



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:09 PM UTC

PDB ID : 8KG2 / pdb_00008kg2
Title : Crystal structure of p97-N/D1 hexamer in complex with FAF1-UBX domain
Authors : Kang, W.
Deposited on : 2023-08-17
Resolution : 3.10 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

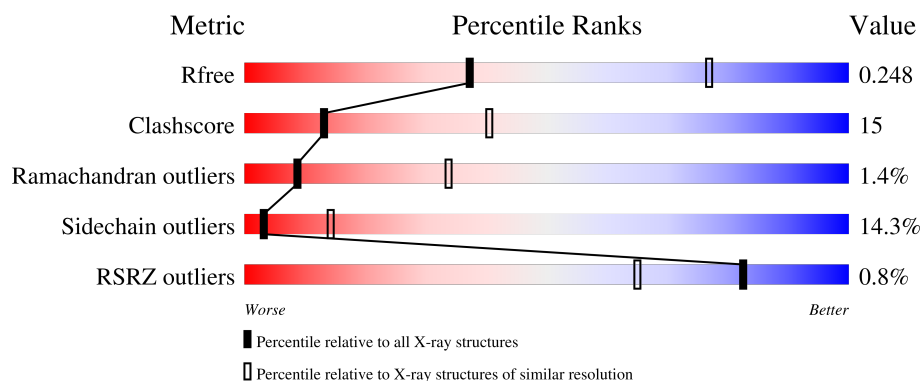
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	% 68% 26% 5% .
1	B	438	% 67% 26% 5% .
1	C	438	 68% 28% . .
1	D	438	 68% 26% . .
1	E	438	 68% 23% 7% .

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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	76	
2	N	76	
2	O	76	
2	P	76	
2	Q	76	
2	R	76	
2	S	76	
2	T	76	
2	U	76	
2	V	76	
2	W	76	
2	X	76	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 48735 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	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	B	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	C	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	D	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	E	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	F	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	G	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	H	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	I	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	J	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	K	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			
1	L	438	Total	C	N	O	S	0	0	0
			3422	2150	609	645	18			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	ALA	GLU	engineered mutation	UNP P55072
A	193	ALA	ASP	engineered mutation	UNP P55072
A	194	ALA	GLU	engineered mutation	UNP P55072
B	192	ALA	GLU	engineered mutation	UNP P55072
B	193	ALA	ASP	engineered mutation	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
B	194	ALA	GLU	engineered mutation	UNP P55072
C	192	ALA	GLU	engineered mutation	UNP P55072
C	193	ALA	ASP	engineered mutation	UNP P55072
C	194	ALA	GLU	engineered mutation	UNP P55072
D	192	ALA	GLU	engineered mutation	UNP P55072
D	193	ALA	ASP	engineered mutation	UNP P55072
D	194	ALA	GLU	engineered mutation	UNP P55072
E	192	ALA	GLU	engineered mutation	UNP P55072
E	193	ALA	ASP	engineered mutation	UNP P55072
E	194	ALA	GLU	engineered mutation	UNP P55072
F	192	ALA	GLU	engineered mutation	UNP P55072
F	193	ALA	ASP	engineered mutation	UNP P55072
F	194	ALA	GLU	engineered mutation	UNP P55072
G	192	ALA	GLU	engineered mutation	UNP P55072
G	193	ALA	ASP	engineered mutation	UNP P55072
G	194	ALA	GLU	engineered mutation	UNP P55072
H	192	ALA	GLU	engineered mutation	UNP P55072
H	193	ALA	ASP	engineered mutation	UNP P55072
H	194	ALA	GLU	engineered mutation	UNP P55072
I	192	ALA	GLU	engineered mutation	UNP P55072
I	193	ALA	ASP	engineered mutation	UNP P55072
I	194	ALA	GLU	engineered mutation	UNP P55072
J	192	ALA	GLU	engineered mutation	UNP P55072
J	193	ALA	ASP	engineered mutation	UNP P55072
J	194	ALA	GLU	engineered mutation	UNP P55072
K	192	ALA	GLU	engineered mutation	UNP P55072
K	193	ALA	ASP	engineered mutation	UNP P55072
K	194	ALA	GLU	engineered mutation	UNP P55072
L	192	ALA	GLU	engineered mutation	UNP P55072
L	193	ALA	ASP	engineered mutation	UNP P55072
L	194	ALA	GLU	engineered mutation	UNP P55072

- Molecule 2 is a protein called FAS-associated factor 1.

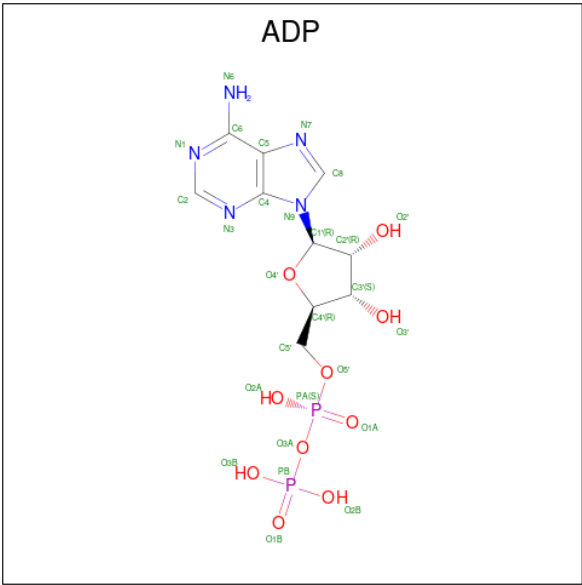
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	N	62	Total	C	N	O	0	0	0
			524	340	89	95			
2	O	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	P	76	Total	C	N	O	0	0	0
			637	417	107	113			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	R	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	S	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	T	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	U	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	V	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	W	53	Total	C	N	O	0	0	0
			453	299	79	75			
2	X	76	Total	C	N	O	0	0	0
			637	417	107	113			

- 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

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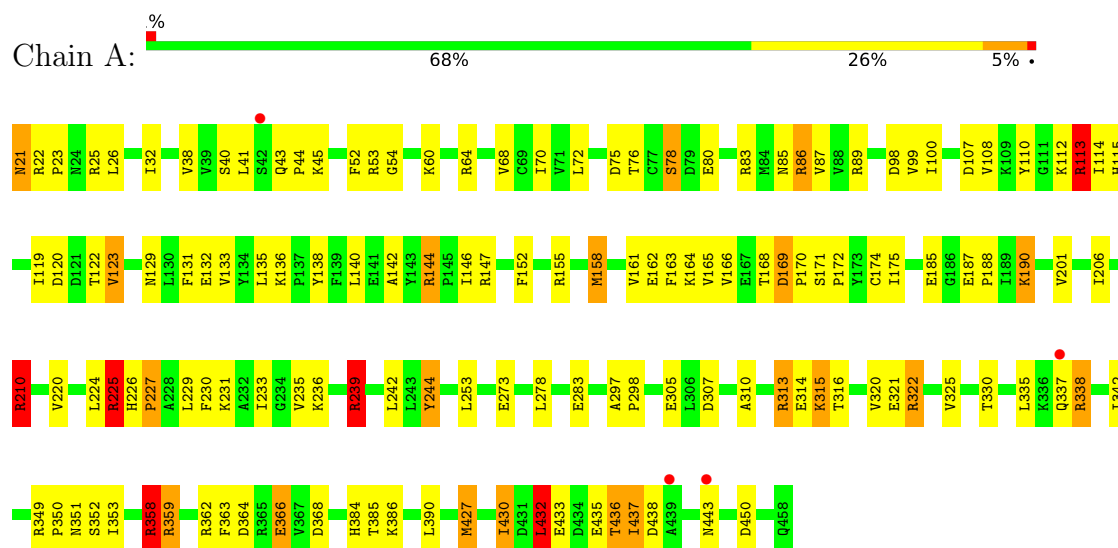
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5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

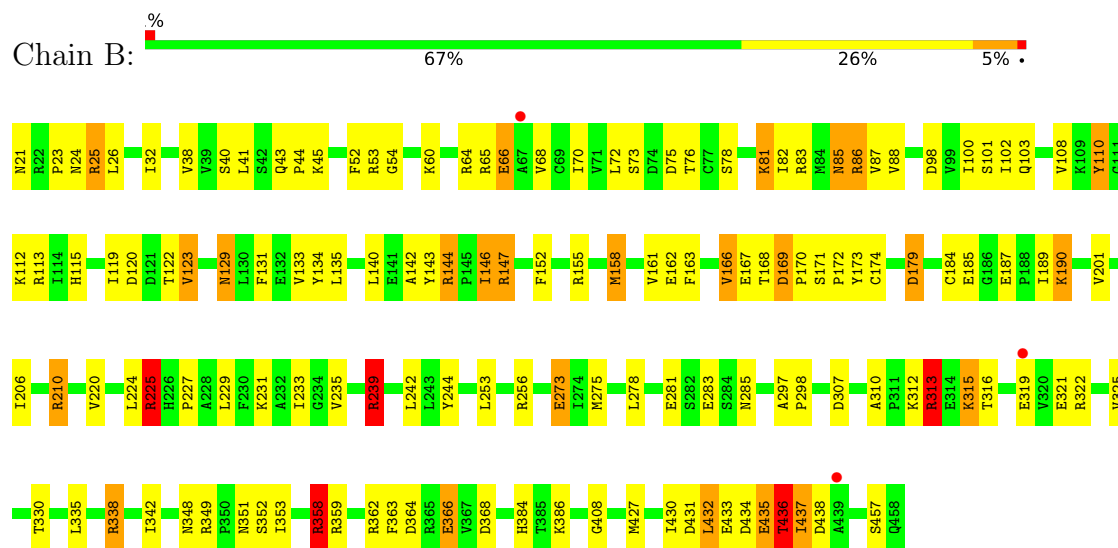
3 Residue-property plots

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

- Molecule 1: Transitional endoplasmic reticulum ATPase

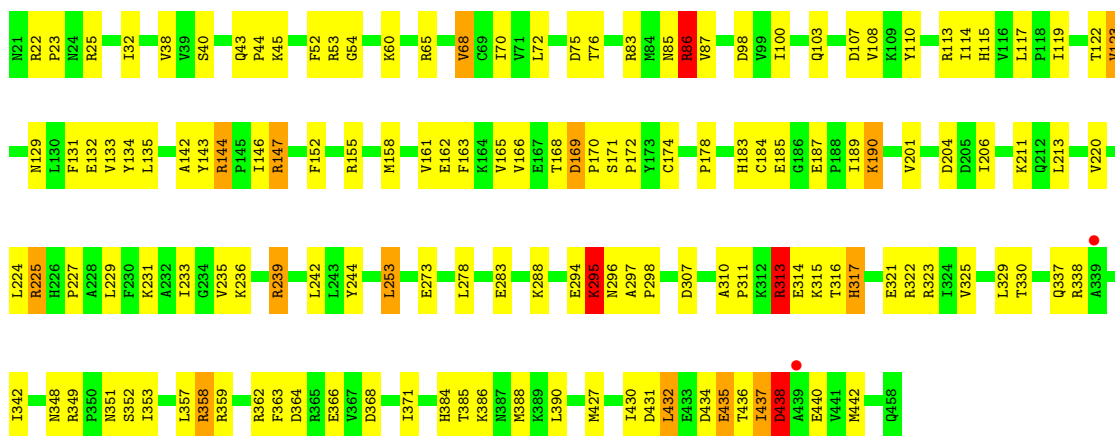


- Molecule 1: Transitional endoplasmic reticulum ATPase



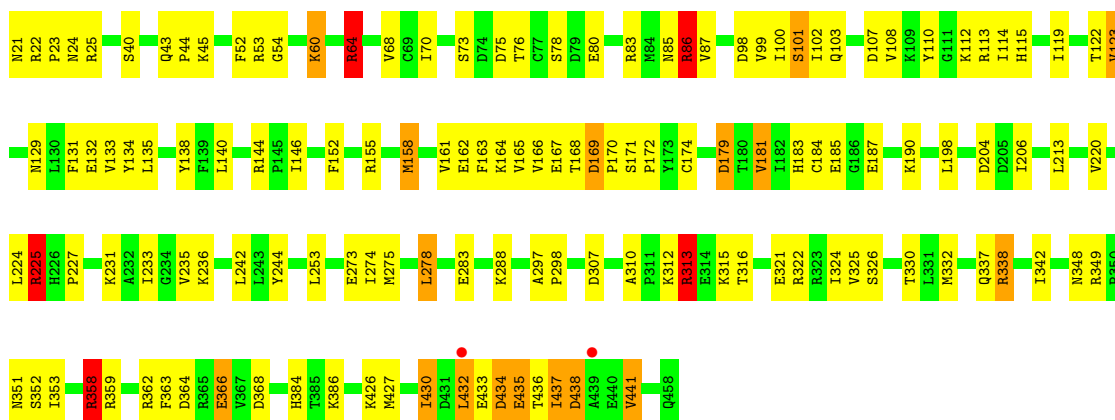
- Molecule 1: Transitional endoplasmic reticulum ATPase





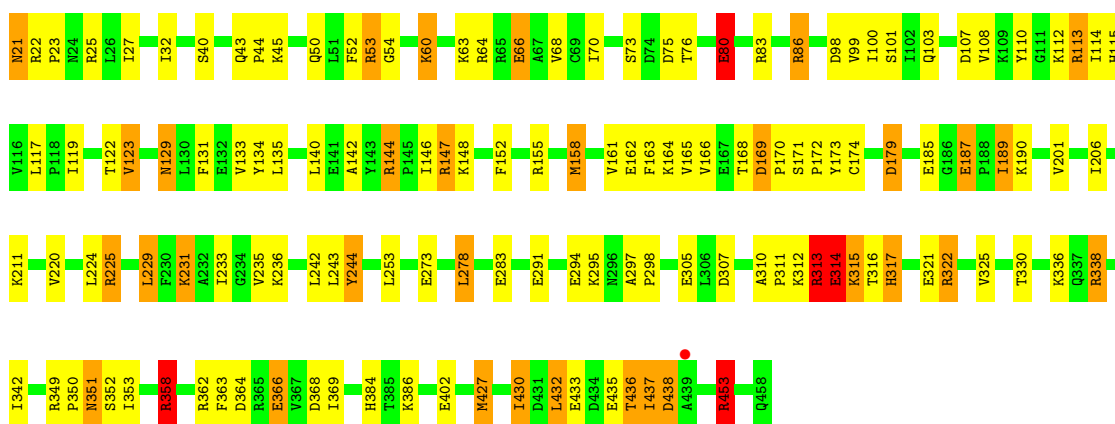
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D: 68% 26% • •



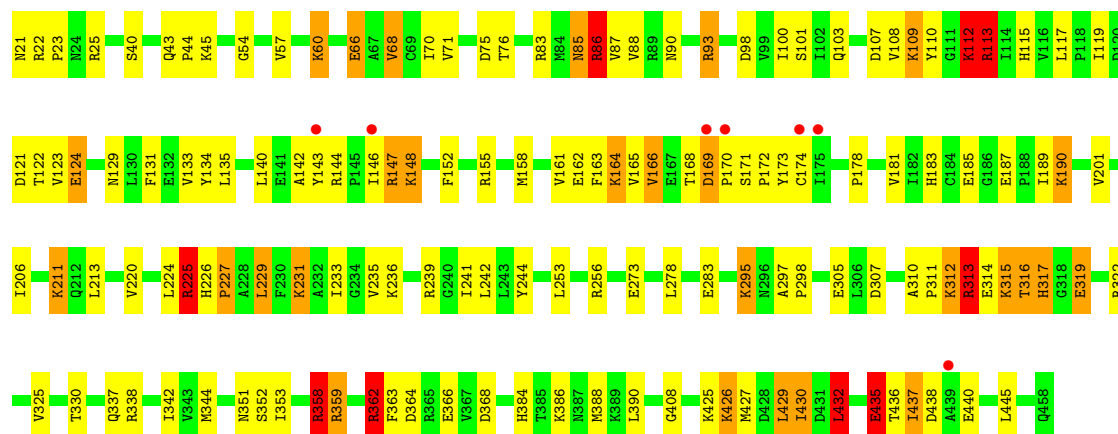
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E: 68% 23% 7% •



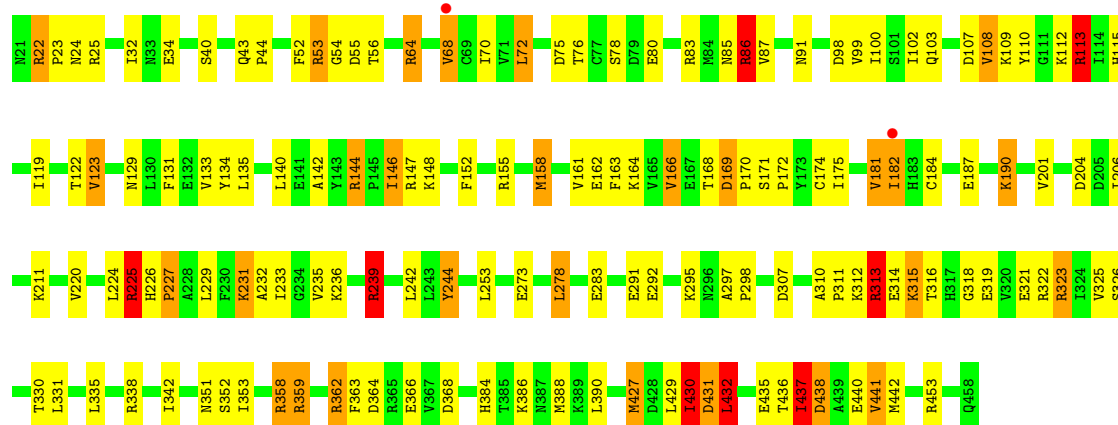
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F: 2% 66% 25% 6% •



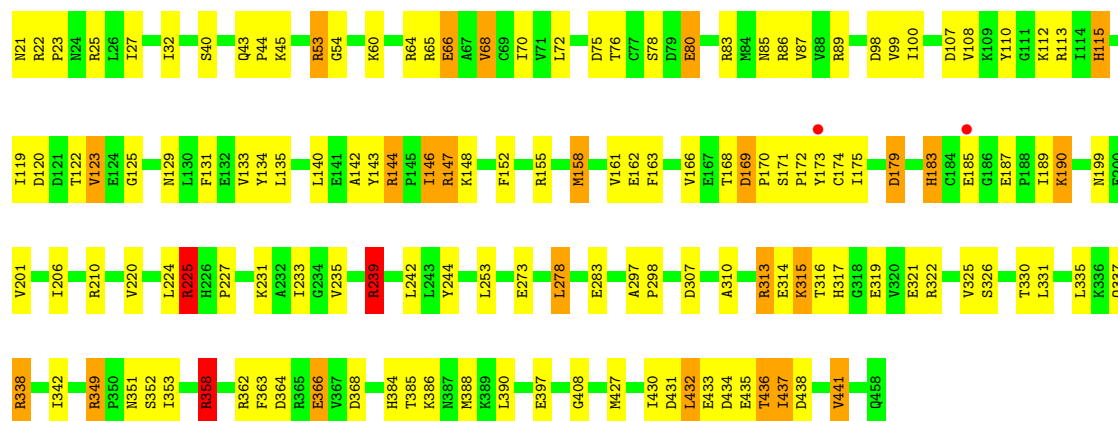
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain G: 66% 25% 6% •



• Molecule 1: Transitional endoplasmic reticulum ATPase

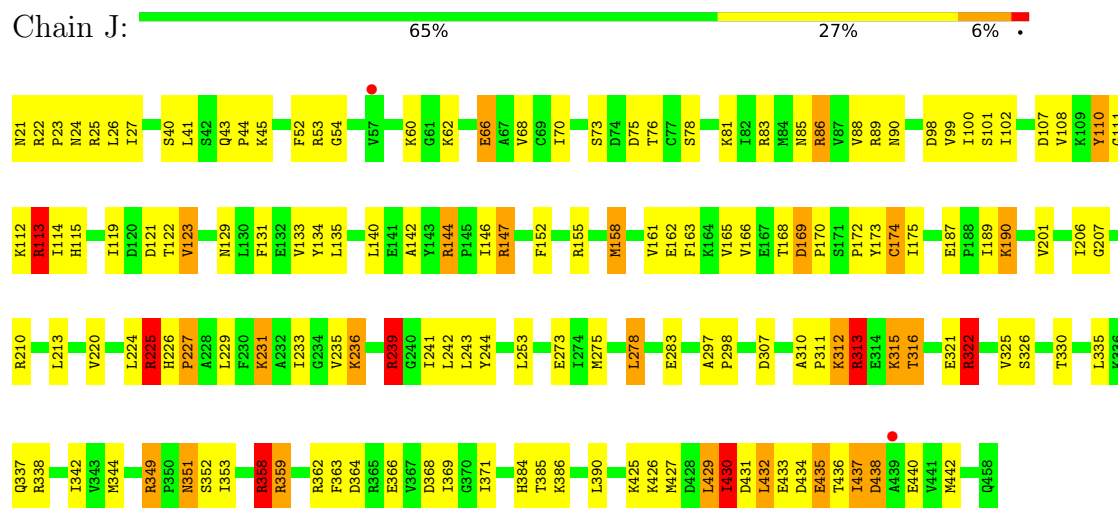
Chain H: 68% 26% 5% •



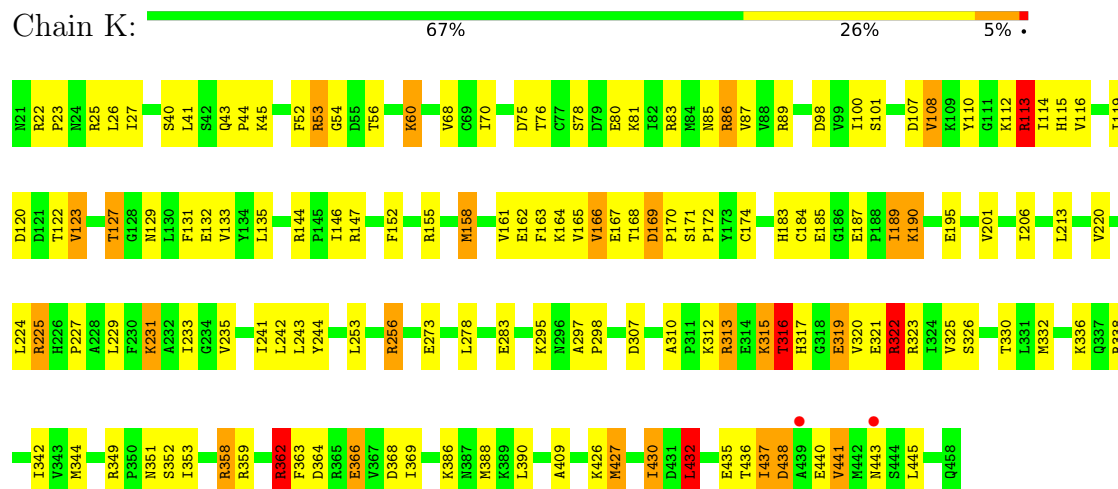
• Molecule 1: Transitional endoplasmic reticulum ATPase



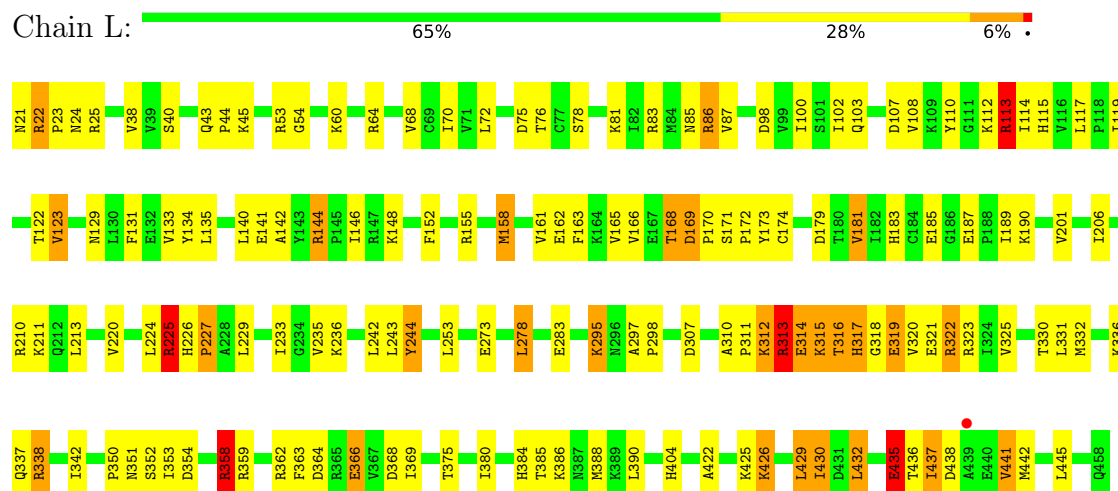
• Molecule 1: Transitional endoplasmic reticulum ATPase



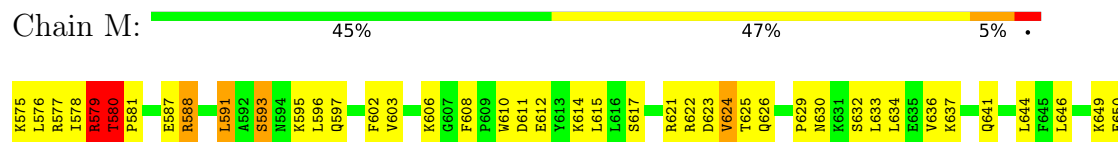
• Molecule 1: Transitional endoplasmic reticulum ATPase



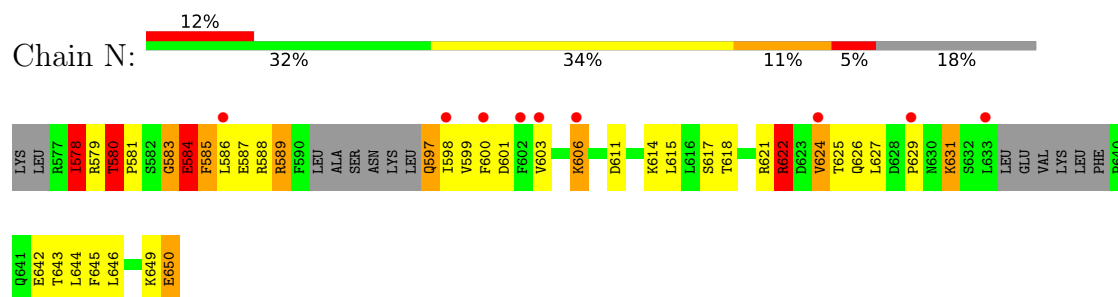
- Molecule 1: Transitional endoplasmic reticulum ATPase



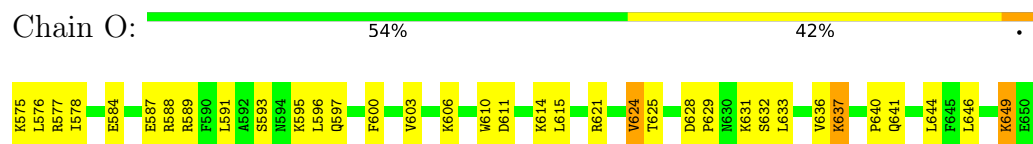
- Molecule 2: FAS-associated factor 1



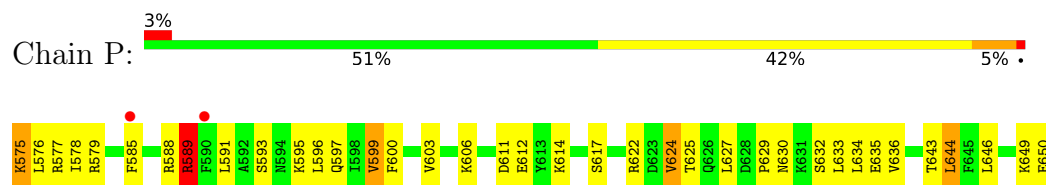
- Molecule 2: FAS-associated factor 1



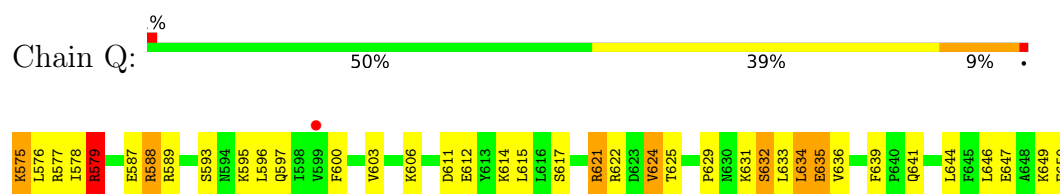
- Molecule 2: FAS-associated factor 1



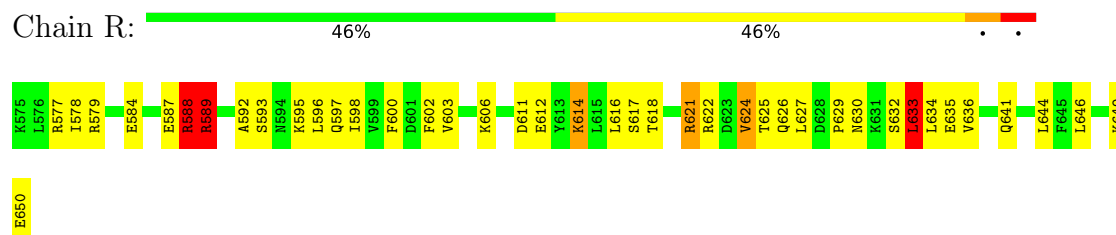
- Molecule 2: FAS-associated factor 1



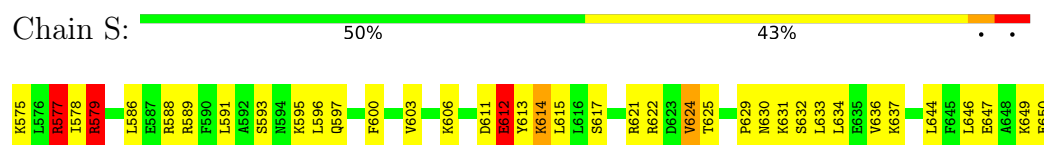
- Molecule 2: FAS-associated factor 1



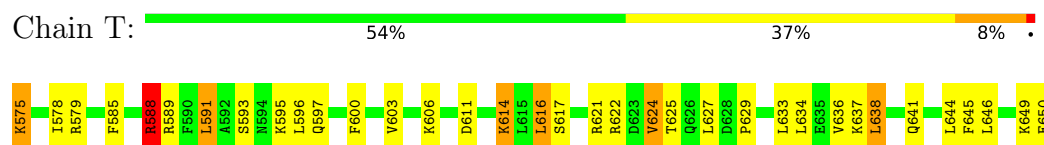
- Molecule 2: FAS-associated factor 1



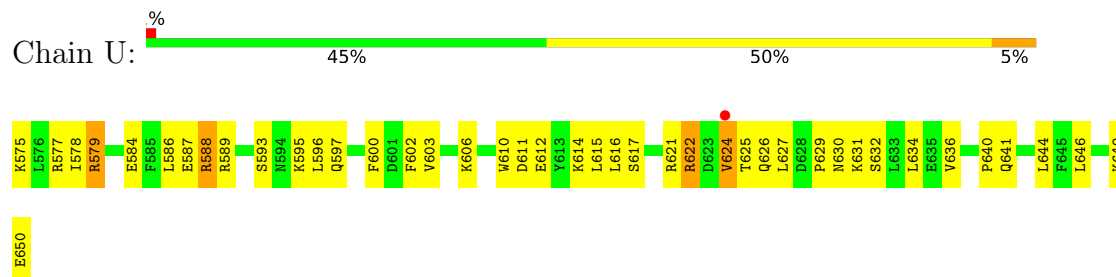
- Molecule 2: FAS-associated factor 1



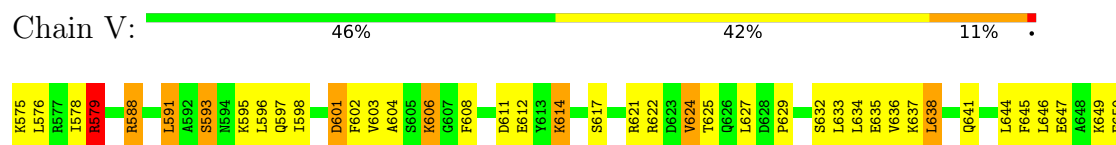
- Molecule 2: FAS-associated factor 1



- Molecule 2: FAS-associated factor 1



- Molecule 2: FAS-associated factor 1



- Molecule 2: FAS-associated factor 1





● Molecule 2: FAS-associated factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	106.67Å 134.48Å 148.22Å 71.52° 80.87° 87.53°	Depositor
Resolution (Å)	48.80 – 3.10 48.80 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.80-3.10) 97.4 (48.80-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.198 , 0.246 0.200 , 0.248	Depositor DCC
R_{free} test set	6798 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	48735	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.54	0/3475	1.15	9/4696 (0.2%)
1	B	0.55	0/3475	1.16	11/4696 (0.2%)
1	C	0.56	0/3475	1.15	7/4696 (0.1%)
1	D	0.55	0/3475	1.15	11/4696 (0.2%)
1	E	0.55	0/3475	1.16	12/4696 (0.3%)
1	F	0.57	0/3475	1.22	16/4696 (0.3%)
1	G	0.54	0/3475	1.16	7/4696 (0.1%)
1	H	0.55	0/3475	1.19	14/4696 (0.3%)
1	I	0.55	0/3475	1.16	11/4696 (0.2%)
1	J	0.56	0/3475	1.17	12/4696 (0.3%)
1	K	0.55	0/3475	1.18	17/4696 (0.4%)
1	L	0.53	0/3475	1.14	10/4696 (0.2%)
2	M	0.46	0/652	1.12	3/878 (0.3%)
2	N	0.74	0/536	1.58	13/719 (1.8%)
2	O	0.51	0/652	1.16	3/878 (0.3%)
2	P	0.50	0/652	1.15	5/878 (0.6%)
2	Q	0.45	0/652	1.15	3/878 (0.3%)
2	R	0.49	0/652	1.23	5/878 (0.6%)
2	S	0.47	0/652	1.13	3/878 (0.3%)
2	T	0.47	0/652	1.13	2/878 (0.2%)
2	U	0.47	0/652	1.14	4/878 (0.5%)
2	V	0.47	0/652	1.12	2/878 (0.2%)
2	W	0.54	0/461	1.31	3/613 (0.5%)
2	X	0.47	0/652	1.18	4/878 (0.5%)
All	All	0.54	0/49217	1.17	187/66464 (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	A	0	12
1	B	0	8
1	C	0	6
1	D	0	7
1	E	0	8
1	F	0	11
1	G	0	11
1	H	0	8
1	I	0	11
1	J	0	9
1	K	0	7
1	L	0	7
2	M	0	2
2	N	0	1
2	Q	0	2
2	R	0	2
2	S	0	3
2	T	0	2
2	U	0	1
2	V	0	1
2	X	0	2
All	All	0	121

There are no bond length outliers.

