Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2023 – 12:21 PM JST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

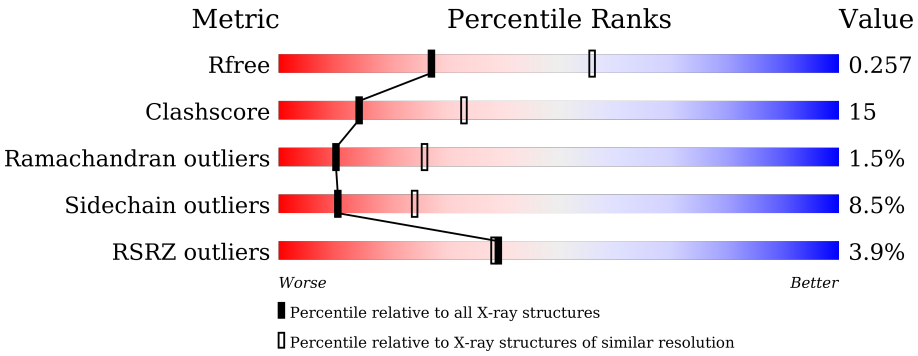
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5% 73% 23% ·
1	B	438	3% 72% 24% ·
1	C	438	3% 71% 24% ·
1	D	438	5% 69% 26% 5%
1	E	438	6% 71% 22% 6% ·
1	F	438	6% 72% 24% ·

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Mol	Chain	Length	Quality of chain
1	G	438	5% 70% 24% 5%
1	H	438	4% 70% 25%
1	I	438	4% 70% 26%
1	J	438	3% 74% 21% 5%
1	K	438	3% 69% 25% 5%
1	L	438	4% 70% 25%
2	M	85	68% 24% 8%
2	N	85	72% 22% 6%
2	O	85	71% 27%
2	P	85	68% 24% 8%
2	Q	85	4% 75% 20% 5%
2	R	85	73% 20% 6%
2	S	85	71% 21% 6%
2	T	85	65% 27% 7%
2	U	85	74% 20% 6%
2	V	85	64% 29% 7%
2	W	85	69% 25% 6%
2	X	85	71% 24% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 49084 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

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

There are 24 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called NSFL1 cofactor p47.

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

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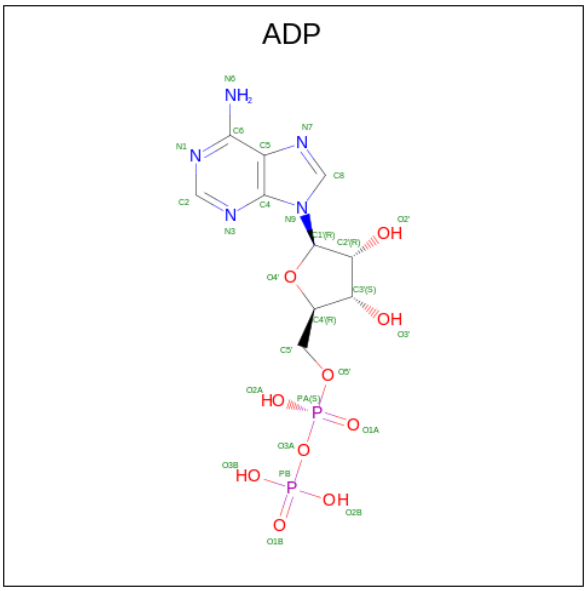
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			
2	X	85	Total	C	N	O	S	0	0	0
			670	422	119	126	3			

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



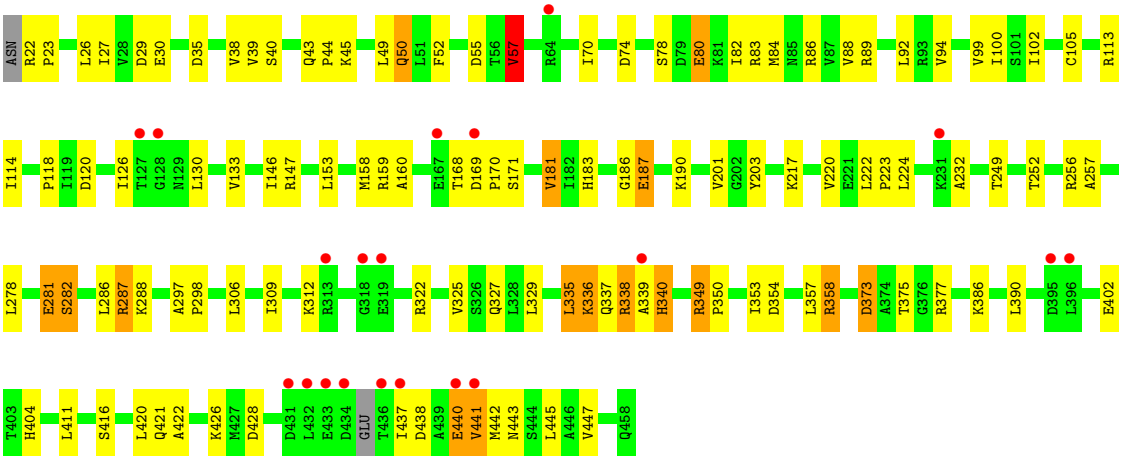
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	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 (i)

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

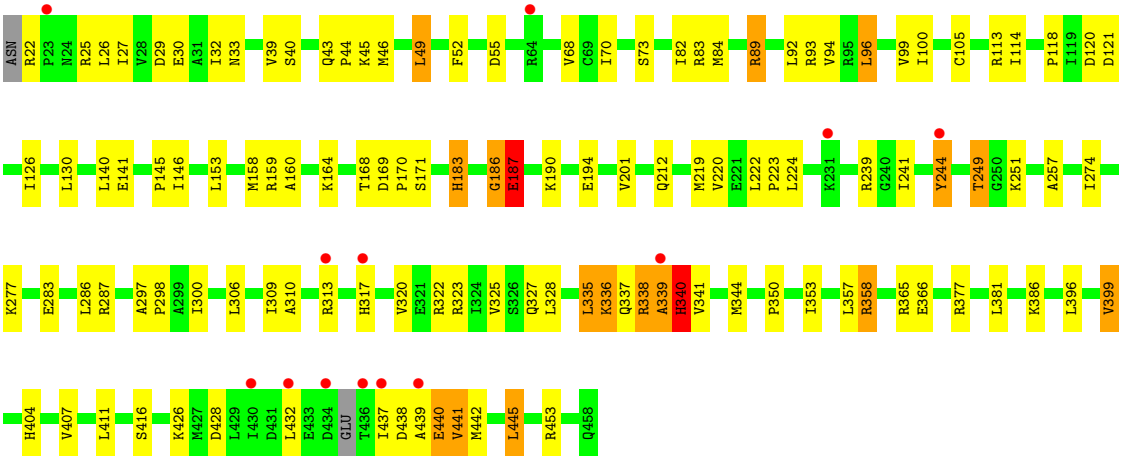
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain A:



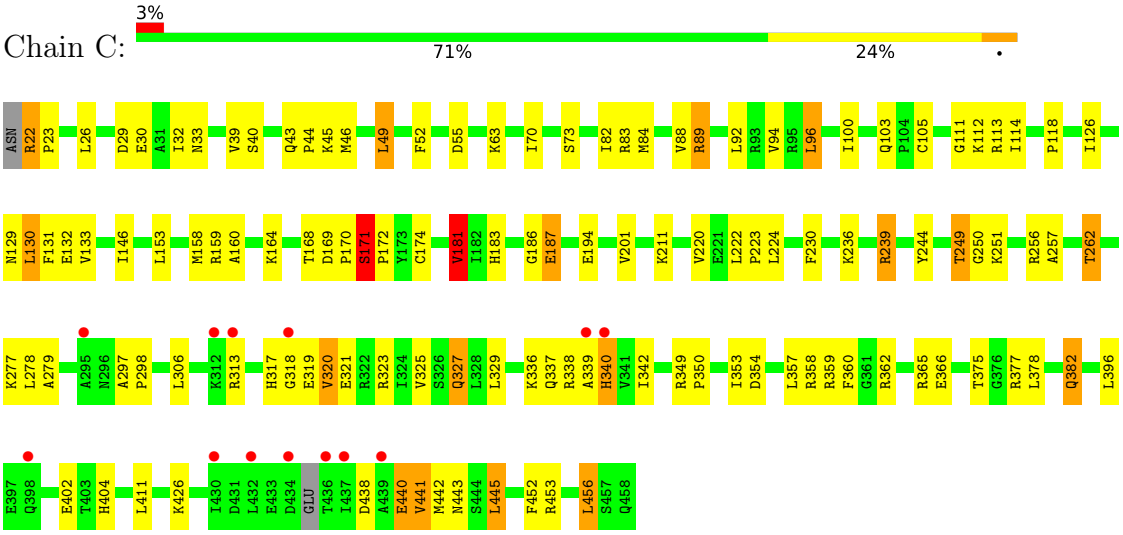
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B:



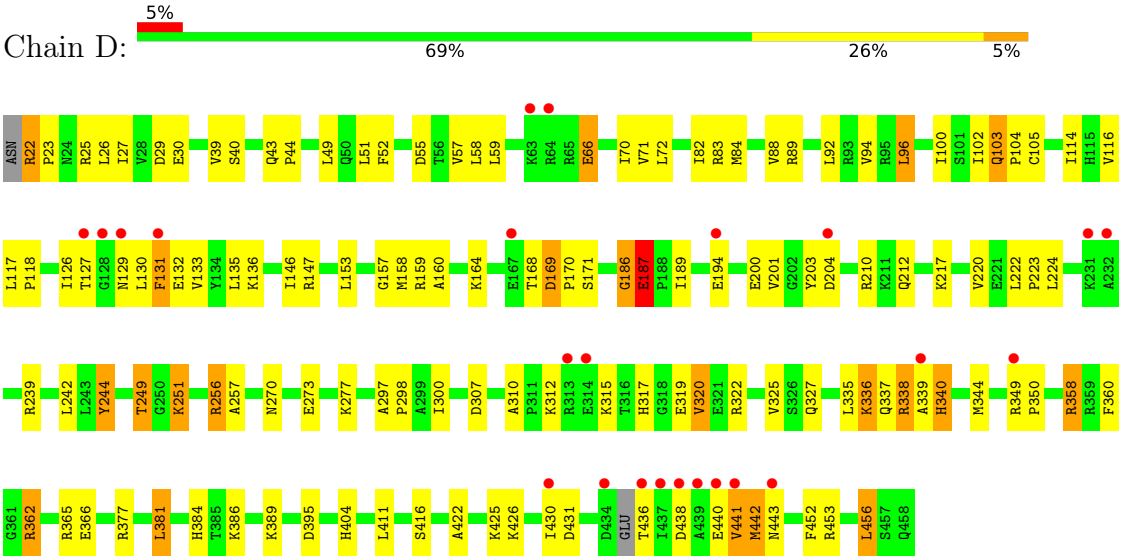
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



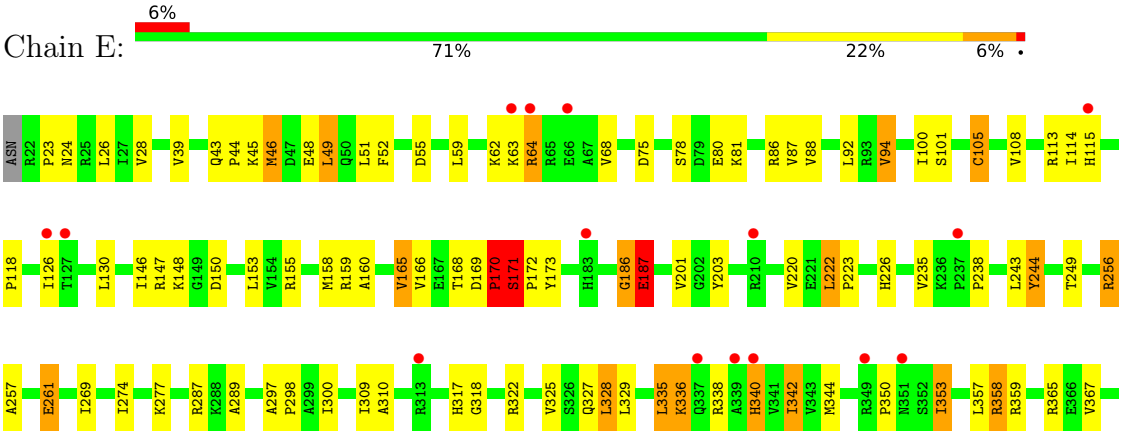
• Molecule 1: Transitional endoplasmic reticulum ATPase

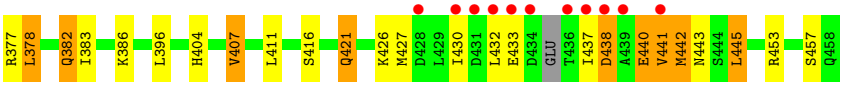
Chain D:



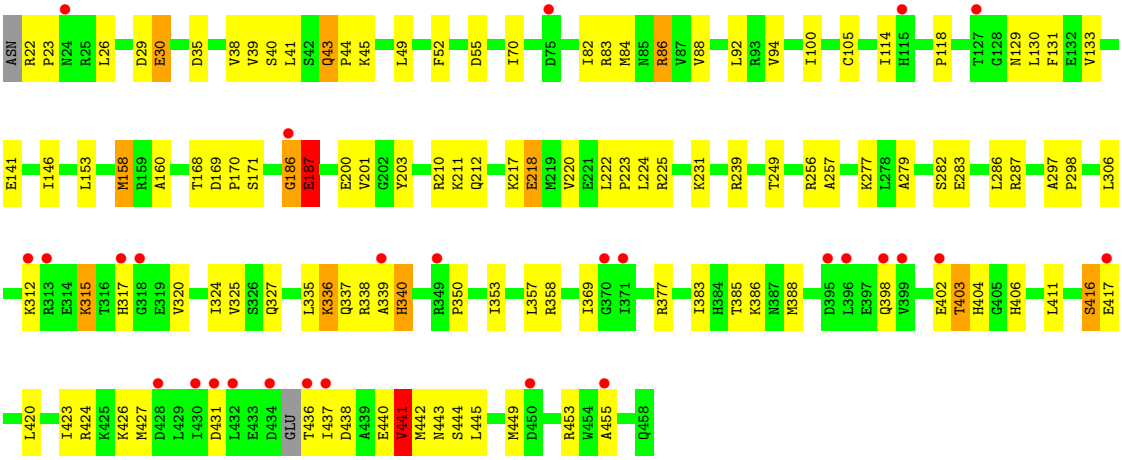
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:

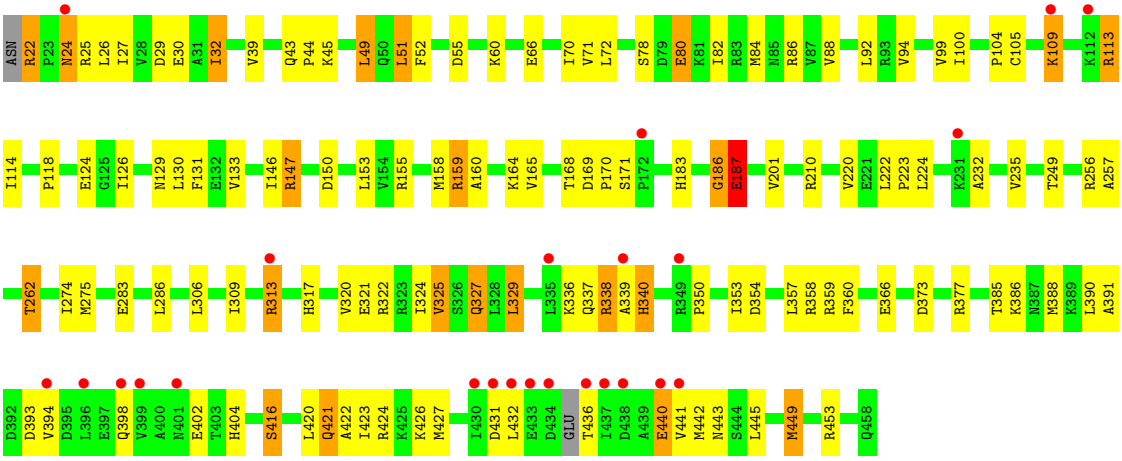




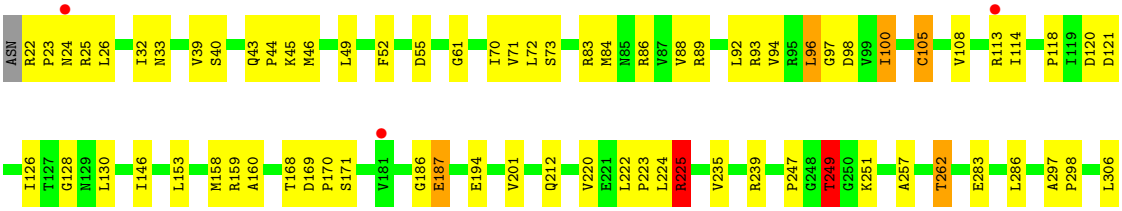
• Molecule 1: Transitional endoplasmic reticulum ATPase

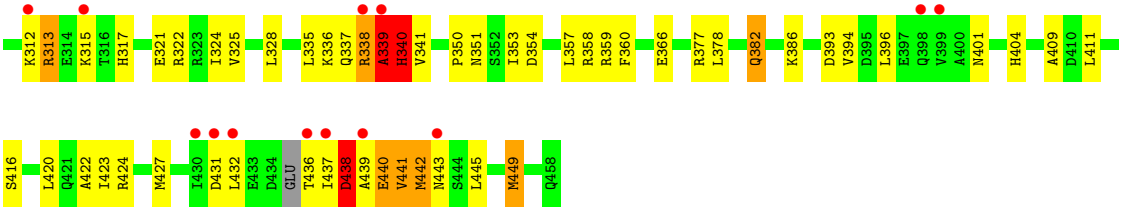


• Molecule 1: Transitional endoplasmic reticulum ATPase

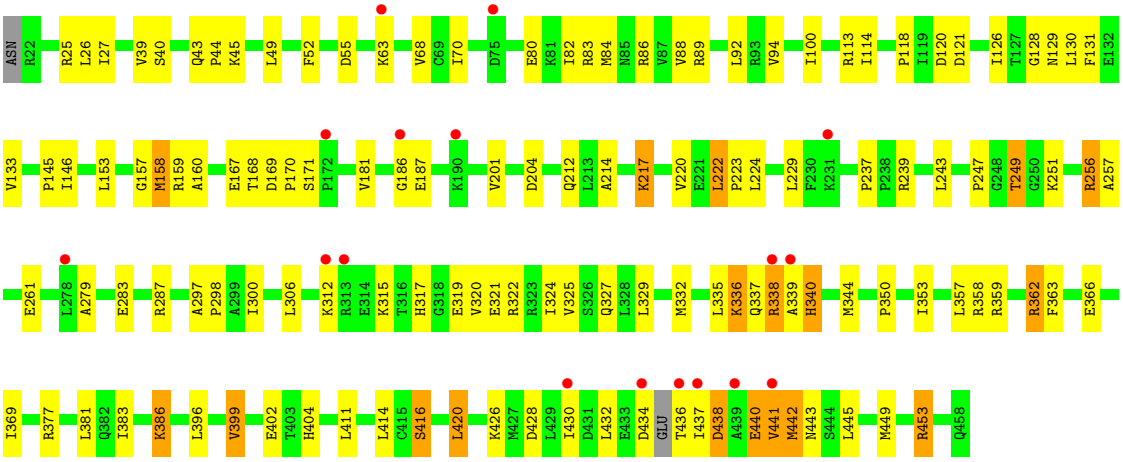


• Molecule 1: Transitional endoplasmic reticulum ATPase

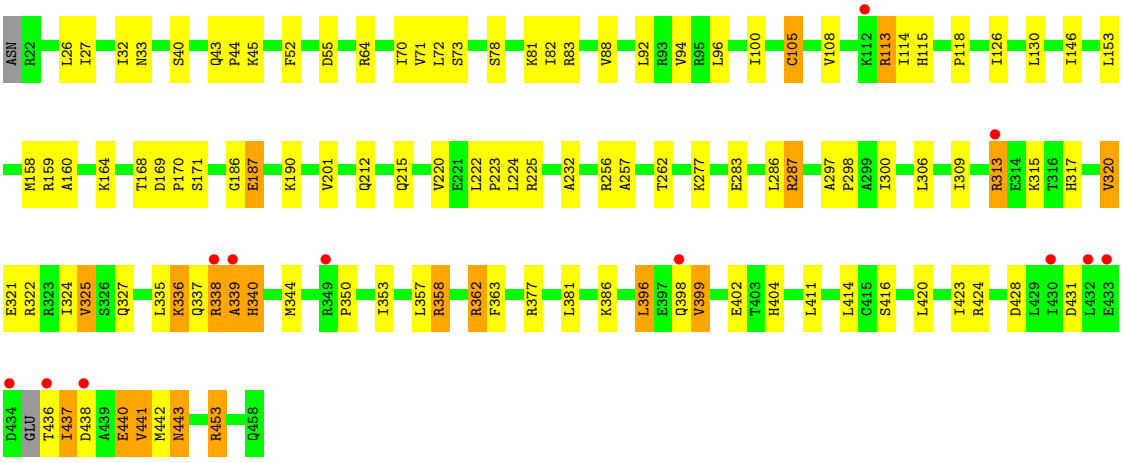




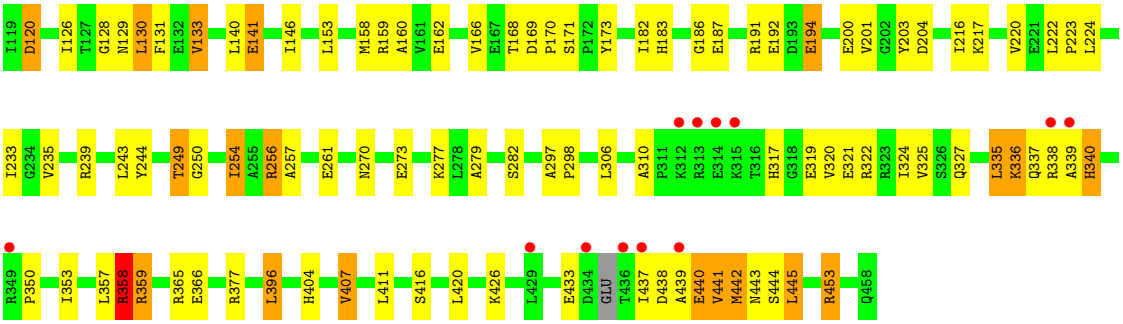
• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase

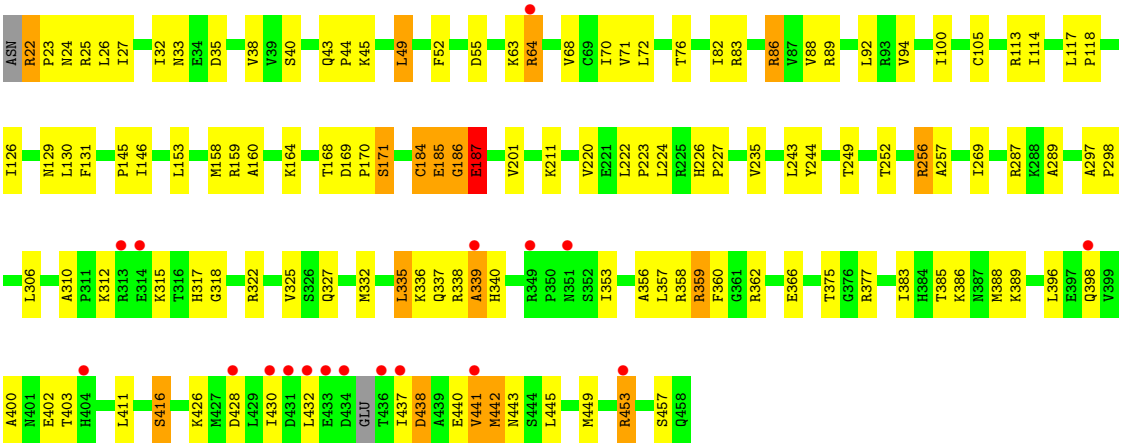


• Molecule 1: Transitional endoplasmic reticulum ATPase



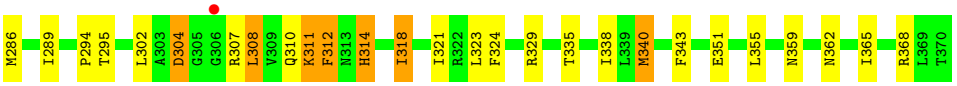
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain L:



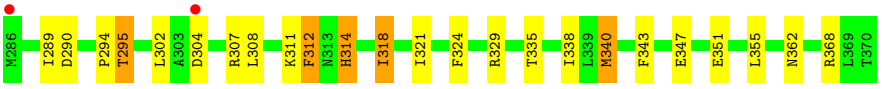
• Molecule 2: NSFL1 cofactor p47

Chain M:



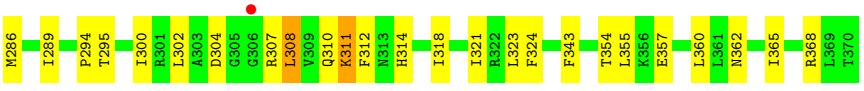
• Molecule 2: NSFL1 cofactor p47

Chain N:



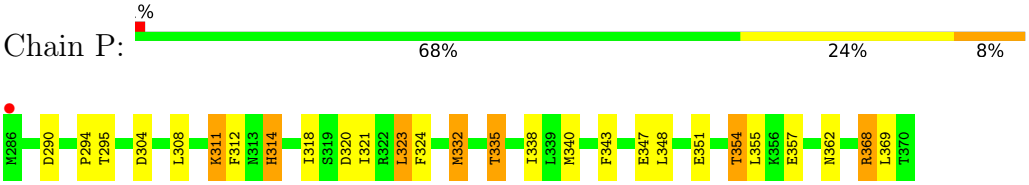
• Molecule 2: NSFL1 cofactor p47

Chain O:



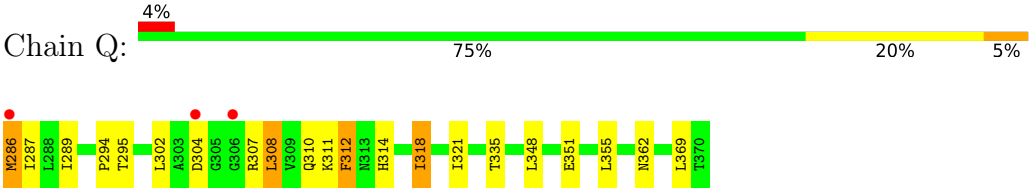
• Molecule 2: NSFL1 cofactor p47

Chain P:



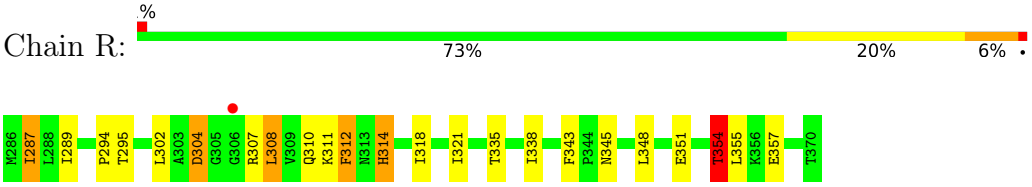
• Molecule 2: NSFL1 cofactor p47

Chain Q:



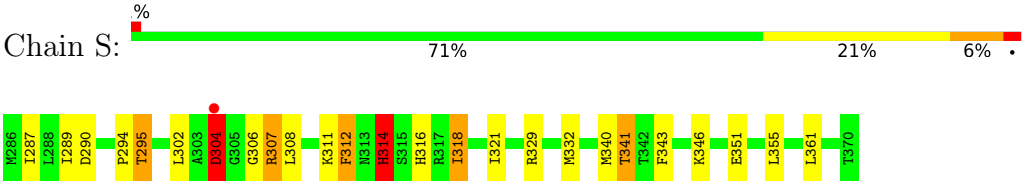
• Molecule 2: NSFL1 cofactor p47

Chain R:



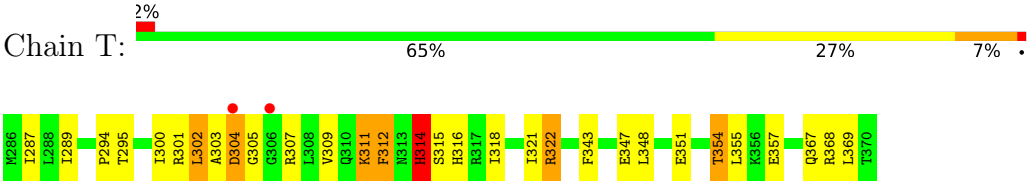
• Molecule 2: NSFL1 cofactor p47

Chain S:



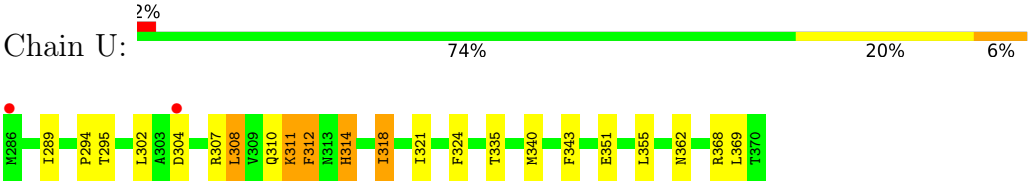
• Molecule 2: NSFL1 cofactor p47

Chain T:



• Molecule 2: NSFL1 cofactor p47

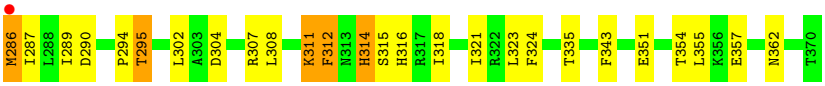
Chain U:



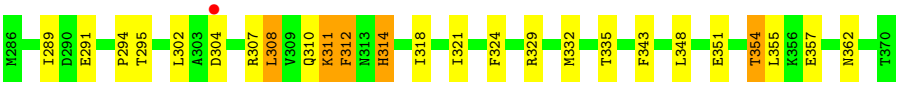
• Molecule 2: NSFL1 cofactor p47

Chain V:

• Molecule 2: NSFL1 cofactor p47



• Molecule 2: NSFL1 cofactor p47



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	170.78Å 178.85Å 171.33Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	40.01 – 2.70 39.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.01-2.70) 99.3 (39.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.213 , 0.256 0.214 , 0.257	Depositor DCC
R_{free} test set	11938 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.049 for -h-l,k,h 0.049 for l,k,-h-l 0.047 for h,-k,-h-l 0.049 for -h-l,-k,l 0.077 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49084	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

