



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:54 PM UTC

PDB ID : 3K0C / pdb_00003k0c
Title : Crystal structure of the phosphorylation-site double mutant S431A/T432E of the KaiC circadian clock protein
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on : 2009-09-24
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

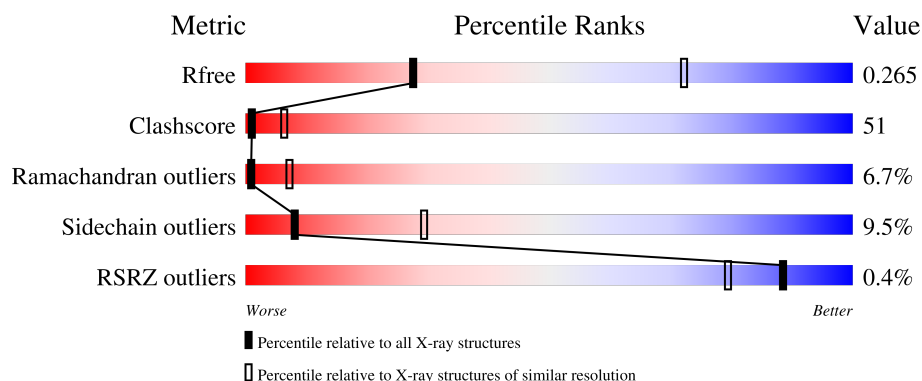
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	519	% 29% 59% 9% • •
1	B	519	28% 55% 11% • 5%
1	E	519	32% 51% 11% • 5%
1	F	519	27% 55% 13% • •
2	C	519	26% 55% 12% • 6%

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Mol	Chain	Length	Quality of chain
2	D	519	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	A	426	-	-	X	-
1	TPO	B	426	-	-	X	-
1	TPO	F	426	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23919 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3990	2510	701	763	1	15			
1	B	491	Total	C	N	O	P	S	0	0	0
			3875	2440	678	741	1	15			
1	E	492	Total	C	N	O	P	S	0	0	0
			3883	2446	679	742	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3990	2510	701	763	1	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ALA	SER	engineered mutation	UNP Q79PF4
A	432	GLU	THR	engineered mutation	UNP Q79PF4
B	431	ALA	SER	engineered mutation	UNP Q79PF4
B	432	GLU	THR	engineered mutation	UNP Q79PF4
E	431	ALA	SER	engineered mutation	UNP Q79PF4
E	432	GLU	THR	engineered mutation	UNP Q79PF4
F	431	ALA	SER	engineered mutation	UNP Q79PF4
F	432	GLU	THR	engineered mutation	UNP Q79PF4

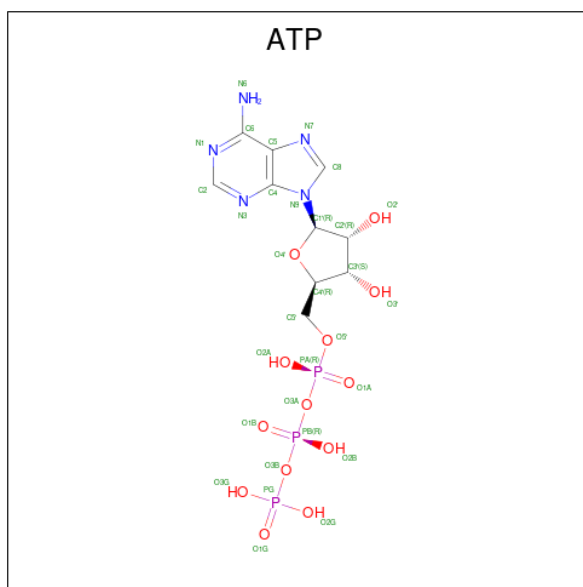
- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	488	Total	C	N	O	S	0	0	0
			3847	2426	674	732	15			
2	D	485	Total	C	N	O	S	0	0	0
			3823	2412	671	725	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	431	ALA	SER	engineered mutation	UNP Q79PF4
C	432	GLU	THR	engineered mutation	UNP Q79PF4
D	431	ALA	SER	engineered mutation	UNP Q79PF4
D	432	GLU	THR	engineered mutation	UNP Q79PF4

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	B	3	Total	Mg	0	0
			3	3		
4	C	4	Total	Mg	0	0
			4	4		
4	D	4	Total	Mg	0	0
			4	4		
4	E	3	Total	Mg	0	0
			3	3		
4	F	3	Total	Mg	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	18	Total	O	0	0
			18	18		
5	C	22	Total	O	0	0
			22	22		
5	D	31	Total	O	0	0
			31	31		
5	E	13	Total	O	0	0
			13	13		
5	F	21	Total	O	0	0
			21	21		

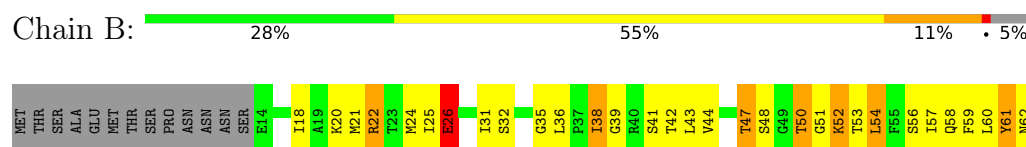
3 Residue-property plots

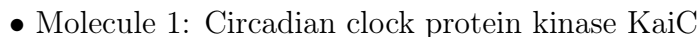
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

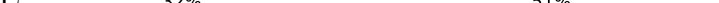
• Molecule 1: Circadian clock protein kinase KaiC

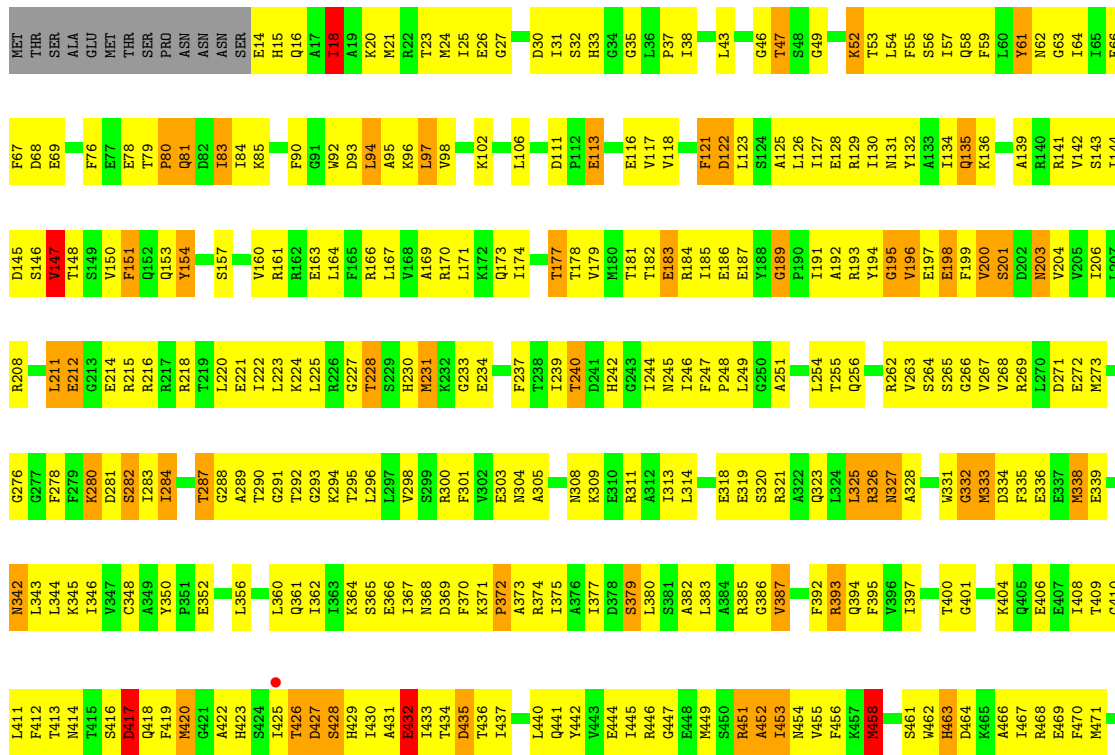


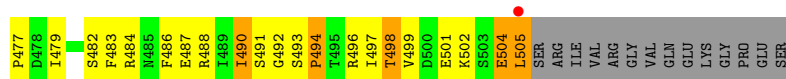
• Molecule 1: Circadian clock protein kinase KaiC





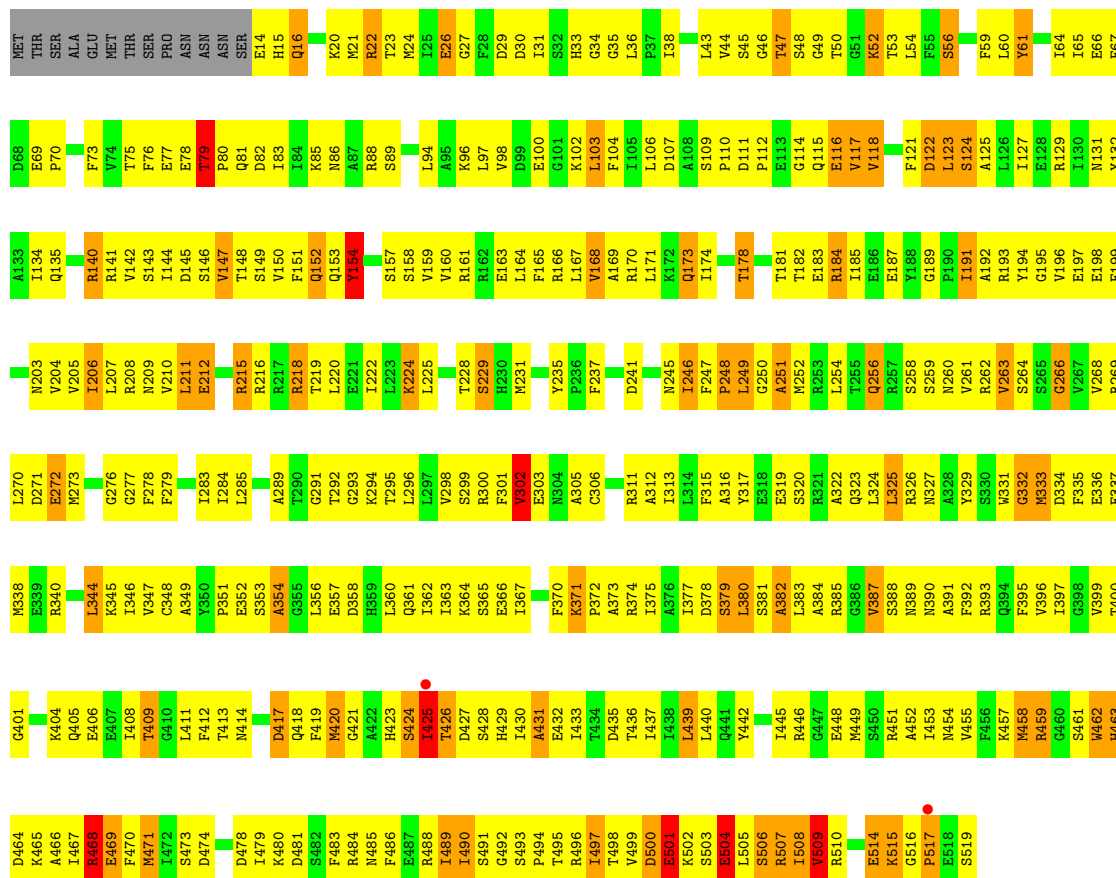
Chain E:  32% 51% 11% • 5%





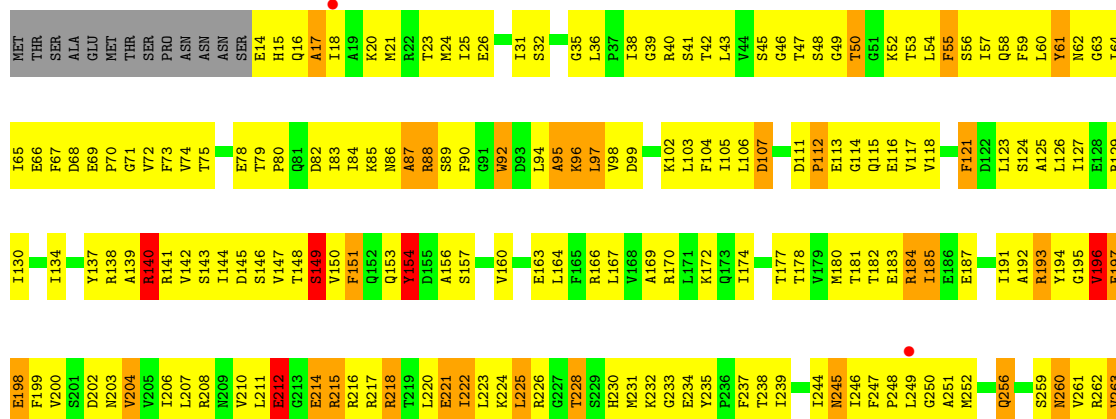
• Molecule 1: Circadian clock protein kinase KaiC

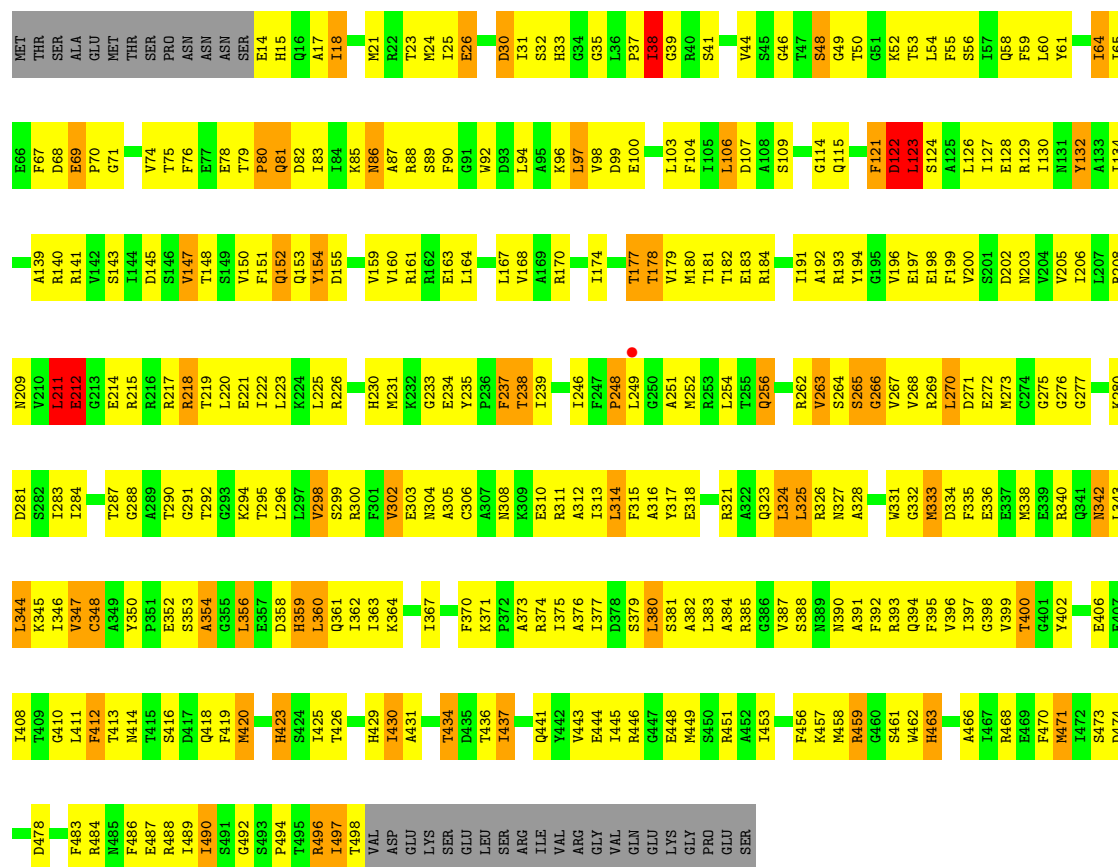
Chain F: 27% 55% 13% . .



• Molecule 2: Circadian clock protein kinase KaiC

Chain C: 26% 55% 12% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.28Å 135.03Å 204.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (30.00-3.30) 90.6 (30.00-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.269 0.239 , 0.265	Depositor DCC
R_{free} test set	5141 reflections (9.44%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23919	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MG, ATP

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	0.49	0/4044	1.03	18/5446 (0.3%)
1	B	0.44	0/3928	0.99	18/5291 (0.3%)
1	E	0.59	0/3936	1.07	18/5302 (0.3%)
1	F	0.56	0/4044	1.09	35/5446 (0.6%)
2	C	0.50	0/3912	1.03	24/5273 (0.5%)
2	D	0.57	0/3888	1.08	24/5240 (0.5%)
All	All	0.53	0/23752	1.05	137/31998 (0.4%)

There are no bond length outliers.

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	380	LEU	N-CA-C	-11.81	98.38	111.14
1	E	380	LEU	N-CA-C	-11.64	97.38	111.69
1	B	502	LYS	N-CA-C	-9.68	99.30	112.94
1	E	214	GLU	N-CA-C	-8.97	103.16	114.56
1	B	266	GLY	N-CA-C	-8.85	102.25	114.64
1	A	266	GLY	N-CA-C	-8.62	103.22	114.85
2	D	178	THR	N-CA-C	8.61	124.02	110.17
1	A	380	LEU	N-CA-C	-8.35	102.36	112.54
1	F	16	GLN	N-CA-C	-8.16	95.85	108.42
1	F	380	LEU	N-CA-C	-8.16	102.39	111.28
1	F	251	ALA	N-CA-C	-8.02	103.40	113.02
2	C	380	LEU	N-CA-C	-7.95	102.21	112.23
1	A	493	SER	CA-C-N	7.34	127.25	120.21
1	A	493	SER	C-N-CA	7.34	127.25	120.21
2	C	369	ASP	N-CA-C	-7.29	104.63	113.97
1	E	458	MET	N-CA-C	-7.29	98.23	109.52
2	D	132	TYR	N-CA-C	-7.15	103.18	110.97
1	B	373	ALA	N-CA-C	-6.98	105.95	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	439	LEU	N-CA-C	6.93	119.81	108.52
1	F	235	TYR	CA-C-N	6.91	127.16	119.90
1	F	235	TYR	C-N-CA	6.91	127.16	119.90
2	D	266	GLY	N-CA-C	-6.90	106.87	115.08
1	A	507	ARG	N-CA-C	-6.75	104.86	113.23
1	E	66	GLU	N-CA-C	6.74	119.98	111.69
1	A	512	VAL	N-CA-C	-6.71	104.28	113.00
1	A	397	ILE	N-CA-C	-6.68	103.00	110.62
1	B	38	ILE	N-CA-C	6.68	117.65	109.30
1	F	498	THR	N-CA-C	6.66	119.80	109.07
1	A	437	ILE	N-CA-C	6.62	117.38	108.11
1	F	268	VAL	N-CA-C	6.57	117.36	110.72
2	D	145	ASP	N-CA-C	6.57	119.43	108.20
2	C	480	LYS	N-CA-C	6.52	118.49	108.12
1	B	382	ALA	N-CA-C	-6.51	105.16	113.23
1	F	241	ASP	N-CA-C	-6.42	105.41	113.18
1	F	382	ALA	N-CA-C	-6.39	103.60	111.40
1	A	459	ARG	N-CA-C	6.28	118.20	111.36
2	C	461	SER	N-CA-C	6.27	116.36	108.45
2	D	69	GLU	CA-C-N	6.27	126.63	119.92
2	D	69	GLU	C-N-CA	6.27	126.63	119.92
1	F	332	GLY	N-CA-C	-6.23	103.78	111.45
2	D	50	THR	N-CA-C	6.20	120.84	113.16
2	D	265	SER	N-CA-C	-6.19	105.37	113.17
1	F	36	LEU	N-CA-C	6.16	118.36	109.48
1	E	373	ALA	N-CA-C	-6.14	105.59	114.12
1	F	474	ASP	N-CA-C	-6.11	104.92	112.38
1	E	94	LEU	N-CA-C	-6.10	103.95	111.33
2	D	410	GLY	N-CA-C	6.09	120.02	110.71
1	F	499	VAL	N-CA-C	-6.08	104.45	113.39
1	B	501	GLU	CB-CA-C	-6.08	108.96	117.23
2	C	331	TRP	N-CA-C	-6.07	105.45	112.92
1	F	123	LEU	N-CA-C	-6.07	104.58	112.23
2	D	64	ILE	N-CA-C	6.04	116.78	110.62
2	C	437	ILE	N-CA-C	6.03	117.37	107.24
1	F	224	LYS	N-CA-C	6.00	119.01	108.75
1	A	57	ILE	CB-CA-C	-5.97	104.20	112.02
1	F	373	ALA	N-CA-C	-5.93	105.35	113.30
1	B	98	VAL	N-CA-C	-5.91	104.02	112.35
1	F	229	SER	N-CA-C	-5.88	100.47	109.41
2	D	459	ARG	N-CA-C	5.87	123.31	110.80
2	D	109	SER	CA-C-N	5.81	126.30	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	109	SER	C-N-CA	5.81	126.30	120.14
2	C	95	ALA	N-CA-C	-5.81	104.30	111.33
2	D	237	PHE	N-CA-C	5.80	117.78	109.14
1	E	206	ILE	N-CA-C	5.80	116.21	107.80
1	E	437	ILE	N-CA-C	5.80	116.98	107.24
2	D	437	ILE	N-CA-C	5.79	115.93	106.72
2	D	64	ILE	CB-CA-C	-5.78	104.34	112.14
1	B	413	THR	N-CA-C	5.78	117.93	108.52
1	B	343	LEU	N-CA-C	-5.76	105.15	114.09
2	C	235	TYR	CA-C-N	5.75	125.70	119.78
2	C	235	TYR	C-N-CA	5.75	125.70	119.78
1	F	266	GLY	N-CA-C	-5.75	106.59	114.64
2	C	92	TRP	N-CA-C	5.71	117.67	107.80
2	C	206	ILE	N-CA-C	5.70	116.06	107.80
1	B	210	VAL	N-CA-C	5.69	116.92	109.58
1	F	302	VAL	N-CA-C	-5.69	104.97	110.72
1	E	272	GLU	N-CA-C	-5.67	104.74	111.03
1	E	452	ALA	N-CA-C	-5.66	100.13	108.79
1	B	439	LEU	N-CA-C	5.65	117.99	107.99
1	F	173	GLN	N-CA-C	-5.64	104.83	110.97
2	C	214	GLU	N-CA-C	-5.63	105.00	112.94
2	C	140	ARG	N-CA-C	-5.60	106.34	114.12
2	C	204	VAL	N-CA-C	5.58	116.62	107.24
2	C	459	ARG	N-CA-C	5.58	118.21	111.40
1	B	131	ASN	N-CA-C	-5.57	105.31	111.71
1	B	178	THR	N-CA-C	5.55	117.94	109.95
1	A	373	ALA	N-CA-C	-5.55	106.67	113.50
1	F	124	SER	N-CA-C	-5.54	105.25	112.23
2	D	238	THR	N-CA-C	5.53	118.11	107.44
1	F	22	ARG	N-CA-C	5.51	118.22	109.96
1	B	206	ILE	N-CA-C	5.51	115.82	108.11
1	A	116	GLU	N-CA-C	5.50	118.67	110.14
1	F	122	ASP	N-CA-C	-5.50	106.07	112.89
2	D	38	ILE	N-CA-C	5.49	120.77	109.34
1	E	147	VAL	N-CA-C	-5.47	104.25	111.09
2	C	492	GLY	N-CA-C	-5.47	107.39	113.79
1	F	79	THR	CA-C-N	5.44	126.64	119.84
1	F	79	THR	C-N-CA	5.44	126.64	119.84
1	E	332	GLY	N-CA-C	-5.40	100.38	113.18
1	B	308	ASN	N-CA-C	-5.40	107.25	112.97
1	F	272	GLU	N-CA-C	-5.39	105.05	111.03
2	C	422	ALA	N-CA-C	-5.38	101.01	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	30	ASP	N-CA-C	-5.38	104.29	112.04
1	F	459	ARG	N-CA-C	5.38	116.83	111.07
2	D	324	LEU	N-CA-C	-5.37	104.67	111.11
1	B	270	LEU	N-CA-C	-5.36	104.86	111.40
1	E	383	LEU	N-CA-C	-5.34	106.27	112.89
1	F	147	VAL	N-CA-C	-5.31	105.20	110.62
1	A	38	ILE	N-CA-C	5.30	115.93	109.30
1	F	417	ASP	N-CA-C	5.30	119.49	113.19
1	F	206	ILE	N-CA-C	5.29	115.48	107.80
1	F	246	ILE	N-CA-C	5.28	116.91	108.89
2	D	288	GLY	N-CA-C	5.23	118.12	110.38
1	B	437	ILE	N-CA-C	5.23	115.59	107.28
1	A	308	ASN	N-CA-C	-5.23	105.61	112.41
2	D	373	ALA	N-CA-C	-5.22	107.29	113.97
2	C	388	SER	N-CA-C	-5.19	103.54	110.55
2	D	298	VAL	N-CA-C	5.16	115.78	110.36
1	F	114	GLY	N-CA-C	5.15	120.39	112.51
1	A	48	SER	N-CA-C	5.14	116.55	109.15
1	A	108	ALA	N-CA-C	-5.12	107.42	113.97
1	E	64	ILE	CB-CA-C	-5.12	105.27	111.87
2	C	355	GLY	N-CA-C	-5.11	104.81	112.89
2	C	493	SER	CA-C-N	5.11	125.11	120.21
2	C	493	SER	C-N-CA	5.11	125.11	120.21
1	E	231	MET	N-CA-C	-5.10	103.30	110.50
2	D	430	ILE	N-CA-C	-5.10	108.32	113.47
1	E	125	ALA	N-CA-C	-5.09	105.73	111.28
1	B	380	LEU	N-CA-C	-5.07	105.45	111.69
2	C	221	GLU	N-CA-C	5.06	116.66	108.26
1	A	448	GLU	N-CA-C	5.05	117.06	109.23
1	A	514	GLU	N-CA-C	-5.05	105.50	113.02
2	C	272	GLU	N-CA-C	-5.04	105.79	111.28
2	C	222	ILE	N-CA-C	-5.03	100.39	107.98
1	F	248	PRO	N-CA-C	-5.01	105.72	112.48
1	E	493	SER	CA-C-N	5.00	126.10	119.84
1	E	493	SER	C-N-CA	5.00	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3990	0	3983	426	0
1	B	3875	0	3861	438	0
1	E	3883	0	3871	396	0
1	F	3990	0	3982	488	0
2	C	3847	0	3839	454	0
2	D	3823	0	3819	387	0
3	A	62	0	24	6	0
3	B	62	0	24	9	0
3	C	62	0	24	8	0
3	D	62	0	24	5	0
3	E	62	0	24	9	0
3	F	62	0	24	4	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
5	A	12	0	0	1	0
5	B	18	0	0	2	0
5	C	22	0	0	4	0
5	D	31	0	0	6	0
5	E	13	0	0	3	0
5	F	21	0	0	6	0
All	All	23919	0	23499	2429	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 51.