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	453	ARG	CG-CD-NE	11.97	138.34	112.00
2	Q	588	ARG	CB-CG-CD	11.23	137.13	111.30
1	F	93	ARG	NE-CZ-NH1	-11.12	110.38	121.50
1	H	115	HIS	CA-CB-CG	-11.05	102.75	113.80
1	H	358	ARG	NE-CZ-NH1	-10.88	110.62	121.50
2	X	623	ASP	CA-CB-CG	10.25	122.85	112.60
1	A	113	ARG	CB-CG-CD	10.24	134.86	111.30
1	H	183	HIS	CB-CG-CD2	10.18	144.44	131.20
2	O	588	ARG	CB-CG-CD	10.17	134.69	111.30
2	N	588	ARG	CG-CD-NE	9.76	133.48	112.00
1	L	435	GLU	CB-CG-CD	9.46	128.68	112.60
1	F	435	GLU	CB-CG-CD	9.28	128.38	112.60
2	N	597	GLN	CB-CA-C	9.23	127.64	110.10
2	S	589	ARG	CB-CG-CD	9.08	132.18	111.30
1	B	436	THR	CA-CB-OG1	8.94	123.01	109.60
1	I	168	THR	OG1-CB-CG2	-8.82	91.65	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	358	ARG	NE-CZ-NH2	8.60	126.94	119.20
1	F	113	ARG	CG-CD-NE	-8.06	94.27	112.00
1	I	168	THR	CA-CB-CG2	7.96	124.03	110.50
1	K	256	ARG	CB-CG-CD	7.88	129.43	111.30
1	F	112	LYS	CB-CA-C	7.87	124.96	110.56
1	K	168	THR	CA-CB-CG2	7.81	123.78	110.50
2	R	588	ARG	CG-CD-NE	7.80	129.16	112.00
1	D	86	ARG	NE-CZ-NH2	-7.75	112.23	119.20
1	D	86	ARG	NE-CZ-NH1	7.66	129.16	121.50
1	H	183	HIS	CB-CG-ND1	-7.53	111.41	122.70
1	K	256	ARG	CG-CD-NE	-7.39	95.73	112.00
1	C	438	ASP	CA-CB-CG	7.15	119.75	112.60
2	N	580	THR	CA-CB-OG1	7.11	120.26	109.60
2	X	579	ARG	CG-CD-NE	7.10	127.63	112.00
2	O	588	ARG	CG-CD-NE	-7.03	96.54	112.00
2	M	588	ARG	CB-CG-CD	7.01	127.42	111.30
1	K	168	THR	OG1-CB-CG2	-6.91	95.48	109.30
1	H	107	ASP	CA-CB-CG	-6.88	105.72	112.60
2	Q	579	ARG	NE-CZ-NH2	6.84	125.36	119.20
1	L	316	THR	CA-CB-OG1	-6.79	99.42	109.60
1	B	239	ARG	CG-CD-NE	6.78	126.93	112.00
1	K	127	THR	CB-CA-C	6.75	121.58	110.17
1	F	112	LYS	N-CA-CB	6.71	120.59	110.19
2	T	588	ARG	CG-CD-NE	-6.66	97.34	112.00
2	N	622	ARG	CB-CG-CD	6.65	126.59	111.30
1	B	103	GLN	CB-CG-CD	6.64	123.89	112.60
1	G	239	ARG	CG-CD-NE	6.63	126.59	112.00
1	C	239	ARG	CG-CD-NE	6.58	126.48	112.00
1	H	239	ARG	CG-CD-NE	6.55	126.42	112.00
1	E	80	GLU	CB-CG-CD	6.54	123.72	112.60
2	N	606	LYS	N-CA-C	6.54	118.74	110.24
1	E	314	GLU	CB-CG-CD	6.51	123.66	112.60
1	F	316	THR	CA-CB-OG1	-6.48	99.88	109.60
2	R	589	ARG	CB-CG-CD	6.48	126.20	111.30
1	L	314	GLU	CB-CG-CD	6.43	123.54	112.60
1	G	323	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	D	426	LYS	CG-CD-CE	6.40	126.01	111.30
1	A	358	ARG	NE-CZ-NH1	-6.33	115.17	121.50
1	J	316	THR	CA-CB-OG1	-6.30	100.15	109.60
2	R	614	LYS	CA-CB-CG	6.26	126.63	114.10
1	B	179	ASP	CA-CB-CG	6.26	118.86	112.60
1	J	358	ARG	NE-CZ-NH1	-6.25	115.25	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ARG	CB-CG-CD	6.25	125.67	111.30
1	H	179	ASP	CA-CB-CG	6.24	118.84	112.60
2	P	579	ARG	CB-CG-CD	6.24	125.64	111.30
2	X	588	ARG	CB-CG-CD	6.21	125.58	111.30
1	F	124	GLU	CB-CA-C	6.20	119.56	110.26
2	X	579	ARG	CB-CG-CD	6.17	125.49	111.30
1	A	239	ARG	CG-CD-NE	6.09	125.39	112.00
2	P	630	ASN	CA-CB-CG	6.07	118.67	112.60
1	I	168	THR	CA-CB-OG1	-6.07	100.50	109.60
2	R	633	LEU	CB-CA-C	6.01	122.20	110.67
1	F	426	LYS	CB-CG-CD	6.00	125.10	111.30
1	G	430	ILE	CB-CA-C	5.95	121.04	111.29
1	K	127	THR	CA-CB-CG2	5.94	120.60	110.50
1	K	168	THR	CA-CB-OG1	-5.90	100.75	109.60
2	P	612	GLU	CB-CG-CD	5.89	122.62	112.60
2	M	580	THR	CA-CB-OG1	5.83	118.34	109.60
1	B	147	ARG	CG-CD-NE	5.82	124.81	112.00
1	B	366	GLU	CB-CG-CD	5.80	122.46	112.60
1	E	50	GLN	CB-CG-CD	5.79	122.44	112.60
1	I	25	ARG	CB-CG-CD	5.78	124.59	111.30
1	K	127	THR	OG1-CB-CG2	-5.77	97.76	109.30
1	J	169	ASP	N-CA-CB	5.73	120.57	110.37
1	E	147	ARG	CG-CD-NE	5.73	124.60	112.00
2	W	606	LYS	CB-CA-C	5.73	121.82	110.42
1	D	179	ASP	CA-CB-CG	5.72	118.33	112.60
2	M	637	LYS	CB-CG-CD	5.72	124.47	111.30
1	H	80	GLU	CB-CG-CD	5.72	122.33	112.60
1	E	453	ARG	NE-CZ-NH2	5.71	124.34	119.20
2	N	585	PHE	CA-CB-CG	5.67	119.47	113.80
1	J	358	ARG	CB-CG-CD	5.65	124.29	111.30
1	F	358	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	B	85	ASN	CA-CB-CG	5.63	118.23	112.60
1	K	86	ARG	CD-NE-CZ	-5.63	116.52	124.40
1	A	358	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	B	52	PHE	CA-CB-CG	-5.61	108.19	113.80
1	C	295	LYS	CA-CB-CG	5.59	125.28	114.10
1	F	147	ARG	CG-CD-NE	5.58	124.28	112.00
2	U	622	ARG	NE-CZ-NH1	-5.57	115.93	121.50
2	N	626	GLN	CB-CG-CD	5.56	122.06	112.60
1	D	227	PRO	CB-CA-C	-5.56	103.54	112.21
1	L	366	GLU	CB-CG-CD	5.55	122.04	112.60
1	H	313	ARG	CB-CG-CD	-5.55	98.54	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	622	ARG	NE-CZ-NH2	5.54	124.19	119.20
2	N	631	LYS	CA-CB-CG	5.54	125.18	114.10
1	H	147	ARG	CG-CD-NE	5.54	124.18	112.00
1	J	86	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	J	147	ARG	CG-CD-NE	5.52	124.15	112.00
1	E	294	GLU	CB-CG-CD	5.52	121.98	112.60
2	N	578	ILE	CA-CB-CG1	5.52	119.78	110.40
2	U	575	LYS	CB-CG-CD	5.52	123.99	111.30
1	F	358	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	J	313	ARG	CB-CG-CD	5.51	123.97	111.30
1	B	81	LYS	CG-CD-CE	5.51	123.97	111.30
1	B	227	PRO	CB-CA-C	-5.50	103.63	112.21
1	D	313	ARG	NE-CZ-NH1	-5.49	116.01	121.50
2	N	650	GLU	CB-CA-C	5.48	120.51	110.10
2	V	601	ASP	CB-CA-C	5.48	120.17	110.85
1	B	358	ARG	CB-CG-CD	5.48	123.90	111.30
1	A	147	ARG	CG-CD-NE	-5.46	99.98	112.00
2	W	578	ILE	CB-CA-C	5.46	117.68	110.91
1	E	21	ASN	CA-C-N	5.45	127.97	120.39
1	E	21	ASN	C-N-CA	5.45	127.97	120.39
1	C	183	HIS	CB-CA-C	5.44	119.67	109.71
1	E	366	GLU	CB-CG-CD	5.43	121.83	112.60
2	S	614	LYS	CA-CB-CG	5.41	124.93	114.10
1	A	358	ARG	CB-CG-CD	5.41	123.75	111.30
1	A	227	PRO	CB-CA-C	-5.41	103.77	112.21
1	I	358	ARG	CB-CG-CD	5.40	123.72	111.30
1	J	113	ARG	CG-CD-NE	-5.39	100.15	112.00
2	Q	635	GLU	CB-CG-CD	5.37	121.74	112.60
1	D	86	ARG	CD-NE-CZ	5.37	131.92	124.40
2	P	612	GLU	CA-CB-CG	5.37	124.83	114.10
1	C	147	ARG	CG-CD-NE	-5.36	100.21	112.00
1	I	124	GLU	CB-CG-CD	5.36	121.71	112.60
1	F	295	LYS	CG-CD-CE	5.35	123.61	111.30
1	J	430	ILE	CB-CA-C	5.35	120.06	111.29
1	J	322	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	L	227	PRO	CB-CA-C	-5.34	103.88	112.21
1	D	183	HIS	CB-CA-C	5.34	119.48	109.71
1	H	366	GLU	CB-CG-CD	5.34	121.67	112.60
1	I	358	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	K	366	GLU	CB-CG-CD	5.31	121.63	112.60
1	H	166	VAL	CA-CB-CG2	5.30	119.41	110.40
2	R	579	ARG	CB-CG-CD	5.30	123.48	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	244	TYR	CB-CA-C	5.26	118.83	109.72
2	U	579	ARG	CG-CD-NE	5.26	123.58	112.00
1	F	227	PRO	CB-CA-C	-5.26	104.00	112.21
2	N	578	ILE	CA-C-O	-5.26	114.95	120.57
2	O	649	LYS	N-CA-CB	5.24	118.16	109.88
1	F	362	ARG	CA-C-O	-5.23	113.03	120.51
1	K	147	ARG	CG-CD-NE	-5.23	100.50	112.00
1	C	294	GLU	CB-CG-CD	5.23	121.49	112.60
1	E	179	ASP	CA-CB-CG	5.21	117.81	112.60
2	N	583	GLY	N-CA-C	5.21	119.25	112.68
1	G	113	ARG	NE-CZ-NH1	-5.21	116.28	121.50
1	L	183	HIS	CB-CA-C	5.20	119.23	109.71
1	D	358	ARG	CB-CG-CD	5.20	123.26	111.30
2	P	589	ARG	CG-CD-NE	-5.20	100.56	112.00
1	L	113	ARG	CB-CG-CD	5.19	123.23	111.30
1	L	426	LYS	CB-CG-CD	5.19	123.23	111.30
1	F	319	GLU	CB-CG-CD	5.18	121.41	112.60
1	L	317	HIS	CA-CB-CG	5.18	118.98	113.80
1	C	227	PRO	CB-CA-C	-5.17	104.14	112.21
1	H	227	PRO	CB-CA-C	-5.17	104.15	112.21
1	J	239	ARG	CG-CD-NE	-5.14	100.70	112.00
1	K	362	ARG	CA-C-O	-5.14	113.17	120.51
2	W	601	ASP	CA-CB-CG	5.13	117.73	112.60
1	K	227	PRO	CB-CA-C	-5.12	104.22	112.21
1	I	366	GLU	CB-CG-CD	5.11	121.29	112.60
1	G	244	TYR	CB-CA-C	5.11	118.56	109.72
1	G	227	PRO	CB-CA-C	-5.11	104.24	112.21
1	F	313	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	J	227	PRO	CB-CA-C	-5.10	104.26	112.21
1	L	244	TYR	CB-CA-C	5.10	118.54	109.72
1	I	227	PRO	CB-CA-C	-5.09	104.23	112.62
1	I	349	ARG	CG-CD-NE	-5.08	100.82	112.00
2	N	597	GLN	CB-CG-CD	5.07	121.21	112.60
1	K	183	HIS	CB-CA-C	5.06	118.98	109.71
1	K	322	ARG	NE-CZ-NH1	-5.06	116.44	121.50
2	T	614	LYS	CA-CB-CG	5.05	124.21	114.10
2	S	612	GLU	CA-CB-CG	5.03	124.17	114.10
2	V	650	GLU	CB-CG-CD	5.03	121.14	112.60
1	K	189	ILE	CA-CB-CG1	5.02	118.94	110.40
1	A	244	TYR	CB-CA-C	5.02	118.41	109.72
1	E	244	TYR	CB-CA-C	5.02	118.40	109.72
1	A	366	GLU	CB-CG-CD	5.01	121.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	366	GLU	CB-CG-CD	5.01	121.12	112.60
1	G	55	ASP	CA-CB-CG	5.00	117.60	112.60
1	K	316	THR	CA-CB-OG1	5.00	117.10	109.60

There are no chirality outliers.

All (121) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	144	ARG	Sidechain
1	A	210	ARG	Sidechain
1	A	22	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	239	ARG	Sidechain
1	A	322	ARG	Sidechain
1	A	358	ARG	Sidechain
1	A	359	ARG	Sidechain
1	A	64	ARG	Sidechain
1	A	86	ARG	Sidechain
1	A	89	ARG	Sidechain
1	B	144	ARG	Sidechain
1	B	225	ARG	Sidechain
1	B	239	ARG	Sidechain
1	B	25	ARG	Sidechain
1	B	313	ARG	Sidechain
1	B	338	ARG	Sidechain
1	B	358	ARG	Sidechain
1	B	86	ARG	Sidechain
1	C	144	ARG	Sidechain
1	C	22	ARG	Sidechain
1	C	239	ARG	Sidechain
1	C	313	ARG	Sidechain
1	C	358	ARG	Sidechain
1	C	86	ARG	Sidechain
1	D	144	ARG	Sidechain
1	D	22	ARG	Sidechain
1	D	225	ARG	Sidechain
1	D	313	ARG	Sidechain
1	D	358	ARG	Sidechain
1	D	53	ARG	Sidechain
1	D	86	ARG	Sidechain
1	E	144	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	313	ARG	Sidechain
1	E	322	ARG	Sidechain
1	E	338	ARG	Sidechain
1	E	358	ARG	Sidechain
1	E	453	ARG	Sidechain
1	E	53	ARG	Sidechain
1	E	86	ARG	Sidechain
1	F	113	ARG	Sidechain
1	F	144	ARG	Sidechain
1	F	22	ARG	Sidechain
1	F	225	ARG	Sidechain
1	F	239	ARG	Sidechain
1	F	313	ARG	Sidechain
1	F	358	ARG	Sidechain
1	F	362	ARG	Mainchain
1	F	85	ASN	Sidechain
1	F	86	ARG	Sidechain
1	F	93	ARG	Sidechain
1	G	113	ARG	Sidechain
1	G	144	ARG	Sidechain
1	G	22	ARG	Sidechain
1	G	225	ARG	Sidechain
1	G	239	ARG	Sidechain
1	G	313	ARG	Sidechain
1	G	323	ARG	Sidechain
1	G	358	ARG	Sidechain
1	G	362	ARG	Mainchain
1	G	53	ARG	Sidechain
1	G	86	ARG	Sidechain
1	H	144	ARG	Sidechain
1	H	21	ASN	Peptide
1	H	22	ARG	Sidechain
1	H	225	ARG	Sidechain
1	H	239	ARG	Sidechain
1	H	338	ARG	Sidechain
1	H	349	ARG	Sidechain
1	H	358	ARG	Sidechain
1	I	144	ARG	Sidechain
1	I	210	ARG	Sidechain
1	I	22	ARG	Sidechain
1	I	25	ARG	Sidechain
1	I	313	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	322	ARG	Sidechain
1	I	338	ARG	Sidechain
1	I	349	ARG	Sidechain
1	I	358	ARG	Sidechain
1	I	359	ARG	Sidechain
1	I	86	ARG	Sidechain
1	J	113	ARG	Sidechain
1	J	144	ARG	Sidechain
1	J	22	ARG	Sidechain
1	J	225	ARG	Sidechain
1	J	239	ARG	Sidechain
1	J	322	ARG	Sidechain
1	J	358	ARG	Sidechain
1	J	359	ARG	Sidechain
1	J	53	ARG	Sidechain
1	K	113	ARG	Sidechain
1	K	144	ARG	Sidechain
1	K	22	ARG	Sidechain
1	K	322	ARG	Sidechain
1	K	358	ARG	Sidechain
1	K	362	ARG	Mainchain,Sidechain
1	L	113	ARG	Sidechain
1	L	144	ARG	Sidechain
1	L	22	ARG	Sidechain
1	L	225	ARG	Sidechain
1	L	313	ARG	Sidechain
1	L	358	ARG	Sidechain
1	L	86	ARG	Sidechain
2	M	579	ARG	Sidechain
2	M	621	ARG	Sidechain
2	N	621	ARG	Sidechain
2	Q	579	ARG	Sidechain
2	Q	621	ARG	Sidechain
2	R	588	ARG	Sidechain
2	R	621	ARG	Sidechain
2	S	577	ARG	Sidechain
2	S	579	ARG	Sidechain
2	S	588	ARG	Sidechain
2	T	579	ARG	Sidechain
2	T	588	ARG	Sidechain
2	U	579	ARG	Sidechain
2	V	579	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	X	577	ARG	Sidechain
2	X	621	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3422	0	3486	97	3
1	B	3422	0	3486	108	0
1	C	3422	0	3486	95	4
1	D	3422	0	3486	93	0
1	E	3422	0	3486	100	0
1	F	3422	0	3486	117	0
1	G	3422	0	3486	109	3
1	H	3422	0	3486	114	4
1	I	3422	0	3486	96	0
1	J	3422	0	3486	117	0
1	K	3422	0	3486	110	0
1	L	3422	0	3486	118	0
2	M	637	0	652	32	0
2	N	524	0	517	32	0
2	O	637	0	652	19	0
2	P	637	0	652	28	0
2	Q	637	0	652	27	0
2	R	637	0	652	25	0
2	S	637	0	652	25	0
2	T	637	0	652	32	0
2	U	637	0	652	35	0
2	V	637	0	652	36	0
2	W	453	0	470	20	0
2	X	637	0	652	36	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
3	G	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	27	0	12	3	0
3	I	27	0	12	1	0
3	J	27	0	12	4	0
3	K	27	0	12	1	0
3	L	27	0	12	2	0
All	All	48735	0	49483	1460	7

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 15.

