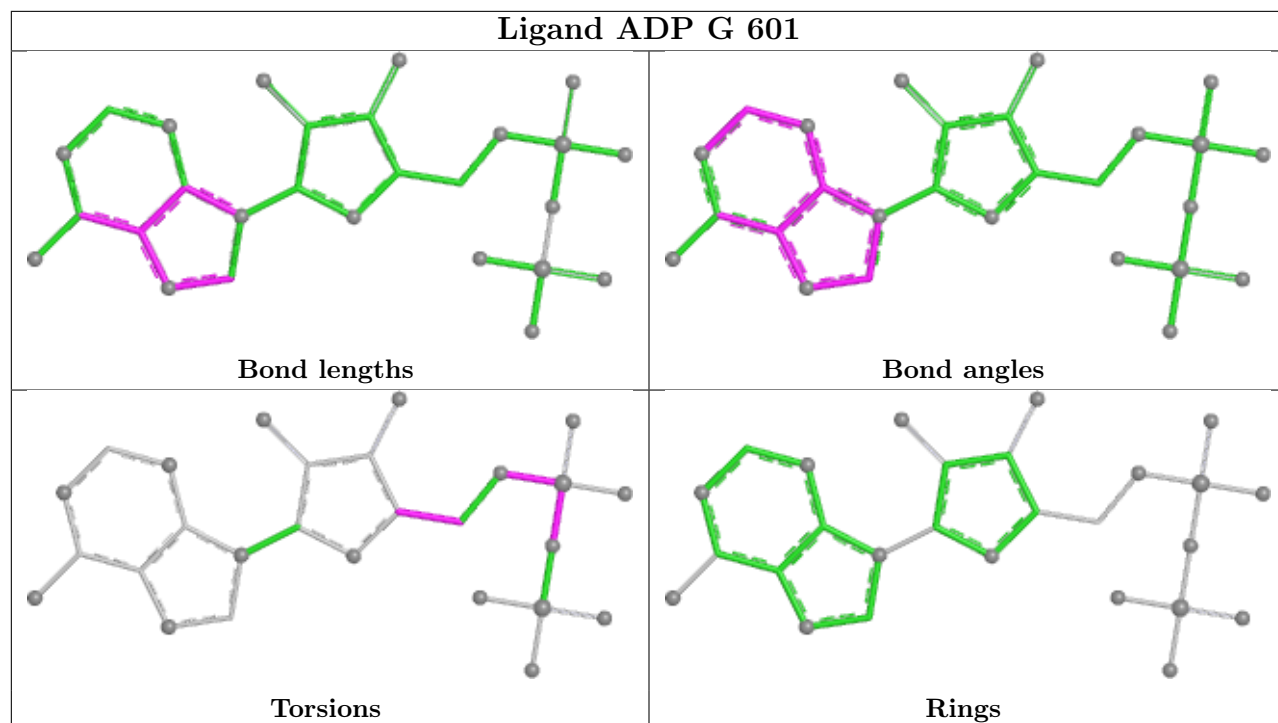
There are no ring outliers.

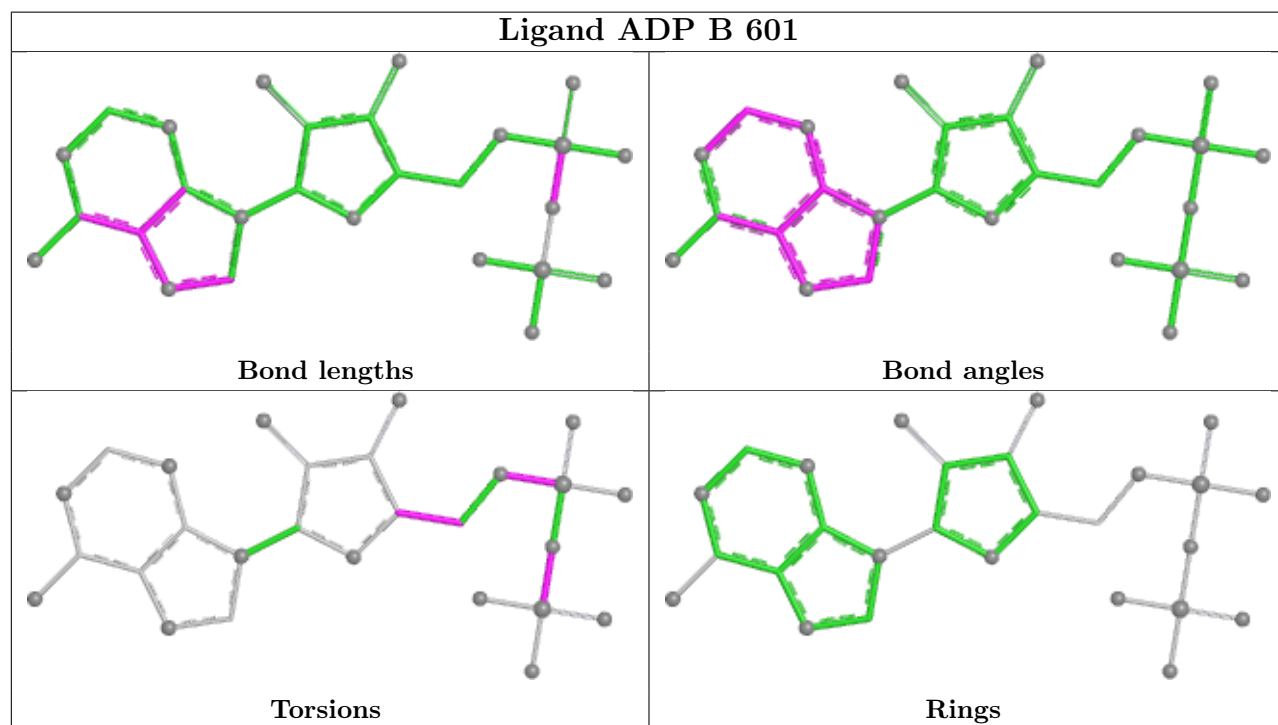
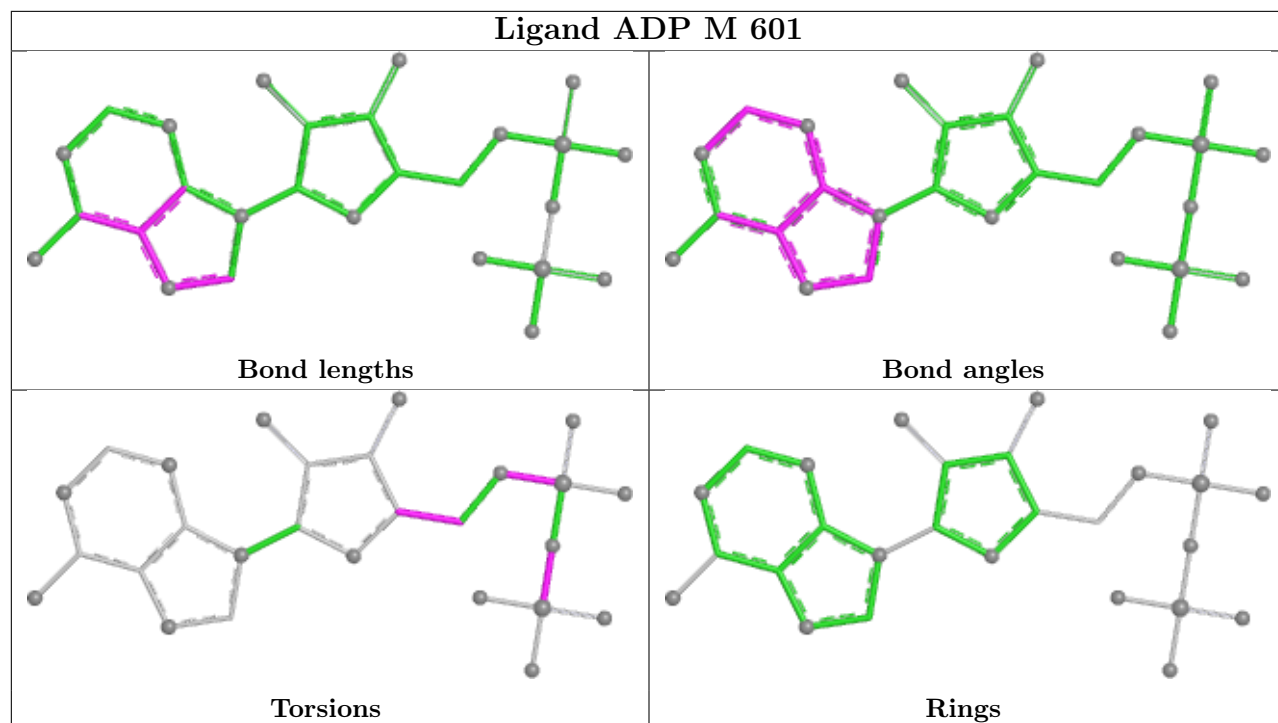
8 monomers are involved in 11 short contacts:

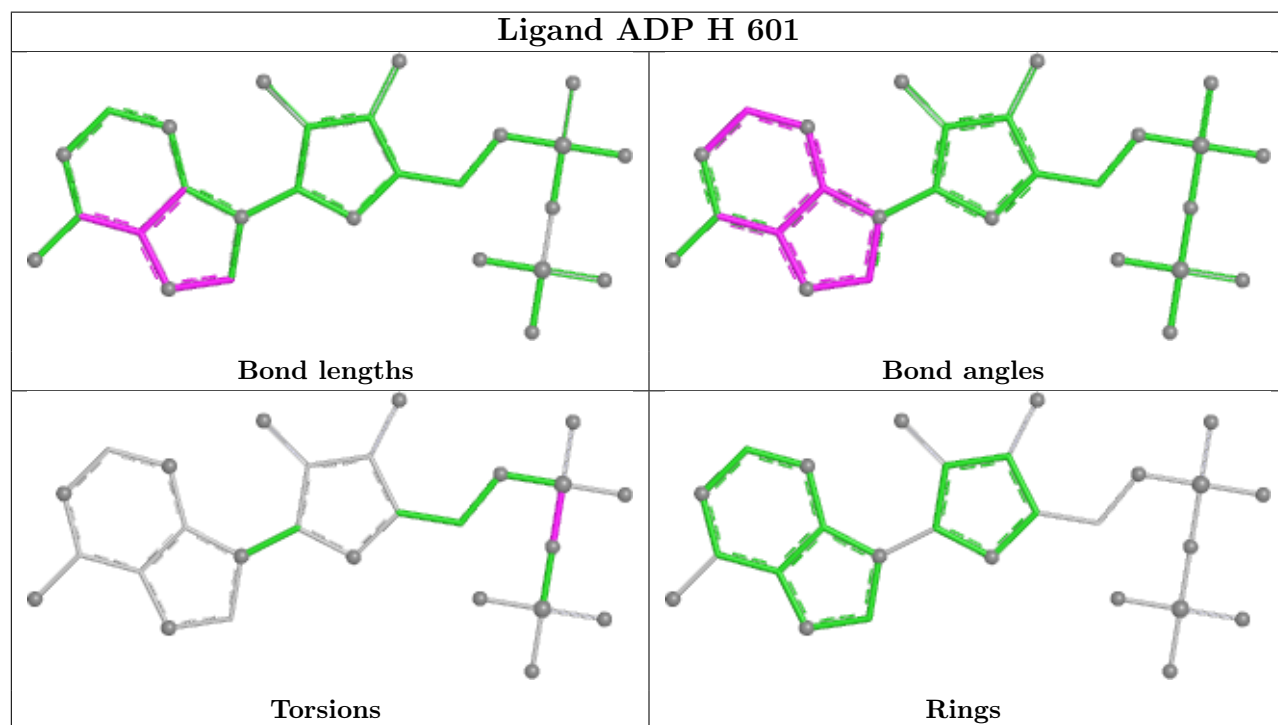
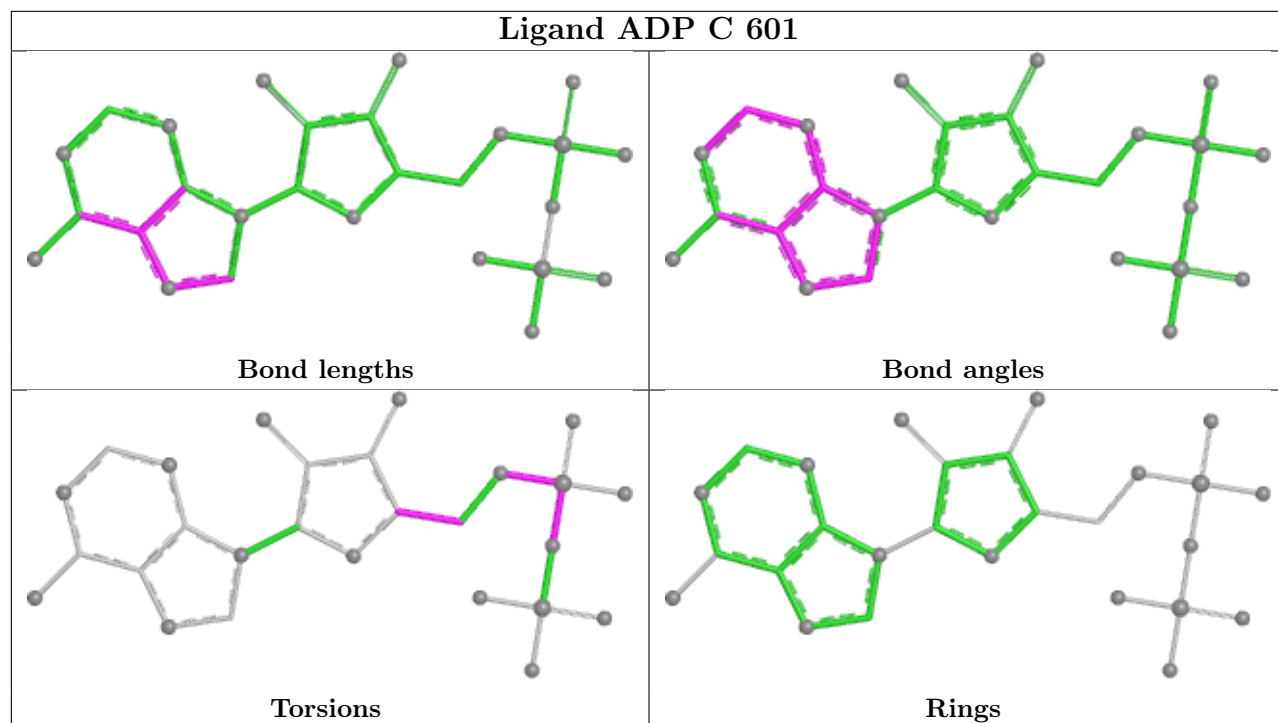
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	2	0
3	K	601	ADP	1	0
3	B	601	ADP	2	0
3	C	601	ADP	2	0
3	L	601	ADP	1	0
3	I	601	ADP	1	0
3	N	601	ADP	1	0
3	D	601	ADP	1	0