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

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.44	0/3456	0.85	5/4670 (0.1%)
1	B	0.43	0/3456	0.87	5/4670 (0.1%)
1	C	0.42	0/3446	0.83	4/4659 (0.1%)
1	D	0.43	0/3450	0.86	7/4663 (0.2%)
1	E	0.45	1/3412 (0.0%)	0.83	4/4619 (0.1%)
1	F	0.43	1/3456 (0.0%)	0.84	2/4670 (0.0%)
1	G	0.43	1/3432 (0.0%)	0.84	4/4643 (0.1%)
1	H	0.42	0/3456	0.85	3/4670 (0.1%)
1	I	0.43	0/3456	0.84	4/4670 (0.1%)
1	J	0.42	0/3450	0.82	0/4663
1	K	0.44	0/3456	0.86	7/4670 (0.1%)
1	L	0.41	0/3436	0.84	5/4647 (0.1%)
2	M	0.45	0/678	0.89	0/917
2	N	0.48	0/672	0.93	0/910
2	O	0.47	0/672	0.92	0/910
2	P	0.46	0/672	0.93	1/910 (0.1%)
2	Q	0.46	0/678	0.95	0/917
2	R	0.45	0/678	0.96	1/917 (0.1%)
2	S	0.46	0/678	0.99	0/917
2	T	0.48	0/678	0.92	2/917 (0.2%)
2	U	0.47	0/678	0.92	0/917
2	V	0.46	0/678	0.93	0/917
2	W	0.45	0/678	0.94	1/917 (0.1%)
2	X	0.49	0/678	0.94	0/917
All	All	0.44	3/49480 (0.0%)	0.86	55/66897 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	261	GLU	CD-OE1	-5.16	1.20	1.25
1	F	30	GLU	CD-OE2	5.11	1.31	1.25
1	G	440	GLU	CD-OE1	-5.08	1.20	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	322	ARG	CG-CD-NE	-11.13	88.44	111.80
2	W	295	THR	CA-CB-OG1	7.86	125.50	109.00
1	E	244	TYR	CB-CA-C	-6.53	97.35	110.40
1	B	183	HIS	CA-CB-CG	6.14	124.04	113.60
1	B	244	TYR	CB-CA-C	-6.11	98.18	110.40
1	L	86	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	T	322	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	A	74	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	L	389	LYS	CB-CG-CD	5.88	126.90	111.60
1	B	89	ARG	CG-CD-NE	-5.84	99.53	111.80
1	K	407	VAL	CA-CB-CG2	5.79	119.59	110.90
1	K	120	ASP	CB-CA-C	-5.76	98.88	110.40
1	K	365	ARG	CG-CD-NE	-5.72	99.78	111.80
1	K	256	ARG	CG-CD-NE	-5.63	99.97	111.80
1	K	365	ARG	CB-CG-CD	5.59	126.14	111.60
1	A	281	GLU	N-CA-C	-5.57	95.95	111.00
1	D	395	ASP	CB-CA-C	5.57	121.54	110.40
1	E	170	PRO	CA-CB-CG	-5.55	93.46	104.00
1	F	218	GLU	CB-CA-C	5.53	121.45	110.40
1	L	256	ARG	CG-CD-NE	5.50	123.35	111.80
1	B	339	ALA	CB-CA-C	5.46	118.30	110.10
1	E	407	VAL	CA-CB-CG2	5.46	119.09	110.90
1	F	403	THR	OG1-CB-CG2	5.45	122.53	110.00
1	D	256	ARG	CG-CD-NE	-5.41	100.43	111.80
1	A	249	THR	CA-CB-OG1	5.40	120.33	109.00
1	G	313	ARG	CB-CG-CD	5.40	125.63	111.60
1	I	256	ARG	CG-CD-NE	5.33	122.98	111.80
1	I	167	GLU	CB-CG-CD	5.29	128.47	114.20
1	H	225	ARG	CG-CD-NE	5.28	122.89	111.80
1	A	57	VAL	CA-CB-CG2	5.27	118.81	110.90
1	A	74	ASP	CB-CG-OD1	5.24	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	407	VAL	CA-CB-CG2	5.24	118.75	110.90
1	D	365	ARG	CG-CD-NE	5.22	122.76	111.80
1	H	249	THR	OG1-CB-CG2	5.22	122.00	110.00
1	G	249	THR	CA-CB-OG1	5.21	119.94	109.00
1	D	88	VAL	CA-CB-CG1	5.20	118.70	110.90
1	I	89	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	G	86	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	I	386	LYS	CA-CB-CG	5.16	124.75	113.40
1	H	339	ALA	CB-CA-C	5.13	117.80	110.10
1	K	358	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	D	251	LYS	CG-CD-CE	-5.11	96.58	111.90
1	D	169	ASP	CB-CG-OD1	5.10	122.89	118.30
1	K	249	THR	CA-CB-OG1	5.10	119.71	109.00
1	C	181	VAL	CA-CB-CG1	5.10	118.55	110.90
1	L	249	THR	CA-CB-OG1	5.09	119.69	109.00
1	C	89	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	365	ARG	CG-CD-NE	5.07	122.45	111.80
1	E	256	ARG	CG-CD-NE	5.05	122.41	111.80
2	R	354	THR	OG1-CB-CG2	5.05	121.63	110.00
2	P	368	ARG	CG-CD-NE	5.04	122.39	111.80
1	L	113	ARG	CB-CG-CD	5.02	124.64	111.60
1	D	244	TYR	CB-CA-C	-5.01	100.37	110.40
1	G	235	VAL	CA-CB-CG2	5.01	118.42	110.90
1	C	362	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	86	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3404	0	3461	93	0
1	B	3404	0	3461	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3394	0	3439	104	0
1	D	3398	0	3450	112	0
1	E	3360	0	3378	116	0
1	F	3404	0	3461	105	0
1	G	3380	0	3411	128	0
1	H	3404	0	3461	115	0
1	I	3404	0	3461	130	0
1	J	3398	0	3450	93	0
1	K	3404	0	3461	117	0
1	L	3384	0	3422	106	0
2	M	670	0	691	23	0
2	N	664	0	680	20	0
2	O	664	0	680	24	0
2	P	664	0	680	27	0
2	Q	670	0	691	20	0
2	R	670	0	691	24	0
2	S	670	0	691	26	0
2	T	670	0	691	31	0
2	U	670	0	691	19	0
2	V	670	0	691	30	0
2	W	670	0	691	28	0
2	X	670	0	691	24	0
3	A	27	0	12	3	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	1	0
3	I	27	0	12	0	0
3	J	27	0	12	0	0
3	K	27	0	12	0	0
3	L	27	0	12	1	0
All	All	49084	0	49719	1529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1529) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:PRO:HB3	1:E:365:ARG:NE	1.47	1.29
1:F:385:THR:HG22	1:F:388:MET:CE	1.73	1.18
1:L:385:THR:HG22	1:L:388:MET:CE	1.74	1.18
1:I:251:LYS:HG2	1:I:369:ILE:HD12	1.25	1.14
1:E:238:PRO:CB	1:E:365:ARG:HE	1.61	1.12
1:C:46:MET:HE1	1:C:73:SER:HB3	1.17	1.10
1:H:46:MET:HE1	1:H:73:SER:HB3	1.22	1.09
1:K:46:MET:HE1	1:K:73:SER:HB3	1.33	1.07
1:C:350:PRO:HB3	1:C:358:ARG:NH2	1.70	1.07
1:B:46:MET:HE1	1:B:73:SER:CB	1.86	1.05
1:B:46:MET:HE1	1:B:73:SER:HB3	1.10	1.05
1:H:46:MET:CE	1:H:73:SER:HB3	1.87	1.04
1:H:339:ALA:O	1:H:340:HIS:CD2	2.12	1.03
1:C:350:PRO:HB3	1:C:358:ARG:HH22	1.18	1.03
1:D:131:PHE:HB3	1:D:136:LYS:NZ	1.73	1.02
1:K:46:MET:CE	1:K:73:SER:HB3	1.89	1.02
1:I:251:LYS:HG2	1:I:369:ILE:CD1	1.90	1.02
1:B:339:ALA:O	1:B:340:HIS:CD2	2.13	1.02
1:G:424:ARG:HG3	1:L:222:LEU:HD21	1.41	0.99
1:J:350:PRO:HB3	1:J:358:ARG:NH2	1.76	0.99
2:U:308:LEU:HD21	2:U:310:GLN:HE21	1.25	0.99
1:D:157:GLY:H	1:D:389:LYS:NZ	1.61	0.98
1:B:46:MET:CE	1:B:73:SER:HB3	1.94	0.97
1:C:113:ARG:HB2	1:C:181:VAL:HG13	1.46	0.97
1:A:113:ARG:HB2	1:A:181:VAL:HG13	1.45	0.97
1:E:92:LEU:HD13	1:E:100:ILE:HD11	1.42	0.96
1:C:46:MET:CE	1:C:73:SER:HB3	1.94	0.96
1:I:332:MET:HB2	1:I:362:ARG:NH1	1.80	0.96
1:I:220:VAL:HG13	1:I:224:LEU:HD22	1.48	0.95
1:A:27:ILE:HD13	1:A:99:VAL:HG22	1.47	0.95
1:A:390:LEU:HD23	1:A:447:VAL:HG12	1.49	0.95
1:E:222:LEU:HD21	1:F:424:ARG:HG3	1.46	0.95
1:B:27:ILE:HD13	1:B:99:VAL:HG22	1.47	0.95
1:G:274:ILE:HG22	1:G:275:MET:CE	1.96	0.94
1:H:440:GLU:O	1:H:442:MET:SD	2.24	0.94
1:J:224:LEU:HB3	1:J:262:THR:HG21	1.49	0.94
1:C:46:MET:HE1	1:C:73:SER:CB	1.96	0.94
1:E:78:SER:HB3	1:E:81:LYS:HE3	1.50	0.94
1:E:427:MET:SD	1:E:430:ILE:HD11	2.08	0.94
1:D:57:VAL:HG21	1:D:102:ILE:CG1	1.98	0.94
1:E:440:GLU:O	1:E:442:MET:SD	2.25	0.93
1:L:377:ARG:HG2	1:L:411:LEU:HD11	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:THR:HG22	1:G:388:MET:CE	1.98	0.93
1:B:426:LYS:HD3	1:B:445:LEU:HD12	1.47	0.93
1:H:220:VAL:HG13	1:H:224:LEU:HD22	1.48	0.93
1:A:339:ALA:O	1:A:340:HIS:ND1	2.02	0.92
2:S:302:LEU:HD12	2:S:307:ARG:HB3	1.47	0.92
1:K:339:ALA:O	1:K:340:HIS:ND1	2.03	0.92
1:F:339:ALA:O	1:F:340:HIS:ND1	2.03	0.92
1:I:339:ALA:O	1:I:340:HIS:ND1	2.02	0.92
1:D:339:ALA:O	1:D:340:HIS:ND1	2.02	0.92
1:G:339:ALA:O	1:G:340:HIS:ND1	2.03	0.92
1:C:111:GLY:HA2	1:C:170:PRO:HD3	1.51	0.92
1:J:339:ALA:O	1:J:340:HIS:ND1	2.03	0.91
1:K:216:ILE:HD13	1:K:254:ILE:HD11	1.52	0.91
1:I:113:ARG:HB2	1:I:181:VAL:CG2	2.00	0.90
1:G:390:LEU:HB3	1:G:394:VAL:HG21	1.51	0.90
1:C:171:SER:HB3	1:C:172:PRO:HD2	1.53	0.90
1:F:385:THR:HG22	1:F:388:MET:HE2	1.54	0.89
1:B:46:MET:CE	1:B:73:SER:CB	2.50	0.89
1:H:46:MET:HE1	1:H:73:SER:CB	2.03	0.89
2:P:318:ILE:HG12	2:P:351:GLU:HA	1.54	0.89
2:Q:318:ILE:CG1	2:Q:351:GLU:HA	2.02	0.89
2:R:318:ILE:HG12	2:R:351:GLU:HA	1.54	0.89
2:S:318:ILE:CG1	2:S:351:GLU:HA	2.03	0.89
2:M:318:ILE:CG1	2:M:351:GLU:HA	2.02	0.88
1:F:403:THR:OG1	1:F:406:HIS:CG	2.25	0.88
2:U:318:ILE:CG1	2:U:351:GLU:HA	2.02	0.88
2:W:318:ILE:HG12	2:W:351:GLU:HA	1.54	0.88
2:W:318:ILE:CG1	2:W:351:GLU:HA	2.04	0.88
2:N:318:ILE:CG1	2:N:351:GLU:HA	2.03	0.88
2:X:318:ILE:HG12	2:X:351:GLU:HA	1.53	0.88
1:A:27:ILE:HD13	1:A:99:VAL:CG2	2.03	0.88
2:T:318:ILE:HG12	2:T:351:GLU:HA	1.55	0.88
2:X:318:ILE:CG1	2:X:351:GLU:HA	2.03	0.87
2:P:318:ILE:CG1	2:P:351:GLU:HA	2.03	0.87
2:R:318:ILE:CG1	2:R:351:GLU:HA	2.03	0.87
1:C:319:GLU:OE1	1:D:320:VAL:CG1	2.23	0.87
1:H:394:VAL:HA	1:H:449:MET:HG2	1.56	0.87
2:T:318:ILE:CG1	2:T:351:GLU:HA	2.04	0.87
1:A:336:LYS:HB2	1:A:338:ARG:NH2	1.88	0.86
1:A:390:LEU:HD23	1:A:447:VAL:CG1	2.05	0.86
1:B:219:MET:HE3	1:B:365:ARG:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HD13	1:B:99:VAL:CG2	2.05	0.86
2:M:302:LEU:HB2	2:M:307:ARG:HB2	1.54	0.86
1:C:350:PRO:CB	1:C:358:ARG:HH22	1.89	0.86
2:T:302:LEU:HB2	2:T:307:ARG:HB2	1.58	0.86
1:G:60:LYS:HD2	1:G:66:GLU:HG2	1.57	0.85
1:J:220:VAL:HG13	1:J:224:LEU:HD12	1.58	0.85
1:B:336:LYS:HB2	1:B:338:ARG:NH2	1.91	0.85
1:G:394:VAL:HA	1:G:449:MET:HG2	1.58	0.85
1:A:113:ARG:HE	1:A:183:HIS:CE1	1.95	0.85
1:G:220:VAL:HG13	1:G:224:LEU:HD12	1.59	0.85
1:K:426:LYS:HD2	1:K:445:LEU:HD12	1.58	0.85
1:D:157:GLY:H	1:D:389:LYS:HZ1	1.22	0.84
1:D:131:PHE:HB3	1:D:136:LYS:HZ2	1.35	0.84
1:J:350:PRO:CB	1:J:358:ARG:NH2	2.41	0.84
1:L:385:THR:HG22	1:L:388:MET:HE2	1.60	0.84
1:L:169:ASP:HB3	1:L:170:PRO:HD3	1.60	0.84
1:C:220:VAL:HG13	1:C:224:LEU:HD12	1.58	0.84
1:F:220:VAL:HG13	1:F:224:LEU:HD12	1.59	0.84
1:E:243:LEU:CD2	1:E:367:VAL:CG1	2.56	0.83
1:C:46:MET:CE	1:C:73:SER:CB	2.54	0.83
1:G:274:ILE:HG22	1:G:275:MET:HE2	1.56	0.83
1:J:313:ARG:HH12	1:J:325:VAL:HG11	1.43	0.83
1:I:332:MET:HB2	1:I:362:ARG:HH12	1.41	0.83
1:E:171:SER:HB3	1:E:172:PRO:HD2	1.61	0.83
1:H:46:MET:CE	1:H:73:SER:CB	2.56	0.83
1:K:169:ASP:HB3	1:K:170:PRO:HD3	1.61	0.83
1:A:220:VAL:HG13	1:A:224:LEU:HD12	1.61	0.83
1:L:220:VAL:HG13	1:L:224:LEU:HD12	1.61	0.83
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.60	0.82
1:D:220:VAL:HG13	1:D:224:LEU:HD12	1.61	0.82
1:K:46:MET:CE	1:K:73:SER:CB	2.57	0.82
1:G:78:SER:HB3	1:G:80:GLU:OE2	1.78	0.82
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.61	0.82
1:A:22:ARG:HG3	1:A:23:PRO:HD2	1.61	0.82
1:C:350:PRO:CB	1:C:358:ARG:NH2	2.41	0.82
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.60	0.82
1:G:169:ASP:HB3	1:G:170:PRO:HD3	1.59	0.82
1:K:220:VAL:HG13	1:K:224:LEU:HD12	1.60	0.82
1:F:169:ASP:HB3	1:F:170:PRO:HD3	1.62	0.82
1:H:169:ASP:HB3	1:H:170:PRO:HD3	1.61	0.82
1:B:220:VAL:HG13	1:B:224:LEU:HD12	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:THR:HG22	1:G:388:MET:HE1	1.60	0.81
1:J:169:ASP:HB3	1:J:170:PRO:HD3	1.61	0.81
1:F:22:ARG:HG3	1:F:23:PRO:HD2	1.60	0.81
1:G:317:HIS:HB2	1:L:322:ARG:HH22	1.43	0.81
1:I:169:ASP:HB3	1:I:170:PRO:HD3	1.61	0.81
1:I:237:PRO:O	1:I:239:ARG:NH1	2.14	0.81
1:E:171:SER:HB3	1:E:172:PRO:CD	2.10	0.80
1:H:224:LEU:HD23	1:H:262:THR:HG21	1.62	0.80
1:H:322:ARG:HH22	1:I:317:HIS:HB2	1.47	0.80
1:G:385:THR:HG22	1:G:388:MET:HE2	1.64	0.80
1:I:332:MET:CB	1:I:362:ARG:NH1	2.45	0.80
1:A:120:ASP:OD2	1:A:190:LYS:HE3	1.82	0.80
1:G:51:LEU:HD11	1:G:104:PRO:HG3	1.62	0.80
1:D:116:VAL:O	1:D:117:LEU:HD12	1.81	0.79
1:K:336:LYS:HB2	1:K:338:ARG:NH2	1.95	0.79
1:A:113:ARG:HE	1:A:183:HIS:HE1	1.30	0.79
1:J:27:ILE:HG23	1:J:81:LYS:HG2	1.64	0.79
1:G:22:ARG:HE	1:G:24:ASN:HB2	1.47	0.78
1:A:281:GLU:O	1:A:282:SER:HB2	1.82	0.78
2:P:311:LYS:NZ	2:P:324:PHE:CE1	2.52	0.78
1:E:243:LEU:CD2	1:E:367:VAL:HG11	2.14	0.78
1:H:313:ARG:NH2	1:H:322:ARG:HG2	1.98	0.78
1:D:126:ILE:HD11	1:D:159:ARG:HD3	1.64	0.78
1:G:222:LEU:HD11	1:H:424:ARG:HG3	1.65	0.78
1:K:113:ARG:HE	1:K:183:HIS:HE1	1.31	0.78
1:A:27:ILE:CD1	1:A:99:VAL:CG2	2.62	0.78
1:C:22:ARG:HG3	1:C:23:PRO:HD2	1.66	0.78
1:J:350:PRO:HB3	1:J:358:ARG:HH21	1.45	0.78
1:K:46:MET:HE1	1:K:73:SER:CB	2.09	0.78
2:M:340:MET:CE	2:M:368:ARG:HH21	1.95	0.78
1:F:282:SER:CB	1:F:324:ILE:HD11	2.14	0.78
2:M:340:MET:HE1	2:M:368:ARG:HH21	1.48	0.78
2:S:302:LEU:HB2	2:S:307:ARG:HB2	1.66	0.78
1:D:300:ILE:HD13	1:D:344:MET:CE	2.13	0.77
1:I:332:MET:HG3	1:I:362:ARG:NH2	2.00	0.77
2:M:318:ILE:HG12	2:M:351:GLU:HA	1.66	0.77
1:D:25:ARG:C	1:D:26:LEU:HD12	2.05	0.77
1:I:357:LEU:HD23	1:I:362:ARG:NH2	1.98	0.77
2:U:318:ILE:HG12	2:U:351:GLU:HA	1.67	0.77
2:O:311:LYS:NZ	2:O:324:PHE:CE1	2.52	0.77
2:Q:318:ILE:HG12	2:Q:351:GLU:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:318:ILE:HG12	2:S:351:GLU:HA	1.67	0.77
1:C:426:LYS:HD2	1:C:445:LEU:HD12	1.67	0.76
1:G:51:LEU:CD1	1:G:104:PRO:HG3	2.14	0.76
1:I:113:ARG:HB2	1:I:181:VAL:HG22	1.66	0.76
1:K:250:GLY:O	1:K:254:ILE:HG23	1.86	0.76
1:L:377:ARG:NH1	1:L:400:ALA:O	2.17	0.76
2:X:295:THR:HA	2:X:314:HIS:HB3	1.67	0.76
1:E:300:ILE:HD13	1:E:344:MET:CE	2.15	0.76
1:J:224:LEU:HB3	1:J:262:THR:CG2	2.16	0.76
1:K:129:ASN:O	1:K:131:PHE:N	2.18	0.76
1:H:313:ARG:HH21	1:H:322:ARG:HG2	1.51	0.76
1:C:114:ILE:HG21	1:C:146:ILE:HD11	1.68	0.76
1:B:27:ILE:CD1	1:B:99:VAL:CG2	2.64	0.76
1:B:46:MET:HE2	1:B:73:SER:HA	1.68	0.76
1:J:300:ILE:HD13	1:J:344:MET:HE1	1.68	0.75
1:E:243:LEU:HD23	1:E:367:VAL:CG1	2.15	0.75
1:D:336:LYS:HB2	1:D:338:ARG:NH2	2.01	0.75
1:G:354:ASP:HB3	1:G:357:LEU:HD23	1.68	0.75
1:B:300:ILE:HD13	1:B:344:MET:HE1	1.68	0.75
1:C:354:ASP:HB3	1:C:357:LEU:HD23	1.68	0.75
1:I:222:LEU:HD23	1:J:420:LEU:HD22	1.69	0.75
1:J:283:GLU:HG3	1:J:324:ILE:HD12	1.68	0.75
1:L:385:THR:HG22	1:L:388:MET:HE1	1.67	0.75
1:G:424:ARG:CG	1:L:222:LEU:HD21	2.16	0.74
1:A:114:ILE:HG21	1:A:146:ILE:HD11	1.70	0.74
2:T:300:ILE:HB	2:T:309:VAL:HG23	1.69	0.74
1:D:131:PHE:HB3	1:D:136:LYS:HZ3	1.51	0.74
1:J:350:PRO:CB	1:J:358:ARG:HH21	1.98	0.74
1:F:417:GLU:HG3	1:F:455:ALA:HB1	1.69	0.74
1:I:114:ILE:HG21	1:I:146:ILE:HD11	1.70	0.74
1:H:283:GLU:HG3	1:H:324:ILE:HD12	1.69	0.74
1:A:373:ASP:O	1:A:377:ARG:HG3	1.87	0.74
1:I:283:GLU:HG3	1:I:324:ILE:HD12	1.69	0.73
1:C:319:GLU:OE1	1:D:320:VAL:HG13	1.88	0.73
1:G:283:GLU:HG3	1:G:324:ILE:HD12	1.69	0.73
1:L:70:ILE:HG13	2:X:343:PHE:CE2	2.22	0.73
1:A:354:ASP:HB3	1:A:357:LEU:HD23	1.69	0.73
1:L:86:ARG:HG2	1:L:89:ARG:NH2	2.03	0.73
1:B:396:LEU:HA	1:B:399:VAL:HG13	1.71	0.73
1:D:70:ILE:HG13	2:P:343:PHE:CE2	2.23	0.73
1:D:319:GLU:OE2	1:E:318:GLY:HA3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:354:THR:HG22	2:X:357:GLU:H	1.53	0.73
1:G:321:GLU:O	1:G:324:ILE:HG22	1.88	0.73
2:N:318:ILE:HG12	2:N:351:GLU:HA	1.68	0.73
1:E:222:LEU:HD21	1:F:424:ARG:CG	2.18	0.73
2:M:308:LEU:HD21	2:M:310:GLN:NE2	2.04	0.73
1:C:319:GLU:CD	1:D:320:VAL:HG13	2.09	0.72
1:I:332:MET:CB	1:I:362:ARG:HH12	2.02	0.72
1:J:440:GLU:OE2	1:J:443:ASN:ND2	2.20	0.72
1:H:114:ILE:HG21	1:H:146:ILE:HD11	1.71	0.72
2:U:308:LEU:HD21	2:U:310:GLN:NE2	2.01	0.72
1:I:321:GLU:O	1:I:324:ILE:HG22	1.88	0.72
1:I:329:LEU:HA	1:I:362:ARG:NH1	2.05	0.72
2:R:354:THR:HG22	2:R:357:GLU:H	1.53	0.72
1:F:114:ILE:HG21	1:F:146:ILE:HD11	1.72	0.72
1:K:86:ARG:HG2	1:K:89:ARG:NH2	2.04	0.72
1:G:402:GLU:OE2	1:G:453:ARG:NH2	2.22	0.72
2:T:354:THR:HG22	2:T:357:GLU:H	1.54	0.72
1:C:129:ASN:HD22	1:C:132:GLU:H	1.36	0.72
2:R:308:LEU:HD21	2:R:310:GLN:NE2	2.05	0.72
1:D:57:VAL:HG21	1:D:102:ILE:HG13	1.72	0.72
1:I:319:GLU:OE1	1:J:320:VAL:CG1	2.38	0.72
1:L:252:THR:HG23	3:L:501:ADP:O3B	1.90	0.72
2:O:308:LEU:HD21	2:O:310:GLN:NE2	2.05	0.72
1:H:322:ARG:NH2	1:I:317:HIS:HB2	2.04	0.71
1:J:114:ILE:HG21	1:J:146:ILE:HD11	1.71	0.71
1:J:321:GLU:O	1:J:324:ILE:HG22	1.89	0.71
1:D:114:ILE:HG21	1:D:146:ILE:HD11	1.70	0.71
1:G:322:ARG:HH22	1:H:317:HIS:HB2	1.55	0.71
1:G:373:ASP:O	1:G:377:ARG:HG3	1.90	0.71
1:I:220:VAL:CG1	1:I:224:LEU:HD22	2.20	0.71
1:J:396:LEU:HA	1:J:399:VAL:HG13	1.73	0.71
1:H:321:GLU:O	1:H:324:ILE:HG22	1.90	0.71
2:P:354:THR:HG22	2:P:357:GLU:H	1.54	0.71
1:J:300:ILE:HD13	1:J:344:MET:CE	2.21	0.71
1:K:114:ILE:HG21	1:K:146:ILE:HD11	1.73	0.71
1:E:426:LYS:HD3	1:E:445:LEU:HD12	1.73	0.71
1:E:114:ILE:HG21	1:E:146:ILE:HD11	1.71	0.71
1:L:114:ILE:HG21	1:L:146:ILE:HD11	1.70	0.71
1:L:227:PRO:HB2	1:L:340:HIS:CE1	2.26	0.71
2:V:308:LEU:HD21	2:V:310:GLN:NE2	2.05	0.71
1:C:46:MET:HE2	1:C:73:SER:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:LYS:HE2	1:D:336:LYS:HA	1.72	0.71
1:G:114:ILE:HG21	1:G:146:ILE:HD11	1.72	0.70
1:L:402:GLU:OE2	1:L:453:ARG:NH2	2.24	0.70
2:V:295:THR:HA	2:V:314:HIS:HB3	1.73	0.70
1:E:92:LEU:HD13	1:E:100:ILE:CD1	2.20	0.70
2:P:295:THR:HA	2:P:314:HIS:HB3	1.73	0.70
1:B:114:ILE:HG21	1:B:146:ILE:HD11	1.72	0.70
1:H:337:GLN:C	1:H:338:ARG:HD3	2.11	0.70
1:J:224:LEU:CB	1:J:262:THR:HG21	2.21	0.70
1:C:170:PRO:HD2	1:C:174:CYS:HB3	1.74	0.70
2:R:295:THR:HA	2:R:314:HIS:HB3	1.74	0.70
1:I:300:ILE:HD13	1:I:344:MET:HE1	1.73	0.70
2:N:295:THR:HA	2:N:314:HIS:HB3	1.74	0.70
1:B:70:ILE:HG13	2:N:343:PHE:CE2	2.27	0.70
2:M:295:THR:HA	2:M:314:HIS:HB3	1.74	0.70
1:A:278:LEU:O	1:A:281:GLU:O	2.09	0.70
1:I:396:LEU:HA	1:I:399:VAL:HG13	1.74	0.69
1:E:243:LEU:HD22	1:E:367:VAL:CG1	2.21	0.69
2:W:354:THR:HG22	2:W:357:GLU:CG	2.21	0.69
1:G:147:ARG:O	1:G:165:VAL:HG11	1.92	0.69
1:L:22:ARG:HG3	1:L:23:PRO:HD2	1.75	0.69
1:D:57:VAL:CG2	1:D:102:ILE:HG13	2.23	0.69
1:J:78:SER:HB2	1:J:81:LYS:HD2	1.75	0.69
2:U:295:THR:HA	2:U:314:HIS:HB3	1.74	0.69
1:I:357:LEU:HA	1:I:362:ARG:HE	1.58	0.69
1:I:402:GLU:OE2	1:I:453:ARG:NH2	2.25	0.69
1:B:274:ILE:HB	1:B:309:ILE:HD11	1.75	0.68
1:D:57:VAL:CG2	1:D:102:ILE:CG1	2.71	0.68
1:C:70:ILE:HG13	2:O:343:PHE:CE2	2.28	0.68
1:H:25:ARG:NH1	1:I:432:LEU:O	2.24	0.68
1:B:140:LEU:O	1:B:141:GLU:HG2	1.93	0.68
1:H:409:ALA:HB2	3:H:501:ADP:H5'1	1.75	0.68
1:I:251:LYS:CG	1:I:369:ILE:HD12	2.16	0.68
1:K:440:GLU:OE1	1:K:440:GLU:HA	1.92	0.68
1:B:437:ILE:HD12	1:B:441:VAL:HG11	1.74	0.68
2:Q:308:LEU:HD21	2:Q:310:GLN:NE2	2.08	0.68
1:E:287:ARG:HE	1:E:327:GLN:HE22	1.41	0.68
1:H:46:MET:HE2	1:H:73:SER:HA	1.75	0.68
1:H:220:VAL:CG1	1:H:224:LEU:HD22	2.21	0.68
1:H:337:GLN:O	1:H:338:ARG:HD3	1.94	0.68
2:O:295:THR:HA	2:O:314:HIS:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:314:HIS:HD1	2:T:315:SER:H	1.42	0.68
1:F:402:GLU:OE2	1:F:453:ARG:NH2	2.21	0.68
1:G:283:GLU:HA	1:G:327:GLN:HE22	1.59	0.68
1:B:219:MET:CE	1:B:365:ARG:HB3	2.23	0.68
2:O:354:THR:HG22	2:O:357:GLU:CG	2.23	0.68
1:K:319:GLU:OE2	1:L:318:GLY:HA3	1.93	0.67
2:S:295:THR:HA	2:S:314:HIS:HB3	1.74	0.67
1:A:70:ILE:HG13	2:M:343:PHE:CE2	2.30	0.67
1:B:300:ILE:HD13	1:B:344:MET:CE	2.24	0.67
1:B:339:ALA:C	1:B:340:HIS:CG	2.68	0.67
1:G:24:ASN:N	1:G:24:ASN:HD22	1.92	0.67
1:F:70:ILE:HG13	2:R:343:PHE:CE2	2.30	0.67
1:A:50:GLN:CG	1:A:50:GLN:O	2.43	0.67
1:D:422:ALA:O	1:D:425:LYS:HG2	1.93	0.67
1:E:28:VAL:HG21	1:E:94:VAL:HG11	1.77	0.67
1:F:282:SER:HB2	1:F:324:ILE:HD11	1.75	0.67
2:W:295:THR:HA	2:W:314:HIS:HB3	1.77	0.67
2:N:318:ILE:CD1	2:N:351:GLU:HA	2.25	0.66
2:O:294:PRO:O	2:O:314:HIS:HB2	1.95	0.66
1:C:224:LEU:HD13	1:C:262:THR:HG21	1.76	0.66
1:G:274:ILE:HG22	1:G:275:MET:HE1	1.76	0.66
1:I:332:MET:HG3	1:I:362:ARG:HH22	1.58	0.66
2:R:318:ILE:CD1	2:R:351:GLU:HA	2.25	0.66
2:X:308:LEU:HD21	2:X:310:GLN:NE2	2.09	0.66
1:E:274:ILE:HB	1:E:309:ILE:HD11	1.78	0.66
1:I:362:ARG:HB3	1:I:362:ARG:CZ	2.25	0.66
2:Q:318:ILE:CD1	2:Q:351:GLU:HA	2.25	0.66
1:E:26:LEU:HD21	1:E:45:LYS:HE3	1.76	0.66
1:E:325:VAL:O	1:E:329:LEU:HD13	1.95	0.66
2:S:318:ILE:CD1	2:S:351:GLU:HA	2.24	0.66
2:X:318:ILE:CD1	2:X:351:GLU:HA	2.25	0.66
1:A:27:ILE:CD1	1:A:99:VAL:HG22	2.24	0.66
1:D:336:LYS:CG	1:D:338:ARG:HH22	2.08	0.66
1:L:186:GLY:O	1:L:187:GLU:HB2	1.93	0.66
2:P:294:PRO:O	2:P:314:HIS:HB2	1.96	0.66
2:R:354:THR:HG22	2:R:357:GLU:HG3	1.78	0.66
2:U:318:ILE:CD1	2:U:351:GLU:HA	2.26	0.66
1:F:282:SER:HB3	1:F:324:ILE:HD11	1.77	0.66
1:G:222:LEU:HD11	1:H:424:ARG:CG	2.26	0.66
2:Q:295:THR:HA	2:Q:314:HIS:HB3	1.75	0.66
1:A:252:THR:HG22	3:A:501:ADP:PA	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:294:PRO:O	2:M:314:HIS:HB2	1.96	0.66
1:C:171:SER:CB	1:C:172:PRO:HD2	2.26	0.66
2:P:318:ILE:CD1	2:P:351:GLU:HA	2.26	0.66
2:V:354:THR:HG22	2:V:357:GLU:CG	2.25	0.66
2:W:286:MET:SD	2:W:287:ILE:HG22	2.35	0.66
2:X:289:ILE:HD13	2:X:312:PHE:HD2	1.61	0.66
1:B:396:LEU:HA	1:B:399:VAL:CG1	2.26	0.66
1:D:157:GLY:N	1:D:389:LYS:HZ1	1.94	0.66
1:F:385:THR:HG22	1:F:388:MET:HE1	1.72	0.66
1:J:43:GLN:HB3	1:J:44:PRO:HD3	1.78	0.66
2:Q:294:PRO:O	2:Q:314:HIS:HB2	1.95	0.66
2:P:354:THR:HG22	2:P:357:GLU:HG3	1.77	0.66
2:S:294:PRO:O	2:S:314:HIS:HB2	1.95	0.66
2:W:321:ILE:HD11	2:W:355:LEU:HD21	1.78	0.66
1:I:332:MET:CG	1:I:362:ARG:HH12	2.09	0.65
1:A:335:LEU:HD12	1:A:338:ARG:HG2	1.79	0.65
1:I:300:ILE:HD13	1:I:344:MET:CE	2.26	0.65
2:M:318:ILE:CD1	2:M:351:GLU:HA	2.26	0.65
2:N:318:ILE:HD11	2:N:351:GLU:HA	1.78	0.65
2:R:294:PRO:O	2:R:314:HIS:HB2	1.96	0.65
2:U:321:ILE:HD11	2:U:355:LEU:HD21	1.79	0.65
1:K:140:LEU:O	1:K:141:GLU:HG3	1.97	0.65
2:T:354:THR:HG22	2:T:357:GLU:HG3	1.78	0.65
1:D:431:ASP:HA	1:D:436:THR:HG22	1.78	0.65
1:G:224:LEU:HD13	1:G:262:THR:HG21	1.78	0.65
1:G:431:ASP:HA	1:G:436:THR:HG22	1.79	0.65
2:W:318:ILE:CD1	2:W:351:GLU:HA	2.26	0.65
2:X:354:THR:HG22	2:X:357:GLU:HG3	1.78	0.65
1:K:113:ARG:HE	1:K:183:HIS:CE1	2.15	0.65
2:S:318:ILE:HD11	2:S:351:GLU:HA	1.78	0.65
2:T:318:ILE:CD1	2:T:351:GLU:HA	2.26	0.65
2:V:294:PRO:O	2:V:314:HIS:HB2	1.96	0.65
1:K:115:HIS:HB3	1:K:166:VAL:HG23	1.78	0.65
1:E:440:GLU:C	1:E:442:MET:H	2.00	0.65
1:G:49:LEU:HB3	1:G:51:LEU:HD22	1.78	0.65
1:J:396:LEU:HA	1:J:399:VAL:CG1	2.27	0.65
1:J:431:ASP:HA	1:J:436:THR:HG22	1.77	0.65
2:N:294:PRO:O	2:N:314:HIS:HB2	1.97	0.65
1:F:431:ASP:HA	1:F:436:THR:HG22	1.79	0.65
1:G:388:MET:HE3	1:G:390:LEU:HD21	1.78	0.65
1:A:322:ARG:HH22	1:B:317:HIS:HB2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:249:THR:HG22	1:I:251:LYS:NZ	2.12	0.65
1:C:440:GLU:C	1:C:442:MET:H	2.01	0.64
2:W:294:PRO:O	2:W:314:HIS:HB2	1.96	0.64
1:B:43:GLN:HB3	1:B:44:PRO:HD3	1.79	0.64
1:K:350:PRO:HB3	1:K:358:ARG:HH12	1.62	0.64
2:R:321:ILE:HD11	2:R:355:LEU:HD21	1.79	0.64
1:B:27:ILE:CD1	1:B:99:VAL:HG22	2.23	0.64
2:S:321:ILE:HD11	2:S:355:LEU:HD21	1.78	0.64
2:U:294:PRO:O	2:U:314:HIS:HB2	1.98	0.64
1:A:27:ILE:CD1	1:A:99:VAL:HG23	2.27	0.64
1:C:220:VAL:CG1	1:C:224:LEU:HD12	2.28	0.64
1:G:43:GLN:HB3	1:G:44:PRO:HD3	1.78	0.64
1:G:220:VAL:CG1	1:G:224:LEU:HD12	2.27	0.64
1:G:317:HIS:HB2	1:L:322:ARG:NH2	2.13	0.64
2:P:321:ILE:HD11	2:P:355:LEU:HD21	1.78	0.64
1:H:431:ASP:HA	1:H:436:THR:HG22	1.80	0.64
1:L:220:VAL:CG1	1:L:224:LEU:HD12	2.28	0.64
1:G:337:GLN:O	1:G:340:HIS:N	2.31	0.64
2:Q:318:ILE:HD11	2:Q:351:GLU:HA	1.79	0.64
1:A:339:ALA:C	1:A:340:HIS:ND1	2.51	0.64
1:B:339:ALA:C	1:B:340:HIS:CD2	2.70	0.64
1:C:43:GLN:HB3	1:C:44:PRO:HD3	1.79	0.64
1:I:357:LEU:HD23	1:I:362:ARG:HH21	1.63	0.64
1:L:440:GLU:C	1:L:442:MET:H	2.01	0.64
1:A:390:LEU:CD2	1:A:447:VAL:CG1	2.76	0.64
1:J:114:ILE:HG22	1:J:168:THR:HG22	1.80	0.64
2:U:318:ILE:HD11	2:U:351:GLU:HA	1.80	0.64
1:E:155:ARG:CZ	1:E:386:LYS:HE2	2.28	0.63
1:F:385:THR:CG2	1:F:388:MET:CE	2.66	0.63
1:B:249:THR:HG22	1:B:251:LYS:NZ	2.13	0.63
1:C:249:THR:HG22	1:C:251:LYS:NZ	2.13	0.63
1:F:339:ALA:C	1:F:340:HIS:ND1	2.52	0.63
1:L:63:LYS:O	1:L:64:ARG:HG2	1.98	0.63
1:B:287:ARG:HG3	1:B:327:GLN:HE22	1.64	0.63
1:F:287:ARG:HE	1:F:327:GLN:HE22	1.43	0.63
1:H:43:GLN:HB3	1:H:44:PRO:HD3	1.79	0.63
1:J:339:ALA:C	1:J:340:HIS:ND1	2.51	0.63
1:K:129:ASN:O	1:K:129:ASN:OD1	2.15	0.63
1:B:283:GLU:HA	1:B:327:GLN:OE1	1.98	0.63
1:D:440:GLU:C	1:D:442:MET:H	2.02	0.63
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:249:THR:HG22	1:H:251:LYS:NZ	2.13	0.63
1:B:287:ARG:HG3	1:B:327:GLN:NE2	2.13	0.63
1:D:43:GLN:HB3	1:D:44:PRO:HD3	1.80	0.63
1:F:220:VAL:CG1	1:F:224:LEU:HD12	2.28	0.63
1:G:385:THR:CG2	1:G:388:MET:HE2	2.29	0.63
1:I:114:ILE:HG22	1:I:168:THR:HG22	1.80	0.63
1:I:339:ALA:C	1:I:340:HIS:ND1	2.52	0.63
1:K:335:LEU:HD12	1:K:338:ARG:HG2	1.80	0.63
2:U:340:MET:HE1	2:U:368:ARG:NH1	2.13	0.63
1:D:339:ALA:C	1:D:340:HIS:ND1	2.52	0.63
1:E:150:ASP:HB2	1:E:165:VAL:CG1	2.29	0.63
1:H:339:ALA:C	1:H:340:HIS:CG	2.71	0.63
1:A:252:THR:HG22	3:A:501:ADP:O1A	1.99	0.63
1:A:349:ARG:HG3	1:A:350:PRO:HD2	1.80	0.63
1:F:114:ILE:HG22	1:F:168:THR:HG22	1.81	0.63
1:I:26:LEU:HD11	1:I:45:LYS:HE2	1.81	0.63
1:J:335:LEU:HA	1:J:338:ARG:HG3	1.79	0.63
1:K:235:VAL:HG23	1:L:416:SER:OG	1.99	0.63
1:L:385:THR:CG2	1:L:388:MET:CE	2.66	0.63
2:M:318:ILE:HD11	2:M:351:GLU:HA	1.81	0.63
1:H:114:ILE:HG22	1:H:168:THR:HG22	1.81	0.62
1:I:396:LEU:HA	1:I:399:VAL:CG1	2.29	0.62
2:Q:321:ILE:HD11	2:Q:355:LEU:HD21	1.80	0.62
2:U:308:LEU:CD2	2:U:310:GLN:HE21	2.08	0.62
2:V:321:ILE:HD11	2:V:355:LEU:HD21	1.81	0.62
1:F:43:GLN:HB3	1:F:44:PRO:HD3	1.80	0.62
1:J:440:GLU:C	1:J:442:MET:H	2.02	0.62
1:K:220:VAL:CG1	1:K:224:LEU:HD12	2.29	0.62
1:L:35:ASP:HB3	1:L:38:VAL:HG13	1.80	0.62
1:B:440:GLU:C	1:B:442:MET:H	2.02	0.62
1:D:220:VAL:CG1	1:D:224:LEU:HD12	2.30	0.62
1:F:440:GLU:C	1:F:442:MET:H	2.02	0.62
1:A:440:GLU:C	1:A:442:MET:H	2.03	0.62
1:D:114:ILE:HG22	1:D:168:THR:HG22	1.82	0.62
1:G:440:GLU:C	1:G:442:MET:H	2.03	0.62
1:H:339:ALA:C	1:H:340:HIS:CD2	2.72	0.62
1:K:339:ALA:C	1:K:340:HIS:ND1	2.53	0.62
2:T:302:LEU:HB3	2:T:304:ASP:OD1	2.00	0.62
