Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:12 am BST

PDB ID	:	1OJL
Title	:	Crystal structure of a sigma54-activator suggests the mechanism for the conformational switch necessary for sigma54 binding
Authors	:	Sallai, L.; Tucker, P.A.
Deposited on	:	2003-07-10
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

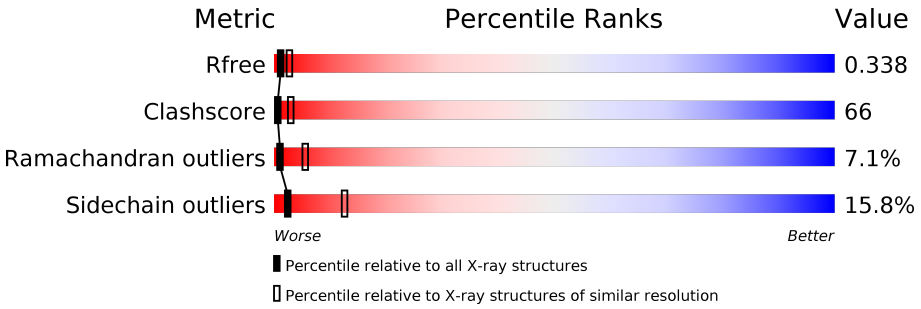
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	304	31% 49% 14% • •
1	B	304	22% 45% 13% • 17%
1	C	304	23% 42% 17% • 17%
1	D	304	32% 50% 14% • •
1	E	304	26% 47% 17% • 6%
1	F	304	19% 45% 15% • 19%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	C	1391	-	-	X	-
2	PO4	D	1442	-	-	X	-
2	PO4	F	1390	-	-	X	-
3	ATP	E	1442	-	-	X	-

2 Entry composition

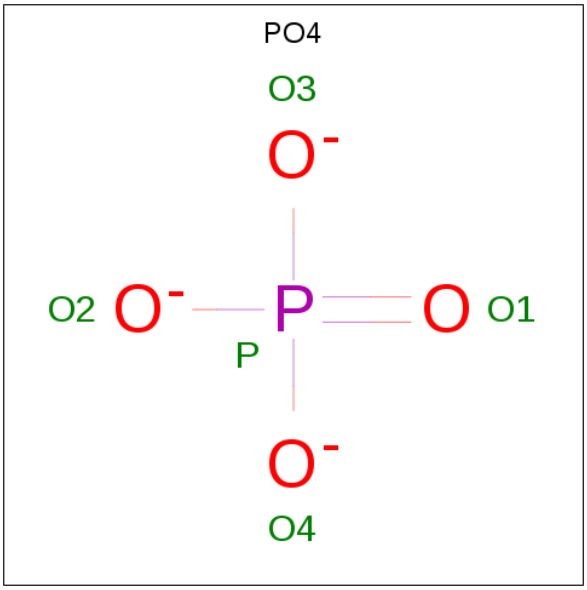
There are 4 unique types of molecules in this entry. The entry contains 12594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSCRIPTIONAL REGULATORY PROTEIN ZRAR.

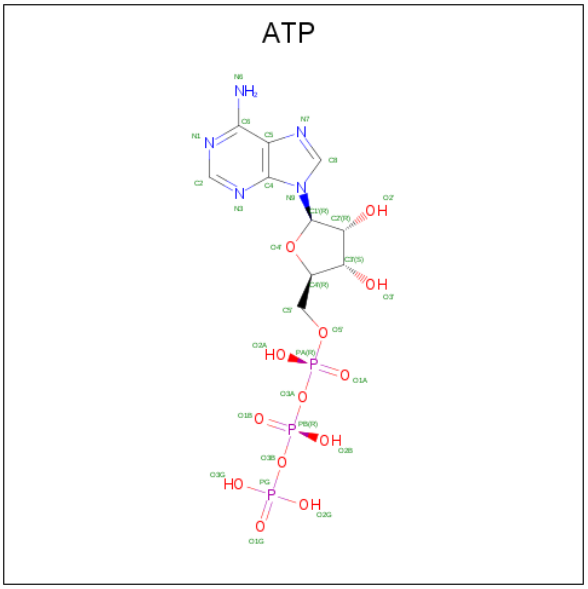
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2234	1396	407	423	8			
1	B	251	Total	C	N	O	S	0	0	0
			1929	1201	357	363	8			
1	C	252	Total	C	N	O	S	0	0	0
			1925	1199	355	363	8			
1	D	297	Total	C	N	O	S	0	0	0
			2270	1416	418	428	8			
1	E	285	Total	C	N	O	S	0	0	0
			2183	1363	400	412	8			
1	F	247	Total	C	N	O	S	0	0	0
			1895	1183	347	357	8			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	0	0
4	B	20	Total O 20 20	0	0
4	C	16	Total O 16 16	0	0

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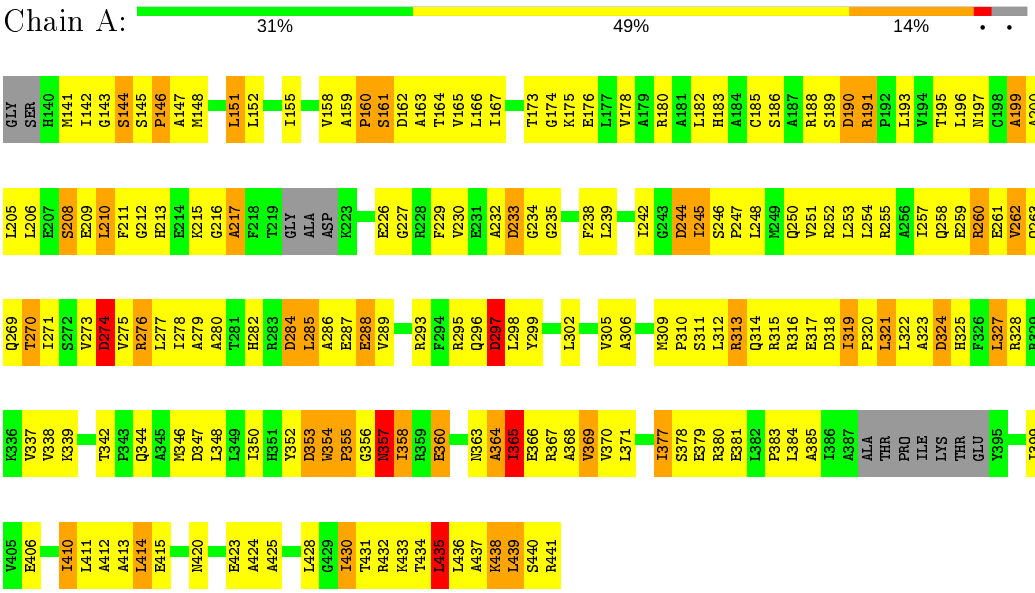
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	23	Total O 23 23	0	0
4	E	17	Total O 17 17	0	0
4	F	10	Total O 10 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

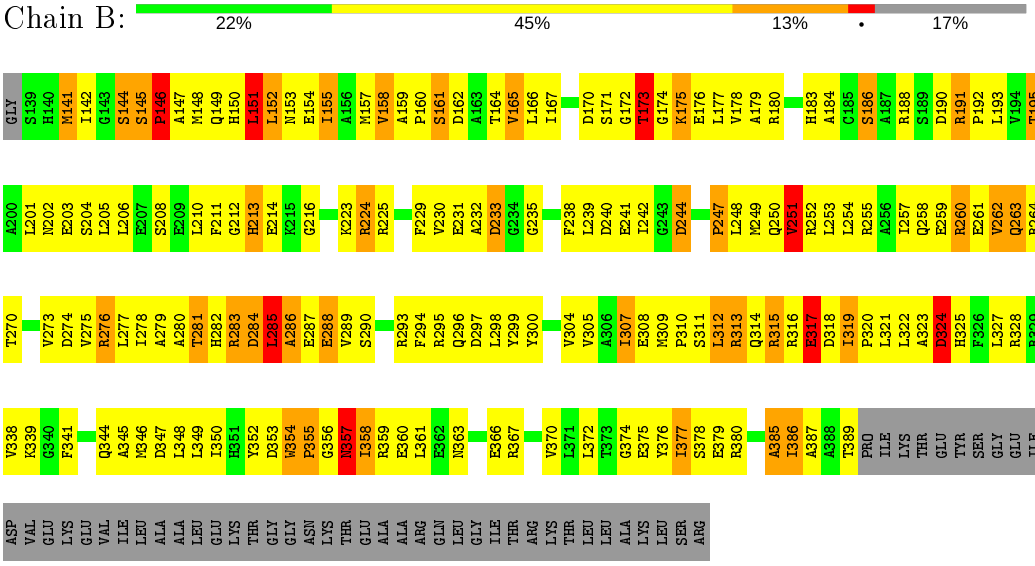
- Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN ZRAR

Chain A:



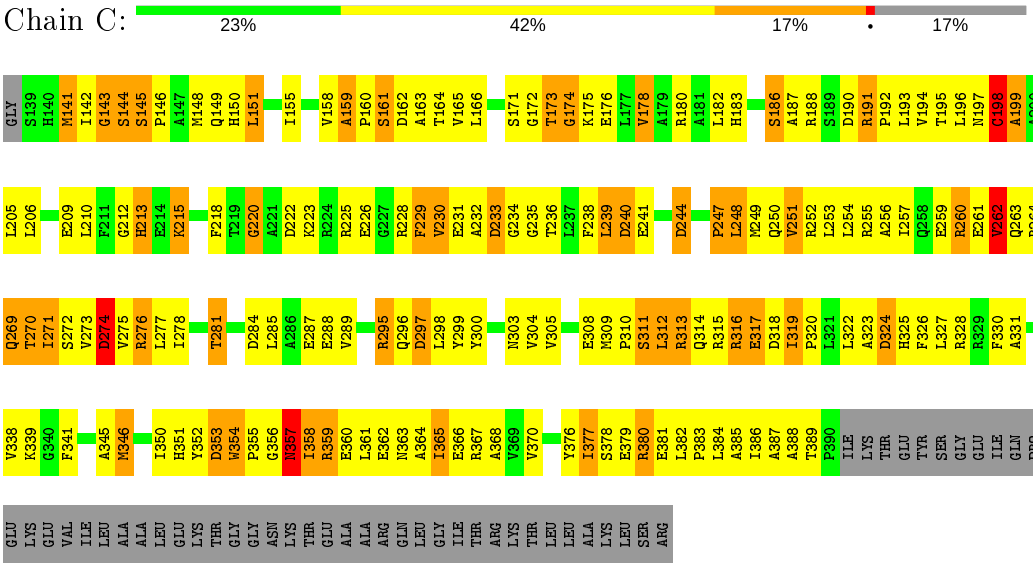
- Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN ZRAR

Chain B:



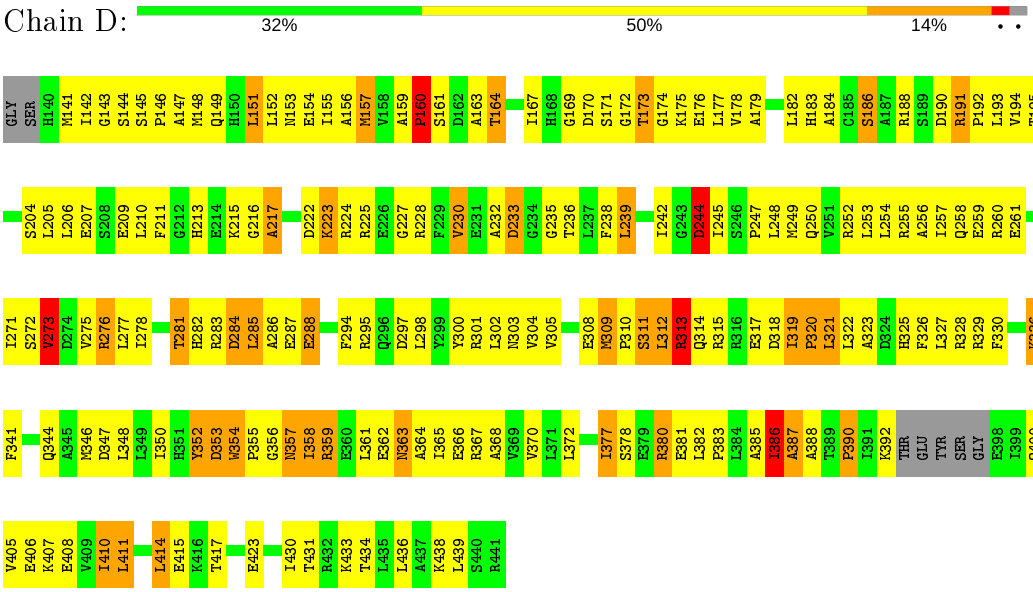
- Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN ZRAR

Chain C:



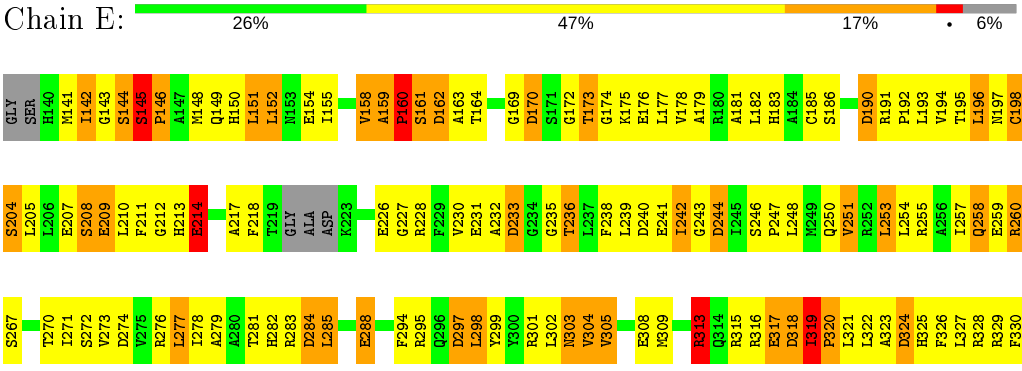
• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN ZRAR

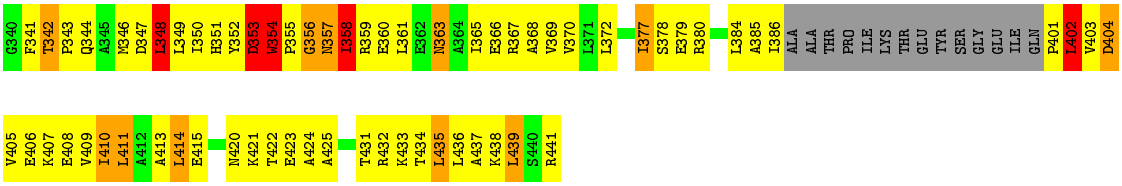
Chain D:



• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN ZRAR

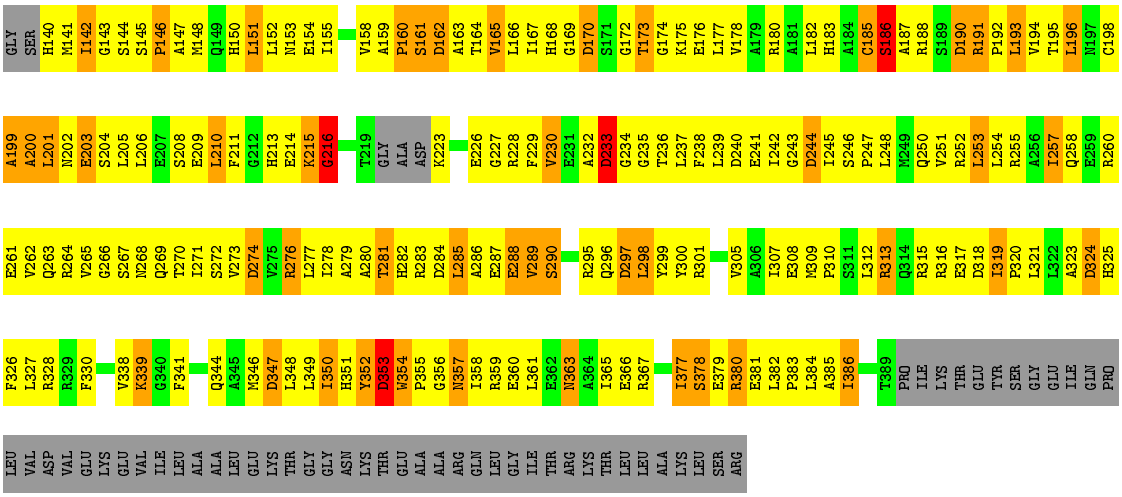
Chain E:





- Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN ZRAR

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.44Å 114.74Å 187.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-3.00) 97.7 (29.68-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.252 , 0.308 0.295 , 0.338	Depositor DCC
R_{free} test set	2290 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	85.4	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12594	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.92	3/2262 (0.1%)	1.19	18/3058 (0.6%)
1	B	0.94	1/1956 (0.1%)	1.28	27/2646 (1.0%)
1	C	0.83	1/1953 (0.1%)	1.19	20/2644 (0.8%)
1	D	0.85	0/2299	1.16	15/3108 (0.5%)
1	E	1.02	7/2210 (0.3%)	1.25	23/2987 (0.8%)
1	F	0.86	1/1922 (0.1%)	1.22	20/2602 (0.8%)
All	All	0.91	13/12602 (0.1%)	1.22	123/17045 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	1
1	E	0	1
All	All	1	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	VAL	CA-CB	-8.23	1.37	1.54
1	E	358	ILE	CA-CB	-6.23	1.40	1.54
1	E	335	ARG	CG-CD	-6.14	1.36	1.51
1	A	251	VAL	CB-CG1	-6.00	1.40	1.52
1	C	251	VAL	CB-CG1	-6.00	1.40	1.52
1	B	286	ALA	CA-CB	-5.89	1.40	1.52
1	E	358	ILE	CB-CG2	-5.71	1.35	1.52
1	F	300	TYR	CE2-CZ	-5.61	1.31	1.38
1	E	335	ARG	CB-CG	-5.49	1.37	1.52
1	E	335	ARG	NE-CZ	-5.46	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	305	VAL	CA-CB	-5.35	1.43	1.54
1	E	304	VAL	CA-CB	-5.21	1.43	1.54
1	A	365	ILE	CA-CB	-5.06	1.43	1.54

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	353	ASP	CB-CG-OD2	11.65	128.78	118.30
1	F	324	ASP	CB-CG-OD2	10.32	127.58	118.30
1	F	233	ASP	CB-CG-OD2	9.53	126.88	118.30
1	D	145	SER	N-CA-C	-9.25	86.03	111.00
1	A	404	ASP	CB-CG-OD2	8.97	126.37	118.30
1	B	170	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	233	ASP	CB-CG-OD2	8.70	126.13	118.30
1	C	220	GLY	N-CA-C	8.65	134.73	113.10
1	D	223	LYS	N-CA-C	-8.21	88.84	111.00
1	E	233	ASP	CB-CG-OD2	8.21	125.68	118.30
1	B	144	SER	N-CA-C	8.17	133.07	111.00
1	C	233	ASP	CB-CG-OD2	7.85	125.37	118.30
1	B	223	LYS	N-CA-C	-7.84	89.83	111.00
1	C	145	SER	N-CA-C	-7.80	89.93	111.00
1	C	144	SER	N-CA-C	7.71	131.82	111.00
1	D	244	ASP	CB-CG-OD2	7.54	125.08	118.30
1	B	146	PRO	N-CD-CG	-7.48	91.99	103.20
1	B	158	VAL	CB-CA-C	-7.39	97.35	111.40
1	E	320	PRO	N-CD-CG	-7.37	92.15	103.20
1	D	233	ASP	CB-CG-OD2	7.34	124.91	118.30
1	B	233	ASP	CB-CG-OD2	7.32	124.89	118.30
1	E	361	LEU	CB-CG-CD2	-7.25	98.67	111.00
1	E	353	ASP	CB-CG-OD2	7.24	124.82	118.30
1	A	402	LEU	CB-CG-CD2	-7.23	98.71	111.00
1	E	367	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	A	324	ASP	CB-CG-OD2	7.16	124.75	118.30
1	E	348	LEU	CA-CB-CG	7.09	131.61	115.30
1	E	324	ASP	CB-CG-OD2	7.05	124.65	118.30
1	E	318	ASP	CB-CG-OD2	7.04	124.64	118.30
1	D	273	VAL	CB-CA-C	-7.02	98.07	111.40
1	D	309	MET	CB-CG-SD	-7.01	91.36	112.40
1	C	297	ASP	CB-CG-OD2	6.90	124.51	118.30
1	E	214	GLU	N-CA-C	6.89	129.60	111.00
1	B	276	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	E	356	GLY	N-CA-C	-6.87	95.91	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284	ASP	CB-CG-OD2	6.78	124.41	118.30
1	A	185	CYS	N-CA-C	6.73	129.18	111.00
1	B	247	PRO	N-CD-CG	-6.72	93.12	103.20
1	A	353	ASP	CB-CG-OD2	6.72	124.35	118.30
1	C	353	ASP	CB-CG-OD2	6.70	124.33	118.30
1	D	353	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	151	LEU	CB-CG-CD1	-6.47	100.00	111.00
1	E	297	ASP	CB-CG-OD2	6.46	124.12	118.30
1	D	247	PRO	N-CD-CG	-6.38	93.63	103.20
1	F	244	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	247	PRO	N-CD-CG	-6.28	93.78	103.20
1	C	218	PHE	N-CA-C	6.25	127.87	111.00
1	C	324	ASP	CB-CG-OD2	6.23	123.91	118.30
1	E	284	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	161	SER	N-CA-C	6.21	127.75	111.00
1	C	270	THR	N-CA-C	-6.15	94.39	111.00
1	B	145	SER	N-CA-C	-6.15	94.39	111.00
1	D	210	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	F	162	ASP	CB-CG-OD2	6.11	123.80	118.30
1	E	347	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	297	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	E	274	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	198	CYS	CA-CB-SG	-5.97	103.25	114.00
1	C	161	SER	N-CA-C	5.96	127.08	111.00
1	F	289	VAL	CB-CA-C	-5.91	100.17	111.40
1	C	274	ASP	CB-CG-OD2	5.82	123.54	118.30
1	F	201	LEU	CA-CB-CG	-5.77	102.02	115.30
1	F	185	CYS	N-CA-C	5.76	126.56	111.00
1	F	170	ASP	CB-CG-OD2	5.75	123.48	118.30
1	D	144	SER	N-CA-C	5.75	126.53	111.00
1	A	274	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	284	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	244	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	404	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	251	VAL	CB-CA-C	-5.66	100.65	111.40
1	A	369	VAL	CA-CB-CG1	-5.66	102.41	110.90
1	F	353	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	F	347	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	151	LEU	CA-CB-CG	5.56	128.08	115.30
1	E	251	VAL	CB-CA-C	-5.55	100.85	111.40
1	E	367	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	A	161	SER	N-CA-C	5.54	125.96	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	170	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	361	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	364	ALA	C-N-CA	-5.48	107.99	121.70
1	C	144	SER	CA-C-N	-5.47	105.16	117.20
1	A	262	VAL	CB-CA-C	-5.45	101.06	111.40
1	B	295	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	216	GLY	N-CA-C	5.41	126.63	113.10
1	A	284	ASP	CB-CG-OD2	5.39	123.16	118.30
1	E	244	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	324	ASP	CB-CG-OD2	5.38	123.14	118.30
1	F	274	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	142	ILE	N-CA-C	5.36	125.47	111.00
1	A	355	PRO	N-CD-CG	-5.35	95.18	103.20
1	F	201	LEU	N-CA-C	-5.32	96.65	111.00
1	B	162	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	173	THR	CA-CB-CG2	-5.30	104.98	112.40
1	C	281	THR	CA-CB-CG2	-5.29	104.99	112.40
1	E	313	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	A	435	LEU	CA-CB-CG	5.29	127.46	115.30
1	F	247	PRO	N-CD-CG	-5.25	95.33	103.20
1	B	144	SER	CA-C-N	-5.23	105.69	117.20
1	F	161	SER	N-CA-C	5.23	125.12	111.00
1	B	307	ILE	CB-CA-C	-5.22	101.17	111.60
1	E	170	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	145	SER	N-CA-C	-5.19	96.98	111.00
1	C	262	VAL	CB-CA-C	-5.17	101.57	111.40
1	B	165	VAL	CB-CA-C	-5.16	101.61	111.40
1	F	187	ALA	N-CA-C	5.15	124.91	111.00
1	B	155	ILE	CB-CA-C	-5.15	101.30	111.60
1	E	190	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	186	SER	N-CA-C	5.13	124.85	111.00
1	B	347	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	347	ASP	CB-CG-OD2	5.11	122.90	118.30
1	F	142	ILE	CB-CA-C	-5.09	101.41	111.60
1	B	244	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	217	ALA	N-CA-C	-5.08	97.27	111.00
1	F	162	ASP	N-CA-C	5.08	124.72	111.00
1	A	347	ASP	CB-CG-OD2	5.06	122.86	118.30
1	C	271	ILE	N-CA-C	-5.06	97.34	111.00
1	C	223	LYS	N-CA-C	-5.05	97.37	111.00
1	C	240	ASP	CB-CG-OD2	5.03	122.82	118.30
1	B	285	LEU	CB-CG-CD1	-5.02	102.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	297	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	162	ASP	CB-CG-OD2	5.01	122.81	118.30
1	F	216	GLY	N-CA-C	5.01	125.64	113.10
1	B	355	PRO	N-CD-CG	-5.00	95.69	103.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	144	SER	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	143	GLY	Peptide
1	E	354	TRP	Peptide

