



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2024 – 10:18 AM JST

PDB ID : 8KG2
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

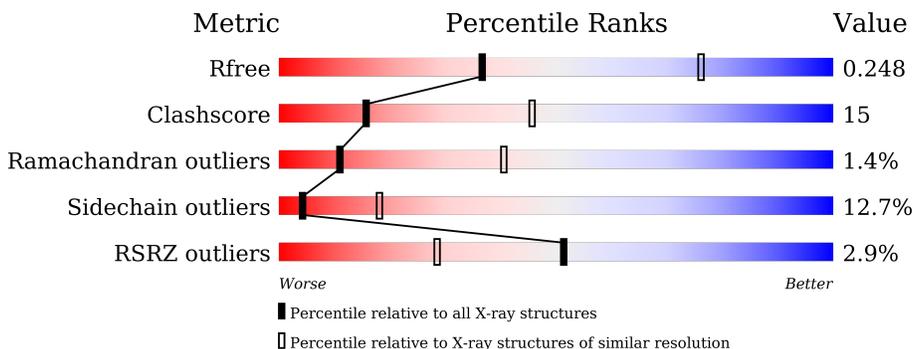
1 Overall quality at a glance

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.



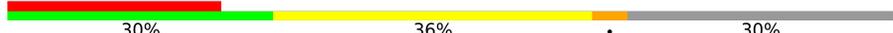
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	 70% 25% 5% 2%
1	B	438	 69% 25% 5% 1%
1	C	438	 70% 26% 4% 2%
1	D	438	 71% 24% 3% 2%
1	E	438	 71% 22% 6% 1%
1	F	438	 67% 26% 5% 2%

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Mol	Chain	Length	Quality of chain
1	G	438	 67% 26% 5% .
1	H	438	 70% 24% 5% .
1	I	438	 68% 26% 5% .
1	J	438	 67% 27% . .
1	K	438	 68% 26% 5% .
1	L	438	 66% 28% . .
2	M	76	 47% 45% 7% .
2	N	76	 9% 36% 36% 7% . 18%
2	O	76	 55% 42% .
2	P	76	 11% 55% 38% 5% .
2	Q	76	 11% 51% 39% 8% .
2	R	76	 12% 46% 46% 5% .
2	S	76	 11% 50% 42% 5% .
2	T	76	 21% 53% 41% 5% .
2	U	76	 16% 46% 47% 5% .
2	V	76	 30% 50% 43% 5% .
2	W	76	 24% 30% 36% . 30%
2	X	76	 25% 42% 43% 14%

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	438	3422	2150	609	645	18	0	0	0
1	B	438	3422	2150	609	645	18	0	0	0
1	C	438	3422	2150	609	645	18	0	0	0
1	D	438	3422	2150	609	645	18	0	0	0
1	E	438	3422	2150	609	645	18	0	0	0
1	F	438	3422	2150	609	645	18	0	0	0
1	G	438	3422	2150	609	645	18	0	0	0
1	H	438	3422	2150	609	645	18	0	0	0
1	I	438	3422	2150	609	645	18	0	0	0
1	J	438	3422	2150	609	645	18	0	0	0
1	K	438	3422	2150	609	645	18	0	0	0
1	L	438	3422	2150	609	645	18	0	0	0

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.

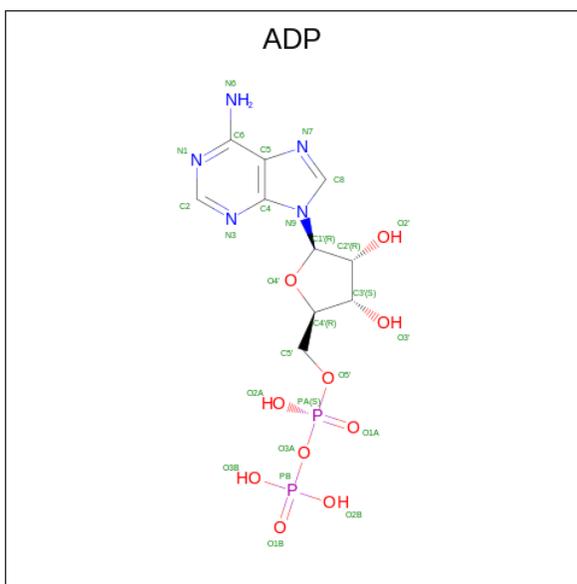
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	N	62	Total	C	N	O	0	0	0
			524	340	89	95			
2	O	76	Total	C	N	O	0	0	0
			637	417	107	113			
2	P	76	Total	C	N	O	0	0	0
			637	417	107	113			

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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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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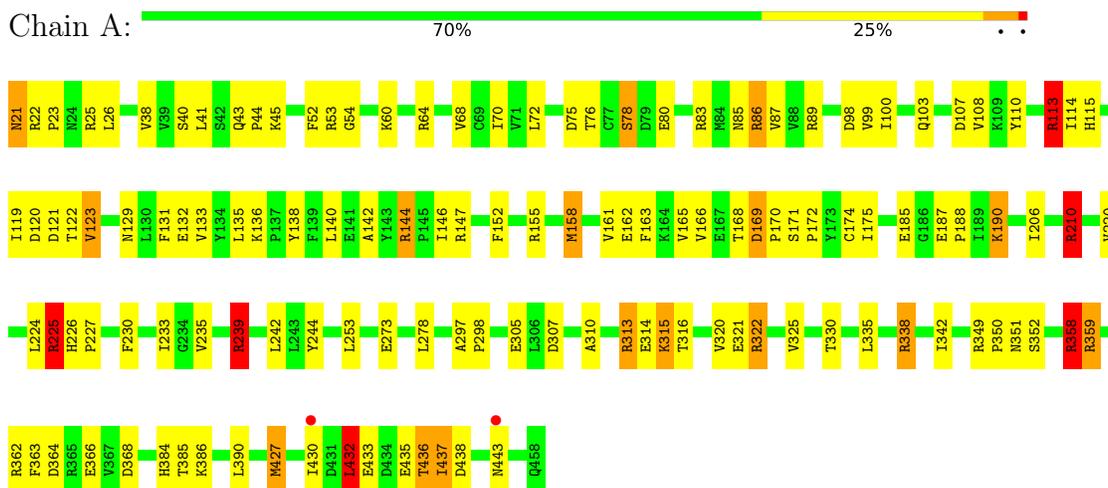
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5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

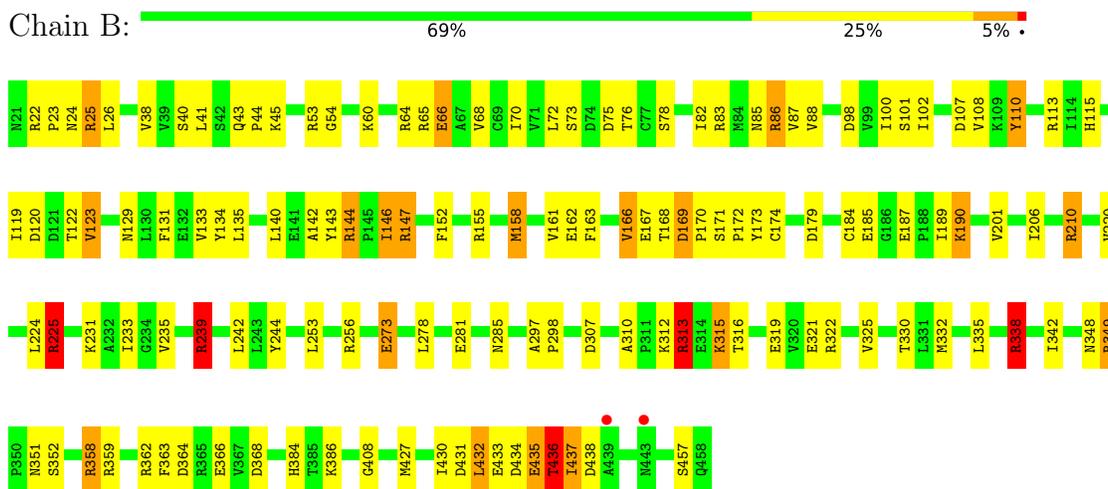
3 Residue-property plots

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



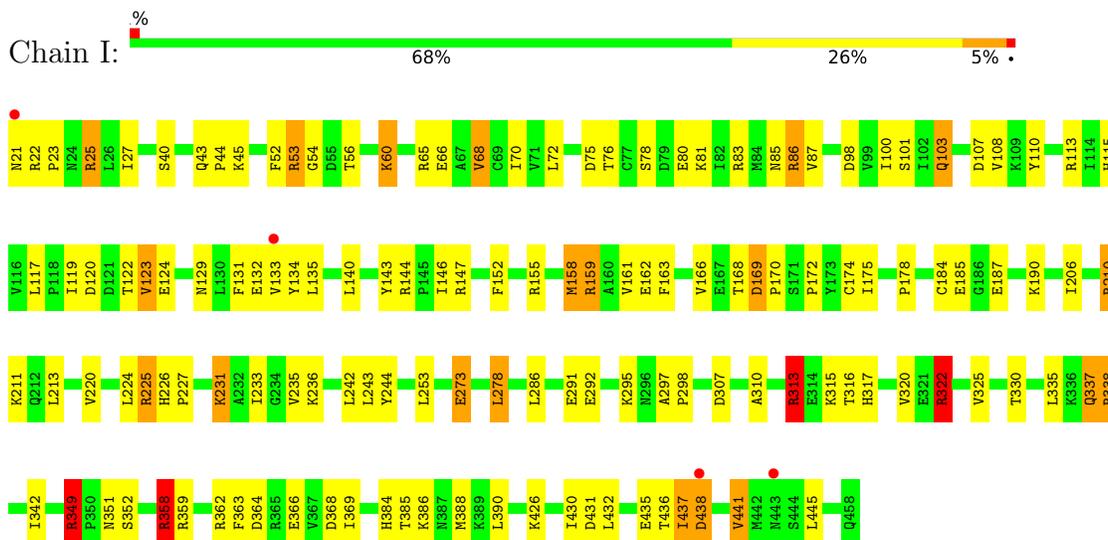
- Molecule 1: Transitional endoplasmic reticulum ATPase



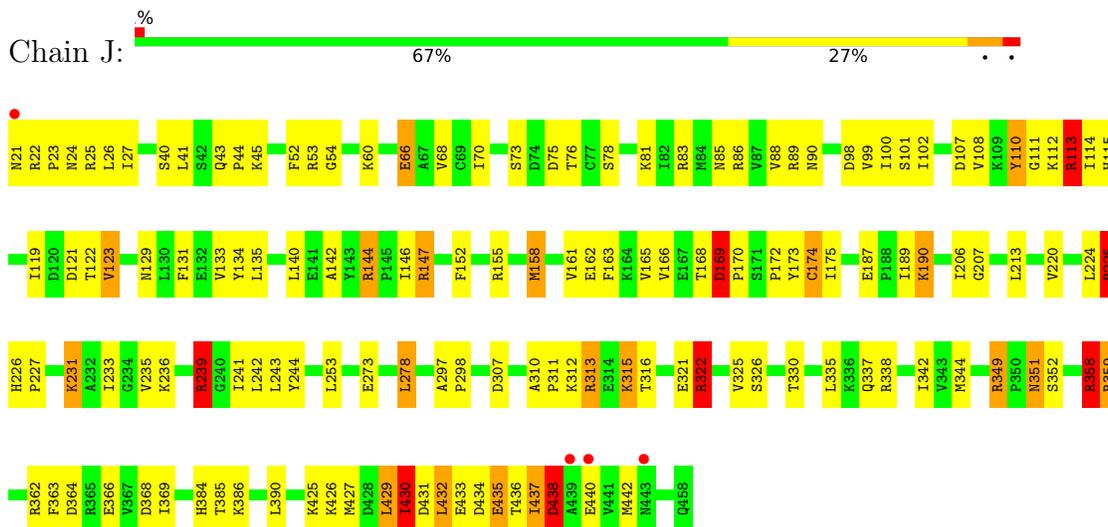
- Molecule 1: Transitional endoplasmic reticulum ATPase



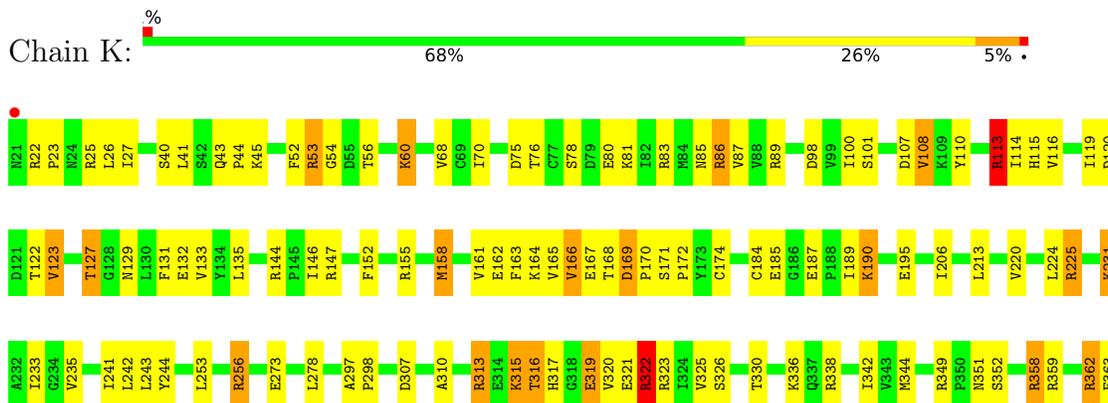
- Molecule 1: Transitional endoplasmic reticulum ATPase

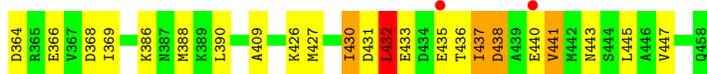


- Molecule 1: Transitional endoplasmic reticulum ATPase

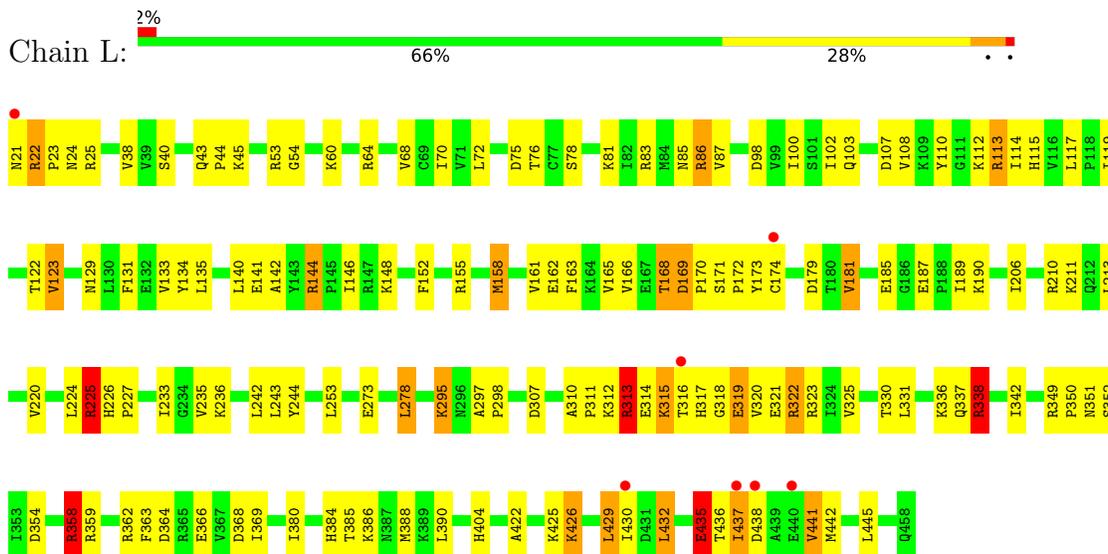


- Molecule 1: Transitional endoplasmic reticulum ATPase

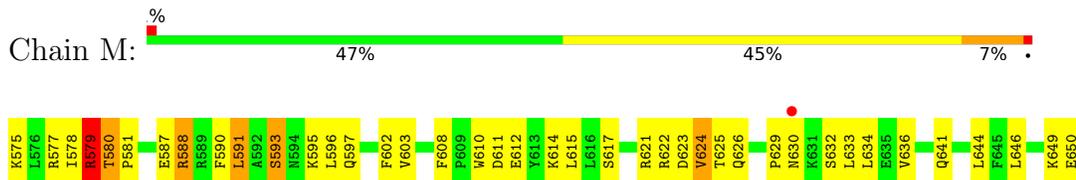




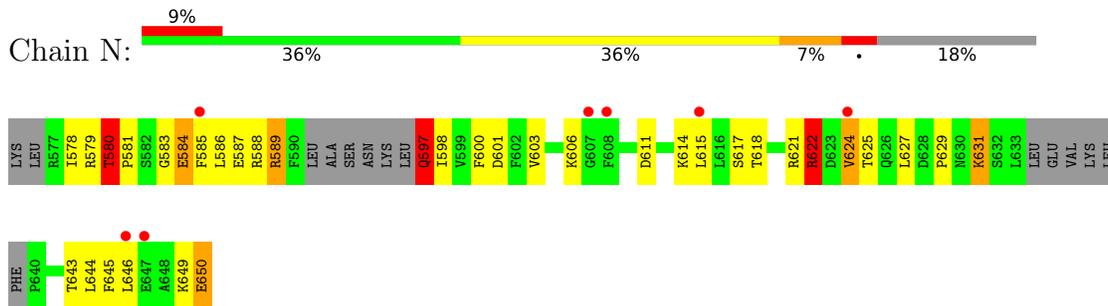
- Molecule 1: Transitional endoplasmic reticulum ATPase