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

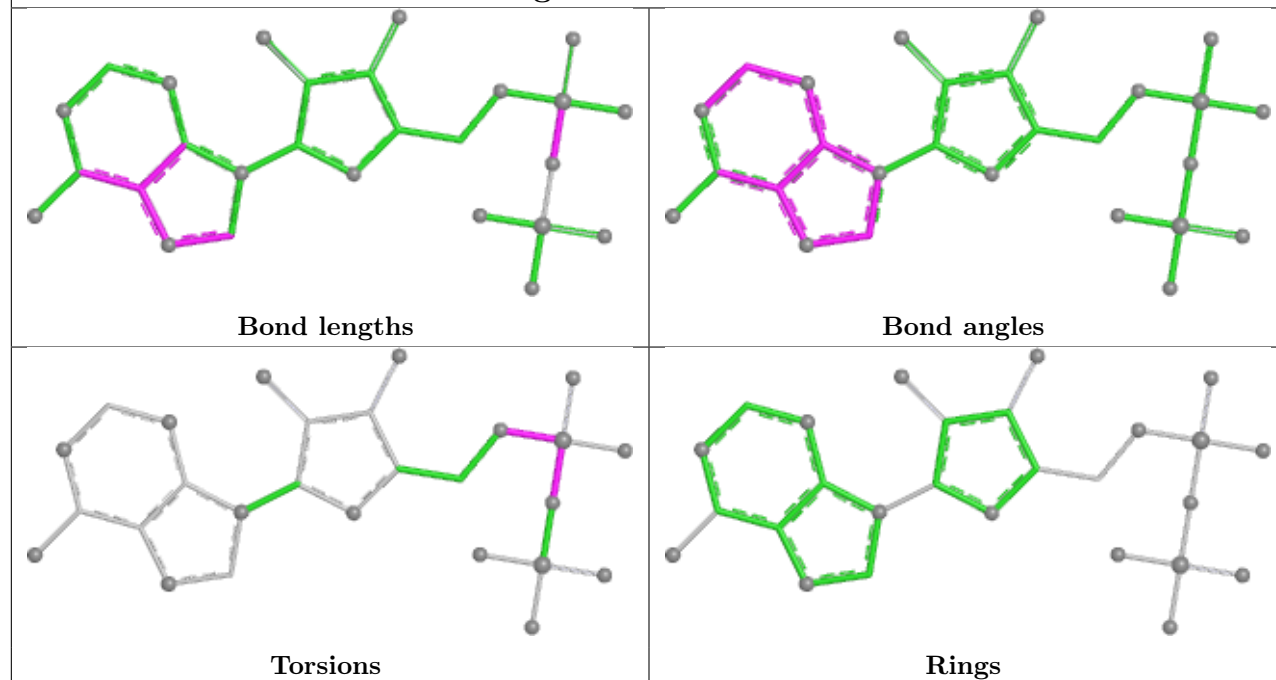




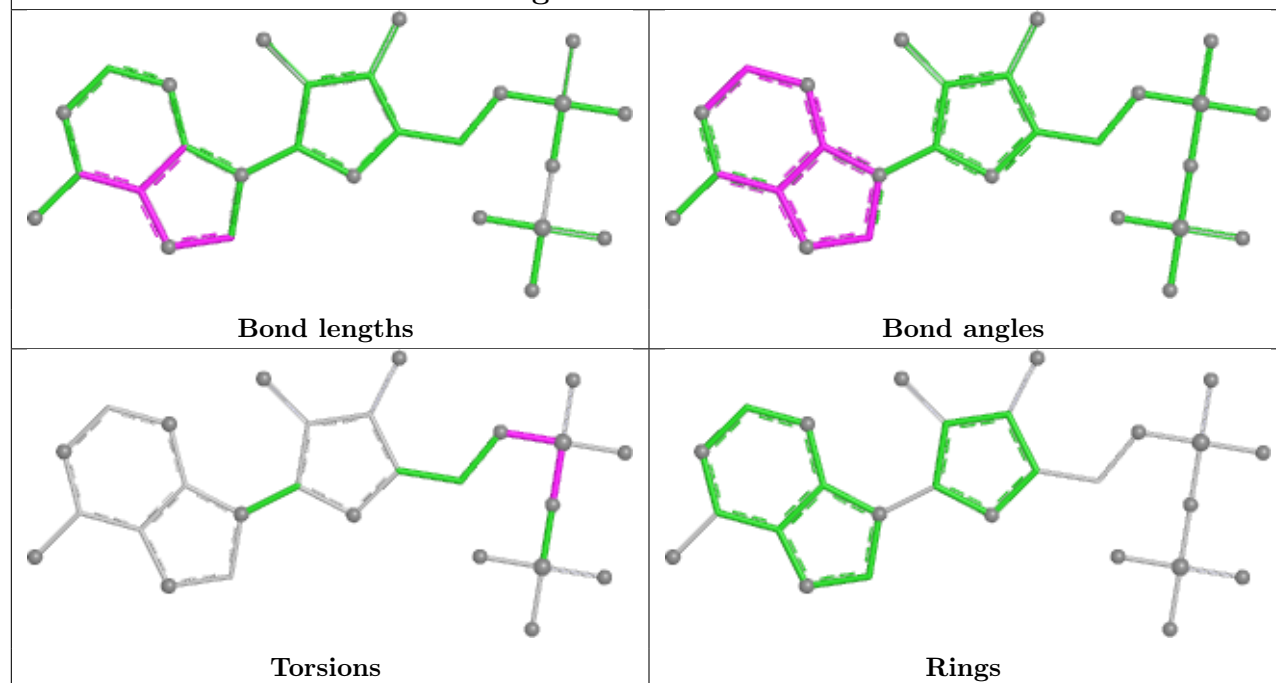




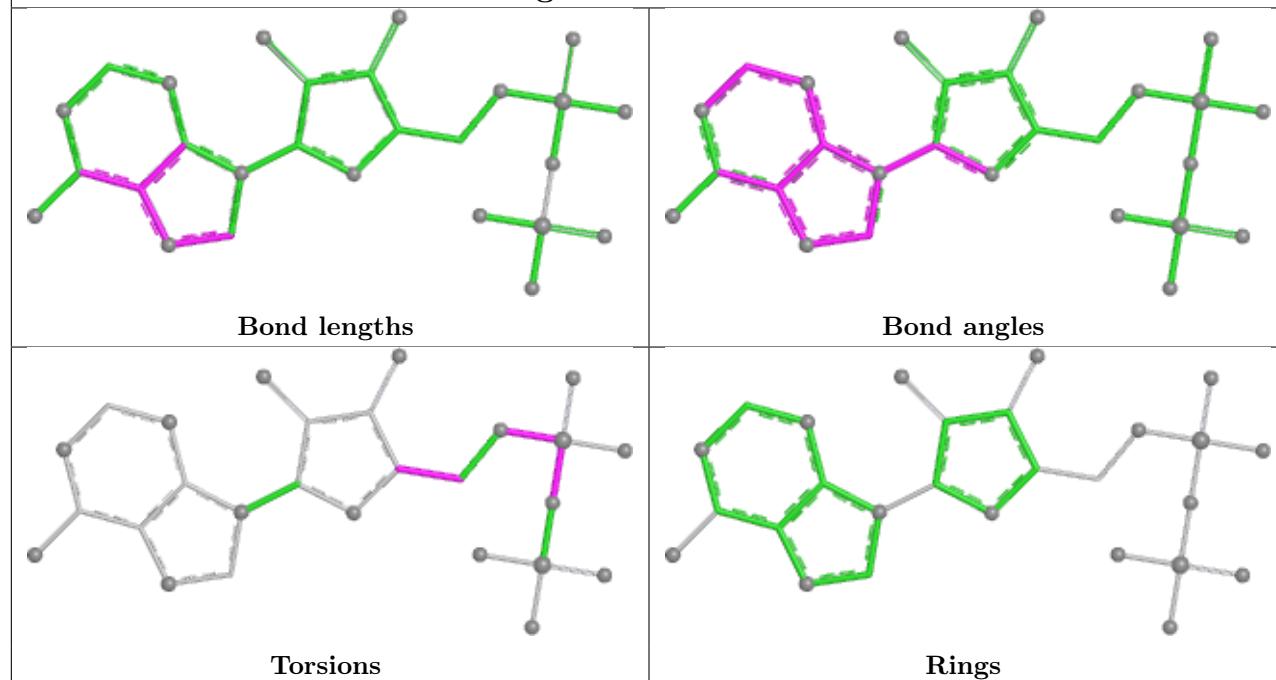
Ligand ADP J 601



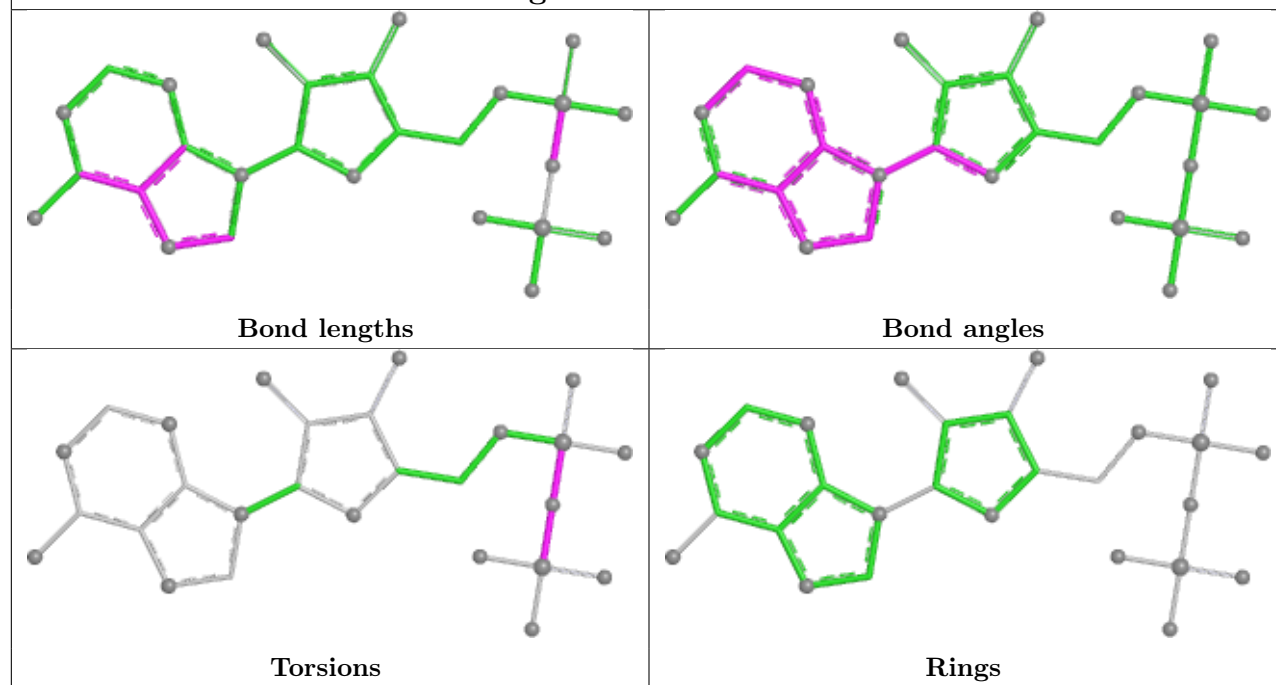
Ligand ADP L 601

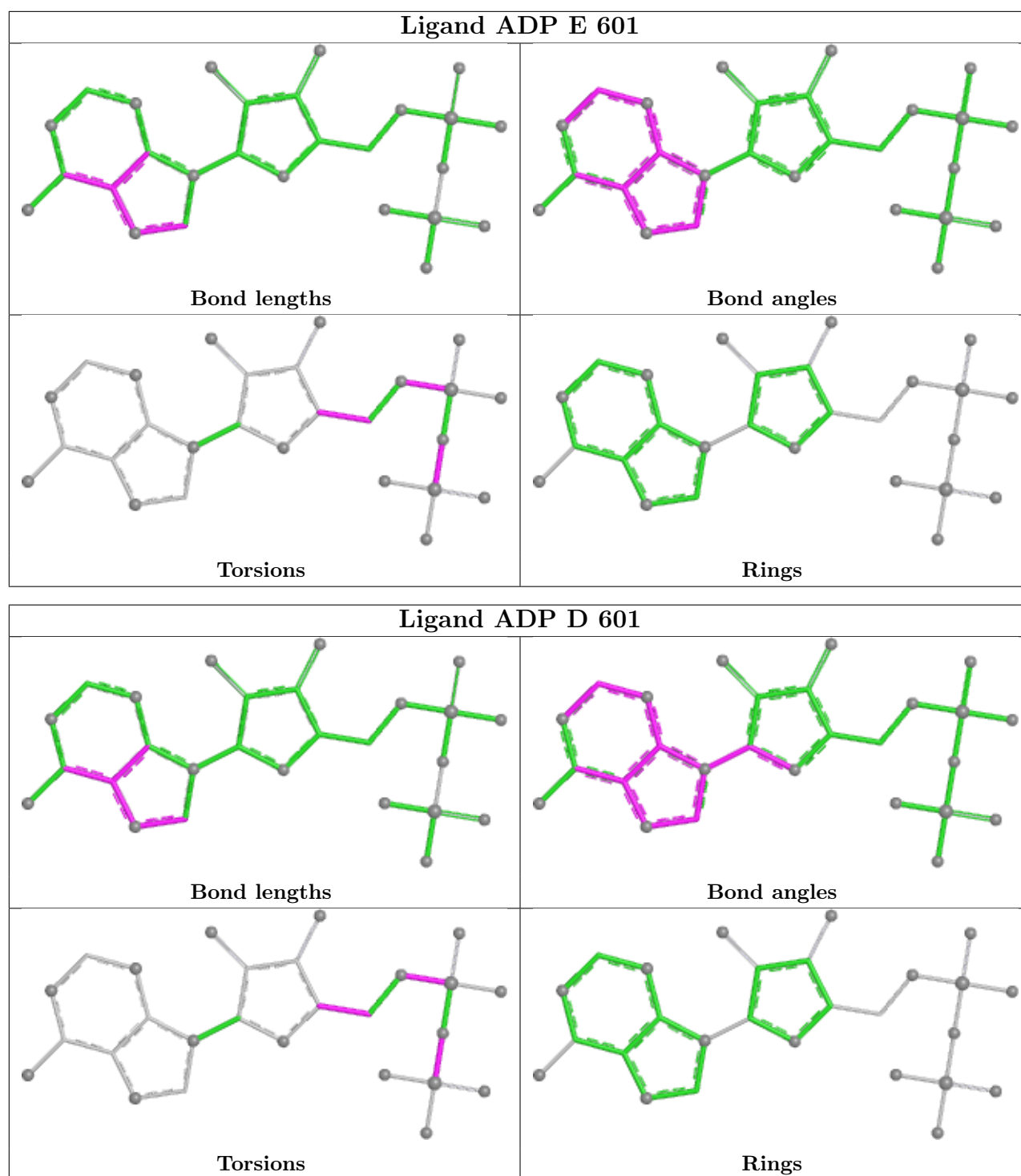


Ligand ADP I 601



Ligand ADP N 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%)	-0.02	2 (0%) 88 78	65, 112, 194, 225	0
1	B	526/558 (94%)	0.14	11 (2%) 63 42	66, 116, 232, 279	0
1	C	526/558 (94%)	-0.09	1 (0%) 91 84	66, 108, 169, 217	0
1	D	526/558 (94%)	-0.02	4 (0%) 82 66	61, 107, 195, 228	0
1	E	526/558 (94%)	0.03	5 (0%) 79 62	66, 106, 202, 226	0
1	F	526/558 (94%)	-0.08	5 (0%) 79 62	67, 110, 166, 192	0
1	G	526/558 (94%)	-0.05	2 (0%) 88 78	67, 102, 153, 196	0
1	H	526/558 (94%)	-0.08	1 (0%) 91 84	66, 103, 160, 191	0
1	I	526/558 (94%)	-0.10	1 (0%) 91 84	64, 103, 179, 203	0
1	J	526/558 (94%)	-0.06	4 (0%) 82 66	65, 107, 164, 191	0
1	K	526/558 (94%)	-0.09	3 (0%) 85 72	61, 106, 167, 207	0
1	L	526/558 (94%)	-0.04	8 (1%) 72 52	66, 101, 151, 182	0
1	M	526/558 (94%)	-0.07	1 (0%) 91 84	66, 112, 169, 207	0
1	N	526/558 (94%)	0.02	11 (2%) 63 42	70, 110, 165, 202	0
2	1	100/114 (87%)	-0.23	0 100 100	94, 117, 179, 210	0
2	2	104/114 (91%)	-0.02	0 100 100	101, 135, 185, 200	0
2	O	100/114 (87%)	-0.06	0 100 100	107, 139, 185, 194	0
2	P	105/114 (92%)	-0.11	0 100 100	93, 121, 199, 209	0
2	Q	100/114 (87%)	-0.20	0 100 100	84, 114, 179, 199	0
2	R	100/114 (87%)	-0.05	1 (1%) 79 62	97, 136, 187, 201	0