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	2234	0	2233	283	3
1	B	1929	0	1905	268	1
1	C	1925	0	1899	265	2
1	D	2270	0	2280	278	0
1	E	2183	0	2185	299	1
1	F	1895	0	1871	265	1
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	3	0
2	D	5	0	0	3	0
2	F	5	0	0	2	0
3	E	31	0	12	11	0
4	A	16	0	0	11	0
4	B	20	0	0	16	0
4	C	16	0	0	12	0
4	D	23	0	0	16	0
4	E	17	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	10	0	0	6	0
All	All	12594	0	12385	1635	4

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 66.

All (1635) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:TYR:CD2	1:E:353:ASP:N	1.80	1.48
1:A:377:ILE:HD12	1:A:378:SER:N	1.44	1.30
1:D:352:TYR:CD2	1:D:353:ASP:N	2.01	1.27
1:D:255:ARG:HD2	4:D:2005:HOH:O	1.30	1.27
1:B:354:TRP:HB2	1:B:355:PRO:CD	1.62	1.25
1:E:377:ILE:HD12	1:E:377:ILE:C	1.41	1.24
1:A:377:ILE:HD12	1:A:377:ILE:C	1.55	1.23
1:F:215:LYS:HA	1:F:223:LYS:CB	1.72	1.20
1:E:377:ILE:HD12	1:E:378:SER:N	1.54	1.20
1:A:327:LEU:HD12	1:A:327:LEU:O	1.36	1.19
1:A:313:ARG:HH12	1:A:354:TRP:HB3	1.03	1.19
1:A:215:LYS:CB	1:A:269:GLN:HE22	1.56	1.18
1:D:377:ILE:HD12	1:D:377:ILE:C	1.64	1.17
1:E:352:TYR:HA	1:E:354:TRP:NE1	1.57	1.17
1:A:352:TYR:HA	1:A:354:TRP:HE1	1.05	1.15
1:C:357:ASN:ND2	1:C:357:ASN:H	1.26	1.15
1:F:164:THR:HG23	1:F:277:LEU:HB3	1.25	1.14
1:C:357:ASN:HD22	1:C:357:ASN:N	1.33	1.14
1:B:321:LEU:HB2	4:B:2015:HOH:O	1.48	1.12
1:D:377:ILE:HD12	1:D:378:SER:N	1.65	1.12
1:D:359:ARG:HG3	1:D:359:ARG:HH11	1.01	1.11
1:B:214:GLU:HG2	1:B:224:ARG:HH21	0.95	1.11
1:E:352:TYR:O	1:E:353:ASP:HB2	1.37	1.11
1:B:377:ILE:C	1:B:377:ILE:HD12	1.70	1.11
1:E:327:LEU:HD11	1:E:338:VAL:HG11	1.32	1.10
1:A:352:TYR:HA	1:A:354:TRP:NE1	1.64	1.10
1:D:352:TYR:HA	1:D:354:TRP:NE1	1.66	1.09
1:C:359:ARG:HH11	1:C:359:ARG:HG3	1.13	1.09
1:A:199:ALA:HB1	1:B:251:VAL:HG11	1.24	1.08
1:B:313:ARG:HH12	1:B:354:TRP:HB3	1.09	1.08
1:B:352:TYR:CD2	1:B:353:ASP:N	2.21	1.08
1:B:214:GLU:CG	1:B:224:ARG:HH21	1.66	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:TYR:CD2	1:F:353:ASP:N	2.21	1.08
1:C:191:ARG:HH11	1:C:191:ARG:HG2	1.07	1.08
1:B:313:ARG:NH1	1:B:354:TRP:HB3	1.69	1.08
1:A:352:TYR:CD2	1:A:353:ASP:N	2.22	1.07
1:C:365:ILE:HG22	1:C:366:GLU:N	1.58	1.07
1:A:164:THR:HG23	1:A:277:LEU:HB3	1.38	1.06
1:D:233:ASP:OD2	1:D:273:VAL:HA	1.54	1.05
1:B:359:ARG:HH11	1:B:359:ARG:HG3	1.20	1.04
1:F:313:ARG:HH11	1:F:313:ARG:HB3	1.21	1.04
1:A:366:GLU:O	1:A:370:VAL:HG23	1.58	1.04
1:E:191:ARG:HB3	1:E:192:PRO:HD2	1.36	1.04
1:F:248:LEU:HD23	1:F:248:LEU:O	1.57	1.04
1:E:251:VAL:HG21	1:F:200:ALA:HB3	1.38	1.04
1:C:158:VAL:HG11	1:C:305:VAL:HG11	1.37	1.03
1:B:354:TRP:HB2	1:B:355:PRO:HD2	1.39	1.03
1:B:250:GLN:CG	1:B:250:GLN:CA	2.37	1.03
1:F:211:PHE:O	1:F:227:GLY:HA3	1.59	1.03
1:C:352:TYR:HE1	4:C:2016:HOH:O	1.40	1.02
1:A:354:TRP:HB2	1:A:355:PRO:CD	1.88	1.02
1:F:383:PRO:O	1:F:386:ILE:HG22	1.57	1.02
1:D:313:ARG:HH12	1:D:354:TRP:HB3	1.17	1.02
1:C:313:ARG:HB3	1:C:313:ARG:HH11	1.22	1.02
1:F:148:MET:HE3	1:F:152:LEU:HD21	1.36	1.02
1:A:199:ALA:CB	1:B:251:VAL:HG11	1.91	1.01
1:D:353:ASP:OD2	1:D:361:LEU:HD13	1.59	1.01
1:F:354:TRP:HB2	1:F:355:PRO:CD	1.89	1.01
1:E:352:TYR:CA	1:E:354:TRP:NE1	2.22	1.00
1:D:155:ILE:HG23	1:D:182:LEU:HD23	1.40	1.00
1:A:215:LYS:CB	1:A:269:GLN:NE2	2.25	0.99
1:B:352:TYR:HA	1:B:354:TRP:NE1	1.77	0.99
1:F:316:ARG:HH22	1:F:354:TRP:HZ2	1.09	0.99
1:E:377:ILE:C	1:E:377:ILE:CD1	2.27	0.98
1:A:313:ARG:NH1	1:A:354:TRP:HB3	1.78	0.98
1:F:209:GLU:O	1:F:228:ARG:HG2	1.62	0.97
1:B:214:GLU:HG2	1:B:224:ARG:NH2	1.78	0.97
1:F:167:ILE:HB	1:F:280:ALA:HB2	1.42	0.97
1:E:304:VAL:HA	1:F:363:ASN:ND2	1.80	0.96
1:E:145:SER:HB3	1:E:317:GLU:HB2	1.47	0.96
1:A:148:MET:CE	1:A:152:LEU:HD21	1.95	0.96
1:B:159:ALA:HB1	1:B:186:SER:HB2	1.48	0.96
1:E:352:TYR:HD2	1:E:353:ASP:N	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ARG:HB3	1:D:192:PRO:HD2	1.44	0.95
1:E:143:GLY:HA3	1:E:318:ASP:OD1	1.65	0.95
1:D:309:MET:SD	1:D:310:PRO:HD2	2.07	0.95
1:D:352:TYR:HA	1:D:354:TRP:HE1	1.23	0.95
1:E:142:ILE:HD12	3:E:1442:ATP:C2	2.00	0.95
1:A:313:ARG:HH11	1:A:313:ARG:HB3	1.30	0.95
1:C:352:TYR:CG	1:C:353:ASP:N	2.30	0.94
1:C:382:LEU:HB3	1:C:386:ILE:HG21	1.49	0.94
1:B:313:ARG:HH12	1:B:354:TRP:CB	1.80	0.94
1:B:352:TYR:HA	1:B:354:TRP:HE1	1.33	0.94
1:D:313:ARG:NH1	1:D:354:TRP:HB3	1.84	0.93
1:C:191:ARG:CG	1:C:191:ARG:HH11	1.81	0.93
1:B:354:TRP:CB	1:B:355:PRO:CD	2.45	0.93
1:C:367:ARG:HB3	4:C:2015:HOH:O	1.67	0.93
1:E:313:ARG:HH12	1:E:354:TRP:HB3	1.34	0.93
1:D:141:MET:HG3	1:D:148:MET:HE1	1.49	0.93
1:B:276:ARG:HH11	1:B:276:ARG:HG2	1.33	0.93
1:D:352:TYR:HD2	1:D:353:ASP:H	0.93	0.92
1:B:377:ILE:HD12	1:B:378:SER:N	1.84	0.92
1:A:357:ASN:H	1:A:357:ASN:ND2	1.56	0.92
1:A:321:LEU:HD12	1:A:321:LEU:O	1.70	0.92
1:B:257:ILE:HD11	1:B:277:LEU:CD2	1.99	0.92
1:C:142:ILE:HG22	1:C:318:ASP:HB3	1.50	0.92
1:C:174:GLY:O	1:C:178:VAL:HG23	1.68	0.92
1:D:359:ARG:HG3	1:D:359:ARG:NH1	1.82	0.91
1:F:148:MET:CE	1:F:152:LEU:HD21	1.99	0.91
1:E:338:VAL:HG22	1:E:372:LEU:HD23	1.51	0.91
1:B:150:HIS:CE1	1:B:154:GLU:OE1	2.24	0.91
1:E:253:LEU:O	1:E:257:ILE:HG13	1.70	0.91
1:E:313:ARG:NH1	1:E:354:TRP:HB3	1.85	0.91
1:A:167:ILE:HB	1:A:280:ALA:CB	2.01	0.90
1:A:431:THR:HG22	1:A:433:LYS:H	1.33	0.90
1:B:193:LEU:O	1:B:193:LEU:HG	1.72	0.90
1:B:239:LEU:CD1	1:B:277:LEU:HD11	2.02	0.90
1:A:199:ALA:HB1	1:B:251:VAL:CG1	2.02	0.90
1:B:354:TRP:HB2	1:B:355:PRO:HD3	1.54	0.89
1:B:276:ARG:CG	1:B:276:ARG:HH11	1.84	0.89
1:D:359:ARG:HH11	1:D:359:ARG:CG	1.86	0.89
1:E:352:TYR:O	1:E:353:ASP:CB	2.18	0.89
1:D:354:TRP:HB2	1:D:355:PRO:HD3	1.54	0.89
1:C:359:ARG:CG	1:C:359:ARG:HH11	1.84	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ILE:CD1	1:A:378:SER:N	2.35	0.88
1:E:359:ARG:HH11	1:E:359:ARG:HG3	1.35	0.88
1:F:352:TYR:HD2	1:F:353:ASP:H	1.15	0.88
1:B:158:VAL:C	1:B:160:PRO:HD2	1.94	0.88
1:E:233:ASP:OD2	1:E:273:VAL:HG12	1.74	0.88
1:C:313:ARG:NH1	1:C:313:ARG:HB3	1.89	0.87
1:E:304:VAL:HA	1:F:363:ASN:HD22	1.37	0.87
1:B:155:ILE:HG22	1:B:155:ILE:O	1.74	0.87
1:A:309:MET:HE3	1:A:310:PRO:HD2	1.55	0.87
1:A:425:ALA:HB1	1:A:430:ILE:O	1.75	0.87
1:F:282:HIS:CD2	1:F:282:HIS:O	2.27	0.87
1:C:248:LEU:HD23	1:C:248:LEU:O	1.74	0.87
1:C:297:ASP:OD1	1:C:298:LEU:N	2.07	0.87
1:D:321:LEU:HD12	1:D:321:LEU:O	1.74	0.87
1:D:153:ASN:O	1:D:156:ALA:HB3	1.74	0.87
1:E:355:PRO:HD2	1:E:360:GLU:OE1	1.75	0.87
1:A:377:ILE:C	1:A:377:ILE:CD1	2.36	0.87
1:E:352:TYR:CA	1:E:354:TRP:HE1	1.84	0.87
1:F:377:ILE:HD12	1:F:377:ILE:C	1.95	0.87
1:E:212:GLY:O	1:E:264:ARG:HA	1.75	0.86
1:D:250:GLN:HE22	1:D:294:PHE:HA	1.40	0.86
1:D:312:LEU:O	1:D:315:ARG:N	2.07	0.86
1:D:252:ARG:HH11	1:D:252:ARG:HG2	1.36	0.86
1:D:305:VAL:HG12	1:D:305:VAL:O	1.75	0.86
1:C:311:SER:H	1:C:314:GLN:NE2	1.74	0.86
1:C:379:GLU:HB2	4:C:2014:HOH:O	1.75	0.86
1:D:175:LYS:NZ	2:D:1442:PO4:O4	2.08	0.86
1:C:312:LEU:HD12	1:C:357:ASN:C	1.96	0.86
1:E:327:LEU:HD11	1:E:338:VAL:CG1	2.06	0.85
1:A:148:MET:HE3	1:A:152:LEU:HD21	1.58	0.85
1:F:377:ILE:HD12	1:F:378:SER:N	1.91	0.85
1:E:211:PHE:O	1:E:227:GLY:HA3	1.76	0.85
1:E:261:GLU:HB3	1:E:270:THR:CG2	2.05	0.85
1:E:435:LEU:HD23	1:E:435:LEU:C	1.97	0.85
1:A:260:ARG:HB3	1:A:273:VAL:O	1.75	0.85
1:B:158:VAL:O	1:B:160:PRO:HD2	1.75	0.85
1:F:175:LYS:HG2	1:F:309:MET:HG3	1.57	0.85
1:A:309:MET:CE	1:A:310:PRO:HD2	2.06	0.85
1:F:276:ARG:HH11	1:F:276:ARG:CG	1.87	0.85
1:C:386:ILE:HG13	1:C:387:ALA:H	1.42	0.84
1:C:352:TYR:CD2	1:C:353:ASP:N	2.44	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:TRP:CB	1:F:355:PRO:CD	2.49	0.84
1:B:191:ARG:HB3	1:B:192:PRO:HD2	1.59	0.84
1:C:195:THR:O	1:C:195:THR:HG23	1.74	0.84
1:B:318:ASP:C	1:B:320:PRO:HD2	1.98	0.84
1:D:297:ASP:OD1	1:D:298:LEU:N	2.10	0.84
1:D:310:PRO:HA	4:D:2014:HOH:O	1.77	0.84
1:D:191:ARG:HB3	1:D:192:PRO:CD	2.08	0.83
1:E:304:VAL:HG12	1:E:305:VAL:HG23	1.59	0.83
1:E:158:VAL:O	1:E:160:PRO:HD2	1.77	0.83
1:C:155:ILE:HG23	1:C:182:LEU:HD23	1.60	0.83
1:E:142:ILE:HD12	3:E:1442:ATP:N1	1.94	0.83
1:C:387:ALA:HB2	4:C:2013:HOH:O	1.78	0.83
1:A:327:LEU:HD12	1:A:327:LEU:C	1.95	0.83
1:C:142:ILE:HD13	1:C:322:LEU:HD12	1.61	0.82
1:C:142:ILE:HG22	1:C:318:ASP:CB	2.08	0.82
1:C:386:ILE:HG13	1:C:387:ALA:N	1.92	0.82
1:C:259:GLU:O	1:C:261:GLU:N	2.13	0.82
1:E:226:GLU:HG2	1:E:230:VAL:HG21	1.61	0.82
1:F:214:GLU:O	1:F:216:GLY:N	2.13	0.82
1:F:145:SER:HB3	1:F:317:GLU:HB2	1.62	0.81
1:C:142:ILE:HD13	1:C:322:LEU:CD1	2.08	0.81
1:E:149:GLN:HA	1:E:152:LEU:HD12	1.61	0.81
1:B:159:ALA:C	1:B:186:SER:OG	2.19	0.81
1:D:141:MET:CG	1:D:148:MET:HE1	2.10	0.81
1:B:159:ALA:CB	1:B:186:SER:HB2	2.11	0.81
1:F:354:TRP:HB2	1:F:355:PRO:HD3	1.61	0.81
1:A:365:ILE:O	1:A:368:ALA:N	2.14	0.81
1:F:354:TRP:HB2	1:F:355:PRO:HD2	1.63	0.80
1:A:167:ILE:HB	1:A:280:ALA:HB2	1.61	0.80
1:C:142:ILE:CG2	1:C:318:ASP:HB3	2.10	0.80
1:D:160:PRO:N	1:D:186:SER:OG	2.13	0.80
1:E:377:ILE:CD1	1:E:378:SER:N	2.40	0.80
1:A:313:ARG:HH12	1:A:354:TRP:CB	1.91	0.80
1:D:239:LEU:CD1	1:D:277:LEU:HD11	2.12	0.80
1:A:352:TYR:HD2	1:A:353:ASP:H	1.25	0.80
1:E:209:GLU:O	1:E:228:ARG:HG2	1.80	0.80
1:D:250:GLN:NE2	1:D:294:PHE:HA	1.96	0.80
1:E:145:SER:HB2	1:E:146:PRO:CD	2.12	0.80
1:D:336:LYS:HA	1:D:336:LYS:HE3	1.64	0.80
1:F:167:ILE:HB	1:F:280:ALA:CB	2.12	0.80
1:F:341:PHE:HD2	1:F:377:ILE:HG13	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ILE:O	1:D:323:ALA:N	2.13	0.79
1:B:354:TRP:CB	1:B:355:PRO:HD2	2.06	0.79
1:C:316:ARG:HB2	1:C:317:GLU:OE2	1.83	0.79
1:A:354:TRP:HB2	1:A:355:PRO:HD3	1.62	0.79
1:E:410:ILE:HD12	1:E:435:LEU:HG	1.64	0.79
1:A:148:MET:HE1	1:A:152:LEU:HD21	1.64	0.79
1:D:148:MET:O	1:D:152:LEU:HG	1.81	0.79
1:A:431:THR:HG22	1:A:433:LYS:N	1.97	0.79
1:D:148:MET:CE	1:D:152:LEU:HD21	2.12	0.79
1:C:284:ASP:O	1:C:287:GLU:N	2.15	0.78
1:D:148:MET:HE2	1:D:152:LEU:HD21	1.63	0.78
1:A:410:ILE:HD11	1:A:439:LEU:CG	2.13	0.78
1:C:160:PRO:N	1:C:186:SER:OG	2.16	0.78
1:C:239:LEU:CD1	1:C:277:LEU:HD11	2.12	0.78
1:F:188:ARG:HB3	1:F:191:ARG:HD3	1.65	0.78
1:D:215:LYS:HG2	1:D:222:ASP:O	1.82	0.78
1:B:159:ALA:C	1:B:186:SER:CB	2.52	0.78
1:E:251:VAL:CG2	1:F:200:ALA:HB3	2.13	0.78
1:E:356:GLY:O	1:E:360:GLU:HB3	1.83	0.78
1:A:352:TYR:CA	1:A:354:TRP:HE1	1.92	0.78
1:E:212:GLY:O	1:E:264:ARG:CA	2.32	0.78
1:B:377:ILE:C	1:B:377:ILE:CD1	2.46	0.77
1:A:270:THR:HG22	1:A:270:THR:O	1.83	0.77
1:E:212:GLY:O	1:E:264:ARG:CB	2.32	0.77
1:E:191:ARG:HB3	1:E:192:PRO:CD	2.14	0.77
1:F:183:HIS:CG	1:F:193:LEU:HD22	2.20	0.77
1:A:410:ILE:HD11	1:A:439:LEU:HD23	1.66	0.77
1:F:140:HIS:O	1:F:177:LEU:HD13	1.84	0.77
1:A:324:ASP:CG	1:A:328:ARG:HH12	1.86	0.77
1:E:202:ASN:O	1:E:204:SER:N	2.18	0.77
1:A:357:ASN:ND2	1:A:357:ASN:N	2.32	0.77
1:F:261:GLU:HB3	1:F:270:THR:HG23	1.65	0.77
1:C:204:SER:OG	1:C:205:LEU:N	2.17	0.77
1:F:235:GLY:HA3	4:F:2004:HOH:O	1.83	0.77
1:A:257:ILE:HG22	4:A:2005:HOH:O	1.85	0.77
1:E:261:GLU:OE1	1:E:270:THR:HG21	1.84	0.77
1:E:352:TYR:HA	1:E:354:TRP:CE2	2.21	0.76
1:B:213:HIS:CE1	1:B:225:ARG:HB2	2.20	0.76
1:E:151:LEU:O	1:E:151:LEU:HD22	1.85	0.76
1:F:164:THR:CG2	1:F:277:LEU:HB3	2.13	0.76
1:B:285:LEU:HB3	1:B:299:TYR:CE1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:O	1:A:276:ARG:NH1	2.17	0.76
1:C:172:GLY:H	2:C:1391:PO4:P	2.08	0.76
1:C:312:LEU:HB2	1:C:357:ASN:HB3	1.68	0.76
1:E:246:SER:O	1:E:250:GLN:HG3	1.86	0.76
1:F:211:PHE:O	1:F:227:GLY:CA	2.32	0.76
1:A:239:LEU:CD1	1:A:277:LEU:HD11	2.16	0.76
1:A:360:GLU:HB2	1:B:300:TYR:CZ	2.21	0.75
1:B:341:PHE:CD2	1:B:377:ILE:HG13	2.21	0.75
1:C:178:VAL:O	1:C:182:LEU:HG	1.86	0.75
1:F:341:PHE:CD2	1:F:377:ILE:HG13	2.21	0.75
1:D:353:ASP:OD2	1:D:361:LEU:CD1	2.34	0.75
1:C:358:ILE:N	1:C:358:ILE:HD12	2.02	0.75
1:E:178:VAL:HG21	1:E:309:MET:SD	2.25	0.75
1:B:359:ARG:NH1	1:B:359:ARG:HG3	1.98	0.75
1:F:276:ARG:HG2	1:F:276:ARG:HH11	1.50	0.75
1:A:246:SER:O	1:A:250:GLN:HG3	1.87	0.75
1:B:213:HIS:ND1	1:B:225:ARG:HB2	2.02	0.75
1:D:377:ILE:CD1	1:D:377:ILE:C	2.42	0.75
1:A:321:LEU:HD12	1:A:321:LEU:C	2.04	0.75
1:D:142:ILE:HG23	1:D:321:LEU:HG	1.69	0.75
1:D:248:LEU:HD23	1:D:248:LEU:C	2.07	0.75
1:B:214:GLU:CG	1:B:224:ARG:NH2	2.41	0.74
1:F:313:ARG:NH1	1:F:313:ARG:HB3	1.99	0.74