1:E:427:MET:HA	1:E:430:ILE:HG12	1.81	0.62
1:G:339:ALA:C	1:G:340:HIS:ND1	2.53	0.62
2:O:321:ILE:HD11	2:O:355:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HG22	1:A:168:THR:HG22	1.82	0.62
1:B:335:LEU:HD12	1:B:338:ARG:HG2	1.81	0.62
1:B:114:ILE:HG22	1:B:168:THR:HG22	1.82	0.62
1:H:440:GLU:C	1:H:442:MET:H	2.02	0.62
1:J:220:VAL:CG1	1:J:224:LEU:HD12	2.28	0.62
1:K:53:ARG:HH12	1:K:73:SER:H	1.48	0.62
1:L:385:THR:HG22	1:L:388:MET:HE3	1.78	0.62
2:X:289:ILE:HD13	2:X:312:PHE:CD2	2.34	0.62
1:I:440:GLU:C	1:I:442:MET:H	2.03	0.62
1:K:440:GLU:C	1:K:442:MET:H	2.02	0.62
2:N:321:ILE:HD11	2:N:355:LEU:HD21	1.80	0.62
1:E:114:ILE:HG22	1:E:168:THR:HG22	1.81	0.62
1:E:421:GLN:HE21	1:E:421:GLN:HA	1.64	0.62
1:J:350:PRO:CA	1:J:358:ARG:HH21	2.13	0.61
1:B:46:MET:CE	1:B:73:SER:CA	2.78	0.61
1:J:27:ILE:HG23	1:J:81:LYS:CG	2.30	0.61
1:K:114:ILE:HG22	1:K:168:THR:HG22	1.83	0.61
1:C:230:PHE:HB2	1:C:340:HIS:NE2	2.15	0.61
1:F:35:ASP:HB3	1:F:38:VAL:HG13	1.83	0.61
1:K:377:ARG:HG2	1:K:411:LEU:HD11	1.82	0.61
1:L:426:LYS:HD2	1:L:445:LEU:HD23	1.82	0.61
1:C:220:VAL:HG22	1:C:342:ILE:HD13	1.83	0.61
1:H:239:ARG:NH1	1:H:335:LEU:O	2.33	0.61
1:L:222:LEU:HB2	1:L:223:PRO:HD3	1.82	0.61
1:D:57:VAL:HG21	1:D:102:ILE:HG12	1.78	0.61
1:C:377:ARG:HG2	1:C:411:LEU:HD11	1.82	0.61
1:I:43:GLN:HB3	1:I:44:PRO:HD3	1.81	0.61
1:J:70:ILE:HG13	2:V:343:PHE:CE2	2.34	0.61
2:S:341:THR:HG22	2:S:346:LYS:HB3	1.83	0.61
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.83	0.61
1:C:350:PRO:CA	1:C:358:ARG:NH2	2.64	0.61
1:F:377:ARG:HE	1:F:403:THR:HG23	1.66	0.61
1:A:220:VAL:CG1	1:A:224:LEU:HD12	2.29	0.60
1:E:377:ARG:HG2	1:E:411:LEU:HD11	1.83	0.60
1:J:377:ARG:HG2	1:J:411:LEU:HD11	1.82	0.60
1:L:43:GLN:HB3	1:L:44:PRO:HD3	1.81	0.60
2:W:354:THR:HG22	2:W:357:GLU:HG3	1.82	0.60
1:H:377:ARG:HG2	1:H:411:LEU:HD11	1.83	0.60
1:I:86:ARG:HH21	1:I:204:ASP:CG	2.04	0.60
1:I:287:ARG:HE	1:I:327:GLN:HE22	1.47	0.60
1:D:377:ARG:HG2	1:D:411:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:ILE:HG13	2:T:343:PHE:CE2	2.36	0.60
1:K:243:LEU:N	1:K:243:LEU:HD12	2.17	0.60
1:L:287:ARG:HE	1:L:327:GLN:HE22	1.47	0.60
1:A:27:ILE:HG12	1:B:432:LEU:HD13	1.83	0.60
1:A:35:ASP:HB3	1:A:38:VAL:HG13	1.82	0.60
1:F:385:THR:HG22	1:F:388:MET:HE3	1.76	0.60
1:A:350:PRO:HB3	1:A:358:ARG:HH12	1.67	0.60
1:F:377:ARG:HG2	1:F:411:LEU:HD11	1.84	0.60
1:E:222:LEU:HB2	1:E:223:PRO:HD3	1.83	0.60
1:F:249:THR:HG22	1:F:369:ILE:HG22	1.84	0.60
1:G:114:ILE:HG22	1:G:168:THR:HG22	1.82	0.60
1:G:424:ARG:HH11	1:L:222:LEU:CD2	2.15	0.60
1:A:281:GLU:O	1:A:282:SER:CB	2.48	0.60
1:H:52:PHE:O	1:H:55:ASP:HB2	2.02	0.60
1:K:108:VAL:HG12	1:K:173:TYR:CE1	2.37	0.60
1:A:339:ALA:C	1:A:340:HIS:CG	2.76	0.59
1:D:339:ALA:C	1:D:340:HIS:CG	2.76	0.59
1:F:52:PHE:O	1:F:55:ASP:HB2	2.03	0.59
1:F:403:THR:OG1	1:F:406:HIS:CD2	2.55	0.59
1:I:332:MET:HG3	1:I:362:ARG:CZ	2.31	0.59
1:C:239:ARG:NH1	1:C:336:LYS:HA	2.17	0.59
1:H:22:ARG:HG2	1:H:23:PRO:HD2	1.83	0.59
1:J:339:ALA:C	1:J:340:HIS:CG	2.75	0.59
2:Q:286:MET:HG2	2:Q:287:ILE:H	1.67	0.59
1:G:339:ALA:C	1:G:340:HIS:CG	2.76	0.59
1:G:385:THR:CG2	1:G:388:MET:CE	2.77	0.59
2:V:302:LEU:HB2	2:V:307:ARG:HB2	1.84	0.59
1:A:50:GLN:O	1:A:50:GLN:HG3	2.02	0.59
1:B:27:ILE:CD1	1:B:99:VAL:HG23	2.31	0.59
1:F:335:LEU:HD23	1:F:338:ARG:HG2	1.84	0.59
1:D:52:PHE:O	1:D:55:ASP:HB2	2.02	0.59
1:I:377:ARG:HG2	1:I:411:LEU:HD11	1.84	0.59
1:B:377:ARG:HG2	1:B:411:LEU:HD11	1.84	0.59
1:G:52:PHE:O	1:G:55:ASP:HB2	2.02	0.59
1:K:339:ALA:C	1:K:340:HIS:CG	2.76	0.59
1:F:239:ARG:NH2	1:F:336:LYS:HA	2.17	0.59
2:X:318:ILE:HD11	2:X:351:GLU:HA	1.84	0.59
1:B:220:VAL:CG1	1:B:224:LEU:HD12	2.30	0.59
1:E:322:ARG:HH22	1:F:317:HIS:HB2	1.68	0.59
1:K:32:ILE:HD12	1:K:33:ASN:N	2.18	0.59
2:R:318:ILE:HD11	2:R:351:GLU:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:140:LEU:HG	1:K:141:GLU:HG2	1.83	0.59
2:S:361:LEU:HD12	2:S:361:LEU:H	1.68	0.59
1:C:32:ILE:HD12	1:C:33:ASN:N	2.18	0.59
1:D:389:LYS:HE2	1:D:443:ASN:CG	2.24	0.59
1:C:113:ARG:HD3	1:C:183:HIS:CE1	2.37	0.58
1:E:243:LEU:HD22	1:E:367:VAL:HG11	1.81	0.58
1:G:70:ILE:HG13	2:S:343:PHE:CE2	2.38	0.58
1:G:393:ASP:O	1:G:449:MET:CG	2.51	0.58
1:I:52:PHE:O	1:I:55:ASP:HB2	2.01	0.58
1:I:249:THR:HG22	1:I:251:LYS:HZ2	1.67	0.58
1:L:52:PHE:O	1:L:55:ASP:HB2	2.03	0.58
1:D:389:LYS:CD	1:D:443:ASN:O	2.51	0.58
1:F:339:ALA:C	1:F:340:HIS:CG	2.76	0.58
1:L:32:ILE:HD12	1:L:33:ASN:N	2.19	0.58
1:B:350:PRO:HB3	1:B:358:ARG:HH12	1.68	0.58
1:H:32:ILE:HD12	1:H:33:ASN:N	2.17	0.58
1:J:52:PHE:O	1:J:55:ASP:HB2	2.03	0.58
1:A:336:LYS:HB2	1:A:338:ARG:HH22	1.67	0.58
1:B:52:PHE:O	1:B:55:ASP:HB2	2.02	0.58
1:C:52:PHE:O	1:C:55:ASP:HB2	2.02	0.58
1:H:339:ALA:O	1:H:340:HIS:CG	2.57	0.58
1:K:52:PHE:O	1:K:55:ASP:HB2	2.02	0.58
1:K:70:ILE:HG13	2:W:343:PHE:CE2	2.38	0.58
2:T:318:ILE:HD11	2:T:351:GLU:HA	1.84	0.58
1:H:222:LEU:HB2	1:H:223:PRO:HD3	1.86	0.58
1:I:339:ALA:C	1:I:340:HIS:CG	2.76	0.58
2:R:318:ILE:HG12	2:R:351:GLU:CA	2.32	0.58
1:G:222:LEU:HB2	1:G:223:PRO:HD3	1.85	0.58
1:D:157:GLY:N	1:D:389:LYS:NZ	2.44	0.58
1:F:249:THR:CG2	1:F:369:ILE:HG22	2.34	0.58
1:G:22:ARG:NE	1:G:24:ASN:HB2	2.16	0.58
2:O:354:THR:HG22	2:O:357:GLU:HG3	1.85	0.58
2:R:302:LEU:HD12	2:R:307:ARG:HB3	1.86	0.58
2:W:318:ILE:HD11	2:W:351:GLU:HA	1.84	0.58
1:A:339:ALA:O	1:A:340:HIS:CG	2.57	0.58
1:G:126:ILE:HD11	1:G:159:ARG:HG2	1.85	0.58
1:K:43:GLN:HB3	1:K:44:PRO:HD3	1.85	0.58
1:L:22:ARG:HB3	1:L:25:ARG:HH21	1.68	0.58
1:D:335:LEU:HD12	1:D:338:ARG:HG2	1.84	0.58
1:G:385:THR:CB	1:G:388:MET:HE2	2.34	0.58
1:K:80:GLU:HG2	1:L:432:LEU:CD1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:HIS:CE1	1:F:427:MET:HE1	2.39	0.57
1:F:339:ALA:O	1:F:340:HIS:CG	2.57	0.57
1:I:339:ALA:O	1:I:340:HIS:CG	2.57	0.57
2:U:302:LEU:HB2	2:U:307:ARG:HB2	1.86	0.57
2:W:287:ILE:HD11	2:W:316:HIS:NE2	2.19	0.57
1:A:86:ARG:HG2	1:A:89:ARG:NH2	2.19	0.57
2:P:318:ILE:HD11	2:P:351:GLU:HA	1.85	0.57
1:B:322:ARG:HH22	1:C:317:HIS:HB2	1.69	0.57
2:X:302:LEU:HD12	2:X:307:ARG:HB3	1.86	0.57
1:G:339:ALA:O	1:G:340:HIS:CG	2.58	0.57
1:C:46:MET:CE	1:C:73:SER:CA	2.82	0.57
1:C:378:LEU:O	1:C:382:GLN:HG2	2.05	0.57
1:H:336:LYS:O	1:H:338:ARG:HD2	2.05	0.57
1:J:335:LEU:HD23	1:J:338:ARG:HG3	1.87	0.57
1:K:222:LEU:HB2	1:K:223:PRO:HD3	1.86	0.57
1:K:339:ALA:O	1:K:340:HIS:CG	2.57	0.57
2:O:311:LYS:NZ	2:O:324:PHE:HE1	2.00	0.57
2:Q:302:LEU:HB2	2:Q:307:ARG:HB2	1.84	0.57
2:R:302:LEU:HB2	2:R:307:ARG:HB2	1.86	0.57
1:D:339:ALA:O	1:D:340:HIS:CG	2.57	0.57
1:H:22:ARG:HB2	1:H:25:ARG:NH2	2.20	0.57
1:J:113:ARG:NH1	1:J:115:HIS:HB2	2.20	0.57
2:R:294:PRO:O	2:R:314:HIS:CB	2.52	0.57
2:W:302:LEU:HB2	2:W:307:ARG:HB2	1.87	0.57
1:H:393:ASP:O	1:H:449:MET:CG	2.53	0.57
1:I:335:LEU:HD23	1:I:338:ARG:HG2	1.86	0.57
1:D:129:ASN:OD1	1:D:132:GLU:HG2	2.04	0.57
1:E:80:GLU:HG2	1:E:81:LYS:HG3	1.87	0.57
1:E:378:LEU:O	1:E:382:GLN:HG2	2.05	0.57
1:J:339:ALA:O	1:J:340:HIS:CG	2.57	0.57
2:W:311:LYS:HD3	2:W:324:PHE:CE1	2.40	0.57
1:C:249:THR:HG22	1:C:251:LYS:HZ2	1.69	0.56
1:G:222:LEU:HD12	1:G:222:LEU:H	1.70	0.56
1:I:332:MET:CG	1:I:362:ARG:NH1	2.67	0.56
1:C:46:MET:HE2	1:C:73:SER:CA	2.35	0.56
1:C:319:GLU:OE1	1:D:320:VAL:HG12	2.03	0.56
1:H:359:ARG:HG3	1:H:360:PHE:H	1.70	0.56
1:J:222:LEU:HB2	1:J:223:PRO:HD3	1.87	0.56
1:K:282:SER:CB	1:K:324:ILE:HD11	2.35	0.56
2:N:311:LYS:HD3	2:N:324:PHE:CE1	2.40	0.56
2:U:311:LYS:HD3	2:U:324:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HB2	1:A:223:PRO:HD3	1.87	0.56
1:B:222:LEU:HB2	1:B:223:PRO:HD3	1.87	0.56
1:F:210:ARG:NH2	1:F:211:LYS:HE3	2.20	0.56
1:G:322:ARG:NH2	1:H:317:HIS:HB2	2.20	0.56
2:M:311:LYS:HD3	2:M:324:PHE:CE1	2.40	0.56
2:Q:294:PRO:O	2:Q:314:HIS:CB	2.53	0.56
2:W:294:PRO:O	2:W:314:HIS:CB	2.53	0.56
1:D:27:ILE:HG13	1:E:432:LEU:HD13	1.87	0.56
1:E:108:VAL:HG12	1:E:173:TYR:CE1	2.41	0.56
1:F:222:LEU:HB2	1:F:223:PRO:HD3	1.88	0.56
1:F:239:ARG:CZ	1:F:335:LEU:O	2.53	0.56
1:H:46:MET:CE	1:H:73:SER:CA	2.83	0.56
2:T:318:ILE:HG12	2:T:351:GLU:CA	2.34	0.56
2:X:302:LEU:HB2	2:X:307:ARG:HB2	1.86	0.56
1:B:339:ALA:O	1:B:340:HIS:CG	2.57	0.56
1:G:359:ARG:HG3	1:G:360:PHE:H	1.71	0.56
1:I:335:LEU:CD2	1:I:338:ARG:HG2	2.36	0.56
2:M:304:ASP:O	2:M:307:ARG:HG2	2.05	0.56
2:S:294:PRO:O	2:S:314:HIS:CB	2.53	0.56
1:B:322:ARG:NH2	1:C:317:HIS:HB2	2.21	0.56
1:C:113:ARG:HB2	1:C:181:VAL:CG1	2.31	0.56
1:H:378:LEU:O	1:H:382:GLN:HG2	2.06	0.56
2:O:294:PRO:O	2:O:314:HIS:CB	2.53	0.56
2:V:311:LYS:HD3	2:V:324:PHE:CE1	2.41	0.56
1:I:357:LEU:CD2	1:I:362:ARG:NH2	2.67	0.56
1:L:312:LYS:HB3	1:L:315:LYS:HG3	1.87	0.56
1:A:113:ARG:NE	1:A:183:HIS:HE1	2.00	0.56
1:E:243:LEU:HD23	1:E:367:VAL:HG12	1.88	0.56
1:I:402:GLU:CD	1:I:453:ARG:HH22	2.08	0.56
1:L:356:ALA:O	1:L:359:ARG:HB2	2.06	0.56
1:F:417:GLU:HG3	1:F:455:ALA:CB	2.34	0.56
1:G:71:VAL:O	1:G:72:LEU:HD12	2.06	0.56
1:E:328:LEU:HD13	1:E:357:LEU:HD21	1.86	0.56
1:J:437:ILE:HD13	1:J:441:VAL:HG11	1.88	0.56
2:M:294:PRO:O	2:M:314:HIS:CB	2.53	0.56
2:O:354:THR:CG2	2:O:357:GLU:H	2.19	0.56
1:C:279:ALA:HB1	1:C:320:VAL:HG21	1.87	0.55
1:D:126:ILE:HG12	1:D:159:ARG:NH1	2.20	0.55
1:D:244:TYR:CE1	1:D:350:PRO:HA	2.41	0.55
1:E:43:GLN:HB3	1:E:44:PRO:HD3	1.86	0.55
2:N:290:ASP:N	2:N:314:HIS:HE1	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:294:PRO:O	2:P:314:HIS:CB	2.54	0.55
2:S:287:ILE:HD11	2:S:316:HIS:NE2	2.21	0.55
1:C:354:ASP:HB3	1:C:357:LEU:CD2	2.37	0.55
1:K:82:ILE:HG21	1:K:100:ILE:HD11	1.88	0.55
2:V:289:ILE:O	2:V:291:GLU:OE1	2.24	0.55
1:D:71:VAL:O	1:D:72:LEU:HD12	2.07	0.55
1:L:71:VAL:O	1:L:72:LEU:HD12	2.06	0.55
1:D:222:LEU:HB2	1:D:223:PRO:HD3	1.89	0.55
1:D:242:LEU:HD13	1:D:244:TYR:OH	2.06	0.55
1:A:52:PHE:O	1:A:55:ASP:HB2	2.06	0.55
2:Q:302:LEU:HD12	2:Q:307:ARG:HB3	1.87	0.55
2:U:294:PRO:O	2:U:314:HIS:CB	2.53	0.55
1:C:129:ASN:O	1:C:131:PHE:N	2.38	0.55
1:D:157:GLY:H	1:D:389:LYS:HZ3	1.54	0.55
1:H:437:ILE:HD12	1:H:441:VAL:HG11	1.88	0.55
1:K:131:PHE:HE1	1:K:182:ILE:HG23	1.72	0.55
1:L:82:ILE:HG21	1:L:100:ILE:HD11	1.89	0.55
2:P:311:LYS:NZ	2:P:324:PHE:HE1	2.00	0.55
2:V:302:LEU:HD12	2:V:307:ARG:HB3	1.87	0.55
2:W:302:LEU:HD12	2:W:307:ARG:HB3	1.87	0.55
1:G:354:ASP:HB3	1:G:357:LEU:CD2	2.35	0.55
1:I:357:LEU:CD2	1:I:362:ARG:HH21	2.19	0.55
1:K:115:HIS:O	1:K:166:VAL:HG22	2.07	0.55
2:V:287:ILE:HD12	2:V:287:ILE:H	1.72	0.55
2:X:289:ILE:CD1	2:X:312:PHE:CD2	2.90	0.55
1:A:322:ARG:NH2	1:B:317:HIS:HB2	2.21	0.55
1:F:336:LYS:HD2	1:F:337:GLN:HG3	1.89	0.55
1:H:239:ARG:NH2	1:H:335:LEU:O	2.40	0.55
2:P:318:ILE:HG12	2:P:351:GLU:CA	2.33	0.55
2:T:300:ILE:HB	2:T:309:VAL:CG2	2.35	0.55
2:V:294:PRO:O	2:V:314:HIS:CB	2.54	0.55
2:X:318:ILE:HG12	2:X:351:GLU:CA	2.32	0.55
1:H:239:ARG:CZ	1:H:335:LEU:O	2.55	0.54
2:V:354:THR:CG2	2:V:357:GLU:H	2.20	0.54
1:E:329:LEU:N	1:E:329:LEU:CD1	2.70	0.54
2:X:311:LYS:HD3	2:X:324:PHE:CE1	2.42	0.54
1:A:78:SER:HB3	1:A:80:GLU:OE2	2.07	0.54
1:E:150:ASP:H	1:E:165:VAL:HG13	1.72	0.54
1:I:63:LYS:HE2	1:I:63:LYS:H	1.73	0.54
2:X:294:PRO:O	2:X:314:HIS:HB2	2.07	0.54
1:B:82:ILE:HG21	1:B:100:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LYS:N	1:C:169:ASP:O	2.38	0.54
1:H:71:VAL:O	1:H:72:LEU:HD12	2.08	0.54
1:H:359:ARG:HD3	1:I:247:PRO:HB3	1.89	0.54
1:I:82:ILE:HG21	1:I:100:ILE:HD11	1.90	0.54
1:J:71:VAL:O	1:J:72:LEU:HD12	2.07	0.54
1:J:82:ILE:HG21	1:J:100:ILE:HD11	1.90	0.54
2:N:294:PRO:O	2:N:314:HIS:CB	2.55	0.54
1:E:115:HIS:O	1:E:166:VAL:HG22	2.07	0.54
1:H:239:ARG:HH22	1:H:336:LYS:HA	1.73	0.54
1:L:22:ARG:HB3	1:L:25:ARG:NH2	2.22	0.54
1:L:332:MET:O	1:L:335:LEU:HB2	2.07	0.54
1:B:244:TYR:OH	1:B:358:ARG:NH1	2.41	0.54
1:I:332:MET:HG3	1:I:362:ARG:NH1	2.22	0.54
1:L:35:ASP:HB3	1:L:38:VAL:CG1	2.37	0.54
1:B:68:VAL:HG13	1:B:145:PRO:HB2	1.90	0.54
1:D:249:THR:HG22	1:D:251:LYS:HE2	1.89	0.54
1:G:22:ARG:HG3	1:G:24:ASN:H	1.72	0.54
2:W:354:THR:CG2	2:W:357:GLU:H	2.21	0.54
1:C:222:LEU:HB2	1:C:223:PRO:HD3	1.89	0.54
1:D:350:PRO:HB3	1:D:358:ARG:HH12	1.73	0.54
1:K:249:THR:HG23	1:K:407:VAL:HG21	1.90	0.54
1:E:249:THR:CG2	1:E:407:VAL:CG2	2.85	0.54
1:F:22:ARG:HG3	1:F:23:PRO:CD	2.36	0.54
1:H:22:ARG:HH21	1:H:24:ASN:HB2	1.73	0.54
1:I:402:GLU:CD	1:I:453:ARG:NH2	2.62	0.54
1:L:357:LEU:C	1:L:359:ARG:H	2.12	0.54
1:H:249:THR:HG22	1:H:251:LYS:HZ2	1.71	0.53
2:W:354:THR:HG23	2:W:357:GLU:H	1.72	0.53
1:A:82:ILE:HG21	1:A:100:ILE:HD11	1.90	0.53
1:B:46:MET:HE1	1:B:73:SER:CA	2.36	0.53
1:E:350:PRO:HB2	1:E:358:ARG:HH21	1.72	0.53
1:H:98:ASP:OD1	1:H:225:ARG:NH2	2.41	0.53
1:J:32:ILE:HD12	1:J:33:ASN:N	2.23	0.53
1:K:233:ILE:CD1	1:K:235:VAL:HG12	2.37	0.53
1:K:249:THR:CG2	1:K:407:VAL:CG2	2.86	0.53
2:O:354:THR:HG23	2:O:357:GLU:H	1.73	0.53
2:T:314:HIS:CE1	2:T:316:HIS:CE1	2.96	0.53
1:D:82:ILE:HG21	1:D:100:ILE:HD11	1.89	0.53
1:G:283:GLU:HA	1:G:327:GLN:NE2	2.22	0.53
1:A:354:ASP:HB3	1:A:357:LEU:CD2	2.37	0.53
1:E:249:THR:HG23	1:E:407:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:80:GLU:HG2	1:L:432:LEU:HD11	1.91	0.53
2:P:290:ASP:N	2:P:314:HIS:HE1	2.06	0.53
2:W:290:ASP:N	2:W:314:HIS:HE1	2.06	0.53
1:G:49:LEU:CB	1:G:51:LEU:HD22	2.39	0.53
1:B:336:LYS:HB2	1:B:338:ARG:HH22	1.68	0.53
2:V:354:THR:HG23	2:V:357:GLU:H	1.72	0.53
1:F:239:ARG:HH21	1:F:336:LYS:HA	1.74	0.53
1:K:440:GLU:O	1:K:442:MET:N	2.42	0.53
2:N:290:ASP:H	2:N:314:HIS:HE1	1.57	0.53
2:O:300:ILE:HD13	2:O:365:ILE:HB	1.90	0.53
1:F:283:GLU:HG3	1:F:324:ILE:HD13	1.90	0.53
1:K:26:LEU:HD21	1:K:45:LYS:HE3	1.89	0.53
2:O:289:ILE:HG23	2:O:314:HIS:CD2	2.44	0.53
2:Q:318:ILE:HG12	2:Q:351:GLU:CA	2.39	0.53
1:C:82:ILE:HG21	1:C:100:ILE:HD11	1.91	0.53
1:J:440:GLU:HA	1:J:440:GLU:OE1	2.08	0.53
2:P:320:ASP:HA	2:P:323:LEU:HG	1.89	0.53
2:V:347:GLU:OE2	2:V:368:ARG:NH2	2.41	0.53
1:F:335:LEU:CD2	1:F:338:ARG:HG2	2.39	0.53
2:V:354:THR:HG22	2:V:357:GLU:HG3	1.90	0.53
1:B:89:ARG:HD3	1:B:96:LEU:HD13	1.92	0.52
1:K:128:GLY:HA2	1:K:440:GLU:OE2	2.09	0.52
2:S:290:ASP:N	2:S:314:HIS:HE1	2.06	0.52
1:B:32:ILE:HD12	1:B:33:ASN:N	2.24	0.52
1:E:68:VAL:HG22	1:E:147:ARG:HB2	1.91	0.52
1:F:35:ASP:HB3	1:F:38:VAL:CG1	2.39	0.52
1:I:319:GLU:OE1	1:J:320:VAL:HG11	2.08	0.52
1:D:452:PHE:O	1:D:456:LEU:HD23	2.08	0.52
1:K:46:MET:HE1	1:K:73:SER:CA	2.40	0.52
1:A:35:ASP:HB3	1:A:38:VAL:CG1	2.40	0.52
1:A:113:ARG:HB2	1:A:181:VAL:CG1	2.31	0.52
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.91	0.52
1:H:338:ARG:NH1	1:H:340:HIS:HA	2.24	0.52
1:H:350:PRO:C	1:H:358:ARG:HH22	2.12	0.52
1:L:377:ARG:HD3	1:L:403:THR:OG1	2.10	0.52
2:M:359:ASN:OD1	2:M:359:ASN:O	2.28	0.52
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.45	0.52
1:E:249:THR:HG23	1:E:407:VAL:CG2	2.40	0.52
1:L:440:GLU:O	1:L:442:MET:N	2.43	0.52
2:Q:289:ILE:HG23	2:Q:314:HIS:CD2	2.45	0.52
2:X:354:THR:CG2	2:X:357:GLU:H	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:PRO:HD2	1:C:174:CYS:CB	2.39	0.52
1:F:282:SER:HB3	1:F:324:ILE:CD1	2.40	0.52
1:L:68:VAL:HG13	1:L:145:PRO:HB2	1.92	0.52
1:D:244:TYR:HE2	1:D:366:GLU:HB3	1.74	0.52
1:E:115:HIS:HB2	1:E:166:VAL:HG23	1.90	0.52
1:L:269:ILE:HD11	1:L:289:ALA:HB2	1.91	0.52
2:M:318:ILE:HG12	2:M:351:GLU:CA	2.39	0.52
2:T:354:THR:CG2	2:T:357:GLU:H	2.21	0.52
1:G:150:ASP:O	1:G:165:VAL:HG12	2.10	0.52
1:J:322:ARG:NH1	1:K:321:GLU:OE2	2.43	0.52
1:K:282:SER:HB3	1:K:324:ILE:HD11	1.91	0.52
1:E:453:ARG:HH21	1:H:401:ASN:HB3	1.73	0.52
1:H:440:GLU:O	1:H:442:MET:N	2.43	0.52
1:L:169:ASP:HB3	1:L:170:PRO:CD	2.37	0.52
1:C:350:PRO:CA	1:C:358:ARG:HH21	2.24	0.51
1:E:353:ILE:CD1	1:E:353:ILE:C	2.79	0.51
1:E:377:ARG:CG	1:E:411:LEU:HD11	2.40	0.51
1:F:239:ARG:NH2	1:F:335:LEU:O	2.43	0.51
1:G:440:GLU:O	1:G:442:MET:N	2.43	0.51
1:I:440:GLU:O	1:I:442:MET:N	2.43	0.51
2:R:354:THR:CG2	2:R:357:GLU:H	2.22	0.51
1:E:440:GLU:O	1:E:442:MET:N	2.43	0.51
1:H:239:ARG:NH2	1:H:336:LYS:HA	2.26	0.51
1:L:244:TYR:HE2	1:L:366:GLU:HB2	1.75	0.51
1:L:339:ALA:C	1:L:340:HIS:CG	2.84	0.51
2:T:303:ALA:O	2:T:305:GLY:N	2.40	0.51
2:V:300:ILE:HD13	2:V:365:ILE:HB	1.91	0.51
1:F:283:GLU:OE1	1:F:324:ILE:HG12	2.09	0.51
1:H:322:ARG:HD2	1:I:321:GLU:OE2	2.11	0.51
1:I:350:PRO:C	1:I:358:ARG:HH22	2.13	0.51
1:K:113:ARG:NE	1:K:183:HIS:HE1	2.05	0.51
1:F:306:LEU:HD23	1:F:353:ILE:HD13	1.91	0.51
1:J:222:LEU:HD12	1:K:420:LEU:HD22	1.91	0.51
1:K:26:LEU:HD21	1:K:45:LYS:CE	2.41	0.51
1:L:117:LEU:HD21	1:L:185:GLU:O	2.10	0.51
2:N:290:ASP:H	2:N:314:HIS:CE1	2.28	0.51
1:B:169:ASP:HB3	1:B:170:PRO:CD	2.37	0.51
1:C:250:GLY:HA2	3:C:501:ADP:O2A	2.11	0.51
1:J:377:ARG:CG	1:J:411:LEU:HD11	2.41	0.51
1:J:440:GLU:O	1:J:442:MET:N	2.43	0.51
1:L:22:ARG:HG3	1:L:23:PRO:CD	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:318:ILE:HG12	2:U:351:GLU:CA	2.39	0.51
1:D:440:GLU:O	1:D:442:MET:N	2.43	0.51
1:F:350:PRO:C	1:F:358:ARG:HH22	2.13	0.51
1:G:391:ALA:O	1:G:394:VAL:HG22	2.10	0.51
1:F:440:GLU:O	1:F:442:MET:N	2.43	0.51
1:I:336:LYS:HG3	1:I:337:GLN:H	1.75	0.51
2:P:354:THR:CG2	2:P:357:GLU:H	2.22	0.51
1:B:377:ARG:CG	1:B:411:LEU:HD11	2.41	0.51
1:C:350:PRO:HA	1:C:358:ARG:HH21	1.76	0.51
1:E:48:GLU:HG2	1:E:49:LEU:HD13	1.92	0.51
1:F:153:LEU:HD11	1:F:160:ALA:HB1	1.91	0.51
1:H:26:LEU:HD21	1:H:45:LYS:CE	2.41	0.51
1:K:140:LEU:HG	1:K:141:GLU:CG	2.41	0.51
1:K:233:ILE:HG13	1:K:235:VAL:HG12	1.93	0.51
1:A:440:GLU:O	1:A:442:MET:N	2.44	0.51
1:C:338:ARG:C	1:C:340:HIS:H	2.14	0.51
1:D:300:ILE:HD13	1:D:344:MET:HE3	1.93	0.51
1:E:329:LEU:N	1:E:329:LEU:HD12	2.26	0.51
2:T:321:ILE:HD11	2:T:355:LEU:HD11	1.93	0.51
1:D:29:ASP:OD1	1:D:30:GLU:N	2.40	0.51
1:E:62:LYS:HG3	1:E:94:VAL:HG23	1.92	0.51
1:E:336:LYS:C	1:E:338:ARG:N	2.62	0.51
2:P:290:ASP:H	2:P:314:HIS:CE1	2.29	0.51
1:C:339:ALA:O	1:C:340:HIS:HB2	2.09	0.50
1:C:440:GLU:O	1:C:442:MET:N	2.44	0.50
1:E:238:PRO:HB3	1:E:365:ARG:CZ	2.34	0.50
1:F:82:ILE:HG21	1:F:100:ILE:HD11	1.93	0.50
1:H:335:LEU:HD22	1:H:338:ARG:HB2	1.93	0.50
2:V:300:ILE:CD1	2:V:365:ILE:HB	2.41	0.50
1:D:26:LEU:HD12	1:D:26:LEU:N	2.25	0.50
1:E:269:ILE:HD11	1:E:289:ALA:HB2	1.93	0.50
1:F:377:ARG:CG	1:F:411:LEU:HD11	2.41	0.50
1:K:377:ARG:CG	1:K:411:LEU:HD11	2.41	0.50
1:L:22:ARG:HH21	1:L:24:ASN:HB2	1.76	0.50
1:C:236:LYS:O	1:C:236:LYS:HG3	2.11	0.50
1:C:402:GLU:OE1	1:J:398:GLN:OE1	2.29	0.50
1:K:46:MET:CE	1:K:73:SER:CA	2.89	0.50
1:K:336:LYS:HB2	1:K:338:ARG:HH22	1.71	0.50
2:S:304:ASP:OD1	2:S:304:ASP:O	2.30	0.50
1:H:46:MET:HE2	1:H:73:SER:CA	2.38	0.50
2:T:322:ARG:NH1	2:T:351:GLU:OE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ARG:NH2	1:B:341:VAL:O	2.44	0.50
1:C:377:ARG:CG	1:C:411:LEU:HD11	2.41	0.50
1:D:57:VAL:HG21	1:D:102:ILE:CD1	2.40	0.50
1:H:306:LEU:HD23	1:H:353:ILE:HD13	1.93	0.50
1:I:377:ARG:CG	1:I:411:LEU:HD11	2.41	0.50
1:J:306:LEU:HD23	1:J:353:ILE:HD13	1.94	0.50
1:J:336:LYS:HG3	1:J:338:ARG:H	1.76	0.50
2:R:302:LEU:HD12	2:R:307:ARG:CB	2.41	0.50
1:D:377:ARG:CG	1:D:411:LEU:HD11	2.41	0.50
1:G:222:LEU:CD1	1:H:424:ARG:HH11	2.24	0.50
1:K:216:ILE:CD1	1:K:254:ILE:HD11	2.33	0.50
1:D:384:HIS:HE1	3:D:501:ADP:N3	2.10	0.50
1:E:287:ARG:HE	1:E:327:GLN:NE2	2.09	0.50
1:F:398:GLN:HE22	1:G:453:ARG:HE	1.60	0.50
1:G:26:LEU:HD11	1:G:45:LYS:HE3	1.93	0.50
1:I:68:VAL:HG13	1:I:145:PRO:HB2	1.93	0.50
1:I:438:ASP:O	1:I:442:MET:SD	2.70	0.50
1:J:381:LEU:HD11	1:J:399:VAL:HG22	1.93	0.50
1:L:310:ALA:HA	1:L:325:VAL:HG22	1.92	0.50
1:B:26:LEU:HD21	1:B:45:LYS:HE3	1.94	0.50
1:G:126:ILE:HG13	1:G:159:ARG:NH1	2.27	0.50
1:I:129:ASN:O	1:I:131:PHE:N	2.45	0.50
1:L:26:LEU:HD21	1:L:45:LYS:CE	2.42	0.50
1:C:22:ARG:HG3	1:C:23:PRO:CD	2.39	0.50
1:E:118:PRO:HG3	1:E:130:LEU:CD2	2.42	0.50
1:I:359:ARG:NH1	1:I:362:ARG:HD3	2.27	0.50
1:H:26:LEU:HD21	1:H:45:LYS:HE3	1.92	0.49
1:I:214:ALA:O	1:I:217:LYS:HG2	2.12	0.49
1:K:131:PHE:HE1	1:K:182:ILE:CG2	2.25	0.49
1:H:377:ARG:CG	1:H:411:LEU:HD11	2.41	0.49
2:M:340:MET:HE3	2:M:368:ARG:HH21	1.75	0.49
2:W:318:ILE:HG12	2:W:351:GLU:CA	2.32	0.49
1:E:238:PRO:CA	1:E:365:ARG:HH21	2.25	0.49
1:G:113:ARG:NH1	1:G:183:HIS:NE2	2.52	0.49
1:I:426:LYS:HD2	1:I:445:LEU:HD23	1.93	0.49
1:B:26:LEU:HD21	1:B:45:LYS:CE	2.43	0.49
1:B:249:THR:HG22	1:B:251:LYS:HZ2	1.77	0.49
1:E:78:SER:CB	1:E:81:LYS:HE3	2.32	0.49
1:G:325:VAL:O	1:G:329:LEU:HD22	2.12	0.49
1:G:358:ARG:HD3	1:G:366:GLU:OE2	2.12	0.49
1:B:322:ARG:HD2	1:C:321:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:PHE:C	1:D:362:ARG:H	2.16	0.49
1:G:393:ASP:O	1:G:449:MET:HG2	2.12	0.49
1:K:453:ARG:HG3	1:K:453:ARG:HH11	1.78	0.49
1:L:211:LYS:O	1:L:211:LYS:NZ	2.43	0.49
1:L:310:ALA:HB1	1:L:357:LEU:HD11	1.93	0.49
2:O:300:ILE:CD1	2:O:365:ILE:HB	2.42	0.49
1:A:26:LEU:HD21	1:A:45:LYS:HE3	1.94	0.49
1:E:39:VAL:HG11	1:E:59:LEU:HD11	1.93	0.49
1:G:109:LYS:HE2	2:S:306:GLY:HA3	1.94	0.49
1:K:426:LYS:HD2	1:K:445:LEU:CD1	2.35	0.49
1:C:452:PHE:O	1:C:456:LEU:HD23	2.13	0.49
1:E:169:ASP:HB3	1:E:170:PRO:CD	2.42	0.49
1:I:306:LEU:HD23	1:I:353:ILE:HD13	1.95	0.49
1:K:131:PHE:CE1	1:K:182:ILE:HG23	2.48	0.49
1:L:430:ILE:CD1	1:L:441:VAL:HG11	2.42	0.49
2:S:290:ASP:H	2:S:314:HIS:HE1	1.61	0.49
2:V:287:ILE:HD12	2:V:287:ILE:N	2.26	0.49
1:B:440:GLU:O	1:B:442:MET:N	2.46	0.49
1:D:438:ASP:O	1:D:442:MET:SD	2.71	0.49
1:E:329:LEU:CD1	1:E:329:LEU:H	2.24	0.49
1:F:287:ARG:HE	1:F:327:GLN:NE2	2.10	0.49
1:H:313:ARG:NH1	1:H:354:ASP:OD2	2.46	0.49
2:S:290:ASP:H	2:S:314:HIS:CE1	2.30	0.49
1:F:312:LYS:HB3	1:F:315:LYS:HG2	1.95	0.49
1:F:437:ILE:HB	1:F:441:VAL:CG2	2.43	0.49
1:H:128:GLY:HA2	1:H:440:GLU:OE2	2.13	0.49
1:I:70:ILE:HG13	2:U:343:PHE:CE1	2.47	0.49
1:A:402:GLU:CD	1:L:398:GLN:HE22	2.15	0.49
1:C:171:SER:HB3	1:C:172:PRO:CD	2.25	0.49
1:C:359:ARG:HG2	1:C:360:PHE:H	1.78	0.49
1:I:118:PRO:HG3	1:I:130:LEU:CD2	2.42	0.49
2:P:290:ASP:H	2:P:314:HIS:HE1	1.60	0.49
1:A:27:ILE:HD13	1:A:99:VAL:HG23	1.89	0.48
1:B:29:ASP:OD1	1:B:30:GLU:N	2.40	0.48
1:I:358:ARG:HD3	1:I:366:GLU:OE2	2.12	0.48
1:J:26:LEU:HD21	1:J:45:LYS:HE3	1.94	0.48
2:P:354:THR:HG22	2:P:357:GLU:CG	2.43	0.48
2:Q:302:LEU:HD12	2:Q:307:ARG:CB	2.43	0.48
1:D:169:ASP:HB3	1:D:170:PRO:CD	2.39	0.48
1:G:169:ASP:HB3	1:G:170:PRO:CD	2.37	0.48
1:K:310:ALA:HA	1:K:325:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:290:ASP:H	2:W:314:HIS:CE1	2.30	0.48
2:X:354:THR:HG22	2:X:357:GLU:CG	2.44	0.48
1:F:306:LEU:HD21	1:F:357:LEU:HD13	1.95	0.48
1:G:150:ASP:HB2	1:G:165:VAL:HG11	1.94	0.48
1:G:393:ASP:O	1:G:449:MET:HG3	2.13	0.48
1:J:287:ARG:HG3	1:J:327:GLN:NE2	2.27	0.48
1:K:115:HIS:ND1	1:K:166:VAL:HG21	2.29	0.48
1:A:306:LEU:HD23	1:A:353:ILE:HD13	1.96	0.48
1:C:113:ARG:HD3	1:C:183:HIS:HE1	1.79	0.48
1:I:157:GLY:C	1:I:158:MET:HG2	2.33	0.48
1:I:381:LEU:HD11	1:I:399:VAL:HG22	1.95	0.48
1:A:349:ARG:HG3	1:A:350:PRO:CD	2.43	0.48
1:A:437:ILE:HD12	1:A:441:VAL:HG11	1.95	0.48
1:E:300:ILE:HD13	1:E:344:MET:HE3	1.94	0.48
1:G:306:LEU:HD23	1:G:353:ILE:HD13	1.94	0.48
1:I:434:ASP:CG	1:I:436:THR:HG22	2.33	0.48
1:K:133:VAL:HG23	1:K:443:ASN:CG	2.33	0.48
1:K:169:ASP:HB3	1:K:170:PRO:CD	2.38	0.48
1:F:417:GLU:CG	1:F:455:ALA:HB1	2.39	0.48
1:G:82:ILE:HG21	1:G:100:ILE:HD11	1.94	0.48
1:I:128:GLY:HA2	1:I:440:GLU:OE2	2.12	0.48
2:V:287:ILE:HD13	2:V:311:LYS:HE3	1.96	0.48
2:X:302:LEU:HD12	2:X:307:ARG:CB	2.44	0.48
1:A:26:LEU:HD21	1:A:45:LYS:CE	2.43	0.48
1:D:338:ARG:HA	1:D:338:ARG:NE	2.29	0.48
1:J:26:LEU:HD21	1:J:45:LYS:CE	2.43	0.48
1:J:313:ARG:HH12	1:J:325:VAL:CG1	2.22	0.48
2:M:321:ILE:HD11	2:M:355:LEU:HD11	1.94	0.48
1:H:96:LEU:O	1:H:225:ARG:NH1	2.46	0.48
1:H:338:ARG:HG2	1:H:341:VAL:H	1.79	0.48
1:K:440:GLU:C	1:K:442:MET:N	2.67	0.48
2:N:347:GLU:OE2	2:N:368:ARG:NH2	2.46	0.48
2:W:302:LEU:HD12	2:W:307:ARG:CB	2.44	0.48
1:F:377:ARG:NE	1:F:403:THR:HG23	2.27	0.48
2:N:302:LEU:HD12	2:N:307:ARG:CB	2.43	0.48
2:W:290:ASP:H	2:W:314:HIS:HE1	1.61	0.48
1:I:306:LEU:HD21	1:I:357:LEU:HD13	1.96	0.48
1:K:306:LEU:HD23	1:K:353:ILE:HD13	1.94	0.48
2:X:321:ILE:HD11	2:X:355:LEU:HD11	1.96	0.48
1:H:393:ASP:O	1:H:449:MET:HG3	2.14	0.47
1:K:249:THR:HG23	1:K:407:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:311:LYS:NZ	2:T:312:PHE:H	2.12	0.47
1:B:219:MET:CE	1:B:365:ARG:CB	2.91	0.47
1:J:440:GLU:C	1:J:442:MET:N	2.68	0.47
1:K:437:ILE:HB	1:K:441:VAL:CG2	2.44	0.47
1:C:318:GLY:O	1:D:317:HIS:HE1	1.96	0.47
1:E:338:ARG:C	1:E:340:HIS:H	2.16	0.47
1:H:358:ARG:HD3	1:H:366:GLU:OE2	2.14	0.47
1:J:169:ASP:HB3	1:J:170:PRO:CD	2.38	0.47
2:R:287:ILE:N	2:R:287:ILE:HD12	2.29	0.47
1:A:286:LEU:HD11	1:A:309:ILE:HD11	1.96	0.47
1:F:26:LEU:HD21	1:F:45:LYS:CE	2.45	0.47
1:H:335:LEU:HD22	1:H:338:ARG:CB	2.44	0.47
1:B:381:LEU:HD11	1:B:399:VAL:HG22	1.96	0.47
1:D:57:VAL:CG2	1:D:102:ILE:HG12	2.41	0.47
1:D:336:LYS:CB	1:D:338:ARG:NH2	2.74	0.47
1:G:26:LEU:HD11	1:G:45:LYS:CE	2.45	0.47
1:L:243:LEU:HD12	1:L:243:LEU:N	2.30	0.47
2:T:295:THR:HA	2:T:314:HIS:HB3	1.97	0.47
1:A:92:LEU:O	1:A:94:VAL:HG13	2.15	0.47
1:B:306:LEU:HD21	1:B:357:LEU:HD13	1.96	0.47
1:D:92:LEU:O	1:D:94:VAL:HG13	2.15	0.47