2	S	100/114 (87%)	0.07	0 100 100	127, 158, 194, 202	0
2	T	100/114 (87%)	-0.04	0 100 100	123, 157, 195, 224	0
2	U	102/114 (89%)	-0.04	1 (0%) 79 62	121, 145, 193, 223	0
2	V	100/114 (87%)	-0.14	0 100 100	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%)	-0.10	0	100	100	118, 145, 182, 197	0
2	X	100/114 (87%)	-0.19	0	100	100	118, 141, 201, 210	0
2	Y	100/114 (87%)	-0.21	0	100	100	97, 124, 181, 216	0
2	Z	108/114 (94%)	-0.09	0	100	100	91, 118, 170, 216	0
All	All	8783/9408 (93%)	-0.05	61 (0%)	84	69	61, 113, 185, 279	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	234	VAL	4.4
1	D	219	TYR	4.0
1	N	235	PRO	3.9
1	N	272	GLN	3.7
1	L	371	ALA	3.6
1	J	171	ARG	3.4
1	G	342	GLN	3.2
1	L	231	GLN	3.1
1	K	357	THR	3.1
1	D	236	ALA	3.0
1	G	8	PHE	2.9
2	U	104	LEU	2.9
1	J	231	GLN	2.8
1	M	380	LEU	2.8
1	F	240	ALA	2.8
1	K	305	GLY	2.8
1	H	356	VAL	2.8
1	N	231	GLN	2.7
1	B	370	LEU	2.7
1	E	248	VAL	2.7
1	L	373	LEU	2.6
1	B	262	LEU	2.6
1	N	240	ALA	2.6
1	N	238	GLU	2.6
1	B	236	ALA	2.6
1	B	213	CYS	2.6
1	F	231	GLN	2.5
1	N	218	ALA	2.5
1	L	374	SER	2.5
1	F	350	ILE	2.5
1	E	275	ALA	2.5
1	N	239	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	255	ASP	2.3
1	L	171	ARG	2.3
1	E	276	VAL	2.3
1	B	254	VAL	2.2
1	F	368	GLU	2.2
1	N	262	LEU	2.2
1	B	222	LEU	2.2
1	D	416	GLY	2.2
2	R	9	PHE	2.2
1	D	356	VAL	2.1
1	L	416	GLY	2.1
1	L	206	ASN	2.1
1	B	300	VAL	2.1
1	N	215	PHE	2.1
1	B	269	VAL	2.1
1	N	308	LEU	2.1
1	B	465	LEU	2.1
1	C	370	LEU	2.1
1	I	368	GLU	2.1
1	B	271	LEU	2.1
1	A	223	SER	2.0
