



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:35 PM EDT

PDB ID : 4P69 / pdb_00004p69
Title : Acek (D477A) ICDH complex
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Deposited on : 2014-03-22
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

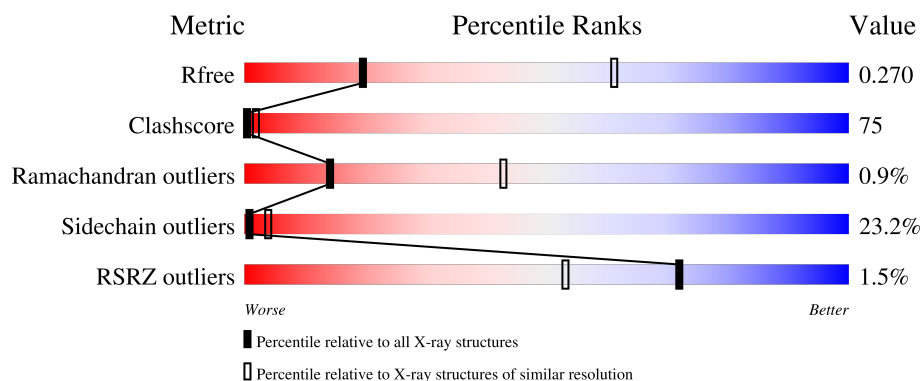
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	568	
1	B	568	
2	C	415	
2	D	415	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	B	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15755 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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4575	2946	799	809	21			
1	B	561	Total	C	N	O	S	0	0	0
			4649	2992	815	821	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ALA	ASP	engineered mutation	UNP Q8X607
B	477	ALA	ASP	engineered mutation	UNP Q8X607

- Molecule 2 is a protein called Isocitrate dehydrogenase [NADP].

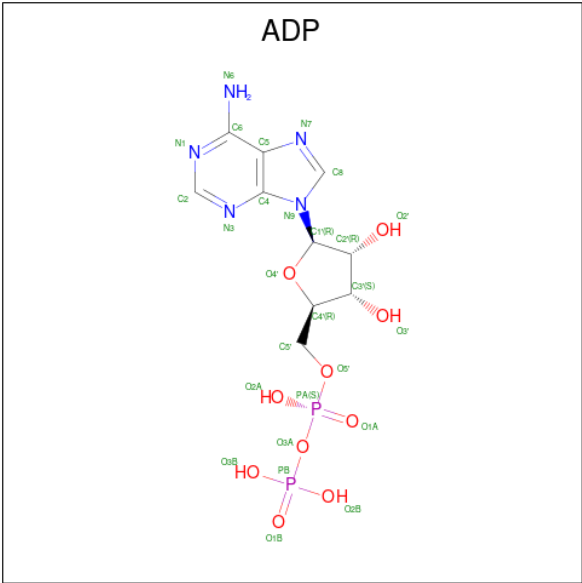
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	415	Total	C	N	O	S	0	0	0
			3205	2040	539	608	18			
2	D	415	Total	C	N	O	S	0	0	0
			3205	2040	539	608	18			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

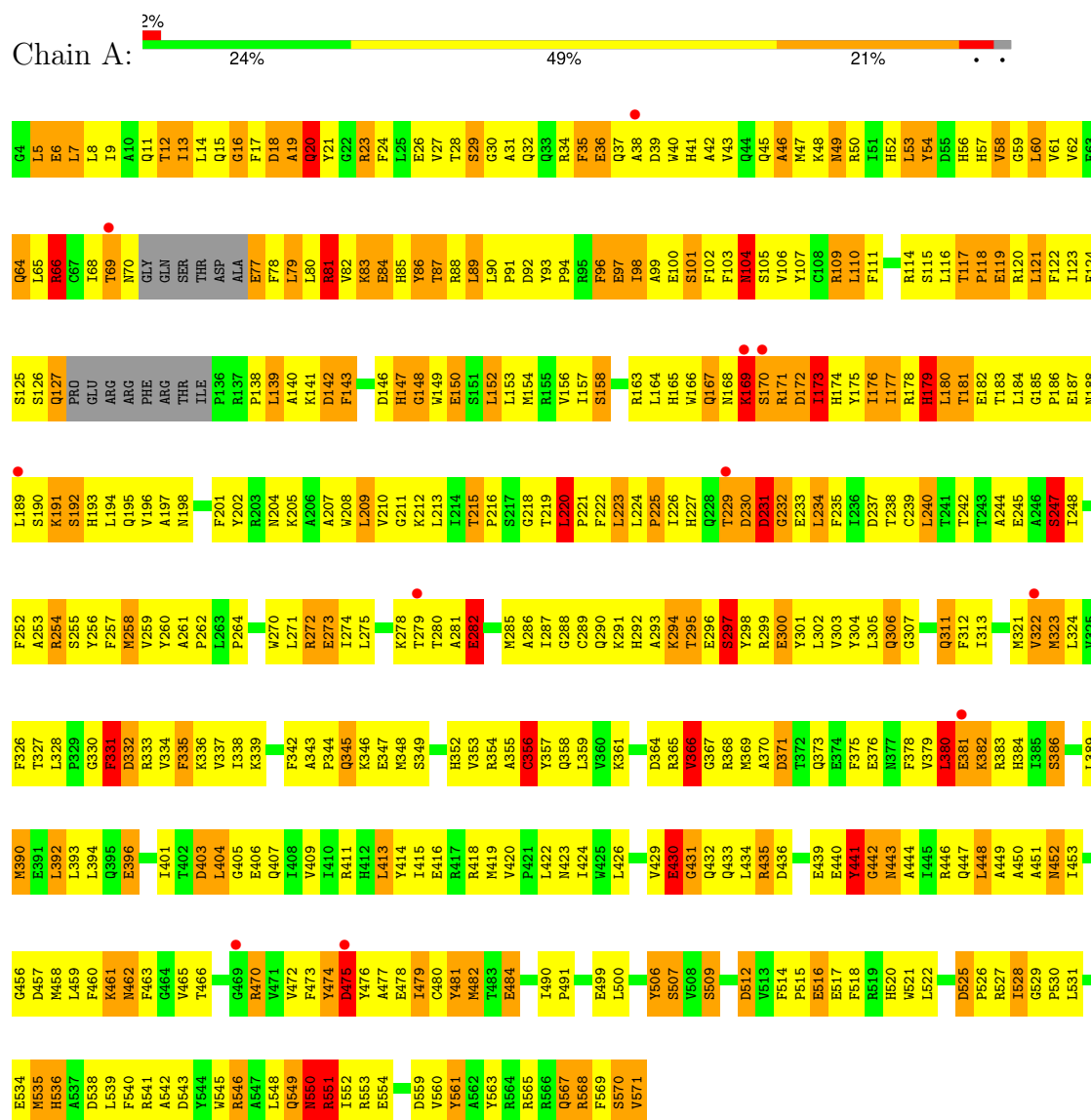
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	4	Total 4	O 4	0	0
5	C	7	Total 7	O 7	0	0
5	D	7	Total 7	O 7	0	0