1:C:383:PRO:O	1:C:386:ILE:HG12	1.86	0.74
1:E:144:SER:O	1:E:145:SER:O	2.05	0.74
1:A:215:LYS:O	1:A:217:ALA:N	2.20	0.74
1:E:253:LEU:O	1:E:253:LEU:HD12	1.87	0.74
1:E:304:VAL:HG12	1:E:305:VAL:N	2.00	0.74
1:F:264:ARG:O	1:F:266:GLY:N	2.20	0.74
1:A:313:ARG:CB	1:A:313:ARG:HH11	2.00	0.74
1:D:194:VAL:CG2	1:D:232:ALA:HB2	2.17	0.74
1:D:239:LEU:HD12	1:D:277:LEU:HD11	1.68	0.74
1:D:232:ALA:O	1:D:235:GLY:N	2.19	0.74
1:E:151:LEU:O	1:E:155:ILE:HG13	1.87	0.74
1:E:254:LEU:O	1:E:257:ILE:N	2.20	0.74
1:E:358:ILE:HG22	1:E:359:ARG:N	1.95	0.74
1:C:354:TRP:HB2	1:C:355:PRO:HD3	1.69	0.74
1:A:356:GLY:O	1:A:357:ASN:C	2.25	0.74
1:D:259:GLU:O	1:D:261:GLU:N	2.20	0.74
1:A:367:ARG:HD3	4:B:2012:HOH:O	1.88	0.73
1:B:178:VAL:HG21	1:B:309:MET:SD	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PRO:N	1:B:186:SER:OG	2.21	0.73
1:C:352:TYR:O	1:C:354:TRP:CD1	2.41	0.73
1:A:276:ARG:HA	4:A:2006:HOH:O	1.88	0.73
1:D:253:LEU:O	1:D:257:ILE:HG13	1.88	0.73
1:F:151:LEU:O	1:F:155:ILE:HG13	1.89	0.73
1:A:158:VAL:HG11	1:A:305:VAL:HG11	1.68	0.73
1:E:352:TYR:CD2	1:E:353:ASP:CA	2.70	0.73
1:D:269:GLN:O	1:D:271:ILE:HG13	1.89	0.73
1:D:357:ASN:H	1:D:357:ASN:ND2	1.82	0.73
1:C:191:ARG:NH1	1:C:191:ARG:HG2	1.89	0.73
1:D:159:ALA:HB1	1:D:186:SER:HB2	1.71	0.73
1:E:326:PHE:HZ	3:E:1442:ATP:H1'	1.51	0.73
1:F:145:SER:CB	1:F:317:GLU:HB2	2.19	0.73
1:F:384:LEU:O	1:F:386:ILE:N	2.21	0.73
1:B:316:ARG:HA	1:B:319:ILE:HD12	1.70	0.73
1:C:230:VAL:O	1:C:233:ASP:N	2.16	0.73
1:B:288:GLU:CD	1:B:293:ARG:HH21	1.91	0.73
1:B:357:ASN:ND2	1:B:357:ASN:H	1.86	0.72
1:F:168:HIS:CD2	4:F:2002:HOH:O	2.40	0.72
1:F:191:ARG:HG3	1:F:191:ARG:HH11	1.53	0.72
1:F:237:LEU:HD12	1:F:238:PHE:H	1.52	0.72
1:C:248:LEU:C	1:C:248:LEU:CD2	2.57	0.72
1:A:183:HIS:CD2	1:A:193:LEU:HD13	2.25	0.72
1:A:358:ILE:N	1:A:358:ILE:CD1	2.52	0.72
1:C:385:ALA:HA	1:C:388:ALA:HB3	1.71	0.72
1:E:158:VAL:O	1:E:160:PRO:CD	2.38	0.72
1:B:164:THR:HG23	1:B:277:LEU:HB3	1.72	0.72
1:C:320:PRO:O	1:C:323:ALA:HB3	1.90	0.72
1:B:191:ARG:HB3	1:B:192:PRO:CD	2.19	0.72
1:D:352:TYR:CG	1:D:353:ASP:N	2.46	0.72
1:F:168:HIS:NE2	4:F:2002:HOH:O	2.23	0.72
1:B:352:TYR:CG	1:B:353:ASP:N	2.39	0.72
1:E:405:VAL:O	1:E:408:GLU:HB3	1.90	0.72
1:B:197:ASN:OD1	1:B:199:ALA:HB2	1.88	0.72
1:E:239:LEU:CD1	1:E:277:LEU:HD11	2.19	0.72
1:F:151:LEU:HD13	1:F:155:ILE:HD11	1.70	0.72
1:F:163:ALA:O	1:F:276:ARG:NH1	2.22	0.71
1:A:167:ILE:HB	1:A:280:ALA:HB1	1.72	0.71
1:B:261:GLU:HB3	1:B:270:THR:HG22	1.71	0.71
1:C:358:ILE:N	1:C:358:ILE:CD1	2.54	0.71
1:D:141:MET:SD	1:D:148:MET:HE1	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:LEU:C	1:F:248:LEU:HD23	2.09	0.71
1:B:239:LEU:HD12	1:B:277:LEU:HD11	1.70	0.71
1:E:212:GLY:HA3	1:E:226:GLU:O	1.90	0.71
1:E:146:PRO:HD3	1:E:317:GLU:OE1	1.90	0.71
1:D:160:PRO:CA	1:D:186:SER:OG	2.38	0.71
1:D:174:GLY:O	1:D:178:VAL:HG23	1.90	0.71
1:B:166:LEU:HD21	1:B:285:LEU:HD23	1.72	0.71
1:F:352:TYR:O	1:F:354:TRP:CD1	2.44	0.71
1:C:354:TRP:CD1	1:C:354:TRP:N	2.55	0.70
1:D:417:THR:HG22	4:D:2021:HOH:O	1.91	0.70
1:F:252:ARG:HH11	1:F:252:ARG:HG2	1.55	0.70
1:B:244:ASP:OD2	1:B:283:ARG:NH1	2.24	0.70
1:C:248:LEU:HB2	4:C:2002:HOH:O	1.91	0.70
1:D:141:MET:HG3	1:D:148:MET:CE	2.22	0.70
1:D:173:THR:OG1	1:D:174:GLY:N	2.22	0.70
1:D:160:PRO:HA	1:D:186:SER:OG	1.90	0.70
1:E:326:PHE:CZ	3:E:1442:ATP:H1'	2.27	0.70
1:C:356:GLY:O	1:C:360:GLU:N	2.23	0.70
1:C:143:GLY:HA2	1:C:148:MET:HG2	1.74	0.70
1:D:164:THR:HG23	1:D:277:LEU:HB3	1.74	0.70
1:D:383:PRO:O	1:D:386:ILE:HG22	1.92	0.70
1:E:260:ARG:HB3	1:E:273:VAL:O	1.92	0.70
1:A:254:LEU:O	1:A:257:ILE:N	2.25	0.70
1:A:313:ARG:NH1	1:A:313:ARG:HB3	2.05	0.70
1:A:232:ALA:O	1:A:235:GLY:N	2.25	0.69
1:A:410:ILE:HD11	1:A:439:LEU:CD2	2.22	0.69
1:E:191:ARG:CB	1:E:192:PRO:HD2	2.19	0.69
1:F:183:HIS:HD2	1:F:236:THR:OG1	1.75	0.69
1:A:357:ASN:H	1:A:357:ASN:HD22	1.38	0.69
1:E:420:ASN:C	1:E:420:ASN:OD1	2.30	0.69
1:F:232:ALA:O	1:F:235:GLY:N	2.24	0.69
1:B:385:ALA:O	1:B:387:ALA:N	2.25	0.69
1:C:310:PRO:O	4:C:2008:HOH:O	2.10	0.69
1:C:327:LEU:HD22	1:C:341:PHE:CE1	2.28	0.69
1:C:382:LEU:CB	1:C:386:ILE:HG21	2.22	0.69
1:D:336:LYS:HA	1:D:336:LYS:CE	2.22	0.69
1:B:159:ALA:O	1:B:186:SER:CB	2.41	0.69
1:E:346:MET:HG3	1:E:346:MET:O	1.93	0.69
1:F:252:ARG:NH1	1:F:252:ARG:HG2	2.08	0.69
1:A:254:LEU:CD2	1:A:297:ASP:HB2	2.22	0.69
1:D:191:ARG:CG	1:D:191:ARG:HH11	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ALA:O	1:B:235:GLY:N	2.25	0.69
1:C:269:GLN:HB3	1:C:271:ILE:CD1	2.23	0.69
1:F:155:ILE:HG23	1:F:182:LEU:HD23	1.74	0.68
1:C:320:PRO:HD3	1:C:350:ILE:HG12	1.73	0.68
1:C:248:LEU:C	1:C:248:LEU:HD23	2.08	0.68
1:D:352:TYR:CA	1:D:354:TRP:HE1	2.03	0.68
1:B:386:ILE:HA	1:B:389:THR:CB	2.24	0.68
1:C:253:LEU:O	1:C:256:ALA:HB3	1.94	0.68
1:E:321:LEU:HD12	1:E:321:LEU:O	1.93	0.68
1:D:271:ILE:HG22	1:D:272:SER:H	1.59	0.68
1:E:164:THR:HG23	1:E:277:LEU:HB3	1.74	0.68
1:F:327:LEU:HD22	1:F:341:PHE:CZ	2.28	0.68
1:C:315:ARG:O	1:C:316:ARG:C	2.31	0.68
1:C:158:VAL:CG1	1:C:305:VAL:HG11	2.18	0.68
1:F:142:ILE:HD12	1:F:142:ILE:H	1.58	0.68
1:A:352:TYR:CA	1:A:354:TRP:NE1	2.51	0.68
1:C:151:LEU:HD22	1:C:151:LEU:O	1.94	0.68
1:B:318:ASP:O	1:B:319:ILE:C	2.32	0.68
1:D:356:GLY:O	1:D:357:ASN:C	2.32	0.67
1:F:236:THR:HG22	1:F:276:ARG:HB3	1.75	0.67
1:F:167:ILE:O	1:F:280:ALA:HB1	1.94	0.67
1:B:158:VAL:CG1	1:B:158:VAL:O	2.41	0.67
1:B:248:LEU:O	1:B:251:VAL:HG23	1.94	0.67
1:F:281:THR:OG1	1:F:283:ARG:N	2.27	0.67
1:B:155:ILE:CG2	1:B:155:ILE:O	2.41	0.67
1:A:151:LEU:HD22	1:A:151:LEU:O	1.95	0.67
1:C:308:GLU:CB	4:C:2007:HOH:O	2.42	0.67
1:E:211:PHE:O	1:E:227:GLY:CA	2.42	0.67
1:D:261:GLU:OE1	1:D:270:THR:HG23	1.94	0.67
1:D:372:LEU:O	4:D:2016:HOH:O	2.12	0.67
1:E:352:TYR:C	1:E:354:TRP:CD1	2.68	0.67
1:E:338:VAL:CG2	1:E:372:LEU:HD23	2.23	0.67
1:C:158:VAL:C	1:C:160:PRO:HD2	2.14	0.67
1:C:239:LEU:HD11	1:C:277:LEU:HD11	1.76	0.67
1:A:142:ILE:HG21	1:A:321:LEU:HG	1.76	0.67
1:B:158:VAL:HG12	1:B:158:VAL:O	1.94	0.67
1:B:257:ILE:HD11	1:B:277:LEU:HD21	1.77	0.67
1:C:166:LEU:HD21	1:C:285:LEU:HD22	1.77	0.67
1:A:238:PHE:HD1	1:A:278:ILE:HG22	1.60	0.66
1:B:188:ARG:NH1	1:B:235:GLY:O	2.28	0.66
1:C:230:VAL:O	1:C:232:ALA:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:VAL:HG22	1:E:372:LEU:CD2	2.23	0.66
1:F:142:ILE:HD12	1:F:142:ILE:N	2.10	0.66
1:F:359:ARG:HG3	1:F:359:ARG:HH11	1.60	0.66
1:C:351:HIS:O	1:C:351:HIS:CD2	2.48	0.66
1:C:261:GLU:HA	1:C:272:SER:HA	1.77	0.66
1:D:194:VAL:HG23	1:D:232:ALA:HB2	1.78	0.66
1:D:188:ARG:HB3	1:D:191:ARG:HD3	1.78	0.66
1:D:206:LEU:HD23	1:D:249:MET:HG3	1.77	0.66
1:C:247:PRO:O	1:C:250:GLN:N	2.27	0.66
1:E:146:PRO:CD	1:E:317:GLU:OE1	2.43	0.66
1:F:174:GLY:O	1:F:178:VAL:HG23	1.95	0.66
1:F:193:LEU:HD12	1:F:193:LEU:C	2.16	0.66
1:A:211:PHE:O	1:A:227:GLY:HA3	1.96	0.66
1:C:252:ARG:HH11	1:C:252:ARG:HG2	1.61	0.66
1:D:431:THR:O	1:D:434:THR:HB	1.96	0.66
1:E:160:PRO:HD3	1:E:186:SER:OG	1.96	0.66
1:A:166:LEU:HA	1:A:279:ALA:O	1.96	0.66
1:A:311:SER:H	1:A:314:GLN:NE2	1.94	0.66
1:D:248:LEU:O	1:D:248:LEU:HD23	1.96	0.66
1:D:276:ARG:HH11	1:D:276:ARG:HG2	1.60	0.66
1:C:365:ILE:O	1:C:368:ALA:N	2.29	0.66
1:B:359:ARG:CG	1:B:359:ARG:HH11	2.01	0.65
1:D:269:GLN:HG3	4:D:2006:HOH:O	1.95	0.65
1:E:261:GLU:HB3	1:E:270:THR:HG23	1.77	0.65
1:F:233:ASP:OD2	1:F:273:VAL:HA	1.95	0.65
1:A:309:MET:HE3	1:A:310:PRO:CD	2.25	0.65
1:B:288:GLU:OE1	1:B:293:ARG:NH2	2.27	0.65
1:C:143:GLY:O	1:C:318:ASP:OD1	2.14	0.65
1:C:239:LEU:HD12	1:C:277:LEU:HD11	1.77	0.65
1:C:313:ARG:NH1	1:C:354:TRP:HB3	2.10	0.65
1:A:316:ARG:NE	4:A:2010:HOH:O	2.24	0.65
1:D:276:ARG:CG	1:D:276:ARG:HH11	2.09	0.65
1:D:309:MET:SD	1:D:310:PRO:CD	2.84	0.65
1:E:341:PHE:CD2	1:E:377:ILE:HG13	2.31	0.65
1:C:247:PRO:HG2	4:C:2002:HOH:O	1.96	0.65
1:F:319:ILE:O	1:F:323:ALA:N	2.21	0.65
1:F:384:LEU:C	1:F:386:ILE:H	1.99	0.65
1:A:410:ILE:HD11	1:A:439:LEU:HB3	1.77	0.65
1:B:285:LEU:HB3	1:B:299:TYR:HE1	1.60	0.65
1:A:165:VAL:HG11	1:A:182:LEU:CD1	2.27	0.65
1:C:359:ARG:NH1	1:C:359:ARG:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:HIS:HB3	4:D:2003:HOH:O	1.97	0.65
1:D:320:PRO:O	1:D:323:ALA:N	2.30	0.65
1:F:244:ASP:OD2	1:F:283:ARG:NH1	2.30	0.65
1:C:309:MET:SD	1:C:310:PRO:HD2	2.37	0.65
1:F:196:LEU:O	1:F:196:LEU:HG	1.91	0.65
1:D:344:GLN:HB3	4:D:2015:HOH:O	1.97	0.64
1:D:356:GLY:O	1:D:357:ASN:O	2.15	0.64
1:E:264:ARG:O	1:E:266:GLY:N	2.30	0.64
1:A:352:TYR:C	1:A:354:TRP:CD1	2.71	0.64
1:A:352:TYR:CG	1:A:353:ASP:N	2.49	0.64
1:B:318:ASP:O	1:B:321:LEU:N	2.26	0.64
1:D:377:ILE:CD1	1:D:378:SER:N	2.54	0.64
1:D:406:GLU:CD	1:D:438:LYS:HD3	2.18	0.64
1:C:248:LEU:CD2	1:C:248:LEU:O	2.45	0.64
1:F:313:ARG:HB3	1:F:354:TRP:CD1	2.32	0.64
1:A:182:LEU:HD12	1:A:278:ILE:HD13	1.77	0.64
1:D:252:ARG:HG2	1:D:252:ARG:NH1	2.07	0.64
1:A:285:LEU:O	1:A:286:ALA:C	2.32	0.64
1:B:259:GLU:O	1:B:261:GLU:N	2.30	0.64
1:D:382:LEU:HA	4:D:2019:HOH:O	1.98	0.64
1:E:155:ILE:HD11	1:E:178:VAL:HG13	1.77	0.64
1:F:237:LEU:HD12	1:F:238:PHE:N	2.12	0.64
1:B:276:ARG:NH1	1:B:276:ARG:CG	2.52	0.64
1:F:169:GLY:HA2	4:F:2002:HOH:O	1.97	0.64
1:B:284:ASP:O	1:B:285:LEU:C	2.35	0.64
1:B:309:MET:CE	1:B:310:PRO:HD2	2.27	0.64
1:C:308:GLU:HB3	4:C:2007:HOH:O	1.97	0.64
1:C:359:ARG:NH1	1:C:359:ARG:CG	2.50	0.64
1:C:377:ILE:HD11	1:C:382:LEU:HD21	1.80	0.64
1:D:352:TYR:CA	1:D:354:TRP:NE1	2.53	0.64
1:D:380:ARG:HD3	1:D:380:ARG:H	1.63	0.64
1:A:288:GLU:CD	1:A:293:ARG:HH21	2.01	0.64
1:E:352:TYR:N	1:E:354:TRP:HE1	1.95	0.64
1:F:282:HIS:O	1:F:282:HIS:CG	2.49	0.64
1:A:363:ASN:OD1	1:B:304:VAL:HA	1.97	0.63
1:D:302:LEU:O	1:D:304:VAL:N	2.31	0.63
1:E:212:GLY:CA	1:E:226:GLU:O	2.46	0.63
1:F:176:GLU:HG2	1:F:180:ARG:NH2	2.13	0.63
1:E:242:ILE:HD12	1:E:279:ALA:HB1	1.79	0.63
1:F:377:ILE:HD11	1:F:382:LEU:HD21	1.80	0.63
1:A:348:LEU:N	1:A:348:LEU:HD12	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:MET:SD	1:C:148:MET:CE	2.87	0.63
1:F:356:GLY:O	1:F:357:ASN:C	2.34	0.63
1:D:239:LEU:HB2	1:D:242:ILE:HD12	1.81	0.63
1:D:285:LEU:O	1:D:286:ALA:C	2.35	0.63
1:A:166:LEU:HD12	1:A:279:ALA:O	1.99	0.63
1:A:377:ILE:HD12	1:A:378:SER:CA	2.29	0.63
1:C:313:ARG:CB	1:C:313:ARG:HH11	2.02	0.63
1:A:148:MET:O	1:A:152:LEU:HG	1.99	0.62
1:A:312:LEU:O	1:A:315:ARG:N	2.20	0.62
1:D:204:SER:O	1:D:205:LEU:C	2.36	0.62
1:D:352:TYR:CD2	1:D:353:ASP:CA	2.82	0.62
1:D:354:TRP:HB2	1:D:355:PRO:CD	2.29	0.62
1:D:392:LYS:HE3	1:D:392:LYS:HA	1.80	0.62
1:F:313:ARG:HH11	1:F:313:ARG:CB	2.06	0.62
1:D:366:GLU:O	1:D:370:VAL:HG23	1.99	0.62
1:A:165:VAL:HG11	1:A:182:LEU:HD11	1.80	0.62
1:A:197:ASN:OD1	1:A:199:ALA:N	2.28	0.62
1:C:356:GLY:O	1:C:360:GLU:CB	2.47	0.62
1:B:357:ASN:ND2	1:B:357:ASN:N	2.46	0.62
1:E:301:ARG:NH2	4:E:2006:HOH:O	2.30	0.62
1:E:194:VAL:CG2	1:E:232:ALA:HB2	2.29	0.62
1:E:319:ILE:O	1:E:323:ALA:N	2.28	0.62
1:F:232:ALA:O	1:F:233:ASP:C	2.36	0.62
1:B:257:ILE:HD11	1:B:277:LEU:HD23	1.79	0.62
1:C:173:THR:O	1:C:175:LYS:N	2.32	0.62
1:C:367:ARG:NH2	1:C:383:PRO:HA	2.14	0.62
1:E:145:SER:HB2	1:E:146:PRO:HD2	1.80	0.62
1:C:319:ILE:O	1:C:323:ALA:N	2.30	0.62
1:D:313:ARG:HH12	1:D:354:TRP:CB	2.03	0.62
1:C:352:TYR:HA	1:C:354:TRP:HE1	1.65	0.62
1:C:364:ALA:HB2	4:C:2011:HOH:O	2.00	0.62
1:D:295:ARG:NH2	1:D:297:ASP:OD2	2.32	0.62
1:E:406:GLU:O	1:E:407:LYS:C	2.35	0.62
1:A:367:ARG:HG3	1:B:305:VAL:HG22	1.82	0.62
1:F:142:ILE:CG2	1:F:143:GLY:N	2.63	0.62
1:B:318:ASP:O	1:B:320:PRO:N	2.33	0.62
1:A:356:GLY:O	1:A:357:ASN:O	2.18	0.61
1:A:430:ILE:HG12	1:A:430:ILE:O	2.00	0.61
1:B:141:MET:HG3	1:B:148:MET:CE	2.30	0.61
1:C:191:ARG:NH1	1:C:191:ARG:CG	2.50	0.61
1:F:285:LEU:O	1:F:286:ALA:C	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:O	1:A:323:ALA:N	2.26	0.61
1:B:146:PRO:O	1:B:147:ALA:C	2.38	0.61
1:C:232:ALA:O	1:C:235:GLY:N	2.33	0.61
1:F:285:LEU:HB3	1:F:299:TYR:CE1	2.35	0.61
1:E:368:ALA:O	1:E:369:VAL:C	2.35	0.61
1:A:367:ARG:CD	4:B:2012:HOH:O	2.46	0.61
1:C:377:ILE:C	1:C:377:ILE:HD12	2.21	0.61
1:D:359:ARG:NH1	1:D:359:ARG:CG	2.51	0.61
1:F:215:LYS:CA	1:F:223:LYS:CB	2.64	0.61
1:F:352:TYR:CG	1:F:353:ASP:N	2.69	0.61
1:A:311:SER:HB2	1:A:314:GLN:HE21	1.65	0.61
1:C:386:ILE:CG1	1:C:387:ALA:H	2.13	0.61
1:F:316:ARG:NH1	1:F:354:TRP:HE1	1.99	0.61