1:L:211:LYS:HD2	1:L:211:LYS:HA	1.52	0.47
2:M:340:MET:HE3	2:M:368:ARG:NH2	2.30	0.47
2:O:318:ILE:HD13	2:O:318:ILE:HG21	1.73	0.47
2:S:307:ARG:HA	2:S:307:ARG:HD3	1.51	0.47
1:C:452:PHE:O	1:C:456:LEU:CD2	2.63	0.47
1:D:22:ARG:N	1:D:23:PRO:HD2	2.30	0.47
1:F:403:THR:HG23	1:F:403:THR:O	2.14	0.47
1:G:421:GLN:O	1:G:422:ALA:C	2.51	0.47
1:K:249:THR:HG22	1:K:407:VAL:CG2	2.45	0.47
1:K:306:LEU:HD21	1:K:357:LEU:HD13	1.96	0.47
1:L:26:LEU:HD21	1:L:45:LYS:HE3	1.96	0.47
1:L:92:LEU:O	1:L:94:VAL:HG13	2.15	0.47
1:L:168:THR:HG23	1:L:171:SER:HA	1.96	0.47
2:O:300:ILE:HD11	2:O:321:ILE:CG2	2.44	0.47
2:P:340:MET:CE	2:P:368:ARG:HE	2.27	0.47
2:S:302:LEU:HD12	2:S:307:ARG:CB	2.32	0.47
1:D:360:PHE:O	1:D:362:ARG:N	2.44	0.47
1:E:426:LYS:CD	1:E:445:LEU:HD12	2.43	0.47
1:F:336:LYS:CB	1:F:338:ARG:NH2	2.78	0.47
1:F:337:GLN:O	1:F:340:HIS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ASP:HB2	1:G:165:VAL:CG1	2.45	0.47
1:G:313:ARG:HD2	1:G:313:ARG:O	2.14	0.47
1:G:423:ILE:O	1:G:427:MET:HG2	2.15	0.47
1:K:46:MET:HE2	1:K:73:SER:HA	1.96	0.47
1:K:203:TYR:CE2	1:K:217:LYS:HD3	2.49	0.47
1:L:256:ARG:HD2	1:L:256:ARG:HA	1.63	0.47
1:L:440:GLU:C	1:L:442:MET:N	2.67	0.47
2:T:354:THR:HG22	2:T:357:GLU:CG	2.43	0.47
2:V:300:ILE:HD11	2:V:321:ILE:CG2	2.45	0.47
1:A:169:ASP:HB3	1:A:170:PRO:CD	2.37	0.47
1:B:306:LEU:HD23	1:B:353:ILE:HD13	1.97	0.47
1:E:287:ARG:NE	1:E:327:GLN:HE22	2.12	0.47
1:E:383:ILE:O	1:E:386:LYS:HG3	2.15	0.47
1:E:440:GLU:C	1:E:442:MET:N	2.68	0.47
1:G:394:VAL:HG23	1:G:394:VAL:O	2.14	0.47
1:I:336:LYS:CB	1:I:338:ARG:NH2	2.77	0.47
1:J:126:ILE:HG13	1:J:159:ARG:NH1	2.30	0.47
2:M:340:MET:CE	2:M:368:ARG:NH2	2.73	0.47
2:T:289:ILE:HG23	2:T:314:HIS:CD2	2.50	0.47
1:B:440:GLU:C	1:B:442:MET:N	2.68	0.47
1:E:153:LEU:HD11	1:E:160:ALA:HB1	1.97	0.47
1:J:306:LEU:HD21	1:J:357:LEU:HD13	1.97	0.47
1:D:350:PRO:HB3	1:D:358:ARG:NH1	2.30	0.46
1:F:437:ILE:HB	1:F:441:VAL:HG22	1.97	0.46
1:G:24:ASN:N	1:G:24:ASN:ND2	2.62	0.46
1:H:440:GLU:C	1:H:442:MET:N	2.68	0.46
1:I:414:LEU:C	1:I:414:LEU:HD13	2.36	0.46
1:A:43:GLN:HB2	1:A:44:PRO:HD3	1.96	0.46
1:G:388:MET:HE3	1:G:390:LEU:CD2	2.45	0.46
1:H:306:LEU:HD21	1:H:357:LEU:HD13	1.96	0.46
1:H:393:ASP:O	1:H:449:MET:HG2	2.15	0.46
1:I:402:GLU:OE1	1:I:453:ARG:NH2	2.48	0.46
1:J:27:ILE:CG2	1:J:81:LYS:HG2	2.41	0.46
1:J:256:ARG:HD2	1:J:256:ARG:HA	1.61	0.46
2:O:302:LEU:HD12	2:O:307:ARG:CB	2.46	0.46
2:T:294:PRO:O	2:T:314:HIS:HB3	2.15	0.46
2:V:302:LEU:HD12	2:V:307:ARG:CB	2.44	0.46
1:A:337:GLN:O	1:A:340:HIS:N	2.48	0.46
1:C:306:LEU:HD23	1:C:353:ILE:HD13	1.97	0.46
1:C:440:GLU:C	1:C:442:MET:N	2.67	0.46
1:F:26:LEU:HD21	1:F:45:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:427:MET:CE	1:L:226:HIS:CE1	2.97	0.46
1:I:126:ILE:HG13	1:I:159:ARG:NH1	2.30	0.46
1:A:113:ARG:HH21	1:A:183:HIS:HE1	1.62	0.46
1:B:249:THR:HG22	1:B:251:LYS:HZ3	1.80	0.46
1:E:46:MET:HG2	1:E:51:LEU:HB2	1.97	0.46
2:P:321:ILE:HD11	2:P:355:LEU:CD2	2.45	0.46
1:A:440:GLU:C	1:A:442:MET:N	2.68	0.46
1:D:116:VAL:C	1:D:117:LEU:HD12	2.36	0.46
1:D:440:GLU:C	1:D:442:MET:N	2.67	0.46
1:H:235:VAL:HG13	1:I:416:SER:OG	2.15	0.46
1:I:440:GLU:C	1:I:442:MET:N	2.68	0.46
1:J:350:PRO:HB3	1:J:358:ARG:HH22	1.73	0.46
2:S:318:ILE:HG12	2:S:351:GLU:CA	2.39	0.46
1:H:22:ARG:CG	1:H:23:PRO:HD2	2.44	0.46
1:I:169:ASP:HB3	1:I:170:PRO:CD	2.38	0.46
1:J:437:ILE:HG22	1:J:440:GLU:HB3	1.97	0.46
2:N:318:ILE:HG12	2:N:351:GLU:CA	2.40	0.46
1:D:239:ARG:HH21	1:D:337:GLN:HA	1.81	0.46
1:E:243:LEU:HD22	1:E:367:VAL:HG13	1.96	0.46
1:F:287:ARG:NE	1:F:327:GLN:HE22	2.11	0.46
1:G:22:ARG:HD3	1:G:25:ARG:HG3	1.98	0.46
1:G:432:LEU:HD13	1:L:27:ILE:HG13	1.98	0.46
2:N:321:ILE:HD11	2:N:355:LEU:CD2	2.45	0.46
2:T:347:GLU:OE2	2:T:368:ARG:NH2	2.48	0.46
2:X:294:PRO:O	2:X:314:HIS:CB	2.63	0.46
1:B:92:LEU:O	1:B:94:VAL:HG13	2.15	0.46
1:E:377:ARG:CZ	1:E:404:HIS:HA	2.46	0.46
1:G:92:LEU:O	1:G:94:VAL:HG13	2.15	0.46
1:G:388:MET:CE	1:G:390:LEU:HD21	2.44	0.46
1:D:249:THR:CG2	1:D:251:LYS:HE2	2.46	0.46
1:F:92:LEU:O	1:F:94:VAL:HG13	2.16	0.46
1:F:440:GLU:C	1:F:442:MET:N	2.68	0.46
1:K:46:MET:HE2	1:K:73:SER:CB	2.44	0.46
1:K:153:LEU:HD11	1:K:160:ALA:HB1	1.97	0.46
1:L:287:ARG:HE	1:L:327:GLN:NE2	2.13	0.46
1:F:141:GLU:O	2:R:345:ASN:ND2	2.39	0.46
1:G:153:LEU:HD11	1:G:160:ALA:HB1	1.98	0.46
1:H:92:LEU:O	1:H:94:VAL:HG13	2.16	0.46
1:H:336:LYS:HG3	1:H:337:GLN:H	1.81	0.46
1:K:337:GLN:O	1:K:340:HIS:N	2.49	0.46
2:R:354:THR:HG22	2:R:357:GLU:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:VAL:HG13	1:D:443:ASN:CG	2.36	0.45
1:D:337:GLN:O	1:D:340:HIS:N	2.48	0.45
1:I:92:LEU:O	1:I:94:VAL:HG13	2.16	0.45
1:I:322:ARG:HH22	1:J:317:HIS:HB2	1.80	0.45
1:J:337:GLN:O	1:J:340:HIS:N	2.48	0.45
2:O:289:ILE:HG23	2:O:314:HIS:HD2	1.80	0.45
2:R:287:ILE:HD12	2:R:287:ILE:H	1.80	0.45
1:A:402:GLU:CD	1:L:398:GLN:NE2	2.70	0.45
1:J:386:LYS:HB2	1:J:386:LYS:HE2	1.68	0.45
2:T:302:LEU:HD12	2:T:367:GLN:OE1	2.17	0.45
1:B:320:VAL:HG22	1:B:323:ARG:HH12	1.80	0.45
1:C:239:ARG:HH12	1:C:336:LYS:HA	1.80	0.45
1:E:350:PRO:CB	1:E:358:ARG:HH21	2.29	0.45
1:G:222:LEU:HD22	1:H:420:LEU:HD22	1.98	0.45
1:G:440:GLU:C	1:G:442:MET:N	2.68	0.45
1:I:26:LEU:HD11	1:I:45:LYS:CE	2.45	0.45
1:J:92:LEU:O	1:J:94:VAL:HG13	2.16	0.45
1:J:225:ARG:HG2	1:J:262:THR:HG23	1.98	0.45
1:A:421:GLN:O	1:A:422:ALA:C	2.54	0.45
1:I:287:ARG:HE	1:I:327:GLN:NE2	2.13	0.45
1:I:322:ARG:NH2	1:J:317:HIS:HB2	2.31	0.45
1:L:126:ILE:HG13	1:L:159:ARG:NH1	2.31	0.45
2:O:321:ILE:HD11	2:O:355:LEU:CD2	2.47	0.45
1:A:287:ARG:HD3	1:A:327:GLN:HE22	1.81	0.45
1:B:153:LEU:HD11	1:B:160:ALA:HB1	1.98	0.45
1:C:46:MET:HE1	1:C:73:SER:CA	2.43	0.45
1:C:63:LYS:NZ	1:C:194:GLU:OE2	2.49	0.45
1:E:238:PRO:N	1:E:365:ARG:HH21	2.14	0.45
1:F:383:ILE:O	1:F:386:LYS:HG3	2.16	0.45
1:G:129:ASN:O	1:G:131:PHE:N	2.48	0.45
1:H:422:ALA:HB1	1:H:445:LEU:HD11	1.97	0.45
2:V:318:ILE:HA	2:V:321:ILE:HD12	1.99	0.45
1:C:118:PRO:HG3	1:C:130:LEU:CD2	2.47	0.45
1:D:452:PHE:O	1:D:456:LEU:CD2	2.64	0.45
1:F:441:VAL:HG12	1:F:444:SER:OG	2.17	0.45
1:G:274:ILE:CG2	1:G:275:MET:HE2	2.36	0.45
1:L:402:GLU:CD	1:L:453:ARG:HH22	2.19	0.45
2:Q:289:ILE:HG23	2:Q:314:HIS:HD2	1.81	0.45
1:B:126:ILE:HG13	1:B:159:ARG:NH1	2.32	0.45
1:C:126:ILE:HG13	1:C:159:ARG:NH1	2.31	0.45
1:H:169:ASP:HB3	1:H:170:PRO:CD	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:337:GLN:O	1:I:340:HIS:N	2.49	0.45
1:J:118:PRO:HG3	1:J:130:LEU:CD2	2.47	0.45
1:E:256:ARG:HD2	1:E:256:ARG:HA	1.63	0.45
1:G:222:LEU:HD11	1:H:424:ARG:HH11	1.82	0.45
1:I:287:ARG:NE	1:I:327:GLN:HE22	2.14	0.45
1:J:322:ARG:HH22	1:K:317:HIS:HB3	1.82	0.45
1:K:441:VAL:HG12	1:K:444:SER:OG	2.17	0.45
2:V:321:ILE:HD13	2:V:365:ILE:HD12	1.99	0.45
1:A:232:ALA:HB2	1:B:439:ALA:HB1	1.98	0.45
1:C:92:LEU:O	1:C:94:VAL:HG13	2.16	0.45
1:F:403:THR:HG1	1:F:406:HIS:CG	2.31	0.45
1:G:155:ARG:NH1	1:G:386:LYS:HE3	2.31	0.45
1:I:249:THR:CG2	1:I:251:LYS:HZ2	2.29	0.45
1:J:153:LEU:HD11	1:J:160:ALA:HB1	1.98	0.45
1:K:92:LEU:O	1:K:94:VAL:HG13	2.16	0.45
1:L:287:ARG:NE	1:L:327:GLN:HE22	2.15	0.45
1:L:383:ILE:O	1:L:386:LYS:HG3	2.17	0.45
2:P:320:ASP:HA	2:P:323:LEU:CG	2.46	0.45
2:P:332:MET:HA	2:P:335:THR:OG1	2.17	0.45
1:A:27:ILE:HD11	1:A:99:VAL:CG2	2.47	0.45
1:A:153:LEU:HD11	1:A:160:ALA:HB1	1.99	0.45
1:B:46:MET:CE	1:B:73:SER:HA	2.38	0.45
1:D:57:VAL:HG23	1:D:103:GLN:O	2.17	0.45
1:D:127:THR:O	1:D:440:GLU:HG3	2.17	0.45
1:I:153:LEU:HD11	1:I:160:ALA:HB1	1.99	0.45
1:I:201:VAL:HG12	1:I:257:ALA:HB2	1.99	0.45
1:I:437:ILE:HD12	1:I:441:VAL:HG11	1.99	0.45
1:J:338:ARG:C	1:J:340:HIS:H	2.21	0.45
1:K:244:TYR:HE2	1:K:366:GLU:HB3	1.82	0.45
2:X:308:LEU:HD21	2:X:310:GLN:HE22	1.78	0.45
1:A:386:LYS:HE2	1:A:386:LYS:HB2	1.77	0.44
1:D:377:ARG:O	1:D:381:LEU:HD22	2.16	0.44
1:G:27:ILE:HG12	1:H:432:LEU:HD13	2.00	0.44
1:J:396:LEU:O	1:J:399:VAL:HG13	2.17	0.44
1:K:126:ILE:HG13	1:K:159:ARG:NH1	2.31	0.44
1:L:153:LEU:HD11	1:L:160:ALA:HB1	1.99	0.44
1:C:440:GLU:OE1	1:C:440:GLU:HA	2.17	0.44
1:F:338:ARG:C	1:F:340:HIS:H	2.21	0.44
1:G:22:ARG:HG2	1:G:25:ARG:HG3	1.99	0.44
1:H:126:ILE:HG13	1:H:159:ARG:NH1	2.32	0.44
1:J:286:LEU:HD11	1:J:309:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:322:ARG:HD2	1:K:321:GLU:OE2	2.16	0.44
1:K:338:ARG:C	1:K:340:HIS:H	2.21	0.44
1:L:306:LEU:HD23	1:L:353:ILE:HD13	1.99	0.44
1:A:57:VAL:HG21	1:A:102:ILE:HD11	1.99	0.44
1:C:171:SER:CB	1:C:172:PRO:CD	2.93	0.44
1:E:235:VAL:HG23	1:F:158:MET:HG2	1.99	0.44
1:E:438:ASP:O	1:E:442:MET:SD	2.76	0.44
1:G:359:ARG:HD3	1:H:247:PRO:HB3	1.99	0.44
1:G:416:SER:OG	1:L:235:VAL:HG13	2.18	0.44
1:J:201:VAL:HG12	1:J:257:ALA:HB2	1.99	0.44
2:R:321:ILE:HD11	2:R:355:LEU:CD2	2.45	0.44
1:A:203:TYR:CE2	1:A:217:LYS:HD3	2.52	0.44
1:B:201:VAL:HG12	1:B:257:ALA:HB2	1.99	0.44
1:D:338:ARG:C	1:D:340:HIS:H	2.21	0.44
1:E:249:THR:HG22	1:E:407:VAL:CG2	2.47	0.44
1:E:350:PRO:O	1:E:353:ILE:HD12	2.17	0.44
1:G:25:ARG:C	1:G:26:LEU:HD22	2.37	0.44
1:H:46:MET:HE1	1:H:73:SER:CA	2.44	0.44
2:Q:289:ILE:HD13	2:Q:312:PHE:HB3	2.00	0.44
2:U:321:ILE:HD11	2:U:355:LEU:CD2	2.46	0.44
1:A:126:ILE:HG13	1:A:159:ARG:NH1	2.32	0.44
1:C:320:VAL:HG23	1:C:323:ARG:NH1	2.32	0.44
1:D:430:ILE:HD11	1:D:441:VAL:HG11	1.98	0.44
1:E:52:PHE:O	1:E:55:ASP:HB2	2.17	0.44
1:E:126:ILE:HG13	1:E:159:ARG:NH1	2.32	0.44
1:E:329:LEU:HD13	1:E:329:LEU:H	1.82	0.44
1:I:27:ILE:CD1	1:J:428:ASP:HB3	2.48	0.44
1:K:39:VAL:HG12	1:K:84:MET:HB3	1.99	0.44
1:A:338:ARG:C	1:A:340:HIS:H	2.21	0.44
1:D:186:GLY:O	1:D:187:GLU:HB2	2.18	0.44
1:D:389:LYS:HD3	1:D:443:ASN:O	2.18	0.44
1:G:147:ARG:O	1:G:165:VAL:CG1	2.64	0.44
1:D:244:TYR:CE2	1:D:366:GLU:HB3	2.52	0.44
1:E:24:ASN:O	1:E:101:SER:HA	2.18	0.44
1:E:105:CYS:SG	1:E:108:VAL:CG1	3.06	0.44
1:G:256:ARG:HD2	1:G:256:ARG:HA	1.62	0.44
1:H:438:ASP:O	1:H:442:MET:SD	2.76	0.44
1:F:336:LYS:HB2	1:F:338:ARG:NH2	2.33	0.44
1:L:338:ARG:O	1:L:340:HIS:N	2.51	0.44
1:L:385:THR:HA	1:L:388:MET:HE2	1.99	0.44
1:H:201:VAL:HG12	1:H:257:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:338:ARG:C	1:I:340:HIS:H	2.21	0.44
1:J:105:CYS:SG	1:J:108:VAL:CG2	3.05	0.44
1:K:239:ARG:HH21	1:K:336:LYS:HA	1.82	0.44
2:T:305:GLY:O	2:T:307:ARG:N	2.46	0.44
2:V:321:ILE:HD11	2:V:355:LEU:CD2	2.48	0.44
1:C:339:ALA:C	1:C:340:HIS:HD1	2.21	0.43
1:K:53:ARG:HH22	1:K:73:SER:CB	2.31	0.43
2:R:289:ILE:HD13	2:R:312:PHE:HB3	2.00	0.43
1:B:396:LEU:O	1:B:399:VAL:HG13	2.18	0.43
1:C:89:ARG:HD3	1:C:96:LEU:HD13	2.00	0.43
1:D:57:VAL:HG21	1:D:102:ILE:HD11	1.99	0.43
1:K:270:ASN:HB3	1:K:273:GLU:HB3	2.00	0.43
1:K:322:ARG:NH2	1:L:317:HIS:HB2	2.32	0.43
1:L:118:PRO:HG3	1:L:130:LEU:CD1	2.48	0.43
2:V:318:ILE:HD13	2:V:318:ILE:HG21	1.73	0.43
1:B:220:VAL:HG13	1:B:224:LEU:CD1	2.42	0.43
1:C:26:LEU:HD21	1:C:45:LYS:HE3	2.00	0.43
1:C:201:VAL:HG12	1:C:257:ALA:HB2	1.99	0.43
1:D:201:VAL:HG12	1:D:257:ALA:HB2	2.00	0.43
1:D:336:LYS:CB	1:D:338:ARG:HH22	2.31	0.43
1:E:64:ARG:HA	1:E:64:ARG:HD3	1.63	0.43
1:I:243:LEU:HD13	1:I:369:ILE:HD11	2.00	0.43
1:K:235:VAL:CG2	1:L:416:SER:OG	2.64	0.43
1:E:335:LEU:HD12	1:E:335:LEU:HA	1.77	0.43
1:G:336:LYS:H	1:G:338:ARG:CB	2.31	0.43
1:I:396:LEU:O	1:I:399:VAL:HG13	2.18	0.43
1:K:22:ARG:CG	1:K:23:PRO:HD2	2.49	0.43
2:P:338:ILE:HD13	2:P:347:GLU:HG3	1.99	0.43
1:F:40:SER:HB2	1:F:83:ARG:HB2	2.00	0.43
1:H:153:LEU:HD11	1:H:160:ALA:HB1	2.00	0.43
1:L:337:GLN:O	1:L:338:ARG:C	2.56	0.43
2:R:318:ILE:HD12	2:R:348:LEU:HB3	1.99	0.43
1:A:201:VAL:HG12	1:A:257:ALA:HB2	2.01	0.43
1:C:249:THR:CG2	1:C:251:LYS:HZ2	2.31	0.43
1:D:153:LEU:HD11	1:D:160:ALA:HB1	2.00	0.43
1:D:310:ALA:HA	1:D:325:VAL:HG22	2.00	0.43
1:D:336:LYS:HE2	1:D:336:LYS:CA	2.43	0.43
1:I:359:ARG:CZ	1:I:362:ARG:HD3	2.48	0.43
1:I:442:MET:N	1:I:442:MET:SD	2.91	0.43
1:J:315:LYS:HB3	1:J:315:LYS:HE2	1.83	0.43
1:L:201:VAL:HG12	1:L:257:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:269:ILE:HD13	1:L:269:ILE:HA	1.78	0.43
1:A:113:ARG:NE	1:A:183:HIS:CE1	2.75	0.43
1:G:350:PRO:O	1:G:358:ARG:NH2	2.52	0.43
1:I:113:ARG:HB2	1:I:181:VAL:HG23	1.93	0.43
1:K:118:PRO:HG3	1:K:130:LEU:CD1	2.49	0.43
1:L:438:ASP:O	1:L:442:MET:SD	2.77	0.43
2:S:304:ASP:O	2:S:307:ARG:HG2	2.18	0.43
1:A:40:SER:HB2	1:A:83:ARG:HB2	2.00	0.43
1:B:39:VAL:HG12	1:B:84:MET:HB3	2.01	0.43
1:E:235:VAL:HG13	1:F:416:SER:OG	2.18	0.43
1:L:184:CYS:O	1:L:185:GLU:C	2.57	0.43
2:O:318:ILE:HA	2:O:321:ILE:HD12	2.01	0.43
1:C:338:ARG:C	1:C:340:HIS:N	2.71	0.43
1:G:232:ALA:HB2	1:H:439:ALA:HB1	1.99	0.43
1:H:39:VAL:HG12	1:H:84:MET:HB3	2.00	0.43
1:H:40:SER:HB2	1:H:83:ARG:HB2	2.01	0.43
1:I:63:LYS:HE2	1:I:63:LYS:N	2.33	0.43
1:J:220:VAL:HG13	1:J:224:LEU:CD1	2.39	0.43
1:D:442:MET:N	1:D:442:MET:SD	2.91	0.43
1:E:201:VAL:HG12	1:E:257:ALA:HB2	2.01	0.43
1:F:423:ILE:O	1:F:427:MET:HG2	2.19	0.43
1:I:279:ALA:CB	1:I:320:VAL:HG11	2.49	0.43
1:J:232:ALA:HB2	1:K:439:ALA:HB1	2.01	0.43
1:K:89:ARG:HD3	1:K:96:LEU:HD13	2.01	0.43
1:A:287:ARG:HG3	1:A:327:GLN:NE2	2.34	0.42
1:A:402:GLU:OE2	1:L:398:GLN:NE2	2.52	0.42
1:C:29:ASP:OD1	1:C:30:GLU:N	2.50	0.42
1:D:220:VAL:HG13	1:D:224:LEU:CD1	2.42	0.42
1:E:169:ASP:O	1:E:170:PRO:C	2.55	0.42
1:E:357:LEU:C	1:E:359:ARG:H	2.21	0.42
1:F:377:ARG:HH11	1:F:377:ARG:HD3	1.73	0.42
1:K:105:CYS:SG	1:K:108:VAL:CG1	3.07	0.42
2:W:354:THR:CG2	2:W:357:GLU:HG3	2.49	0.42
1:C:39:VAL:HG12	1:C:84:MET:HB3	2.01	0.42
1:F:169:ASP:HB3	1:F:170:PRO:CD	2.39	0.42
1:G:26:LEU:HD22	1:G:26:LEU:N	2.34	0.42
1:G:150:ASP:H	1:G:165:VAL:CG1	2.32	0.42
1:G:286:LEU:HD11	1:G:309:ILE:HD11	2.01	0.42
1:H:423:ILE:O	1:H:427:MET:HG2	2.18	0.42
1:J:420:LEU:HD23	1:J:420:LEU:HA	1.89	0.42
1:K:192:GLU:HB3	1:K:194:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:442:MET:N	1:L:442:MET:SD	2.91	0.42
2:Q:321:ILE:HD11	2:Q:355:LEU:CD2	2.47	0.42
1:A:256:ARG:HD2	1:A:256:ARG:HA	1.61	0.42
1:C:129:ASN:ND2	1:C:132:GLU:H	2.11	0.42
1:D:336:LYS:HG2	1:D:338:ARG:HH22	1.81	0.42
1:F:377:ARG:HE	1:F:403:THR:CG2	2.32	0.42
1:H:249:THR:CG2	1:H:251:LYS:HZ2	2.31	0.42
1:I:40:SER:HB2	1:I:83:ARG:HB2	2.01	0.42
1:I:426:LYS:NZ	1:I:430:ILE:HD11	2.34	0.42
1:J:402:GLU:OE1	1:J:453:ARG:NH2	2.50	0.42
1:K:162:GLU:OE1	1:K:191:ARG:NH2	2.53	0.42
1:K:201:VAL:HG12	1:K:257:ALA:HB2	2.00	0.42
2:T:294:PRO:O	2:T:314:HIS:CB	2.67	0.42
2:V:354:THR:HG22	2:V:357:GLU:CD	2.39	0.42
1:A:39:VAL:HG12	1:A:84:MET:HB3	2.02	0.42
1:A:252:THR:CG2	3:A:501:ADP:O1A	2.66	0.42
1:C:26:LEU:HD21	1:C:45:LYS:CE	2.49	0.42
1:C:153:LEU:HD11	1:C:160:ALA:HB1	2.01	0.42
1:F:29:ASP:OD1	1:F:30:GLU:N	2.49	0.42
1:F:201:VAL:HG12	1:F:257:ALA:HB2	1.99	0.42
1:F:297:ALA:HA	1:F:298:PRO:C	2.40	0.42
1:F:377:ARG:CZ	1:F:404:HIS:HA	2.50	0.42
1:G:286:LEU:HD23	1:G:286:LEU:HA	1.88	0.42
1:H:105:CYS:SG	1:H:108:VAL:CG2	3.08	0.42
1:I:251:LYS:HG2	1:I:369:ILE:HD13	1.89	0.42
2:X:318:ILE:HD12	2:X:348:LEU:HB3	2.01	0.42
1:D:39:VAL:HG12	1:D:84:MET:HB3	2.00	0.42
1:E:23:PRO:HA	1:E:45:LYS:HZ1	1.85	0.42
1:F:336:LYS:H	1:F:338:ARG:NH2	2.17	0.42
1:K:80:GLU:CG	1:L:432:LEU:HD11	2.49	0.42
1:L:310:ALA:CB	1:L:357:LEU:HD11	2.50	0.42
2:T:318:ILE:HA	2:T:321:ILE:HD12	2.01	0.42
2:V:308:LEU:HD21	2:V:310:GLN:HE22	1.82	0.42
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.89	0.42
1:C:426:LYS:CD	1:C:445:LEU:HD12	2.45	0.42
1:G:338:ARG:C	1:G:340:HIS:H	2.23	0.42
1:K:336:LYS:H	1:K:338:ARG:NH2	2.18	0.42
2:P:320:ASP:OD1	2:P:323:LEU:HD21	2.19	0.42
1:C:49:LEU:HD13	1:C:49:LEU:HA	1.94	0.42
1:D:322:ARG:HH22	1:E:317:HIS:HB2	1.84	0.42
1:D:377:ARG:CZ	1:D:404:HIS:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:ILE:HD13	1:E:269:ILE:HA	1.77	0.42
1:E:442:MET:SD	1:E:442:MET:N	2.92	0.42
1:G:60:LYS:HD2	1:G:66:GLU:CG	2.40	0.42
1:H:61:GLY:HA2	1:H:100:ILE:HD12	2.02	0.42
1:I:39:VAL:HG12	1:I:84:MET:HB3	2.02	0.42
1:J:362:ARG:HB2	1:J:363:PHE:H	1.47	0.42
1:L:360:PHE:C	1:L:362:ARG:H	2.23	0.42
2:V:300:ILE:HD11	2:V:321:ILE:HG21	2.01	0.42
1:A:29:ASP:OD1	1:A:30:GLU:N	2.50	0.42
1:C:244:TYR:HE2	1:C:366:GLU:HB3	1.84	0.42
1:G:201:VAL:HG12	1:G:257:ALA:HB2	2.01	0.42
1:H:297:ALA:HA	1:H:298:PRO:C	2.40	0.42
1:I:297:ALA:HA	1:I:298:PRO:C	2.40	0.42
1:K:377:ARG:CZ	1:K:404:HIS:HA	2.50	0.42
1:K:396:LEU:HD12	1:K:396:LEU:HA	1.91	0.42
1:L:437:ILE:HG22	1:L:440:GLU:HB3	2.01	0.42
2:M:289:ILE:HD13	2:M:312:PHE:HB3	2.01	0.42
1:D:270:ASN:HB3	1:D:273:GLU:HB3	2.00	0.42
1:D:297:ALA:HA	1:D:298:PRO:C	2.40	0.42
1:D:386:LYS:HB2	1:D:386:LYS:HE2	1.80	0.42
1:E:28:VAL:HG21	1:E:94:VAL:CG1	2.48	0.42
1:F:133:VAL:HG13	1:F:443:ASN:CG	2.40	0.42
1:G:133:VAL:HG13	1:G:443:ASN:CG	2.40	0.42
1:G:377:ARG:CZ	1:G:404:HIS:HA	2.50	0.42
1:K:297:ALA:HA	1:K:298:PRO:C	2.40	0.42
1:B:22:ARG:HB2	1:B:25:ARG:HD3	2.02	0.42
1:D:51:LEU:HD23	1:D:104:PRO:HG3	2.02	0.42
1:D:164:LYS:HD3	1:D:189:ILE:HD11	2.02	0.42
1:D:203:TYR:CE2	1:D:217:LYS:HD3	2.55	0.42
1:E:244:TYR:CE1	1:E:350:PRO:HA	2.55	0.42
1:I:312:LYS:HB3	1:I:315:LYS:HG2	2.02	0.42
1:J:113:ARG:CZ	1:J:115:HIS:HB2	2.50	0.42
2:M:307:ARG:HD3	2:M:307:ARG:HA	1.79	0.42
2:N:340:MET:HE1	2:N:368:ARG:NH1	2.34	0.42
1:A:118:PRO:HG3	1:A:130:LEU:CD1	2.49	0.41
1:C:256:ARG:HA	1:C:256:ARG:HD2	1.60	0.41
1:H:120:ASP:OD1	1:H:121:ASP:N	2.53	0.41
1:B:120:ASP:OD1	1:B:121:ASP:N	2.53	0.41
1:B:297:ALA:HA	1:B:298:PRO:C	2.41	0.41
1:E:287:ARG:HG3	1:E:327:GLN:NE2	2.34	0.41
1:E:353:ILE:HD12	1:E:353:ILE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:ARG:HG3	1:F:327:GLN:NE2	2.35	0.41
1:G:118:PRO:HG3	1:G:130:LEU:CD1	2.50	0.41
1:H:97:GLY:HA3	1:H:225:ARG:HH12	1.84	0.41
1:I:229:LEU:HD21	1:J:423:ILE:HD13	2.02	0.41
2:T:302:LEU:HD23	2:T:307:ARG:HB3	2.01	0.41
1:A:297:ALA:HA	1:A:298:PRO:C	2.40	0.41
1:A:377:ARG:CZ	1:A:404:HIS:HA	2.50	0.41
1:C:40:SER:HB2	1:C:83:ARG:HB2	2.01	0.41
1:C:297:ALA:HA	1:C:298:PRO:C	2.41	0.41
1:D:312:LYS:HB3	1:D:315:LYS:HG2	2.03	0.41
1:E:45:LYS:HD3	1:E:45:LYS:HA	1.82	0.41
1:E:357:LEU:HD23	1:E:357:LEU:HA	1.78	0.41
1:G:124:GLU:O	1:G:159:ARG:NH2	2.50	0.41
1:H:86:ARG:HG3	1:H:89:ARG:NH2	2.36	0.41
1:I:120:ASP:OD1	1:I:121:ASP:N	2.53	0.41
1:I:287:ARG:HG3	1:I:327:GLN:NE2	2.35	0.41
1:K:115:HIS:ND1	1:K:166:VAL:CG2	2.83	0.41
1:K:279:ALA:CB	1:K:320:VAL:HG11	2.50	0.41
1:L:339:ALA:O	1:L:340:HIS:CD2	2.73	0.41
2:O:300:ILE:HD11	2:O:321:ILE:HG21	2.01	0.41
2:V:297:ASN:OD1	2:V:312:PHE:HD1	2.04	0.41
1:F:256:ARG:HD2	1:F:256:ARG:HA	1.63	0.41
1:G:274:ILE:CG2	1:G:275:MET:CE	2.85	0.41
1:G:385:THR:HB	1:G:388:MET:HE2	2.02	0.41
1:J:40:SER:HB2	1:J:83:ARG:HB2	2.01	0.41
1:K:140:LEU:C	1:K:141:GLU:HG3	2.41	0.41
2:Q:295:THR:HG22	2:Q:314:HIS:HD2	1.86	0.41
1:A:329:LEU:HD23	1:A:357:LEU:HD13	2.03	0.41
1:B:93:ARG:HE	1:B:194:GLU:HG3	1.85	0.41
1:B:140:LEU:C	1:B:141:GLU:HG2	2.41	0.41
1:C:329:LEU:HD23	1:C:357:LEU:HD13	2.03	0.41
1:D:118:PRO:HG3	1:D:130:LEU:CD1	2.51	0.41
1:F:279:ALA:CB	1:F:320:VAL:HG11	2.50	0.41
1:G:29:ASP:OD1	1:G:30:GLU:N	2.50	0.41
1:H:312:LYS:HB3	1:H:315:LYS:HG2	2.03	0.41
1:H:339:ALA:O	1:H:340:HIS:HD2	1.88	0.41
1:H:442:MET:SD	1:H:442:MET:N	2.93	0.41
1:I:336:LYS:HB2	1:I:338:ARG:NH2	2.34	0.41
1:K:49:LEU:HD13	1:K:49:LEU:HA	1.93	0.41
1:B:336:LYS:H	1:B:338:ARG:NH2	2.18	0.41
1:B:426:LYS:HE2	1:B:426:LYS:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:SER:HB2	1:D:83:ARG:HB2	2.02	0.41
1:E:297:ALA:HA	1:E:298:PRO:C	2.41	0.41
1:H:118:PRO:HG3	1:H:130:LEU:CD1	2.50	0.41
1:I:86:ARG:NH2	1:I:204:ASP:OD2	2.52	0.41
2:N:289:ILE:HD13	2:N:312:PHE:HB3	2.03	0.41
2:S:302:LEU:HB2	2:S:307:ARG:CB	2.45	0.41
2:W:318:ILE:HA	2:W:321:ILE:HD12	2.03	0.41
2:W:354:THR:HG22	2:W:357:GLU:CD	2.40	0.41
1:F:186:GLY:O	1:F:187:GLU:HB2	2.20	0.41
1:H:377:ARG:CZ	1:H:404:HIS:HA	2.51	0.41
1:I:377:ARG:CZ	1:I:404:HIS:HA	2.50	0.41
1:I:383:ILE:O	1:I:386:LYS:HG2	2.20	0.41
1:L:129:ASN:O	1:L:131:PHE:N	2.50	0.41
1:B:219:MET:HE1	1:B:241:ILE:HG12	2.03	0.41
1:B:283:GLU:CA	1:B:327:GLN:OE1	2.68	0.41
1:D:66:GLU:HG3	1:D:147:ARG:HE	1.86	0.41
1:E:186:GLY:O	1:E:187:GLU:HB2	2.21	0.41
1:F:129:ASN:O	1:F:131:PHE:N	2.46	0.41
1:H:89:ARG:HD3	1:H:96:LEU:HD13	2.03	0.41
1:I:25:ARG:O	1:I:26:LEU:HD13	2.21	0.41
1:K:22:ARG:HG2	1:K:23:PRO:HD2	2.01	0.41
1:L:356:ALA:O	1:L:362:ARG:HD2	2.21	0.41
1:L:430:ILE:HD13	1:L:441:VAL:HG11	2.01	0.41
1:A:336:LYS:H	1:A:338:ARG:NH2	2.18	0.41
1:B:244:TYR:OH	1:B:366:GLU:OE1	2.39	0.41
1:B:337:GLN:O	1:B:340:HIS:N	2.53	0.41
1:B:386:LYS:HB2	1:B:386:LYS:HE2	1.76	0.41
1:C:133:VAL:HG13	1:C:443:ASN:CG	2.40	0.41
1:C:327:GLN:CA	1:C:327:GLN:HE21	2.34	0.41
1:C:377:ARG:CZ	1:C:404:HIS:HA	2.50	0.41
1:D:89:ARG:HD3	1:D:96:LEU:HD13	2.03	0.41
1:E:86:ARG:O	1:E:87:VAL:C	2.58	0.41
1:E:437:ILE:HG22	1:E:440:GLU:HB3	2.01	0.41
1:F:210:ARG:HH22	1:F:211:LYS:HE3	1.85	0.41
1:G:186:GLY:O	1:G:187:GLU:HB2	2.21	0.41
1:G:385:THR:HA	1:G:388:MET:HE2	2.03	0.41
1:H:93:ARG:HE	1:H:194:GLU:HG3	1.86	0.41
1:I:25:ARG:C	1:I:26:LEU:HD22	2.41	0.41
1:J:297:ALA:HA	1:J:298:PRO:C	2.41	0.41
1:L:40:SER:HB2	1:L:83:ARG:HB2	2.01	0.41
1:L:359:ARG:HD3	1:L:359:ARG:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:453:ARG:HG3	1:L:453:ARG:HH11	1.86	0.41
2:Q:318:ILE:HD12	2:Q:348:LEU:HB3	2.03	0.41
2:S:321:ILE:HD11	2:S:355:LEU:CD2	2.45	0.41
2:T:318:ILE:HD12	2:T:348:LEU:HB3	2.02	0.41
2:W:289:ILE:HD13	2:W:312:PHE:HB3	2.03	0.41
1:I:416:SER:O	1:I:420:LEU:HD22	2.21	0.41
1:K:233:ILE:CG1	1:K:235:VAL:HG12	2.51	0.41
2:O:295:THR:HG22	2:O:314:HIS:HD2	1.85	0.41
2:U:289:ILE:HD13	2:U:312:PHE:HB3	2.02	0.41
1:B:40:SER:HB2	1:B:83:ARG:HB2	2.02	0.40
1:B:118:PRO:HG3	1:B:130:LEU:CD1	2.51	0.40
1:E:23:PRO:HA	1:E:45:LYS:NZ	2.36	0.40
1:I:336:LYS:H	1:I:338:ARG:NH2	2.18	0.40
1:J:377:ARG:CZ	1:J:404:HIS:HA	2.50	0.40
1:K:40:SER:HB2	1:K:83:ARG:HB2	2.03	0.40
1:L:287:ARG:HG3	1:L:327:GLN:NE2	2.35	0.40
1:L:297:ALA:HA	1:L:298:PRO:C	2.41	0.40
2:W:321:ILE:HD11	2:W:355:LEU:CD2	2.48	0.40
1:G:286:LEU:HD12	1:G:327:GLN:NE2	2.35	0.40
1:H:437:ILE:O	1:H:438:ASP:OD1	2.39	0.40
1:I:222:LEU:HB2	1:I:223:PRO:HD3	2.04	0.40
1:L:220:VAL:HG13	1:L:224:LEU:CD1	2.42	0.40
2:M:318:ILE:HA	2:M:321:ILE:HD12	2.04	0.40
2:S:289:ILE:HD13	2:S:312:PHE:HB3	2.04	0.40
1:B:49:LEU:HD13	1:B:49:LEU:HA	1.95	0.40
1:B:377:ARG:CZ	1:B:404:HIS:HA	2.50	0.40
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.85	0.40
1:F:40:SER:O	1:F:41:LEU:HD12	2.21	0.40
1:F:118:PRO:HG3	1:F:130:LEU:CD1	2.51	0.40
1:F:203:TYR:CE2	1:F:217:LYS:HD3	2.57	0.40
1:G:32:ILE:HD12	1:G:32:ILE:O	2.21	0.40
1:G:39:VAL:HG12	1:G:84:MET:HB3	2.02	0.40
2:O:360:LEU:HD22	2:O:365:ILE:HD11	2.03	0.40
1:A:133:VAL:HG13	1:A:443:ASN:CG	2.41	0.40
1:B:186:GLY:O	1:B:187:GLU:HB2	2.21	0.40
1:C:249:THR:HG22	1:C:251:LYS:HZ3	1.86	0.40
1:E:220:VAL:HG12	1:E:342:ILE:HD12	2.04	0.40
1:I:217:LYS:HE3	1:I:217:LYS:HB3	1.79	0.40
1:I:256:ARG:HD2	1:I:256:ARG:HA	1.61	0.40
2:U:318:ILE:HA	2:U:321:ILE:HD12	2.04	0.40
1:A:420:LEU:HD22	1:F:222:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:GLY:HA2	1:C:170:PRO:CD	2.35	0.40
1:E:226:HIS:CE1	1:F:427:MET:CE	3.04	0.40
1:F:39:VAL:HG12	1:F:84:MET:HB3	2.02	0.40
1:H:386:LYS:HB2	1:H:386:LYS:HE2	1.77	0.40
1:I:362:ARG:HB2	1:I:363:PHE:H	1.59	0.40
1:I:377:ARG:HH11	1:I:377:ARG:HD3	1.74	0.40
1:K:46:MET:HE2	1:K:73:SER:CA	2.52	0.40
1:L:49:LEU:HD13	1:L:49:LEU:HA	1.94	0.40
2:N:340:MET:CE	2:N:368:ARG:NH1	2.85	0.40
2:P:318:ILE:HD12	2:P:348:LEU:HB3	2.03	0.40
2:T:304:ASP:O	2:T:307:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (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	432/438 (99%)	400 (93%)	25 (6%)	7 (2%)	9 24
1	B	432/438 (99%)	404 (94%)	22 (5%)	6 (1%)	11 28
1	C	432/438 (99%)	403 (93%)	22 (5%)	7 (2%)	9 24
1	D	432/438 (99%)	396 (92%)	31 (7%)	5 (1%)	13 32
1	E	432/438 (99%)	397 (92%)	27 (6%)	8 (2%)	8 20
1	F	432/438 (99%)	403 (93%)	23 (5%)	6 (1%)	11 28
1	G	432/438 (99%)	404 (94%)	23 (5%)	5 (1%)	13 32
1	H	432/438 (99%)	403 (93%)	23 (5%)	6 (1%)	11 28
1	I	432/438 (99%)	404 (94%)	22 (5%)	6 (1%)	11 28
1	J	432/438 (99%)	403 (93%)	22 (5%)	7 (2%)	9 24
1	K	432/438 (99%)	403 (93%)	21 (5%)	8 (2%)	8 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	432/438 (99%)	400 (93%)	25 (6%)	7 (2%)	9	24
2	M	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	N	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	O	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	P	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	Q	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	R	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	S	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	6	15
2	T	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	6	15
2	U	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	V	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	W	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
2	X	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	32
All	All	6180/6276 (98%)	5745 (93%)	343 (6%)	92 (2%)	10	26