3 Residue-property plots

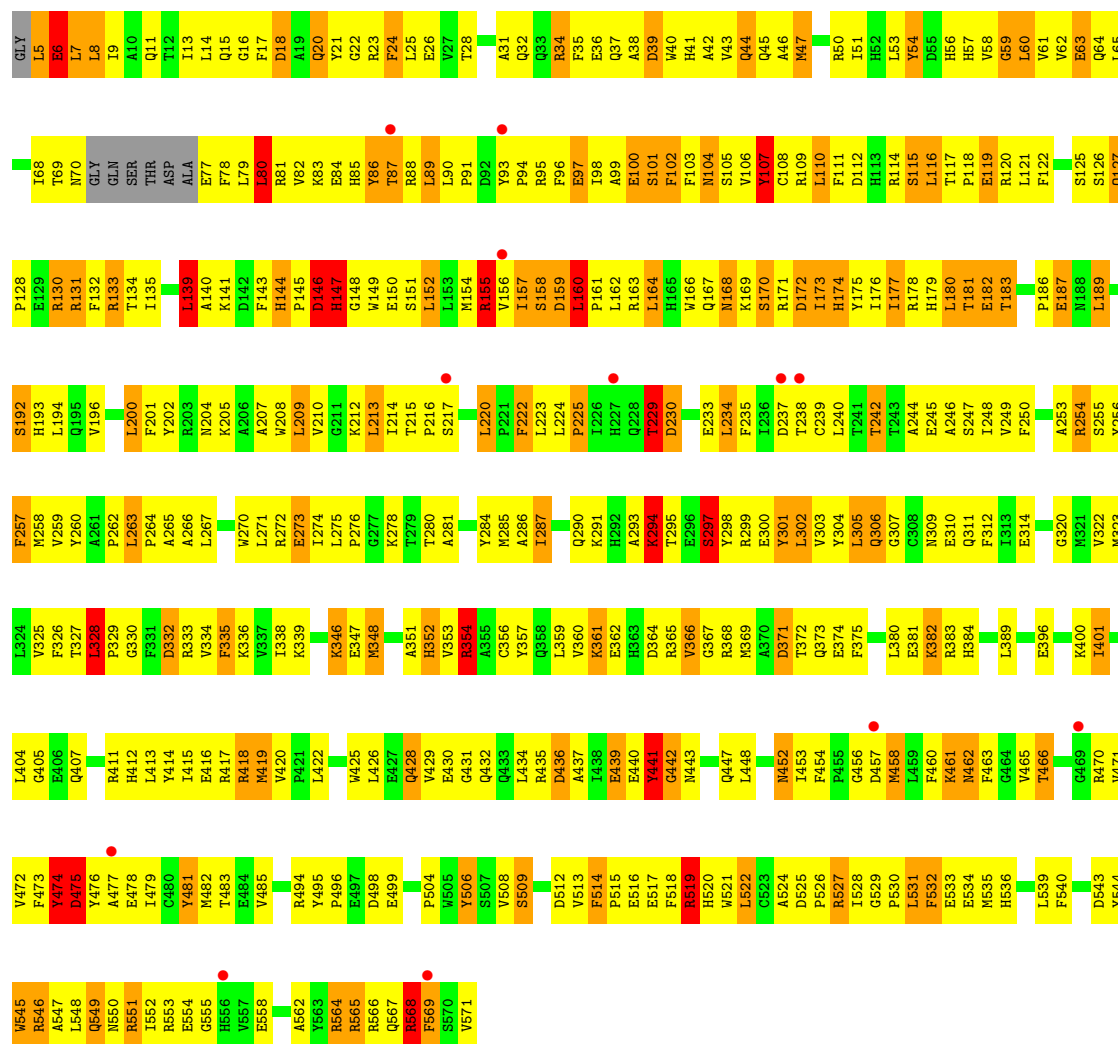
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase

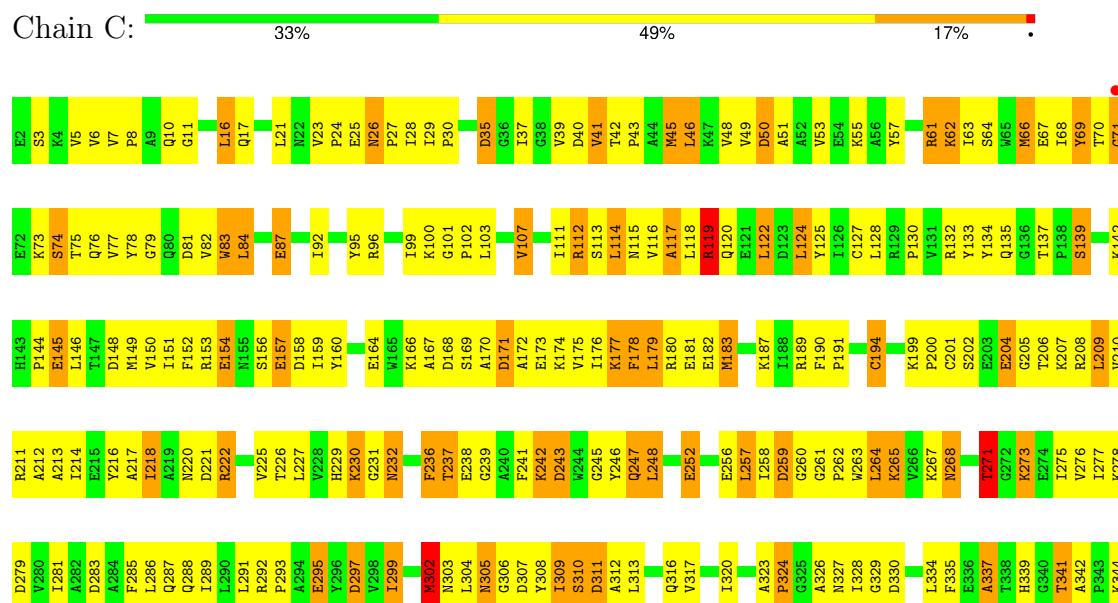


- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



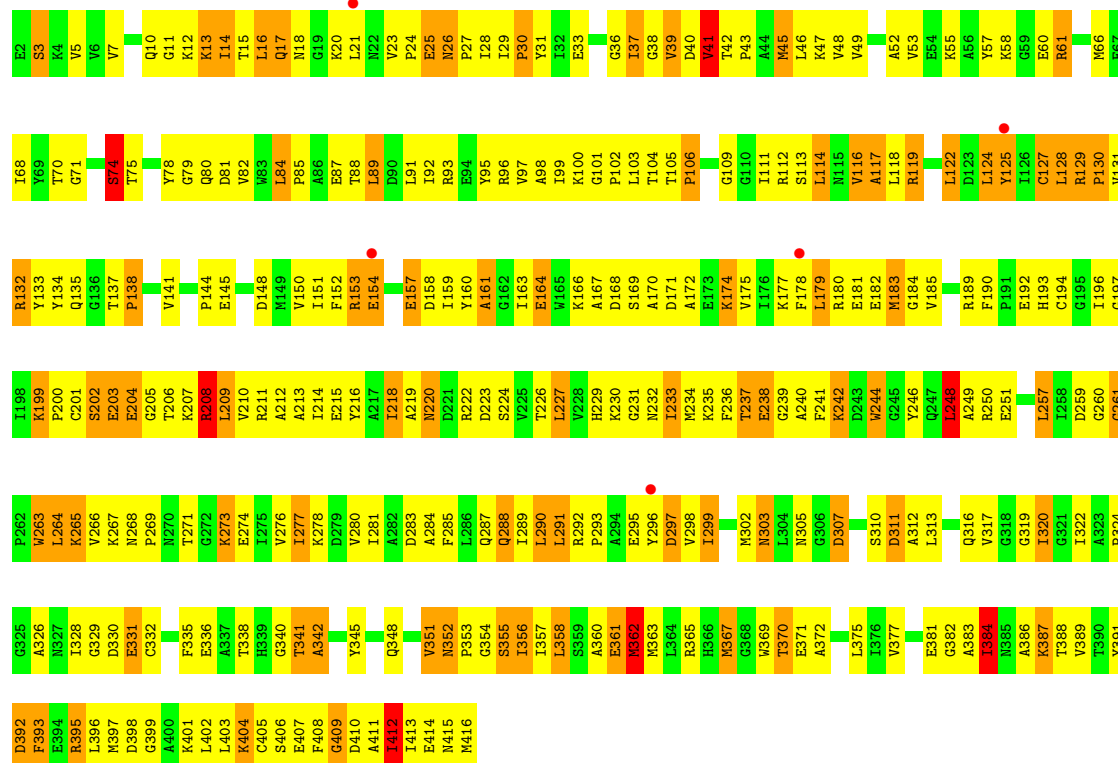


• Molecule 2: Isocitrate dehydrogenase [NADP]





• Molecule 2: Isocitrate dehydrogenase [NADP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	198.16Å 198.16Å 156.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 3.30 29.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.97-3.30) 99.2 (29.97-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.177 , 0.247 0.221 , 0.270	Depositor DCC
R_{free} test set	2657 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	99.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15755	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.30	0/4699	1.22	64/6367 (1.0%)
1	B	1.31	0/4776	1.17	58/6473 (0.9%)
2	C	1.45	0/3266	1.25	38/4417 (0.9%)
2	D	1.38	2/3266 (0.1%)	1.26	43/4417 (1.0%)
All	All	1.35	2/16007 (0.0%)	1.22	203/21674 (0.9%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	342	ALA	C-O	-5.81	1.21	1.23
2	D	342	ALA	CA-C	-5.05	1.49	1.53

