



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:48 PM UTC

PDB ID : 8HRZ / pdb_00008hrz
Title : Crystal structure of the p97-N/D1 hexamer in complex with six p47-UBX domains
Authors : Nguyen, T.Q.; Kang, W.
Deposited on : 2022-12-16
Resolution : 2.70 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:

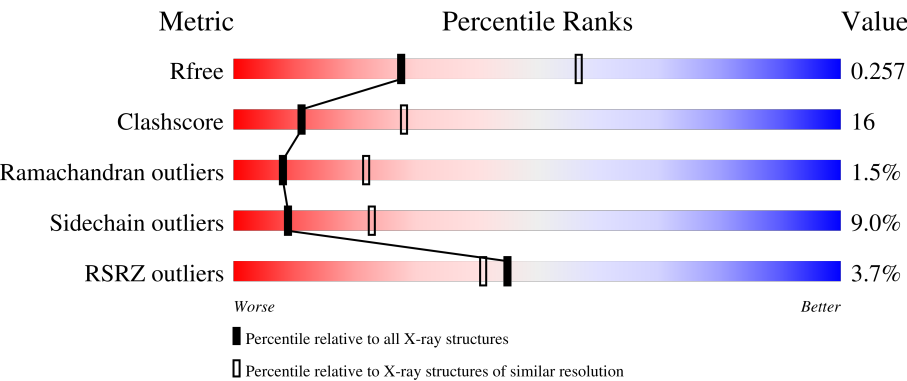
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	438	3% 72% 23% .
1	B	438	3% 70% 26% ..
1	C	438	3% 71% 24% ..
1	D	438	5% 67% 26% 6%
1	E	438	5% 67% 25% 6% .

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Mol	Chain	Length	Quality of chain
1	F	438	
1	G	438	
1	H	438	
1	I	438	
1	J	438	
1	K	438	
1	L	438	
2	M	85	
2	N	85	
2	O	85	
2	P	85	
2	Q	85	
2	R	85	
2	S	85	
2	T	85	
2	U	85	
2	V	85	
2	W	85	
2	X	85	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49084 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3404	2139	605	642	18			
1	B	436	Total	C	N	O	S	0	0	0
			3404	2139	605	642	18			
1	C	436	Total	C	N	O	S	0	0	0
			3394	2133	601	642	18			
1	D	436	Total	C	N	O	S	0	0	0
			3398	2136	602	642	18			
1	E	436	Total	C	N	O	S	0	0	0
			3360	2116	585	641	18			
1	F	436	Total	C	N	O	S	0	0	0
			3404	2139	605	642	18			
1	G	436	Total	C	N	O	S	0	0	0
			3380	2125	596	641	18			
1	H	436	Total	C	N	O	S	0	0	0
			3404	2139	605	642	18			
1	I	436	Total	C	N	O	S	0	0	0
			3404	2139	605	642	18			
1	J	436	Total	C	N	O	S	0	0	0
			3398	2136	602	642	18			
1	K	436	Total	C	N	O	S	0	0	0
			3404	2139	605	642	18			
1	L	436	Total	C	N	O	S	0	0	0
			3384	2128	597	641	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	ALA	GLU	engineered mutation	UNP P55072
A	295	ALA	LYS	engineered mutation	UNP P55072
B	294	ALA	GLU	engineered mutation	UNP P55072
B	295	ALA	LYS	engineered mutation	UNP P55072
C	294	ALA	GLU	engineered mutation	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
C	295	ALA	LYS	engineered mutation	UNP P55072
D	294	ALA	GLU	engineered mutation	UNP P55072
D	295	ALA	LYS	engineered mutation	UNP P55072
E	294	ALA	GLU	engineered mutation	UNP P55072
E	295	ALA	LYS	engineered mutation	UNP P55072
F	294	ALA	GLU	engineered mutation	UNP P55072
F	295	ALA	LYS	engineered mutation	UNP P55072
G	294	ALA	GLU	engineered mutation	UNP P55072
G	295	ALA	LYS	engineered mutation	UNP P55072
H	294	ALA	GLU	engineered mutation	UNP P55072
H	295	ALA	LYS	engineered mutation	UNP P55072
I	294	ALA	GLU	engineered mutation	UNP P55072
I	295	ALA	LYS	engineered mutation	UNP P55072
J	294	ALA	GLU	engineered mutation	UNP P55072
J	295	ALA	LYS	engineered mutation	UNP P55072
K	294	ALA	GLU	engineered mutation	UNP P55072
K	295	ALA	LYS	engineered mutation	UNP P55072
L	294	ALA	GLU	engineered mutation	UNP P55072
L	295	ALA	LYS	engineered mutation	UNP P55072

- Molecule 2 is a protein called NSFL1 cofactor p47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			
2	N	85	Total	C	N	O	S	0	0	0
			664	419	116	126	3			
2	O	85	Total	C	N	O	S	0	0	0
			664	419	116	126	3			
2	P	85	Total	C	N	O	S	0	0	0
			664	419	116	126	3			
2	Q	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			
2	R	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			
2	S	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			
2	T	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			
2	U	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			
2	V	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			

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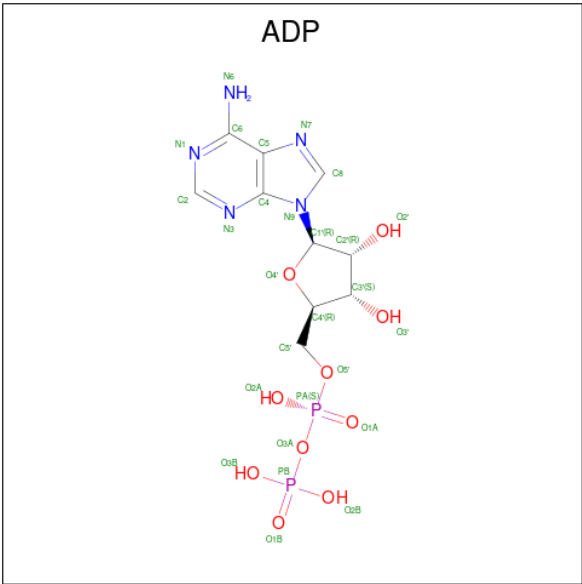
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			
2	X	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	286	MET	-	initiating methionine	UNP Q9UNZ2
N	286	MET	-	initiating methionine	UNP Q9UNZ2
O	286	MET	-	initiating methionine	UNP Q9UNZ2
P	286	MET	-	initiating methionine	UNP Q9UNZ2
Q	286	MET	-	initiating methionine	UNP Q9UNZ2
R	286	MET	-	initiating methionine	UNP Q9UNZ2
S	286	MET	-	initiating methionine	UNP Q9UNZ2
T	286	MET	-	initiating methionine	UNP Q9UNZ2
U	286	MET	-	initiating methionine	UNP Q9UNZ2
V	286	MET	-	initiating methionine	UNP Q9UNZ2
W	286	MET	-	initiating methionine	UNP Q9UNZ2
X	286	MET	-	initiating methionine	UNP Q9UNZ2

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

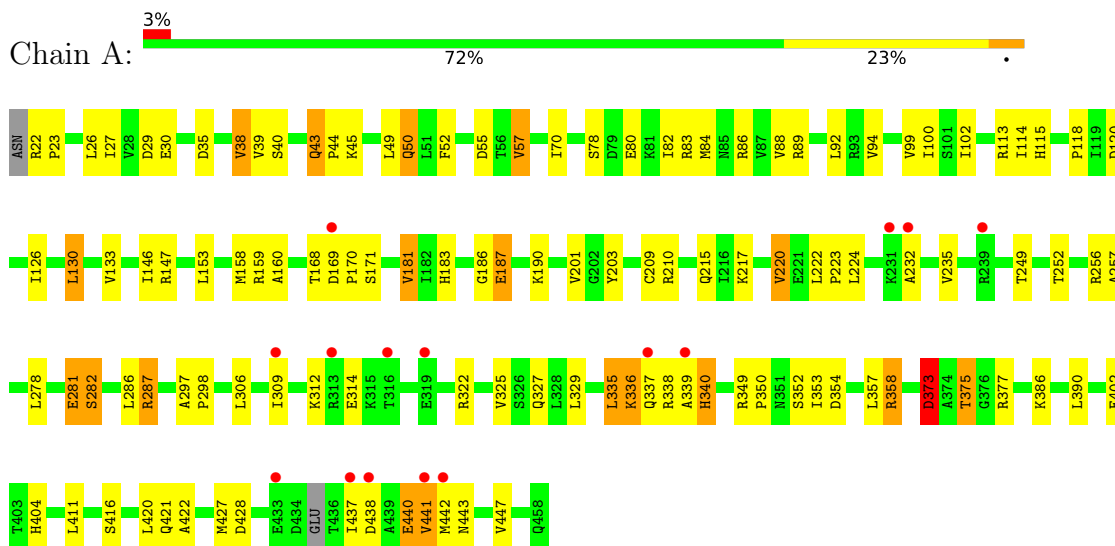


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0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

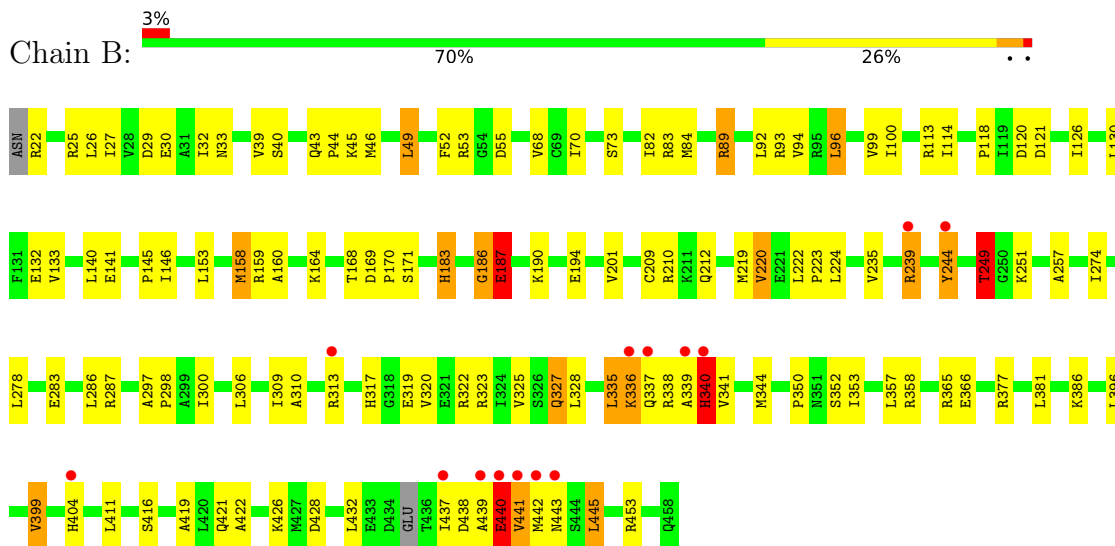
3 Residue-property plots [i](#)

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

- Molecule 1: Transitional endoplasmic reticulum ATPase

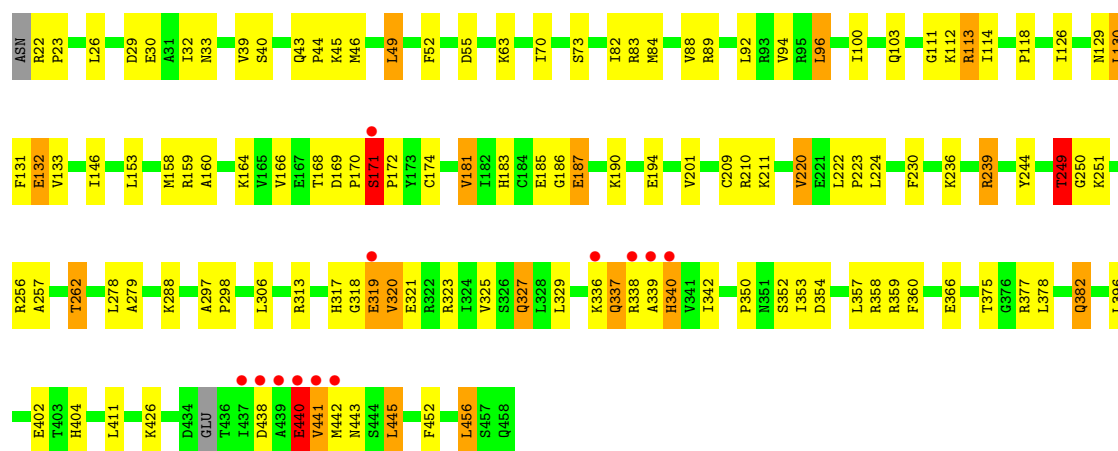


- Molecule 1: Transitional endoplasmic reticulum ATPase

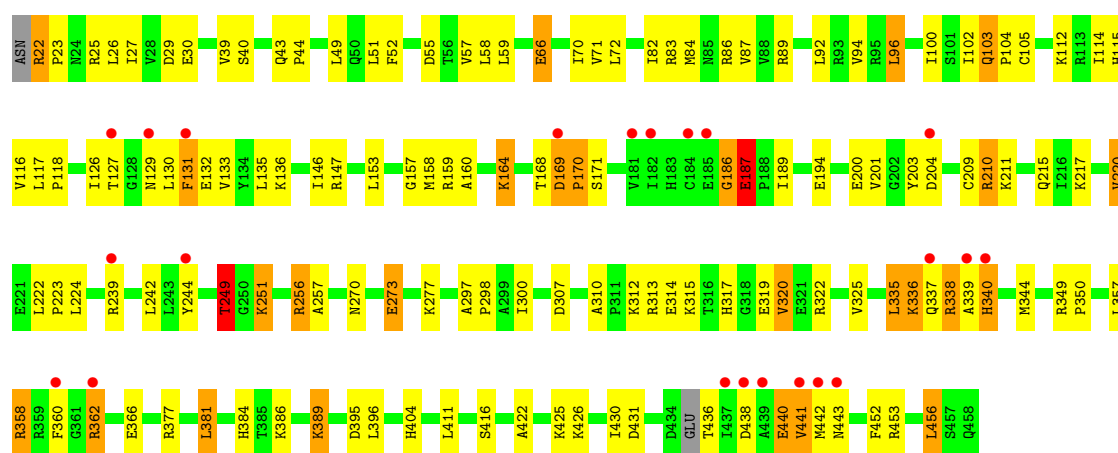


- Molecule 1: Transitional endoplasmic reticulum ATPase





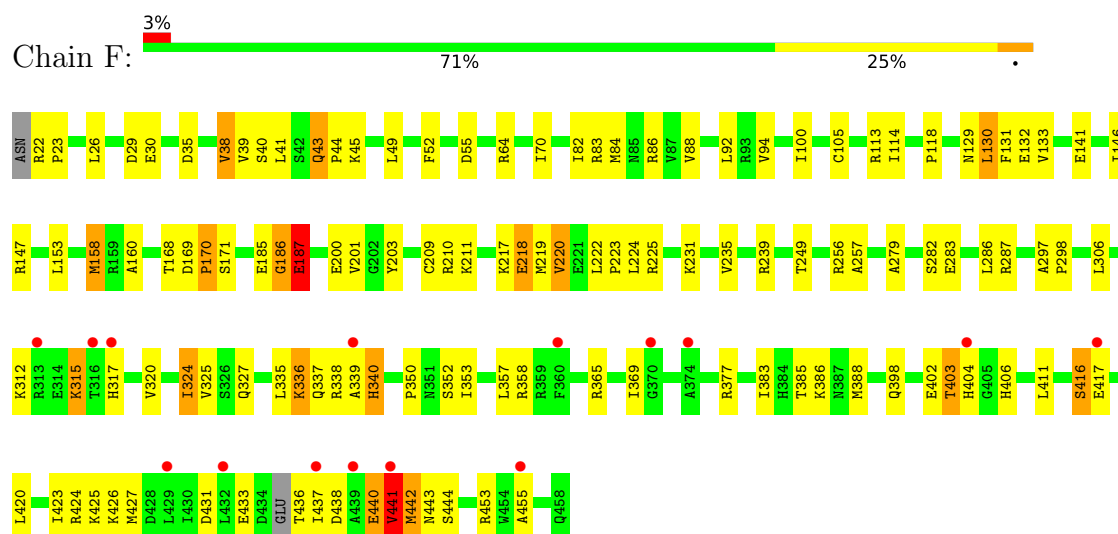
• Molecule 1: Transitional endoplasmic reticulum ATPase



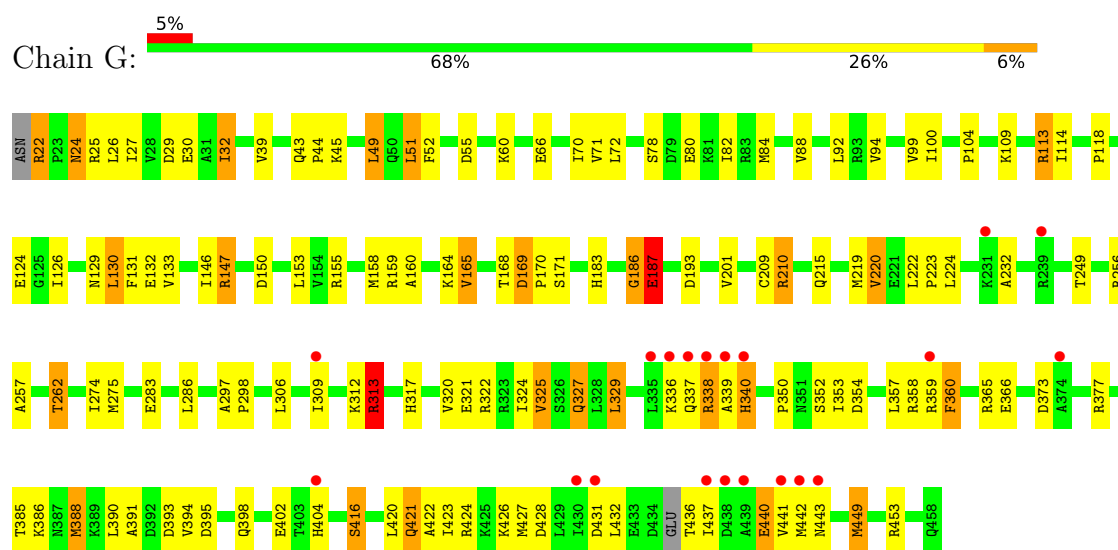
• Molecule 1: Transitional endoplasmic reticulum ATPase



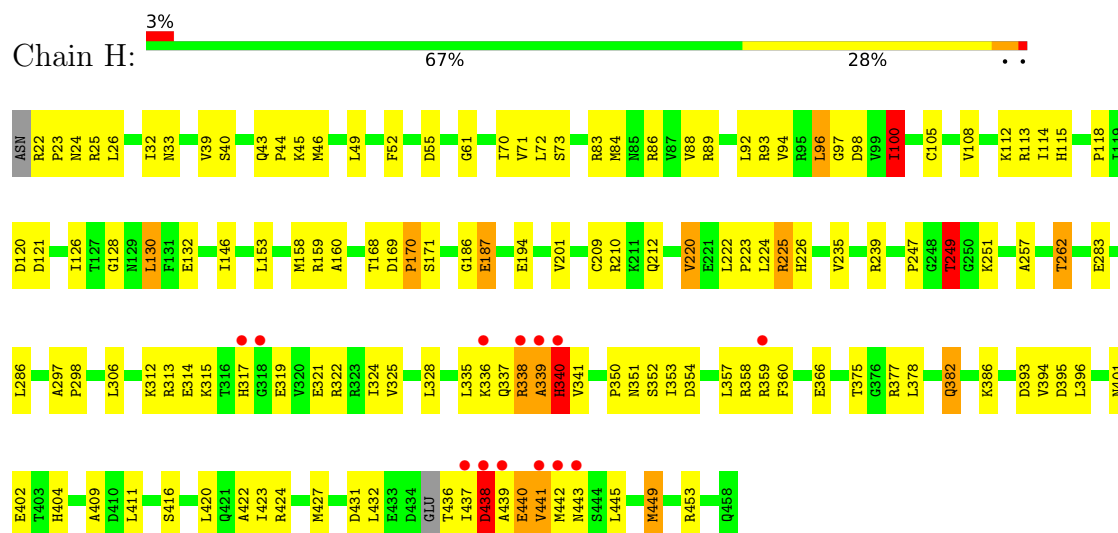
• Molecule 1: Transitional endoplasmic reticulum ATPase



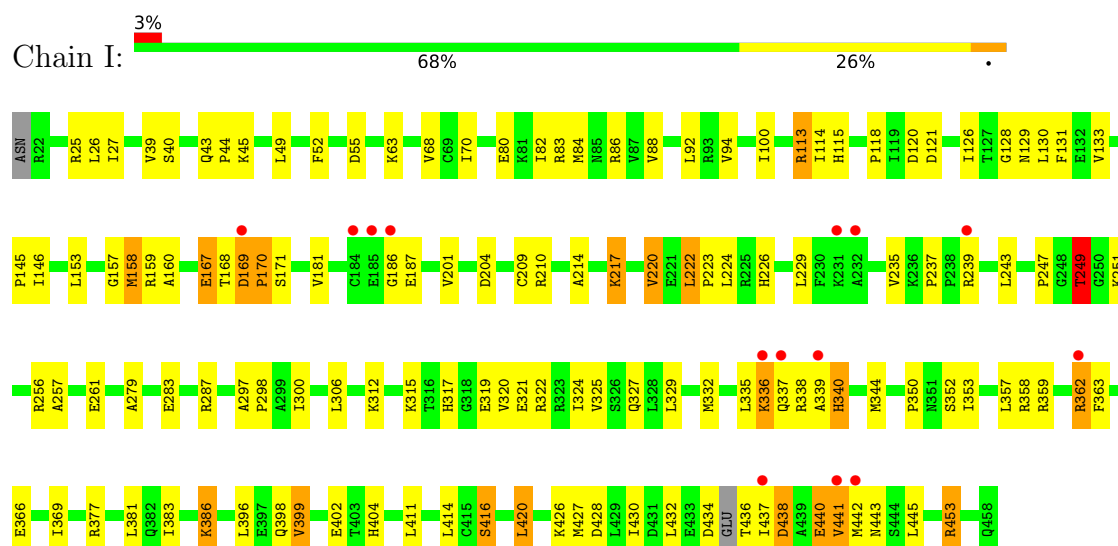
• Molecule 1: Transitional endoplasmic reticulum ATPase



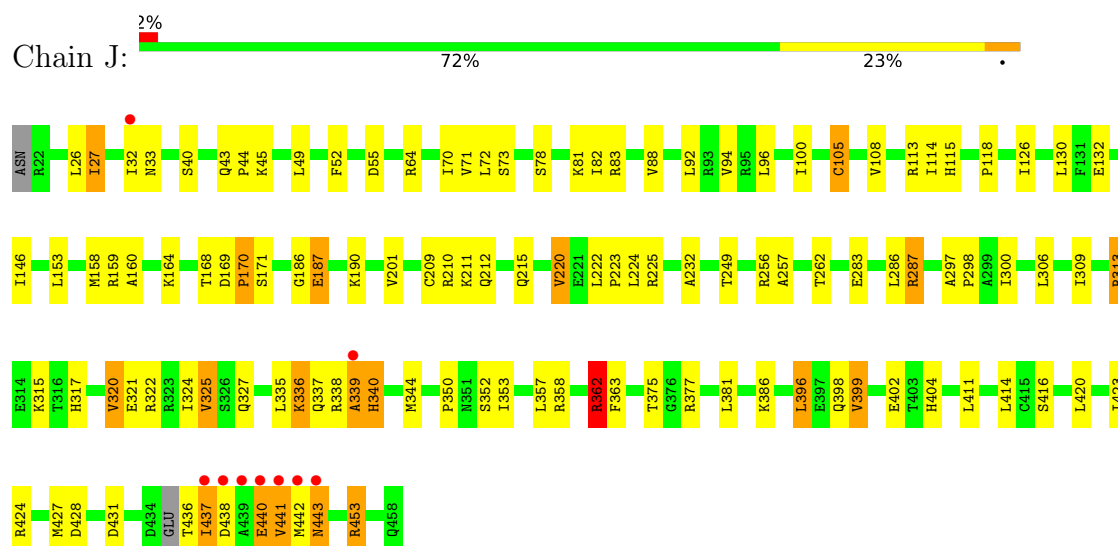
• Molecule 1: Transitional endoplasmic reticulum ATPase



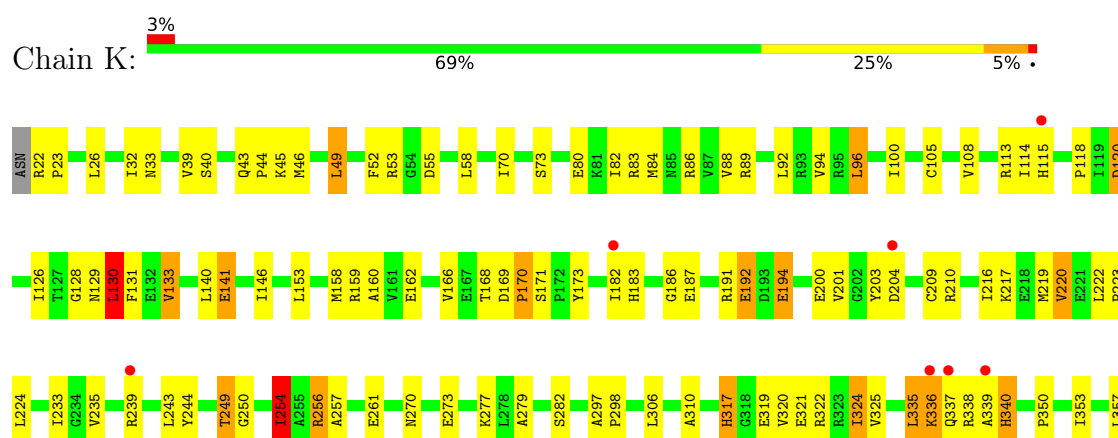
• Molecule 1: Transitional endoplasmic reticulum ATPase

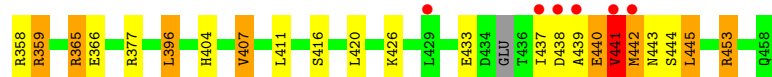


• Molecule 1: Transitional endoplasmic reticulum ATPase

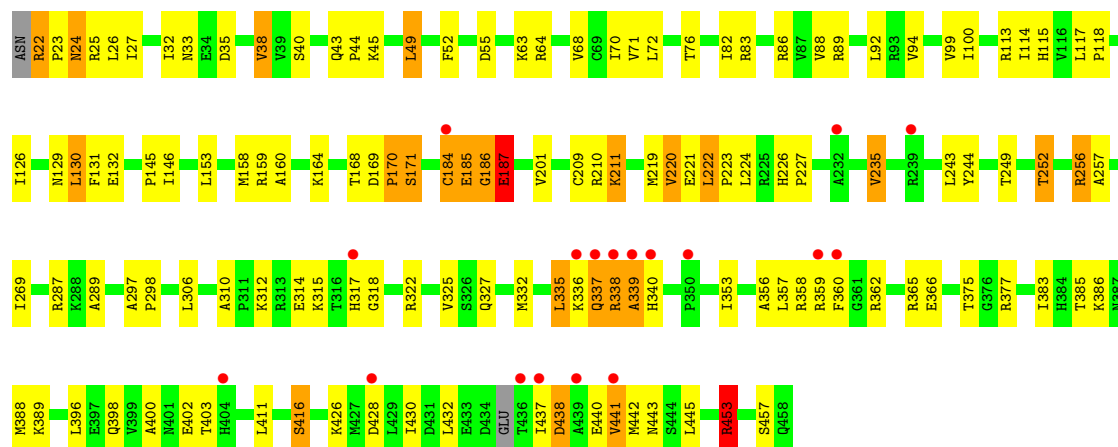


• Molecule 1: Transitional endoplasmic reticulum ATPase

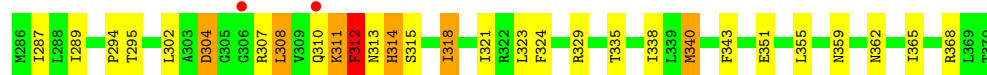




- Molecule 1: Transitional endoplasmic reticulum ATPase



- Molecule 2: NSFL1 cofactor p47



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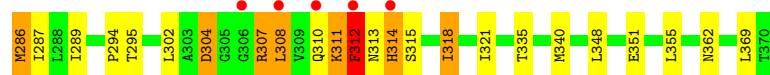
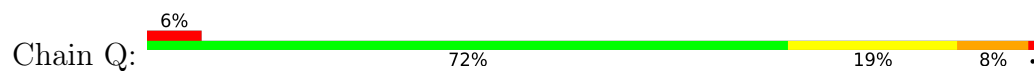
- Molecule 2: NSFL1 cofactor p47



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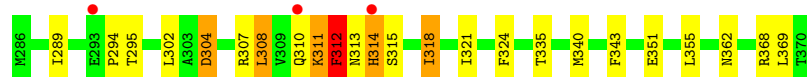
• Molecule 2: NSFL1 cofactor p47



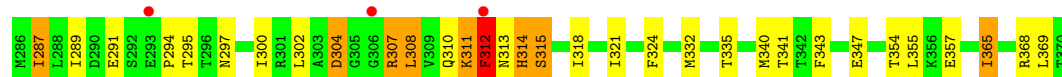
• Molecule 2: NSFL1 cofactor p47



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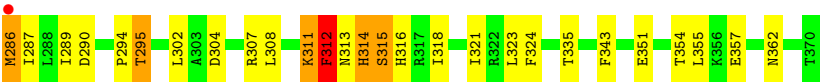