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLY
1	A	282	SER
1	A	340	HIS
1	B	340	HIS
1	B	441	VAL
1	C	186	GLY
1	C	340	HIS
1	C	441	VAL
1	D	340	HIS
1	E	171	SER
1	E	186	GLY
1	E	441	VAL
1	F	186	GLY
1	F	340	HIS
1	G	186	GLY
1	G	340	HIS
1	H	186	GLY
1	H	340	HIS
1	H	441	VAL

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Mol	Chain	Res	Type
1	I	186	GLY
1	I	340	HIS
1	J	340	HIS
1	J	441	VAL
1	K	340	HIS
1	L	187	GLU
2	R	304	ASP
2	S	304	ASP
1	A	441	VAL
1	B	186	GLY
1	C	171	SER
1	D	186	GLY
1	D	441	VAL
1	E	340	HIS
1	F	441	VAL
1	G	441	VAL
1	H	339	ALA
1	I	441	VAL
1	J	186	GLY
1	K	130	LEU
1	K	186	GLY
1	K	441	VAL
1	L	186	GLY
1	L	336	LYS
1	L	441	VAL
2	M	304	ASP
2	N	304	ASP
2	O	304	ASP
2	P	304	ASP
2	Q	304	ASP
2	T	304	ASP
2	U	304	ASP
2	V	304	ASP
2	W	304	ASP
2	X	304	ASP
1	B	438	ASP
1	C	130	LEU
1	G	338	ARG
1	J	336	LYS
1	K	359	ARG
1	A	187	GLU
1	A	336	LYS