All (2429) 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:A:425:ILE:O	1:A:426:TPO:HG22	1.25	1.24
1:B:300:ARG:HA	1:B:333:MET:HE1	1.23	1.20
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.26	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:379:SER:H	2:D:413:THR:HB	0.97	1.09
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.30	1.07
1:F:426:TPO:CG2	1:F:430:ILE:H	1.66	1.07
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.38	1.06
1:F:191:ILE:HG13	1:F:206:ILE:HD11	1.35	1.04
1:A:379:SER:H	1:A:413:THR:HB	1.19	1.04
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.18	1.04
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.24	1.03
2:C:45:SER:HB3	2:C:182:THR:HB	1.41	1.03
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.37	1.03
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.39	1.02
1:A:211:LEU:O	1:A:212:GLU:HB3	1.58	1.02
1:A:425:ILE:O	1:A:426:TPO:CG2	2.08	1.01
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.42	1.01
1:A:380:LEU:HD11	1:A:412:PHE:CD2	1.96	1.00
2:C:215:ARG:HA	2:C:215:ARG:HE	1.26	1.00
2:D:379:SER:N	2:D:413:THR:HB	1.76	1.00
1:F:426:TPO:HG21	1:F:430:ILE:N	1.77	1.00
1:E:18:ILE:HD11	1:E:227:GLY:HA3	1.43	0.98
1:F:426:TPO:HG21	1:F:430:ILE:H	1.26	0.98
1:B:25:ILE:HG12	1:B:58:GLN:HE21	1.27	0.97
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.29	0.97
1:F:127:ILE:HD11	1:F:167:LEU:HA	1.44	0.97
1:A:14:GLU:HG3	1:A:15:HIS:H	1.30	0.96
1:F:283:ILE:HG23	1:F:412:PHE:HE1	1.31	0.96
1:E:320:SER:HA	1:F:254:LEU:HG	1.47	0.96
1:B:273:MET:O	1:B:463:HIS:HA	1.66	0.95
1:E:24:MET:HA	1:E:24:MET:HE3	1.48	0.95
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.46	0.95
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.49	0.94
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.46	0.94
2:C:231:MET:HE1	2:C:251:ALA:HB2	1.49	0.93
2:C:70:PRO:HB2	2:C:139:ALA:HA	1.51	0.93
1:F:486:PHE:HE2	1:F:496:ARG:HH11	1.10	0.92
1:B:25:ILE:HG23	1:B:58:GLN:HE22	1.32	0.92
1:E:356:LEU:HD11	1:E:387:VAL:HG21	1.52	0.92
1:E:426:TPO:HG21	1:E:431:ALA:H	1.34	0.91
1:A:380:LEU:HD11	1:A:412:PHE:HD2	1.36	0.90
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.54	0.89
1:F:515:LYS:HG3	1:F:516:GLY:H	1.39	0.88
1:B:221:GLU:HG3	1:B:233:GLY:O	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:GLY:HA2	1:E:304:ASN:HD22	1.37	0.88
1:E:344:LEU:HD22	1:E:345:LYS:H	1.36	0.88
1:A:350:TYR:CZ	1:B:254:LEU:HD13	2.09	0.88
1:E:426:TPO:HG21	1:E:431:ALA:N	1.89	0.88
1:A:265:SER:O	1:A:301:PHE:HA	1.73	0.88
1:A:429:HIS:HB3	5:F:522:HOH:O	1.73	0.87
2:D:148:THR:HG21	2:D:193:ARG:HD2	1.55	0.87
1:E:263:VAL:HG12	1:E:374:ARG:NH2	1.89	0.87
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.38	0.87
2:C:261:VAL:HG12	2:C:262:ARG:H	1.39	0.86
1:A:266:GLY:HA3	1:A:300:ARG:O	1.76	0.86
1:B:146:SER:H	1:B:181:THR:HB	1.39	0.86
1:B:497:ILE:HD12	1:B:498:THR:N	1.91	0.86
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.58	0.85
1:B:218:ARG:HD3	1:B:237:PHE:CE1	2.10	0.85
1:B:426:TPO:O1P	1:B:429:HIS:HA	1.77	0.85
1:A:147:VAL:O	1:A:150:VAL:HG12	1.75	0.85
1:F:312:ALA:HA	1:F:372:PRO:HB3	1.58	0.85
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.42	0.85
1:B:449:MET:HE3	2:C:467:ILE:HD11	1.57	0.84
1:A:263:VAL:CG1	1:A:374:ARG:HH21	1.90	0.84
2:C:220:LEU:HD13	2:C:246:ILE:HD11	1.59	0.84
2:C:451:ARG:HG2	2:C:451:ARG:HH11	1.41	0.84
1:F:313:ILE:HG13	1:F:372:PRO:HG2	1.58	0.84
1:F:500:ASP:O	1:F:501:GLU:HB3	1.75	0.84
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.60	0.84
1:F:171:LEU:HD13	1:F:178:THR:HG21	1.58	0.84
1:B:140:ARG:HB3	1:B:140:ARG:NH1	1.92	0.84
1:E:379:SER:H	1:E:413:THR:HB	1.43	0.84
1:F:170:ARG:HH12	1:F:174:ILE:HG12	1.42	0.83
1:A:264:SER:HA	1:A:271:ASP:OD1	1.78	0.83
1:F:142:VAL:HB	1:F:178:THR:HG23	1.61	0.82
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.13	0.82
1:A:323:GLN:HG2	1:A:327:ASN:HD21	1.42	0.82
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.60	0.82
1:E:294:LYS:HB2	3:E:901:ATP:O1B	1.79	0.82
2:C:182:THR:HG22	2:C:183:GLU:H	1.45	0.82
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.44	0.82
1:A:65:ILE:O	1:A:66:GLU:HG2	1.79	0.82
1:A:211:LEU:HG	1:A:212:GLU:H	1.43	0.82
1:A:299:SER:C	1:A:333:MET:HE1	2.04	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.93	0.82
1:A:451:ARG:HD2	1:A:451:ARG:N	1.95	0.81
2:D:52:LYS:HB2	5:D:550:HOH:O	1.80	0.81
2:D:18:ILE:H	2:D:18:ILE:HD12	1.42	0.81
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.59	0.81
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.63	0.81
1:E:418:GLN:HB2	1:F:423:HIS:O	1.81	0.81
2:C:45:SER:CB	2:C:182:THR:HB	2.11	0.81
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.11	0.81
2:C:431:ALA:O	2:C:434:THR:HG22	1.79	0.81
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.62	0.81
2:C:287:THR:HG21	2:C:425:ILE:O	1.81	0.81
2:D:436:THR:HG23	2:D:458:MET:HG2	1.62	0.81
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.46	0.81
2:C:409:THR:HA	5:C:539:HOH:O	1.80	0.81
3:B:901:ATP:H3'	2:C:458:MET:O	1.82	0.80
2:C:344:LEU:HD22	2:C:345:LYS:H	1.46	0.80
2:C:245:ASN:C	2:C:245:ASN:HD22	1.88	0.80
1:A:72:VAL:HB	1:A:142:VAL:HG22	1.64	0.80
1:B:300:ARG:HA	1:B:333:MET:CE	2.08	0.80
1:E:14:GLU:HG3	1:E:16:GLN:H	1.47	0.80
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.63	0.80
1:E:283:ILE:HG13	1:E:400:THR:HG23	1.63	0.80
1:E:293:GLY:HA2	3:E:901:ATP:O1A	1.81	0.80
1:A:425:ILE:C	1:A:426:TPO:O1P	2.24	0.80
1:B:25:ILE:HG23	1:B:58:GLN:NE2	1.97	0.79
2:C:384:ALA:HB2	2:C:392:PHE:CE1	2.16	0.79
1:A:467:ILE:HD11	1:F:449:MET:HE3	1.63	0.79
2:D:31:ILE:HA	2:D:231:MET:SD	2.23	0.79
2:D:164:LEU:HD22	2:D:180:MET:HE1	1.64	0.79
2:C:446:ARG:HG2	2:C:496:ARG:NH2	1.97	0.79
2:D:419:PHE:CE2	1:E:425:ILE:HG13	2.16	0.79
2:D:471:MET:HE2	2:D:478:ASP:HB2	1.63	0.79
1:F:299:SER:C	1:F:333:MET:HE1	2.06	0.79
1:A:446:ARG:HA	1:A:496:ARG:NH2	1.98	0.79
1:F:303:GLU:OE2	1:F:333:MET:HB3	1.82	0.79
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.12	0.79
1:F:344:LEU:HD22	1:F:345:LYS:H	1.47	0.79
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.19	0.78
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.63	0.78
1:E:263:VAL:CG1	1:E:374:ARG:HH21	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:C	1:A:426:TPO:HG22	2.07	0.78
5:D:538:HOH:O	1:E:432:GLU:HG2	1.84	0.78
1:F:377:ILE:HD11	1:F:399:VAL:HG11	1.66	0.78
1:F:383:LEU:HD13	1:F:395:PHE:CE2	2.18	0.78
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.65	0.78
2:D:347:VAL:HG12	2:D:348:CYS:N	1.98	0.78
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.49	0.78
2:D:294:LYS:O	2:D:298:VAL:HG23	1.83	0.78
1:E:382:ALA:O	1:E:385:ARG:HG3	1.84	0.78
1:F:393:ARG:O	1:F:397:ILE:HG12	1.84	0.77
1:A:273:MET:HE3	1:A:468:ARG:HD2	1.65	0.77
2:D:21:MET:HE3	2:D:59:PHE:HZ	1.49	0.77
2:D:170:ARG:O	2:D:174:ILE:HG12	1.84	0.77
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.14	0.77
1:F:514:GLU:CD	1:F:515:LYS:H	1.92	0.77
1:A:14:GLU:CG	1:A:15:HIS:H	1.97	0.77
2:C:72:VAL:HG22	2:C:104:PHE:HB3	1.65	0.77
1:B:492:GLY:O	1:B:494:PRO:HD3	1.83	0.77
2:C:42:THR:HA	2:C:203:ASN:HB2	1.66	0.77
1:E:313:ILE:CD1	1:E:372:PRO:HG2	2.15	0.77
1:E:445:ILE:HG22	1:E:446:ARG:HD2	1.67	0.77
1:E:497:ILE:HG22	1:E:498:THR:H	1.48	0.77
2:C:371:LYS:O	2:C:371:LYS:HD2	1.84	0.77
2:C:300:ARG:N	2:C:333:MET:HE1	1.99	0.77
1:E:464:ASP:OD2	1:E:466:ALA:HB3	1.83	0.77
1:B:116:GLU:HG2	1:B:117:VAL:H	1.50	0.77
1:B:496:ARG:HG2	1:B:498:THR:HG23	1.67	0.77
2:D:212:GLU:HG2	2:D:212:GLU:O	1.84	0.77
1:A:64:ILE:HD11	1:A:103:LEU:HB2	1.65	0.77
2:C:182:THR:HG22	2:C:183:GLU:N	2.00	0.77
2:D:377:ILE:HG22	2:D:377:ILE:O	1.84	0.77
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.00	0.76
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.20	0.76
1:A:16:GLN:O	1:F:88:ARG:HD2	1.85	0.76
1:B:25:ILE:HG12	1:B:58:GLN:NE2	1.99	0.76
1:E:326:ARG:HD3	1:F:258:SER:OG	1.85	0.76
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.68	0.76
2:C:299:SER:HB3	2:C:333:MET:HE2	1.68	0.76
1:E:313:ILE:HG13	1:E:372:PRO:CG	2.16	0.76
1:E:294:LYS:HB3	1:E:413:THR:HG23	1.67	0.76
1:E:504:GLU:HG2	1:E:505:LEU:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:SER:HA	1:B:254:LEU:HG	1.68	0.75
2:C:422:ALA:HB1	5:C:536:HOH:O	1.86	0.75
2:D:214:GLU:HB3	1:E:234:GLU:HB2	1.67	0.75
1:F:344:LEU:HD22	1:F:345:LYS:N	2.00	0.75
2:D:371:LYS:HD2	2:D:371:LYS:O	1.85	0.75
1:F:381:SER:HB3	1:F:414:ASN:OD1	1.87	0.75
1:E:323:GLN:HE21	1:F:459:ARG:HD3	1.50	0.75
1:E:191:ILE:HB	1:E:198:GLU:CG	2.16	0.75
1:B:191:ILE:HB	1:B:198:GLU:CG	2.16	0.75
1:A:323:GLN:HG2	1:A:327:ASN:ND2	2.01	0.75
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.69	0.75
1:A:386:GLY:HA2	1:B:390:ASN:OD1	1.86	0.75
1:B:52:LYS:H	1:B:207:LEU:HD12	1.51	0.74
1:B:191:ILE:HB	1:B:198:GLU:CD	2.12	0.74
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.70	0.74
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.51	0.74
1:B:56:SER:O	1:B:59:PHE:HB3	1.87	0.74
1:E:148:THR:OG1	1:E:182:THR:HG23	1.85	0.74
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.17	0.74
1:B:358:ASP:O	1:B:362:ILE:HG12	1.88	0.74
1:B:50:THR:HB	1:B:207:LEU:HB3	1.68	0.74
1:B:426:TPO:O1P	1:B:429:HIS:CA	2.35	0.74
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.69	0.74
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.53	0.74
1:E:461:SER:OG	1:E:462:TRP:N	2.19	0.74
1:A:50:THR:HG22	1:A:209:ASN:HB2	1.70	0.74
1:E:20:LYS:HE3	1:E:228:THR:HG21	1.70	0.74
1:B:263:VAL:HG12	1:B:374:ARG:NH2	2.03	0.73
1:B:379:SER:H	1:B:413:THR:HB	1.53	0.73
1:E:304:ASN:HB3	1:E:374:ARG:HH12	1.53	0.73
2:C:140:ARG:HB3	2:C:140:ARG:NH1	2.01	0.73
1:F:20:LYS:HE2	1:F:228:THR:HG21	1.69	0.73
1:B:214:GLU:HB3	2:C:234:GLU:HB2	1.70	0.73
2:C:50:THR:HG21	2:C:207:LEU:C	2.13	0.73
2:D:221:GLU:HG3	2:D:233:GLY:O	1.88	0.73
2:D:304:ASN:HB3	2:D:374:ARG:HH12	1.51	0.73
2:D:220:LEU:HD23	2:D:221:GLU:N	2.02	0.73
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.68	0.73
1:B:196:VAL:O	1:B:200:VAL:HG23	1.89	0.73
1:B:316:ALA:HA	1:B:378:ASP:HB3	1.70	0.73
2:D:497:ILE:HD12	2:D:497:ILE:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:232:LYS:HD2	2:C:232:LYS:N	2.02	0.73
2:C:296:LEU:HD21	2:C:477:PRO:HB3	1.70	0.73
1:B:458:MET:HB2	1:B:463:HIS:HD2	1.54	0.73
1:B:21:MET:HB2	1:B:38:ILE:HG12	1.71	0.72
1:B:184:ARG:HH22	1:B:187:GLU:C	1.98	0.72
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.18	0.72
2:C:215:ARG:HA	2:C:215:ARG:NE	2.03	0.72
1:B:195:GLY:HA2	1:B:198:GLU:OE2	1.88	0.72
1:F:383:LEU:HD13	1:F:395:PHE:HE2	1.53	0.72
1:B:318:GLU:OE2	2:C:432:GLU:HB3	1.90	0.72
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.04	0.72
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.04	0.72
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.53	0.72
2:D:18:ILE:HD12	2:D:18:ILE:N	2.04	0.72
1:F:79:THR:HG23	1:F:81:GLN:H	1.54	0.72
1:B:503:SER:O	1:B:504:GLU:HB2	1.88	0.72
2:D:114:GLY:O	2:D:115:GLN:HG3	1.89	0.72
1:E:134:ILE:HG23	1:E:139:ALA:HB3	1.72	0.72
1:A:436:THR:CG2	1:A:458:MET:HG2	2.19	0.72
1:B:140:ARG:HB3	1:B:140:ARG:HH11	1.54	0.72
1:B:184:ARG:HD2	1:B:191:ILE:O	1.89	0.72
1:B:451:ARG:HH11	1:B:451:ARG:HG2	1.54	0.72
1:E:123:LEU:HD13	1:E:163:GLU:OE2	1.90	0.71
1:E:313:ILE:HG13	1:E:372:PRO:HG3	1.72	0.71
2:C:300:ARG:HA	2:C:333:MET:HE1	1.73	0.71
2:D:164:LEU:CD2	2:D:180:MET:HE1	2.19	0.71
1:A:258:SER:OG	1:F:326:ARG:HD3	1.89	0.71
1:B:300:ARG:CA	1:B:333:MET:HE1	2.12	0.71
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.25	0.71
1:A:84:ILE:HG23	1:A:94:LEU:HB2	1.73	0.71
1:E:436:THR:HG23	1:E:458:MET:HG2	1.72	0.71
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.72	0.71
1:F:497:ILE:O	1:F:497:ILE:HG13	1.88	0.71
2:C:261:VAL:HG12	2:C:262:ARG:N	2.01	0.71
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.91	0.71
1:A:447:GLY:HA2	1:B:489:ILE:CD1	2.20	0.71
1:F:191:ILE:HG13	1:F:206:ILE:CD1	2.18	0.71
1:B:84:ILE:HA	1:B:94:LEU:HD12	1.72	0.71
1:B:169:ALA:O	1:B:173:GLN:HG3	1.91	0.71
2:D:67:PHE:HB3	2:D:69:GLU:HG3	1.72	0.71
1:E:344:LEU:HD22	1:E:345:LYS:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLU:HB2	2:C:199:PHE:CE1	2.25	0.70
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.55	0.70
2:C:146:SER:H	2:C:181:THR:HB	1.55	0.70
2:D:64:ILE:HG21	2:D:97:LEU:HD13	1.71	0.70
2:D:221:GLU:HG3	2:D:233:GLY:C	2.16	0.70
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.73	0.70
2:D:344:LEU:HD13	2:D:344:LEU:C	2.16	0.70
1:E:451:ARG:HG2	1:E:451:ARG:HH11	1.56	0.70
1:A:126:LEU:O	1:A:130:ILE:HG13	1.92	0.70
1:A:379:SER:N	1:A:413:THR:HB	2.02	0.70
2:C:483:PHE:HB2	2:C:489:ILE:HD13	1.74	0.70
1:E:24:MET:HE3	1:E:24:MET:CA	2.18	0.70
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.73	0.70
2:C:293:GLY:HA2	3:C:901:ATP:O1A	1.90	0.70
1:E:300:ARG:HA	1:E:333:MET:HE1	1.73	0.70
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.22	0.70
1:B:341:GLN:O	1:B:343:LEU:HG	1.92	0.70
1:E:441:GLN:NE2	1:E:490:ILE:HD13	2.06	0.70
1:F:106:LEU:HD11	1:F:129:ARG:CZ	2.22	0.70
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.72	0.69
1:B:379:SER:HA	1:B:413:THR:O	1.92	0.69
2:D:287:THR:HG21	2:D:425:ILE:O	1.92	0.69
2:C:41:SER:HB3	2:C:178:THR:HB	1.73	0.69
1:A:148:THR:OG1	1:A:182:THR:HG23	1.92	0.69
2:C:220:LEU:HD13	2:C:246:ILE:CD1	2.21	0.69
1:A:79:THR:HG23	1:A:80:PRO:HD2	1.74	0.69
1:A:438:ILE:HD11	1:A:455:VAL:HG22	1.74	0.69
1:F:303:GLU:HB2	1:F:333:MET:HE3	1.74	0.69
1:F:325:LEU:HD23	1:F:335:PHE:HB2	1.74	0.69
1:B:75:THR:O	1:B:108:ALA:HB3	1.92	0.69
1:F:78:GLU:HB3	1:F:83:ILE:HD11	1.75	0.69
1:B:263:VAL:CG1	1:B:374:ARG:HH21	2.05	0.69
2:C:300:ARG:CA	2:C:333:MET:HE1	2.22	0.69
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.23	0.69
1:F:336:GLU:HB3	1:F:340:ARG:HH21	1.57	0.69
1:A:43:LEU:HD11	1:A:182:THR:OG1	1.92	0.69
1:A:488:ARG:HE	1:F:488:ARG:HH12	1.41	0.69
2:C:269:ARG:O	2:C:273:MET:HG3	1.91	0.69
2:D:354:ALA:HB3	2:D:359:HIS:NE2	2.06	0.69
1:B:161:ARG:NH2	1:B:199:PHE:HB2	2.07	0.69
1:A:487:GLU:OE1	1:F:495:THR:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:TPO:O1P	1:B:430:ILE:N	2.26	0.69
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.57	0.69
2:D:64:ILE:HG22	2:D:65:ILE:HD13	1.75	0.69
1:B:56:SER:HB2	1:B:143:SER:HB3	1.75	0.68
2:C:451:ARG:HG2	2:C:451:ARG:NH1	2.08	0.68
1:E:199:PHE:C	1:E:201:SER:H	2.01	0.68
1:E:303:GLU:OE1	1:E:333:MET:HE3	1.93	0.68
1:F:49:GLY:O	1:F:218:ARG:NH2	2.26	0.68
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.56	0.68
1:B:194:TYR:O	1:B:196:VAL:HG23	1.93	0.68
2:C:214:GLU:OE2	2:D:217:ARG:NH1	2.26	0.68
2:D:56:SER:HB2	2:D:143:SER:HB3	1.75	0.68
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.58	0.68
1:A:210:VAL:HG12	1:A:211:LEU:O	1.93	0.68
1:B:130:ILE:O	1:B:134:ILE:HG13	1.92	0.68
2:D:21:MET:HE1	2:D:177:THR:HB	1.74	0.68
2:D:387:VAL:HG12	2:D:388:SER:N	2.08	0.68
2:C:17:ALA:C	2:C:18:ILE:HD12	2.19	0.68
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.23	0.68
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.75	0.68
1:E:462:TRP:O	1:E:463:HIS:O	2.11	0.68
1:A:371:LYS:O	1:A:371:LYS:HD2	1.92	0.68
1:B:151:PHE:C	1:B:153:GLN:H	2.02	0.68
2:C:52:LYS:HD2	2:C:182:THR:O	1.93	0.68
2:D:347:VAL:O	2:D:348:CYS:HB2	1.94	0.68
1:F:266:GLY:HA3	1:F:300:ARG:HG3	1.76	0.68
1:F:426:TPO:O1P	1:F:431:ALA:HB3	1.94	0.68
1:F:516:GLY:N	1:F:517:PRO:HD2	2.08	0.68
1:B:155:ASP:OD1	1:B:159:VAL:HG11	1.93	0.68
2:C:308:ASN:O	2:C:310:GLU:HG3	1.92	0.68
2:C:488:ARG:HH22	2:D:488:ARG:HH21	1.41	0.68
1:E:147:VAL:O	1:E:150:VAL:HG12	1.94	0.68
1:E:281:ASP:O	1:E:282:SER:HB3	1.91	0.68
1:B:293:GLY:HA2	3:B:901:ATP:O1A	1.93	0.68
2:C:50:THR:HB	2:C:207:LEU:HB3	1.74	0.68
3:C:903:ATP:HO2'	2:D:230:HIS:CE1	2.10	0.68
1:E:221:GLU:HG3	1:E:233:GLY:O	1.94	0.68
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.73	0.68
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.76	0.68
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.58	0.68
2:D:152:GLN:HG3	1:E:161:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:LEU:HD11	2:C:197:GLU:HG3	1.76	0.68
1:B:64:ILE:HG22	1:B:65:ILE:HD13	1.75	0.67
1:B:315:PHE:CE2	1:B:347:VAL:HG21	2.29	0.67
1:E:319:GLU:O	1:F:254:LEU:HD21	1.94	0.67
1:F:47:THR:HG22	1:F:50:THR:CG2	2.24	0.67
1:F:79:THR:HG22	1:F:82:ASP:H	1.58	0.67
1:F:44:VAL:HG22	1:F:205:VAL:HB	1.76	0.67
1:F:170:ARG:HH22	1:F:174:ILE:HD11	1.57	0.67
1:F:353:SER:O	1:F:354:ALA:HB2	1.93	0.67
1:F:464:ASP:OD2	1:F:466:ALA:HB3	1.94	0.67
2:D:88:ARG:HD3	1:E:15:HIS:O	1.94	0.67
2:D:496:ARG:HG2	1:E:487:GLU:OE1	1.94	0.67
1:E:131:ASN:O	1:E:135:GLN:HB2	1.93	0.67
3:E:901:ATP:H3'	1:F:458:MET:O	1.94	0.67
1:B:326:ARG:HG3	2:C:260:ASN:ND2	2.10	0.67
2:D:220:LEU:HD13	2:D:246:ILE:CD1	2.25	0.67
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.59	0.67
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.76	0.67
1:A:65:ILE:O	1:A:65:ILE:HG22	1.92	0.67
2:C:488:ARG:NH2	2:D:488:ARG:HH21	1.93	0.67
1:A:348:CYS:SG	1:B:254:LEU:HD23	2.35	0.67
2:D:89:SER:HB2	1:E:227:GLY:O	1.95	0.67
1:E:304:ASN:HB3	1:E:374:ARG:NH1	2.10	0.67
1:B:129:ARG:O	1:B:132:TYR:HB3	1.95	0.67
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.77	0.67
1:B:81:GLN:HE21	1:B:81:GLN:H	1.42	0.67
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.77	0.67
1:E:309:LYS:HA	1:E:343:LEU:HD13	1.75	0.67
2:C:25:ILE:HG23	2:C:58:GLN:NE2	2.09	0.66
2:D:332:GLY:O	2:D:333:MET:HG2	1.94	0.66
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.76	0.66
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.78	0.66
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.59	0.66
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.59	0.66
1:E:289:ALA:CB	1:E:419:PHE:HA	2.25	0.66
1:F:24:MET:HE2	1:F:66:GLU:OE2	1.96	0.66
2:C:87:ALA:C	2:C:89:SER:H	2.04	0.66
1:F:338:MET:HB3	1:F:344:LEU:HB3	1.78	0.66
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.76	0.66
1:A:14:GLU:HG3	1:A:15:HIS:N	2.08	0.66
1:A:274:CYS:HG	1:A:278:PHE:HE2	1.39	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ILE:O	1:B:248:PRO:HD3	1.95	0.66
1:B:471:MET:HB3	1:B:480:LYS:HZ1	1.60	0.66
2:C:70:PRO:HD2	2:C:140:ARG:HG2	1.78	0.66
1:E:431:ALA:O	1:E:434:THR:HG22	1.94	0.66
1:B:164:LEU:HD22	1:B:180:MET:HE1	1.77	0.66
1:B:304:ASN:HB3	1:B:374:ARG:HH12	1.61	0.66
1:E:94:LEU:O	1:E:98:VAL:HG23	1.96	0.66
1:F:260:ASN:HA	1:F:279:PHE:HE2	1.61	0.66
2:C:21:MET:HB2	2:C:38:ILE:HG13	1.78	0.66
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.76	0.66
1:E:194:TYR:O	1:E:196:VAL:N	2.29	0.66
1:F:197:GLU:OE2	1:F:197:GLU:N	2.25	0.66
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.18	0.66
1:F:96:LYS:O	1:F:100:GLU:HG3	1.96	0.66
1:A:45:SER:CB	1:A:182:THR:HB	2.26	0.66
1:B:334:ASP:OD1	1:B:336:GLU:HB2	1.96	0.66
2:D:178:THR:HG22	2:D:179:VAL:N	2.11	0.66
1:E:313:ILE:HG22	1:E:314:LEU:N	2.10	0.66
1:F:313:ILE:CG1	1:F:372:PRO:HG2	2.26	0.66
1:F:263:VAL:HG12	1:F:374:ARG:NH2	2.12	0.65
1:A:431:ALA:O	1:A:434:THR:HB	1.97	0.65
1:B:178:THR:HG22	1:B:179:VAL:H	1.60	0.65
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.31	0.65
1:F:118:VAL:HG22	1:F:122:ASP:OD1	1.96	0.65
1:A:191:ILE:N	1:A:191:ILE:HD12	2.11	0.65
2:C:221:GLU:HG3	2:C:233:GLY:O	1.96	0.65
1:A:14:GLU:HG3	1:A:16:GLN:OE1	1.96	0.65
1:A:227:GLY:O	1:F:89:SER:HB2	1.96	0.65
2:C:202:ASP:HA	2:C:226:ARG:HD2	1.77	0.65
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.24	0.65
1:F:144:ILE:HD13	1:F:167:LEU:HD21	1.79	0.65
1:F:377:ILE:CD1	1:F:399:VAL:HG11	2.26	0.65
2:C:52:LYS:N	3:C:903:ATP:O1B	2.29	0.65
1:E:446:ARG:HH21	1:E:496:ARG:HH22	1.45	0.65
1:E:225:LEU:HB2	1:E:230:HIS:HD2	1.61	0.65
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.31	0.65
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.79	0.65
1:E:123:LEU:O	1:E:127:ILE:HG13	1.96	0.65
1:E:142:VAL:HB	1:E:178:THR:HG23	1.77	0.65
1:F:370:PHE:HD2	1:F:372:PRO:HG3	1.61	0.65
1:A:161:ARG:HD2	1:A:196:VAL:HG13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:MET:HE3	2:D:59:PHE:CZ	2.29	0.65
1:E:452:ALA:HA	1:E:469:GLU:HA	1.78	0.65
1:E:504:GLU:HG2	1:E:505:LEU:N	2.10	0.65
1:F:313:ILE:HG13	1:F:372:PRO:CG	2.26	0.65
1:F:509:VAL:HG12	1:F:510:ARG:H	1.61	0.65
1:A:425:ILE:HG23	1:F:419:PHE:CE2	2.30	0.65
1:B:80:PRO:HA	1:B:83:ILE:HD13	1.79	0.65
2:C:444:GLU:OE2	2:D:489:ILE:HG12	1.97	0.65
2:D:436:THR:CG2	2:D:458:MET:HG2	2.27	0.65
2:D:486:PHE:CE2	2:D:496:ARG:HD3	2.32	0.65
1:F:46:GLY:HA2	1:F:184:ARG:HD2	1.79	0.65
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.61	0.65
1:A:426:TPO:O	1:A:427:ASP:HB2	1.97	0.64
2:D:81:GLN:H	2:D:81:GLN:CD	2.05	0.64
1:E:212:GLU:O	1:E:212:GLU:HG2	1.96	0.64
1:F:248:PRO:C	1:F:250:GLY:H	2.06	0.64
1:A:31:ILE:HA	1:A:231:MET:SD	2.37	0.64
1:F:197:GLU:H	1:F:197:GLU:CD	2.03	0.64
1:F:400:THR:HG21	1:F:433:ILE:CG2	2.27	0.64
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.12	0.64
2:D:194:TYR:O	2:D:196:VAL:HG23	1.96	0.64
2:D:338:MET:HE2	2:D:338:MET:HA	1.78	0.64
1:A:164:LEU:HD11	1:A:197:GLU:HG3	1.79	0.64
1:E:367:ILE:HG12	1:E:375:ILE:HD11	1.79	0.64
1:E:451:ARG:H	1:E:451:ARG:HD2	1.62	0.64
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.33	0.64
1:F:452:ALA:HA	1:F:469:GLU:HA	1.79	0.64
1:A:273:MET:O	1:A:463:HIS:HA	1.97	0.64
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.10	0.64
1:A:327:ASN:HB3	5:A:531:HOH:O	1.96	0.64
1:B:147:VAL:HG11	1:B:180:MET:CE	2.27	0.64
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.62	0.64
2:D:225:LEU:HD12	2:D:230:HIS:HB3	1.80	0.64
1:E:153:GLN:C	1:F:158:SER:HB2	2.22	0.64
1:E:393:ARG:O	1:E:397:ILE:HG12	1.96	0.64
1:E:425:ILE:HG22	1:E:425:ILE:O	1.97	0.64
1:A:130:ILE:O	1:A:134:ILE:HG13	1.97	0.64
1:B:52:LYS:O	1:B:53:THR:C	2.41	0.64
2:D:267:VAL:HG22	2:D:300:ARG:HG2	1.79	0.64
2:D:489:ILE:HA	2:D:494:PRO:HG3	1.79	0.64
1:A:161:ARG:NH1	1:F:183:GLU:OE2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HD13	1:B:123:LEU:O	1.98	0.64
1:B:191:ILE:HB	1:B:198:GLU:HG3	1.79	0.64
1:E:427:ASP:O	1:E:428:SER:HB3	1.96	0.64
1:A:436:THR:HG23	1:A:458:MET:HG2	1.80	0.64
1:A:488:ARG:HE	1:F:488:ARG:NH1	1.95	0.64
2:C:25:ILE:CG1	2:C:58:GLN:HE21	2.07	0.64
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.79	0.64
1:E:24:MET:HA	1:E:24:MET:CE	2.26	0.64
1:F:298:VAL:O	1:F:301:PHE:HB3	1.98	0.64
1:B:145:ASP:OD2	1:B:181:THR:HG21	1.98	0.64
2:D:18:ILE:H	2:D:18:ILE:CD1	2.11	0.64
1:A:27:GLY:O	1:A:30:ASP:HB2	1.98	0.63
1:A:356:LEU:HD11	1:A:387:VAL:HG21	1.80	0.63
2:D:147:VAL:HG11	2:D:180:MET:HE2	1.80	0.63
1:A:299:SER:HB3	1:A:333:MET:CE	2.28	0.63
1:B:148:THR:C	1:B:150:VAL:H	2.07	0.63
1:B:426:TPO:O3P	1:B:426:TPO:O	2.16	0.63
2:D:449:MET:HE2	2:D:449:MET:HA	1.80	0.63
1:E:146:SER:H	1:E:181:THR:HB	1.61	0.63
1:E:294:LYS:N	3:E:901:ATP:O1B	2.30	0.63
1:F:458:MET:SD	1:F:461:SER:HB3	2.37	0.63
1:A:41:SER:HA	1:A:178:THR:O	1.98	0.63
1:B:123:LEU:HD12	1:B:166:ARG:HD2	1.80	0.63
1:E:332:GLY:O	1:E:333:MET:HG2	1.99	0.63
2:C:380:LEU:HD11	2:C:412:PHE:HD2	1.63	0.63
1:E:18:ILE:HD11	1:E:227:GLY:CA	2.25	0.63
1:F:293:GLY:HA2	3:F:901:ATP:O1A	1.98	0.63
1:F:317:TYR:HA	1:F:349:ALA:O	1.97	0.63
1:A:166:ARG:HG3	1:F:112:PRO:O	1.97	0.63
1:F:220:LEU:HD23	1:F:220:LEU:C	2.23	0.63
1:F:370:PHE:C	1:F:372:PRO:HD3	2.23	0.63
1:F:453:ILE:HG12	1:F:454:ASN:H	1.63	0.63
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.62	0.63
2:C:54:LEU:HD23	2:C:244:ILE:HG13	1.81	0.63
2:C:74:VAL:HG22	2:C:106:LEU:HD23	1.80	0.63
1:E:323:GLN:HG2	1:E:327:ASN:HD21	1.63	0.63
1:E:458:MET:SD	1:E:461:SER:HB3	2.38	0.63
1:F:61:TYR:CZ	1:F:65:ILE:HG13	2.34	0.63
1:A:183:GLU:HB2	1:B:199:PHE:CZ	2.34	0.63
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.99	0.63
1:F:461:SER:OG	1:F:462:TRP:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLN:O	1:B:342:ASN:C	2.41	0.63
2:D:283:ILE:HG13	2:D:400:THR:HG23	1.79	0.63
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.81	0.63
1:A:231:MET:HB3	1:A:235:TYR:OH	1.99	0.63
1:A:360:LEU:O	1:A:360:LEU:HD22	1.98	0.63
1:B:88:ARG:HG2	1:B:88:ARG:HH11	1.64	0.63
1:B:192:ALA:O	1:B:194:TYR:N	2.32	0.63
2:C:344:LEU:HD22	2:C:345:LYS:N	2.13	0.63
2:D:496:ARG:HD2	5:D:546:HOH:O	1.97	0.63
1:F:315:PHE:CE1	1:F:375:ILE:HD11	2.34	0.63
1:A:442:TYR:HE1	1:B:456:PHE:CZ	2.17	0.62
1:F:247:PHE:HB3	1:F:249:LEU:CD2	2.29	0.62
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.81	0.62
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.34	0.62
2:D:379:SER:HA	2:D:413:THR:O	1.98	0.62
1:F:80:PRO:HG2	1:F:107:ASP:HB2	1.80	0.62
2:C:211:LEU:O	2:C:212:GLU:HB3	1.99	0.62
2:C:316:ALA:O	2:C:348:CYS:HA	1.98	0.62
1:F:264:SER:O	1:F:374:ARG:NH2	2.31	0.62
1:A:50:THR:CG2	1:A:209:ASN:HB2	2.28	0.62
1:B:18:ILE:HB	1:B:228:THR:CG2	2.30	0.62
2:C:299:SER:C	2:C:333:MET:HE1	2.24	0.62
2:D:151:PHE:C	2:D:153:GLN:H	2.07	0.62
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.30	0.62
2:D:60:LEU:HD22	2:D:71:GLY:HA3	1.82	0.62
2:D:79:THR:HG22	2:D:82:ASP:OD2	2.00	0.62
1:E:21:MET:HE1	1:E:141:ARG:HG2	1.82	0.62
1:E:294:LYS:HB3	1:E:413:THR:CG2	2.30	0.62
1:F:168:VAL:HG12	1:F:169:ALA:N	2.14	0.62
1:F:445:ILE:HG13	1:F:483:PHE:HE2	1.63	0.62
2:D:196:VAL:O	2:D:200:VAL:HG23	1.99	0.62
1:E:291:GLY:C	1:E:442:TYR:OH	2.42	0.62
1:F:147:VAL:O	1:F:150:VAL:HG12	2.00	0.62
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.81	0.62
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.30	0.62
2:C:25:ILE:HG23	2:C:58:GLN:HE22	1.64	0.62
1:A:284:ILE:HD12	1:A:436:THR:HB	1.82	0.62
1:B:469:GLU:HB3	1:B:483:PHE:CZ	2.35	0.62
2:C:137:TYR:O	2:C:138:ARG:HB2	1.98	0.62
2:C:471:MET:HE2	2:C:478:ASP:H	1.64	0.62
2:D:266:GLY:HA3	2:D:300:ARG:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:446:ARG:HB3	1:E:484:ARG:HG3	1.82	0.62
1:E:284:ILE:HB	1:E:411:LEU:HD12	1.82	0.62
1:E:301:PHE:HZ	1:E:409:THR:HG22	1.65	0.62
1:A:356:LEU:HD23	1:A:395:PHE:HB2	1.80	0.62
1:B:36:LEU:HD12	1:B:59:PHE:CZ	2.35	0.62
1:B:315:PHE:CD2	1:B:347:VAL:HG21	2.34	0.62
2:C:46:GLY:HA2	2:C:184:ARG:HD2	1.79	0.62
1:E:52:LYS:HB3	1:E:181:THR:HG23	1.80	0.62
1:F:504:GLU:O	1:F:505:LEU:HB2	1.98	0.62
1:A:427:ASP:O	1:A:429:HIS:ND1	2.31	0.61
2:C:121:PHE:O	2:C:125:ALA:HB3	2.00	0.61
2:C:311:ARG:HD2	2:C:371:LYS:HE3	1.81	0.61
1:E:21:MET:HE3	1:E:141:ARG:NE	2.15	0.61
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.30	0.61
1:E:311:ARG:HD2	1:E:371:LYS:HE3	1.81	0.61
1:F:344:LEU:C	1:F:344:LEU:HD13	2.25	0.61
1:A:400:THR:HG21	1:A:433:ILE:HG22	1.82	0.61
1:B:297:LEU:HD12	1:B:440:LEU:HD11	1.83	0.61
2:C:41:SER:HA	2:C:178:THR:O	2.00	0.61
1:B:220:LEU:HD13	1:B:246:ILE:CD1	2.30	0.61
2:D:147:VAL:CG2	2:D:148:THR:N	2.63	0.61
1:B:31:ILE:HA	1:B:231:MET:SD	2.41	0.61
2:C:24:MET:HB2	2:C:62:ASN:ND2	2.15	0.61
2:D:127:ILE:HG12	2:D:167:LEU:HD13	1.81	0.61
2:D:334:ASP:OD1	2:D:336:GLU:N	2.33	0.61
1:E:27:GLY:O	1:E:30:ASP:HB2	2.01	0.61
1:F:103:LEU:C	1:F:103:LEU:HD12	2.26	0.61
2:C:182:THR:CG2	2:C:183:GLU:H	2.11	0.61
2:C:267:VAL:HB	2:C:270:LEU:HB2	1.82	0.61
1:A:79:THR:HB	1:A:82:ASP:OD2	2.01	0.61
1:B:461:SER:OG	1:B:462:TRP:N	2.34	0.61
2:C:98:VAL:HG13	2:C:103:LEU:O	2.01	0.61
2:D:80:PRO:HG2	2:D:107:ASP:HB2	1.82	0.61
2:D:273:MET:SD	2:D:468:ARG:HD2	2.39	0.61
1:E:38:ILE:HA	1:E:177:THR:HG23	1.81	0.61
1:E:184:ARG:HD2	1:E:191:ILE:O	2.01	0.61
1:F:171:LEU:CD1	1:F:178:THR:HG21	2.31	0.61
1:A:24:MET:N	1:A:29:ASP:OD2	2.33	0.61
1:A:508:ILE:H	1:A:508:ILE:HD13	1.65	0.61
1:B:170:ARG:O	1:B:174:ILE:HG12	1.99	0.61
2:D:23:THR:HB	2:D:25:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:375:ILE:HG13	2:D:408:ILE:HG21	1.82	0.61
1:A:45:SER:HB2	1:A:182:THR:HB	1.83	0.61
1:B:187:GLU:OE2	1:B:208:ARG:HA	2.01	0.61
2:C:347:VAL:O	2:C:348:CYS:HB2	1.99	0.61
2:D:218:ARG:HG3	2:D:237:PHE:O	2.00	0.61
1:F:115:GLN:CG	1:F:116:GLU:H	2.13	0.61
1:F:363:ILE:O	1:F:367:ILE:HG13	2.00	0.61
2:D:123:LEU:O	2:D:127:ILE:HG13	2.00	0.61
1:E:469:GLU:HB3	1:E:483:PHE:CE1	2.36	0.61
1:F:313:ILE:CD1	1:F:372:PRO:HG2	2.31	0.61
1:B:112:PRO:O	2:C:166:ARG:HG3	2.01	0.61
2:C:170:ARG:O	2:C:174:ILE:HG12	2.01	0.61
1:E:31:ILE:HA	1:E:231:MET:HG3	1.83	0.61
1:E:93:ASP:OD1	1:E:95:ALA:HB3	2.01	0.61
1:F:484:ARG:HB3	1:F:484:ARG:HH11	1.66	0.61
2:C:283:ILE:HG13	2:C:400:THR:HG23	1.81	0.60
2:C:315:PHE:HA	2:C:347:VAL:HB	1.83	0.60
1:E:303:GLU:CD	1:E:333:MET:HE3	2.26	0.60
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.66	0.60
1:F:64:ILE:HG22	1:F:65:ILE:HD13	1.82	0.60
1:B:326:ARG:HD3	2:C:259:SER:O	2.01	0.60
2:C:488:ARG:O	2:C:491:SER:HB3	2.01	0.60
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.36	0.60
1:F:194:TYR:O	1:F:196:VAL:HG23	2.00	0.60
1:A:191:ILE:HB	1:A:198:GLU:CG	2.31	0.60
1:A:418:GLN:HB2	1:B:423:HIS:O	2.02	0.60
1:B:414:ASN:ND2	1:B:426:TPO:HG23	2.17	0.60
1:E:170:ARG:O	1:E:174:ILE:HG12	2.01	0.60
1:A:79:THR:HG22	1:A:81:GLN:HG2	1.83	0.60
2:C:20:LYS:C	2:C:38:ILE:HD11	2.27	0.60
2:C:315:PHE:HE2	2:C:363:ILE:HA	1.62	0.60
1:A:32:SER:OG	1:A:35:GLY:N	2.34	0.60
1:A:52:LYS:HD2	1:A:181:THR:HG23	1.84	0.60
1:B:202:ASP:HA	1:B:226:ARG:HD2	1.82	0.60
1:B:311:ARG:HD2	1:B:371:LYS:HE3	1.84	0.60
2:C:48:SER:HB2	2:D:199:PHE:CE1	2.36	0.60
2:C:245:ASN:C	2:C:245:ASN:ND2	2.60	0.60
2:D:48:SER:HA	5:D:526:HOH:O	2.01	0.60
1:B:451:ARG:HB3	1:B:470:PHE:CE2	2.36	0.60
2:C:156:ALA:O	2:C:160:VAL:HG23	2.01	0.60
1:A:344:LEU:HD13	1:A:344:LEU:C	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:PRO:HG2	2:C:138:ARG:O	2.02	0.60
2:D:380:LEU:N	2:D:413:THR:O	2.32	0.60
1:E:455:VAL:HG11	1:E:463:HIS:HB2	1.82	0.60
1:F:269:ARG:O	1:F:272:GLU:HB2	2.01	0.60
1:F:471:MET:HE2	1:F:478:ASP:HB2	1.84	0.60
1:A:273:MET:O	1:A:464:ASP:N	2.30	0.60
2:C:393:ARG:NH2	2:C:429:HIS:HB2	2.17	0.60
2:D:163:GLU:HA	2:D:163:GLU:OE2	2.01	0.60
1:E:52:LYS:HB3	1:E:181:THR:CG2	2.31	0.60
1:F:247:PHE:HB3	1:F:249:LEU:HD21	1.81	0.60
1:F:451:ARG:HG2	1:F:451:ARG:HH11	1.67	0.60
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.32	0.60
2:C:389:ASN:HD21	2:C:428:SER:HB2	1.67	0.60
1:E:283:ILE:HD12	1:E:412:PHE:HE1	1.66	0.60
1:F:260:ASN:HA	1:F:279:PHE:CE2	2.36	0.60
1:B:294:LYS:HB3	1:B:413:THR:HG23	1.83	0.60
1:F:329:TYR:HA	1:F:332:GLY:O	2.01	0.60
1:A:230:HIS:CE1	1:A:232:LYS:HG3	2.37	0.59
1:B:62:ASN:O	1:B:66:GLU:HB2	2.02	0.59
1:E:392:PHE:O	1:E:395:PHE:N	2.35	0.59
1:F:53:THR:OG1	1:F:145:ASP:OD1	2.20	0.59
2:C:464:ASP:OD1	2:C:466:ALA:N	2.35	0.59
1:F:471:MET:HE1	1:F:473:SER:HB3	1.83	0.59
2:C:386:GLY:HA2	2:D:390:ASN:HD21	1.66	0.59
2:C:404:LYS:C	2:C:406:GLU:H	2.09	0.59
1:A:446:ARG:HA	1:A:496:ARG:HH22	1.67	0.59
1:E:164:LEU:HD11	1:E:197:GLU:HG3	1.85	0.59
1:F:47:THR:CG2	1:F:50:THR:CG2	2.80	0.59
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.82	0.59
1:A:448:GLU:HG2	1:B:466:ALA:HB2	1.84	0.59
1:B:31:ILE:HG23	1:B:231:MET:HB2	1.85	0.59
2:C:21:MET:HE3	2:C:141:ARG:CZ	2.33	0.59
2:C:358:ASP:O	2:C:362:ILE:HG12	2.02	0.59
1:E:153:GLN:O	1:F:158:SER:HB2	2.02	0.59
1:F:78:GLU:CB	1:F:83:ILE:HD11	2.32	0.59
1:F:82:ASP:HA	1:F:85:LYS:HB3	1.84	0.59
1:B:221:GLU:HG2	1:B:222:ILE:N	2.15	0.59
1:B:415:THR:HB	2:C:432:GLU:OE2	2.02	0.59
1:B:490:ILE:HG22	1:B:491:SER:N	2.18	0.59
2:D:152:GLN:HG3	1:E:161:ARG:HH11	1.67	0.59
1:E:467:ILE:O	1:E:467:ILE:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.33	0.59
1:B:123:LEU:O	1:B:127:ILE:HG13	2.02	0.59
2:D:155:ASP:OD1	2:D:159:VAL:HG11	2.01	0.59
2:D:399:VAL:O	2:D:400:THR:C	2.45	0.59
1:E:267:VAL:HG21	1:E:477:PRO:HG3	1.85	0.59
1:B:50:THR:HB	1:B:207:LEU:CB	2.33	0.59
2:D:81:GLN:H	2:D:81:GLN:NE2	2.01	0.59
2:D:262:ARG:NH1	2:D:275:GLY:O	2.36	0.59
1:E:501:GLU:O	1:E:502:LYS:HG3	2.03	0.59
1:F:501:GLU:HG3	1:F:502:LYS:N	2.17	0.59
1:A:211:LEU:CG	1:A:212:GLU:H	2.08	0.59
1:B:363:ILE:O	1:B:367:ILE:HG13	2.03	0.59
1:E:419:PHE:CE2	1:F:425:ILE:HG13	2.37	0.59
1:F:453:ILE:HG12	1:F:454:ASN:N	2.18	0.59
1:A:18:ILE:N	1:A:18:ILE:HD12	2.18	0.58
1:E:84:ILE:HG21	1:E:95:ALA:HB2	1.84	0.58
1:F:315:PHE:CE2	1:F:347:VAL:HG21	2.38	0.58
1:A:429:HIS:CD2	1:F:417:ASP:CG	2.81	0.58
1:B:36:LEU:HD12	1:B:59:PHE:CE1	2.38	0.58
1:B:140:ARG:HH11	1:B:140:ARG:CB	2.15	0.58
1:B:185:ILE:HD13	1:B:185:ILE:N	2.19	0.58
2:C:461:SER:OG	2:C:462:TRP:N	2.33	0.58
2:D:86:ASN:O	2:D:88:ARG:N	2.36	0.58
2:D:263:VAL:HG12	2:D:374:ARG:HH21	1.67	0.58
1:E:184:ARG:NH2	1:E:187:GLU:O	2.36	0.58
1:E:342:ASN:O	1:E:343:LEU:HD23	2.02	0.58
1:E:385:ARG:HA	1:F:393:ARG:NH1	2.19	0.58
1:F:187:GLU:OE2	1:F:208:ARG:HA	2.03	0.58
1:B:193:ARG:NH2	2:C:196:VAL:HG23	2.19	0.58
2:C:220:LEU:HD23	2:C:221:GLU:N	2.17	0.58
2:C:379:SER:H	2:C:413:THR:HB	1.68	0.58
1:E:344:LEU:HD13	1:E:345:LYS:N	2.19	0.58
1:F:150:VAL:HG13	1:F:151:PHE:N	2.17	0.58
1:F:294:LYS:HB3	1:F:413:THR:HG23	1.83	0.58
1:A:286:ALA:HA	1:A:438:ILE:O	2.03	0.58
2:D:150:VAL:O	2:D:153:GLN:HG3	2.02	0.58
1:E:81:GLN:NE2	1:E:81:GLN:H	2.02	0.58
1:A:348:CYS:SG	1:B:254:LEU:CD2	2.91	0.58
2:C:185:ILE:HD13	2:C:185:ILE:N	2.19	0.58
1:E:420:MET:SD	1:F:490:ILE:HG13	2.44	0.58
1:F:191:ILE:HB	1:F:198:GLU:CG	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:HE3	1:B:18:ILE:HD13	1.85	0.58
1:B:150:VAL:O	1:B:153:GLN:HG3	2.04	0.58
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.69	0.58
2:C:106:LEU:CD2	2:C:130:ILE:HG12	2.34	0.58
2:C:311:ARG:HD3	2:C:370:PHE:O	2.04	0.58
1:E:492:GLY:O	1:E:494:PRO:HD3	2.03	0.58
1:A:254:LEU:HG	1:F:320:SER:HA	1.86	0.58
2:C:493:SER:OG	2:D:488:ARG:HG2	2.04	0.58
1:E:311:ARG:HD2	1:E:371:LYS:CE	2.33	0.58
2:C:344:LEU:HD11	2:C:346:ILE:HG13	1.85	0.58
2:D:83:ILE:H	2:D:83:ILE:HD12	1.67	0.58
1:E:126:LEU:O	1:E:130:ILE:HG13	2.04	0.58
1:F:248:PRO:O	1:F:250:GLY:N	2.36	0.58
1:A:360:LEU:HD21	1:A:398:GLY:O	2.03	0.58
1:B:31:ILE:O	1:B:231:MET:HG3	2.04	0.58
1:B:462:TRP:O	1:B:463:HIS:O	2.21	0.58
2:D:21:MET:O	2:D:35:GLY:HA3	2.03	0.58
2:D:147:VAL:HG11	2:D:180:MET:CE	2.32	0.58
2:D:182:THR:HG22	2:D:183:GLU:N	2.18	0.58
2:D:312:ALA:O	2:D:344:LEU:HD22	2.04	0.58
2:D:318:GLU:OE2	1:E:432:GLU:HB3	2.03	0.58
2:D:367:ILE:HD11	2:D:375:ILE:CD1	2.34	0.58
1:E:33:HIS:HD2	1:E:230:HIS:HA	1.69	0.58
1:E:200:VAL:O	1:E:200:VAL:HG12	2.04	0.58
1:E:323:GLN:HG2	1:E:327:ASN:ND2	2.19	0.58
1:F:231:MET:CE	1:F:251:ALA:HB2	2.34	0.58
1:B:24:MET:CB	1:B:62:ASN:HD22	2.17	0.58
2:C:38:ILE:H	2:C:38:ILE:HD12	1.68	0.58
2:C:486:PHE:CE2	2:C:496:ARG:HG2	2.39	0.58
1:F:353:SER:O	1:F:354:ALA:CB	2.51	0.58
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.69	0.58
1:B:81:GLN:H	1:B:81:GLN:NE2	2.01	0.57
2:C:147:VAL:O	2:C:150:VAL:HG12	2.04	0.57
2:C:265:SER:O	2:C:301:PHE:HA	2.04	0.57
1:A:316:ALA:O	1:A:348:CYS:HA	2.04	0.57
1:A:469:GLU:HG3	1:A:470:PHE:N	2.18	0.57
2:C:38:ILE:HG22	2:C:39:GLY:N	2.18	0.57
1:F:406:GLU:O	1:F:408:ILE:HG13	2.04	0.57
1:A:274:CYS:SG	1:A:278:PHE:HE2	2.27	0.57
1:B:147:VAL:O	1:B:150:VAL:HG12	2.03	0.57
1:B:164:LEU:CD2	1:B:180:MET:HE1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:MET:HE1	2:C:141:ARG:HG2	1.85	0.57
2:C:493:SER:OG	2:D:488:ARG:HA	2.05	0.57
2:D:294:LYS:N	3:D:901:ATP:O1B	2.36	0.57
1:A:152:GLN:HG3	1:B:161:ARG:HH11	1.70	0.57
1:A:284:ILE:CD1	1:A:436:THR:HB	2.34	0.57
2:C:71:GLY:O	2:C:104:PHE:N	2.37	0.57
2:C:151:PHE:C	2:C:153:GLN:H	2.12	0.57
2:C:182:THR:CG2	2:C:183:GLU:N	2.68	0.57
2:C:298:VAL:O	2:C:301:PHE:HB3	2.04	0.57
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.34	0.57
2:C:497:ILE:HD12	2:C:497:ILE:O	2.04	0.57
2:D:305:ALA:O	2:D:310:GLU:O	2.22	0.57
2:D:332:GLY:O	2:D:333:MET:O	2.22	0.57
1:E:132:TYR:HE2	1:E:136:LYS:HD2	1.69	0.57
1:A:27:GLY:O	1:A:30:ASP:N	2.33	0.57
1:A:251:ALA:O	1:A:252:MET:C	2.47	0.57
2:C:70:PRO:HB2	2:C:139:ALA:CA	2.30	0.57
2:C:164:LEU:HD22	2:C:180:MET:HE1	1.85	0.57
2:C:464:ASP:OD1	2:C:464:ASP:C	2.47	0.57
2:D:225:LEU:HB2	2:D:230:HIS:CD2	2.40	0.57
1:F:311:ARG:HD2	1:F:371:LYS:HE3	1.86	0.57
1:B:191:ILE:HD12	1:B:191:ILE:N	2.20	0.57
1:B:436:THR:HA	1:B:457:LYS:O	2.04	0.57
2:C:294:LYS:O	2:C:298:VAL:HG23	2.04	0.57
2:C:296:LEU:CD2	2:C:477:PRO:HB3	2.35	0.57
2:C:389:ASN:O	2:C:392:PHE:N	2.38	0.57
2:D:31:ILE:HA	2:D:231:MET:CG	2.35	0.57
2:D:214:GLU:HG2	1:E:234:GLU:OE1	2.04	0.57
1:E:23:THR:O	1:E:24:MET:HB2	2.04	0.57
1:F:435:ASP:OD1	1:F:459:ARG:NH1	2.37	0.57
1:A:70:PRO:HA	1:A:102:LYS:O	2.04	0.57
1:A:191:ILE:HD13	1:A:198:GLU:OE2	2.04	0.57
1:A:377:ILE:HD12	1:A:412:PHE:CE2	2.40	0.57
2:C:149:SER:HB3	2:D:161:ARG:NH2	2.19	0.57
2:D:249:LEU:HD12	2:D:394:GLN:OE1	2.04	0.57
2:D:295:THR:HA	2:D:298:VAL:CG2	2.35	0.57
1:E:416:SER:C	1:E:418:GLN:H	2.12	0.57
1:F:52:LYS:HB3	1:F:181:THR:HG23	1.86	0.57
1:F:379:SER:OG	1:F:382:ALA:HB2	2.04	0.57
1:F:515:LYS:HG3	1:F:516:GLY:N	2.14	0.57