1:B:313:ARG:HH12	1:B:354:TRP:CA	2.14	0.61
1:B:359:ARG:NH1	1:C:297:ASP:HB3	2.15	0.61
1:D:261:GLU:OE1	1:D:270:THR:CG2	2.48	0.61
1:E:209:GLU:O	1:E:228:ARG:CG	2.47	0.61
1:E:295:ARG:NH2	1:E:297:ASP:OD2	2.33	0.61
1:A:188:ARG:NH1	1:A:235:GLY:O	2.32	0.61
1:E:155:ILE:HG23	1:E:182:LEU:HD23	1.83	0.61
1:E:284:ASP:O	1:E:285:LEU:C	2.39	0.61
1:C:285:LEU:O	1:C:289:VAL:HG23	2.00	0.61
1:D:238:PHE:CD1	1:D:278:ILE:HG22	2.36	0.61
1:B:284:ASP:O	1:B:287:GLU:N	2.34	0.60
1:B:145:SER:HB3	1:B:317:GLU:HB2	1.83	0.60
1:E:339:LYS:C	4:E:2011:HOH:O	2.40	0.60
1:F:175:LYS:HG2	1:F:309:MET:CG	2.31	0.60
1:C:377:ILE:CD1	1:C:382:LEU:HD21	2.31	0.60
1:D:352:TYR:C	1:D:354:TRP:CD1	2.75	0.60
1:F:214:GLU:O	1:F:215:LYS:C	2.40	0.60
1:F:251:VAL:O	1:F:254:LEU:HB3	2.00	0.60
1:A:238:PHE:HA	1:A:278:ILE:O	2.01	0.60
1:B:248:LEU:HD23	1:B:248:LEU:C	2.21	0.60
1:B:311:SER:HB3	4:B:2013:HOH:O	2.01	0.60
1:B:377:ILE:O	1:B:377:ILE:HD12	2.01	0.60
1:F:195:THR:HG23	1:F:195:THR:O	2.01	0.60
1:F:295:ARG:NH2	1:F:297:ASP:OD2	2.32	0.60
1:D:191:ARG:CB	1:D:192:PRO:HD2	2.26	0.60
1:C:352:TYR:C	1:C:354:TRP:CD1	2.75	0.60
1:C:383:PRO:O	1:C:386:ILE:HG23	2.02	0.60
1:D:233:ASP:OD2	1:D:273:VAL:CA	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ILE:HB	1:D:320:PRO:CD	2.31	0.60
1:A:151:LEU:O	1:A:155:ILE:HG13	2.01	0.60
1:C:191:ARG:HB3	1:C:192:PRO:HD2	1.83	0.60
1:C:142:ILE:HD13	1:C:322:LEU:HD13	1.83	0.60
1:D:382:LEU:HB3	1:D:383:PRO:HD2	1.84	0.60
1:E:208:SER:O	1:E:210:LEU:N	2.34	0.60
1:E:316:ARG:O	1:E:318:ASP:N	2.35	0.60
1:F:248:LEU:CD2	1:F:248:LEU:C	2.69	0.60
1:F:356:GLY:O	1:F:360:GLU:HB3	2.02	0.60
1:B:165:VAL:HG12	1:B:166:LEU:N	2.15	0.60
1:B:206:LEU:CD2	1:B:249:MET:HE2	2.31	0.60
1:C:188:ARG:HB3	1:C:191:ARG:HD2	1.82	0.60
1:C:269:GLN:HB3	1:C:271:ILE:HD11	1.82	0.60
1:C:367:ARG:HH21	1:C:383:PRO:HA	1.67	0.60
1:F:252:ARG:O	1:F:253:LEU:C	2.39	0.60
1:E:319:ILE:HB	1:E:320:PRO:CD	2.32	0.59
1:B:230:VAL:HG23	1:B:231:GLU:H	1.66	0.59
1:B:385:ALA:C	1:B:387:ALA:H	2.05	0.59
1:C:255:ARG:O	1:C:256:ALA:C	2.40	0.59
1:D:173:THR:O	2:D:1442:PO4:O1	2.20	0.59
1:D:239:LEU:HD11	1:D:277:LEU:HD11	1.81	0.59
1:B:159:ALA:O	1:B:186:SER:HB3	2.03	0.59
1:B:259:GLU:HG3	1:B:259:GLU:O	2.02	0.59
1:B:284:ASP:O	1:B:286:ALA:N	2.35	0.59
1:C:212:GLY:O	1:C:265:VAL:N	2.25	0.59
1:D:222:ASP:C	1:D:223:LYS:O	2.36	0.59
1:E:144:SER:C	1:E:145:SER:O	2.39	0.59
1:A:439:LEU:HD12	1:A:439:LEU:C	2.22	0.59
1:C:365:ILE:O	1:C:366:GLU:C	2.41	0.59
1:D:172:GLY:O	1:D:358:ILE:N	2.34	0.59
1:A:260:ARG:O	1:A:273:VAL:HG22	2.03	0.59
1:B:348:LEU:HD12	1:B:348:LEU:H	1.68	0.59
1:B:370:VAL:HG21	1:C:163:ALA:HB2	1.83	0.59
1:C:352:TYR:O	1:C:354:TRP:HD1	1.85	0.59
1:D:382:LEU:HD12	1:D:386:ILE:HD12	1.85	0.59
1:E:158:VAL:C	1:E:160:PRO:HD2	2.23	0.59
1:A:330:PHE:CZ	1:A:366:GLU:HB2	2.37	0.59
1:B:318:ASP:O	1:B:320:PRO:HD2	2.03	0.59
1:B:370:VAL:HG12	1:B:370:VAL:O	2.02	0.59
1:C:272:SER:C	1:C:273:VAL:HG13	2.23	0.59
1:A:183:HIS:HD2	1:A:193:LEU:HD13	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:SER:O	1:A:209:GLU:C	2.40	0.59
1:B:197:ASN:O	1:B:201:LEU:HD11	2.02	0.59
1:A:367:ARG:HG3	1:B:305:VAL:CG2	2.33	0.59
1:C:313:ARG:HH12	1:C:354:TRP:HB3	1.65	0.59
1:D:346:MET:O	1:D:346:MET:HE2	2.02	0.59
1:E:305:VAL:HG22	1:F:367:ARG:HG3	1.84	0.59
1:A:173:THR:O	1:A:175:LYS:N	2.35	0.59
1:D:367:ARG:HH21	1:D:382:LEU:C	2.06	0.59
1:E:271:ILE:HG22	1:E:273:VAL:HG13	1.83	0.59
1:E:359:ARG:NH1	1:E:359:ARG:HG3	2.10	0.59
1:D:354:TRP:N	1:D:354:TRP:CD1	2.68	0.58
1:F:148:MET:O	1:F:152:LEU:HG	2.03	0.58
1:F:162:ASP:O	1:F:162:ASP:CG	2.40	0.58
1:F:175:LYS:CG	1:F:309:MET:HG3	2.31	0.58
1:D:176:GLU:O	1:D:179:ALA:N	2.36	0.58
1:C:195:THR:CG2	1:C:195:THR:O	2.46	0.58
1:E:194:VAL:HG21	1:E:232:ALA:HB2	1.85	0.58
1:E:261:GLU:HB3	1:E:270:THR:HG22	1.84	0.58
1:A:410:ILE:HD11	1:A:439:LEU:CB	2.33	0.58
1:C:377:ILE:HD12	1:C:378:SER:N	2.18	0.58
1:F:183:HIS:CB	1:F:193:LEU:HD22	2.33	0.58
1:A:354:TRP:HB2	1:A:355:PRO:HD2	1.78	0.58
1:E:344:GLN:O	1:E:348:LEU:HD12	2.04	0.58
1:E:354:TRP:N	1:E:354:TRP:CD1	2.67	0.58
1:F:271:ILE:O	1:F:273:VAL:HG13	2.03	0.58
1:A:423:GLU:HA	1:A:423:GLU:OE1	2.02	0.58
1:C:252:ARG:NH1	1:C:252:ARG:HG2	2.16	0.58
1:C:356:GLY:O	1:C:360:GLU:HB3	2.04	0.58
1:E:339:LYS:HG3	4:E:2011:HOH:O	2.03	0.58
1:F:354:TRP:H	1:F:355:PRO:HD2	1.68	0.58
1:A:344:GLN:HA	1:A:344:GLN:OE1	2.04	0.58
1:E:172:GLY:O	1:E:358:ILE:HB	2.02	0.58
1:E:434:THR:HG22	1:E:435:LEU:N	2.17	0.58
1:C:382:LEU:HB2	1:C:386:ILE:HD13	1.86	0.58
1:D:196:LEU:O	1:D:196:LEU:HD23	2.03	0.58
1:E:178:VAL:CG2	1:E:309:MET:SD	2.92	0.58
1:C:284:ASP:OD1	1:C:287:GLU:N	2.36	0.58
1:F:178:VAL:HG21	1:F:309:MET:SD	2.44	0.58
1:F:248:LEU:CD2	1:F:248:LEU:O	2.43	0.58
1:F:313:ARG:NH1	1:F:354:TRP:CG	2.71	0.58
1:C:174:GLY:O	1:C:178:VAL:CG2	2.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ASP:CG	1:C:328:ARG:HH12	2.07	0.58
1:E:240:ASP:OD2	1:E:241:GLU:N	2.37	0.58
1:C:141:MET:CG	1:C:148:MET:HE2	2.33	0.57
1:A:410:ILE:HD11	1:A:439:LEU:HG	1.85	0.57
1:D:318:ASP:O	1:D:319:ILE:C	2.41	0.57
1:E:242:ILE:O	1:E:242:ILE:HG23	2.05	0.57
1:A:439:LEU:CD1	1:A:439:LEU:C	2.73	0.57
1:E:401:PRO:O	1:E:402:LEU:C	2.43	0.57
1:B:145:SER:O	1:B:146:PRO:C	2.41	0.57
1:D:191:ARG:HG3	1:D:191:ARG:HH11	1.69	0.57
1:D:402:LEU:O	1:D:405:VAL:N	2.37	0.57
1:B:354:TRP:CD1	1:B:354:TRP:N	2.66	0.57
1:C:354:TRP:HB2	1:C:355:PRO:CD	2.35	0.57
1:F:239:LEU:N	1:F:239:LEU:HD12	2.19	0.57
1:B:341:PHE:HD2	1:B:377:ILE:HG13	1.67	0.57
1:D:344:GLN:O	1:D:348:LEU:HD12	2.04	0.57
1:E:163:ALA:O	1:E:276:ARG:NH1	2.38	0.57
1:A:247:PRO:O	1:A:248:LEU:C	2.41	0.57
1:C:176:GLU:HG2	1:C:180:ARG:NH2	2.20	0.57
1:E:159:ALA:HB1	1:E:186:SER:HB2	1.86	0.57
1:A:167:ILE:CB	1:A:280:ALA:HB2	2.34	0.57
1:F:153:ASN:ND2	4:F:2001:HOH:O	2.38	0.57
1:D:254:LEU:HD13	1:D:298:LEU:HA	1.86	0.57
1:D:300:TYR:CZ	1:E:360:GLU:HB2	2.39	0.57
1:E:359:ARG:CZ	3:E:1442:ATP:O1A	2.53	0.57
1:E:422:THR:O	1:E:425:ALA:HB3	2.04	0.57
1:C:172:GLY:O	1:C:357:ASN:HB2	2.04	0.57
1:E:277:LEU:HD12	1:E:278:ILE:H	1.69	0.57
1:F:232:ALA:O	1:F:233:ASP:O	2.23	0.57
1:A:319:ILE:HB	1:A:320:PRO:HD3	1.87	0.56
1:E:407:LYS:NZ	1:E:441:ARG:HB2	2.20	0.56
1:A:178:VAL:O	1:A:182:LEU:HG	2.05	0.56
1:A:318:ASP:O	1:A:319:ILE:C	2.44	0.56
1:B:252:ARG:HH11	1:B:252:ARG:HG2	1.70	0.56
1:E:352:TYR:CD2	1:E:352:TYR:C	2.66	0.56
1:F:160:PRO:HA	1:F:186:SER:HB3	1.87	0.56
1:F:183:HIS:CD2	1:F:193:LEU:HD22	2.40	0.56
1:F:319:ILE:HB	1:F:320:PRO:CD	2.34	0.56
1:B:261:GLU:HB3	1:B:270:THR:CG2	2.36	0.56
1:B:346:MET:HE3	1:B:346:MET:O	2.05	0.56
1:E:406:GLU:O	1:E:408:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ARG:HD2	4:D:2012:HOH:O	2.05	0.56
1:E:324:ASP:CG	1:E:328:ARG:NH1	2.58	0.56
1:B:202:ASN:OD1	1:B:205:LEU:HG	2.04	0.56
1:B:313:ARG:HH11	1:B:313:ARG:HB3	1.71	0.56
1:B:379:GLU:O	4:B:2019:HOH:O	2.17	0.56
1:C:358:ILE:CD1	1:C:358:ILE:H	2.17	0.56
1:D:321:LEU:HD12	1:D:321:LEU:C	2.21	0.56
1:A:437:ALA:O	1:A:439:LEU:N	2.38	0.56
1:B:352:TYR:O	1:B:353:ASP:HB2	2.05	0.56
1:D:164:THR:HG23	4:D:2007:HOH:O	2.04	0.56
1:D:381:GLU:O	4:D:2019:HOH:O	2.18	0.56
1:E:202:ASN:O	1:E:203:GLU:C	2.43	0.56
1:E:354:TRP:HB2	1:E:355:PRO:HD3	1.85	0.56
1:C:209:GLU:O	1:C:228:ARG:HG2	2.05	0.56
1:F:354:TRP:N	1:F:355:PRO:HD2	2.20	0.56
1:B:174:GLY:O	1:B:175:LYS:C	2.43	0.56
1:C:281:THR:HG23	1:C:281:THR:O	2.06	0.56
1:D:341:PHE:CD2	1:D:377:ILE:HG13	2.41	0.56
1:C:215:LYS:HA	1:C:222:ASP:HA	1.87	0.56
1:D:295:ARG:NE	1:D:297:ASP:OD2	2.39	0.56
1:A:191:ARG:HG3	1:A:191:ARG:HH11	1.71	0.56
1:A:354:TRP:CD1	1:A:354:TRP:N	2.71	0.56
1:C:234:GLY:N	1:C:274:ASP:O	2.38	0.56
1:C:379:GLU:N	4:C:2014:HOH:O	2.33	0.56
1:E:261:GLU:HA	1:E:272:SER:HA	1.88	0.56
1:E:352:TYR:HA	1:E:354:TRP:CD1	2.38	0.56
1:E:254:LEU:HD21	1:E:297:ASP:HB2	1.86	0.56
1:A:247:PRO:O	1:A:250:GLN:N	2.39	0.55
1:B:232:ALA:O	1:B:233:ASP:C	2.45	0.55
1:B:242:ILE:HD11	1:B:253:LEU:CD2	2.36	0.55
1:B:285:LEU:HB3	1:B:299:TYR:CD1	2.41	0.55
1:B:355:PRO:HG2	1:B:360:GLU:OE1	2.06	0.55
1:D:175:LYS:HG3	2:D:1442:PO4:O4	2.05	0.55
1:E:159:ALA:O	1:E:160:PRO:C	2.44	0.55
1:F:348:LEU:O	1:F:349:LEU:C	2.43	0.55
1:B:318:ASP:O	1:B:320:PRO:CD	2.55	0.55
1:B:313:ARG:NH1	1:B:354:TRP:CB	2.50	0.55
1:D:353:ASP:CG	1:D:361:LEU:HD13	2.25	0.55
1:A:262:VAL:HG12	1:A:263:GLN:O	2.07	0.55
1:A:324:ASP:CG	1:A:328:ARG:NH1	2.59	0.55
1:A:338:VAL:O	1:A:339:LYS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:N	1:A:358:ILE:HD12	2.20	0.55
1:C:268:ASN:O	1:C:270:THR:N	2.39	0.55
1:E:232:ALA:O	1:E:235:GLY:N	2.40	0.55
1:F:142:ILE:HG22	1:F:143:GLY:N	2.21	0.55
1:F:348:LEU:HD12	1:F:348:LEU:H	1.71	0.55
1:A:286:ALA:O	1:A:289:VAL:N	2.40	0.55
1:A:399:ILE:HD12	1:A:399:ILE:H	1.70	0.55
1:B:377:ILE:CD1	1:B:378:SER:N	2.65	0.55
1:C:285:LEU:HB3	1:C:299:TYR:CE1	2.42	0.55
1:D:357:ASN:ND2	1:D:357:ASN:N	2.54	0.55
1:D:407:LYS:O	1:D:411:LEU:HB2	2.06	0.55
1:E:142:ILE:CD1	3:E:1442:ATP:C2	2.84	0.55
1:A:165:VAL:HB	1:A:278:ILE:HG12	1.88	0.55
1:B:252:ARG:NH1	1:B:252:ARG:HG2	2.22	0.55
1:B:297:ASP:OD1	1:B:298:LEU:N	2.39	0.55
1:B:372:LEU:HD22	1:B:377:ILE:HG22	1.89	0.55
1:D:405:VAL:O	1:D:408:GLU:HB3	2.06	0.55
1:A:188:ARG:NH2	1:A:274:ASP:OD1	2.35	0.55
1:A:403:VAL:HG13	1:A:441:ARG:HH11	1.72	0.55
1:E:420:ASN:O	1:E:420:ASN:OD1	2.23	0.55
1:A:355:PRO:HG2	1:A:360:GLU:OE1	2.06	0.55
1:B:308:GLU:OE2	1:B:309:MET:O	2.25	0.55
1:B:318:ASP:C	1:B:320:PRO:CD	2.74	0.55
1:B:359:ARG:NH1	1:B:359:ARG:CG	2.64	0.55
1:C:141:MET:SD	1:C:148:MET:HE2	2.47	0.55
1:D:252:ARG:CG	1:D:252:ARG:NH1	2.66	0.55
1:E:178:VAL:O	1:E:182:LEU:HG	2.07	0.55
1:B:348:LEU:HD12	1:B:348:LEU:N	2.21	0.55
1:B:358:ILE:N	1:B:358:ILE:CD1	2.69	0.55
1:C:327:LEU:HD22	1:C:341:PHE:CZ	2.42	0.55
1:C:312:LEU:HD12	1:C:357:ASN:O	2.06	0.55
1:E:260:ARG:NH2	4:E:2003:HOH:O	2.33	0.55
1:E:435:LEU:CD2	1:E:435:LEU:C	2.73	0.55
1:F:359:ARG:NH2	2:F:1390:PO4:O3	2.40	0.55
1:F:170:ASP:O	1:F:173:THR:CG2	2.55	0.55
1:B:202:ASN:OD1	1:B:204:SER:OG	2.22	0.55
1:D:193:LEU:HG	1:D:193:LEU:O	2.06	0.55
1:A:204:SER:OG	1:A:205:LEU:N	2.39	0.55
1:A:322:LEU:O	1:A:325:HIS:N	2.40	0.55
1:C:357:ASN:ND2	1:C:357:ASN:N	2.07	0.55
1:E:406:GLU:O	1:E:409:VAL:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ASP:O	1:C:274:ASP:OD1	2.25	0.54
1:C:313:ARG:HH12	1:C:354:TRP:HA	1.73	0.54
1:D:358:ILE:CD1	1:D:358:ILE:N	2.69	0.54
1:F:281:THR:OG1	1:F:283:ARG:HB2	2.07	0.54
1:F:318:ASP:O	1:F:319:ILE:C	2.45	0.54
1:A:316:ARG:HA	1:A:319:ILE:HD12	1.87	0.54
1:C:318:ASP:O	1:C:319:ILE:C	2.46	0.54
1:E:158:VAL:O	1:E:160:PRO:N	2.41	0.54
1:E:352:TYR:CA	1:E:354:TRP:CD1	2.89	0.54
1:F:354:TRP:CB	1:F:355:PRO:HD3	2.29	0.54
1:F:330:PHE:CZ	1:F:366:GLU:HB2	2.42	0.54
1:E:377:ILE:HD12	1:E:377:ILE:O	2.00	0.54
1:A:252:ARG:CD	4:A:2004:HOH:O	2.55	0.54
1:B:145:SER:OG	1:B:148:MET:CB	2.56	0.54
1:B:339:LYS:C	4:B:2018:HOH:O	2.46	0.54
1:E:160:PRO:CD	1:E:186:SER:OG	2.55	0.54
1:E:259:GLU:O	1:E:261:GLU:N	2.40	0.54
1:E:406:GLU:C	1:E:408:GLU:N	2.59	0.54
1:F:206:LEU:O	1:F:210:LEU:HB2	2.08	0.54
1:B:257:ILE:CD1	1:B:277:LEU:CD2	2.81	0.54
1:F:367:ARG:HH21	1:F:382:LEU:C	2.10	0.54
1:A:358:ILE:N	1:A:358:ILE:HD13	2.23	0.54
1:B:281:THR:OG1	1:B:283:ARG:N	2.39	0.54
1:C:209:GLU:O	1:C:228:ARG:CG	2.56	0.54
1:D:358:ILE:O	1:D:359:ARG:C	2.45	0.54
1:E:352:TYR:HD2	1:E:353:ASP:CA	2.15	0.54
1:A:346:MET:HE2	1:A:346:MET:O	2.08	0.54
1:B:296:GLN:O	1:B:299:TYR:N	2.40	0.54
1:C:264:ARG:O	1:C:266:GLY:N	2.41	0.54
1:D:176:GLU:O	1:D:179:ALA:HB3	2.08	0.54
1:D:194:VAL:HG21	1:D:232:ALA:HB2	1.89	0.54
1:D:386:ILE:HG23	1:D:387:ALA:N	2.23	0.54
1:A:239:LEU:O	1:A:279:ALA:HA	2.08	0.54
1:B:307:ILE:O	1:B:307:ILE:HG22	2.04	0.54
1:C:141:MET:SD	1:C:148:MET:HE1	2.46	0.54
1:C:352:TYR:HA	1:C:354:TRP:NE1	2.22	0.54
1:D:191:ARG:CG	1:D:191:ARG:NH1	2.67	0.54
1:E:431:THR:HG22	1:E:433:LYS:H	1.72	0.54
1:B:206:LEU:HD23	1:B:249:MET:HG3	1.90	0.54
1:B:370:VAL:O	1:B:370:VAL:CG1	2.55	0.54
1:C:194:VAL:HG21	1:C:232:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:LEU:O	1:E:386:ILE:N	2.41	0.54
1:B:213:HIS:ND1	1:B:213:HIS:O	2.41	0.54
1:C:263:GLN:HA	1:C:269:GLN:O	2.07	0.54
1:C:295:ARG:NH2	1:C:297:ASP:OD2	2.36	0.54
1:D:281:THR:HG23	1:D:281:THR:O	2.08	0.54