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Mol	Chain	Res	Type
1	B	187	GLU
1	B	336	LYS
1	C	187	GLU
1	E	187	GLU
1	E	336	LYS
1	F	336	LYS
1	G	187	GLU
1	H	187	GLU
1	I	336	LYS
1	J	187	GLU
1	J	339	ALA
1	K	336	LYS
1	L	185	GLU
1	L	339	ALA
2	T	314	HIS
1	C	438	ASP
1	D	187	GLU
1	F	187	GLU
1	I	187	GLU
1	J	438	ASP
1	K	438	ASP
1	A	438	ASP
1	D	336	LYS
1	E	438	ASP
1	F	438	ASP
1	H	438	ASP
1	I	438	ASP
1	K	187	GLU
1	L	438	ASP
2	S	314	HIS
1	E	170	PRO

5.3.2 Protein sidechains (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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/373 (99%)	343 (93%)	27 (7%)	14	33
1	B	370/373 (99%)	345 (93%)	25 (7%)	16	36
1	C	368/373 (99%)	337 (92%)	31 (8%)	11	25
1	D	369/373 (99%)	335 (91%)	34 (9%)	9	21
1	E	362/373 (97%)	328 (91%)	34 (9%)	8	20
1	F	370/373 (99%)	347 (94%)	23 (6%)	18	40
1	G	365/373 (98%)	335 (92%)	30 (8%)	11	26
1	H	370/373 (99%)	342 (92%)	28 (8%)	13	30
1	I	370/373 (99%)	347 (94%)	23 (6%)	18	40
1	J	369/373 (99%)	339 (92%)	30 (8%)	11	27
1	K	370/373 (99%)	342 (92%)	28 (8%)	13	30
1	L	366/373 (98%)	343 (94%)	23 (6%)	18	40
2	M	75/75 (100%)	62 (83%)	13 (17%)	2	5
2	N	74/75 (99%)	64 (86%)	10 (14%)	4	9
2	O	74/75 (99%)	67 (90%)	7 (10%)	8	20
2	P	74/75 (99%)	64 (86%)	10 (14%)	4	9
2	Q	75/75 (100%)	67 (89%)	8 (11%)	6	15
2	R	75/75 (100%)	66 (88%)	9 (12%)	5	11
2	S	75/75 (100%)	63 (84%)	12 (16%)	2	6
2	T	75/75 (100%)	67 (89%)	8 (11%)	6	15
2	U	75/75 (100%)	67 (89%)	8 (11%)	6	15
2	V	75/75 (100%)	63 (84%)	12 (16%)	2	6
2	W	75/75 (100%)	66 (88%)	9 (12%)	5	11
2	X	75/75 (100%)	65 (87%)	10 (13%)	4	9
All	All	5316/5376 (99%)	4864 (92%)	452 (8%)	10	24

All (452) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	50	GLN
1	A	57	VAL

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Mol	Chain	Res	Type
1	A	80	GLU
1	A	88	VAL
1	A	105	CYS
1	A	147	ARG
1	A	158	MET
1	A	171	SER
1	A	181	VAL
1	A	187	GLU
1	A	287	ARG
1	A	288	LYS
1	A	312	LYS
1	A	325	VAL
1	A	335	LEU
1	A	338	ARG
1	A	349	ARG
1	A	358	ARG
1	A	373	ASP
1	A	375	THR
1	A	411	LEU
1	A	416	SER
1	A	426	LYS
1	A	428	ASP
1	A	440	GLU
1	A	445	LEU
1	B	49	LEU
1	B	96	LEU
1	B	105	CYS
1	B	113	ARG
1	B	158	MET
1	B	164	LYS
1	B	171	SER
1	B	183	HIS
1	B	187	GLU
1	B	190	LYS
1	B	212	GLN
1	B	249	THR
1	B	277	LYS
1	B	313	ARG
1	B	328	LEU
1	B	335	LEU
1	B	338	ARG
1	B	340	HIS

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Mol	Chain	Res	Type
1	B	358	ARG
1	B	399	VAL
1	B	416	SER
1	B	428	ASP
1	B	440	GLU
1	B	445	LEU
1	B	453	ARG
1	C	22	ARG
1	C	49	LEU
1	C	88	VAL
1	C	96	LEU
1	C	103	GLN
1	C	105	CYS
1	C	158	MET
1	C	164	LYS
1	C	168	THR
1	C	171	SER
1	C	181	VAL
1	C	187	GLU
1	C	211	LYS
1	C	239	ARG
1	C	249	THR
1	C	262	THR
1	C	277	LYS
1	C	313	ARG
1	C	320	VAL
1	C	325	VAL
1	C	327	GLN
1	C	337	GLN
1	C	349	ARG
1	C	375	THR
1	C	382	GLN
1	C	396	LEU
1	C	440	GLU
1	C	441	VAL
1	C	445	LEU
1	C	453	ARG
1	C	456	LEU
1	D	22	ARG
1	D	49	LEU
1	D	58	LEU
1	D	59	LEU

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Mol	Chain	Res	Type
1	D	66	GLU
1	D	96	LEU
1	D	103	GLN
1	D	105	CYS
1	D	131	PHE
1	D	135	LEU
1	D	158	MET
1	D	171	SER
1	D	187	GLU
1	D	194	GLU
1	D	200	GLU
1	D	204	ASP
1	D	210	ARG
1	D	212	GLN
1	D	249	THR
1	D	256	ARG
1	D	277	LYS
1	D	307	ASP
1	D	320	VAL
1	D	327	GLN
1	D	338	ARG
1	D	349	ARG
1	D	358	ARG
1	D	362	ARG
1	D	381	LEU
1	D	416	SER
1	D	426	LYS
1	D	442	MET
1	D	453	ARG
1	D	456	LEU
1	E	46	MET
1	E	49	LEU
1	E	63	LYS
1	E	64	ARG
1	E	75	ASP
1	E	88	VAL
1	E	94	VAL
1	E	105	CYS
1	E	113	ARG
1	E	148	LYS
1	E	158	MET
1	E	165	VAL

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Mol	Chain	Res	Type
1	E	170	PRO
1	E	171	SER
1	E	187	GLU
1	E	222	LEU
1	E	277	LYS
1	E	328	LEU
1	E	335	LEU
1	E	342	ILE
1	E	353	ILE
1	E	358	ARG
1	E	378	LEU
1	E	382	GLN
1	E	396	LEU
1	E	416	SER
1	E	421	GLN
1	E	433	GLU
1	E	440	GLU
1	E	441	VAL
1	E	442	MET
1	E	443	ASN
1	E	445	LEU
1	E	457	SER
1	F	43	GLN
1	F	49	LEU
1	F	86	ARG
1	F	88	VAL
1	F	105	CYS
1	F	158	MET
1	F	171	SER
1	F	187	GLU
1	F	200	GLU
1	F	212	GLN
1	F	218	GLU
1	F	225	ARG
1	F	231	LYS
1	F	277	LYS
1	F	286	LEU
1	F	315	LYS
1	F	325	VAL
1	F	416	SER
1	F	420	LEU
1	F	426	LYS

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Mol	Chain	Res	Type
1	F	441	VAL
1	F	445	LEU
1	F	449	MET
1	G	22	ARG
1	G	24	ASN
1	G	32	ILE
1	G	49	LEU
1	G	51	LEU
1	G	80	GLU
1	G	88	VAL
1	G	99	VAL
1	G	105	CYS
1	G	109	LYS
1	G	113	ARG
1	G	147	ARG
1	G	158	MET
1	G	159	ARG
1	G	164	LYS
1	G	171	SER
1	G	187	GLU
1	G	210	ARG
1	G	262	THR
1	G	320	VAL
1	G	325	VAL
1	G	327	GLN
1	G	329	LEU
1	G	398	GLN
1	G	416	SER
1	G	420	LEU
1	G	421	GLN
1	G	426	LYS
1	G	445	LEU
1	G	449	MET
1	H	49	LEU
1	H	88	VAL
1	H	96	LEU
1	H	100	ILE
1	H	105	CYS
1	H	113	ARG
1	H	158	MET
1	H	171	SER
1	H	187	GLU

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Mol	Chain	Res	Type
1	H	212	GLN
1	H	225	ARG
1	H	249	THR
1	H	262	THR
1	H	286	LEU
1	H	313	ARG
1	H	325	VAL
1	H	328	LEU
1	H	338	ARG
1	H	340	HIS
1	H	351	ASN
1	H	382	GLN
1	H	396	LEU
1	H	416	SER
1	H	438	ASP
1	H	440	GLU
1	H	442	MET
1	H	443	ASN
1	H	449	MET
1	I	49	LEU
1	I	80	GLU
1	I	88	VAL
1	I	133	VAL
1	I	158	MET
1	I	171	SER
1	I	212	GLN
1	I	217	LYS
1	I	222	LEU
1	I	249	THR
1	I	261	GLU
1	I	325	VAL
1	I	338	ARG
1	I	362	ARG
1	I	399	VAL
1	I	416	SER
1	I	420	LEU
1	I	428	ASP
1	I	440	GLU
1	I	442	MET
1	I	443	ASN
1	I	449	MET
1	I	453	ARG

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Mol	Chain	Res	Type
1	J	64	ARG
1	J	73	SER
1	J	88	VAL
1	J	96	LEU
1	J	105	CYS
1	J	113	ARG
1	J	158	MET
1	J	164	LYS
1	J	171	SER
1	J	187	GLU
1	J	190	LYS
1	J	212	GLN
1	J	215	GLN
1	J	277	LYS
1	J	287	ARG
1	J	313	ARG
1	J	320	VAL
1	J	325	VAL
1	J	338	ARG
1	J	358	ARG
1	J	362	ARG
1	J	396	LEU
1	J	399	VAL
1	J	414	LEU
1	J	416	SER
1	J	424	ARG
1	J	437	ILE
1	J	440	GLU
1	J	443	ASN
1	J	453	ARG
1	K	49	LEU
1	K	58	LEU
1	K	88	VAL
1	K	96	LEU
1	K	105	CYS
1	K	120	ASP
1	K	133	VAL
1	K	141	GLU
1	K	158	MET
1	K	171	SER
1	K	194	GLU
1	K	200	GLU

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Mol	Chain	Res	Type
1	K	204	ASP
1	K	254	ILE
1	K	256	ARG
1	K	261	GLU
1	K	277	LYS
1	K	327	GLN
1	K	335	LEU
1	K	358	ARG
1	K	359	ARG
1	K	396	LEU
1	K	416	SER
1	K	433	GLU
1	K	440	GLU
1	K	442	MET
1	K	445	LEU
1	K	453	ARG
1	L	22	ARG
1	L	49	LEU
1	L	64	ARG
1	L	76	THR
1	L	88	VAL
1	L	105	CYS
1	L	158	MET
1	L	164	LYS
1	L	171	SER
1	L	184	CYS
1	L	187	GLU
1	L	335	LEU
1	L	358	ARG
1	L	359	ARG
1	L	375	THR
1	L	396	LEU
1	L	416	SER
1	L	428	ASP
1	L	442	MET
1	L	443	ASN
1	L	449	MET
1	L	453	ARG
1	L	457	SER
2	M	286	MET
2	M	308	LEU
2	M	311	LYS

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

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Mol	Chain	Res	Type
2	Q	335	THR
2	Q	362	ASN
2	Q	369	LEU
2	R	287	ILE
2	R	304	ASP
2	R	308	LEU
2	R	311	LYS
2	R	312	PHE
2	R	314	HIS
2	R	335	THR
2	R	338	ILE
2	R	354	THR
2	S	295	THR
2	S	304	ASP
2	S	307	ARG
2	S	308	LEU
2	S	311	LYS
2	S	312	PHE
2	S	314	HIS
2	S	318	ILE
2	S	329	ARG
2	S	332	MET
2	S	340	MET
2	S	341	THR
2	T	287	ILE
2	T	301	ARG
2	T	302	LEU
2	T	311	LYS
2	T	312	PHE
2	T	314	HIS
2	T	354	THR
2	T	369	LEU
2	U	308	LEU
2	U	311	LYS
2	U	312	PHE
2	U	314	HIS
2	U	318	ILE
2	U	335	THR
2	U	362	ASN
2	U	369	LEU
2	V	286	MET
2	V	287	ILE

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Mol	Chain	Res	Type
2	V	308	LEU
2	V	311	LYS
2	V	312	PHE
2	V	314	HIS
2	V	315	SER
2	V	332	MET
2	V	335	THR
2	V	341	THR
2	V	365	ILE
2	V	369	LEU
2	W	286	MET
2	W	308	LEU
2	W	311	LYS
2	W	312	PHE
2	W	314	HIS
2	W	315	SER
2	W	323	LEU
2	W	335	THR
2	W	362	ASN
2	X	291	GLU
2	X	308	LEU
2	X	311	LYS
2	X	312	PHE
2	X	314	HIS
2	X	329	ARG
2	X	332	MET
2	X	335	THR
2	X	354	THR
2	X	362	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	285	ASN
1	A	327	GLN
1	B	212	GLN
1	B	340	HIS
1	C	129	ASN
1	C	183	HIS
1	C	398	GLN
1	D	103	GLN

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Mol	Chain	Res	Type
1	D	285	ASN
1	D	384	HIS
1	E	43	GLN
1	E	115	HIS
1	E	183	HIS
1	E	270	ASN
1	E	285	ASN
1	E	327	GLN
1	E	340	HIS
1	E	351	ASN
1	E	421	GLN
1	F	327	GLN
1	G	24	ASN
1	G	50	GLN
1	G	327	GLN
1	G	421	GLN
1	H	212	GLN
1	H	340	HIS
1	I	129	ASN
1	I	270	ASN
1	I	327	GLN
1	J	398	GLN
1	K	129	ASN
1	K	183	HIS
1	L	327	GLN
1	L	398	GLN
1	L	443	ASN
2	M	359	ASN
2	N	314	HIS
2	P	299	GLN
2	P	314	HIS
2	Q	299	GLN
2	S	314	HIS
2	T	313	ASN
2	U	299	GLN
2	U	310	GLN
2	V	299	GLN
2	W	299	GLN
2	W	314	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	0.60	0	29,45,45	0.88	1 (3%)
3	ADP	G	501	-	24,29,29	0.65	0	29,45,45	0.83	1 (3%)
3	ADP	H	501	-	24,29,29	0.67	0	29,45,45	0.84	0
3	ADP	I	501	-	24,29,29	0.56	0	29,45,45	0.98	3 (10%)
3	ADP	A	501	-	24,29,29	0.54	0	29,45,45	1.02	1 (3%)
3	ADP	K	501	-	24,29,29	0.60	0	29,45,45	1.01	1 (3%)
3	ADP	F	501	-	24,29,29	0.64	0	29,45,45	0.84	1 (3%)
3	ADP	J	501	-	24,29,29	0.63	0	29,45,45	0.88	0
3	ADP	L	501	-	24,29,29	0.68	0	29,45,45	1.01	2 (6%)
3	ADP	D	501	-	24,29,29	0.69	0	29,45,45	0.93	1 (3%)
3	ADP	E	501	-	24,29,29	0.66	0	29,45,45	0.97	2 (6%)
3	ADP	C	501	-	24,29,29	0.65	0	29,45,45	1.10	3 (10%)

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	-	-	4/12/32/32	0/3/3/3
3	ADP	G	501	-	-	2/12/32/32	0/3/3/3
3	ADP	H	501	-	-	5/12/32/32	0/3/3/3
3	ADP	I	501	-	-	7/12/32/32	0/3/3/3
3	ADP	A	501	-	-	4/12/32/32	0/3/3/3
3	ADP	K	501	-	-	6/12/32/32	0/3/3/3
3	ADP	F	501	-	-	4/12/32/32	0/3/3/3
3	ADP	J	501	-	-	5/12/32/32	0/3/3/3
3	ADP	L	501	-	-	4/12/32/32	0/3/3/3
3	ADP	D	501	-	-	4/12/32/32	0/3/3/3
3	ADP	E	501	-	-	3/12/32/32	0/3/3/3
3	ADP	C	501	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	ADP	O2B-PB-O3A	3.35	115.86	104.64
3	E	501	ADP	C5-C6-N6	2.93	124.81	120.35
3	B	501	ADP	C5-C6-N6	2.67	124.41	120.35
3	F	501	ADP	C5-C6-N6	2.67	124.41	120.35
3	C	501	ADP	O3A-PB-O1B	-2.65	96.51	111.19
3	I	501	ADP	C5-C6-N6	2.56	124.24	120.35
3	G	501	ADP	C5-C6-N6	2.49	124.14	120.35
3	L	501	ADP	O2B-PB-O3A	2.31	112.37	104.64
3	D	501	ADP	C5-C6-N6	2.24	123.76	120.35
3	E	501	ADP	PA-O3A-PB	-2.16	125.42	132.83
3	K	501	ADP	O3'-C3'-C4'	2.15	117.27	111.05
3	A	501	ADP	C5-C6-N6	2.13	123.59	120.35
3	L	501	ADP	C5-C6-N6	2.09	123.52	120.35
3	I	501	ADP	O2B-PB-O3A	2.04	111.47	104.64
3	C	501	ADP	C5-C6-N6	2.02	123.42	120.35
3	I	501	ADP	O3A-PB-O1B	-2.00	100.09	111.19

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O3A
3	B	501	ADP	C5'-O5'-PA-O2A
3	B	501	ADP	C5'-O5'-PA-O3A
3	D	501	ADP	C5'-O5'-PA-O1A
3	D	501	ADP	C5'-O5'-PA-O2A
3	E	501	ADP	C5'-O5'-PA-O1A
3	F	501	ADP	C5'-O5'-PA-O3A
3	G	501	ADP	C5'-O5'-PA-O2A
3	G	501	ADP	C5'-O5'-PA-O3A
3	H	501	ADP	C5'-O5'-PA-O1A
3	H	501	ADP	C5'-O5'-PA-O2A
3	I	501	ADP	PA-O3A-PB-O3B
3	I	501	ADP	C5'-O5'-PA-O1A
3	J	501	ADP	C5'-O5'-PA-O3A
3	K	501	ADP	PA-O3A-PB-O2B
3	K	501	ADP	C5'-O5'-PA-O2A
3	L	501	ADP	C5'-O5'-PA-O1A
3	H	501	ADP	O4'-C4'-C5'-O5'
3	C	501	ADP	PA-O3A-PB-O1B
3	H	501	ADP	C3'-C4'-C5'-O5'
3	E	501	ADP	C5'-O5'-PA-O3A
3	I	501	ADP	C5'-O5'-PA-O3A
3	K	501	ADP	C5'-O5'-PA-O3A
3	L	501	ADP	C5'-O5'-PA-O3A
3	E	501	ADP	PB-O3A-PA-O2A
3	J	501	ADP	PB-O3A-PA-O2A
3	L	501	ADP	PB-O3A-PA-O1A
3	A	501	ADP	C5'-O5'-PA-O1A
3	F	501	ADP	C5'-O5'-PA-O1A
3	I	501	ADP	C5'-O5'-PA-O2A
3	J	501	ADP	C5'-O5'-PA-O1A
3	J	501	ADP	C5'-O5'-PA-O2A
3	K	501	ADP	C5'-O5'-PA-O1A
3	K	501	ADP	C3'-C4'-C5'-O5'
3	A	501	ADP	C4'-C5'-O5'-PA
3	L	501	ADP	C4'-C5'-O5'-PA
3	A	501	ADP	PB-O3A-PA-O2A
3	B	501	ADP	PB-O3A-PA-O1A
3	F	501	ADP	PB-O3A-PA-O2A
3	I	501	ADP	C3'-C4'-C5'-O5'
3	K	501	ADP	PA-O3A-PB-O1B
3	D	501	ADP	C3'-C4'-C5'-O5'
3	I	501	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	C	501	ADP	C5'-O5'-PA-O3A
3	D	501	ADP	C5'-O5'-PA-O3A
3	H	501	ADP	C5'-O5'-PA-O3A
3	B	501	ADP	PB-O3A-PA-O2A
3	J	501	ADP	PB-O3A-PA-O1A
3	F	501	ADP	C5'-O5'-PA-O2A
3	I	501	ADP	PA-O3A-PB-O1B

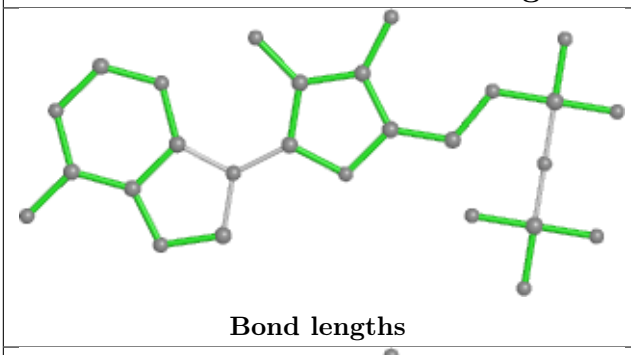
There are no ring outliers.

5 monomers are involved in 7 short contacts:

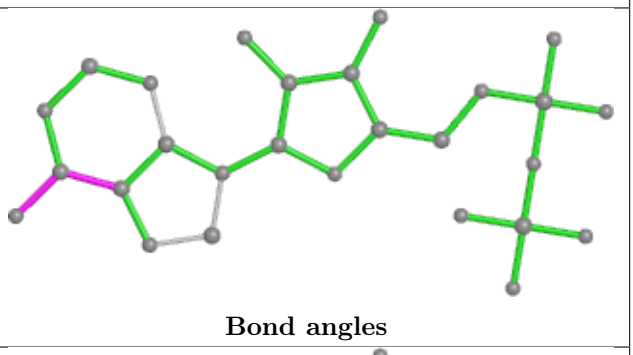
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	501	ADP	1	0
3	A	501	ADP	3	0
3	L	501	ADP	1	0
3	D	501	ADP	1	0
3	C	501	ADP	1	0