1:B:126:LEU:HD12	1:B:129:ARG:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ALA:HA	1:B:434:THR:HG22	1.86	0.57
2:C:212:GLU:O	2:C:212:GLU:HG2	2.04	0.57
2:C:323:GLN:NE2	2:D:459:ARG:HD3	2.20	0.57
1:F:446:ARG:H	1:F:496:ARG:NH2	2.03	0.57
2:D:353:SER:O	2:D:354:ALA:HB2	2.05	0.57
1:E:287:THR:CG2	1:E:414:ASN:HD22	2.18	0.57
1:E:445:ILE:HG22	1:E:445:ILE:O	2.04	0.57
1:F:418:GLN:HE21	1:F:421:GLY:C	2.13	0.57
1:F:435:ASP:HA	1:F:459:ARG:HD2	1.87	0.57
1:A:458:MET:O	3:F:901:ATP:H3'	2.05	0.56
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.87	0.56
2:D:151:PHE:O	2:D:153:GLN:N	2.32	0.56
1:E:283:ILE:HD12	1:E:412:PHE:CE1	2.40	0.56
1:B:36:LEU:HD22	1:B:42:THR:HG21	1.86	0.56
1:B:294:LYS:N	3:B:901:ATP:O1B	2.38	0.56
1:B:326:ARG:C	1:B:328:ALA:H	2.12	0.56
1:E:273:MET:SD	1:E:479:ILE:HD13	2.45	0.56
1:F:305:ALA:HB2	1:F:374:ARG:CD	2.28	0.56
1:A:24:MET:HA	1:A:24:MET:HE3	1.86	0.56
1:A:188:TYR:HE2	1:F:211:LEU:HD23	1.69	0.56
1:A:298:VAL:HG23	1:A:411:LEU:HD23	1.88	0.56
1:B:404:LYS:C	1:B:406:GLU:H	2.14	0.56
2:C:24:MET:CB	2:C:62:ASN:HD22	2.16	0.56
2:C:425:ILE:HD12	2:C:425:ILE:H	1.70	0.56
2:D:96:LYS:O	2:D:100:GLU:HG3	2.05	0.56
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.86	0.56
2:D:382:ALA:O	2:D:385:ARG:HG3	2.04	0.56
2:D:461:SER:OG	2:D:462:TRP:N	2.39	0.56
1:E:266:GLY:HA3	1:E:300:ARG:HG3	1.86	0.56
1:E:364:LYS:O	1:E:368:ASN:ND2	2.38	0.56
1:E:444:GLU:OE1	1:F:489:ILE:HB	2.05	0.56
1:E:451:ARG:HD2	1:E:451:ARG:N	2.20	0.56
1:F:379:SER:H	1:F:413:THR:HB	1.70	0.56
1:F:471:MET:HE1	1:F:473:SER:CB	2.35	0.56
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.87	0.56
1:B:308:ASN:O	1:B:310:GLU:HG3	2.05	0.56
1:B:379:SER:N	1:B:413:THR:HB	2.21	0.56
2:C:488:ARG:HH22	2:D:488:ARG:NH2	2.03	0.56
1:B:192:ALA:HB3	1:B:197:GLU:OE2	2.05	0.56
2:C:60:LEU:O	2:C:61:TYR:C	2.47	0.56
2:D:170:ARG:HH12	2:D:174:ILE:HD11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:ARG:CA	1:E:333:MET:HE1	2.36	0.56
1:F:45:SER:HB3	1:F:182:THR:HB	1.87	0.56
1:A:509:VAL:O	1:A:511:GLY:N	2.37	0.56
2:C:150:VAL:HG13	2:C:151:PHE:N	2.20	0.56
2:C:191:ILE:HD12	2:C:191:ILE:H	1.70	0.56
2:C:197:GLU:H	2:C:197:GLU:CD	2.13	0.56
1:F:111:ASP:OD1	1:F:112:PRO:HD2	2.04	0.56
1:F:426:TPO:C	1:F:428:SER:H	2.19	0.56
1:B:117:VAL:O	1:B:117:VAL:HG12	2.06	0.56
1:B:150:VAL:HG13	1:B:151:PHE:N	2.20	0.56
1:B:334:ASP:O	1:B:338:MET:HG2	2.06	0.56
1:B:347:VAL:O	1:B:348:CYS:HB2	2.06	0.56
2:C:315:PHE:HB3	2:C:317:TYR:HE1	1.69	0.56
2:C:357:GLU:HG3	2:C:358:ASP:N	2.20	0.56
1:E:146:SER:HA	1:E:181:THR:O	2.06	0.56
1:A:471:MET:CG	1:A:478:ASP:HB3	2.35	0.56
1:B:130:ILE:HG22	1:B:134:ILE:HD11	1.86	0.56
2:C:261:VAL:CG1	2:C:262:ARG:H	2.16	0.56
1:E:379:SER:N	1:E:413:THR:HB	2.19	0.56
1:F:192:ALA:HB3	1:F:197:GLU:OE2	2.06	0.56
1:A:64:ILE:CD1	1:A:103:LEU:HB2	2.34	0.56
1:B:64:ILE:HG21	1:B:97:LEU:HD13	1.86	0.56
1:B:123:LEU:HG	1:B:163:GLU:HB3	1.87	0.56
1:B:360:LEU:C	1:B:360:LEU:HD13	2.31	0.56
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.46	0.56
2:D:346:ILE:CG2	2:D:347:VAL:N	2.68	0.56
1:E:221:GLU:HG2	1:E:222:ILE:N	2.19	0.56
1:E:371:LYS:HD2	1:E:371:LYS:O	2.05	0.56
1:F:426:TPO:HG21	1:F:429:HIS:C	2.30	0.56
1:A:219:THR:HA	1:A:235:TYR:O	2.06	0.56
1:B:502:LYS:HG3	1:B:504:GLU:O	2.06	0.56
2:D:468:ARG:HG2	2:D:468:ARG:HH11	1.71	0.56
1:F:300:ARG:N	1:F:333:MET:HE1	2.19	0.56
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.19	0.56
1:A:254:LEU:HD23	1:F:348:CYS:SG	2.46	0.55
1:A:318:GLU:OE2	1:B:432:GLU:HB3	2.05	0.55
2:C:471:MET:SD	2:C:478:ASP:HB3	2.46	0.55
2:D:294:LYS:H	2:D:294:LYS:HD3	1.71	0.55
2:D:350:TYR:CE1	1:E:254:LEU:HD13	2.42	0.55
1:F:362:ILE:O	1:F:365:SER:HB3	2.06	0.55
1:F:396:VAL:HG11	1:F:430:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:LEU:HD23	1:F:454:ASN:HD22	1.71	0.55
1:F:514:GLU:O	1:F:515:LYS:HB2	2.05	0.55
1:B:237:PHE:HB2	1:B:246:ILE:HG12	1.88	0.55
1:B:325:LEU:O	1:B:328:ALA:HB3	2.06	0.55
1:B:486:PHE:CE2	1:B:496:ARG:HB2	2.41	0.55
1:E:194:TYR:O	1:E:195:GLY:C	2.49	0.55
1:E:311:ARG:HD3	1:E:370:PHE:CE1	2.40	0.55
1:E:417:ASP:OD2	1:F:429:HIS:CE1	2.60	0.55
1:F:191:ILE:HB	1:F:198:GLU:HG2	1.88	0.55
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.46	0.55
1:F:514:GLU:O	1:F:515:LYS:CB	2.53	0.55
1:A:426:TPO:CG2	1:A:426:TPO:O3P	2.55	0.55
1:E:167:LEU:HG	1:E:171:LEU:HD12	1.89	0.55
1:A:199:PHE:CZ	1:F:183:GLU:HB2	2.41	0.55
1:A:483:PHE:HB2	1:A:489:ILE:CD1	2.36	0.55
1:B:150:VAL:CG1	1:B:151:PHE:N	2.69	0.55
2:C:63:GLY:HA3	2:C:141:ARG:CZ	2.36	0.55
2:C:71:GLY:O	2:C:103:LEU:HA	2.05	0.55
2:C:191:ILE:HD12	2:C:191:ILE:N	2.21	0.55
1:F:45:SER:CB	1:F:182:THR:HB	2.37	0.55
1:F:408:ILE:HG22	1:F:408:ILE:O	2.06	0.55
2:C:142:VAL:O	2:C:178:THR:HA	2.07	0.55
2:C:311:ARG:HA	2:C:343:LEU:O	2.06	0.55
2:D:334:ASP:O	2:D:338:MET:HG2	2.07	0.55
2:D:358:ASP:O	2:D:361:GLN:N	2.40	0.55
1:F:323:GLN:HG2	1:F:327:ASN:HD21	1.71	0.55
1:F:515:LYS:HB3	1:F:517:PRO:HD2	1.89	0.55
1:A:317:TYR:HA	1:A:349:ALA:O	2.06	0.55
1:A:350:TYR:OH	1:B:254:LEU:HD13	2.07	0.55
1:A:362:ILE:O	1:A:366:GLU:HB2	2.07	0.55
1:A:414:ASN:ND2	1:A:426:TPO:HA	2.21	0.55
2:D:220:LEU:HD13	2:D:246:ILE:HD11	1.89	0.55
1:E:170:ARG:HD2	1:E:173:GLN:OE1	2.07	0.55
1:A:52:LYS:HB3	1:A:181:THR:HG23	1.88	0.55
1:B:383:LEU:HD13	1:B:395:PHE:CE2	2.42	0.55
2:C:261:VAL:O	2:C:262:ARG:HG2	2.07	0.55
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.22	0.55
2:D:347:VAL:CG1	2:D:348:CYS:N	2.70	0.55
2:D:354:ALA:HB3	2:D:359:HIS:CE1	2.40	0.55
1:B:284:ILE:CD1	1:B:436:THR:HB	2.37	0.55
2:C:94:LEU:O	2:C:98:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:ARG:HG3	2:C:217:ARG:O	2.06	0.55
1:E:441:GLN:HE22	1:E:490:ILE:HA	1.71	0.55
1:F:508:ILE:H	1:F:508:ILE:HD12	1.71	0.55
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.22	0.55
2:C:31:ILE:HG23	2:C:231:MET:HB2	1.89	0.55
2:D:23:THR:O	2:D:24:MET:HB2	2.07	0.55
2:D:387:VAL:CG1	2:D:388:SER:N	2.68	0.55
1:E:417:ASP:O	1:F:424:SER:HB3	2.06	0.55
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.72	0.55
1:B:291:GLY:HA3	1:B:442:TYR:OH	2.06	0.55
1:F:203:ASN:OD1	1:F:225:LEU:HA	2.06	0.55
1:A:211:LEU:O	1:A:212:GLU:CB	2.44	0.54
1:A:483:PHE:HB2	1:A:489:ILE:HD11	1.88	0.54
1:B:284:ILE:HD12	1:B:436:THR:HB	1.88	0.54
2:D:147:VAL:O	2:D:150:VAL:HG12	2.07	0.54
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.72	0.54
1:A:82:ASP:O	1:A:83:ILE:C	2.49	0.54
1:A:363:ILE:O	1:A:367:ILE:HG13	2.07	0.54
1:A:379:SER:O	1:A:382:ALA:HB3	2.08	0.54
1:A:419:PHE:CD2	1:B:425:ILE:HD12	2.43	0.54
1:B:167:LEU:O	1:B:170:ARG:N	2.40	0.54
2:C:379:SER:HA	2:C:413:THR:O	2.07	0.54
1:E:54:LEU:HD13	1:E:90:PHE:CE1	2.42	0.54
1:E:203:ASN:CB	1:E:225:LEU:HD23	2.29	0.54
1:E:451:ARG:HH11	1:E:451:ARG:CG	2.18	0.54
1:F:183:GLU:HG3	1:F:193:ARG:HE	1.72	0.54
1:A:442:TYR:CE1	1:B:456:PHE:CZ	2.95	0.54
1:A:501:GLU:O	1:A:503:SER:N	2.39	0.54
2:C:354:ALA:HB1	2:C:358:ASP:HB2	1.90	0.54
1:E:294:LYS:CB	1:E:413:THR:HG23	2.37	0.54
1:F:397:ILE:CD1	1:F:433:ILE:HG12	2.38	0.54
1:A:87:ALA:HB1	1:A:92:TRP:CD1	2.42	0.54
1:A:389:ASN:ND2	1:A:428:SER:HB2	2.23	0.54
1:B:51:GLY:O	1:B:54:LEU:HB3	2.08	0.54
2:C:418:GLN:HB2	2:D:423:HIS:O	2.07	0.54
2:D:82:ASP:O	2:D:83:ILE:C	2.49	0.54
2:D:94:LEU:O	2:D:98:VAL:HG23	2.07	0.54
2:D:332:GLY:C	2:D:333:MET:HG2	2.33	0.54
1:E:132:TYR:CE2	1:E:136:LYS:HD2	2.42	0.54
1:E:290:THR:HG21	1:F:431:ALA:HB1	1.88	0.54
1:F:21:MET:HE3	1:F:59:PHE:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:LEU:HD13	1:F:360:LEU:C	2.32	0.54
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.88	0.54
2:D:31:ILE:HA	2:D:231:MET:HG3	1.89	0.54
1:F:418:GLN:NE2	1:F:421:GLY:O	2.40	0.54
1:A:218:ARG:O	1:A:236:PRO:HA	2.07	0.54
1:B:121:PHE:H	1:B:121:PHE:HD1	1.54	0.54
1:B:451:ARG:N	1:B:451:ARG:HD2	2.23	0.54
2:C:72:VAL:HG13	2:C:104:PHE:HD2	1.72	0.54
2:C:426:THR:HG22	2:C:427:ASP:N	2.23	0.54
2:C:462:TRP:O	2:C:463:HIS:O	2.26	0.54
2:D:273:MET:CE	2:D:468:ARG:HD2	2.37	0.54
1:F:436:THR:HG23	1:F:458:MET:HG2	1.89	0.54
3:A:903:ATP:O3'	1:B:224:LYS:HA	2.07	0.54
1:B:131:ASN:HA	1:B:134:ILE:HD12	1.90	0.54
1:B:193:ARG:NH2	2:C:195:GLY:O	2.41	0.54
1:B:293:GLY:O	1:B:296:LEU:HB3	2.08	0.54
2:C:95:ALA:O	2:C:99:ASP:HB2	2.08	0.54
2:D:313:ILE:HG12	2:D:345:LYS:HB3	1.89	0.54
1:F:78:GLU:HB3	1:F:83:ILE:CD1	2.38	0.54
1:F:426:TPO:HG21	1:F:429:HIS:CA	2.38	0.54
1:B:48:SER:OG	2:C:224:LYS:HD3	2.07	0.54
2:D:347:VAL:HG12	2:D:348:CYS:H	1.71	0.54
1:E:106:LEU:HD11	1:E:129:ARG:CZ	2.38	0.54
1:E:344:LEU:HD13	1:E:344:LEU:C	2.33	0.54
1:A:426:TPO:O3P	1:A:426:TPO:HG21	2.08	0.54
1:A:430:ILE:O	1:A:431:ALA:C	2.51	0.54
1:B:25:ILE:CG1	1:B:58:GLN:HE21	2.12	0.54
2:C:87:ALA:O	2:C:89:SER:N	2.40	0.54
1:E:169:ALA:O	1:E:173:GLN:HG3	2.06	0.54
1:E:447:GLY:HA2	1:F:467:ILE:HD12	1.90	0.54
1:F:163:GLU:HA	1:F:163:GLU:OE2	2.07	0.54
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.37	0.54
2:D:486:PHE:HE2	2:D:496:ARG:HD3	1.70	0.54
1:A:147:VAL:CG1	1:A:180:MET:HE3	2.25	0.53
1:A:272:GLU:O	1:A:462:TRP:HZ3	1.91	0.53
1:B:287:THR:HG21	1:B:425:ILE:O	2.08	0.53
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.91	0.53
2:C:144:ILE:HG22	2:C:147:VAL:HG12	1.89	0.53
2:D:49:GLY:HA2	1:E:224:LYS:HB3	1.90	0.53
2:D:178:THR:CG2	2:D:179:VAL:N	2.71	0.53
1:E:318:GLU:OE2	1:F:432:GLU:OE1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:ASP:N	1:E:435:ASP:OD1	2.41	0.53
1:F:170:ARG:HD2	1:F:173:GLN:OE1	2.08	0.53
1:F:504:GLU:HA	1:F:507:ARG:HG3	1.89	0.53
2:C:38:ILE:HG23	2:C:177:THR:OG1	2.08	0.53
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.89	0.53
2:D:370:PHE:O	2:D:371:LYS:HG3	2.08	0.53
1:E:499:VAL:O	1:E:499:VAL:HG12	2.07	0.53
1:E:504:GLU:CG	1:E:505:LEU:H	2.14	0.53
1:F:64:ILE:HG21	1:F:97:LEU:HD13	1.90	0.53
1:F:256:GLN:HB3	1:F:405:GLN:HA	1.90	0.53
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.43	0.53
1:A:89:SER:HB2	1:B:227:GLY:O	2.08	0.53
1:A:315:PHE:HE1	1:A:375:ILE:HG12	1.74	0.53
2:C:54:LEU:O	2:C:57:ILE:N	2.42	0.53
2:D:60:LEU:O	2:D:61:TYR:C	2.52	0.53
1:E:67:PHE:O	1:E:69:GLU:HG3	2.09	0.53
1:F:420:MET:HE3	1:F:492:GLY:O	2.08	0.53
1:F:453:ILE:CG1	1:F:454:ASN:H	2.21	0.53
1:A:459:ARG:NH1	1:F:319:GLU:HG2	2.23	0.53
1:B:289:ALA:HB2	1:B:419:PHE:HA	1.91	0.53
2:C:218:ARG:HD2	5:C:526:HOH:O	2.08	0.53
2:C:310:GLU:O	2:C:343:LEU:HB3	2.08	0.53
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.39	0.53
1:E:194:TYR:O	1:E:196:VAL:HB	2.09	0.53
1:E:497:ILE:HG22	1:E:498:THR:N	2.21	0.53
1:F:52:LYS:HB3	1:F:181:THR:CG2	2.39	0.53
1:B:247:PHE:HZ	1:B:361:GLN:HG3	1.74	0.53
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.74	0.53
2:C:38:ILE:HG22	2:C:39:GLY:H	1.73	0.53
2:D:264:SER:HA	2:D:271:ASP:OD1	2.08	0.53
1:F:316:ALA:HB2	1:F:324:LEU:HD11	1.89	0.53
1:F:437:ILE:HD12	1:F:457:LYS:HG2	1.90	0.53
1:A:24:MET:CB	1:A:62:ASN:HD22	2.21	0.53
1:A:188:TYR:HE2	1:F:211:LEU:CD2	2.22	0.53
2:C:248:PRO:O	2:C:250:GLY:N	2.42	0.53
1:F:191:ILE:HB	1:F:198:GLU:CD	2.33	0.53
2:C:386:GLY:CA	2:D:390:ASN:HD21	2.21	0.53
2:D:44:VAL:HG22	2:D:205:VAL:CB	2.39	0.53
2:D:443:VAL:HG13	2:D:494:PRO:HG2	1.89	0.53
1:E:406:GLU:O	1:E:408:ILE:HG13	2.09	0.53
1:F:44:VAL:O	1:F:181:THR:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:THR:HG22	1:F:50:THR:HG22	1.89	0.53
1:F:262:ARG:HD2	1:F:276:GLY:O	2.08	0.53
2:C:23:THR:O	2:C:24:MET:HB2	2.08	0.53
2:C:299:SER:C	2:C:333:MET:CE	2.82	0.53
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.90	0.53
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.90	0.53
1:B:286:ALA:HA	1:B:438:ILE:O	2.09	0.53
2:C:170:ARG:HB3	2:C:170:ARG:NH1	2.24	0.53
2:C:248:PRO:O	2:C:251:ALA:N	2.42	0.53
1:E:220:LEU:HD13	1:E:246:ILE:HD11	1.91	0.53
1:E:262:ARG:HD2	1:E:276:GLY:O	2.09	0.53
1:F:118:VAL:O	1:F:118:VAL:HG13	2.08	0.53
1:F:147:VAL:HG23	1:F:148:THR:N	2.24	0.53
1:A:375:ILE:O	1:A:410:GLY:HA2	2.09	0.53
1:A:396:VAL:HG21	1:A:430:ILE:HD12	1.91	0.53
1:B:43:LEU:HD12	1:B:180:MET:HB2	1.92	0.53
2:C:71:GLY:N	2:C:102:LYS:O	2.41	0.53
2:D:451:ARG:H	2:D:451:ARG:HD2	1.74	0.53
1:F:451:ARG:HD2	1:F:451:ARG:N	2.24	0.53
1:B:50:THR:HG21	1:B:207:LEU:O	2.09	0.52
1:B:344:LEU:HD13	1:B:344:LEU:C	2.35	0.52
2:C:334:ASP:O	2:C:338:MET:HG2	2.09	0.52
2:C:426:THR:HG22	2:C:428:SER:H	1.73	0.52
2:D:52:LYS:HE3	5:D:550:HOH:O	2.07	0.52
2:D:468:ARG:HG2	2:D:468:ARG:NH1	2.23	0.52
1:E:303:GLU:OE2	1:E:333:MET:HB3	2.09	0.52
1:E:313:ILE:HD12	1:E:372:PRO:HG2	1.90	0.52
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.90	0.52
1:A:162:ARG:O	1:A:165:PHE:HB3	2.09	0.52
1:A:257:ARG:NH2	1:A:407:GLU:HG2	2.23	0.52
1:A:379:SER:HA	1:A:413:THR:O	2.09	0.52
2:C:50:THR:HG21	2:C:207:LEU:O	2.08	0.52
1:E:451:ARG:HG2	1:E:470:PHE:CE1	2.45	0.52
1:E:497:ILE:O	1:E:498:THR:OG1	2.21	0.52
1:F:73:PHE:HE2	1:F:75:THR:HB	1.74	0.52
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.39	0.52
1:F:131:ASN:O	1:F:135:GLN:HB2	2.09	0.52
1:F:514:GLU:OE1	1:F:515:LYS:N	2.42	0.52
1:A:296:LEU:HD13	1:A:331:TRP:CE2	2.45	0.52
1:B:316:ALA:O	1:B:348:CYS:HA	2.09	0.52
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:THR:HG23	5:E:527:HOH:O	2.09	0.52
1:F:94:LEU:O	1:F:98:VAL:HG23	2.10	0.52
1:F:127:ILE:HD13	1:F:167:LEU:HD12	1.91	0.52
1:A:220:LEU:HD23	1:A:220:LEU:C	2.34	0.52
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.90	0.52
1:A:436:THR:OG1	1:A:458:MET:HG2	2.08	0.52
1:B:385:ARG:NH1	2:C:397:ILE:HD11	2.24	0.52
2:C:123:LEU:CD2	2:C:167:LEU:HB2	2.40	0.52
2:C:323:GLN:HE22	2:D:459:ARG:HD3	1.75	0.52
2:C:389:ASN:O	2:C:390:ASN:C	2.52	0.52
2:D:74:VAL:HA	2:D:106:LEU:HB3	1.91	0.52
2:D:296:LEU:HD12	2:D:296:LEU:O	2.08	0.52
1:E:266:GLY:HA2	1:E:304:ASN:ND2	2.15	0.52
1:F:436:THR:CG2	1:F:458:MET:HG2	2.39	0.52
1:B:497:ILE:HD12	1:B:498:THR:H	1.71	0.52
2:C:98:VAL:HA	2:C:103:LEU:O	2.10	0.52
2:C:296:LEU:HD13	2:C:331:TRP:CE2	2.44	0.52
2:C:395:PHE:O	2:C:399:VAL:HG23	2.09	0.52
2:D:183:GLU:HB2	1:E:199:PHE:CE1	2.44	0.52
1:E:313:ILE:CG1	1:E:372:PRO:HG2	2.39	0.52
1:F:115:GLN:CG	1:F:116:GLU:N	2.72	0.52
1:F:150:VAL:CG1	1:F:151:PHE:N	2.72	0.52
1:F:270:LEU:O	1:F:273:MET:N	2.42	0.52
1:F:289:ALA:O	1:F:292:THR:HG23	2.09	0.52
1:A:344:LEU:HD13	1:A:345:LYS:N	2.25	0.52
1:B:74:VAL:HG13	1:B:106:LEU:HG	1.90	0.52
2:C:14:GLU:OE2	2:C:16:GLN:HB2	2.10	0.52
2:C:42:THR:HG23	2:C:203:ASN:CB	2.40	0.52
2:C:54:LEU:O	2:C:55:PHE:C	2.52	0.52
2:D:313:ILE:HG21	2:D:315:PHE:CZ	2.44	0.52
1:E:346:ILE:HG22	1:E:348:CYS:SG	2.49	0.52
1:A:199:PHE:CE1	1:F:183:GLU:HB2	2.44	0.52
1:A:371:LYS:N	1:A:372:PRO:HD3	2.24	0.52
1:B:51:GLY:O	1:B:52:LYS:C	2.53	0.52
1:B:320:SER:HB3	2:C:256:GLN:HG2	1.91	0.52
2:C:174:ILE:HG22	2:C:174:ILE:O	2.10	0.52
2:C:363:ILE:O	2:C:367:ILE:HG13	2.10	0.52
1:E:53:THR:O	1:E:54:LEU:C	2.52	0.52
1:E:352:GLU:CD	1:E:352:GLU:H	2.17	0.52
1:F:299:SER:HB3	1:F:333:MET:HE2	1.92	0.52
1:A:44:VAL:HA	1:A:205:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.45	0.52
1:B:152:GLN:NE2	1:B:194:TYR:OH	2.43	0.52
2:C:357:GLU:CG	2:C:358:ASP:N	2.73	0.52
1:E:255:THR:HG22	1:E:255:THR:O	2.08	0.52
2:C:53:THR:HG23	2:C:145:ASP:OD1	2.10	0.52
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.90	0.52
2:D:206:ILE:HD11	2:D:223:LEU:HD12	1.92	0.52
2:D:371:LYS:O	2:D:371:LYS:CD	2.56	0.52
1:E:339:GLU:HG2	1:E:344:LEU:HD12	1.91	0.52
1:A:31:ILE:HG23	1:A:231:MET:HB2	1.92	0.52
1:A:230:HIS:HE1	1:A:232:LYS:HG3	1.74	0.52
1:A:385:ARG:HG2	1:B:393:ARG:CZ	2.40	0.52
1:B:197:GLU:CD	1:B:197:GLU:H	2.17	0.52
2:C:56:SER:O	2:C:59:PHE:HB3	2.09	0.52
2:C:72:VAL:HG13	2:C:104:PHE:CD2	2.44	0.52
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.90	0.52
2:C:387:VAL:HG12	2:C:388:SER:O	2.10	0.52
2:D:219:THR:HA	2:D:235:TYR:O	2.10	0.52
1:E:21:MET:O	1:E:35:GLY:HA3	2.10	0.52
1:E:313:ILE:HG13	1:E:372:PRO:HG2	1.88	0.52
1:E:325:LEU:HD21	1:E:336:GLU:H	1.75	0.52
1:E:404:LYS:C	1:E:406:GLU:H	2.17	0.52
1:F:47:THR:N	1:F:50:THR:HG21	2.25	0.52
1:F:379:SER:O	1:F:382:ALA:HB3	2.10	0.52
1:A:104:PHE:CD1	1:A:104:PHE:C	2.86	0.51
1:B:83:ILE:H	1:B:83:ILE:HD12	1.76	0.51
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.20	0.51
1:E:43:LEU:HD23	1:E:204:VAL:HG13	1.92	0.51
1:A:498:THR:O	1:A:499:VAL:C	2.54	0.51
1:B:148:THR:O	1:B:150:VAL:N	2.42	0.51
2:C:50:THR:HB	2:C:207:LEU:CB	2.39	0.51
2:C:320:SER:HB3	2:D:256:GLN:HG2	1.92	0.51
2:C:419:PHE:O	2:C:420:MET:HB2	2.10	0.51
1:E:199:PHE:O	1:E:201:SER:N	2.44	0.51
1:F:80:PRO:CG	1:F:107:ASP:HB2	2.40	0.51
1:F:302:VAL:HG12	1:F:303:GLU:N	2.25	0.51
1:B:87:ALA:C	1:B:89:SER:H	2.18	0.51
1:B:119:GLY:C	1:B:121:PHE:H	2.18	0.51
1:B:220:LEU:HD13	1:B:246:ILE:HD11	1.91	0.51
1:B:418:GLN:HB2	2:C:423:HIS:O	2.10	0.51
2:C:32:SER:HB3	2:C:222:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:TYR:C	1:E:63:GLY:N	2.66	0.51
1:F:20:LYS:HB3	1:F:35:GLY:O	2.09	0.51
1:F:20:LYS:CE	1:F:228:THR:HG21	2.39	0.51
1:F:420:MET:HE3	1:F:492:GLY:C	2.36	0.51
1:B:53:THR:HB	3:B:903:ATP:PA	2.50	0.51
2:C:261:VAL:CG1	2:C:262:ARG:N	2.73	0.51
1:E:444:GLU:O	1:E:494:PRO:HD2	2.11	0.51
1:A:317:TYR:CD2	1:A:349:ALA:O	2.63	0.51
1:B:65:ILE:O	1:B:65:ILE:HG22	2.10	0.51
1:B:194:TYR:O	1:B:196:VAL:N	2.44	0.51
1:B:321:ARG:NH1	5:B:535:HOH:O	2.44	0.51
1:B:486:PHE:HE2	1:B:496:ARG:HB2	1.75	0.51
2:C:359:HIS:O	2:C:363:ILE:HG13	2.10	0.51
2:D:164:LEU:CD1	2:D:197:GLU:HG3	2.41	0.51
1:E:56:SER:HB2	1:E:143:SER:HB3	1.91	0.51
1:E:321:ARG:HG2	1:E:348:CYS:SG	2.51	0.51
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.91	0.51
1:F:471:MET:HE3	1:F:471:MET:C	2.36	0.51
1:B:72:VAL:HB	1:B:142:VAL:HG13	1.93	0.51
1:B:237:PHE:CB	1:B:246:ILE:HG12	2.40	0.51
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.91	0.51
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.92	0.51
1:E:335:PHE:HA	1:E:338:MET:HG3	1.91	0.51
1:F:273:MET:O	1:F:463:HIS:HB2	2.10	0.51
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.93	0.51
1:A:266:GLY:C	1:A:300:ARG:HG3	2.35	0.51
1:B:54:LEU:CD2	1:B:244:ILE:HG13	2.40	0.51
1:B:268:VAL:O	1:B:271:ASP:N	2.44	0.51
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.92	0.51
1:E:25:ILE:HG23	1:E:58:GLN:NE2	2.25	0.51
1:F:231:MET:HE1	1:F:251:ALA:HB2	1.91	0.51
1:A:51:GLY:O	1:A:52:LYS:C	2.54	0.51
1:A:94:LEU:HD22	1:A:103:LEU:CD2	2.40	0.51
1:A:164:LEU:HD11	1:A:197:GLU:CG	2.41	0.51
1:B:39:GLY:H	1:B:177:THR:CB	2.24	0.51
1:B:247:PHE:HE2	1:B:364:LYS:HD2	1.76	0.51
1:B:294:LYS:H	1:B:294:LYS:HD3	1.74	0.51
2:C:295:THR:HG22	2:C:331:TRP:CH2	2.46	0.51
1:F:20:LYS:C	1:F:38:ILE:CD1	2.84	0.51
1:F:211:LEU:HD12	1:F:215:ARG:O	2.10	0.51
1:F:334:ASP:OD1	1:F:336:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:430:ILE:O	1:F:432:GLU:N	2.44	0.51
1:A:164:LEU:CD1	1:A:197:GLU:HG3	2.39	0.51
1:B:61:TYR:CE1	1:B:92:TRP:HB2	2.45	0.51
1:B:65:ILE:O	1:B:66:GLU:HG2	2.11	0.51
1:B:145:ASP:HA	1:B:181:THR:HB	1.92	0.51
2:C:90:PHE:N	2:C:90:PHE:CD1	2.78	0.51
2:D:67:PHE:O	2:D:68:ASP:HB3	2.11	0.51
2:D:323:GLN:O	2:D:326:ARG:HB3	2.11	0.51
1:E:97:LEU:N	1:E:97:LEU:HD23	2.25	0.51
1:E:453:ILE:HG22	1:E:470:PHE:HD2	1.76	0.51
1:F:329:TYR:O	1:F:332:GLY:N	2.36	0.51
1:A:483:PHE:N	1:A:483:PHE:CD1	2.79	0.51
2:D:393:ARG:O	2:D:397:ILE:HG12	2.11	0.51
1:E:265:SER:HB3	1:E:278:PHE:CZ	2.46	0.51
1:E:292:THR:N	1:E:442:TYR:OH	2.43	0.51
1:F:316:ALA:O	1:F:348:CYS:HA	2.11	0.51
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.41	0.50
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.76	0.50
1:B:194:TYR:C	1:B:196:VAL:N	2.68	0.50
1:B:357:GLU:CG	1:B:358:ASP:N	2.74	0.50
1:F:38:ILE:H	1:F:38:ILE:HD12	1.76	0.50
1:F:149:SER:O	1:F:152:GLN:HB2	2.11	0.50
1:A:52:LYS:HB2	3:A:903:ATP:O1B	2.11	0.50
1:A:332:GLY:O	1:A:333:MET:C	2.54	0.50
1:B:183:GLU:HG3	1:B:193:ARG:HD2	1.94	0.50
1:B:197:GLU:O	1:B:200:VAL:N	2.39	0.50
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.45	0.50
2:C:82:ASP:O	2:C:85:LYS:N	2.44	0.50
2:D:64:ILE:CD1	2:D:97:LEU:HD13	2.41	0.50
2:D:182:THR:CG2	2:D:183:GLU:N	2.74	0.50
1:F:311:ARG:HG3	1:F:371:LYS:NZ	2.26	0.50
1:F:505:LEU:O	1:F:506:SER:HB3	2.11	0.50
1:A:131:ASN:HD21	1:A:135:GLN:NE2	2.09	0.50
1:B:79:THR:O	1:B:83:ILE:HD12	2.11	0.50
2:D:184:ARG:HG2	2:D:191:ILE:O	2.11	0.50
1:E:451:ARG:CG	1:E:451:ARG:NH1	2.72	0.50
1:F:56:SER:O	1:F:59:PHE:HB3	2.11	0.50
1:A:359:HIS:O	1:A:363:ILE:HG13	2.11	0.50
1:A:396:VAL:O	1:A:397:ILE:C	2.55	0.50
1:B:193:ARG:NH1	5:B:525:HOH:O	2.44	0.50
1:B:248:PRO:O	1:B:251:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:HG22	1:B:288:GLY:N	2.27	0.50
2:D:445:ILE:HA	2:D:496:ARG:HH12	1.75	0.50
2:D:484:ARG:CB	2:D:484:ARG:NH1	2.75	0.50
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.31	0.50
1:F:370:PHE:HB3	1:F:372:PRO:HD3	1.94	0.50
1:F:486:PHE:HB2	1:F:489:ILE:HD11	1.94	0.50
1:F:515:LYS:CB	1:F:517:PRO:HD2	2.41	0.50
2:D:39:GLY:N	2:D:177:THR:HG23	2.25	0.50
2:D:152:GLN:HB3	1:E:161:ARG:HD3	1.93	0.50
1:E:425:ILE:HD12	1:E:456:PHE:CE2	2.45	0.50
1:E:441:GLN:HG3	1:E:441:GLN:O	2.12	0.50
1:F:357:GLU:HG3	1:F:358:ASP:N	2.27	0.50
1:B:53:THR:HA	1:B:145:ASP:OD1	2.11	0.50
1:B:146:SER:N	1:B:181:THR:HB	2.18	0.50
1:B:161:ARG:HH21	1:B:199:PHE:HB2	1.77	0.50
1:B:273:MET:O	1:B:464:ASP:N	2.45	0.50
2:D:486:PHE:HB3	2:D:489:ILE:CD1	2.41	0.50
1:E:445:ILE:HG13	1:E:483:PHE:HE2	1.77	0.50
1:F:59:PHE:CE1	1:F:141:ARG:HD3	2.46	0.50
1:F:294:LYS:O	1:F:295:THR:C	2.54	0.50
1:F:311:ARG:HG3	1:F:371:LYS:HZ1	1.77	0.50
1:A:52:LYS:O	1:A:55:PHE:N	2.45	0.50
1:A:145:ASP:O	1:A:146:SER:OG	2.26	0.50
1:A:326:ARG:HD3	1:B:258:SER:OG	2.11	0.50
2:C:116:GLU:C	2:C:118:VAL:H	2.20	0.50
2:C:263:VAL:HG12	2:C:374:ARG:HH21	1.77	0.50
2:C:340:ARG:C	2:C:342:ASN:N	2.68	0.50
1:E:61:TYR:CZ	1:E:92:TRP:CD1	3.00	0.50
1:E:178:THR:HG22	1:E:179:VAL:N	2.27	0.50
1:E:323:GLN:CG	1:E:327:ASN:HD21	2.25	0.50
1:F:103:LEU:HD12	1:F:104:PHE:N	2.27	0.50
1:A:299:SER:HB3	1:A:333:MET:HE2	1.94	0.50
1:B:232:LYS:H	1:B:232:LYS:HD2	1.77	0.50
1:B:426:TPO:O3P	1:B:426:TPO:C	2.60	0.50
2:C:49:GLY:O	2:C:218:ARG:NH2	2.45	0.50
2:C:54:LEU:O	2:C:56:SER:N	2.44	0.50
2:C:87:ALA:C	2:C:89:SER:N	2.70	0.50
2:D:425:ILE:HD11	2:D:456:PHE:CE2	2.47	0.50
2:D:451:ARG:HD2	2:D:451:ARG:N	2.27	0.50
1:E:313:ILE:CG2	1:E:314:LEU:N	2.75	0.50
1:A:153:GLN:O	1:A:154:TYR:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.27	0.50
2:C:193:ARG:NH2	2:D:199:PHE:HE2	2.10	0.50
2:D:222:ILE:CG2	2:D:225:LEU:HG	2.42	0.50
2:D:270:LEU:O	2:D:270:LEU:HD23	2.12	0.50
2:D:358:ASP:O	2:D:359:HIS:C	2.54	0.50
2:D:425:ILE:HG22	2:D:426:THR:HG23	1.94	0.50
1:E:303:GLU:OE2	1:E:333:MET:CB	2.60	0.50
1:E:418:GLN:CB	1:F:423:HIS:O	2.57	0.50
1:F:59:PHE:CZ	1:F:141:ARG:HD3	2.47	0.50
1:F:73:PHE:C	1:F:73:PHE:CD2	2.90	0.50
1:A:183:GLU:OE2	1:B:161:ARG:NH2	2.44	0.49
1:A:294:LYS:HB3	1:A:413:THR:HG23	1.94	0.49
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.12	0.49
1:B:182:THR:HG21	1:B:192:ALA:CB	2.37	0.49
1:B:359:HIS:O	1:B:360:LEU:C	2.56	0.49
2:C:452:ALA:HA	2:C:469:GLU:HA	1.92	0.49
2:D:103:LEU:HD12	2:D:104:PHE:N	2.26	0.49
1:E:84:ILE:O	1:E:85:LYS:C	2.54	0.49
1:E:262:ARG:HH12	1:E:461:SER:HB2	1.77	0.49
1:E:386:GLY:O	1:E:387:VAL:C	2.55	0.49
1:A:426:TPO:O2P	1:A:429:HIS:HA	2.11	0.49
2:C:87:ALA:HB1	2:C:92:TRP:CD1	2.47	0.49
2:D:191:ILE:HB	2:D:198:GLU:CG	2.41	0.49
2:D:324:LEU:C	2:D:326:ARG:H	2.18	0.49
1:F:294:LYS:N	3:F:901:ATP:O1B	2.46	0.49
1:F:516:GLY:N	1:F:517:PRO:CD	2.74	0.49
1:B:216:ARG:HH21	2:C:221:GLU:CD	2.19	0.49
1:B:335:PHE:O	1:B:336:GLU:C	2.56	0.49
2:D:121:PHE:N	2:D:121:PHE:CD1	2.80	0.49
2:D:334:ASP:OD1	2:D:334:ASP:C	2.55	0.49
2:D:412:PHE:N	2:D:412:PHE:CD1	2.79	0.49
2:D:437:ILE:O	2:D:437:ILE:HG22	2.12	0.49
1:F:52:LYS:HB2	3:F:903:ATP:O1B	2.13	0.49
1:F:298:VAL:HA	1:F:411:LEU:CD2	2.42	0.49
1:A:148:THR:HG1	1:A:182:THR:HG23	1.78	0.49
1:A:167:LEU:O	1:A:168:VAL:C	2.56	0.49
1:B:284:ILE:N	1:B:410:GLY:O	2.34	0.49
1:E:215:ARG:HD3	5:F:528:HOH:O	2.11	0.49
1:F:361:GLN:O	1:F:362:ILE:C	2.56	0.49
1:F:467:ILE:O	1:F:467:ILE:HG22	2.12	0.49
1:A:191:ILE:N	1:A:191:ILE:CD1	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:LEU:HD11	2:D:197:GLU:HG3	1.95	0.49
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.94	0.49
1:A:87:ALA:HB1	1:A:92:TRP:HD1	1.77	0.49
1:B:326:ARG:C	1:B:328:ALA:N	2.71	0.49
2:C:217:ARG:O	2:C:217:ARG:CG	2.59	0.49
2:C:295:THR:HB	3:C:901:ATP:O3A	2.12	0.49
2:C:469:GLU:HB3	2:C:483:PHE:CE1	2.47	0.49
1:E:386:GLY:O	1:E:387:VAL:O	2.30	0.49
1:E:433:ILE:HD12	1:E:433:ILE:N	2.28	0.49
1:A:215:ARG:NH2	1:B:234:GLU:O	2.46	0.49
1:A:402:TYR:O	1:A:406:GLU:HB2	2.13	0.49
1:B:75:THR:HG21	1:B:78:GLU:O	2.12	0.49
1:B:445:ILE:HD12	1:B:486:PHE:CE1	2.47	0.49
2:C:21:MET:O	2:C:35:GLY:HA3	2.13	0.49
2:C:299:SER:CB	2:C:333:MET:HE2	2.40	0.49
2:C:311:ARG:CD	2:C:371:LYS:HE3	2.43	0.49
2:D:52:LYS:HD2	2:D:182:THR:O	2.13	0.49
2:D:262:ARG:HD2	2:D:276:GLY:O	2.13	0.49
1:E:245:ASN:ND2	1:E:247:PHE:CE2	2.81	0.49
1:F:27:GLY:O	1:F:31:ILE:HG13	2.12	0.49
1:B:106:LEU:O	1:B:107:ASP:C	2.55	0.49
2:C:381:SER:C	2:C:383:LEU:N	2.70	0.49
1:A:371:LYS:O	1:A:371:LYS:CD	2.59	0.49
1:B:350:TYR:CE1	2:C:252:MET:HE3	2.46	0.49
2:C:220:LEU:HD23	2:C:220:LEU:C	2.38	0.49
2:D:271:ASP:O	2:D:277:GLY:N	2.36	0.49
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.43	0.49
1:E:311:ARG:HD2	1:E:371:LYS:NZ	2.28	0.49
1:F:47:THR:HG23	1:F:48:SER:N	2.27	0.49
1:F:83:ILE:N	1:F:83:ILE:HD12	2.28	0.49
1:F:303:GLU:CD	1:F:333:MET:HB3	2.38	0.49
1:F:462:TRP:O	1:F:463:HIS:O	2.31	0.49
1:F:463:HIS:CE1	1:F:465:LYS:HD3	2.48	0.49
1:A:18:ILE:HD11	1:F:86:ASN:HA	1.94	0.49
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.48	0.49
1:A:64:ILE:HG21	1:A:97:LEU:HD22	1.95	0.49
1:A:189:GLY:O	1:A:190:PRO:C	2.56	0.49
1:A:199:PHE:HE2	1:F:193:ARG:NH2	2.11	0.49
1:A:356:LEU:HB3	1:A:395:PHE:HD1	1.78	0.49
1:B:52:LYS:H	1:B:207:LEU:CD1	2.24	0.49
1:B:148:THR:C	1:B:150:VAL:N	2.68	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PHE:C	1:B:237:PHE:CD1	2.90	0.49
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.48	0.49
2:C:215:ARG:HE	2:C:215:ARG:CA	2.11	0.49
2:C:453:ILE:HG12	2:C:454:ASN:N	2.28	0.49
2:D:130:ILE:O	2:D:134:ILE:HG13	2.12	0.49
2:D:264:SER:OG	2:D:265:SER:N	2.46	0.49
1:E:54:LEU:HD13	1:E:90:PHE:CZ	2.48	0.49
1:F:379:SER:HA	1:F:413:THR:O	2.12	0.49
1:F:380:LEU:C	1:F:382:ALA:N	2.71	0.49
1:F:486:PHE:HE2	1:F:496:ARG:NH1	1.93	0.49
1:A:207:LEU:CD2	1:A:220:LEU:HD12	2.41	0.48
1:A:357:GLU:HG3	1:A:358:ASP:N	2.28	0.48
1:B:215:ARG:NH2	2:C:234:GLU:O	2.46	0.48
1:B:385:ARG:HD3	2:C:393:ARG:HD3	1.94	0.48
2:C:73:PHE:HD1	2:C:143:SER:HB2	1.78	0.48
2:C:121:PHE:N	2:C:121:PHE:CD1	2.81	0.48
2:C:149:SER:HB3	2:D:161:ARG:CZ	2.43	0.48
1:E:295:THR:O	1:E:298:VAL:HB	2.13	0.48
1:F:31:ILE:CD1	1:F:246:ILE:HG21	2.43	0.48
1:F:164:LEU:O	1:F:167:LEU:N	2.46	0.48
1:A:166:ARG:O	1:A:167:LEU:C	2.56	0.48
1:A:379:SER:OG	1:A:382:ALA:HB2	2.14	0.48
1:A:483:PHE:H	1:A:483:PHE:HD1	1.60	0.48
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.43	0.48
2:D:268:VAL:O	2:D:271:ASP:HB2	2.13	0.48
1:E:167:LEU:O	1:E:171:LEU:HB2	2.12	0.48
1:E:289:ALA:O	1:E:292:THR:HG23	2.13	0.48
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.94	0.48
1:A:448:GLU:HG2	1:B:466:ALA:CB	2.43	0.48
1:B:32:SER:HB3	1:B:222:ILE:HD11	1.95	0.48
1:B:127:ILE:O	1:B:127:ILE:HG22	2.12	0.48
1:B:273:MET:HE3	1:B:468:ARG:HD2	1.95	0.48
1:B:380:LEU:HB3	1:B:392:PHE:HZ	1.78	0.48
2:C:86:ASN:O	2:C:87:ALA:C	2.56	0.48
2:C:471:MET:HE1	2:C:473:SER:OG	2.13	0.48
3:C:903:ATP:O2'	2:D:230:HIS:CE1	2.65	0.48
2:D:212:GLU:O	2:D:212:GLU:CG	2.58	0.48
2:D:411:LEU:HD12	2:D:412:PHE:N	2.29	0.48
1:F:20:LYS:C	1:F:38:ILE:HD11	2.39	0.48
1:F:20:LYS:HD3	1:F:35:GLY:O	2.13	0.48
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:VAL:HG12	1:B:391:ALA:HB3	1.95	0.48
2:C:396:VAL:HG11	2:C:430:ILE:CG2	2.43	0.48
1:E:32:SER:OG	1:E:35:GLY:N	2.45	0.48
1:E:294:LYS:HG2	1:E:413:THR:HG23	1.93	0.48
1:F:380:LEU:C	1:F:382:ALA:H	2.19	0.48
1:F:408:ILE:O	1:F:409:THR:C	2.56	0.48
1:F:430:ILE:C	1:F:432:GLU:H	2.20	0.48
1:A:104:PHE:HD2	1:A:133:ALA:HB1	1.79	0.48
1:A:231:MET:HE1	1:A:251:ALA:HB2	1.96	0.48
1:A:273:MET:HA	1:A:464:ASP:HB2	1.95	0.48
1:B:21:MET:CB	1:B:38:ILE:HG12	2.42	0.48
2:C:123:LEU:HD12	2:C:163:GLU:OE2	2.14	0.48
2:C:184:ARG:NH1	2:C:187:GLU:O	2.47	0.48
2:C:281:ASP:OD1	2:C:407:GLU:HA	2.14	0.48
2:C:340:ARG:C	2:C:342:ASN:H	2.21	0.48
2:C:384:ALA:HB2	2:C:392:PHE:CZ	2.47	0.48
2:C:430:ILE:O	2:C:431:ALA:C	2.56	0.48
1:E:265:SER:O	1:E:301:PHE:HA	2.13	0.48
1:F:23:THR:O	1:F:24:MET:HB2	2.13	0.48
1:A:161:ARG:HD3	1:F:152:GLN:HB3	1.95	0.48
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.49	0.48
1:B:25:ILE:CG1	1:B:58:GLN:NE2	2.75	0.48
1:B:64:ILE:C	1:B:66:GLU:H	2.21	0.48
1:B:146:SER:H	1:B:181:THR:CB	2.17	0.48
1:B:220:LEU:HD13	1:B:246:ILE:HD13	1.96	0.48
2:C:237:PHE:CB	2:C:246:ILE:HA	2.43	0.48
2:C:304:ASN:HB3	2:C:374:ARG:HH12	1.77	0.48
2:D:21:MET:CE	2:D:177:THR:HB	2.43	0.48
2:D:486:PHE:CB	2:D:489:ILE:HD11	2.43	0.48
1:E:416:SER:C	1:E:418:GLN:N	2.71	0.48
1:F:16:GLN:NE2	1:F:33:HIS:HB3	2.27	0.48
1:F:449:MET:HE2	1:F:449:MET:HA	1.94	0.48
1:A:299:SER:C	1:A:301:PHE:N	2.71	0.48
1:A:426:TPO:O3P	1:A:431:ALA:HB2	2.14	0.48
1:B:64:ILE:O	1:B:66:GLU:N	2.44	0.48
1:A:366:GLU:HA	1:A:366:GLU:OE2	2.13	0.48
1:A:449:MET:HE2	1:A:449:MET:HA	1.96	0.48
1:B:273:MET:C	1:B:275:GLY:H	2.20	0.48
2:C:42:THR:HG23	2:C:203:ASN:HB2	1.95	0.48
2:C:42:THR:HG22	2:C:43:LEU:N	2.28	0.48
2:C:404:LYS:C	2:C:406:GLU:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:VAL:HG23	2:D:148:THR:N	2.29	0.48
1:E:199:PHE:C	1:E:201:SER:N	2.66	0.48
1:E:308:ASN:O	1:E:309:LYS:HB2	2.14	0.48
1:E:311:ARG:HB3	1:E:370:PHE:CE2	2.49	0.48
1:F:154:TYR:O	1:F:154:TYR:HD1	1.97	0.48
1:F:273:MET:SD	1:F:468:ARG:HD2	2.53	0.48
1:A:21:MET:HE1	1:A:59:PHE:HZ	1.77	0.48
1:A:306:CYS:SG	1:A:338:MET:SD	3.12	0.48
1:A:377:ILE:HD11	1:A:399:VAL:HG11	1.96	0.48
2:C:53:THR:HG22	2:C:53:THR:O	2.14	0.48
2:C:123:LEU:O	2:C:127:ILE:HG13	2.14	0.48
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.14	0.48
2:C:419:PHE:O	2:C:419:PHE:CG	2.67	0.48
2:C:483:PHE:HB2	2:C:489:ILE:CD1	2.43	0.48
2:D:269:ARG:O	2:D:272:GLU:HB2	2.13	0.48
1:F:426:TPO:HG23	1:F:429:HIS:N	2.28	0.48
1:A:90:PHE:HB2	1:A:92:TRP:NE1	2.29	0.48
1:A:426:TPO:O	1:A:427:ASP:CB	2.60	0.48
1:A:458:MET:HB2	1:A:463:HIS:HD2	1.78	0.48
1:B:52:LYS:HB2	3:B:903:ATP:O1B	2.14	0.48
1:B:273:MET:O	1:B:463:HIS:CA	2.52	0.48
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.44	0.48
2:D:484:ARG:NH1	2:D:484:ARG:HB2	2.28	0.48
1:E:231:MET:HE1	1:E:251:ALA:HB2	1.94	0.48
1:B:183:GLU:HB2	2:C:199:PHE:CZ	2.48	0.47
1:B:211:LEU:HD13	1:B:216:ARG:NE	2.28	0.47
1:B:371:LYS:O	1:B:371:LYS:CD	2.62	0.47
1:B:437:ILE:HD12	1:B:457:LYS:HG2	1.96	0.47
2:C:340:ARG:O	2:C:342:ASN:N	2.47	0.47
2:C:353:SER:O	2:C:354:ALA:HB2	2.14	0.47
2:D:122:ASP:O	2:D:123:LEU:C	2.57	0.47
2:D:380:LEU:O	2:D:382:ALA:N	2.47	0.47
1:E:31:ILE:HA	1:E:231:MET:CG	2.43	0.47
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.37	0.47
1:E:360:LEU:HD13	1:E:360:LEU:C	2.39	0.47
1:E:362:ILE:O	1:E:365:SER:HB3	2.14	0.47
3:E:903:ATP:O3'	1:F:224:LYS:HB2	2.14	0.47
1:A:52:LYS:O	1:A:53:THR:C	2.56	0.47
1:B:323:GLN:HG3	1:B:326:ARG:NH2	2.30	0.47
2:C:246:ILE:HG22	2:C:247:PHE:N	2.28	0.47
2:C:256:GLN:HG3	2:C:404:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:MET:HE2	2:D:177:THR:HG21	1.95	0.47
1:E:183:GLU:OE2	1:F:161:ARG:NH1	2.40	0.47
1:E:430:ILE:O	1:E:431:ALA:C	2.56	0.47
1:F:263:VAL:CG1	1:F:374:ARG:NH2	2.69	0.47
1:F:296:LEU:HD13	1:F:331:TRP:CE2	2.49	0.47
1:F:471:MET:HE3	1:F:471:MET:O	2.15	0.47
1:F:504:GLU:HA	1:F:507:ARG:HE	1.80	0.47
1:A:264:SER:HB3	1:A:304:ASN:HD21	1.79	0.47
1:A:299:SER:O	1:A:333:MET:HE1	2.13	0.47
1:A:504:GLU:C	1:A:506:SER:H	2.22	0.47
1:B:148:THR:HG21	1:B:193:ARG:HD2	1.95	0.47
1:B:269:ARG:O	1:B:273:MET:HG3	2.13	0.47
1:B:304:ASN:HB3	1:B:374:ARG:NH1	2.26	0.47
2:C:344:LEU:HD13	2:C:345:LYS:N	2.28	0.47
2:D:25:ILE:HG23	2:D:58:GLN:NE2	2.29	0.47
2:D:67:PHE:CB	2:D:69:GLU:HG3	2.41	0.47
1:E:160:VAL:HG21	1:E:194:TYR:CD2	2.48	0.47
1:E:446:ARG:HE	1:E:496:ARG:HH22	1.62	0.47
1:A:332:GLY:O	1:A:333:MET:O	2.32	0.47
1:A:393:ARG:NH1	1:F:385:ARG:HA	2.30	0.47
1:B:195:GLY:HA2	1:B:198:GLU:CD	2.39	0.47
1:B:264:SER:HA	1:B:271:ASP:OD1	2.14	0.47
2:C:64:ILE:HG12	2:C:69:GLU:O	2.14	0.47
2:C:146:SER:C	2:C:148:THR:H	2.23	0.47
2:D:484:ARG:CB	2:D:484:ARG:HH11	2.28	0.47
1:E:294:LYS:CB	3:E:901:ATP:O1B	2.57	0.47
1:E:313:ILE:CG1	1:E:372:PRO:CG	2.89	0.47
1:F:79:THR:HG22	1:F:82:ASP:OD2	2.14	0.47
1:F:312:ALA:HA	1:F:374:ARG:O	2.15	0.47
1:B:32:SER:OG	1:B:35:GLY:HA2	2.15	0.47
1:B:148:THR:HA	1:B:151:PHE:CE1	2.49	0.47
1:B:326:ARG:O	1:B:328:ALA:N	2.48	0.47
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.28	0.47
2:C:231:MET:HE1	2:C:251:ALA:CB	2.32	0.47
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.96	0.47
2:D:431:ALA:O	2:D:434:THR:HG23	2.15	0.47
2:D:449:MET:HE3	1:E:467:ILE:HD11	1.95	0.47
1:E:67:PHE:O	1:E:68:ASP:C	2.58	0.47
1:E:352:GLU:CD	1:E:352:GLU:N	2.72	0.47
1:E:356:LEU:CD2	1:E:392:PHE:HA	2.44	0.47
1:E:446:ARG:HE	1:E:496:ARG:NH2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ILE:HD11	1:F:97:LEU:HD11	1.97	0.47
1:F:334:ASP:O	1:F:338:MET:HG2	2.14	0.47
1:F:446:ARG:H	1:F:496:ARG:HH22	1.63	0.47
1:A:111:ASP:C	1:A:113:GLU:H	2.22	0.47
1:A:211:LEU:CG	1:A:212:GLU:N	2.78	0.47
1:A:420:MET:CE	1:B:490:ILE:HG21	2.45	0.47
1:B:63:GLY:HA3	1:B:141:ARG:HD2	1.97	0.47
1:B:72:VAL:HG23	1:B:139:ALA:CB	2.45	0.47
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.96	0.47
1:B:315:PHE:HE1	1:B:375:ILE:HD11	1.80	0.47
2:C:197:GLU:OE2	2:C:197:GLU:N	2.26	0.47
2:D:81:GLN:CD	2:D:81:GLN:N	2.71	0.47
2:D:151:PHE:CE1	2:D:160:VAL:HG13	2.50	0.47
2:D:314:LEU:O	2:D:314:LEU:HG	2.13	0.47
2:D:383:LEU:HD13	2:D:395:PHE:CE2	2.49	0.47
1:E:21:MET:HB2	1:E:38:ILE:HG12	1.97	0.47
1:E:31:ILE:HG22	1:E:222:ILE:CD1	2.45	0.47
1:E:371:LYS:O	1:E:371:LYS:CD	2.63	0.47
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.49	0.47
1:F:364:LYS:O	1:F:365:SER:C	2.55	0.47
1:A:320:SER:O	1:A:324:LEU:HG	2.15	0.47
1:A:418:GLN:CB	1:B:423:HIS:O	2.63	0.47
1:B:284:ILE:HG23	1:B:436:THR:HB	1.97	0.47
2:C:148:THR:C	2:C:150:VAL:H	2.21	0.47
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.47	0.47
1:E:488:ARG:O	1:E:491:SER:OG	2.29	0.47
1:F:31:ILE:HD11	1:F:246:ILE:HG21	1.96	0.47
1:A:299:SER:HB3	1:A:333:MET:HE1	1.97	0.47
1:B:240:THR:HG21	1:B:361:GLN:HE22	1.79	0.47
1:B:283:ILE:HD13	1:B:410:GLY:HA3	1.96	0.47
2:C:123:LEU:O	2:C:124:SER:C	2.58	0.47
2:C:493:SER:HG	2:D:488:ARG:HA	1.79	0.47
2:D:30:ASP:OD2	2:D:30:ASP:N	2.48	0.47
2:D:44:VAL:HA	2:D:205:VAL:O	2.15	0.47
2:D:361:GLN:O	2:D:362:ILE:C	2.56	0.47
2:D:420:MET:HE3	2:D:492:GLY:O	2.14	0.47
2:D:471:MET:HE2	2:D:478:ASP:CB	2.39	0.47
1:E:58:GLN:HG2	1:E:62:ASN:ND2	2.30	0.47
1:E:61:TYR:O	1:E:62:ASN:C	2.58	0.47
1:E:183:GLU:H	1:E:183:GLU:HG2	1.56	0.47
1:E:313:ILE:CD1	1:E:372:PRO:CG	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:PHE:O	1:F:109:SER:HA	2.15	0.47
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.97	0.47
1:F:325:LEU:CD2	1:F:335:PHE:HB2	2.44	0.47
1:F:371:LYS:N	1:F:372:PRO:HD3	2.29	0.47
1:A:382:ALA:O	1:A:385:ARG:HG3	2.15	0.47
2:D:106:LEU:HD11	2:D:129:ARG:HH21	1.80	0.47
1:E:417:ASP:HB2	1:E:427:ASP:OD2	2.14	0.47
1:E:431:ALA:O	1:E:432:GLU:C	2.58	0.47
1:F:98:VAL:HA	1:F:103:LEU:O	2.15	0.47
1:F:115:GLN:HG3	1:F:116:GLU:N	2.29	0.47
1:F:315:PHE:HE1	1:F:375:ILE:HD11	1.76	0.47
1:F:338:MET:HE1	5:F:540:HOH:O	2.14	0.47
1:F:486:PHE:HD2	1:F:494:PRO:HB2	1.80	0.47
1:A:229:SER:O	1:A:230:HIS:HB3	2.14	0.46
2:C:191:ILE:H	2:C:191:ILE:CD1	2.28	0.46
2:D:14:GLU:CD	2:D:15:HIS:H	2.23	0.46
2:D:328:ALA:O	2:D:332:GLY:O	2.34	0.46
1:E:121:PHE:O	1:E:122:ASP:C	2.58	0.46
1:E:246:ILE:HG22	1:E:247:PHE:N	2.29	0.46
1:E:264:SER:O	1:E:374:ARG:NH2	2.48	0.46
1:F:211:LEU:O	1:F:212:GLU:HB3	2.15	0.46
1:F:484:ARG:NH1	1:F:484:ARG:CB	2.78	0.46
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.45	0.46
1:A:440:LEU:HA	1:A:452:ALA:O	2.15	0.46
1:A:451:ARG:HD2	1:A:451:ARG:H	1.75	0.46
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.97	0.46
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.96	0.46
2:C:111:ASP:O	2:C:113:GLU:N	2.43	0.46
2:C:315:PHE:CZ	2:C:363:ILE:HG23	2.51	0.46
2:D:316:ALA:O	2:D:348:CYS:HA	2.14	0.46
2:D:445:ILE:O	2:D:446:ARG:HB2	2.15	0.46
1:F:204:VAL:HG23	1:F:224:LYS:HG2	1.98	0.46
1:F:453:ILE:CG1	1:F:454:ASN:N	2.77	0.46
1:A:121:PHE:HD1	1:A:122:ASP:N	2.14	0.46
1:A:162:ARG:HH11	1:A:162:ARG:HG3	1.80	0.46
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.48	0.46
1:B:290:THR:O	1:B:442:TYR:HE1	1.99	0.46
1:B:392:PHE:C	1:B:394:GLN:N	2.71	0.46
1:B:471:MET:HE1	1:B:473:SER:HB3	1.96	0.46
2:D:58:GLN:OE1	2:D:92:TRP:HH2	1.99	0.46