All (1460) 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:147:ARG:NH2	1:E:173:TYR:HD2	1.14	1.44
1:G:430:ILE:CD1	1:G:431:ASP:H	1.31	1.43
1:B:147:ARG:NH2	1:B:173:TYR:HD2	1.13	1.43
1:H:147:ARG:NH2	1:H:173:TYR:HD2	1.14	1.43
1:G:430:ILE:HD12	1:G:431:ASP:N	1.28	1.43
1:J:430:ILE:HD12	1:J:431:ASP:N	1.26	1.42
1:F:147:ARG:NH2	1:F:173:TYR:HD2	1.17	1.40
1:J:147:ARG:NH2	1:J:173:TYR:HD2	1.14	1.40
1:J:430:ILE:CD1	1:J:431:ASP:H	1.39	1.36
1:B:147:ARG:NH2	1:B:173:TYR:CD2	2.06	1.24
1:E:147:ARG:NH2	1:E:173:TYR:CD2	2.07	1.23
1:H:147:ARG:NH2	1:H:173:TYR:CD2	2.07	1.22
1:F:147:ARG:NH2	1:F:173:TYR:CD2	2.08	1.21
1:J:147:ARG:NH2	1:J:173:TYR:CD2	2.06	1.21
1:H:115:HIS:NE2	1:H:183:HIS:HB3	1.64	1.12
2:U:616:LEU:HD22	2:U:621:ARG:HH22	1.18	1.06
1:J:169:ASP:CG	1:J:170:PRO:HD3	1.82	1.04
2:O:614:LYS:HG3	2:O:649:LYS:HG2	1.38	1.03
1:J:313:ARG:HB2	1:J:322:ARG:HH22	1.19	1.03
1:C:325:VAL:O	1:C:329:LEU:HD13	1.61	1.01
1:K:437:ILE:HG23	1:K:441:VAL:HG22	1.42	1.01
1:D:437:ILE:HG23	1:D:441:VAL:HG22	1.43	1.00
1:H:437:ILE:HG23	1:H:441:VAL:HG22	1.43	1.00
1:J:112:LYS:H	1:J:169:ASP:CG	1.70	0.99
1:I:437:ILE:HG23	1:I:441:VAL:HG22	1.43	0.97
2:V:614:LYS:HG3	2:V:649:LYS:HG2	1.45	0.97
1:D:274:ILE:HG22	1:D:275:MET:HE2	1.47	0.97
2:Q:614:LYS:HG3	2:Q:649:LYS:HG2	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:614:LYS:HG3	2:N:649:LYS:HG2	1.43	0.96
2:U:614:LYS:HG3	2:U:649:LYS:HG2	1.46	0.96
2:P:614:LYS:HG3	2:P:649:LYS:HG2	1.48	0.95
1:J:112:LYS:N	1:J:169:ASP:OD1	2.00	0.95
2:M:614:LYS:HG3	2:M:649:LYS:HG2	1.46	0.94
2:X:614:LYS:HG3	2:X:649:LYS:HG2	1.45	0.94
1:J:437:ILE:HG23	1:J:438:ASP:H	1.33	0.93
1:L:114:ILE:HD12	1:L:168:THR:HB	1.50	0.93
1:C:329:LEU:HG	1:C:362:ARG:CZ	1.98	0.93
1:H:115:HIS:CD2	1:H:183:HIS:HB3	2.04	0.93
1:H:143:TYR:CE2	2:T:616:LEU:HD11	2.03	0.92
1:J:169:ASP:OD2	1:J:170:PRO:HD3	1.68	0.92
1:G:169:ASP:OD2	1:G:170:PRO:HD3	1.71	0.91
1:F:169:ASP:OD2	1:F:170:PRO:HD3	1.71	0.91
1:F:121:ASP:O	1:F:124:GLU:OE1	1.88	0.91
1:B:432:LEU:HA	1:D:21:ASN:HD22	1.34	0.91
1:E:169:ASP:OD2	1:E:170:PRO:HD3	1.71	0.91
1:K:316:THR:HG23	1:K:321:GLU:HG2	1.54	0.90
1:A:169:ASP:OD2	1:A:170:PRO:HD3	1.71	0.90
1:B:322:ARG:NH2	1:E:317:HIS:HD2	1.70	0.90
2:P:596:LEU:O	2:P:599:VAL:HG13	1.72	0.90
1:K:169:ASP:OD2	1:K:170:PRO:HD3	1.71	0.90
1:J:147:ARG:HH21	1:J:173:TYR:HD2	0.94	0.90
1:D:169:ASP:OD2	1:D:170:PRO:HD3	1.71	0.89
2:M:580:THR:HG23	2:M:608:PHE:CZ	2.07	0.89
1:L:422:ALA:O	1:L:425:LYS:HG2	1.73	0.89
1:B:169:ASP:OD2	1:B:170:PRO:HD3	1.71	0.89
1:H:169:ASP:OD2	1:H:170:PRO:HD3	1.71	0.89
1:B:110:TYR:HH	2:N:645:PHE:HD1	0.90	0.89
1:C:169:ASP:OD2	1:C:170:PRO:HD3	1.71	0.89
1:A:230:PHE:O	1:A:338:ARG:NH1	2.04	0.88
1:C:359:ARG:NH1	1:C:362:ARG:CD	2.36	0.88
1:K:316:THR:HG23	1:K:321:GLU:CG	2.04	0.88
1:L:169:ASP:OD2	1:L:170:PRO:HD3	1.72	0.88
1:A:129:ASN:ND2	1:A:132:GLU:HG2	1.90	0.87
1:H:147:ARG:HH22	1:H:173:TYR:HD2	1.21	0.87
2:T:616:LEU:CD1	2:T:645:PHE:HB2	2.04	0.87
1:D:129:ASN:ND2	1:D:132:GLU:HG2	1.89	0.87
1:A:133:VAL:HG13	1:A:443:ASN:CG	1.99	0.87
1:H:115:HIS:NE2	1:H:183:HIS:CB	2.36	0.87
1:I:129:ASN:ND2	1:I:132:GLU:HG2	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ASN:ND2	1:C:132:GLU:HG2	1.89	0.87
1:J:425:LYS:O	1:J:429:LEU:HD22	1.74	0.87
1:H:432:LEU:HB3	1:J:21:ASN:HD22	1.40	0.86
1:G:135:LEU:HD13	1:G:182:ILE:HD11	1.56	0.86
1:J:147:ARG:HH22	1:J:173:TYR:HD2	1.21	0.86
1:E:147:ARG:HH22	1:E:173:TYR:HD2	1.22	0.86
1:B:321:GLU:OE2	1:D:322:ARG:HD3	1.76	0.85
1:L:78:SER:HB2	1:L:81:LYS:HD3	1.58	0.85
1:B:147:ARG:HH22	1:B:173:TYR:HD2	1.21	0.85
1:K:129:ASN:ND2	1:K:132:GLU:HG2	1.90	0.85
1:F:147:ARG:HH22	1:F:173:TYR:HD2	1.23	0.85
1:H:147:ARG:HH21	1:H:173:TYR:HD2	0.95	0.85
1:D:275:MET:HE1	1:D:324:ILE:HG21	1.58	0.85
1:E:147:ARG:HH21	1:E:173:TYR:HD2	0.95	0.84
1:G:113:ARG:HA	1:G:181:VAL:HG13	1.59	0.84
1:K:313:ARG:HH12	1:L:315:LYS:HB3	1.42	0.83
1:F:85:ASN:HD21	1:F:87:VAL:HG23	1.44	0.82
1:I:169:ASP:HB3	1:I:170:PRO:HD3	1.62	0.82
1:B:110:TYR:OH	2:N:645:PHE:HD1	1.62	0.81
1:G:318:GLY:HA3	1:L:319:GLU:OE2	1.79	0.81
1:D:113:ARG:HA	1:D:181:VAL:HG13	1.62	0.81
2:W:578:ILE:HG23	2:W:586:LEU:HB2	1.63	0.81
1:A:313:ARG:HA	1:A:316:THR:HG22	1.63	0.81
1:L:113:ARG:HA	1:L:181:VAL:HG13	1.62	0.81
1:B:432:LEU:HB3	1:D:21:ASN:HB2	1.62	0.81
1:C:329:LEU:HG	1:C:362:ARG:NH1	1.96	0.80
1:J:168:THR:HG21	1:J:174:CYS:HB3	1.62	0.80
1:C:359:ARG:NH1	1:C:362:ARG:HD2	1.96	0.80
1:H:143:TYR:HE2	2:T:616:LEU:CD1	1.94	0.80
1:G:321:GLU:OE2	1:L:322:ARG:HD2	1.81	0.80
1:L:114:ILE:CD1	1:L:168:THR:HA	2.12	0.80
2:U:627:LEU:HD13	2:U:636:VAL:HG13	1.63	0.79
1:B:432:LEU:CA	1:D:21:ASN:HD22	1.95	0.79
1:C:313:ARG:HA	1:C:316:THR:HG22	1.65	0.78
2:M:580:THR:HG23	2:M:608:PHE:HZ	1.46	0.78
2:R:633:LEU:HA	2:R:636:VAL:HG22	1.66	0.78
2:U:600:PHE:HB3	2:U:610:TRP:NE1	1.99	0.78
1:H:143:TYR:CE2	2:T:616:LEU:CD1	2.65	0.77
1:J:384:HIS:HE1	3:J:501:ADP:N3	1.83	0.76
1:K:437:ILE:HG23	1:K:441:VAL:CG2	2.15	0.76
1:A:432:LEU:HB3	1:F:21:ASN:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:ARG:HH21	1:F:173:TYR:HD2	0.97	0.76
1:D:437:ILE:HG23	1:D:441:VAL:CG2	2.16	0.76
1:H:430:ILE:HG22	1:H:430:ILE:O	1.86	0.75
2:N:583:GLY:O	2:N:584:GLU:HB2	1.85	0.75
2:T:616:LEU:HD11	2:T:645:PHE:HB2	1.68	0.75
1:C:437:ILE:O	1:C:438:ASP:HB3	1.86	0.75
1:F:57:VAL:HG11	1:F:71:VAL:HG21	1.68	0.75
1:H:113:ARG:H	1:H:169:ASP:HB2	1.51	0.75
1:A:313:ARG:HH12	1:C:311:PRO:HG3	1.50	0.75
2:P:643:THR:O	2:P:644:LEU:HD13	1.87	0.75
2:N:615:LEU:O	2:N:624:VAL:HG23	1.87	0.74
1:H:437:ILE:HG23	1:H:441:VAL:CG2	2.16	0.74
2:U:588:ARG:CZ	2:U:602:PHE:HB3	2.17	0.74
1:L:114:ILE:HD12	1:L:168:THR:CB	2.17	0.74
1:C:359:ARG:NH1	1:C:362:ARG:HD3	2.03	0.74
1:G:232:ALA:HA	1:I:159:ARG:NH2	2.02	0.74
1:F:113:ARG:NH2	1:F:183:HIS:HB3	2.01	0.74
1:E:437:ILE:HG22	1:E:438:ASP:H	1.53	0.74
1:F:113:ARG:H	1:F:169:ASP:HB2	1.51	0.74
1:B:430:ILE:O	1:B:430:ILE:HG22	1.87	0.74
2:V:633:LEU:HD13	2:V:638:LEU:HD21	1.69	0.74
1:K:133:VAL:HG13	1:K:443:ASN:CG	2.12	0.73
1:G:113:ARG:H	1:G:169:ASP:HB2	1.53	0.73
1:I:437:ILE:HG23	1:I:441:VAL:CG2	2.16	0.73
1:B:113:ARG:H	1:B:169:ASP:HB2	1.53	0.73
1:L:384:HIS:HE1	3:L:501:ADP:N3	1.86	0.73
1:C:430:ILE:HG22	1:C:430:ILE:O	1.89	0.73
1:L:113:ARG:H	1:L:169:ASP:HB2	1.54	0.73
1:E:435:GLU:HG2	1:E:436:THR:H	1.54	0.73
1:D:113:ARG:H	1:D:169:ASP:HB2	1.54	0.72
2:T:633:LEU:HD13	2:T:638:LEU:HD21	1.69	0.72
1:H:115:HIS:CE1	1:H:183:HIS:HB3	2.23	0.72
1:K:437:ILE:CG2	1:K:441:VAL:HG22	2.19	0.72
1:A:113:ARG:H	1:A:169:ASP:HB2	1.54	0.72
1:C:113:ARG:H	1:C:169:ASP:HB2	1.53	0.72
1:E:113:ARG:H	1:E:169:ASP:HB2	1.54	0.72
1:H:437:ILE:HG22	1:H:438:ASP:H	1.54	0.72
1:L:114:ILE:HD13	1:L:168:THR:HA	1.71	0.71
1:J:430:ILE:CD1	1:J:431:ASP:N	2.17	0.71
2:N:578:ILE:HD12	2:N:644:LEU:HB2	1.71	0.71
1:A:349:ARG:NH2	1:A:350:PRO:HD2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:437:ILE:HG23	1:G:438:ASP:H	1.56	0.71
1:A:133:VAL:HG13	1:A:443:ASN:OD1	1.91	0.71
1:A:437:ILE:CG2	1:F:229:LEU:HD11	2.21	0.71
1:A:322:ARG:HH22	1:C:317:HIS:CD2	2.09	0.70
1:A:437:ILE:HG22	1:F:229:LEU:CD1	2.21	0.70
1:I:437:ILE:CG2	1:I:441:VAL:HG22	2.20	0.70
1:K:113:ARG:H	1:K:169:ASP:HB2	1.54	0.70
2:X:594:ASN:HB3	2:X:598:ILE:HG21	1.72	0.70
1:L:141:GLU:HB2	2:X:621:ARG:NH2	2.07	0.70
1:H:437:ILE:CG2	1:H:441:VAL:HG22	2.22	0.70
1:B:312:LYS:HD3	1:B:315:LYS:HE2	1.73	0.69
1:D:437:ILE:HG22	1:D:438:ASP:H	1.56	0.69
1:E:384:HIS:HE1	3:E:501:ADP:N3	1.90	0.69
1:G:437:ILE:HG13	1:G:441:VAL:HG22	1.74	0.69
2:U:627:LEU:CD1	2:U:636:VAL:HG13	2.21	0.69
2:W:598:ILE:HD13	2:W:601:ASP:OD2	1.92	0.69
1:G:437:ILE:CD1	1:G:441:VAL:HG22	2.23	0.69
2:X:580:THR:HG23	2:X:586:LEU:HD21	1.74	0.69
1:D:274:ILE:CG2	1:D:275:MET:HE2	2.20	0.69
1:K:437:ILE:HG22	1:K:438:ASP:H	1.57	0.69
2:S:612:GLU:HG3	2:S:613:TYR:CD2	2.27	0.69
1:L:437:ILE:HG23	1:L:438:ASP:H	1.58	0.69
1:B:319:GLU:OE1	1:E:321:GLU:HG2	1.92	0.69
2:M:588:ARG:HD3	2:M:602:PHE:CD1	2.27	0.69
1:B:60:LYS:NZ	1:B:64:ARG:HA	2.08	0.68
1:A:52:PHE:CZ	2:M:641:GLN:HB3	2.28	0.68
1:C:388:MET:CE	1:C:390:LEU:HD21	2.23	0.68
1:I:384:HIS:HE1	3:I:501:ADP:N3	1.92	0.68
1:I:437:ILE:HG22	1:I:438:ASP:H	1.57	0.68
1:L:388:MET:CE	1:L:390:LEU:HD21	2.23	0.68
1:C:329:LEU:HG	1:C:362:ARG:NH2	2.07	0.68
1:F:388:MET:CE	1:F:390:LEU:HD21	2.23	0.68
1:H:143:TYR:HE2	2:T:616:LEU:HD11	1.54	0.68
1:E:402:GLU:OE2	1:E:453:ARG:NH2	2.26	0.68
1:F:311:PRO:HG2	1:F:316:THR:HG22	1.76	0.68
1:G:437:ILE:HG12	1:G:442:MET:HE2	1.75	0.68
1:A:158:MET:HG2	1:F:235:VAL:HG23	1.74	0.68
1:L:437:ILE:HG13	1:L:441:VAL:HG22	1.75	0.68
2:V:638:LEU:HD12	2:V:638:LEU:O	1.93	0.68
1:C:322:ARG:HD3	1:D:321:GLU:OE2	1.94	0.68
1:H:388:MET:CE	1:H:390:LEU:HD21	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:ILE:HG12	1:F:253:LEU:HD23	1.76	0.68
1:D:437:ILE:CG2	1:D:441:VAL:HG22	2.22	0.67
1:L:311:PRO:HG2	1:L:316:THR:HG22	1.74	0.67
1:F:85:ASN:HD21	1:F:87:VAL:CG2	2.06	0.67
1:H:430:ILE:HG23	1:H:434:ASP:HB3	1.76	0.67
1:A:437:ILE:HG23	1:A:438:ASP:H	1.60	0.67
1:K:430:ILE:HD12	1:K:430:ILE:C	2.20	0.67
2:N:603:VAL:HG11	2:N:615:LEU:CD2	2.24	0.67
1:I:388:MET:CE	1:I:390:LEU:HD21	2.25	0.67
1:B:158:MET:HG2	1:D:235:VAL:HG23	1.77	0.67
1:I:113:ARG:H	1:I:169:ASP:HB2	1.57	0.67
2:W:596:LEU:HD22	2:W:600:PHE:CZ	2.30	0.67
1:G:388:MET:CE	1:G:390:LEU:HD21	2.25	0.67
1:K:388:MET:CE	1:K:390:LEU:HD21	2.25	0.67
1:H:27:ILE:HD13	1:H:99:VAL:HG22	1.76	0.66
1:A:349:ARG:NH2	1:A:350:PRO:CD	2.59	0.66
1:A:52:PHE:CE1	2:M:641:GLN:HB3	2.31	0.66
1:E:169:ASP:CG	1:E:170:PRO:HD3	2.21	0.66
1:H:115:HIS:HD2	1:H:185:GLU:OE2	1.78	0.66
1:H:317:HIS:CE1	1:J:313:ARG:HH12	2.13	0.66
1:C:169:ASP:CG	1:C:170:PRO:HD3	2.21	0.66
1:F:169:ASP:CG	1:F:170:PRO:HD3	2.20	0.66
1:F:437:ILE:HG23	1:F:438:ASP:H	1.59	0.66
1:H:169:ASP:CG	1:H:170:PRO:HD3	2.20	0.66
1:C:430:ILE:HG23	1:C:434:ASP:HB3	1.77	0.66
1:E:430:ILE:C	1:E:430:ILE:HD12	2.20	0.66
1:A:436:THR:HG22	1:F:226:HIS:HD2	1.59	0.66
1:G:437:ILE:CG1	1:G:441:VAL:HG22	2.26	0.66
1:A:169:ASP:CG	1:A:170:PRO:HD3	2.21	0.66
1:D:169:ASP:CG	1:D:170:PRO:HD3	2.21	0.66
1:G:319:GLU:OE2	1:I:320:VAL:HG12	1.95	0.65
1:C:329:LEU:HA	1:C:362:ARG:NH2	2.12	0.65
1:K:316:THR:HG23	1:K:321:GLU:HG3	1.77	0.65
1:G:169:ASP:CG	1:G:170:PRO:HD3	2.20	0.65
1:L:169:ASP:CG	1:L:170:PRO:HD3	2.21	0.65
2:M:591:LEU:HD11	2:U:589:ARG:HB3	1.79	0.65
1:K:169:ASP:CG	1:K:170:PRO:HD3	2.20	0.65
1:G:430:ILE:HD12	1:G:431:ASP:CA	2.24	0.65
1:H:206:ILE:HG12	1:H:253:LEU:HD23	1.78	0.65
1:L:437:ILE:CG1	1:L:441:VAL:HG22	2.27	0.65
1:A:129:ASN:HD22	1:A:132:GLU:CG	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASP:CG	1:B:170:PRO:HD3	2.21	0.65
1:B:115:HIS:CE1	1:B:185:GLU:HB2	2.32	0.65
1:F:384:HIS:HE1	3:F:501:ADP:N3	1.94	0.65
1:I:129:ASN:HD22	1:I:132:GLU:CG	2.10	0.65
1:K:129:ASN:HD22	1:K:132:GLU:CG	2.10	0.65
1:L:206:ILE:HG12	1:L:253:LEU:HD23	1.78	0.65
1:H:436:THR:HG22	1:J:226:HIS:HD2	1.62	0.64
1:A:53:ARG:HG3	1:A:72:LEU:HD23	1.79	0.64
1:E:435:GLU:HG2	1:E:436:THR:N	2.12	0.64
1:I:120:ASP:OD2	1:I:190:LYS:HD2	1.97	0.64
1:A:437:ILE:HG22	1:F:229:LEU:HD12	1.79	0.64
1:B:430:ILE:HG23	1:B:434:ASP:HB3	1.79	0.64
1:D:206:ILE:HG12	1:D:253:LEU:HD23	1.79	0.64
1:I:129:ASN:ND2	1:I:132:GLU:CG	2.61	0.64
1:C:129:ASN:ND2	1:C:132:GLU:CG	2.61	0.64
1:D:129:ASN:HD22	1:D:132:GLU:CG	2.09	0.64
1:I:236:LYS:HD2	1:I:337:GLN:OE1	1.97	0.64
1:K:26:LEU:HD13	1:K:41:LEU:HD21	1.79	0.64
1:L:437:ILE:CD1	1:L:441:VAL:HG22	2.27	0.64
1:L:437:ILE:HG12	1:L:442:MET:HE2	1.80	0.64
1:I:206:ILE:HG12	1:I:253:LEU:HD23	1.80	0.64
1:K:313:ARG:NH1	1:L:315:LYS:HB3	2.12	0.64
1:E:27:ILE:HD13	1:E:99:VAL:HG22	1.79	0.64
1:K:129:ASN:ND2	1:K:132:GLU:CG	2.62	0.64
1:K:316:THR:CG2	1:K:321:GLU:CG	2.76	0.63
1:J:206:ILE:HG12	1:J:253:LEU:HD23	1.80	0.63
1:K:206:ILE:HG12	1:K:253:LEU:HD23	1.80	0.63
2:Q:614:LYS:HG3	2:Q:649:LYS:CG	2.27	0.63
1:L:122:THR:HG21	1:L:162:GLU:HB2	1.79	0.63
2:U:614:LYS:HG3	2:U:649:LYS:CG	2.27	0.63
1:A:129:ASN:ND2	1:A:132:GLU:CG	2.61	0.63
1:B:322:ARG:NH2	1:E:317:HIS:CD2	2.59	0.63
2:N:603:VAL:HG11	2:N:615:LEU:HD22	1.78	0.63
1:G:437:ILE:HD11	1:G:441:VAL:HG22	1.77	0.63
1:J:243:LEU:HD22	1:J:369:ILE:HD11	1.79	0.63
1:K:243:LEU:HD22	1:K:369:ILE:HD11	1.78	0.63
1:A:122:THR:HG21	1:A:162:GLU:HB2	1.80	0.63
1:B:26:LEU:HD13	1:B:41:LEU:HD21	1.81	0.63
2:N:617:SER:HB3	2:N:622:ARG:HG2	1.81	0.63
1:C:129:ASN:HD22	1:C:132:GLU:CG	2.10	0.63
1:E:122:THR:HG21	1:E:162:GLU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:THR:HG21	1:G:162:GLU:HB2	1.80	0.63
1:H:122:THR:HG21	1:H:162:GLU:HB2	1.81	0.63
1:J:122:THR:HG21	1:J:162:GLU:HB2	1.80	0.63
1:J:311:PRO:HG2	1:J:316:THR:HG22	1.80	0.63
1:C:206:ILE:HG12	1:C:253:LEU:HD23	1.80	0.63
1:E:206:ILE:HG12	1:E:253:LEU:HD23	1.80	0.63
1:H:98:ASP:OD1	1:H:225:ARG:NH2	2.31	0.63
2:T:638:LEU:O	2:T:638:LEU:HD12	1.99	0.63
2:U:617:SER:HB3	2:U:622:ARG:HG2	1.81	0.63
1:B:147:ARG:HH21	1:B:173:TYR:HB3	1.64	0.62
1:G:98:ASP:OD1	1:G:225:ARG:NH2	2.30	0.62
1:L:243:LEU:HD22	1:L:369:ILE:HD11	1.80	0.62
1:B:432:LEU:HA	1:D:21:ASN:ND2	2.09	0.62
1:D:129:ASN:ND2	1:D:132:GLU:CG	2.61	0.62
1:J:147:ARG:HH21	1:J:173:TYR:HB3	1.64	0.62
1:K:122:THR:HG21	1:K:162:GLU:HB2	1.81	0.62
1:B:122:THR:HG21	1:B:162:GLU:HB2	1.81	0.62
2:N:600:PHE:CZ	2:N:627:LEU:O	2.51	0.62
2:R:617:SER:HB3	2:R:622:ARG:HG2	1.80	0.62
1:J:427:MET:O	1:J:430:ILE:HG13	2.00	0.62
1:L:437:ILE:HD11	1:L:441:VAL:HG22	1.80	0.62
2:W:587:GLU:OE2	2:W:589:ARG:HG3	2.00	0.62
1:F:57:VAL:HG21	1:F:71:VAL:HG22	1.80	0.62
1:H:187:GLU:N	1:H:187:GLU:OE1	2.31	0.62
1:H:235:VAL:HG23	1:K:158:MET:HG2	1.81	0.62
1:L:114:ILE:CD1	1:L:168:THR:CB	2.77	0.62
1:L:236:LYS:NZ	1:L:337:GLN:HG3	2.14	0.62
1:D:122:THR:HG21	1:D:162:GLU:HB2	1.81	0.62
1:A:206:ILE:HG12	1:A:253:LEU:HD23	1.81	0.62
2:R:588:ARG:HH11	2:R:588:ARG:HB3	1.65	0.62
1:G:99:VAL:HG21	1:I:431:ASP:HB2	1.80	0.62
1:G:206:ILE:HG12	1:G:253:LEU:HD23	1.80	0.62
1:I:108:VAL:HG22	1:I:175:ILE:HG13	1.82	0.62
1:H:115:HIS:CD2	1:H:185:GLU:OE2	2.52	0.62
2:T:649:LYS:O	2:T:650:GLU:C	2.43	0.62
2:U:616:LEU:HD22	2:U:621:ARG:NH2	2.03	0.62
1:E:427:MET:HE2	1:E:430:ILE:CG1	2.30	0.61
1:H:27:ILE:CD1	1:H:99:VAL:HG22	2.29	0.61
1:I:122:THR:HG21	1:I:162:GLU:HB2	1.80	0.61
1:E:147:ARG:HH21	1:E:173:TYR:HB3	1.65	0.61
2:S:617:SER:HB3	2:S:622:ARG:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:HG2	1:D:235:VAL:CG2	2.30	0.61
1:C:122:THR:HG21	1:C:162:GLU:HB2	1.82	0.61
1:H:108:VAL:HG22	1:H:175:ILE:HG13	1.82	0.61
1:H:147:ARG:HH21	1:H:173:TYR:HB3	1.65	0.61
1:J:113:ARG:H	1:J:169:ASP:HB3	1.64	0.61
1:B:235:VAL:HG23	1:E:158:MET:HG2	1.82	0.61
1:J:168:THR:CG2	1:J:174:CYS:HB3	2.30	0.61
2:Q:617:SER:HB3	2:Q:622:ARG:HG2	1.83	0.61
1:J:175:ILE:HD12	2:V:579:ARG:NH2	2.15	0.61
1:F:122:THR:HG21	1:F:162:GLU:HB2	1.81	0.61
1:I:21:ASN:N	1:J:432:LEU:HD22	2.16	0.61
2:P:614:LYS:HG3	2:P:649:LYS:CG	2.27	0.61
2:X:578:ILE:O	2:X:586:LEU:HD22	2.01	0.61
2:S:649:LYS:O	2:S:650:GLU:C	2.43	0.61
1:A:320:VAL:HG11	1:F:319:GLU:HG3	1.83	0.60
1:E:27:ILE:CD1	1:E:99:VAL:HG22	2.31	0.60
1:A:384:HIS:HE1	3:A:501:ADP:N3	1.99	0.60
1:E:427:MET:HA	1:E:430:ILE:HG13	1.82	0.60
2:N:578:ILE:HG23	2:N:615:LEU:HD11	1.83	0.60
1:A:322:ARG:HD2	1:C:321:GLU:OE2	2.00	0.60
1:B:437:ILE:HG23	1:B:438:ASP:H	1.65	0.60
1:C:53:ARG:HG3	1:C:72:LEU:HD23	1.81	0.60
1:I:98:ASP:OD1	1:I:225:ARG:NH2	2.31	0.60
2:U:615:LEU:O	2:U:624:VAL:HG23	2.01	0.60
2:V:614:LYS:HG3	2:V:649:LYS:CG	2.25	0.60
1:C:325:VAL:O	1:C:329:LEU:CD1	2.44	0.60
1:J:98:ASP:OD1	1:J:225:ARG:NH2	2.32	0.60
2:U:636:VAL:HG12	2:U:636:VAL:O	2.01	0.60
2:X:617:SER:HB3	2:X:622:ARG:HG2	1.83	0.60
1:G:427:MET:O	1:G:430:ILE:HG13	2.00	0.60
2:M:649:LYS:O	2:M:650:GLU:C	2.44	0.60
1:H:108:VAL:CG2	1:H:175:ILE:HG13	2.32	0.60
1:B:53:ARG:HG2	1:B:72:LEU:HD23	1.82	0.60
1:B:66:GLU:OE2	1:B:147:ARG:HD3	2.02	0.60
1:E:243:LEU:HD22	1:E:369:ILE:HD11	1.83	0.60
2:O:615:LEU:O	2:O:624:VAL:HG23	2.02	0.60
1:J:60:LYS:HB2	1:J:101:SER:OG	2.02	0.60
1:K:427:MET:HA	1:K:430:ILE:HG13	1.84	0.60
1:B:206:ILE:HG12	1:B:253:LEU:HD23	1.83	0.60
1:C:357:LEU:HD23	1:C:362:ARG:NH2	2.17	0.60
1:I:243:LEU:HD22	1:I:369:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:614:LYS:HG3	2:X:649:LYS:CG	2.25	0.60
2:X:649:LYS:O	2:X:650:GLU:C	2.45	0.60
1:H:437:ILE:HG22	1:H:438:ASP:N	2.17	0.59
2:T:588:ARG:NH1	2:T:589:ARG:H	2.00	0.59
1:D:437:ILE:HG22	1:D:438:ASP:N	2.17	0.59
1:G:86:ARG:HD2	1:G:204:ASP:OD2	2.03	0.59
1:H:66:GLU:CD	1:H:147:ARG:HD3	2.27	0.59
1:H:432:LEU:CB	1:J:21:ASN:HD22	2.14	0.59
1:A:158:MET:HG2	1:F:235:VAL:CG2	2.32	0.59
1:K:220:VAL:HG12	1:K:342:ILE:HD12	1.84	0.59
1:K:427:MET:HE3	1:K:430:ILE:HD11	1.84	0.59
1:E:66:GLU:CD	1:E:147:ARG:HD3	2.28	0.59
1:F:66:GLU:CD	1:F:147:ARG:HD3	2.28	0.59
2:P:617:SER:HB3	2:P:622:ARG:HG2	1.84	0.59
2:R:649:LYS:O	2:R:650:GLU:C	2.45	0.59
2:U:649:LYS:O	2:U:650:GLU:C	2.45	0.59
1:A:322:ARG:HH22	1:C:317:HIS:HD2	1.48	0.59
1:G:52:PHE:HE1	2:S:575:LYS:HE3	1.67	0.59
1:H:66:GLU:OE2	1:H:147:ARG:HD3	2.03	0.59
1:L:114:ILE:HD12	1:L:168:THR:HA	1.81	0.59
1:F:425:LYS:O	1:F:429:LEU:HD22	2.02	0.59
1:I:108:VAL:CG2	1:I:175:ILE:HG13	2.33	0.59
1:J:66:GLU:CD	1:J:147:ARG:HD3	2.27	0.59
1:A:133:VAL:CG1	1:A:443:ASN:CG	2.74	0.59
1:B:98:ASP:OD1	1:B:225:ARG:NH2	2.32	0.59
1:F:316:THR:O	1:F:316:THR:OG1	2.21	0.59
1:I:437:ILE:HG22	1:I:438:ASP:N	2.17	0.59
1:K:133:VAL:HG13	1:K:443:ASN:OD1	2.03	0.59
2:P:575:LYS:N	2:P:575:LYS:HD2	2.18	0.59
1:J:66:GLU:OE2	1:J:147:ARG:HD3	2.02	0.59
1:E:66:GLU:OE2	1:E:147:ARG:HD3	2.02	0.59
1:E:164:LYS:HE2	1:E:189:ILE:HD12	1.84	0.59
2:Q:575:LYS:HD2	2:Q:589:ARG:HE	1.68	0.59
1:G:56:THR:HG21	1:G:108:VAL:HG11	1.85	0.59
1:E:98:ASP:OD1	1:E:225:ARG:NH2	2.31	0.59
2:P:596:LEU:HD12	2:P:599:VAL:HG11	1.83	0.59
1:H:431:ASP:HB2	1:J:99:VAL:HG21	1.85	0.59
1:H:120:ASP:OD2	1:H:190:LYS:HD2	2.03	0.58
1:K:129:ASN:HD22	1:K:132:GLU:HG2	1.67	0.58
1:L:437:ILE:HG23	1:L:438:ASP:N	2.18	0.58
2:Q:649:LYS:O	2:Q:650:GLU:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:ASP:CG	1:J:170:PRO:CD	2.69	0.58
1:L:220:VAL:HG12	1:L:342:ILE:HD12	1.84	0.58
1:A:437:ILE:HG23	1:A:438:ASP:N	2.18	0.58
1:E:231:LYS:HE2	1:E:338:ARG:HG3	1.84	0.58
2:Q:632:SER:HB3	2:Q:635:GLU:HG2	1.85	0.58
2:N:600:PHE:HZ	2:N:627:LEU:O	1.87	0.58
2:T:617:SER:HB3	2:T:622:ARG:HG2	1.85	0.58
2:V:617:SER:HB3	2:V:622:ARG:HG2	1.84	0.58
1:B:66:GLU:CD	1:B:147:ARG:HD3	2.28	0.58
1:C:86:ARG:HD2	1:C:204:ASP:OD2	2.03	0.58
2:O:628:ASP:OD1	2:O:631:LYS:HG2	2.04	0.58
1:B:60:LYS:HB3	1:B:101:SER:OG	2.03	0.58
1:F:437:ILE:HG23	1:F:438:ASP:N	2.18	0.58
2:Q:589:ARG:HB3	2:T:591:LEU:HD11	1.83	0.58
2:X:633:LEU:HA	2:X:636:VAL:HG22	1.86	0.58
1:A:98:ASP:OD1	1:A:225:ARG:NH2	2.31	0.58
1:F:86:ARG:O	1:F:90:ASN:ND2	2.34	0.58
2:V:633:LEU:HA	2:V:636:VAL:HG22	1.86	0.58
1:F:147:ARG:HH21	1:F:173:TYR:HB3	1.69	0.58
1:I:169:ASP:HB3	1:I:170:PRO:CD	2.31	0.58
1:J:430:ILE:HD12	1:J:431:ASP:CA	2.25	0.58
1:A:220:VAL:HG12	1:A:342:ILE:HD12	1.86	0.58
2:P:633:LEU:HA	2:P:636:VAL:HG22	1.86	0.58
1:L:98:ASP:OD1	1:L:225:ARG:NH2	2.30	0.58
1:G:437:ILE:HG23	1:G:438:ASP:N	2.17	0.58
1:L:244:TYR:CZ	1:L:368:ASP:HB2	2.39	0.58
1:K:437:ILE:HG22	1:K:438:ASP:N	2.18	0.57
2:S:633:LEU:HA	2:S:636:VAL:HG22	1.85	0.57
1:F:85:ASN:ND2	1:F:87:VAL:HG23	2.18	0.57
2:M:588:ARG:HD3	2:M:602:PHE:CE1	2.38	0.57
1:J:316:THR:O	1:J:316:THR:OG1	2.22	0.57
1:K:244:TYR:CZ	1:K:368:ASP:HB2	2.39	0.57
2:T:633:LEU:HA	2:T:636:VAL:HG22	1.86	0.57
2:X:580:THR:CG2	2:X:586:LEU:HD21	2.34	0.57
1:F:57:VAL:CG1	1:F:71:VAL:HG21	2.33	0.57
1:H:115:HIS:NE2	1:H:183:HIS:CG	2.72	0.57
1:I:220:VAL:HG12	1:I:342:ILE:HD12	1.87	0.57
1:J:220:VAL:HG12	1:J:342:ILE:HD12	1.85	0.57
1:L:425:LYS:O	1:L:429:LEU:HD22	2.05	0.57
1:D:98:ASP:OD1	1:D:225:ARG:NH2	2.31	0.57
1:J:244:TYR:CZ	1:J:368:ASP:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:VAL:HG12	1:D:342:ILE:HD12	1.85	0.57
1:E:220:VAL:HG12	1:E:342:ILE:HD12	1.85	0.57
2:M:633:LEU:HA	2:M:636:VAL:HG22	1.85	0.57
1:G:220:VAL:HG12	1:G:342:ILE:HD12	1.87	0.57
1:B:120:ASP:OD2	1:B:190:LYS:HD2	2.04	0.57
1:E:244:TYR:CZ	1:E:368:ASP:HB2	2.39	0.57
1:F:244:TYR:CZ	1:F:368:ASP:HB2	2.39	0.57
2:N:580:THR:HG22	2:N:581:PRO:HD2	1.87	0.57
1:G:52:PHE:CE2	2:S:577:ARG:HG2	2.40	0.57
1:G:244:TYR:CZ	1:G:368:ASP:HB2	2.39	0.57
1:A:244:TYR:CZ	1:A:368:ASP:HB2	2.39	0.57
1:C:98:ASP:OD1	1:C:225:ARG:NH2	2.31	0.57
2:Q:633:LEU:HA	2:Q:636:VAL:HG22	1.85	0.57
1:I:244:TYR:CZ	1:I:368:ASP:HB2	2.39	0.57
1:K:120:ASP:OD2	1:K:190:LYS:HD2	2.04	0.57
1:B:244:TYR:CZ	1:B:368:ASP:HB2	2.40	0.57
1:G:311:PRO:HB2	1:G:315:LYS:HD3	1.87	0.57
2:X:623:ASP:OD1	2:X:626:GLN:HG2	2.04	0.57
1:F:220:VAL:HG12	1:F:342:ILE:HD12	1.87	0.57
2:N:614:LYS:HG3	2:N:649:LYS:CG	2.26	0.57
2:O:575:LYS:HE2	2:O:589:ARG:HD3	1.86	0.57
1:H:143:TYR:HE2	2:T:616:LEU:HD13	1.68	0.57
2:X:615:LEU:HB3	2:X:624:VAL:HG22	1.87	0.57
2:M:614:LYS:HG3	2:M:649:LYS:CG	2.27	0.57
1:G:52:PHE:CE1	2:S:575:LYS:HE3	2.39	0.57
1:H:244:TYR:CZ	1:H:368:ASP:HB2	2.39	0.57
1:J:26:LEU:HD13	1:J:41:LEU:HD21	1.87	0.57
1:K:146:ILE:HD12	1:K:165:VAL:HG11	1.87	0.57
1:D:244:TYR:CZ	1:D:368:ASP:HB2	2.39	0.56
1:F:66:GLU:OE2	1:F:147:ARG:HD3	2.04	0.56
2:W:579:ARG:N	2:W:644:LEU:O	2.37	0.56
2:X:585:PHE:C	2:X:586:LEU:HD13	2.30	0.56
1:A:52:PHE:CE1	2:M:575:LYS:HD2	2.40	0.56
1:B:437:ILE:HG23	1:B:438:ASP:N	2.20	0.56
1:D:60:LYS:HB2	1:D:101:SER:OG	2.05	0.56
1:E:427:MET:CE	1:E:430:ILE:HG12	2.35	0.56
1:F:98:ASP:OD1	1:F:225:ARG:NH2	2.31	0.56
2:R:589:ARG:HB2	2:V:591:LEU:HD11	1.87	0.56
2:N:583:GLY:O	2:N:584:GLU:CB	2.53	0.56
1:G:384:HIS:HE1	3:G:501:ADP:N3	2.04	0.56
1:K:56:THR:HG21	1:K:108:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:615:LEU:HB3	2:S:624:VAL:HG22	1.88	0.56
1:C:220:VAL:HG12	1:C:342:ILE:HD12	1.86	0.56
1:D:146:ILE:HD12	1:D:165:VAL:HG11	1.88	0.56
1:K:115:HIS:CE1	1:K:185:GLU:HB2	2.40	0.56
2:O:633:LEU:HA	2:O:636:VAL:HG22	1.86	0.56
1:K:316:THR:CG2	1:K:321:GLU:HG2	2.33	0.56
2:T:616:LEU:CG	2:T:645:PHE:HB2	2.34	0.56
1:C:244:TYR:CZ	1:C:368:ASP:HB2	2.39	0.56
1:G:169:ASP:CB	1:G:170:PRO:HD3	2.36	0.56
1:A:26:LEU:HD13	1:A:41:LEU:HD21	1.87	0.56
1:E:60:LYS:HB2	1:E:101:SER:OG	2.05	0.56
2:M:617:SER:HB3	2:M:622:ARG:HG2	1.86	0.56
1:G:430:ILE:HD12	1:G:431:ASP:H	0.45	0.56
1:H:169:ASP:CB	1:H:170:PRO:HD3	2.36	0.56
1:J:52:PHE:HA	2:V:641:GLN:OE1	2.06	0.56
2:V:638:LEU:HD12	2:V:638:LEU:C	2.31	0.56
2:X:575:LYS:HD2	2:X:589:ARG:HE	1.71	0.56
1:G:53:ARG:CZ	1:G:72:LEU:HD23	2.36	0.55
1:G:158:MET:HG2	1:L:235:VAL:HG23	1.88	0.55
1:K:233:ILE:HG22	1:L:442:MET:HG2	1.87	0.55
1:K:316:THR:CG2	1:K:321:GLU:HG3	2.35	0.55
1:K:53:ARG:O	2:W:643:THR:OG1	2.06	0.55
1:L:236:LYS:HZ2	1:L:337:GLN:HG3	1.70	0.55
2:W:580:THR:HG22	2:W:586:LEU:HD11	1.88	0.55
1:F:113:ARG:NH2	1:F:115:HIS:HB2	2.21	0.55
1:K:133:VAL:HG11	1:K:443:ASN:ND2	2.21	0.55
1:L:437:ILE:HD11	1:L:441:VAL:CG2	2.36	0.55
1:B:384:HIS:HE1	3:B:501:ADP:N3	2.04	0.55
1:E:437:ILE:O	1:E:438:ASP:HB2	2.05	0.55
1:B:430:ILE:O	1:B:430:ILE:CG2	2.55	0.55
2:Q:596:LEU:HD13	2:Q:636:VAL:HG21	1.89	0.55
2:Q:615:LEU:HB3	2:Q:624:VAL:HG22	1.87	0.55
1:G:437:ILE:CD1	1:G:441:VAL:CG2	2.84	0.55
1:I:60:LYS:HB2	1:I:101:SER:OG	2.07	0.55
1:J:437:ILE:CG2	1:J:438:ASP:H	2.11	0.55
1:K:133:VAL:CG1	1:K:443:ASN:CG	2.78	0.55
1:K:235:VAL:HG23	1:L:158:MET:HG2	1.89	0.55
1:C:359:ARG:CZ	1:C:362:ARG:CD	2.84	0.55
1:D:113:ARG:CA	1:D:181:VAL:HG13	2.36	0.55
1:J:113:ARG:HH12	1:J:115:HIS:HB2	1.71	0.55
1:G:362:ARG:O	1:G:364:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:316:THR:O	1:L:316:THR:OG1	2.24	0.55
1:F:57:VAL:CG2	1:F:71:VAL:CG2	2.84	0.55
1:F:362:ARG:O	1:F:364:ASP:N	2.40	0.55
2:M:615:LEU:HB3	2:M:624:VAL:HG22	1.87	0.55
1:G:113:ARG:CA	1:G:181:VAL:HG13	2.34	0.55
1:F:388:MET:HE2	1:F:390:LEU:HD21	1.89	0.55
2:R:596:LEU:HD13	2:R:636:VAL:HG21	1.88	0.55
1:H:384:HIS:HE1	3:H:501:ADP:N3	2.05	0.55
1:J:129:ASN:O	1:J:133:VAL:HG22	2.07	0.55
1:C:359:ARG:CZ	1:C:362:ARG:HD3	2.36	0.55
1:C:384:HIS:HE1	3:C:501:ADP:N3	2.05	0.54
1:E:21:ASN:HB2	1:F:432:LEU:HA	1.88	0.54
1:F:169:ASP:CB	1:F:170:PRO:HD3	2.37	0.54
2:R:589:ARG:CB	2:V:591:LEU:HD11	2.37	0.54
1:H:220:VAL:HG12	1:H:342:ILE:HD12	1.89	0.54
1:I:129:ASN:O	1:I:133:VAL:HG22	2.08	0.54
1:I:430:ILE:CG2	1:I:430:ILE:O	2.55	0.54
1:K:60:LYS:HB2	1:K:101:SER:OG	2.07	0.54
1:K:362:ARG:O	1:K:364:ASP:N	2.40	0.54
1:F:60:LYS:HB2	1:F:101:SER:OG	2.06	0.54
1:G:235:VAL:HG23	1:I:158:MET:HG2	1.88	0.54
1:J:349:ARG:HE	1:J:351:ASN:ND2	2.06	0.54
2:T:638:LEU:HD12	2:T:638:LEU:C	2.32	0.54
1:B:169:ASP:CB	1:B:170:PRO:HD3	2.37	0.54
1:C:235:VAL:HG23	1:D:158:MET:HG2	1.88	0.54
1:C:295:LYS:HG2	1:C:296:ASN:OD1	2.06	0.54
2:N:587:GLU:OE1	2:N:589:ARG:NH1	2.40	0.54
1:L:169:ASP:CB	1:L:170:PRO:HD3	2.38	0.54
2:W:603:VAL:O	2:W:608:PHE:HB2	2.07	0.54
1:L:437:ILE:CD1	1:L:441:VAL:CG2	2.85	0.54
1:F:57:VAL:CG1	1:F:71:VAL:CG2	2.86	0.54
1:H:408:GLY:HA3	3:H:501:ADP:C8	2.43	0.54
1:J:123:VAL:HG13	1:J:161:VAL:HG13	1.88	0.54
1:J:146:ILE:HD12	1:J:165:VAL:HG11	1.89	0.54
1:K:169:ASP:CB	1:K:170:PRO:HD3	2.37	0.54
1:A:437:ILE:HG21	1:F:229:LEU:HD11	1.89	0.54
1:C:129:ASN:O	1:C:133:VAL:HG22	2.08	0.54
1:C:169:ASP:CB	1:C:170:PRO:HD3	2.37	0.54
1:E:169:ASP:CB	1:E:170:PRO:HD3	2.37	0.54
2:T:596:LEU:HD13	2:T:636:VAL:HG21	1.90	0.54
1:B:123:VAL:HG13	1:B:161:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:ILE:HG22	1:E:438:ASP:N	2.21	0.54
1:G:129:ASN:O	1:G:133:VAL:HG22	2.08	0.54
1:G:175:ILE:HD12	2:S:579:ARG:NH2	2.23	0.54
1:D:169:ASP:CB	1:D:170:PRO:HD3	2.37	0.54
1:D:274:ILE:HG22	1:D:275:MET:CE	2.31	0.54
1:I:21:ASN:HB2	1:J:432:LEU:HD21	1.90	0.54
1:K:23:PRO:O	1:K:45:LYS:NZ	2.40	0.54
2:S:596:LEU:HD13	2:S:636:VAL:HG21	1.90	0.54
1:C:430:ILE:O	1:C:430:ILE:CG2	2.55	0.54
1:F:146:ILE:HD12	1:F:165:VAL:HG11	1.88	0.54
2:X:594:ASN:ND2	2:X:598:ILE:HD12	2.23	0.54
1:D:129:ASN:O	1:D:133:VAL:HG22	2.08	0.54
2:M:596:LEU:HD13	2:M:636:VAL:HG21	1.90	0.54
1:H:319:GLU:OE1	1:K:320:VAL:HG23	2.07	0.54
2:U:600:PHE:HB3	2:U:610:TRP:CE2	2.43	0.54
2:V:596:LEU:HD13	2:V:636:VAL:HG21	1.90	0.54
2:X:596:LEU:HD13	2:X:636:VAL:HG21	1.90	0.54
1:A:146:ILE:HD12	1:A:165:VAL:HG11	1.89	0.53
2:N:580:THR:OG1	2:N:583:GLY:O	2.16	0.53
2:Q:615:LEU:HD23	2:Q:624:VAL:HG21	1.90	0.53
1:L:146:ILE:HD12	1:L:165:VAL:HG11	1.90	0.53
1:L:430:ILE:CG2	1:L:430:ILE:O	2.55	0.53
2:T:595:LYS:HB3	2:T:629:PRO:O	2.08	0.53
2:U:595:LYS:HB3	2:U:629:PRO:O	2.08	0.53
1:A:169:ASP:CB	1:A:170:PRO:HD3	2.37	0.53
1:D:430:ILE:CG2	1:D:430:ILE:O	2.55	0.53
2:O:595:LYS:HB3	2:O:629:PRO:O	2.08	0.53
1:J:437:ILE:HG12	1:J:442:MET:SD	2.48	0.53
1:L:114:ILE:CD1	1:L:168:THR:CA	2.85	0.53
2:U:586:LEU:HD21	2:U:588:ARG:CZ	2.37	0.53
2:X:595:LYS:O	2:X:598:ILE:HG22	2.08	0.53
1:A:123:VAL:HG13	1:A:161:VAL:HG13	1.90	0.53
1:E:129:ASN:O	1:E:133:VAL:HG22	2.08	0.53
1:F:113:ARG:HH11	1:F:181:VAL:HG12	1.74	0.53
1:H:23:PRO:O	1:H:45:LYS:NZ	2.41	0.53
1:H:129:ASN:O	1:H:133:VAL:HG22	2.08	0.53
1:J:111:GLY:C	1:J:169:ASP:OD1	2.52	0.53
1:L:129:ASN:O	1:L:133:VAL:HG22	2.08	0.53
1:L:313:ARG:NH1	1:L:354:ASP:OD1	2.41	0.53
1:L:337:GLN:HE21	1:L:338:ARG:HG2	1.74	0.53
2:S:615:LEU:HD23	2:S:624:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:595:LYS:HB2	2:V:629:PRO:O	2.08	0.53
2:X:595:LYS:HB2	2:X:629:PRO:O	2.09	0.53
1:B:166:VAL:O	1:B:167:GLU:HG3	2.09	0.53
1:C:388:MET:HE2	1:C:390:LEU:HD21	1.90	0.53
2:P:595:LYS:HB3	2:P:629:PRO:O	2.08	0.53
1:J:113:ARG:NH1	1:J:115:HIS:HB2	2.23	0.53
1:L:23:PRO:O	1:L:45:LYS:NZ	2.41	0.53
2:S:595:LYS:HB3	2:S:629:PRO:O	2.08	0.53
2:T:616:LEU:HG	2:T:645:PHE:HB2	1.91	0.53
2:U:588:ARG:NH1	2:U:602:PHE:HB3	2.23	0.53
1:D:437:ILE:O	1:D:438:ASP:HB2	2.09	0.53
1:J:326:SER:O	1:J:330:THR:HG23	2.09	0.53
1:K:98:ASP:OD1	1:K:225:ARG:NH2	2.32	0.53
1:L:123:VAL:HG13	1:L:161:VAL:HG13	1.91	0.53
1:B:85:ASN:OD1	1:B:88:VAL:HG23	2.07	0.53
1:C:123:VAL:HG13	1:C:161:VAL:HG13	1.91	0.53
1:D:23:PRO:O	1:D:45:LYS:NZ	2.41	0.53
1:G:430:ILE:CD1	1:G:431:ASP:N	2.16	0.53
1:B:129:ASN:O	1:B:133:VAL:HG22	2.08	0.53
2:N:578:ILE:CG2	2:N:615:LEU:HD11	2.38	0.53
1:D:384:HIS:HE1	3:D:501:ADP:N3	2.07	0.53
1:E:123:VAL:HG13	1:E:161:VAL:HG13	1.91	0.53
2:M:615:LEU:HD23	2:M:624:VAL:HG21	1.89	0.53
2:P:624:VAL:HG22	2:P:627:LEU:HD12	1.90	0.53
1:B:322:ARG:HD2	1:E:321:GLU:OE2	2.09	0.53
1:C:146:ILE:HD12	1:C:165:VAL:HG11	1.90	0.53
1:D:123:VAL:HG13	1:D:161:VAL:HG13	1.91	0.53
2:M:595:LYS:HB3	2:M:629:PRO:O	2.08	0.53
2:N:624:VAL:HA	2:N:627:LEU:HG	1.91	0.53
2:Q:595:LYS:HB2	2:Q:629:PRO:O	2.09	0.53
1:G:437:ILE:HD11	1:G:441:VAL:CG2	2.39	0.53
1:H:326:SER:O	1:H:330:THR:HG23	2.08	0.53
1:J:23:PRO:O	1:J:45:LYS:NZ	2.40	0.53
1:K:330:THR:HG21	1:L:273:GLU:HA	1.91	0.53
1:H:430:ILE:O	1:H:430:ILE:CG2	2.55	0.53
2:W:616:LEU:HD12	2:W:622:ARG:C	2.34	0.53
1:F:115:HIS:O	1:F:166:VAL:HG13	2.09	0.52
1:H:53:ARG:HD2	2:T:641:GLN:O	2.09	0.52
1:E:146:ILE:HD12	1:E:165:VAL:HG11	1.91	0.52
1:F:23:PRO:O	1:F:45:LYS:NZ	2.41	0.52
1:F:57:VAL:HG21	1:F:71:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:VAL:HG13	1:I:161:VAL:HG13	1.90	0.52
1:I:438:ASP:HB3	1:I:441:VAL:CG1	2.39	0.52
1:B:220:VAL:HG12	1:B:342:ILE:HD12	1.92	0.52
2:P:596:LEU:HD13	2:P:636:VAL:HG21	1.91	0.52
2:R:595:LYS:HB2	2:R:629:PRO:O	2.08	0.52
1:G:115:HIS:O	1:G:166:VAL:HG13	2.09	0.52
1:G:123:VAL:HG13	1:G:161:VAL:HG13	1.90	0.52
1:I:292:GLU:HA	1:I:295:LYS:HE2	1.92	0.52
1:I:322:ARG:HH11	1:J:275:MET:HE3	1.74	0.52
2:V:606:LYS:HD2	2:V:606:LYS:N	2.24	0.52
2:X:615:LEU:HD23	2:X:624:VAL:HG21	1.91	0.52
2:O:577:ARG:HG2	2:O:587:GLU:HG2	1.90	0.52
1:H:158:MET:HG2	1:J:235:VAL:HG23	1.92	0.52
1:K:166:VAL:O	1:K:167:GLU:HG3	2.09	0.52
1:K:427:MET:HE3	1:K:430:ILE:CG1	2.39	0.52
2:V:632:SER:HB2	2:V:635:GLU:HG3	1.91	0.52
1:K:326:SER:O	1:K:330:THR:HG23	2.09	0.52
2:P:575:LYS:NZ	2:X:591:LEU:HB3	2.24	0.52
1:G:326:SER:O	1:G:330:THR:HG23	2.09	0.52
2:X:597:GLN:HB2	2:X:629:PRO:HB2	1.92	0.52
1:F:312:LYS:O	1:F:316:THR:HG23	2.09	0.52
2:N:587:GLU:OE2	2:N:589:ARG:HG3	2.10	0.52
2:O:597:GLN:HB2	2:O:629:PRO:HB2	1.90	0.52
1:I:388:MET:HE2	1:I:390:LEU:HD21	1.92	0.52
1:J:312:LYS:O	1:J:316:THR:HG23	2.08	0.52
2:U:597:GLN:HB2	2:U:629:PRO:HB2	1.92	0.52
1:A:23:PRO:O	1:A:45:LYS:NZ	2.41	0.52
1:B:23:PRO:O	1:B:45:LYS:NZ	2.41	0.52
1:C:23:PRO:O	1:C:45:LYS:NZ	2.41	0.52
1:G:99:VAL:CG2	1:I:431:ASP:HB2	2.39	0.52
1:G:330:THR:HG21	1:I:273:GLU:HA	1.92	0.52
1:D:326:SER:O	1:D:330:THR:HG23	2.09	0.52
1:I:235:VAL:HG23	1:J:158:MET:HG2	1.91	0.52
1:L:312:LYS:O	1:L:316:THR:HG23	2.09	0.52
1:E:23:PRO:O	1:E:45:LYS:NZ	2.41	0.52
2:P:596:LEU:C	2:P:599:VAL:HG13	2.35	0.52
1:G:232:ALA:HA	1:I:159:ARG:HH21	1.72	0.52
1:H:123:VAL:HG13	1:H:161:VAL:HG13	1.91	0.52
1:K:437:ILE:O	1:K:438:ASP:HB2	2.10	0.52
2:V:633:LEU:HD22	2:V:638:LEU:CD2	2.40	0.52
1:A:430:ILE:O	1:A:430:ILE:CG2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:596:LEU:HB3	2:Q:629:PRO:HA	1.93	0.51
1:A:321:GLU:OE2	1:F:322:ARG:HD2	2.10	0.51
1:E:402:GLU:CD	1:E:453:ARG:HH21	2.18	0.51
1:E:427:MET:HE2	1:E:430:ILE:HD11	1.92	0.51
2:P:632:SER:HB2	2:P:635:GLU:HG3	1.91	0.51
2:U:596:LEU:HB3	2:U:629:PRO:HA	1.93	0.51
1:F:129:ASN:O	1:F:133:VAL:HG22	2.08	0.51
1:K:123:VAL:HG13	1:K:161:VAL:HG13	1.92	0.51
1:H:388:MET:HE2	1:H:390:LEU:HD21	1.91	0.51
2:V:596:LEU:HB3	2:V:629:PRO:HA	1.93	0.51
2:P:596:LEU:HB3	2:P:629:PRO:HA	1.93	0.51
2:X:623:ASP:CG	2:X:626:GLN:HG2	2.36	0.51
1:F:430:ILE:O	1:F:430:ILE:CG2	2.58	0.51
2:P:643:THR:C	2:P:644:LEU:HD13	2.36	0.51
2:S:597:GLN:HB2	2:S:629:PRO:HB2	1.93	0.51
1:F:85:ASN:OD1	1:F:88:VAL:HG23	2.10	0.51
2:O:596:LEU:HB3	2:O:629:PRO:HA	1.92	0.51
1:L:388:MET:HE2	1:L:390:LEU:HD21	1.91	0.51
1:B:431:ASP:HB2	1:D:99:VAL:HG21	1.92	0.51
1:B:437:ILE:O	1:B:438:ASP:HB2	2.10	0.51
1:E:427:MET:HE2	1:E:430:ILE:HG12	1.93	0.51
1:B:41:LEU:HG	1:B:82:ILE:CD1	2.41	0.51
1:B:147:ARG:HH21	1:B:173:TYR:CB	2.23	0.51
1:F:437:ILE:O	1:F:438:ASP:HB2	2.11	0.51
2:Q:577:ARG:HG2	2:Q:587:GLU:HG2	1.93	0.51
1:H:147:ARG:HH21	1:H:173:TYR:CB	2.24	0.51
1:H:235:VAL:CG2	1:K:158:MET:HG2	2.40	0.51
1:G:388:MET:HE2	1:G:390:LEU:HD21	1.93	0.50
1:K:114:ILE:HG21	1:K:146:ILE:HD11	1.92	0.50
1:B:60:LYS:HZ1	1:B:64:ARG:HA	1.76	0.50
2:R:596:LEU:HB3	2:R:629:PRO:HA	1.93	0.50
1:G:54:GLY:HA2	1:G:70:ILE:HG23	1.93	0.50
1:A:115:HIS:CE1	1:A:185:GLU:HB2	2.47	0.50
2:Q:615:LEU:HD23	2:Q:624:VAL:CG2	2.41	0.50
1:G:292:GLU:HA	1:G:295:LYS:HE2	1.92	0.50
1:H:321:GLU:OE2	1:J:322:ARG:HD3	2.11	0.50
1:L:113:ARG:CA	1:L:181:VAL:HG13	2.37	0.50
2:T:596:LEU:HB3	2:T:629:PRO:HA	1.92	0.50
1:F:233:ILE:HD12	1:F:235:VAL:HB	1.93	0.50
2:M:596:LEU:HB3	2:M:629:PRO:HA	1.93	0.50
1:G:158:MET:HG2	1:L:235:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:614:LYS:NZ	2:W:622:ARG:O	2.44	0.50
1:E:147:ARG:HH21	1:E:173:TYR:CB	2.24	0.50
1:F:113:ARG:CZ	1:F:183:HIS:HB3	2.41	0.50
2:M:615:LEU:HD23	2:M:624:VAL:CG2	2.41	0.50
1:I:437:ILE:O	1:I:438:ASP:HB2	2.11	0.50
1:J:86:ARG:O	1:J:90:ASN:ND2	2.36	0.50
1:G:432:LEU:HA	1:L:21:ASN:HB2	1.93	0.50
1:J:297:ALA:HA	1:J:298:PRO:C	2.37	0.50
1:K:297:ALA:HA	1:K:298:PRO:C	2.37	0.50
1:L:40:SER:HB2	1:L:83:ARG:HB2	1.94	0.50
1:L:297:ALA:HA	1:L:298:PRO:C	2.37	0.50
2:S:615:LEU:HD23	2:S:624:VAL:CG2	2.42	0.50
1:F:148:LYS:NZ	1:F:171:SER:OG	2.38	0.50
1:G:437:ILE:O	1:G:438:ASP:HB2	2.11	0.50
1:H:185:GLU:HB2	1:H:187:GLU:OE1	2.12	0.50
1:K:53:ARG:NH2	2:W:643:THR:O	2.45	0.50
2:W:596:LEU:HA	2:W:633:LEU:HD21	1.94	0.50
1:A:437:ILE:CG2	1:F:229:LEU:CD1	2.83	0.50
1:B:235:VAL:CG2	1:E:158:MET:HG2	2.40	0.50
1:B:244:TYR:HE2	1:B:366:GLU:HB3	1.77	0.50
1:J:147:ARG:HH21	1:J:173:TYR:CB	2.24	0.50
1:A:78:SER:OG	1:A:80:GLU:OE1	2.30	0.50