• Molecule 2: NSFL1 cofactor p47



• Molecule 2: NSFL1 cofactor p47





● Molecule 2: NSFL1 cofactor p47



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	170.78Å 178.85Å 171.33Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	40.01 – 2.70 40.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.01-2.70) 99.3 (40.01-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.213 , 0.256 0.214 , 0.257	Depositor DCC
R_{free} test set	11938 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.049 for -h-l,k,h 0.049 for l,k,-h-l 0.047 for h,-k,-h-l 0.049 for -h-l,-k,l 0.077 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49084	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9479e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.59	0/3456	1.16	9/4670 (0.2%)
1	B	0.59	0/3456	1.17	11/4670 (0.2%)
1	C	0.60	0/3446	1.14	6/4659 (0.1%)
1	D	0.60	0/3450	1.18	12/4663 (0.3%)
1	E	0.64	0/3412	1.18	14/4619 (0.3%)
1	F	0.58	0/3456	1.16	10/4670 (0.2%)
1	G	0.58	0/3432	1.16	8/4643 (0.2%)
1	H	0.58	0/3456	1.16	10/4670 (0.2%)
1	I	0.58	0/3456	1.14	6/4670 (0.1%)
1	J	0.59	0/3450	1.13	5/4663 (0.1%)
1	K	0.59	0/3456	1.16	10/4670 (0.2%)
1	L	0.58	0/3436	1.16	14/4647 (0.3%)
2	M	0.64	0/678	1.24	3/917 (0.3%)
2	N	0.64	0/672	1.30	4/910 (0.4%)
2	O	0.67	0/672	1.29	4/910 (0.4%)
2	P	0.66	0/672	1.29	3/910 (0.3%)
2	Q	0.66	0/678	1.28	7/917 (0.8%)
2	R	0.64	0/678	1.29	6/917 (0.7%)
2	S	0.65	0/678	1.34	7/917 (0.8%)
2	T	0.69	0/678	1.27	3/917 (0.3%)
2	U	0.64	0/678	1.25	3/917 (0.3%)
2	V	0.65	0/678	1.29	4/917 (0.4%)
2	W	0.65	0/678	1.30	4/917 (0.4%)
2	X	0.69	0/678	1.28	5/917 (0.5%)
All	All	0.60	0/49480	1.18	168/66897 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	322	ARG	CG-CD-NE	-10.71	88.44	112.00
2	W	295	THR	CA-CB-OG1	10.60	125.50	109.60
2	N	312	PHE	CA-CB-CG	10.59	124.39	113.80
1	B	183	HIS	CA-CB-CG	10.24	124.04	113.80
2	V	312	PHE	CA-CB-CG	9.70	123.50	113.80
1	I	167	GLU	CB-CG-CD	9.34	128.47	112.60
2	S	312	PHE	CA-CB-CG	9.21	123.01	113.80
2	O	312	PHE	CA-CB-CG	9.06	122.86	113.80
1	A	373	ASP	CA-CB-CG	8.90	121.50	112.60
2	Q	312	PHE	CA-CB-CG	8.89	122.69	113.80
2	P	312	PHE	CA-CB-CG	8.79	122.58	113.80
2	R	312	PHE	CA-CB-CG	8.71	122.51	113.80
2	W	312	PHE	CA-CB-CG	8.61	122.41	113.80
2	U	312	PHE	CA-CB-CG	8.46	122.26	113.80
2	M	312	PHE	CA-CB-CG	8.43	122.23	113.80
2	O	313	ASN	CA-CB-CG	8.33	120.93	112.60
1	A	281	GLU	N-CA-C	-8.21	95.95	108.67
2	U	313	ASN	CA-CB-CG	8.16	120.77	112.60
2	X	312	PHE	CA-CB-CG	8.13	121.93	113.80
2	M	313	ASN	CA-CB-CG	8.13	120.73	112.60
2	N	313	ASN	CA-CB-CG	8.12	120.72	112.60
1	L	314	GLU	CB-CG-CD	8.06	126.31	112.60
2	P	313	ASN	CA-CB-CG	8.04	120.64	112.60
2	S	313	ASN	CA-CB-CG	8.03	120.63	112.60
2	R	313	ASN	CA-CB-CG	8.00	120.60	112.60
2	W	313	ASN	CA-CB-CG	7.95	120.55	112.60
2	Q	313	ASN	CA-CB-CG	7.62	120.22	112.60
1	E	32	ILE	N-CA-C	-7.61	105.35	112.96
2	V	313	ASN	CA-CB-CG	7.58	120.18	112.60
1	G	193	ASP	CA-CB-CG	7.52	120.12	112.60
2	X	313	ASN	CA-CB-CG	7.37	119.97	112.60
1	G	169	ASP	N-CA-CB	7.19	117.22	110.39
1	D	395	ASP	N-CA-C	7.16	120.13	111.40
1	A	249	THR	CA-CB-OG1	7.16	120.33	109.60
1	K	120	ASP	CB-CA-C	-7.14	98.88	110.74
1	H	438	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	43	GLN	CB-CG-CD	-7.06	100.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	ASP	N-CA-CB	6.96	117.00	110.39
1	G	249	THR	CA-CB-OG1	6.89	119.94	109.60
1	A	115	HIS	CA-CB-CG	6.87	120.67	113.80
1	L	389	LYS	CB-CG-CD	6.78	126.90	111.30
1	K	249	THR	CA-CB-OG1	6.74	119.71	109.60
1	L	337	GLN	N-CA-C	-6.74	104.32	112.54
1	F	218	GLU	CB-CA-C	6.74	121.45	110.88
1	L	249	THR	CA-CB-OG1	6.73	119.69	109.60
2	M	315	SER	N-CA-C	-6.71	103.68	112.41
1	E	115	HIS	CA-CB-CG	6.71	120.50	113.80
2	W	315	SER	N-CA-C	-6.67	103.74	112.41
1	I	169	ASP	N-CA-CB	6.66	116.72	110.39
1	F	403	THR	OG1-CB-CG2	6.62	122.53	109.30
1	J	375	THR	CA-CB-OG1	-6.58	99.73	109.60
1	E	314	GLU	CB-CG-CD	6.54	123.72	112.60
1	H	115	HIS	CA-CB-CG	6.48	120.28	113.80
1	E	249	THR	CA-CB-OG1	6.48	119.31	109.60
2	R	315	SER	N-CA-C	-6.47	104.00	112.41
2	X	315	SER	N-CA-C	-6.46	104.01	112.41
1	A	314	GLU	CB-CG-CD	6.45	123.57	112.60
1	K	365	ARG	CB-CG-CD	6.45	126.14	111.30
2	N	295	THR	CA-CB-OG1	6.45	119.28	109.60
2	V	315	SER	N-CA-C	-6.44	104.04	112.41
2	O	315	SER	N-CA-C	-6.41	104.07	112.41
2	P	315	SER	N-CA-C	-6.41	104.08	112.41
1	D	251	LYS	CG-CD-CE	-6.40	96.58	111.30
1	D	395	ASP	CB-CA-C	6.40	121.54	110.79
2	T	315	SER	N-CA-C	-6.40	104.09	112.41
1	H	249	THR	OG1-CB-CG2	6.35	122.00	109.30
1	J	249	THR	CA-CB-OG1	6.34	119.11	109.60
1	F	403	THR	CA-CB-OG1	-6.33	100.11	109.60
1	H	314	GLU	CB-CG-CD	6.31	123.33	112.60
1	E	339	ALA	N-CA-C	-6.25	106.03	113.21
1	G	313	ARG	CB-CG-CD	6.23	125.63	111.30
2	N	315	SER	N-CA-C	-6.22	104.32	112.41
1	D	115	HIS	CA-CB-CG	6.21	120.01	113.80
1	K	254	ILE	CB-CA-C	6.21	120.52	112.14
1	I	115	HIS	CA-CB-CG	6.17	119.97	113.80
2	R	354	THR	OG1-CB-CG2	6.16	121.63	109.30
2	S	295	THR	CA-CB-OG1	6.16	118.84	109.60
2	U	315	SER	N-CA-C	-6.16	104.41	112.41
2	S	315	SER	N-CA-C	-6.14	104.43	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	244	TYR	CB-CA-C	-6.08	97.35	109.33
1	L	252	THR	CA-CB-OG1	-6.08	100.48	109.60
1	B	249	THR	OG1-CB-CG2	6.06	121.42	109.30
2	Q	315	SER	N-CA-C	-6.04	104.56	112.41
1	E	100	ILE	N-CA-CB	-6.00	102.39	112.47
2	S	341	THR	OG1-CB-CG2	5.89	121.09	109.30
1	D	249	THR	OG1-CB-CG2	5.87	121.04	109.30
1	H	100	ILE	N-CA-CB	-5.85	102.64	112.47
1	C	249	THR	OG1-CB-CG2	5.85	121.00	109.30
1	E	337	GLN	N-CA-C	-5.85	104.74	112.34
1	E	170	PRO	CA-CB-CG	-5.81	93.46	104.50
1	B	327	GLN	CA-CB-CG	-5.81	102.48	114.10
1	L	113	ARG	CB-CG-CD	5.80	124.64	111.30
1	D	314	GLU	CB-CG-CD	5.77	122.42	112.60
1	J	362	ARG	CB-CA-C	-5.76	108.12	116.54
1	H	340	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	L	132	GLU	CB-CG-CD	5.74	122.36	112.60
1	F	170	PRO	CB-CA-C	5.69	120.95	111.56
1	B	340	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	B	89	ARG	CG-CD-NE	-5.67	99.53	112.00
1	B	244	TYR	CB-CA-C	-5.66	98.18	109.33
2	O	314	HIS	CA-CB-CG	5.66	119.46	113.80
2	T	354	THR	OG1-CB-CG2	5.64	120.59	109.30
1	H	375	THR	CA-CB-OG1	-5.64	101.14	109.60
1	I	249	THR	OG1-CB-CG2	5.61	120.52	109.30
1	C	132	GLU	CB-CG-CD	5.60	122.13	112.60
2	Q	314	HIS	CA-CB-CG	5.56	119.36	113.80
1	K	365	ARG	CG-CD-NE	-5.55	99.78	112.00
1	G	428	ASP	CA-CB-CG	5.53	118.13	112.60
2	Q	307	ARG	CB-CG-CD	5.53	124.01	111.30
1	F	132	GLU	CB-CG-CD	5.52	121.99	112.60
1	G	132	GLU	CB-CG-CD	5.47	121.89	112.60
1	K	256	ARG	CG-CD-NE	-5.47	99.97	112.00
2	Q	311	LYS	CB-CG-CD	5.46	123.86	111.30
1	H	170	PRO	CB-CA-C	5.42	120.50	111.56
1	K	407	VAL	CA-CB-CG2	5.41	119.59	110.40
1	D	215	GLN	CB-CG-CD	-5.38	103.45	112.60
1	L	24	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	373	ASP	N-CA-CB	-5.38	102.70	110.45
1	L	22	ARG	CB-CG-CD	5.35	123.61	111.30
1	L	338	ARG	N-CA-C	-5.34	104.04	111.30
2	X	354	THR	OG1-CB-CG2	5.34	119.98	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	386	LYS	CA-CB-CG	5.33	124.75	114.10
1	E	100	ILE	CA-CB-CG1	5.32	119.44	110.40
1	B	239	ARG	CB-CG-CD	5.31	123.52	111.30
1	D	164	LYS	CG-CD-CE	5.30	123.49	111.30
1	B	132	GLU	CB-CG-CD	5.29	121.60	112.60
1	E	362	ARG	CB-CA-C	-5.28	108.83	116.54
1	E	132	GLU	CB-CG-CD	5.27	121.57	112.60
1	L	115	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	D	256	ARG	CG-CD-NE	-5.26	100.43	112.00
1	A	375	THR	CB-CA-C	5.24	119.18	110.90
1	J	132	GLU	CB-CG-CD	5.24	121.50	112.60
1	A	215	GLN	CB-CG-CD	-5.22	103.73	112.60
1	D	170	PRO	CB-CA-C	5.22	120.17	111.56
1	L	453	ARG	CB-CG-CD	5.22	123.30	111.30
1	B	319	GLU	N-CA-C	-5.21	107.47	113.88
1	I	170	PRO	CB-CA-C	5.21	120.16	111.56
1	C	319	GLU	N-CA-C	-5.21	107.48	113.88
2	R	311	LYS	CB-CG-CD	5.20	123.27	111.30
1	F	433	GLU	N-CA-CB	5.18	116.85	110.53
1	D	313	ARG	CB-CG-CD	5.18	123.21	111.30
1	H	132	GLU	CB-CG-CD	5.17	121.39	112.60
1	L	256	ARG	CG-CD-NE	5.16	123.35	112.00
1	C	185	GLU	CA-C-N	5.15	131.50	121.41
1	C	185	GLU	C-N-CA	5.15	131.50	121.41
1	G	360	PHE	CB-CA-C	5.14	119.60	110.85
1	C	440	GLU	CA-C-O	-5.13	116.49	120.19
2	S	311	LYS	CB-CG-CD	5.13	123.11	111.30
1	F	64	ARG	CB-CG-CD	5.13	123.10	111.30
1	H	319	GLU	N-CA-C	-5.12	107.17	113.41
2	V	307	ARG	CB-CG-CD	5.11	123.06	111.30
1	B	440	GLU	CA-C-O	-5.11	115.43	120.80
1	E	407	VAL	CA-CB-CG2	5.11	119.09	110.40
1	F	185	GLU	CA-C-N	5.09	131.40	121.41
1	F	185	GLU	C-N-CA	5.09	131.40	121.41
1	G	215	GLN	CB-CG-CD	-5.09	103.94	112.60
1	K	317	HIS	CB-CG-CD2	5.09	137.81	131.20
1	L	170	PRO	CB-CA-C	5.08	119.94	111.56
2	Q	314	HIS	N-CA-C	5.08	121.61	110.80
1	J	170	PRO	CB-CA-C	5.07	119.93	111.56
2	S	341	THR	CA-CB-OG1	5.07	117.21	109.60
1	K	170	PRO	CB-CA-C	5.06	119.91	111.56
1	E	365	ARG	CB-CG-CD	5.06	122.94	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ARG	CB-CG-CD	5.02	122.85	111.30
1	F	442	MET	CB-CG-SD	-5.02	97.64	112.70
2	R	314	HIS	CA-CB-CG	5.02	118.82	113.80
1	K	192	GLU	CB-CG-CD	5.01	121.12	112.60
2	X	314	HIS	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	86	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3404	0	3461	96	0
1	B	3404	0	3461	106	0
1	C	3394	0	3439	106	0
1	D	3398	0	3450	119	0
1	E	3360	0	3378	132	0
1	F	3404	0	3461	115	0
1	G	3380	0	3411	132	0
1	H	3404	0	3461	119	0
1	I	3404	0	3461	135	0
1	J	3398	0	3450	98	0
1	K	3404	0	3461	119	0
1	L	3384	0	3422	109	0
2	M	670	0	691	23	0
2	N	664	0	680	23	0
2	O	664	0	680	26	0
2	P	664	0	680	31	0
2	Q	670	0	691	22	0
2	R	670	0	691	24	0
2	S	670	0	691	26	0
2	T	670	0	691	32	0
2	U	670	0	691	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	670	0	691	32	0
2	W	670	0	691	28	0
2	X	670	0	691	26	0
3	A	27	0	12	3	0
3	B	27	0	12	0	0
3	C	27	0	12	1	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	1	0
3	I	27	0	12	0	0
3	J	27	0	12	0	0
3	K	27	0	12	0	0
3	L	27	0	12	1	0
All	All	49084	0	49719	1606	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 16.