2:D:121:PHE:O	2:D:124:SER:OG	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LEU:HD23	1:E:123:LEU:C	2.40	0.46
1:F:356:LEU:HD13	1:F:387:VAL:HG21	1.98	0.46
1:F:388:SER:O	1:F:389:ASN:C	2.57	0.46
1:A:21:MET:CE	1:A:59:PHE:HZ	2.28	0.46
1:A:283:ILE:HD12	1:A:412:PHE:CE1	2.51	0.46
1:A:426:TPO:HG21	1:A:431:ALA:H	1.80	0.46
2:D:90:PHE:N	2:D:90:PHE:CD1	2.83	0.46
2:D:436:THR:HA	2:D:457:LYS:O	2.16	0.46
2:D:492:GLY:O	2:D:494:PRO:HD3	2.16	0.46
1:F:29:ASP:O	1:F:34:GLY:N	2.45	0.46
1:F:144:ILE:HG21	1:F:147:VAL:HG12	1.97	0.46
1:A:237:PHE:HB3	1:A:246:ILE:HG12	1.96	0.46
1:A:434:THR:O	1:A:457:LYS:NZ	2.47	0.46
2:C:53:THR:HG21	2:C:78:GLU:OE2	2.15	0.46
2:C:123:LEU:HD11	2:C:163:GLU:HA	1.97	0.46
2:C:344:LEU:HD13	2:C:344:LEU:C	2.40	0.46
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.97	0.46
2:D:313:ILE:HD11	2:D:370:PHE:HB3	1.96	0.46
1:E:24:MET:HB2	1:E:62:ASN:HB3	1.98	0.46
1:E:27:GLY:HA3	1:E:246:ILE:HB	1.97	0.46
1:E:186:GLU:OE1	1:E:189:GLY:N	2.48	0.46
1:E:211:LEU:CD1	1:E:216:ARG:HG2	2.45	0.46
1:F:47:THR:HB	5:F:523:HOH:O	2.15	0.46
1:F:146:SER:H	1:F:181:THR:HB	1.79	0.46
1:F:218:ARG:HG3	1:F:237:PHE:O	2.14	0.46
1:F:247:PHE:CE1	1:F:360:LEU:HD12	2.51	0.46
1:A:96:LYS:O	1:A:100:GLU:HG3	2.14	0.46
1:A:299:SER:C	1:A:301:PHE:H	2.22	0.46
1:B:44:VAL:HG22	1:B:205:VAL:HG11	1.98	0.46
1:B:371:LYS:N	1:B:372:PRO:HD3	2.30	0.46
1:B:428:SER:O	1:B:429:HIS:HB2	2.15	0.46
2:C:88:ARG:NH2	2:D:15:HIS:ND1	2.64	0.46
2:C:396:VAL:HG11	2:C:430:ILE:HG23	1.96	0.46
2:C:448:GLU:HA	2:D:466:ALA:HA	1.98	0.46
2:D:37:PRO:HD2	2:D:203:ASN:ND2	2.31	0.46
1:E:382:ALA:O	1:E:385:ARG:CG	2.59	0.46
1:A:227:GLY:O	1:F:89:SER:CB	2.64	0.46
2:C:54:LEU:C	2:C:56:SER:N	2.74	0.46
2:C:232:LYS:N	2:C:232:LYS:CD	2.76	0.46
2:C:248:PRO:C	2:C:250:GLY:N	2.72	0.46
2:C:404:LYS:O	2:C:406:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:GLY:O	2:D:218:ARG:NH2	2.48	0.46
2:D:222:ILE:HG21	2:D:225:LEU:HG	1.97	0.46
2:D:346:ILE:HG22	2:D:347:VAL:N	2.29	0.46
1:E:184:ARG:C	1:E:185:ILE:HD13	2.41	0.46
1:E:326:ARG:O	1:E:328:ALA:N	2.48	0.46
1:E:470:PHE:CD1	1:E:470:PHE:C	2.94	0.46
1:F:231:MET:SD	1:F:251:ALA:HB2	2.55	0.46
1:F:266:GLY:HA3	1:F:300:ARG:O	2.16	0.46
1:F:425:ILE:HG21	1:F:439:LEU:HD13	1.98	0.46
1:F:451:ARG:HG2	1:F:451:ARG:NH1	2.30	0.46
1:A:129:ARG:O	1:A:130:ILE:C	2.59	0.46
1:A:129:ARG:O	1:A:132:TYR:HB3	2.15	0.46
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.98	0.46
1:A:302:VAL:HG12	1:A:303:GLU:N	2.30	0.46
1:B:65:ILE:HD11	1:B:97:LEU:HD11	1.98	0.46
1:B:245:ASN:ND2	1:B:247:PHE:CZ	2.84	0.46
2:C:261:VAL:C	2:C:262:ARG:HG2	2.40	0.46
2:D:53:THR:C	2:D:55:PHE:N	2.73	0.46
2:D:193:ARG:HG2	2:D:193:ARG:HH11	1.80	0.46
2:D:306:CYS:C	2:D:308:ASN:N	2.74	0.46
2:D:358:ASP:O	2:D:360:LEU:N	2.49	0.46
1:E:218:ARG:NH1	1:E:239:ILE:HD12	2.31	0.46
1:E:296:LEU:HD13	1:E:331:TRP:CE2	2.51	0.46
1:E:332:GLY:O	1:E:333:MET:O	2.33	0.46
1:E:392:PHE:O	1:E:395:PHE:HB3	2.16	0.46
1:E:446:ARG:NH2	1:E:496:ARG:HH22	2.11	0.46
1:A:27:GLY:O	1:A:28:PHE:C	2.58	0.46
1:A:429:HIS:CD2	1:F:417:ASP:OD2	2.68	0.46
1:B:191:ILE:CB	1:B:198:GLU:HG3	2.46	0.46
1:B:211:LEU:O	1:B:212:GLU:HB3	2.15	0.46
2:C:96:LYS:O	2:C:99:ASP:N	2.49	0.46
2:C:311:ARG:HH11	2:C:371:LYS:HG3	1.81	0.46
1:E:377:ILE:O	1:E:377:ILE:HG22	2.14	0.46
1:E:453:ILE:CG2	1:E:470:PHE:HD2	2.28	0.46
1:A:161:ARG:NH1	1:F:152:GLN:HG3	2.30	0.46
1:A:200:VAL:O	1:A:200:VAL:HG12	2.16	0.46
1:A:383:LEU:C	1:A:385:ARG:H	2.23	0.46
1:B:18:ILE:HB	1:B:228:THR:HG23	1.96	0.46
1:B:162:ARG:NH1	1:B:162:ARG:HB2	2.31	0.46
1:B:166:ARG:O	1:B:170:ARG:HG2	2.16	0.46
2:C:469:GLU:CG	2:C:480:LYS:HE3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:ILE:HG23	2:D:39:GLY:N	2.31	0.46
2:D:396:VAL:HG11	2:D:430:ILE:HG21	1.98	0.46
1:E:191:ILE:HG21	1:E:198:GLU:HG3	1.98	0.46
1:F:367:ILE:HD11	1:F:375:ILE:CD1	2.46	0.46
1:A:392:PHE:O	1:A:393:ARG:C	2.57	0.45
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.98	0.45
2:C:440:LEU:CD2	2:C:453:ILE:HG13	2.46	0.45
1:E:197:GLU:O	1:E:199:PHE:N	2.49	0.45
1:A:266:GLY:O	1:A:300:ARG:HG3	2.16	0.45
1:A:442:TYR:HE1	1:B:456:PHE:CE2	2.34	0.45
2:C:21:MET:HE3	2:C:141:ARG:NE	2.31	0.45
2:C:211:LEU:O	2:C:212:GLU:CB	2.64	0.45
2:C:335:PHE:HA	2:C:338:MET:HG3	1.99	0.45
2:C:435:ASP:HA	2:C:459:ARG:HD2	1.97	0.45
2:D:94:LEU:HD23	2:D:94:LEU:N	2.31	0.45
2:D:303:GLU:C	2:D:305:ALA:H	2.23	0.45
1:F:298:VAL:HA	1:F:411:LEU:HD23	1.98	0.45
1:F:426:TPO:HG23	1:F:430:ILE:H	1.70	0.45
1:A:188:TYR:CE2	1:F:211:LEU:HD23	2.50	0.45
1:B:93:ASP:OD1	1:B:95:ALA:HB3	2.16	0.45
1:B:340:ARG:C	1:B:342:ASN:H	2.24	0.45
2:C:64:ILE:HG22	2:C:65:ILE:HD13	1.97	0.45
2:C:123:LEU:HD11	2:C:163:GLU:O	2.16	0.45
2:C:350:TYR:CE1	2:D:252:MET:HE3	2.51	0.45
2:D:67:PHE:HD1	2:D:141:ARG:NH2	2.14	0.45
2:D:315:PHE:HA	2:D:347:VAL:HB	1.98	0.45
2:D:317:TYR:CD2	2:D:383:LEU:HD21	2.50	0.45
2:D:471:MET:CG	2:D:478:ASP:HB3	2.46	0.45
1:E:118:VAL:O	1:E:118:VAL:HG12	2.17	0.45
1:E:416:SER:O	1:E:418:GLN:N	2.49	0.45
1:E:446:ARG:O	1:E:447:GLY:C	2.57	0.45
1:F:161:ARG:NH2	1:F:199:PHE:HB2	2.32	0.45
1:F:256:GLN:H	1:F:256:GLN:HG2	1.58	0.45
1:F:514:GLU:HG2	1:F:519:SER:HB3	1.98	0.45
1:A:61:TYR:CE1	1:A:97:LEU:HD11	2.52	0.45
1:B:71:GLY:O	1:B:103:LEU:HA	2.17	0.45
1:B:151:PHE:C	1:B:153:GLN:N	2.68	0.45
1:B:151:PHE:O	1:B:153:GLN:N	2.45	0.45
1:B:167:LEU:O	1:B:168:VAL:C	2.59	0.45
1:B:247:PHE:CE2	1:B:364:LYS:HD2	2.51	0.45
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:191:ILE:HB	2:C:198:GLU:CG	2.47	0.45
2:D:220:LEU:HD13	2:D:246:ILE:HD13	1.97	0.45
2:D:406:GLU:HB3	2:D:408:ILE:HG13	1.98	0.45
1:E:350:TYR:CE1	1:F:254:LEU:HD13	2.51	0.45
1:F:170:ARG:HB3	1:F:170:ARG:NH1	2.32	0.45
1:F:367:ILE:O	1:F:367:ILE:HG22	2.16	0.45
1:F:379:SER:CB	1:F:382:ALA:HB2	2.46	0.45
1:F:418:GLN:HG3	1:F:418:GLN:O	2.17	0.45
1:A:28:PHE:H	1:A:246:ILE:HD12	1.82	0.45
1:A:165:PHE:CE2	1:F:110:PRO:HB2	2.52	0.45
1:A:420:MET:HE1	1:B:490:ILE:HG21	1.99	0.45
1:B:20:LYS:HG2	1:B:35:GLY:O	2.16	0.45
1:B:70:PRO:HA	1:B:102:LYS:O	2.17	0.45
1:B:74:VAL:HB	1:B:144:ILE:HG23	1.98	0.45
1:B:311:ARG:HA	1:B:343:LEU:O	2.17	0.45
1:B:311:ARG:HG2	1:B:343:LEU:HA	1.98	0.45
1:B:350:TYR:CZ	2:C:252:MET:HE3	2.51	0.45
2:C:392:PHE:O	2:C:395:PHE:HB3	2.15	0.45
1:F:293:GLY:O	1:F:296:LEU:HB3	2.17	0.45
1:F:371:LYS:C	1:F:371:LYS:HD2	2.41	0.45
1:A:254:LEU:HD11	5:F:535:HOH:O	2.15	0.45
1:B:216:ARG:NE	2:C:221:GLU:OE1	2.41	0.45
1:B:307:ALA:C	1:B:309:LYS:H	2.24	0.45
2:C:126:LEU:O	2:C:129:ARG:N	2.50	0.45
2:C:287:THR:HG22	2:C:288:GLY:N	2.32	0.45
2:D:85:LYS:O	2:D:86:ASN:C	2.60	0.45
2:D:306:CYS:C	2:D:308:ASN:H	2.23	0.45
1:E:21:MET:CE	1:E:141:ARG:HG2	2.46	0.45
1:F:127:ILE:CD1	1:F:167:LEU:HA	2.31	0.45
1:F:170:ARG:HH12	1:F:174:ILE:CG1	2.19	0.45
1:F:430:ILE:O	1:F:430:ILE:HG22	2.16	0.45
1:F:504:GLU:HA	1:F:507:ARG:CG	2.47	0.45
1:A:45:SER:HB3	1:A:182:THR:HB	1.96	0.45
1:A:267:VAL:CG1	1:A:270:LEU:HB2	2.47	0.45
1:B:305:ALA:CB	1:B:374:ARG:HD2	2.29	0.45
1:B:371:LYS:O	1:B:371:LYS:HD2	2.16	0.45
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.43	0.45
2:C:382:ALA:O	2:C:385:ARG:HG3	2.17	0.45
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.98	0.45
2:D:231:MET:HE1	2:D:251:ALA:HB2	1.98	0.45
1:E:281:ASP:O	1:E:282:SER:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:384:ALA:HB2	1:F:392:PHE:CE1	2.51	0.45
1:A:80:PRO:HB3	1:A:105:ILE:HG21	1.99	0.45
1:A:426:TPO:OG1	1:A:427:ASP:N	2.50	0.45
1:B:87:ALA:C	1:B:89:SER:N	2.74	0.45
1:B:232:LYS:HD2	1:B:232:LYS:N	2.32	0.45
1:B:283:ILE:HD12	1:B:412:PHE:CE1	2.52	0.45
2:C:46:GLY:HA2	2:C:184:ARG:CD	2.47	0.45
2:C:312:ALA:N	2:C:343:LEU:O	2.43	0.45
2:D:152:GLN:CB	1:E:161:ARG:HD3	2.45	0.45
1:E:33:HIS:HD2	1:E:230:HIS:CA	2.30	0.45
1:E:160:VAL:O	1:E:161:ARG:C	2.58	0.45
1:E:247:PHE:HZ	1:E:361:GLN:HG3	1.82	0.45
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.98	0.45
1:F:299:SER:HB3	1:F:333:MET:CE	2.46	0.45
1:A:52:LYS:HB3	1:A:181:THR:CG2	2.46	0.45
1:A:290:THR:HG23	1:A:290:THR:O	2.17	0.45
1:A:425:ILE:O	1:A:425:ILE:HG13	2.15	0.45
2:C:54:LEU:HD23	2:C:244:ILE:CG1	2.45	0.45
2:C:360:LEU:O	2:C:360:LEU:HD23	2.16	0.45
2:D:52:LYS:N	3:D:903:ATP:O1B	2.47	0.45
2:D:387:VAL:CG1	2:D:388:SER:H	2.29	0.45
2:D:397:ILE:O	2:D:398:GLY:C	2.60	0.45
2:D:490:ILE:C	2:D:492:GLY:H	2.25	0.45
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.99	0.45
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.47	0.45
1:A:273:MET:O	1:A:463:HIS:CA	2.64	0.45
1:A:293:GLY:HA2	3:A:901:ATP:O1A	2.16	0.45
1:B:119:GLY:C	1:B:121:PHE:N	2.72	0.45
2:C:107:ASP:C	2:C:107:ASP:OD1	2.59	0.45
2:C:263:VAL:HG12	2:C:374:ARG:NH2	2.32	0.45
1:E:52:LYS:O	1:E:55:PHE:HB3	2.16	0.45
1:E:301:PHE:O	1:E:374:ARG:NH1	2.49	0.45
1:E:323:GLN:NE2	1:F:459:ARG:CD	2.78	0.45
1:E:325:LEU:CD2	1:E:335:PHE:HB2	2.47	0.45
1:F:252:MET:CE	1:F:401:GLY:HA3	2.46	0.45
1:F:332:GLY:O	1:F:333:MET:O	2.35	0.45
1:F:426:TPO:HG21	1:F:429:HIS:HA	1.99	0.45
1:A:140:ARG:HB3	1:A:140:ARG:HH11	1.81	0.44
1:A:247:PHE:O	1:A:249:LEU:N	2.50	0.44
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.81	0.44
1:A:361:GLN:O	1:A:362:ILE:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.44	0.44
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.98	0.44
2:C:295:THR:HB	3:C:901:ATP:PA	2.57	0.44
2:C:370:PHE:O	2:C:371:LYS:C	2.59	0.44
2:C:468:ARG:HA	2:C:481:ASP:O	2.17	0.44
2:D:99:ASP:HA	5:D:545:HOH:O	2.17	0.44
2:D:484:ARG:HH11	2:D:484:ARG:HB3	1.82	0.44
1:E:18:ILE:CD1	1:E:227:GLY:HA3	2.31	0.44
1:E:46:GLY:HA2	1:E:184:ARG:HD3	1.99	0.44
1:E:150:VAL:HG13	1:E:151:PHE:N	2.32	0.44
1:F:61:TYR:O	1:F:64:ILE:HB	2.17	0.44
1:F:351:PRO:HD2	1:F:352:GLU:OE1	2.17	0.44
1:A:154:TYR:O	1:A:154:TYR:HD1	2.00	0.44
1:A:184:ARG:NH2	1:A:186:GLU:O	2.50	0.44
1:A:295:THR:O	1:A:296:LEU:C	2.60	0.44
1:A:344:LEU:HD11	1:A:346:ILE:HG13	1.97	0.44
1:A:356:LEU:N	1:A:356:LEU:HD12	2.32	0.44
1:B:393:ARG:O	1:B:397:ILE:HG12	2.17	0.44
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.27	0.44
2:C:385:ARG:C	2:C:387:VAL:H	2.24	0.44
2:D:64:ILE:HD12	2:D:97:LEU:HD13	1.99	0.44
1:E:21:MET:HE1	1:E:177:THR:HB	2.00	0.44
1:A:52:LYS:HD3	1:A:182:THR:O	2.17	0.44
1:A:106:LEU:C	1:A:106:LEU:HD12	2.43	0.44
1:A:430:ILE:O	1:A:432:GLU:N	2.51	0.44
2:D:140:ARG:HB3	2:D:140:ARG:NH1	2.31	0.44
2:D:380:LEU:C	2:D:382:ALA:N	2.75	0.44
2:D:402:TYR:O	2:D:406:GLU:HB2	2.18	0.44
1:E:193:ARG:NH2	1:F:195:GLY:O	2.48	0.44
1:E:266:GLY:CA	1:E:300:ARG:HG3	2.47	0.44
1:E:375:ILE:O	1:E:410:GLY:HA2	2.16	0.44
1:F:160:VAL:HG21	1:F:194:TYR:CD2	2.51	0.44
2:C:295:THR:HG22	2:C:331:TRP:HH2	1.83	0.44
2:C:315:PHE:HB3	2:C:317:TYR:CE1	2.50	0.44
2:D:32:SER:O	2:D:33:HIS:C	2.59	0.44
2:D:64:ILE:HD12	2:D:97:LEU:CD1	2.48	0.44
1:E:197:GLU:C	1:E:199:PHE:H	2.25	0.44
1:E:211:LEU:HD12	1:E:211:LEU:HA	1.72	0.44
1:F:269:ARG:HG2	1:F:479:ILE:CG2	2.47	0.44
1:F:382:ALA:O	1:F:385:ARG:HG3	2.17	0.44
1:F:507:ARG:O	1:F:508:ILE:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:O	1:A:59:PHE:HB3	2.16	0.44
1:A:351:PRO:CG	1:A:382:ALA:O	2.66	0.44
1:B:182:THR:CG2	1:B:192:ALA:HB1	2.43	0.44
1:B:357:GLU:HG3	1:B:358:ASP:N	2.33	0.44
1:B:418:GLN:HG3	1:B:418:GLN:O	2.17	0.44
1:B:464:ASP:OD2	1:B:468:ARG:NE	2.50	0.44
2:C:66:GLU:C	2:C:67:PHE:CD1	2.95	0.44
2:C:72:VAL:HA	2:C:104:PHE:O	2.18	0.44
2:D:191:ILE:HB	2:D:198:GLU:HG2	1.97	0.44
2:D:302:VAL:HG21	2:D:314:LEU:HB2	1.99	0.44
2:D:315:PHE:CE2	2:D:347:VAL:HG21	2.52	0.44
2:D:324:LEU:C	2:D:326:ARG:N	2.74	0.44
1:E:280:LYS:O	1:E:409:THR:OG1	2.33	0.44
1:E:367:ILE:O	1:E:367:ILE:HG22	2.16	0.44
1:F:164:LEU:O	1:F:165:PHE:C	2.60	0.44
1:F:187:GLU:CD	1:F:209:ASN:H	2.25	0.44
1:A:82:ASP:O	1:A:85:LYS:N	2.51	0.44
1:A:118:VAL:HG23	1:A:118:VAL:O	2.18	0.44
1:A:221:GLU:HG2	1:A:222:ILE:N	2.32	0.44
2:D:272:GLU:O	2:D:275:GLY:N	2.45	0.44
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.52	0.44
3:D:901:ATP:O2'	1:E:463:HIS:NE2	2.46	0.44
1:F:65:ILE:O	1:F:65:ILE:HG22	2.17	0.44
1:F:148:THR:HG21	1:F:183:GLU:CG	2.48	0.44
1:F:486:PHE:CE2	1:F:496:ARG:CD	3.00	0.44
1:A:492:GLY:O	1:A:494:PRO:HD3	2.17	0.44
1:B:86:ASN:HD21	2:C:40:ARG:HH22	1.64	0.44
1:B:480:LYS:HB3	1:B:481:ASP:H	1.62	0.44
1:B:498:THR:O	1:B:499:VAL:C	2.61	0.44
2:C:111:ASP:OD2	2:C:113:GLU:HG2	2.18	0.44
2:C:396:VAL:O	2:C:400:THR:HB	2.17	0.44
2:D:223:LEU:HD23	2:D:223:LEU:C	2.42	0.44
1:A:194:TYR:O	1:A:196:VAL:HG23	2.18	0.44
1:A:322:ALA:HB3	1:B:256:GLN:O	2.18	0.44
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.53	0.44
1:B:88:ARG:HG2	1:B:88:ARG:NH1	2.31	0.44
1:B:171:LEU:HA	1:B:174:ILE:HG12	2.00	0.44
1:B:452:ALA:HA	1:B:469:GLU:HA	2.00	0.44
2:C:21:MET:HB2	2:C:38:ILE:CG1	2.47	0.44
2:D:52:LYS:HB2	2:D:52:LYS:HE3	1.84	0.44
1:E:192:ALA:HB3	1:E:197:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:ARG:HG2	1:E:468:ARG:HH11	1.83	0.44
1:F:61:TYR:CE2	1:F:65:ILE:HG13	2.53	0.44
1:F:79:THR:CG2	1:F:82:ASP:H	2.26	0.44
1:A:163:GLU:HA	1:A:163:GLU:OE2	2.18	0.44
1:A:311:ARG:HA	1:A:343:LEU:O	2.18	0.44
1:B:44:VAL:HG22	1:B:205:VAL:CG1	2.47	0.44
1:B:54:LEU:HD13	1:B:90:PHE:CE1	2.53	0.44
1:B:364:LYS:O	1:B:365:SER:C	2.61	0.44
2:C:80:PRO:HB3	2:C:105:ILE:HG21	1.99	0.44
2:D:150:VAL:CG1	2:D:151:PHE:N	2.81	0.44
2:D:358:ASP:C	2:D:360:LEU:N	2.74	0.44
1:E:128:GLU:O	1:E:129:ARG:C	2.60	0.44
1:E:397:ILE:O	1:E:401:GLY:N	2.35	0.44
1:F:38:ILE:HD12	1:F:38:ILE:N	2.32	0.44
1:F:142:VAL:HB	1:F:178:THR:CG2	2.41	0.44
1:A:230:HIS:C	1:A:230:HIS:HD1	2.25	0.43
1:B:21:MET:HE1	1:B:59:PHE:CZ	2.52	0.43
1:B:291:GLY:C	3:B:901:ATP:O2B	2.60	0.43
1:B:414:ASN:ND2	1:B:426:TPO:CG2	2.81	0.43
2:C:232:LYS:HD2	2:C:232:LYS:H	1.80	0.43
2:C:294:LYS:HB2	3:C:901:ATP:O1B	2.17	0.43
2:C:471:MET:HE2	2:C:478:ASP:CB	2.48	0.43
2:D:52:LYS:CD	2:D:182:THR:O	2.66	0.43
2:D:266:GLY:C	2:D:300:ARG:HG3	2.42	0.43
2:D:430:ILE:O	2:D:431:ALA:C	2.60	0.43
1:E:123:LEU:HD21	1:E:166:ARG:HG2	2.00	0.43
1:E:144:ILE:HD11	1:E:171:LEU:HD11	1.99	0.43
1:E:294:LYS:CG	1:E:413:THR:HG23	2.48	0.43
1:E:386:GLY:HA2	1:F:390:ASN:OD1	2.18	0.43
1:E:447:GLY:C	1:F:467:ILE:HD12	2.43	0.43
1:F:116:GLU:O	1:F:117:VAL:CB	2.66	0.43
1:F:154:TYR:O	1:F:154:TYR:CD1	2.71	0.43
1:F:352:GLU:N	1:F:352:GLU:CD	2.76	0.43
1:B:25:ILE:CG2	1:B:58:GLN:NE2	2.75	0.43
2:D:46:GLY:O	2:D:183:GLU:HA	2.18	0.43
1:E:121:PHE:CD1	1:E:121:PHE:N	2.87	0.43
1:F:124:SER:OG	1:F:166:ARG:NH1	2.51	0.43
1:F:507:ARG:O	1:F:508:ILE:O	2.36	0.43
1:B:36:LEU:CD1	1:B:59:PHE:CE1	3.01	0.43
1:B:57:ILE:C	1:B:59:PHE:N	2.74	0.43
1:B:274:CYS:HG	1:B:278:PHE:HE2	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:PHE:O	1:B:485:ASN:N	2.51	0.43
2:C:79:THR:HG23	2:C:82:ASP:H	1.84	0.43
2:C:111:ASP:C	2:C:113:GLU:H	2.26	0.43
2:C:118:VAL:O	2:C:118:VAL:HG12	2.18	0.43
2:C:311:ARG:HD2	2:C:371:LYS:CD	2.49	0.43
2:C:347:VAL:HG12	2:C:348:CYS:N	2.33	0.43
2:D:38:ILE:HA	2:D:177:THR:HG23	2.00	0.43
2:D:161:ARG:CB	2:D:196:VAL:HG11	2.46	0.43
2:D:263:VAL:CG2	2:D:280:LYS:HA	2.48	0.43
1:E:102:LYS:HA	1:E:102:LYS:HD3	1.55	0.43
1:E:150:VAL:CG1	1:E:151:PHE:N	2.81	0.43
1:E:392:PHE:O	1:E:394:GLN:N	2.50	0.43
1:E:404:LYS:C	1:E:406:GLU:N	2.73	0.43
1:A:487:GLU:OE1	1:F:496:ARG:HG2	2.18	0.43
1:B:146:SER:O	1:B:149:SER:OG	2.34	0.43
1:B:194:TYR:O	1:B:195:GLY:C	2.60	0.43
1:B:437:ILE:HB	1:B:456:PHE:HB3	2.00	0.43
2:C:126:LEU:O	2:C:129:ARG:HB2	2.18	0.43
2:C:302:VAL:HG12	2:C:303:GLU:N	2.33	0.43
2:C:381:SER:C	2:C:383:LEU:H	2.25	0.43
2:D:78:GLU:HB3	2:D:83:ILE:HD11	2.01	0.43
2:D:223:LEU:HD23	2:D:223:LEU:O	2.18	0.43
2:D:436:THR:OG1	2:D:458:MET:HE3	2.18	0.43
1:E:197:GLU:C	1:E:199:PHE:N	2.75	0.43
1:E:198:GLU:O	1:E:224:LYS:HE2	2.19	0.43
1:F:98:VAL:HG22	1:F:103:LEU:HG	1.99	0.43
1:A:269:ARG:O	1:A:272:GLU:HB2	2.19	0.43
1:A:425:ILE:HD12	1:A:437:ILE:HG21	2.00	0.43
1:A:451:ARG:HH11	1:A:451:ARG:CG	2.28	0.43
1:B:52:LYS:N	3:B:903:ATP:O1B	2.51	0.43
1:B:419:PHE:CD2	2:C:425:ILE:HD12	2.53	0.43
2:C:31:ILE:HA	2:C:231:MET:SD	2.58	0.43
2:C:64:ILE:O	2:C:68:ASP:HA	2.19	0.43
2:C:70:PRO:CG	2:C:138:ARG:O	2.66	0.43
2:C:252:MET:HE1	2:C:397:ILE:HG22	2.00	0.43
2:C:329:TYR:CD2	2:C:329:TYR:O	2.71	0.43
2:C:435:ASP:OD1	2:C:459:ARG:NH1	2.51	0.43
2:C:443:VAL:O	2:C:444:GLU:C	2.61	0.43
2:D:31:ILE:O	2:D:231:MET:HG3	2.18	0.43
2:D:67:PHE:CD1	2:D:141:ARG:NH2	2.86	0.43
2:D:332:GLY:O	2:D:333:MET:CG	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:338:MET:HB3	2:D:344:LEU:HB3	2.00	0.43
2:D:443:VAL:HG13	2:D:494:PRO:CG	2.49	0.43
2:D:446:ARG:HB3	1:E:484:ARG:CG	2.46	0.43
1:E:332:GLY:C	1:E:333:MET:HG2	2.44	0.43
1:F:169:ALA:O	1:F:173:GLN:HG3	2.18	0.43
1:F:212:GLU:O	1:F:212:GLU:OE2	2.37	0.43
1:A:334:ASP:OD1	1:A:336:GLU:HB2	2.18	0.43
1:A:441:GLN:HG3	1:A:441:GLN:O	2.18	0.43
1:B:103:LEU:HD12	1:B:104:PHE:N	2.34	0.43
1:B:291:GLY:O	1:B:293:GLY:N	2.52	0.43
1:B:380:LEU:O	1:B:383:LEU:HB2	2.18	0.43
1:B:483:PHE:O	1:B:484:ARG:C	2.62	0.43
2:C:194:TYR:HD1	2:C:197:GLU:OE1	2.01	0.43
1:F:33:HIS:CD2	1:F:229:SER:OG	2.72	0.43
1:F:191:ILE:CG1	1:F:206:ILE:HD11	2.26	0.43
1:A:71:GLY:O	1:A:103:LEU:HA	2.18	0.43
1:B:82:ASP:O	1:B:83:ILE:C	2.60	0.43
2:C:127:ILE:HG12	2:C:167:LEU:HD13	2.01	0.43
2:D:315:PHE:CE1	2:D:363:ILE:HG23	2.54	0.43
2:D:340:ARG:C	2:D:342:ASN:N	2.77	0.43
2:D:352:GLU:C	2:D:354:ALA:H	2.26	0.43
1:E:37:PRO:HG2	1:E:225:LEU:HD22	2.01	0.43
1:E:191:ILE:HB	1:E:198:GLU:HG3	1.98	0.43
1:F:21:MET:HE3	1:F:59:PHE:HE1	1.84	0.43
1:F:22:ARG:HA	1:F:29:ASP:OD2	2.18	0.43
1:A:109:SER:HA	1:A:110:PRO:HD3	1.80	0.43
1:A:153:GLN:O	1:A:154:TYR:CB	2.66	0.43
1:A:206:ILE:HD11	1:A:223:LEU:CD1	2.49	0.43
1:A:248:PRO:HB2	1:A:251:ALA:CB	2.46	0.43
1:A:358:ASP:O	1:A:361:GLN:N	2.52	0.43
1:B:26:GLU:HB3	1:B:245:ASN:OD1	2.19	0.43
1:B:116:GLU:HG2	1:B:117:VAL:N	2.27	0.43
1:B:145:ASP:HA	1:B:181:THR:CB	2.48	0.43
1:B:451:ARG:HB3	1:B:452:ALA:H	1.69	0.43
2:C:278:PHE:CE1	2:C:284:ILE:HG21	2.54	0.43
2:C:316:ALA:HB2	2:C:324:LEU:HD11	2.01	0.43
2:C:378:ASP:O	2:C:379:SER:HB3	2.19	0.43
2:C:400:THR:O	2:C:402:TYR:N	2.52	0.43
2:D:295:THR:HA	2:D:298:VAL:HG23	2.00	0.43
2:D:418:GLN:HB2	1:E:423:HIS:O	2.19	0.43
1:E:61:TYR:O	1:E:63:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:THR:HB	1:E:440:LEU:HB3	2.01	0.43
1:F:116:GLU:O	1:F:117:VAL:HG23	2.18	0.43
1:F:181:THR:HG22	1:F:182:THR:N	2.34	0.43
1:F:256:GLN:HE21	1:F:404:LYS:HB3	1.82	0.43
1:A:22:ARG:NH2	1:A:24:MET:HE1	2.34	0.43
1:A:383:LEU:C	1:A:385:ARG:N	2.77	0.43
1:A:426:TPO:O1P	1:A:426:TPO:N	2.51	0.43
1:B:50:THR:O	1:B:207:LEU:HD13	2.19	0.43
1:B:396:VAL:C	1:B:398:GLY:N	2.73	0.43
1:B:497:ILE:C	1:B:499:VAL:N	2.77	0.43
2:C:211:LEU:HA	2:C:216:ARG:HD3	2.00	0.43
2:C:252:MET:CE	2:C:397:ILE:HG22	2.49	0.43
2:C:294:LYS:NZ	2:C:415:THR:HG23	2.34	0.43
2:D:79:THR:O	2:D:79:THR:HG23	2.18	0.43
2:D:237:PHE:CD1	2:D:237:PHE:C	2.97	0.43
2:D:304:ASN:O	2:D:308:ASN:ND2	2.44	0.43
2:D:384:ALA:HB2	2:D:392:PHE:CE1	2.54	0.43
3:D:901:ATP:H3'	1:E:458:MET:O	2.19	0.43
1:E:326:ARG:C	1:E:328:ALA:N	2.75	0.43
1:F:452:ALA:CB	1:F:469:GLU:HA	2.49	0.43
1:A:213:GLY:C	1:A:215:ARG:H	2.27	0.43
1:A:379:SER:CB	1:A:382:ALA:HB2	2.49	0.43
1:A:425:ILE:N	1:A:426:TPO:O1P	2.52	0.43
1:A:447:GLY:HA2	1:B:489:ILE:HD13	2.00	0.43
1:B:240:THR:CG2	1:B:361:GLN:HE22	2.32	0.43
2:C:311:ARG:NE	2:C:371:LYS:HE3	2.34	0.43
2:C:323:GLN:HE21	2:C:327:ASN:HD21	1.66	0.43
2:D:344:LEU:C	2:D:344:LEU:CD1	2.86	0.43
1:F:262:ARG:HA	1:F:278:PHE:O	2.18	0.43
1:F:289:ALA:HB2	1:F:419:PHE:HA	2.00	0.43
1:A:52:LYS:N	3:A:903:ATP:O1B	2.52	0.42
1:A:88:ARG:O	1:A:89:SER:C	2.62	0.42
1:A:225:LEU:O	1:A:226:ARG:C	2.61	0.42
1:B:54:LEU:HD21	1:B:244:ILE:HG13	2.01	0.42
1:B:191:ILE:N	1:B:191:ILE:CD1	2.83	0.42
2:D:380:LEU:C	2:D:382:ALA:H	2.27	0.42
2:D:443:VAL:CG1	2:D:494:PRO:HG2	2.49	0.42
1:E:191:ILE:CB	1:E:198:GLU:CG	2.93	0.42
1:E:194:TYR:CD1	1:E:194:TYR:N	2.87	0.42
1:F:29:ASP:OD1	1:F:29:ASP:N	2.51	0.42
1:F:222:ILE:HG21	1:F:225:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:471:MET:HG2	1:F:480:LYS:HE2	2.01	0.42
1:A:199:PHE:CE2	1:F:193:ARG:NH2	2.86	0.42
1:A:389:ASN:HD21	1:A:428:SER:HB2	1.85	0.42
1:B:22:ARG:O	1:B:141:ARG:NH2	2.52	0.42
1:B:42:THR:O	1:B:179:VAL:HA	2.19	0.42
1:B:335:PHE:HA	1:B:338:MET:CG	2.49	0.42
1:B:359:HIS:O	1:B:361:GLN:N	2.51	0.42
2:C:43:LEU:HD11	2:C:182:THR:OG1	2.18	0.42
2:C:82:ASP:C	2:C:84:ILE:N	2.76	0.42
2:C:170:ARG:HB3	2:C:170:ARG:HH11	1.82	0.42
2:C:208:ARG:HG3	5:C:535:HOH:O	2.18	0.42
2:C:400:THR:HG22	2:C:401:GLY:N	2.34	0.42
2:C:483:PHE:CD1	2:C:483:PHE:N	2.87	0.42
2:D:220:LEU:HD23	2:D:220:LEU:C	2.43	0.42
2:D:291:GLY:CA	3:D:901:ATP:O2B	2.68	0.42
2:D:451:ARG:HG2	2:D:451:ARG:HH11	1.84	0.42
1:E:356:LEU:HD12	1:E:356:LEU:N	2.34	0.42
1:F:332:GLY:O	1:F:333:MET:C	2.62	0.42
1:F:500:ASP:O	1:F:501:GLU:CB	2.54	0.42
1:A:184:ARG:HH22	1:A:188:TYR:CA	2.32	0.42
1:A:435:ASP:HA	1:A:459:ARG:HD2	2.01	0.42
1:B:179:VAL:O	1:B:179:VAL:HG12	2.20	0.42
1:B:317:TYR:CE2	1:B:383:LEU:HD21	2.54	0.42
1:B:423:HIS:O	1:B:424:SER:HB3	2.19	0.42
1:B:451:ARG:NH1	1:B:451:ARG:CG	2.80	0.42
1:B:490:ILE:HA	1:B:490:ILE:HD13	1.82	0.42
2:C:73:PHE:HE2	2:C:83:ILE:HD13	1.83	0.42
2:C:163:GLU:OE2	2:C:163:GLU:HA	2.19	0.42
2:C:185:ILE:N	2:C:185:ILE:CD1	2.81	0.42
2:C:263:VAL:CG1	2:C:374:ARG:HH21	2.32	0.42
2:D:305:ALA:CB	2:D:374:ARG:HD2	2.33	0.42
1:E:266:GLY:O	1:E:300:ARG:NE	2.52	0.42
1:F:129:ARG:O	1:F:132:TYR:HB3	2.19	0.42
1:F:294:LYS:HD3	1:F:294:LYS:H	1.84	0.42
1:F:356:LEU:CD1	1:F:387:VAL:HG21	2.49	0.42
1:B:148:THR:HA	1:B:151:PHE:HE1	1.84	0.42
1:B:193:ARG:HG2	1:B:193:ARG:NH1	2.33	0.42
1:B:404:LYS:C	1:B:406:GLU:N	2.77	0.42
2:C:202:ASP:CA	2:C:226:ARG:HD2	2.47	0.42
2:C:204:VAL:HG21	2:C:224:LYS:HE2	2.02	0.42
2:C:248:PRO:C	2:C:250:GLY:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:364:LYS:HE2	2:C:402:TYR:CD1	2.54	0.42
2:C:425:ILE:HD12	2:C:425:ILE:N	2.32	0.42
2:D:361:GLN:O	2:D:364:LYS:N	2.52	0.42
1:E:78:GLU:HB2	1:E:83:ILE:HD11	2.02	0.42
1:F:312:ALA:HB2	1:F:374:ARG:HB2	2.00	0.42
1:F:337:GLU:O	1:F:338:MET:C	2.63	0.42
1:F:485:ASN:O	1:F:486:PHE:CD1	2.72	0.42
1:A:146:SER:H	1:A:181:THR:HB	1.85	0.42
1:B:284:ILE:O	1:B:411:LEU:HA	2.19	0.42
3:B:901:ATP:O3'	2:C:457:LYS:HB2	2.19	0.42
2:C:192:ALA:O	2:C:193:ARG:C	2.63	0.42
2:D:219:THR:HB	2:D:234:GLU:HB3	2.00	0.42
2:D:380:LEU:O	2:D:383:LEU:N	2.52	0.42
2:D:385:ARG:O	2:D:387:VAL:HG23	2.20	0.42
1:E:420:MET:HE1	1:F:490:ILE:HB	2.02	0.42
1:F:47:THR:HG22	1:F:50:THR:HG21	2.00	0.42
1:F:53:THR:O	1:F:54:LEU:C	2.63	0.42
1:F:271:ASP:OD1	1:F:277:GLY:HA2	2.19	0.42
1:F:360:LEU:HD13	1:F:360:LEU:O	2.19	0.42
1:A:49:GLY:HA2	3:A:903:ATP:O2B	2.20	0.42
1:A:51:GLY:O	1:A:54:LEU:HB3	2.18	0.42
1:B:90:PHE:HA	1:B:241:ASP:O	2.19	0.42
1:B:94:LEU:O	1:B:95:ALA:C	2.62	0.42
1:B:445:ILE:CD1	1:B:494:PRO:HG2	2.50	0.42
2:C:24:MET:CB	2:C:62:ASN:ND2	2.79	0.42
2:C:88:ARG:CZ	2:D:15:HIS:HA	2.49	0.42
2:C:123:LEU:HD13	2:C:166:ARG:HD2	2.02	0.42
2:C:204:VAL:CG2	2:C:224:LYS:HE2	2.49	0.42
2:D:123:LEU:HD11	2:D:167:LEU:HB2	2.00	0.42
1:E:58:GLN:CG	1:E:62:ASN:ND2	2.83	0.42
1:E:81:GLN:H	1:E:81:GLN:CD	2.26	0.42
1:E:298:VAL:O	1:E:301:PHE:HB3	2.20	0.42
1:E:393:ARG:NH2	5:E:524:HOH:O	2.52	0.42
1:F:389:ASN:O	1:F:392:PHE:N	2.53	0.42
1:A:14:GLU:CG	1:A:15:HIS:N	2.66	0.42
1:A:32:SER:OG	1:A:35:GLY:CA	2.68	0.42
1:A:49:GLY:CA	3:A:903:ATP:O2B	2.68	0.42
1:A:131:ASN:O	1:A:132:TYR:C	2.62	0.42
1:A:183:GLU:H	1:A:183:GLU:HG2	1.67	0.42
1:A:209:ASN:ND2	1:A:218:ARG:HG3	2.34	0.42
1:A:420:MET:SD	1:B:490:ILE:HG13	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:O	1:B:237:PHE:HZ	2.02	0.42
1:B:278:PHE:CD1	1:B:301:PHE:HE1	2.37	0.42
2:C:61:TYR:CD1	2:C:97:LEU:HD11	2.54	0.42
2:D:38:ILE:HA	2:D:177:THR:CG2	2.50	0.42
2:D:161:ARG:HD2	2:D:196:VAL:HG13	2.02	0.42
2:D:303:GLU:C	2:D:305:ALA:N	2.77	0.42
1:E:269:ARG:HG2	1:E:479:ILE:HB	2.02	0.42
1:F:116:GLU:O	1:F:117:VAL:HB	2.19	0.42
1:F:134:ILE:HD11	1:F:142:VAL:HG21	2.01	0.42
1:F:399:VAL:O	1:F:400:THR:C	2.63	0.42
1:A:191:ILE:HD12	1:A:191:ILE:H	1.83	0.42
1:A:306:CYS:CB	1:A:338:MET:SD	3.07	0.42
1:A:380:LEU:O	1:A:392:PHE:HE1	2.03	0.42
1:B:41:SER:O	1:B:203:ASN:ND2	2.53	0.42
1:B:51:GLY:O	1:B:54:LEU:N	2.53	0.42
1:B:60:LEU:O	1:B:61:TYR:C	2.62	0.42
1:B:268:VAL:C	1:B:270:LEU:N	2.77	0.42
1:B:370:PHE:C	1:B:372:PRO:HD3	2.45	0.42
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.82	0.42
2:C:87:ALA:HB1	2:C:92:TRP:HD1	1.82	0.42
2:C:151:PHE:C	2:C:153:GLN:N	2.77	0.42
2:C:169:ALA:O	2:C:172:LYS:HB3	2.20	0.42
2:C:378:ASP:O	2:C:379:SER:CB	2.67	0.42
2:C:397:ILE:O	2:C:398:GLY:C	2.60	0.42
2:D:299:SER:CB	2:D:333:MET:HE1	2.50	0.42
1:E:237:PHE:CD1	1:E:237:PHE:C	2.97	0.42
1:E:249:LEU:CD1	1:E:394:GLN:HG2	2.50	0.42
1:E:331:TRP:NE1	3:E:901:ATP:N7	2.68	0.42
1:F:315:PHE:CD2	1:F:347:VAL:HG21	2.55	0.42
1:F:387:VAL:HG13	1:F:391:ALA:HB3	2.02	0.42
1:F:503:SER:O	1:F:504:GLU:C	2.62	0.42
1:F:515:LYS:C	1:F:517:PRO:HD2	2.45	0.42
1:A:94:LEU:O	1:A:97:LEU:N	2.52	0.42
1:B:52:LYS:HB2	1:B:52:LYS:HE3	1.81	0.42
1:B:52:LYS:HE3	3:B:903:ATP:O3B	2.20	0.42
1:B:215:ARG:NE	1:B:215:ARG:HA	2.33	0.42
1:B:266:GLY:O	1:B:300:ARG:CG	2.68	0.42
1:B:284:ILE:HB	1:B:411:LEU:HD12	2.01	0.42
1:B:356:LEU:N	1:B:356:LEU:CD1	2.82	0.42
2:C:123:LEU:HD21	2:C:167:LEU:HB2	2.01	0.42
2:C:332:GLY:O	2:C:333:MET:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:384:ALA:HB2	2:C:392:PHE:CD1	2.54	0.42
2:D:304:ASN:O	2:D:304:ASN:OD1	2.37	0.42
1:F:140:ARG:HH11	1:F:140:ARG:CB	2.30	0.42
1:A:53:THR:O	1:A:54:LEU:C	2.60	0.42
1:A:508:ILE:HD13	1:A:508:ILE:N	2.33	0.42
2:C:73:PHE:CD1	2:C:143:SER:HB2	2.55	0.42
2:C:75:THR:HB	2:C:83:ILE:HD11	2.02	0.42
2:C:82:ASP:O	2:C:83:ILE:C	2.62	0.42
2:C:191:ILE:HB	2:C:198:GLU:HG2	2.02	0.42
2:C:196:VAL:HG12	2:C:197:GLU:N	2.34	0.42
2:C:445:ILE:O	2:C:445:ILE:HG22	2.19	0.42
2:D:128:GLU:O	2:D:132:TYR:N	2.49	0.42
2:D:317:TYR:HE2	2:D:383:LEU:HD21	1.80	0.42
2:D:396:VAL:HG11	2:D:430:ILE:CG2	2.50	0.42
1:E:49:GLY:HA2	3:E:903:ATP:O2B	2.20	0.42
1:E:288:GLY:O	1:E:294:LYS:NZ	2.48	0.42
1:F:79:THR:HA	1:F:80:PRO:HD3	1.87	0.42
1:F:437:ILE:HD11	1:F:457:LYS:HE2	2.01	0.42
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.81	0.41
1:A:184:ARG:O	1:A:185:ILE:HD13	2.19	0.41
1:A:281:ASP:OD1	1:A:407:GLU:OE1	2.38	0.41
1:A:356:LEU:CD1	1:A:356:LEU:N	2.83	0.41
1:A:445:ILE:HD12	1:A:486:PHE:CE2	2.54	0.41
2:C:303:GLU:C	2:C:303:GLU:OE1	2.63	0.41
2:C:316:ALA:HB3	2:C:348:CYS:SG	2.60	0.41
2:C:400:THR:C	2:C:402:TYR:N	2.78	0.41
2:C:480:LYS:HE3	2:C:480:LYS:HB2	1.93	0.41
2:D:76:PHE:CZ	2:D:126:LEU:CD2	3.03	0.41
2:D:441:GLN:HE22	2:D:490:ILE:HD12	1.85	0.41
1:F:60:LEU:HD23	1:F:60:LEU:HA	1.73	0.41
1:A:264:SER:HB3	1:A:304:ASN:ND2	2.36	0.41
1:A:448:GLU:HA	1:B:466:ALA:HA	2.02	0.41
1:B:76:PHE:HE1	1:B:144:ILE:CG2	2.33	0.41
2:C:60:LEU:O	2:C:62:ASN:N	2.53	0.41
2:C:164:LEU:HB3	2:C:200:VAL:HG11	2.02	0.41
2:D:237:PHE:HE1	2:D:239:ILE:HG13	1.86	0.41
2:D:323:GLN:HG2	2:D:327:ASN:ND2	2.35	0.41
1:E:496:ARG:O	1:E:497:ILE:HD13	2.20	0.41
1:F:170:ARG:O	1:F:174:ILE:HG12	2.20	0.41
1:F:246:ILE:HG22	1:F:247:PHE:N	2.34	0.41
1:F:377:ILE:HD12	1:F:412:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:TPO:CG2	1:F:429:HIS:CA	2.99	0.41
1:A:384:ALA:HB2	1:A:392:PHE:CE1	2.55	0.41
1:A:419:PHE:O	1:A:420:MET:HB2	2.20	0.41
1:B:38:ILE:HA	1:B:177:THR:CG2	2.51	0.41
1:B:122:ASP:C	1:B:124:SER:N	2.77	0.41
1:B:324:LEU:O	1:B:325:LEU:C	2.63	0.41
2:C:126:LEU:O	2:C:127:ILE:C	2.63	0.41
2:C:245:ASN:ND2	2:C:247:PHE:CZ	2.88	0.41
2:D:54:LEU:HD13	2:D:90:PHE:CZ	2.55	0.41
2:D:78:GLU:HB3	2:D:83:ILE:CD1	2.50	0.41
1:F:252:MET:HE3	1:F:401:GLY:HA3	2.02	0.41
1:F:504:GLU:HB2	1:F:505:LEU:H	1.49	0.41
1:A:65:ILE:HD11	1:A:97:LEU:HD21	2.03	0.41
1:A:395:PHE:C	1:A:395:PHE:CD2	2.98	0.41
1:B:218:ARG:HD3	1:B:237:PHE:CZ	2.53	0.41
2:C:166:ARG:O	2:C:166:ARG:HG2	2.19	0.41
2:C:317:TYR:N	2:C:317:TYR:CD1	2.88	0.41
2:C:356:LEU:O	2:C:357:GLU:C	2.63	0.41
2:D:76:PHE:HZ	2:D:126:LEU:CD2	2.34	0.41
1:E:54:LEU:CD2	1:E:244:ILE:HG13	2.50	0.41
1:E:283:ILE:HG23	1:E:412:PHE:CE1	2.55	0.41
3:E:903:ATP:O3G	1:F:224:LYS:NZ	2.44	0.41
1:F:61:TYR:O	1:F:64:ILE:N	2.41	0.41
1:F:145:ASP:O	1:F:146:SER:OG	2.30	0.41
1:F:462:TRP:CE3	1:F:463:HIS:N	2.88	0.41
1:A:256:GLN:O	1:F:322:ALA:HB3	2.20	0.41
1:B:84:ILE:O	1:B:85:LYS:C	2.62	0.41
1:B:425:ILE:HD12	1:B:425:ILE:H	1.85	0.41
2:C:111:ASP:HA	2:C:112:PRO:HD3	1.93	0.41
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.49	0.41
2:C:335:PHE:O	2:C:339:GLU:HG3	2.20	0.41
2:C:420:MET:HE3	2:C:492:GLY:O	2.21	0.41
1:F:312:ALA:CA	1:F:372:PRO:HB3	2.40	0.41
1:A:18:ILE:N	1:A:18:ILE:CD1	2.83	0.41
1:A:294:LYS:O	1:A:295:THR:C	2.64	0.41
1:B:167:LEU:O	1:B:170:ARG:HB2	2.21	0.41
1:B:311:ARG:O	1:B:372:PRO:HA	2.20	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.94	0.41
2:C:297:LEU:O	2:C:298:VAL:C	2.63	0.41
2:C:320:SER:HA	2:D:254:LEU:HG	2.03	0.41
2:D:182:THR:HG21	2:D:192:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:LEU:HD13	2:D:345:LYS:N	2.36	0.41
2:D:486:PHE:CB	2:D:489:ILE:CD1	2.98	0.41
2:D:487:GLU:O	2:D:494:PRO:HA	2.21	0.41
1:E:61:TYR:C	1:E:63:GLY:H	2.29	0.41
1:E:218:ARG:HG3	1:E:237:PHE:O	2.20	0.41
1:E:334:ASP:HA	5:E:525:HOH:O	2.19	0.41
1:E:348:CYS:HB3	1:F:254:LEU:HD23	2.03	0.41
1:F:117:VAL:HA	1:F:154:TYR:OH	2.20	0.41
1:F:218:ARG:HB2	1:F:237:PHE:CE2	2.55	0.41
1:F:317:TYR:OH	1:F:363:ILE:HD11	2.20	0.41
1:F:490:ILE:H	1:F:490:ILE:HG12	1.61	0.41
1:A:71:GLY:HA2	1:A:141:ARG:O	2.20	0.41
1:A:267:VAL:HG22	1:A:300:ARG:HG2	2.02	0.41
1:A:313:ILE:HD12	1:A:372:PRO:HG2	2.03	0.41
1:B:359:HIS:C	1:B:361:GLN:N	2.77	0.41
1:B:451:ARG:HB2	1:B:470:PHE:O	2.21	0.41
1:B:503:SER:O	1:B:504:GLU:CB	2.66	0.41
2:C:150:VAL:CG1	2:C:151:PHE:N	2.82	0.41
2:C:352:GLU:C	2:C:354:ALA:H	2.29	0.41
2:D:208:ARG:O	2:D:218:ARG:HA	2.21	0.41
2:D:471:MET:HE1	2:D:473:SER:OG	2.20	0.41
2:D:490:ILE:C	2:D:492:GLY:N	2.78	0.41
1:F:153:GLN:O	1:F:154:TYR:CB	2.69	0.41
1:F:259:SER:C	1:F:261:VAL:H	2.27	0.41
1:F:284:ILE:HB	1:F:411:LEU:HA	2.03	0.41
1:F:426:TPO:HG23	1:F:429:HIS:H	1.86	0.41
1:A:79:THR:O	1:A:82:ASP:HB2	2.20	0.41
1:A:125:ALA:O	1:A:129:ARG:HG3	2.20	0.41
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.36	0.41
1:A:358:ASP:O	1:A:359:HIS:C	2.63	0.41
1:A:396:VAL:C	1:A:398:GLY:N	2.75	0.41
2:C:64:ILE:HG23	2:C:102:LYS:HB3	2.03	0.41
2:C:231:MET:CE	2:C:251:ALA:HB2	2.35	0.41
2:D:167:LEU:O	2:D:168:VAL:C	2.61	0.41
1:E:81:GLN:H	1:E:81:GLN:HE21	1.66	0.41
1:F:47:THR:N	5:F:523:HOH:O	2.54	0.41
1:F:67:PHE:CB	1:F:69:GLU:HG3	2.51	0.41
1:F:171:LEU:O	1:F:174:ILE:HB	2.20	0.41
1:F:291:GLY:C	1:F:442:TYR:OH	2.64	0.41
1:F:295:THR:HA	1:F:378:ASP:OD2	2.20	0.41
1:A:96:LYS:HE2	1:A:100:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:HG21	1:A:180:MET:CE	2.50	0.41
1:A:249:LEU:HD13	1:A:394:GLN:HG2	2.02	0.41
1:A:421:GLY:O	1:A:422:ALA:C	2.63	0.41
1:B:337:GLU:O	1:B:338:MET:C	2.64	0.41
2:C:46:GLY:O	2:C:52:LYS:HD3	2.21	0.41
2:C:153:GLN:O	2:C:154:TYR:HB3	2.21	0.41
2:C:187:GLU:OE2	2:C:208:ARG:HA	2.21	0.41
2:C:289:ALA:HB2	2:C:419:PHE:HA	2.02	0.41
2:C:295:THR:HG22	2:C:296:LEU:N	2.34	0.41
2:C:429:HIS:C	2:C:430:ILE:HD13	2.45	0.41
2:C:451:ARG:NH1	2:C:451:ARG:CG	2.74	0.41
2:D:75:THR:HG23	2:D:75:THR:O	2.21	0.41
2:D:151:PHE:C	2:D:153:GLN:N	2.71	0.41
2:D:208:ARG:NE	2:D:234:GLU:OE2	2.54	0.41
2:D:223:LEU:C	2:D:223:LEU:CD2	2.94	0.41
2:D:265:SER:N	2:D:271:ASP:OD1	2.52	0.41
2:D:267:VAL:HG12	2:D:270:LEU:H	1.86	0.41
2:D:331:TRP:O	2:D:333:MET:HG2	2.20	0.41
2:D:356:LEU:HD23	2:D:391:ALA:O	2.20	0.41
2:D:392:PHE:O	2:D:395:PHE:HB3	2.21	0.41
2:D:486:PHE:HB3	2:D:489:ILE:HD11	2.02	0.41
2:D:496:ARG:NH2	1:E:486:PHE:O	2.54	0.41
1:E:57:ILE:HA	1:E:57:ILE:HD13	1.85	0.41
1:E:80:PRO:HB2	1:E:81:GLN:NE2	2.36	0.41
1:E:362:ILE:O	1:E:365:SER:N	2.51	0.41
1:E:370:PHE:C	1:E:372:PRO:HD3	2.45	0.41
1:E:371:LYS:HD2	1:E:371:LYS:C	2.46	0.41
1:F:208:ARG:O	1:F:218:ARG:HA	2.20	0.41
1:F:237:PHE:HA	1:F:245:ASN:O	2.21	0.41
1:F:425:ILE:N	1:F:425:ILE:HD12	2.36	0.41
1:F:426:TPO:CG2	1:F:429:HIS:N	2.84	0.41
1:F:489:ILE:O	1:F:491:SER:N	2.54	0.41
1:A:21:MET:HE2	1:A:177:THR:HG21	2.03	0.41
1:A:191:ILE:CD1	1:A:191:ILE:H	2.33	0.41
1:B:47:THR:O	1:B:48:SER:C	2.63	0.41
2:C:50:THR:CB	2:C:207:LEU:HB3	2.47	0.41
2:C:146:SER:C	2:C:148:THR:N	2.78	0.41
2:C:239:ILE:HG22	3:C:903:ATP:N3	2.36	0.41
2:D:376:ALA:HA	2:D:411:LEU:O	2.21	0.41
2:D:483:PHE:O	2:D:484:ARG:C	2.63	0.41
1:E:79:THR:O	1:E:80:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ASN:OD1	1:E:135:GLN:NE2	2.54	0.41
1:F:21:MET:CE	1:F:59:PHE:CZ	3.04	0.41
1:F:191:ILE:N	1:F:191:ILE:CD1	2.84	0.41
1:F:419:PHE:O	1:F:420:MET:O	2.39	0.41
1:A:150:VAL:HG13	1:A:151:PHE:N	2.35	0.40
1:A:156:ALA:O	1:A:157:SER:C	2.65	0.40
1:A:211:LEU:HA	1:A:216:ARG:HD3	2.03	0.40
1:A:441:GLN:NE2	1:A:490:ILE:HD13	2.21	0.40
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.86	0.40
1:B:273:MET:HA	1:B:464:ASP:HB2	2.03	0.40
1:B:306:CYS:CB	1:B:338:MET:SD	3.09	0.40
1:B:313:ILE:HG22	1:B:314:LEU:N	2.36	0.40
2:C:42:THR:HG23	2:C:203:ASN:HB3	2.03	0.40
2:D:44:VAL:HG22	2:D:205:VAL:CG1	2.52	0.40
2:D:299:SER:HB3	2:D:333:MET:CE	2.51	0.40
2:D:444:GLU:HA	2:D:448:GLU:O	2.21	0.40
1:E:21:MET:CE	1:E:59:PHE:CZ	3.04	0.40
1:E:145:ASP:O	1:E:146:SER:OG	2.37	0.40
1:E:191:ILE:CB	1:E:198:GLU:HG2	2.42	0.40
1:E:426:TPO:O3P	1:E:429:HIS:HA	2.22	0.40
1:F:60:LEU:O	1:F:61:TYR:C	2.64	0.40
1:F:70:PRO:HA	1:F:102:LYS:O	2.21	0.40
1:F:117:VAL:O	1:F:118:VAL:HB	2.20	0.40
1:F:170:ARG:CA	1:F:170:ARG:HH11	2.34	0.40
1:F:294:LYS:CB	1:F:413:THR:HG23	2.48	0.40
1:A:69:GLU:HB3	1:A:140:ARG:HB2	2.02	0.40
1:A:121:PHE:CD1	1:A:122:ASP:N	2.89	0.40
1:A:161:ARG:HH11	1:F:152:GLN:HG3	1.86	0.40
1:A:312:ALA:O	1:A:344:LEU:HD22	2.21	0.40
1:B:86:ASN:O	1:B:89:SER:N	2.48	0.40
1:B:220:LEU:HD23	1:B:220:LEU:C	2.46	0.40
1:B:291:GLY:O	1:B:292:THR:C	2.64	0.40
1:B:397:ILE:O	1:B:397:ILE:HG22	2.20	0.40
2:C:48:SER:HB2	2:D:199:PHE:CD1	2.55	0.40
2:C:57:ILE:HD13	2:C:57:ILE:HA	1.94	0.40
2:C:64:ILE:CD1	2:C:103:LEU:HB2	2.52	0.40
2:C:393:ARG:O	2:C:396:VAL:N	2.54	0.40
2:D:225:LEU:CB	2:D:230:HIS:HD2	2.31	0.40
1:F:209:ASN:O	1:F:216:ARG:NH1	2.54	0.40
1:F:256:GLN:NE2	1:F:404:LYS:HB3	2.36	0.40
1:F:371:LYS:O	1:F:371:LYS:CD	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:ASP:OD1	1:F:413:THR:HG21	2.21	0.40
1:F:430:ILE:C	1:F:432:GLU:N	2.79	0.40
1:F:433:ILE:N	1:F:433:ILE:HD12	2.36	0.40
1:F:470:PHE:CD1	1:F:470:PHE:C	3.00	0.40
1:A:287:THR:HG23	1:A:414:ASN:HB3	2.03	0.40
1:A:438:ILE:HD13	1:A:455:VAL:HA	2.04	0.40
1:B:356:LEU:HD23	1:B:395:PHE:HB2	2.04	0.40
2:C:412:PHE:N	2:C:412:PHE:CD1	2.89	0.40
2:C:443:VAL:HG12	2:C:445:ILE:HG12	2.04	0.40
1:E:47:THR:O	1:E:52:LYS:HE2	2.21	0.40
1:E:360:LEU:HD13	1:E:360:LEU:O	2.22	0.40
1:E:454:ASN:ND2	1:E:456:PHE:HD1	2.19	0.40
1:F:47:THR:CG2	1:F:50:THR:HG22	2.51	0.40
1:F:263:VAL:HG12	1:F:264:SER:H	1.86	0.40
1:F:440:LEU:HD23	1:F:453:ILE:HG13	2.03	0.40
1:A:31:ILE:HD11	1:A:246:ILE:CG2	2.40	0.40
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.86	0.40
1:A:255:THR:O	1:A:255:THR:HG22	2.22	0.40
1:A:488:ARG:HA	1:F:493:SER:HB2	2.02	0.40
1:B:266:GLY:O	1:B:300:ARG:HG2	2.20	0.40
1:B:400:THR:HG21	1:B:433:ILE:CG2	2.51	0.40
2:C:106:LEU:O	2:C:106:LEU:HG	2.21	0.40
2:C:196:VAL:C	2:C:198:GLU:N	2.79	0.40
2:C:370:PHE:O	2:C:371:LYS:HG3	2.21	0.40
2:C:420:MET:HE3	2:C:492:GLY:C	2.47	0.40
2:D:41:SER:HA	2:D:178:THR:O	2.22	0.40
2:D:80:PRO:HA	2:D:83:ILE:HD13	2.03	0.40
2:D:311:ARG:HA	2:D:343:LEU:O	2.20	0.40
2:D:443:VAL:HG11	2:D:483:PHE:CE2	2.57	0.40
1:E:262:ARG:NH1	1:E:461:SER:HB2	2.36	0.40
1:E:311:ARG:HA	1:E:343:LEU:O	2.21	0.40
1:E:356:LEU:CD1	1:E:356:LEU:H	2.35	0.40
1:F:452:ALA:CA	1:F:469:GLU:HA	2.50	0.40
1:A:59:PHE:HD2	1:A:143:SER:OG	2.05	0.40
1:A:94:LEU:O	1:A:95:ALA:C	2.64	0.40
1:B:39:GLY:N	1:B:177:THR:OG1	2.39	0.40
1:B:251:ALA:O	1:B:252:MET:C	2.65	0.40
1:B:444:GLU:O	1:B:494:PRO:HD2	2.22	0.40
2:C:18:ILE:HD12	2:C:18:ILE:N	2.37	0.40
2:C:123:LEU:C	2:C:127:ILE:HG13	2.47	0.40
2:C:208:ARG:O	2:C:218:ARG:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:ARG:NH1	2:C:472:ILE:HD12	2.37	0.40
2:D:193:ARG:NH2	1:E:195:GLY:O	2.45	0.40
2:D:211:LEU:HD12	2:D:215:ARG:O	2.22	0.40
2:D:263:VAL:CG1	2:D:374:ARG:HH21	2.34	0.40
1:E:67:PHE:CB	1:E:69:GLU:HG3	2.51	0.40
1:E:111:ASP:C	1:E:113:GLU:H	2.30	0.40
1:E:240:THR:C	1:E:242:HIS:N	2.79	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	503/519 (97%)	377 (75%)	92 (18%)	34 (7%)	1	7
1	B	488/519 (94%)	365 (75%)	82 (17%)	41 (8%)	0	4
1	E	489/519 (94%)	375 (77%)	79 (16%)	35 (7%)	1	6
1	F	503/519 (97%)	399 (79%)	70 (14%)	34 (7%)	1	7
2	C	486/519 (94%)	373 (77%)	81 (17%)	32 (7%)	1	7
2	D	483/519 (93%)	392 (81%)	69 (14%)	22 (5%)	2	13
All	All	2952/3114 (95%)	2281 (77%)	473 (16%)	198 (7%)	1	7