1:A:305:GLU:OE1	1:F:359:ARG:NH1	2.45	0.50
1:H:297:ALA:HA	1:H:298:PRO:C	2.37	0.50
1:L:115:HIS:CE1	1:L:185:GLU:HB2	2.47	0.50
2:V:597:GLN:HB2	2:V:629:PRO:HB2	1.94	0.50
2:V:633:LEU:HD22	2:V:638:LEU:HD21	1.93	0.50
1:A:297:ALA:HA	1:A:298:PRO:C	2.37	0.49
1:B:220:VAL:HB	1:B:224:LEU:HD12	1.94	0.49
1:F:297:ALA:HA	1:F:298:PRO:C	2.37	0.49
1:G:297:ALA:HA	1:G:298:PRO:C	2.37	0.49
1:H:54:GLY:HA2	1:H:70:ILE:HG23	1.94	0.49
2:S:612:GLU:HG3	2:S:613:TYR:CE2	2.47	0.49
2:T:633:LEU:HD22	2:T:638:LEU:CD2	2.41	0.49
1:C:297:ALA:HA	1:C:298:PRO:C	2.37	0.49
1:D:220:VAL:HB	1:D:224:LEU:HD12	1.94	0.49
1:E:297:ALA:HA	1:E:298:PRO:C	2.37	0.49
1:E:349:ARG:NH1	1:E:351:ASN:OD1	2.45	0.49
2:O:596:LEU:HD13	2:O:636:VAL:HG21	1.94	0.49
1:I:40:SER:HB2	1:I:83:ARG:HB2	1.94	0.49
1:K:438:ASP:HB3	1:K:441:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:596:LEU:HB3	2:X:629:PRO:HA	1.93	0.49
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.94	0.49
1:D:297:ALA:HA	1:D:298:PRO:C	2.37	0.49
1:D:438:ASP:HB3	1:D:441:VAL:CG1	2.42	0.49
1:G:40:SER:HB2	1:G:83:ARG:HB2	1.94	0.49
1:H:40:SER:HB2	1:H:83:ARG:HB2	1.95	0.49
2:T:624:VAL:HG22	2:T:627:LEU:HD12	1.93	0.49
2:U:600:PHE:C	2:U:610:TRP:HE1	2.20	0.49
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.93	0.49
1:B:321:GLU:OE2	1:D:322:ARG:CD	2.53	0.49
1:F:244:TYR:HE2	1:F:366:GLU:HB3	1.77	0.49
2:R:635:GLU:OE1	2:R:635:GLU:HA	2.12	0.49
2:W:576:LEU:HA	2:W:642:GLU:N	2.27	0.49
1:B:273:GLU:HA	1:D:330:THR:HG21	1.94	0.49
1:G:52:PHE:CE2	2:S:577:ARG:CG	2.95	0.49
1:A:133:VAL:HG11	1:A:443:ASN:ND2	2.27	0.49
1:A:437:ILE:O	1:A:438:ASP:HB2	2.12	0.49
1:C:53:ARG:CZ	1:C:72:LEU:HD22	2.42	0.49
1:C:329:LEU:HA	1:C:362:ARG:CZ	2.42	0.49
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.95	0.49
1:E:115:HIS:CE1	1:E:185:GLU:HB2	2.48	0.49
1:F:54:GLY:HA2	1:F:70:ILE:HG23	1.95	0.49
2:M:580:THR:HG22	2:M:581:PRO:HD2	1.93	0.49
2:M:597:GLN:HB2	2:M:629:PRO:HB2	1.94	0.49
1:K:231:LYS:HA	1:K:338:ARG:HE	1.76	0.49
1:B:297:ALA:HA	1:B:298:PRO:C	2.37	0.49
1:C:115:HIS:CE1	1:C:185:GLU:HB2	2.47	0.49
1:C:313:ARG:CA	1:C:316:THR:HG22	2.41	0.49
2:N:578:ILE:HD12	2:N:644:LEU:HD12	1.95	0.49
1:I:54:GLY:HA2	1:I:70:ILE:HG23	1.94	0.49
1:I:297:ALA:HA	1:I:298:PRO:C	2.37	0.49
1:J:40:SER:HB2	1:J:83:ARG:HB2	1.94	0.49
1:K:244:TYR:HE2	1:K:366:GLU:HB3	1.78	0.49
1:K:388:MET:HE2	1:K:390:LEU:HD21	1.93	0.49
1:L:244:TYR:HE2	1:L:366:GLU:HB3	1.78	0.49
1:B:362:ARG:HH22	1:E:305:GLU:CD	2.21	0.49
1:L:437:ILE:O	1:L:438:ASP:HB2	2.11	0.49
2:U:617:SER:O	2:U:621:ARG:NH1	2.41	0.49
1:B:166:VAL:C	1:B:167:GLU:HG3	2.38	0.49
1:D:115:HIS:CE1	1:D:185:GLU:HB2	2.48	0.49
1:E:244:TYR:HE2	1:E:366:GLU:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:597:GLN:HB2	2:Q:629:PRO:HB2	1.94	0.49
1:L:114:ILE:HD12	1:L:168:THR:CA	2.43	0.49
1:C:131:PHE:HA	1:C:135:LEU:HB2	1.95	0.49
2:P:597:GLN:HB2	2:P:629:PRO:HB2	1.93	0.49
1:I:115:HIS:CE1	1:I:185:GLU:HB2	2.48	0.49
2:S:596:LEU:HB3	2:S:629:PRO:HA	1.93	0.49
2:T:578:ILE:HG13	2:T:644:LEU:HB2	1.95	0.49
1:D:231:LYS:HA	1:D:338:ARG:HE	1.77	0.48
1:E:220:VAL:HB	1:E:224:LEU:HD12	1.95	0.48
1:F:115:HIS:CE1	1:F:185:GLU:HB2	2.48	0.48
1:F:147:ARG:HH21	1:F:173:TYR:CB	2.26	0.48
1:I:56:THR:HG21	1:I:108:VAL:HG11	1.94	0.48
1:J:313:ARG:HB2	1:J:322:ARG:NH2	2.04	0.48
1:L:310:ALA:HA	1:L:325:VAL:HG22	1.95	0.48
1:D:64:ARG:HA	1:D:64:ARG:HH21	1.77	0.48
1:I:23:PRO:O	1:I:45:LYS:NZ	2.42	0.48
1:L:380:ILE:HG12	3:L:501:ADP:N1	2.28	0.48
1:L:438:ASP:HB3	1:L:441:VAL:CG1	2.43	0.48
1:C:244:TYR:HE2	1:C:366:GLU:HB3	1.78	0.48
1:B:244:TYR:CE2	1:B:366:GLU:HB3	2.49	0.48
1:G:278:LEU:HD23	1:L:323:ARG:NH2	2.28	0.48
1:H:244:TYR:HE2	1:H:366:GLU:HB3	1.78	0.48
1:H:437:ILE:O	1:H:438:ASP:HB2	2.11	0.48
1:J:168:THR:CG2	1:J:174:CYS:CB	2.91	0.48
1:K:430:ILE:C	1:K:430:ILE:CD1	2.86	0.48
2:X:615:LEU:HD23	2:X:624:VAL:CG2	2.42	0.48
1:D:54:GLY:HA2	1:D:70:ILE:HG23	1.95	0.48
1:D:362:ARG:O	1:D:364:ASP:N	2.47	0.48
1:E:54:GLY:HA2	1:E:70:ILE:HG23	1.96	0.48
1:E:131:PHE:HA	1:E:135:LEU:HB2	1.96	0.48
1:E:313:ARG:HA	1:E:313:ARG:HD3	1.75	0.48
1:G:231:LYS:O	1:I:159:ARG:NH2	2.47	0.48
1:H:438:ASP:HB3	1:H:441:VAL:CG1	2.43	0.48
1:A:54:GLY:HA2	1:A:70:ILE:HG23	1.95	0.48
1:B:131:PHE:HA	1:B:135:LEU:HB2	1.96	0.48
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.95	0.48
1:G:430:ILE:C	1:G:432:LEU:H	2.22	0.48
1:G:438:ASP:HB3	1:G:441:VAL:CG1	2.43	0.48
1:K:166:VAL:C	1:K:167:GLU:HG3	2.39	0.48
1:A:131:PHE:CE2	1:A:136:LYS:HE3	2.48	0.48
1:D:131:PHE:HA	1:D:135:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:337:GLN:NE2	1:I:338:ARG:HE	2.11	0.48
1:B:85:ASN:HD21	1:B:87:VAL:CG2	2.27	0.48
1:D:244:TYR:HE2	1:D:366:GLU:HB3	1.78	0.48
1:D:432:LEU:HD12	1:D:434:ASP:OD2	2.13	0.48
1:I:362:ARG:O	1:I:364:ASP:N	2.47	0.48
1:K:244:TYR:CE2	1:K:366:GLU:HB3	2.49	0.48
1:L:131:PHE:HA	1:L:135:LEU:HB2	1.95	0.48
1:L:362:ARG:O	1:L:364:ASP:N	2.47	0.48
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.95	0.48
1:C:54:GLY:HA2	1:C:70:ILE:HG23	1.96	0.48
1:C:359:ARG:CZ	1:C:362:ARG:HD2	2.44	0.48
1:F:244:TYR:CE2	1:F:366:GLU:HB3	2.49	0.48
2:P:575:LYS:HE2	2:X:593:SER:OG	2.12	0.48
1:J:131:PHE:HA	1:J:135:LEU:HB2	1.96	0.48
1:J:362:ARG:O	1:J:364:ASP:N	2.47	0.48
2:T:633:LEU:HD22	2:T:638:LEU:HD21	1.95	0.48
2:U:577:ARG:HG2	2:U:587:GLU:HG2	1.96	0.48
1:A:320:VAL:CG1	1:F:319:GLU:HG3	2.43	0.48
1:B:362:ARG:O	1:B:364:ASP:N	2.47	0.48
1:E:52:PHE:CE1	2:Q:641:GLN:HB3	2.48	0.48
1:E:362:ARG:O	1:E:364:ASP:N	2.47	0.48
1:H:125:GLY:HA3	1:J:231:LYS:HD3	1.94	0.48
1:I:244:TYR:HE2	1:I:366:GLU:HB3	1.78	0.48
1:K:323:ARG:NH2	1:L:278:LEU:HD23	2.29	0.48
1:L:54:GLY:HA2	1:L:70:ILE:HG23	1.96	0.48
1:A:362:ARG:O	1:A:364:ASP:N	2.47	0.47
1:C:244:TYR:CE2	1:C:366:GLU:HB3	2.49	0.47
1:F:131:PHE:HA	1:F:135:LEU:HB2	1.96	0.47
1:H:362:ARG:O	1:H:364:ASP:N	2.47	0.47
1:J:437:ILE:HG23	1:J:438:ASP:N	2.15	0.47
1:C:323:ARG:NH2	1:D:278:LEU:HD23	2.29	0.47
1:E:322:ARG:HH22	1:F:317:HIS:HD2	1.62	0.47
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.94	0.47
1:J:85:ASN:OD1	1:J:88:VAL:HG23	2.15	0.47
1:J:111:GLY:CA	1:J:169:ASP:OD1	2.62	0.47
1:J:220:VAL:HB	1:J:224:LEU:HD12	1.97	0.47
1:K:40:SER:HB2	1:K:83:ARG:HB2	1.95	0.47
1:L:438:ASP:HB3	1:L:441:VAL:HG12	1.96	0.47
1:D:60:LYS:HG2	1:D:64:ARG:HH12	1.78	0.47
1:H:220:VAL:HB	1:H:224:LEU:HD12	1.96	0.47
2:T:597:GLN:HB2	2:T:629:PRO:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLY:HA2	1:B:70:ILE:HG23	1.95	0.47
1:D:244:TYR:CE2	1:D:366:GLU:HB3	2.50	0.47
1:F:68:VAL:HG22	1:F:147:ARG:HB2	1.96	0.47
1:G:442:MET:HG2	1:L:233:ILE:HG22	1.97	0.47
1:H:436:THR:CG2	1:J:226:HIS:HD2	2.26	0.47
2:W:577:ARG:O	2:W:643:THR:HA	2.14	0.47
1:A:133:VAL:CG1	1:A:443:ASN:ND2	2.78	0.47
1:C:220:VAL:HB	1:C:224:LEU:HD12	1.97	0.47
2:M:623:ASP:O	2:M:626:GLN:HG2	2.15	0.47
2:T:575:LYS:HD2	2:T:589:ARG:HE	1.79	0.47
1:I:244:TYR:CE2	1:I:366:GLU:HB3	2.50	0.47
1:J:114:ILE:HG21	1:J:146:ILE:HD11	1.97	0.47
1:J:244:TYR:CE2	1:J:366:GLU:HB3	2.50	0.47
1:L:220:VAL:HB	1:L:224:LEU:HD12	1.97	0.47
1:A:244:TYR:CE2	1:A:366:GLU:HB3	2.50	0.47
1:A:244:TYR:HE2	1:A:366:GLU:HB3	1.78	0.47
1:B:210:ARG:NH1	1:B:210:ARG:HG2	2.30	0.47
1:B:432:LEU:HD23	1:D:21:ASN:HB2	1.97	0.47
1:E:244:TYR:CE2	1:E:366:GLU:HB3	2.49	0.47
1:F:57:VAL:CG2	1:F:71:VAL:HG22	2.45	0.47
1:F:220:VAL:HB	1:F:224:LEU:HD12	1.96	0.47
2:O:614:LYS:O	2:O:646:LEU:HA	2.15	0.47
2:R:577:ARG:HG2	2:R:587:GLU:HG2	1.97	0.47
1:G:220:VAL:HB	1:G:224:LEU:HD12	1.95	0.47
1:G:430:ILE:O	1:G:431:ASP:OD2	2.32	0.47
1:I:131:PHE:HA	1:I:135:LEU:HB2	1.96	0.47
1:J:244:TYR:HE2	1:J:366:GLU:HB3	1.78	0.47
1:K:319:GLU:OE2	1:L:318:GLY:HA3	2.15	0.47
1:F:236:LYS:HA	1:F:236:LYS:HD3	1.66	0.47
1:G:244:TYR:HE2	1:G:366:GLU:HB3	1.79	0.47
1:J:54:GLY:HA2	1:J:70:ILE:HG23	1.97	0.47
1:J:239:ARG:HD3	1:J:335:LEU:HB2	1.97	0.47
1:K:220:VAL:HB	1:K:224:LEU:HD12	1.97	0.47
1:K:235:VAL:CG2	1:L:158:MET:HG2	2.45	0.47
1:K:330:THR:CG2	1:L:273:GLU:HA	2.45	0.47
1:A:349:ARG:CZ	1:A:350:PRO:HD2	2.44	0.47
2:N:579:ARG:HA	2:N:585:PHE:HB3	1.96	0.47
2:Q:578:ILE:HG13	2:Q:644:LEU:HB2	1.96	0.47
1:G:131:PHE:HA	1:G:135:LEU:HB2	1.97	0.47
2:V:578:ILE:HG13	2:V:644:LEU:HB2	1.97	0.47
2:W:596:LEU:HD22	2:W:600:PHE:HZ	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:603:VAL:CG1	2:M:608:PHE:HB2	2.44	0.47
2:R:597:GLN:HB2	2:R:629:PRO:HB2	1.97	0.47
1:G:244:TYR:CE2	1:G:366:GLU:HB3	2.50	0.47
1:G:437:ILE:HG13	1:G:441:VAL:CG2	2.44	0.47
1:J:110:TYR:OH	2:V:645:PHE:HD1	1.98	0.47
2:V:603:VAL:CG1	2:V:608:PHE:HB2	2.45	0.47
1:C:362:ARG:O	1:C:364:ASP:N	2.47	0.46
1:E:233:ILE:HD12	1:E:235:VAL:HB	1.97	0.46
2:O:578:ILE:HG13	2:O:644:LEU:HB2	1.97	0.46
1:H:244:TYR:CE2	1:H:366:GLU:HB3	2.49	0.46
1:K:54:GLY:HA2	1:K:70:ILE:HG23	1.95	0.46
1:L:244:TYR:CE2	1:L:366:GLU:HB3	2.49	0.46
2:M:614:LYS:O	2:M:646:LEU:HA	2.16	0.46
1:K:131:PHE:HA	1:K:135:LEU:HB2	1.97	0.46
1:E:430:ILE:C	1:E:430:ILE:CD1	2.87	0.46
2:N:598:ILE:O	2:N:601:ASP:OD1	2.33	0.46
1:I:220:VAL:HB	1:I:224:LEU:HD12	1.97	0.46
1:K:322:ARG:HD2	1:L:321:GLU:OE2	2.15	0.46
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.98	0.46
1:B:313:ARG:HD2	1:B:322:ARG:HD3	1.98	0.46
1:C:348:ASN:HB2	1:C:349:ARG:HH11	1.81	0.46
1:D:310:ALA:HA	1:D:325:VAL:HG22	1.98	0.46
1:H:131:PHE:HA	1:H:135:LEU:HB2	1.96	0.46
1:G:438:ASP:HB3	1:G:441:VAL:HG12	1.97	0.46
1:J:429:LEU:O	1:J:430:ILE:O	2.34	0.46
1:A:38:VAL:CG1	1:A:72:LEU:HD12	2.46	0.46
1:B:60:LYS:HZ3	1:B:64:ARG:HA	1.80	0.46
1:F:57:VAL:HG11	1:F:71:VAL:CG2	2.41	0.46
1:H:322:ARG:NH2	1:K:321:GLU:HB2	2.31	0.46
1:I:337:GLN:HE21	1:I:338:ARG:HE	1.62	0.46
1:J:133:VAL:HG23	1:J:134:TYR:CD2	2.51	0.46
1:I:133:VAL:HG23	1:I:134:TYR:CD2	2.51	0.46
1:I:169:ASP:CB	1:I:170:PRO:HD3	2.39	0.46
1:B:40:SER:O	1:B:82:ILE:HD12	2.16	0.46
1:E:322:ARG:HH12	1:F:317:HIS:HD2	1.64	0.46
1:F:109:LYS:HG3	1:F:170:PRO:HG2	1.98	0.46
2:P:578:ILE:HG13	2:P:644:LEU:HB2	1.98	0.46
1:C:235:VAL:CG2	1:D:158:MET:HG2	2.45	0.46
1:E:185:GLU:OE1	1:E:187:GLU:HB2	2.16	0.46
1:F:142:ALA:O	2:R:618:THR:HG21	2.16	0.46
2:R:624:VAL:HG22	2:R:627:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:LEU:HB3	1:I:366:GLU:HG2	1.98	0.46
1:J:66:GLU:OE1	1:J:147:ARG:NH1	2.39	0.46
1:K:41:LEU:HD23	1:K:41:LEU:HA	1.77	0.46
1:L:25:ARG:HA	1:L:100:ILE:O	2.16	0.46
1:L:313:ARG:HA	1:L:313:ARG:HD3	1.60	0.46
1:L:426:LYS:HD2	1:L:445:LEU:HD13	1.98	0.46
1:A:220:VAL:HB	1:A:224:LEU:HD12	1.97	0.45
1:B:38:VAL:CG1	1:B:72:LEU:HD12	2.46	0.45
1:B:85:ASN:ND2	1:B:87:VAL:HG23	2.31	0.45
1:C:242:LEU:HB3	1:C:366:GLU:HG2	1.98	0.45
1:D:348:ASN:HB2	1:D:349:ARG:HH11	1.80	0.45
1:B:133:VAL:HG23	1:B:134:TYR:CD2	2.51	0.45
2:M:578:ILE:HG13	2:M:644:LEU:HB2	1.98	0.45
1:I:322:ARG:HH12	1:J:321:GLU:CG	2.29	0.45
1:K:435:GLU:O	1:K:437:ILE:N	2.49	0.45
1:L:236:LYS:HA	1:L:236:LYS:HD3	1.59	0.45
2:U:578:ILE:HG13	2:U:644:LEU:HB2	1.98	0.45
2:V:614:LYS:O	2:V:646:LEU:HA	2.16	0.45
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.98	0.45
1:C:133:VAL:HG23	1:C:134:TYR:CD2	2.52	0.45
1:D:129:ASN:HD22	1:D:132:GLU:HG2	1.65	0.45
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.99	0.45
2:P:614:LYS:O	2:P:646:LEU:HA	2.16	0.45
1:H:317:HIS:HE1	1:J:313:ARG:HH22	1.65	0.45
1:L:38:VAL:CG1	1:L:72:LEU:HD12	2.46	0.45
1:A:131:PHE:HA	1:A:135:LEU:HB2	1.96	0.45
1:D:52:PHE:CD2	2:P:577:ARG:HD3	2.51	0.45
1:E:430:ILE:HD12	1:E:430:ILE:O	2.15	0.45
1:H:435:GLU:O	1:H:437:ILE:N	2.50	0.45
1:I:438:ASP:HB3	1:I:441:VAL:HG12	1.99	0.45
1:L:112:LYS:O	1:L:181:VAL:HG12	2.16	0.45
2:X:603:VAL:HG21	2:X:646:LEU:HD21	1.98	0.45
1:E:427:MET:HE2	1:E:430:ILE:CD1	2.47	0.45
1:H:152:PHE:CE2	1:H:163:PHE:HB2	2.51	0.45
1:H:233:ILE:HD12	1:H:235:VAL:HB	1.97	0.45
1:I:233:ILE:HD12	1:I:235:VAL:HB	1.98	0.45
1:K:25:ARG:HA	1:K:100:ILE:O	2.16	0.45
1:L:133:VAL:HG23	1:L:134:TYR:CD2	2.52	0.45
2:S:578:ILE:HG13	2:S:644:LEU:HB2	1.98	0.45
2:W:576:LEU:O	2:W:577:ARG:HG2	2.16	0.45
1:E:152:PHE:CE2	1:E:163:PHE:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:VAL:HG23	1:F:134:TYR:CD2	2.51	0.45
1:G:235:VAL:CG2	1:I:158:MET:HG2	2.46	0.45
1:H:273:GLU:HA	1:J:330:THR:HG21	1.97	0.45
1:J:437:ILE:O	1:J:438:ASP:CB	2.63	0.45
1:K:427:MET:CE	1:K:430:ILE:HD11	2.45	0.45
2:U:614:LYS:O	2:U:646:LEU:HA	2.16	0.45
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.98	0.45
1:E:114:ILE:HG21	1:E:146:ILE:HD11	1.97	0.45
1:K:427:MET:O	1:K:430:ILE:HG13	2.17	0.45
1:L:242:LEU:HB3	1:L:366:GLU:HG2	1.99	0.45
1:A:435:GLU:O	1:A:437:ILE:N	2.50	0.45
1:C:38:VAL:CG1	1:C:72:LEU:HD12	2.46	0.45
1:C:316:THR:HG23	1:C:316:THR:O	2.17	0.45
1:C:329:LEU:CG	1:C:362:ARG:NH2	2.77	0.45
2:R:578:ILE:HG13	2:R:644:LEU:HB2	1.99	0.45
2:R:588:ARG:HG3	2:R:602:PHE:HD2	1.82	0.45
1:G:25:ARG:HA	1:G:100:ILE:O	2.17	0.45
1:G:429:LEU:O	1:G:430:ILE:O	2.35	0.45
1:H:278:LEU:H	1:H:278:LEU:HG	1.66	0.45
1:I:231:LYS:HB2	1:I:231:LYS:HE2	1.80	0.45
1:K:133:VAL:CG1	1:K:443:ASN:ND2	2.80	0.45
1:K:242:LEU:HB3	1:K:366:GLU:HG2	1.99	0.45
1:L:53:ARG:CZ	1:L:72:LEU:HD22	2.47	0.45
2:Q:614:LYS:O	2:Q:646:LEU:HA	2.16	0.45
1:G:52:PHE:CD2	2:S:577:ARG:HD2	2.52	0.45
1:L:43:GLN:N	1:L:44:PRO:HD2	2.32	0.45
1:L:437:ILE:HG13	1:L:441:VAL:CG2	2.44	0.45
2:W:580:THR:HG23	2:W:584:GLU:O	2.16	0.45
1:A:152:PHE:CE2	1:A:163:PHE:HB2	2.51	0.45
1:A:427:MET:SD	1:F:226:HIS:CD2	3.09	0.45
1:B:281:GLU:O	1:B:285:ASN:ND2	2.50	0.45
1:E:133:VAL:HG23	1:E:134:TYR:CD2	2.52	0.45
1:F:25:ARG:HA	1:F:100:ILE:O	2.17	0.45
1:I:152:PHE:CE2	1:I:163:PHE:HB2	2.51	0.45
1:J:25:ARG:HA	1:J:100:ILE:O	2.17	0.45
1:K:427:MET:HE3	1:K:430:ILE:CD1	2.45	0.45
2:X:614:LYS:O	2:X:646:LEU:HA	2.16	0.45
1:A:313:ARG:NH2	1:C:321:GLU:OE1	2.50	0.44
1:D:25:ARG:HA	1:D:100:ILE:O	2.17	0.44
1:F:113:ARG:NH1	1:F:181:VAL:HG12	2.30	0.44
1:G:435:GLU:O	1:G:437:ILE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:207:GLY:O	3:J:501:ADP:N6	2.49	0.44
1:K:43:GLN:N	1:K:44:PRO:HD2	2.32	0.44
2:S:614:LYS:O	2:S:646:LEU:HA	2.16	0.44
1:B:152:PHE:CE2	1:B:163:PHE:HB2	2.52	0.44
1:D:86:ARG:HG3	1:D:204:ASP:OD2	2.17	0.44
1:D:112:LYS:O	1:D:181:VAL:HG12	2.17	0.44
1:D:152:PHE:CE2	1:D:163:PHE:HB2	2.53	0.44
1:D:435:GLU:O	1:D:437:ILE:N	2.50	0.44
2:M:577:ARG:HG2	2:M:587:GLU:HG2	1.97	0.44
1:H:25:ARG:HA	1:H:100:ILE:O	2.18	0.44
1:H:310:ALA:HA	1:H:325:VAL:HG22	1.99	0.44
1:L:295:LYS:HD2	1:L:295:LYS:HA	1.78	0.44
2:V:575:LYS:C	2:V:576:LEU:HD12	2.43	0.44
1:C:43:GLN:N	1:C:44:PRO:HD2	2.32	0.44
1:C:190:LYS:HE3	1:C:190:LYS:HB3	1.81	0.44
1:C:437:ILE:O	1:C:438:ASP:CB	2.63	0.44
1:E:25:ARG:HA	1:E:100:ILE:O	2.17	0.44
1:G:142:ALA:HB1	1:G:144:ARG:HG3	2.00	0.44
1:J:310:ALA:HA	1:J:325:VAL:HG22	1.99	0.44
1:E:278:LEU:H	1:E:278:LEU:HG	1.66	0.44
1:G:112:LYS:O	1:G:181:VAL:HG12	2.18	0.44
2:T:616:LEU:HD11	2:T:645:PHE:CB	2.44	0.44
2:X:626:GLN:HE22	2:X:649:LYS:HE2	1.81	0.44
1:C:437:ILE:HG21	1:C:442:MET:SD	2.58	0.44
1:F:242:LEU:HB3	1:F:366:GLU:HG2	1.99	0.44
2:P:614:LYS:HG2	2:P:649:LYS:HE2	1.99	0.44
2:R:614:LYS:O	2:R:646:LEU:HA	2.17	0.44
1:I:435:GLU:O	1:I:437:ILE:N	2.50	0.44
2:U:596:LEU:HD22	2:U:636:VAL:HG21	2.00	0.44
2:U:636:VAL:O	2:U:636:VAL:CG1	2.65	0.44
2:X:631:LYS:HA	2:X:631:LYS:HD3	1.68	0.44
1:A:25:ARG:HA	1:A:100:ILE:O	2.17	0.44
1:E:362:ARG:HH22	1:F:305:GLU:CD	2.26	0.44
1:F:152:PHE:CE2	1:F:163:PHE:HB2	2.52	0.44
2:N:614:LYS:O	2:N:646:LEU:HA	2.18	0.44
2:R:589:ARG:NH1	2:V:593:SER:OG	2.51	0.44
1:H:85:ASN:ND2	1:H:87:VAL:HB	2.32	0.44
1:J:242:LEU:HB3	1:J:366:GLU:HG2	1.99	0.44
1:J:384:HIS:CE1	3:J:501:ADP:N3	2.74	0.44
1:L:233:ILE:HD12	1:L:235:VAL:HB	2.00	0.44
1:L:435:GLU:O	1:L:437:ILE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:614:LYS:O	2:T:646:LEU:HA	2.17	0.44
1:B:242:LEU:HB3	1:B:366:GLU:HG2	1.99	0.44
1:C:152:PHE:CE2	1:C:163:PHE:HB2	2.52	0.44
1:E:313:ARG:HD2	1:E:322:ARG:HD3	1.99	0.44
1:F:435:GLU:O	1:F:437:ILE:N	2.51	0.44
1:H:242:LEU:HB3	1:H:366:GLU:HG2	1.99	0.44
1:K:85:ASN:ND2	1:K:87:VAL:HB	2.33	0.44
1:B:41:LEU:HG	1:B:82:ILE:HD12	2.00	0.44
1:B:143:TYR:HB2	2:N:618:THR:HG21	2.00	0.44
1:B:408:GLY:HA3	3:B:501:ADP:C8	2.53	0.44
1:C:114:ILE:HG21	1:C:146:ILE:HD11	1.99	0.44
2:N:649:LYS:O	2:N:650:GLU:C	2.61	0.44
2:O:600:PHE:HB3	2:O:610:TRP:CE3	2.52	0.44
1:J:152:PHE:CE2	1:J:163:PHE:HB2	2.53	0.44
1:K:315:LYS:HB3	1:K:315:LYS:HE3	1.84	0.44
1:L:155:ARG:CZ	1:L:386:LYS:HD3	2.48	0.44
2:V:624:VAL:HG22	2:V:627:LEU:HD22	2.00	0.44
1:B:25:ARG:HA	1:B:100:ILE:O	2.17	0.44
1:B:146:ILE:HD13	1:B:146:ILE:HA	1.91	0.44
1:D:114:ILE:HG21	1:D:146:ILE:HD11	1.98	0.44
1:F:432:LEU:H	1:F:432:LEU:HG	1.68	0.44
2:R:588:ARG:HD2	2:R:588:ARG:HA	1.71	0.44
1:G:152:PHE:CE2	1:G:163:PHE:HB2	2.53	0.44
1:G:242:LEU:HB3	1:G:366:GLU:HG2	2.00	0.44
1:L:112:LYS:O	1:L:181:VAL:CG1	2.66	0.44
1:B:312:LYS:CD	1:B:315:LYS:HE2	2.45	0.43
1:B:313:ARG:HD3	1:B:313:ARG:HA	1.75	0.43
1:B:348:ASN:HB2	1:B:349:ARG:HH11	1.83	0.43
1:D:133:VAL:HG23	1:D:134:TYR:CD2	2.53	0.43
1:E:63:LYS:O	1:E:64:ARG:HG2	2.17	0.43
1:E:427:MET:O	1:E:430:ILE:HG13	2.17	0.43
1:F:211:LYS:HB3	1:F:211:LYS:HE3	1.72	0.43
1:G:233:ILE:HD12	1:G:235:VAL:HB	2.00	0.43
1:H:43:GLN:N	1:H:44:PRO:HD2	2.33	0.43
1:H:317:HIS:CE1	1:J:313:ARG:NH1	2.85	0.43
1:L:432:LEU:H	1:L:432:LEU:HG	1.64	0.43
1:A:43:GLN:N	1:A:44:PRO:HD2	2.33	0.43
1:A:53:ARG:CZ	1:A:72:LEU:HD22	2.48	0.43
1:A:114:ILE:HG21	1:A:146:ILE:HD11	1.99	0.43
1:F:113:ARG:HH21	1:F:115:HIS:HB2	1.83	0.43
2:P:600:PHE:O	2:P:603:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:VAL:HG23	1:G:134:TYR:CD2	2.53	0.43
1:G:310:ALA:HA	1:G:325:VAL:HG22	1.99	0.43
1:J:236:LYS:HD3	1:J:236:LYS:HA	1.64	0.43
2:V:603:VAL:HG13	2:V:608:PHE:HB2	1.99	0.43
1:A:155:ARG:CZ	1:A:386:LYS:HD3	2.48	0.43
1:B:435:GLU:O	1:B:437:ILE:N	2.51	0.43
1:C:155:ARG:CZ	1:C:386:LYS:HD3	2.48	0.43
1:H:146:ILE:HD13	1:H:146:ILE:HA	1.91	0.43
1:H:158:MET:HG2	1:J:235:VAL:CG2	2.48	0.43
1:I:278:LEU:O	1:I:278:LEU:HG	2.18	0.43
1:I:310:ALA:HA	1:I:325:VAL:HG22	2.01	0.43
1:J:315:LYS:HB3	1:J:315:LYS:HE3	1.54	0.43
1:L:152:PHE:CE2	1:L:163:PHE:HB2	2.53	0.43
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.73	0.43
1:F:430:ILE:O	1:F:430:ILE:HG23	2.18	0.43
2:M:603:VAL:HG13	2:M:608:PHE:HB2	2.01	0.43
1:G:146:ILE:HD13	1:G:146:ILE:HA	1.91	0.43
1:G:239:ARG:HD3	1:G:335:LEU:HB2	2.00	0.43
1:I:426:LYS:HD2	1:I:445:LEU:HD13	1.99	0.43
1:B:24:ASN:HB2	1:B:102:ILE:O	2.19	0.43
1:C:25:ARG:HA	1:C:100:ILE:O	2.18	0.43
1:C:233:ILE:HD12	1:C:235:VAL:HB	2.00	0.43
1:C:329:LEU:HD12	1:C:362:ARG:HH22	1.84	0.43
1:D:43:GLN:N	1:D:44:PRO:HD2	2.33	0.43
1:D:430:ILE:O	1:D:430:ILE:HG23	2.19	0.43
2:Q:575:LYS:C	2:Q:576:LEU:HD12	2.44	0.43
1:G:135:LEU:CD1	1:G:182:ILE:HD11	2.39	0.43
1:H:330:THR:HG21	1:K:273:GLU:HA	1.99	0.43
1:I:155:ARG:CZ	1:I:386:LYS:HD3	2.48	0.43
1:J:435:GLU:O	1:J:437:ILE:N	2.52	0.43
2:U:588:ARG:CD	2:U:602:PHE:HD2	2.31	0.43
2:V:606:LYS:HB2	2:V:608:PHE:CD2	2.54	0.43
1:A:313:ARG:CA	1:A:316:THR:HG22	2.40	0.43
1:B:155:ARG:CZ	1:B:386:LYS:HD3	2.49	0.43
1:B:432:LEU:CD2	1:D:21:ASN:HB2	2.48	0.43
1:D:242:LEU:HB3	1:D:366:GLU:HG2	2.00	0.43
1:E:435:GLU:O	1:E:437:ILE:N	2.52	0.43
1:F:310:ALA:HA	1:F:325:VAL:HG22	2.01	0.43
1:K:310:ALA:HA	1:K:325:VAL:HG22	2.00	0.43
1:C:385:THR:HB	1:C:390:LEU:HD11	1.99	0.43
1:E:242:LEU:HB3	1:E:366:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:592:ALA:HA	2:R:633:LEU:HG	1.99	0.43
1:G:313:ARG:HD2	1:G:322:ARG:HD3	2.00	0.43
1:K:27:ILE:HB	1:K:81:LYS:HG2	1.99	0.43
2:T:600:PHE:O	2:T:603:VAL:HG22	2.19	0.43
2:U:595:LYS:HD3	2:U:630:ASN:HA	2.00	0.43
1:A:210:ARG:HE	1:A:210:ARG:HA	1.84	0.43
1:B:43:GLN:N	1:B:44:PRO:HD2	2.33	0.43
1:E:311:PRO:HB2	1:E:315:LYS:HD2	2.01	0.43
1:G:322:ARG:HH22	1:I:317:HIS:HB2	1.84	0.43
1:K:52:PHE:CE1	2:W:575:LYS:HE3	2.54	0.43
1:L:430:ILE:O	1:L:430:ILE:HG23	2.19	0.43
2:V:633:LEU:O	2:V:638:LEU:HG	2.18	0.43
1:B:275:MET:HE3	1:D:322:ARG:HH12	1.83	0.43
1:C:435:GLU:O	1:C:437:ILE:N	2.52	0.43
1:F:43:GLN:N	1:F:44:PRO:HD2	2.33	0.43
2:P:589:ARG:HH22	2:X:593:SER:HB2	1.83	0.43
1:H:65:ARG:HE	1:H:65:ARG:HB3	1.68	0.43
1:J:155:ARG:CZ	1:J:386:LYS:HD3	2.49	0.43
2:X:578:ILE:HG13	2:X:644:LEU:HB2	1.99	0.43
1:A:315:LYS:HE3	1:A:315:LYS:HB3	1.82	0.43
1:A:432:LEU:H	1:A:432:LEU:HG	1.68	0.43
1:C:68:VAL:HG22	1:C:147:ARG:HB2	2.01	0.43
1:C:313:ARG:HA	1:C:316:THR:CG2	2.44	0.43
1:C:329:LEU:CD1	1:C:362:ARG:HH22	2.32	0.43
1:F:155:ARG:CZ	1:F:386:LYS:HD3	2.49	0.43
1:F:190:LYS:HA	1:F:190:LYS:HD2	1.75	0.43
1:G:43:GLN:N	1:G:44:PRO:HD2	2.34	0.43
1:H:169:ASP:HB3	1:H:170:PRO:HD3	2.01	0.43
1:H:315:LYS:HE3	1:H:315:LYS:HB3	1.76	0.43
2:V:598:ILE:O	2:V:601:ASP:OD1	2.37	0.43
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.86	0.42
1:E:43:GLN:N	1:E:44:PRO:HD2	2.33	0.42
1:E:155:ARG:CZ	1:E:386:LYS:HD3	2.49	0.42
1:E:350:PRO:O	1:E:358:ARG:NH2	2.52	0.42
2:P:575:LYS:C	2:P:576:LEU:HD12	2.44	0.42
1:G:135:LEU:HB3	1:G:182:ILE:CD1	2.49	0.42
1:G:169:ASP:HB3	1:G:170:PRO:HD3	2.01	0.42
1:H:66:GLU:OE1	1:H:147:ARG:NH1	2.38	0.42
1:I:52:PHE:CZ	2:U:577:ARG:HG3	2.53	0.42
1:K:152:PHE:CE2	1:K:163:PHE:HB2	2.54	0.42
1:L:332:MET:HE3	1:L:332:MET:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:MET:HE3	1:D:332:MET:HB3	1.91	0.42
1:E:432:LEU:H	1:E:432:LEU:HG	1.69	0.42
2:P:588:ARG:HD3	2:P:588:ARG:HA	1.80	0.42
1:J:384:HIS:HE1	3:J:501:ADP:C2	2.37	0.42
1:L:24:ASN:HB2	1:L:102:ILE:O	2.19	0.42
2:X:575:LYS:C	2:X:576:LEU:HD12	2.43	0.42
1:D:112:LYS:O	1:D:181:VAL:CG1	2.67	0.42
2:O:591:LEU:HD23	2:S:591:LEU:HD23	2.00	0.42
2:R:614:LYS:HD2	2:R:616:LEU:HD21	2.00	0.42
2:U:600:PHE:O	2:U:603:VAL:HG22	2.19	0.42
1:B:435:GLU:H	1:B:435:GLU:HG3	1.43	0.42
2:N:578:ILE:HG23	2:N:615:LEU:CD1	2.48	0.42
2:Q:647:GLU:OE1	2:Q:647:GLU:HA	2.19	0.42
2:R:588:ARG:HG3	2:R:602:PHE:CD2	2.54	0.42
2:R:600:PHE:O	2:R:603:VAL:HG22	2.19	0.42
1:H:190:LYS:HD2	1:H:190:LYS:HA	1.89	0.42
1:H:432:LEU:H	1:H:432:LEU:HG	1.65	0.42
1:I:25:ARG:HA	1:I:100:ILE:O	2.20	0.42
1:I:68:VAL:HG12	1:I:147:ARG:HB2	2.00	0.42
1:J:43:GLN:N	1:J:44:PRO:HD2	2.33	0.42
1:J:233:ILE:HD12	1:J:235:VAL:HB	2.01	0.42
2:S:647:GLU:OE1	2:S:647:GLU:HA	2.20	0.42
1:A:85:ASN:ND2	1:A:87:VAL:HB	2.35	0.42
1:A:233:ILE:HD12	1:A:235:VAL:HB	2.00	0.42
1:A:242:LEU:HB3	1:A:366:GLU:HG2	2.00	0.42
1:A:385:THR:HB	1:A:390:LEU:HD11	2.01	0.42
1:B:142:ALA:HB1	1:B:144:ARG:HG3	2.02	0.42
1:E:53:ARG:NH2	2:Q:639:PHE:CE2	2.87	0.42
1:H:155:ARG:CZ	1:H:386:LYS:HD3	2.50	0.42
1:H:169:ASP:CB	1:H:170:PRO:CD	2.98	0.42
1:K:225:ARG:HH11	1:K:225:ARG:HD2	1.72	0.42
1:K:319:GLU:OE1	1:L:320:VAL:CG1	2.68	0.42
2:X:596:LEU:HD22	2:X:636:VAL:HG11	2.02	0.42
1:B:431:ASP:HB2	1:D:99:VAL:CG2	2.49	0.42
2:Q:600:PHE:O	2:Q:603:VAL:HG22	2.18	0.42
2:Q:634:LEU:HD21	2:Q:635:GLU:OE2	2.19	0.42
1:G:112:LYS:O	1:G:181:VAL:CG1	2.67	0.42
1:H:185:GLU:C	1:H:187:GLU:OE1	2.62	0.42
1:I:65:ARG:HE	1:I:65:ARG:HB3	1.69	0.42
1:K:190:LYS:HD2	1:K:190:LYS:HA	1.89	0.42
2:S:600:PHE:O	2:S:603:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:633:LEU:O	2:T:638:LEU:HG	2.20	0.42
2:X:634:LEU:CD2	2:X:635:GLU:OE2	2.67	0.42
1:B:457:SER:O	1:L:404:HIS:HE1	2.01	0.42
1:E:80:GLU:H	1:E:80:GLU:HG3	1.17	0.42
1:E:229:LEU:CD1	1:F:437:ILE:HG21	2.50	0.42
1:E:322:ARG:HH22	1:F:317:HIS:CD2	2.37	0.42
2:M:575:LYS:C	2:M:576:LEU:HD12	2.44	0.42
2:N:579:ARG:HG2	2:N:585:PHE:CD2	2.54	0.42
2:Q:614:LYS:HE3	2:Q:614:LYS:HB2	1.83	0.42
1:G:331:LEU:HD23	1:G:331:LEU:HA	1.92	0.42
1:I:430:ILE:O	1:I:430:ILE:HG23	2.20	0.42
1:K:53:ARG:HD3	2:W:642:GLU:OE1	2.19	0.42
2:S:595:LYS:HD3	2:S:630:ASN:HA	2.01	0.42
1:D:233:ILE:HD12	1:D:235:VAL:HB	2.01	0.42
1:F:117:LEU:HD21	1:F:185:GLU:HB3	2.02	0.42
1:F:426:LYS:HD2	1:F:445:LEU:HD13	2.02	0.42
2:O:575:LYS:C	2:O:576:LEU:HD12	2.45	0.42
1:I:43:GLN:N	1:I:44:PRO:HD2	2.33	0.42
1:J:24:ASN:HB2	1:J:102:ILE:O	2.20	0.42
1:A:430:ILE:O	1:A:430:ILE:HG23	2.19	0.42
1:D:24:ASN:HB2	1:D:102:ILE:O	2.20	0.42
1:F:429:LEU:N	1:F:429:LEU:HD13	2.35	0.42
1:G:24:ASN:HB2	1:G:102:ILE:O	2.19	0.42
1:G:291:GLU:O	1:G:295:LYS:HG3	2.20	0.42
1:H:239:ARG:HD3	1:H:335:LEU:HB2	2.02	0.42
1:H:331:LEU:HD23	1:H:331:LEU:HA	1.94	0.42
1:I:235:VAL:CG2	1:J:158:MET:HG2	2.50	0.42
1:K:155:ARG:CZ	1:K:386:LYS:HD3	2.50	0.42
2:U:586:LEU:HD21	2:U:588:ARG:NH1	2.34	0.42
1:D:155:ARG:CZ	1:D:386:LYS:HD3	2.50	0.42
1:H:78:SER:OG	1:H:80:GLU:OE1	2.35	0.42
1:I:213:LEU:HD12	1:I:213:LEU:HA	1.85	0.42
1:I:313:ARG:HA	1:I:313:ARG:HD3	1.75	0.42
1:K:86:ARG:HG3	1:K:89:ARG:HH21	1.85	0.42
1:K:213:LEU:HD12	1:K:213:LEU:HA	1.86	0.42
1:K:426:LYS:HD2	1:K:445:LEU:HD13	2.02	0.42
2:U:626:GLN:HE22	2:U:649:LYS:HE2	1.84	0.42
2:V:647:GLU:OE1	2:V:647:GLU:HA	2.20	0.42
1:D:85:ASN:ND2	1:D:87:VAL:HB	2.35	0.41
1:G:169:ASP:CB	1:G:170:PRO:CD	2.98	0.41
1:H:438:ASP:HB3	1:H:441:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:ARG:HE	1:I:53:ARG:HB3	1.71	0.41
1:I:291:GLU:O	1:I:295:LYS:HG3	2.20	0.41
1:J:86:ARG:HG3	1:J:89:ARG:HH21	1.85	0.41
1:J:113:ARG:HH12	1:J:115:HIS:CB	2.33	0.41
1:K:233:ILE:CG2	1:L:442:MET:HG2	2.50	0.41
1:B:231:LYS:HA	1:B:338:ARG:HE	1.85	0.41
1:C:142:ALA:HB1	1:C:144:ARG:HG3	2.02	0.41
1:F:143:TYR:CE1	1:F:178:PRO:HD3	2.55	0.41
1:F:169:ASP:CB	1:F:170:PRO:CD	2.98	0.41
2:N:650:GLU:HG3	2:N:650:GLU:O	2.20	0.41
1:H:384:HIS:NE2	3:H:501:ADP:O2'	2.42	0.41
1:I:225:ARG:HH11	1:I:225:ARG:HD2	1.71	0.41
1:J:52:PHE:CZ	2:V:641:GLN:HB3	2.55	0.41
1:L:350:PRO:O	1:L:358:ARG:NH2	2.53	0.41
2:U:586:LEU:HD21	2:U:588:ARG:NH2	2.35	0.41
1:A:175:ILE:HD12	2:M:579:ARG:NH2	2.35	0.41
1:A:190:LYS:HE3	1:A:190:LYS:HB3	1.67	0.41
1:D:78:SER:OG	1:D:80:GLU:OE1	2.36	0.41
1:D:86:ARG:HD3	1:D:204:ASP:CG	2.45	0.41
1:E:430:ILE:CD1	1:E:430:ILE:O	2.67	0.41
1:F:112:LYS:H	1:F:169:ASP:CG	2.29	0.41
1:F:164:LYS:HE2	1:F:164:LYS:HB2	1.78	0.41
1:G:155:ARG:CZ	1:G:386:LYS:HD3	2.49	0.41
1:L:142:ALA:HB1	1:L:144:ARG:HG3	2.03	0.41
2:W:578:ILE:O	2:W:586:LEU:N	2.50	0.41
2:X:647:GLU:OE1	2:X:647:GLU:HA	2.20	0.41
1:B:201:VAL:HG11	1:B:256:ARG:HB3	2.01	0.41
1:B:233:ILE:HD12	1:B:235:VAL:HB	2.02	0.41
1:B:273:GLU:HA	1:D:330:THR:CG2	2.49	0.41
1:C:169:ASP:CB	1:C:170:PRO:CD	2.99	0.41
1:H:68:VAL:HG22	1:H:147:ARG:HB2	2.02	0.41
1:H:133:VAL:HG23	1:H:134:TYR:CD2	2.54	0.41
1:H:431:ASP:OD1	1:J:21:ASN:ND2	2.54	0.41
1:I:335:LEU:HD23	1:I:335:LEU:HA	1.97	0.41
1:L:85:ASN:ND2	1:L:87:VAL:HB	2.35	0.41
1:A:239:ARG:HD3	1:A:335:LEU:HB2	2.01	0.41
1:A:316:THR:HG23	1:A:316:THR:O	2.21	0.41
1:B:321:GLU:OE2	1:D:322:ARG:NH1	2.52	0.41
1:C:52:PHE:HA	2:O:641:GLN:OE1	2.19	0.41
1:D:169:ASP:HB3	1:D:170:PRO:HD3	2.02	0.41
1:J:278:LEU:H	1:J:278:LEU:HG	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:429:LEU:N	1:L:429:LEU:HD13	2.35	0.41
1:B:432:LEU:H	1:B:432:LEU:HG	1.66	0.41
1:C:52:PHE:CE1	2:O:641:GLN:HB3	2.55	0.41
1:E:142:ALA:HB1	1:E:144:ARG:HG3	2.03	0.41
2:M:593:SER:OG	2:U:589:ARG:NH1	2.53	0.41
2:N:600:PHE:O	2:N:603:VAL:HG22	2.21	0.41
2:P:596:LEU:HA	2:P:599:VAL:HG13	2.03	0.41
2:Q:634:LEU:CD2	2:Q:635:GLU:OE2	2.68	0.41
1:H:112:LYS:H	1:H:169:ASP:CG	2.29	0.41
1:K:164:LYS:NZ	1:K:195:GLU:OE2	2.54	0.41
2:V:588:ARG:HG3	2:V:602:PHE:CD2	2.55	0.41
2:V:601:ASP:HA	2:V:604:ALA:HB3	2.02	0.41
2:V:614:LYS:HB2	2:V:614:LYS:HE2	1.71	0.41
1:C:117:LEU:HD21	1:C:185:GLU:HB3	2.03	0.41
1:F:213:LEU:HD12	1:F:213:LEU:HA	1.86	0.41
1:J:190:LYS:HB3	1:J:190:LYS:HE3	1.83	0.41
1:K:332:MET:HE3	1:K:332:MET:HB3	1.90	0.41
1:K:430:ILE:HD12	1:K:430:ILE:O	2.20	0.41
1:K:432:LEU:H	1:K:432:LEU:HG	1.69	0.41
1:K:438:ASP:HB3	1:K:441:VAL:HG12	2.02	0.41
1:A:313:ARG:HA	1:A:316:THR:CG2	2.42	0.41
1:B:65:ARG:HE	1:B:65:ARG:HB3	1.68	0.41
1:B:143:TYR:HD2	2:N:618:THR:CG2	2.34	0.41
1:B:169:ASP:CB	1:B:170:PRO:CD	2.99	0.41
1:C:85:ASN:ND2	1:C:87:VAL:HB	2.35	0.41
1:F:201:VAL:HG11	1:F:256:ARG:HB3	2.03	0.41
2:N:597:GLN:N	2:N:629:PRO:CB	2.84	0.41
1:G:359:ARG:HH11	1:G:359:ARG:HD3	1.78	0.41
1:I:85:ASN:ND2	1:I:87:VAL:HB	2.36	0.41
1:I:226:HIS:N	1:I:227:PRO:HD3	2.36	0.41
1:K:78:SER:OG	1:K:80:GLU:OE1	2.36	0.41
1:A:142:ALA:HB1	1:A:144:ARG:HG3	2.01	0.41
1:A:313:ARG:O	1:A:316:THR:HG22	2.21	0.41
1:B:322:ARG:HH11	1:E:321:GLU:CD	2.28	0.41
1:D:169:ASP:CB	1:D:170:PRO:CD	2.99	0.41
1:E:117:LEU:HD21	1:E:185:GLU:HB3	2.02	0.41
1:F:315:LYS:H	1:F:315:LYS:HG2	1.67	0.41
2:O:637:LYS:HA	2:O:637:LYS:HD2	1.96	0.41
2:R:598:ILE:O	2:R:602:PHE:HD1	2.04	0.41
1:G:78:SER:OG	1:G:80:GLU:OE1	2.36	0.41
1:G:313:ARG:HA	1:G:313:ARG:HD3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:SER:OG	1:I:80:GLU:OE1	2.36	0.41
1:I:117:LEU:HD21	1:I:185:GLU:HB3	2.03	0.41
1:J:385:THR:HB	1:J:390:LEU:HD11	2.02	0.41
1:L:112:LYS:H	1:L:169:ASP:CG	2.29	0.41
1:L:117:LEU:HD21	1:L:185:GLU:HB3	2.03	0.41
1:L:385:THR:HB	1:L:390:LEU:HD11	2.02	0.41
2:U:627:LEU:CD1	2:U:636:VAL:CG1	2.96	0.41
2:X:590:PHE:HD1	2:X:598:ILE:HD13	1.86	0.41
1:A:226:HIS:N	1:A:227:PRO:HD3	2.36	0.41
1:E:231:LYS:HA	1:E:338:ARG:HE	1.84	0.41
2:M:595:LYS:HD3	2:M:630:ASN:HA	2.03	0.41
1:G:190:LYS:HE3	1:G:190:LYS:HB3	1.85	0.41
1:H:86:ARG:HG3	1:H:89:ARG:HH21	1.86	0.41
1:I:66:GLU:OE1	1:I:147:ARG:NH2	2.52	0.41
1:K:241:ILE:O	1:K:344:MET:HA	2.22	0.41
1:L:114:ILE:HG13	1:L:146:ILE:HD11	2.03	0.41
1:A:45:LYS:HD2	1:A:45:LYS:HA	1.98	0.40
1:B:112:LYS:H	1:B:169:ASP:CG	2.29	0.40
1:C:65:ARG:HE	1:C:65:ARG:HB3	1.68	0.40
1:D:213:LEU:HD12	1:D:213:LEU:HA	1.85	0.40
1:D:438:ASP:HB3	1:D:441:VAL:HG12	2.03	0.40
1:E:112:LYS:H	1:E:169:ASP:CG	2.29	0.40
1:F:169:ASP:HB3	1:F:170:PRO:HD3	2.02	0.40
2:R:596:LEU:HD22	2:R:636:VAL:HG11	2.03	0.40
1:G:22:ARG:HA	1:G:23:PRO:HD3	1.97	0.40
1:G:226:HIS:N	1:G:227:PRO:HD3	2.36	0.40
1:I:143:TYR:CE1	1:I:178:PRO:HD3	2.56	0.40
1:I:286:LEU:HD23	1:I:286:LEU:HA	1.98	0.40
1:J:241:ILE:O	1:J:344:MET:HA	2.21	0.40
1:L:213:LEU:HD12	1:L:213:LEU:HA	1.86	0.40
1:A:99:VAL:HG21	1:C:431:ASP:HB2	2.04	0.40
1:E:169:ASP:CB	1:E:170:PRO:CD	2.98	0.40
1:E:322:ARG:HH12	1:F:317:HIS:CD2	2.38	0.40
1:F:408:GLY:HA3	3:F:501:ADP:C8	2.56	0.40
2:O:600:PHE:O	2:O:603:VAL:HG22	2.20	0.40
1:G:242:LEU:HD12	1:G:242:LEU:HA	1.90	0.40
1:I:27:ILE:HB	1:I:81:LYS:HG2	2.03	0.40
1:I:385:THR:HB	1:I:390:LEU:HD11	2.03	0.40
1:K:323:ARG:HH22	1:L:278:LEU:HD23	1.86	0.40
1:L:331:LEU:HD23	1:L:331:LEU:HA	1.94	0.40
1:A:112:LYS:H	1:A:169:ASP:CG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:CE2	1:A:152:PHE:CD1	3.09	0.40
1:A:169:ASP:CB	1:A:170:PRO:CD	2.99	0.40
1:C:329:LEU:HD12	1:C:362:ARG:NH2	2.36	0.40
1:E:322:ARG:NH2	1:F:317:HIS:HD2	2.19	0.40
1:F:231:LYS:HB2	1:F:231:LYS:HE2	1.90	0.40
2:M:580:THR:CG2	2:M:608:PHE:HZ	2.27	0.40
2:P:634:LEU:HD12	2:P:634:LEU:HA	1.69	0.40
2:Q:589:ARG:HD3	2:T:591:LEU:HD13	2.02	0.40
1:H:335:LEU:HD23	1:H:335:LEU:HA	1.97	0.40
1:H:385:THR:HB	1:H:390:LEU:HD11	2.04	0.40
1:J:27:ILE:HB	1:J:81:LYS:HG2	2.03	0.40
1:K:409:ALA:HB2	3:K:501:ADP:H5'1	2.04	0.40
1:L:169:ASP:CB	1:L:170:PRO:CD	2.99	0.40
1:L:242:LEU:HD12	1:L:242:LEU:HA	1.89	0.40
1:B:239:ARG:HD3	1:B:335:LEU:HB2	2.03	0.40
1:D:138:TYR:CE2	1:D:152:PHE:CD1	3.10	0.40
1:E:314:GLU:CD	1:E:314:GLU:N	2.80	0.40
1:F:241:ILE:O	1:F:344:MET:HA	2.22	0.40
1:G:68:VAL:HG22	1:G:147:ARG:HB2	2.03	0.40
1:G:85:ASN:ND2	1:G:87:VAL:HB	2.36	0.40
1:H:431:ASP:HB2	1:J:99:VAL:CG2	2.50	0.40
1:I:21:ASN:CB	1:J:432:LEU:HD11	2.52	0.40
1:J:213:LEU:HD12	1:J:213:LEU:HA	1.86	0.40
1:K:112:LYS:H	1:K:169:ASP:CG	2.29	0.40
1:L:169:ASP:HB3	1:L:170:PRO:HD3	2.03	0.40
2:V:596:LEU:HD22	2:V:636:VAL:HG11	2.03	0.40
1:C:143:TYR:CE1	1:C:178:PRO:HD3	2.57	0.40
1:C:432:LEU:H	1:C:432:LEU:HG	1.65	0.40
1:E:291:GLU:O	1:E:295:LYS:HG3	2.22	0.40
1:F:226:HIS:N	1:F:227:PRO:HD3	2.37	0.40
1:G:91:ASN:HD22	1:G:91:ASN:HA	1.33	0.40
1:H:142:ALA:HB1	1:H:144:ARG:HG3	2.03	0.40
1:I:53:ARG:CZ	1:I:72:LEU:HD23	2.52	0.40
1:I:244:TYR:CE1	1:I:368:ASP:HB2	2.57	0.40
1:J:142:ALA:HB1	1:J:144:ARG:HG3	2.04	0.40
1:J:226:HIS:N	1:J:227:PRO:HD3	2.37	0.40
1:L:226:HIS:N	1:L:227:PRO:HD3	2.37	0.40
2:S:596:LEU:HD22	2:S:636:VAL:HG11	2.04	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ASN:OD1	1:H:185:GLU:OE2[1_565]	1.41	0.79
1:A:120:ASP:OD2	1:G:64:ARG:NH2[1_655]	1.79	0.41
1:A:188:PRO:O	1:G:64:ARG:NH1[1_655]	1.81	0.39
1:C:296:ASN:OD1	1:H:185:GLU:CD[1_565]	1.81	0.39
1:A:190:LYS:CA	1:G:64:ARG:NH2[1_655]	2.13	0.07
1:C:296:ASN:OD1	1:H:185:GLU:OE1[1_565]	2.14	0.06
1:C:295:LYS:CE	1:H:115:HIS:NE2[1_565]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/438 (100%)	415 (95%)	14 (3%)	7 (2%)	7	30
1	B	436/438 (100%)	417 (96%)	13 (3%)	6 (1%)	9	34
1	C	436/438 (100%)	413 (95%)	16 (4%)	7 (2%)	7	30
1	D	436/438 (100%)	416 (95%)	13 (3%)	7 (2%)	7	30
1	E	436/438 (100%)	417 (96%)	12 (3%)	7 (2%)	7	30
1	F	436/438 (100%)	415 (95%)	14 (3%)	7 (2%)	7	30
1	G	436/438 (100%)	415 (95%)	11 (2%)	10 (2%)	5	23
1	H	436/438 (100%)	415 (95%)	15 (3%)	6 (1%)	9	34
1	I	436/438 (100%)	418 (96%)	11 (2%)	7 (2%)	7	30
1	J	436/438 (100%)	415 (95%)	14 (3%)	7 (2%)	7	30
1	K	436/438 (100%)	416 (95%)	12 (3%)	8 (2%)	6	28
1	L	436/438 (100%)	416 (95%)	14 (3%)	6 (1%)	9	34
2	M	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	N	56/76 (74%)	50 (89%)	4 (7%)	2 (4%)	2	16
2	O	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
2	P	74/76 (97%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	R	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	S	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	T	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	U	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	V	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	W	45/76 (59%)	43 (96%)	2 (4%)	0	100	100
2	X	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
All	All	6073/6168 (98%)	5790 (95%)	196 (3%)	87 (1%)	9	34