1:E:316:ARG:NH1	1:E:351:HIS:HA	2.23	0.54
1:F:140:HIS:O	1:F:141:MET:HB3	2.08	0.54
1:C:164:THR:HG23	1:C:277:LEU:HB3	1.90	0.53
1:C:260:ARG:HB3	1:C:273:VAL:O	2.08	0.53
1:D:197:ASN:OD1	1:D:199:ALA:HB2	2.07	0.53
1:E:155:ILE:CD1	1:E:178:VAL:HG13	2.39	0.53
1:B:199:ALA:HB1	1:C:251:VAL:HG21	1.91	0.53
1:C:276:ARG:HG2	1:C:276:ARG:HH11	1.74	0.53
1:C:275:VAL:HG12	1:C:276:ARG:N	2.22	0.53
1:D:312:LEU:HD13	1:D:353:ASP:HB3	1.90	0.53
1:A:141:MET:HG2	1:A:148:MET:HE2	1.90	0.53
1:B:287:GLU:OE2	4:B:2010:HOH:O	2.18	0.53
1:C:155:ILE:HD11	1:C:178:VAL:HG13	1.89	0.53
1:D:326:PHE:O	1:D:327:LEU:C	2.47	0.53
1:D:400:GLN:HA	1:D:400:GLN:OE1	2.07	0.53
1:A:213:HIS:O	1:A:213:HIS:CG	2.61	0.53
1:A:239:LEU:HD12	1:A:277:LEU:HD11	1.89	0.53
1:B:327:LEU:HD22	1:B:341:PHE:CE1	2.43	0.53
1:C:254:LEU:O	1:C:257:ILE:N	2.42	0.53
1:E:423:GLU:O	1:E:424:ALA:C	2.46	0.53
1:F:312:LEU:O	1:F:315:ARG:N	2.27	0.53
1:A:274:ASP:OD1	1:A:274:ASP:O	2.27	0.53
1:A:365:ILE:O	1:A:366:GLU:C	2.47	0.53
1:E:277:LEU:HD12	1:E:278:ILE:N	2.24	0.53
1:E:357:ASN:H	1:E:357:ASN:ND2	2.07	0.53
1:B:281:THR:OG1	1:B:282:HIS:N	2.41	0.53
1:E:142:ILE:HD12	3:E:1442:ATP:H2	1.70	0.53
1:E:177:LEU:O	1:E:181:ALA:N	2.31	0.53
1:A:202:ASN:HD21	1:A:205:LEU:CD1	2.21	0.53
1:A:276:ARG:HG2	4:A:2002:HOH:O	2.08	0.53
1:A:354:TRP:CB	1:A:355:PRO:CD	2.66	0.53
1:B:360:GLU:HB2	1:C:300:TYR:CZ	2.43	0.53
1:C:320:PRO:HA	1:C:346:MET:SD	2.49	0.53
1:D:319:ILE:HB	1:D:320:PRO:HD2	1.90	0.53
1:D:406:GLU:O	1:D:410:ILE:HG23	2.09	0.53
1:E:363:ASN:C	1:E:363:ASN:OD1	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:N	1:A:348:LEU:CD1	2.72	0.53
1:A:410:ILE:CD1	1:A:439:LEU:HB3	2.38	0.53
1:C:322:LEU:O	1:C:325:HIS:HB3	2.09	0.53
1:D:242:ILE:O	1:D:245:ILE:HG23	2.08	0.53
1:D:207:GLU:HA	1:D:249:MET:HE1	1.91	0.53
1:D:385:ALA:O	1:D:386:ILE:C	2.44	0.53
1:D:402:LEU:O	1:D:404:ASP:N	2.42	0.53
1:E:315:ARG:O	1:E:318:ASP:HB2	2.08	0.53
1:A:252:ARG:NE	4:A:2004:HOH:O	2.42	0.53
1:A:161:SER:O	1:A:276:ARG:HG3	2.08	0.53
1:B:151:LEU:O	1:B:155:ILE:HG13	2.08	0.53
1:B:230:VAL:HG23	1:B:231:GLU:N	2.24	0.53
1:A:238:PHE:CD1	1:A:278:ILE:HG22	2.41	0.52
1:B:356:GLY:O	1:B:357:ASN:C	2.48	0.52
1:C:161:SER:O	1:C:276:ARG:HG3	2.10	0.52
1:D:188:ARG:CB	1:D:191:ARG:HD3	2.39	0.52
1:F:316:ARG:HA	1:F:319:ILE:HG13	1.90	0.52
1:A:232:ALA:O	1:A:233:ASP:C	2.46	0.52
1:B:173:THR:OG1	1:B:174:GLY:N	2.41	0.52
1:B:214:GLU:HA	1:B:224:ARG:HB2	1.90	0.52
1:E:324:ASP:CG	1:E:328:ARG:HH12	2.13	0.52
4:E:2006:HOH:O	1:F:363:ASN:HB2	2.09	0.52
1:F:367:ARG:NH2	1:F:382:LEU:O	2.42	0.52
1:C:285:LEU:HB3	1:C:299:TYR:HE1	1.73	0.52
1:D:259:GLU:O	1:D:259:GLU:HG3	2.09	0.52
1:A:312:LEU:HD22	1:A:319:ILE:HG12	1.91	0.52
1:B:248:LEU:HA	1:B:251:VAL:HG23	1.91	0.52
1:C:272:SER:O	1:C:273:VAL:CG1	2.58	0.52
1:E:358:ILE:HG21	3:E:1442:ATP:O4'	2.08	0.52
1:F:145:SER:O	1:F:148:MET:N	2.42	0.52
1:F:202:ASN:OD1	1:F:205:LEU:HG	2.08	0.52
1:F:173:THR:OG1	1:F:309:MET:HE2	2.10	0.52
1:A:182:LEU:HD13	1:A:278:ILE:HD11	1.91	0.52
1:A:365:ILE:HG22	1:A:366:GLU:N	2.22	0.52
1:B:289:VAL:HA	1:B:294:PHE:O	2.09	0.52
1:B:312:LEU:O	1:B:315:ARG:N	2.37	0.52
1:D:160:PRO:CD	1:D:186:SER:OG	2.57	0.52
1:E:142:ILE:O	1:E:142:ILE:CG2	2.58	0.52
1:E:302:LEU:O	1:E:304:VAL:N	2.35	0.52
1:E:341:PHE:HZ	1:E:365:ILE:HD13	1.74	0.52
1:A:259:GLU:O	1:A:261:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:O	1:A:369:VAL:HG12	2.07	0.52
1:B:213:HIS:HD1	1:B:225:ARG:HB2	1.71	0.52
1:C:313:ARG:HH12	1:C:354:TRP:CB	2.22	0.52
1:D:154:GLU:O	1:D:157:MET:N	2.43	0.52
1:E:259:GLU:HG3	1:E:259:GLU:O	2.10	0.52
1:F:191:ARG:HH11	1:F:191:ARG:CG	2.19	0.52
1:F:287:GLU:HA	1:F:290:SER:OG	2.08	0.52
1:A:414:LEU:HD12	1:A:424:ALA:HB2	1.92	0.52
1:C:272:SER:C	1:C:273:VAL:CG1	2.78	0.52
1:C:354:TRP:O	1:C:357:ASN:ND2	2.43	0.52
1:A:415:GLU:HA	1:A:415:GLU:OE1	2.08	0.52
1:E:410:ILE:CD1	1:E:435:LEU:HG	2.39	0.52
1:A:254:LEU:O	1:A:255:ARG:C	2.47	0.52
1:C:296:GLN:O	1:C:299:TYR:N	2.43	0.52
1:D:312:LEU:O	1:D:314:GLN:N	2.43	0.52
1:D:377:ILE:HD12	1:D:378:SER:CA	2.39	0.52
1:F:341:PHE:CD2	1:F:377:ILE:CG1	2.91	0.52
1:B:358:ILE:N	1:B:358:ILE:HD13	2.25	0.52
1:E:258:GLN:OE1	1:E:301:ARG:HD2	2.10	0.52
1:F:169:GLY:O	1:F:175:LYS:NZ	2.42	0.52
1:A:285:LEU:HB3	1:A:299:TYR:CD1	2.45	0.51
1:A:337:VAL:HG12	1:A:337:VAL:O	2.08	0.51
1:A:430:ILE:HD11	1:A:435:LEU:HB2	1.90	0.51
1:C:159:ALA:C	1:C:186:SER:OG	2.48	0.51
1:C:319:ILE:HB	1:C:320:PRO:CD	2.40	0.51
1:E:150:HIS:CE1	1:E:154:GLU:OE1	2.63	0.51
1:B:264:ARG:O	1:B:266:GLY:N	2.42	0.51
1:C:389:THR:HG22	1:C:389:THR:O	2.10	0.51
1:D:315:ARG:NE	1:D:318:ASP:OD2	2.31	0.51
1:E:148:MET:O	1:E:152:LEU:HD11	2.10	0.51
1:E:303:ASN:O	1:E:303:ASN:CG	2.48	0.51
1:D:148:MET:HE3	1:D:152:LEU:HD21	1.88	0.51
1:D:320:PRO:O	1:D:321:LEU:C	2.48	0.51
3:E:1442:ATP:O3G	3:E:1442:ATP:O1A	2.28	0.51
1:E:325:HIS:HE1	1:E:329:ARG:HH21	1.56	0.51
1:F:190:ASP:OD2	1:F:191:ARG:HD2	2.10	0.51
1:C:163:ALA:O	1:C:276:ARG:NH1	2.43	0.51
1:D:327:LEU:HD22	1:D:341:PHE:CE1	2.46	0.51
1:F:173:THR:OG1	1:F:309:MET:CE	2.59	0.51
1:F:263:GLN:NE2	1:F:268:ASN:OD1	2.44	0.51
1:F:318:ASP:O	1:F:321:LEU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:PRO:HA	1:F:346:MET:HE1	1.93	0.51
1:D:352:TYR:HD2	1:D:353:ASP:N	1.69	0.51
1:D:365:ILE:HG22	1:D:366:GLU:N	2.24	0.51
1:E:175:LYS:HG2	1:E:309:MET:HG3	1.91	0.51
1:E:316:ARG:HH12	1:E:354:TRP:HE1	1.57	0.51
1:F:172:GLY:N	2:F:1390:PO4:O1	2.31	0.51
1:F:353:ASP:OD2	1:F:361:LEU:HD13	2.11	0.51
1:E:379:GLU:HB2	4:E:2016:HOH:O	2.10	0.51
1:A:248:LEU:C	1:A:248:LEU:HD23	2.31	0.51
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.75	0.51
1:B:250:GLN:O	1:B:251:VAL:C	2.47	0.51
1:D:169:GLY:O	1:D:175:LYS:HE3	2.11	0.51
1:D:368:ALA:HA	4:D:2017:HOH:O	2.10	0.51
1:E:162:ASP:O	1:E:162:ASP:CG	2.48	0.51
1:E:191:ARG:CB	1:E:192:PRO:CD	2.83	0.51
1:E:203:GLU:OE2	1:E:248:LEU:HB3	2.11	0.51
1:E:365:ILE:O	1:E:366:GLU:C	2.48	0.51
1:F:341:PHE:HD2	1:F:377:ILE:CG1	2.21	0.51
1:A:242:ILE:HG12	1:A:245:ILE:HD13	1.91	0.51
1:B:175:LYS:O	1:B:178:VAL:HB	2.11	0.51
1:C:145:SER:HB2	1:C:317:GLU:OE1	2.11	0.51
1:C:304:VAL:HG12	1:C:305:VAL:N	2.26	0.51
1:D:213:HIS:HA	1:D:265:VAL:H	1.76	0.51
1:E:202:ASN:C	1:E:204:SER:N	2.60	0.51
1:F:191:ARG:HB3	1:F:192:PRO:HD2	1.93	0.51
1:F:204:SER:O	1:F:205:LEU:C	2.49	0.51
1:A:178:VAL:HG21	1:A:309:MET:SD	2.51	0.51
1:A:202:ASN:HD21	1:A:205:LEU:HD12	1.76	0.51
1:E:148:MET:O	1:E:152:LEU:CD1	2.59	0.51
1:E:213:HIS:HB2	1:E:265:VAL:CB	2.41	0.51
1:A:364:ALA:O	1:A:365:ILE:C	2.46	0.51
1:B:257:ILE:CD1	1:B:277:LEU:HD23	2.39	0.51
1:C:337:VAL:C	1:C:338:VAL:HG23	2.30	0.51
1:E:154:GLU:O	1:E:155:ILE:C	2.48	0.51
1:E:370:VAL:O	1:E:370:VAL:HG12	2.11	0.51
1:F:252:ARG:O	1:F:254:LEU:N	2.44	0.51
1:A:254:LEU:HD22	1:A:297:ASP:HB2	1.92	0.50
1:A:309:MET:CA	1:A:309:MET:HE3	2.41	0.50
1:B:321:LEU:CB	4:B:2015:HOH:O	2.25	0.50
1:D:151:LEU:O	1:D:151:LEU:HD22	2.10	0.50
1:A:146:PRO:O	1:A:147:ALA:C	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:CD	1:A:438:LYS:HD3	2.31	0.50
1:C:330:PHE:O	1:C:331:ALA:C	2.49	0.50
1:C:354:TRP:CB	1:C:355:PRO:HD3	2.41	0.50
1:E:434:THR:O	1:E:437:ALA:N	2.41	0.50
1:F:352:TYR:CE2	1:F:353:ASP:HA	2.47	0.50
1:C:259:GLU:HG3	1:C:259:GLU:O	2.12	0.50
1:C:276:ARG:CG	1:C:276:ARG:HH11	2.24	0.50
1:C:320:PRO:HD3	1:C:350:ILE:CG1	2.42	0.50
1:C:365:ILE:O	1:C:367:ARG:N	2.44	0.50
1:E:247:PRO:O	1:E:251:VAL:HG23	2.12	0.50
1:E:238:PHE:HD1	1:E:278:ILE:HG22	1.77	0.50
1:F:276:ARG:NH1	1:F:276:ARG:CG	2.57	0.50
1:F:313:ARG:HH12	1:F:354:TRP:CB	2.25	0.50
1:A:285:LEU:HB3	1:A:299:TYR:CE1	2.47	0.50
1:A:434:THR:O	1:A:437:ALA:N	2.43	0.50
1:E:248:LEU:HD21	4:E:2001:HOH:O	2.10	0.50
1:F:151:LEU:HD22	1:F:151:LEU:O	2.11	0.50
1:F:321:LEU:O	1:F:321:LEU:HD12	2.11	0.50
1:C:352:TYR:HD2	1:C:353:ASP:OD1	1.94	0.50
1:D:244:ASP:OD2	1:D:283:ARG:CZ	2.59	0.50
1:F:246:SER:O	1:F:250:GLN:HG3	2.11	0.50
1:A:202:ASN:ND2	1:A:205:LEU:HD12	2.26	0.50
1:A:311:SER:CB	1:A:314:GLN:HE21	2.23	0.50
1:A:354:TRP:CB	1:A:355:PRO:HD2	2.40	0.50
1:B:338:VAL:HG13	1:B:372:LEU:CD2	2.42	0.50
1:E:439:LEU:C	1:E:439:LEU:HD12	2.32	0.50
1:F:298:LEU:O	1:F:301:ARG:N	2.43	0.50
1:D:154:GLU:O	1:D:155:ILE:C	2.50	0.50
1:D:312:LEU:CD2	1:D:319:ILE:HG12	2.42	0.50
1:E:179:ALA:HA	1:E:182:LEU:HD12	1.94	0.50
1:F:165:VAL:HA	1:F:305:VAL:O	2.12	0.50
1:A:284:ASP:O	1:A:285:LEU:C	2.50	0.49
1:B:262:VAL:HG12	1:B:262:VAL:O	2.11	0.49
1:C:358:ILE:O	1:C:359:ARG:C	2.49	0.49
1:D:319:ILE:CB	1:D:320:PRO:CD	2.90	0.49
1:D:367:ARG:HG2	4:D:2017:HOH:O	2.11	0.49
1:E:250:GLN:HE22	1:E:294:PHE:HA	1.76	0.49
1:E:352:TYR:CE2	1:E:353:ASP:N	2.65	0.49
1:F:348:LEU:O	1:F:351:HIS:N	2.43	0.49
1:F:359:ARG:HG3	1:F:359:ARG:NH1	2.26	0.49
1:A:274:ASP:OD1	1:A:274:ASP:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ILE:N	1:B:279:ALA:O	2.37	0.49
1:D:232:ALA:O	1:D:233:ASP:C	2.50	0.49
1:D:276:ARG:CG	1:D:276:ARG:NH1	2.71	0.49
1:F:309:MET:SD	1:F:310:PRO:HD2	2.52	0.49
1:F:324:ASP:O	1:F:325:HIS:C	2.49	0.49
1:B:261:GLU:C	1:B:262:VAL:HG23	2.32	0.49
1:E:141:MET:SD	1:E:148:MET:HE1	2.52	0.49
1:A:357:ASN:HD22	1:A:357:ASN:N	2.02	0.49
1:D:177:LEU:O	1:D:178:VAL:C	2.45	0.49
1:D:164:THR:CG2	1:D:277:LEU:HB3	2.42	0.49
1:D:320:PRO:HD3	1:D:350:ILE:HG12	1.94	0.49
1:E:213:HIS:CG	1:E:213:HIS:O	2.65	0.49
1:E:230:VAL:HG23	1:E:231:GLU:H	1.76	0.49
1:F:319:ILE:HD12	1:F:350:ILE:HA	1.94	0.49
1:B:304:VAL:HG12	1:B:305:VAL:HG23	1.95	0.49
1:D:163:ALA:O	1:D:276:ARG:NH1	2.46	0.49
1:D:250:GLN:OE1	1:D:295:ARG:HG2	2.12	0.49
1:D:382:LEU:CD1	1:D:386:ILE:HD12	2.43	0.49
1:E:244:ASP:OD1	1:E:283:ARG:NH1	2.45	0.49
1:F:234:GLY:N	1:F:274:ASP:O	2.45	0.49
1:A:212:GLY:O	1:A:264:ARG:CB	2.60	0.49
1:B:312:LEU:HD13	1:B:353:ASP:HB3	1.94	0.49
1:B:379:GLU:HG2	4:B:2019:HOH:O	2.12	0.49
1:D:149:GLN:HA	1:D:152:LEU:HD12	1.95	0.49
1:D:193:LEU:HD12	1:D:236:THR:O	2.13	0.49
1:D:287:GLU:HA	1:D:287:GLU:OE1	2.13	0.49
1:D:320:PRO:HD3	1:D:350:ILE:CG1	2.42	0.49
1:E:173:THR:OG1	1:E:174:GLY:N	2.44	0.49
1:B:145:SER:OG	1:B:148:MET:HB2	2.13	0.49
1:B:191:ARG:HH11	1:B:191:ARG:HG2	1.76	0.49
1:D:213:HIS:CE1	1:D:225:ARG:CB	2.96	0.49
1:E:196:LEU:HD21	1:E:239:LEU:HD23	1.94	0.49
1:E:431:THR:HG22	1:E:433:LYS:N	2.27	0.49
1:F:198:CYS:SG	1:F:239:LEU:HB3	2.53	0.49
1:B:202:ASN:O	1:B:203:GLU:C	2.49	0.49
1:B:213:HIS:CE1	1:B:225:ARG:CG	2.95	0.49
1:C:175:LYS:NZ	2:C:1391:PO4:O4	2.46	0.49
1:C:262:VAL:HG12	1:C:262:VAL:O	2.11	0.49
1:E:288:GLU:OE1	1:E:288:GLU:HA	2.12	0.49
1:F:182:LEU:HD12	1:F:278:ILE:HD13	1.94	0.49
1:B:348:LEU:O	1:B:349:LEU:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ASP:N	1:C:244:ASP:OD1	2.45	0.49
1:C:389:THR:CG2	1:C:389:THR:O	2.60	0.49
1:F:309:MET:CE	1:F:310:PRO:HD2	2.41	0.49
1:A:159:ALA:O	1:A:160:PRO:C	2.51	0.49
1:A:164:THR:CG2	1:A:277:LEU:HB3	2.26	0.49
1:A:254:LEU:HD21	1:A:297:ASP:HB2	1.94	0.49
1:C:313:ARG:HH12	1:C:354:TRP:CA	2.26	0.49
1:E:160:PRO:N	1:E:186:SER:OG	2.46	0.49
1:E:288:GLU:OE1	1:E:288:GLU:CA	2.60	0.49
1:E:415:GLU:OE1	1:E:415:GLU:HA	2.12	0.49
1:F:151:LEU:HD21	1:F:307:ILE:HG21	1.95	0.49
1:A:423:GLU:O	1:A:424:ALA:C	2.49	0.48
1:A:439:LEU:HD12	1:A:440:SER:N	2.28	0.48
1:B:244:ASP:CG	1:B:283:ARG:NH1	2.66	0.48
1:C:284:ASP:O	1:C:285:LEU:C	2.50	0.48
1:E:354:TRP:HB2	1:E:355:PRO:CD	2.42	0.48
1:A:155:ILE:HG23	1:A:182:LEU:HD23	1.95	0.48
1:B:214:GLU:HG3	1:B:224:ARG:NH2	2.24	0.48
1:C:172:GLY:N	2:C:1391:PO4:O4	2.42	0.48
1:D:252:ARG:O	1:D:253:LEU:C	2.51	0.48
1:E:145:SER:CB	1:E:146:PRO:CD	2.84	0.48
1:E:377:ILE:HD12	1:E:378:SER:CA	2.40	0.48
1:B:239:LEU:HD11	1:B:277:LEU:HD11	1.91	0.48
1:E:149:GLN:O	1:E:150:HIS:C	2.51	0.48
1:C:254:LEU:HD21	1:C:297:ASP:HB2	1.94	0.48
1:B:167:ILE:O	1:B:280:ALA:HA	2.14	0.48
1:B:262:VAL:O	1:B:263:GLN:O	2.31	0.48
1:C:162:ASP:OD1	1:C:162:ASP:O	2.31	0.48
1:C:272:SER:O	1:C:273:VAL:HG12	2.13	0.48
1:E:316:ARG:HA	1:E:319:ILE:HG13	1.96	0.48
1:E:351:HIS:O	1:E:354:TRP:CZ2	2.67	0.48
1:B:375:GLU:O	4:B:2018:HOH:O	2.19	0.48
1:E:370:VAL:CG1	1:E:370:VAL:O	2.58	0.48
1:F:142:ILE:CD1	1:F:142:ILE:H	2.25	0.48
1:A:183:HIS:CG	1:A:193:LEU:HD22	2.49	0.48
1:D:148:MET:HE3	1:D:152:LEU:CD2	2.43	0.48
1:E:356:GLY:O	1:E:357:ASN:O	2.31	0.48