All (198) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	65	ILE
1	A	154	TYR
1	A	212	GLU
1	A	333	MET

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Mol	Chain	Res	Type
1	A	427	ASP
1	A	499	VAL
1	A	502	LYS
1	A	510	ARG
1	B	52	LYS
1	B	65	ILE
1	B	154	TYR
1	B	193	ARG
1	B	461	SER
1	B	463	HIS
2	C	17	ALA
2	C	88	ARG
2	C	117	VAL
2	C	154	TYR
2	C	333	MET
2	C	463	HIS
2	D	87	ALA
2	D	122	ASP
2	D	154	TYR
2	D	333	MET
1	E	122	ASP
1	E	154	TYR
1	E	157	SER
1	E	195	GLY
1	E	333	MET
1	E	372	PRO
1	E	387	VAL
1	E	428	SER
1	E	463	HIS
1	F	26	GLU
1	F	117	VAL
1	F	118	VAL
1	F	154	TYR
1	F	249	LEU
1	F	333	MET
1	F	354	ALA
1	F	431	ALA
1	F	463	HIS
1	F	504	GLU
1	F	506	SER
1	F	507	ARG
1	F	508	ILE

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Mol	Chain	Res	Type
1	F	515	LYS
1	A	17	ALA
1	A	167	LEU
1	A	189	GLY
1	A	387	VAL
1	A	420	MET
1	A	429	HIS
1	A	431	ALA
1	A	463	HIS
1	B	26	GLU
1	B	119	GLY
1	B	132	TYR
1	B	149	SER
1	B	249	LEU
1	B	292	THR
1	B	342	ASN
1	B	370	PHE
1	B	372	PRO
1	B	420	MET
1	B	484	ARG
2	C	47	THR
2	C	115	GLN
2	C	149	SER
2	C	193	ARG
2	C	249	LEU
2	C	405	GLN
2	D	17	ALA
2	D	152	GLN
2	D	211	LEU
2	D	381	SER
2	D	400	THR
1	E	117	VAL
1	E	198	GLU
1	E	200	VAL
1	E	282	SER
1	E	327	ASN
1	E	393	ARG
1	E	417	ASP
1	E	420	MET
1	E	422	ALA
1	E	427	ASP
1	E	494	PRO