1	A	370	LEU	2.0
1	K	380	LEU	2.0
1	B	306	LEU	2.0
1	J	371	ALA	2.0
1	E	368	GLU	2.0
1	J	368	GLU	2.0
1	L	370	LEU	2.0
1	F	230	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

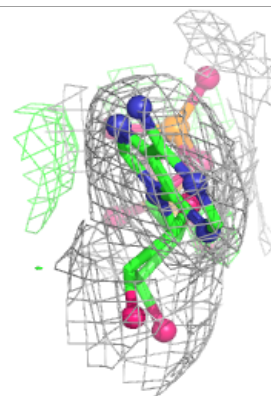
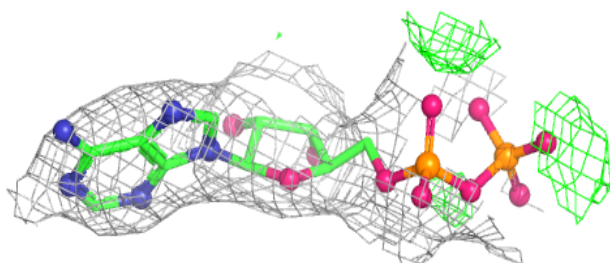
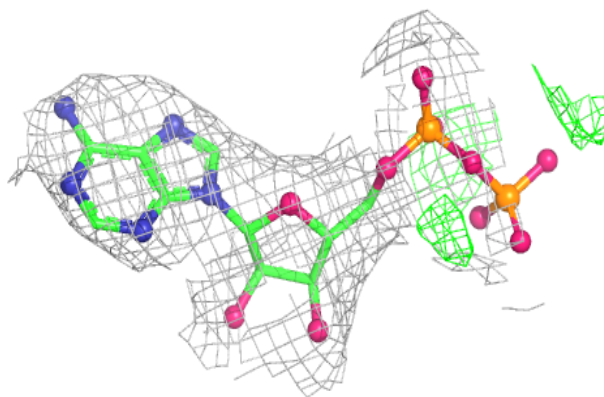
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	C	602	1/1	0.86	0.15	84,84,84,84	0
4	MG	D	602	1/1	0.88	0.15	77,77,77,77	0
4	MG	N	602	1/1	0.89	0.16	81,81,81,81	0
4	MG	J	602	1/1	0.90	0.15	66,66,66,66	0
4	MG	I	602	1/1	0.91	0.12	60,60,60,60	0
4	MG	L	602	1/1	0.92	0.11	72,72,72,72	0
4	MG	B	602	1/1	0.93	0.12	74,74,74,74	0
4	MG	H	602	1/1	0.93	0.13	73,73,73,73	0
4	MG	G	602	1/1	0.94	0.13	67,67,67,67	0
3	ADP	J	601	27/27	0.94	0.09	69,88,94,105	0
3	ADP	N	601	27/27	0.94	0.09	72,87,97,99	0
3	ADP	A	601	27/27	0.94	0.09	68,90,102,104	0
3	ADP	E	601	27/27	0.94	0.09	69,80,89,93	0
3	ADP	F	601	27/27	0.94	0.10	62,87,92,94	0
3	ADP	I	601	27/27	0.95	0.09	61,86,93,96	0
3	ADP	D	601	27/27	0.95	0.10	62,86,98,100	0
3	ADP	B	601	27/27	0.95	0.08	74,98,105,115	0
3	ADP	C	601	27/27	0.95	0.08	69,90,104,110	0
3	ADP	G	601	27/27	0.95	0.10	65,81,90,97	0
4	MG	M	602	1/1	0.95	0.15	60,60,60,60	0
3	ADP	H	601	27/27	0.95	0.09	75,87,95,98	0
4	MG	K	602	1/1	0.96	0.09	61,61,61,61	0
4	MG	E	602	1/1	0.96	0.12	62,62,62,62	0
4	MG	F	602	1/1	0.96	0.13	66,66,66,66	0
3	ADP	K	601	27/27	0.96	0.08	67,87,96,104	0
3	ADP	L	601	27/27	0.97	0.07	63,85,94,95	0
4	MG	A	602	1/1	0.97	0.10	72,72,72,72	0
3	ADP	M	601	27/27	0.97	0.07	69,87,93,95	0