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LYS	N-CA-C	-12.84	90.97	110.10
1	A	475	ASP	N-CA-C	-9.46	95.87	109.96
2	D	352	ASN	C-N-CD	-9.41	86.42	125.00
1	B	568	ARG	N-CA-C	-9.35	97.64	110.35
2	D	41	VAL	N-CA-C	9.16	119.14	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	VAL	N-CA-C	9.12	119.93	110.72
2	D	296	TYR	N-CA-C	8.81	124.72	113.88
2	C	10	GLN	N-CA-C	8.31	120.42	111.36
2	C	96	ARG	N-CA-C	8.30	120.41	111.36
2	D	404	LYS	N-CA-C	-8.21	99.67	110.43
1	A	322	VAL	N-CA-C	8.00	118.80	110.72
1	B	475	ASP	N-CA-C	-7.85	97.23	109.25
1	A	36	GLU	N-CA-C	-7.73	102.80	111.07
1	A	282	GLU	N-CA-C	-7.59	102.95	111.07
1	A	148	GLY	N-CA-C	-7.59	103.21	111.93
1	A	279	THR	N-CA-C	-7.37	100.80	110.53
2	C	236	PHE	N-CA-C	7.33	119.35	111.36
1	A	66	ARG	N-CA-C	-7.30	103.26	111.07
2	D	101	GLY	N-CA-C	-7.26	103.44	112.23
1	B	474	TYR	N-CA-C	7.20	126.14	110.80
1	A	59	GLY	N-CA-C	-7.13	104.17	112.73
1	B	437	ALA	N-CA-C	7.13	118.84	111.14
2	C	283	ASP	N-CA-C	-7.10	103.23	110.97
1	A	68	ILE	O-C-N	7.09	128.75	121.87
2	C	396	LEU	N-CA-C	7.05	119.05	111.36
2	C	142	LYS	N-CA-C	7.03	118.94	111.28
2	D	312	ALA	N-CA-C	7.00	119.00	111.36
2	C	252	GLU	N-CA-C	6.91	118.60	111.14
2	D	203	GLU	N-CA-C	-6.90	103.69	111.14
2	D	305	ASN	N-CA-C	-6.89	103.77	111.28
2	C	77	VAL	N-CA-C	6.89	117.00	110.53
1	A	229	THR	N-CA-C	-6.88	101.45	110.53
2	C	261	GLY	N-CA-C	-6.88	98.31	112.34
1	A	442	GLY	N-CA-C	-6.85	104.51	112.73
2	C	302	MET	N-CA-C	-6.83	101.72	110.19
2	D	261	GLY	N-CA-C	-6.83	98.40	112.34
2	C	117	ALA	N-CA-C	-6.78	103.81	111.07
1	A	232	GLY	N-CA-C	6.76	120.73	111.54
1	A	81	ARG	N-CA-C	-6.75	103.92	111.28
1	A	173	ILE	N-CA-C	-6.72	103.76	110.62
1	B	86	TYR	N-CA-C	-6.70	103.98	111.28
1	B	15	GLN	N-CA-C	-6.69	103.98	111.28
1	A	147	HIS	N-CA-C	-6.69	100.06	109.69
2	D	157	GLU	N-CA-C	6.64	118.68	110.91
1	B	101	SER	N-CA-C	-6.63	103.97	111.07
2	C	83	TRP	N-CA-C	6.61	118.27	111.14
1	B	532	PHE	N-CA-C	-6.59	104.02	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	GLU	N-CA-C	-6.57	104.12	111.28
1	B	18	ASP	N-CA-C	-6.55	104.14	111.28
2	D	109	GLY	N-CA-C	6.54	120.09	112.50
2	D	178	PHE	N-CA-C	-6.52	104.10	111.07
2	D	74	SER	N-CA-C	-6.50	104.19	111.28
1	B	144	HIS	CA-C-N	6.46	126.22	119.05
1	B	144	HIS	C-N-CA	6.46	126.22	119.05
2	C	157	GLU	N-CA-C	6.45	123.08	114.12
1	A	441	TYR	N-CA-C	-6.44	104.18	111.07
1	B	353	VAL	N-CA-C	-6.39	104.10	110.62
1	A	35	PHE	N-CA-C	-6.35	104.36	111.28
1	B	514	PHE	C-N-CD	-6.35	98.96	125.00
2	D	14	ILE	N-CA-C	-6.34	99.76	109.78
1	B	22	GLY	N-CA-C	-6.34	105.12	112.73
1	A	150	GLU	N-CA-C	-6.32	104.40	111.28
1	B	441	TYR	N-CA-C	-6.29	104.42	111.28
1	A	481	TYR	N-CA-C	-6.26	102.27	110.53
1	A	15	GLN	N-CA-C	-6.22	104.50	111.28
1	B	439	GLU	N-CA-C	-6.18	104.45	111.07
1	B	160	LEU	CA-C-N	6.16	125.72	119.19
1	B	160	LEU	C-N-CA	6.16	125.72	119.19
1	B	545	TRP	N-CA-C	-6.12	104.61	111.28
1	A	431	GLY	N-CA-C	6.11	119.59	112.50
1	B	51	ILE	N-CA-C	-6.10	104.56	110.42
1	A	521	TRP	N-CA-C	6.08	117.99	111.36
1	A	179	HIS	N-CA-C	-6.03	104.70	111.28
1	B	139	LEU	N-CA-C	6.03	117.65	111.14
2	C	218	ILE	N-CA-C	-6.03	104.47	110.62
1	A	553	ARG	N-CA-C	-6.03	104.71	111.28
1	B	428	GLN	N-CA-C	6.02	117.64	111.14
1	B	59	GLY	N-CA-C	-6.01	105.51	112.73
2	C	337	ALA	N-CA-C	-6.01	102.59	110.53
2	D	393	PHE	N-CA-C	5.98	117.60	111.14
1	A	231	ASP	N-CA-C	-5.96	103.17	111.39
2	C	246	TYR	N-CA-C	-5.96	104.79	111.28
1	B	273	GLU	N-CA-C	-5.96	104.79	111.28
2	C	408	PHE	N-CA-C	-5.93	104.81	111.28
1	A	294	LYS	N-CA-C	-5.92	104.82	111.28
1	B	352	HIS	N-CA-C	-5.92	104.83	111.28
2	C	71	GLY	N-CA-C	5.92	122.12	115.08
1	B	63	GLU	N-CA-C	-5.91	104.84	111.28
1	A	358	GLN	N-CA-C	-5.90	104.85	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	ASP	N-CA-C	-5.90	100.92	109.59
1	A	58	VAL	N-CA-C	-5.89	104.61	110.62
1	A	512	ASP	N-CA-C	-5.88	101.15	109.96
1	B	102	PHE	N-CA-C	-5.87	104.89	111.28
1	A	20	GLN	N-CA-C	-5.85	104.81	111.07
1	B	294	LYS	N-CA-C	-5.83	104.83	111.07
2	C	311	ASP	N-CA-C	-5.83	104.93	111.28
2	D	223	ASP	N-CA-C	5.80	117.68	111.36
1	B	147	HIS	N-CA-C	-5.78	104.84	112.24
1	B	44	GLN	N-CA-C	-5.78	104.99	111.28
1	A	146	ASP	N-CA-C	-5.75	105.01	111.28
1	A	550	ASN	N-CA-C	-5.75	104.70	110.97
2	D	384	ILE	CB-CA-C	-5.75	104.61	111.97
2	D	362	MET	N-CA-C	-5.72	105.05	111.28
2	D	320	ILE	N-CA-C	-5.71	104.80	110.62
1	A	98	ILE	N-CA-C	-5.71	104.80	110.62