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Mol	Chain	Res	Type
1	E	498	THR
1	E	504	GLU
1	F	47	THR
1	F	189	GLY
1	F	420	MET
1	F	501	GLU
1	A	157	SER
1	A	422	ALA
1	A	480	LYS
1	B	22	ARG
1	B	61	TYR
1	B	211	LEU
1	B	327	ASN
1	B	354	ALA
1	B	424	SER
1	B	429	HIS
2	C	55	PHE
2	C	61	TYR
2	C	96	LYS
2	C	97	LEU
2	C	107	ASP
2	C	112	PRO
2	C	114	GLY
2	C	157	SER
2	C	341	GLN
2	C	398	GLY
2	D	86	ASN
2	D	123	LEU
2	D	420	MET
1	E	211	LEU
1	E	326	ARG
1	E	342	ASN
1	E	432	GLU
1	F	52	LYS
1	F	490	ILE
1	A	347	VAL
1	A	384	ALA
1	A	428	SER
1	B	167	LEU
1	B	189	GLY
1	B	326	ARG
1	B	405	GLN

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Mol	Chain	Res	Type
1	B	452	ALA
1	B	498	THR
2	C	197	GLU
2	C	289	ALA
2	C	477	PRO
2	D	325	LEU
2	D	429	HIS
1	E	18	ILE
1	E	47	THR
1	E	52	LYS
1	E	379	SER
1	E	482	SER
1	E	490	ILE
1	F	61	TYR
1	F	116	GLU
1	F	379	SER
1	F	468	ARG
1	A	120	GLY
1	A	211	LEU
1	A	289	ALA
1	B	54	LEU
1	B	152	GLN
1	B	198	GLU
1	B	268	VAL
1	B	289	ALA
1	B	309	LYS
2	C	212	GLU
2	C	379	SER
2	C	386	GLY
2	D	26	GLU
2	D	212	GLU
2	D	348	CYS
2	D	463	HIS
1	E	61	TYR
1	F	157	SER
1	F	211	LEU
1	F	500	ASP
1	F	517	PRO
1	A	112	PRO
1	A	117	VAL
1	A	268	VAL
1	A	348	CYS

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Mol	Chain	Res	Type
1	B	85	LYS
2	C	87	ALA
2	C	348	CYS
2	C	420	MET
2	D	248	PRO
2	D	354	ALA
2	D	359	HIS
1	F	152	GLN
1	F	409	THR
1	B	84	ILE
1	B	117	VAL
1	B	195	GLY
1	F	425	ILE
1	F	489	ILE
1	F	509	VAL
1	A	509	VAL
2	C	196	VAL
2	D	347	VAL
1	E	80	PRO
1	A	168	VAL
1	B	179	VAL
1	F	371	LYS
1	A	433	ILE
1	A	83	ILE
1	E	189	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/442 (97%)	396 (92%)	34 (8%)	11	36
1	B	417/442 (94%)	388 (93%)	29 (7%)	14	41
1	E	418/442 (95%)	378 (90%)	40 (10%)	8	29
1	F	430/442 (97%)	385 (90%)	45 (10%)	6	25
2	C	415/443 (94%)	370 (89%)	45 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	412/443 (93%)	365 (89%)	47 (11%)	5	21
All	All	2522/2654 (95%)	2282 (90%)	240 (10%)	8	29

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	30	ASP
1	A	33	HIS
1	A	50	THR
1	A	75	THR
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	115	GLN
1	A	191	ILE
1	A	198	GLU
1	A	212	GLU
1	A	219	THR
1	A	238	THR
1	A	270	LEU
1	A	280	LYS
1	A	287	THR
1	A	298	VAL
1	A	302	VAL
1	A	335	PHE
1	A	342	ASN
1	A	360	LEU
1	A	366	GLU
1	A	375	ILE
1	A	427	ASP
1	A	429	HIS
1	A	434	THR
1	A	439	LEU
1	A	451	ARG
1	A	463	HIS
1	A	469	GLU
1	A	471	MET
1	A	508	ILE
1	A	518	GLU
1	B	26	GLU
1	B	47	THR

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Mol	Chain	Res	Type
1	B	50	THR
1	B	77	GLU
1	B	81	GLN
1	B	103	LEU
1	B	111	ASP
1	B	151	PHE
1	B	154	TYR
1	B	178	THR
1	B	182	THR
1	B	185	ILE
1	B	186	GLU
1	B	193	ARG
1	B	203	ASN
1	B	205	VAL
1	B	212	GLU
1	B	223	LEU
1	B	239	ILE
1	B	256	GLN
1	B	270	LEU
1	B	283	ILE
1	B	295	THR
1	B	302	VAL
1	B	333	MET
1	B	411	LEU
1	B	474	ASP
1	B	490	ILE
1	B	499	VAL
2	C	15	HIS
2	C	26	GLU
2	C	50	THR
2	C	121	PHE
2	C	140	ARG
2	C	149	SER
2	C	151	PHE
2	C	154	TYR
2	C	184	ARG
2	C	185	ILE
2	C	196	VAL
2	C	198	GLU
2	C	210	VAL
2	C	212	GLU
2	C	215	ARG

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Mol	Chain	Res	Type
2	C	218	ARG
2	C	223	LEU
2	C	225	LEU
2	C	228	THR
2	C	238	THR
2	C	245	ASN
2	C	256	GLN
2	C	260	ASN
2	C	263	VAL
2	C	270	LEU
2	C	290	THR
2	C	295	THR
2	C	302	VAL
2	C	303	GLU
2	C	317	TYR
2	C	333	MET
2	C	336	GLU
2	C	342	ASN
2	C	356	LEU
2	C	366	GLU
2	C	375	ILE
2	C	383	LEU
2	C	413	THR
2	C	454	ASN
2	C	458	MET
2	C	470	PHE
2	C	471	MET
2	C	477	PRO
2	C	491	SER
2	C	498	THR
2	D	18	ILE
2	D	26	GLU
2	D	30	ASP
2	D	38	ILE
2	D	48	SER
2	D	80	PRO
2	D	81	GLN
2	D	97	LEU
2	D	106	LEU
2	D	121	PHE
2	D	122	ASP
2	D	123	LEU

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Mol	Chain	Res	Type
2	D	147	VAL
2	D	154	TYR
2	D	177	THR
2	D	181	THR
2	D	209	ASN
2	D	211	LEU
2	D	212	GLU
2	D	218	ARG
2	D	238	THR
2	D	256	GLN
2	D	263	VAL
2	D	270	LEU
2	D	281	ASP
2	D	284	ILE
2	D	290	THR
2	D	292	THR
2	D	302	VAL
2	D	314	LEU
2	D	321	ARG
2	D	342	ASN
2	D	344	LEU
2	D	356	LEU
2	D	360	LEU
2	D	412	PHE
2	D	416	SER
2	D	423	HIS
2	D	434	THR
2	D	453	ILE
2	D	463	HIS
2	D	471	MET
2	D	474	ASP
2	D	490	ILE
2	D	496	ARG
2	D	497	ILE
2	D	498	THR
1	E	18	ILE
1	E	26	GLU
1	E	81	GLN
1	E	83	ILE
1	E	97	LEU
1	E	113	GLU
1	E	116	GLU

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Mol	Chain	Res	Type
1	E	121	PHE
1	E	135	GLN
1	E	147	VAL
1	E	151	PHE
1	E	154	TYR
1	E	177	THR
1	E	183	GLU
1	E	196	VAL
1	E	201	SER
1	E	203	ASN
1	E	212	GLU
1	E	223	LEU
1	E	228	THR
1	E	240	THR
1	E	256	GLN
1	E	268	VAL
1	E	271	ASP
1	E	280	LYS
1	E	284	ILE
1	E	287	THR
1	E	325	LEU
1	E	338	MET
1	E	366	GLU
1	E	369	ASP
1	E	417	ASP
1	E	432	GLU
1	E	435	ASP
1	E	449	MET
1	E	451	ARG
1	E	453	ILE
1	E	458	MET
1	E	471	MET
1	E	505	LEU
1	F	15	HIS
1	F	26	GLU
1	F	43	LEU
1	F	56	SER
1	F	77	GLU
1	F	79	THR
1	F	103	LEU
1	F	121	PHE
1	F	123	LEU

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Mol	Chain	Res	Type
1	F	140	ARG
1	F	143	SER
1	F	154	TYR
1	F	159	VAL
1	F	168	VAL
1	F	178	THR
1	F	184	ARG
1	F	185	ILE
1	F	191	ILE
1	F	210	VAL
1	F	212	GLU
1	F	215	ARG
1	F	218	ARG
1	F	219	THR
1	F	256	GLN
1	F	263	VAL
1	F	285	LEU
1	F	302	VAL
1	F	325	LEU
1	F	344	LEU
1	F	366	GLU
1	F	387	VAL
1	F	424	SER
1	F	425	ILE
1	F	427	ASP
1	F	458	MET
1	F	462	TRP
1	F	468	ARG
1	F	469	GLU
1	F	471	MET
1	F	481	ASP
1	F	497	ILE
1	F	501	GLU
1	F	504	GLU
1	F	509	VAL
1	F	514	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	33	HIS

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Mol	Chain	Res	Type
1	A	62	ASN
1	A	131	ASN
1	A	135	GLN
1	A	152	GLN
1	A	209	ASN
1	A	304	ASN
1	A	308	ASN
1	A	323	GLN
1	A	327	ASN
1	A	359	HIS
1	A	414	ASN
1	A	441	GLN
1	B	16	GLN
1	B	58	GLN
1	B	62	ASN
1	B	81	GLN
1	B	152	GLN
1	B	203	ASN
1	B	342	ASN
1	B	359	HIS
1	B	361	GLN
1	B	368	ASN
1	B	441	GLN
2	C	33	HIS
2	C	58	GLN
2	C	62	ASN
2	C	152	GLN
2	C	153	GLN
2	C	203	ASN
2	C	209	ASN
2	C	245	ASN
2	C	260	ASN
2	C	323	GLN
2	C	389	ASN
2	C	414	ASN
2	C	423	HIS
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	260	ASN
2	D	323	GLN
2	D	341	GLN

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Mol	Chain	Res	Type
2	D	342	ASN
2	D	390	ASN
2	D	414	ASN
2	D	441	GLN
1	E	33	HIS
1	E	62	ASN
1	E	81	GLN
1	E	135	GLN
1	E	209	ASN
1	E	260	ASN
1	E	323	GLN
1	E	368	ASN
1	E	405	GLN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	16	GLN
1	F	33	HIS
1	F	81	GLN
1	F	209	ASN
1	F	256	GLN
1	F	260	ASN
1	F	327	ASN
1	F	342	ASN
1	F	418	GLN
1	F	441	GLN
1	F	454	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	TPO	B	426	1	8,10,11	1.58	2 (25%)	10,14,16	2.62	3 (30%)
1	TPO	A	426	1	8,10,11	1.16	1 (12%)	10,14,16	0.91	0
1	TPO	F	426	1	8,10,11	1.54	1 (12%)	10,14,16	2.46	5 (50%)
1	TPO	E	426	1	8,10,11	0.98	0	10,14,16	1.84	2 (20%)

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
1	TPO	B	426	1	-	4/9/11/13	-
1	TPO	A	426	1	-	2/9/11/13	-
1	TPO	F	426	1	-	3/9/11/13	-
1	TPO	E	426	1	-	3/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	426	TPO	CB-CA	3.24	1.60	1.53
1	B	426	TPO	CG2-CB	3.15	1.59	1.51
1	A	426	TPO	P-OG1	-2.41	1.55	1.59
1	B	426	TPO	P-O1P	-2.08	1.44	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	TPO	P-OG1-CB	-6.19	106.50	123.33
1	B	426	TPO	CG2-CB-CA	-4.02	105.42	113.26
1	E	426	TPO	P-OG1-CB	-3.97	112.55	123.33
1	F	426	TPO	CG2-CB-CA	-3.62	106.22	113.26
1	F	426	TPO	P-OG1-CB	-3.59	113.57	123.33
1	E	426	TPO	CG2-CB-CA	-3.55	106.34	113.26
1	F	426	TPO	O2P-P-O1P	-3.51	97.14	110.83
1	F	426	TPO	O2P-P-OG1	3.40	119.09	105.85
1	B	426	TPO	O2P-P-OG1	2.89	117.13	105.85
1	F	426	TPO	O3P-P-O2P	2.68	117.85	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	426	TPO	CG2-CB-OG1-P
1	B	426	TPO	N-CA-CB-CG2
1	B	426	TPO	N-CA-CB-OG1
1	B	426	TPO	C-CA-CB-CG2
1	E	426	TPO	N-CA-CB-CG2
1	E	426	TPO	N-CA-CB-OG1
1	E	426	TPO	C-CA-CB-CG2
1	F	426	TPO	N-CA-CB-OG1
1	A	426	TPO	CA-CB-OG1-P
1	B	426	TPO	O-C-CA-CB
1	F	426	TPO	O-C-CA-CB
1	F	426	TPO	N-CA-CB-CG2

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	426	TPO	7	0
1	A	426	TPO	15	0
1	F	426	TPO	13	0
1	E	426	TPO	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	901	4	32,33,33	1.14	2 (6%)	48,52,52	2.04	12 (25%)
3	ATP	E	901	4	32,33,33	1.12	2 (6%)	48,52,52	2.17	16 (33%)
3	ATP	A	901	4	32,33,33	1.18	3 (9%)	48,52,52	2.03	13 (27%)
3	ATP	E	903	4	32,33,33	1.38	4 (12%)	48,52,52	2.09	13 (27%)
3	ATP	C	901	4	32,33,33	1.36	3 (9%)	48,52,52	2.15	15 (31%)
3	ATP	D	903	4	32,33,33	1.21	4 (12%)	48,52,52	2.04	9 (18%)
3	ATP	C	903	4	32,33,33	1.33	4 (12%)	48,52,52	2.12	11 (22%)
3	ATP	F	903	4	32,33,33	1.14	2 (6%)	48,52,52	2.08	14 (29%)
3	ATP	B	903	4	32,33,33	1.22	5 (15%)	48,52,52	2.05	12 (25%)
3	ATP	A	903	4	32,33,33	1.46	4 (12%)	48,52,52	1.96	11 (22%)
3	ATP	D	901	4	32,33,33	1.26	5 (15%)	48,52,52	2.06	15 (31%)
3	ATP	F	901	4	32,33,33	1.16	3 (9%)	48,52,52	2.04	13 (27%)

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	ATP	B	901	4	-	5/22/38/38	0/3/3/3
3	ATP	E	901	4	-	9/22/38/38	0/3/3/3
3	ATP	A	901	4	-	6/22/38/38	0/3/3/3
3	ATP	E	903	4	-	7/22/38/38	0/3/3/3
3	ATP	C	901	4	-	8/22/38/38	0/3/3/3
3	ATP	D	903	4	-	7/22/38/38	0/3/3/3
3	ATP	C	903	4	-	8/22/38/38	0/3/3/3
3	ATP	F	903	4	-	8/22/38/38	0/3/3/3
3	ATP	B	903	4	-	9/22/38/38	0/3/3/3
3	ATP	A	903	4	-	8/22/38/38	0/3/3/3
3	ATP	D	901	4	-	9/22/38/38	0/3/3/3
3	ATP	F	901	4	-	7/22/38/38	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	ATP	PB-O3A	-4.30	1.54	1.59
3	A	903	ATP	PB-O3A	4.15	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	ATP	PB-O3A	-3.88	1.55	1.59
3	A	903	ATP	PA-O3A	3.81	1.63	1.59
3	E	903	ATP	PA-O3A	3.62	1.63	1.59
3	E	903	ATP	PB-O3B	-3.29	1.55	1.59
3	E	903	ATP	PB-O3A	2.96	1.62	1.59
3	D	901	ATP	C2-N3	2.87	1.39	1.33
3	F	903	ATP	C2-N3	2.86	1.39	1.33
3	D	903	ATP	C4-N3	2.84	1.39	1.34
3	C	901	ATP	C2-N3	2.81	1.38	1.33
3	A	901	ATP	C2-N3	2.81	1.38	1.33
3	F	901	ATP	C2-N3	2.72	1.38	1.33
3	B	903	ATP	C2-N3	2.70	1.38	1.33
3	C	901	ATP	PA-O3A	-2.68	1.56	1.59
3	B	903	ATP	PB-O3B	-2.64	1.56	1.59
3	D	901	ATP	C2-N1	2.64	1.38	1.33
3	E	901	ATP	C2-N3	2.61	1.38	1.33
3	D	903	ATP	C2-N3	2.59	1.38	1.33
3	C	903	ATP	C2-N3	2.57	1.38	1.33
3	D	903	ATP	PB-O3B	-2.54	1.56	1.59
3	B	903	ATP	C1'-N9	2.53	1.53	1.46
3	F	901	ATP	C2-N1	2.49	1.38	1.33
3	F	903	ATP	C2-N1	2.49	1.38	1.33
3	A	903	ATP	C2-N3	2.47	1.38	1.33
3	A	903	ATP	C2-N1	2.47	1.38	1.33
3	A	901	ATP	PB-O3B	-2.40	1.56	1.59
3	C	903	ATP	PA-O3A	-2.37	1.56	1.59
3	D	901	ATP	PA-O3A	2.37	1.62	1.59
3	B	901	ATP	PA-O3A	2.36	1.62	1.59
3	B	903	ATP	C2-N1	2.33	1.38	1.33
3	B	903	ATP	C4-N3	2.29	1.38	1.34
3	E	903	ATP	C2-N3	2.28	1.38	1.33
3	A	901	ATP	C2-N1	2.28	1.38	1.33
3	B	901	ATP	C2-N1	2.24	1.37	1.33
3	D	903	ATP	C2-N1	2.20	1.37	1.33
3	C	903	ATP	C2-N1	2.18	1.37	1.33
3	D	901	ATP	C4-N3	2.11	1.38	1.34
3	F	901	ATP	C4-N3	2.08	1.38	1.34
3	E	901	ATP	C2-N1	2.03	1.37	1.33
3	D	901	ATP	C5-N7	-2.01	1.35	1.39

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ATP	N3-C2-N1	-5.68	119.98	128.58
3	E	901	ATP	N3-C2-N1	-5.68	119.99	128.58
3	D	903	ATP	N3-C2-N1	-5.66	120.01	128.58
3	E	903	ATP	N3-C2-N1	-5.63	120.06	128.58
3	B	903	ATP	N3-C2-N1	-5.61	120.08	128.58
3	B	901	ATP	N3-C2-N1	-5.60	120.10	128.58
3	C	903	ATP	N3-C2-N1	-5.57	120.15	128.58
3	C	901	ATP	N3-C2-N1	-5.47	120.30	128.58
3	F	901	ATP	N3-C2-N1	-5.47	120.31	128.58
3	A	903	ATP	N3-C2-N1	-5.39	120.42	128.58
3	F	903	ATP	N3-C2-N1	-5.37	120.45	128.58
3	B	903	ATP	C5-N7-C8	5.36	111.87	103.45
3	C	901	ATP	C5-N7-C8	5.36	111.87	103.45
3	D	903	ATP	C5-N7-C8	5.35	111.86	103.45
3	F	903	ATP	C5-N7-C8	5.34	111.85	103.45
3	B	901	ATP	C5-N7-C8	5.31	111.80	103.45
3	A	901	ATP	N3-C2-N1	-5.26	120.62	128.58
3	F	901	ATP	C5-N7-C8	5.26	111.71	103.45
3	C	903	ATP	C5-N7-C8	5.25	111.69	103.45
3	E	903	ATP	N9-C8-N7	-5.21	106.55	113.94
3	E	903	ATP	C5-N7-C8	5.20	111.62	103.45
3	A	901	ATP	C5-N7-C8	5.19	111.61	103.45
3	E	901	ATP	C5-N7-C8	5.17	111.58	103.45
3	D	901	ATP	C5-N7-C8	5.11	111.48	103.45
3	C	903	ATP	N9-C8-N7	-5.07	106.75	113.94
3	B	903	ATP	C4-C5-N7	-5.06	104.79	110.58
3	C	903	ATP	C4-C5-N7	-4.98	104.88	110.58
3	D	903	ATP	C4-C5-N7	-4.94	104.94	110.58
3	F	901	ATP	C4-C5-N7	-4.90	104.98	110.58
3	C	901	ATP	C4-C5-N7	-4.87	105.01	110.58
3	A	903	ATP	C5-N7-C8	4.85	111.07	103.45
3	D	903	ATP	N9-C8-N7	-4.84	107.07	113.94
3	A	901	ATP	C4-C5-N7	-4.82	105.08	110.58
3	B	901	ATP	C4-C5-N7	-4.78	105.11	110.58
3	F	903	ATP	C4-C5-N7	-4.76	105.14	110.58
3	E	901	ATP	N9-C8-N7	-4.74	107.21	113.94
3	E	903	ATP	C4-C5-N7	-4.73	105.17	110.58
3	E	901	ATP	C4-C5-N7	-4.67	105.25	110.58
3	C	901	ATP	N9-C8-N7	-4.64	107.36	113.94
3	B	901	ATP	N9-C8-N7	-4.62	107.38	113.94
3	A	903	ATP	C4-C5-N7	-4.60	105.32	110.58
3	F	903	ATP	N9-C8-N7	-4.57	107.45	113.94
3	B	903	ATP	N9-C8-N7	-4.56	107.47	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	ATP	N9-C8-N7	-4.54	107.49	113.94
3	F	901	ATP	N9-C8-N7	-4.53	107.51	113.94
3	D	901	ATP	N9-C8-N7	-4.44	107.64	113.94
3	D	901	ATP	C4-C5-N7	-4.38	105.58	110.58
3	A	901	ATP	N9-C8-N7	-4.36	107.75	113.94
3	C	901	ATP	C5-C4-N3	-3.49	121.92	126.72
3	E	901	ATP	O2B-PB-O3B	3.48	116.68	107.27
3	C	901	ATP	O2B-PB-O3B	3.44	116.57	107.27
3	A	901	ATP	C5-C4-N3	-3.35	122.10	126.72
3	B	901	ATP	O2B-PB-O3B	3.35	116.33	107.27
3	F	903	ATP	C5-C4-N3	-3.30	122.17	126.72
3	B	903	ATP	C5-C4-N3	-3.24	122.25	126.72
3	D	901	ATP	O2B-PB-O3B	3.20	115.94	107.27
3	D	903	ATP	C6-C5-N7	3.20	138.26	132.09
3	E	901	ATP	O3A-PB-O1B	-3.19	101.11	110.70
3	B	903	ATP	C6-C5-N7	3.19	138.23	132.09
3	F	901	ATP	C5-C4-N3	-3.19	122.33	126.72
3	B	903	ATP	C2-N3-C4	3.18	119.61	111.83
3	D	903	ATP	C5-C4-N3	-3.18	122.33	126.72
3	E	903	ATP	C4-N9-C8	3.16	109.06	105.74
3	D	903	ATP	C2-N3-C4	3.13	119.48	111.83
3	C	901	ATP	C2-N3-C4	3.12	119.45	111.83
3	E	903	ATP	C2'-C1'-N9	3.10	121.00	113.30
3	C	903	ATP	C2-N3-C4	3.09	119.38	111.83
3	E	901	ATP	C2-N3-C4	3.08	119.35	111.83
3	E	901	ATP	C5-C4-N3	-3.08	122.48	126.72
3	C	903	ATP	C6-C5-N7	3.03	137.94	132.09
3	B	901	ATP	C2-N3-C4	3.03	119.23	111.83
3	F	901	ATP	C2-N3-C4	3.02	119.21	111.83
3	D	901	ATP	C5-C4-N3	-3.02	122.56	126.72
3	C	903	ATP	O2B-PB-O3B	3.01	115.40	107.27
3	A	901	ATP	C2-N3-C4	3.00	119.16	111.83
3	D	903	ATP	C2'-C1'-N9	3.00	120.76	113.30
3	B	901	ATP	C6-C5-N7	2.96	137.80	132.09
3	F	903	ATP	C2-N3-C4	2.96	119.05	111.83
3	D	901	ATP	C2-N3-C4	2.95	119.03	111.83
3	F	901	ATP	C6-C5-N7	2.93	137.74	132.09
3	A	903	ATP	C2-N3-C4	2.91	118.95	111.83
3	C	903	ATP	C5-C4-N3	-2.91	122.71	126.72
3	C	903	ATP	C4-N9-C8	2.90	108.78	105.74
3	E	903	ATP	C2-N3-C4	2.88	118.86	111.83
3	C	901	ATP	C6-C5-N7	2.87	137.62	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	ATP	C5-C4-N3	-2.87	122.77	126.72
3	E	903	ATP	C6-C5-N7	2.87	137.61	132.09
3	A	901	ATP	C6-C5-N7	2.86	137.59	132.09
3	A	903	ATP	C6-C5-N7	2.85	137.59	132.09
3	A	903	ATP	C5-C4-N3	-2.84	122.81	126.72
3	E	901	ATP	C6-C5-N7	2.83	137.54	132.09
3	E	901	ATP	O3B-PB-O1B	-2.82	102.22	110.70
3	C	901	ATP	C2'-C1'-N9	2.79	120.23	113.30
3	C	903	ATP	C2'-C1'-N9	2.79	120.23	113.30
3	D	901	ATP	O3A-PB-O1B	-2.78	102.36	110.70
3	F	901	ATP	O2B-PB-O3B	2.77	114.76	107.27
3	F	903	ATP	C6-C5-N7	2.75	137.40	132.09
3	F	903	ATP	O3A-PB-O1B	-2.72	102.51	110.70
3	F	903	ATP	C2'-C1'-N9	2.71	120.04	113.30
3	E	903	ATP	C5-C4-N3	-2.70	123.00	126.72
3	F	903	ATP	O2B-PB-O3B	2.69	114.55	107.27
3	A	901	ATP	O2B-PB-O3B	2.69	114.53	107.27
3	A	901	ATP	C2'-C1'-N9	2.68	119.95	113.30
3	E	901	ATP	C4-N9-C8	2.67	108.54	105.74
3	C	901	ATP	O4'-C1'-N9	-2.64	103.01	108.09
3	B	903	ATP	C2'-C1'-N9	2.61	119.80	113.30
3	E	901	ATP	O2'-C2'-C3'	2.61	120.18	111.82
3	D	901	ATP	O3B-PB-O1B	-2.60	102.88	110.70
3	A	903	ATP	C4-N9-C8	2.59	108.46	105.74
3	D	903	ATP	C4-N9-C8	2.56	108.42	105.74
3	D	901	ATP	C6-C5-N7	2.51	136.93	132.09
3	B	901	ATP	O3A-PB-O1B	-2.51	103.16	110.70
3	C	901	ATP	C4-N9-C8	2.45	108.31	105.74
3	E	901	ATP	O2G-PG-O3B	2.41	112.72	104.64
3	D	901	ATP	C4-N9-C8	2.41	108.27	105.74
3	A	903	ATP	C2'-C1'-N9	2.39	119.23	113.30
3	A	903	ATP	O2B-PB-O3B	2.38	113.70	107.27
3	F	901	ATP	O3B-PB-O1B	-2.37	103.58	110.70
3	A	903	ATP	O2'-C2'-C3'	2.37	119.40	111.82
3	D	901	ATP	C2'-C1'-N9	2.36	119.18	113.30
3	F	901	ATP	C2'-C1'-N9	2.36	119.17	113.30
3	B	901	ATP	O3B-PB-O1B	-2.36	103.60	110.70
3	E	903	ATP	O4'-C1'-N9	-2.35	103.58	108.09
3	B	901	ATP	C4-N9-C8	2.32	108.17	105.74
3	F	901	ATP	O2'-C2'-C3'	2.31	119.23	111.82
3	F	903	ATP	C2'-C3'-C4'	2.29	107.04	102.61
3	F	901	ATP	C4-N9-C8	2.29	108.14	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ATP	O4'-C1'-N9	-2.28	103.70	108.09
3	E	903	ATP	O2B-PB-O3B	2.26	113.37	107.27
3	F	903	ATP	C4-N9-C8	2.24	108.09	105.74
3	B	901	ATP	C2'-C1'-N9	2.21	118.78	113.30
3	F	903	ATP	N6-C6-N1	-2.20	113.47	118.38
3	B	903	ATP	O2B-PB-O3B	2.18	113.17	107.27
3	E	903	ATP	O2B-PB-O3A	2.18	113.17	107.27
3	A	901	ATP	C4-N9-C8	2.18	108.03	105.74
3	C	901	ATP	C2'-C3'-C4'	2.16	106.78	102.61
3	B	903	ATP	N6-C6-N1	-2.16	113.57	118.38
3	F	903	ATP	O2G-PG-O3B	2.16	111.87	104.64
3	A	901	ATP	C2'-C3'-C4'	2.15	106.77	102.61
3	E	901	ATP	C2'-C1'-N9	2.14	118.63	113.30
3	F	901	ATP	O3A-PB-O1B	-2.13	104.29	110.70
3	D	901	ATP	C2'-C3'-C4'	2.13	106.73	102.61
3	D	901	ATP	O2G-PG-O3B	2.10	111.67	104.64
3	B	903	ATP	O2'-C2'-C3'	2.09	118.53	111.82
3	C	901	ATP	O3A-PA-O1A	-2.09	104.41	110.70
3	A	901	ATP	O3B-PB-O1B	-2.07	104.47	110.70
3	E	901	ATP	C2'-C3'-C4'	2.06	106.59	102.61
3	B	903	ATP	C5-C4-N9	2.06	108.05	105.81
3	C	903	ATP	N6-C6-N1	-2.05	113.81	118.38
3	C	901	ATP	O2'-C2'-C3'	2.05	118.38	111.82
3	E	901	ATP	O2B-PB-O3A	2.04	112.78	107.27
3	C	901	ATP	N3-C4-N9	2.03	130.63	127.17
3	E	903	ATP	O2G-PG-O3B	2.02	111.42	104.64
3	A	901	ATP	N6-C6-N1	-2.01	113.91	118.38