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	THR
1	C	438	ASP
1	D	436	THR
1	E	363	PHE
1	F	363	PHE
1	G	363	PHE
1	G	430	ILE
1	H	110	TYR
1	H	436	THR
1	I	110	TYR
1	I	436	THR
1	J	430	ILE
1	J	438	ASP
1	K	363	PHE
1	L	363	PHE
1	L	436	THR
1	A	110	TYR
1	A	363	PHE
1	B	110	TYR
1	B	172	PRO
1	B	363	PHE
1	B	436	THR
1	C	110	TYR
1	C	363	PHE
1	C	436	THR
1	C	437	ILE

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Mol	Chain	Res	Type
1	D	110	TYR
1	D	172	PRO
1	D	363	PHE
1	E	110	TYR
1	E	172	PRO
1	E	436	THR
1	F	110	TYR
1	F	432	LEU
1	F	436	THR
2	N	584	GLU
1	G	110	TYR
1	G	436	THR
1	H	172	PRO
1	H	363	PHE
1	I	363	PHE
1	J	110	TYR
1	J	172	PRO
1	J	363	PHE
1	J	436	THR
1	J	437	ILE
1	K	110	TYR
1	K	436	THR
1	L	110	TYR
1	L	172	PRO
1	A	172	PRO
1	A	437	ILE
1	B	437	ILE
1	C	172	PRO
1	D	437	ILE
1	F	172	PRO
1	F	437	ILE
1	G	172	PRO
1	G	431	ASP
1	G	432	LEU
1	G	437	ILE
1	H	437	ILE
1	I	172	PRO
1	I	437	ILE
1	K	172	PRO
1	K	437	ILE
1	L	437	ILE
1	A	432	LEU