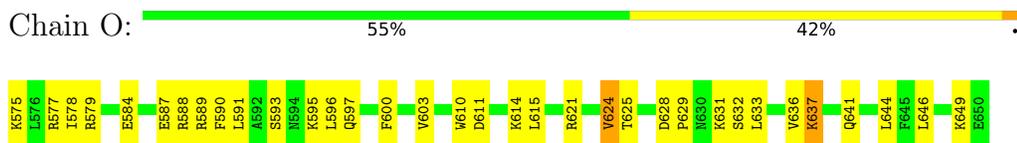
- Molecule 2: FAS-associated factor 1



- Molecule 2: FAS-associated factor 1



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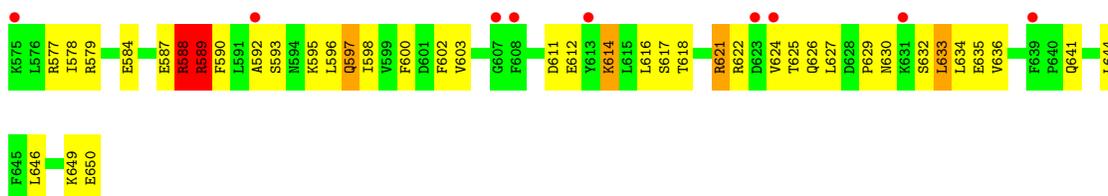




- Molecule 2: FAS-associated factor 1



- Molecule 2: FAS-associated factor 1



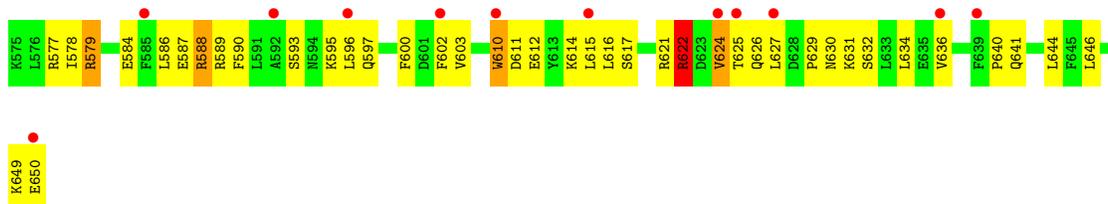
- Molecule 2: FAS-associated factor 1



- Molecule 2: FAS-associated factor 1

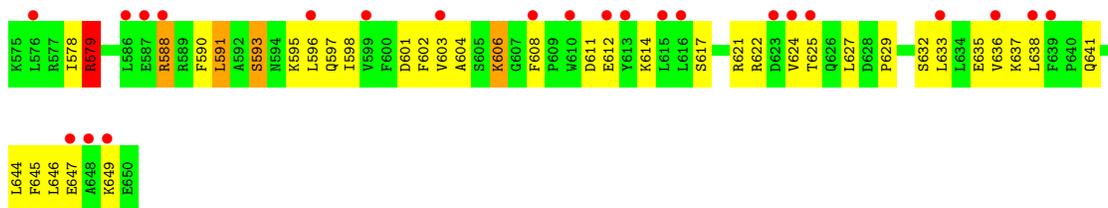


- Molecule 2: FAS-associated factor 1

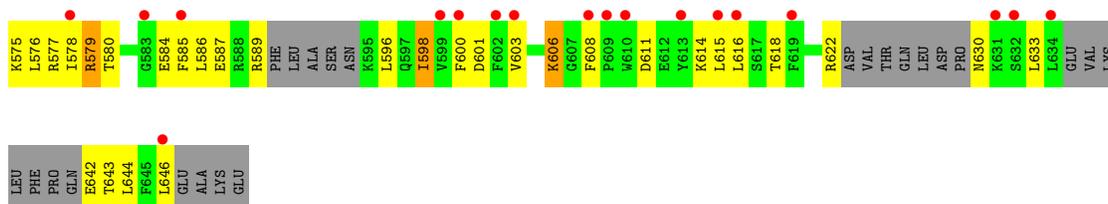


- Molecule 2: FAS-associated factor 1

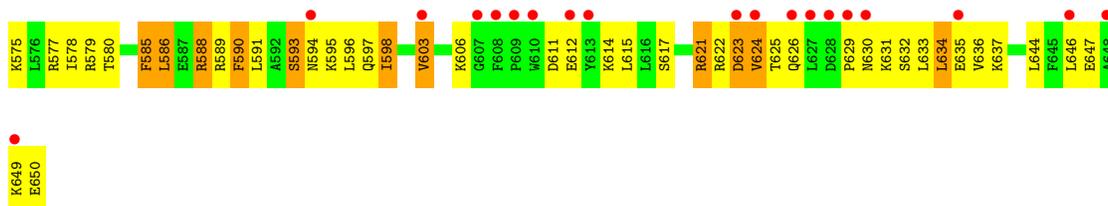




- Molecule 2: FAS-associated factor 1



- 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)	Xtrriage
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 (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

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	0.39	0/3475	0.83	5/4696 (0.1%)
1	B	0.39	0/3475	0.82	3/4696 (0.1%)
1	C	0.39	0/3475	0.83	6/4696 (0.1%)
1	D	0.40	0/3475	0.89	9/4696 (0.2%)
1	E	0.40	0/3475	0.85	6/4696 (0.1%)
1	F	0.41	1/3475 (0.0%)	0.95	13/4696 (0.3%)
1	G	0.39	0/3475	0.86	10/4696 (0.2%)
1	H	0.39	0/3475	0.90	8/4696 (0.2%)
1	I	0.39	0/3475	0.83	7/4696 (0.1%)
1	J	0.40	0/3475	0.87	10/4696 (0.2%)
1	K	0.40	0/3475	0.87	9/4696 (0.2%)
1	L	0.37	0/3475	0.82	5/4696 (0.1%)
2	M	0.34	0/652	0.82	1/878 (0.1%)
2	N	0.53	0/536	1.26	6/719 (0.8%)
2	O	0.39	0/652	0.92	3/878 (0.3%)
2	P	0.39	0/652	0.88	3/878 (0.3%)
2	Q	0.33	0/652	0.91	3/878 (0.3%)
2	R	0.40	0/652	0.95	5/878 (0.6%)
2	S	0.36	0/652	0.89	3/878 (0.3%)
2	T	0.37	0/652	0.88	1/878 (0.1%)
2	U	0.35	0/652	0.95	3/878 (0.3%)
2	V	0.35	0/652	0.81	0/878
2	W	0.39	0/461	0.97	1/613 (0.2%)
2	X	0.36	0/652	0.87	3/878 (0.3%)
All	All	0.39	1/49217 (0.0%)	0.87	123/66464 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	167	GLU	CD-OE2	-6.63	1.18	1.25

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	93	ARG	NE-CZ-NH1	-19.83	110.38	120.30
1	H	358	ARG	NE-CZ-NH1	-19.37	110.62	120.30
1	D	86	ARG	NE-CZ-NH1	17.71	129.16	120.30
1	D	86	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	H	358	ARG	NE-CZ-NH2	13.29	126.94	120.30
1	E	453	ARG	CG-CD-NE	12.64	138.34	111.80
1	E	358	ARG	NE-CZ-NH1	12.09	126.35	120.30
1	L	358	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	G	323	ARG	NE-CZ-NH1	-10.42	115.09	120.30
2	N	588	ARG	CG-CD-NE	10.32	133.48	111.80
1	A	358	ARG	NE-CZ-NH1	-10.26	115.17	120.30
2	Q	579	ARG	NE-CZ-NH2	10.11	125.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	358	ARG	NE-CZ-NH1	-10.11	115.25	120.30
1	C	358	ARG	NE-CZ-NH2	-9.87	115.36	120.30
2	Q	588	ARG	CB-CG-CD	9.82	137.13	111.60
1	G	358	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	E	358	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	A	113	ARG	CB-CG-CD	8.95	134.86	111.60
2	O	588	ARG	CB-CG-CD	8.88	134.69	111.60
2	U	622	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	F	358	ARG	NE-CZ-NH1	-8.63	115.99	120.30
2	N	597	GLN	CB-CA-C	8.62	127.64	110.40
1	D	313	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	F	113	ARG	CG-CD-NE	-8.35	94.27	111.80
1	L	358	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	I	168	THR	CA-CB-CG2	8.31	124.03	112.40
1	J	322	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	R	588	ARG	CG-CD-NE	8.27	129.16	111.80
1	I	358	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	K	168	THR	CA-CB-CG2	8.12	123.78	112.40
1	E	453	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	G	113	ARG	NE-CZ-NH1	-8.03	116.28	120.30
1	I	168	THR	OG1-CB-CG2	-7.98	91.65	110.00
1	F	358	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	A	358	ARG	NE-CZ-NH2	7.93	124.27	120.30
2	S	589	ARG	CB-CG-CD	7.91	132.18	111.60
1	F	313	ARG	NE-CZ-NH1	-7.80	116.40	120.30
2	U	622	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	K	322	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	K	256	ARG	CG-CD-NE	-7.65	95.73	111.80
2	X	579	ARG	CG-CD-NE	7.54	127.63	111.80
1	F	112	LYS	CB-CA-C	7.28	124.96	110.40
2	O	588	ARG	CG-CD-NE	-7.26	96.54	111.80
1	B	239	ARG	CG-CD-NE	7.20	126.93	111.80
1	G	239	ARG	CG-CD-NE	7.04	126.59	111.80
1	C	239	ARG	CG-CD-NE	6.99	126.48	111.80
1	J	169	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	H	239	ARG	CG-CD-NE	6.96	126.42	111.80
2	T	588	ARG	CG-CD-NE	-6.89	97.34	111.80
1	K	256	ARG	CB-CG-CD	6.86	129.43	111.60
1	B	436	THR	CA-CB-OG1	6.67	123.01	109.00
1	J	358	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	I	358	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	239	ARG	CG-CD-NE	6.47	125.39	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	115	HIS	CA-CB-CG	-6.38	102.75	113.60
1	G	287	ARG	NE-CZ-NH2	6.35	123.48	120.30
2	R	633	LEU	CB-CA-C	6.32	122.20	110.20
1	K	168	THR	OG1-CB-CG2	-6.31	95.48	110.00
1	B	147	ARG	CG-CD-NE	6.19	124.81	111.80
1	E	147	ARG	CG-CD-NE	6.09	124.60	111.80
2	M	588	ARG	CB-CG-CD	6.08	127.42	111.60
1	G	323	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	D	53	ARG	NE-CZ-NH1	-6.04	117.28	120.30
2	R	614	LYS	CA-CB-CG	6.01	126.63	113.40
1	J	169	ASP	CB-CG-OD2	6.00	123.69	118.30
1	F	147	ARG	CG-CD-NE	5.94	124.28	111.80
1	D	86	ARG	CD-NE-CZ	5.94	131.92	123.60
1	H	147	ARG	CG-CD-NE	5.89	124.18	111.80
1	J	147	ARG	CG-CD-NE	5.88	124.15	111.80
1	K	127	THR	CA-CB-CG2	5.86	120.60	112.40
2	S	577	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	G	358	ARG	NE-CZ-NH1	5.77	123.18	120.30
2	N	622	ARG	CB-CG-CD	5.77	126.59	111.60
1	C	358	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	W	606	LYS	CB-CA-C	5.71	121.82	110.40
1	F	313	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	H	166	VAL	CA-CB-CG2	5.67	119.41	110.90
1	H	431	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	D	432	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	E	453	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	147	ARG	CG-CD-NE	-5.63	99.98	111.80
2	R	589	ARG	CB-CG-CD	5.62	126.20	111.60
2	U	579	ARG	CG-CD-NE	5.61	123.58	111.80
1	D	313	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	F	112	LYS	N-CA-CB	5.55	120.59	110.60
1	J	113	ARG	CG-CD-NE	-5.55	100.15	111.80
2	O	579	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	J	169	ASP	N-CA-CB	5.54	120.57	110.60
1	C	147	ARG	CG-CD-NE	-5.52	100.21	111.80
1	L	426	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	D	64	ARG	CB-CG-CD	5.41	125.67	111.60
2	P	579	ARG	CB-CG-CD	5.40	125.64	111.60
1	C	295	LYS	CA-CB-CG	5.40	125.28	113.40
1	K	147	ARG	CG-CD-NE	-5.38	100.50	111.80
2	X	588	ARG	CB-CG-CD	5.38	125.58	111.60
1	L	435	GLU	CB-CG-CD	5.36	128.68	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	580	THR	CA-CB-OG1	5.36	120.26	109.00
2	N	631	LYS	CA-CB-CG	5.35	125.18	113.40
2	P	589	ARG	CG-CD-NE	-5.35	100.56	111.80
2	X	579	ARG	CB-CG-CD	5.34	125.49	111.60
1	G	287	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	L	338	ARG	CG-CD-NE	5.33	122.99	111.80
1	K	127	THR	OG1-CB-CG2	-5.32	97.76	110.00
1	C	158	MET	CA-CB-CG	5.32	122.34	113.30
2	R	579	ARG	CG-CD-NE	5.30	122.94	111.80
1	F	158	MET	CA-CB-CG	5.30	122.31	113.30
1	J	239	ARG	CG-CD-NE	-5.29	100.70	111.80
1	F	435	GLU	CB-CG-CD	5.25	128.38	114.20
1	I	68	VAL	CA-CB-CG2	5.25	118.78	110.90
2	S	614	LYS	CA-CB-CG	5.24	124.93	113.40
1	G	323	ARG	CD-NE-CZ	5.23	130.93	123.60
1	I	349	ARG	CG-CD-NE	-5.23	100.82	111.80
2	P	612	GLU	CA-CB-CG	5.20	124.83	113.40
1	F	426	LYS	CB-CG-CD	5.19	125.10	111.60
1	D	256	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	I	68	VAL	CG1-CB-CG2	5.13	119.11	110.90
1	F	338	ARG	CG-CD-NE	5.13	122.57	111.80
1	G	86	ARG	NE-CZ-NH1	-5.10	117.75	120.30
2	Q	579	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	J	438	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	K	86	ARG	CD-NE-CZ	-5.06	116.52	123.60
2	N	650	GLU	CB-CA-C	5.06	120.51	110.40
1	H	313	ARG	CB-CG-CD	-5.02	98.54	111.60

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
1	K	322	ARG	Sidechain
1	K	358	ARG	Sidechain
1	K	362	ARG	Sidechain,Mainchain
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
2	X	577	ARG	Sidechain
2	X	621	ARG	Sidechain