All (1606) 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:E:238:PRO:HB3	1:E:365:ARG:NE	1.47	1.29
1:F:385:THR:HG22	1:F:388:MET:CE	1.73	1.18
1:L:385:THR:HG22	1:L:388:MET:CE	1.74	1.18
1:I:251:LYS:HG2	1:I:369:ILE:HD12	1.25	1.14
1:E:238:PRO:CB	1:E:365:ARG:HE	1.61	1.12
1:K:46:MET:HE1	1:K:73:SER:HB3	1.33	1.11
1:H:46:MET:HE1	1:H:73:SER:HB3	1.24	1.10
1:C:46:MET:HE1	1:C:73:SER:HB3	1.20	1.09
1:B:46:MET:HE1	1:B:73:SER:CB	1.82	1.08
1:B:46:MET:HE1	1:B:73:SER:HB3	1.15	1.08
1:C:350:PRO:HB3	1:C:358:ARG:NH2	1.70	1.07
1:G:274:ILE:HG22	1:G:275:MET:HE2	1.36	1.06
1:H:46:MET:CE	1:H:73:SER:HB3	1.87	1.04
1:H:339:ALA:O	1:H:340:HIS:CD2	2.12	1.03
1:C:350:PRO:HB3	1:C:358:ARG:HH22	1.18	1.03
1:D:131:PHE:HB3	1:D:136:LYS:NZ	1.73	1.02
1:K:46:MET:CE	1:K:73:SER:HB3	1.89	1.02
1:I:251:LYS:HG2	1:I:369:ILE:CD1	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ALA:O	1:B:340:HIS:CD2	2.13	1.02
1:C:46:MET:HE1	1:C:73:SER:CB	1.90	1.01
1:G:424:ARG:HG3	1:L:222:LEU:HD21	1.41	0.99
1:J:350:PRO:HB3	1:J:358:ARG:NH2	1.76	0.99
2:U:308:LEU:HD21	2:U:310:GLN:HE21	1.25	0.99
1:D:157:GLY:H	1:D:389:LYS:NZ	1.61	0.98
1:B:46:MET:CE	1:B:73:SER:HB3	1.94	0.97
1:C:113:ARG:HB2	1:C:181:VAL:HG13	1.46	0.97
1:A:113:ARG:HB2	1:A:181:VAL:HG13	1.45	0.97
1:E:92:LEU:HD13	1:E:100:ILE:HD11	1.42	0.96
1:C:46:MET:CE	1:C:73:SER:HB3	1.94	0.96
1:I:332:MET:HB2	1:I:362:ARG:NH1	1.80	0.96
1:I:220:VAL:HG13	1:I:224:LEU:HD22	1.48	0.95
1:A:27:ILE:HD13	1:A:99:VAL:HG22	1.47	0.95
1:A:390:LEU:HD23	1:A:447:VAL:HG12	1.49	0.95
1:E:222:LEU:HD21	1:F:424:ARG:HG3	1.46	0.95
1:B:27:ILE:HD13	1:B:99:VAL:HG22	1.47	0.95
1:G:274:ILE:HG22	1:G:275:MET:CE	1.96	0.94
1:H:440:GLU:O	1:H:442:MET:SD	2.24	0.94
1:J:224:LEU:HB3	1:J:262:THR:HG21	1.49	0.94
1:E:78:SER:HB3	1:E:81:LYS:HE3	1.50	0.94
1:E:427:MET:SD	1:E:430:ILE:HD11	2.08	0.94
1:D:57:VAL:HG21	1:D:102:ILE:CG1	1.98	0.94
1:E:440:GLU:O	1:E:442:MET:SD	2.25	0.93
1:L:377:ARG:HG2	1:L:411:LEU:HD11	1.50	0.93
1:G:385:THR:HG22	1:G:388:MET:CE	1.98	0.93
1:B:426:LYS:HD3	1:B:445:LEU:HD12	1.47	0.93
1:H:220:VAL:HG13	1:H:224:LEU:HD22	1.48	0.93
1:A:339:ALA:O	1:A:340:HIS:ND1	2.02	0.92
2:S:302:LEU:HD12	2:S:307:ARG:HB3	1.47	0.92
1:K:339:ALA:O	1:K:340:HIS:ND1	2.03	0.92
1:F:339:ALA:O	1:F:340:HIS:ND1	2.03	0.92
1:I:339:ALA:O	1:I:340:HIS:ND1	2.02	0.92
1:D:339:ALA:O	1:D:340:HIS:ND1	2.02	0.92
1:G:339:ALA:O	1:G:340:HIS:ND1	2.03	0.92
1:C:111:GLY:HA2	1:C:170:PRO:HD3	1.51	0.92
1:J:339:ALA:O	1:J:340:HIS:ND1	2.03	0.91
1:K:216:ILE:HD13	1:K:254:ILE:HD11	1.52	0.91
1:H:46:MET:HE1	1:H:73:SER:CB	2.00	0.90
1:I:113:ARG:HB2	1:I:181:VAL:CG2	2.00	0.90
1:G:390:LEU:HB3	1:G:394:VAL:HG21	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:PHE:HB3	1:D:136:LYS:HZ2	1.26	0.90
1:C:171:SER:HB3	1:C:172:PRO:HD2	1.53	0.90
1:B:46:MET:CE	1:B:73:SER:CB	2.50	0.89
2:P:318:ILE:HG12	2:P:351:GLU:HA	1.54	0.89
2:Q:318:ILE:CG1	2:Q:351:GLU:HA	2.02	0.89
2:R:318:ILE:HG12	2:R:351:GLU:HA	1.54	0.89
2:S:318:ILE:CG1	2:S:351:GLU:HA	2.03	0.89
2:M:318:ILE:CG1	2:M:351:GLU:HA	2.02	0.88
1:F:403:THR:OG1	1:F:406:HIS:CG	2.25	0.88
2:U:318:ILE:CG1	2:U:351:GLU:HA	2.02	0.88
2:W:318:ILE:HG12	2:W:351:GLU:HA	1.54	0.88
2:W:318:ILE:CG1	2:W:351:GLU:HA	2.04	0.88
2:N:318:ILE:CG1	2:N:351:GLU:HA	2.03	0.88
2:X:318:ILE:HG12	2:X:351:GLU:HA	1.53	0.88
1:A:27:ILE:HD13	1:A:99:VAL:CG2	2.03	0.88
2:T:318:ILE:HG12	2:T:351:GLU:HA	1.55	0.88
2:X:318:ILE:CG1	2:X:351:GLU:HA	2.03	0.87
2:P:318:ILE:CG1	2:P:351:GLU:HA	2.03	0.87
2:R:318:ILE:CG1	2:R:351:GLU:HA	2.03	0.87
1:C:319:GLU:OE1	1:D:320:VAL:CG1	2.23	0.87
1:H:394:VAL:HA	1:H:449:MET:HG2	1.56	0.87
2:T:318:ILE:CG1	2:T:351:GLU:HA	2.04	0.87
1:A:336:LYS:HB2	1:A:338:ARG:NH2	1.88	0.86
1:A:390:LEU:HD23	1:A:447:VAL:CG1	2.05	0.86
1:B:27:ILE:HD13	1:B:99:VAL:CG2	2.05	0.86
2:M:302:LEU:HB2	2:M:307:ARG:HB2	1.54	0.86
1:C:350:PRO:CB	1:C:358:ARG:HH22	1.89	0.86
2:T:302:LEU:HB2	2:T:307:ARG:HB2	1.58	0.86
1:G:60:LYS:HD2	1:G:66:GLU:HG2	1.57	0.85
1:J:220:VAL:HG13	1:J:224:LEU:HD12	1.58	0.85
1:B:336:LYS:HB2	1:B:338:ARG:NH2	1.91	0.85
1:G:394:VAL:HA	1:G:449:MET:HG2	1.58	0.85
1:A:113:ARG:HE	1:A:183:HIS:CE1	1.95	0.85
1:G:220:VAL:HG13	1:G:224:LEU:HD12	1.59	0.85
1:K:426:LYS:HD2	1:K:445:LEU:HD12	1.58	0.85
1:D:157:GLY:H	1:D:389:LYS:HZ1	1.22	0.84
1:J:350:PRO:CB	1:J:358:ARG:NH2	2.41	0.84
1:L:169:ASP:HB3	1:L:170:PRO:HD3	1.60	0.84
1:C:220:VAL:HG13	1:C:224:LEU:HD12	1.58	0.84
1:F:220:VAL:HG13	1:F:224:LEU:HD12	1.59	0.84
1:E:243:LEU:CD2	1:E:367:VAL:CG1	2.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:MET:CE	1:C:73:SER:CB	2.54	0.83
1:J:313:ARG:HH12	1:J:325:VAL:HG11	1.43	0.83
1:I:332:MET:HB2	1:I:362:ARG:HH12	1.41	0.83
1:E:171:SER:HB3	1:E:172:PRO:HD2	1.61	0.83
1:F:385:THR:HG22	1:F:388:MET:HE2	1.58	0.83
1:H:46:MET:CE	1:H:73:SER:CB	2.56	0.83
1:K:169:ASP:HB3	1:K:170:PRO:HD3	1.61	0.83
1:B:219:MET:HE1	1:B:365:ARG:HB3	1.60	0.83
1:A:220:VAL:HG13	1:A:224:LEU:HD12	1.61	0.83
1:L:220:VAL:HG13	1:L:224:LEU:HD12	1.61	0.83
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.60	0.82
1:D:220:VAL:HG13	1:D:224:LEU:HD12	1.61	0.82
1:G:385:THR:HG22	1:G:388:MET:HE1	1.59	0.82
1:K:46:MET:CE	1:K:73:SER:CB	2.57	0.82
1:G:78:SER:HB3	1:G:80:GLU:OE2	1.78	0.82
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.61	0.82
1:A:22:ARG:HG3	1:A:23:PRO:HD2	1.61	0.82
1:C:350:PRO:CB	1:C:358:ARG:NH2	2.41	0.82
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.60	0.82
1:G:169:ASP:HB3	1:G:170:PRO:HD3	1.59	0.82
1:K:220:VAL:HG13	1:K:224:LEU:HD12	1.60	0.82
1:F:169:ASP:HB3	1:F:170:PRO:HD3	1.62	0.82
1:H:169:ASP:HB3	1:H:170:PRO:HD3	1.61	0.82
1:B:220:VAL:HG13	1:B:224:LEU:HD12	1.61	0.81
1:J:169:ASP:HB3	1:J:170:PRO:HD3	1.61	0.81
1:F:22:ARG:HG3	1:F:23:PRO:HD2	1.60	0.81
1:G:317:HIS:HB2	1:L:322:ARG:HH22	1.43	0.81
1:I:169:ASP:HB3	1:I:170:PRO:HD3	1.61	0.81
1:L:385:THR:HG22	1:L:388:MET:HE2	1.61	0.81
1:I:237:PRO:O	1:I:239:ARG:NH1	2.14	0.81
1:D:25:ARG:C	1:D:26:LEU:HD12	2.05	0.81
1:E:171:SER:HB3	1:E:172:PRO:CD	2.10	0.80
1:H:224:LEU:HD23	1:H:262:THR:HG21	1.62	0.80
1:H:322:ARG:HH22	1:I:317:HIS:HB2	1.47	0.80
1:I:332:MET:CB	1:I:362:ARG:NH1	2.45	0.80
1:A:120:ASP:OD2	1:A:190:LYS:HE3	1.82	0.80
1:G:51:LEU:HD11	1:G:104:PRO:HG3	1.62	0.80
1:D:116:VAL:O	1:D:117:LEU:HD12	1.81	0.79
1:K:336:LYS:HB2	1:K:338:ARG:NH2	1.95	0.79
1:A:113:ARG:HE	1:A:183:HIS:HE1	1.30	0.79
1:J:27:ILE:HG23	1:J:81:LYS:HG2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:ARG:HE	1:G:24:ASN:HB2	1.47	0.78
1:A:281:GLU:O	1:A:282:SER:HB2	1.82	0.78
2:P:311:LYS:NZ	2:P:324:PHE:CE1	2.52	0.78
1:E:243:LEU:CD2	1:E:367:VAL:HG11	2.14	0.78
1:G:385:THR:HG22	1:G:388:MET:HE2	1.66	0.78
1:H:313:ARG:NH2	1:H:322:ARG:HG2	1.98	0.78
1:D:126:ILE:HD11	1:D:159:ARG:HD3	1.64	0.78
1:G:222:LEU:HD11	1:H:424:ARG:HG3	1.65	0.78
1:K:113:ARG:HE	1:K:183:HIS:HE1	1.31	0.78
1:A:27:ILE:CD1	1:A:99:VAL:CG2	2.62	0.78
1:C:22:ARG:HG3	1:C:23:PRO:HD2	1.66	0.78
1:J:350:PRO:HB3	1:J:358:ARG:HH21	1.45	0.78
2:M:340:MET:CE	2:M:368:ARG:HH21	1.95	0.78
1:F:282:SER:CB	1:F:324:ILE:HD11	2.14	0.78
2:S:302:LEU:HB2	2:S:307:ARG:HB2	1.66	0.78
1:D:300:ILE:HD13	1:D:344:MET:CE	2.13	0.77
1:I:332:MET:HG3	1:I:362:ARG:NH2	2.00	0.77
2:M:318:ILE:HG12	2:M:351:GLU:HA	1.66	0.77
1:C:319:GLU:CD	1:D:320:VAL:HG13	2.09	0.77
1:I:357:LEU:HD23	1:I:362:ARG:NH2	1.98	0.77
2:U:318:ILE:HG12	2:U:351:GLU:HA	1.67	0.77
2:O:311:LYS:NZ	2:O:324:PHE:CE1	2.52	0.77
2:Q:318:ILE:HG12	2:Q:351:GLU:HA	1.67	0.77
2:S:318:ILE:HG12	2:S:351:GLU:HA	1.67	0.77
1:C:426:LYS:HD2	1:C:445:LEU:HD12	1.67	0.76
1:F:385:THR:HG22	1:F:388:MET:HE1	1.64	0.76
1:K:46:MET:HE1	1:K:73:SER:CB	2.13	0.76
1:G:51:LEU:CD1	1:G:104:PRO:HG3	2.14	0.76
1:I:113:ARG:HB2	1:I:181:VAL:HG22	1.66	0.76
1:K:250:GLY:O	1:K:254:ILE:HG23	1.86	0.76
1:L:377:ARG:NH1	1:L:400:ALA:O	2.17	0.76
2:X:295:THR:HA	2:X:314:HIS:HB3	1.67	0.76
1:E:300:ILE:HD13	1:E:344:MET:CE	2.15	0.76
1:J:224:LEU:HB3	1:J:262:THR:CG2	2.16	0.76
1:K:129:ASN:O	1:K:131:PHE:N	2.18	0.76
1:H:313:ARG:HH21	1:H:322:ARG:HG2	1.51	0.76
1:C:114:ILE:HG21	1:C:146:ILE:HD11	1.68	0.76
1:H:337:GLN:C	1:H:338:ARG:HD3	2.11	0.76
1:B:27:ILE:CD1	1:B:99:VAL:CG2	2.64	0.76
1:E:243:LEU:HD23	1:E:367:VAL:CG1	2.15	0.75
1:D:336:LYS:HB2	1:D:338:ARG:NH2	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:354:ASP:HB3	1:G:357:LEU:HD23	1.68	0.75
2:M:340:MET:HE3	2:M:368:ARG:HH21	1.52	0.75
1:C:354:ASP:HB3	1:C:357:LEU:HD23	1.68	0.75
1:I:222:LEU:HD23	1:J:420:LEU:HD22	1.69	0.75
1:J:283:GLU:HG3	1:J:324:ILE:HD12	1.68	0.75
1:L:385:THR:HG22	1:L:388:MET:HE1	1.65	0.75
1:G:424:ARG:CG	1:L:222:LEU:HD21	2.16	0.74
1:A:114:ILE:HG21	1:A:146:ILE:HD11	1.70	0.74
1:B:46:MET:HE1	1:B:73:SER:CA	2.17	0.74
2:T:300:ILE:HB	2:T:309:VAL:HG23	1.69	0.74
1:J:350:PRO:CB	1:J:358:ARG:HH21	1.98	0.74
1:F:417:GLU:HG3	1:F:455:ALA:HB1	1.69	0.74
1:I:114:ILE:HG21	1:I:146:ILE:HD11	1.70	0.74
1:H:283:GLU:HG3	1:H:324:ILE:HD12	1.69	0.74
1:A:373:ASP:O	1:A:377:ARG:HG3	1.87	0.74
1:I:283:GLU:HG3	1:I:324:ILE:HD12	1.69	0.73
1:C:319:GLU:OE1	1:D:320:VAL:HG13	1.88	0.73
1:G:283:GLU:HG3	1:G:324:ILE:HD12	1.69	0.73
1:L:70:ILE:HG13	2:X:343:PHE:CE2	2.22	0.73
1:A:354:ASP:HB3	1:A:357:LEU:HD23	1.69	0.73
1:L:86:ARG:HG2	1:L:89:ARG:NH2	2.03	0.73
1:B:396:LEU:HA	1:B:399:VAL:HG13	1.71	0.73
1:D:70:ILE:HG13	2:P:343:PHE:CE2	2.23	0.73
1:D:319:GLU:OE2	1:E:318:GLY:HA3	1.89	0.73
2:X:354:THR:HG22	2:X:357:GLU:H	1.53	0.73
1:G:321:GLU:O	1:G:324:ILE:HG22	1.88	0.73
2:N:318:ILE:HG12	2:N:351:GLU:HA	1.68	0.73
1:E:222:LEU:HD21	1:F:424:ARG:CG	2.18	0.73
2:M:308:LEU:HD21	2:M:310:GLN:NE2	2.04	0.73
1:I:332:MET:CB	1:I:362:ARG:HH12	2.02	0.72
1:J:440:GLU:OE2	1:J:443:ASN:ND2	2.20	0.72
1:H:114:ILE:HG21	1:H:146:ILE:HD11	1.71	0.72
2:U:308:LEU:HD21	2:U:310:GLN:NE2	2.01	0.72
1:I:321:GLU:O	1:I:324:ILE:HG22	1.88	0.72
1:I:329:LEU:HA	1:I:362:ARG:NH1	2.05	0.72
2:R:354:THR:HG22	2:R:357:GLU:H	1.53	0.72
1:F:114:ILE:HG21	1:F:146:ILE:HD11	1.72	0.72
1:K:86:ARG:HG2	1:K:89:ARG:NH2	2.04	0.72
1:G:402:GLU:OE2	1:G:453:ARG:NH2	2.22	0.72
2:T:354:THR:HG22	2:T:357:GLU:H	1.54	0.72
1:C:129:ASN:HD22	1:C:132:GLU:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:308:LEU:HD21	2:R:310:GLN:NE2	2.05	0.72
1:D:57:VAL:HG21	1:D:102:ILE:HG13	1.72	0.72
1:I:319:GLU:OE1	1:J:320:VAL:CG1	2.38	0.72
1:L:252:THR:HG23	3:L:501:ADP:O3B	1.90	0.72
2:O:308:LEU:HD21	2:O:310:GLN:NE2	2.05	0.72
1:H:322:ARG:NH2	1:I:317:HIS:HB2	2.04	0.71
1:J:114:ILE:HG21	1:J:146:ILE:HD11	1.71	0.71
1:J:321:GLU:O	1:J:324:ILE:HG22	1.89	0.71
1:D:114:ILE:HG21	1:D:146:ILE:HD11	1.70	0.71
1:G:322:ARG:HH22	1:H:317:HIS:HB2	1.55	0.71
1:G:373:ASP:O	1:G:377:ARG:HG3	1.90	0.71
1:I:220:VAL:CG1	1:I:224:LEU:HD22	2.20	0.71
1:J:396:LEU:HA	1:J:399:VAL:HG13	1.73	0.71
1:H:321:GLU:O	1:H:324:ILE:HG22	1.90	0.71
2:P:354:THR:HG22	2:P:357:GLU:H	1.54	0.71
1:J:300:ILE:HD13	1:J:344:MET:CE	2.21	0.71
1:K:114:ILE:HG21	1:K:146:ILE:HD11	1.73	0.71
1:E:426:LYS:HD3	1:E:445:LEU:HD12	1.73	0.71
1:E:114:ILE:HG21	1:E:146:ILE:HD11	1.71	0.71
1:L:114:ILE:HG21	1:L:146:ILE:HD11	1.70	0.71
1:L:227:PRO:HB2	1:L:340:HIS:CE1	2.26	0.71
2:V:308:LEU:HD21	2:V:310:GLN:NE2	2.05	0.71
1:D:336:LYS:HE2	1:D:336:LYS:HA	1.72	0.71
1:G:114:ILE:HG21	1:G:146:ILE:HD11	1.72	0.70
1:L:402:GLU:OE2	1:L:453:ARG:NH2	2.24	0.70
2:V:295:THR:HA	2:V:314:HIS:HB3	1.73	0.70
1:B:339:ALA:C	1:B:340:HIS:CG	2.68	0.70
1:E:92:LEU:HD13	1:E:100:ILE:CD1	2.20	0.70
2:P:295:THR:HA	2:P:314:HIS:HB3	1.73	0.70
1:B:114:ILE:HG21	1:B:146:ILE:HD11	1.72	0.70
1:J:224:LEU:CB	1:J:262:THR:HG21	2.21	0.70
1:C:170:PRO:HD2	1:C:174:CYS:HB3	1.74	0.70
2:R:295:THR:HA	2:R:314:HIS:HB3	1.74	0.70
2:N:295:THR:HA	2:N:314:HIS:HB3	1.74	0.70
1:B:70:ILE:HG13	2:N:343:PHE:CE2	2.27	0.70
2:M:295:THR:HA	2:M:314:HIS:HB3	1.74	0.70
1:A:278:LEU:O	1:A:281:GLU:O	2.09	0.70
1:I:396:LEU:HA	1:I:399:VAL:HG13	1.74	0.69
1:E:243:LEU:HD22	1:E:367:VAL:CG1	2.21	0.69
2:W:354:THR:HG22	2:W:357:GLU:CG	2.21	0.69
1:C:440:GLU:C	1:C:442:MET:H	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:ARG:O	1:G:165:VAL:HG11	1.92	0.69
1:L:22:ARG:HG3	1:L:23:PRO:HD2	1.75	0.69
1:D:57:VAL:CG2	1:D:102:ILE:HG13	2.23	0.69
1:E:440:GLU:C	1:E:442:MET:H	2.00	0.69
1:J:78:SER:HB2	1:J:81:LYS:HD2	1.75	0.69
1:L:440:GLU:C	1:L:442:MET:H	2.01	0.69
2:U:295:THR:HA	2:U:314:HIS:HB3	1.74	0.69
1:A:339:ALA:C	1:A:340:HIS:ND1	2.51	0.69
1:B:339:ALA:C	1:B:340:HIS:CD2	2.70	0.69
1:I:357:LEU:HA	1:I:362:ARG:HE	1.58	0.69
1:I:402:GLU:OE2	1:I:453:ARG:NH2	2.25	0.69
1:B:274:ILE:HB	1:B:309:ILE:HD11	1.75	0.68
1:D:57:VAL:CG2	1:D:102:ILE:CG1	2.71	0.68
1:C:70:ILE:HG13	2:O:343:PHE:CE2	2.28	0.68
1:H:25:ARG:NH1	1:I:432:LEU:O	2.24	0.68
1:B:140:LEU:O	1:B:141:GLU:HG2	1.93	0.68
1:H:409:ALA:HB2	3:H:501:ADP:H5'1	1.75	0.68
1:I:251:LYS:CG	1:I:369:ILE:HD12	2.16	0.68
1:K:440:GLU:OE1	1:K:440:GLU:HA	1.92	0.68
1:B:437:ILE:HD12	1:B:441:VAL:HG11	1.74	0.68
1:F:339:ALA:C	1:F:340:HIS:ND1	2.52	0.68
2:Q:308:LEU:HD21	2:Q:310:GLN:NE2	2.08	0.68
1:E:287:ARG:HE	1:E:327:GLN:HE22	1.41	0.68
1:H:220:VAL:CG1	1:H:224:LEU:HD22	2.21	0.68
1:J:339:ALA:C	1:J:340:HIS:ND1	2.51	0.68
1:H:337:GLN:O	1:H:338:ARG:HD3	1.94	0.68
2:O:295:THR:HA	2:O:314:HIS:HB3	1.75	0.68
1:D:440:GLU:C	1:D:442:MET:H	2.02	0.68
1:I:339:ALA:C	1:I:340:HIS:ND1	2.52	0.68
2:T:314:HIS:HD1	2:T:315:SER:H	1.42	0.68
1:F:402:GLU:OE2	1:F:453:ARG:NH2	2.21	0.68
1:G:283:GLU:HA	1:G:327:GLN:HE22	1.59	0.68
1:B:219:MET:CE	1:B:365:ARG:HB3	2.23	0.68
1:D:339:ALA:C	1:D:340:HIS:ND1	2.52	0.68
2:O:354:THR:HG22	2:O:357:GLU:CG	2.23	0.68
1:K:319:GLU:OE2	1:L:318:GLY:HA3	1.93	0.67
1:B:300:ILE:HD13	1:B:344:MET:CE	2.24	0.67
1:H:339:ALA:C	1:H:340:HIS:CG	2.71	0.67
2:S:295:THR:HA	2:S:314:HIS:HB3	1.74	0.67
1:A:70:ILE:HG13	2:M:343:PHE:CE2	2.30	0.67
1:A:440:GLU:C	1:A:442:MET:H	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:440:GLU:C	1:F:442:MET:H	2.02	0.67
1:G:24:ASN:N	1:G:24:ASN:HD22	1.92	0.67
2:M:340:MET:HE3	2:M:368:ARG:NH2	2.09	0.67
1:B:440:GLU:C	1:B:442:MET:H	2.02	0.67
1:J:440:GLU:C	1:J:442:MET:H	2.02	0.67
1:C:46:MET:HE1	1:C:73:SER:CA	2.24	0.67
1:F:70:ILE:HG13	2:R:343:PHE:CE2	2.30	0.67
1:G:440:GLU:C	1:G:442:MET:H	2.03	0.67
1:H:339:ALA:C	1:H:340:HIS:CD2	2.72	0.67
1:K:339:ALA:C	1:K:340:HIS:ND1	2.53	0.67
1:A:50:GLN:CG	1:A:50:GLN:O	2.43	0.67
1:D:422:ALA:O	1:D:425:LYS:HG2	1.93	0.67
1:E:28:VAL:HG21	1:E:94:VAL:HG11	1.77	0.67
1:F:282:SER:HB2	1:F:324:ILE:HD11	1.75	0.67
1:G:339:ALA:C	1:G:340:HIS:ND1	2.53	0.67
1:I:440:GLU:C	1:I:442:MET:H	2.03	0.67
2:W:295:THR:HA	2:W:314:HIS:HB3	1.77	0.67
1:H:440:GLU:C	1:H:442:MET:H	2.02	0.66
1:K:440:GLU:C	1:K:442:MET:H	2.02	0.66
2:N:318:ILE:CD1	2:N:351:GLU:HA	2.25	0.66
2:O:294:PRO:O	2:O:314:HIS:HB2	1.95	0.66
1:C:224:LEU:HD13	1:C:262:THR:HG21	1.76	0.66
1:I:332:MET:HG3	1:I:362:ARG:HH22	1.58	0.66
2:R:318:ILE:CD1	2:R:351:GLU:HA	2.25	0.66
2:X:308:LEU:HD21	2:X:310:GLN:NE2	2.09	0.66
1:E:274:ILE:HB	1:E:309:ILE:HD11	1.78	0.66
1:I:362:ARG:HB3	1:I:362:ARG:CZ	2.25	0.66
2:Q:318:ILE:CD1	2:Q:351:GLU:HA	2.25	0.66
1:E:26:LEU:HD21	1:E:45:LYS:HE3	1.76	0.66
1:E:325:VAL:O	1:E:329:LEU:HD13	1.95	0.66
2:S:318:ILE:CD1	2:S:351:GLU:HA	2.24	0.66
2:X:318:ILE:CD1	2:X:351:GLU:HA	2.25	0.66
1:A:27:ILE:CD1	1:A:99:VAL:HG22	2.24	0.66
1:D:336:LYS:CG	1:D:338:ARG:HH22	2.08	0.66
1:L:186:GLY:O	1:L:187:GLU:HB2	1.93	0.66
2:P:294:PRO:O	2:P:314:HIS:HB2	1.96	0.66
2:R:354:THR:HG22	2:R:357:GLU:HG3	1.78	0.66
2:U:318:ILE:CD1	2:U:351:GLU:HA	2.26	0.66
1:F:282:SER:HB3	1:F:324:ILE:HD11	1.77	0.66
1:G:222:LEU:HD11	1:H:424:ARG:CG	2.26	0.66
2:Q:295:THR:HA	2:Q:314:HIS:HB3	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:THR:HG22	3:A:501:ADP:PA	2.36	0.66
2:M:294:PRO:O	2:M:314:HIS:HB2	1.96	0.66
1:C:171:SER:CB	1:C:172:PRO:HD2	2.26	0.66
2:P:318:ILE:CD1	2:P:351:GLU:HA	2.26	0.66
2:V:354:THR:HG22	2:V:357:GLU:CG	2.25	0.66
2:W:286:MET:SD	2:W:287:ILE:HG22	2.35	0.66
2:X:289:ILE:HD13	2:X:312:PHE:HD2	1.61	0.66
1:B:396:LEU:HA	1:B:399:VAL:CG1	2.26	0.66
1:D:157:GLY:N	1:D:389:LYS:HZ1	1.94	0.66
1:J:43:GLN:HB3	1:J:44:PRO:HD3	1.78	0.66
2:Q:294:PRO:O	2:Q:314:HIS:HB2	1.95	0.66
2:P:354:THR:HG22	2:P:357:GLU:HG3	1.77	0.66
2:S:294:PRO:O	2:S:314:HIS:HB2	1.95	0.66
2:W:321:ILE:HD11	2:W:355:LEU:HD21	1.78	0.66
1:I:332:MET:CG	1:I:362:ARG:HH12	2.09	0.65
1:A:335:LEU:HD12	1:A:338:ARG:HG2	1.79	0.65
1:I:300:ILE:HD13	1:I:344:MET:CE	2.26	0.65
2:M:318:ILE:CD1	2:M:351:GLU:HA	2.26	0.65
2:N:318:ILE:HD11	2:N:351:GLU:HA	1.78	0.65
2:R:294:PRO:O	2:R:314:HIS:HB2	1.96	0.65
2:U:321:ILE:HD11	2:U:355:LEU:HD21	1.79	0.65
1:G:388:MET:HE3	1:G:390:LEU:HD21	1.78	0.65
1:K:140:LEU:O	1:K:141:GLU:HG3	1.97	0.65
2:T:354:THR:HG22	2:T:357:GLU:HG3	1.78	0.65
1:D:431:ASP:HA	1:D:436:THR:HG22	1.78	0.65
1:G:224:LEU:HD13	1:G:262:THR:HG21	1.78	0.65
1:G:431:ASP:HA	1:G:436:THR:HG22	1.79	0.65
2:W:318:ILE:CD1	2:W:351:GLU:HA	2.26	0.65
2:X:354:THR:HG22	2:X:357:GLU:HG3	1.78	0.65
1:I:86:ARG:HH21	1:I:204:ASP:CG	2.04	0.65
1:K:113:ARG:HE	1:K:183:HIS:CE1	2.15	0.65
2:S:318:ILE:HD11	2:S:351:GLU:HA	1.78	0.65
2:T:318:ILE:CD1	2:T:351:GLU:HA	2.26	0.65
2:V:294:PRO:O	2:V:314:HIS:HB2	1.96	0.65
1:K:115:HIS:HB3	1:K:166:VAL:HG23	1.78	0.65
2:U:340:MET:HE1	2:U:368:ARG:NH1	2.11	0.65
1:G:49:LEU:HB3	1:G:51:LEU:HD22	1.78	0.65
1:J:396:LEU:HA	1:J:399:VAL:CG1	2.27	0.65
1:J:431:ASP:HA	1:J:436:THR:HG22	1.77	0.65
2:N:294:PRO:O	2:N:314:HIS:HB2	1.97	0.65
1:F:431:ASP:HA	1:F:436:THR:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ARG:HH22	1:B:317:HIS:HB2	1.61	0.65
1:I:249:THR:HG22	1:I:251:LYS:NZ	2.12	0.65
2:W:294:PRO:O	2:W:314:HIS:HB2	1.96	0.64
1:B:43:GLN:HB3	1:B:44:PRO:HD3	1.79	0.64
1:K:350:PRO:HB3	1:K:358:ARG:HH12	1.62	0.64
2:R:321:ILE:HD11	2:R:355:LEU:HD21	1.79	0.64
1:A:339:ALA:C	1:A:340:HIS:CG	2.76	0.64
1:B:27:ILE:CD1	1:B:99:VAL:HG22	2.23	0.64
1:D:131:PHE:HB3	1:D:136:LYS:HZ3	1.60	0.64
2:S:321:ILE:HD11	2:S:355:LEU:HD21	1.78	0.64
2:U:294:PRO:O	2:U:314:HIS:HB2	1.98	0.64
1:A:27:ILE:CD1	1:A:99:VAL:HG23	2.27	0.64
1:C:220:VAL:CG1	1:C:224:LEU:HD12	2.28	0.64
1:G:43:GLN:HB3	1:G:44:PRO:HD3	1.78	0.64
1:G:220:VAL:CG1	1:G:224:LEU:HD12	2.27	0.64
1:G:317:HIS:HB2	1:L:322:ARG:NH2	2.13	0.64
1:J:339:ALA:C	1:J:340:HIS:CG	2.75	0.64
2:P:321:ILE:HD11	2:P:355:LEU:HD21	1.78	0.64
1:D:300:ILE:HG21	1:D:344:MET:HE3	1.78	0.64
1:D:339:ALA:C	1:D:340:HIS:CG	2.76	0.64
1:H:431:ASP:HA	1:H:436:THR:HG22	1.80	0.64
1:L:220:VAL:CG1	1:L:224:LEU:HD12	2.28	0.64
1:G:337:GLN:O	1:G:340:HIS:N	2.31	0.64
1:G:339:ALA:C	1:G:340:HIS:CG	2.76	0.64
2:Q:318:ILE:HD11	2:Q:351:GLU:HA	1.79	0.64
1:C:43:GLN:HB3	1:C:44:PRO:HD3	1.79	0.64
1:I:357:LEU:HD23	1:I:362:ARG:HH21	1.63	0.64
1:A:390:LEU:CD2	1:A:447:VAL:CG1	2.76	0.64
1:E:300:ILE:HG21	1:E:344:MET:HE3	1.77	0.64
1:J:114:ILE:HG22	1:J:168:THR:HG22	1.80	0.64
2:U:318:ILE:HD11	2:U:351:GLU:HA	1.80	0.64
1:E:155:ARG:CZ	1:E:386:LYS:HE2	2.28	0.63
1:F:385:THR:CG2	1:F:388:MET:CE	2.66	0.63
1:K:339:ALA:C	1:K:340:HIS:CG	2.76	0.63
1:B:249:THR:HG22	1:B:251:LYS:NZ	2.13	0.63
1:C:249:THR:HG22	1:C:251:LYS:NZ	2.13	0.63
1:D:389:LYS:HE2	1:D:443:ASN:CG	2.24	0.63
1:I:339:ALA:C	1:I:340:HIS:CG	2.76	0.63
1:L:63:LYS:O	1:L:64:ARG:HG2	1.98	0.63
1:B:287:ARG:HG3	1:B:327:GLN:HE22	1.64	0.63
1:F:287:ARG:HE	1:F:327:GLN:HE22	1.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:GLN:HB3	1:H:44:PRO:HD3	1.79	0.63
1:K:129:ASN:O	1:K:129:ASN:OD1	2.15	0.63
1:B:283:GLU:HA	1:B:327:GLN:OE1	1.98	0.63
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.79	0.63
1:F:339:ALA:C	1:F:340:HIS:CG	2.76	0.63
1:H:249:THR:HG22	1:H:251:LYS:NZ	2.13	0.63
1:B:287:ARG:HG3	1:B:327:GLN:NE2	2.13	0.63
1:D:43:GLN:HB3	1:D:44:PRO:HD3	1.80	0.63
1:F:220:VAL:CG1	1:F:224:LEU:HD12	2.28	0.63
1:I:114:ILE:HG22	1:I:168:THR:HG22	1.80	0.63
1:K:335:LEU:HD12	1:K:338:ARG:HG2	1.80	0.63
1:E:150:ASP:HB2	1:E:165:VAL:CG1	2.29	0.63
1:H:249:THR:HG22	1:H:251:LYS:HZ2	1.63	0.63
1:A:252:THR:HG22	3:A:501:ADP:O1A	1.99	0.63
1:A:349:ARG:HG3	1:A:350:PRO:HD2	1.80	0.63
1:F:114:ILE:HG22	1:F:168:THR:HG22	1.81	0.63
1:I:26:LEU:HD11	1:I:45:LYS:HE2	1.81	0.63
1:J:335:LEU:HA	1:J:338:ARG:HG3	1.79	0.63
1:K:235:VAL:HG23	1:L:416:SER:OG	1.99	0.63
1:L:385:THR:CG2	1:L:388:MET:CE	2.66	0.63
2:M:318:ILE:HD11	2:M:351:GLU:HA	1.81	0.63
1:H:114:ILE:HG22	1:H:168:THR:HG22	1.81	0.62
1:I:396:LEU:HA	1:I:399:VAL:CG1	2.29	0.62
2:Q:321:ILE:HD11	2:Q:355:LEU:HD21	1.80	0.62
2:U:308:LEU:CD2	2:U:310:GLN:HE21	2.08	0.62
2:V:321:ILE:HD11	2:V:355:LEU:HD21	1.81	0.62
1:F:43:GLN:HB3	1:F:44:PRO:HD3	1.80	0.62
1:K:220:VAL:CG1	1:K:224:LEU:HD12	2.29	0.62
1:L:35:ASP:HB3	1:L:38:VAL:HG13	1.80	0.62
1:D:220:VAL:CG1	1:D:224:LEU:HD12	2.30	0.62
1:D:114:ILE:HG22	1:D:168:THR:HG22	1.82	0.62
2:T:302:LEU:HB3	2:T:304:ASP:OD1	2.00	0.62
1:E:427:MET:HA	1:E:430:ILE:HG12	1.81	0.62
2:O:321:ILE:HD11	2:O:355:LEU:HD21	1.81	0.62
1:A:114:ILE:HG22	1:A:168:THR:HG22	1.82	0.62
1:B:335:LEU:HD12	1:B:338:ARG:HG2	1.81	0.62
1:E:233:ILE:CG2	1:F:442:MET:HE2	2.29	0.62
1:B:114:ILE:HG22	1:B:168:THR:HG22	1.82	0.62
1:J:220:VAL:CG1	1:J:224:LEU:HD12	2.28	0.62
1:K:53:ARG:HH12	1:K:73:SER:H	1.48	0.62
2:X:289:ILE:HD13	2:X:312:PHE:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:THR:CG2	1:G:388:MET:HE2	2.30	0.62
1:L:385:THR:HG22	1:L:388:MET:HE3	1.78	0.62
2:N:321:ILE:HD11	2:N:355:LEU:HD21	1.80	0.62
1:E:114:ILE:HG22	1:E:168:THR:HG22	1.81	0.62
1:E:421:GLN:HE21	1:E:421:GLN:HA	1.64	0.62
1:J:350:PRO:CA	1:J:358:ARG:HH21	2.13	0.61
1:J:27:ILE:HG23	1:J:81:LYS:CG	2.30	0.61
1:K:114:ILE:HG22	1:K:168:THR:HG22	1.83	0.61
1:C:230:PHE:HB2	1:C:340:HIS:NE2	2.15	0.61
1:F:35:ASP:HB3	1:F:38:VAL:HG13	1.83	0.61
1:K:377:ARG:HG2	1:K:411:LEU:HD11	1.82	0.61
1:L:426:LYS:HD2	1:L:445:LEU:HD23	1.82	0.61
1:B:300:ILE:HD13	1:B:344:MET:HE3	1.82	0.61
1:C:220:VAL:HG22	1:C:342:ILE:HD13	1.83	0.61
1:H:239:ARG:NH1	1:H:335:LEU:O	2.33	0.61
1:L:222:LEU:HB2	1:L:223:PRO:HD3	1.82	0.61
1:D:57:VAL:HG21	1:D:102:ILE:HG12	1.78	0.61
1:C:377:ARG:HG2	1:C:411:LEU:HD11	1.82	0.61
1:I:43:GLN:HB3	1:I:44:PRO:HD3	1.81	0.61
1:J:70:ILE:HG13	2:V:343:PHE:CE2	2.34	0.61
2:S:341:THR:HG22	2:S:346:LYS:HB3	1.83	0.61
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.83	0.61
1:C:350:PRO:CA	1:C:358:ARG:NH2	2.64	0.61
1:F:377:ARG:HE	1:F:403:THR:HG23	1.66	0.61
1:A:220:VAL:CG1	1:A:224:LEU:HD12	2.29	0.60
1:E:377:ARG:HG2	1:E:411:LEU:HD11	1.83	0.60
1:J:377:ARG:HG2	1:J:411:LEU:HD11	1.82	0.60
1:L:43:GLN:HB3	1:L:44:PRO:HD3	1.81	0.60
2:W:354:THR:HG22	2:W:357:GLU:HG3	1.82	0.60
1:H:377:ARG:HG2	1:H:411:LEU:HD11	1.83	0.60
1:I:287:ARG:HE	1:I:327:GLN:HE22	1.47	0.60
1:I:402:GLU:CD	1:I:453:ARG:HH22	2.08	0.60
1:D:377:ARG:HG2	1:D:411:LEU:HD11	1.84	0.60
1:H:70:ILE:HG13	2:T:343:PHE:CE2	2.36	0.60
1:K:243:LEU:N	1:K:243:LEU:HD12	2.17	0.60
1:L:287:ARG:HE	1:L:327:GLN:HE22	1.47	0.60
1:A:27:ILE:HG12	1:B:432:LEU:HD13	1.83	0.60
1:A:35:ASP:HB3	1:A:38:VAL:HG13	1.82	0.60
1:G:275:MET:HE1	1:G:324:ILE:HG12	1.82	0.60
1:A:350:PRO:HB3	1:A:358:ARG:HH12	1.67	0.60
1:F:377:ARG:HG2	1:F:411:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:LEU:HB2	1:E:223:PRO:HD3	1.83	0.60
1:F:249:THR:HG22	1:F:369:ILE:HG22	1.84	0.60
1:G:114:ILE:HG22	1:G:168:THR:HG22	1.82	0.60
1:G:424:ARG:HH11	1:L:222:LEU:CD2	2.15	0.60
1:A:281:GLU:O	1:A:282:SER:CB	2.48	0.60
1:H:52:PHE:O	1:H:55:ASP:HB2	2.02	0.60
1:K:108:VAL:HG12	1:K:173:TYR:CE1	2.37	0.60
1:F:52:PHE:O	1:F:55:ASP:HB2	2.03	0.59
1:F:403:THR:OG1	1:F:406:HIS:CD2	2.55	0.59
1:I:332:MET:HG3	1:I:362:ARG:CZ	2.31	0.59
1:C:239:ARG:NH1	1:C:336:LYS:HA	2.17	0.59
1:H:22:ARG:HG2	1:H:23:PRO:HD2	1.83	0.59
2:Q:286:MET:HG2	2:Q:287:ILE:H	1.67	0.59
1:G:385:THR:CG2	1:G:388:MET:CE	2.77	0.59
1:H:46:MET:HE1	1:H:73:SER:CA	2.32	0.59
2:V:302:LEU:HB2	2:V:307:ARG:HB2	1.84	0.59
1:A:50:GLN:O	1:A:50:GLN:HG3	2.02	0.59
1:B:27:ILE:CD1	1:B:99:VAL:HG23	2.31	0.59
1:F:335:LEU:HD23	1:F:338:ARG:HG2	1.84	0.59
1:D:52:PHE:O	1:D:55:ASP:HB2	2.02	0.59
1:I:377:ARG:HG2	1:I:411:LEU:HD11	1.84	0.59
1:B:377:ARG:HG2	1:B:411:LEU:HD11	1.84	0.59
1:G:52:PHE:O	1:G:55:ASP:HB2	2.02	0.59
1:F:239:ARG:NH2	1:F:336:LYS:HA	2.17	0.59
2:X:318:ILE:HD11	2:X:351:GLU:HA	1.84	0.59
1:B:220:VAL:CG1	1:B:224:LEU:HD12	2.30	0.59
1:E:322:ARG:HH22	1:F:317:HIS:HB2	1.68	0.59
1:K:32:ILE:HD12	1:K:33:ASN:N	2.18	0.59
2:R:318:ILE:HD11	2:R:351:GLU:HA	1.83	0.59
1:K:140:LEU:HG	1:K:141:GLU:HG2	1.83	0.59