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	C3'-C4'-C5'-O5'
3	A	903	ATP	PB-O3B-PG-O3G
3	B	901	ATP	C5'-O5'-PA-O1A
3	B	903	ATP	PB-O3B-PG-O3G
3	B	903	ATP	O4'-C4'-C5'-O5'
3	B	903	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	PB-O3B-PG-O2G
3	C	901	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
3	C	901	ATP	C5'-O5'-PA-O3A
3	C	901	ATP	O4'-C4'-C5'-O5'
3	C	903	ATP	PB-O3B-PG-O3G
3	C	903	ATP	C5'-O5'-PA-O1A
3	C	903	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	C5'-O5'-PA-O3A
3	D	901	ATP	C3'-C4'-C5'-O5'
3	D	903	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	PB-O3B-PG-O3G
3	E	901	ATP	PB-O3A-PA-O5'
3	E	901	ATP	C5'-O5'-PA-O3A
3	E	903	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	C5'-O5'-PA-O3A
3	F	903	ATP	PB-O3B-PG-O3G
3	F	903	ATP	C5'-O5'-PA-O1A
3	F	903	ATP	O4'-C4'-C5'-O5'
3	A	903	ATP	C3'-C4'-C5'-O5'
3	B	901	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	C3'-C4'-C5'-O5'
3	D	903	ATP	C3'-C4'-C5'-O5'
3	E	901	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	C3'-C4'-C5'-O5'
3	F	903	ATP	C3'-C4'-C5'-O5'
3	A	901	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	O4'-C4'-C5'-O5'
3	C	903	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	O4'-C4'-C5'-O5'
3	E	903	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	F	901	ATP	O4'-C4'-C5'-O5'
3	A	903	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	PB-O3A-PA-O5'
3	A	903	ATP	PB-O3A-PA-O5'
3	B	901	ATP	PB-O3A-PA-O5'
3	B	903	ATP	PB-O3A-PA-O5'
3	C	901	ATP	PB-O3A-PA-O5'
3	C	903	ATP	PB-O3A-PA-O5'
3	D	901	ATP	PB-O3A-PA-O5'
3	D	903	ATP	PB-O3A-PA-O5'
3	E	903	ATP	PB-O3A-PA-O5'
3	F	901	ATP	PB-O3A-PA-O5'
3	F	903	ATP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
3	D	903	ATP	PB-O3B-PG-O1G
3	E	901	ATP	PB-O3B-PG-O2G
3	A	901	ATP	PA-O3A-PB-O2B
3	A	903	ATP	PA-O3A-PB-O2B
3	B	901	ATP	PA-O3A-PB-O2B
3	B	903	ATP	PA-O3A-PB-O2B
3	C	901	ATP	PA-O3A-PB-O2B
3	C	903	ATP	PA-O3A-PB-O2B
3	D	901	ATP	PA-O3A-PB-O2B
3	D	903	ATP	PA-O3A-PB-O2B
3	E	901	ATP	PA-O3A-PB-O2B
3	E	903	ATP	PA-O3A-PB-O2B
3	E	903	ATP	PB-O3A-PA-O1A
3	F	901	ATP	PA-O3A-PB-O2B
3	F	903	ATP	PA-O3A-PB-O2B
3	A	903	ATP	C5'-O5'-PA-O1A
3	B	903	ATP	C5'-O5'-PA-O1A
3	C	901	ATP	C5'-O5'-PA-O1A
3	D	901	ATP	C5'-O5'-PA-O1A
3	D	903	ATP	C5'-O5'-PA-O1A
3	E	901	ATP	C5'-O5'-PA-O1A
3	E	903	ATP	C5'-O5'-PA-O1A
3	F	901	ATP	C5'-O5'-PA-O1A
3	F	903	ATP	PB-O3B-PG-O1G
3	C	903	ATP	PB-O3B-PG-O1G
3	E	903	ATP	PB-O3B-PG-O1G
3	A	903	ATP	PB-O3B-PG-O2G
3	D	901	ATP	PB-O3B-PG-O2G
3	B	903	ATP	PA-O3A-PB-O1B
3	B	903	ATP	PB-O3A-PA-O1A
3	C	903	ATP	PB-O3A-PA-O2A
3	D	903	ATP	PA-O3A-PB-O1B
3	B	903	ATP	PB-O3B-PG-O1G
3	E	901	ATP	PB-O3B-PG-O1G
3	A	903	ATP	PB-O3A-PA-O2A
3	D	901	ATP	PA-O3A-PB-O1B
3	D	901	ATP	PB-O3A-PA-O2A
3	F	901	ATP	PB-O3A-PA-O2A
3	F	903	ATP	PB-O3A-PA-O1A

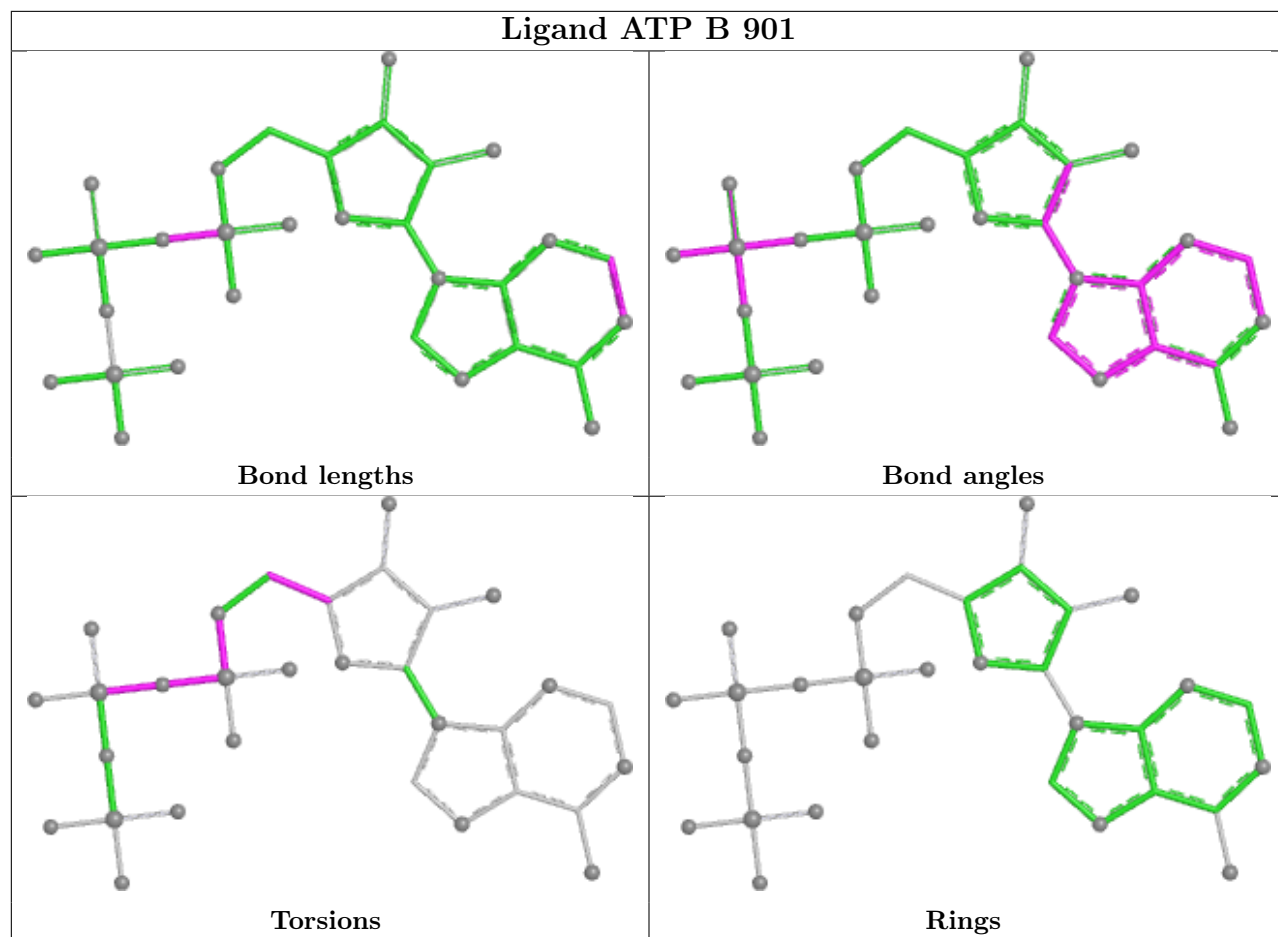
There are no ring outliers.

12 monomers are involved in 41 short contacts:

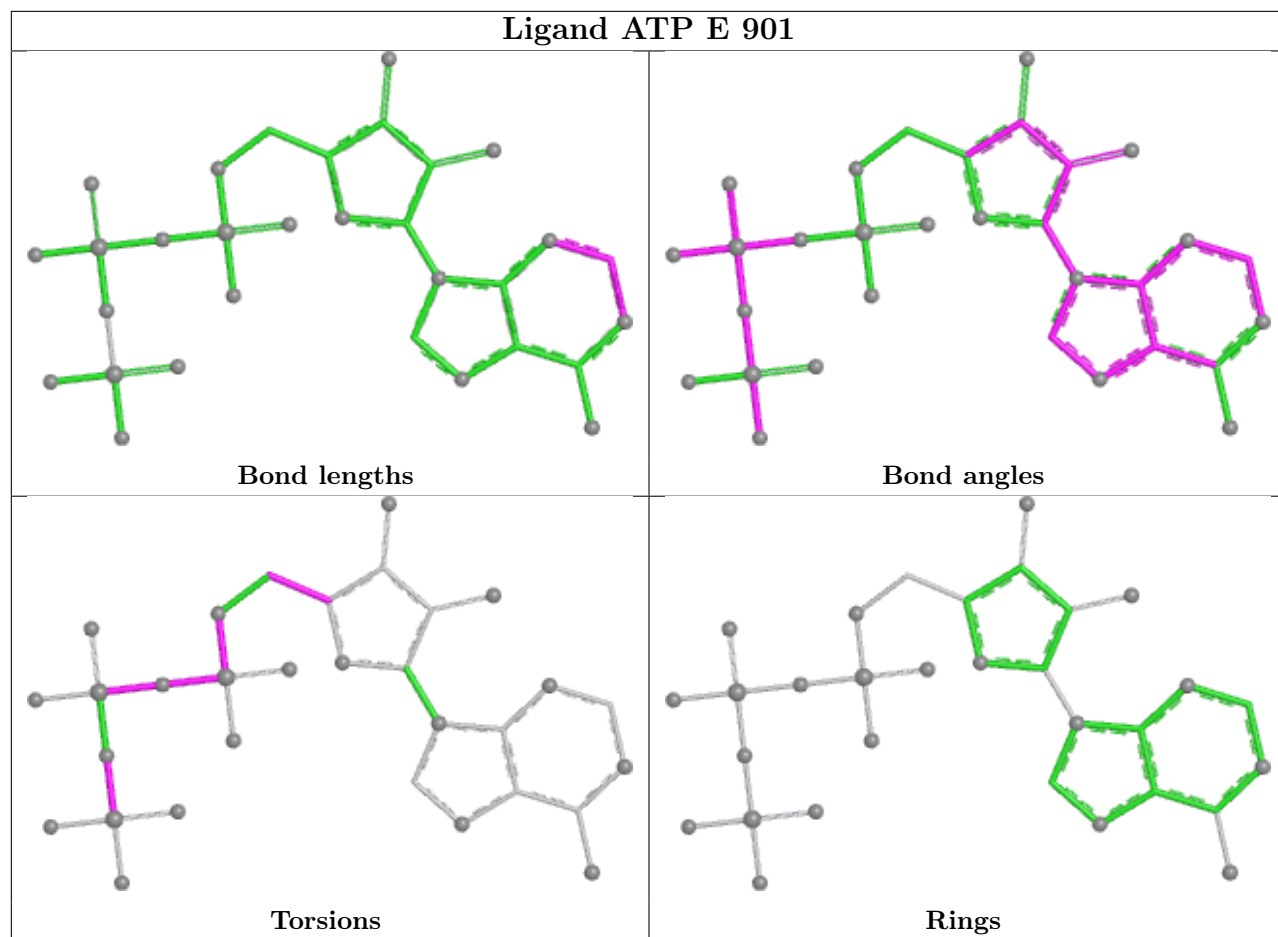
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	ATP	5	0
3	E	901	ATP	6	0
3	A	901	ATP	1	0
3	E	903	ATP	3	0
3	C	901	ATP	4	0
3	D	903	ATP	1	0
3	C	903	ATP	4	0
3	F	903	ATP	1	0
3	B	903	ATP	4	0
3	A	903	ATP	5	0
3	D	901	ATP	4	0
3	F	901	ATP	3	0

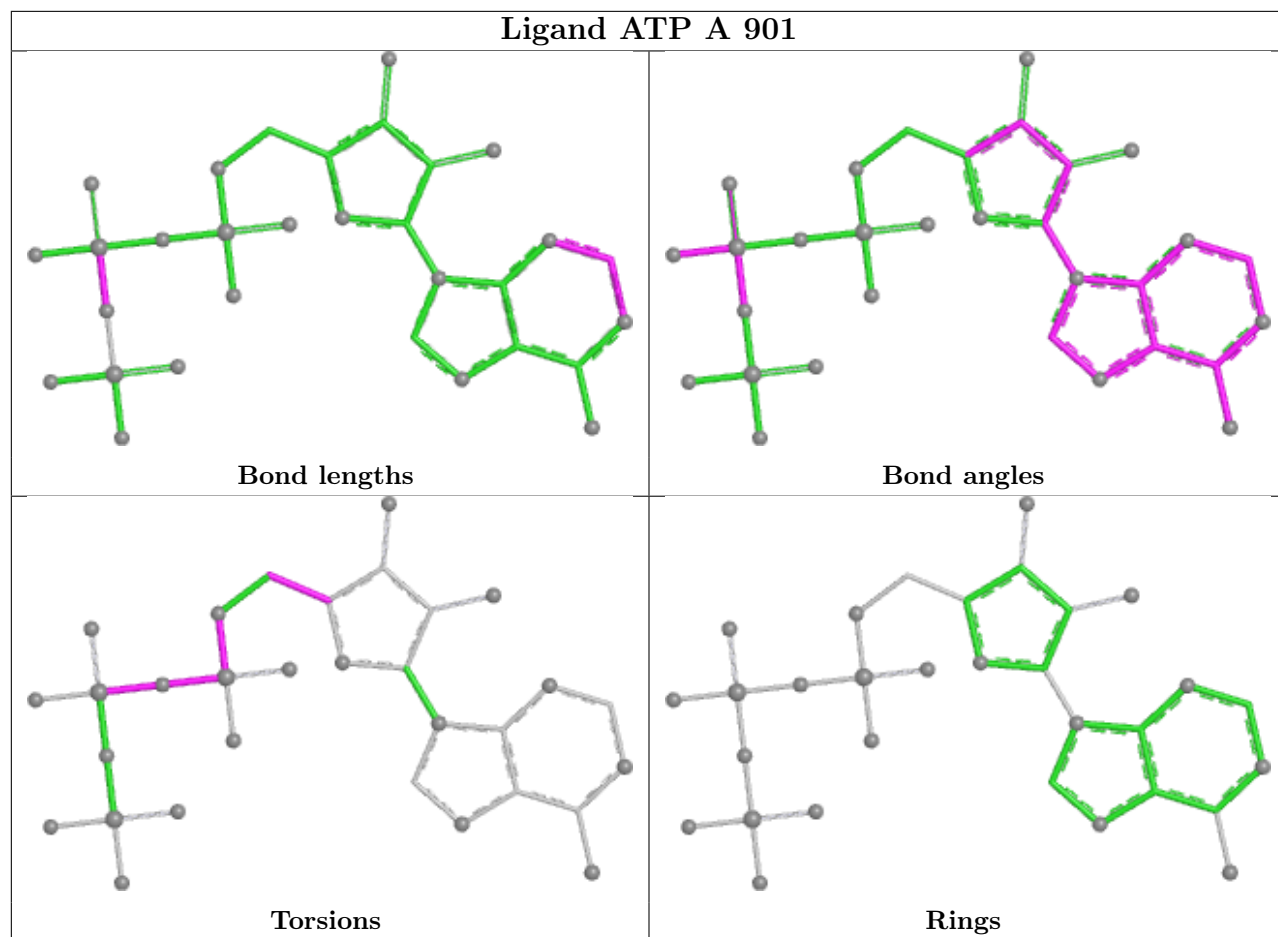
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ATP B 901