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3422	0	3486	96	3
1	B	3422	0	3486	106	0
1	C	3422	0	3486	96	4
1	D	3422	0	3486	92	0
1	E	3422	0	3486	96	0
1	F	3422	0	3486	115	0
1	G	3422	0	3486	109	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3422	0	3486	115	4
1	I	3422	0	3486	96	0
1	J	3422	0	3486	116	0
1	K	3422	0	3486	106	0
1	L	3422	0	3486	116	0
2	M	637	0	652	31	0
2	N	524	0	517	31	0
2	O	637	0	652	18	0
2	P	637	0	652	27	0
2	Q	637	0	652	26	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	35	0
2	W	453	0	470	20	0
2	X	637	0	652	35	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
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	1442	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 (1442) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:169:ASP:CG	1:J:170:PRO:HD3	1.82	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
2:Q:614:LYS:HG3	2:Q:649:LYS:HG2	1.46	0.97
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:112:LYS:H	1:J:169:ASP:CG	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:133:VAL:HG13	1:A:443:ASN:CG	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:437:ILE:HG23	1:L:438:ASP:H	1.58	0.69
1:K:133:VAL:HG13	1:K:443:ASN:CG	2.12	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: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
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
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: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:F:437:ILE:HG23	1:F:438:ASP:H	1.59	0.66
1:C:430:ILE:HG23	1:C:434:ASP:HB3	1.77	0.66
1:A:436:THR:HG22	1:F:226:HIS:HD2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:437:ILE:CG1	1:G:441:VAL:HG22	2.26	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
2:M:591:LEU:HD11	2:U:589:ARG:HB3	1.79	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:HG12	1:L:442:MET:HE2	1.77	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
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:427:MET:HE2	1:E:430:ILE:HD11	1.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:430:ILE:HD12	1:K:430:ILE:C	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:616:LEU:HD22	2:U:621:ARG:NH2	2.03	0.62
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
1:E:169:ASP:CG	1:E:170:PRO:HD3	2.21	0.61
2:S:617:SER:HB3	2:S:622:ARG:HG2	1.82	0.61
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:F:169:ASP:CG	1:F:170:PRO:HD3	2.20	0.61
1:H:147:ARG:HH21	1:H:173:TYR:HB3	1.65	0.61
1:H:169:ASP:CG	1:H:170:PRO:HD3	2.20	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:C:169:ASP:CG	1:C:170:PRO:HD3	2.21	0.61
1:D:274:ILE:HG22	1:D:275:MET:CE	2.31	0.61
1:E:430:ILE:C	1:E:430:ILE:HD12	2.20	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:H:115:HIS:HE2	1:H:183:HIS:CG	2.18	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
1:D:169:ASP:CG	1:D:170:PRO:HD3	2.21	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
1:A:169:ASP:CG	1:A:170:PRO:HD3	2.21	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:G:169:ASP:CG	1:G:170:PRO:HD3	2.20	0.60
1:L:169:ASP:CG	1:L:170:PRO:HD3	2.21	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:K:169:ASP:CG	1:K:170:PRO:HD3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:169:ASP:CG	1:B:170:PRO:HD3	2.21	0.60
1:C:325:VAL:O	1:C:329:LEU:CD1	2.44	0.60
1:G:437:ILE:HG12	1:G:442:MET:HE2	1.83	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
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
2:X:614:LYS:HG3	2:X:649:LYS:CG	2.25	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: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
2:P:617:SER:HB3	2:P:622:ARG:HG2	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:D:274:ILE:HG22	1:D:275:MET:HE1	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:T:649:LYS:O	2:T:650:GLU:C	2.43	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:N:580:THR:OG1	2:N:583:GLY:O	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:S:649:LYS:O	2:S:650:GLU:C	2.43	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: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
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:J:316:THR:O	1:J:316:THR:OG1	2.22	0.55
1:B:430:ILE:O	1:B:430:ILE:CG2	2.55	0.55
1:F:388:MET:HE2	1:F:390:LEU:HD21	1.89	0.55
2:M:649:LYS:O	2:M:650:GLU:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:66:GLU:CD	1:H:147:ARG:HD3	2.27	0.55
1:J:113:ARG:HH12	1:J:115:HIS:HB2	1.71	0.55
2:X:649:LYS:O	2:X:650:GLU:C	2.45	0.55
1:G:362:ARG:O	1:G:364:ASP:N	2.40	0.55
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
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:E:66:GLU:CD	1:E:147:ARG:HD3	2.28	0.55
1:F:66:GLU:CD	1:F:147:ARG:HD3	2.28	0.55
2:R:649:LYS:O	2:R:650:GLU:C	2.45	0.55
2:U:649:LYS:O	2:U:650:GLU:C	2.45	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
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

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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	0.54
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:B:66:GLU:CD	1:B:147:ARG:HD3	2.28	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
1:J:66:GLU:CD	1:J:147:ARG:HD3	2.27	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
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
2:Q:649:LYS:O	2:Q:650:GLU:C	2.45	0.54
1:I:21:ASN:HB2	1:J:432:LEU:HD21	1.90	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
1:C:388:MET:HE2	1:C:390:LEU:HD21	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:129:ASN:O	1:H:133:VAL:HG22	2.08	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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:236:LYS:HZ2	1:L:337:GLN:HG3	1.73	0.53
1:H:430:ILE:O	1:H:430:ILE:CG2	2.55	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:57:VAL:HG21	1:F:71:VAL:CG2	2.39	0.52
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
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
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:D:427:MET:HE1	1:D:436:THR:HA	1.91	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:J:312:LYS:O	1:J:316:THR:HG23	2.08	0.52
1:L:388:MET:HE2	1:L:390:LEU:HD21	1.91	0.52
2:U:597:GLN:HB2	2:U:629:PRO:HB2	1.92	0.52
1:B:23:PRO:O	1:B: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:I:388:MET:HE2	1:I:390:LEU:HD21	1.92	0.52
2:X:585:PHE:C	2:X:586:LEU:HD13	2.30	0.52
1:D:23:PRO:O	1:D:45:LYS:NZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:F:430:ILE:O	1:F:430:ILE:CG2	2.58	0.51
1:K:133:VAL:CG1	1:K:443:ASN:CG	2.78	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: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:A:133:VAL:CG1	1:A:443:ASN:CG	2.74	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:A:23:PRO:O	1:A:45:LYS:NZ	2.41	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:G:388:MET:HE2	1:G:390:LEU:HD21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:321:GLU:OE2	1:J:322:ARG:HD3	2.11	0.50
1:H:437:ILE:O	1:H:438:ASP:HB2	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
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:L:40:SER:HB2	1:L:83:ARG:HB2	1.94	0.50
2:S:615:LEU:HD23	2:S:624:VAL:CG2	2.42	0.50
2:V:638:LEU:HD12	2:V:638:LEU:C	2.31	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
1:K:388:MET:HE2	1:K:390:LEU:HD21	1.93	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:L:115:HIS:CE1	1:L:185:GLU:HB2	2.47	0.50
2:T:638:LEU:HD12	2:T:638:LEU:C	2.32	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:B:220:VAL:HB	1:B:224:LEU:HD12	1.94	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:D:220:VAL:HB	1:D:224:LEU:HD12	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:438:ASP:HB3	1:K:441:VAL:CG1	2.42	0.49
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: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
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:HA	2:R:635:GLU:OE1	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: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: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:L:244:TYR:HE2	1:L:366:GLU:HB3	1.78	0.49
1:E:427:MET:HE2	1:E:430:ILE:CD1	2.42	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: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
1:E:427:MET:HE3	1:E:430:ILE:HG12	1.94	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:GLY:C	1:J:169:ASP:OD1	2.52	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:D:275:MET:CE	1:D:324:ILE:HG21	2.43	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:J:168:THR:CG2	1:J:174:CYS:CB	2.91	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:D:275:MET:HE3	1:D:324:ILE:HG21	1.95	0.48
1:G:438:ASP:HB3	1:G:441:VAL:CG1	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:W:616:LEU:HD12	2:W:622:ARG:C	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:427:MET:HE2	1:E:430:ILE:CG1	2.44	0.47
2:M:623:ASP:O	2:M:626:GLN:HG2	2.15	0.47
1:I:60:LYS:HZ3	1:I:103:GLN:HB2	1.79	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:P:596:LEU:C	2:P:599:VAL:HG13	2.35	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:23:PRO:O	1:K:45:LYS:NZ	2.40	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)
1:E:402:GLU:CD	1:E:453:ARG:HH21	2.18	0.47
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:L:23:PRO:O	1:L:45:LYS:NZ	2.41	0.46
2:X:623:ASP:CG	2:X:626:GLN:HG2	2.36	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
2:P:643:THR:C	2:P:644:LEU:HD13	2.36	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:K:427:MET:CE	1:K:430:ILE:HD11	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:23:PRO:O	1:H:45:LYS:NZ	2.41	0.46
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:J:297:ALA:HA	1:J:298:PRO:C	2.37	0.45
1:K:297:ALA:HA	1:K:298:PRO:C	2.37	0.45
1:L:38:VAL:CG1	1:L:72:LEU:HD12	2.46	0.45
1:L:297:ALA:HA	1:L:298:PRO:C	2.37	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:D:274:ILE:HG22	1:D:275:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:23:PRO:O	1:F:45:LYS:NZ	2.41	0.45
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
2:U:614:LYS:O	2:U:646:LEU:HA	2.16	0.45
1:A:297:ALA:HA	1:A:298:PRO:C	2.37	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:F:297:ALA:HA	1:F:298:PRO:C	2.37	0.45
1:G:297:ALA:HA	1:G:298:PRO:C	2.37	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:297:ALA:HA	1:C:298:PRO:C	2.37	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
1:E:297:ALA:HA	1:E:298:PRO:C	2.37	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
1:D:297:ALA:HA	1:D:298:PRO:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:600:PHE:C	2:U:610:TRP:HE1	2.20	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:H:297:ALA:HA	1:H:298:PRO:C	2.37	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
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
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
1:B:297:ALA:HA	1:B:298:PRO:C	2.37	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:B:166:VAL:C	1:B:167:GLU:HG3	2.38	0.44
1:B:362:ARG:HH22	1:E:305:GLU:CD	2.21	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
1:I:297:ALA:HA	1:I:298:PRO:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:K:430:ILE:C	1:K:430:ILE:CD1	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:166:VAL:C	1:K:167:GLU:HG3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:G:430:ILE:C	1:G:432:LEU:H	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:H:427:MET:HE1	1:H:436:THR:HA	2.01	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
1:D:112:LYS:O	1:D:181:VAL:CG1	2.67	0.42
1:E:430:ILE:C	1:E:430:ILE:CD1	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:HIS:HE2	1:H:183:HIS:CB	2.22	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: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
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: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:C:388:MET:HE3	1:C:388:MET:HB3	1.93	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
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:C:23:PRO:O	1:C:45:LYS:NZ	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:430:ILE:CD1	1:E:430:ILE:O	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:332:MET:HE2	1:B:362:ARG:HA	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:388:MET:HE3	1:K:447:VAL:HG21	2.04	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%)	9 37
1	B	436/438 (100%)	417 (96%)	13 (3%)	6 (1%)	11 40
1	C	436/438 (100%)	413 (95%)	16 (4%)	7 (2%)	9 37
1	D	436/438 (100%)	416 (95%)	13 (3%)	7 (2%)	9 37
1	E	436/438 (100%)	417 (96%)	12 (3%)	7 (2%)	9 37
1	F	436/438 (100%)	415 (95%)	14 (3%)	7 (2%)	9 37
1	G	436/438 (100%)	415 (95%)	11 (2%)	10 (2%)	6 28
1	H	436/438 (100%)	415 (95%)	15 (3%)	6 (1%)	11 40
1	I	436/438 (100%)	418 (96%)	11 (2%)	7 (2%)	9 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	436/438 (100%)	415 (95%)	14 (3%)	7 (2%)	9	37
1	K	436/438 (100%)	416 (95%)	12 (3%)	8 (2%)	8	34
1	L	436/438 (100%)	416 (95%)	14 (3%)	6 (1%)	11	40
2	M	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	N	56/76 (74%)	50 (89%)	4 (7%)	2 (4%)	3	20
2	O	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
2	P	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
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%)	11	40

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	372/372 (100%)	333 (90%)	39 (10%)	7 26
1	B	372/372 (100%)	328 (88%)	44 (12%)	5 21
1	C	372/372 (100%)	330 (89%)	42 (11%)	6 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	372/372 (100%)	327 (88%)	45 (12%)	5	20
1	E	372/372 (100%)	327 (88%)	45 (12%)	5	20
1	F	372/372 (100%)	328 (88%)	44 (12%)	5	21
1	G	372/372 (100%)	321 (86%)	51 (14%)	3	16
1	H	372/372 (100%)	332 (89%)	40 (11%)	6	25
1	I	372/372 (100%)	335 (90%)	37 (10%)	8	29
1	J	372/372 (100%)	331 (89%)	41 (11%)	6	25
1	K	372/372 (100%)	330 (89%)	42 (11%)	6	23
1	L	372/372 (100%)	323 (87%)	49 (13%)	4	17
2	M	71/71 (100%)	59 (83%)	12 (17%)	2	9
2	N	58/71 (82%)	48 (83%)	10 (17%)	2	9
2	O	71/71 (100%)	62 (87%)	9 (13%)	4	18
2	P	71/71 (100%)	60 (84%)	11 (16%)	2	11
2	Q	71/71 (100%)	58 (82%)	13 (18%)	1	7
2	R	71/71 (100%)	56 (79%)	15 (21%)	1	5
2	S	71/71 (100%)	56 (79%)	15 (21%)	1	5
2	T	71/71 (100%)	58 (82%)	13 (18%)	1	7
2	U	71/71 (100%)	56 (79%)	15 (21%)	1	5
2	V	71/71 (100%)	60 (84%)	11 (16%)	2	11
2	W	50/71 (70%)	41 (82%)	9 (18%)	1	7
2	X	71/71 (100%)	54 (76%)	17 (24%)	0	2
All	All	5282/5316 (99%)	4613 (87%)	669 (13%)	4	18

All (669) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
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	103	GLN
1	A	107	ASP

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Mol	Chain	Res	Type
1	A	108	VAL
1	A	113	ARG
1	A	119	ILE
1	A	121	ASP
1	A	123	VAL
1	A	140	LEU
1	A	158	MET
1	A	166	VAL
1	A	168	THR
1	A	171	SER
1	A	174	CYS
1	A	187	GLU
1	A	190	LYS
1	A	210	ARG
1	A	225	ARG
1	A	273	GLU
1	A	278	LEU
1	A	307	ASP
1	A	313	ARG
1	A	314	GLU
1	A	315	LYS
1	A	330	THR
1	A	338	ARG
1	A	351	ASN
1	A	352	SER
1	A	358	ARG
1	A	359	ARG
1	A	427	MET
1	A	432	LEU
1	A	433	GLU
1	B	22	ARG
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	86	ARG
1	B	107	ASP
1	B	108	VAL
1	B	119	ILE
1	B	123	VAL

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Mol	Chain	Res	Type
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	273	GLU
1	B	278	LEU
1	B	307	ASP
1	B	313	ARG
1	B	315	LYS
1	B	316	THR
1	B	330	THR
1	B	338	ARG
1	B	349	ARG
1	B	351	ASN
1	B	352	SER
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	60	LYS
1	C	68	VAL
1	C	75	ASP
1	C	76	THR
1	C	86	ARG
1	C	103	GLN
1	C	107	ASP
1	C	108	VAL
1	C	119	ILE
1	C	123	VAL

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Mol	Chain	Res	Type
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	210	ARG
1	C	211	LYS
1	C	225	ARG
1	C	231	LYS
1	C	273	GLU
1	C	278	LEU
1	C	295	LYS
1	C	307	ASP
1	C	313	ARG
1	C	315	LYS
1	C	317	HIS
1	C	330	THR
1	C	337	GLN
1	C	338	ARG
1	C	349	ARG
1	C	351	ASN
1	C	352	SER
1	C	358	ARG
1	C	427	MET
1	C	432	LEU
1	C	433	GLU
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	103	GLN
1	D	107	ASP
1	D	108	VAL
1	D	112	LYS