2:S:361:LEU:HD12	2:S:361:LEU:H	1.68	0.59
1:C:32:ILE:HD12	1:C:33:ASN:N	2.18	0.59
1:C:113:ARG:HD3	1:C:183:HIS:CE1	2.37	0.58
1:E:243:LEU:HD22	1:E:367:VAL:HG11	1.81	0.58
1:G:70:ILE:HG13	2:S:343:PHE:CE2	2.38	0.58
1:G:393:ASP:O	1:G:449:MET:CG	2.51	0.58
1:I:52:PHE:O	1:I:55:ASP:HB2	2.01	0.58
1:I:249:THR:HG22	1:I:251:LYS:HZ2	1.67	0.58
1:L:52:PHE:O	1:L:55:ASP:HB2	2.03	0.58
1:D:389:LYS:CD	1:D:443:ASN:O	2.51	0.58
1:L:32:ILE:HD12	1:L:33:ASN:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:MET:CE	1:B:73:SER:CA	2.78	0.58
1:B:350:PRO:HB3	1:B:358:ARG:HH12	1.68	0.58
1:H:32:ILE:HD12	1:H:33:ASN:N	2.17	0.58
1:J:52:PHE:O	1:J:55:ASP:HB2	2.03	0.58
1:A:336:LYS:HB2	1:A:338:ARG:HH22	1.67	0.58
1:B:52:PHE:O	1:B:55:ASP:HB2	2.02	0.58
1:C:52:PHE:O	1:C:55:ASP:HB2	2.02	0.58
1:F:385:THR:HA	1:F:388:MET:HE2	1.85	0.58
1:H:339:ALA:O	1:H:340:HIS:CG	2.57	0.58
1:I:402:GLU:CD	1:I:453:ARG:NH2	2.62	0.58
1:K:52:PHE:O	1:K:55:ASP:HB2	2.02	0.58
1:K:70:ILE:HG13	2:W:343:PHE:CE2	2.38	0.58
1:L:357:LEU:C	1:L:359:ARG:H	2.12	0.58
2:T:318:ILE:HD11	2:T:351:GLU:HA	1.84	0.58
1:H:222:LEU:HB2	1:H:223:PRO:HD3	1.86	0.58
2:R:318:ILE:HG12	2:R:351:GLU:CA	2.32	0.58
1:G:222:LEU:HB2	1:G:223:PRO:HD3	1.85	0.58
1:D:157:GLY:N	1:D:389:LYS:NZ	2.44	0.58
1:F:249:THR:CG2	1:F:369:ILE:HG22	2.34	0.58
1:G:22:ARG:NE	1:G:24:ASN:HB2	2.16	0.58
2:O:354:THR:HG22	2:O:357:GLU:HG3	1.85	0.58
2:R:302:LEU:HD12	2:R:307:ARG:HB3	1.86	0.58
2:W:318:ILE:HD11	2:W:351:GLU:HA	1.84	0.58
1:A:339:ALA:O	1:A:340:HIS:CG	2.57	0.58
1:G:126:ILE:HD11	1:G:159:ARG:HG2	1.85	0.58
1:K:43:GLN:HB3	1:K:44:PRO:HD3	1.85	0.58
1:L:22:ARG:HB3	1:L:25:ARG:HH21	1.68	0.58
1:D:335:LEU:HD12	1:D:338:ARG:HG2	1.84	0.58
1:K:80:GLU:HG2	1:L:432:LEU:CD1	2.34	0.58
1:F:339:ALA:O	1:F:340:HIS:CG	2.57	0.57
1:H:46:MET:HE2	1:H:73:SER:HA	1.85	0.57
1:I:339:ALA:O	1:I:340:HIS:CG	2.57	0.57
2:U:302:LEU:HB2	2:U:307:ARG:HB2	1.86	0.57
2:W:287:ILE:HD11	2:W:316:HIS:NE2	2.19	0.57
1:A:86:ARG:HG2	1:A:89:ARG:NH2	2.19	0.57
1:C:249:THR:HG22	1:C:251:LYS:HZ2	1.68	0.57
2:P:318:ILE:HD11	2:P:351:GLU:HA	1.85	0.57
1:B:322:ARG:HH22	1:C:317:HIS:HB2	1.69	0.57
2:X:302:LEU:HD12	2:X:307:ARG:HB3	1.86	0.57
1:G:339:ALA:O	1:G:340:HIS:CG	2.58	0.57
1:G:385:THR:CB	1:G:388:MET:HE2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:MET:CE	1:C:73:SER:CA	2.82	0.57
1:C:378:LEU:O	1:C:382:GLN:HG2	2.05	0.57
1:H:336:LYS:O	1:H:338:ARG:HD2	2.05	0.57
1:J:335:LEU:HD23	1:J:338:ARG:HG3	1.87	0.57
1:K:222:LEU:HB2	1:K:223:PRO:HD3	1.86	0.57
1:K:339:ALA:O	1:K:340:HIS:CG	2.57	0.57
2:O:311:LYS:NZ	2:O:324:PHE:HE1	2.00	0.57
2:Q:302:LEU:HB2	2:Q:307:ARG:HB2	1.84	0.57
2:R:302:LEU:HB2	2:R:307:ARG:HB2	1.86	0.57
1:D:339:ALA:O	1:D:340:HIS:CG	2.57	0.57
1:H:22:ARG:HB2	1:H:25:ARG:NH2	2.20	0.57
1:J:113:ARG:NH1	1:J:115:HIS:HB2	2.20	0.57
2:R:294:PRO:O	2:R:314:HIS:CB	2.52	0.57
2:W:302:LEU:HB2	2:W:307:ARG:HB2	1.87	0.57
1:H:393:ASP:O	1:H:449:MET:CG	2.53	0.57
1:I:335:LEU:HD23	1:I:338:ARG:HG2	1.86	0.57
1:D:129:ASN:OD1	1:D:132:GLU:HG2	2.04	0.57
1:E:80:GLU:HG2	1:E:81:LYS:HG3	1.87	0.57
1:H:350:PRO:C	1:H:358:ARG:HH22	2.12	0.57
1:E:378:LEU:O	1:E:382:GLN:HG2	2.05	0.57
1:J:339:ALA:O	1:J:340:HIS:CG	2.57	0.57
2:W:311:LYS:HD3	2:W:324:PHE:CE1	2.40	0.57
1:E:233:ILE:HG21	1:F:442:MET:HE2	1.86	0.56
1:G:222:LEU:HD12	1:G:222:LEU:H	1.70	0.56
1:I:332:MET:CG	1:I:362:ARG:NH1	2.67	0.56
1:C:319:GLU:OE1	1:D:320:VAL:HG12	2.03	0.56
1:H:359:ARG:HG3	1:H:360:PHE:H	1.70	0.56
1:J:222:LEU:HB2	1:J:223:PRO:HD3	1.87	0.56
1:K:282:SER:CB	1:K:324:ILE:HD11	2.35	0.56
2:N:311:LYS:HD3	2:N:324:PHE:CE1	2.40	0.56
2:U:311:LYS:HD3	2:U:324:PHE:CE1	2.40	0.56
1:A:222:LEU:HB2	1:A:223:PRO:HD3	1.87	0.56
1:B:222:LEU:HB2	1:B:223:PRO:HD3	1.87	0.56
1:F:210:ARG:NH2	1:F:211:LYS:HE3	2.20	0.56
1:G:322:ARG:NH2	1:H:317:HIS:HB2	2.20	0.56
2:M:311:LYS:HD3	2:M:324:PHE:CE1	2.40	0.56
2:Q:294:PRO:O	2:Q:314:HIS:CB	2.53	0.56
2:W:294:PRO:O	2:W:314:HIS:CB	2.53	0.56
1:D:27:ILE:HG13	1:E:432:LEU:HD13	1.87	0.56
1:E:108:VAL:HG12	1:E:173:TYR:CE1	2.41	0.56
1:E:353:ILE:CD1	1:E:353:ILE:C	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:LEU:HB2	1:F:223:PRO:HD3	1.88	0.56
1:F:239:ARG:CZ	1:F:335:LEU:O	2.53	0.56
1:H:46:MET:CE	1:H:73:SER:CA	2.83	0.56
1:K:46:MET:HE2	1:K:73:SER:HA	1.88	0.56
2:T:318:ILE:HG12	2:T:351:GLU:CA	2.34	0.56
2:X:302:LEU:HB2	2:X:307:ARG:HB2	1.86	0.56
1:G:359:ARG:HG3	1:G:360:PHE:H	1.71	0.56
1:I:335:LEU:CD2	1:I:338:ARG:HG2	2.36	0.56
1:L:339:ALA:C	1:L:340:HIS:CG	2.84	0.56
2:M:304:ASP:O	2:M:307:ARG:HG2	2.05	0.56
2:S:294:PRO:O	2:S:314:HIS:CB	2.53	0.56
1:B:322:ARG:NH2	1:C:317:HIS:HB2	2.21	0.56
1:C:113:ARG:HB2	1:C:181:VAL:CG1	2.31	0.56
1:H:378:LEU:O	1:H:382:GLN:HG2	2.06	0.56
1:I:300:ILE:HD13	1:I:344:MET:HE3	1.87	0.56
1:I:350:PRO:C	1:I:358:ARG:HH22	2.13	0.56
2:O:294:PRO:O	2:O:314:HIS:CB	2.53	0.56
2:V:311:LYS:HD3	2:V:324:PHE:CE1	2.41	0.56
1:I:357:LEU:CD2	1:I:362:ARG:NH2	2.67	0.56
1:L:312:LYS:HB3	1:L:315:LYS:HG3	1.87	0.56
1:A:113:ARG:NE	1:A:183:HIS:HE1	2.00	0.56
1:A:427:MET:HE2	1:A:427:MET:HA	1.87	0.56
1:B:219:MET:HE3	1:B:365:ARG:CZ	2.35	0.56
1:E:243:LEU:HD23	1:E:367:VAL:HG12	1.88	0.56
1:F:350:PRO:C	1:F:358:ARG:HH22	2.13	0.56
1:L:356:ALA:O	1:L:359:ARG:HB2	2.06	0.56
1:F:417:GLU:HG3	1:F:455:ALA:CB	2.34	0.56
1:G:71:VAL:O	1:G:72:LEU:HD12	2.06	0.56
1:H:395:ASP:H	1:H:449:MET:HE2	1.70	0.56
1:E:328:LEU:HD13	1:E:357:LEU:HD21	1.86	0.56
1:J:437:ILE:HD13	1:J:441:VAL:HG11	1.88	0.56
2:M:294:PRO:O	2:M:314:HIS:CB	2.53	0.56
2:O:354:THR:CG2	2:O:357:GLU:H	2.19	0.56
1:C:279:ALA:HB1	1:C:320:VAL:HG21	1.87	0.55
1:D:126:ILE:HG12	1:D:159:ARG:NH1	2.20	0.55
1:D:244:TYR:CE1	1:D:350:PRO:HA	2.41	0.55
1:E:43:GLN:HB3	1:E:44:PRO:HD3	1.86	0.55
2:N:290:ASP:N	2:N:314:HIS:HE1	2.04	0.55
2:P:294:PRO:O	2:P:314:HIS:CB	2.54	0.55
2:P:340:MET:HE3	2:P:368:ARG:HE	1.70	0.55
2:S:287:ILE:HD11	2:S:316:HIS:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ARG:C	1:C:340:HIS:H	2.14	0.55
1:C:354:ASP:HB3	1:C:357:LEU:CD2	2.37	0.55
1:K:82:ILE:HG21	1:K:100:ILE:HD11	1.88	0.55
2:V:289:ILE:O	2:V:291:GLU:OE1	2.24	0.55
1:D:71:VAL:O	1:D:72:LEU:HD12	2.07	0.55
1:E:336:LYS:C	1:E:338:ARG:N	2.62	0.55
1:L:71:VAL:O	1:L:72:LEU:HD12	2.06	0.55
1:D:222:LEU:HB2	1:D:223:PRO:HD3	1.89	0.55
1:D:242:LEU:HD13	1:D:244:TYR:OH	2.06	0.55
1:A:52:PHE:O	1:A:55:ASP:HB2	2.06	0.55
1:B:46:MET:HE2	1:B:73:SER:HA	1.87	0.55
2:Q:302:LEU:HD12	2:Q:307:ARG:HB3	1.87	0.55
2:U:294:PRO:O	2:U:314:HIS:CB	2.53	0.55
1:C:129:ASN:O	1:C:131:PHE:N	2.38	0.55
1:D:157:GLY:H	1:D:389:LYS:HZ3	1.54	0.55
1:H:437:ILE:HD12	1:H:441:VAL:HG11	1.88	0.55
1:K:131:PHE:HE1	1:K:182:ILE:HG23	1.72	0.55
1:L:82:ILE:HG21	1:L:100:ILE:HD11	1.89	0.55
2:P:311:LYS:NZ	2:P:324:PHE:HE1	2.00	0.55
2:V:302:LEU:HD12	2:V:307:ARG:HB3	1.87	0.55
2:W:302:LEU:HD12	2:W:307:ARG:HB3	1.87	0.55
1:G:354:ASP:HB3	1:G:357:LEU:CD2	2.35	0.55
1:G:427:MET:HE2	1:L:226:HIS:CE1	2.42	0.55
1:I:357:LEU:CD2	1:I:362:ARG:HH21	2.19	0.55
1:K:115:HIS:O	1:K:166:VAL:HG22	2.07	0.55
2:V:287:ILE:HD12	2:V:287:ILE:H	1.72	0.55
2:X:289:ILE:CD1	2:X:312:PHE:CD2	2.90	0.55
1:A:322:ARG:NH2	1:B:317:HIS:HB2	2.21	0.55
1:F:336:LYS:HD2	1:F:337:GLN:HG3	1.89	0.55
1:H:239:ARG:NH2	1:H:335:LEU:O	2.40	0.55
2:P:318:ILE:HG12	2:P:351:GLU:CA	2.33	0.55
2:T:300:ILE:HB	2:T:309:VAL:CG2	2.35	0.55
2:V:294:PRO:O	2:V:314:HIS:CB	2.54	0.55
2:X:318:ILE:HG12	2:X:351:GLU:CA	2.32	0.55
1:H:239:ARG:CZ	1:H:335:LEU:O	2.55	0.54
2:V:354:THR:CG2	2:V:357:GLU:H	2.20	0.54
1:E:329:LEU:N	1:E:329:LEU:CD1	2.70	0.54
2:X:311:LYS:HD3	2:X:324:PHE:CE1	2.42	0.54
1:A:78:SER:HB3	1:A:80:GLU:OE2	2.07	0.54
1:E:150:ASP:H	1:E:165:VAL:HG13	1.72	0.54
1:I:63:LYS:HE2	1:I:63:LYS:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:294:PRO:O	2:X:314:HIS:HB2	2.07	0.54
1:B:82:ILE:HG21	1:B:100:ILE:HD11	1.89	0.54
1:C:112:LYS:N	1:C:169:ASP:O	2.38	0.54
1:H:71:VAL:O	1:H:72:LEU:HD12	2.08	0.54
1:H:359:ARG:HD3	1:I:247:PRO:HB3	1.89	0.54
1:I:82:ILE:HG21	1:I:100:ILE:HD11	1.90	0.54
1:J:71:VAL:O	1:J:72:LEU:HD12	2.07	0.54
1:J:82:ILE:HG21	1:J:100:ILE:HD11	1.90	0.54
2:N:294:PRO:O	2:N:314:HIS:CB	2.55	0.54
1:E:115:HIS:O	1:E:166:VAL:HG22	2.07	0.54
1:H:239:ARG:HH22	1:H:336:LYS:HA	1.73	0.54
1:J:300:ILE:HD13	1:J:344:MET:HE3	1.89	0.54
1:L:22:ARG:HB3	1:L:25:ARG:NH2	2.22	0.54
1:L:332:MET:O	1:L:335:LEU:HB2	2.07	0.54
1:B:244:TYR:OH	1:B:358:ARG:NH1	2.41	0.54
1:C:46:MET:HE2	1:C:73:SER:HA	1.89	0.54
1:I:332:MET:HG3	1:I:362:ARG:NH1	2.22	0.54
1:K:219:MET:HE2	1:K:365:ARG:CZ	2.38	0.54
1:L:35:ASP:HB3	1:L:38:VAL:CG1	2.37	0.54
1:B:68:VAL:HG13	1:B:145:PRO:HB2	1.90	0.54
1:D:249:THR:HG22	1:D:251:LYS:HE2	1.89	0.54
1:D:360:PHE:C	1:D:362:ARG:H	2.16	0.54
1:G:22:ARG:HG3	1:G:24:ASN:H	1.72	0.54
2:W:354:THR:CG2	2:W:357:GLU:H	2.21	0.54
1:C:222:LEU:HB2	1:C:223:PRO:HD3	1.89	0.54
1:D:350:PRO:HB3	1:D:358:ARG:HH12	1.73	0.54
1:K:249:THR:HG23	1:K:407:VAL:HG21	1.90	0.54
1:E:249:THR:CG2	1:E:407:VAL:CG2	2.85	0.54
1:F:22:ARG:HG3	1:F:23:PRO:CD	2.36	0.54
1:H:22:ARG:HH21	1:H:24:ASN:HB2	1.73	0.54
1:B:339:ALA:O	1:B:340:HIS:CG	2.57	0.53
1:K:133:VAL:HG23	1:K:443:ASN:CG	2.33	0.53
2:W:354:THR:HG23	2:W:357:GLU:H	1.72	0.53
1:A:82:ILE:HG21	1:A:100:ILE:HD11	1.90	0.53
1:A:402:GLU:CD	1:L:398:GLN:HE22	2.15	0.53
1:E:350:PRO:HB2	1:E:358:ARG:HH21	1.72	0.53
1:H:98:ASP:OD1	1:H:225:ARG:NH2	2.41	0.53
1:I:434:ASP:CG	1:I:436:THR:HG22	2.33	0.53
1:J:32:ILE:HD12	1:J:33:ASN:N	2.23	0.53
1:K:233:ILE:CD1	1:K:235:VAL:HG12	2.37	0.53
1:K:249:THR:CG2	1:K:407:VAL:CG2	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:354:THR:HG23	2:O:357:GLU:H	1.73	0.53
2:T:314:HIS:CE1	2:T:316:HIS:CE1	2.96	0.53
1:D:82:ILE:HG21	1:D:100:ILE:HD11	1.89	0.53
1:G:283:GLU:HA	1:G:327:GLN:NE2	2.22	0.53
1:L:385:THR:HA	1:L:388:MET:HE2	1.90	0.53
1:A:354:ASP:HB3	1:A:357:LEU:CD2	2.37	0.53
1:E:249:THR:HG23	1:E:407:VAL:HG21	1.90	0.53
1:K:80:GLU:HG2	1:L:432:LEU:HD11	1.91	0.53
2:P:290:ASP:N	2:P:314:HIS:HE1	2.06	0.53
2:W:290:ASP:N	2:W:314:HIS:HE1	2.06	0.53
1:G:49:LEU:CB	1:G:51:LEU:HD22	2.39	0.53
1:B:336:LYS:HB2	1:B:338:ARG:HH22	1.68	0.53
2:V:354:THR:HG23	2:V:357:GLU:H	1.72	0.53
1:F:239:ARG:HH21	1:F:336:LYS:HA	1.74	0.53
1:K:440:GLU:O	1:K:442:MET:N	2.42	0.53
2:M:340:MET:HE1	2:M:368:ARG:HH21	1.70	0.53
2:N:290:ASP:H	2:N:314:HIS:HE1	1.57	0.53
2:O:300:ILE:HD13	2:O:365:ILE:HB	1.90	0.53
1:F:283:GLU:HG3	1:F:324:ILE:HD13	1.90	0.53
1:K:26:LEU:HD21	1:K:45:LYS:HE3	1.89	0.53
1:K:440:GLU:C	1:K:442:MET:N	2.67	0.53
2:O:289:ILE:HG23	2:O:314:HIS:CD2	2.44	0.53
2:Q:318:ILE:HG12	2:Q:351:GLU:CA	2.39	0.53
1:C:82:ILE:HG21	1:C:100:ILE:HD11	1.91	0.53
1:J:300:ILE:HG21	1:J:344:MET:HE3	1.91	0.53
1:J:440:GLU:HA	1:J:440:GLU:OE1	2.08	0.53
2:P:320:ASP:HA	2:P:323:LEU:HG	1.89	0.53
2:V:347:GLU:OE2	2:V:368:ARG:NH2	2.41	0.53
1:F:335:LEU:CD2	1:F:338:ARG:HG2	2.39	0.53
1:G:395:ASP:H	1:G:449:MET:HE2	1.72	0.53
2:V:354:THR:HG22	2:V:357:GLU:HG3	1.90	0.53
1:B:89:ARG:HD3	1:B:96:LEU:HD13	1.92	0.52
1:K:128:GLY:HA2	1:K:440:GLU:OE2	2.09	0.52
2:S:290:ASP:N	2:S:314:HIS:HE1	2.06	0.52
1:B:32:ILE:HD12	1:B:33:ASN:N	2.24	0.52
1:B:46:MET:CE	1:B:73:SER:HA	2.38	0.52
1:E:68:VAL:HG22	1:E:147:ARG:HB2	1.91	0.52
1:F:35:ASP:HB3	1:F:38:VAL:CG1	2.39	0.52
1:I:319:GLU:OE1	1:J:320:VAL:HG11	2.08	0.52
1:D:452:PHE:O	1:D:456:LEU:HD23	2.08	0.52
1:F:385:THR:HG22	1:F:388:MET:HE3	1.80	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:GLY:C	1:I:158:MET:HG2	2.33	0.52
1:A:35:ASP:HB3	1:A:38:VAL:CG1	2.40	0.52
1:A:113:ARG:HB2	1:A:181:VAL:CG1	2.31	0.52
1:B:219:MET:HE1	1:B:365:ARG:CB	2.33	0.52
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.91	0.52
1:H:338:ARG:NH1	1:H:340:HIS:HA	2.24	0.52
1:L:377:ARG:HD3	1:L:403:THR:OG1	2.10	0.52
2:M:359:ASN:OD1	2:M:359:ASN:O	2.28	0.52
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.45	0.52
1:E:249:THR:HG23	1:E:407:VAL:CG2	2.40	0.52
1:E:338:ARG:C	1:E:340:HIS:H	2.16	0.52
1:L:440:GLU:O	1:L:442:MET:N	2.43	0.52
2:Q:289:ILE:HG23	2:Q:314:HIS:CD2	2.45	0.52
2:X:354:THR:CG2	2:X:357:GLU:H	2.20	0.52
1:C:170:PRO:HD2	1:C:174:CYS:CB	2.39	0.52
1:F:282:SER:HB3	1:F:324:ILE:CD1	2.40	0.52
1:L:68:VAL:HG13	1:L:145:PRO:HB2	1.92	0.52
1:D:244:TYR:HE2	1:D:366:GLU:HB3	1.74	0.52
1:E:115:HIS:HB2	1:E:166:VAL:HG23	1.90	0.52
1:L:269:ILE:HD11	1:L:289:ALA:HB2	1.91	0.52
2:M:318:ILE:HG12	2:M:351:GLU:CA	2.39	0.52
2:T:354:THR:CG2	2:T:357:GLU:H	2.21	0.52
1:E:226:HIS:CD2	1:F:427:MET:HE2	2.45	0.52
1:G:150:ASP:O	1:G:165:VAL:HG12	2.10	0.52
1:G:421:GLN:O	1:G:422:ALA:C	2.51	0.52
1:J:322:ARG:NH1	1:K:321:GLU:OE2	2.43	0.52
1:K:282:SER:HB3	1:K:324:ILE:HD11	1.91	0.52
1:E:453:ARG:HH21	1:H:401:ASN:HB3	1.73	0.52
1:H:440:GLU:O	1:H:442:MET:N	2.43	0.52
1:L:169:ASP:HB3	1:L:170:PRO:CD	2.37	0.52
1:C:350:PRO:CA	1:C:358:ARG:HH21	2.24	0.51
1:E:377:ARG:CG	1:E:411:LEU:HD11	2.40	0.51
1:F:239:ARG:NH2	1:F:335:LEU:O	2.43	0.51
1:F:440:GLU:C	1:F:442:MET:N	2.68	0.51
1:G:440:GLU:O	1:G:442:MET:N	2.43	0.51
1:I:440:GLU:O	1:I:442:MET:N	2.43	0.51
2:R:354:THR:CG2	2:R:357:GLU:H	2.22	0.51
1:E:440:GLU:O	1:E:442:MET:N	2.43	0.51
1:H:239:ARG:NH2	1:H:336:LYS:HA	2.26	0.51
1:J:440:GLU:C	1:J:442:MET:N	2.68	0.51
1:L:244:TYR:HE2	1:L:366:GLU:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:303:ALA:O	2:T:305:GLY:N	2.40	0.51
2:V:300:ILE:HD13	2:V:365:ILE:HB	1.91	0.51
1:B:440:GLU:C	1:B:442:MET:N	2.68	0.51
1:F:283:GLU:OE1	1:F:324:ILE:HG12	2.09	0.51
1:H:322:ARG:HD2	1:I:321:GLU:OE2	2.11	0.51
1:K:113:ARG:NE	1:K:183:HIS:HE1	2.05	0.51
1:F:306:LEU:HD23	1:F:353:ILE:HD13	1.91	0.51
1:J:222:LEU:HD12	1:K:420:LEU:HD22	1.91	0.51
1:K:26:LEU:HD21	1:K:45:LYS:CE	2.41	0.51
1:L:117:LEU:HD21	1:L:185:GLU:O	2.10	0.51
2:N:290:ASP:H	2:N:314:HIS:CE1	2.28	0.51
1:B:169:ASP:HB3	1:B:170:PRO:CD	2.37	0.51
1:C:250:GLY:HA2	3:C:501:ADP:O2A	2.11	0.51
1:I:414:LEU:C	1:I:414:LEU:HD13	2.36	0.51
1:J:300:ILE:HD13	1:J:344:MET:HE1	1.92	0.51
1:J:377:ARG:CG	1:J:411:LEU:HD11	2.41	0.51
1:J:440:GLU:O	1:J:442:MET:N	2.43	0.51
1:L:22:ARG:HG3	1:L:23:PRO:CD	2.39	0.51
2:U:318:ILE:HG12	2:U:351:GLU:CA	2.39	0.51
1:D:440:GLU:O	1:D:442:MET:N	2.43	0.51
1:G:391:ALA:O	1:G:394:VAL:HG22	2.10	0.51
1:F:440:GLU:O	1:F:442:MET:N	2.43	0.51
1:I:336:LYS:HG3	1:I:337:GLN:H	1.75	0.51
2:P:354:THR:CG2	2:P:357:GLU:H	2.22	0.51
1:B:377:ARG:CG	1:B:411:LEU:HD11	2.41	0.51
1:C:350:PRO:HA	1:C:358:ARG:HH21	1.76	0.51
1:D:116:VAL:C	1:D:117:LEU:HD12	2.36	0.51
1:E:48:GLU:HG2	1:E:49:LEU:HD13	1.92	0.51
1:F:153:LEU:HD11	1:F:160:ALA:HB1	1.91	0.51
1:H:26:LEU:HD21	1:H:45:LYS:CE	2.41	0.51
1:H:440:GLU:C	1:H:442:MET:N	2.68	0.51
1:K:140:LEU:HG	1:K:141:GLU:CG	2.41	0.51
1:K:233:ILE:HG13	1:K:235:VAL:HG12	1.93	0.51
1:A:440:GLU:O	1:A:442:MET:N	2.44	0.51
1:E:329:LEU:N	1:E:329:LEU:HD12	2.26	0.51
2:T:321:ILE:HD11	2:T:355:LEU:HD11	1.93	0.51
1:D:29:ASP:OD1	1:D:30:GLU:N	2.40	0.51
1:E:62:LYS:HG3	1:E:94:VAL:HG23	1.92	0.51
2:P:290:ASP:H	2:P:314:HIS:CE1	2.29	0.51
1:C:339:ALA:O	1:C:340:HIS:HB2	2.09	0.50
1:C:440:GLU:O	1:C:442:MET:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:PRO:HB3	1:E:365:ARG:CZ	2.34	0.50
1:F:82:ILE:HG21	1:F:100:ILE:HD11	1.93	0.50
1:H:335:LEU:HD22	1:H:338:ARG:HB2	1.93	0.50
2:V:300:ILE:CD1	2:V:365:ILE:HB	2.41	0.50
1:D:26:LEU:HD12	1:D:26:LEU:N	2.25	0.50
1:E:269:ILE:HD11	1:E:289:ALA:HB2	1.93	0.50
1:F:377:ARG:CG	1:F:411:LEU:HD11	2.41	0.50
1:K:377:ARG:CG	1:K:411:LEU:HD11	2.41	0.50
1:L:22:ARG:HH21	1:L:24:ASN:HB2	1.76	0.50
1:B:300:ILE:HD13	1:B:344:MET:HE1	1.94	0.50
1:C:236:LYS:O	1:C:236:LYS:HG3	2.11	0.50
1:C:402:GLU:OE1	1:J:398:GLN:OE1	2.29	0.50
1:K:46:MET:CE	1:K:73:SER:CA	2.89	0.50
1:K:336:LYS:HB2	1:K:338:ARG:HH22	1.71	0.50
2:S:304:ASP:OD1	2:S:304:ASP:O	2.30	0.50
1:A:402:GLU:CD	1:L:398:GLN:NE2	2.70	0.50
2:T:322:ARG:NH1	2:T:351:GLU:OE2	2.44	0.50
1:B:239:ARG:NH2	1:B:341:VAL:O	2.44	0.50
1:C:377:ARG:CG	1:C:411:LEU:HD11	2.41	0.50
1:D:57:VAL:HG21	1:D:102:ILE:CD1	2.40	0.50
1:H:306:LEU:HD23	1:H:353:ILE:HD13	1.93	0.50
1:I:377:ARG:CG	1:I:411:LEU:HD11	2.41	0.50
1:J:306:LEU:HD23	1:J:353:ILE:HD13	1.94	0.50
1:J:336:LYS:HG3	1:J:338:ARG:H	1.76	0.50
2:R:302:LEU:HD12	2:R:307:ARG:CB	2.41	0.50
1:A:421:GLN:O	1:A:422:ALA:C	2.54	0.50
1:D:377:ARG:CG	1:D:411:LEU:HD11	2.41	0.50
1:G:222:LEU:CD1	1:H:424:ARG:HH11	2.24	0.50
1:K:216:ILE:CD1	1:K:254:ILE:HD11	2.33	0.50
1:D:384:HIS:HE1	3:D:501:ADP:N3	2.10	0.50
1:E:226:HIS:NE2	1:F:427:MET:HE2	2.27	0.50
1:E:287:ARG:HE	1:E:327:GLN:NE2	2.09	0.50
1:F:398:GLN:HE22	1:G:453:ARG:HE	1.60	0.50
1:G:26:LEU:HD11	1:G:45:LYS:HE3	1.93	0.50
1:I:68:VAL:HG13	1:I:145:PRO:HB2	1.93	0.50
1:I:438:ASP:O	1:I:442:MET:SD	2.70	0.50
1:J:381:LEU:HD11	1:J:399:VAL:HG22	1.93	0.50
1:L:310:ALA:HA	1:L:325:VAL:HG22	1.92	0.50
1:B:26:LEU:HD21	1:B:45:LYS:HE3	1.94	0.50
1:D:133:VAL:HG13	1:D:443:ASN:CG	2.36	0.50
1:G:126:ILE:HG13	1:G:159:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:249:THR:CG2	1:H:251:LYS:HZ2	2.24	0.50
1:I:129:ASN:O	1:I:131:PHE:N	2.45	0.50
1:L:26:LEU:HD21	1:L:45:LYS:CE	2.42	0.50
1:C:22:ARG:HG3	1:C:23:PRO:CD	2.39	0.50
1:E:118:PRO:HG3	1:E:130:LEU:CD2	2.42	0.50
1:G:440:GLU:C	1:G:442:MET:N	2.68	0.50
1:I:359:ARG:NH1	1:I:362:ARG:HD3	2.27	0.50
1:L:402:GLU:CD	1:L:453:ARG:HH22	2.19	0.50
1:H:26:LEU:HD21	1:H:45:LYS:HE3	1.92	0.49
1:I:214:ALA:O	1:I:217:LYS:HG2	2.12	0.49
1:K:131:PHE:HE1	1:K:182:ILE:CG2	2.25	0.49
1:H:377:ARG:CG	1:H:411:LEU:HD11	2.41	0.49
2:W:318:ILE:HG12	2:W:351:GLU:CA	2.32	0.49
1:E:238:PRO:CA	1:E:365:ARG:HH21	2.25	0.49
1:G:113:ARG:NH1	1:G:183:HIS:NE2	2.52	0.49
1:I:426:LYS:HD2	1:I:445:LEU:HD23	1.93	0.49
1:K:46:MET:HE2	1:K:73:SER:CA	2.43	0.49
1:B:26:LEU:HD21	1:B:45:LYS:CE	2.43	0.49
1:E:78:SER:CB	1:E:81:LYS:HE3	2.32	0.49
1:G:325:VAL:O	1:G:329:LEU:HD22	2.12	0.49
1:G:358:ARG:HD3	1:G:366:GLU:OE2	2.12	0.49
1:J:338:ARG:C	1:J:340:HIS:H	2.21	0.49
1:B:322:ARG:HD2	1:C:321:GLU:OE2	2.13	0.49
1:G:393:ASP:O	1:G:449:MET:HG2	2.12	0.49
1:K:453:ARG:HG3	1:K:453:ARG:HH11	1.78	0.49
1:L:310:ALA:HB1	1:L:357:LEU:HD11	1.93	0.49
2:O:300:ILE:CD1	2:O:365:ILE:HB	2.42	0.49
1:A:26:LEU:HD21	1:A:45:LYS:HE3	1.94	0.49
1:E:39:VAL:HG11	1:E:59:LEU:HD11	1.93	0.49
1:F:338:ARG:C	1:F:340:HIS:H	2.21	0.49
1:G:109:LYS:HE2	2:S:306:GLY:HA3	1.94	0.49
1:K:338:ARG:C	1:K:340:HIS:H	2.21	0.49
1:K:426:LYS:HD2	1:K:445:LEU:CD1	2.35	0.49
1:C:452:PHE:O	1:C:456:LEU:HD23	2.13	0.49
1:D:338:ARG:C	1:D:340:HIS:H	2.21	0.49
1:E:169:ASP:HB3	1:E:170:PRO:CD	2.42	0.49
1:G:25:ARG:C	1:G:26:LEU:HD22	2.37	0.49
1:I:306:LEU:HD23	1:I:353:ILE:HD13	1.95	0.49
1:K:131:PHE:CE1	1:K:182:ILE:HG23	2.48	0.49
1:L:430:ILE:CD1	1:L:441:VAL:HG11	2.42	0.49
2:S:290:ASP:H	2:S:314:HIS:HE1	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:287:ILE:HD12	2:V:287:ILE:N	2.26	0.49
1:B:440:GLU:O	1:B:442:MET:N	2.46	0.49
1:C:46:MET:CE	1:C:73:SER:HA	2.43	0.49
1:D:438:ASP:O	1:D:442:MET:SD	2.71	0.49
1:E:329:LEU:CD1	1:E:329:LEU:H	2.24	0.49
1:F:287:ARG:HE	1:F:327:GLN:NE2	2.10	0.49
1:H:313:ARG:NH1	1:H:354:ASP:OD2	2.46	0.49
2:S:290:ASP:H	2:S:314:HIS:CE1	2.30	0.49
1:F:312:LYS:HB3	1:F:315:LYS:HG2	1.95	0.49
1:F:437:ILE:HB	1:F:441:VAL:CG2	2.43	0.49
1:H:128:GLY:HA2	1:H:440:GLU:OE2	2.13	0.49
1:I:70:ILE:HG13	2:U:343:PHE:CE1	2.47	0.49
1:A:338:ARG:C	1:A:340:HIS:H	2.21	0.49
1:C:171:SER:HB3	1:C:172:PRO:CD	2.25	0.49
1:C:359:ARG:HG2	1:C:360:PHE:H	1.78	0.49
1:I:118:PRO:HG3	1:I:130:LEU:CD2	2.42	0.49
1:K:46:MET:HE2	1:K:73:SER:CB	2.39	0.49
2:P:290:ASP:H	2:P:314:HIS:HE1	1.60	0.49
1:A:27:ILE:HD13	1:A:99:VAL:HG23	1.89	0.48
1:B:29:ASP:OD1	1:B:30:GLU:N	2.40	0.48
1:I:358:ARG:HD3	1:I:366:GLU:OE2	2.12	0.48
1:J:26:LEU:HD21	1:J:45:LYS:HE3	1.94	0.48
2:P:354:THR:HG22	2:P:357:GLU:CG	2.43	0.48
2:Q:302:LEU:HD12	2:Q:307:ARG:CB	2.43	0.48
1:D:169:ASP:HB3	1:D:170:PRO:CD	2.39	0.48
1:G:169:ASP:HB3	1:G:170:PRO:CD	2.37	0.48
1:K:310:ALA:HA	1:K:325:VAL:HG22	1.95	0.48
2:W:290:ASP:H	2:W:314:HIS:CE1	2.30	0.48
2:X:354:THR:HG22	2:X:357:GLU:CG	2.44	0.48
1:B:249:THR:HG22	1:B:251:LYS:HZ2	1.78	0.48
1:F:306:LEU:HD21	1:F:357:LEU:HD13	1.95	0.48
1:G:150:ASP:HB2	1:G:165:VAL:HG11	1.94	0.48
1:G:393:ASP:O	1:G:449:MET:HG3	2.13	0.48
1:I:338:ARG:C	1:I:340:HIS:H	2.21	0.48
1:J:287:ARG:HG3	1:J:327:GLN:NE2	2.27	0.48
1:K:115:HIS:ND1	1:K:166:VAL:HG21	2.29	0.48
1:A:306:LEU:HD23	1:A:353:ILE:HD13	1.96	0.48
1:C:113:ARG:HD3	1:C:183:HIS:HE1	1.79	0.48
1:C:440:GLU:C	1:C:442:MET:N	2.67	0.48
1:I:381:LEU:HD11	1:I:399:VAL:HG22	1.95	0.48
1:A:349:ARG:HG3	1:A:350:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ILE:HD12	1:A:441:VAL:HG11	1.95	0.48
1:C:339:ALA:C	1:C:340:HIS:HD1	2.21	0.48
1:G:306:LEU:HD23	1:G:353:ILE:HD13	1.94	0.48
1:K:169:ASP:HB3	1:K:170:PRO:CD	2.38	0.48
1:F:417:GLU:CG	1:F:455:ALA:HB1	2.39	0.48
1:G:82:ILE:HG21	1:G:100:ILE:HD11	1.94	0.48
1:I:128:GLY:HA2	1:I:440:GLU:OE2	2.12	0.48
2:V:287:ILE:HD13	2:V:311:LYS:HE3	1.96	0.48
2:X:302:LEU:HD12	2:X:307:ARG:CB	2.44	0.48
1:A:26:LEU:HD21	1:A:45:LYS:CE	2.43	0.48
1:D:338:ARG:HA	1:D:338:ARG:NE	2.29	0.48
1:J:26:LEU:HD21	1:J:45:LYS:CE	2.43	0.48
1:J:313:ARG:HH12	1:J:325:VAL:CG1	2.22	0.48
2:M:321:ILE:HD11	2:M:355:LEU:HD11	1.94	0.48
1:H:96:LEU:O	1:H:225:ARG:NH1	2.46	0.48
1:H:338:ARG:HG2	1:H:341:VAL:H	1.79	0.48
1:L:219:MET:HE2	1:L:365:ARG:HE	1.79	0.48
1:L:337:GLN:O	1:L:338:ARG:C	2.56	0.48
2:N:347:GLU:OE2	2:N:368:ARG:NH2	2.46	0.48
2:W:302:LEU:HD12	2:W:307:ARG:CB	2.44	0.48
1:F:377:ARG:NE	1:F:403:THR:HG23	2.27	0.48
2:N:302:LEU:HD12	2:N:307:ARG:CB	2.43	0.48
2:W:290:ASP:H	2:W:314:HIS:HE1	1.61	0.48
1:D:300:ILE:HD13	1:D:344:MET:HE3	1.94	0.48
1:I:306:LEU:HD21	1:I:357:LEU:HD13	1.96	0.48
1:K:306:LEU:HD23	1:K:353:ILE:HD13	1.94	0.48
2:X:321:ILE:HD11	2:X:355:LEU:HD11	1.96	0.48
1:H:393:ASP:O	1:H:449:MET:HG3	2.14	0.47
1:K:249:THR:HG23	1:K:407:VAL:CG2	2.44	0.47
1:L:184:CYS:O	1:L:185:GLU:C	2.57	0.47
2:N:340:MET:HE1	2:N:368:ARG:NH1	2.29	0.47
2:T:311:LYS:NZ	2:T:312:PHE:H	2.12	0.47
1:B:219:MET:CE	1:B:365:ARG:CB	2.91	0.47
1:K:437:ILE:HB	1:K:441:VAL:CG2	2.44	0.47
2:X:304:ASP:OD1	2:X:332:MET:HE1	2.14	0.47
1:C:318:GLY:O	1:D:317:HIS:HE1	1.96	0.47
1:H:358:ARG:HD3	1:H:366:GLU:OE2	2.14	0.47
1:J:169:ASP:HB3	1:J:170:PRO:CD	2.38	0.47
2:R:287:ILE:N	2:R:287:ILE:HD12	2.29	0.47
1:A:286:LEU:HD11	1:A:309:ILE:HD11	1.96	0.47
1:E:357:LEU:C	1:E:359:ARG:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:LEU:HD21	1:F:45:LYS:CE	2.45	0.47
1:H:335:LEU:HD22	1:H:338:ARG:CB	2.44	0.47
1:B:381:LEU:HD11	1:B:399:VAL:HG22	1.96	0.47
1:D:57:VAL:CG2	1:D:102:ILE:HG12	2.41	0.47
1:D:336:LYS:CB	1:D:338:ARG:NH2	2.74	0.47
1:E:169:ASP:O	1:E:170:PRO:C	2.55	0.47
1:G:26:LEU:HD11	1:G:45:LYS:CE	2.45	0.47
1:L:243:LEU:HD12	1:L:243:LEU:N	2.30	0.47
2:T:295:THR:HA	2:T:314:HIS:HB3	1.97	0.47
1:A:92:LEU:O	1:A:94:VAL:HG13	2.15	0.47
1:B:249:THR:HG22	1:B:251:LYS:HZ3	1.79	0.47
1:B:306:LEU:HD21	1:B:357:LEU:HD13	1.96	0.47
1:D:92:LEU:O	1:D:94:VAL:HG13	2.15	0.47
1:F:219:MET:HE2	1:F:365:ARG:NH1	2.30	0.47
1:L:211:LYS:HD2	1:L:211:LYS:HA	1.52	0.47
2:O:318:ILE:HD13	2:O:318:ILE:HG21	1.73	0.47
2:S:307:ARG:HA	2:S:307:ARG:HD3	1.51	0.47
2:V:354:THR:HG22	2:V:357:GLU:CD	2.39	0.47
1:C:452:PHE:O	1:C:456:LEU:CD2	2.63	0.47
1:D:22:ARG:N	1:D:23:PRO:HD2	2.30	0.47
1:F:297:ALA:HA	1:F:298:PRO:C	2.40	0.47
1:K:249:THR:HG22	1:K:407:VAL:CG2	2.45	0.47
1:K:306:LEU:HD21	1:K:357:LEU:HD13	1.96	0.47
1:L:26:LEU:HD21	1:L:45:LYS:HE3	1.96	0.47
1:L:92:LEU:O	1:L:94:VAL:HG13	2.15	0.47
1:L:168:THR:HG23	1:L:171:SER:HA	1.96	0.47
2:O:300:ILE:HD11	2:O:321:ILE:CG2	2.44	0.47
2:P:340:MET:CE	2:P:368:ARG:HE	2.27	0.47
2:S:302:LEU:HD12	2:S:307:ARG:CB	2.32	0.47
1:D:360:PHE:O	1:D:362:ARG:N	2.44	0.47
1:E:426:LYS:CD	1:E:445:LEU:HD12	2.43	0.47
1:F:336:LYS:CB	1:F:338:ARG:NH2	2.78	0.47
1:F:337:GLN:O	1:F:340:HIS:N	2.48	0.47
1:F:403:THR:HG23	1:F:403:THR:O	2.14	0.47
1:G:150:ASP:HB2	1:G:165:VAL:CG1	2.45	0.47
1:G:313:ARG:HD2	1:G:313:ARG:O	2.14	0.47
1:G:338:ARG:C	1:G:340:HIS:H	2.23	0.47
1:G:388:MET:HE3	1:G:390:LEU:CD2	2.45	0.47
1:G:423:ILE:O	1:G:427:MET:HG2	2.15	0.47
1:K:203:TYR:CE2	1:K:217:LYS:HD3	2.49	0.47
1:L:256:ARG:HD2	1:L:256:ARG:HA	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:354:THR:HG22	2:T:357:GLU:CG	2.43	0.47
2:V:300:ILE:HD11	2:V:321:ILE:CG2	2.45	0.47
1:A:169:ASP:HB3	1:A:170:PRO:CD	2.37	0.47
1:B:306:LEU:HD23	1:B:353:ILE:HD13	1.97	0.47
1:E:287:ARG:NE	1:E:327:GLN:HE22	2.12	0.47