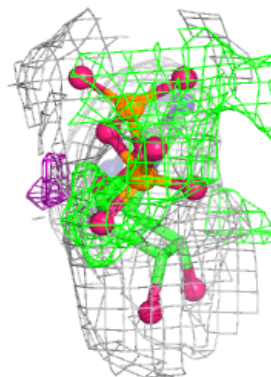
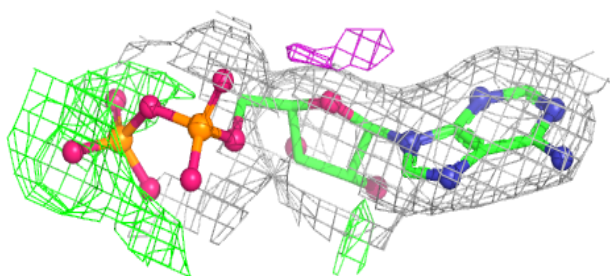
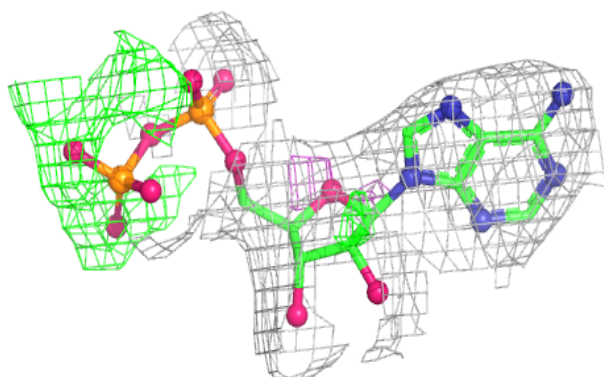
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP 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)

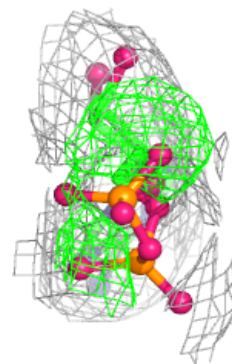
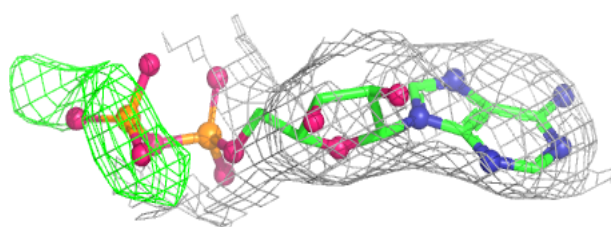
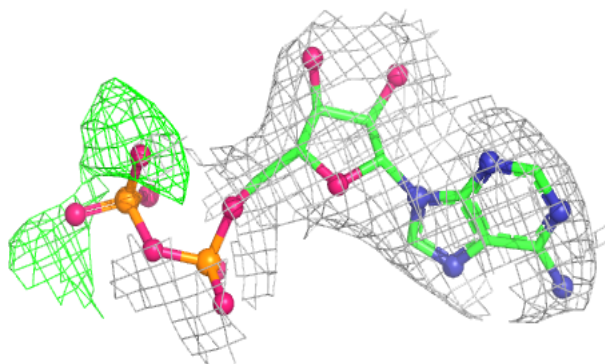
**Electron density around ADP N 601:**

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

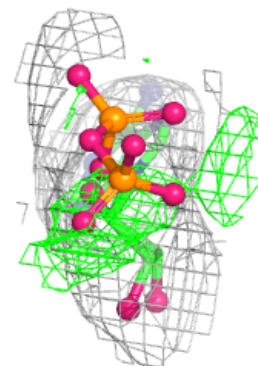
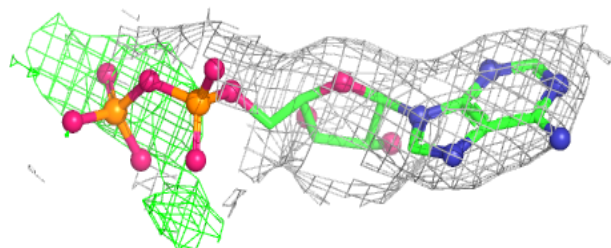
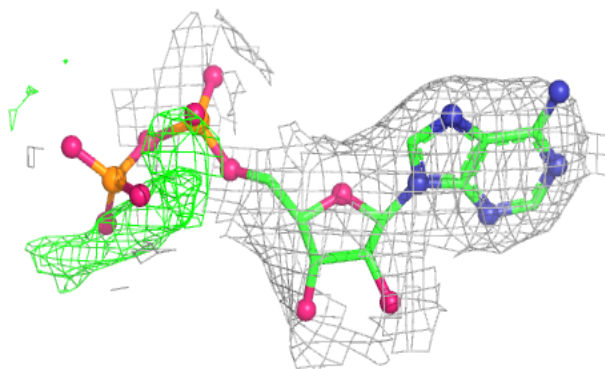


Electron density around ADP A 601:

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

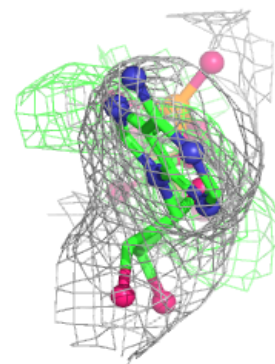
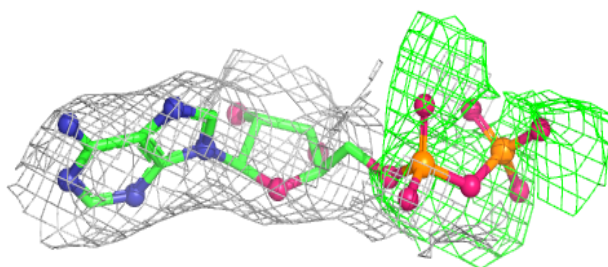
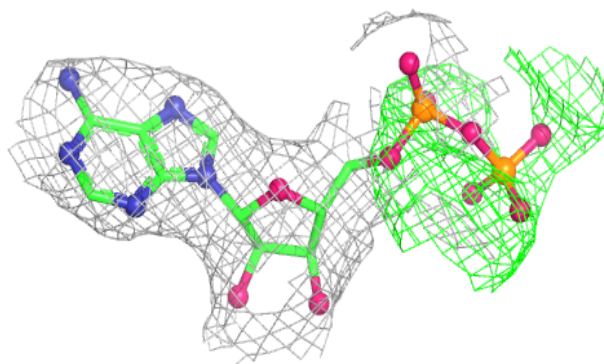
**Electron density around ADP E 601:**