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

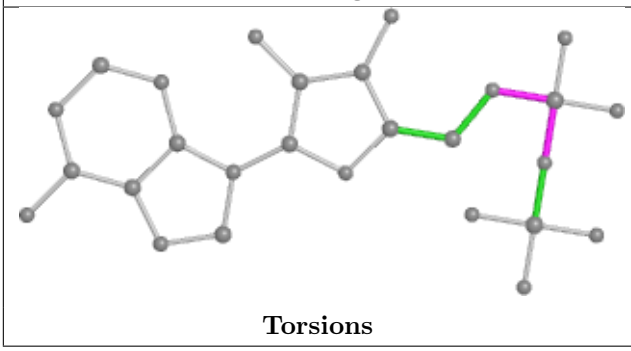
Ligand ADP B 501



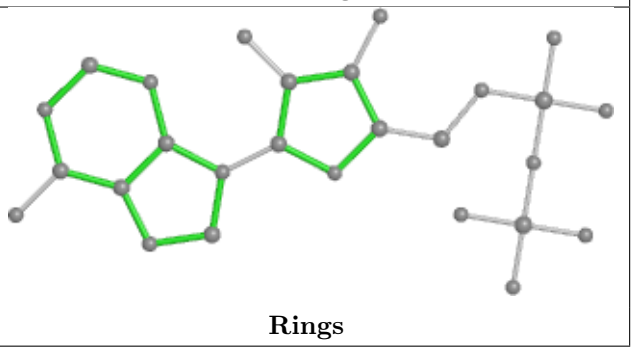
Bond lengths



Bond angles

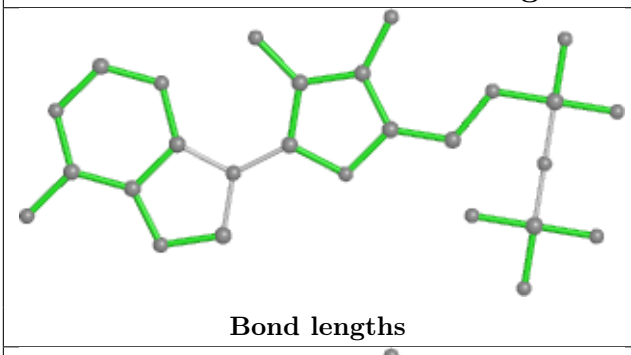


Torsions

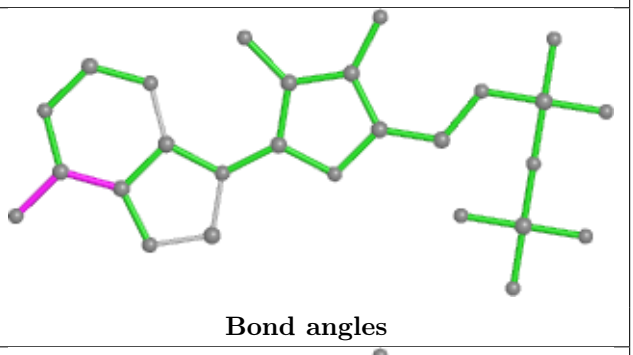


Rings

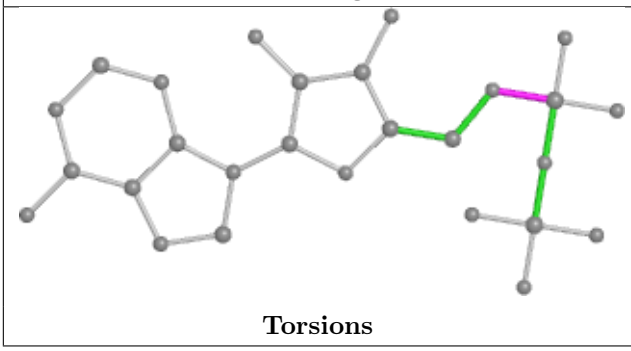
Ligand ADP G 501



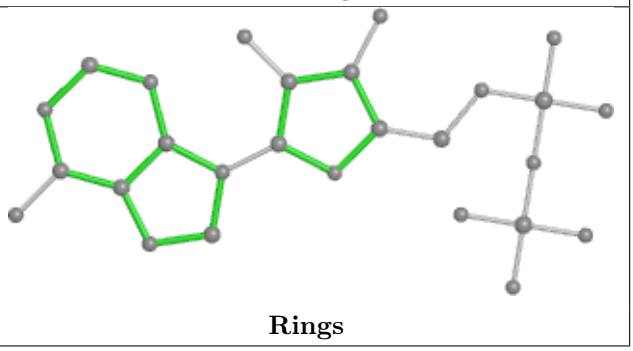
Bond lengths



Bond angles

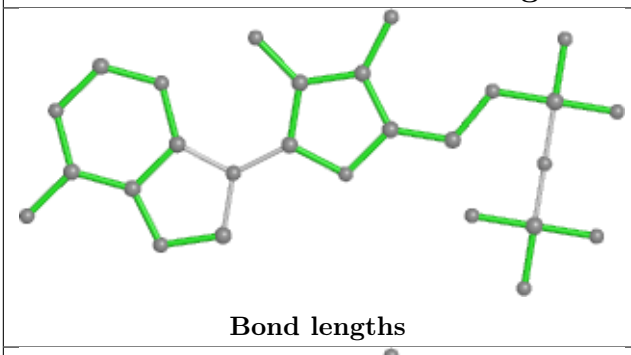


Torsions

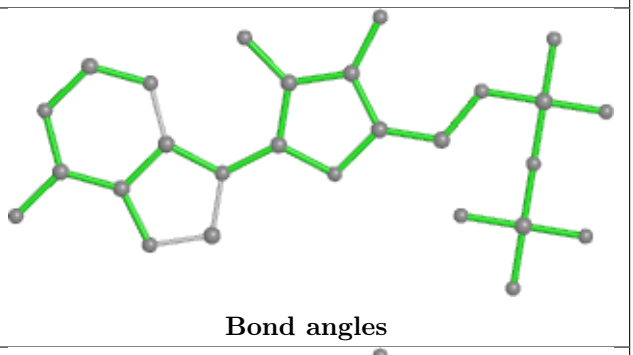


Rings

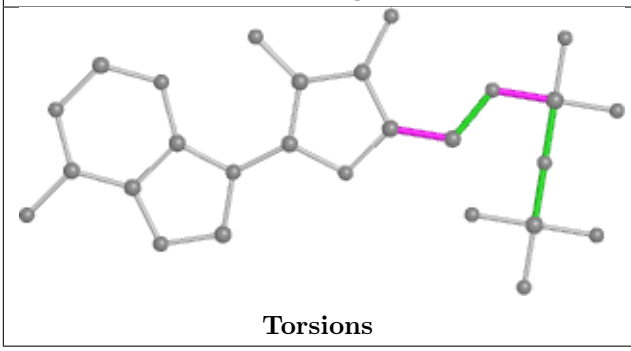
Ligand ADP H 501



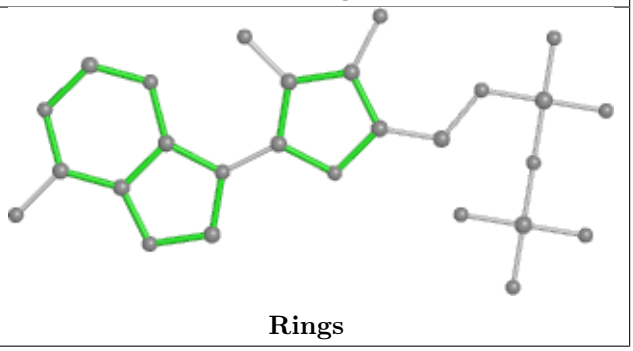
Bond lengths



Bond angles

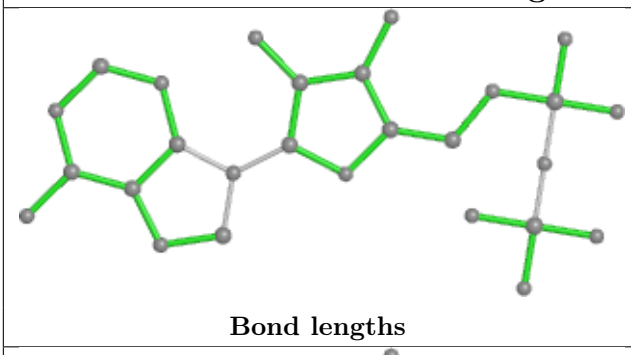


Torsions

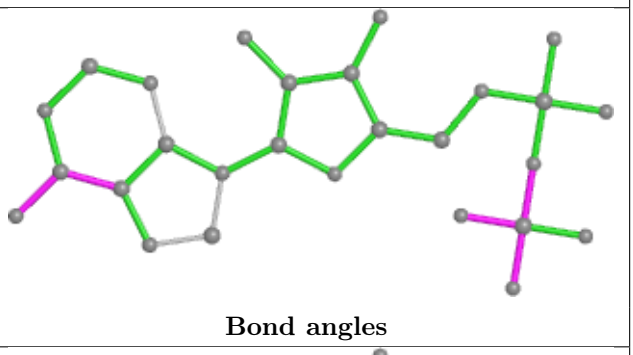


Rings

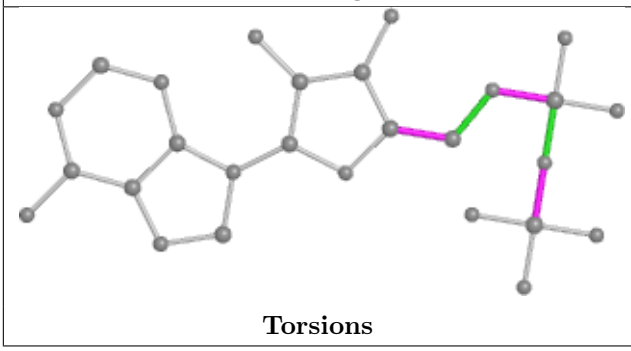
Ligand ADP I 501



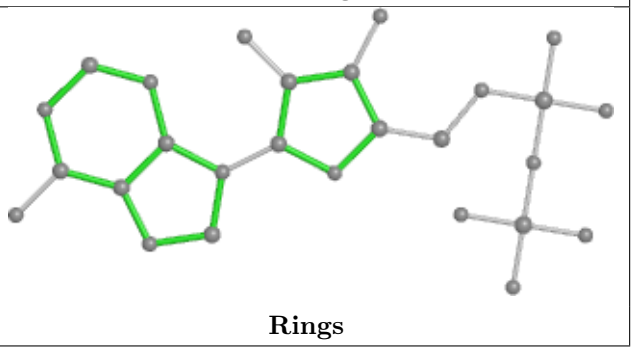
Bond lengths



Bond angles

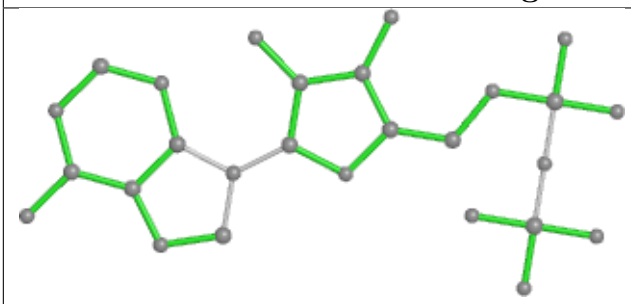


Torsions

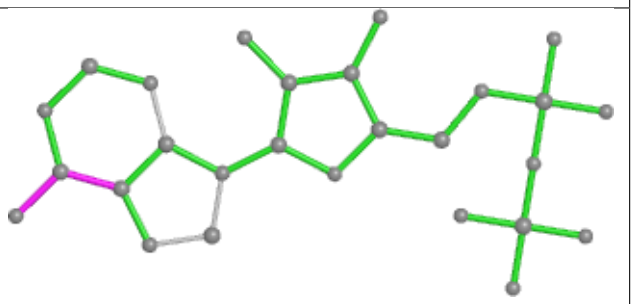


Rings

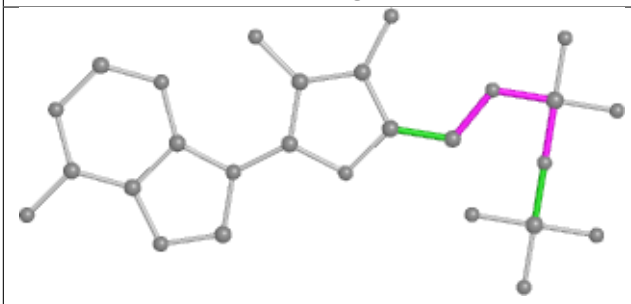
Ligand ADP A 501



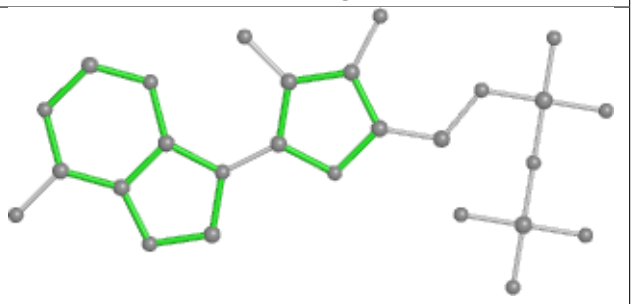
Bond lengths



Bond angles

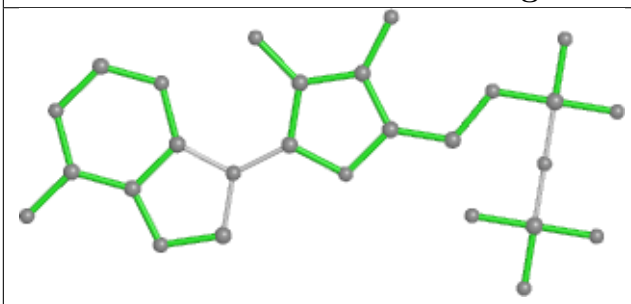


Torsions

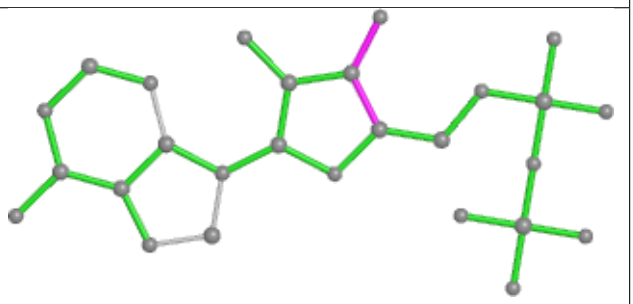


Rings

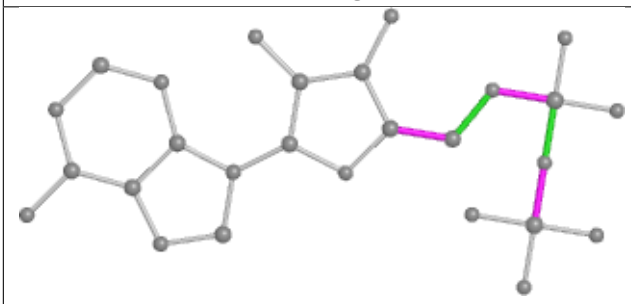
Ligand ADP K 501



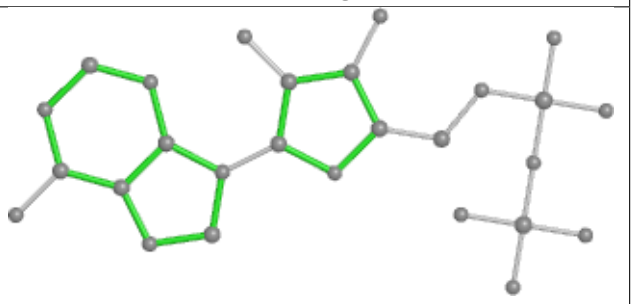
Bond lengths



Bond angles

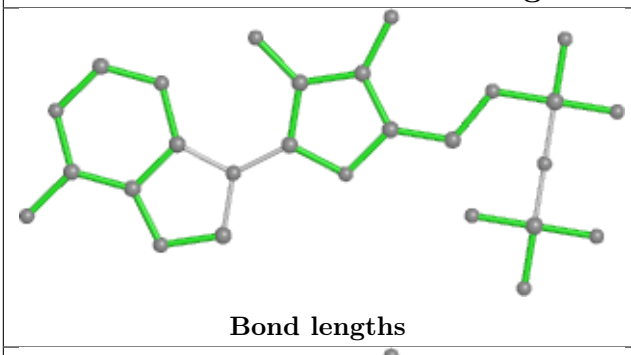


Torsions

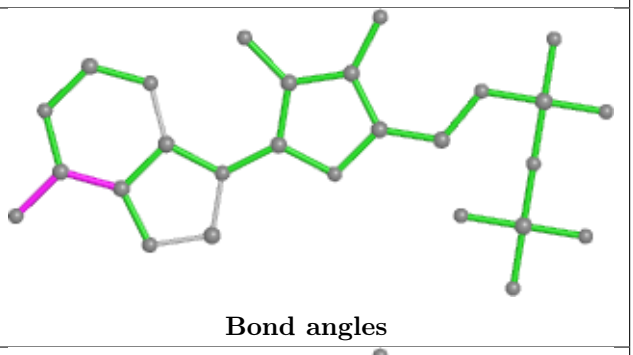


Rings

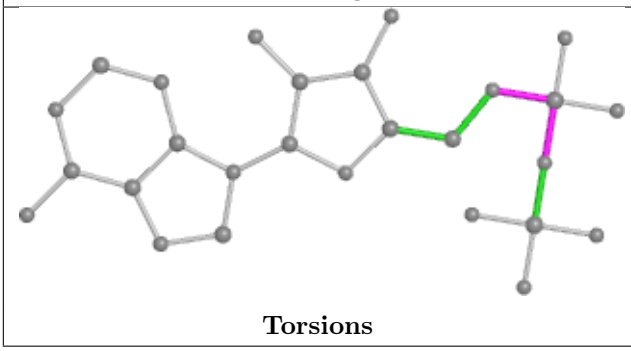
Ligand ADP F 501



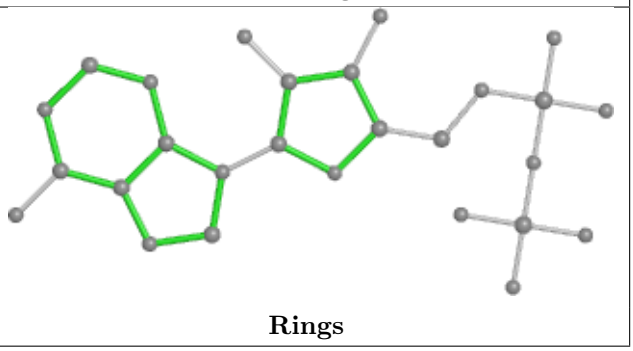
Bond lengths



Bond angles

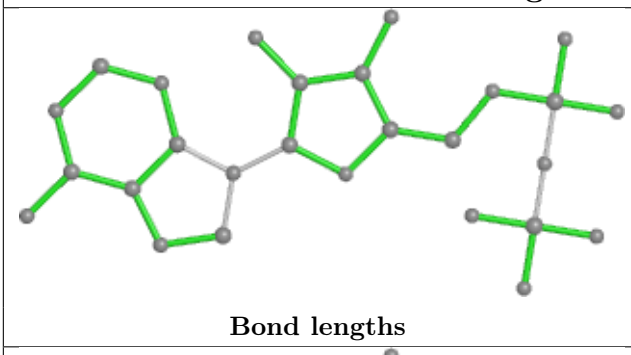


Torsions

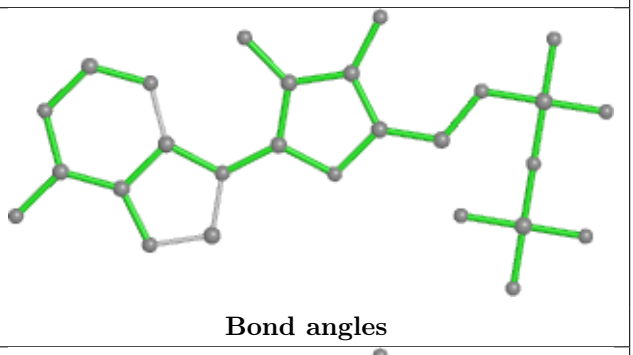


Rings

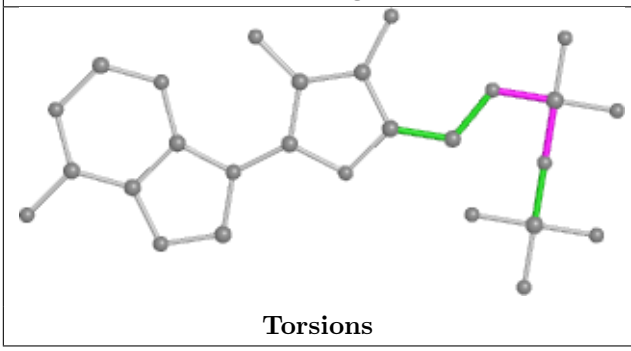
Ligand ADP J 501



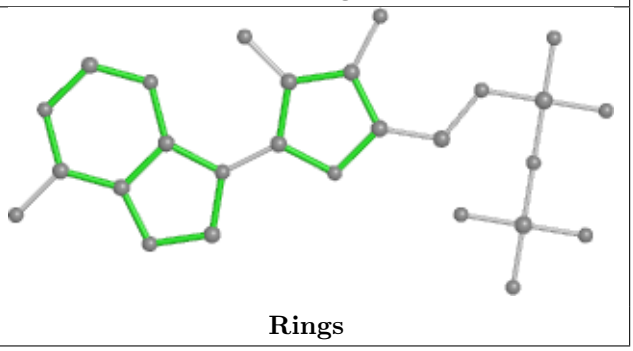
Bond lengths



Bond angles

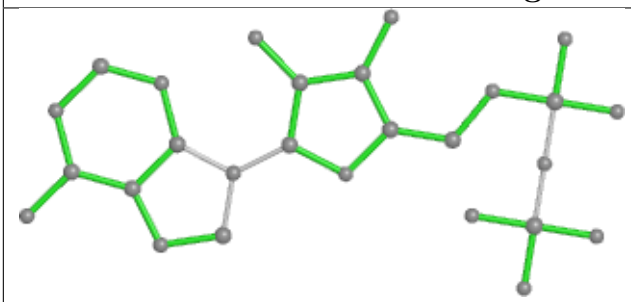


Torsions

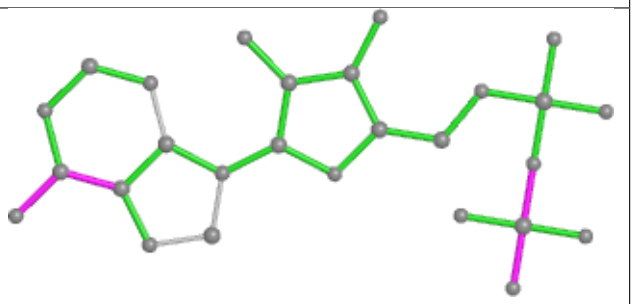


Rings

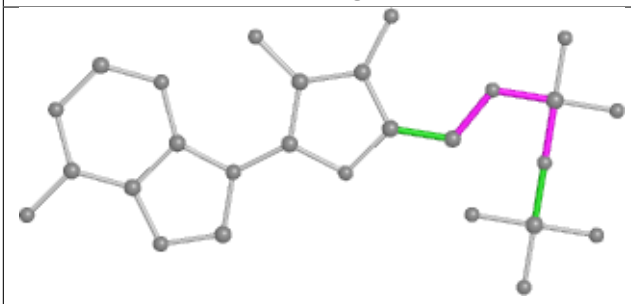
Ligand ADP L 501



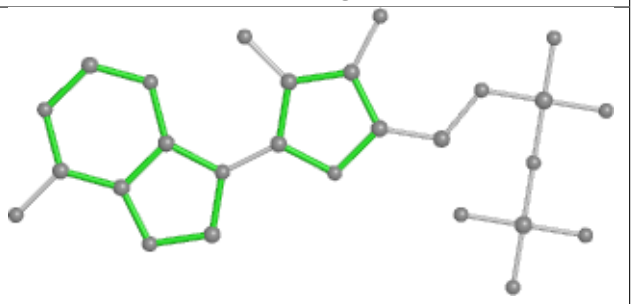
Bond lengths



Bond angles

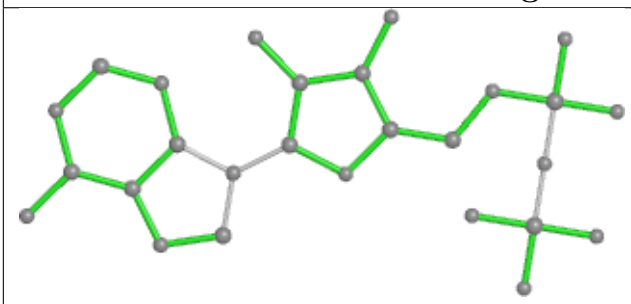


Torsions

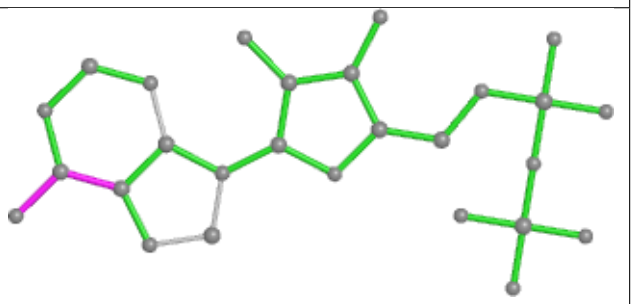


Rings

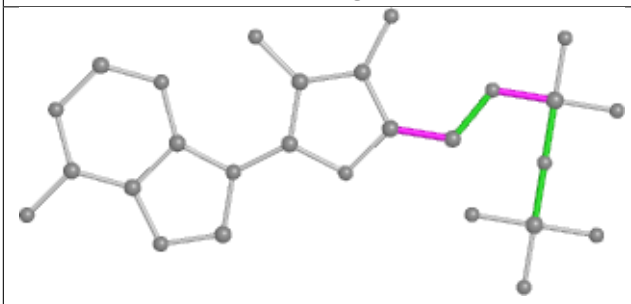
Ligand ADP D 501



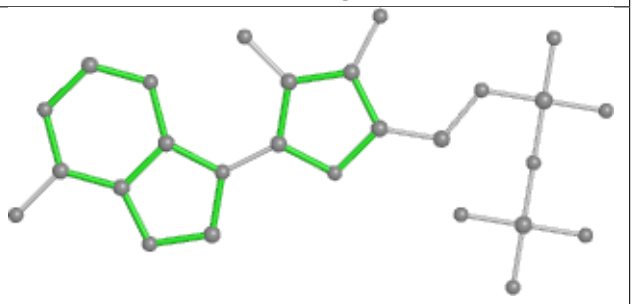
Bond lengths



Bond angles

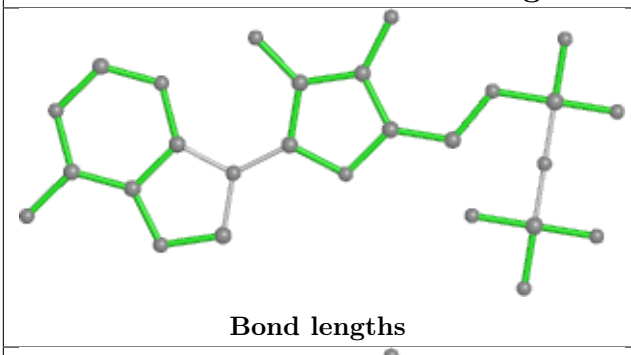


Torsions

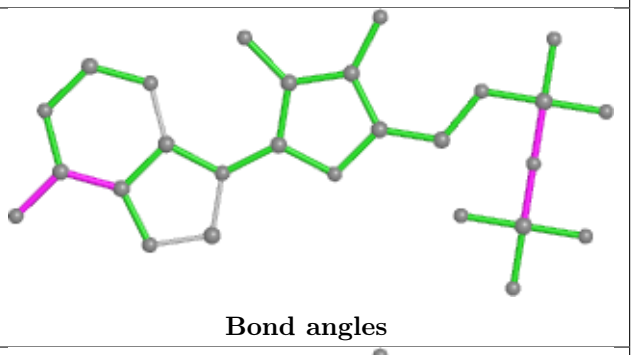


Rings

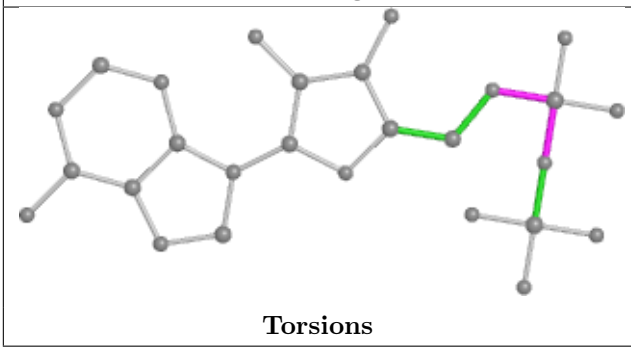
Ligand ADP E 501



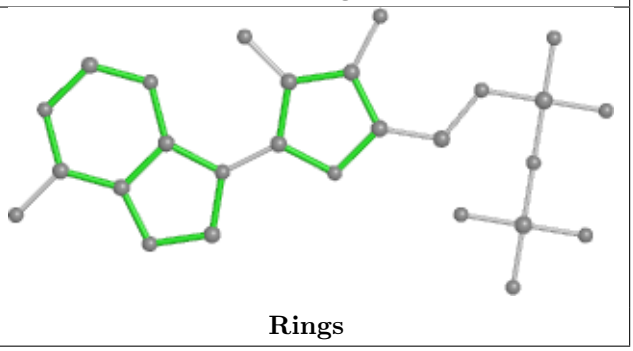
Bond lengths



Bond angles

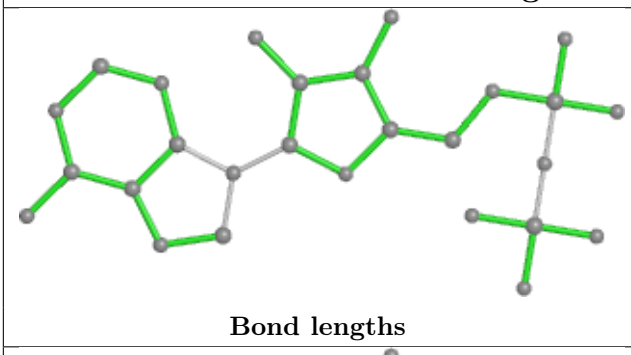


Torsions

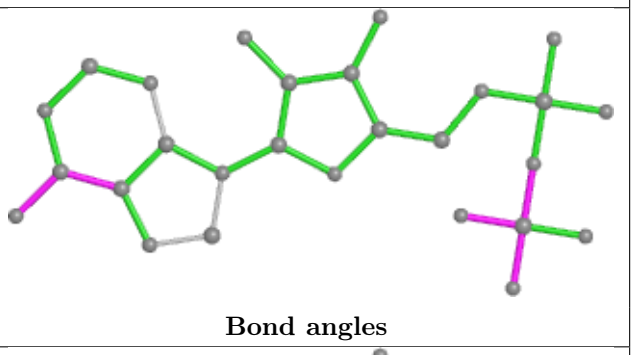


Rings

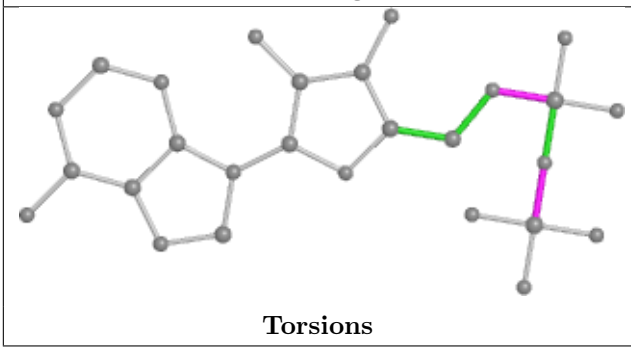
Ligand ADP C 501



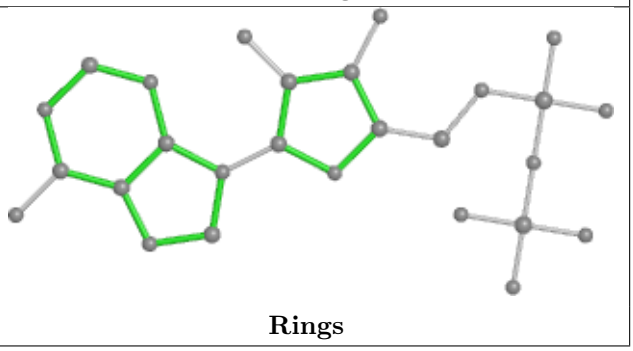
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	436/438 (99%)	0.11	20 (4%)	32	31	35, 66, 127, 193	0
1	B	436/438 (99%)	0.07	13 (2%)	50	51	33, 58, 121, 219	0
1	C	436/438 (99%)	0.06	13 (2%)	50	51	35, 58, 116, 196	0
1	D	436/438 (99%)	0.24	24 (5%)	25	24	39, 67, 133, 224	0
1	E	436/438 (99%)	0.36	26 (5%)	21	20	30, 77, 132, 206	0
1	F	436/438 (99%)	0.23	28 (6%)	19	18	35, 66, 133, 211	0
1	G	436/438 (99%)	0.23	24 (5%)	25	24	46, 71, 132, 203	0
1	H	436/438 (99%)	0.06	16 (3%)	41	41	40, 63, 126, 202	0
1	I	436/438 (99%)	0.09	17 (3%)	39	38	36, 66, 125, 186	0
1	J	436/438 (99%)	0.10	12 (2%)	53	54	34, 61, 119, 197	0
1	K	436/438 (99%)	0.07	14 (3%)	47	48	35, 61, 117, 182	0
1	L	436/438 (99%)	0.10	18 (4%)	37	36	36, 67, 124, 207	0
2	M	85/85 (100%)	-0.15	1 (1%)	79	80	37, 60, 99, 119	0
2	N	85/85 (100%)	-0.08	2 (2%)	59	60	42, 63, 104, 138	0
2	O	85/85 (100%)	-0.16	1 (1%)	79	80	40, 57, 93, 119	0
2	P	85/85 (100%)	-0.04	1 (1%)	79	80	37, 60, 102, 136	0
2	Q	85/85 (100%)	-0.04	3 (3%)	44	44	44, 63, 99, 137	0
2	R	85/85 (100%)	-0.30	1 (1%)	79	80	35, 53, 88, 124	0
2	S	85/85 (100%)	-0.10	1 (1%)	79	80	50, 69, 107, 130	0
2	T	85/85 (100%)	-0.15	2 (2%)	59	60	36, 56, 92, 123	0
2	U	85/85 (100%)	-0.12	2 (2%)	59	60	37, 59, 100, 131	0
2	V	85/85 (100%)	0.04	1 (1%)	79	80	39, 64, 101, 132	0
2	W	85/85 (100%)	-0.20	1 (1%)	79	80	38, 59, 92, 129	0
2	X	85/85 (100%)	-0.17	1 (1%)	79	80	38, 56, 98, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	6252/6276 (99%)	0.10	242 (3%) 39 38	30, 64, 122, 224	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	436	THR	10.1
1	B	437	ILE	9.4
1	B	436	THR	9.2
1	D	436	THR	8.9
1	F	313	ARG	7.3
1	J	436	THR	7.0
1	F	339	ALA	6.7
1	K	339	ALA	6.2
1	L	313	ARG	6.2
1	D	438	ASP	6.1
1	A	436	THR	6.1
1	K	439	ALA	5.8
1	C	436	THR	5.7
1	F	432	LEU	5.6
1	G	441	VAL	5.4
1	D	437	ILE	5.4
1	I	436	THR	5.3
1	C	437	ILE	5.3
1	D	439	ALA	5.2
1	E	339	ALA	5.0
1	F	430	ILE	4.9
1	K	313	ARG	4.9
1	G	339	ALA	4.8
1	J	339	ALA	4.8
1	B	439	ALA	4.7
2	Q	286	MET	4.6
1	E	432	LEU	4.5
1	L	436	THR	4.5
1	F	398	GLN	4.5
1	G	399	VAL	4.4
1	L	430	ILE	4.4
1	L	441	VAL	4.4
1	K	436	THR	4.3
1	E	438	ASP	4.3
1	L	433	GLU	4.3
1	F	437	ILE	4.2
1	C	313	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	436	THR	4.2
1	E	337	GLN	4.1
1	E	349	ARG	3.9
1	B	434	ASP	3.9
1	F	127	THR	3.9
1	J	338	ARG	3.9
1	I	437	ILE	3.9
2	V	304	ASP	3.9
1	C	339	ALA	3.8
1	E	433	GLU	3.8
2	N	286	MET	3.8
1	F	431	ASP	3.8
1	I	439	ALA	3.7
1	G	231	LYS	3.7
1	L	432	LEU	3.7
1	D	434	ASP	3.7
1	K	312	LYS	3.7
1	F	312	LYS	3.6
1	L	339	ALA	3.6
1	E	434	ASP	3.6
1	G	313	ARG	3.6
1	H	436	THR	3.6
1	B	313	ARG	3.6
1	B	339	ALA	3.6
1	F	402	GLU	3.5
1	A	169	ASP	3.5
1	F	428	ASP	3.5
1	F	434	ASP	3.5
1	G	438	ASP	3.4
1	D	440	GLU	3.4
1	G	431	ASP	3.4
1	D	313	ARG	3.4
1	L	437	ILE	3.3
1	J	349	ARG	3.3
1	D	127	THR	3.3
1	D	441	VAL	3.3
1	L	398	GLN	3.3
1	E	127	THR	3.3
1	K	437	ILE	3.3
1	E	437	ILE	3.3
1	A	339	ALA	3.3
2	N	304	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	335	LEU	3.2
1	B	432	LEU	3.2
1	G	432	LEU	3.2
1	A	434	ASP	3.1
1	G	394	VAL	3.1
1	A	64	ARG	3.1
1	K	429	LEU	3.1
1	D	339	ALA	3.1
1	J	434	ASP	3.1
1	D	349	ARG	3.1
1	F	399	VAL	3.1
1	F	75	ASP	3.0
1	J	438	ASP	3.0
1	D	129	ASN	3.0
1	A	437	ILE	2.9
1	D	231	LYS	2.9
1	K	349	ARG	2.9
1	E	441	VAL	2.9
1	A	433	GLU	2.9
1	E	430	ILE	2.9
1	F	318	GLY	2.9
1	K	314	GLU	2.9
1	D	314	GLU	2.9
1	C	430	ILE	2.9
1	C	340	HIS	2.9
1	H	430	ILE	2.9
1	B	64	ARG	2.9
1	A	432	LEU	2.8
2	T	304	ASP	2.8
1	H	439	ALA	2.8
1	K	315	LYS	2.8
1	H	339	ALA	2.8
1	E	115	HIS	2.8
1	E	126	ILE	2.7
1	D	131	PHE	2.7
1	A	395	ASP	2.7
2	U	304	ASP	2.7
1	H	431	ASP	2.7
2	R	306	GLY	2.7
1	D	443	ASN	2.7
1	E	431	ASP	2.7
1	L	349	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	439	ALA	2.6
2	T	306	GLY	2.6
1	E	351	ASN	2.6
1	K	434	ASP	2.6
1	A	318	GLY	2.6
1	D	430	ILE	2.6
1	F	317	HIS	2.6
1	C	432	LEU	2.6
1	K	338	ARG	2.6
1	B	317	HIS	2.6
1	C	434	ASP	2.6
2	X	304	ASP	2.6
1	G	398	GLN	2.6
1	G	172	PRO	2.6
1	E	237	PRO	2.6
1	H	312	LYS	2.6
1	C	398	GLN	2.5
1	L	404	HIS	2.5
1	H	181	VAL	2.5
1	G	349	ARG	2.5
1	A	231	LYS	2.5
1	F	417	GLU	2.5
1	J	313	ARG	2.5
1	H	315	LYS	2.5
1	E	313	ARG	2.5
1	I	441	VAL	2.4
1	I	313	ARG	2.4
1	I	339	ALA	2.4
1	L	428	ASP	2.4
1	G	430	ILE	2.4
1	F	450	ASP	2.4
1	D	194	GLU	2.4
1	A	128	GLY	2.4
1	A	441	VAL	2.4
1	E	66	GLU	2.4
1	H	398	GLN	2.4
1	I	186	GLY	2.4
1	A	319	GLU	2.4
1	H	338	ARG	2.4
1	L	453	ARG	2.3
1	I	434	ASP	2.3
1	F	455	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	428	ASP	2.3
1	A	167	GLU	2.3
1	D	128	GLY	2.3
1	F	370	GLY	2.3
1	J	433	GLU	2.3
2	Q	306	GLY	2.3
2	S	304	ASP	2.3
1	F	186	GLY	2.3
2	W	286	MET	2.3
1	D	64	ARG	2.3
1	G	401	ASN	2.3
1	G	437	ILE	2.3
1	D	167	GLU	2.3
1	L	314	GLU	2.3
1	F	395	ASP	2.3
2	M	306	GLY	2.3
1	E	63	LYS	2.3
1	A	396	LEU	2.3
1	G	436	THR	2.3
1	E	183	HIS	2.3
1	H	432	LEU	2.3
1	K	64	ARG	2.3
1	G	434	ASP	2.3
1	L	431	ASP	2.3
1	H	443	ASN	2.2
1	L	351	ASN	2.2
1	D	63	LYS	2.2
1	I	63	LYS	2.2
1	I	231	LYS	2.2
1	A	313	ARG	2.2
1	I	312	LYS	2.2
1	H	113	ARG	2.2
1	J	432	LEU	2.2
1	A	440	GLU	2.2
1	J	398	GLN	2.2
1	B	430	ILE	2.2
1	C	295	ALA	2.2
1	C	312	LYS	2.2
2	O	306	GLY	2.2
1	B	244	TYR	2.2
1	E	210	ARG	2.2
1	G	24	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	109	LYS	2.1
1	F	371	ILE	2.1
1	I	430	ILE	2.1
1	I	172	PRO	2.1
1	L	434	ASP	2.1
1	E	64	ARG	2.1
1	J	112	LYS	2.1
2	P	286	MET	2.1
1	A	431	ASP	2.1
1	C	318	GLY	2.1
1	I	338	ARG	2.1
1	J	430	ILE	2.1
2	U	286	MET	2.1
1	G	396	LEU	2.1
1	G	433	GLU	2.1
1	F	24	ASN	2.1
1	B	23	PRO	2.1
1	D	204	ASP	2.1
1	L	64	ARG	2.1
1	G	440	GLU	2.1
1	I	75	ASP	2.1
2	Q	304	ASP	2.1
1	F	396	LEU	2.0
1	H	399	VAL	2.0
1	H	437	ILE	2.0
1	D	232	ALA	2.0
1	B	231	LYS	2.0
1	E	340	HIS	2.0
1	F	349	ARG	2.0
1	C	439	ALA	2.0
1	A	127	THR	2.0
1	G	112	LYS	2.0
1	I	278	LEU	2.0
1	F	115	HIS	2.0
1	K	115	HIS	2.0
1	H	24	ASN	2.0
1	I	190	LYS	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)