1	A	354	ARG	N-CA-C	-5.69	105.08	111.28
1	B	107	TYR	N-CA-C	-5.69	104.99	111.07
1	B	442	GLY	N-CA-C	-5.68	105.92	112.73
2	C	87	GLU	N-CA-C	-5.67	105.09	111.28
1	B	328	LEU	N-CA-C	-5.66	102.04	110.20
2	D	361	GLU	N-CA-C	-5.66	105.02	111.07
2	C	243	ASP	N-CA-C	-5.65	105.02	111.07
1	A	118	PRO	N-CA-C	-5.65	105.68	113.53
1	B	6	GLU	N-CA-C	-5.63	105.04	111.07
1	A	331	PHE	N-CA-C	5.62	117.78	110.53
1	A	18	ASP	N-CA-C	-5.60	105.08	111.07
1	B	133	ARG	N-CA-C	-5.60	105.09	111.14
1	A	356	CYS	N-CA-C	-5.57	105.11	111.07
1	A	474	TYR	N-CA-C	5.53	122.58	110.80
2	C	350	LYS	N-CA-C	5.53	117.31	111.28
1	B	146	ASP	N-CA-C	-5.53	103.34	110.19
2	D	174	LYS	N-CA-C	-5.49	105.29	111.28
1	B	170	SER	N-CA-C	-5.48	105.30	111.28
2	D	358	LEU	N-CA-C	-5.47	105.42	111.71
2	C	247	GLN	N-CA-C	-5.45	105.44	111.71
1	B	519	ARG	N-CA-C	-5.45	105.34	111.28
1	B	157	ILE	N-CA-C	5.44	115.64	110.53
2	D	288	GLN	N-CA-C	5.44	117.29	111.36
2	D	311	ASP	N-CA-C	-5.44	105.35	111.28
1	A	247	SER	N-CA-C	-5.43	105.36	111.28
1	B	216	PRO	N-CA-C	-5.43	106.31	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	211	ARG	N-CA-C	-5.43	105.46	111.71
1	A	300	GLU	N-CA-C	-5.43	105.36	111.28
1	B	229	THR	N-CA-C	-5.43	103.73	110.41
2	D	116	VAL	CB-CA-C	-5.43	104.81	112.14
2	C	409	GLY	N-CA-C	-5.42	106.14	113.24
1	A	53	LEU	N-CA-C	5.42	116.99	111.14
2	D	248	LEU	N-CA-C	-5.41	105.39	111.28
1	B	247	SER	N-CA-C	-5.41	105.39	111.28
1	A	50	ARG	N-CA-C	-5.40	105.50	111.71
1	A	19	ALA	N-CA-C	-5.40	105.39	111.28
1	A	297	SER	N-CA-C	-5.40	105.39	111.28
2	C	395	ARG	N-CA-C	-5.40	105.50	111.71
1	B	522	LEU	N-CA-C	5.39	117.24	111.36
2	C	119	ARG	N-CA-C	-5.39	105.31	111.07
2	C	404	LYS	N-CA-C	-5.38	103.59	110.53
2	D	307	ASP	N-CA-C	-5.38	105.31	111.07
1	A	16	GLY	N-CA-C	-5.38	106.28	112.73
1	A	104	ASN	N-CA-C	-5.35	105.45	111.28
2	D	406	SER	N-CA-C	-5.34	105.46	111.28
2	D	251	GLU	N-CA-C	5.33	117.17	111.36
2	D	211	ARG	N-CA-C	-5.33	105.47	111.28
2	D	161	ALA	N-CA-C	-5.31	105.50	111.28
2	C	232	ASN	N-CA-C	5.30	116.87	111.14
1	B	553	ARG	N-CA-C	-5.30	105.50	111.28
2	D	411	ALA	N-CA-C	-5.29	105.51	111.28
1	A	430	GLU	N-CA-C	-5.28	103.07	110.35
2	D	117	ALA	N-CA-C	-5.26	105.54	111.28
2	C	412	ILE	N-CA-C	-5.26	105.26	110.62
1	B	150	GLU	N-CA-C	-5.24	105.68	111.71
1	B	24	PHE	N-CA-C	-5.23	105.48	111.07
1	A	443	ASN	N-CA-C	-5.22	105.71	111.71
1	A	64	GLN	N-CA-C	-5.22	105.49	111.07
1	B	481	TYR	N-CA-C	-5.21	103.66	110.53
1	B	47	MET	N-CA-C	-5.20	105.61	111.28
2	D	89	LEU	N-CA-C	-5.19	105.62	111.28
2	D	365	ARG	N-CA-C	-5.19	105.62	111.28
1	B	297	SER	N-CA-C	-5.19	105.63	111.28
2	D	48	VAL	CB-CA-C	-5.19	105.33	111.97
1	A	13	ILE	CB-CA-C	-5.17	105.35	111.97
1	A	380	LEU	N-CA-C	-5.15	101.24	109.07
1	B	155	ARG	N-CA-C	-5.15	105.79	111.71
2	C	305	ASN	N-CA-C	-5.14	105.80	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	LEU	N-CA-C	-5.13	105.69	111.28
2	C	63	ILE	CB-CA-C	-5.13	103.95	110.98
2	D	208	ARG	N-CA-C	-5.13	105.69	111.28
1	A	551	ARG	N-CA-C	5.13	116.95	111.36
1	A	187	GLU	N-CA-C	-5.12	105.70	111.28
1	A	86	TYR	N-CA-C	-5.10	105.72	111.28
1	A	62	VAL	N-CA-C	-5.10	105.42	110.62
2	C	309	ILE	N-CA-C	5.09	115.32	110.53
2	D	412	ILE	CB-CA-C	-5.09	105.45	111.97
2	C	207	LYS	N-CA-C	-5.09	105.74	111.28
2	D	52	ALA	N-CA-C	-5.08	105.74	111.28
1	A	46	ALA	N-CA-C	-5.08	105.75	111.28
2	D	87	GLU	N-CA-C	-5.06	105.76	111.28
2	D	370	THR	N-CA-C	-5.06	105.76	111.28
1	A	68	ILE	CB-CA-C	-5.05	105.32	112.14
2	D	409	GLY	N-CA-C	-5.05	106.67	112.73
2	C	358	LEU	N-CA-C	-5.05	105.77	111.28
2	C	365	ARG	N-CA-C	-5.05	105.77	111.28
1	B	383	ARG	N-CA-C	-5.04	105.78	111.28
1	B	551	ARG	N-CA-C	-5.04	105.67	111.07
2	C	137	THR	N-CA-C	-5.03	103.25	109.64
2	D	395	ARG	N-CA-C	-5.03	105.79	111.28
1	B	382	LYS	N-CA-C	-5.03	105.92	111.71
1	A	58	VAL	CB-CA-C	-5.03	105.35	112.14
1	A	220	LEU	N-CA-C	5.03	116.39	108.55
1	B	354	ARG	N-CA-C	-5.02	105.81	111.28
1	B	104	ASN	N-CA-C	-5.02	105.81	111.28
1	A	306	GLN	N-CA-C	-5.01	105.82	111.28
2	C	271	THR	N-CA-C	5.01	116.55	111.14
1	A	355	ALA	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	GLU	Peptide
2	C	70	THR	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	4575	0	4464	781	3
1	B	4649	0	4550	716	0
2	C	3205	0	3213	437	2
2	D	3205	0	3211	462	3
3	A	23	0	12	2	0
3	B	23	0	12	7	0
4	A	27	0	12	7	0
4	B	27	0	12	7	0
5	A	3	0	0	0	0
5	B	4	0	0	1	0
5	C	7	0	0	2	0
5	D	7	0	0	3	0
All	All	15755	0	15486	2354	5