1:E:383:ILE:O	1:E:386:LYS:HG3	2.15	0.47
1:G:394:VAL:HG23	1:G:394:VAL:O	2.14	0.47
1:I:336:LYS:CB	1:I:338:ARG:NH2	2.77	0.47
1:J:126:ILE:HG13	1:J:159:ARG:NH1	2.30	0.47
1:L:360:PHE:C	1:L:362:ARG:H	2.23	0.47
2:T:289:ILE:HG23	2:T:314:HIS:CD2	2.50	0.47
1:C:338:ARG:C	1:C:340:HIS:N	2.71	0.47
1:E:153:LEU:HD11	1:E:160:ALA:HB1	1.97	0.47
1:H:297:ALA:HA	1:H:298:PRO:C	2.40	0.47
1:J:306:LEU:HD21	1:J:357:LEU:HD13	1.97	0.47
1:D:297:ALA:HA	1:D:298:PRO:C	2.40	0.46
1:D:350:PRO:HB3	1:D:358:ARG:NH1	2.30	0.46
1:F:437:ILE:HB	1:F:441:VAL:HG22	1.97	0.46
1:G:24:ASN:N	1:G:24:ASN:ND2	2.62	0.46
1:K:297:ALA:HA	1:K:298:PRO:C	2.40	0.46
1:A:43:GLN:HB2	1:A:44:PRO:HD3	1.96	0.46
1:F:158:MET:SD	1:F:442:MET:HE1	2.55	0.46
1:G:133:VAL:HG13	1:G:443:ASN:CG	2.40	0.46
1:H:306:LEU:HD21	1:H:357:LEU:HD13	1.96	0.46
1:H:393:ASP:O	1:H:449:MET:HG2	2.15	0.46
1:I:402:GLU:OE1	1:I:453:ARG:NH2	2.48	0.46
1:J:27:ILE:CG2	1:J:81:LYS:HG2	2.41	0.46
1:J:256:ARG:HD2	1:J:256:ARG:HA	1.61	0.46
2:O:302:LEU:HD12	2:O:307:ARG:CB	2.46	0.46
2:T:294:PRO:O	2:T:314:HIS:HB3	2.15	0.46
2:V:302:LEU:HD12	2:V:307:ARG:CB	2.44	0.46
1:A:337:GLN:O	1:A:340:HIS:N	2.48	0.46
1:C:306:LEU:HD23	1:C:353:ILE:HD13	1.97	0.46
1:F:26:LEU:HD21	1:F:45:LYS:HE3	1.96	0.46
1:G:427:MET:CE	1:L:226:HIS:CE1	2.97	0.46
1:I:126:ILE:HG13	1:I:159:ARG:NH1	2.30	0.46
1:A:113:ARG:HH21	1:A:183:HIS:HE1	1.62	0.46
1:B:297:ALA:HA	1:B:298:PRO:C	2.41	0.46
1:E:46:MET:HG2	1:E:51:LEU:HB2	1.97	0.46
2:P:321:ILE:HD11	2:P:355:LEU:CD2	2.45	0.46
1:C:297:ALA:HA	1:C:298:PRO:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:VAL:HG13	1:I:416:SER:OG	2.15	0.46
1:J:350:PRO:HB3	1:J:358:ARG:HH22	1.73	0.46
2:S:318:ILE:HG12	2:S:351:GLU:CA	2.39	0.46
1:H:22:ARG:CG	1:H:23:PRO:HD2	2.44	0.46
1:I:169:ASP:HB3	1:I:170:PRO:CD	2.38	0.46
1:J:437:ILE:HG22	1:J:440:GLU:HB3	1.97	0.46
1:K:140:LEU:C	1:K:141:GLU:HG3	2.41	0.46
2:N:318:ILE:HG12	2:N:351:GLU:CA	2.40	0.46
1:B:140:LEU:C	1:B:141:GLU:HG2	2.41	0.46
1:D:239:ARG:HH21	1:D:337:GLN:HA	1.81	0.46
1:E:243:LEU:HD22	1:E:367:VAL:HG13	1.96	0.46
1:F:287:ARG:NE	1:F:327:GLN:HE22	2.11	0.46
1:G:22:ARG:HD3	1:G:25:ARG:HG3	1.98	0.46
1:G:432:LEU:HD13	1:L:27:ILE:HG13	1.98	0.46
1:I:300:ILE:HD13	1:I:344:MET:HE1	1.98	0.46
2:N:321:ILE:HD11	2:N:355:LEU:CD2	2.45	0.46
2:T:347:GLU:OE2	2:T:368:ARG:NH2	2.48	0.46
2:X:294:PRO:O	2:X:314:HIS:CB	2.63	0.46
1:B:92:LEU:O	1:B:94:VAL:HG13	2.15	0.46
1:C:133:VAL:HG13	1:C:443:ASN:CG	2.40	0.46
1:D:440:GLU:C	1:D:442:MET:N	2.67	0.46
1:E:233:ILE:HG22	1:F:442:MET:HE2	1.96	0.46
1:E:297:ALA:HA	1:E:298:PRO:C	2.41	0.46
1:E:377:ARG:CZ	1:E:404:HIS:HA	2.46	0.46
1:G:92:LEU:O	1:G:94:VAL:HG13	2.15	0.46
1:G:388:MET:CE	1:G:390:LEU:HD21	2.44	0.46
2:W:354:THR:HG22	2:W:357:GLU:CD	2.40	0.46
1:D:249:THR:CG2	1:D:251:LYS:HE2	2.46	0.46
1:E:300:ILE:CG2	1:E:344:MET:HE3	2.45	0.46
1:F:92:LEU:O	1:F:94:VAL:HG13	2.16	0.46
1:F:133:VAL:HG13	1:F:443:ASN:CG	2.40	0.46
1:J:300:ILE:CG2	1:J:344:MET:HE3	2.46	0.46
1:K:153:LEU:HD11	1:K:160:ALA:HB1	1.97	0.46
1:L:287:ARG:HE	1:L:327:GLN:NE2	2.13	0.46
1:A:297:ALA:HA	1:A:298:PRO:C	2.40	0.46
1:F:141:GLU:O	2:R:345:ASN:ND2	2.39	0.46
1:G:153:LEU:HD11	1:G:160:ALA:HB1	1.98	0.46
1:H:92:LEU:O	1:H:94:VAL:HG13	2.16	0.46
1:H:336:LYS:HG3	1:H:337:GLN:H	1.81	0.46
1:K:337:GLN:O	1:K:340:HIS:N	2.49	0.46
2:R:354:THR:HG22	2:R:357:GLU:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:GLN:O	1:D:340:HIS:N	2.48	0.45
1:E:86:ARG:O	1:E:87:VAL:C	2.58	0.45
1:I:25:ARG:C	1:I:26:LEU:HD22	2.41	0.45
1:I:92:LEU:O	1:I:94:VAL:HG13	2.16	0.45
1:I:297:ALA:HA	1:I:298:PRO:C	2.40	0.45
1:I:322:ARG:HH22	1:J:317:HIS:HB2	1.80	0.45
1:J:297:ALA:HA	1:J:298:PRO:C	2.41	0.45
1:J:337:GLN:O	1:J:340:HIS:N	2.48	0.45
2:O:289:ILE:HG23	2:O:314:HIS:HD2	1.80	0.45
2:R:287:ILE:HD12	2:R:287:ILE:H	1.80	0.45
1:J:386:LYS:HB2	1:J:386:LYS:HE2	1.68	0.45
2:T:302:LEU:HD12	2:T:367:GLN:OE1	2.17	0.45
1:B:320:VAL:HG22	1:B:323:ARG:HH12	1.80	0.45
1:C:239:ARG:HH12	1:C:336:LYS:HA	1.80	0.45
1:E:350:PRO:CB	1:E:358:ARG:HH21	2.29	0.45
1:G:222:LEU:HD22	1:H:420:LEU:HD22	1.98	0.45
1:I:26:LEU:HD11	1:I:45:LYS:CE	2.45	0.45
1:J:92:LEU:O	1:J:94:VAL:HG13	2.16	0.45
1:J:225:ARG:HG2	1:J:262:THR:HG23	1.98	0.45
1:I:287:ARG:HE	1:I:327:GLN:NE2	2.13	0.45
1:I:322:ARG:NH2	1:J:317:HIS:HB2	2.31	0.45
1:L:126:ILE:HG13	1:L:159:ARG:NH1	2.31	0.45
1:L:297:ALA:HA	1:L:298:PRO:C	2.41	0.45
2:O:321:ILE:HD11	2:O:355:LEU:CD2	2.47	0.45
1:A:287:ARG:HD3	1:A:327:GLN:HE22	1.81	0.45
1:B:153:LEU:HD11	1:B:160:ALA:HB1	1.98	0.45
1:C:63:LYS:NZ	1:C:194:GLU:OE2	2.49	0.45
1:E:238:PRO:N	1:E:365:ARG:HH21	2.14	0.45
1:F:383:ILE:O	1:F:386:LYS:HG3	2.16	0.45
1:G:129:ASN:O	1:G:131:PHE:N	2.48	0.45
1:H:422:ALA:HB1	1:H:445:LEU:HD11	1.97	0.45
2:V:318:ILE:HA	2:V:321:ILE:HD12	1.99	0.45
1:C:118:PRO:HG3	1:C:130:LEU:CD2	2.47	0.45
1:D:452:PHE:O	1:D:456:LEU:CD2	2.64	0.45
1:F:441:VAL:HG12	1:F:444:SER:OG	2.17	0.45
2:Q:289:ILE:HG23	2:Q:314:HIS:HD2	1.81	0.45
1:A:133:VAL:HG13	1:A:443:ASN:CG	2.41	0.45
1:B:126:ILE:HG13	1:B:159:ARG:NH1	2.32	0.45
1:C:126:ILE:HG13	1:C:159:ARG:NH1	2.31	0.45
1:F:158:MET:HE2	1:F:388:MET:HA	1.98	0.45
1:H:169:ASP:HB3	1:H:170:PRO:CD	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:337:GLN:O	1:I:340:HIS:N	2.49	0.45
1:J:118:PRO:HG3	1:J:130:LEU:CD2	2.47	0.45
1:A:440:GLU:C	1:A:442:MET:N	2.68	0.45
1:E:256:ARG:HD2	1:E:256:ARG:HA	1.63	0.45
1:G:222:LEU:HD11	1:H:424:ARG:HH11	1.82	0.45
1:I:287:ARG:NE	1:I:327:GLN:HE22	2.14	0.45
1:J:322:ARG:HH22	1:K:317:HIS:HB3	1.82	0.45
1:K:441:VAL:HG12	1:K:444:SER:OG	2.17	0.45
2:V:321:ILE:HD13	2:V:365:ILE:HD12	1.99	0.45
1:A:232:ALA:HB2	1:B:439:ALA:HB1	1.98	0.45
1:B:133:VAL:HG13	1:B:443:ASN:CG	2.42	0.45
1:C:92:LEU:O	1:C:94:VAL:HG13	2.16	0.45
1:E:42:SER:O	1:E:43:GLN:C	2.60	0.45
1:G:155:ARG:NH1	1:G:386:LYS:HE3	2.31	0.45
1:I:249:THR:CG2	1:I:251:LYS:HZ2	2.29	0.45
1:J:153:LEU:HD11	1:J:160:ALA:HB1	1.98	0.45
1:K:92:LEU:O	1:K:94:VAL:HG13	2.16	0.45
1:L:287:ARG:NE	1:L:327:GLN:HE22	2.15	0.45
1:L:383:ILE:O	1:L:386:LYS:HG3	2.17	0.45
2:P:320:ASP:HA	2:P:323:LEU:CG	2.46	0.45
2:P:332:MET:HA	2:P:335:THR:OG1	2.17	0.45
1:A:27:ILE:HD11	1:A:99:VAL:CG2	2.47	0.45
1:A:153:LEU:HD11	1:A:160:ALA:HB1	1.99	0.45
1:D:57:VAL:HG23	1:D:103:GLN:O	2.17	0.45
1:D:127:THR:O	1:D:440:GLU:HG3	2.17	0.45
1:G:297:ALA:HA	1:G:298:PRO:C	2.41	0.45
1:I:153:LEU:HD11	1:I:160:ALA:HB1	1.99	0.45
1:I:201:VAL:HG12	1:I:257:ALA:HB2	1.99	0.45
1:I:437:ILE:HD12	1:I:441:VAL:HG11	1.99	0.45
1:K:244:TYR:HE2	1:K:366:GLU:HB3	1.82	0.45
2:X:308:LEU:HD21	2:X:310:GLN:HE22	1.78	0.45
1:A:386:LYS:HE2	1:A:386:LYS:HB2	1.77	0.44
1:D:300:ILE:CG2	1:D:344:MET:HE3	2.46	0.44
1:D:377:ARG:O	1:D:381:LEU:HD22	2.16	0.44
1:G:27:ILE:HG12	1:H:432:LEU:HD13	2.00	0.44
1:J:396:LEU:O	1:J:399:VAL:HG13	2.17	0.44
1:K:126:ILE:HG13	1:K:159:ARG:NH1	2.31	0.44
1:L:153:LEU:HD11	1:L:160:ALA:HB1	1.99	0.44
1:C:440:GLU:OE1	1:C:440:GLU:HA	2.17	0.44
1:G:22:ARG:HG2	1:G:25:ARG:HG3	1.99	0.44
1:H:126:ILE:HG13	1:H:159:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:LEU:HD11	1:J:309:ILE:HD11	2.00	0.44
1:J:322:ARG:HD2	1:K:321:GLU:OE2	2.16	0.44
1:L:306:LEU:HD23	1:L:353:ILE:HD13	1.99	0.44
1:A:57:VAL:HG21	1:A:102:ILE:HD11	1.99	0.44
1:C:171:SER:CB	1:C:172:PRO:CD	2.93	0.44
1:E:46:MET:HE1	1:E:73:SER:CB	2.47	0.44
1:E:235:VAL:HG23	1:F:158:MET:HG2	1.99	0.44
1:E:438:ASP:O	1:E:442:MET:SD	2.76	0.44
1:G:359:ARG:HD3	1:H:247:PRO:HB3	1.99	0.44
1:G:416:SER:OG	1:L:235:VAL:HG13	2.18	0.44
1:J:201:VAL:HG12	1:J:257:ALA:HB2	1.99	0.44
2:R:321:ILE:HD11	2:R:355:LEU:CD2	2.45	0.44
1:A:203:TYR:CE2	1:A:217:LYS:HD3	2.52	0.44
1:B:201:VAL:HG12	1:B:257:ALA:HB2	1.99	0.44
1:E:249:THR:HG22	1:E:407:VAL:CG2	2.47	0.44
1:E:350:PRO:O	1:E:353:ILE:HD12	2.17	0.44
2:Q:289:ILE:HD13	2:Q:312:PHE:HB3	2.00	0.44
2:U:321:ILE:HD11	2:U:355:LEU:CD2	2.46	0.44
1:A:126:ILE:HG13	1:A:159:ARG:NH1	2.32	0.44
1:C:249:THR:CG2	1:C:251:LYS:HZ2	2.30	0.44
1:C:320:VAL:HG23	1:C:323:ARG:NH1	2.32	0.44
1:D:430:ILE:HD11	1:D:441:VAL:HG11	1.98	0.44
1:E:52:PHE:O	1:E:55:ASP:HB2	2.17	0.44
1:E:126:ILE:HG13	1:E:159:ARG:NH1	2.32	0.44
1:E:329:LEU:HD13	1:E:329:LEU:H	1.82	0.44
1:I:27:ILE:CD1	1:J:428:ASP:HB3	2.48	0.44
1:K:39:VAL:HG12	1:K:84:MET:HB3	1.99	0.44
1:D:186:GLY:O	1:D:187:GLU:HB2	2.18	0.44
1:D:389:LYS:HD3	1:D:443:ASN:O	2.18	0.44
1:G:147:ARG:O	1:G:165:VAL:CG1	2.64	0.44
2:O:354:THR:HG22	2:O:357:GLU:CD	2.42	0.44
1:D:244:TYR:CE2	1:D:366:GLU:HB3	2.52	0.44
1:E:24:ASN:O	1:E:101:SER:HA	2.18	0.44
1:E:46:MET:HE3	1:E:46:MET:HB2	1.72	0.44
1:E:105:CYS:SG	1:E:108:VAL:CG1	3.06	0.44
1:G:256:ARG:HD2	1:G:256:ARG:HA	1.62	0.44
1:H:438:ASP:O	1:H:442:MET:SD	2.76	0.44
1:I:440:GLU:C	1:I:442:MET:N	2.68	0.44
1:F:336:LYS:HB2	1:F:338:ARG:NH2	2.33	0.44
1:J:209:CYS:O	1:J:210:ARG:C	2.61	0.44
1:L:338:ARG:O	1:L:340:HIS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ILE:C	1:D:103:GLN:HG3	2.43	0.44
1:H:201:VAL:HG12	1:H:257:ALA:HB2	1.99	0.44
1:I:226:HIS:CE1	1:J:427:MET:HE2	2.53	0.44
1:J:105:CYS:SG	1:J:108:VAL:CG2	3.05	0.44
1:K:239:ARG:HH21	1:K:336:LYS:HA	1.82	0.44
1:L:357:LEU:C	1:L:359:ARG:N	2.76	0.44
2:T:305:GLY:O	2:T:307:ARG:N	2.46	0.44
2:V:321:ILE:HD11	2:V:355:LEU:CD2	2.48	0.44
1:K:53:ARG:HH22	1:K:73:SER:CB	2.31	0.43
1:L:440:GLU:C	1:L:442:MET:N	2.67	0.43
2:R:289:ILE:HD13	2:R:312:PHE:HB3	2.00	0.43
1:B:158:MET:HE2	1:B:419:ALA:HB1	2.00	0.43
1:B:396:LEU:O	1:B:399:VAL:HG13	2.18	0.43
1:C:89:ARG:HD3	1:C:96:LEU:HD13	2.00	0.43
1:C:209:CYS:O	1:C:210:ARG:C	2.61	0.43
1:D:57:VAL:HG21	1:D:102:ILE:HD11	1.99	0.43
1:K:270:ASN:HB3	1:K:273:GLU:HB3	2.00	0.43
1:K:322:ARG:NH2	1:L:317:HIS:HB2	2.32	0.43
1:L:118:PRO:HG3	1:L:130:LEU:CD1	2.48	0.43
2:V:318:ILE:HD13	2:V:318:ILE:HG21	1.73	0.43
1:B:220:VAL:HG13	1:B:224:LEU:CD1	2.42	0.43
1:C:26:LEU:HD21	1:C:45:LYS:HE3	2.00	0.43
1:C:201:VAL:HG12	1:C:257:ALA:HB2	1.99	0.43
1:D:201:VAL:HG12	1:D:257:ALA:HB2	2.00	0.43
1:D:336:LYS:CB	1:D:338:ARG:HH22	2.31	0.43
1:E:64:ARG:HA	1:E:64:ARG:HD3	1.63	0.43
1:I:243:LEU:HD13	1:I:369:ILE:HD11	2.00	0.43
1:K:235:VAL:CG2	1:L:416:SER:OG	2.64	0.43
1:A:209:CYS:O	1:A:210:ARG:C	2.61	0.43
1:E:335:LEU:HD12	1:E:335:LEU:HA	1.77	0.43
1:G:336:LYS:H	1:G:338:ARG:CB	2.31	0.43
1:H:209:CYS:O	1:H:210:ARG:C	2.61	0.43
1:I:396:LEU:O	1:I:399:VAL:HG13	2.18	0.43
1:K:22:ARG:CG	1:K:23:PRO:HD2	2.49	0.43
2:P:338:ILE:HD13	2:P:347:GLU:HG3	1.99	0.43
1:F:40:SER:HB2	1:F:83:ARG:HB2	2.00	0.43
1:H:153:LEU:HD11	1:H:160:ALA:HB1	2.00	0.43
1:H:402:GLU:CD	1:H:453:ARG:HH12	2.27	0.43
1:K:46:MET:HE1	1:K:73:SER:CA	2.49	0.43
2:P:332:MET:HE3	2:P:367:GLN:HE22	1.83	0.43
2:R:318:ILE:HD12	2:R:348:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HG12	1:A:257:ALA:HB2	2.01	0.43
1:D:153:LEU:HD11	1:D:160:ALA:HB1	2.00	0.43
1:D:310:ALA:HA	1:D:325:VAL:HG22	2.00	0.43
1:D:336:LYS:HE2	1:D:336:LYS:CA	2.43	0.43
1:I:359:ARG:CZ	1:I:362:ARG:HD3	2.48	0.43
1:I:442:MET:N	1:I:442:MET:SD	2.91	0.43
1:J:315:LYS:HB3	1:J:315:LYS:HE2	1.83	0.43
1:L:201:VAL:HG12	1:L:257:ALA:HB2	2.00	0.43
1:L:269:ILE:HD13	1:L:269:ILE:HA	1.78	0.43
1:A:113:ARG:NE	1:A:183:HIS:CE1	2.75	0.43
1:F:209:CYS:O	1:F:210:ARG:C	2.61	0.43
1:F:442:MET:HE3	1:F:442:MET:HB3	1.48	0.43
1:G:350:PRO:O	1:G:358:ARG:NH2	2.52	0.43
1:H:226:HIS:CG	1:I:427:MET:HE2	2.53	0.43
1:I:113:ARG:HB2	1:I:181:VAL:HG23	1.93	0.43
1:K:118:PRO:HG3	1:K:130:LEU:CD1	2.49	0.43
1:L:438:ASP:O	1:L:442:MET:SD	2.77	0.43
2:S:304:ASP:O	2:S:307:ARG:HG2	2.18	0.43
1:A:40:SER:HB2	1:A:83:ARG:HB2	2.00	0.43
1:B:39:VAL:HG12	1:B:84:MET:HB3	2.01	0.43
1:E:235:VAL:HG13	1:F:416:SER:OG	2.18	0.43
1:I:209:CYS:O	1:I:210:ARG:C	2.61	0.43
2:O:318:ILE:HA	2:O:321:ILE:HD12	2.01	0.43
1:B:209:CYS:O	1:B:210:ARG:C	2.62	0.43
1:G:232:ALA:HB2	1:H:439:ALA:HB1	1.99	0.43
1:H:39:VAL:HG12	1:H:84:MET:HB3	2.00	0.43
1:H:40:SER:HB2	1:H:83:ARG:HB2	2.01	0.43
1:I:63:LYS:HE2	1:I:63:LYS:N	2.33	0.43
1:J:220:VAL:HG13	1:J:224:LEU:CD1	2.39	0.43
1:D:442:MET:N	1:D:442:MET:SD	2.91	0.43
1:E:201:VAL:HG12	1:E:257:ALA:HB2	2.01	0.43
1:F:423:ILE:O	1:F:427:MET:HG2	2.19	0.43
1:I:279:ALA:CB	1:I:320:VAL:HG11	2.49	0.43
1:J:232:ALA:HB2	1:K:439:ALA:HB1	2.01	0.43
1:K:89:ARG:HD3	1:K:96:LEU:HD13	2.01	0.43
1:A:287:ARG:HG3	1:A:327:GLN:NE2	2.34	0.42
1:A:402:GLU:OE2	1:L:398:GLN:NE2	2.52	0.42
1:C:29:ASP:OD1	1:C:30:GLU:N	2.50	0.42
1:D:209:CYS:O	1:D:210:ARG:C	2.61	0.42
1:D:220:VAL:HG13	1:D:224:LEU:CD1	2.42	0.42
1:F:377:ARG:HH11	1:F:377:ARG:HD3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:CYS:SG	1:K:108:VAL:CG1	3.07	0.42
1:K:209:CYS:O	1:K:210:ARG:C	2.61	0.42
1:L:209:CYS:O	1:L:210:ARG:C	2.61	0.42
2:W:354:THR:CG2	2:W:357:GLU:HG3	2.49	0.42
1:A:441:VAL:HG23	1:A:442:MET:HE2	2.01	0.42
1:C:39:VAL:HG12	1:C:84:MET:HB3	2.01	0.42
1:F:169:ASP:HB3	1:F:170:PRO:CD	2.39	0.42
1:G:26:LEU:HD22	1:G:26:LEU:N	2.34	0.42
1:G:150:ASP:H	1:G:165:VAL:CG1	2.32	0.42
1:G:286:LEU:HD11	1:G:309:ILE:HD11	2.01	0.42
1:H:423:ILE:O	1:H:427:MET:HG2	2.18	0.42
1:J:420:LEU:HD23	1:J:420:LEU:HA	1.89	0.42
1:K:192:GLU:HB3	1:K:194:GLU:OE2	2.19	0.42
1:L:442:MET:N	1:L:442:MET:SD	2.91	0.42
2:Q:321:ILE:HD11	2:Q:355:LEU:CD2	2.47	0.42
1:A:256:ARG:HD2	1:A:256:ARG:HA	1.61	0.42
1:B:421:GLN:O	1:B:422:ALA:C	2.62	0.42
1:C:129:ASN:ND2	1:C:132:GLU:H	2.11	0.42
1:D:336:LYS:HG2	1:D:338:ARG:HH22	1.81	0.42
1:F:377:ARG:HE	1:F:403:THR:CG2	2.32	0.42
1:I:40:SER:HB2	1:I:83:ARG:HB2	2.01	0.42
1:I:426:LYS:NZ	1:I:430:ILE:HD11	2.34	0.42
1:J:402:GLU:OE1	1:J:453:ARG:NH2	2.50	0.42
1:K:162:GLU:OE1	1:K:191:ARG:NH2	2.53	0.42
1:K:201:VAL:HG12	1:K:257:ALA:HB2	2.00	0.42
2:T:294:PRO:O	2:T:314:HIS:CB	2.67	0.42
1:A:39:VAL:HG12	1:A:84:MET:HB3	2.02	0.42
1:A:252:THR:CG2	3:A:501:ADP:O1A	2.66	0.42
1:C:26:LEU:HD21	1:C:45:LYS:CE	2.49	0.42
1:C:153:LEU:HD11	1:C:160:ALA:HB1	2.01	0.42
1:E:440:GLU:C	1:E:442:MET:N	2.68	0.42
1:F:29:ASP:OD1	1:F:30:GLU:N	2.49	0.42
1:F:201:VAL:HG12	1:F:257:ALA:HB2	1.99	0.42
1:F:377:ARG:CZ	1:F:404:HIS:HA	2.50	0.42
1:G:286:LEU:HD23	1:G:286:LEU:HA	1.88	0.42
1:H:105:CYS:SG	1:H:108:VAL:CG2	3.08	0.42
1:I:251:LYS:HG2	1:I:369:ILE:HD13	1.89	0.42
2:N:304:ASP:O	2:N:304:ASP:CG	2.63	0.42
2:X:318:ILE:HD12	2:X:348:LEU:HB3	2.01	0.42
1:D:39:VAL:HG12	1:D:84:MET:HB3	2.00	0.42
1:E:209:CYS:O	1:E:210:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:LYS:H	1:F:338:ARG:NH2	2.17	0.42
1:H:46:MET:CE	1:H:73:SER:HA	2.47	0.42
1:K:80:GLU:CG	1:L:432:LEU:HD11	2.49	0.42
1:L:310:ALA:CB	1:L:357:LEU:HD11	2.50	0.42
2:T:318:ILE:HA	2:T:321:ILE:HD12	2.01	0.42
2:V:308:LEU:HD21	2:V:310:GLN:HE22	1.82	0.42
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.89	0.42
1:C:426:LYS:CD	1:C:445:LEU:HD12	2.45	0.42
1:E:336:LYS:O	1:E:337:GLN:C	2.63	0.42
1:K:336:LYS:H	1:K:338:ARG:NH2	2.18	0.42
2:P:320:ASP:OD1	2:P:323:LEU:HD21	2.19	0.42
1:C:49:LEU:HD13	1:C:49:LEU:HA	1.94	0.42
1:D:322:ARG:HH22	1:E:317:HIS:HB2	1.84	0.42
1:D:377:ARG:CZ	1:D:404:HIS:HA	2.50	0.42
1:E:269:ILE:HD13	1:E:269:ILE:HA	1.77	0.42
1:E:442:MET:SD	1:E:442:MET:N	2.92	0.42
1:F:385:THR:CG2	1:F:388:MET:HE2	2.39	0.42
1:G:60:LYS:HD2	1:G:66:GLU:CG	2.40	0.42
1:H:61:GLY:HA2	1:H:100:ILE:HD12	2.02	0.42
1:I:39:VAL:HG12	1:I:84:MET:HB3	2.02	0.42
1:J:362:ARG:HB2	1:J:363:PHE:H	1.47	0.42
2:T:322:ARG:NH1	2:T:351:GLU:CD	2.78	0.42
2:V:300:ILE:HD11	2:V:321:ILE:HG21	2.01	0.42
1:A:29:ASP:OD1	1:A:30:GLU:N	2.50	0.42
1:C:244:TYR:HE2	1:C:366:GLU:HB3	1.84	0.42
1:E:338:ARG:C	1:E:340:HIS:N	2.78	0.42
1:G:201:VAL:HG12	1:G:257:ALA:HB2	2.01	0.42
1:G:209:CYS:O	1:G:210:ARG:C	2.62	0.42
1:K:377:ARG:CZ	1:K:404:HIS:HA	2.50	0.42
1:K:396:LEU:HD12	1:K:396:LEU:HA	1.91	0.42
1:L:437:ILE:HG22	1:L:440:GLU:HB3	2.01	0.42
2:M:289:ILE:HD13	2:M:312:PHE:HB3	2.01	0.42
1:D:270:ASN:HB3	1:D:273:GLU:HB3	2.00	0.42
1:D:386:LYS:HB2	1:D:386:LYS:HE2	1.80	0.42
1:E:28:VAL:HG21	1:E:94:VAL:CG1	2.48	0.42
1:G:377:ARG:CZ	1:G:404:HIS:HA	2.50	0.42
2:P:304:ASP:O	2:P:304:ASP:CG	2.63	0.42
1:B:22:ARG:HB2	1:B:25:ARG:HD3	2.02	0.42
1:D:51:LEU:HD23	1:D:104:PRO:HG3	2.02	0.42
1:D:164:LYS:HD3	1:D:189:ILE:HD11	2.02	0.42
1:D:203:TYR:CE2	1:D:217:LYS:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:TYR:CE1	1:E:350:PRO:HA	2.55	0.42
1:I:312:LYS:HB3	1:I:315:LYS:HG2	2.02	0.42
1:J:113:ARG:CZ	1:J:115:HIS:HB2	2.50	0.42
2:M:307:ARG:HD3	2:M:307:ARG:HA	1.79	0.42
1:A:118:PRO:HG3	1:A:130:LEU:CD1	2.49	0.41
1:C:256:ARG:HA	1:C:256:ARG:HD2	1.60	0.41
1:E:300:ILE:HD13	1:E:344:MET:HE3	1.98	0.41
1:H:120:ASP:OD1	1:H:121:ASP:N	2.53	0.41
2:N:286:MET:HE3	2:N:286:MET:HB3	1.90	0.41
1:B:120:ASP:OD1	1:B:121:ASP:N	2.53	0.41
1:E:287:ARG:HG3	1:E:327:GLN:NE2	2.34	0.41
1:E:353:ILE:HD12	1:E:353:ILE:O	2.19	0.41
1:F:287:ARG:HG3	1:F:327:GLN:NE2	2.35	0.41
1:G:118:PRO:HG3	1:G:130:LEU:CD1	2.50	0.41
1:H:97:GLY:HA3	1:H:225:ARG:HH12	1.84	0.41
1:I:229:LEU:HD21	1:J:423:ILE:HD13	2.02	0.41
2:T:302:LEU:HD23	2:T:307:ARG:HB3	2.01	0.41
1:A:377:ARG:CZ	1:A:404:HIS:HA	2.50	0.41
1:C:40:SER:HB2	1:C:83:ARG:HB2	2.01	0.41
1:D:312:LYS:HB3	1:D:315:LYS:HG2	2.03	0.41
1:E:45:LYS:HD3	1:E:45:LYS:HA	1.82	0.41
1:E:357:LEU:HD23	1:E:357:LEU:HA	1.78	0.41
1:G:124:GLU:O	1:G:159:ARG:NH2	2.50	0.41
1:H:86:ARG:HG3	1:H:89:ARG:NH2	2.36	0.41
1:I:120:ASP:OD1	1:I:121:ASP:N	2.53	0.41
1:I:287:ARG:HG3	1:I:327:GLN:NE2	2.35	0.41
1:K:115:HIS:ND1	1:K:166:VAL:CG2	2.83	0.41
1:K:279:ALA:CB	1:K:320:VAL:HG11	2.50	0.41
1:L:339:ALA:O	1:L:340:HIS:CD2	2.73	0.41
2:O:300:ILE:HD11	2:O:321:ILE:HG21	2.01	0.41
2:V:297:ASN:OD1	2:V:312:PHE:HD1	2.04	0.41
1:F:256:ARG:HD2	1:F:256:ARG:HA	1.63	0.41
1:G:274:ILE:CG2	1:G:275:MET:CE	2.85	0.41
1:G:385:THR:HB	1:G:388:MET:HE2	2.02	0.41
1:J:40:SER:HB2	1:J:83:ARG:HB2	2.01	0.41
2:Q:295:THR:HG22	2:Q:314:HIS:HD2	1.86	0.41
1:A:329:LEU:HD23	1:A:357:LEU:HD13	2.03	0.41
1:B:93:ARG:HE	1:B:194:GLU:HG3	1.85	0.41
1:C:329:LEU:HD23	1:C:357:LEU:HD13	2.03	0.41
1:D:118:PRO:HG3	1:D:130:LEU:CD1	2.51	0.41
1:E:357:LEU:C	1:E:359:ARG:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:ALA:CB	1:F:320:VAL:HG11	2.50	0.41
1:G:29:ASP:OD1	1:G:30:GLU:N	2.50	0.41
1:H:312:LYS:HB3	1:H:315:LYS:HG2	2.03	0.41
1:H:339:ALA:O	1:H:340:HIS:HD2	1.88	0.41
1:H:442:MET:SD	1:H:442:MET:N	2.93	0.41
1:I:336:LYS:HB2	1:I:338:ARG:NH2	2.34	0.41
1:K:49:LEU:HD13	1:K:49:LEU:HA	1.93	0.41
2:V:304:ASP:O	2:V:304:ASP:CG	2.64	0.41
2:X:304:ASP:O	2:X:304:ASP:CG	2.64	0.41
1:B:336:LYS:H	1:B:338:ARG:NH2	2.18	0.41
1:B:426:LYS:HE2	1:B:426:LYS:HB3	1.90	0.41
1:D:40:SER:HB2	1:D:83:ARG:HB2	2.02	0.41
1:H:118:PRO:HG3	1:H:130:LEU:CD1	2.50	0.41
1:I:86:ARG:NH2	1:I:204:ASP:OD2	2.52	0.41
2:N:289:ILE:HD13	2:N:312:PHE:HB3	2.03	0.41
2:S:302:LEU:HB2	2:S:307:ARG:CB	2.45	0.41
2:W:318:ILE:HA	2:W:321:ILE:HD12	2.03	0.41
1:E:143:TYR:HE2	2:Q:340:MET:HE1	1.85	0.41
1:F:186:GLY:O	1:F:187:GLU:HB2	2.20	0.41
1:H:377:ARG:CZ	1:H:404:HIS:HA	2.51	0.41
1:I:377:ARG:CZ	1:I:404:HIS:HA	2.50	0.41
1:I:383:ILE:O	1:I:386:LYS:HG2	2.20	0.41
1:L:129:ASN:O	1:L:131:PHE:N	2.50	0.41
1:B:283:GLU:CA	1:B:327:GLN:OE1	2.68	0.41
1:D:66:GLU:HG3	1:D:147:ARG:HE	1.86	0.41
1:E:186:GLY:O	1:E:187:GLU:HB2	2.21	0.41
1:F:129:ASN:O	1:F:131:PHE:N	2.46	0.41
1:H:89:ARG:HD3	1:H:96:LEU:HD13	2.03	0.41
1:I:25:ARG:O	1:I:26:LEU:HD13	2.21	0.41
1:K:22:ARG:HG2	1:K:23:PRO:HD2	2.01	0.41
1:L:356:ALA:O	1:L:362:ARG:HD2	2.21	0.41
1:L:430:ILE:HD13	1:L:441:VAL:HG11	2.01	0.41
1:A:336:LYS:H	1:A:338:ARG:NH2	2.18	0.41
1:B:244:TYR:OH	1:B:366:GLU:OE1	2.39	0.41
1:B:337:GLN:O	1:B:340:HIS:N	2.53	0.41
1:B:386:LYS:HB2	1:B:386:LYS:HE2	1.76	0.41
1:C:327:GLN:CA	1:C:327:GLN:HE21	2.34	0.41
1:C:377:ARG:CZ	1:C:404:HIS:HA	2.50	0.41
1:D:89:ARG:HD3	1:D:96:LEU:HD13	2.03	0.41
1:D:360:PHE:C	1:D:362:ARG:N	2.79	0.41
1:E:353:ILE:C	1:E:353:ILE:HD13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:ILE:HG22	1:E:440:GLU:HB3	2.01	0.41
1:F:210:ARG:HH22	1:F:211:LYS:HE3	1.85	0.41
1:G:186:GLY:O	1:G:187:GLU:HB2	2.21	0.41
1:G:219:MET:HE2	1:G:365:ARG:NH2	2.35	0.41
1:H:93:ARG:HE	1:H:194:GLU:HG3	1.86	0.41
1:L:40:SER:HB2	1:L:83:ARG:HB2	2.01	0.41
1:L:359:ARG:HD3	1:L:359:ARG:HA	1.74	0.41
1:L:453:ARG:HG3	1:L:453:ARG:HH11	1.86	0.41
2:M:304:ASP:O	2:M:304:ASP:CG	2.64	0.41
2:Q:304:ASP:CG	2:Q:304:ASP:O	2.63	0.41
2:Q:318:ILE:HD12	2:Q:348:LEU:HB3	2.03	0.41
2:S:321:ILE:HD11	2:S:355:LEU:CD2	2.45	0.41
2:T:318:ILE:HD12	2:T:348:LEU:HB3	2.02	0.41
2:U:304:ASP:CG	2:U:304:ASP:O	2.64	0.41
2:V:311:LYS:HZ2	2:V:311:LYS:HG3	1.69	0.41
2:W:289:ILE:HD13	2:W:312:PHE:HB3	2.03	0.41
1:E:402:GLU:CD	1:E:453:ARG:HH22	2.29	0.41
1:I:416:SER:O	1:I:420:LEU:HD22	2.21	0.41
1:K:233:ILE:CG1	1:K:235:VAL:HG12	2.51	0.41
2:N:304:ASP:OD1	2:N:332:MET:HE1	2.21	0.41
2:O:295:THR:HG22	2:O:314:HIS:HD2	1.85	0.41
2:U:289:ILE:HD13	2:U:312:PHE:HB3	2.02	0.41
1:B:40:SER:HB2	1:B:83:ARG:HB2	2.02	0.40
1:B:118:PRO:HG3	1:B:130:LEU:CD1	2.51	0.40
1:C:336:LYS:O	1:C:337:GLN:C	2.64	0.40
1:D:116:VAL:C	1:D:117:LEU:CD1	2.94	0.40
1:E:23:PRO:HA	1:E:45:LYS:NZ	2.36	0.40
1:G:385:THR:HA	1:G:388:MET:HE2	2.03	0.40
1:I:100:ILE:C	1:I:100:ILE:HD12	2.46	0.40
1:I:336:LYS:H	1:I:338:ARG:NH2	2.18	0.40
1:J:377:ARG:CZ	1:J:404:HIS:HA	2.50	0.40
1:K:40:SER:HB2	1:K:83:ARG:HB2	2.03	0.40
1:L:287:ARG:HG3	1:L:327:GLN:NE2	2.35	0.40
2:O:304:ASP:O	2:O:304:ASP:CG	2.63	0.40
2:W:321:ILE:HD11	2:W:355:LEU:CD2	2.48	0.40
1:G:286:LEU:HD12	1:G:327:GLN:NE2	2.35	0.40
1:H:437:ILE:O	1:H:438:ASP:OD1	2.39	0.40
1:I:222:LEU:HB2	1:I:223:PRO:HD3	2.04	0.40
1:L:220:VAL:HG13	1:L:224:LEU:CD1	2.42	0.40
2:M:318:ILE:HA	2:M:321:ILE:HD12	2.04	0.40
2:S:289:ILE:HD13	2:S:312:PHE:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD13	1:B:49:LEU:HA	1.95	0.40
1:B:100:ILE:C	1:B:100:ILE:HD12	2.46	0.40
1:B:377:ARG:CZ	1:B:404:HIS:HA	2.50	0.40
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.85	0.40
1:F:40:SER:O	1:F:41:LEU:HD12	2.21	0.40
1:F:118:PRO:HG3	1:F:130:LEU:CD1	2.51	0.40
1:F:203:TYR:CE2	1:F:217:LYS:HD3	2.57	0.40
1:G:32:ILE:HD12	1:G:32:ILE:O	2.21	0.40
1:G:39:VAL:HG12	1:G:84:MET:HB3	2.02	0.40
2:O:360:LEU:HD22	2:O:365:ILE:HD11	2.03	0.40
1:B:186:GLY:O	1:B:187:GLU:HB2	2.21	0.40
1:D:86:ARG:O	1:D:87:VAL:C	2.64	0.40
1:E:220:VAL:HG12	1:E:342:ILE:HD12	2.04	0.40
1:I:217:LYS:HE3	1:I:217:LYS:HB3	1.79	0.40
1:I:256:ARG:HD2	1:I:256:ARG:HA	1.61	0.40
2:P:329:ARG:HB2	2:P:332:MET:HE2	2.04	0.40
2:U:318:ILE:HA	2:U:321:ILE:HD12	2.04	0.40
1:A:420:LEU:HD22	1:F:222:LEU:HD12	2.03	0.40
1:C:100:ILE:C	1:C:100:ILE:HD12	2.46	0.40
1:C:111:GLY:HA2	1:C:170:PRO:CD	2.35	0.40
1:E:226:HIS:CE1	1:F:427:MET:CE	3.04	0.40
1:E:300:ILE:HD13	1:E:344:MET:HE1	2.01	0.40
1:F:39:VAL:HG12	1:F:84:MET:HB3	2.02	0.40
1:H:386:LYS:HB2	1:H:386:LYS:HE2	1.77	0.40
1:I:362:ARG:HB2	1:I:363:PHE:H	1.59	0.40
1:I:377:ARG:HH11	1:I:377:ARG:HD3	1.74	0.40
1:L:49:LEU:HD13	1:L:49:LEU:HA	1.94	0.40
2:N:340:MET:CE	2:N:368:ARG:NH1	2.85	0.40
2:P:318:ILE:HD12	2:P:348:LEU:HB3	2.03	0.40
2:T:304:ASP:O	2:T:307:ARG:HG2	2.22	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	432/438 (99%)	400 (93%)	25 (6%)	7 (2%)	7	20
1	B	432/438 (99%)	404 (94%)	22 (5%)	6 (1%)	9	23
1	C	432/438 (99%)	403 (93%)	22 (5%)	7 (2%)	7	20
1	D	432/438 (99%)	396 (92%)	31 (7%)	5 (1%)	10	27
1	E	432/438 (99%)	397 (92%)	27 (6%)	8 (2%)	6	17
1	F	432/438 (99%)	403 (93%)	23 (5%)	6 (1%)	9	23
1	G	432/438 (99%)	404 (94%)	23 (5%)	5 (1%)	10	27
1	H	432/438 (99%)	403 (93%)	23 (5%)	6 (1%)	9	23
1	I	432/438 (99%)	404 (94%)	22 (5%)	6 (1%)	9	23
1	J	432/438 (99%)	403 (93%)	22 (5%)	7 (2%)	7	20
1	K	432/438 (99%)	403 (93%)	21 (5%)	8 (2%)	6	17
1	L	432/438 (99%)	400 (93%)	25 (6%)	7 (2%)	7	20
2	M	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	N	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	O	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	P	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	Q	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	R	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	S	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	4	12
2	T	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	12
2	U	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	V	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	W	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
2	X	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	27
All	All	6180/6276 (98%)	5745 (93%)	343 (6%)	92 (2%)	8	22