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Mol	Chain	Res	Type
1	E	437	ILE
1	K	432	LEU
1	A	169	ASP
1	B	169	ASP
1	C	169	ASP
1	D	169	ASP
1	D	438	ASP
1	E	169	ASP
1	E	438	ASP
1	F	169	ASP
2	N	643	THR
1	G	169	ASP
1	G	438	ASP
1	H	169	ASP
1	I	169	ASP
1	I	438	ASP
1	K	169	ASP
1	K	438	ASP
1	L	169	ASP

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	372/372 (100%)	324 (87%)	48 (13%)	4	18
1	B	372/372 (100%)	325 (87%)	47 (13%)	4	19
1	C	372/372 (100%)	322 (87%)	50 (13%)	4	17
1	D	372/372 (100%)	321 (86%)	51 (14%)	3	15
1	E	372/372 (100%)	318 (86%)	54 (14%)	3	14
1	F	372/372 (100%)	319 (86%)	53 (14%)	3	14
1	G	372/372 (100%)	315 (85%)	57 (15%)	3	12
1	H	372/372 (100%)	327 (88%)	45 (12%)	5	20
1	I	372/372 (100%)	327 (88%)	45 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	372/372 (100%)	323 (87%)	49 (13%)	4	17
1	K	372/372 (100%)	325 (87%)	47 (13%)	4	19
1	L	372/372 (100%)	317 (85%)	55 (15%)	3	13
2	M	71/71 (100%)	59 (83%)	12 (17%)	2	10
2	N	58/71 (82%)	45 (78%)	13 (22%)	1	4
2	O	71/71 (100%)	61 (86%)	10 (14%)	3	15
2	P	71/71 (100%)	59 (83%)	12 (17%)	2	10
2	Q	71/71 (100%)	58 (82%)	13 (18%)	2	8
2	R	71/71 (100%)	55 (78%)	16 (22%)	1	4
2	S	71/71 (100%)	57 (80%)	14 (20%)	1	6
2	T	71/71 (100%)	58 (82%)	13 (18%)	2	8
2	U	71/71 (100%)	58 (82%)	13 (18%)	2	8
2	V	71/71 (100%)	57 (80%)	14 (20%)	1	6
2	W	50/71 (70%)	40 (80%)	10 (20%)	1	6
2	X	71/71 (100%)	55 (78%)	16 (22%)	1	4
All	All	5282/5316 (99%)	4525 (86%)	757 (14%)	3	14

All (757) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	32	ILE
1	A	60	LYS
1	A	68	VAL
1	A	75	ASP
1	A	76	THR
1	A	78	SER
1	A	86	ARG
1	A	107	ASP
1	A	108	VAL
1	A	113	ARG
1	A	119	ILE
1	A	123	VAL
1	A	140	LEU
1	A	158	MET
1	A	164	LYS
1	A	166	VAL

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Mol	Chain	Res	Type
1	A	168	THR
1	A	171	SER
1	A	174	CYS
1	A	187	GLU
1	A	190	LYS
1	A	201	VAL
1	A	210	ARG
1	A	225	ARG
1	A	229	LEU
1	A	231	LYS
1	A	236	LYS
1	A	273	GLU
1	A	278	LEU
1	A	283	GLU
1	A	307	ASP
1	A	313	ARG
1	A	314	GLU
1	A	315	LYS
1	A	330	THR
1	A	337	GLN
1	A	338	ARG
1	A	351	ASN
1	A	352	SER
1	A	353	ILE
1	A	358	ARG
1	A	359	ARG
1	A	427	MET
1	A	430	ILE
1	A	432	LEU
1	A	433	GLU
1	A	450	ASP
1	B	21	ASN
1	B	32	ILE
1	B	66	GLU
1	B	68	VAL
1	B	73	SER
1	B	75	ASP
1	B	76	THR
1	B	78	SER
1	B	81	LYS
1	B	86	ARG
1	B	108	VAL

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Mol	Chain	Res	Type
1	B	119	ILE
1	B	123	VAL
1	B	129	ASN
1	B	140	LEU
1	B	146	ILE
1	B	158	MET
1	B	166	VAL
1	B	168	THR
1	B	171	SER
1	B	174	CYS
1	B	179	ASP
1	B	184	CYS
1	B	187	GLU
1	B	189	ILE
1	B	190	LYS
1	B	210	ARG
1	B	225	ARG
1	B	229	LEU
1	B	273	GLU
1	B	278	LEU
1	B	283	GLU
1	B	307	ASP
1	B	313	ARG
1	B	315	LYS
1	B	316	THR
1	B	330	THR
1	B	351	ASN
1	B	352	SER
1	B	353	ILE
1	B	358	ARG
1	B	359	ARG
1	B	427	MET
1	B	432	LEU
1	B	433	GLU
1	B	435	GLU
1	B	436	THR
1	C	32	ILE
1	C	60	LYS
1	C	68	VAL
1	C	75	ASP
1	C	76	THR
1	C	86	ARG

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Mol	Chain	Res	Type
1	C	103	GLN
1	C	107	ASP
1	C	108	VAL
1	C	119	ILE
1	C	123	VAL
1	C	158	MET
1	C	166	VAL
1	C	168	THR
1	C	171	SER
1	C	174	CYS
1	C	184	CYS
1	C	187	GLU
1	C	189	ILE
1	C	190	LYS
1	C	201	VAL
1	C	211	LYS
1	C	225	ARG
1	C	229	LEU
1	C	231	LYS
1	C	236	LYS
1	C	253	LEU
1	C	273	GLU
1	C	278	LEU
1	C	283	GLU
1	C	288	LYS
1	C	295	LYS
1	C	307	ASP
1	C	313	ARG
1	C	314	GLU
1	C	315	LYS
1	C	317	HIS
1	C	330	THR
1	C	337	GLN
1	C	338	ARG
1	C	351	ASN
1	C	352	SER
1	C	353	ILE
1	C	358	ARG
1	C	371	ILE
1	C	427	MET
1	C	432	LEU
1	C	435	GLU

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Mol	Chain	Res	Type
1	C	438	ASP
1	C	440	GLU
1	D	60	LYS
1	D	64	ARG
1	D	68	VAL
1	D	73	SER
1	D	75	ASP
1	D	76	THR
1	D	101	SER
1	D	103	GLN
1	D	107	ASP
1	D	108	VAL
1	D	119	ILE
1	D	123	VAL
1	D	140	LEU
1	D	158	MET
1	D	164	LYS
1	D	166	VAL
1	D	167	GLU
1	D	168	THR
1	D	171	SER
1	D	174	CYS
1	D	179	ASP
1	D	181	VAL
1	D	184	CYS
1	D	187	GLU
1	D	190	LYS
1	D	198	LEU
1	D	225	ARG
1	D	236	LYS
1	D	273	GLU
1	D	278	LEU
1	D	283	GLU
1	D	288	LYS
1	D	307	ASP
1	D	312	LYS
1	D	313	ARG
1	D	315	LYS
1	D	316	THR
1	D	337	GLN
1	D	338	ARG
1	D	351	ASN

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Mol	Chain	Res	Type
1	D	352	SER
1	D	353	ILE
1	D	358	ARG
1	D	359	ARG
1	D	427	MET
1	D	430	ILE
1	D	432	LEU
1	D	433	GLU
1	D	434	ASP
1	D	435	GLU
1	D	441	VAL
1	E	22	ARG
1	E	32	ILE
1	E	60	LYS
1	E	66	GLU
1	E	68	VAL
1	E	73	SER
1	E	75	ASP
1	E	76	THR
1	E	80	GLU
1	E	86	ARG
1	E	103	GLN
1	E	107	ASP
1	E	108	VAL
1	E	113	ARG
1	E	119	ILE
1	E	123	VAL
1	E	129	ASN
1	E	140	LEU
1	E	148	LYS
1	E	158	MET
1	E	166	VAL
1	E	168	THR
1	E	171	SER
1	E	174	CYS
1	E	179	ASP
1	E	187	GLU
1	E	189	ILE
1	E	190	LYS
1	E	201	VAL
1	E	211	LYS
1	E	225	ARG

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Mol	Chain	Res	Type
1	E	229	LEU
1	E	231	LYS
1	E	236	LYS
1	E	273	GLU
1	E	278	LEU
1	E	283	GLU
1	E	307	ASP
1	E	312	LYS
1	E	313	ARG
1	E	314	GLU
1	E	315	LYS
1	E	316	THR
1	E	317	HIS
1	E	330	THR
1	E	336	LYS
1	E	351	ASN
1	E	352	SER
1	E	353	ILE
1	E	358	ARG
1	E	427	MET
1	E	430	ILE
1	E	432	LEU
1	E	433	GLU
1	F	60	LYS
1	F	66	GLU
1	F	68	VAL
1	F	75	ASP
1	F	76	THR
1	F	86	ARG
1	F	103	GLN
1	F	107	ASP
1	F	108	VAL
1	F	109	LYS
1	F	112	LYS
1	F	113	ARG
1	F	119	ILE
1	F	123	VAL
1	F	140	LEU
1	F	148	LYS
1	F	158	MET
1	F	161	VAL
1	F	164	LYS

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Mol	Chain	Res	Type
1	F	166	VAL
1	F	168	THR
1	F	174	CYS
1	F	187	GLU
1	F	189	ILE
1	F	190	LYS
1	F	211	LYS
1	F	225	ARG
1	F	229	LEU
1	F	231	LYS
1	F	273	GLU
1	F	278	LEU
1	F	283	GLU
1	F	295	LYS
1	F	307	ASP
1	F	312	LYS
1	F	313	ARG
1	F	314	GLU
1	F	315	LYS
1	F	317	HIS
1	F	330	THR
1	F	337	GLN
1	F	338	ARG
1	F	351	ASN
1	F	352	SER
1	F	353	ILE
1	F	358	ARG
1	F	359	ARG
1	F	427	MET
1	F	429	LEU
1	F	430	ILE
1	F	432	LEU
1	F	435	GLU
1	F	440	GLU
2	M	579	ARG
2	M	580	THR
2	M	591	LEU
2	M	593	SER
2	M	606	LYS
2	M	610	TRP
2	M	611	ASP
2	M	612	GLU

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Mol	Chain	Res	Type
2	M	624	VAL
2	M	625	THR
2	M	632	SER
2	M	634	LEU
2	N	578	ILE
2	N	580	THR
2	N	584	GLU
2	N	586	LEU
2	N	589	ARG
2	N	599	VAL
2	N	606	LYS
2	N	611	ASP
2	N	622	ARG
2	N	624	VAL
2	N	625	THR
2	N	631	LYS
2	N	642	GLU
2	O	584	GLU
2	O	593	SER
2	O	606	LYS
2	O	611	ASP
2	O	621	ARG
2	O	624	VAL
2	O	625	THR
2	O	632	SER
2	O	637	LYS
2	O	640	PRO
2	P	575	LYS
2	P	585	PHE
2	P	589	ARG
2	P	591	LEU
2	P	593	SER
2	P	599	VAL
2	P	606	LYS
2	P	611	ASP
2	P	624	VAL
2	P	625	THR
2	P	644	LEU
2	P	650	GLU
2	Q	575	LYS
2	Q	579	ARG
2	Q	588	ARG

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Mol	Chain	Res	Type
2	Q	593	SER
2	Q	606	LYS
2	Q	611	ASP
2	Q	612	GLU
2	Q	621	ARG
2	Q	624	VAL
2	Q	625	THR
2	Q	631	LYS
2	Q	632	SER
2	Q	634	LEU
2	R	584	GLU
2	R	588	ARG
2	R	589	ARG
2	R	593	SER
2	R	606	LYS
2	R	611	ASP
2	R	612	GLU
2	R	621	ARG
2	R	624	VAL
2	R	625	THR
2	R	626	GLN
2	R	630	ASN
2	R	632	SER
2	R	633	LEU
2	R	634	LEU
2	R	641	GLN
1	G	32	ILE
1	G	34	GLU
1	G	64	ARG
1	G	68	VAL
1	G	72	LEU
1	G	75	ASP
1	G	76	THR
1	G	86	ARG
1	G	103	GLN
1	G	107	ASP
1	G	108	VAL
1	G	109	LYS
1	G	113	ARG
1	G	119	ILE
1	G	123	VAL
1	G	140	LEU

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Mol	Chain	Res	Type
1	G	146	ILE
1	G	148	LYS
1	G	158	MET
1	G	164	LYS
1	G	166	VAL
1	G	168	THR
1	G	171	SER
1	G	174	CYS
1	G	181	VAL
1	G	182	ILE
1	G	184	CYS
1	G	187	GLU
1	G	190	LYS
1	G	201	VAL
1	G	211	LYS
1	G	225	ARG
1	G	229	LEU
1	G	231	LYS
1	G	236	LYS
1	G	273	GLU
1	G	278	LEU
1	G	283	GLU
1	G	307	ASP
1	G	312	LYS
1	G	313	ARG
1	G	314	GLU
1	G	315	LYS
1	G	316	THR
1	G	338	ARG
1	G	351	ASN
1	G	352	SER
1	G	353	ILE
1	G	358	ARG
1	G	359	ARG
1	G	427	MET
1	G	430	ILE
1	G	432	LEU
1	G	437	ILE
1	G	440	GLU
1	G	441	VAL
1	G	453	ARG
1	H	32	ILE

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Mol	Chain	Res	Type
1	H	53	ARG
1	H	60	LYS
1	H	64	ARG
1	H	66	GLU
1	H	68	VAL
1	H	72	LEU
1	H	75	ASP
1	H	76	THR
1	H	119	ILE
1	H	123	VAL
1	H	140	LEU
1	H	146	ILE
1	H	148	LYS
1	H	158	MET
1	H	168	THR
1	H	171	SER
1	H	174	CYS
1	H	179	ASP
1	H	189	ILE
1	H	190	LYS
1	H	199	ASN
1	H	201	VAL
1	H	210	ARG
1	H	225	ARG
1	H	231	LYS
1	H	278	LEU
1	H	283	GLU
1	H	307	ASP
1	H	313	ARG
1	H	314	GLU
1	H	315	LYS
1	H	316	THR
1	H	337	GLN
1	H	338	ARG
1	H	349	ARG
1	H	351	ASN
1	H	352	SER
1	H	353	ILE
1	H	358	ARG
1	H	397	GLU
1	H	427	MET
1	H	432	LEU

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Mol	Chain	Res	Type
1	H	433	GLU
1	H	441	VAL
1	I	32	ILE
1	I	53	ARG
1	I	60	LYS
1	I	68	VAL
1	I	75	ASP
1	I	76	THR
1	I	86	ARG
1	I	103	GLN
1	I	107	ASP
1	I	119	ILE
1	I	123	VAL
1	I	124	GLU
1	I	140	LEU
1	I	146	ILE
1	I	158	MET
1	I	159	ARG
1	I	164	LYS
1	I	166	VAL
1	I	174	CYS
1	I	184	CYS
1	I	187	GLU
1	I	210	ARG
1	I	211	LYS
1	I	225	ARG
1	I	229	LEU
1	I	231	LYS
1	I	273	GLU
1	I	278	LEU
1	I	283	GLU
1	I	307	ASP
1	I	313	ARG
1	I	315	LYS
1	I	316	THR
1	I	322	ARG
1	I	330	THR
1	I	337	GLN
1	I	349	ARG
1	I	351	ASN
1	I	352	SER
1	I	353	ILE

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Mol	Chain	Res	Type
1	I	358	ARG
1	I	430	ILE
1	I	432	LEU
1	I	440	GLU
1	I	441	VAL
1	J	62	LYS
1	J	66	GLU
1	J	68	VAL
1	J	73	SER
1	J	75	ASP
1	J	76	THR
1	J	78	SER
1	J	107	ASP
1	J	108	VAL
1	J	119	ILE
1	J	121	ASP
1	J	123	VAL
1	J	140	LEU
1	J	158	MET
1	J	166	VAL
1	J	174	CYS
1	J	187	GLU
1	J	189	ILE
1	J	190	LYS
1	J	201	VAL
1	J	210	ARG
1	J	225	ARG
1	J	229	LEU
1	J	231	LYS
1	J	236	LYS
1	J	273	GLU
1	J	278	LEU
1	J	283	GLU
1	J	307	ASP
1	J	312	LYS
1	J	313	ARG
1	J	315	LYS
1	J	337	GLN
1	J	338	ARG
1	J	349	ARG
1	J	351	ASN
1	J	352	SER

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Mol	Chain	Res	Type
1	J	353	ILE
1	J	358	ARG
1	J	359	ARG
1	J	371	ILE
1	J	426	LYS
1	J	429	LEU
1	J	430	ILE
1	J	432	LEU
1	J	433	GLU
1	J	434	ASP
1	J	435	GLU
1	J	440	GLU
1	K	53	ARG
1	K	60	LYS
1	K	68	VAL
1	K	75	ASP
1	K	76	THR
1	K	107	ASP
1	K	108	VAL
1	K	113	ARG
1	K	116	VAL
1	K	119	ILE
1	K	123	VAL
1	K	127	THR
1	K	158	MET
1	K	166	VAL
1	K	171	SER
1	K	174	CYS
1	K	184	CYS
1	K	187	GLU
1	K	189	ILE
1	K	190	LYS
1	K	201	VAL
1	K	225	ARG
1	K	229	LEU
1	K	231	LYS
1	K	256	ARG
1	K	278	LEU
1	K	283	GLU
1	K	295	LYS
1	K	307	ASP
1	K	312	LYS

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Mol	Chain	Res	Type
1	K	313	ARG
1	K	315	LYS
1	K	316	THR
1	K	317	HIS
1	K	319	GLU
1	K	336	LYS
1	K	349	ARG
1	K	351	ASN
1	K	352	SER
1	K	353	ILE
1	K	358	ARG
1	K	359	ARG
1	K	427	MET
1	K	430	ILE
1	K	432	LEU
1	K	440	GLU
1	K	441	VAL
1	L	22	ARG
1	L	60	LYS
1	L	64	ARG
1	L	68	VAL
1	L	75	ASP
1	L	76	THR
1	L	86	ARG
1	L	103	GLN
1	L	107	ASP
1	L	108	VAL
1	L	119	ILE
1	L	123	VAL
1	L	140	LEU
1	L	148	LYS
1	L	158	MET
1	L	166	VAL
1	L	168	THR
1	L	171	SER
1	L	173	TYR
1	L	174	CYS
1	L	179	ASP
1	L	181	VAL
1	L	187	GLU
1	L	189	ILE
1	L	190	LYS

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Mol	Chain	Res	Type
1	L	201	VAL
1	L	210	ARG
1	L	211	LYS
1	L	225	ARG
1	L	229	LEU
1	L	278	LEU
1	L	283	GLU
1	L	295	LYS
1	L	307	ASP
1	L	312	LYS
1	L	313	ARG
1	L	314	GLU
1	L	315	LYS
1	L	317	HIS
1	L	319	GLU
1	L	322	ARG
1	L	330	THR
1	L	336	LYS
1	L	338	ARG
1	L	351	ASN
1	L	352	SER
1	L	353	ILE
1	L	358	ARG
1	L	359	ARG
1	L	375	THR
1	L	429	LEU
1	L	430	ILE
1	L	432	LEU
1	L	435	GLU
1	L	441	VAL
2	S	577	ARG
2	S	579	ARG
2	S	586	LEU
2	S	593	SER
2	S	606	LYS
2	S	611	ASP
2	S	612	GLU
2	S	621	ARG
2	S	624	VAL
2	S	625	THR
2	S	631	LYS
2	S	632	SER

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Mol	Chain	Res	Type
2	S	634	LEU
2	S	637	LYS
2	T	575	LYS
2	T	585	PHE
2	T	591	LEU
2	T	593	SER
2	T	606	LYS
2	T	611	ASP
2	T	616	LEU
2	T	621	ARG
2	T	624	VAL
2	T	625	THR
2	T	634	LEU
2	T	637	LYS
2	T	638	LEU
2	U	584	GLU
2	U	588	ARG
2	U	593	SER
2	U	606	LYS
2	U	611	ASP
2	U	612	GLU
2	U	624	VAL
2	U	625	THR
2	U	631	LYS
2	U	632	SER
2	U	634	LEU
2	U	640	PRO
2	U	641	GLN
2	V	579	ARG
2	V	588	ARG
2	V	591	LEU
2	V	593	SER
2	V	606	LYS
2	V	611	ASP
2	V	612	GLU
2	V	614	LYS
2	V	621	ARG
2	V	624	VAL
2	V	625	THR
2	V	634	LEU
2	V	637	LYS
2	V	638	LEU

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Mol	Chain	Res	Type
2	W	578	ILE
2	W	579	ARG
2	W	585	PHE
2	W	587	GLU
2	W	598	ILE
2	W	606	LYS
2	W	611	ASP
2	W	615	LEU
2	W	618	THR
2	W	630	ASN
2	X	586	LEU
2	X	588	ARG
2	X	593	SER
2	X	598	ILE
2	X	603	VAL
2	X	606	LYS
2	X	611	ASP
2	X	612	GLU
2	X	623	ASP
2	X	624	VAL
2	X	625	THR
2	X	630	ASN
2	X	631	LYS
2	X	632	SER
2	X	634	LEU
2	X	637	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	115	HIS
1	A	129	ASN
1	A	215	GLN
1	A	285	ASN
1	A	317	HIS
1	A	348	ASN
1	A	406	HIS
1	B	85	ASN
1	B	103	GLN
1	B	115	HIS
1	B	199	ASN

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Mol	Chain	Res	Type
1	B	215	GLN
1	B	285	ASN
1	B	348	ASN
1	B	351	ASN
1	C	115	HIS
1	C	129	ASN
1	C	183	HIS
1	C	285	ASN
1	C	317	HIS
1	C	337	GLN
1	D	21	ASN
1	D	115	HIS
1	D	129	ASN
1	D	183	HIS
1	D	215	GLN
1	D	351	ASN
1	D	443	ASN
1	E	115	HIS
1	E	317	HIS
1	F	85	ASN
1	F	115	HIS
1	F	226	HIS
1	F	285	ASN
1	F	317	HIS
1	F	351	ASN
1	F	384	HIS
2	M	597	GLN
2	N	597	GLN
2	N	626	GLN
2	N	641	GLN
2	O	597	GLN
2	O	626	GLN
2	O	630	ASN
2	Q	597	GLN
2	R	626	GLN
1	G	91	ASN
1	G	215	GLN
1	G	384	HIS
1	H	103	GLN
1	H	285	ASN
1	H	317	HIS
1	H	327	GLN

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Mol	Chain	Res	Type
1	H	398	GLN
1	I	115	HIS
1	I	129	ASN
1	I	285	ASN
1	I	317	HIS
1	I	384	HIS
1	J	21	ASN
1	J	199	ASN
1	J	226	HIS
1	J	285	ASN
1	J	317	HIS
1	J	337	GLN
1	J	351	ASN
1	J	384	HIS
1	J	443	ASN
1	K	115	HIS
1	K	129	ASN
1	K	215	GLN
1	K	285	ASN
1	K	348	ASN
1	K	398	GLN
1	L	115	HIS
1	L	183	HIS
1	L	337	GLN
1	L	348	ASN
1	L	351	ASN
2	S	597	GLN
2	T	597	GLN
2	U	626	GLN
2	U	630	ASN
2	V	597	GLN
2	W	597	GLN
2	X	594	ASN
2	X	597	GLN
2	X	626	GLN

5.3.3 RNA ⓘ

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	H	501	-	28,29,29	0.43	0	43,45,45	0.72	0
3	ADP	E	501	-	28,29,29	0.45	0	43,45,45	0.65	1 (2%)
3	ADP	L	501	-	28,29,29	0.49	0	43,45,45	0.72	0
3	ADP	G	501	-	28,29,29	0.41	0	43,45,45	0.66	0
3	ADP	D	501	-	28,29,29	0.40	0	43,45,45	0.68	0
3	ADP	I	501	-	28,29,29	0.62	1 (3%)	43,45,45	0.61	0
3	ADP	B	501	-	28,29,29	0.47	0	43,45,45	0.85	0
3	ADP	A	501	-	28,29,29	0.43	0	43,45,45	0.73	0
3	ADP	J	501	-	28,29,29	0.52	0	43,45,45	0.84	1 (2%)
3	ADP	K	501	-	28,29,29	0.46	0	43,45,45	0.62	0
3	ADP	F	501	-	28,29,29	0.44	0	43,45,45	0.78	0
3	ADP	C	501	-	28,29,29	0.40	0	43,45,45	0.67	1 (2%)

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	H	501	-	-	3/16/32/32	0/3/3/3
3	ADP	E	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	L	501	-	-	3/16/32/32	0/3/3/3
3	ADP	G	501	-	-	5/16/32/32	0/3/3/3
3	ADP	D	501	-	-	3/16/32/32	0/3/3/3
3	ADP	I	501	-	-	4/16/32/32	0/3/3/3
3	ADP	B	501	-	-	1/16/32/32	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	K	501	-	-	5/16/32/32	0/3/3/3
3	ADP	F	501	-	-	4/16/32/32	0/3/3/3
3	ADP	C	501	-	-	2/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

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

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	501	ADP	O3'-C3'-C2'	-2.51	103.78	111.82
3	C	501	ADP	O3'-C3'-C2'	-2.11	105.04	111.82
3	E	501	ADP	O3B-PB-O2B	2.00	115.32	107.80

There are no chirality outliers.