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Mol	Chain	Res	Type
1	D	119	ILE
1	D	123	VAL
1	D	140	LEU
1	D	158	MET
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	288	LYS
1	D	307	ASP
1	D	313	ARG
1	D	315	LYS
1	D	338	ARG
1	D	349	ARG
1	D	351	ASN
1	D	352	SER
1	D	358	ARG
1	D	359	ARG
1	D	427	MET
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	60	LYS
1	E	66	GLU
1	E	68	VAL
1	E	73	SER
1	E	75	ASP
1	E	76	THR

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Mol	Chain	Res	Type
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	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	204	ASP
1	E	211	LYS
1	E	225	ARG
1	E	231	LYS
1	E	278	LEU
1	E	307	ASP
1	E	313	ARG
1	E	314	GLU
1	E	315	LYS
1	E	317	HIS
1	E	330	THR
1	E	336	LYS
1	E	338	ARG
1	E	351	ASN
1	E	352	SER
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

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Mol	Chain	Res	Type
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	158	MET
1	F	161	VAL
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	273	GLU
1	F	278	LEU
1	F	288	LYS
1	F	295	LYS
1	F	307	ASP
1	F	313	ARG
1	F	315	LYS
1	F	317	HIS
1	F	330	THR
1	F	337	GLN
1	F	351	ASN
1	F	352	SER
1	F	358	ARG
1	F	359	ARG
1	F	429	LEU
1	F	431	ASP
1	F	432	LEU
1	F	435	GLU
2	M	579	ARG
2	M	580	THR

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Mol	Chain	Res	Type
2	M	590	PHE
2	M	591	LEU
2	M	593	SER
2	M	610	TRP
2	M	611	ASP
2	M	612	GLU
2	M	624	VAL
2	M	625	THR
2	M	632	SER
2	M	634	LEU
2	N	580	THR
2	N	586	LEU
2	N	589	ARG
2	N	597	GLN
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	O	584	GLU
2	O	590	PHE
2	O	593	SER
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	P	575	LYS
2	P	585	PHE
2	P	588	ARG
2	P	589	ARG
2	P	591	LEU
2	P	593	SER
2	P	599	VAL
2	P	611	ASP
2	P	625	THR
2	P	644	LEU
2	P	650	GLU
2	Q	575	LYS
2	Q	579	ARG

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Mol	Chain	Res	Type
2	Q	588	ARG
2	Q	590	PHE
2	Q	593	SER
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	590	PHE
2	R	593	SER
2	R	597	GLN
2	R	611	ASP
2	R	612	GLU
2	R	621	ARG
2	R	625	THR
2	R	626	GLN
2	R	630	ASN
2	R	632	SER
2	R	634	LEU
2	R	641	GLN
1	G	34	GLU
1	G	60	LYS
1	G	68	VAL
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
1	G	146	ILE
1	G	148	LYS

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Mol	Chain	Res	Type
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	211	LYS
1	G	225	ARG
1	G	231	LYS
1	G	236	LYS
1	G	273	GLU
1	G	278	LEU
1	G	288	LYS
1	G	307	ASP
1	G	313	ARG
1	G	315	LYS
1	G	316	THR
1	G	337	GLN
1	G	338	ARG
1	G	351	ASN
1	G	352	SER
1	G	358	ARG
1	G	359	ARG
1	G	427	MET
1	G	430	ILE
1	G	432	LEU
1	G	433	GLU
1	G	440	GLU
1	G	441	VAL
1	G	453	ARG
1	H	21	ASN
1	H	53	ARG
1	H	60	LYS
1	H	64	ARG
1	H	66	GLU
1	H	68	VAL
1	H	75	ASP

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Mol	Chain	Res	Type
1	H	76	THR
1	H	109	LYS
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	210	ARG
1	H	225	ARG
1	H	231	LYS
1	H	278	LEU
1	H	307	ASP
1	H	313	ARG
1	H	315	LYS
1	H	337	GLN
1	H	338	ARG
1	H	349	ARG
1	H	351	ASN
1	H	352	SER
1	H	358	ARG
1	H	397	GLU
1	H	427	MET
1	H	432	LEU
1	H	433	GLU
1	H	441	VAL
1	I	53	ARG
1	I	60	LYS
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

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Mol	Chain	Res	Type
1	I	124	GLU
1	I	140	LEU
1	I	146	ILE
1	I	158	MET
1	I	159	ARG
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	231	LYS
1	I	273	GLU
1	I	278	LEU
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	358	ARG
1	I	432	LEU
1	I	441	VAL
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

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Mol	Chain	Res	Type
1	J	169	ASP
1	J	174	CYS
1	J	187	GLU
1	J	189	ILE
1	J	190	LYS
1	J	225	ARG
1	J	231	LYS
1	J	273	GLU
1	J	278	LEU
1	J	307	ASP
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
1	J	358	ARG
1	J	359	ARG
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

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Mol	Chain	Res	Type
1	K	174	CYS
1	K	184	CYS
1	K	187	GLU
1	K	189	ILE
1	K	190	LYS
1	K	225	ARG
1	K	231	LYS
1	K	256	ARG
1	K	278	LEU
1	K	307	ASP
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	358	ARG
1	K	359	ARG
1	K	430	ILE
1	K	431	ASP
1	K	432	LEU
1	K	433	GLU
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

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Mol	Chain	Res	Type
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
1	L	210	ARG
1	L	211	LYS
1	L	225	ARG
1	L	278	LEU
1	L	295	LYS
1	L	307	ASP
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	349	ARG
1	L	351	ASN
1	L	352	SER
1	L	358	ARG
1	L	359	ARG
1	L	429	LEU
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	588	ARG
2	S	590	PHE
2	S	593	SER
2	S	610	TRP
2	S	611	ASP

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Mol	Chain	Res	Type
2	S	612	GLU
2	S	621	ARG
2	S	624	VAL
2	S	625	THR
2	S	632	SER
2	S	634	LEU
2	S	637	LYS
2	T	575	LYS
2	T	585	PHE
2	T	590	PHE
2	T	591	LEU
2	T	593	SER
2	T	606	LYS
2	T	611	ASP
2	T	612	GLU
2	T	616	LEU
2	T	621	ARG
2	T	624	VAL
2	T	625	THR
2	T	634	LEU
2	U	584	GLU
2	U	588	ARG
2	U	590	PHE
2	U	593	SER
2	U	610	TRP
2	U	611	ASP
2	U	612	GLU
2	U	622	ARG
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	590	PHE
2	V	591	LEU
2	V	593	SER
2	V	606	LYS
2	V	611	ASP

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Mol	Chain	Res	Type
2	V	612	GLU
2	V	621	ARG
2	V	625	THR
2	V	637	LYS
2	W	579	ARG
2	W	585	PHE
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	W	646	LEU
2	X	585	PHE
2	X	586	LEU
2	X	588	ARG
2	X	590	PHE
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	632	SER
2	X	634	LEU
2	X	637	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	129	ASN
1	A	348	ASN
1	B	285	ASN
1	B	348	ASN
1	C	129	ASN
1	C	183	HIS
1	C	317	HIS

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Mol	Chain	Res	Type
1	C	337	GLN
1	D	21	ASN
1	D	129	ASN
1	D	183	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	O	626	GLN
2	R	626	GLN
1	G	91	ASN
1	G	337	GLN
1	G	384	HIS
1	H	226	HIS
1	H	285	ASN
1	H	317	HIS
1	H	327	GLN
1	I	129	ASN
1	J	21	ASN
1	J	226	HIS
1	J	351	ASN
1	J	384	HIS
1	J	443	ASN
1	K	129	ASN
1	K	285	ASN
1	K	348	ASN
1	L	183	HIS
1	L	337	GLN
1	L	348	ASN
2	U	626	GLN
2	X	594	ASN
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 monosaccharides 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	B	501	-	24,29,29	0.72	0	29,45,45	1.10	1 (3%)
3	ADP	D	501	-	24,29,29	0.66	0	29,45,45	0.87	0
3	ADP	L	501	-	24,29,29	0.68	0	29,45,45	0.97	1 (3%)
3	ADP	J	501	-	24,29,29	0.72	0	29,45,45	1.07	2 (6%)
3	ADP	C	501	-	24,29,29	0.64	0	29,45,45	0.91	2 (6%)
3	ADP	A	501	-	24,29,29	0.69	0	29,45,45	1.01	1 (3%)
3	ADP	E	501	-	24,29,29	0.66	0	29,45,45	0.93	2 (6%)
3	ADP	G	501	-	24,29,29	0.66	0	29,45,45	0.97	2 (6%)
3	ADP	H	501	-	24,29,29	0.67	0	29,45,45	0.99	1 (3%)
3	ADP	F	501	-	24,29,29	0.66	0	29,45,45	1.07	1 (3%)
3	ADP	K	501	-	24,29,29	0.68	0	29,45,45	0.90	1 (3%)
3	ADP	I	501	-	24,29,29	0.76	0	29,45,45	0.84	1 (3%)

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	B	501	-	-	2/12/32/32	0/3/3/3
3	ADP	D	501	-	-	3/12/32/32	0/3/3/3
3	ADP	L	501	-	-	3/12/32/32	0/3/3/3
3	ADP	J	501	-	-	5/12/32/32	0/3/3/3
3	ADP	C	501	-	-	2/12/32/32	0/3/3/3
3	ADP	A	501	-	-	4/12/32/32	0/3/3/3
3	ADP	E	501	-	-	3/12/32/32	0/3/3/3
3	ADP	G	501	-	-	4/12/32/32	0/3/3/3
3	ADP	H	501	-	-	3/12/32/32	0/3/3/3
3	ADP	F	501	-	-	4/12/32/32	0/3/3/3
3	ADP	K	501	-	-	5/12/32/32	0/3/3/3
3	ADP	I	501	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	ADP	C5-C6-N6	2.85	124.69	120.35
3	J	501	ADP	C5-C6-N6	2.80	124.60	120.35
3	A	501	ADP	C3'-C2'-C1'	2.63	104.93	100.98
3	B	501	ADP	C3'-C2'-C1'	2.50	104.75	100.98
3	J	501	ADP	O3'-C3'-C2'	-2.49	103.78	111.82
3	F	501	ADP	C5-C6-N6	2.42	124.03	120.35
3	C	501	ADP	C5-C6-N6	2.33	123.89	120.35
3	H	501	ADP	C5-C6-N6	2.30	123.85	120.35
3	L	501	ADP	C3'-C2'-C1'	2.24	104.34	100.98
3	I	501	ADP	C5-C6-N6	2.20	123.70	120.35
3	K	501	ADP	C5-C6-N6	2.14	123.60	120.35
3	G	501	ADP	PA-O3A-PB	-2.13	125.51	132.83
3	E	501	ADP	C5-C6-N6	2.12	123.58	120.35
3	C	501	ADP	O3'-C3'-C2'	-2.10	105.04	111.82
3	E	501	ADP	O3B-PB-O2B	2.01	115.32	107.64

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	C	501	ADP	C5'-O5'-PA-O2A

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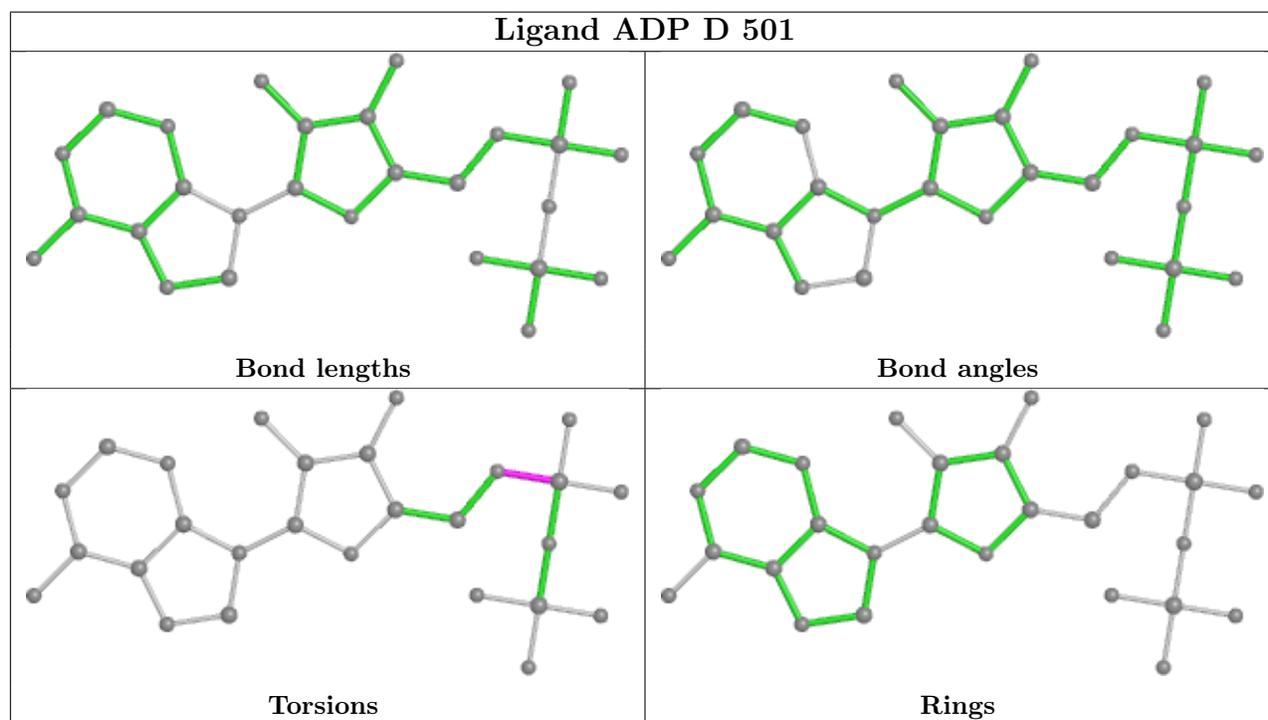
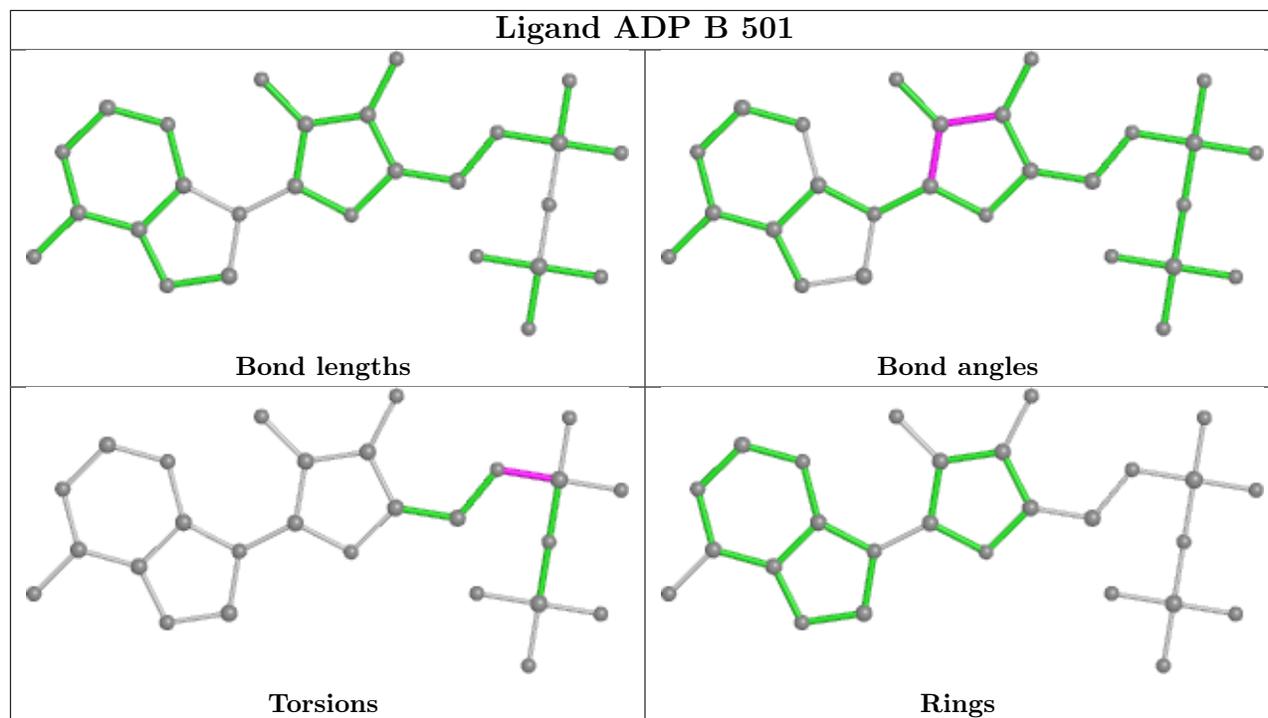
Mol	Chain	Res	Type	Atoms
3	C	501	ADP	C5'-O5'-PA-O3A
3	D	501	ADP	C5'-O5'-PA-O1A
3	D	501	ADP	C5'-O5'-PA-O2A
3	E	501	ADP	C5'-O5'-PA-O3A
3	F	501	ADP	C5'-O5'-PA-O3A
3	G	501	ADP	C5'-O5'-PA-O1A
3	G	501	ADP	C5'-O5'-PA-O2A
3	H	501	ADP	C5'-O5'-PA-O1A
3	I	501	ADP	C5'-O5'-PA-O1A
3	I	501	ADP	C5'-O5'-PA-O2A
3	J	501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