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 75.

All (2354) 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)
2:D:261:GLY:HA3	2:D:263:TRP:CZ3	1.26	1.69
1:A:7:LEU:CD1	1:A:85:HIS:CD2	1.76	1.66
1:B:40:TRP:CZ3	1:B:205:LYS:HE2	1.36	1.59
2:D:154:GLU:C	2:D:303:ASN:HD21	1.04	1.56
1:A:525:ASP:CB	1:A:528:ILE:HD12	1.31	1.54
2:D:106:PRO:HB2	2:D:111:ILE:CD1	1.42	1.47
2:D:119:ARG:HA	2:D:124:LEU:CD1	1.44	1.47
2:D:240:ALA:O	2:D:244:TRP:CD1	1.69	1.46
1:A:525:ASP:CB	1:A:528:ILE:CD1	1.94	1.44
1:A:525:ASP:CA	1:A:528:ILE:HD11	1.45	1.44
1:A:336:LYS:NZ	1:A:416:GLU:CD	1.74	1.43
1:A:7:LEU:CD1	1:A:85:HIS:HD2	1.08	1.43
1:A:7:LEU:HD12	1:A:85:HIS:CD2	1.35	1.42
2:C:118:LEU:O	2:C:122:LEU:CD1	1.64	1.41
1:B:365:ARG:NH1	1:B:371:ASP:HB2	1.14	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LYS:O	1:B:173:ILE:CD1	1.67	1.40
1:A:219:THR:C	1:A:220:LEU:HD23	1.46	1.38
1:A:444:ALA:O	1:A:448:LEU:CD1	1.73	1.36
1:A:509:SER:OG	1:A:512:ASP:CG	1.69	1.36
2:C:153:ARG:CD	2:C:306:GLY:HA3	1.55	1.36
2:C:100:LYS:NZ	2:C:115:ASN:OD1	1.60	1.35
1:A:23:ARG:NH2	1:B:18:ASP:OD2	1.57	1.34
1:A:254:ARG:NH2	1:A:470:ARG:NH1	1.74	1.34
2:C:263:TRP:C	2:C:264:LEU:HD23	1.52	1.34
1:A:525:ASP:C	1:A:528:ILE:HD11	1.51	1.33
1:B:176:ILE:O	1:B:180:LEU:HD12	1.16	1.33
2:D:202:SER:OG	2:D:205:GLY:N	1.60	1.33
1:A:525:ASP:C	1:A:528:ILE:CD1	2.04	1.31
1:B:229:THR:HG22	1:B:233:GLU:C	1.56	1.30
1:B:237:ASP:OD1	1:B:568:ARG:HD2	1.27	1.30
1:A:294:LYS:C	1:A:297:SER:HG	1.38	1.30
1:A:7:LEU:O	1:A:11:GLN:HG3	1.33	1.29
1:A:294:LYS:C	1:A:297:SER:OG	1.76	1.29
2:D:106:PRO:CB	2:D:111:ILE:CD1	2.10	1.28
1:B:237:ASP:OD1	1:B:568:ARG:CD	1.81	1.28
1:A:509:SER:HG	1:A:512:ASP:CG	1.36	1.27
1:B:253:ALA:O	1:B:367:GLY:HA2	1.15	1.27
2:C:37:ILE:HG23	2:C:341:THR:O	1.15	1.27
1:A:525:ASP:O	1:A:528:ILE:CD1	1.82	1.27
1:A:422:LEU:O	1:A:426:LEU:HD12	1.34	1.27
2:C:258:ILE:HG22	2:C:259:ASP:OD1	1.29	1.27
2:C:262:PRO:O	2:C:264:LEU:HD21	1.30	1.27
2:C:271:THR:CG2	2:C:273:LYS:HE3	1.64	1.26
2:D:92:ILE:HG22	2:D:332:CYS:SG	1.73	1.26
1:A:163:ARG:O	1:A:164:LEU:HD12	1.10	1.26
1:B:253:ALA:O	1:B:367:GLY:CA	1.82	1.26
1:B:242:THR:OG1	1:B:245:GLU:CD	1.77	1.26
2:C:353:PRO:O	2:C:357:ILE:CD1	1.84	1.26
2:C:214:ILE:O	2:C:218:ILE:HD12	1.12	1.25
2:D:154:GLU:O	2:D:303:ASN:CG	1.77	1.25
2:D:261:GLY:CA	2:D:263:TRP:CZ3	2.16	1.25
2:C:353:PRO:O	2:C:357:ILE:HD12	1.15	1.24
1:B:192:SER:OG	1:B:215:THR:HA	1.08	1.24
2:C:124:LEU:CD1	2:C:327:ASN:C	2.11	1.24
2:D:106:PRO:CB	2:D:111:ILE:HD11	1.65	1.24
1:B:242:THR:CB	1:B:245:GLU:OE2	1.84	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:THR:HG22	1:B:233:GLU:O	1.10	1.24
1:A:525:ASP:HB3	1:A:528:ILE:CD1	1.59	1.23
2:C:124:LEU:HD12	2:C:327:ASN:CB	1.68	1.23
2:C:153:ARG:HD3	2:C:306:GLY:CA	1.68	1.23
2:D:118:LEU:O	2:D:122:LEU:HD12	1.33	1.22
1:A:7:LEU:HD11	1:A:85:HIS:CD2	1.54	1.22
1:A:509:SER:CB	1:A:512:ASP:OD2	1.86	1.22
1:A:368:ARG:NH2	1:A:440:GLU:OE2	1.72	1.22
2:C:262:PRO:O	2:C:264:LEU:CD2	1.86	1.22
2:D:382:GLY:C	2:D:415:ASN:HD22	1.45	1.21
1:B:204:ASN:ND2	1:B:364:ASP:OD2	1.73	1.21
2:C:92:ILE:O	2:C:95:TYR:O	1.56	1.21
1:A:542:ALA:O	1:A:546:ARG:HD2	1.41	1.20
2:C:214:ILE:O	2:C:218:ILE:CD1	1.89	1.20
1:B:163:ARG:O	1:B:164:LEU:CD2	1.88	1.19
1:B:242:THR:HG1	1:B:245:GLU:CD	1.47	1.19
2:D:214:ILE:O	2:D:218:ILE:HG13	1.41	1.19
1:B:551:ARG:NH2	1:B:558:GLU:OE1	1.75	1.19
1:A:294:LYS:CA	1:A:297:SER:OG	1.92	1.18
2:D:203:GLU:HB2	2:D:244:TRP:CZ3	1.77	1.18
2:C:222:ARG:NH1	2:C:297:ASP:OD2	1.77	1.18
2:C:323:ALA:O	2:C:355:SER:OG	1.57	1.18
1:B:192:SER:OG	1:B:215:THR:CA	1.90	1.18
2:D:382:GLY:C	2:D:415:ASN:ND2	2.01	1.18
1:B:229:THR:HG21	1:B:233:GLU:CB	1.74	1.17
1:A:551:ARG:O	1:A:554:GLU:N	1.76	1.17
1:B:365:ARG:HH11	1:B:371:ASP:CB	1.57	1.16
2:D:119:ARG:CA	2:D:124:LEU:CD1	2.23	1.16
1:B:173:ILE:O	1:B:177:ILE:HD11	1.45	1.16