All (42) 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-O1A
3	C	501	ADP	C5'-O5'-PA-O2A
3	C	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-O3A
3	F	501	ADP	C5'-O5'-PA-O3A
3	G	501	ADP	C5'-O5'-PA-O1A
3	G	501	ADP	C5'-O5'-PA-O2A
3	G	501	ADP	C5'-O5'-PA-O3A

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

There are no ring outliers.

12 monomers are involved in 20 short contacts:

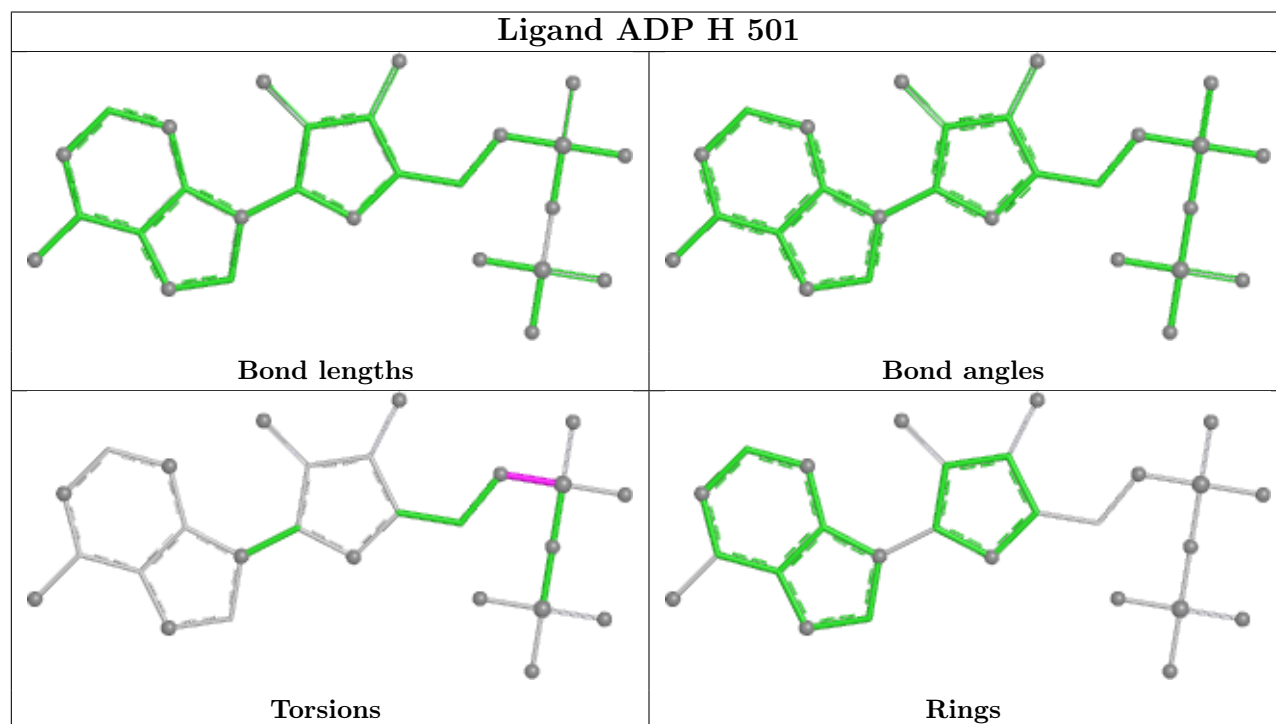
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	501	ADP	3	0
3	E	501	ADP	1	0
3	L	501	ADP	2	0
3	G	501	ADP	1	0
3	D	501	ADP	1	0
3	I	501	ADP	1	0
3	B	501	ADP	2	0

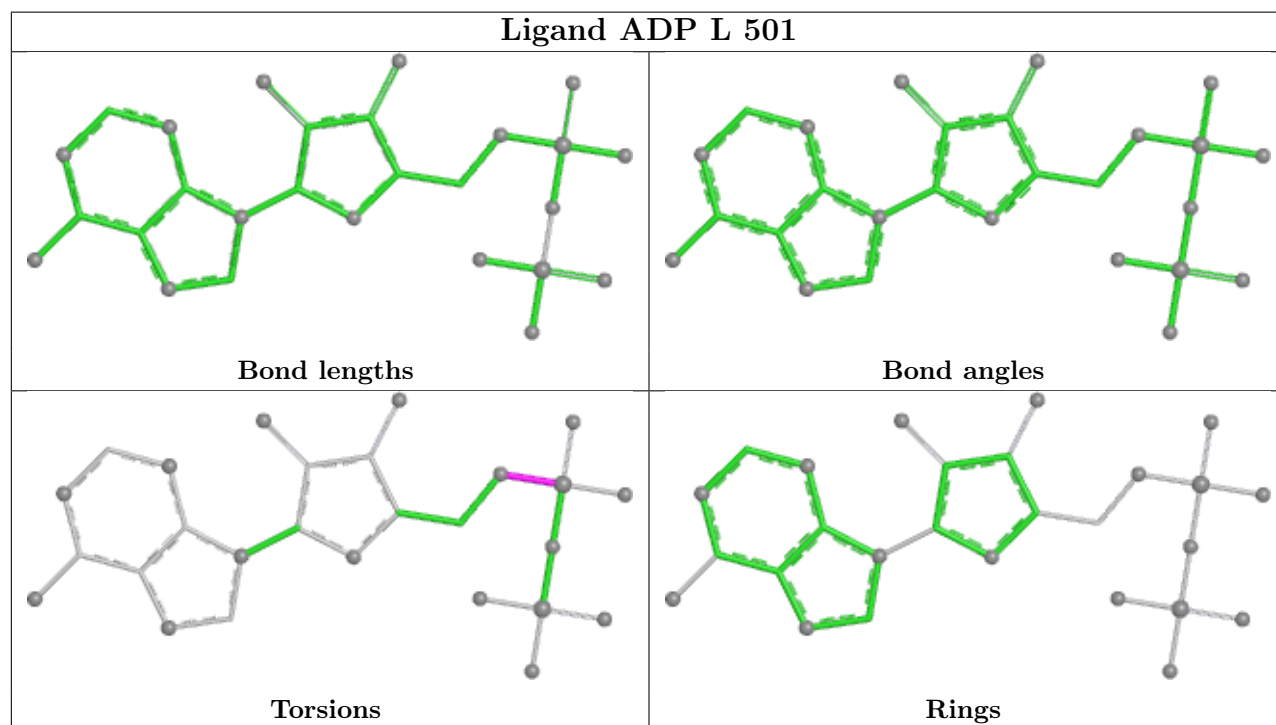
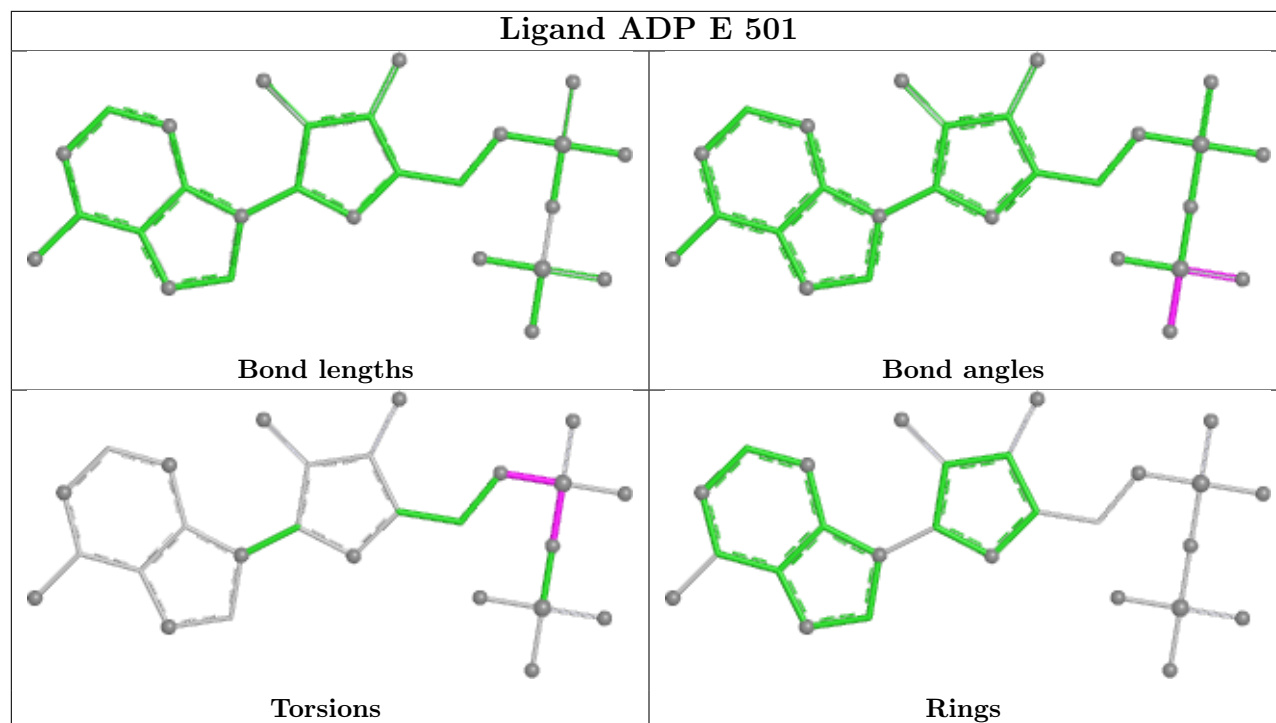
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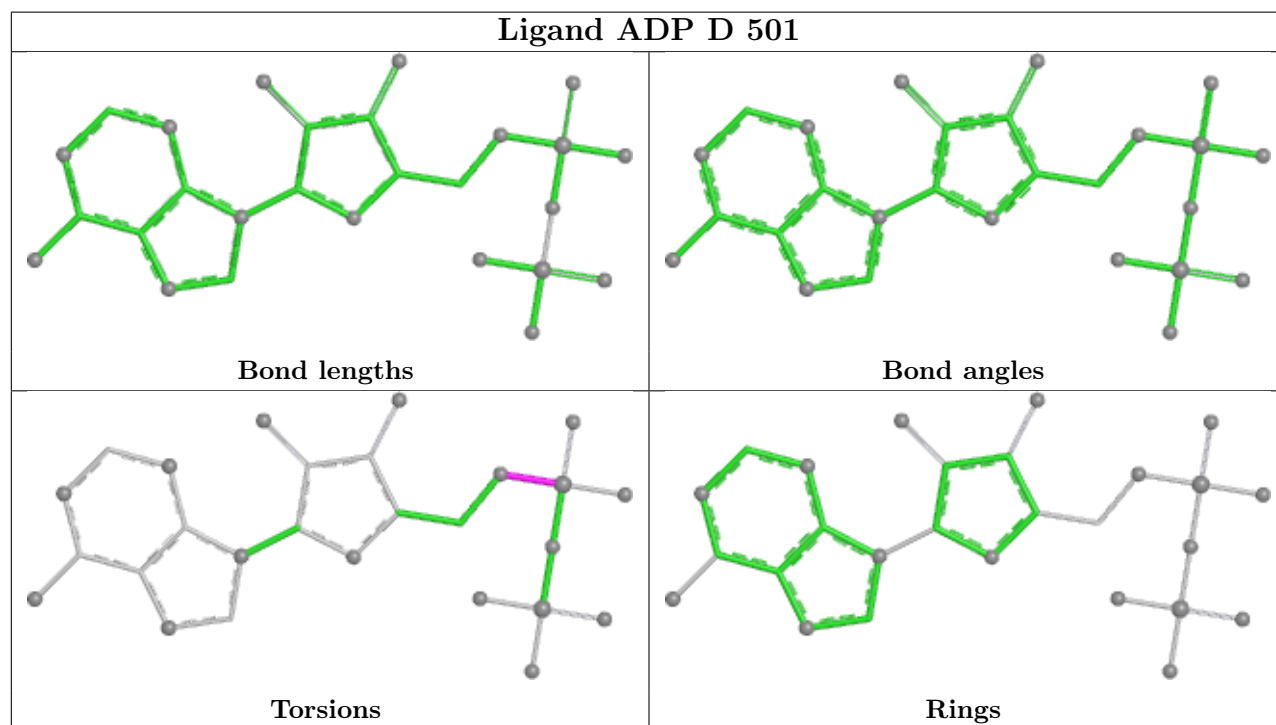
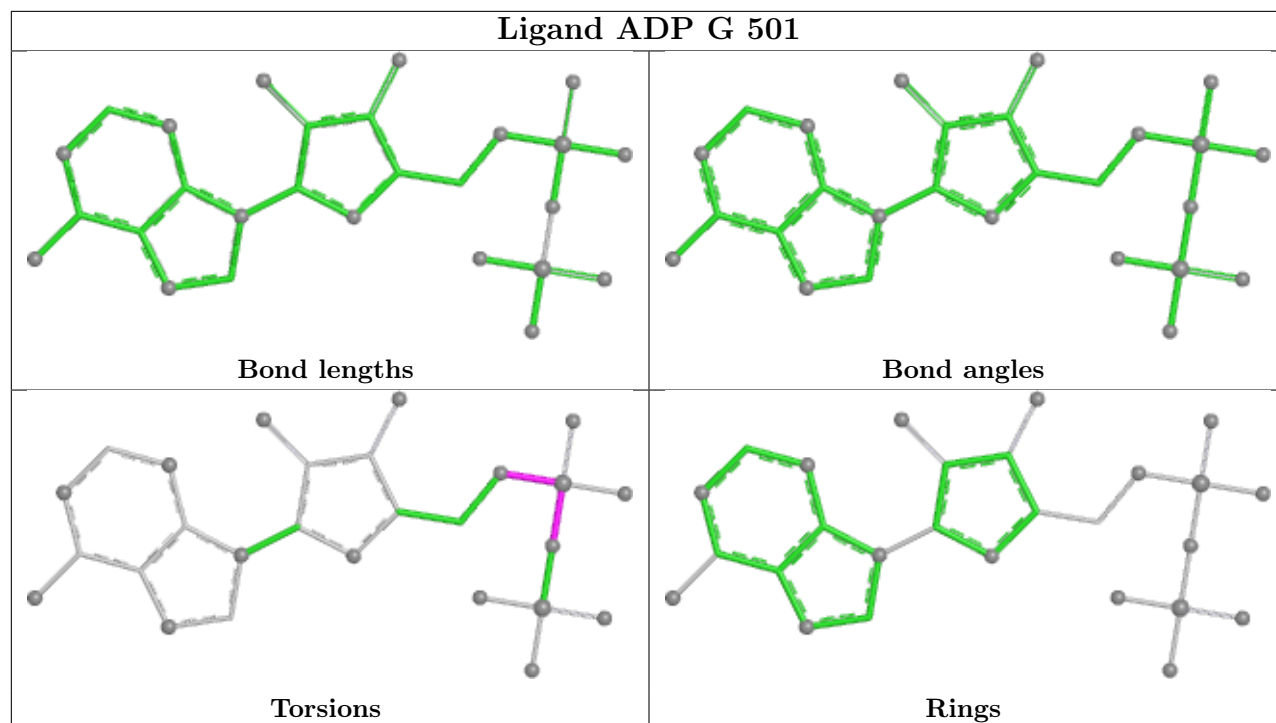
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ADP	1	0
3	J	501	ADP	4	0
3	K	501	ADP	1	0
3	F	501	ADP	2	0
3	C	501	ADP	1	0

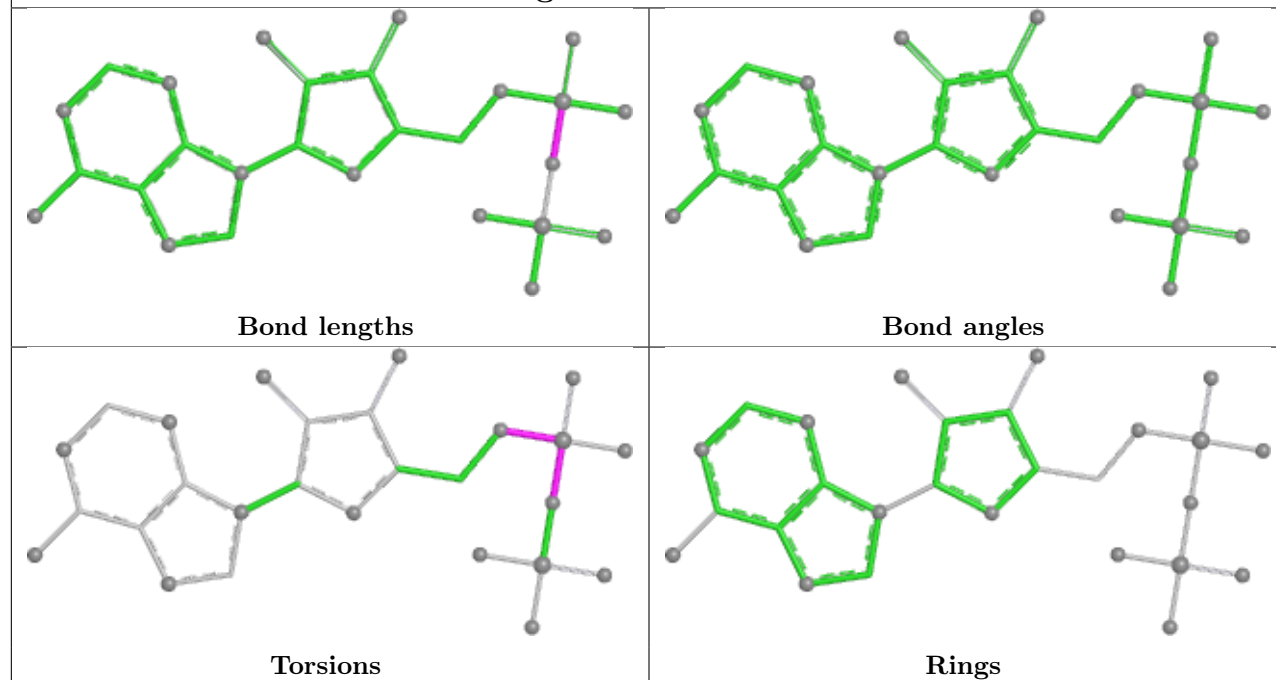
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



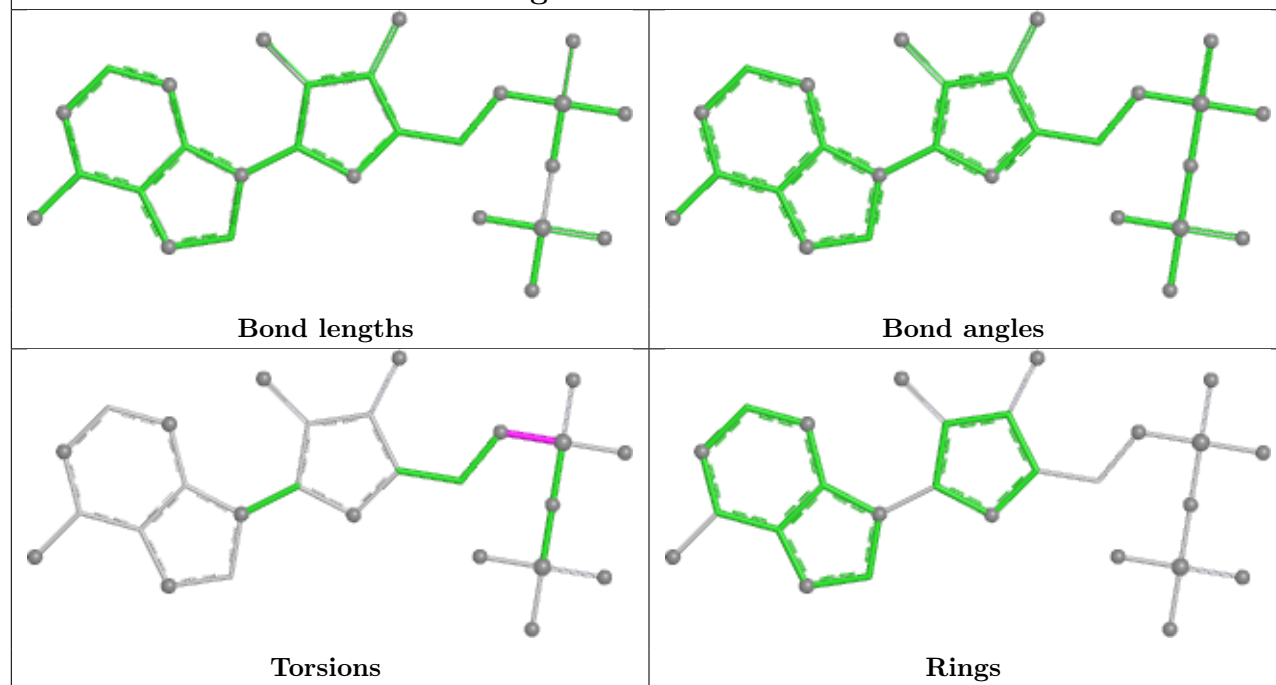


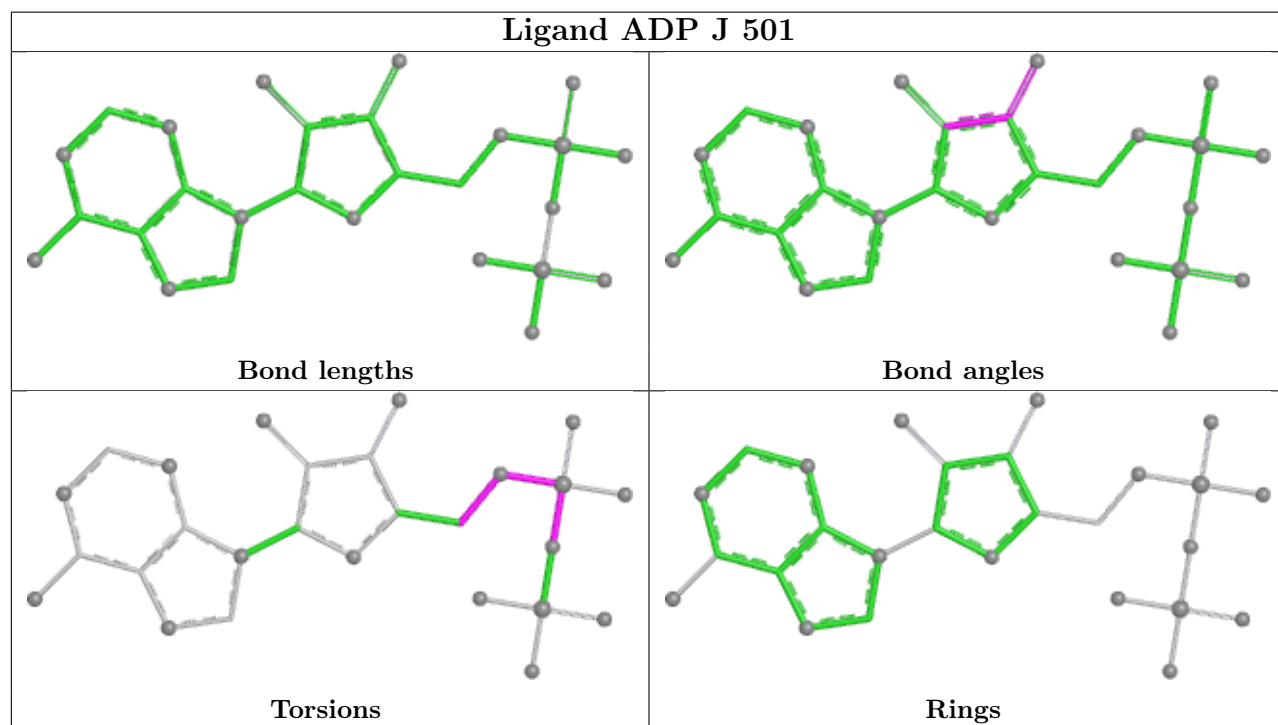
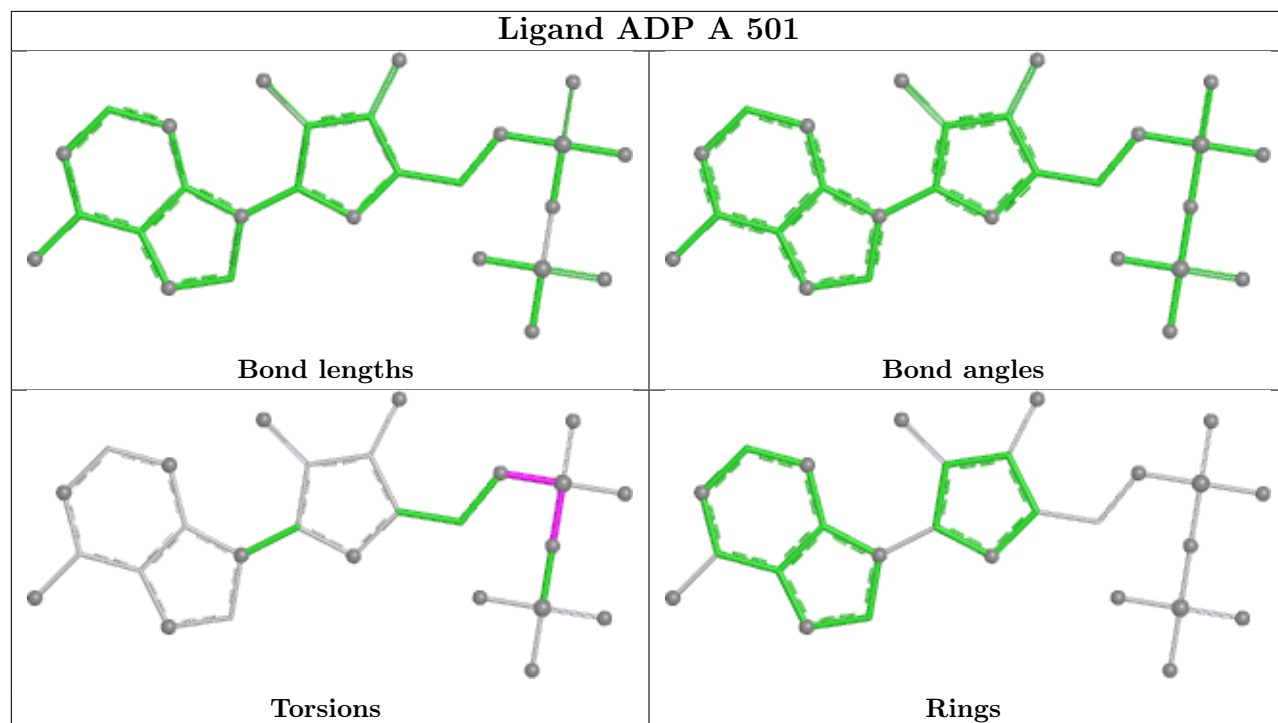


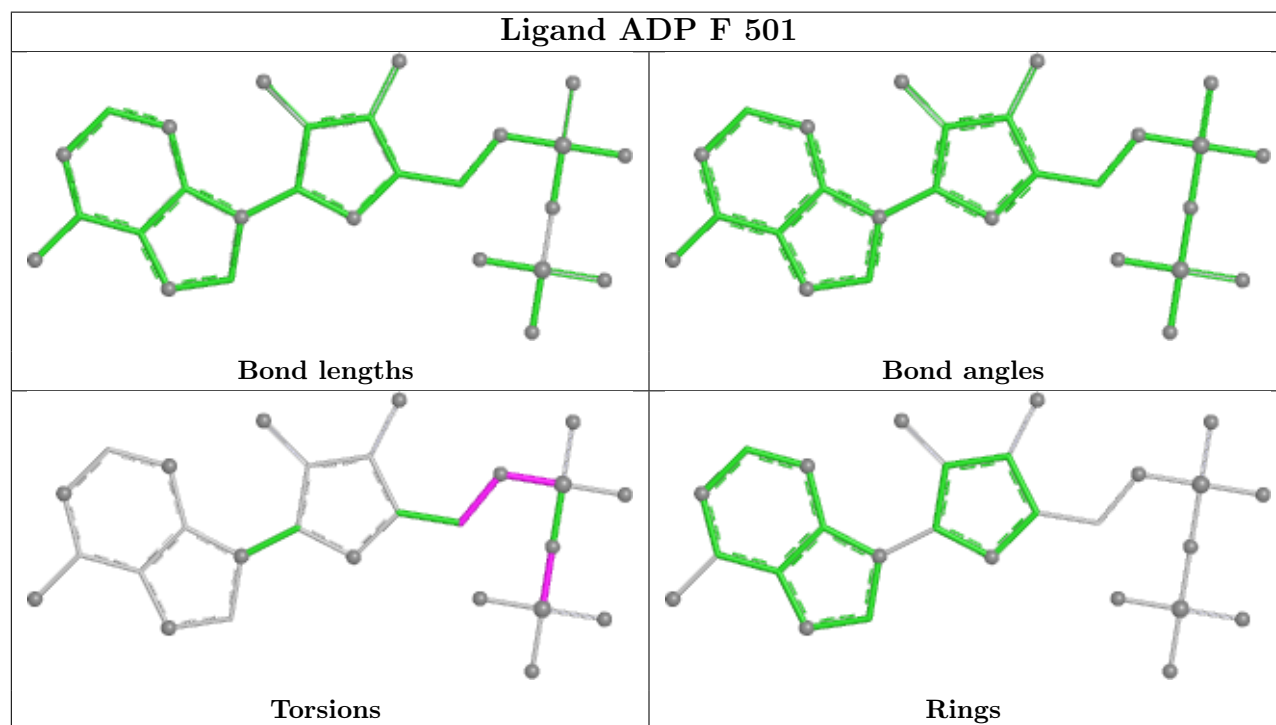
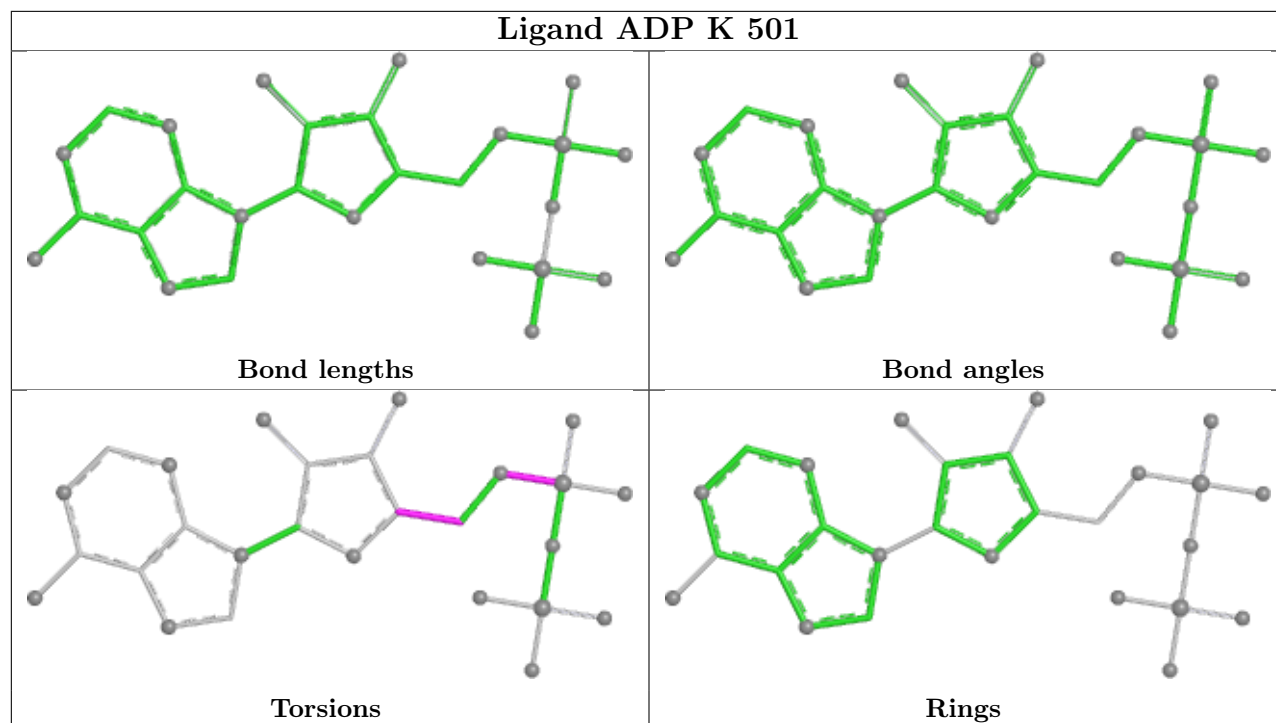
Ligand ADP I 501