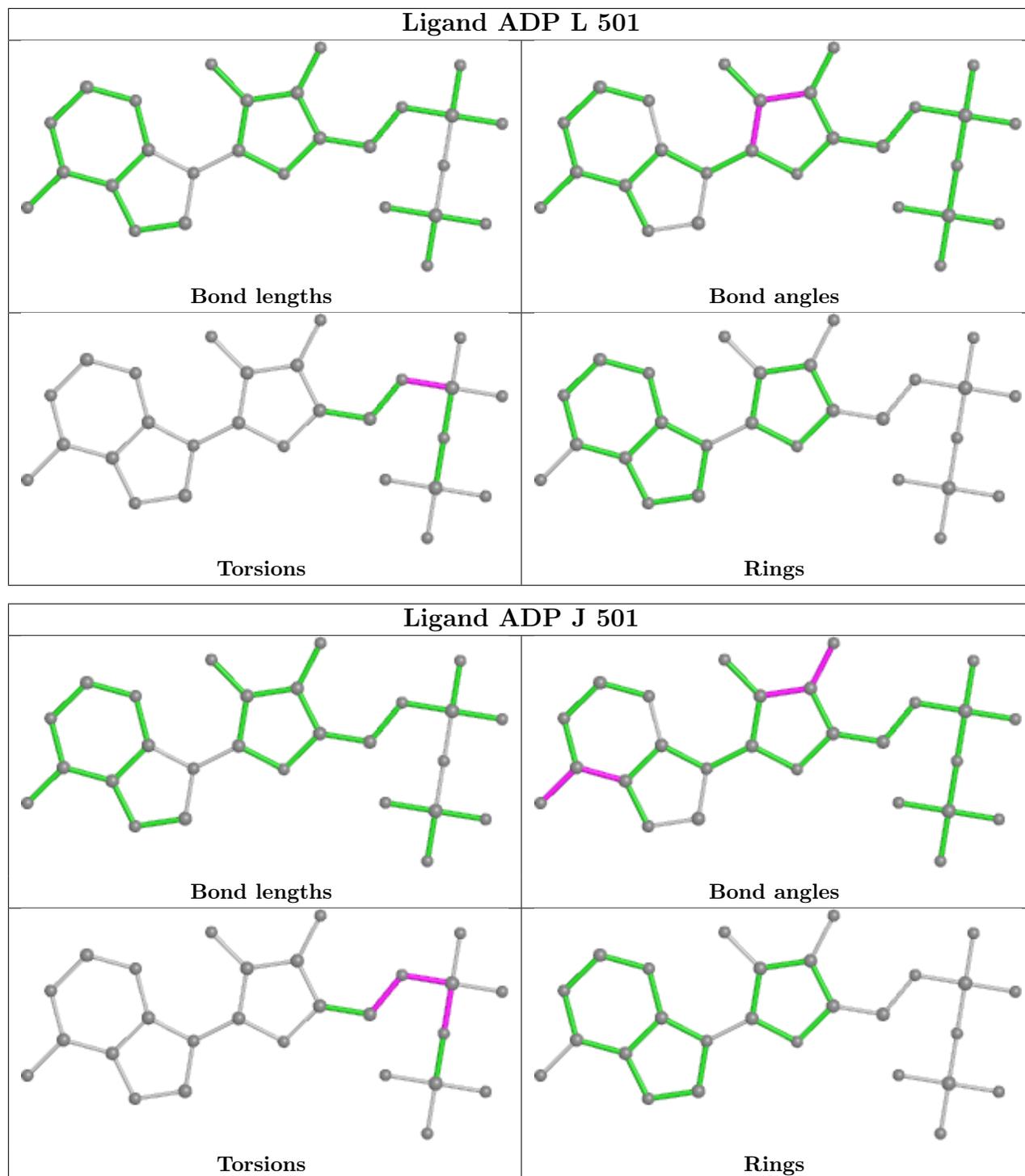
There are no ring outliers.

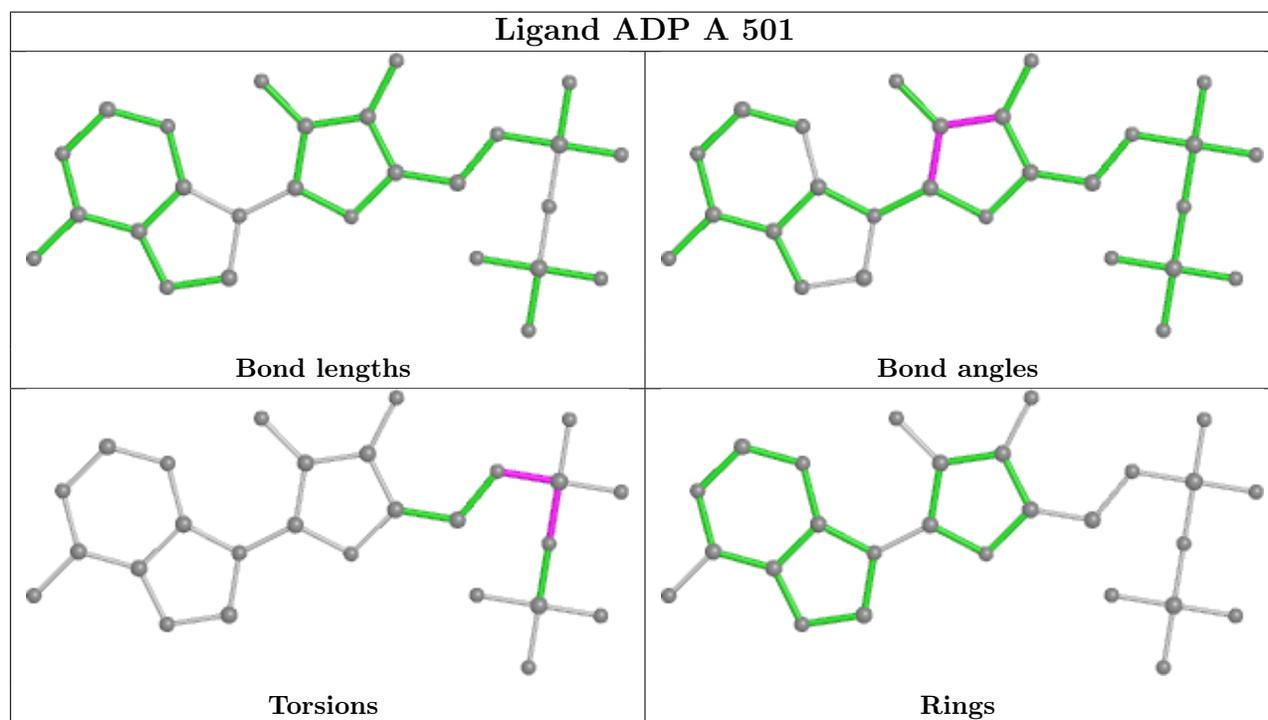
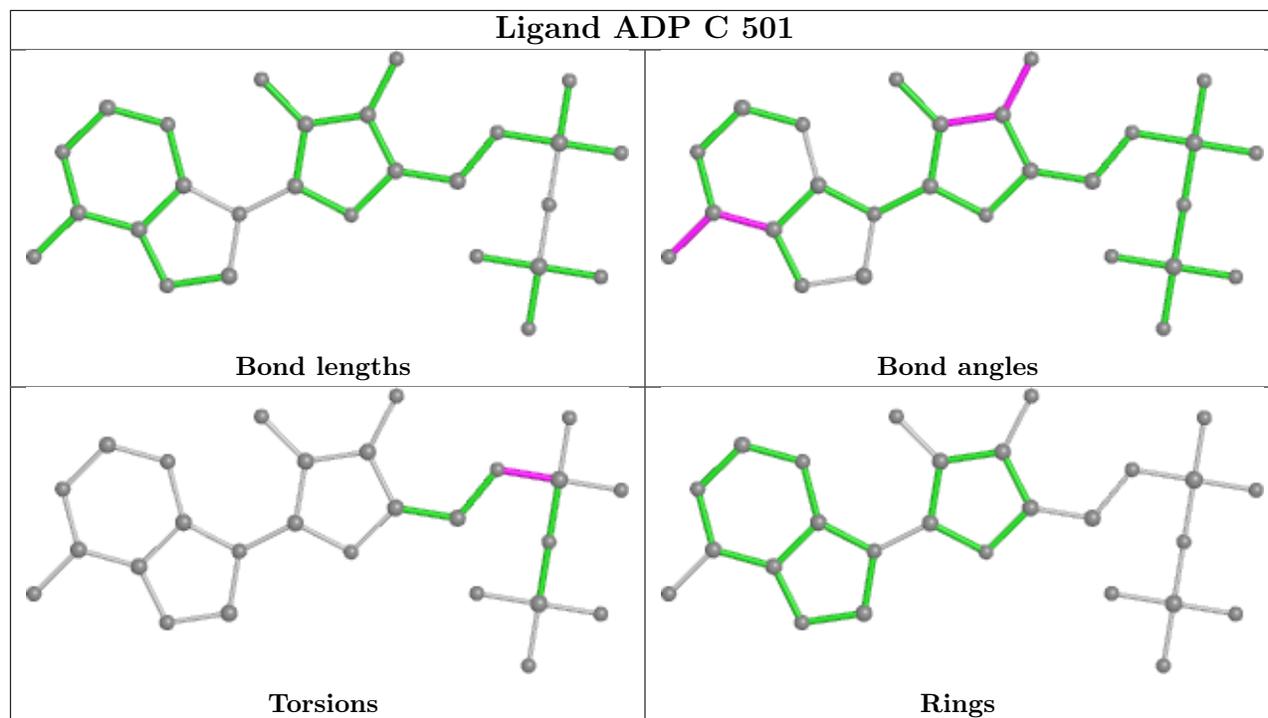
12 monomers are involved in 20 short contacts:

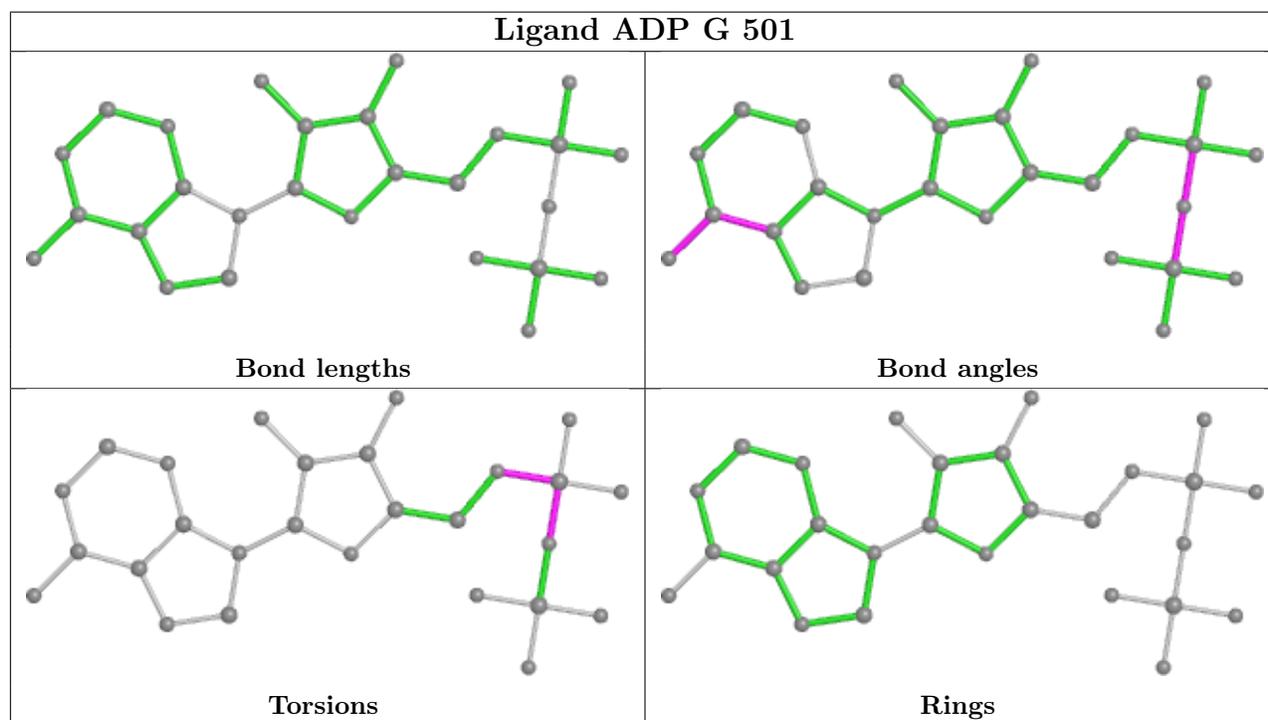
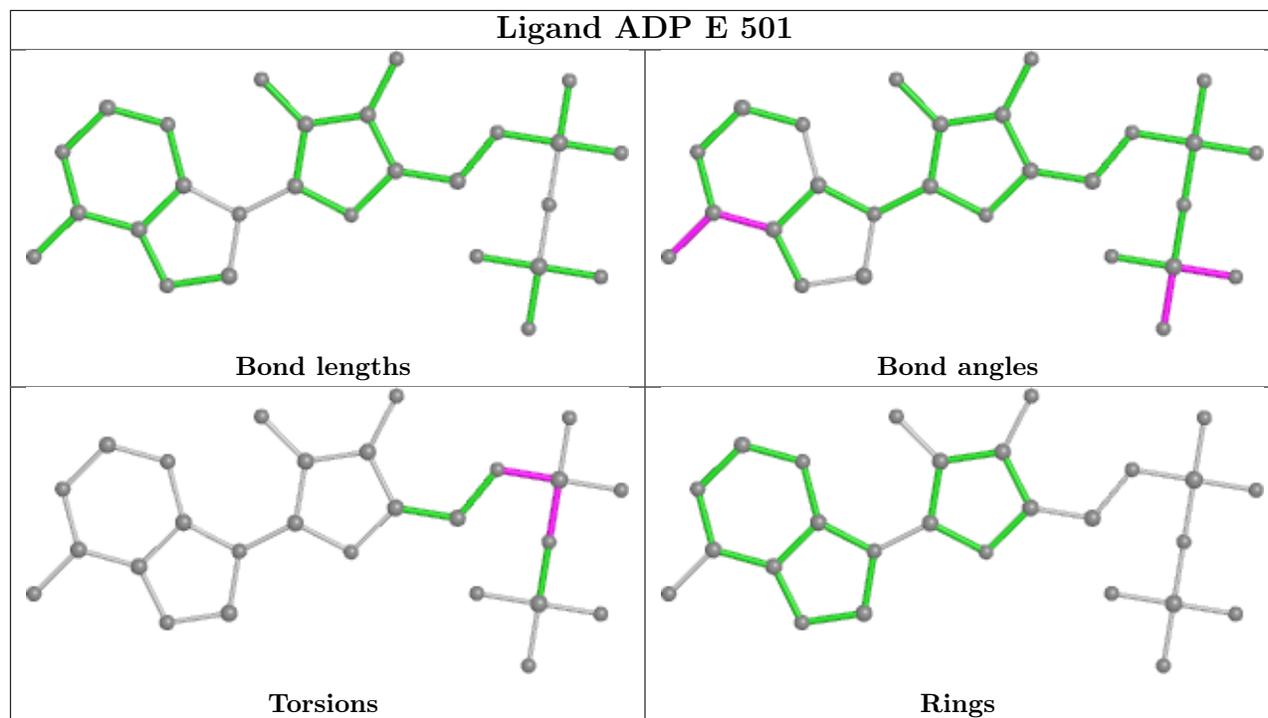
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	ADP	2	0
3	D	501	ADP	1	0
3	L	501	ADP	2	0
3	J	501	ADP	4	0
3	C	501	ADP	1	0
3	A	501	ADP	1	0
3	E	501	ADP	1	0
3	G	501	ADP	1	0
3	H	501	ADP	3	0
3	F	501	ADP	2	0
3	K	501	ADP	1	0
3	I	501	ADP	1	0