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLY
1	A	282	SER
1	A	340	HIS

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Mol	Chain	Res	Type
1	B	340	HIS
1	B	441	VAL
1	C	186	GLY
1	C	340	HIS
1	C	441	VAL
1	D	340	HIS
1	E	171	SER
1	E	186	GLY
1	E	441	VAL
1	F	186	GLY
1	F	340	HIS
1	G	186	GLY
1	G	340	HIS
1	H	186	GLY
1	H	340	HIS
1	H	441	VAL
1	I	186	GLY
1	I	340	HIS
1	J	340	HIS
1	J	441	VAL
1	K	340	HIS
1	L	187	GLU
2	R	304	ASP
2	S	304	ASP
1	A	441	VAL
1	B	186	GLY
1	C	171	SER
1	D	186	GLY
1	D	441	VAL
1	E	340	HIS
1	F	441	VAL
1	G	441	VAL
1	H	339	ALA
1	I	441	VAL
1	J	186	GLY
1	K	130	LEU
1	K	186	GLY
1	K	441	VAL
1	L	186	GLY
1	L	336	LYS
1	L	441	VAL
2	M	304	ASP

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Mol	Chain	Res	Type
2	N	304	ASP
2	O	304	ASP
2	P	304	ASP
2	Q	304	ASP
2	T	304	ASP
2	U	304	ASP
2	V	304	ASP
2	W	304	ASP
2	X	304	ASP
1	B	438	ASP
1	C	130	LEU
1	G	338	ARG
1	J	336	LYS
1	K	359	ARG
1	A	187	GLU
1	A	336	LYS
1	B	187	GLU
1	B	336	LYS
1	C	187	GLU
1	E	187	GLU
1	E	336	LYS
1	F	336	LYS
1	G	187	GLU
1	H	187	GLU
1	I	336	LYS
1	J	187	GLU
1	J	339	ALA
1	K	336	LYS
1	L	185	GLU
1	L	339	ALA
2	T	314	HIS
1	C	438	ASP
1	D	187	GLU
1	F	187	GLU
1	I	187	GLU
1	J	438	ASP
1	K	438	ASP
1	A	438	ASP
1	D	336	LYS
1	E	438	ASP
1	F	438	ASP
1	H	438	ASP

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Mol	Chain	Res	Type
1	I	438	ASP
1	K	187	GLU
1	L	438	ASP
2	S	314	HIS
1	E	170	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/373 (99%)	345 (93%)	25 (7%)	14	35
1	B	370/373 (99%)	345 (93%)	25 (7%)	14	35
1	C	368/373 (99%)	336 (91%)	32 (9%)	9	24
1	D	369/373 (99%)	329 (89%)	40 (11%)	6	16
1	E	362/373 (97%)	325 (90%)	37 (10%)	7	18
1	F	370/373 (99%)	342 (92%)	28 (8%)	12	30
1	G	365/373 (98%)	331 (91%)	34 (9%)	8	21
1	H	370/373 (99%)	341 (92%)	29 (8%)	11	29
1	I	370/373 (99%)	345 (93%)	25 (7%)	14	35
1	J	369/373 (99%)	338 (92%)	31 (8%)	10	26
1	K	370/373 (99%)	341 (92%)	29 (8%)	11	29
1	L	366/373 (98%)	341 (93%)	25 (7%)	14	35
2	M	75/75 (100%)	62 (83%)	13 (17%)	2	5
2	N	74/75 (99%)	64 (86%)	10 (14%)	4	9
2	O	74/75 (99%)	66 (89%)	8 (11%)	6	16
2	P	74/75 (99%)	64 (86%)	10 (14%)	4	9
2	Q	75/75 (100%)	67 (89%)	8 (11%)	6	16
2	R	75/75 (100%)	66 (88%)	9 (12%)	5	12
2	S	75/75 (100%)	62 (83%)	13 (17%)	2	5
2	T	75/75 (100%)	67 (89%)	8 (11%)	6	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U	75/75 (100%)	67 (89%)	8 (11%)	6	16
2	V	75/75 (100%)	63 (84%)	12 (16%)	2	6
2	W	75/75 (100%)	66 (88%)	9 (12%)	5	12
2	X	75/75 (100%)	64 (85%)	11 (15%)	3	8
All	All	5316/5376 (99%)	4837 (91%)	479 (9%)	9	23

All (479) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	49	LEU
1	A	50	GLN
1	A	57	VAL
1	A	88	VAL
1	A	130	LEU
1	A	147	ARG
1	A	158	MET
1	A	171	SER
1	A	181	VAL
1	A	187	GLU
1	A	220	VAL
1	A	235	VAL
1	A	287	ARG
1	A	312	LYS
1	A	325	VAL
1	A	335	LEU
1	A	352	SER
1	A	358	ARG
1	A	373	ASP
1	A	375	THR
1	A	411	LEU
1	A	416	SER
1	A	428	ASP
1	A	440	GLU
1	B	49	LEU
1	B	96	LEU
1	B	113	ARG
1	B	158	MET
1	B	164	LYS
1	B	171	SER
1	B	183	HIS

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Mol	Chain	Res	Type
1	B	187	GLU
1	B	190	LYS
1	B	212	GLN
1	B	220	VAL
1	B	235	VAL
1	B	249	THR
1	B	278	LEU
1	B	313	ARG
1	B	328	LEU
1	B	335	LEU
1	B	340	HIS
1	B	352	SER
1	B	399	VAL
1	B	416	SER
1	B	428	ASP
1	B	440	GLU
1	B	445	LEU
1	B	453	ARG
1	C	49	LEU
1	C	88	VAL
1	C	96	LEU
1	C	103	GLN
1	C	113	ARG
1	C	158	MET
1	C	164	LYS
1	C	166	VAL
1	C	168	THR
1	C	171	SER
1	C	181	VAL
1	C	187	GLU
1	C	190	LYS
1	C	211	LYS
1	C	220	VAL
1	C	239	ARG
1	C	249	THR
1	C	262	THR
1	C	288	LYS
1	C	313	ARG
1	C	320	VAL
1	C	325	VAL
1	C	327	GLN
1	C	337	GLN

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Mol	Chain	Res	Type
1	C	352	SER
1	C	375	THR
1	C	382	GLN
1	C	396	LEU
1	C	440	GLU
1	C	441	VAL
1	C	445	LEU
1	C	456	LEU
1	D	22	ARG
1	D	49	LEU
1	D	58	LEU
1	D	59	LEU
1	D	66	GLU
1	D	96	LEU
1	D	103	GLN
1	D	105	CYS
1	D	112	LYS
1	D	131	PHE
1	D	135	LEU
1	D	158	MET
1	D	171	SER
1	D	187	GLU
1	D	194	GLU
1	D	200	GLU
1	D	204	ASP
1	D	210	ARG
1	D	211	LYS
1	D	220	VAL
1	D	249	THR
1	D	256	ARG
1	D	273	GLU
1	D	277	LYS
1	D	307	ASP
1	D	320	VAL
1	D	335	LEU
1	D	338	ARG
1	D	349	ARG
1	D	357	LEU
1	D	358	ARG
1	D	362	ARG
1	D	381	LEU
1	D	389	LYS

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Mol	Chain	Res	Type
1	D	396	LEU
1	D	416	SER
1	D	426	LYS
1	D	440	GLU
1	D	453	ARG
1	D	456	LEU
1	E	46	MET
1	E	49	LEU
1	E	60	LYS
1	E	63	LYS
1	E	64	ARG
1	E	75	ASP
1	E	88	VAL
1	E	94	VAL
1	E	100	ILE
1	E	113	ARG
1	E	130	LEU
1	E	148	LYS
1	E	158	MET
1	E	165	VAL
1	E	170	PRO
1	E	171	SER
1	E	187	GLU
1	E	222	LEU
1	E	235	VAL
1	E	277	LYS
1	E	328	LEU
1	E	332	MET
1	E	335	LEU
1	E	342	ILE
1	E	352	SER
1	E	353	ILE
1	E	358	ARG
1	E	378	LEU
1	E	382	GLN
1	E	396	LEU
1	E	416	SER
1	E	421	GLN
1	E	433	GLU
1	E	440	GLU
1	E	441	VAL
1	E	443	ASN

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Mol	Chain	Res	Type
1	E	457	SER
1	F	38	VAL
1	F	43	GLN
1	F	49	LEU
1	F	88	VAL
1	F	105	CYS
1	F	113	ARG
1	F	130	LEU
1	F	147	ARG
1	F	158	MET
1	F	171	SER
1	F	187	GLU
1	F	200	GLU
1	F	218	GLU
1	F	220	VAL
1	F	225	ARG
1	F	231	LYS
1	F	235	VAL
1	F	286	LEU
1	F	315	LYS
1	F	324	ILE
1	F	325	VAL
1	F	352	SER
1	F	416	SER
1	F	420	LEU
1	F	425	LYS
1	F	426	LYS
1	F	440	GLU
1	F	441	VAL
1	G	22	ARG
1	G	24	ASN
1	G	32	ILE
1	G	49	LEU
1	G	51	LEU
1	G	88	VAL
1	G	99	VAL
1	G	113	ARG
1	G	130	LEU
1	G	147	ARG
1	G	158	MET
1	G	164	LYS
1	G	165	VAL

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Mol	Chain	Res	Type
1	G	171	SER
1	G	187	GLU
1	G	210	ARG
1	G	220	VAL
1	G	262	THR
1	G	312	LYS
1	G	313	ARG
1	G	320	VAL
1	G	325	VAL
1	G	327	GLN
1	G	329	LEU
1	G	352	SER
1	G	388	MET
1	G	398	GLN
1	G	416	SER
1	G	420	LEU
1	G	421	GLN
1	G	426	LYS
1	G	437	ILE
1	G	440	GLU
1	G	449	MET
1	H	49	LEU
1	H	88	VAL
1	H	96	LEU
1	H	100	ILE
1	H	112	LYS
1	H	113	ARG
1	H	130	LEU
1	H	158	MET
1	H	171	SER
1	H	187	GLU
1	H	212	GLN
1	H	220	VAL
1	H	225	ARG
1	H	249	THR
1	H	262	THR
1	H	286	LEU
1	H	325	VAL
1	H	328	LEU
1	H	338	ARG
1	H	340	HIS
1	H	351	ASN

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Mol	Chain	Res	Type
1	H	352	SER
1	H	382	GLN
1	H	396	LEU
1	H	416	SER
1	H	438	ASP
1	H	440	GLU
1	H	443	ASN
1	H	449	MET
1	I	49	LEU
1	I	80	GLU
1	I	88	VAL
1	I	113	ARG
1	I	133	VAL
1	I	158	MET
1	I	167	GLU
1	I	171	SER
1	I	217	LYS
1	I	220	VAL
1	I	222	LEU
1	I	235	VAL
1	I	249	THR
1	I	261	GLU
1	I	325	VAL
1	I	352	SER
1	I	362	ARG
1	I	398	GLN
1	I	399	VAL
1	I	416	SER
1	I	420	LEU
1	I	428	ASP
1	I	440	GLU
1	I	443	ASN
1	I	453	ARG
1	J	27	ILE
1	J	49	LEU
1	J	64	ARG
1	J	73	SER
1	J	88	VAL
1	J	96	LEU
1	J	105	CYS
1	J	158	MET
1	J	164	LYS

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Mol	Chain	Res	Type
1	J	171	SER
1	J	187	GLU
1	J	190	LYS
1	J	211	LYS
1	J	212	GLN
1	J	215	GLN
1	J	220	VAL
1	J	287	ARG
1	J	313	ARG
1	J	320	VAL
1	J	325	VAL
1	J	352	SER
1	J	362	ARG
1	J	396	LEU
1	J	399	VAL
1	J	414	LEU
1	J	416	SER
1	J	424	ARG
1	J	437	ILE
1	J	440	GLU
1	J	443	ASN
1	J	453	ARG
1	K	49	LEU
1	K	58	LEU
1	K	88	VAL
1	K	96	LEU
1	K	120	ASP
1	K	130	LEU
1	K	133	VAL
1	K	141	GLU
1	K	158	MET
1	K	171	SER
1	K	194	GLU
1	K	200	GLU
1	K	204	ASP
1	K	220	VAL
1	K	254	ILE
1	K	256	ARG
1	K	261	GLU
1	K	277	LYS
1	K	324	ILE
1	K	335	LEU

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Mol	Chain	Res	Type
1	K	359	ARG
1	K	396	LEU
1	K	416	SER
1	K	433	GLU
1	K	440	GLU
1	K	441	VAL
1	K	442	MET
1	K	445	LEU
1	K	453	ARG
1	L	38	VAL
1	L	49	LEU
1	L	76	THR
1	L	88	VAL
1	L	99	VAL
1	L	130	LEU
1	L	158	MET
1	L	164	LYS
1	L	171	SER
1	L	184	CYS
1	L	187	GLU
1	L	211	LYS
1	L	220	VAL
1	L	221	GLU
1	L	222	LEU
1	L	235	VAL
1	L	335	LEU
1	L	358	ARG
1	L	375	THR
1	L	396	LEU
1	L	416	SER
1	L	428	ASP
1	L	443	ASN
1	L	453	ARG
1	L	457	SER
2	M	287	ILE
2	M	308	LEU
2	M	311	LYS
2	M	312	PHE
2	M	314	HIS
2	M	318	ILE
2	M	323	LEU
2	M	329	ARG

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Mol	Chain	Res	Type
2	M	335	THR
2	M	338	ILE
2	M	340	MET
2	M	362	ASN
2	M	365	ILE
2	N	295	THR
2	N	308	LEU
2	N	312	PHE
2	N	314	HIS
2	N	318	ILE
2	N	329	ARG
2	N	335	THR
2	N	338	ILE
2	N	340	MET
2	N	362	ASN
2	O	286	MET
2	O	308	LEU
2	O	311	LYS
2	O	312	PHE
2	O	323	LEU
2	O	340	MET
2	O	362	ASN
2	O	368	ARG
2	P	308	LEU
2	P	311	LYS
2	P	312	PHE
2	P	314	HIS
2	P	323	LEU
2	P	332	MET
2	P	335	THR
2	P	354	THR
2	P	362	ASN
2	P	369	LEU
2	Q	286	MET
2	Q	308	LEU
2	Q	311	LYS
2	Q	312	PHE
2	Q	318	ILE
2	Q	335	THR
2	Q	362	ASN
2	Q	369	LEU
2	R	287	ILE

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Mol	Chain	Res	Type
2	R	304	ASP
2	R	308	LEU
2	R	311	LYS
2	R	312	PHE
2	R	314	HIS
2	R	335	THR
2	R	338	ILE
2	R	354	THR
2	S	295	THR
2	S	304	ASP
2	S	307	ARG
2	S	308	LEU
2	S	311	LYS
2	S	312	PHE
2	S	314	HIS
2	S	318	ILE
2	S	329	ARG
2	S	332	MET
2	S	335	THR
2	S	340	MET
2	S	341	THR
2	T	287	ILE
2	T	301	ARG
2	T	302	LEU
2	T	311	LYS
2	T	312	PHE
2	T	314	HIS
2	T	354	THR
2	T	369	LEU
2	U	308	LEU
2	U	311	LYS
2	U	312	PHE
2	U	314	HIS
2	U	318	ILE
2	U	335	THR
2	U	362	ASN
2	U	369	LEU
2	V	287	ILE
2	V	308	LEU
2	V	311	LYS
2	V	312	PHE
2	V	314	HIS

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Mol	Chain	Res	Type
2	V	315	SER
2	V	332	MET
2	V	335	THR
2	V	340	MET
2	V	341	THR
2	V	365	ILE
2	V	369	LEU
2	W	286	MET
2	W	308	LEU
2	W	311	LYS
2	W	312	PHE
2	W	314	HIS
2	W	315	SER
2	W	323	LEU
2	W	335	THR
2	W	362	ASN
2	X	287	ILE
2	X	289	ILE
2	X	291	GLU
2	X	308	LEU
2	X	311	LYS
2	X	312	PHE
2	X	314	HIS
2	X	332	MET
2	X	335	THR
2	X	354	THR
2	X	362	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	85	ASN
1	A	183	HIS
1	A	270	ASN
1	A	285	ASN
1	A	327	GLN
1	B	36	ASN
1	B	270	ASN
1	B	340	HIS
1	B	443	ASN
1	C	36	ASN

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Mol	Chain	Res	Type
1	C	129	ASN
1	C	183	HIS
1	C	398	GLN
1	C	443	ASN
1	D	103	GLN
1	D	215	GLN
1	D	285	ASN
1	D	384	HIS
1	E	115	HIS
1	E	183	HIS
1	E	226	HIS
1	E	270	ASN
1	E	285	ASN
1	E	327	GLN
1	E	340	HIS
1	E	351	ASN
1	F	50	GLN
1	F	115	HIS
1	F	226	HIS
1	F	327	GLN
1	F	443	ASN
1	G	24	ASN
1	G	36	ASN
1	G	50	GLN
1	G	115	HIS
1	G	327	GLN
1	G	421	GLN
1	H	270	ASN
1	H	340	HIS
1	I	36	ASN
1	I	129	ASN
1	I	270	ASN
1	J	36	ASN
1	J	215	GLN
1	J	270	ASN
1	J	398	GLN
1	K	36	ASN
1	K	129	ASN
1	K	183	HIS
1	K	398	GLN
1	K	443	ASN
1	L	36	ASN

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Mol	Chain	Res	Type
1	L	226	HIS
1	L	398	GLN
1	L	443	ASN
2	M	359	ASN
2	M	362	ASN
2	N	314	HIS
2	N	362	ASN
2	O	362	ASN
2	P	299	GLN
2	P	314	HIS
2	Q	299	GLN
2	S	314	HIS
2	U	299	GLN
2	U	310	GLN
2	V	299	GLN
2	V	362	ASN
2	W	299	GLN
2	W	314	HIS
2	W	362	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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	G	501	-	28,29,29	0.56	0	43,45,45	0.58	0
3	ADP	B	501	-	28,29,29	0.47	0	43,45,45	0.63	0
3	ADP	K	501	-	28,29,29	0.44	0	43,45,45	0.86	2 (4%)
3	ADP	E	501	-	28,29,29	0.57	0	43,45,45	0.63	0
3	ADP	L	501	-	28,29,29	0.55	0	43,45,45	0.76	1 (2%)
3	ADP	D	501	-	28,29,29	0.49	0	43,45,45	0.81	1 (2%)
3	ADP	C	501	-	28,29,29	0.42	0	43,45,45	0.90	2 (4%)
3	ADP	H	501	-	28,29,29	0.51	0	43,45,45	0.68	0
3	ADP	A	501	-	28,29,29	0.54	1 (3%)	43,45,45	0.80	1 (2%)
3	ADP	J	501	-	28,29,29	0.47	0	43,45,45	0.67	0
3	ADP	I	501	-	28,29,29	0.42	0	43,45,45	0.73	2 (4%)
3	ADP	F	501	-	28,29,29	0.73	1 (3%)	43,45,45	0.72	0

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	G	501	-	-	3/16/32/32	0/3/3/3
3	ADP	B	501	-	-	4/16/32/32	0/3/3/3
3	ADP	K	501	-	-	6/16/32/32	0/3/3/3
3	ADP	E	501	-	-	4/16/32/32	0/3/3/3
3	ADP	L	501	-	-	5/16/32/32	0/3/3/3
3	ADP	D	501	-	-	4/16/32/32	0/3/3/3
3	ADP	C	501	-	-	2/16/32/32	0/3/3/3
3	ADP	H	501	-	-	5/16/32/32	0/3/3/3
3	ADP	A	501	-	-	4/16/32/32	0/3/3/3
3	ADP	J	501	-	-	5/16/32/32	0/3/3/3
3	ADP	I	501	-	-	7/16/32/32	0/3/3/3
3	ADP	F	501	-	-	3/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	ADP	PA-O3A	3.06	1.62	1.59
3	A	501	ADP	PA-O3A	2.07	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	ADP	O2B-PB-O3A	3.35	115.86	104.64
3	C	501	ADP	O3A-PB-O1B	-2.76	96.51	111.04
3	D	501	ADP	O4'-C1'-N9	2.71	113.30	108.09
3	L	501	ADP	O2B-PB-O3A	2.31	112.37	104.64
3	A	501	ADP	O2A-PA-O3A	2.21	113.25	107.27
3	K	501	ADP	O3'-C3'-C4'	2.15	117.27	111.08
3	I	501	ADP	O3A-PB-O1B	-2.08	100.09	111.04
3	I	501	ADP	O2B-PB-O3A	2.04	111.47	104.64
3	K	501	ADP	O4'-C1'-N9	2.03	111.99	108.09

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O3A
3	B	501	ADP	C5'-O5'-PA-O2A
3	B	501	ADP	C5'-O5'-PA-O3A
3	D	501	ADP	C5'-O5'-PA-O1A
3	D	501	ADP	C5'-O5'-PA-O2A
3	D	501	ADP	C5'-O5'-PA-O3A
3	E	501	ADP	C5'-O5'-PA-O1A
3	E	501	ADP	C5'-O5'-PA-O3A
3	F	501	ADP	C5'-O5'-PA-O3A
3	G	501	ADP	C5'-O5'-PA-O2A
3	G	501	ADP	C5'-O5'-PA-O3A
3	H	501	ADP	C5'-O5'-PA-O1A
3	H	501	ADP	C5'-O5'-PA-O2A
3	H	501	ADP	C5'-O5'-PA-O3A
3	I	501	ADP	PA-O3A-PB-O3B
3	I	501	ADP	C5'-O5'-PA-O1A
3	I	501	ADP	C5'-O5'-PA-O3A
3	J	501	ADP	C5'-O5'-PA-O3A
3	K	501	ADP	PA-O3A-PB-O2B
3	K	501	ADP	C5'-O5'-PA-O2A
3	K	501	ADP	C5'-O5'-PA-O3A
3	L	501	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	L	501	ADP	C5'-O5'-PA-O3A
3	H	501	ADP	O4'-C4'-C5'-O5'
3	C	501	ADP	PA-O3A-PB-O1B
3	H	501	ADP	C3'-C4'-C5'-O5'
3	K	501	ADP	C3'-C4'-C5'-O5'
3	E	501	ADP	PB-O3A-PA-O2A
3	J	501	ADP	PB-O3A-PA-O2A
3	L	501	ADP	PB-O3A-PA-O1A
3	A	501	ADP	C5'-O5'-PA-O1A
3	F	501	ADP	C5'-O5'-PA-O1A
3	I	501	ADP	C5'-O5'-PA-O2A
3	J	501	ADP	C5'-O5'-PA-O1A
3	J	501	ADP	C5'-O5'-PA-O2A
3	K	501	ADP	C5'-O5'-PA-O1A
3	A	501	ADP	PB-O3A-PA-O2A
3	B	501	ADP	PB-O3A-PA-O1A
3	F	501	ADP	PB-O3A-PA-O2A
3	A	501	ADP	C4'-C5'-O5'-PA
3	L	501	ADP	C4'-C5'-O5'-PA
3	I	501	ADP	C3'-C4'-C5'-O5'
3	D	501	ADP	C3'-C4'-C5'-O5'
3	K	501	ADP	PA-O3A-PB-O1B
3	I	501	ADP	PA-O3A-PB-O2B
3	B	501	ADP	PB-O3A-PA-O2A
3	J	501	ADP	PB-O3A-PA-O1A
3	I	501	ADP	PA-O3A-PB-O1B
3	C	501	ADP	C3'-C4'-C5'-O5'
3	E	501	ADP	PB-O3A-PA-O1A
3	G	501	ADP	PB-O3A-PA-O2A
3	L	501	ADP	PB-O3A-PA-O2A

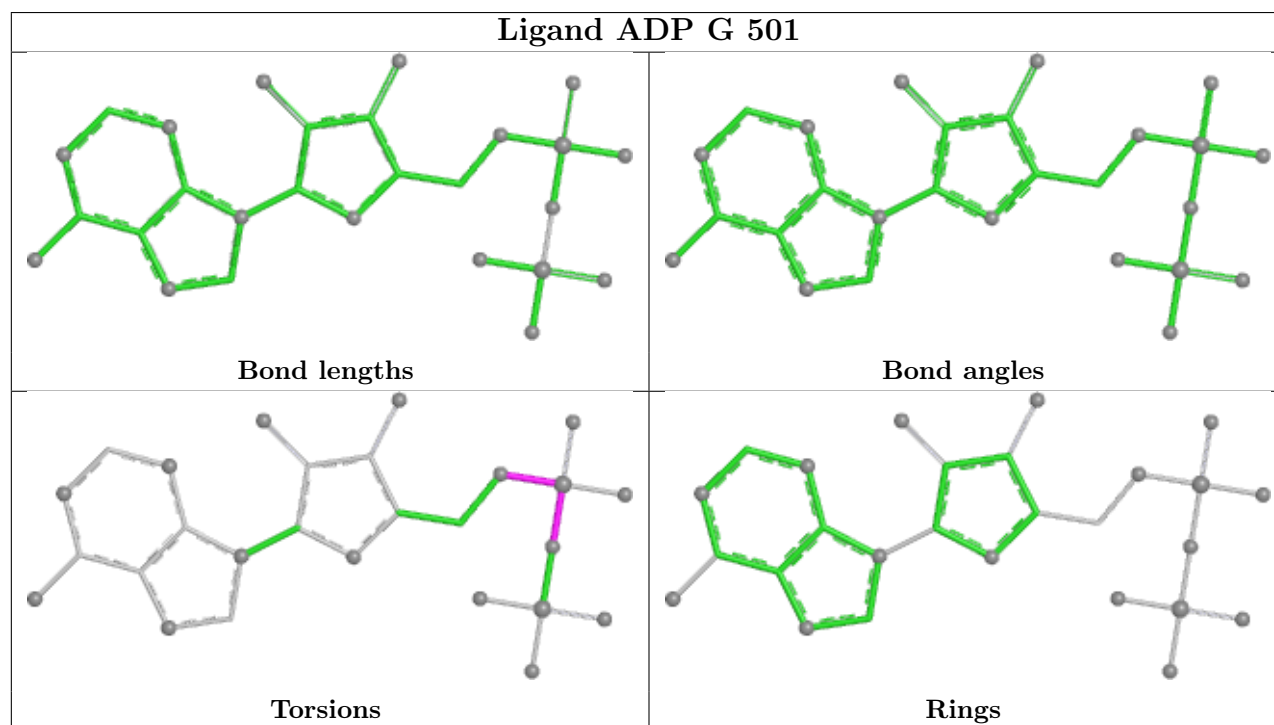
There are no ring outliers.