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

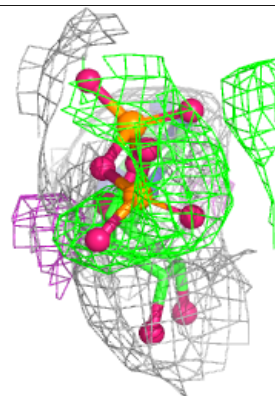
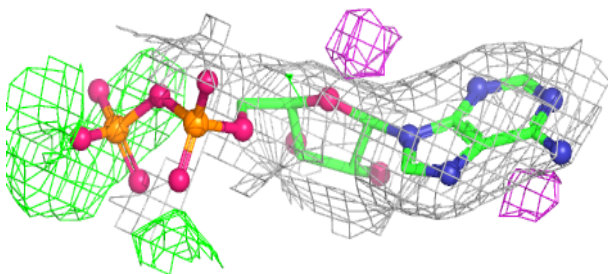
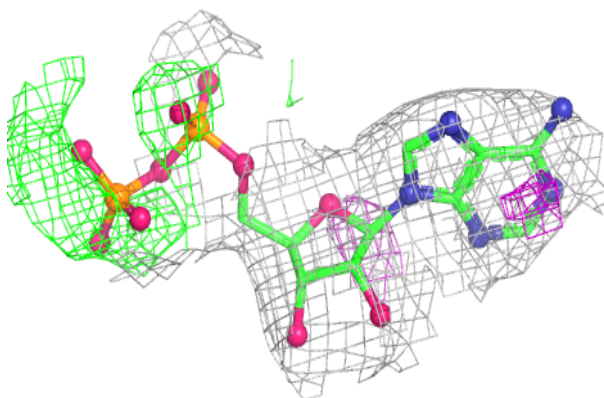


Electron density around ADP F 601:

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

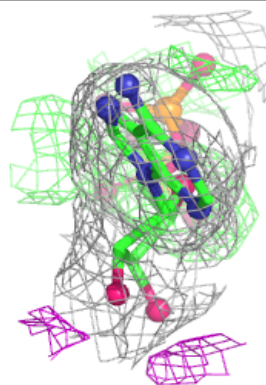
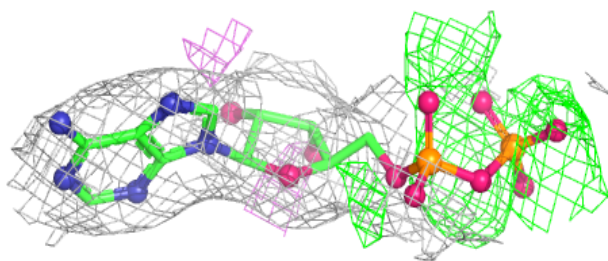
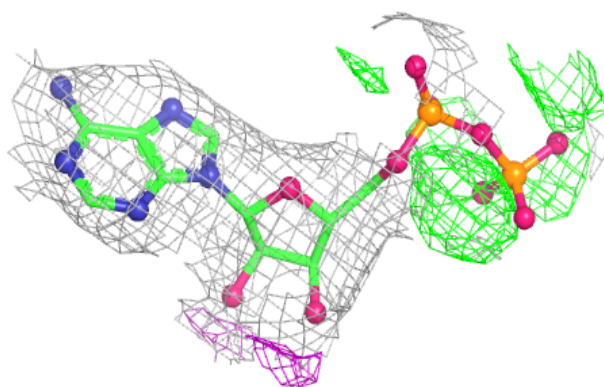
**Electron density around ADP I 601:**

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

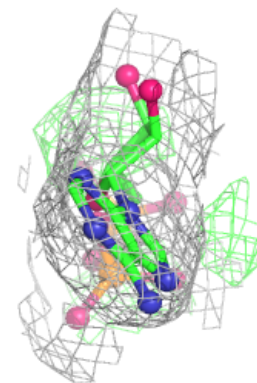
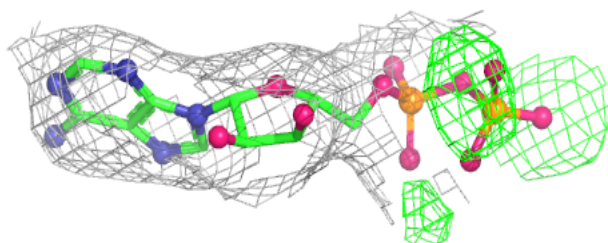
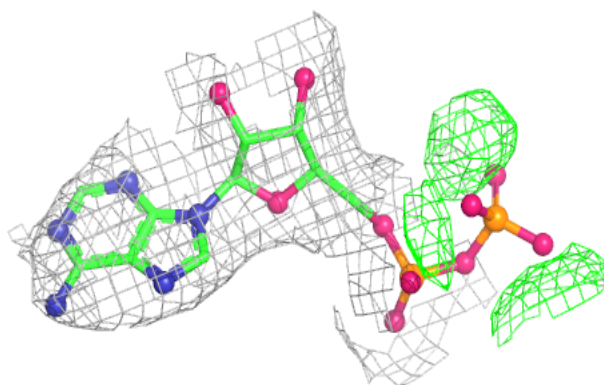


Electron density around ADP D 601:

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

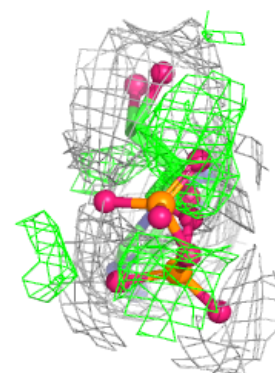
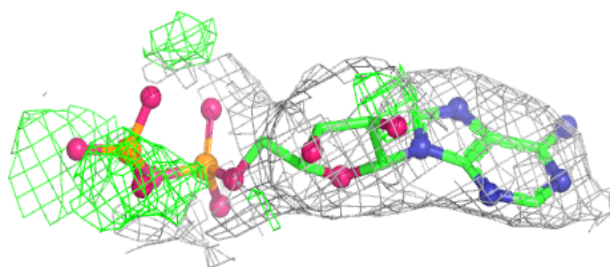
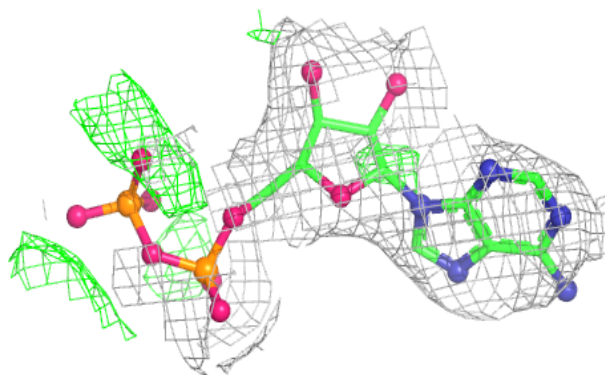
**Electron density around ADP B 601:**