1:F:150:HIS:CE1	1:F:154:GLU:OE1	2.67	0.48
1:A:276:ARG:CG	1:A:276:ARG:HH11	2.27	0.48
1:F:166:LEU:HA	1:F:279:ALA:O	2.13	0.48
1:F:327:LEU:HD22	1:F:341:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HD23	1:A:248:LEU:O	2.14	0.48
1:A:277:LEU:HD12	1:A:278:ILE:N	2.29	0.48
1:A:378:SER:O	1:A:379:GLU:C	2.52	0.48
1:D:273:VAL:HG23	1:D:273:VAL:O	2.11	0.48
1:A:176:GLU:OE1	1:A:180:ARG:NH2	2.47	0.48
1:A:270:THR:CG2	1:A:270:THR:O	2.56	0.48
1:C:158:VAL:O	1:C:160:PRO:HD2	2.14	0.48
1:D:252:ARG:C	1:D:254:LEU:N	2.65	0.48
1:F:145:SER:O	1:F:146:PRO:C	2.52	0.48
1:A:296:GLN:O	1:A:297:ASP:C	2.52	0.47
1:B:213:HIS:CE1	1:B:225:ARG:CB	2.94	0.47
1:B:213:HIS:HE1	1:B:225:ARG:CG	2.27	0.47
1:D:209:GLU:O	1:D:228:ARG:HG2	2.14	0.47
1:D:339:LYS:HD2	1:D:339:LYS:HA	1.56	0.47
1:D:328:ARG:CZ	1:D:339:LYS:HE2	2.44	0.47
1:E:281:THR:OG1	1:E:282:HIS:N	2.47	0.47
1:E:351:HIS:O	1:E:354:TRP:HZ2	1.97	0.47
1:E:359:ARG:CG	1:E:359:ARG:NH1	2.73	0.47
1:F:277:LEU:HD12	1:F:277:LEU:HA	1.70	0.47
1:F:312:LEU:HG	1:F:358:ILE:CD1	2.44	0.47
1:A:369:VAL:O	1:A:370:VAL:C	2.51	0.47
1:A:436:LEU:HA	1:A:436:LEU:HD23	1.42	0.47
1:B:180:ARG:O	1:B:183:HIS:HB3	2.14	0.47
1:E:149:GLN:HA	1:E:152:LEU:CD1	2.39	0.47
1:F:229:PHE:O	1:F:230:VAL:C	2.52	0.47
1:B:145:SER:OG	1:B:148:MET:HB3	2.15	0.47
1:E:161:SER:O	1:E:276:ARG:HG3	2.14	0.47
1:E:435:LEU:HD23	1:E:436:LEU:N	2.30	0.47
1:F:182:LEU:HB3	1:F:278:ILE:HD11	1.94	0.47
1:F:269:GLN:O	1:F:271:ILE:HG13	2.14	0.47
1:F:285:LEU:HB3	1:F:299:TYR:CD1	2.49	0.47
1:B:210:LEU:HD21	1:B:239:LEU:HD21	1.95	0.47
1:C:326:PHE:CD2	1:C:362:GLU:HG3	2.49	0.47
1:E:284:ASP:O	1:E:284:ASP:OD1	2.31	0.47
1:E:354:TRP:H	1:E:355:PRO:HD3	1.79	0.47
1:B:248:LEU:HA	1:B:251:VAL:CG2	2.44	0.47
1:B:316:ARG:HG2	4:B:2014:HOH:O	2.14	0.47
1:C:206:LEU:HD23	1:C:249:MET:SD	2.54	0.47
1:C:386:ILE:CG1	1:C:387:ALA:N	2.66	0.47
1:A:305:VAL:HG12	1:A:305:VAL:O	2.14	0.47
1:E:344:GLN:HB3	4:E:2013:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASN:O	1:A:203:GLU:C	2.52	0.47
1:A:260:ARG:NH1	1:A:275:VAL:H	2.13	0.47
1:A:342:THR:HG23	1:A:377:ILE:O	2.14	0.47
1:A:438:LYS:NZ	4:A:2016:HOH:O	2.31	0.47
1:C:309:MET:CE	1:C:310:PRO:HD2	2.44	0.47
1:C:326:PHE:O	1:C:327:LEU:C	2.51	0.47
1:D:196:LEU:C	1:D:196:LEU:HD23	2.34	0.47
1:C:161:SER:HB2	1:C:187:ALA:HB3	1.97	0.47
1:C:213:HIS:O	1:C:225:ARG:N	2.48	0.47
1:D:146:PRO:O	1:D:149:GLN:N	2.47	0.47
1:E:197:ASN:C	1:E:197:ASN:OD1	2.53	0.47
1:F:166:LEU:HD11	1:F:281:THR:HG22	1.97	0.47
1:F:253:LEU:O	1:F:257:ILE:HG13	2.15	0.47
1:F:356:GLY:O	1:F:357:ASN:O	2.32	0.47
1:A:165:VAL:HG12	1:A:165:VAL:O	2.14	0.47
1:A:206:LEU:O	1:A:210:LEU:HB2	2.15	0.47
1:B:247:PRO:HG2	1:B:248:LEU:H	1.79	0.47
1:C:365:ILE:C	1:C:367:ARG:N	2.66	0.47
1:E:226:GLU:HG2	1:E:230:VAL:CG2	2.37	0.47
1:E:247:PRO:O	1:E:250:GLN:HB2	2.15	0.47
1:F:148:MET:CE	1:F:152:LEU:CD2	2.82	0.47
1:F:169:GLY:O	1:F:170:ASP:C	2.50	0.47
1:F:327:LEU:HD11	1:F:338:VAL:HG11	1.95	0.47
1:A:182:LEU:CD1	1:A:278:ILE:CD1	2.93	0.47
1:B:377:ILE:HD12	1:B:378:SER:CA	2.45	0.47
1:C:230:VAL:C	1:C:232:ALA:H	2.18	0.47
1:C:354:TRP:HD1	1:C:354:TRP:N	2.11	0.47
1:C:378:SER:H	1:C:381:GLU:HG3	1.80	0.47
1:D:312:LEU:HD22	1:D:319:ILE:HG12	1.97	0.47
1:E:230:VAL:HG23	1:E:231:GLU:N	2.29	0.47
1:F:208:SER:HB3	1:F:213:HIS:ND1	2.30	0.47
1:A:250:GLN:OE1	1:A:295:ARG:HG2	2.15	0.47
1:B:146:PRO:O	1:B:149:GLN:N	2.45	0.47
1:C:367:ARG:HH21	1:C:383:PRO:CA	2.27	0.47
1:D:175:LYS:O	1:D:176:GLU:C	2.53	0.47
1:D:233:ASP:OD2	1:D:273:VAL:HG12	2.15	0.47
1:F:330:PHE:CE2	1:F:366:GLU:HB2	2.49	0.47
1:A:284:ASP:O	1:A:287:GLU:N	2.48	0.46
1:A:383:PRO:O	1:A:384:LEU:C	2.54	0.46
1:C:202:ASN:O	1:C:203:GLU:C	2.54	0.46
1:E:323:ALA:O	1:E:324:ASP:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:ALA:O	1:E:414:LEU:C	2.52	0.46
1:A:402:LEU:O	1:A:403:VAL:C	2.52	0.46
1:B:336:LYS:NZ	1:B:372:LEU:O	2.35	0.46
1:C:210:LEU:HA	1:C:210:LEU:HD23	1.68	0.46
1:C:312:LEU:HD12	1:C:357:ASN:CA	2.45	0.46
1:D:318:ASP:O	1:D:320:PRO:N	2.48	0.46
1:E:230:VAL:C	1:E:232:ALA:N	2.68	0.46
1:E:285:LEU:HD12	1:E:285:LEU:HA	1.39	0.46
1:F:165:VAL:HG22	1:F:305:VAL:CG1	2.45	0.46
1:A:148:MET:HE1	1:A:152:LEU:CD2	2.40	0.46
1:B:296:GLN:O	1:B:299:TYR:HB3	2.15	0.46
1:B:339:LYS:N	4:B:2018:HOH:O	2.46	0.46
1:D:216:GLY:O	1:D:217:ALA:C	2.53	0.46
1:D:300:TYR:CE1	1:E:360:GLU:HB2	2.50	0.46
1:D:431:THR:HG22	1:D:433:LYS:H	1.80	0.46
1:E:437:ALA:C	1:E:439:LEU:N	2.68	0.46
1:F:316:ARG:O	1:F:318:ASP:N	2.48	0.46
1:A:346:MET:O	1:A:350:ILE:HG13	2.14	0.46
1:B:141:MET:HG3	1:B:148:MET:HE2	1.97	0.46
1:B:322:LEU:O	1:B:325:HIS:HB3	2.15	0.46
1:D:159:ALA:C	1:D:186:SER:CB	2.84	0.46
1:D:382:LEU:HB2	1:D:386:ILE:HD12	1.98	0.46
1:F:237:LEU:HG	1:F:239:LEU:CD1	2.45	0.46
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.72	0.46
1:C:178:VAL:HG21	1:C:309:MET:SD	2.55	0.46
1:C:188:ARG:NH1	1:C:235:GLY:O	2.48	0.46
1:D:151:LEU:O	1:D:155:ILE:HG13	2.16	0.46
1:D:415:GLU:HA	1:D:415:GLU:OE1	2.16	0.46
1:E:348:LEU:O	1:E:349:LEU:C	2.54	0.46
1:F:154:GLU:O	1:F:155:ILE:C	2.53	0.46
1:F:191:ARG:NH1	1:F:191:ARG:HG3	2.27	0.46
1:A:143:GLY:O	1:A:144:SER:HB3	2.15	0.46
1:C:228:ARG:O	1:C:229:PHE:C	2.52	0.46
1:E:208:SER:O	1:E:209:GLU:C	2.53	0.46
1:C:160:PRO:CA	1:C:186:SER:OG	2.64	0.46
1:C:201:LEU:HG	1:C:201:LEU:H	1.57	0.46
1:D:282:HIS:O	1:D:282:HIS:CD2	2.69	0.46
1:E:421:LYS:O	1:E:422:THR:C	2.53	0.46
1:F:257:ILE:CD1	1:F:277:LEU:HD22	2.46	0.46
1:D:250:GLN:CD	1:D:294:PHE:HA	2.36	0.46
1:F:167:ILE:O	1:F:280:ALA:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:ARG:HH11	1:F:276:ARG:HG3	1.74	0.46
1:B:195:THR:HB	1:B:238:PHE:HB3	1.99	0.45
1:B:229:PHE:HD2	1:B:275:VAL:HG21	1.80	0.45
1:C:197:ASN:OD1	1:C:199:ALA:HB2	2.15	0.45
1:C:377:ILE:CD1	1:C:382:LEU:CD2	2.94	0.45
1:C:364:ALA:HB2	1:C:383:PRO:HG3	1.98	0.45
1:D:319:ILE:HG21	1:D:350:ILE:HA	1.97	0.45
1:E:281:THR:HG23	1:E:283:ARG:H	1.80	0.45
1:F:243:GLY:N	4:F:2005:HOH:O	2.34	0.45
1:B:296:GLN:O	1:B:300:TYR:N	2.42	0.45
1:D:363:ASN:OD1	1:D:364:ALA:N	2.49	0.45
1:E:320:PRO:HG2	1:E:321:LEU:H	1.81	0.45
1:E:341:PHE:HZ	1:E:365:ILE:CD1	2.28	0.45
1:A:309:MET:CA	1:A:309:MET:CE	2.93	0.45
1:B:166:LEU:HD21	1:B:285:LEU:CD2	2.42	0.45
1:C:230:VAL:C	1:C:232:ALA:N	2.66	0.45
1:D:257:ILE:HD13	1:D:277:LEU:HD23	1.99	0.45
1:F:282:HIS:O	1:F:282:HIS:HD2	1.91	0.45
1:F:344:GLN:OE1	1:F:344:GLN:HA	2.17	0.45
1:A:315:ARG:O	1:A:316:ARG:C	2.55	0.45
1:A:322:LEU:O	1:A:323:ALA:C	2.54	0.45
1:A:330:PHE:CE1	1:A:366:GLU:HB2	2.52	0.45
1:D:277:LEU:HD12	1:D:278:ILE:H	1.81	0.45
1:E:159:ALA:CB	1:E:186:SER:OG	2.64	0.45
1:E:254:LEU:O	1:E:255:ARG:C	2.55	0.45
1:E:297:ASP:OD1	1:E:298:LEU:N	2.46	0.45
1:F:242:ILE:HD11	1:F:253:LEU:CD2	2.46	0.45
1:F:257:ILE:HD11	1:F:277:LEU:HD22	1.98	0.45
1:B:188:ARG:NH2	1:B:274:ASP:OD1	2.50	0.45
1:B:385:ALA:C	1:B:387:ALA:N	2.63	0.45
1:C:183:HIS:HD2	1:C:236:THR:HB	1.82	0.45
1:C:284:ASP:O	1:C:284:ASP:OD1	2.35	0.45
1:C:356:GLY:O	1:C:357:ASN:C	2.55	0.45
1:D:213:HIS:HB2	1:D:265:VAL:CB	2.47	0.45
1:D:275:VAL:HG12	1:D:276:ARG:N	2.30	0.45
1:D:313:ARG:HH11	1:D:313:ARG:HB3	1.80	0.45
1:E:239:LEU:HD12	1:E:277:LEU:HD11	1.99	0.45
1:E:365:ILE:O	1:E:368:ALA:N	2.50	0.45
1:F:313:ARG:NH1	1:F:354:TRP:CD1	2.84	0.45
1:F:380:ARG:C	1:F:381:GLU:HG2	2.36	0.45
1:A:159:ALA:O	1:A:276:ARG:NH2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:HIS:CD2	1:A:213:HIS:O	2.69	0.45
1:A:182:LEU:CD1	1:A:278:ILE:HD13	2.44	0.45
1:A:312:LEU:O	1:A:313:ARG:C	2.54	0.45
1:B:260:ARG:HB3	1:B:273:VAL:O	2.15	0.45
1:D:401:PRO:HG2	1:D:404:ASP:OD1	2.17	0.45
1:E:159:ALA:HB1	1:E:186:SER:CB	2.47	0.45
1:E:251:VAL:O	1:E:254:LEU:HB3	2.17	0.45
1:F:262:VAL:HG12	1:F:262:VAL:O	2.15	0.45
1:A:410:ILE:CD1	1:A:439:LEU:HD23	2.41	0.45
1:C:160:PRO:CD	1:C:186:SER:OG	2.64	0.45
1:C:380:ARG:H	1:C:380:ARG:HD3	1.82	0.45
1:D:207:GLU:HA	1:D:249:MET:CE	2.47	0.45
1:D:436:LEU:HA	1:D:436:LEU:HD23	1.71	0.45
1:F:309:MET:HE1	1:F:310:PRO:HD2	1.97	0.45
1:F:339:LYS:HD2	1:F:339:LYS:HA	1.58	0.45
1:A:253:LEU:O	1:A:257:ILE:HG13	2.17	0.45
1:A:267:SER:OG	1:A:269:GLN:HG3	2.16	0.45
1:A:316:ARG:O	1:A:318:ASP:N	2.49	0.45
1:A:348:LEU:H	1:A:348:LEU:CD1	2.30	0.45
1:A:358:ILE:H	1:A:358:ILE:HD13	1.82	0.45
1:B:206:LEU:HD21	1:B:249:MET:HE2	1.97	0.45
1:C:175:LYS:O	1:C:176:GLU:C	2.55	0.45
1:D:312:LEU:O	1:D:313:ARG:C	2.56	0.45
1:E:238:PHE:HA	1:E:278:ILE:O	2.17	0.45
1:F:288:GLU:O	1:F:289:VAL:C	2.50	0.45
1:B:159:ALA:C	1:B:186:SER:HB2	2.36	0.45
1:B:322:LEU:HA	1:B:322:LEU:HD12	1.68	0.45
1:B:359:ARG:HH12	1:C:297:ASP:HB3	1.81	0.45
1:C:238:PHE:HD1	1:C:278:ILE:O	1.98	0.45
1:C:233:ASP:OD2	1:C:273:VAL:HA	2.16	0.45
1:E:141:MET:CE	1:E:148:MET:CE	2.95	0.45
1:E:169:GLY:O	1:E:170:ASP:C	2.52	0.45
1:E:285:LEU:HB3	1:E:299:TYR:CE1	2.52	0.45
1:F:183:HIS:HB2	1:F:193:LEU:HD22	1.99	0.45
1:A:190:ASP:OD2	1:A:191:ARG:HD2	2.17	0.45
1:A:319:ILE:HB	1:A:320:PRO:CD	2.47	0.45
1:C:159:ALA:O	1:C:160:PRO:C	2.54	0.45
1:D:141:MET:SD	1:D:148:MET:CE	3.03	0.45
1:E:313:ARG:HH12	1:E:354:TRP:CB	2.15	0.45
1:F:296:GLN:O	1:F:297:ASP:C	2.53	0.45
1:F:309:MET:HE3	1:F:309:MET:HB3	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:C	1:B:251:VAL:HG23	2.36	0.44
1:C:155:ILE:HD11	1:C:178:VAL:CG1	2.46	0.44
1:C:240:ASP:O	1:C:241:GLU:HB2	2.17	0.44
1:D:318:ASP:O	1:D:321:LEU:N	2.50	0.44
1:D:383:PRO:O	1:D:386:ILE:CG2	2.64	0.44
1:D:430:ILE:HB	1:D:434:THR:HG21	2.00	0.44
1:E:411:LEU:HD13	1:E:411:LEU:HA	1.78	0.44
1:F:319:ILE:HB	1:F:320:PRO:HD3	1.98	0.44
1:A:282:HIS:CD2	1:A:282:HIS:O	2.71	0.44
1:A:431:THR:HG21	1:A:433:LYS:HB3	1.98	0.44
1:B:165:VAL:CG1	1:B:166:LEU:N	2.77	0.44
1:D:146:PRO:O	1:D:147:ALA:C	2.53	0.44
1:D:344:GLN:CB	4:D:2015:HOH:O	2.61	0.44
1:E:304:VAL:CG1	1:E:305:VAL:HG23	2.38	0.44
1:F:158:VAL:HG11	1:F:305:VAL:HG11	1.98	0.44
1:B:179:ALA:O	1:B:180:ARG:C	2.55	0.44
1:B:196:LEU:HD21	1:B:239:LEU:HD23	1.98	0.44
1:B:251:VAL:O	1:B:255:ARG:HG3	2.17	0.44
1:C:277:LEU:C	1:C:278:ILE:HG13	2.38	0.44
1:E:193:LEU:CD1	1:E:236:THR:HG22	2.47	0.44
1:F:226:GLU:HG2	1:F:230:VAL:HG21	1.99	0.44
1:A:296:GLN:O	1:A:299:TYR:N	2.51	0.44
1:B:354:TRP:HZ2	4:B:2017:HOH:O	2.01	0.44
1:C:159:ALA:C	1:C:186:SER:CB	2.86	0.44
1:E:238:PHE:CD1	1:E:278:ILE:HG22	2.53	0.44
1:F:276:ARG:NH1	1:F:276:ARG:HG3	2.30	0.44
1:F:313:ARG:NH1	1:F:354:TRP:CB	2.80	0.44
1:B:153:ASN:HD21	1:E:343:PRO:HA	1.81	0.44
1:B:159:ALA:N	1:B:160:PRO:CD	2.80	0.44
1:B:233:ASP:OD2	1:B:274:ASP:N	2.43	0.44
1:B:248:LEU:CA	1:B:251:VAL:HG23	2.47	0.44
1:B:285:LEU:HA	1:B:285:LEU:HD12	1.26	0.44
1:D:252:ARG:O	1:D:254:LEU:N	2.50	0.44
1:E:432:ARG:HH11	1:E:432:ARG:HG2	1.81	0.44
1:F:202:ASN:O	1:F:203:GLU:C	2.55	0.44
1:F:353:ASP:N	1:F:353:ASP:OD1	2.47	0.44
1:A:191:ARG:HG2	1:A:234:GLY:O	2.18	0.44
1:A:277:LEU:HD12	1:A:278:ILE:H	1.83	0.44
1:A:420:ASN:C	1:A:420:ASN:OD1	2.56	0.44
1:D:271:ILE:HG22	1:D:272:SER:N	2.30	0.44
1:D:284:ASP:OD1	1:D:284:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:TRP:O	1:E:356:GLY:N	2.50	0.44
1:F:316:ARG:CZ	1:F:354:TRP:HE1	2.30	0.44
1:F:365:ILE:O	1:F:366:GLU:C	2.54	0.44
1:A:252:ARG:HD3	4:A:2004:HOH:O	2.18	0.44
1:B:311:SER:HB2	1:B:314:GLN:HE21	1.82	0.44
1:B:330:PHE:CE2	1:B:366:GLU:HB2	2.52	0.44
1:D:233:ASP:CG	1:D:273:VAL:HG12	2.38	0.44
1:E:204:SER:OG	1:E:205:LEU:N	2.50	0.44
1:E:295:ARG:HE	1:E:297:ASP:CG	2.20	0.44
1:F:316:ARG:NH2	1:F:354:TRP:HZ2	1.93	0.44
1:A:412:ALA:O	1:A:413:ALA:C	2.54	0.44
1:A:435:LEU:HD23	1:A:435:LEU:C	2.38	0.44
1:B:176:GLU:O	1:B:179:ALA:N	2.50	0.44
1:B:149:GLN:OE1	4:B:2001:HOH:O	2.21	0.44
1:B:262:VAL:HG12	1:B:263:GLN:O	2.18	0.44
1:C:151:LEU:HD22	1:C:151:LEU:C	2.37	0.44
1:C:188:ARG:CB	1:C:191:ARG:HD2	2.45	0.44
1:C:377:ILE:HD13	1:C:382:LEU:CD2	2.48	0.44
1:D:348:LEU:H	1:D:348:LEU:HD12	1.83	0.44
1:E:349:LEU:O	1:E:350:ILE:C	2.56	0.44
1:F:160:PRO:HD3	1:F:186:SER:HB2	2.00	0.44
1:A:322:LEU:O	1:A:325:HIS:HB3	2.18	0.43
1:B:239:LEU:HD12	1:B:277:LEU:CD1	2.45	0.43
1:B:242:ILE:HG23	1:B:242:ILE:O	2.18	0.43
1:D:354:TRP:CB	1:D:355:PRO:HD3	2.35	0.43
1:A:226:GLU:HG2	1:A:230:VAL:HG21	1.99	0.43
1:A:285:LEU:HA	1:A:285:LEU:HD12	1.33	0.43
1:A:339:LYS:HB3	4:A:2012:HOH:O	2.18	0.43