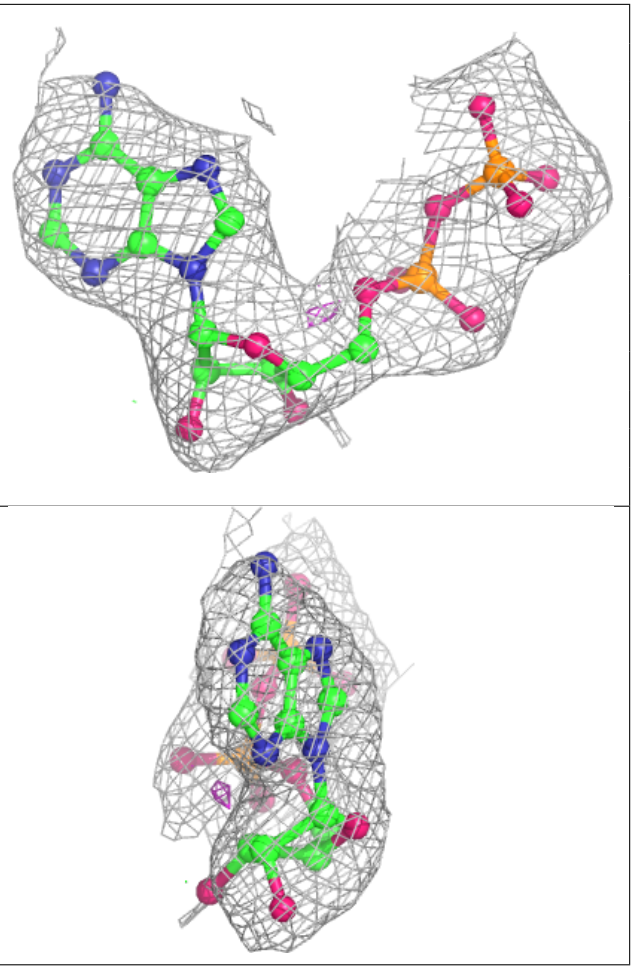
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

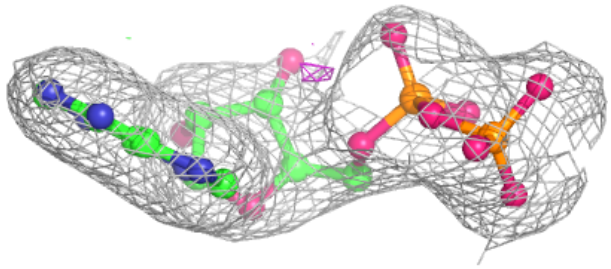
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	F	501	27/27	0.95	0.14	56,68,87,89	0
3	ADP	D	501	27/27	0.96	0.14	53,64,78,88	0
3	ADP	E	501	27/27	0.96	0.13	65,75,88,100	0
3	ADP	A	501	27/27	0.96	0.15	49,68,85,87	0
3	ADP	G	501	27/27	0.96	0.14	62,72,89,90	0
3	ADP	H	501	27/27	0.96	0.16	58,68,75,82	0
3	ADP	I	501	27/27	0.96	0.17	55,67,78,80	0
3	ADP	J	501	27/27	0.96	0.16	53,65,79,81	0
3	ADP	L	501	27/27	0.96	0.14	60,71,87,96	0
3	ADP	C	501	27/27	0.97	0.15	52,61,71,87	0
3	ADP	K	501	27/27	0.98	0.14	49,62,76,86	0
3	ADP	B	501	27/27	0.98	0.13	40,57,69,73	0

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

Electron density around ADP F 501:

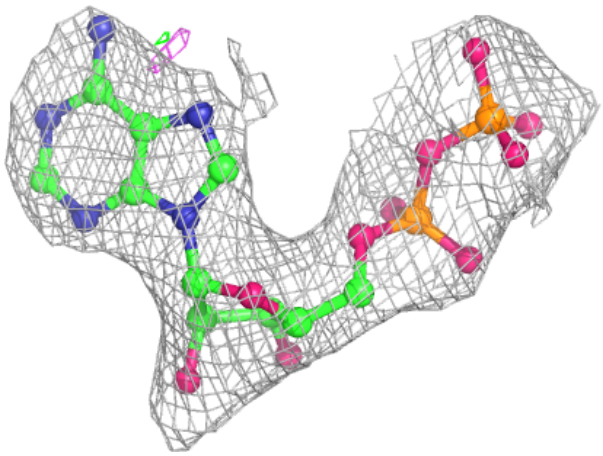
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

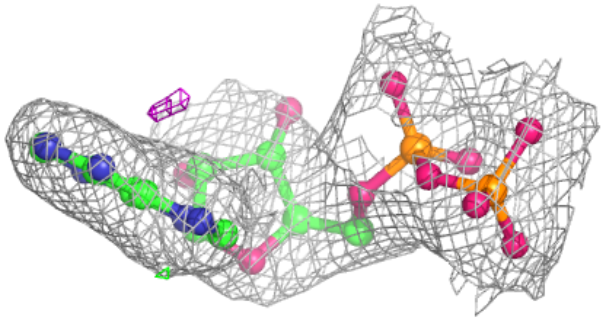


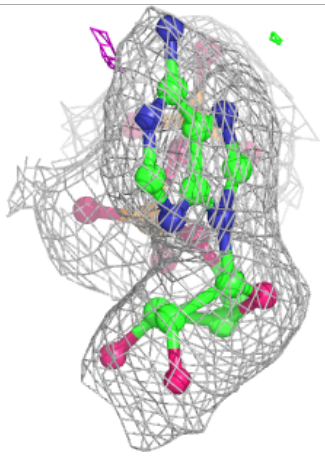


Electron density around ADP D 501:

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

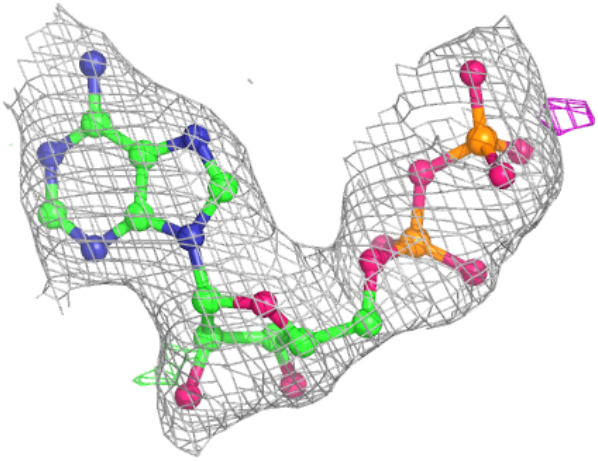


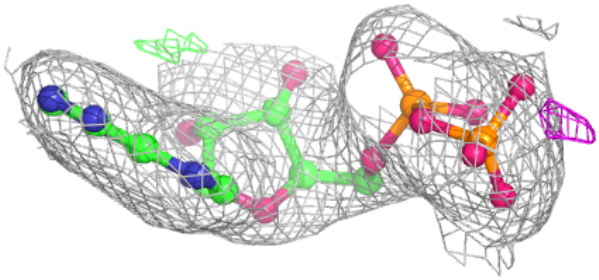


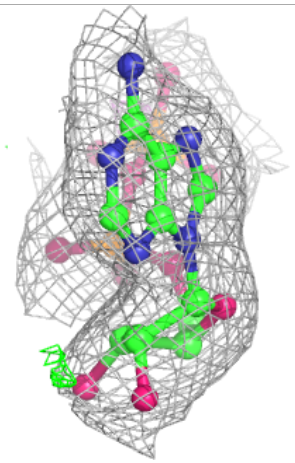


Electron density around ADP E 501:

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

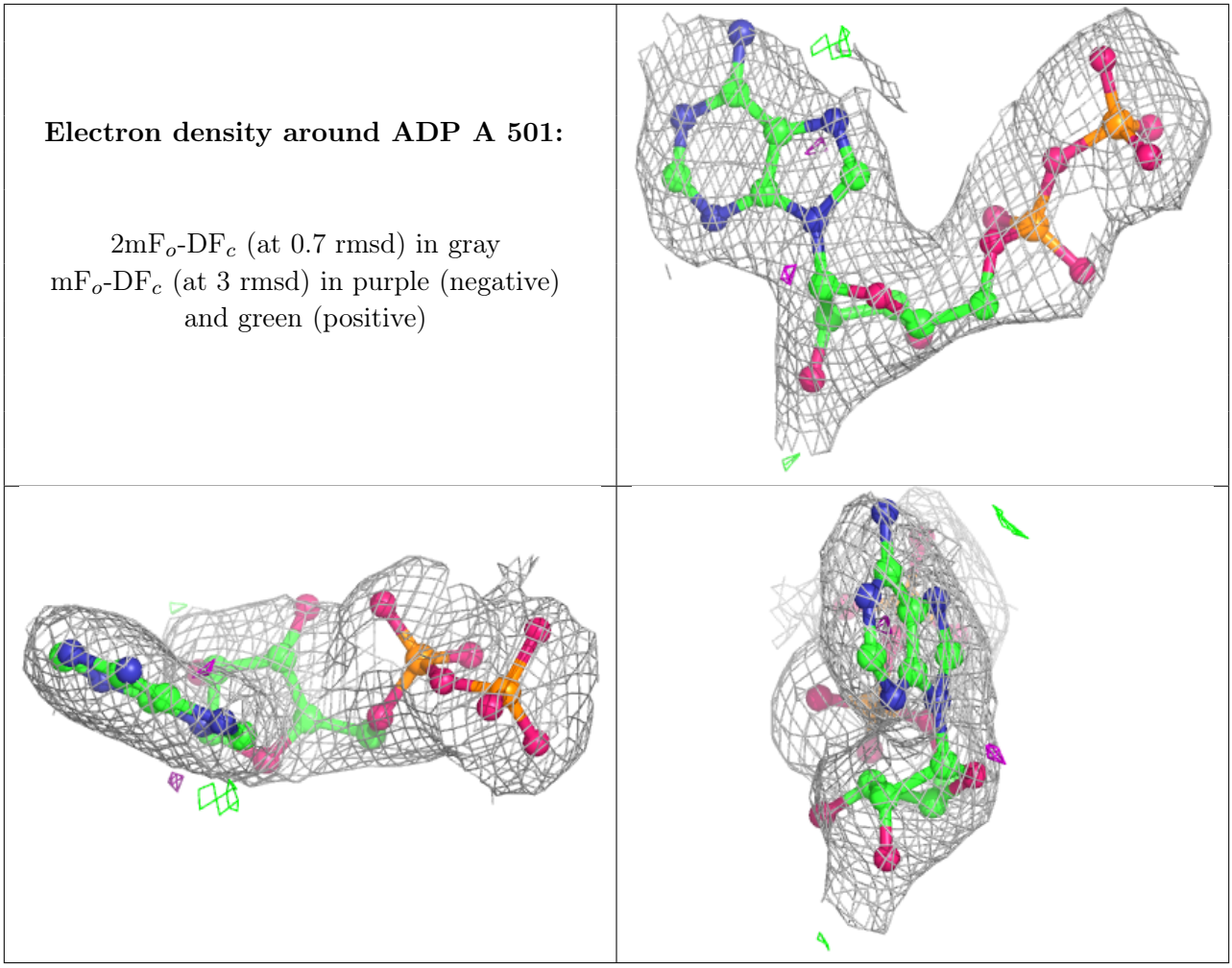






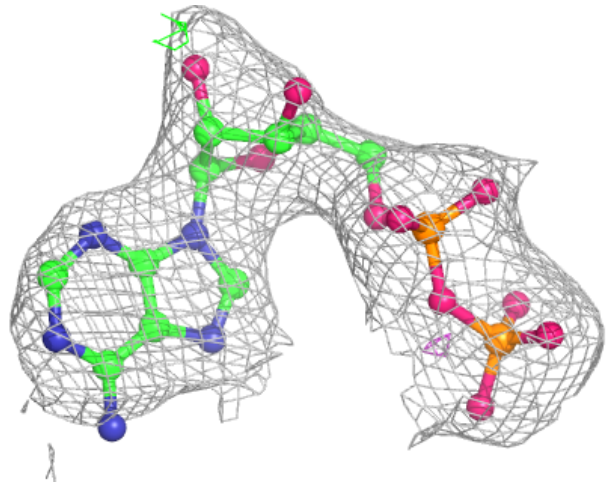
Electron density around ADP A 501:

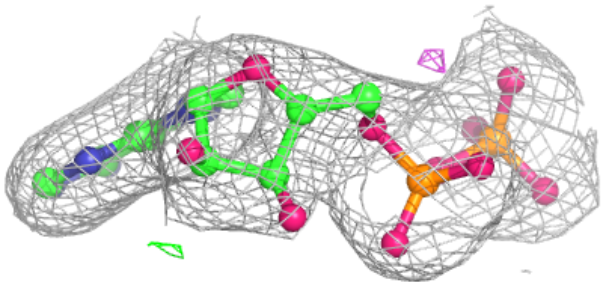
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

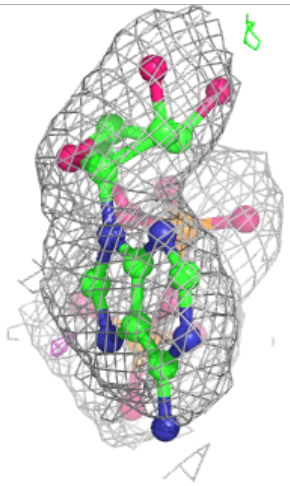


Electron density around ADP G 501:

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

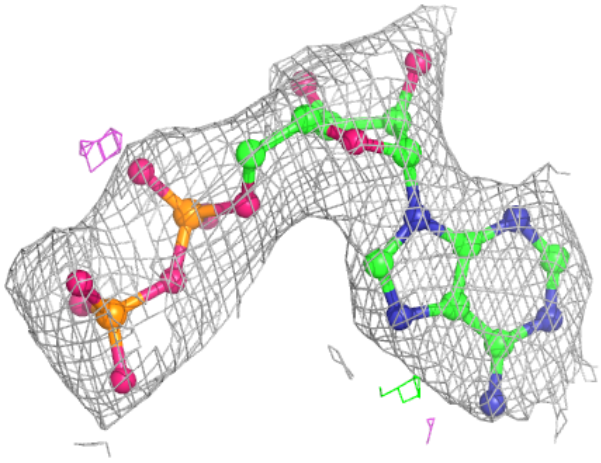


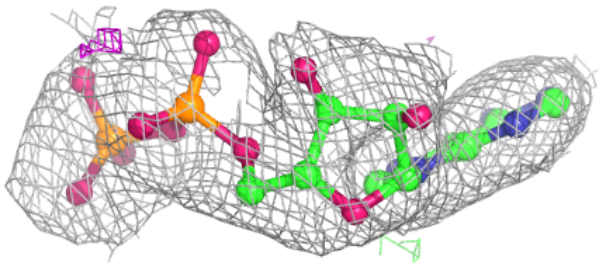


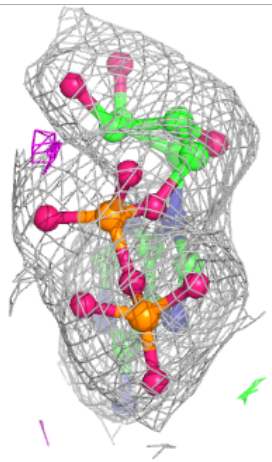


Electron density around ADP H 501:

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

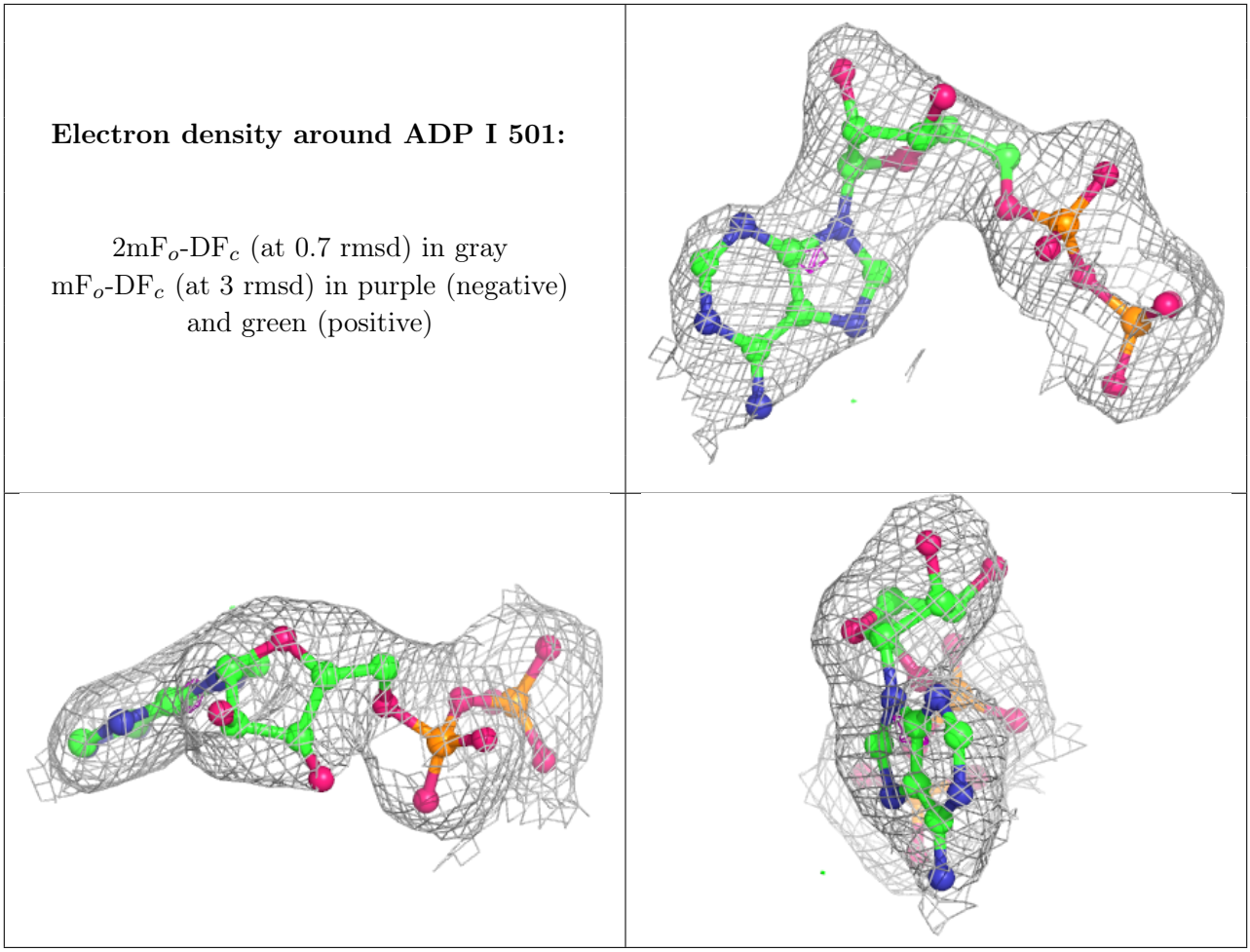






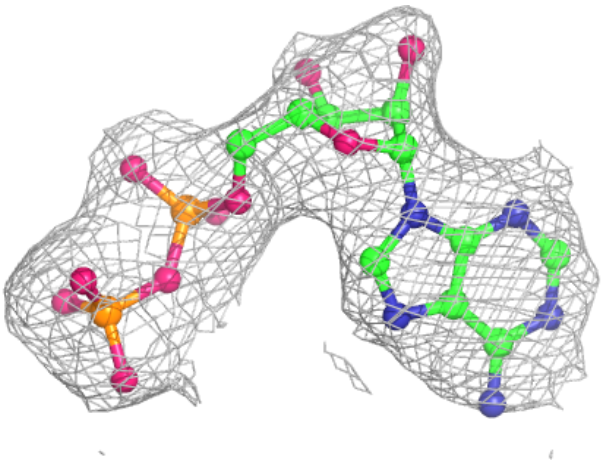
Electron density around ADP I 501:

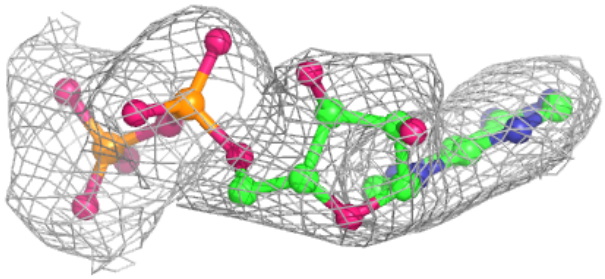
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

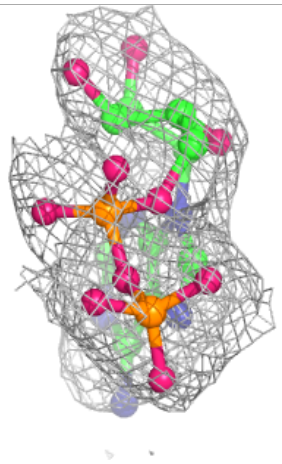


Electron density around ADP J 501:

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

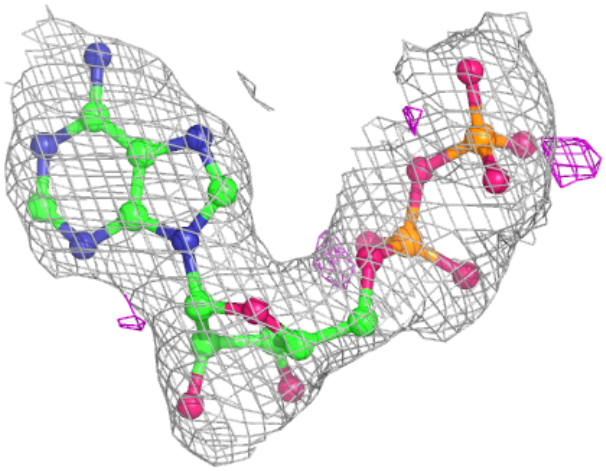


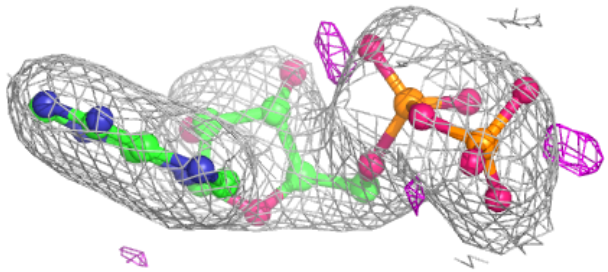


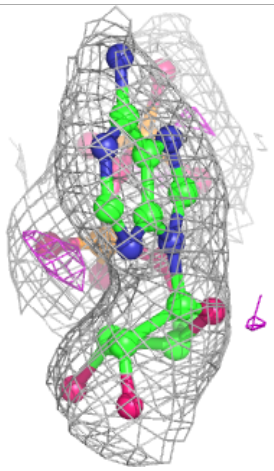


Electron density around ADP L 501:

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

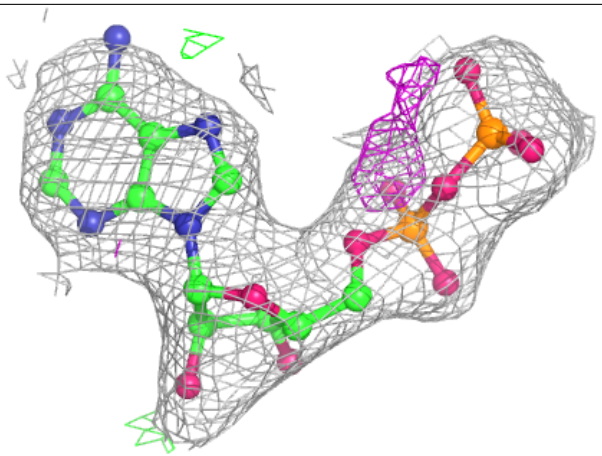


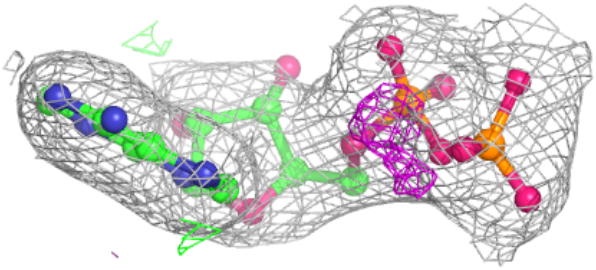


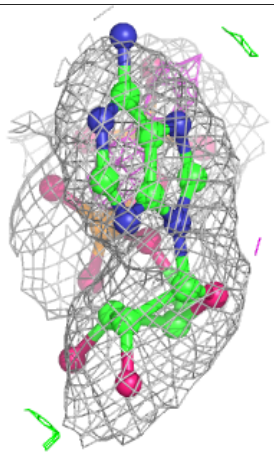


Electron density around ADP C 501:

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

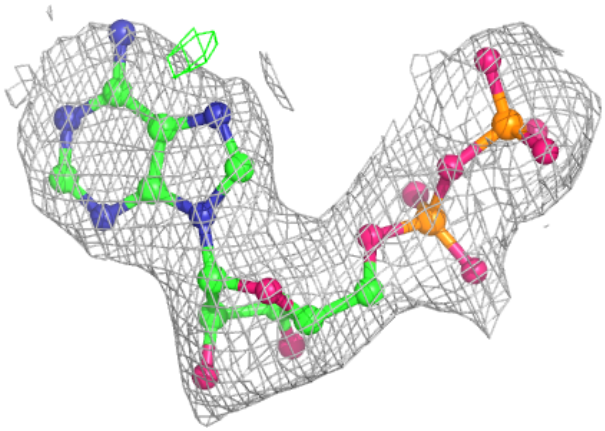


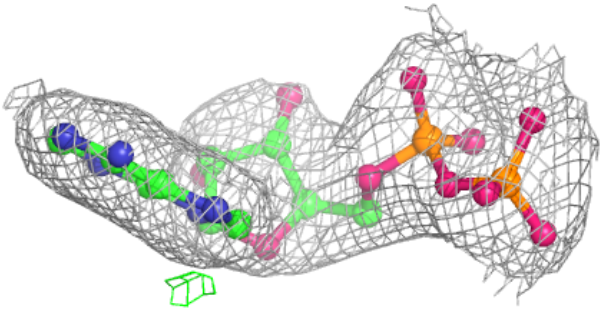


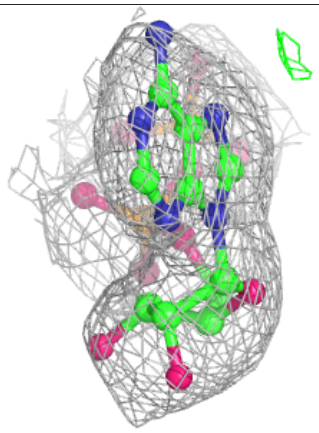


Electron density around ADP K 501:

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

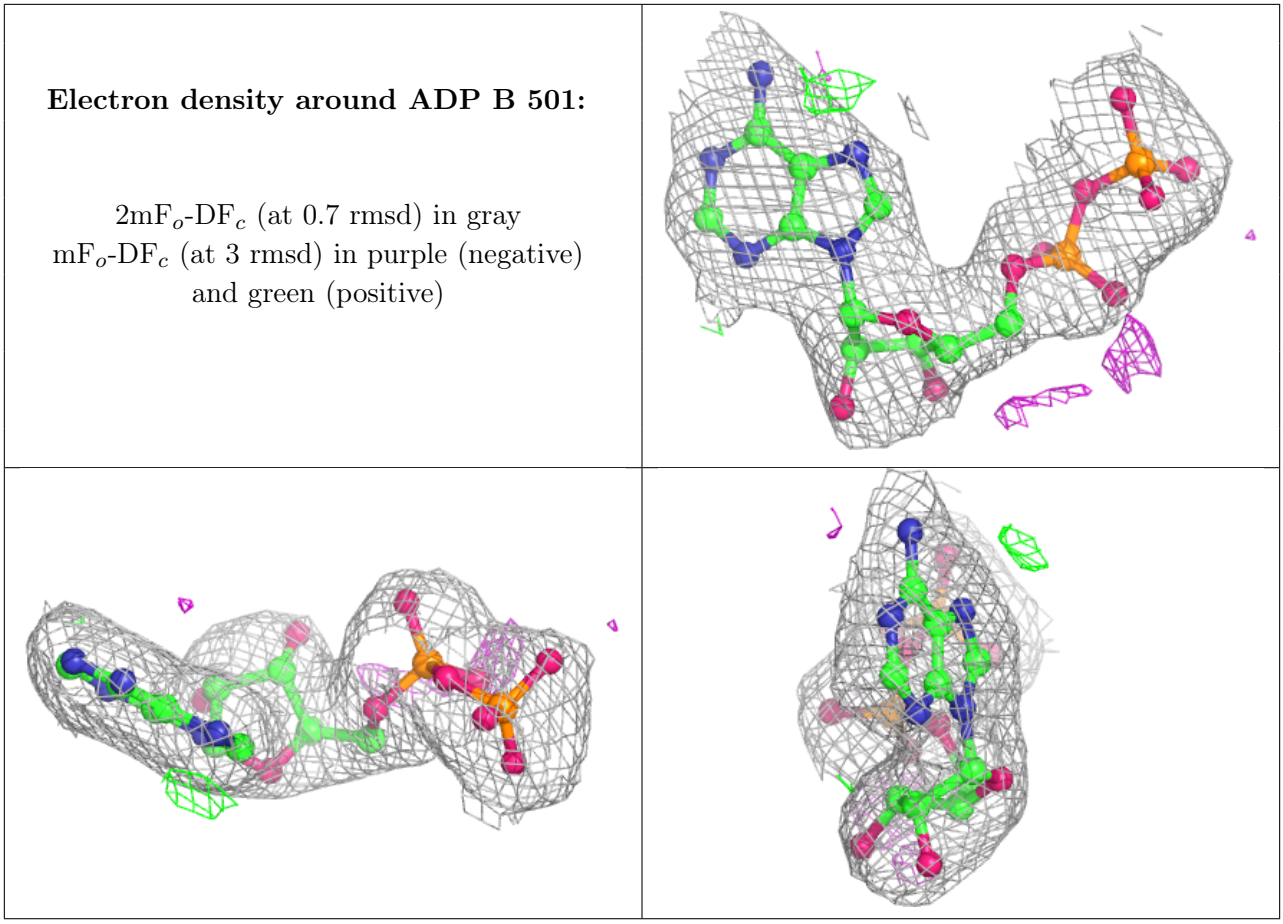






Electron density around ADP B 501:

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



6.5 Other polymers

There are no such residues in this entry.