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

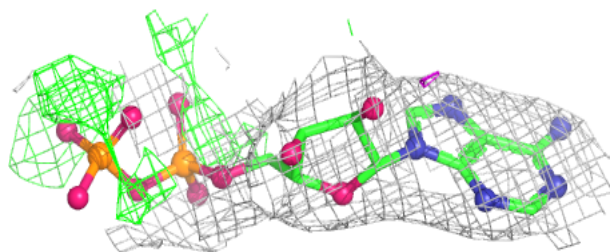
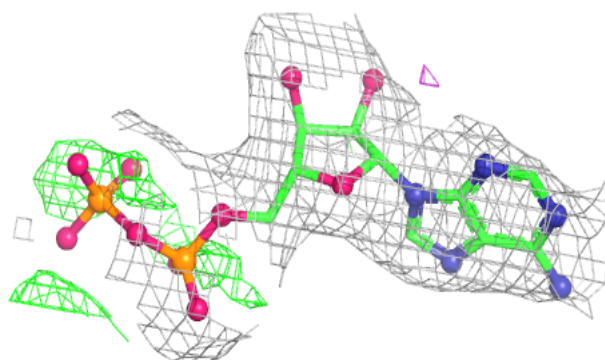


Electron density around ADP C 601:

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

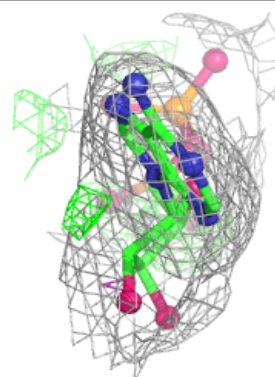
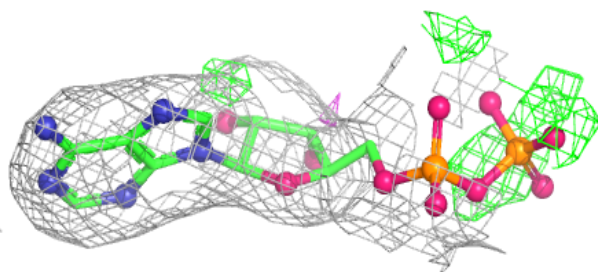
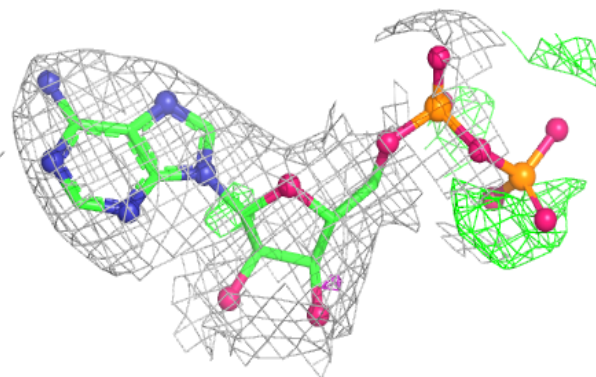
**Electron density around ADP G 601:**

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

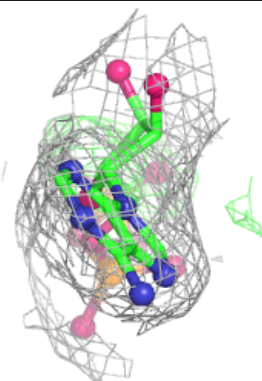
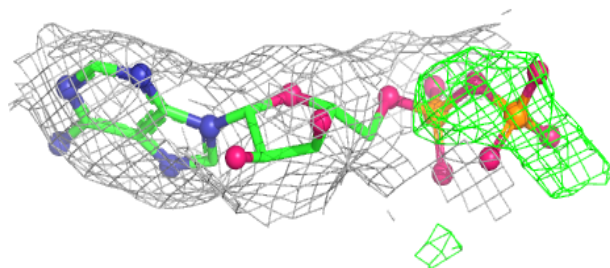
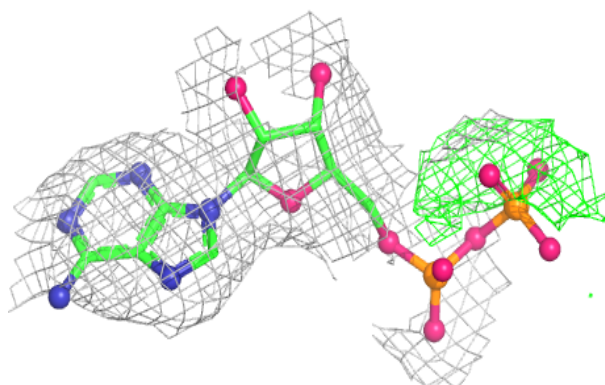


Electron density around ADP H 601:

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

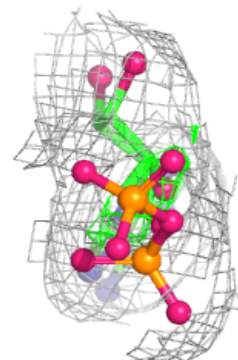
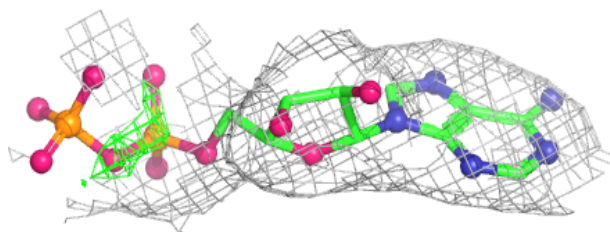
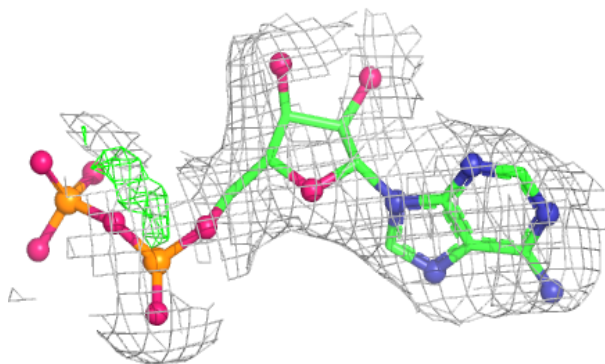
**Electron density around ADP K 601:**

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

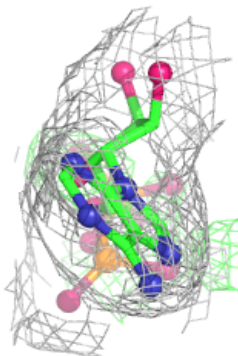
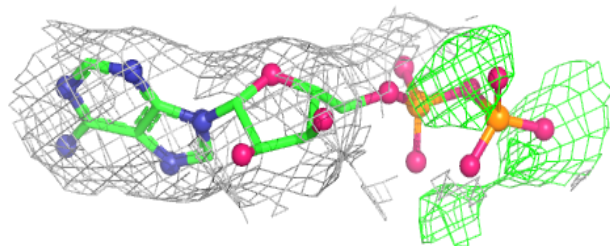
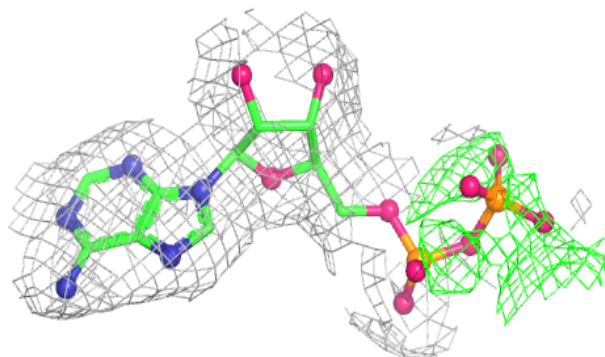


Electron density around ADP L 601:

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

There are no such residues in this entry.