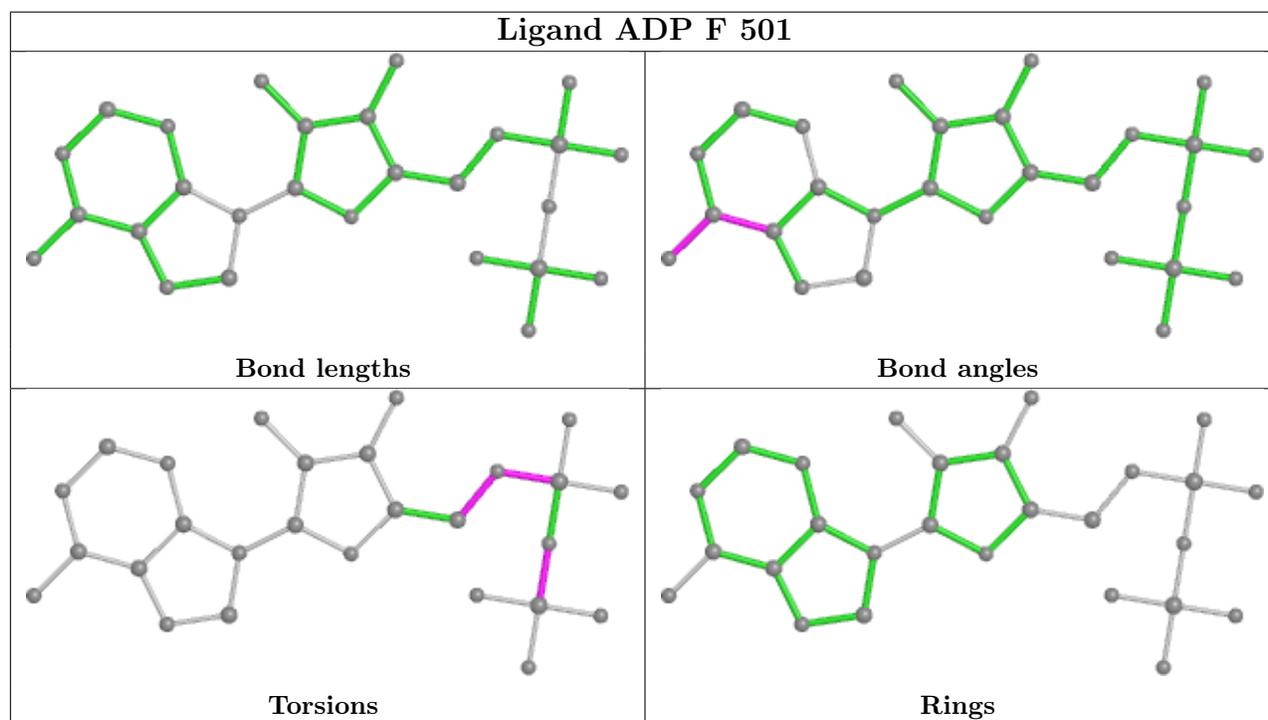
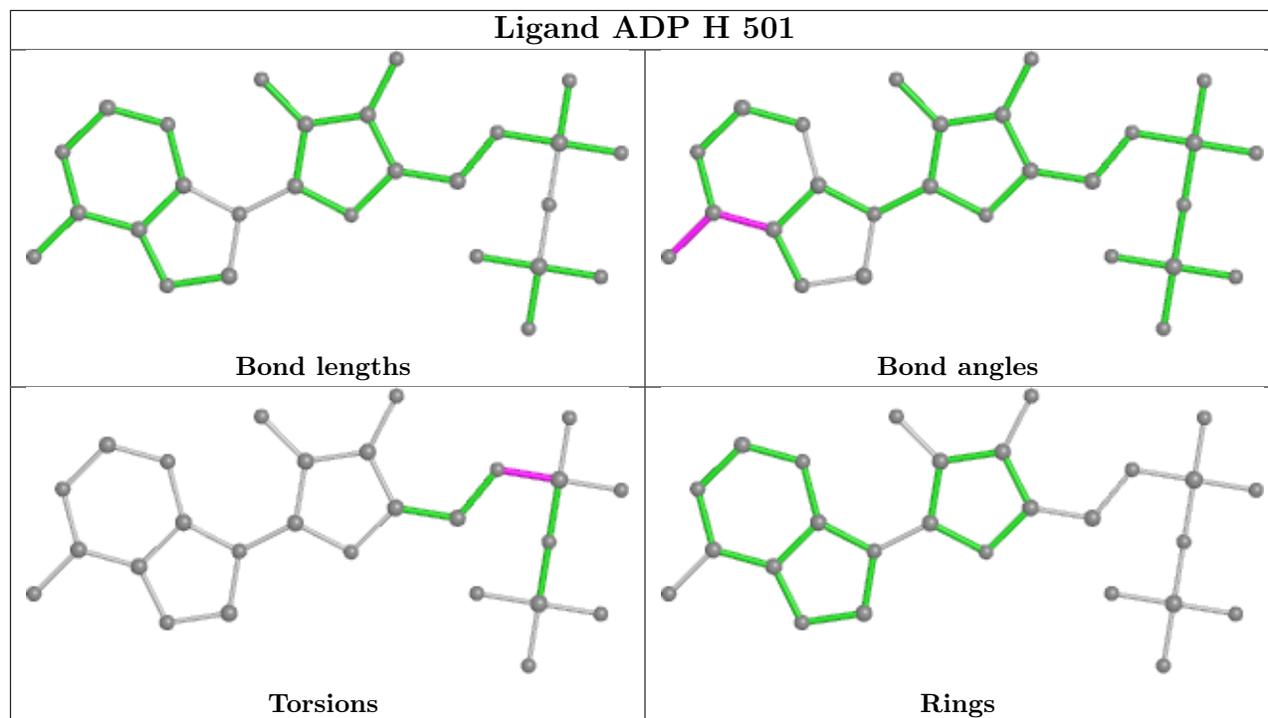
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

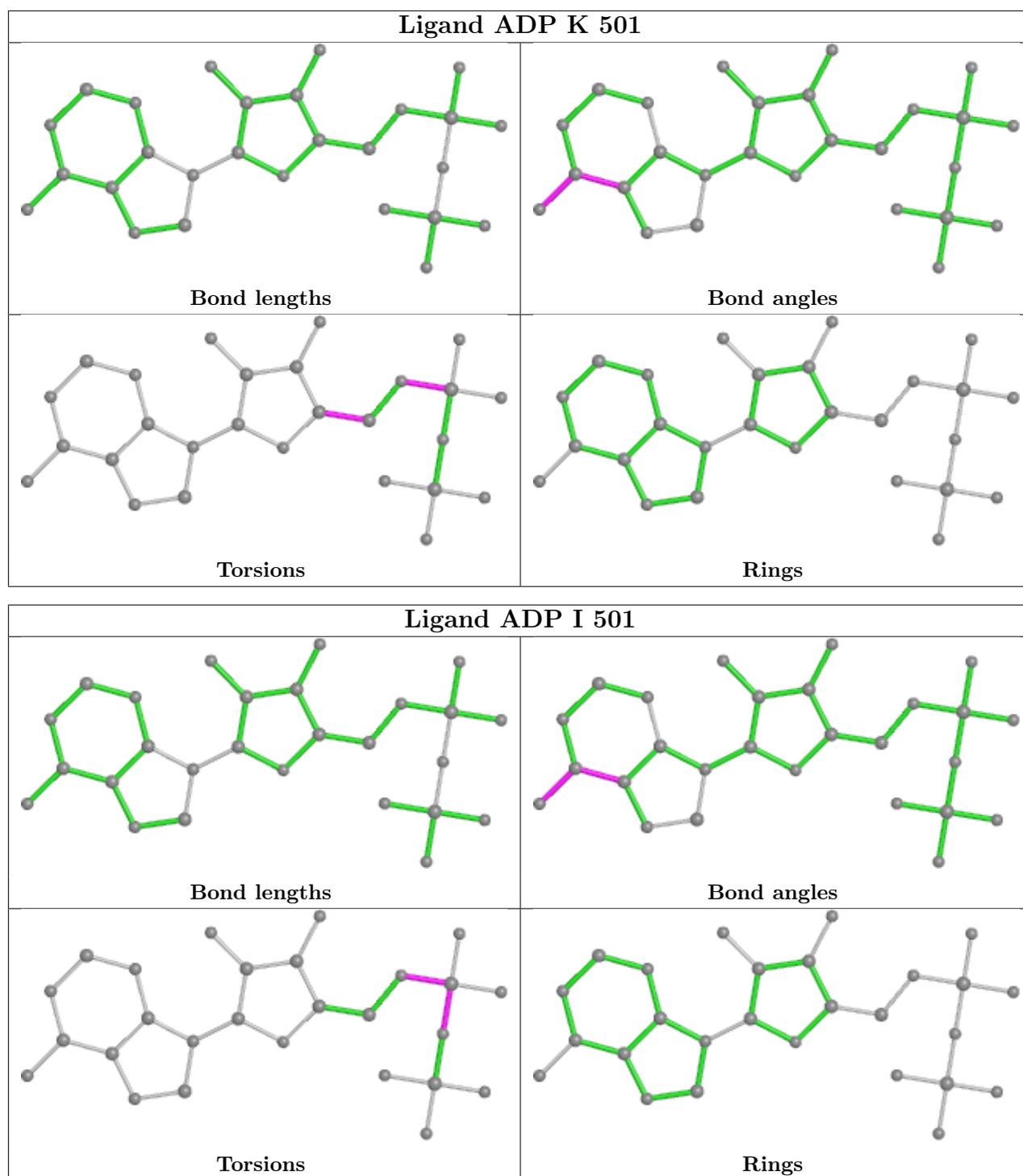












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.25	2 (0%) 91 81	30, 64, 127, 190	0
1	B	438/438 (100%)	-0.29	2 (0%) 91 81	38, 73, 138, 207	0
1	C	438/438 (100%)	-0.26	5 (1%) 80 64	34, 66, 129, 214	0
1	D	438/438 (100%)	-0.24	5 (1%) 80 64	37, 73, 136, 214	0
1	E	438/438 (100%)	-0.23	6 (1%) 75 56	38, 76, 143, 252	0
1	F	438/438 (100%)	-0.09	8 (1%) 68 47	36, 81, 157, 205	0
1	G	438/438 (100%)	-0.24	1 (0%) 95 90	38, 75, 133, 194	0
1	H	438/438 (100%)	-0.24	2 (0%) 91 81	37, 73, 134, 200	0
1	I	438/438 (100%)	-0.26	4 (0%) 84 69	36, 75, 145, 240	0
1	J	438/438 (100%)	-0.23	4 (0%) 84 69	36, 78, 153, 252	0
1	K	438/438 (100%)	-0.25	3 (0%) 87 75	39, 77, 138, 203	0
1	L	438/438 (100%)	-0.14	7 (1%) 72 51	44, 85, 150, 209	0
2	M	76/76 (100%)	-0.21	1 (1%) 77 59	71, 110, 143, 168	0
2	N	62/76 (81%)	0.79	7 (11%) 5 2	91, 133, 172, 194	0
2	O	76/76 (100%)	-0.17	0 100 100	65, 96, 137, 160	0
2	P	76/76 (100%)	0.55	8 (10%) 6 2	97, 148, 188, 229	0
2	Q	76/76 (100%)	0.58	8 (10%) 6 2	109, 159, 192, 233	0
2	R	76/76 (100%)	0.73	9 (11%) 4 2	111, 161, 203, 219	0
2	S	76/76 (100%)	0.43	8 (10%) 6 2	84, 120, 158, 182	0
2	T	76/76 (100%)	1.00	16 (21%) 1 0	114, 157, 197, 216	0
2	U	76/76 (100%)	0.99	12 (15%) 2 1	101, 137, 178, 232	0
2	V	76/76 (100%)	1.17	23 (30%) 0 0	108, 164, 199, 210	0
2	W	53/76 (69%)	1.27	18 (33%) 0 0	80, 133, 195, 219	0
2	X	76/76 (100%)	1.19	19 (25%) 0 0	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%)	-0.10	178 (2%) 51 28	30, 80, 165, 252	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	ASN	5.4
2	U	627	LEU	5.1
2	T	592	ALA	5.0
1	D	21	ASN	5.0
2	W	609	PRO	5.0
1	L	440	GLU	4.8
1	B	439	ALA	4.7
2	W	632	SER	4.7
2	W	608	PHE	4.6
2	P	636	VAL	4.6
1	L	21	ASN	4.5
2	N	647	GLU	4.4
2	V	623	ASP	4.3
2	P	576	LEU	4.3
2	U	610	TRP	4.3
1	I	21	ASN	4.3
2	W	585	PHE	4.2
1	D	186	GLY	4.1
2	V	613	TYR	4.0
2	V	624	VAL	4.0
2	W	615	LEU	3.9
2	U	624	VAL	3.9
2	X	609	PRO	3.9
2	T	631	LYS	3.8
2	X	613	TYR	3.7
2	X	608	PHE	3.7
2	X	603	VAL	3.6
2	V	648	ALA	3.6
1	L	430	ILE	3.6
2	X	623	ASP	3.6
2	T	590	PHE	3.5
2	P	585	PHE	3.4
2	P	586	LEU	3.4
2	U	625	THR	3.4
2	V	603	VAL	3.4
2	V	608	PHE	3.4
1	E	440	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	S	647	GLU	3.3
1	K	440	GLU	3.3
2	X	628	ASP	3.3
2	W	602	PHE	3.3
1	J	440	GLU	3.3
1	J	443	ASN	3.3
2	N	615	LEU	3.2
2	X	610	TRP	3.2
1	E	443	ASN	3.2
2	N	608	PHE	3.2
2	X	630	ASN	3.2
1	E	439	ALA	3.2
1	J	439	ALA	3.2
2	Q	627	LEU	3.1
2	U	615	LEU	3.1
1	C	437	ILE	3.1
2	T	622	ARG	3.1
2	Q	648	ALA	3.0
1	A	430	ILE	3.0
2	S	607	GLY	3.0
2	W	613	TYR	3.0
1	L	438	ASP	3.0
2	V	588	ARG	3.0
1	J	21	ASN	3.0
2	R	575	LYS	3.0
1	K	435	GLU	3.0
2	T	628	ASP	3.0
2	X	649	LYS	2.9
1	E	21	ASN	2.9
2	X	627	LEU	2.9
2	Q	585	PHE	2.9
2	V	625	THR	2.9
2	V	633	LEU	2.9
1	F	182	ILE	2.8
2	W	583	GLY	2.8
2	T	627	LEU	2.8
2	V	647	GLU	2.7
2	V	639	PHE	2.7
2	V	612	GLU	2.7
1	D	176	VAL	2.7
1	B	443	ASN	2.7
2	S	627	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	V	615	LEU	2.7
2	Q	613	TYR	2.7
2	S	624	VAL	2.7
1	I	438	ASP	2.6
2	X	594	ASN	2.6
2	U	650	GLU	2.6
2	V	576	LEU	2.6
2	V	616	LEU	2.6
2	R	639	PHE	2.6
2	X	646	LEU	2.6
2	W	599	VAL	2.6
2	W	603	VAL	2.6
2	U	639	PHE	2.6
2	T	624	VAL	2.6
1	L	437	ILE	2.6
1	E	438	ASP	2.6
2	T	599	VAL	2.6
1	H	433	GLU	2.5
2	Q	649	LYS	2.5
2	W	578	ILE	2.5
2	S	612	GLU	2.5
1	F	105	CYS	2.5
2	X	607	GLY	2.5
2	P	650	GLU	2.5
2	W	616	LEU	2.5
1	I	133	VAL	2.5
2	V	586	LEU	2.5
2	T	613	TYR	2.5
1	D	23	PRO	2.4
2	T	650	GLU	2.4
2	T	638	LEU	2.4
2	R	592	ALA	2.4
1	K	21	ASN	2.4
2	M	630	ASN	2.4
2	Q	637	LYS	2.4
2	R	613	TYR	2.4
1	F	437	ILE	2.4
2	T	593	SER	2.4
2	P	627	LEU	2.4
2	X	635	GLU	2.4
2	W	646	LEU	2.4
2	Q	635	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	V	587	GLU	2.3
1	F	24	ASN	2.3
1	I	443	ASN	2.3
1	L	316	THR	2.3
1	C	434	ASP	2.3
1	F	169	ASP	2.3
2	U	592	ALA	2.3
2	X	648	ALA	2.3
2	R	608	PHE	2.3
1	H	173	TYR	2.3
2	S	613	TYR	2.3
2	R	623	ASP	2.3
2	T	611	ASP	2.3
2	X	624	VAL	2.3
1	C	438	ASP	2.3
2	U	602	PHE	2.3
2	S	614	LYS	2.2
2	X	629	PRO	2.2
2	V	599	VAL	2.2
2	W	634	LEU	2.2
1	C	443	ASN	2.2
2	Q	639	PHE	2.2
2	N	607	GLY	2.2
2	V	610	TRP	2.2
2	T	636	VAL	2.2
1	C	440	GLU	2.2
1	L	174	CYS	2.2
2	V	638	LEU	2.2
2	U	596	LEU	2.2
2	W	631	LYS	2.2
2	W	619	PHE	2.1
2	V	596	LEU	2.1
2	R	607	GLY	2.1
2	N	646	LEU	2.1
1	F	112	LYS	2.1
2	T	616	LEU	2.1
1	F	174	CYS	2.1
2	X	612	GLU	2.1
2	V	649	LYS	2.1
2	U	636	VAL	2.1
1	G	443	ASN	2.1
2	P	623	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	R	624	VAL	2.1
2	V	636	VAL	2.1
2	T	630	ASN	2.1
1	E	23	PRO	2.1
2	N	585	PHE	2.1
2	R	631	LYS	2.0
2	W	610	TRP	2.0
1	D	187	GLU	2.0
2	P	639	PHE	2.0
2	N	624	VAL	2.0
1	F	111	GLY	2.0
2	S	648	ALA	2.0
2	U	585	PHE	2.0
2	W	600	PHE	2.0
2	X	626	GLN	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 monosaccharides 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.