1:B:159:ALA:N	1:B:160:PRO:HD2	2.29	0.43
1:C:194:VAL:CG2	1:C:232:ALA:HB2	2.48	0.43
1:C:232:ALA:O	1:C:233:ASP:C	2.55	0.43
1:C:337:VAL:O	1:C:338:VAL:CG2	2.66	0.43
1:E:174:GLY:O	1:E:175:LYS:C	2.52	0.43
1:E:198:CYS:O	1:E:199:ALA:C	2.57	0.43
1:A:254:LEU:HD11	1:A:258:GLN:NE2	2.34	0.43
1:A:211:PHE:CD2	1:A:262:VAL:HG13	2.53	0.43
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.57	0.43
1:A:377:ILE:HD13	1:A:381:GLU:HB2	1.99	0.43
1:D:142:ILE:CG2	1:D:321:LEU:HG	2.43	0.43
1:D:382:LEU:HD12	1:D:386:ILE:CD1	2.47	0.43
1:E:142:ILE:O	1:E:142:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ARG:NH1	1:F:191:ARG:CG	2.76	0.43
1:F:344:GLN:O	1:F:347:ASP:HB3	2.18	0.43
4:E:2006:HOH:O	1:F:363:ASN:HA	2.18	0.43
1:A:284:ASP:CG	1:A:287:GLU:HB2	2.39	0.43
1:A:312:LEU:CD1	1:A:358:ILE:HD12	2.48	0.43
1:B:353:ASP:OD2	1:B:361:LEU:HD13	2.17	0.43
1:C:276:ARG:CG	1:C:276:ARG:NH1	2.82	0.43
1:C:352:TYR:CD2	1:C:353:ASP:OD1	2.71	0.43
1:D:215:LYS:HE2	1:D:215:LYS:HB3	1.71	0.43
1:D:326:PHE:O	1:D:329:ARG:N	2.51	0.43
1:E:324:ASP:OD1	1:E:328:ARG:NH1	2.48	0.43
1:B:313:ARG:N	4:B:2013:HOH:O	2.28	0.43
1:D:142:ILE:HB	1:D:322:LEU:HD13	2.01	0.43
1:E:356:GLY:O	1:E:357:ASN:C	2.56	0.43
1:A:197:ASN:C	1:A:197:ASN:OD1	2.57	0.43
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.67	0.43
1:B:328:ARG:NH2	1:B:339:LYS:HE2	2.34	0.43
1:B:352:TYR:HA	1:B:354:TRP:CD1	2.49	0.43
1:B:356:GLY:O	1:B:360:GLU:HB3	2.17	0.43
1:D:244:ASP:OD2	1:D:283:ARG:NH1	2.51	0.43
1:D:336:LYS:HE3	1:D:336:LYS:CA	2.38	0.43
1:E:406:GLU:CD	1:E:438:LYS:HD3	2.39	0.43
1:D:211:PHE:O	1:D:227:GLY:HA2	2.18	0.43
1:A:344:GLN:CA	1:A:344:GLN:OE1	2.67	0.43
1:A:435:LEU:O	1:A:439:LEU:HG	2.18	0.43
1:B:259:GLU:CG	1:B:259:GLU:O	2.66	0.43
1:C:352:TYR:CE1	4:C:2016:HOH:O	2.32	0.43
1:C:384:LEU:C	1:C:386:ILE:H	2.21	0.43
1:E:213:HIS:CD2	1:E:213:HIS:O	2.72	0.43
1:E:313:ARG:CG	1:E:313:ARG:HH11	2.30	0.43
1:B:254:LEU:O	1:B:258:GLN:HB2	2.19	0.43
1:B:376:TYR:HA	4:B:2018:HOH:O	2.18	0.43
1:E:142:ILE:HG23	1:E:321:LEU:HG	2.00	0.43
1:A:230:VAL:O	1:A:232:ALA:N	2.51	0.43
1:A:360:GLU:HB2	1:B:300:TYR:CE2	2.53	0.43
1:A:431:THR:HG22	1:A:432:ARG:N	2.34	0.43
1:B:142:ILE:N	1:B:142:ILE:HD12	2.34	0.43
1:E:151:LEU:C	1:E:151:LEU:HD22	2.36	0.43
1:E:330:PHE:CE1	1:E:366:GLU:HB2	2.53	0.43
1:F:257:ILE:HD11	1:F:277:LEU:CD2	2.49	0.43
1:F:278:ILE:HG21	1:F:278:ILE:HD13	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ARG:NH2	1:F:383:PRO:HA	2.33	0.43
1:A:200:ALA:O	1:A:201:LEU:C	2.57	0.42
1:B:230:VAL:O	1:B:233:ASP:N	2.35	0.42
1:B:212:GLY:HA3	1:B:264:ARG:CB	2.48	0.42
1:C:337:VAL:O	1:C:338:VAL:HG23	2.19	0.42
1:C:351:HIS:CG	1:C:351:HIS:O	2.72	0.42
1:F:177:LEU:O	1:F:180:ARG:N	2.52	0.42
1:F:319:ILE:N	1:F:320:PRO:HD2	2.33	0.42
1:A:242:ILE:HD12	1:A:279:ALA:HB1	2.01	0.42
1:A:367:ARG:HB3	4:A:2013:HOH:O	2.19	0.42
1:A:371:LEU:O	1:B:157:MET:HE2	2.19	0.42
1:B:352:TYR:O	1:B:353:ASP:C	2.54	0.42
1:D:184:ALA:N	4:D:2003:HOH:O	2.51	0.42
1:D:285:LEU:O	1:D:288:GLU:N	2.52	0.42
1:D:410:ILE:HD11	1:D:439:LEU:HB3	2.01	0.42
1:E:358:ILE:O	1:E:359:ARG:C	2.56	0.42
1:F:142:ILE:HG22	1:F:143:GLY:CA	2.49	0.42
1:F:194:VAL:HG13	1:F:228:ARG:HH11	1.84	0.42
1:B:312:LEU:HB2	1:B:357:ASN:HB3	2.01	0.42
1:B:323:ALA:O	1:B:324:ASP:C	2.55	0.42
1:C:298:LEU:O	1:C:298:LEU:HD12	2.18	0.42
1:C:364:ALA:CB	1:C:383:PRO:HG3	2.49	0.42
1:D:330:PHE:CE1	1:D:366:GLU:HB2	2.55	0.42
1:F:159:ALA:N	1:F:160:PRO:HD2	2.35	0.42
1:F:254:LEU:O	1:F:255:ARG:C	2.57	0.42
1:F:378:SER:O	1:F:379:GLU:C	2.58	0.42
1:A:339:LYS:HD2	1:A:339:LYS:HA	1.77	0.42
1:B:247:PRO:O	1:B:248:LEU:C	2.57	0.42
1:B:338:VAL:HG22	1:B:372:LEU:HD23	2.00	0.42
1:D:312:LEU:HD12	1:D:357:ASN:HA	2.00	0.42
1:E:342:THR:HG23	1:E:378:SER:HA	2.01	0.42
1:E:378:SER:O	1:E:379:GLU:C	2.57	0.42
1:F:152:LEU:O	1:F:153:ASN:C	2.57	0.42
1:F:312:LEU:HG	1:F:358:ILE:HD11	2.00	0.42
1:A:312:LEU:HD12	1:A:357:ASN:C	2.39	0.42
1:A:352:TYR:CD2	1:A:353:ASP:CA	3.01	0.42
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.16	0.42
1:A:434:THR:HG22	1:A:435:LEU:N	2.34	0.42
1:A:437:ALA:C	1:A:439:LEU:H	2.23	0.42
1:B:166:LEU:CD2	1:B:285:LEU:HD23	2.44	0.42
1:B:158:VAL:HG22	1:B:305:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:THR:HG22	1:C:165:VAL:N	2.34	0.42
1:C:303:ASN:CG	1:C:303:ASN:O	2.58	0.42
1:D:352:TYR:O	1:D:354:TRP:CD1	2.73	0.42
1:F:284:ASP:O	1:F:285:LEU:C	2.56	0.42
1:F:151:LEU:HD21	1:F:307:ILE:CG2	2.49	0.42
1:A:248:LEU:CD2	1:A:252:ARG:HG3	2.49	0.42
1:A:142:ILE:CG2	1:A:321:LEU:HG	2.47	0.42
1:C:260:ARG:O	1:C:273:VAL:N	2.52	0.42
1:C:275:VAL:CG1	1:C:276:ARG:N	2.83	0.42
1:D:213:HIS:CB	1:D:265:VAL:CB	2.97	0.42
1:E:233:ASP:OD2	1:E:273:VAL:CG1	2.57	0.42
1:F:145:SER:HB2	1:F:317:GLU:OE1	2.19	0.42
1:F:242:ILE:HG12	1:F:245:ILE:HD13	2.01	0.42
1:F:238:PHE:HA	1:F:278:ILE:O	2.20	0.42
1:F:296:GLN:O	1:F:299:TYR:N	2.52	0.42
1:F:378:SER:H	1:F:381:GLU:HG3	1.84	0.42
1:B:176:GLU:O	1:B:177:LEU:C	2.57	0.42
1:C:142:ILE:HG22	1:C:318:ASP:CG	2.38	0.42
1:C:159:ALA:O	1:C:186:SER:CB	2.68	0.42
1:C:159:ALA:HB1	1:C:186:SER:HB2	2.02	0.42
1:D:250:GLN:HE22	1:D:294:PHE:CA	2.23	0.42
1:E:243:GLY:O	1:E:244:ASP:OD1	2.37	0.42
1:E:404:ASP:N	1:E:404:ASP:OD1	2.53	0.42
1:F:142:ILE:HG22	1:F:143:GLY:HA3	2.02	0.42
1:A:410:ILE:O	1:A:410:ILE:HG13	2.18	0.42
1:B:296:GLN:O	1:B:297:ASP:C	2.58	0.42
1:C:212:GLY:HA2	1:C:226:GLU:O	2.19	0.42
1:E:204:SER:O	1:E:207:GLU:N	2.53	0.42
1:E:214:GLU:CB	1:E:267:SER:H	2.33	0.42
1:E:239:LEU:HD11	1:E:277:LEU:HD11	2.00	0.42
1:F:352:TYR:CD2	1:F:353:ASP:OD1	2.73	0.42
1:A:437:ALA:C	1:A:439:LEU:N	2.70	0.42
1:D:141:MET:HG2	1:D:141:MET:H	1.73	0.42
1:E:176:GLU:HB3	3:E:1442:ATP:O1B	2.20	0.42
1:E:253:LEU:C	1:E:253:LEU:HD12	2.35	0.42
1:E:315:ARG:HD3	1:E:315:ARG:HH11	1.73	0.42
1:F:199:ALA:O	1:F:200:ALA:HB2	2.20	0.42
1:B:211:PHE:CE1	1:B:252:ARG:HB3	2.55	0.42
1:B:240:ASP:OD2	1:B:241:GLU:N	2.53	0.42
1:B:239:LEU:HB2	1:B:242:ILE:HD12	2.01	0.42
1:C:345:ALA:O	1:C:346:MET:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ILE:HD13	1:C:358:ILE:H	1.84	0.42
1:D:213:HIS:HA	1:D:265:VAL:CB	2.50	0.42
1:D:414:LEU:HD12	1:D:414:LEU:HA	1.64	0.42
1:E:309:MET:HE3	1:E:309:MET:HB3	1.78	0.42
1:F:208:SER:O	1:F:209:GLU:C	2.57	0.42
1:F:238:PHE:HD1	1:F:278:ILE:O	2.03	0.42
1:F:386:ILE:C	1:F:386:ILE:HD12	2.39	0.42
1:A:428:LEU:HA	1:A:428:LEU:HD23	1.94	0.41
1:B:366:GLU:O	1:B:367:ARG:C	2.58	0.41
1:C:193:LEU:HG	1:C:193:LEU:O	2.19	0.41
1:A:297:ASP:OD1	1:A:298:LEU:N	2.48	0.41
1:A:306:ALA:N	4:A:2009:HOH:O	2.50	0.41
1:B:344:GLN:O	1:B:345:ALA:C	2.58	0.41
1:C:198:CYS:O	1:C:199:ALA:C	2.59	0.41
1:C:324:ASP:CG	1:C:328:ARG:NH1	2.72	0.41
1:D:159:ALA:C	1:D:186:SER:HB2	2.40	0.41
1:D:207:GLU:OE1	1:D:252:ARG:NE	2.47	0.41
1:E:251:VAL:HG21	1:F:200:ALA:CB	2.28	0.41
1:F:237:LEU:HG	1:F:239:LEU:HD11	2.01	0.41
1:B:149:GLN:HA	1:B:152:LEU:HD12	2.03	0.41
1:B:197:ASN:OD1	1:B:199:ALA:CB	2.64	0.41
1:C:334:ASN:HB2	1:C:336:LYS:HG3	2.03	0.41
1:D:245:ILE:HD13	1:D:245:ILE:HG21	1.72	0.41
1:D:295:ARG:HE	1:D:297:ASP:CG	2.22	0.41
1:D:361:LEU:O	1:D:362:GLU:C	2.59	0.41
1:E:175:LYS:O	1:E:176:GLU:C	2.56	0.41
1:E:230:VAL:O	1:E:232:ALA:N	2.54	0.41
1:F:254:LEU:O	1:F:257:ILE:N	2.54	0.41
1:B:284:ASP:C	1:B:286:ALA:N	2.72	0.41
1:C:320:PRO:HB3	1:C:346:MET:SD	2.61	0.41
1:D:386:ILE:HG23	1:D:387:ALA:H	1.84	0.41
1:E:202:ASN:C	1:E:204:SER:H	2.23	0.41
1:E:341:PHE:CE2	1:E:377:ILE:HG13	2.55	0.41
1:E:404:ASP:O	1:E:405:VAL:C	2.57	0.41
1:E:437:ALA:O	1:E:439:LEU:N	2.53	0.41
1:A:191:ARG:NH1	1:A:191:ARG:HG3	2.35	0.41
1:B:208:SER:OG	1:B:213:HIS:CD2	2.73	0.41
1:B:230:VAL:O	1:B:233:ASP:HB2	2.21	0.41
1:D:151:LEU:HD22	1:D:151:LEU:C	2.41	0.41
1:D:285:LEU:HA	1:D:285:LEU:HD12	1.83	0.41
1:E:437:ALA:O	1:E:438:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:THR:O	1:F:281:THR:HG23	2.20	0.41
1:A:182:LEU:HD13	1:A:278:ILE:CD1	2.50	0.41
1:A:334:ASN:O	1:A:335:ARG:C	2.59	0.41
1:B:339:LYS:HD2	1:B:339:LYS:HA	1.69	0.41
1:C:182:LEU:O	1:C:183:HIS:C	2.58	0.41
1:E:170:ASP:O	1:E:173:THR:CG2	2.69	0.41
1:F:252:ARG:O	1:F:255:ARG:N	2.54	0.41
1:B:352:TYR:C	1:B:354:TRP:CD1	2.94	0.41
1:D:278:ILE:HD13	1:D:278:ILE:HG21	1.75	0.41
1:D:328:ARG:NH2	1:D:339:LYS:CE	2.83	0.41
1:D:372:LEU:CD1	1:D:381:GLU:OE2	2.69	0.41
1:E:406:GLU:OE1	1:E:441:ARG:NH2	2.54	0.41
1:B:172:GLY:H	2:B:1390:PO4:P	2.43	0.41
1:C:319:ILE:CB	1:C:320:PRO:CD	2.99	0.41
1:E:232:ALA:O	1:E:233:ASP:C	2.59	0.41
1:F:326:PHE:C	1:F:328:ARG:N	2.73	0.41
1:F:313:ARG:HH12	1:F:354:TRP:CA	2.34	0.41
1:C:361:LEU:O	1:C:364:ALA:N	2.54	0.41
1:D:174:GLY:HA3	1:D:177:LEU:HD12	2.03	0.41
1:D:230:VAL:O	1:D:232:ALA:N	2.54	0.41
1:D:387:ALA:HB2	4:D:2020:HOH:O	2.21	0.41
1:E:142:ILE:HD12	1:E:322:LEU:HD12	2.03	0.41
1:F:352:TYR:HD2	1:F:353:ASP:OD1	2.04	0.41
1:A:313:ARG:HG3	1:A:314:GLN:N	2.36	0.41
1:B:275:VAL:HG12	1:B:276:ARG:N	2.35	0.41
1:D:143:GLY:O	1:D:318:ASP:OD1	2.38	0.41
1:D:191:ARG:NH1	1:D:191:ARG:HG2	2.35	0.41
1:E:316:ARG:C	1:E:318:ASP:H	2.25	0.41
1:F:146:PRO:O	1:F:147:ALA:C	2.59	0.41
1:F:188:ARG:CB	1:F:191:ARG:HD3	2.43	0.41
1:F:202:ASN:O	1:F:204:SER:N	2.54	0.41
1:F:240:ASP:OD2	1:F:241:GLU:N	2.54	0.41
1:A:195:THR:HG23	1:A:195:THR:O	2.20	0.41
1:A:365:ILE:O	1:A:367:ARG:N	2.54	0.41
1:B:348:LEU:CD1	1:B:348:LEU:H	2.31	0.41
1:C:149:GLN:O	1:C:150:HIS:C	2.59	0.41
1:C:366:GLU:O	1:C:370:VAL:HG23	2.21	0.41
1:D:325:HIS:HE1	1:D:329:ARG:HH21	1.69	0.41
1:E:335:ARG:HD2	1:E:335:ARG:HA	1.33	0.41
1:F:164:THR:HA	1:F:277:LEU:O	2.20	0.41
1:F:285:LEU:HB3	1:F:299:TYR:HE1	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:LEU:HB3	1:F:383:PRO:HD2	2.03	0.41
1:A:435:LEU:O	1:A:436:LEU:C	2.59	0.40
1:C:377:ILE:HD12	1:C:378:SER:O	2.21	0.40
1:D:311:SER:O	1:D:312:LEU:C	2.58	0.40
1:F:145:SER:HB2	1:F:317:GLU:HB2	2.00	0.40
1:B:142:ILE:HB	1:B:322:LEU:CD1	2.51	0.40
1:B:142:ILE:O	1:B:142:ILE:HG22	2.20	0.40
1:D:352:TYR:O	1:D:354:TRP:HD1	2.03	0.40
1:E:183:HIS:CD2	1:E:193:LEU:HD13	2.56	0.40
1:E:212:GLY:HA2	1:E:226:GLU:O	2.19	0.40
1:E:233:ASP:OD2	1:E:273:VAL:HA	2.21	0.40
1:F:210:LEU:HA	1:F:228:ARG:HB2	2.02	0.40
1:A:167:ILE:O	1:A:280:ALA:HB1	2.22	0.40
1:A:318:ASP:C	1:A:320:PRO:HD2	2.42	0.40
1:B:260:ARG:NH1	1:B:275:VAL:H	2.19	0.40
1:B:278:ILE:HG21	1:B:278:ILE:HD13	1.57	0.40
1:D:255:ARG:O	1:D:256:ALA:C	2.56	0.40
1:D:338:VAL:O	1:D:339:LYS:HB2	2.21	0.40
1:D:380:ARG:HD3	1:D:380:ARG:N	2.31	0.40
1:D:388:ALA:O	1:D:390:PRO:HD3	2.22	0.40
1:E:259:GLU:CG	1:E:259:GLU:O	2.69	0.40
1:E:318:ASP:O	1:E:319:ILE:C	2.60	0.40
1:F:324:ASP:OD2	1:F:339:LYS:NZ	2.55	0.40
1:A:370:VAL:H	1:A:370:VAL:HG23	1.55	0.40
1:B:344:GLN:HA	1:B:344:GLN:OE1	2.21	0.40
1:D:178:VAL:O	1:D:182:LEU:HG	2.22	0.40
1:D:239:LEU:CB	1:D:242:ILE:HD12	2.51	0.40
1:D:344:GLN:O	1:D:348:LEU:CD1	2.68	0.40
1:E:210:LEU:HA	1:E:210:LEU:HD23	1.85	0.40
1:E:322:LEU:HD11	3:E:1442:ATP:C6	2.57	0.40
1:F:230:VAL:C	1:F:232:ALA:N	2.75	0.40
1:F:287:GLU:O	1:F:288:GLU:C	2.59	0.40
1:F:384:LEU:C	1:F:386:ILE:N	2.66	0.40
1:A:147:ALA:O	1:A:148:MET:C	2.58	0.40
1:A:318:ASP:O	1:A:321:LEU:N	2.54	0.40
1:B:214:GLU:OE2	1:B:269:GLN:NE2	2.54	0.40
1:B:298:LEU:O	1:B:299:TYR:C	2.59	0.40
1:B:311:SER:HB2	1:B:314:GLN:NE2	2.35	0.40
1:C:304:VAL:HG12	1:C:305:VAL:HG23	2.04	0.40
1:C:320:PRO:HA	1:C:346:MET:HE1	2.03	0.40
1:D:297:ASP:HB3	1:E:359:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:VAL:HG12	1:D:339:LYS:N	2.36	0.40
1:D:423:GLU:HA	1:D:423:GLU:OE1	2.22	0.40
1:E:407:LYS:O	1:E:411:LEU:HB2	2.22	0.40
1:F:229:PHE:O	1:F:232:ALA:N	2.40	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:GLY:CA	1:C:376:TYR:OH[3_455]	1.96	0.24
1:A:144:SER:OG	1:F:144:SER:O[1_655]	2.02	0.18
1:A:162:ASP:OD2	1:C:334:ASN:OD1[3_555]	2.05	0.15
1:A:287:GLU:OE2	1:E:420:ASN:ND2[4_555]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/304 (94%)	213 (74%)	55 (19%)	18 (6%)	1	7
1	B	249/304 (82%)	185 (74%)	48 (19%)	16 (6%)	1	7
1	C	250/304 (82%)	182 (73%)	51 (20%)	17 (7%)	1	6
1	D	293/304 (96%)	227 (78%)	48 (16%)	18 (6%)	1	8
1	E	279/304 (92%)	201 (72%)	53 (19%)	25 (9%)	1	3
1	F	243/304 (80%)	176 (72%)	48 (20%)	19 (8%)	1	4
All	All	1600/1824 (88%)	1184 (74%)	303 (19%)	113 (7%)	1	5