2:C:154:GLU:OE1	2:C:157:GLU:N	1.79	1.16
1:B:176:ILE:O	1:B:180:LEU:CD1	1.92	1.15
1:B:300:GLU:O	1:B:303:VAL:HG22	1.45	1.15
1:B:365:ARG:NH1	1:B:371:ASP:CB	2.10	1.15
1:B:517:GLU:OE2	2:C:107:VAL:HG23	1.42	1.15
1:B:126:SER:OG	1:B:127:GLN:NE2	1.79	1.15
1:A:525:ASP:CA	1:A:528:ILE:CD1	2.16	1.14
2:C:258:ILE:C	2:C:259:ASP:OD1	1.89	1.14
1:A:439:GLU:O	1:A:443:ASN:ND2	1.79	1.14
2:C:74:SER:OG	2:C:82:VAL:O	1.66	1.14
1:B:40:TRP:CZ3	1:B:205:LYS:CE	2.31	1.13
2:C:306:GLY:O	2:C:310:SER:OG	1.68	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:O	1:A:164:LEU:CD1	1.97	1.12
1:A:294:LYS:O	1:A:297:SER:OG	1.63	1.12
1:B:89:LEU:O	1:B:93:TYR:CD1	2.03	1.12
2:C:153:ARG:HD3	2:C:306:GLY:HA3	1.13	1.11
1:B:346:LYS:HD3	1:B:348:MET:CE	1.81	1.11
2:D:261:GLY:HA3	2:D:263:TRP:CH2	1.85	1.11
1:A:542:ALA:C	1:A:546:ARG:HD2	1.74	1.11
1:B:499:GLU:OE2	2:C:345:TYR:OH	1.67	1.11
1:A:170:SER:H	1:A:173:ILE:CG1	1.62	1.10
2:C:29:ILE:HG21	2:C:363:MET:HE1	1.32	1.10
1:B:17:PHE:HE1	1:B:98:ILE:HG22	1.13	1.10
1:A:163:ARG:C	1:A:164:LEU:HD12	1.75	1.10
1:A:170:SER:N	1:A:173:ILE:HG12	1.50	1.10
1:A:336:LYS:HZ2	1:A:416:GLU:CD	1.41	1.10
2:D:37:ILE:HG12	2:D:341:THR:O	1.49	1.10
1:A:336:LYS:CE	1:A:416:GLU:OE2	2.00	1.09
1:B:163:ARG:O	1:B:164:LEU:HD23	0.92	1.08
2:D:71:GLY:N	2:D:74:SER:OG	1.67	1.08
1:A:444:ALA:O	1:A:448:LEU:HD12	1.53	1.08
1:B:430:GLU:OE1	1:B:431:GLY:N	1.85	1.08
2:C:78:TYR:OH	2:C:87:GLU:OE2	1.68	1.08
1:A:171:ARG:NH1	1:A:175:TYR:HE2	1.51	1.08
1:B:68:ILE:O	1:B:69:THR:OG1	1.70	1.08
1:B:253:ALA:C	1:B:367:GLY:HA2	1.77	1.08
2:C:133:TYR:CE1	2:C:134:TYR:O	2.06	1.08
1:A:100:GLU:OE2	1:A:125:SER:O	1.72	1.08
1:B:50:ARG:HD2	1:B:258:MET:HE2	1.27	1.08
1:A:444:ALA:O	1:A:448:LEU:HD11	1.34	1.07
1:B:176:ILE:HG22	1:B:180:LEU:HD11	1.09	1.07
1:B:237:ASP:OD1	1:B:568:ARG:NE	1.86	1.07
1:A:140:ALA:HB2	1:A:197:ALA:CA	1.84	1.07
1:B:178:ARG:O	1:B:182:GLU:OE2	1.70	1.07
2:C:271:THR:HG21	2:C:273:LYS:CE	1.85	1.07
2:D:157:GLU:OE1	2:D:202:SER:N	1.87	1.07
1:A:6:GLU:OE1	1:A:6:GLU:N	1.88	1.07
2:D:80:GLN:O	2:D:81:ASP:OD1	1.71	1.07
2:D:289:ILE:O	2:D:293:PRO:HG3	1.55	1.07
1:B:169:LYS:O	1:B:173:ILE:HD12	1.27	1.06
2:C:145:GLU:N	2:C:145:GLU:OE1	1.88	1.06
1:B:167:GLN:HG2	1:B:233:GLU:OE1	1.52	1.06
1:B:169:LYS:O	1:B:173:ILE:HD13	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:H	1:A:173:ILE:HG12	0.93	1.06
1:A:422:LEU:O	1:A:426:LEU:CD1	2.04	1.06
1:B:40:TRP:CE3	1:B:205:LYS:HE2	1.89	1.06
2:D:119:ARG:HA	2:D:124:LEU:HD11	1.06	1.06
2:D:154:GLU:C	2:D:303:ASN:ND2	1.79	1.06
1:A:140:ALA:CB	1:A:197:ALA:HA	1.86	1.05
2:C:160:TYR:HB2	2:C:303:ASN:HD22	1.17	1.05
1:A:177:ILE:O	1:A:181:THR:HG23	1.54	1.05
1:B:80:LEU:HD23	1:B:81:ARG:H	1.20	1.05
2:C:37:ILE:CG2	2:C:341:THR:O	2.05	1.05
1:A:119:GLU:N	1:A:119:GLU:OE2	1.89	1.05
2:C:154:GLU:CD	2:C:157:GLU:H	1.63	1.05
2:C:66:MET:HE1	2:C:95:TYR:CE2	1.92	1.05
2:C:258:ILE:CG2	2:C:259:ASP:OD1	2.05	1.05
2:D:153:ARG:NH2	2:D:303:ASN:O	1.88	1.05
1:A:166:TRP:HA	1:A:233:GLU:HG3	1.36	1.04
1:A:254:ARG:HH22	1:A:470:ARG:CZ	1.70	1.04
1:A:525:ASP:HB2	1:A:528:ILE:HD12	1.37	1.04
1:B:173:ILE:O	1:B:177:ILE:CD1	2.05	1.04
1:B:179:HIS:HA	1:B:182:GLU:OE2	1.54	1.04
2:C:153:ARG:HD3	2:C:306:GLY:C	1.82	1.04
2:C:221:ASP:OD2	2:C:271:THR:HG21	1.53	1.04
1:A:429:VAL:HG13	1:A:433:GLN:HB2	1.40	1.04
1:B:89:LEU:O	1:B:93:TYR:CE1	2.11	1.04
1:B:177:ILE:O	1:B:181:THR:OG1	1.76	1.03
2:C:236:PHE:CD2	2:D:164:GLU:OE1	2.11	1.03
1:B:517:GLU:OE2	2:C:107:VAL:N	1.90	1.03
2:C:154:GLU:OE2	2:C:156:SER:N	1.89	1.03
1:A:66:ARG:O	1:A:70:ASN:N	1.90	1.03
1:A:525:ASP:N	1:A:528:ILE:HD11	1.72	1.03
2:C:124:LEU:HD11	2:C:327:ASN:O	1.59	1.03
1:B:154:MET:O	1:B:158:SER:OG	1.76	1.03
2:D:106:PRO:HB2	2:D:111:ILE:HD11	1.03	1.03
1:B:229:THR:HG21	1:B:233:GLU:HB2	1.04	1.03
2:D:106:PRO:CB	2:D:111:ILE:HD12	1.88	1.03
1:A:107:TYR:CE1	1:A:111:PHE:CE2	2.46	1.02