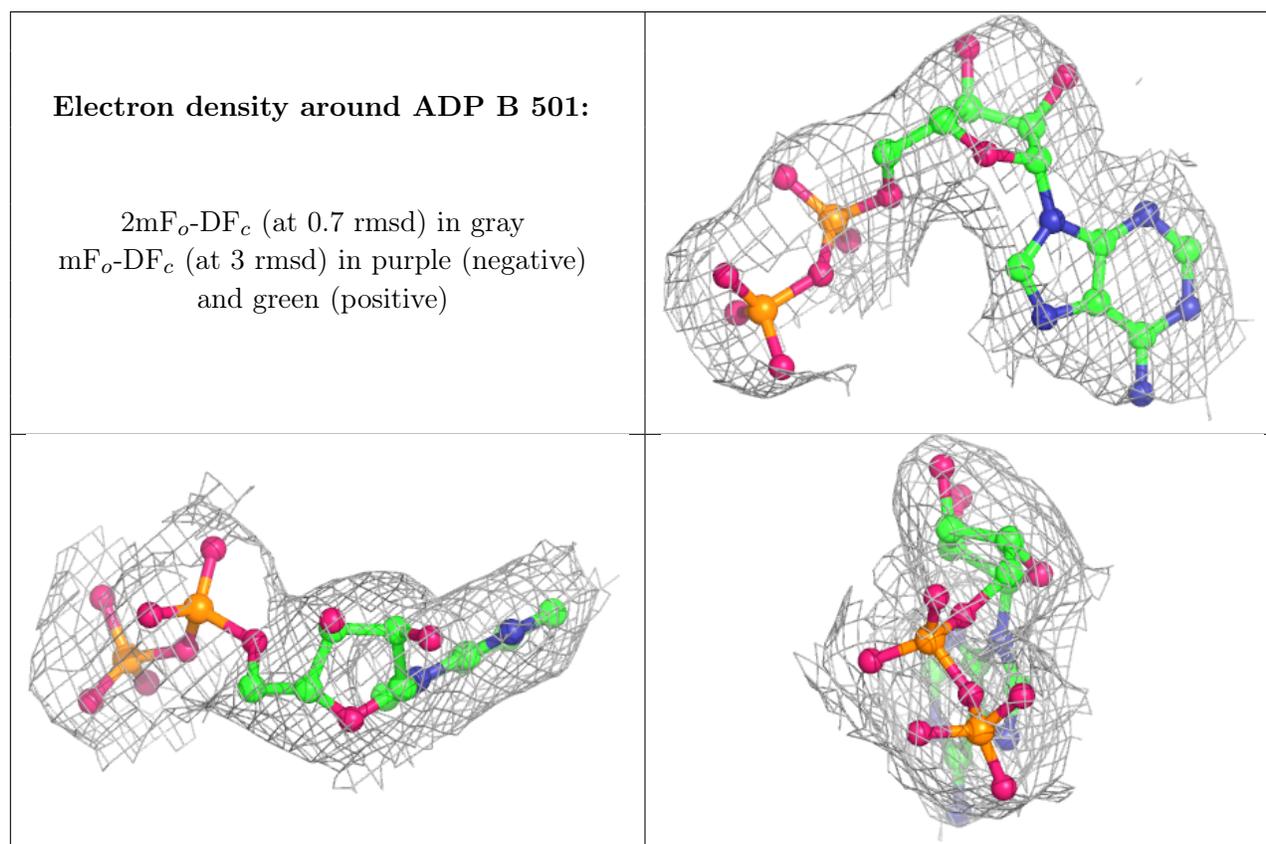
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	B	501	27/27	0.96	0.16	52,62,84,94	0
3	ADP	C	501	27/27	0.97	0.18	45,60,77,94	0
3	ADP	D	501	27/27	0.97	0.16	51,60,76,99	0
3	ADP	E	501	27/27	0.97	0.18	55,63,87,91	0
3	ADP	H	501	27/27	0.97	0.17	55,65,93,109	0
3	ADP	J	501	27/27	0.97	0.19	53,60,79,94	0
3	ADP	L	501	27/27	0.97	0.15	59,75,90,98	0
3	ADP	I	501	27/27	0.98	0.17	45,57,81,83	0

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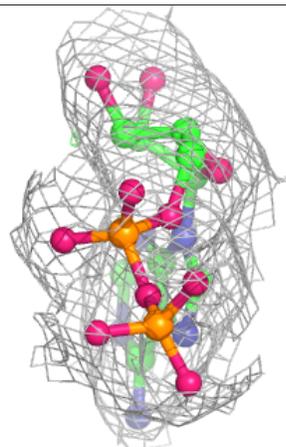
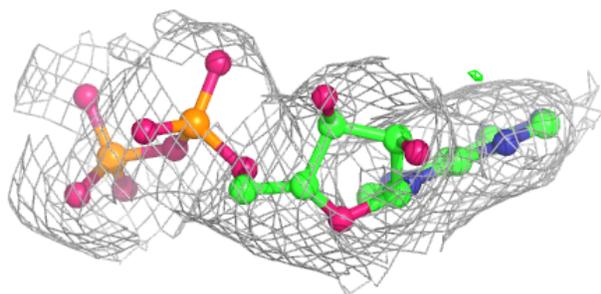
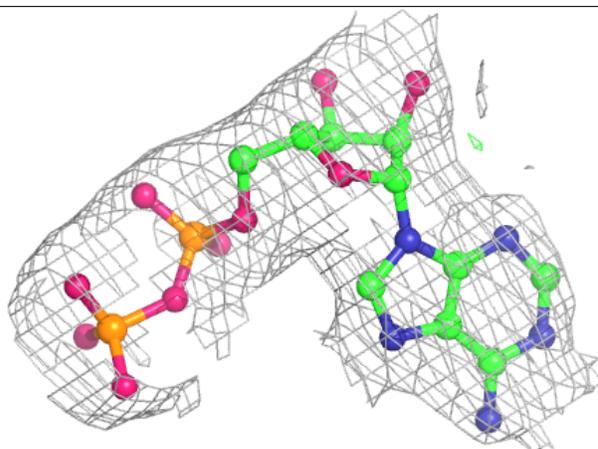
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	G	501	27/27	0.98	0.15	56,69,102,122	0
3	ADP	K	501	27/27	0.98	0.17	55,63,86,108	0
3	ADP	A	501	27/27	0.98	0.17	50,59,74,95	0
3	ADP	F	501	27/27	0.99	0.16	48,54,74,89	0

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.



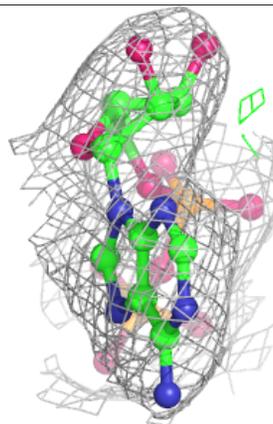
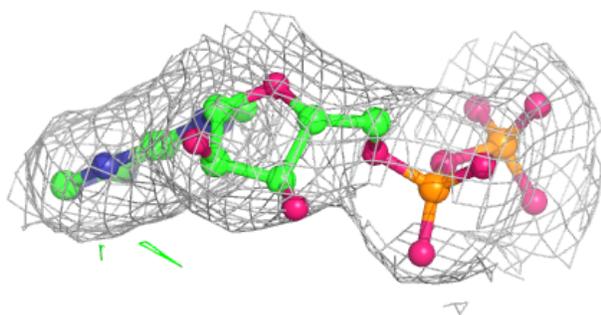
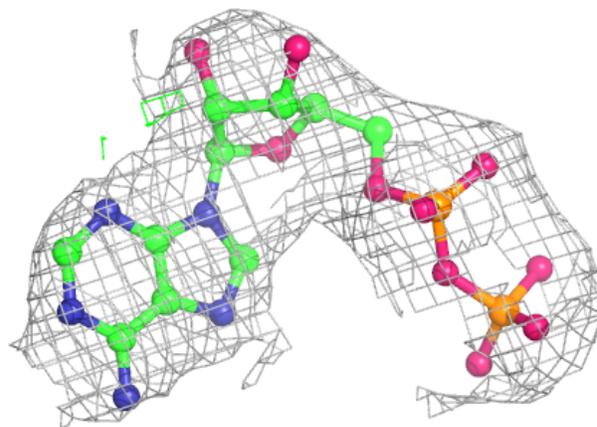
Electron density around ADP C 501:

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



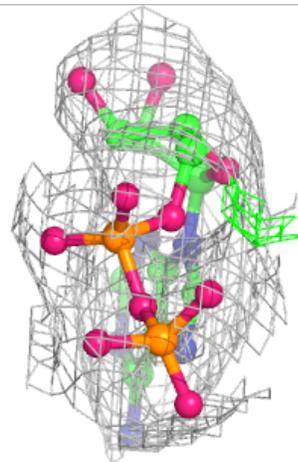
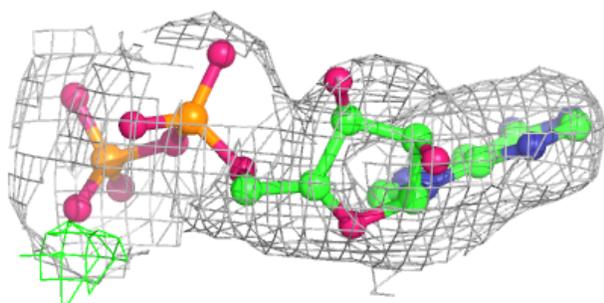
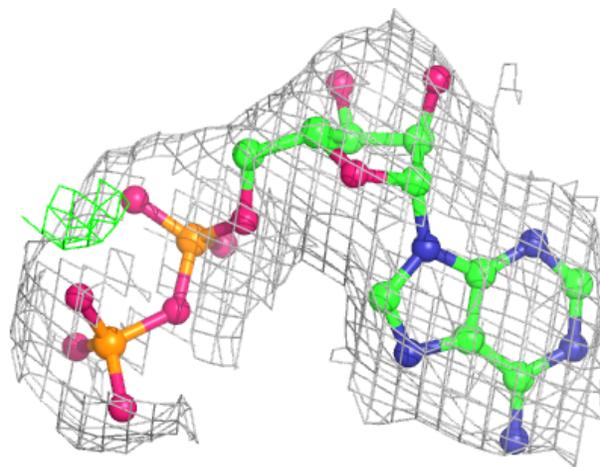
Electron density around ADP D 501:

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



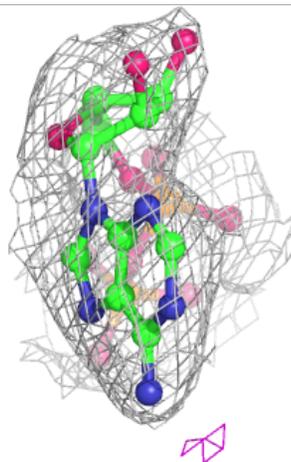
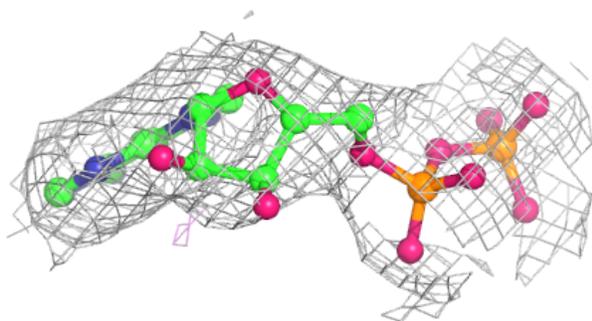
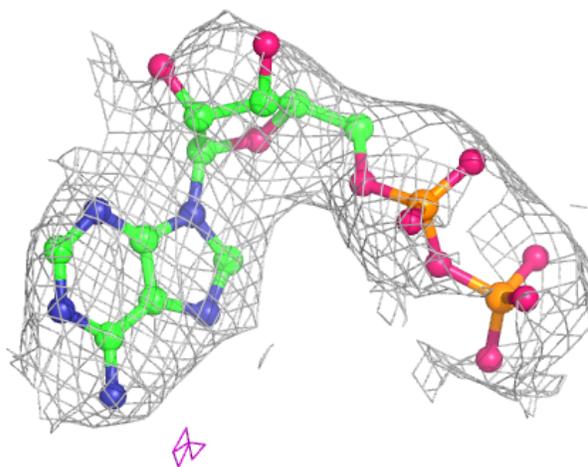
Electron density around ADP E 501:

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



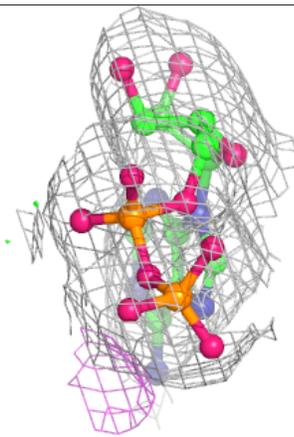
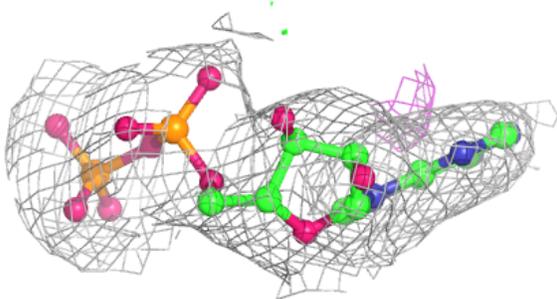
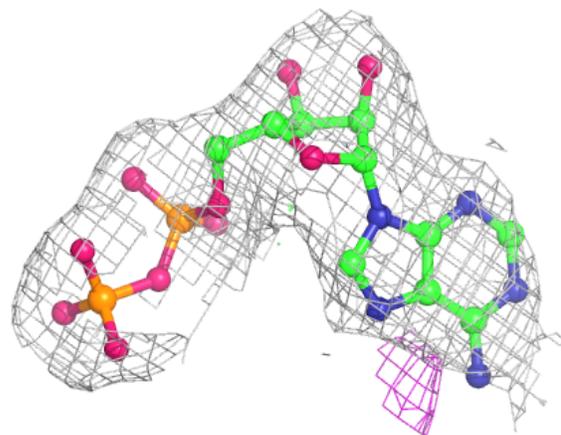
Electron density around ADP H 501:

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



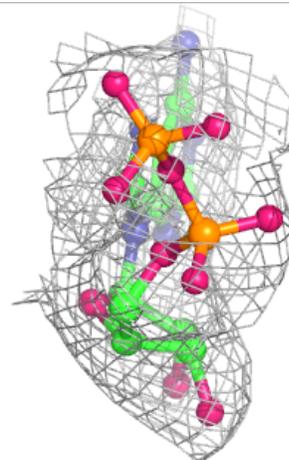
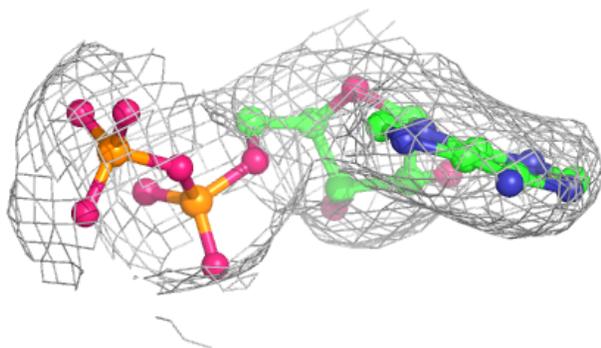
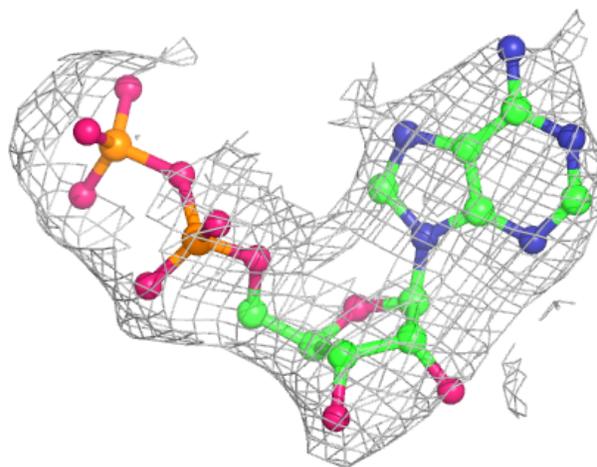
Electron density around ADP J 501:

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



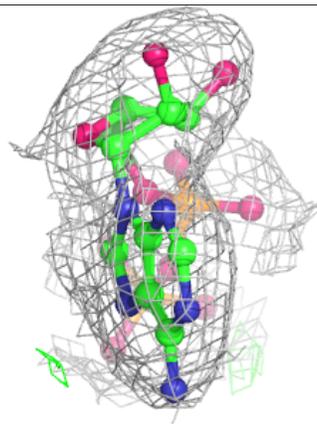
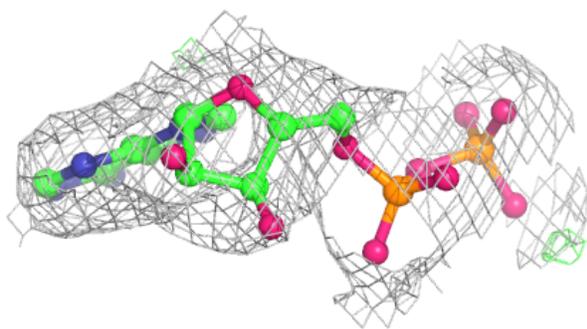
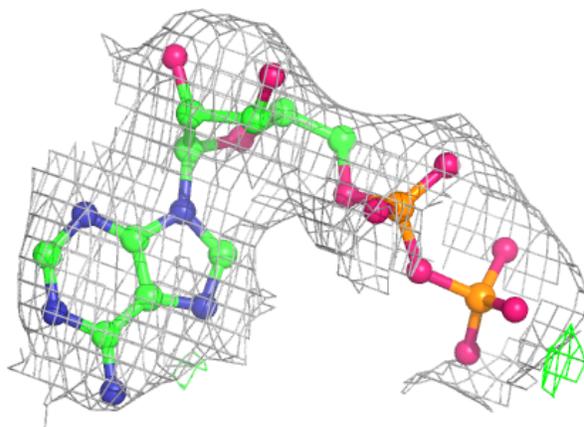
Electron density around ADP L 501:

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



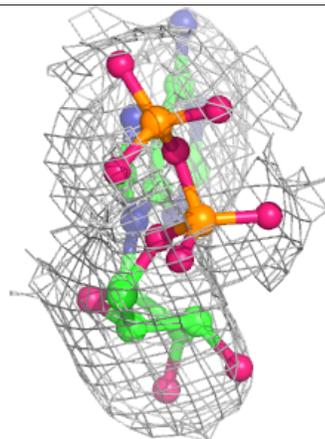
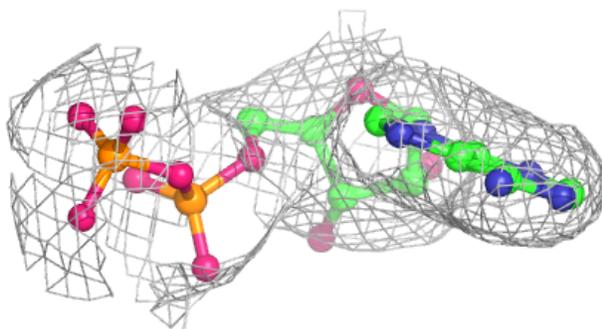
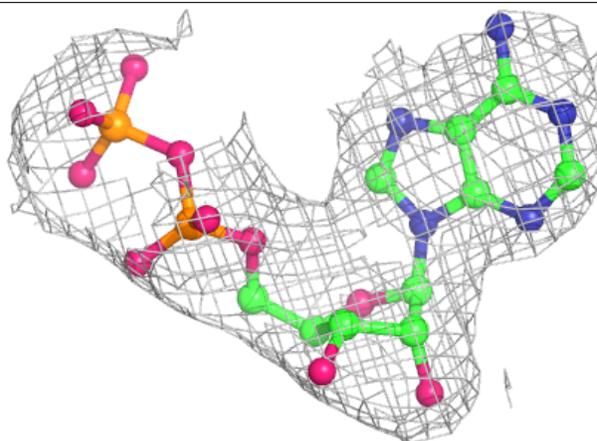
Electron density around ADP I 501:

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



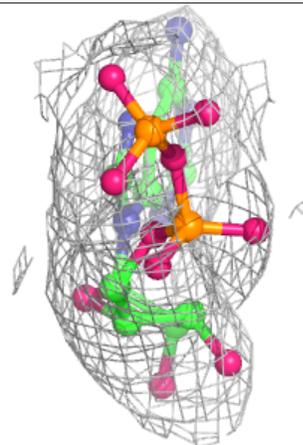
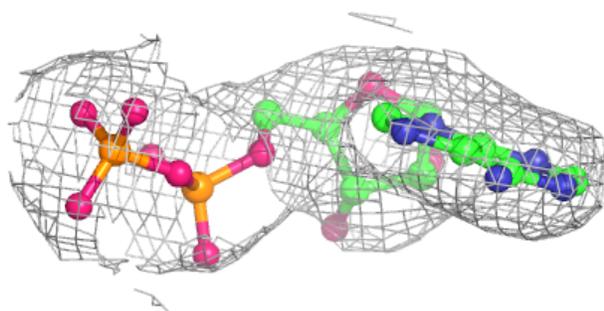
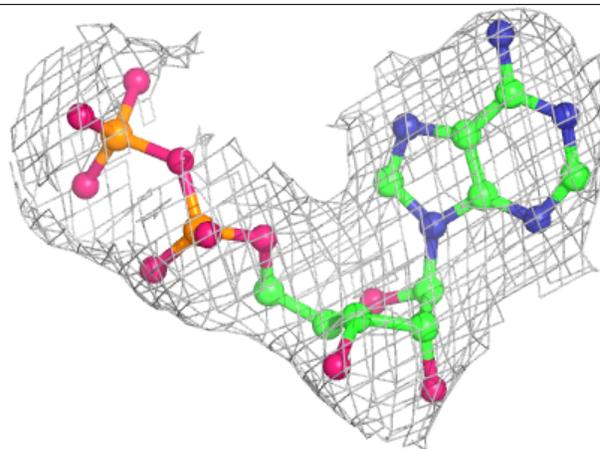
Electron density around ADP G 501:

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



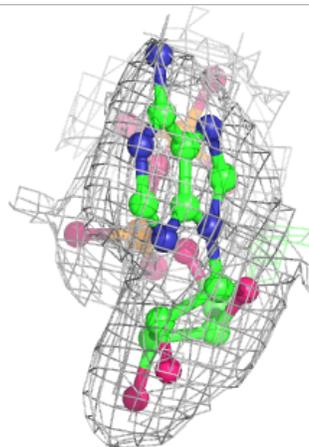
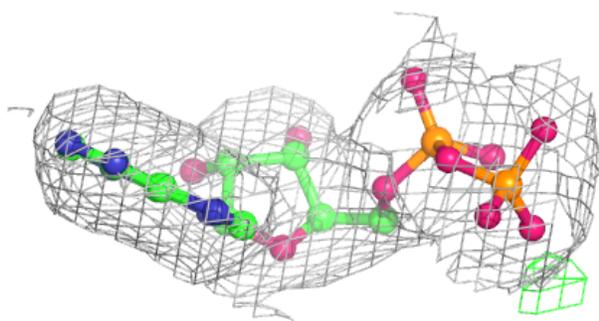
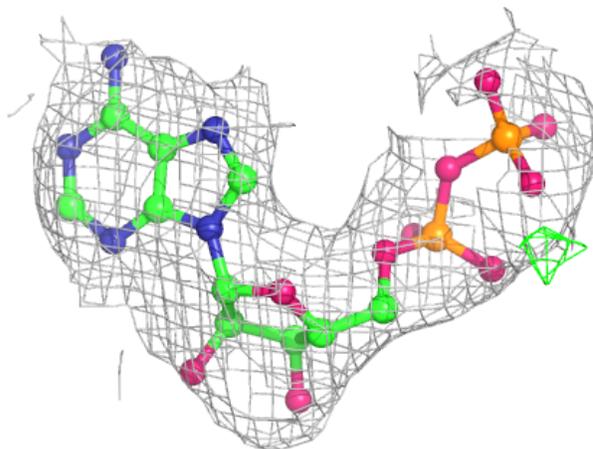
Electron density around ADP K 501:

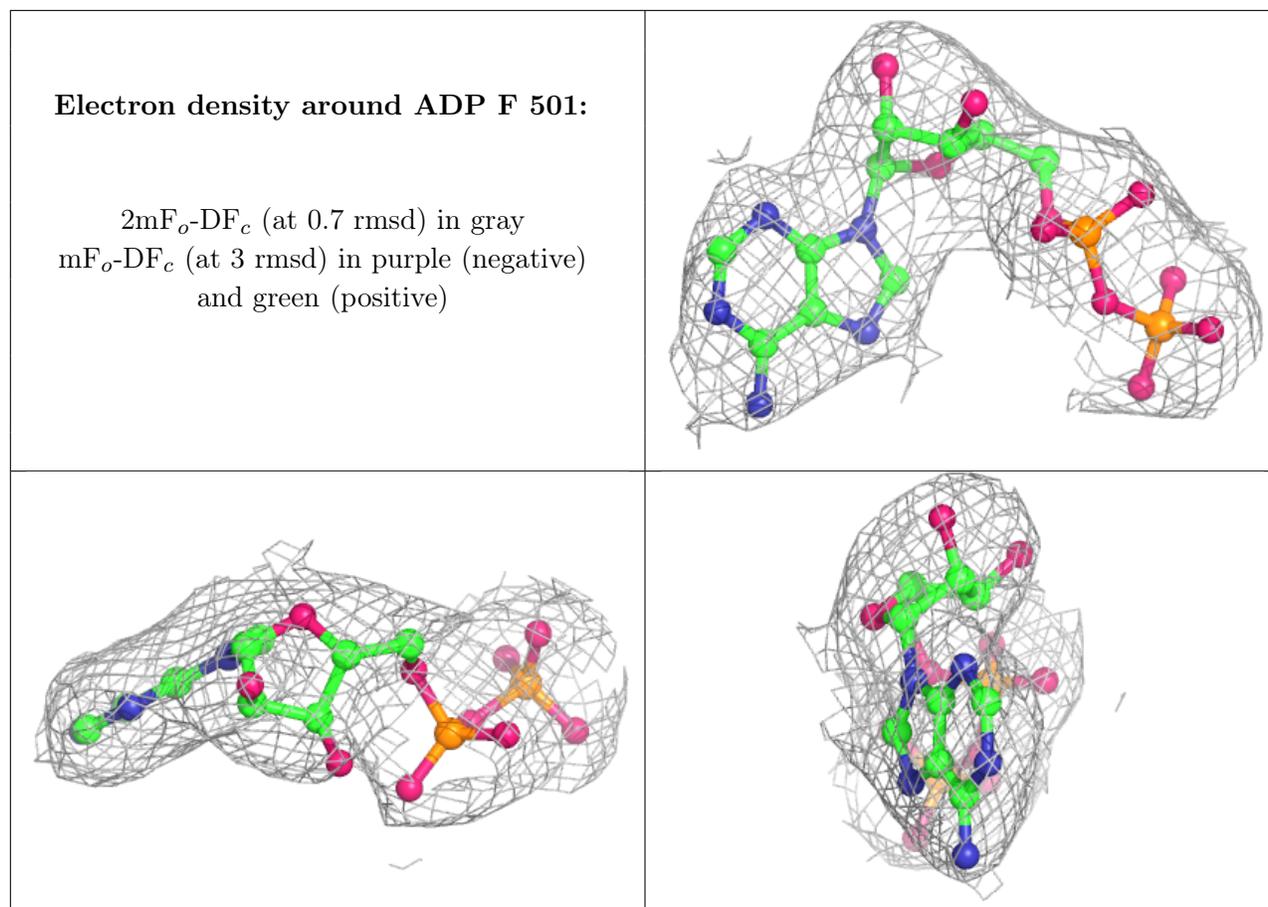
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.