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ALA

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	216	GLY
1	A	260	ARG
1	A	270	THR
1	A	354	TRP
1	A	357	ASN
1	B	144	SER
1	B	199	ALA
1	B	260	ARG
1	B	263	GLN
1	B	354	TRP
1	B	357	ASN
1	B	385	ALA
1	C	144	SER
1	C	174	GLY
1	C	199	ALA
1	C	215	LYS
1	C	220	GLY
1	C	260	ARG
1	C	317	GLU
1	C	357	ASN
1	D	199	ALA
1	D	260	ARG
1	D	319	ILE
1	D	357	ASN
1	D	387	ALA
1	D	403	VAL
1	E	144	SER
1	E	145	SER
1	E	159	ALA
1	E	199	ALA
1	E	203	GLU
1	E	218	PHE
1	E	260	ARG
1	E	357	ASN
1	E	385	ALA
1	F	199	ALA
1	F	215	LYS
1	F	216	GLY
1	F	265	VAL
1	F	357	ASN
1	F	385	ALA

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Mol	Chain	Res	Type
1	A	144	SER
1	A	174	GLY
1	A	217	ALA
1	A	385	ALA
1	B	386	ILE
1	C	159	ALA
1	C	231	GLU
1	D	270	THR
1	D	303	ASN
1	D	313	ARG
1	E	208	SER
1	E	209	GLU
1	E	217	ALA
1	E	265	VAL
1	E	303	ASN
1	E	317	GLU
1	E	353	ASP
1	F	200	ALA
1	F	233	ASP
1	F	260	ARG
1	B	161	SER
1	B	184	ALA
1	B	285	LEU
1	C	265	VAL
1	C	269	GLN
1	D	354	TRP
1	E	319	ILE
1	F	353	ASP
1	A	208	SER
1	A	438	LYS
1	B	146	PRO
1	C	316	ARG
1	D	160	PRO
1	D	161	SER
1	D	317	GLU
1	D	320	PRO
1	E	160	PRO
1	E	161	SER
1	E	214	GLU
1	E	402	LEU
1	F	160	PRO
1	F	161	SER

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Mol	Chain	Res	Type
1	F	354	TRP
1	A	160	PRO
1	A	317	GLU
1	A	319	ILE
1	B	262	VAL
1	B	317	GLU
1	C	146	PRO
1	C	319	ILE
1	C	354	TRP
1	D	339	LYS
1	D	352	TYR
1	D	390	PRO
1	E	354	TRP
1	F	203	GLU
1	F	258	GLN
1	A	271	ILE
1	D	386	ILE
1	E	146	PRO
1	F	253	LEU
1	F	319	ILE
1	C	262	VAL
1	B	265	VAL
1	B	319	ILE
1	E	158	VAL
1	A	146	PRO
1	E	403	VAL
1	F	146	PRO
1	F	165	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	231/251 (92%)	198 (86%)	33 (14%)	3 15
1	B	197/251 (78%)	167 (85%)	30 (15%)	3 14
1	C	197/251 (78%)	163 (83%)	34 (17%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	234/251 (93%)	196 (84%)	38 (16%)	2 12
1	E	226/251 (90%)	190 (84%)	36 (16%)	2 12
1	F	195/251 (78%)	164 (84%)	31 (16%)	2 12
All	All	1280/1506 (85%)	1078 (84%)	202 (16%)	2 12

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	186	SER
1	A	189	SER
1	A	190	ASP
1	A	191	ARG
1	A	196	LEU
1	A	204	SER
1	A	210	LEU
1	A	229	PHE
1	A	244	ASP
1	A	245	ILE
1	A	274	ASP
1	A	276	ARG
1	A	285	LEU
1	A	288	GLU
1	A	297	ASP
1	A	313	ARG
1	A	321	LEU
1	A	327	LEU
1	A	357	ASN
1	A	358	ILE
1	A	360	GLU
1	A	365	ILE
1	A	377	ILE
1	A	380	ARG
1	A	403	VAL
1	A	404	ASP
1	A	410	ILE
1	A	411	LEU
1	A	414	LEU
1	A	430	ILE
1	A	435	LEU
1	A	439	LEU

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Mol	Chain	Res	Type
1	B	141	MET
1	B	151	LEU
1	B	152	LEU
1	B	171	SER
1	B	173	THR
1	B	175	LYS
1	B	186	SER
1	B	190	ASP
1	B	191	ARG
1	B	195	THR
1	B	196	LEU
1	B	213	HIS
1	B	224	ARG
1	B	251	VAL
1	B	281	THR
1	B	283	ARG
1	B	285	LEU
1	B	288	GLU
1	B	290	SER
1	B	312	LEU
1	B	313	ARG
1	B	315	ARG
1	B	317	GLU
1	B	324	ASP
1	B	350	ILE
1	B	357	ASN
1	B	358	ILE
1	B	363	ASN
1	B	377	ILE
1	B	380	ARG
1	C	141	MET
1	C	151	LEU
1	C	171	SER
1	C	173	THR
1	C	178	VAL
1	C	186	SER
1	C	190	ASP
1	C	191	ARG
1	C	196	LEU
1	C	198	CYS
1	C	201	LEU
1	C	213	HIS

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Mol	Chain	Res	Type
1	C	229	PHE
1	C	230	VAL
1	C	239	LEU
1	C	244	ASP
1	C	248	LEU
1	C	268	ASN
1	C	274	ASP
1	C	276	ARG
1	C	288	GLU
1	C	295	ARG
1	C	311	SER
1	C	312	LEU
1	C	313	ARG
1	C	339	LYS
1	C	346	MET
1	C	357	ASN
1	C	358	ILE
1	C	359	ARG
1	C	363	ASN
1	C	365	ILE
1	C	377	ILE
1	C	380	ARG
1	D	151	LEU
1	D	157	MET
1	D	160	PRO
1	D	164	THR
1	D	167	ILE
1	D	171	SER
1	D	173	THR
1	D	186	SER
1	D	190	ASP
1	D	191	ARG
1	D	195	THR
1	D	196	LEU
1	D	198	CYS
1	D	224	ARG
1	D	230	VAL
1	D	239	LEU
1	D	244	ASP
1	D	258	GLN
1	D	273	VAL
1	D	276	ARG

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Mol	Chain	Res	Type
1	D	281	THR
1	D	285	LEU
1	D	288	GLU
1	D	308	GLU
1	D	311	SER
1	D	312	LEU
1	D	313	ARG
1	D	321	LEU
1	D	336	LYS
1	D	358	ILE
1	D	359	ARG
1	D	363	ASN
1	D	377	ILE
1	D	380	ARG
1	D	386	ILE
1	D	410	ILE
1	D	411	LEU
1	D	414	LEU
1	E	145	SER
1	E	151	LEU
1	E	152	LEU
1	E	160	PRO
1	E	173	THR
1	E	185	CYS
1	E	190	ASP
1	E	195	THR
1	E	196	LEU
1	E	198	CYS
1	E	201	LEU
1	E	204	SER
1	E	236	THR
1	E	242	ILE
1	E	253	LEU
1	E	258	GLN
1	E	277	LEU
1	E	285	LEU
1	E	288	GLU
1	E	298	LEU
1	E	308	GLU
1	E	313	ARG
1	E	319	ILE
1	E	342	THR

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Mol	Chain	Res	Type
1	E	348	LEU
1	E	358	ILE
1	E	363	ASN
1	E	377	ILE
1	E	380	ARG
1	E	402	LEU
1	E	404	ASP
1	E	410	ILE
1	E	411	LEU
1	E	414	LEU
1	E	435	LEU
1	E	439	LEU
1	F	151	LEU
1	F	173	THR
1	F	185	CYS
1	F	186	SER
1	F	190	ASP
1	F	191	ARG
1	F	193	LEU
1	F	196	LEU
1	F	201	LEU
1	F	210	LEU
1	F	230	VAL
1	F	257	ILE
1	F	267	SER
1	F	272	SER
1	F	276	ARG
1	F	281	THR
1	F	285	LEU
1	F	288	GLU
1	F	290	SER
1	F	297	ASP
1	F	298	LEU
1	F	308	GLU
1	F	313	ARG
1	F	339	LYS
1	F	350	ILE
1	F	352	TYR
1	F	363	ASN
1	F	377	ILE
1	F	378	SER
1	F	380	ARG

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Mol	Chain	Res	Type
1	F	386	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	183	HIS
1	A	269	GLN
1	A	282	HIS
1	A	314	GLN
1	A	357	ASN
1	B	150	HIS
1	B	183	HIS
1	B	213	HIS
1	B	269	GLN
1	B	314	GLN
1	B	334	ASN
1	B	357	ASN
1	C	149	GLN
1	C	263	GLN
1	C	314	GLN
1	C	351	HIS
1	C	357	ASN
1	D	149	GLN
1	D	269	GLN
1	D	325	HIS
1	D	357	ASN
1	E	149	GLN
1	E	150	HIS
1	E	213	HIS
1	E	325	HIS
1	E	334	ASN
1	E	351	HIS
1	F	183	HIS
1	F	282	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	B	1390	-	4,4,4	0.71	0	6,6,6	0.98	0
2	PO4	A	1442	-	4,4,4	0.84	0	6,6,6	0.95	0
3	ATP	E	1442	-	26,33,33	1.13	2 (7%)	31,52,52	1.78	5 (16%)
2	PO4	F	1390	-	4,4,4	0.74	0	6,6,6	0.39	0
2	PO4	D	1442	-	4,4,4	0.99	0	6,6,6	0.84	0
2	PO4	C	1391	-	4,4,4	0.88	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	1442	-	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1442	ATP	C2-N3	3.63	1.38	1.32
3	E	1442	ATP	C2-N1	2.42	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1442	ATP	N3-C2-N1	-5.69	119.79	128.68
3	E	1442	ATP	C5'-C4'-C3'	-4.48	98.41	115.18
3	E	1442	ATP	PB-O3B-PG	-2.55	124.06	132.83
3	E	1442	ATP	C2'-C3'-C4'	2.12	106.76	102.64
3	E	1442	ATP	PA-O3A-PB	-2.11	125.57	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1442	ATP	PA-O3A-PB-O3B
3	E	1442	ATP	C5'-O5'-PA-O3A
3	E	1442	ATP	PB-O3B-PG-O1G

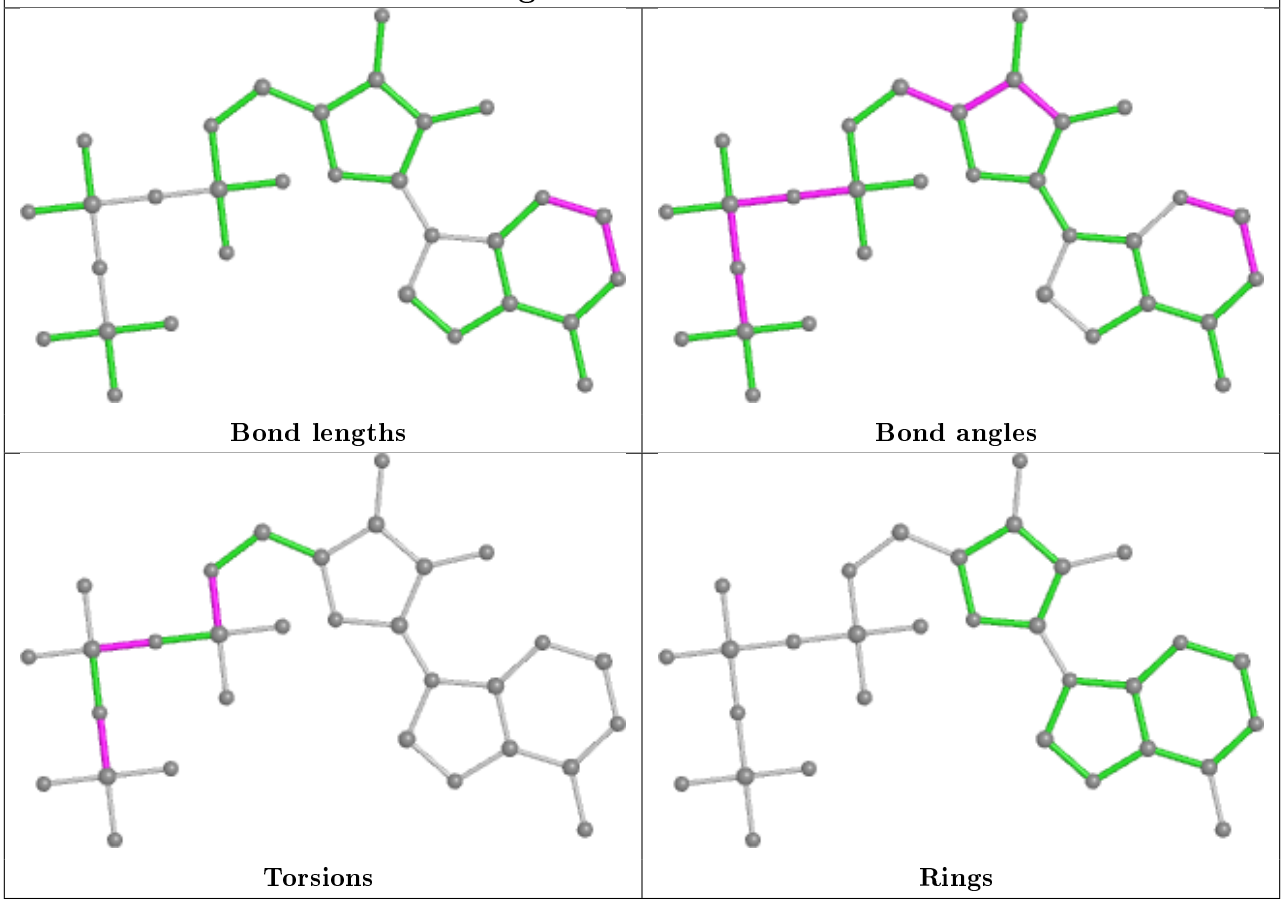
There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1390	PO4	1	0
3	E	1442	ATP	11	0
2	F	1390	PO4	2	0
2	D	1442	PO4	3	0
2	C	1391	PO4	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP E 1442



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

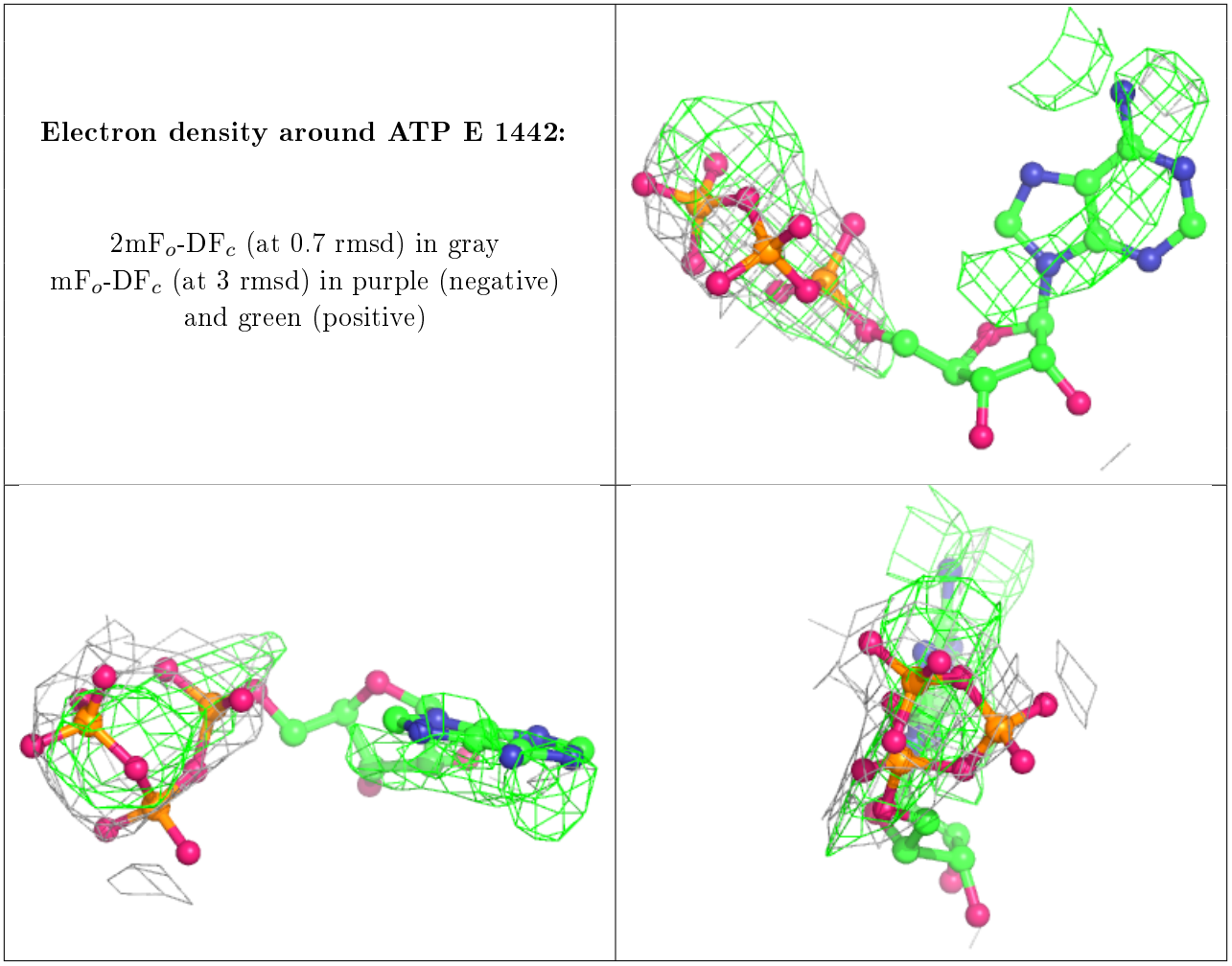
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 E 1442:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.