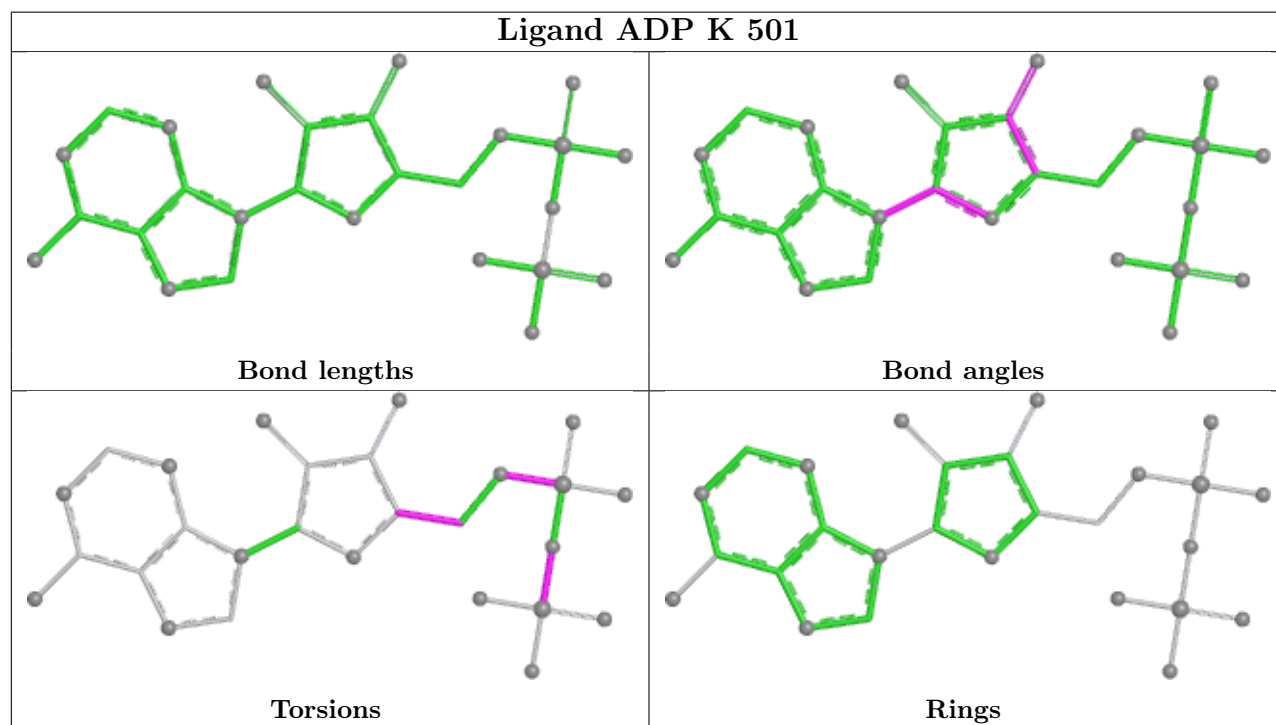
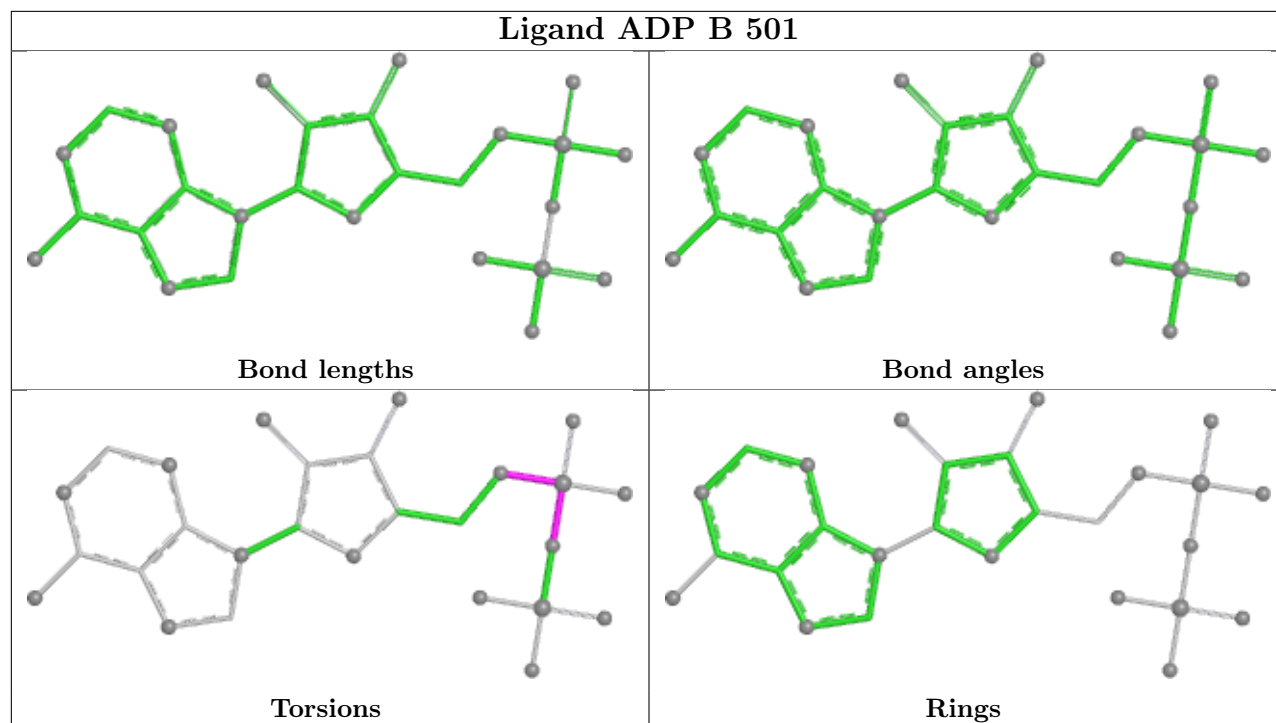
5 monomers are involved in 7 short contacts:

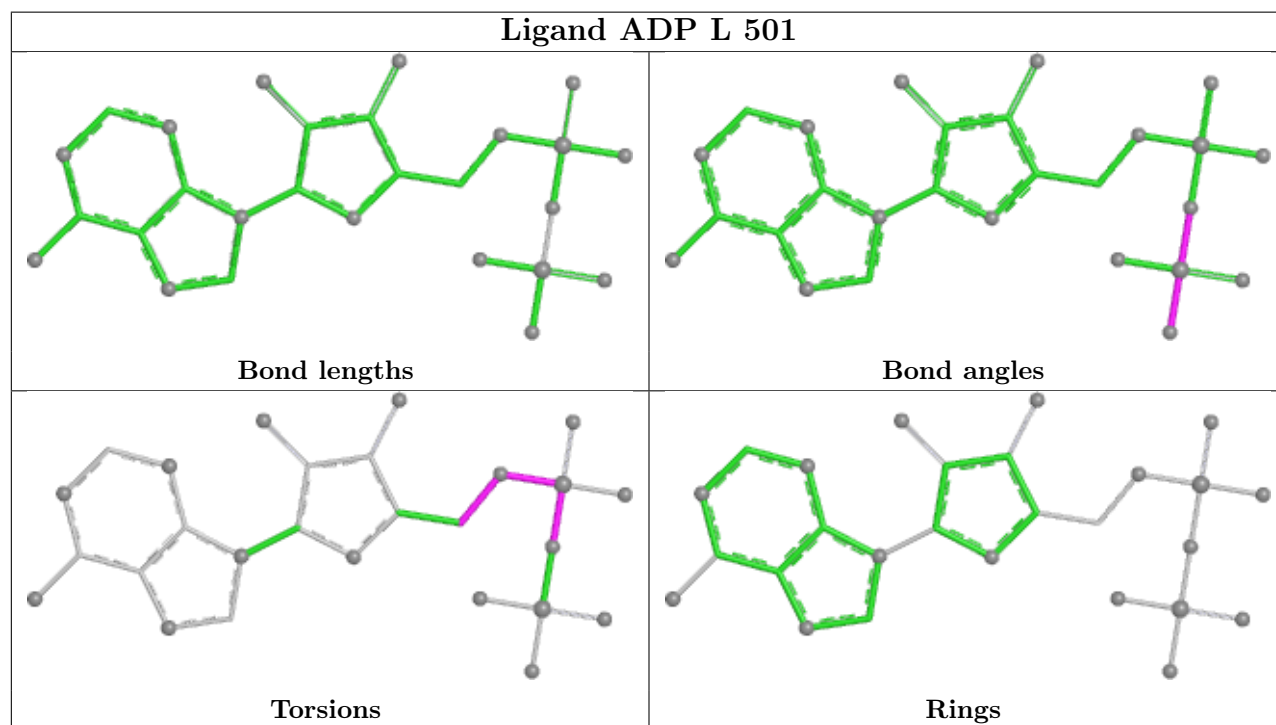
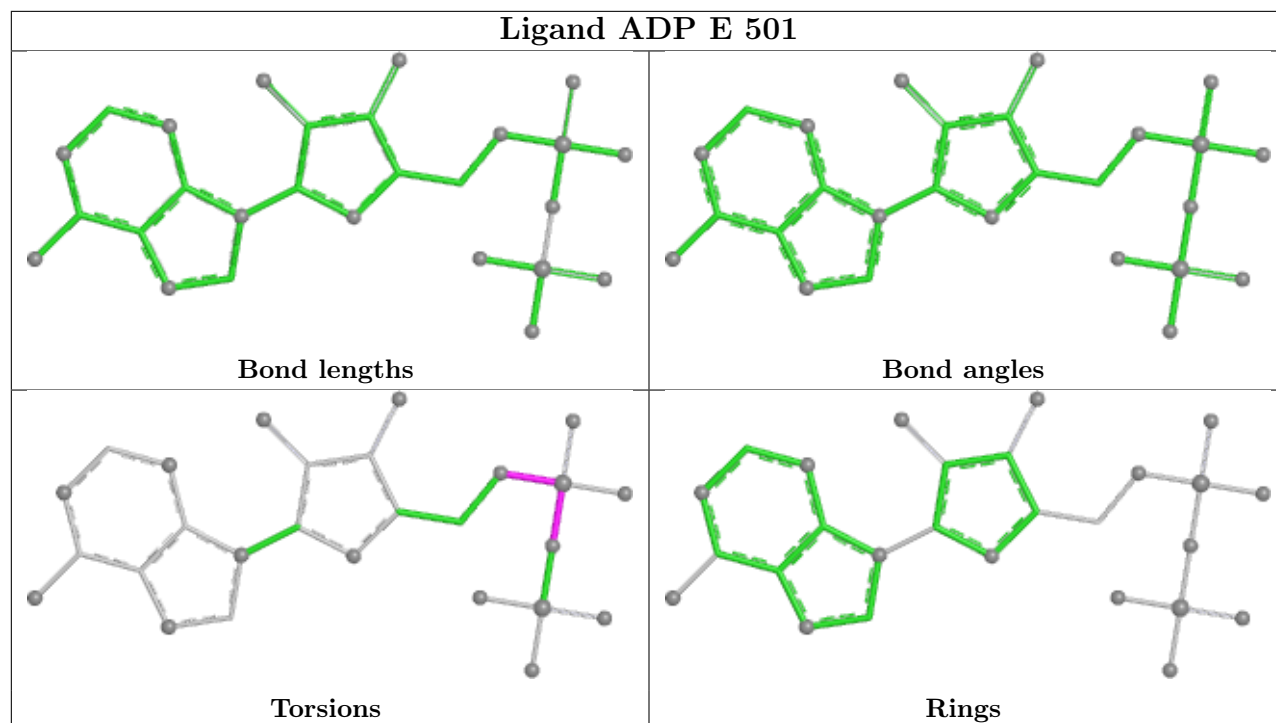
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	501	ADP	1	0
3	D	501	ADP	1	0
3	C	501	ADP	1	0
3	H	501	ADP	1	0
3	A	501	ADP	3	0

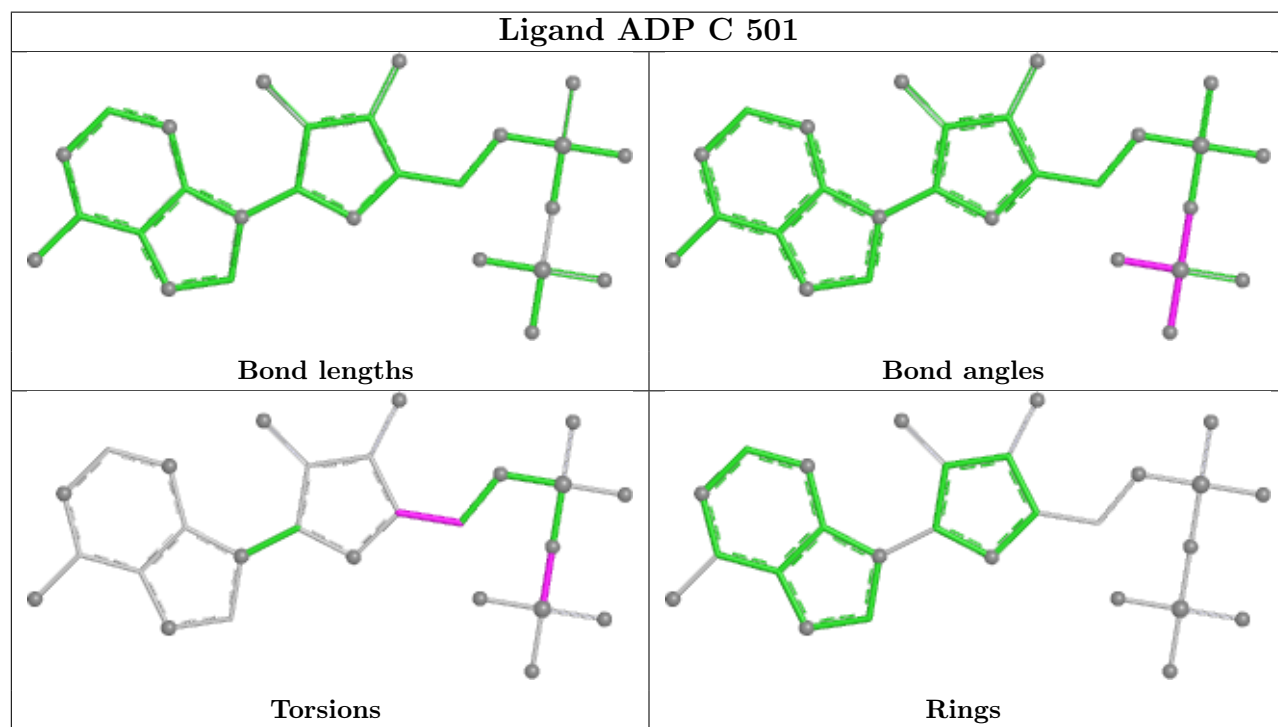
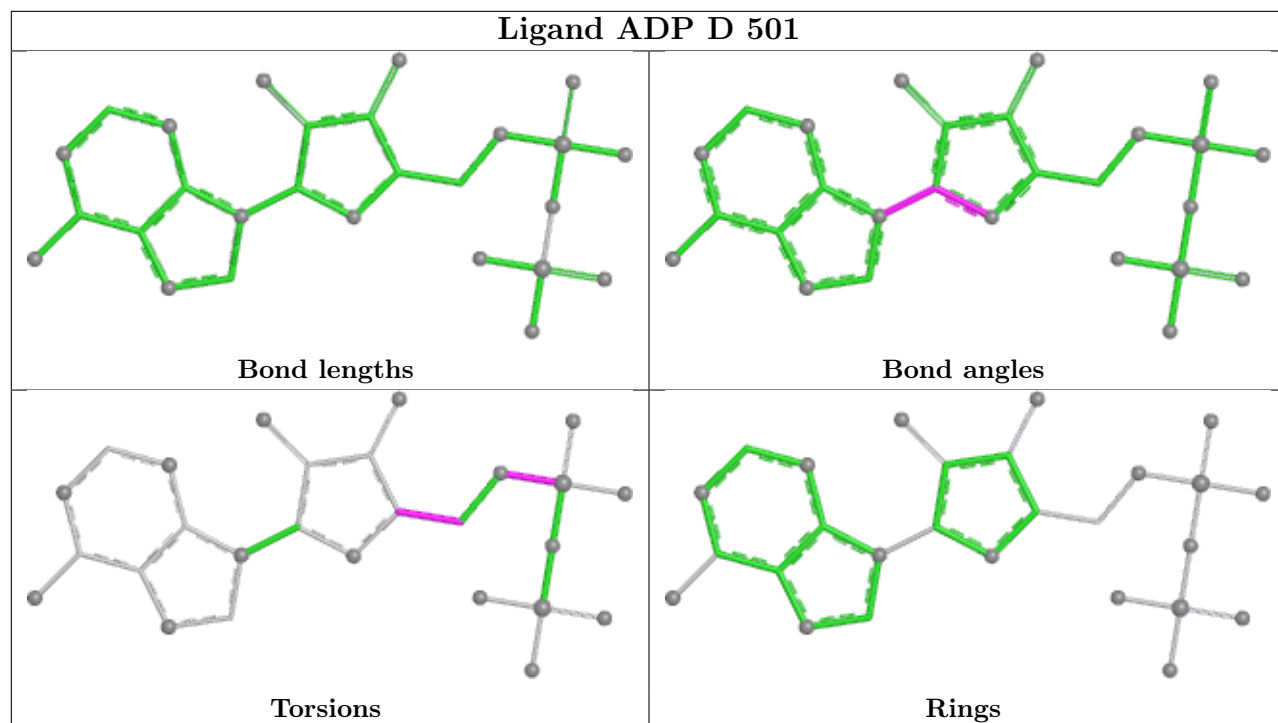
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

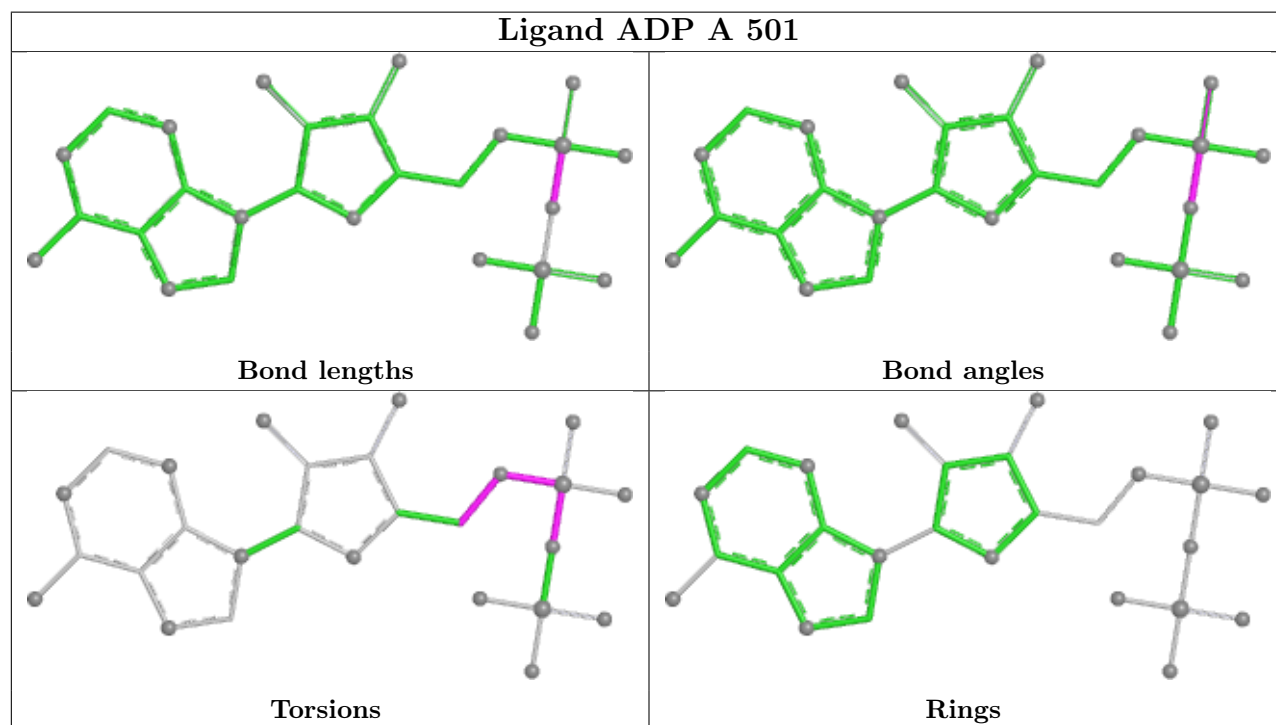
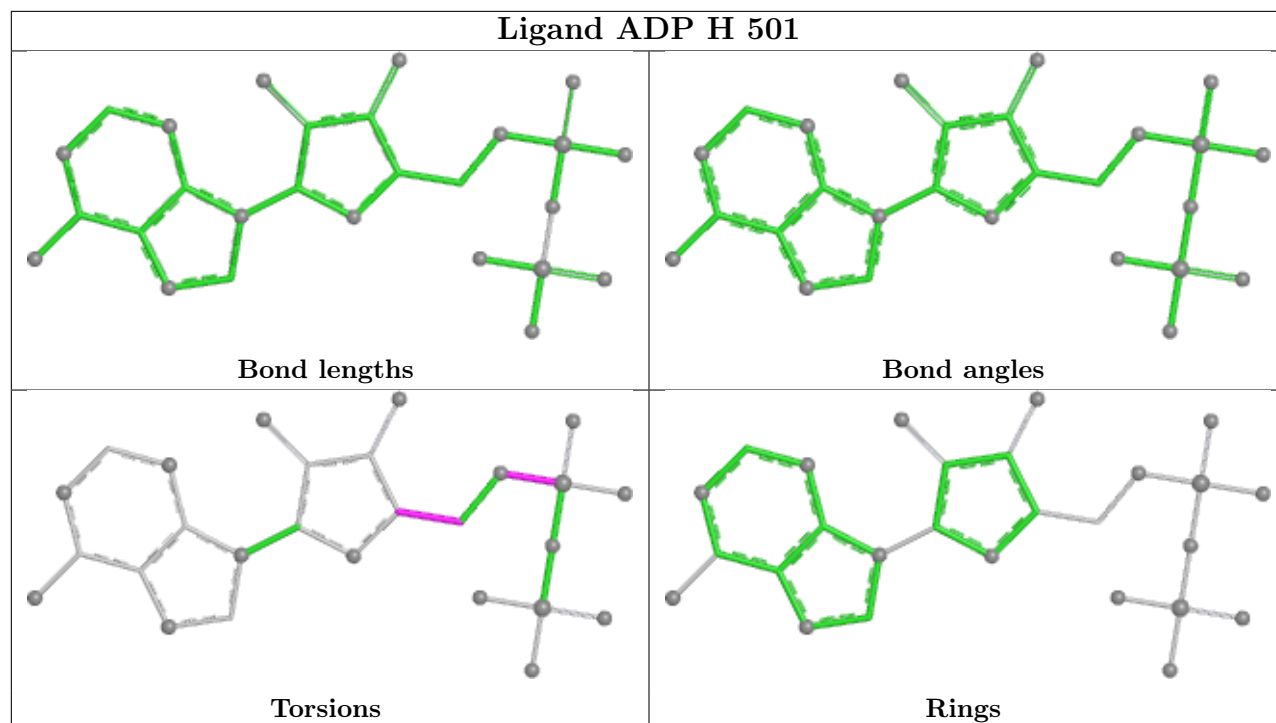
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