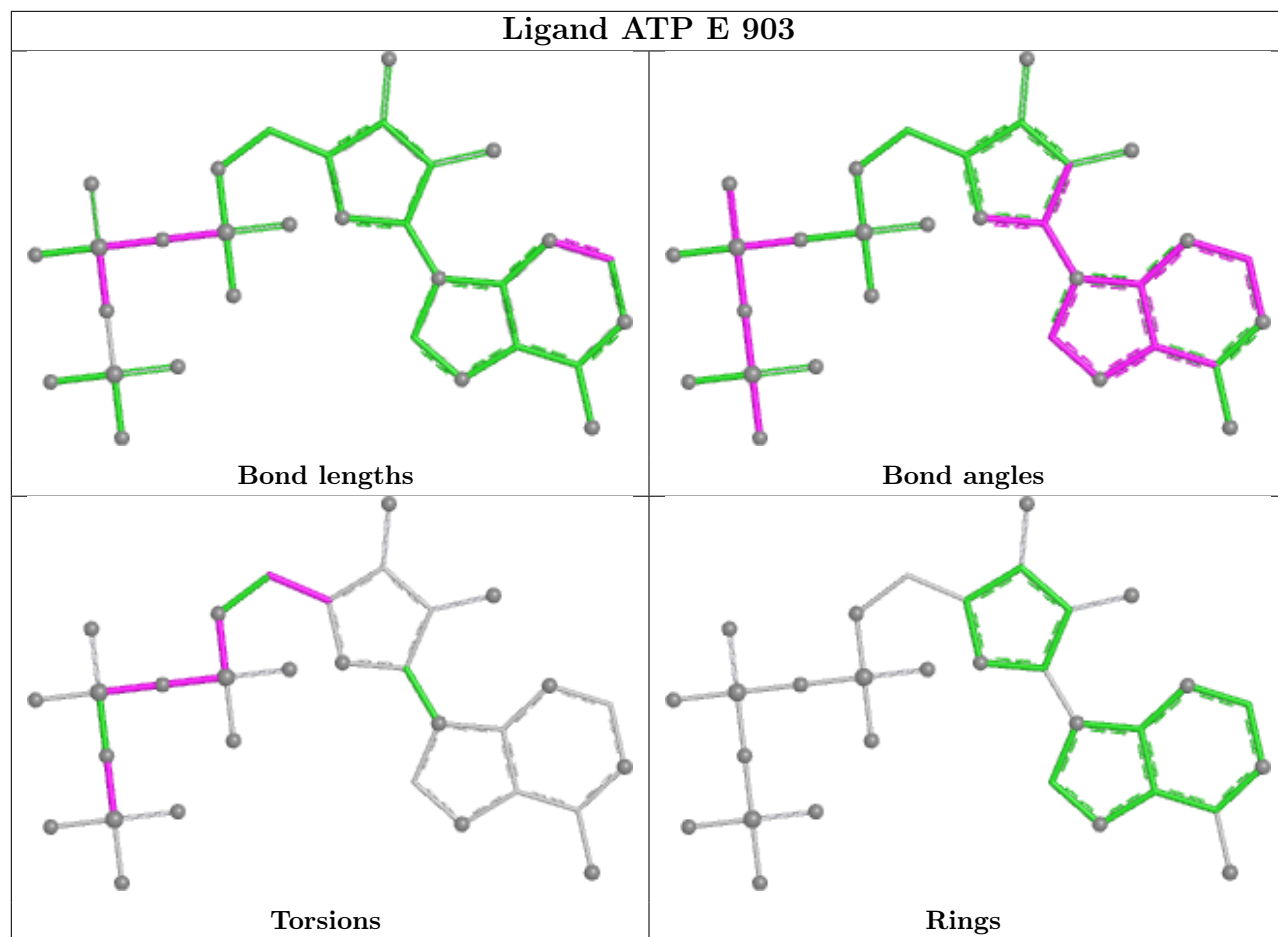


Ligand ATP E 901

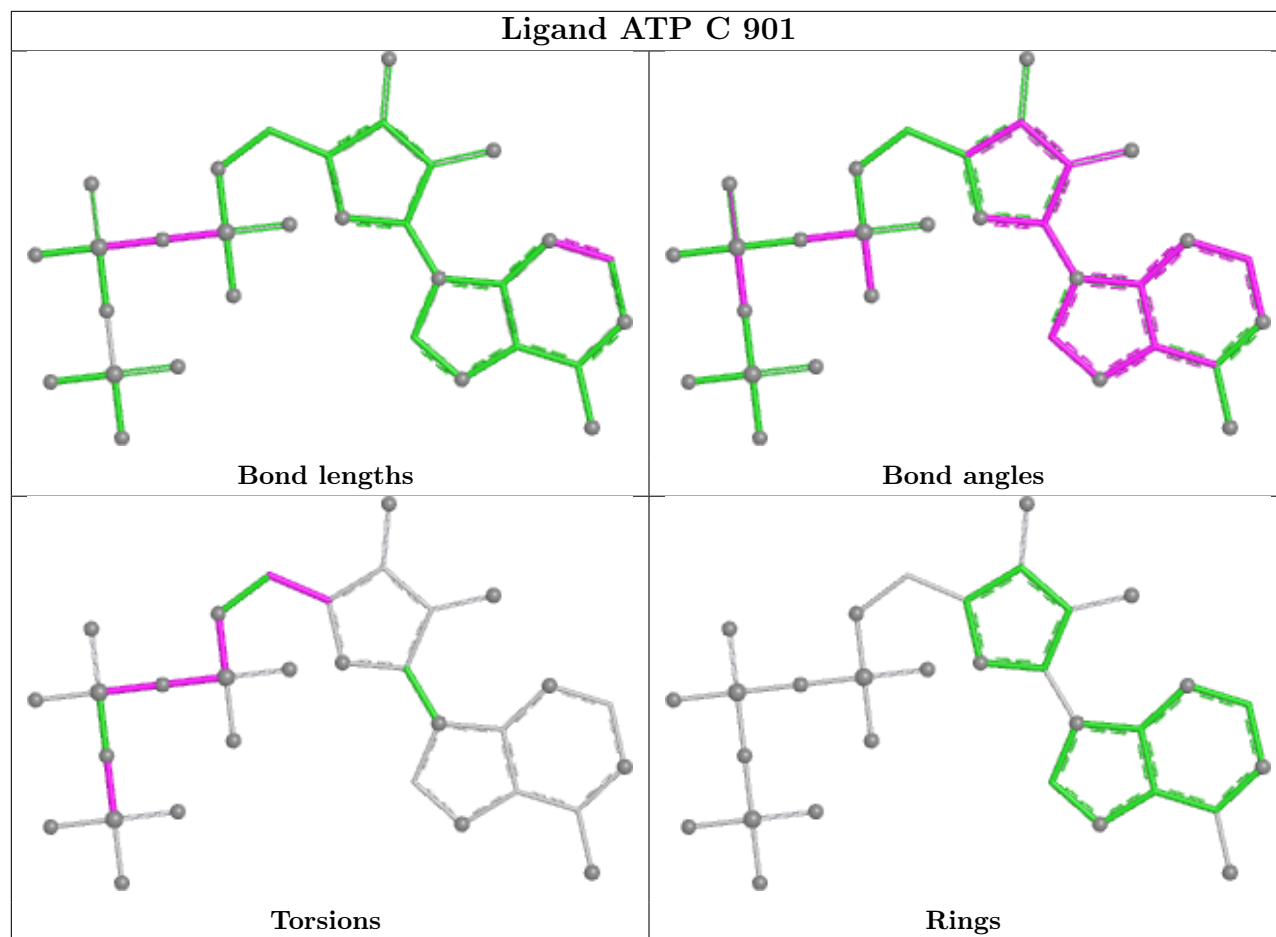




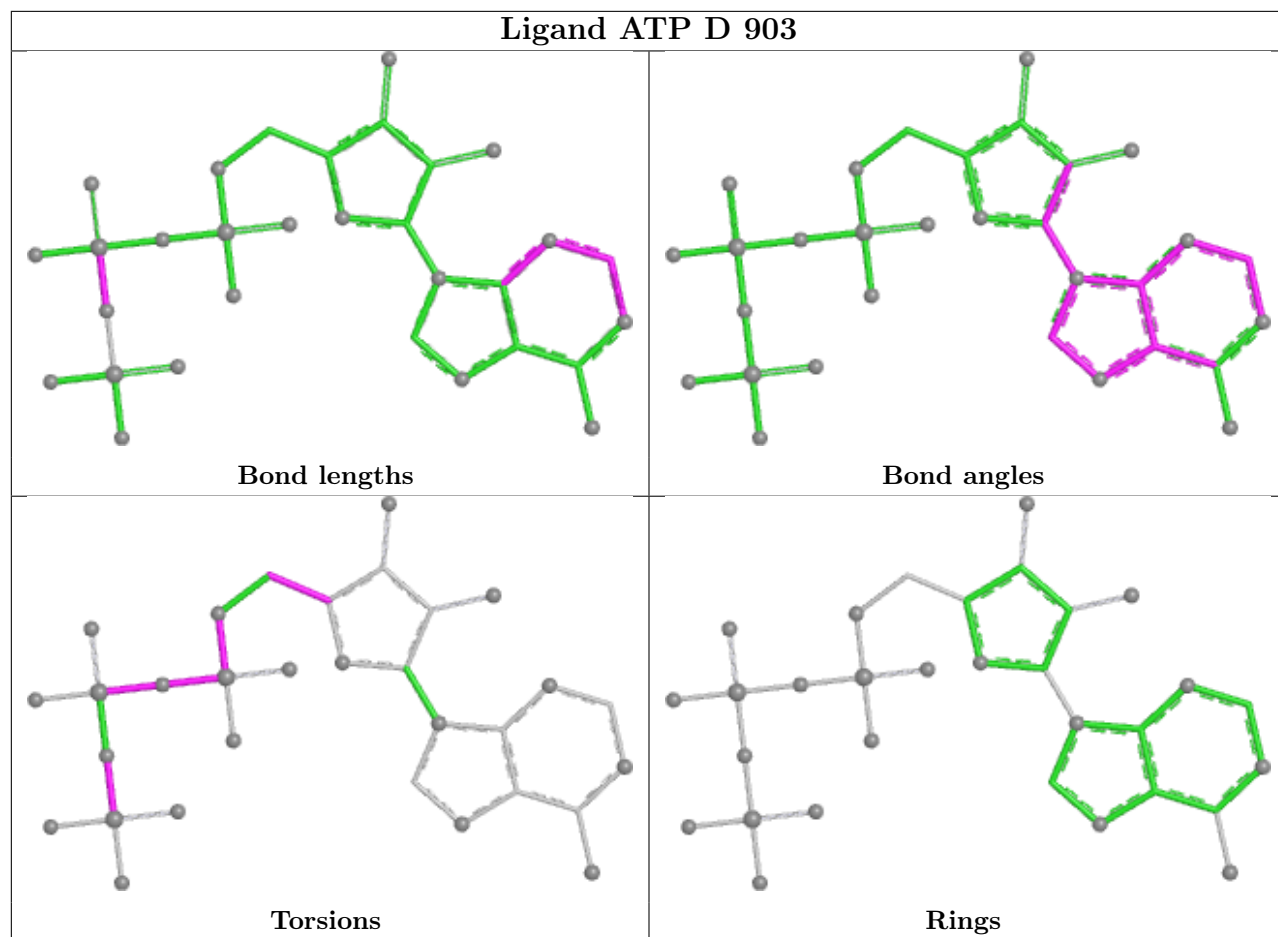
Ligand ATP E 903



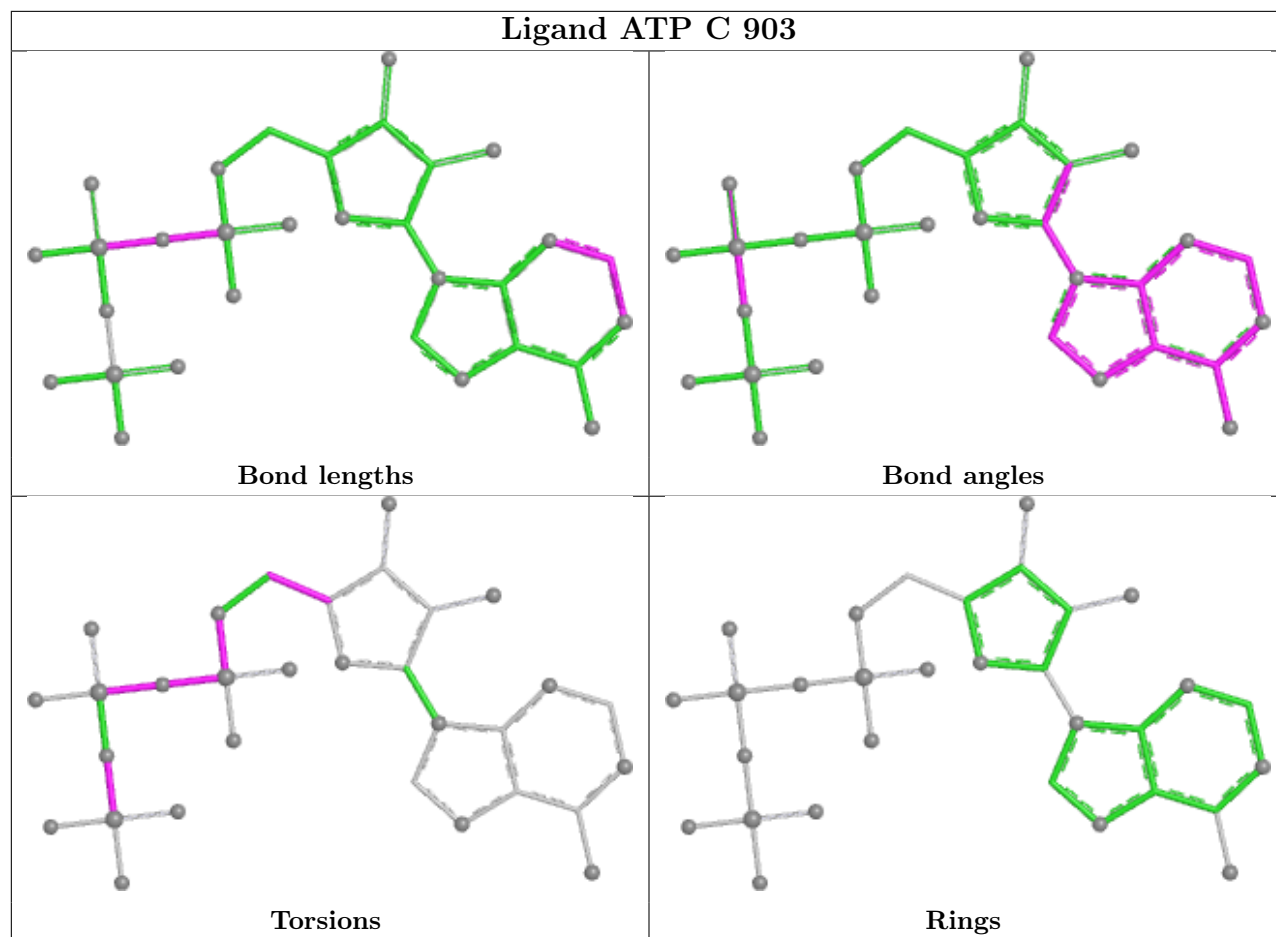
Ligand ATP C 901



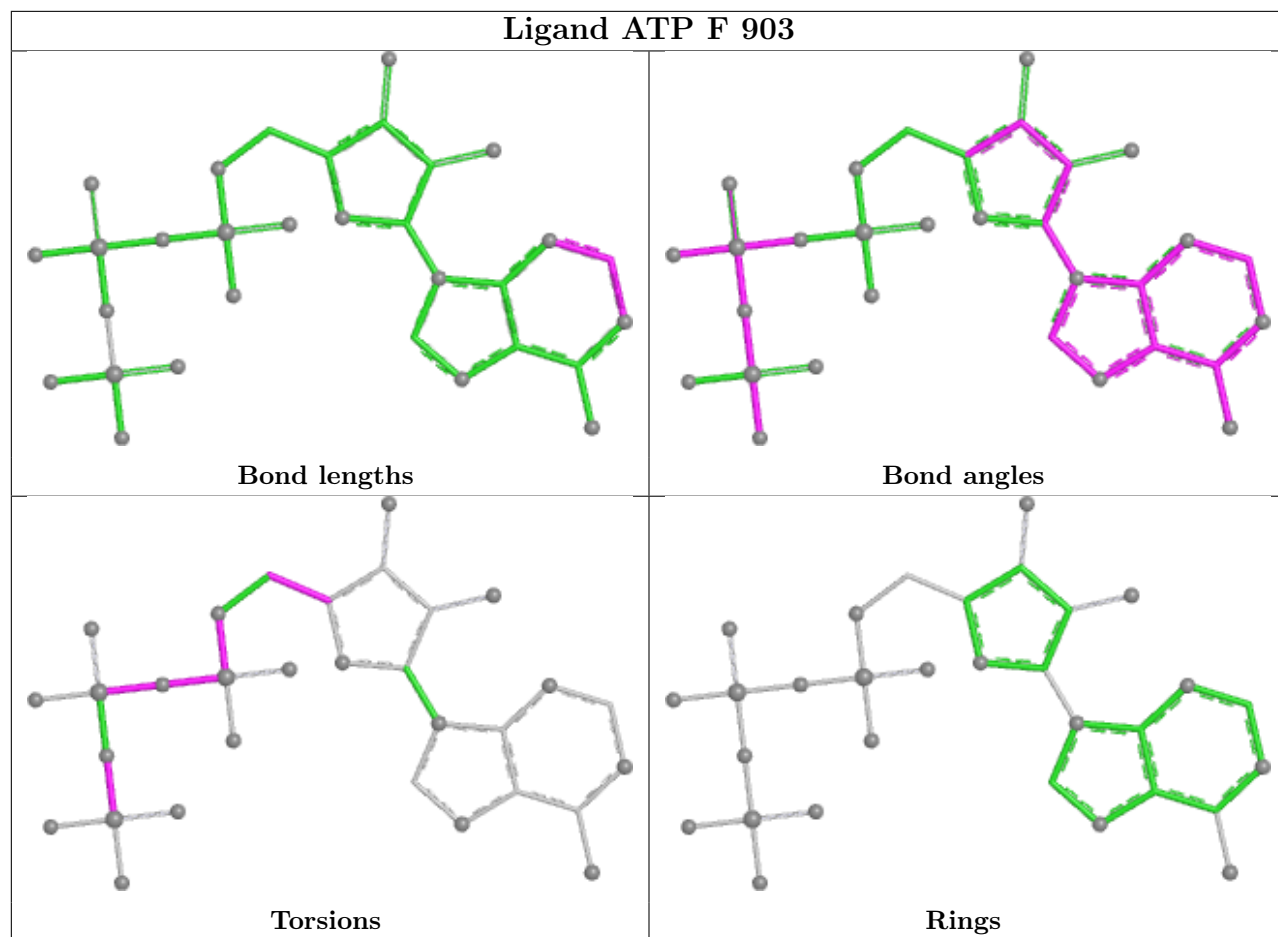
Ligand ATP D 903



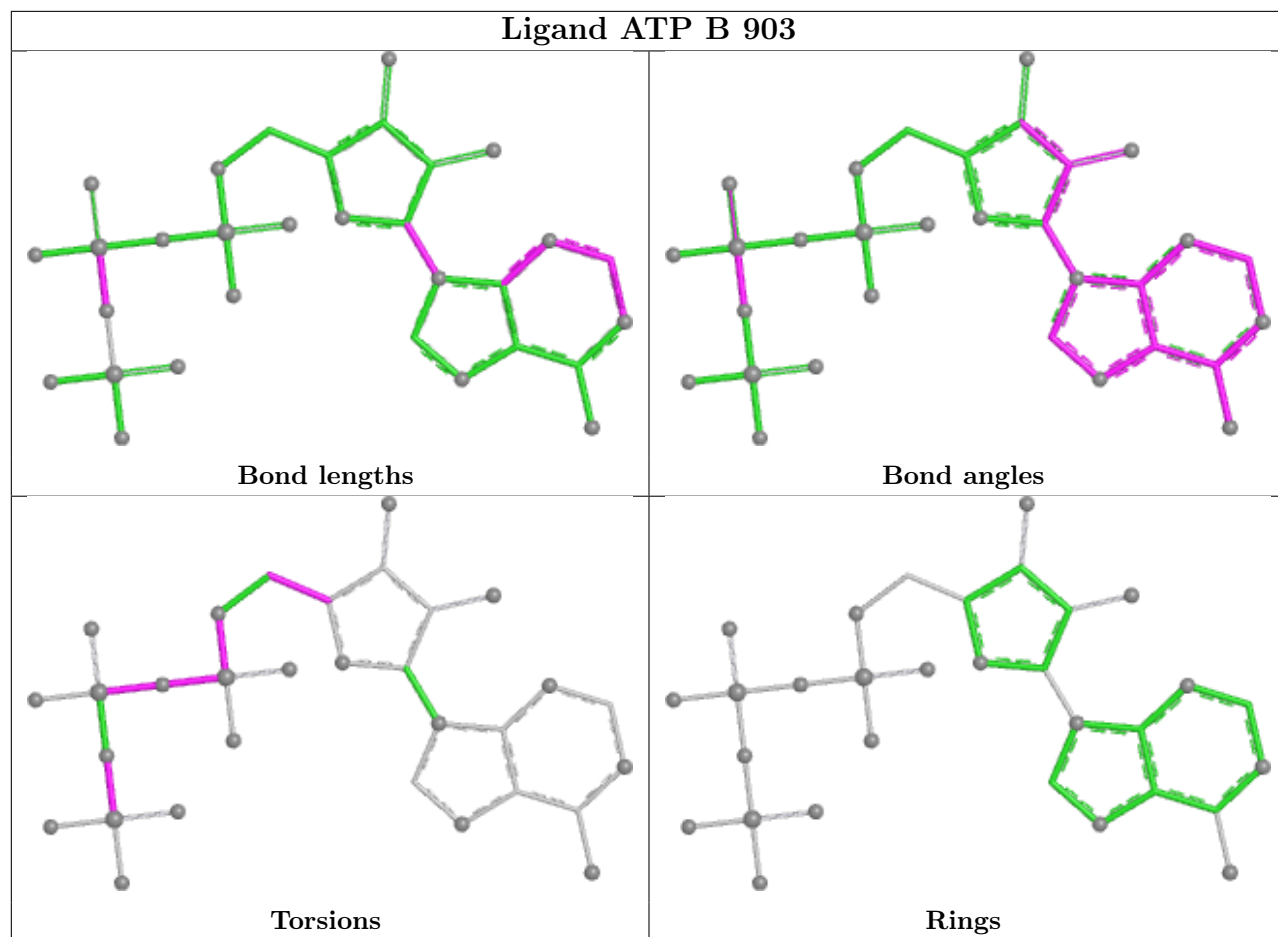
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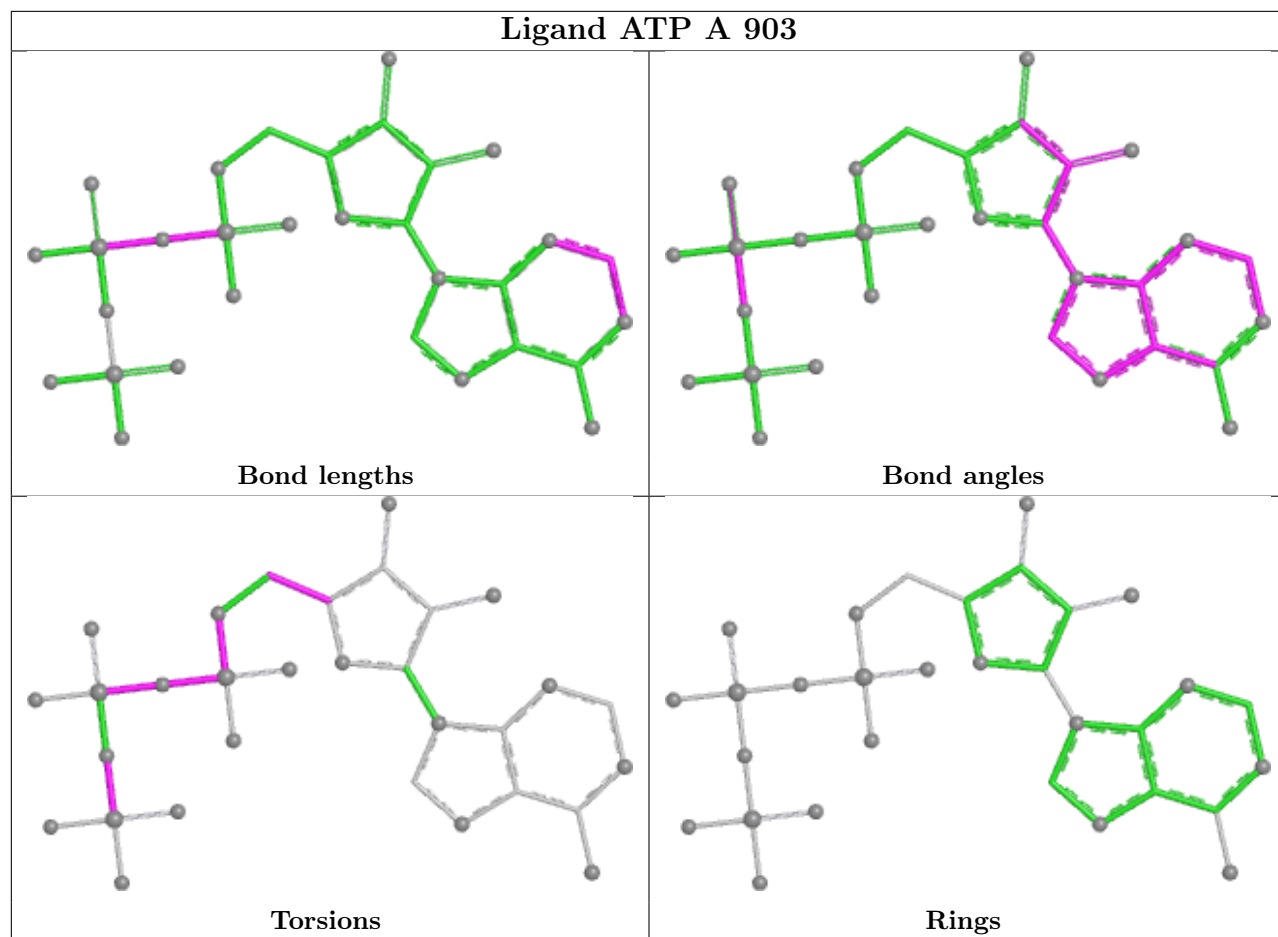
Ligand ATP F 903



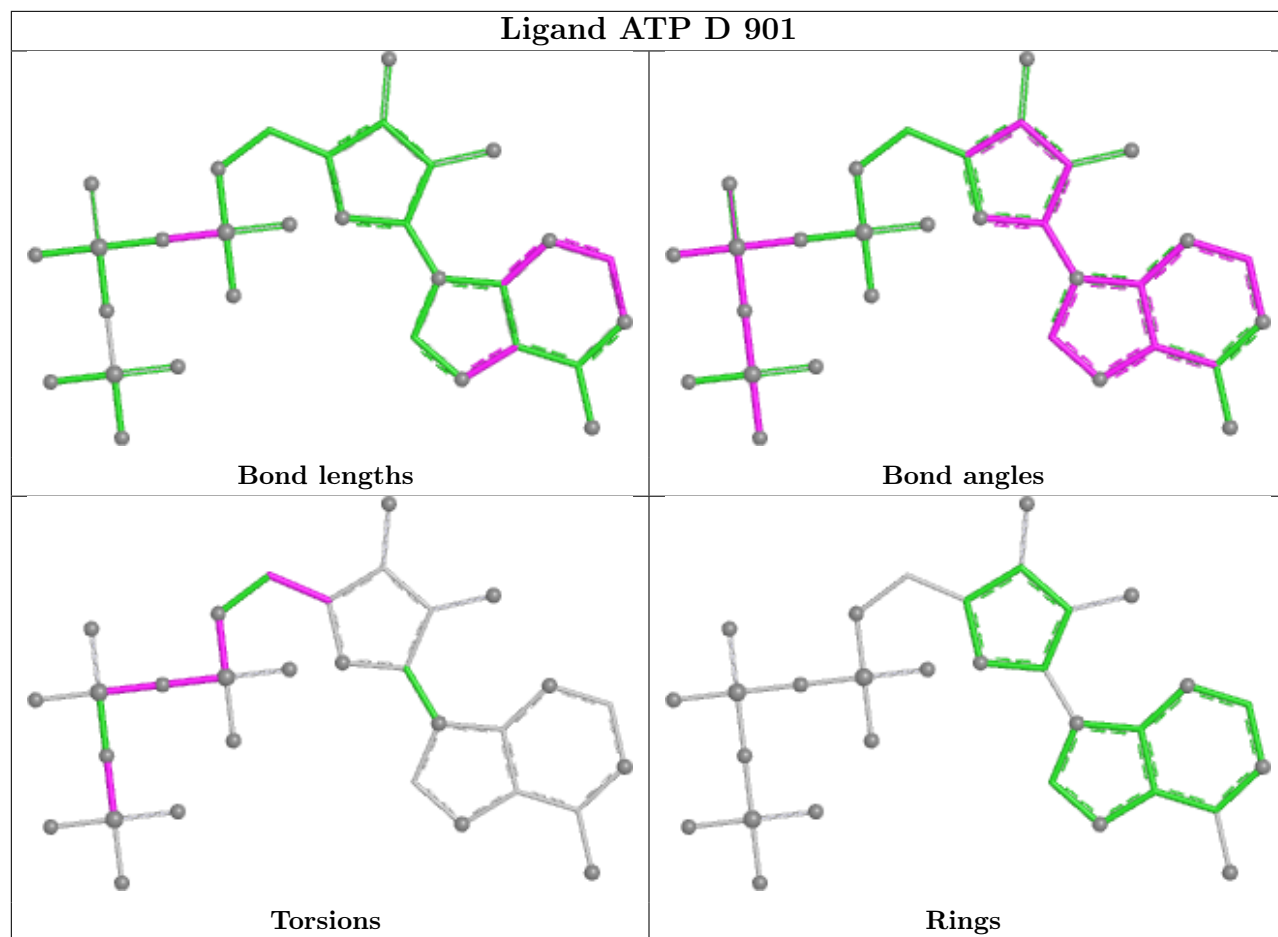
Ligand ATP B 903

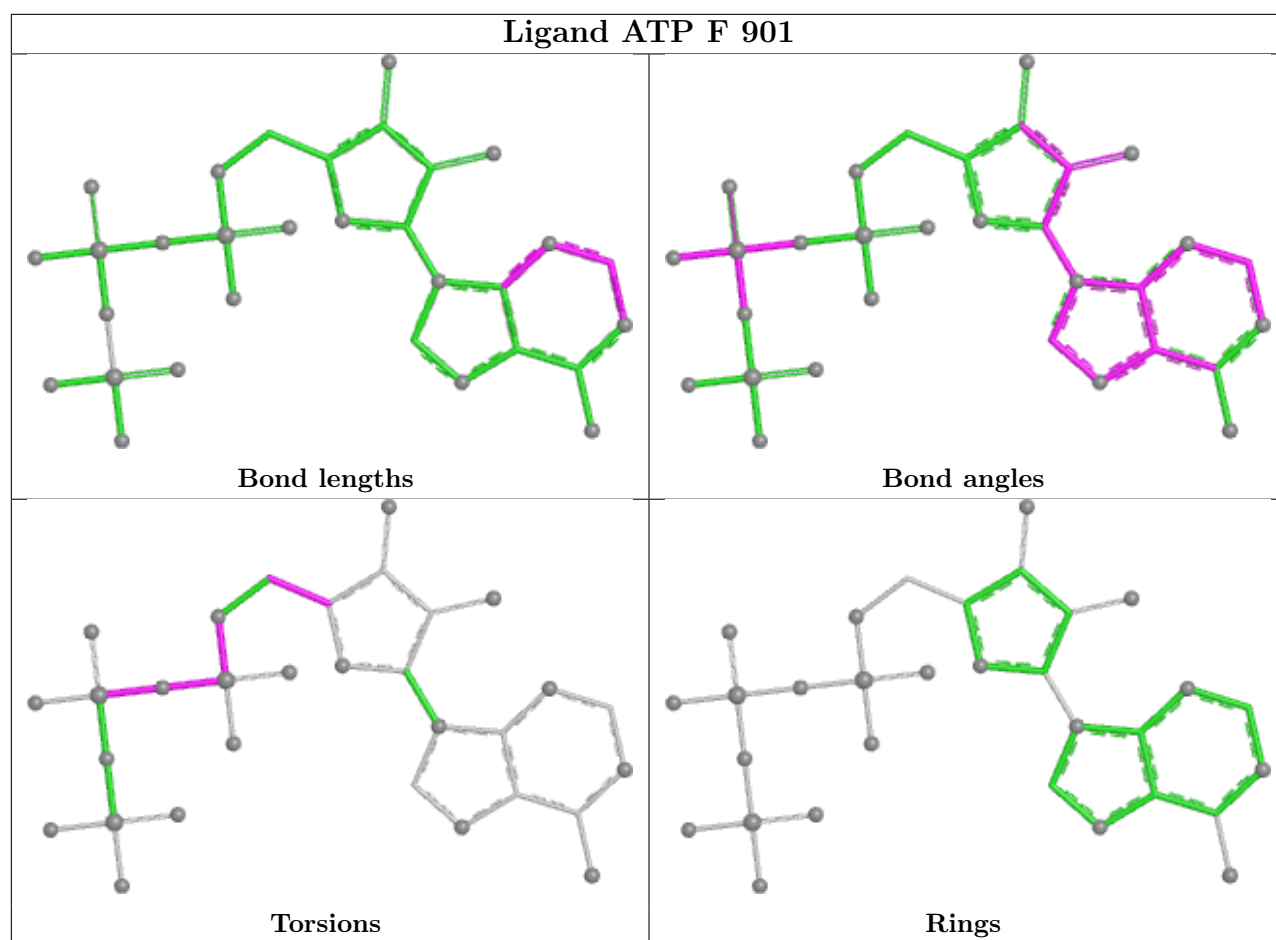


Ligand ATP A 903



Ligand ATP D 901





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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	505/519 (97%)	-0.08	4 (0%) 82 68	20, 75, 128, 156	0
1	B	490/519 (94%)	-0.11	0 100 100	31, 78, 130, 168	0
1	E	491/519 (94%)	-0.43	2 (0%) 88 79	2, 47, 110, 149	0
1	F	505/519 (97%)	-0.33	2 (0%) 88 79	2, 57, 123, 139	0
2	C	488/519 (94%)	-0.25	2 (0%) 88 79	8, 62, 129, 167	0
2	D	485/519 (93%)	-0.49	1 (0%) 91 86	5, 42, 100, 152	0
All	All	2964/3114 (95%)	-0.28	11 (0%) 88 79	2, 62, 126, 168	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	249	LEU	3.4
2	D	249	LEU	2.8
1	E	425	ILE	2.4
1	F	517	PRO	2.4
1	A	117	VAL	2.4
1	A	428	SER	2.2
1	E	505	LEU	2.2
1	A	350	TYR	2.1
1	F	425	ILE	2.0
1	A	518	GLU	2.0
2	C	18	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	F	426	11/12	0.59	0.20	67,68,79,81	0
1	TPO	A	426	11/12	0.79	0.15	74,77,78,78	0
1	TPO	E	426	11/12	0.80	0.20	75,89,101,102	0
1	TPO	B	426	11/12	0.83	0.20	79,85,91,92	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	702	1/1	0.84	0.11	76,76,76,76	0
4	MG	B	701	1/1	0.84	0.07	49,49,49,49	0
4	MG	F	702	1/1	0.85	0.13	62,62,62,62	0
4	MG	D	702	1/1	0.88	0.08	70,70,70,70	0
4	MG	C	701	1/1	0.88	0.07	69,69,69,69	0
3	ATP	B	903	31/31	0.91	0.08	65,69,75,76	0
4	MG	D	801	1/1	0.91	0.15	72,72,72,72	0
4	MG	B	802	1/1	0.92	0.07	61,61,61,61	0
3	ATP	A	903	31/31	0.92	0.07	57,64,69,70	0
4	MG	C	702	1/1	0.93	0.06	67,67,67,67	0
4	MG	D	701	1/1	0.93	0.09	67,67,67,67	0
4	MG	E	702	1/1	0.93	0.12	70,70,70,70	0
4	MG	F	701	1/1	0.93	0.15	29,29,29,29	0
4	MG	A	520	1/1	0.93	0.09	58,58,58,58	0
3	ATP	E	901	31/31	0.94	0.08	35,63,67,68	0
3	ATP	A	901	31/31	0.94	0.07	65,80,87,88	0
4	MG	E	520	1/1	0.94	0.11	23,23,23,23	0
4	MG	A	802	1/1	0.94	0.11	77,77,77,77	0
4	MG	A	701	1/1	0.94	0.07	70,70,70,70	0
3	ATP	C	903	31/31	0.94	0.07	36,41,67,68	0
3	ATP	F	901	31/31	0.95	0.08	53,79,88,88	0
3	ATP	B	901	31/31	0.95	0.06	42,47,53,54	0
3	ATP	D	901	31/31	0.96	0.07	38,43,54,55	0
3	ATP	E	903	31/31	0.96	0.07	16,24,41,42	0
3	ATP	D	903	31/31	0.96	0.06	15,19,42,44	0

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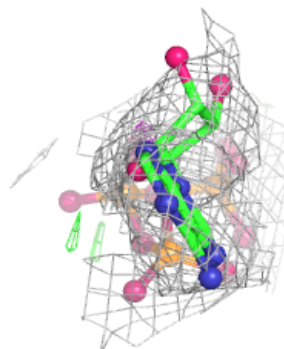
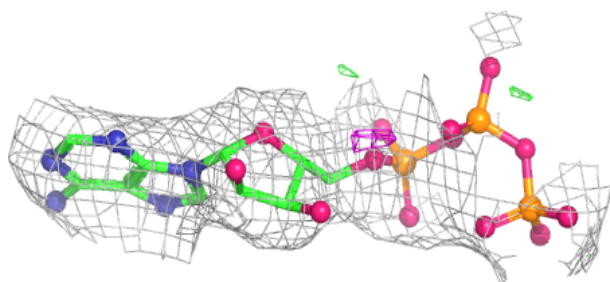
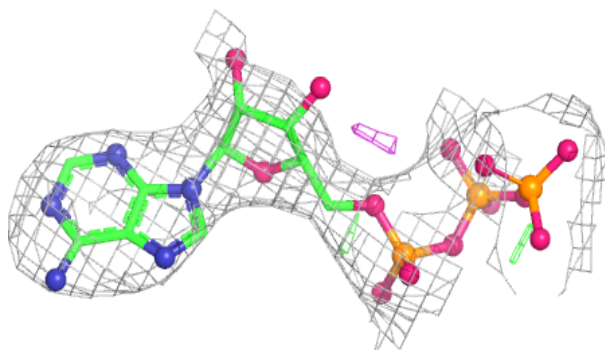
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	F	903	31/31	0.97	0.06	31,36,40,40	0
4	MG	A	801	1/1	0.97	0.06	31,31,31,31	0
4	MG	C	802	1/1	0.97	0.10	19,19,19,19	0
3	ATP	C	901	31/31	0.98	0.06	24,28,38,40	0
4	MG	B	801	1/1	0.98	0.04	10,10,10,10	0
4	MG	F	802	1/1	0.98	0.07	21,21,21,21	0
4	MG	C	801	1/1	1.00	0.06	6,6,6,6	0
4	MG	E	801	1/1	1.00	0.02	1,1,1,1	0
4	MG	D	802	1/1	1.00	0.05	1,1,1,1	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.

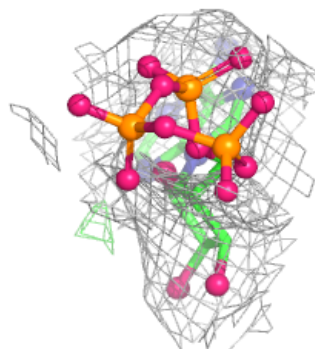
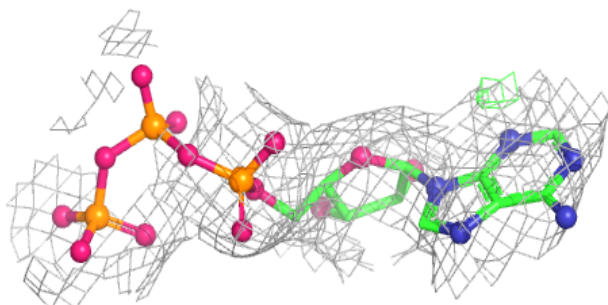
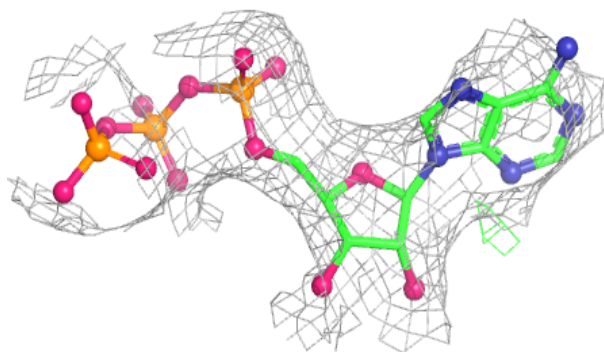
Electron density around ATP B 903:

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

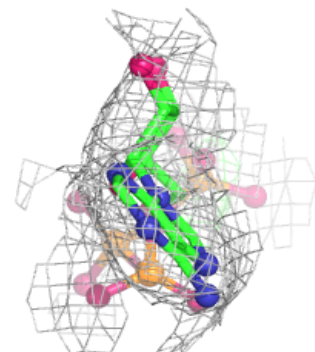
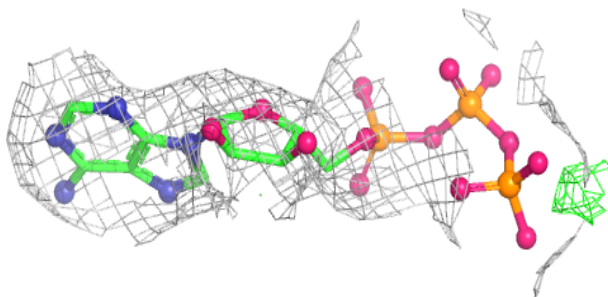
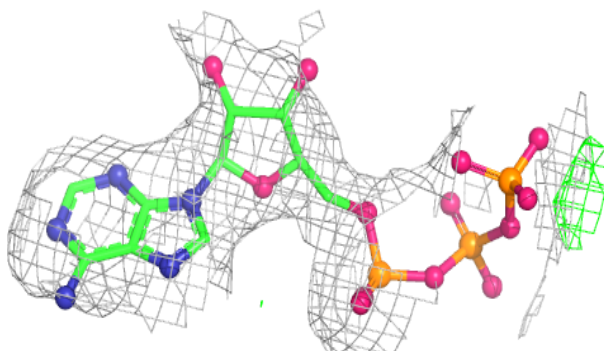


Electron density around ATP A 903:

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and green (positive)

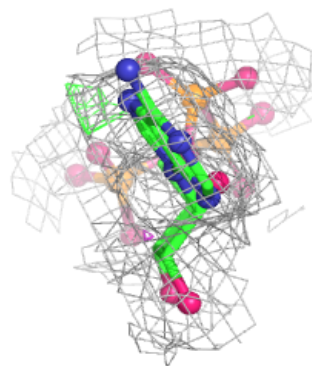
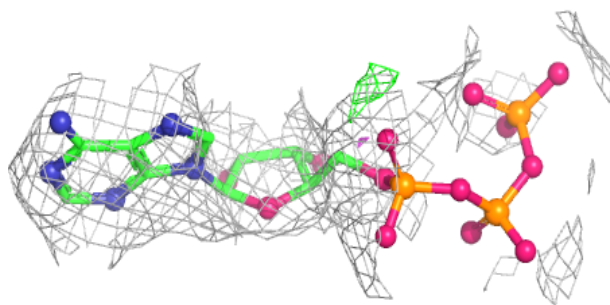
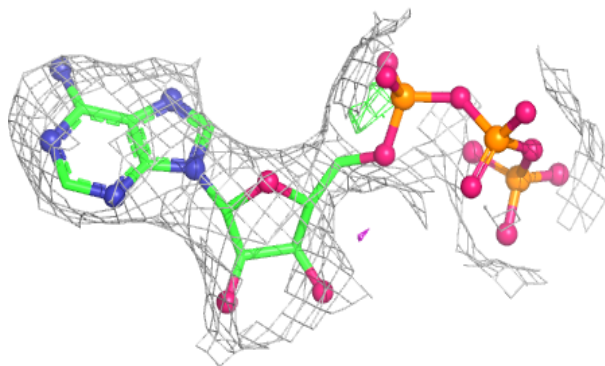
**Electron density around ATP E 901:**

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and green (positive)

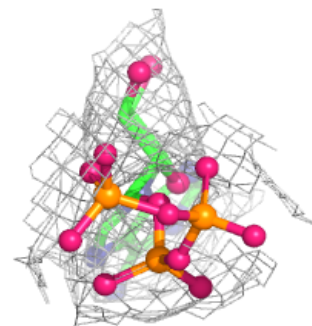
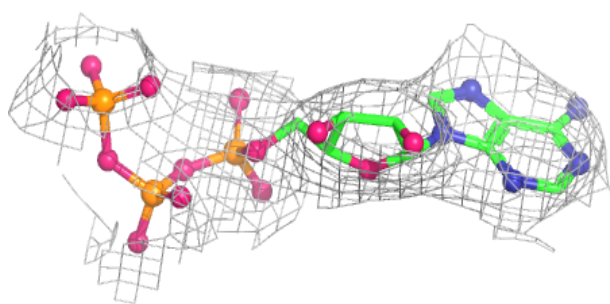
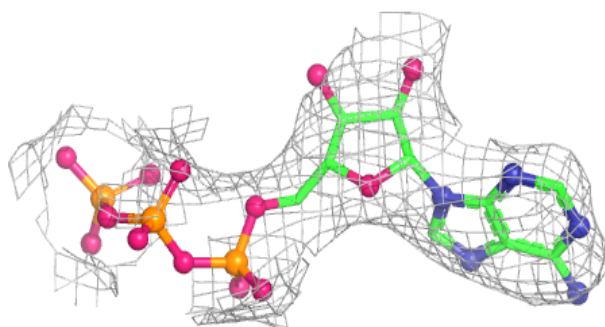


Electron density around ATP A 901:

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and green (positive)

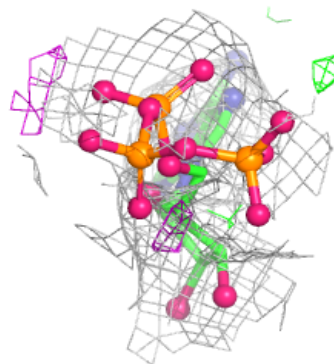
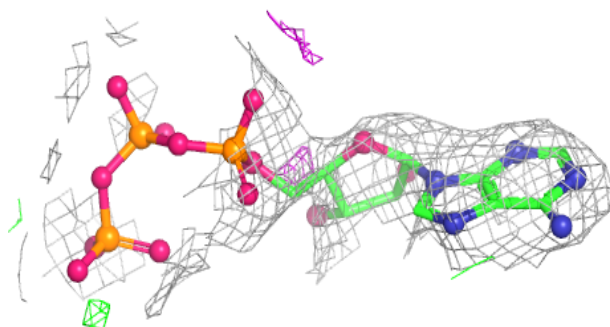
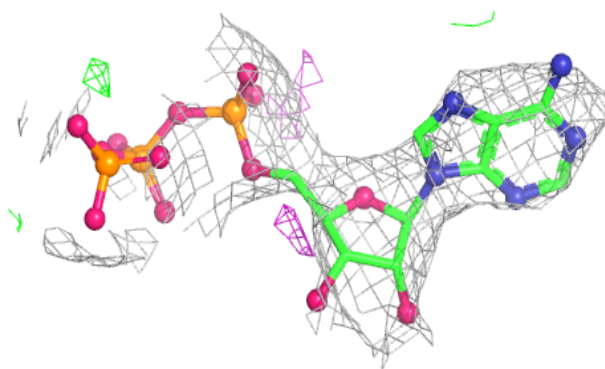
**Electron density around ATP C 903:**

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and green (positive)

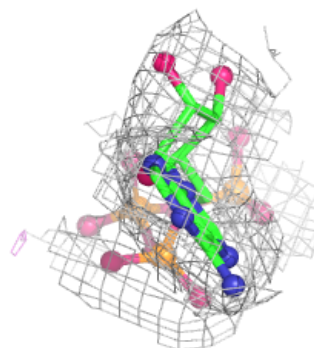
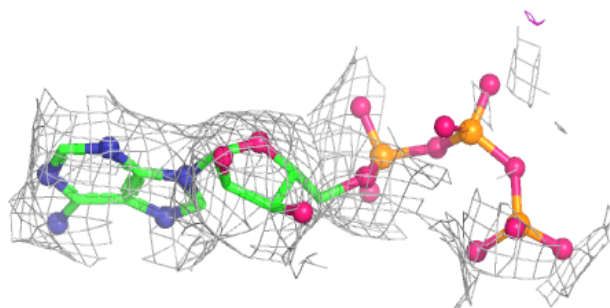
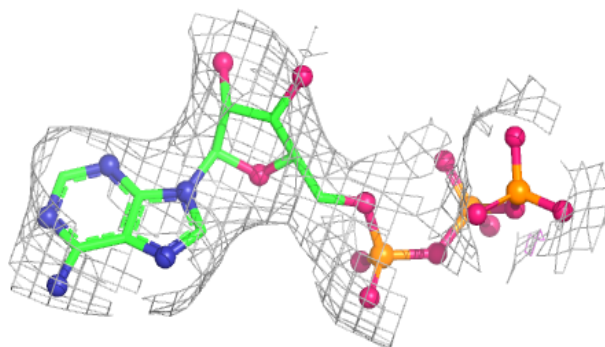


Electron density around ATP F 901:

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and green (positive)

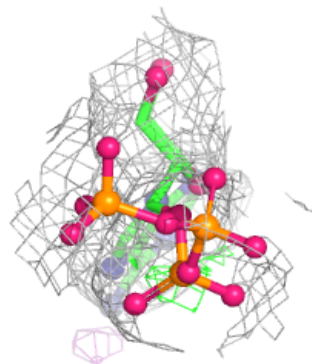
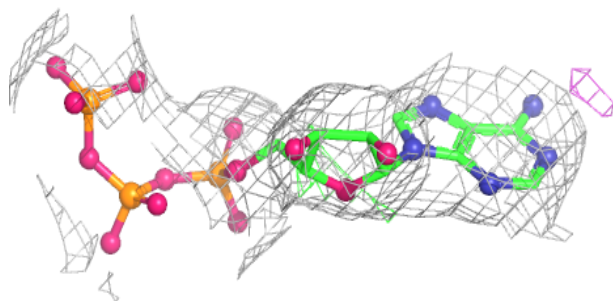
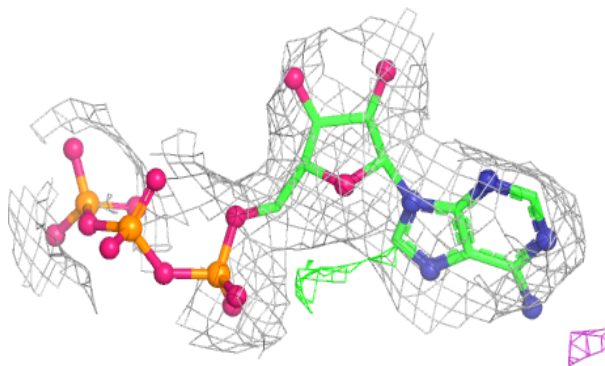
**Electron density around ATP B 901:**

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and green (positive)

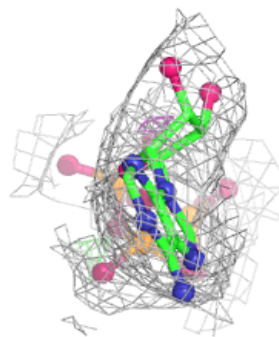
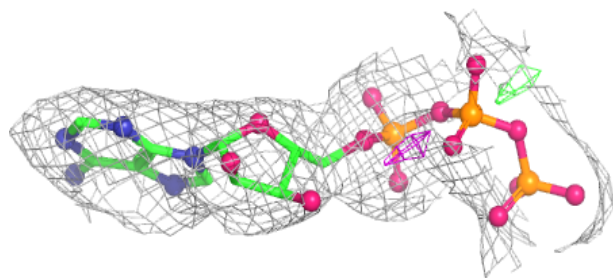
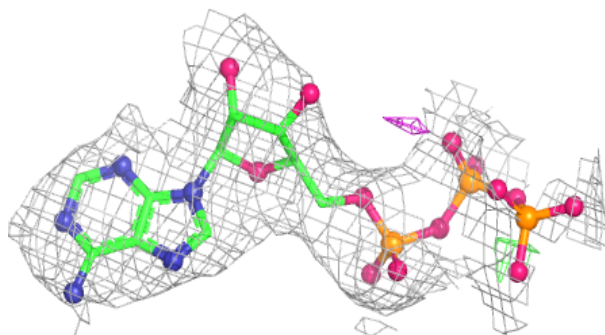


Electron density around ATP D 901:

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and green (positive)

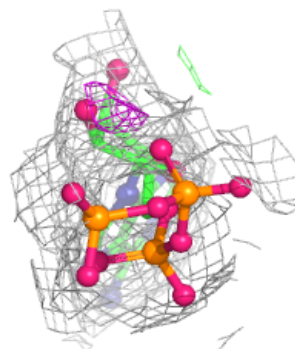
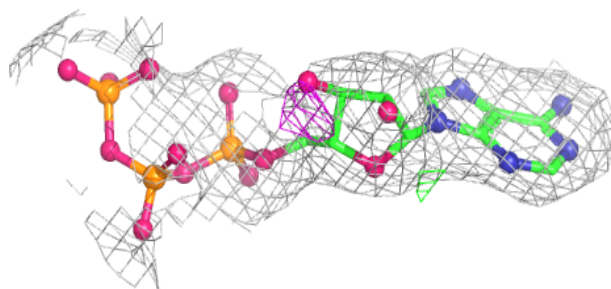
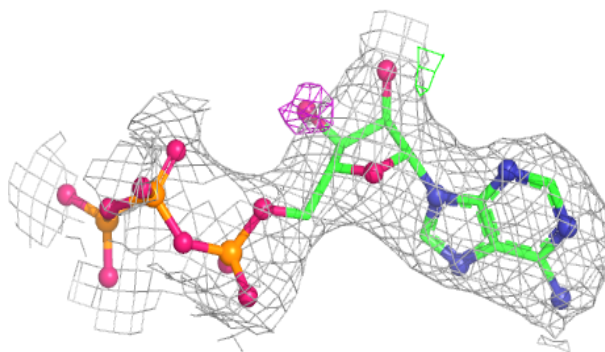
**Electron density around ATP E 903:**

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and green (positive)

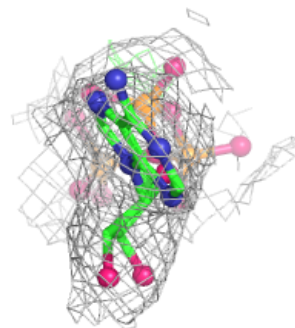
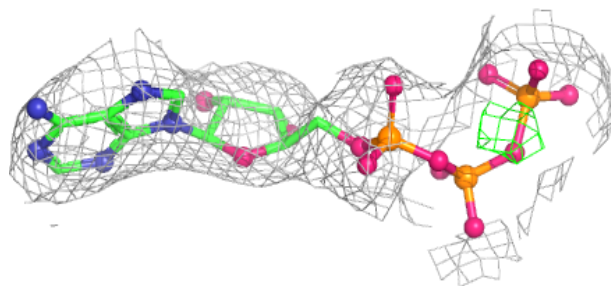
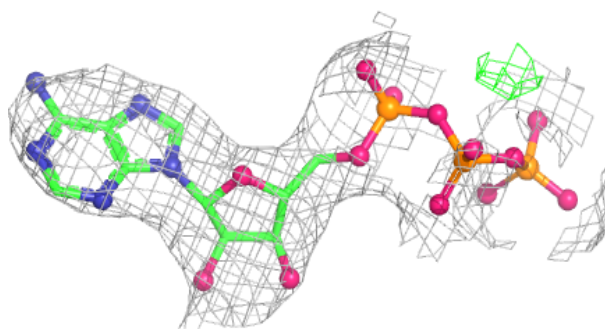


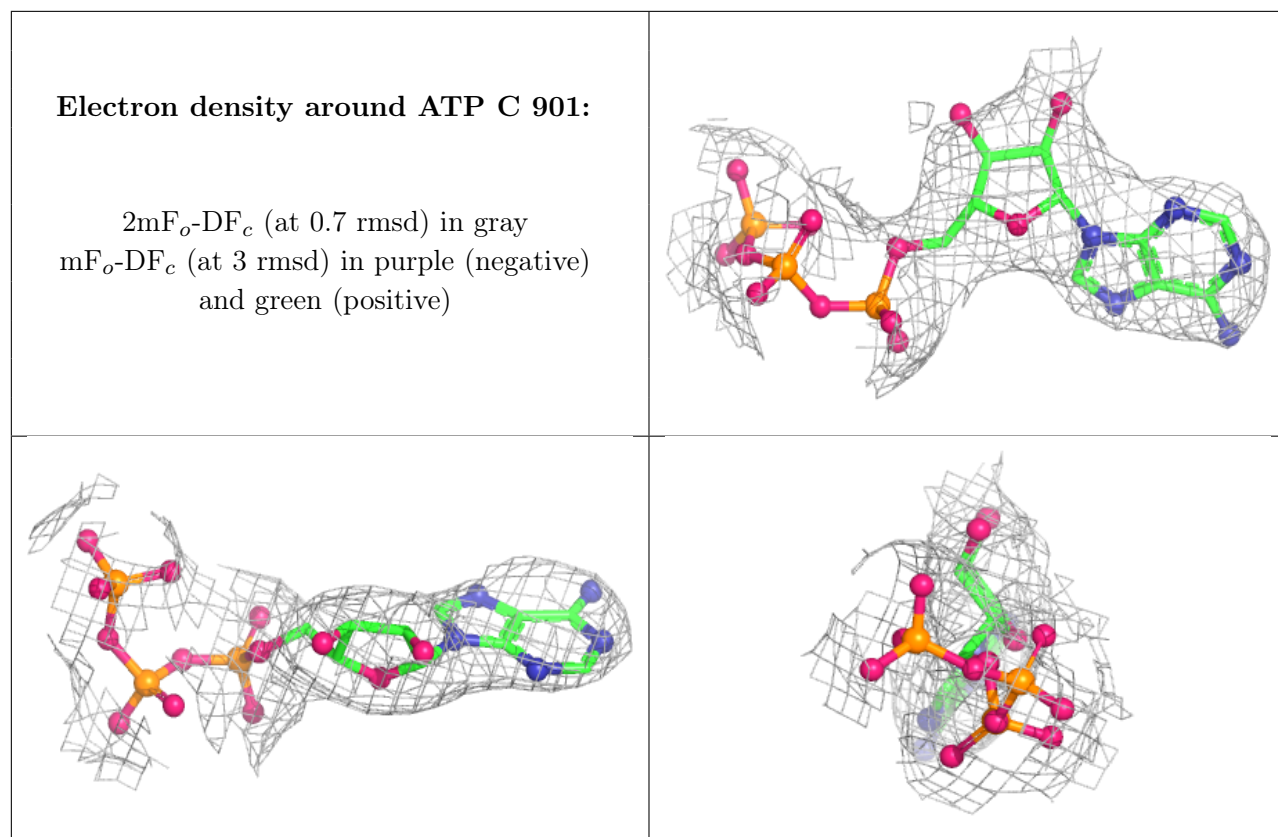
Electron density around ATP D 903:

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

**Electron density around ATP F 903:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.