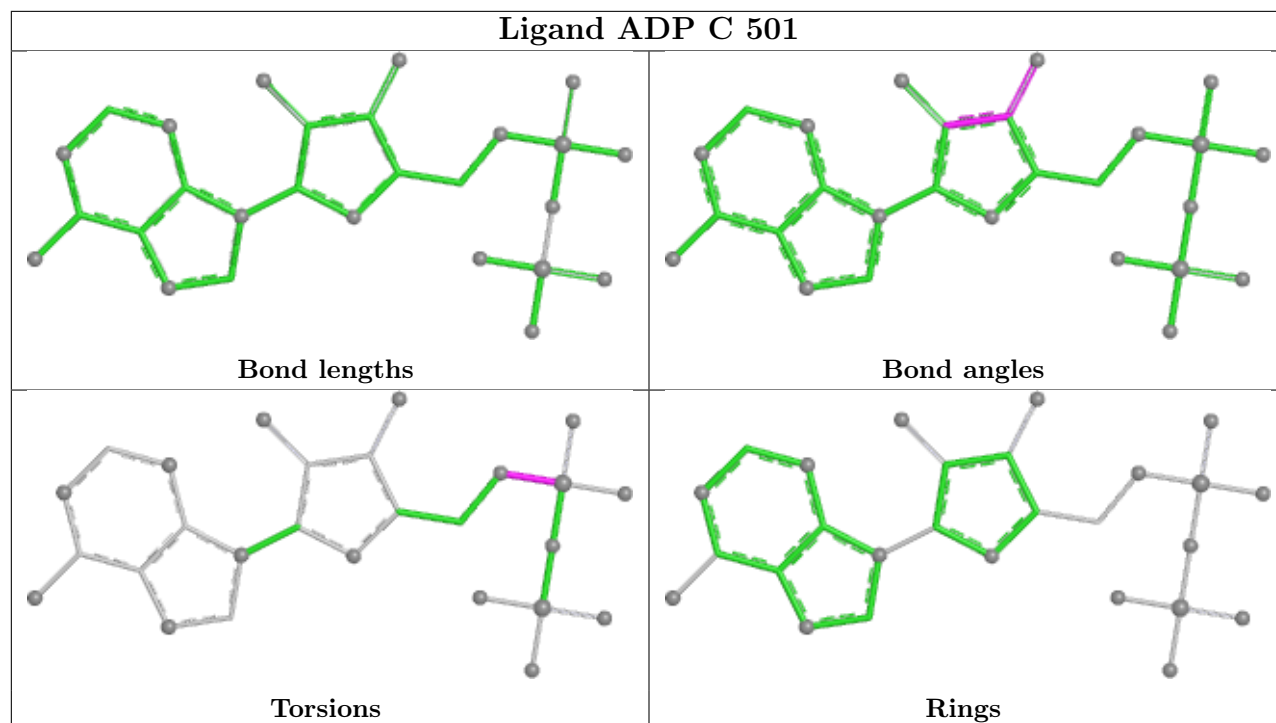


Ligand ADP B 501









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	438/438 (100%)	-0.40	4 (0%) 81 63	30, 64, 127, 190	0
1	B	438/438 (100%)	-0.27	3 (0%) 84 68	38, 73, 138, 207	0
1	C	438/438 (100%)	-0.38	2 (0%) 87 73	34, 66, 129, 214	0
1	D	438/438 (100%)	-0.28	2 (0%) 87 73	37, 73, 136, 214	0
1	E	438/438 (100%)	-0.29	1 (0%) 91 83	38, 76, 143, 252	0
1	F	438/438 (100%)	-0.11	7 (1%) 70 49	36, 81, 157, 205	0
1	G	438/438 (100%)	-0.28	2 (0%) 87 73	38, 75, 133, 194	0
1	H	438/438 (100%)	-0.26	2 (0%) 87 73	37, 73, 134, 200	0
1	I	438/438 (100%)	-0.24	4 (0%) 81 63	36, 75, 145, 240	0
1	J	438/438 (100%)	-0.22	2 (0%) 87 73	36, 78, 153, 252	0
1	K	438/438 (100%)	-0.24	2 (0%) 87 73	39, 77, 138, 203	0
1	L	438/438 (100%)	-0.20	1 (0%) 91 83	44, 85, 150, 209	0
2	M	76/76 (100%)	0.02	0 100 100	71, 110, 143, 168	0
2	N	62/76 (81%)	0.85	9 (14%) 6 3	91, 133, 172, 194	0
2	O	76/76 (100%)	-0.07	0 100 100	65, 96, 137, 160	0
2	P	76/76 (100%)	0.35	2 (2%) 57 36	97, 148, 188, 229	0
2	Q	76/76 (100%)	0.29	1 (1%) 75 56	109, 159, 192, 233	0
2	R	76/76 (100%)	0.31	0 100 100	111, 161, 203, 219	0
2	S	76/76 (100%)	-0.07	0 100 100	84, 120, 158, 182	0
2	T	76/76 (100%)	0.25	0 100 100	114, 157, 197, 216	0
2	U	76/76 (100%)	0.19	1 (1%) 75 56	101, 137, 178, 232	0
2	V	76/76 (100%)	0.20	0 100 100	108, 164, 199, 210	0
2	W	53/76 (69%)	0.65	5 (9%) 14 8	80, 133, 195, 219	0
2	X	76/76 (100%)	0.21	0 100 100	111, 159, 185, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	6131/6168 (99%)	-0.19	50 (0%)	82 65	30, 80, 165, 252	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	439	ALA	5.0
1	J	439	ALA	4.9
1	E	439	ALA	4.6
1	D	439	ALA	3.9
1	B	439	ALA	3.6
1	A	443	ASN	3.5
2	N	624	VAL	3.4
2	N	603	VAL	3.2
2	U	624	VAL	3.0
2	N	598	ILE	3.0
2	W	615	LEU	2.9
1	F	146	ILE	2.7
1	I	146	ILE	2.6
2	N	602	PHE	2.6
2	P	585	PHE	2.6
1	F	175	ILE	2.6
1	G	182	ILE	2.6
1	F	174	CYS	2.6
1	I	443	ASN	2.6
1	K	443	ASN	2.6
1	A	439	ALA	2.6
2	N	629	PRO	2.5
1	L	439	ALA	2.5
1	G	68	VAL	2.4
2	W	608	PHE	2.4
2	Q	599	VAL	2.4
2	N	606	LYS	2.3
1	F	143	TYR	2.3
1	H	173	TYR	2.3
1	B	67	ALA	2.3
1	F	439	ALA	2.3
1	D	432	LEU	2.3
1	C	439	ALA	2.2
1	I	68	VAL	2.2
1	I	171	SER	2.2
2	N	633	LEU	2.2
1	F	170	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	W	599	VAL	2.2
1	A	42	SER	2.2
2	W	610	TRP	2.2
2	P	590	PHE	2.1
1	J	57	VAL	2.1
1	A	337	GLN	2.1
2	N	600	PHE	2.1
2	N	586	LEU	2.1
1	B	319	GLU	2.1
2	W	619	PHE	2.1
1	F	169	ASP	2.0
1	C	339	ALA	2.0
1	H	185	GLU	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	J	501	27/27	0.95	0.07	53,60,79,94	0
3	ADP	I	501	27/27	0.96	0.06	45,57,81,83	0
3	ADP	L	501	27/27	0.96	0.06	59,75,90,98	0
3	ADP	E	501	27/27	0.97	0.05	55,63,87,91	0
3	ADP	F	501	27/27	0.97	0.05	48,54,74,89	0
3	ADP	G	501	27/27	0.97	0.06	56,69,102,122	0
3	ADP	H	501	27/27	0.97	0.05	55,65,93,109	0
3	ADP	A	501	27/27	0.97	0.06	50,59,74,95	0
3	ADP	B	501	27/27	0.97	0.06	52,62,84,94	0
3	ADP	K	501	27/27	0.97	0.06	55,63,86,108	0

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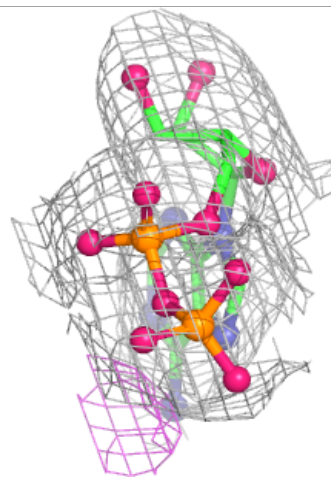
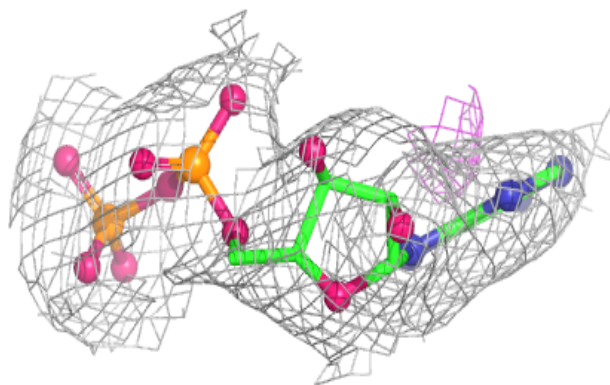
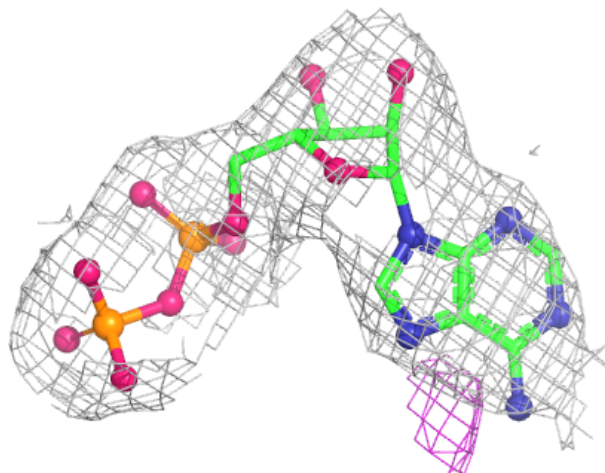
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	C	501	27/27	0.97	0.06	45,60,77,94	0
3	ADP	D	501	27/27	0.98	0.04	51,60,76,99	0

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

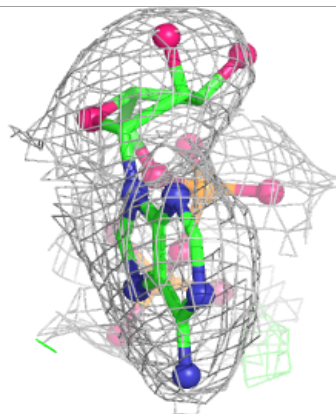
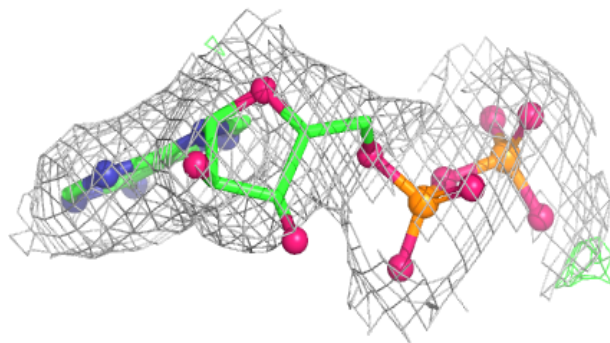
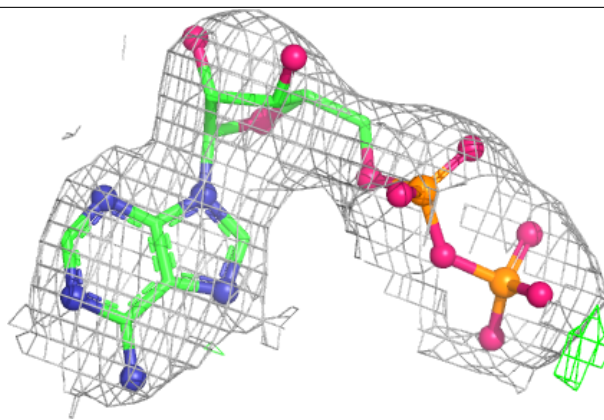
Electron density around ADP J 501:

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



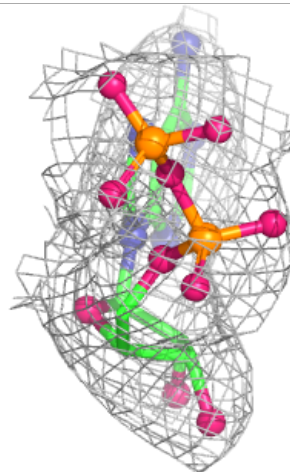
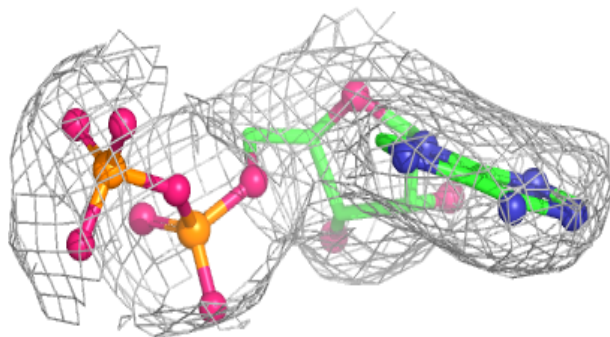
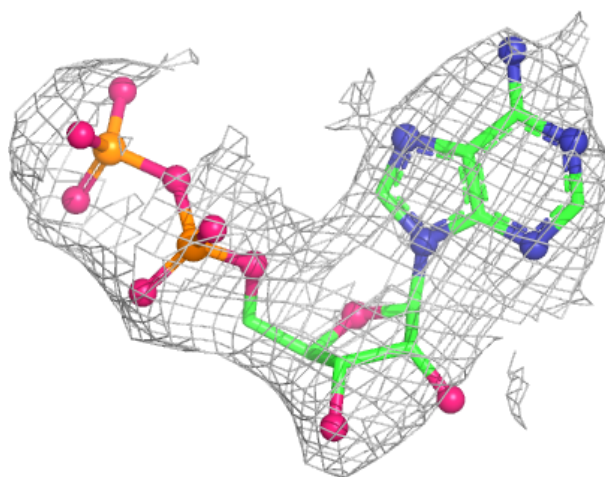
Electron density around ADP I 501:

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



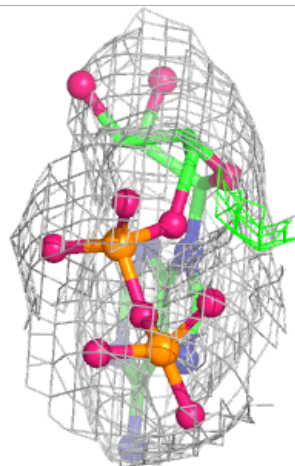
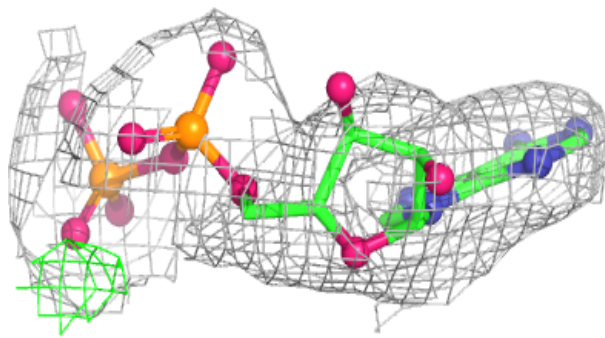
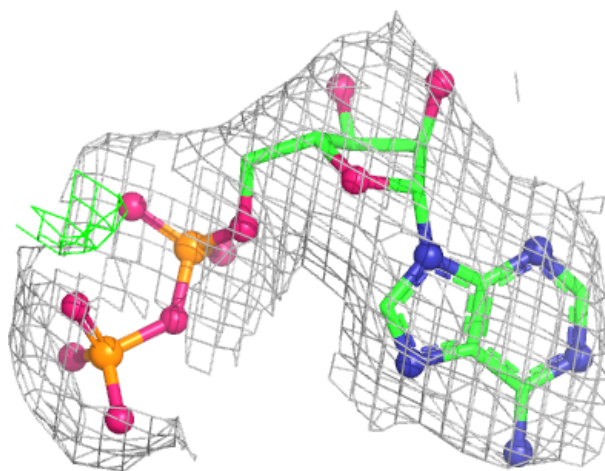
Electron density around ADP L 501:

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



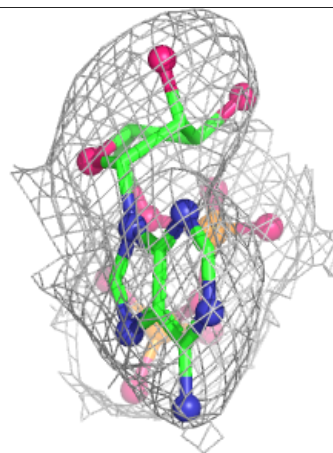
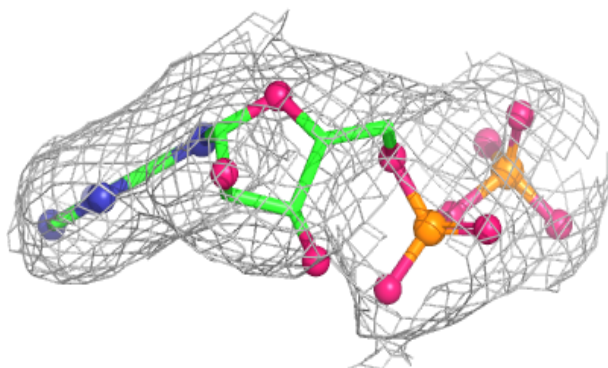
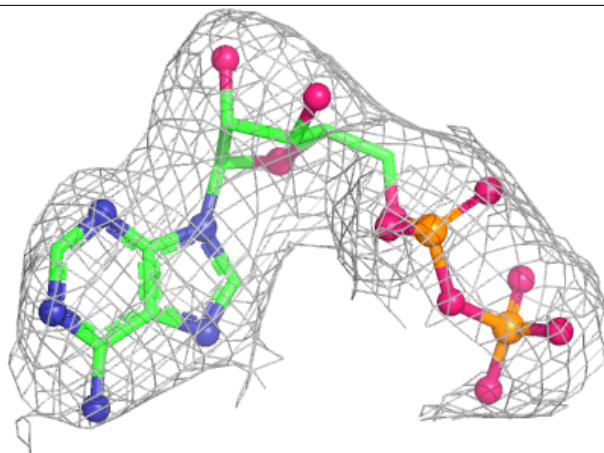
Electron density around ADP E 501:

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



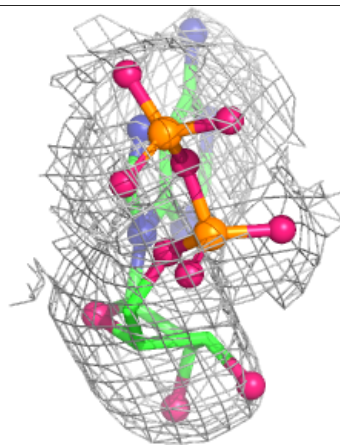
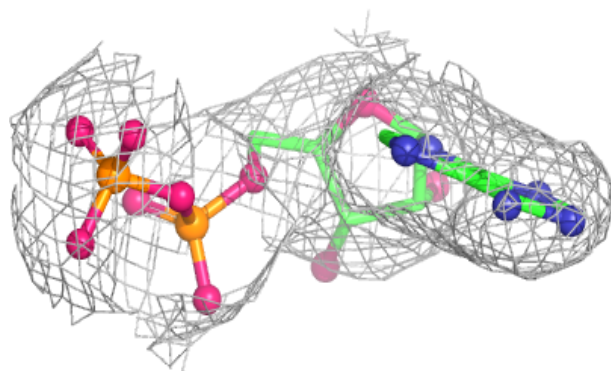
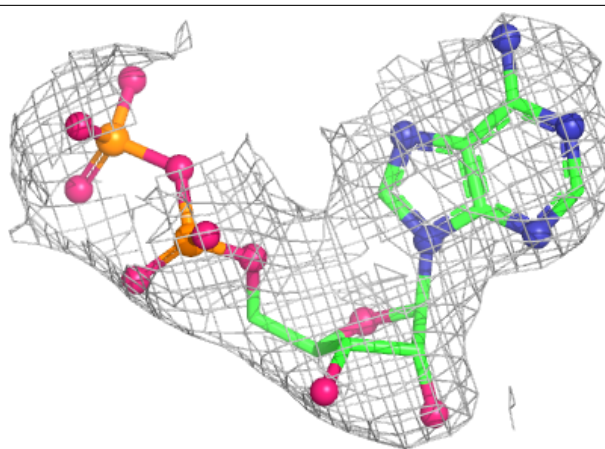
Electron density around ADP F 501:

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



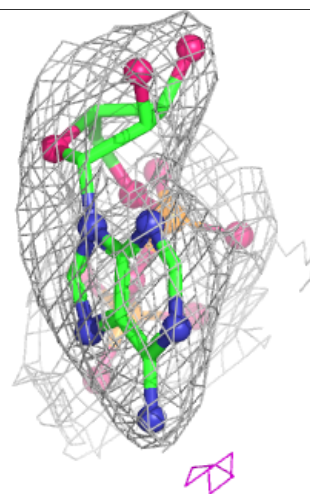
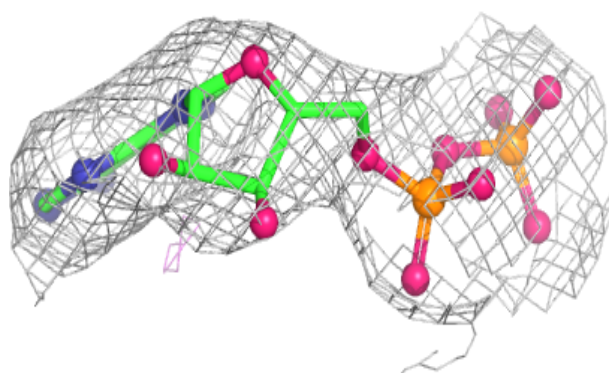
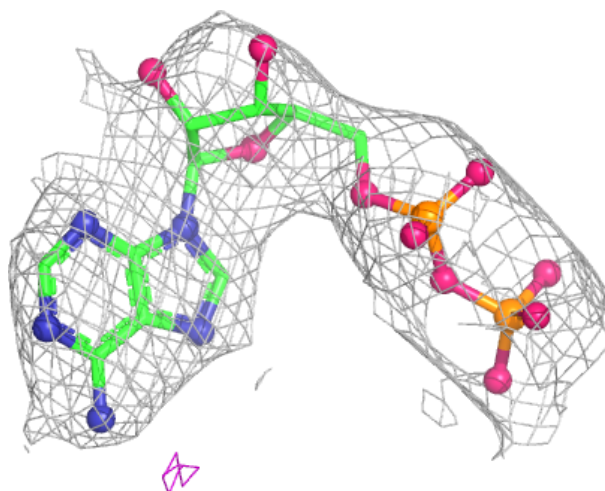
Electron density around ADP G 501:

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



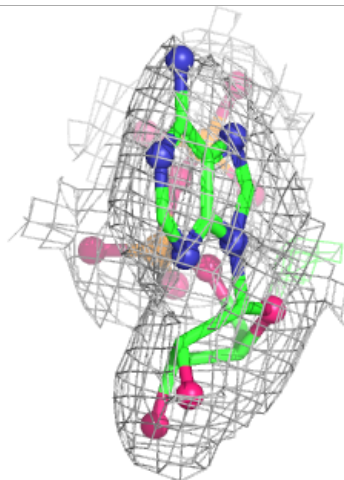
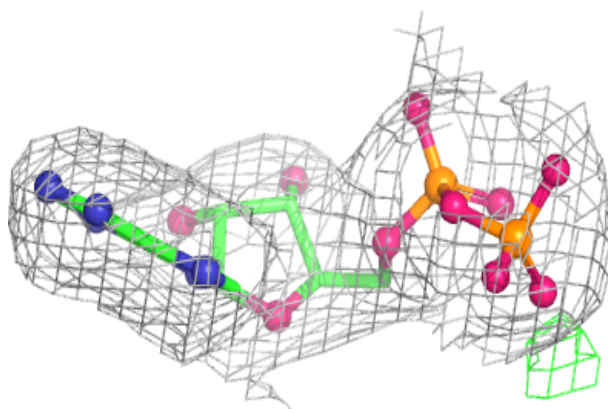
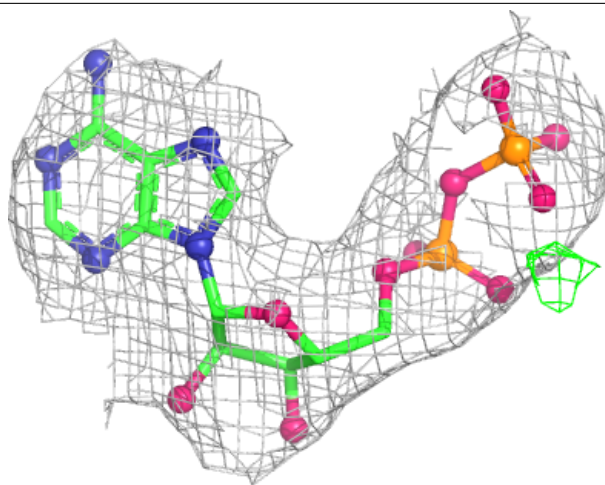
Electron density around ADP H 501:

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



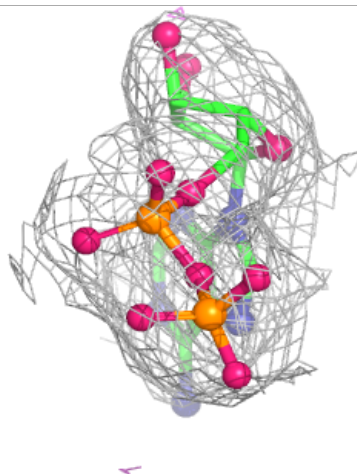
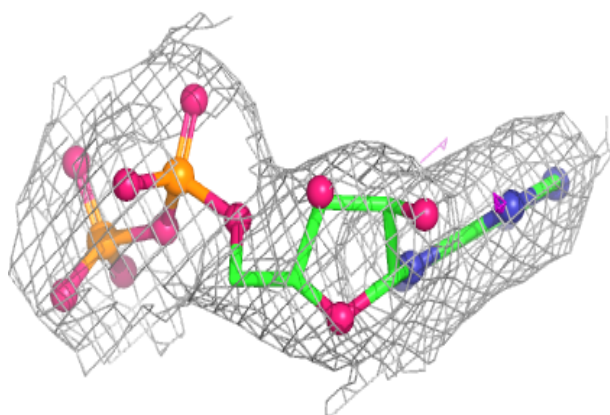
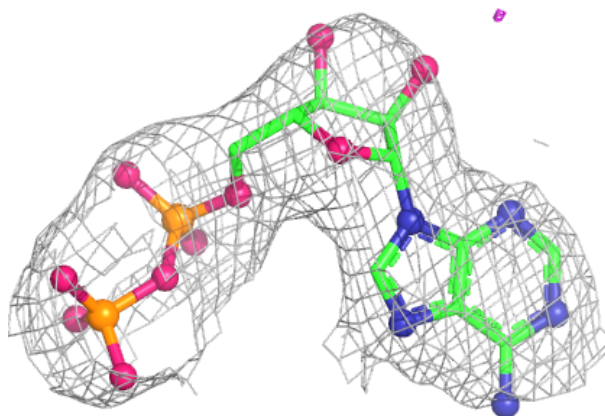
Electron density around ADP A 501:

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



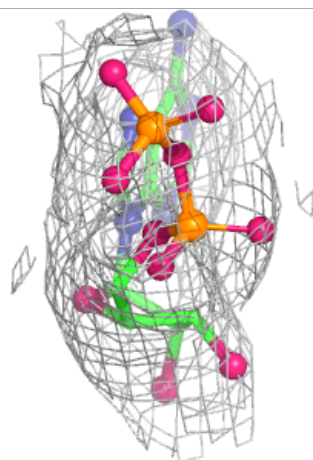
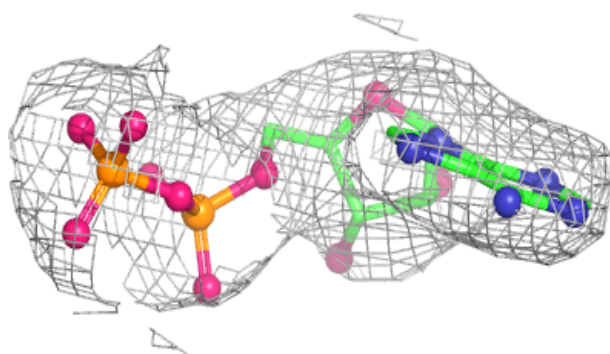
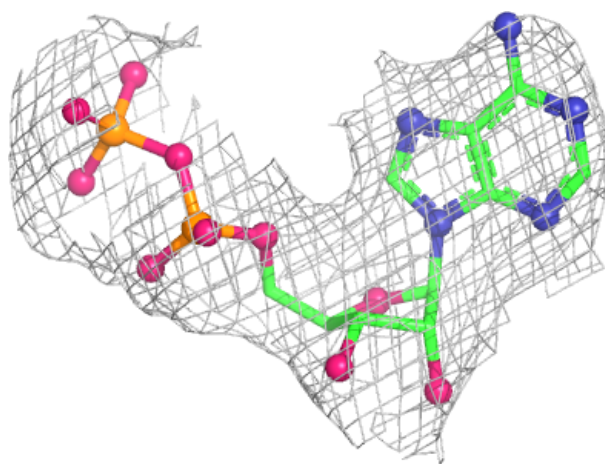
Electron density around ADP B 501:

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



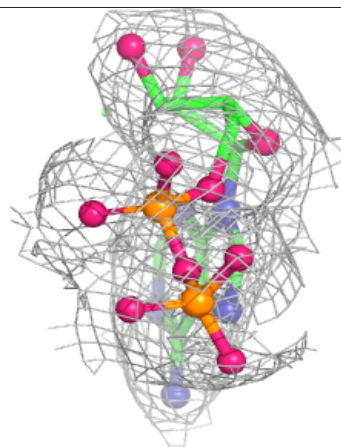
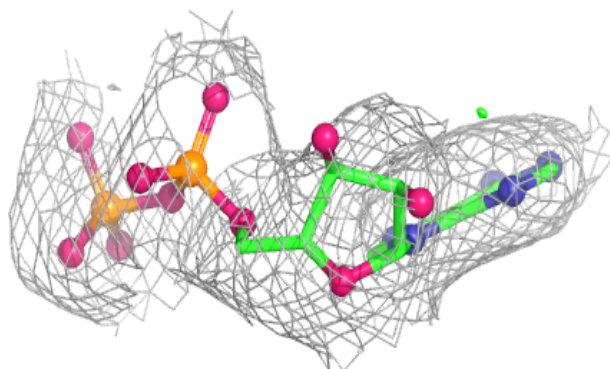
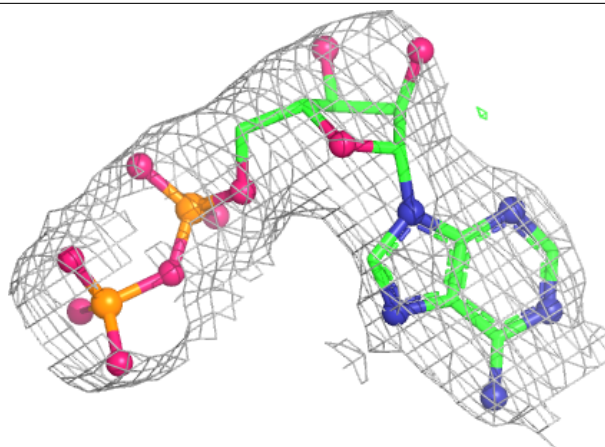
Electron density around ADP K 501:

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



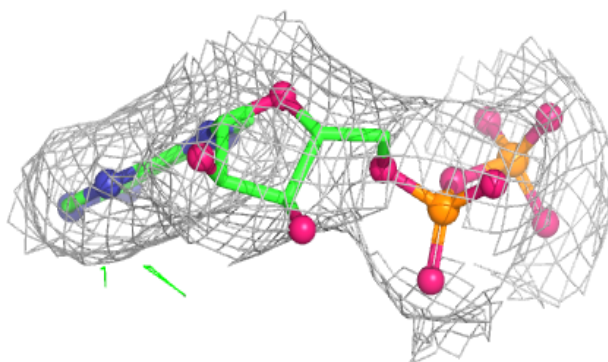
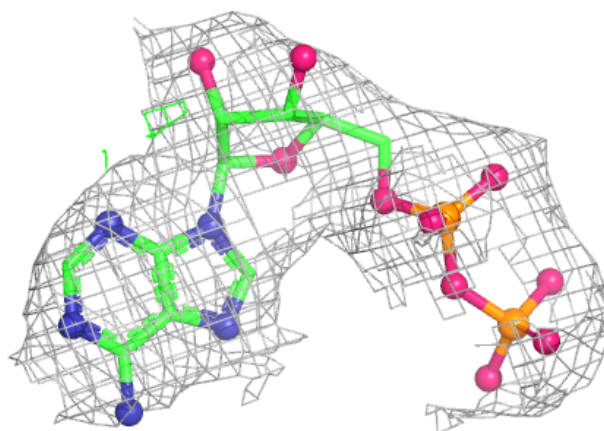
Electron density around ADP C 501:

$2mF_o-DF_c$ (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:

$2mF_o-DF_c$ (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.