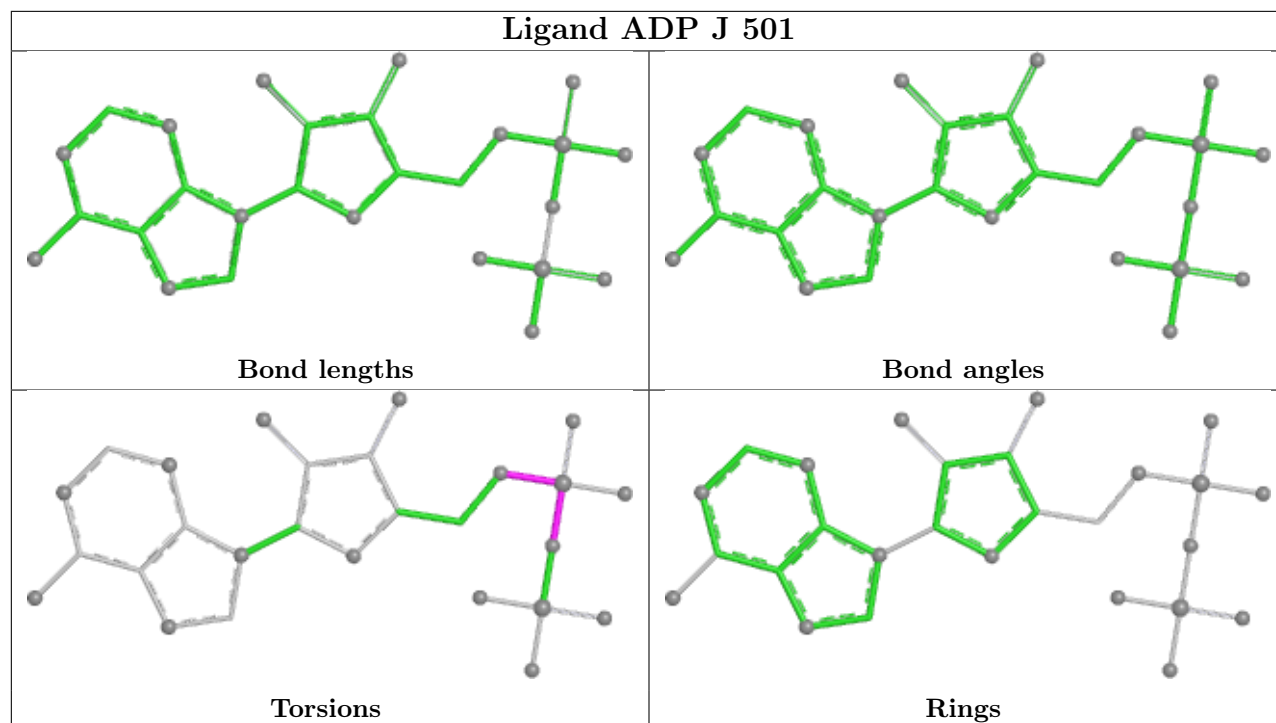




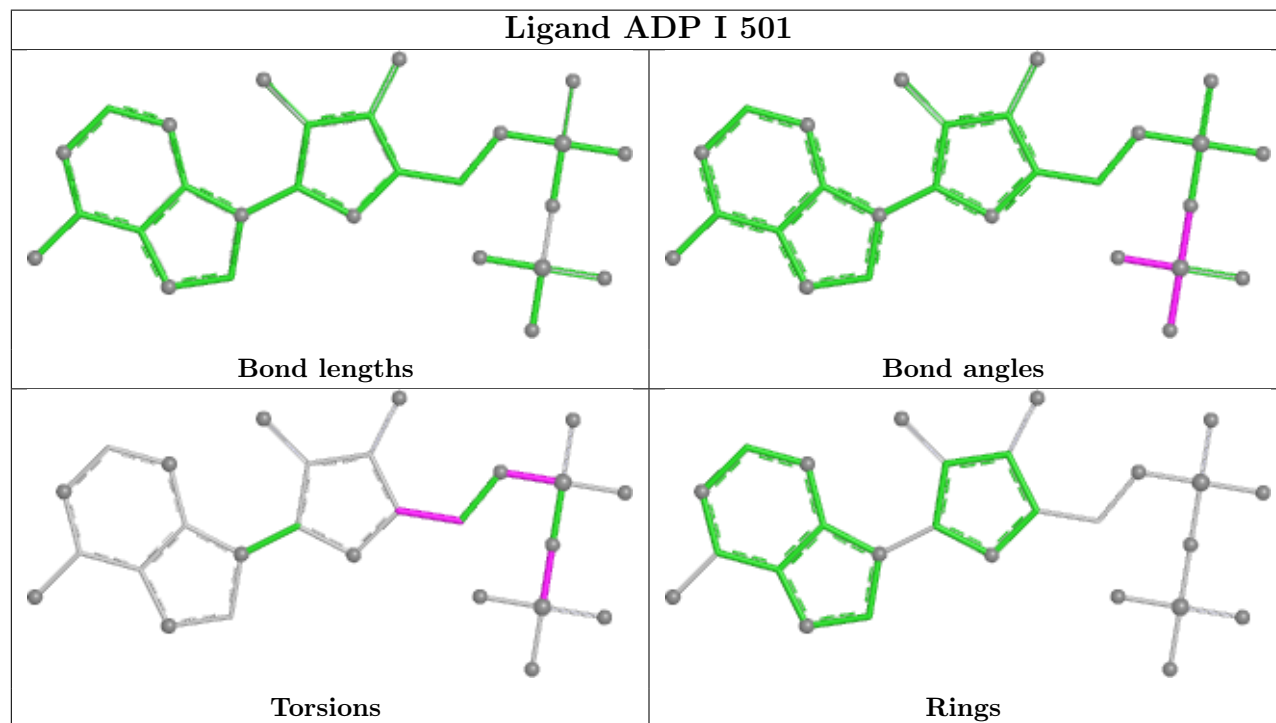


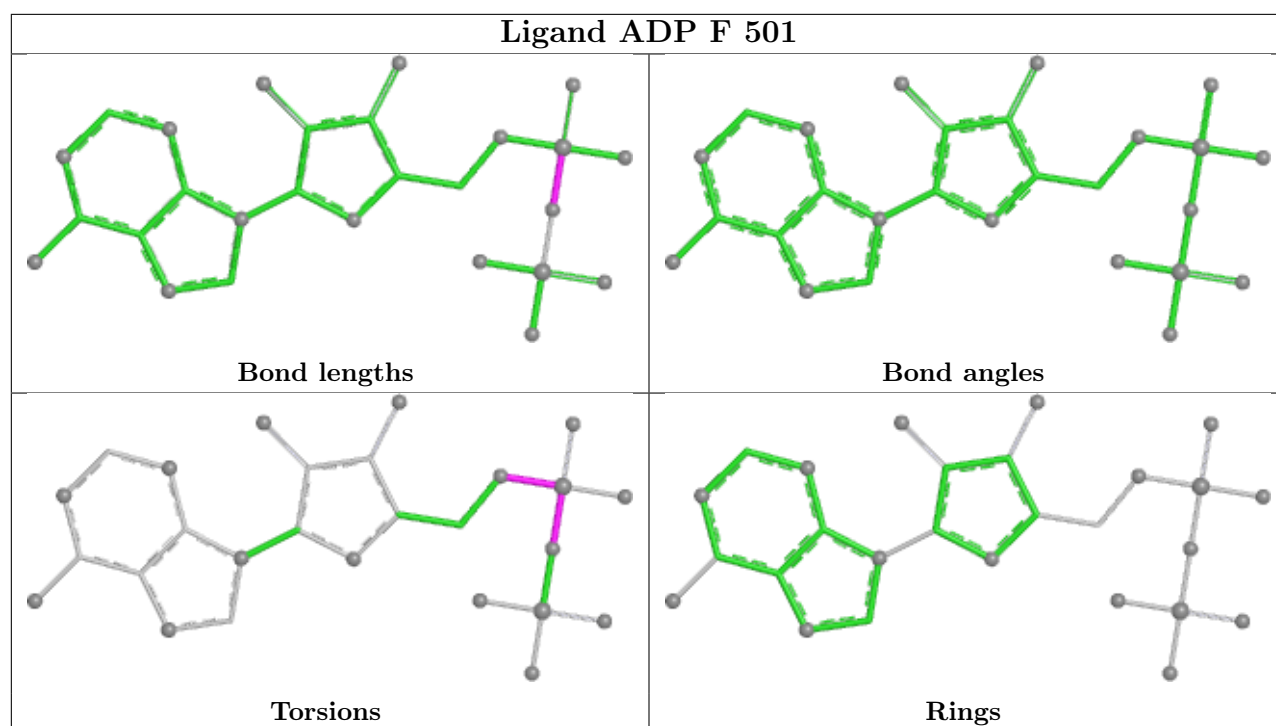


Ligand ADP J 501



Ligand ADP I 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	436/438 (99%)	0.08	15 (3%)	48	44	35, 66, 127, 193	0
1	B	436/438 (99%)	-0.12	14 (3%)	50	46	33, 58, 121, 219	0
1	C	436/438 (99%)	-0.08	12 (2%)	55	51	35, 58, 116, 196	0
1	D	436/438 (99%)	0.22	22 (5%)	34	30	39, 67, 133, 224	0
1	E	436/438 (99%)	0.57	23 (5%)	32	28	30, 77, 132, 206	0
1	F	436/438 (99%)	0.15	15 (3%)	48	44	35, 66, 133, 211	0
1	G	436/438 (99%)	0.23	20 (4%)	37	34	46, 71, 132, 203	0
1	H	436/438 (99%)	-0.02	13 (2%)	52	49	40, 63, 126, 202	0
1	I	436/438 (99%)	0.07	14 (3%)	50	46	36, 66, 125, 186	0
1	J	436/438 (99%)	-0.05	9 (2%)	63	61	34, 61, 119, 197	0
1	K	436/438 (99%)	0.03	13 (2%)	52	49	35, 61, 117, 182	0
1	L	436/438 (99%)	0.16	18 (4%)	41	37	36, 67, 124, 207	0
2	M	85/85 (100%)	-0.02	2 (2%)	59	56	37, 60, 99, 119	0
2	N	85/85 (100%)	0.17	5 (5%)	28	25	42, 63, 104, 138	0
2	O	85/85 (100%)	-0.01	4 (4%)	36	33	40, 57, 93, 119	0
2	P	85/85 (100%)	0.10	4 (4%)	36	33	37, 60, 102, 136	0
2	Q	85/85 (100%)	0.11	5 (5%)	28	25	44, 63, 99, 137	0
2	R	85/85 (100%)	-0.11	5 (5%)	28	25	35, 53, 88, 124	0
2	S	85/85 (100%)	0.26	3 (3%)	47	43	50, 69, 107, 130	0
2	T	85/85 (100%)	-0.00	6 (7%)	22	19	36, 56, 92, 123	0
2	U	85/85 (100%)	-0.00	3 (3%)	47	43	37, 59, 100, 131	0
2	V	85/85 (100%)	0.13	3 (3%)	47	43	39, 64, 101, 132	0
2	W	85/85 (100%)	-0.07	1 (1%)	76	75	38, 59, 92, 129	0
2	X	85/85 (100%)	-0.05	3 (3%)	47	43	38, 56, 98, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	6252/6276 (99%)	0.09	232 (3%)	45	41	30, 64, 122, 224	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	339	ALA	7.5
1	E	337	GLN	6.6
1	B	439	ALA	6.3
1	C	441	VAL	5.4
1	G	337	GLN	4.8
1	J	439	ALA	4.8
1	G	336	LYS	4.6
1	D	339	ALA	4.6
1	C	339	ALA	4.5
1	G	335	LEU	4.4
1	D	131	PHE	4.4
1	E	239	ARG	4.3
1	F	417	GLU	4.3
1	E	340	HIS	4.2
1	A	339	ALA	4.1
1	J	339	ALA	4.1
1	G	239	ARG	4.1
1	G	441	VAL	4.0
1	B	437	ILE	3.9
1	L	337	GLN	3.8
1	A	442	MET	3.8
1	F	441	VAL	3.8
1	A	438	ASP	3.7
1	F	339	ALA	3.7
1	L	239	ARG	3.7
1	D	362	ARG	3.7
2	U	310	GLN	3.7
1	A	239	ARG	3.6
1	G	339	ALA	3.6
1	D	439	ALA	3.6
1	I	441	VAL	3.6
1	C	437	ILE	3.6
1	I	339	ALA	3.6
1	D	437	ILE	3.5
1	C	336	LYS	3.5
1	E	336	LYS	3.5
1	G	437	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	439	ALA	3.5
1	D	182	ILE	3.4
1	H	339	ALA	3.4
1	B	336	LYS	3.4
1	C	438	ASP	3.4
1	K	439	ALA	3.4
1	I	184	CYS	3.4
1	E	360	PHE	3.4
1	E	338	ARG	3.4
1	K	441	VAL	3.4
1	L	339	ALA	3.3
1	J	442	MET	3.3
2	T	306	GLY	3.3
1	F	437	ILE	3.3
1	B	244	TYR	3.3
1	E	362	ARG	3.3
1	L	439	ALA	3.3
1	I	362	ARG	3.2
1	C	340	HIS	3.2
1	F	429	LEU	3.2
1	L	359	ARG	3.2
1	K	339	ALA	3.2
2	T	312	PHE	3.2
1	G	359	ARG	3.1
1	E	22	ARG	3.1
1	A	441	VAL	3.1
1	E	437	ILE	3.1
1	E	359	ARG	3.1
1	A	437	ILE	3.0
1	H	442	MET	3.0
2	P	329	ARG	3.0
1	J	441	VAL	3.0
1	E	244	TYR	3.0
1	L	340	HIS	3.0
1	I	337	GLN	3.0
1	L	336	LYS	3.0
1	D	239	ARG	3.0
1	B	339	ALA	3.0
1	B	440	GLU	2.9
1	H	437	ILE	2.9
2	O	310	GLN	2.9
1	D	438	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	437	ILE	2.9
1	L	437	ILE	2.9
1	I	442	MET	2.9
2	R	310	GLN	2.9
1	C	442	MET	2.9
1	D	442	MET	2.9
1	D	169	ASP	2.9
1	D	441	VAL	2.9
1	E	429	LEU	2.9
1	H	359	ARG	2.8
1	G	442	MET	2.8
1	H	443	ASN	2.8
1	K	438	ASP	2.8
1	A	319	GLU	2.8
1	F	313	ARG	2.8
1	K	337	GLN	2.8
1	F	439	ALA	2.8
1	K	182	ILE	2.8
1	G	431	ASP	2.8
1	B	441	VAL	2.8
1	L	441	VAL	2.8
1	D	184	CYS	2.7
1	I	336	LYS	2.7
1	I	437	ILE	2.7
1	H	441	VAL	2.7
2	U	293	GLU	2.7
1	G	443	ASN	2.7
1	C	439	ALA	2.7
1	D	204	ASP	2.7
1	D	129	ASN	2.7
1	G	439	ALA	2.7
2	M	310	GLN	2.7
2	T	310	GLN	2.7
1	B	337	GLN	2.6
2	O	306	GLY	2.6
2	X	306	GLY	2.6
1	A	232	ALA	2.6
1	A	316	THR	2.6
2	R	312	PHE	2.6
1	J	32	ILE	2.6
1	K	442	MET	2.6
1	I	186	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	V	306	GLY	2.6
1	E	237	PRO	2.6
1	E	436	THR	2.6
1	B	239	ARG	2.6
1	J	440	GLU	2.6
1	F	316	THR	2.6
2	T	304	ASP	2.6
2	P	308	LEU	2.6
2	S	312	PHE	2.6
1	H	338	ARG	2.5
1	L	338	ARG	2.5
1	D	443	ASN	2.5
2	Q	310	GLN	2.5
1	G	231	LYS	2.5
1	E	432	LEU	2.5
2	T	314	HIS	2.5
1	E	439	ALA	2.5
2	X	310	GLN	2.5
1	J	443	ASN	2.5
1	E	222	LEU	2.5
1	D	244	TYR	2.5
1	I	232	ALA	2.5
1	H	438	ASP	2.4
1	L	317	HIS	2.4
1	I	185	GLU	2.4
1	E	441	VAL	2.4
1	G	374	ALA	2.4
1	F	404	HIS	2.4
1	A	169	ASP	2.4
2	N	293	GLU	2.4
1	A	337	GLN	2.4
2	P	312	PHE	2.4
1	B	313	ARG	2.4
1	G	338	ARG	2.4
1	L	428	ASP	2.4
2	O	304	ASP	2.4
1	E	170	PRO	2.4
2	V	312	PHE	2.4
1	K	204	ASP	2.4
1	A	313	ARG	2.4
1	F	374	ALA	2.4
1	L	404	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	443	ASN	2.3
1	J	437	ILE	2.3
1	B	340	HIS	2.3
2	W	286	MET	2.3
1	C	319	GLU	2.3
2	R	304	ASP	2.3
1	F	370	GLY	2.3
1	H	318	GLY	2.3
1	L	232	ALA	2.3
1	L	436	THR	2.3
2	V	293	GLU	2.3
1	C	171	SER	2.3
1	L	350	PRO	2.3
2	T	308	LEU	2.3
2	O	312	PHE	2.3
1	I	169	ASP	2.2
2	M	306	GLY	2.2
2	N	306	GLY	2.2
2	Q	306	GLY	2.2
2	R	306	GLY	2.2
1	D	340	HIS	2.2
1	F	455	ALA	2.2
1	G	430	ILE	2.2
1	K	239	ARG	2.2
1	A	231	LYS	2.2
1	K	336	LYS	2.2
1	B	442	MET	2.2
1	I	239	ARG	2.2
2	N	308	LEU	2.2
2	Q	308	LEU	2.2
2	R	308	LEU	2.2
1	D	181	VAL	2.2
1	E	332	MET	2.2
1	H	317	HIS	2.2
1	K	115	HIS	2.2
1	D	337	GLN	2.2
1	I	231	LYS	2.2
1	G	438	ASP	2.2
1	B	404	HIS	2.2
1	G	309	ILE	2.2
1	G	404	HIS	2.2
2	Q	314	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	433	GLU	2.1
1	D	127	THR	2.1
2	S	308	LEU	2.1
1	A	309	ILE	2.1
1	E	343	VAL	2.1
1	F	317	HIS	2.1
1	F	360	PHE	2.1
1	L	360	PHE	2.1
2	S	293	GLU	2.1
1	H	336	LYS	2.1
2	N	304	ASP	2.1
2	N	312	PHE	2.1
1	C	338	ARG	2.1
1	E	335	LEU	2.1
2	P	323	LEU	2.1
1	G	340	HIS	2.1
2	X	314	HIS	2.1
2	Q	312	PHE	2.1
1	C	440	GLU	2.1
1	H	340	HIS	2.1
1	L	184	CYS	2.1
2	U	314	HIS	2.1
1	D	360	PHE	2.1
1	J	438	ASP	2.0
1	D	185	GLU	2.0
1	F	432	LEU	2.0
1	K	429	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

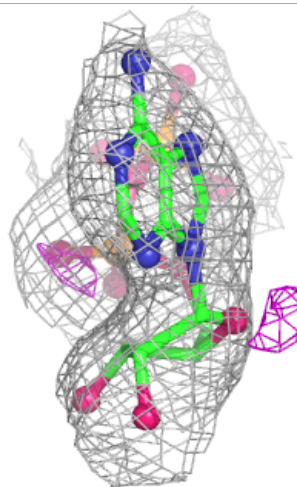
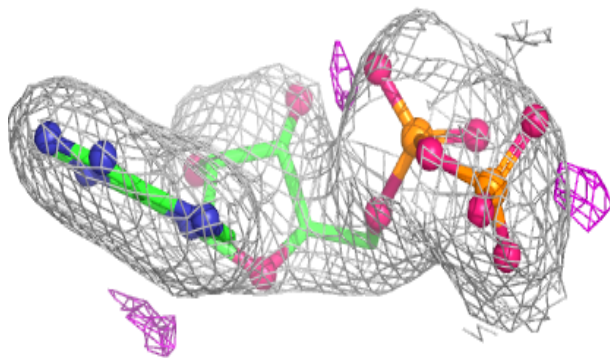
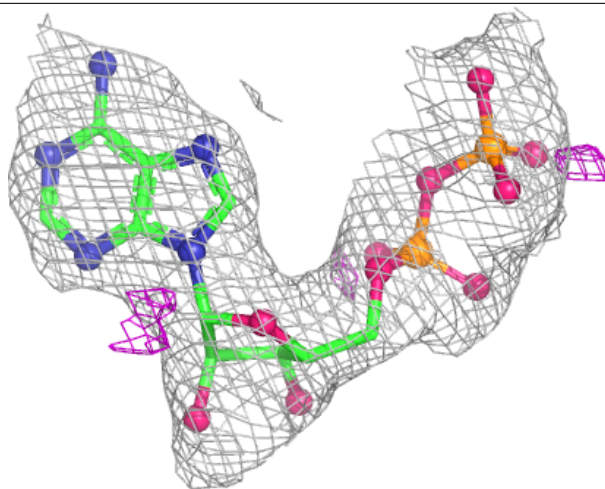
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	L	501	27/27	0.94	0.08	60,71,87,96	0
3	ADP	D	501	27/27	0.95	0.07	53,64,78,88	0
3	ADP	E	501	27/27	0.95	0.07	65,75,88,100	0
3	ADP	G	501	27/27	0.95	0.06	62,72,89,90	0
3	ADP	H	501	27/27	0.95	0.07	58,68,75,82	0
3	ADP	J	501	27/27	0.95	0.07	53,65,79,81	0
3	ADP	A	501	27/27	0.95	0.07	49,68,85,87	0
3	ADP	I	501	27/27	0.96	0.06	55,67,78,80	0
3	ADP	C	501	27/27	0.96	0.07	52,61,71,87	0
3	ADP	K	501	27/27	0.96	0.07	49,62,76,86	0
3	ADP	F	501	27/27	0.96	0.06	56,68,87,89	0
3	ADP	B	501	27/27	0.97	0.06	40,57,69,73	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.

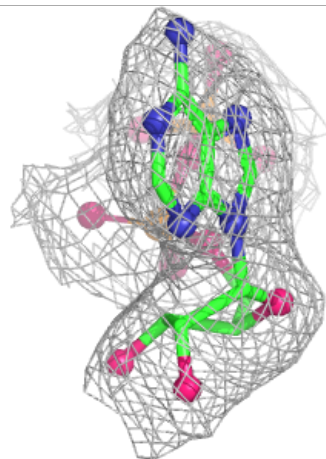
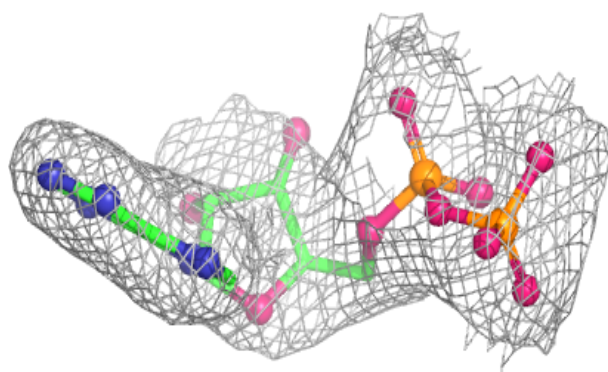
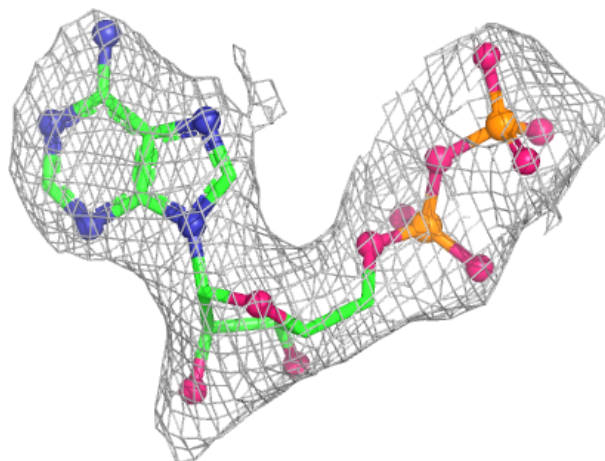
Electron density around ADP L 501:

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



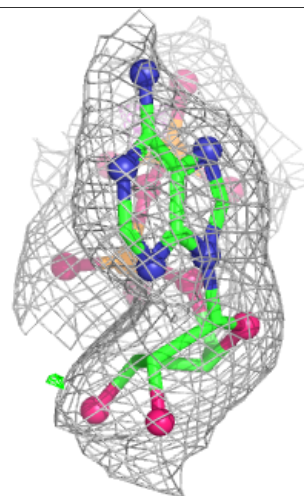
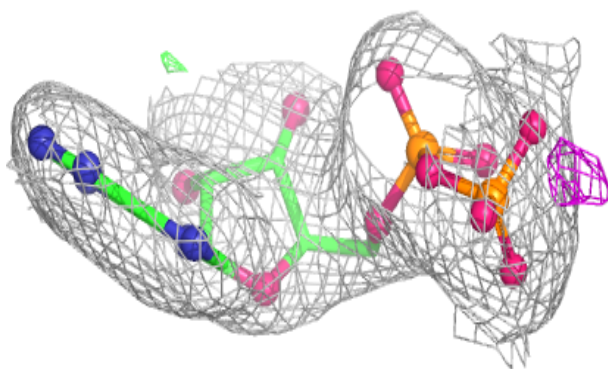
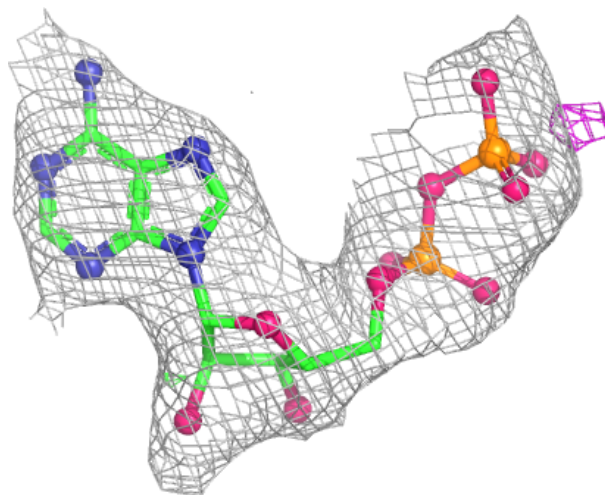
Electron density around ADP D 501:

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and green (positive)



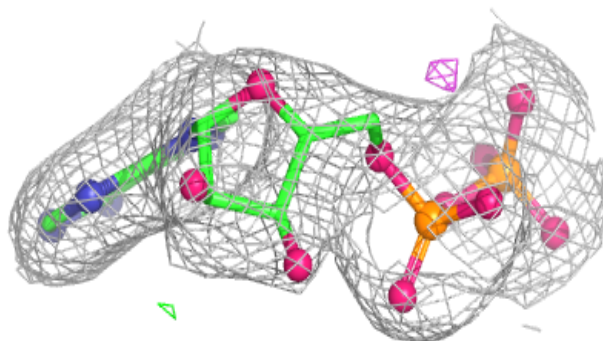
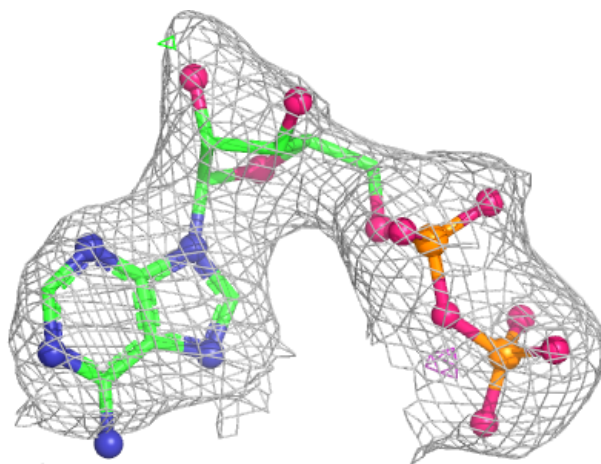
Electron density around ADP E 501:

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and green (positive)



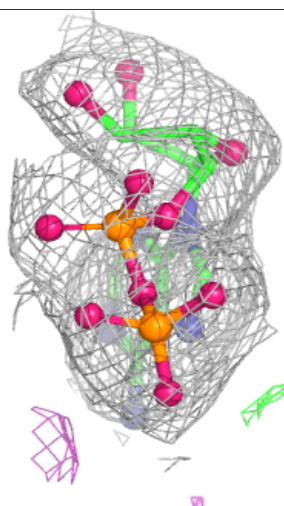
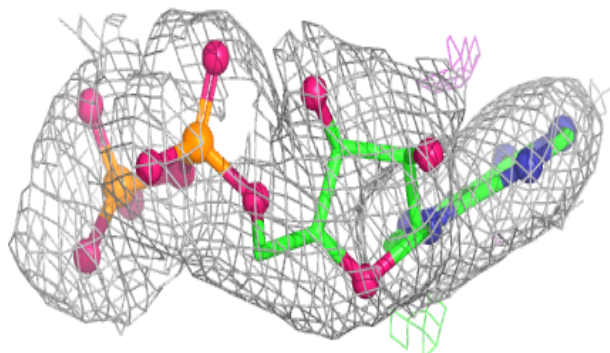
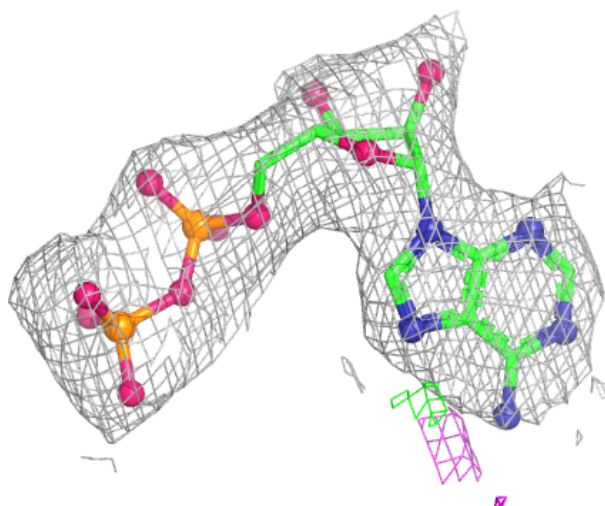
Electron density around ADP G 501:

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and green (positive)



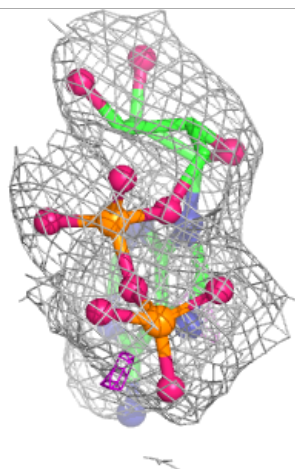
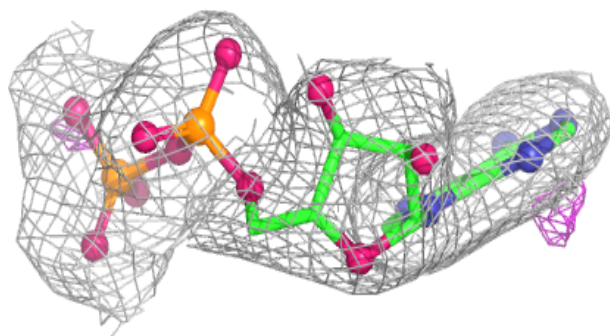
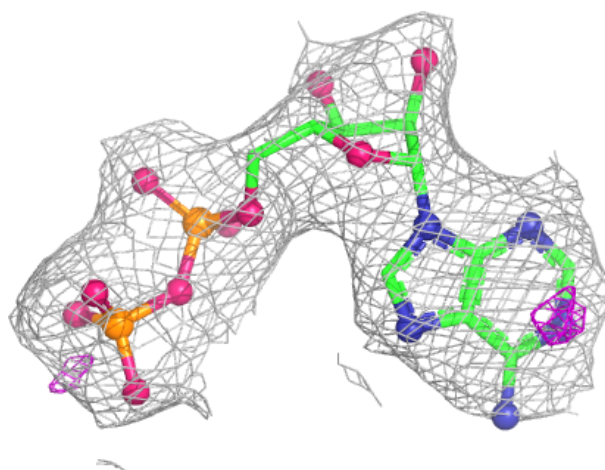
Electron density around ADP H 501:

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



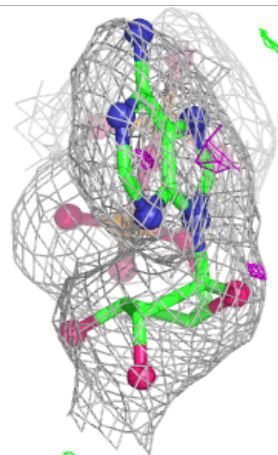
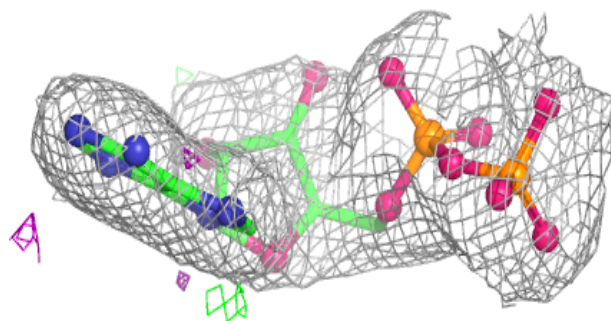
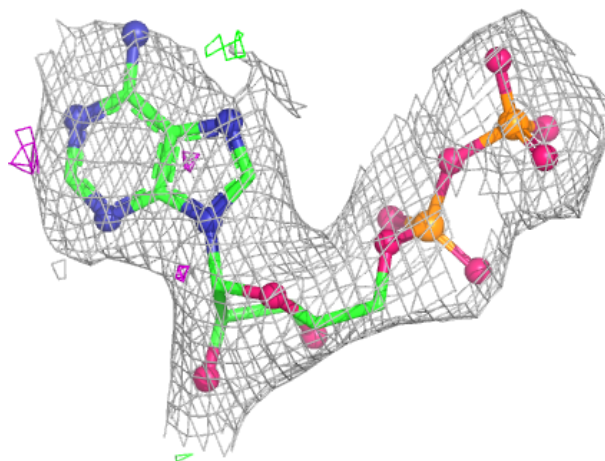
Electron density around ADP J 501:

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and green (positive)



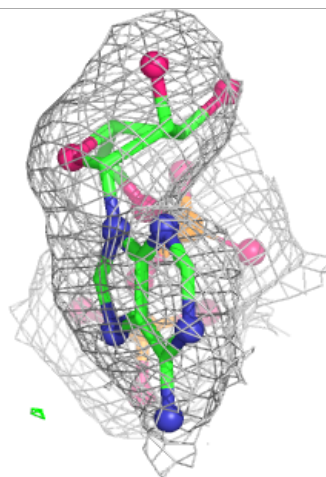
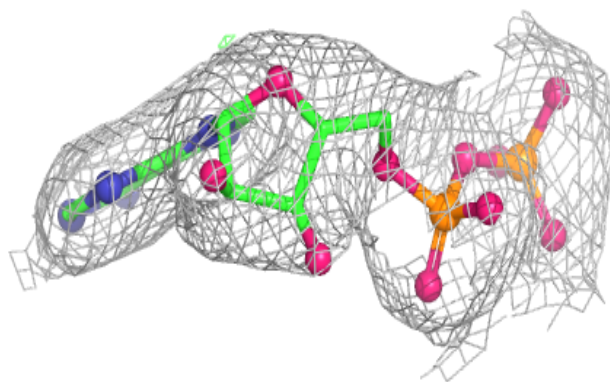
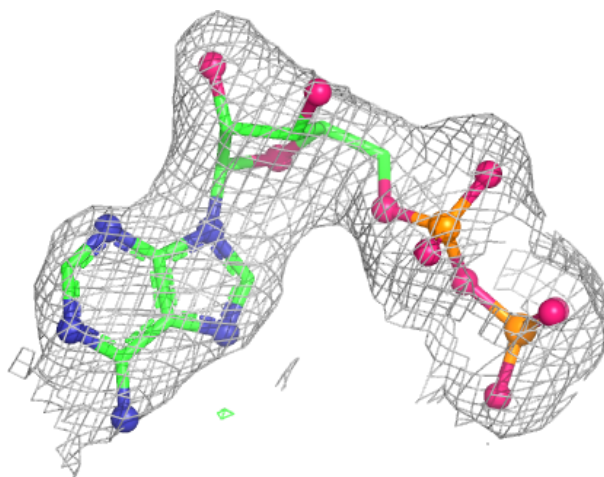
Electron density around ADP A 501:

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



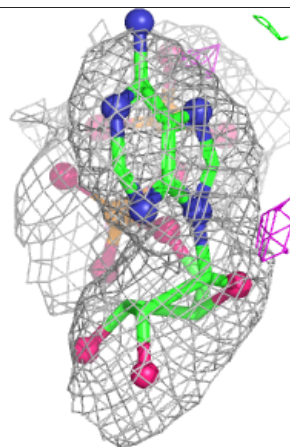
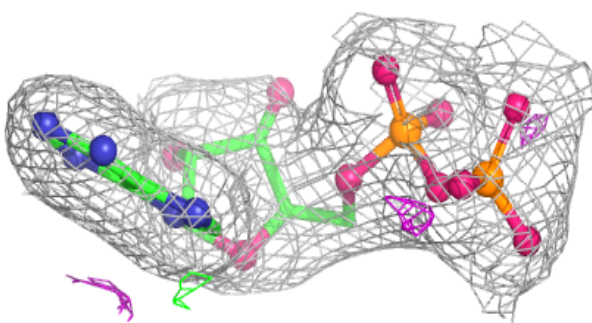
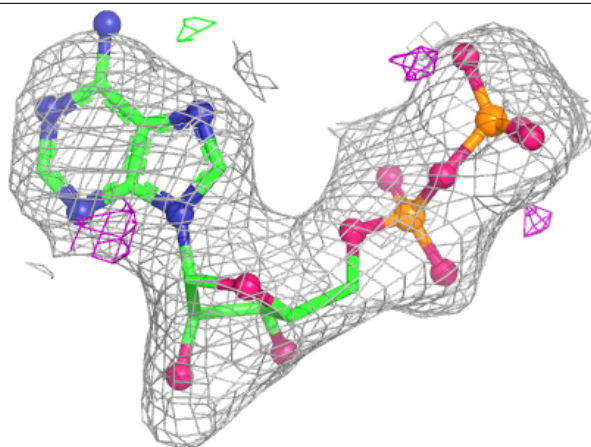
Electron density around ADP I 501:

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



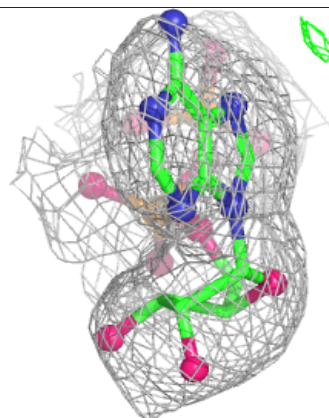
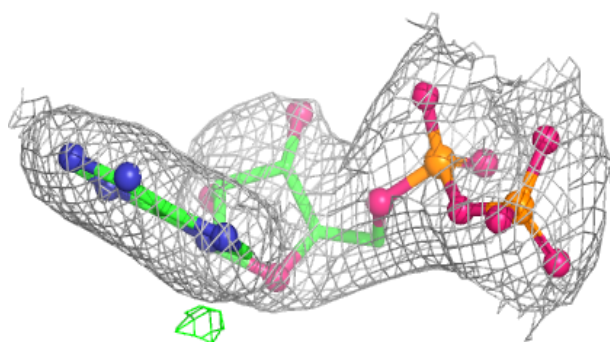
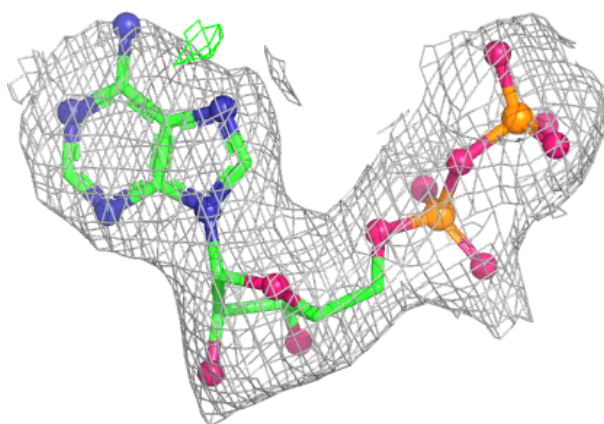
Electron density around ADP C 501:

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



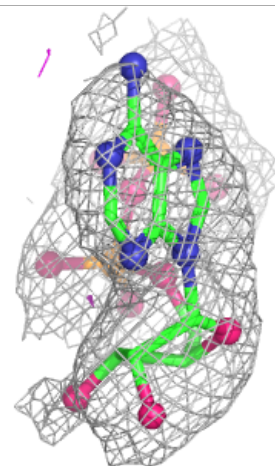
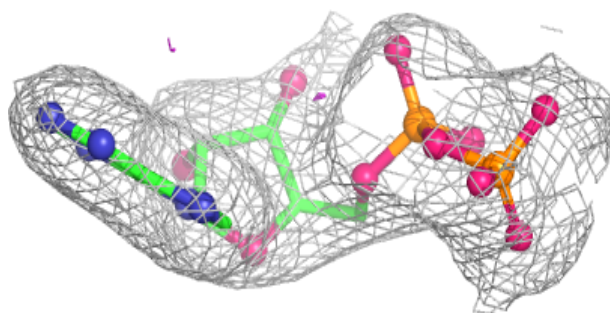
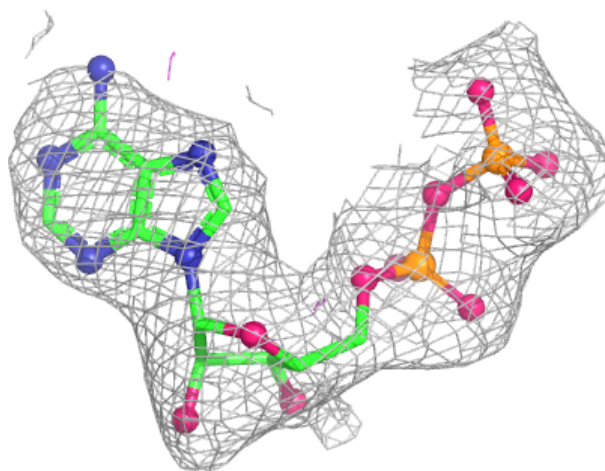
Electron density around ADP K 501:

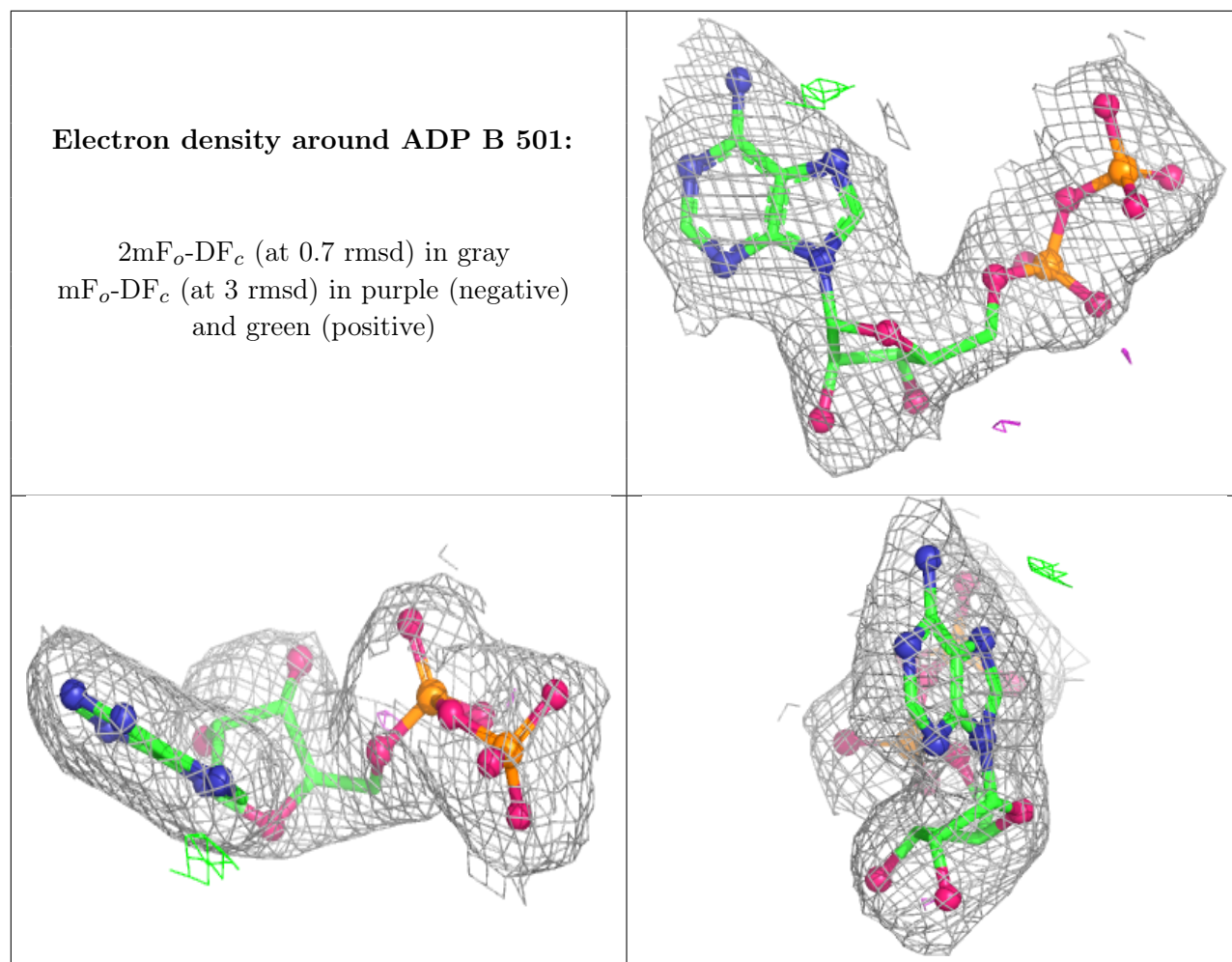
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP F 501:

$2mF_o-DF_c$ (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.