1:A:163:ARG:C	1:A:164:LEU:CD1	2.32	1.02
2:C:71:GLY:O	2:C:83:TRP:CE3	2.12	1.02
1:B:173:ILE:HD13	1:B:173:ILE:H	1.22	1.02
1:A:525:ASP:O	1:A:528:ILE:HD13	1.55	1.02
1:B:86:TYR:HA	1:B:89:LEU:HD13	1.36	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:H	1:A:176:ILE:HD13	1.24	1.01
1:B:229:THR:CG2	1:B:233:GLU:CA	2.38	1.01
1:B:229:THR:CG2	1:B:233:GLU:O	2.07	1.01
2:C:204:GLU:HB3	2:D:190:PHE:CE2	1.94	1.01
1:A:274:ILE:HG22	1:A:275:LEU:CD2	1.90	1.01
1:A:298:TYR:HE2	1:A:302:LEU:HD11	1.22	1.01
1:B:229:THR:CG2	1:B:233:GLU:C	2.34	1.01
2:D:383:ALA:N	2:D:415:ASN:HD22	1.55	1.01
2:D:383:ALA:N	2:D:415:ASN:ND2	2.09	1.01
1:A:8:LEU:O	1:A:12:THR:OG1	1.78	1.00
2:D:180:ARG:O	2:D:184:GLY:HA2	1.61	1.00
2:C:204:GLU:OE1	2:D:190:PHE:CZ	2.13	1.00
1:B:293:ALA:O	1:B:297:SER:OG	1.78	1.00
1:B:83:LYS:O	1:B:87:THR:N	1.88	1.00
2:C:263:TRP:O	2:C:264:LEU:HD23	1.59	1.00
1:B:176:ILE:CG2	1:B:180:LEU:HD11	1.91	0.99
2:C:118:LEU:O	2:C:122:LEU:HD12	0.83	0.99
2:C:402:LEU:HD12	2:C:403:LEU:N	1.77	0.99
1:A:525:ASP:O	1:A:528:ILE:HD11	1.49	0.99
1:B:346:LYS:HD3	1:B:348:MET:HE1	1.41	0.99
1:B:346:LYS:HB3	1:B:348:MET:CE	1.92	0.99
2:D:57:TYR:HE2	2:D:372:ALA:HB2	1.28	0.99
1:B:169:LYS:C	1:B:173:ILE:HD12	1.80	0.99
2:D:298:VAL:C	2:D:299:ILE:HD12	1.86	0.98
1:B:229:THR:CG2	1:B:233:GLU:N	2.26	0.98
1:B:237:ASP:CG	1:B:568:ARG:HD2	1.88	0.98
2:C:124:LEU:HD12	2:C:327:ASN:C	1.83	0.98
1:A:294:LYS:HA	1:A:297:SER:OG	1.63	0.98
1:B:375:PHE:CD1	1:B:415:ILE:CD1	2.47	0.98
1:A:219:THR:O	1:A:220:LEU:HD23	1.61	0.98
2:D:353:PRO:HG3	2:D:405:CYS:SG	2.02	0.98
1:A:7:LEU:HD11	1:A:85:HIS:HD2	0.90	0.98
2:C:124:LEU:CD1	2:C:327:ASN:O	2.10	0.98
1:B:312:PHE:CE1	1:B:328:LEU:CD2	2.47	0.98
2:C:175:VAL:HG22	2:D:183:MET:CE	1.93	0.97
1:A:107:TYR:CE1	1:A:111:PHE:HE2	1.81	0.97
2:D:203:GLU:HB2	2:D:244:TRP:HZ3	1.15	0.97
1:A:452:ASN:O	1:A:452:ASN:ND2	1.95	0.97
1:B:452:ASN:O	1:B:452:ASN:ND2	1.97	0.97
1:B:163:ARG:C	1:B:164:LEU:HD23	1.89	0.97
1:B:298:TYR:CE2	3:B:602:AMP:H2	1.82	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:O	1:A:571:VAL:HG23	1.65	0.97
1:B:187:GLU:OE1	1:B:187:GLU:N	1.97	0.96
2:D:230:LYS:H	2:D:238:GLU:HG2	1.25	0.96
1:A:413:LEU:HD12	1:A:414:TYR:N	1.80	0.96
1:A:119:GLU:HG2	1:A:120:ARG:HG2	1.48	0.96
2:C:125:TYR:OH	2:C:330:ASP:OD1	1.82	0.96
1:A:96:PHE:O	1:A:99:ALA:N	1.98	0.96
1:A:254:ARG:HH21	1:A:470:ARG:NH1	1.56	0.96
1:A:298:TYR:CE2	1:A:302:LEU:HD11	1.99	0.96
2:C:171:ASP:O	2:C:175:VAL:HG23	1.66	0.96
1:B:156:VAL:HG23	1:B:157:ILE:H	1.28	0.95
1:A:166:TRP:CA	1:A:233:GLU:HG3	1.86	0.95
2:C:271:THR:HG21	2:C:273:LYS:HE3	0.99	0.95
2:D:47:LYS:NZ	2:D:410:ASP:OD1	1.99	0.95
2:D:132:ARG:HG2	2:D:132:ARG:HH11	1.31	0.95
2:D:209:LEU:HD23	2:D:210:VAL:N	1.80	0.95
1:B:40:TRP:HZ3	1:B:205:LYS:HE2	1.31	0.95
1:A:149:TRP:CE3	1:A:152:LEU:HD23	2.01	0.95
1:A:303:VAL:O	1:A:306:GLN:HG2	1.66	0.95
2:D:240:ALA:C	2:D:244:TRP:NE1	2.24	0.95
2:D:291:LEU:HD12	2:D:291:LEU:H	1.31	0.95
2:D:129:ARG:NH2	2:D:336:GLU:OE2	2.00	0.95
2:D:209:LEU:HD23	2:D:210:VAL:H	1.29	0.95
1:A:140:ALA:HB2	1:A:197:ALA:HA	0.96	0.94
1:B:212:LYS:HG3	1:B:274:ILE:HD11	1.49	0.94
2:C:124:LEU:HD12	2:C:327:ASN:HB3	1.47	0.94
1:A:78:PHE:O	1:A:80:LEU:N	2.00	0.94
2:C:8:PRO:HG3	2:C:28:ILE:HG23	1.47	0.94
1:B:222:PHE:O	1:B:223:LEU:HD12	1.67	0.94
1:B:17:PHE:HE1	1:B:98:ILE:CG2	1.81	0.94
2:D:118:LEU:O	2:D:122:LEU:CD1	2.15	0.94
2:D:240:ALA:O	2:D:244:TRP:HD1	1.43	0.94
1:A:149:TRP:HA	1:A:152:LEU:HB3	1.48	0.93
1:B:312:PHE:CE1	1:B:328:LEU:HD23	2.02	0.93
1:B:84:GLU:O	1:B:88:ARG:N	2.02	0.93
1:A:432:GLN:O	1:A:436:ASP:OD2	1.86	0.93
1:A:171:ARG:NH1	1:A:175:TYR:CE2	2.37	0.93
1:A:336:LYS:HZ1	1:A:416:GLU:CD	1.55	0.93
1:B:57:HIS:O	1:B:61:VAL:HG23	1.68	0.93
1:B:361:LYS:HE2	1:B:372:THR:O	1.69	0.93
1:B:539:LEU:O	1:B:545:TRP:NE1	2.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:236:PHE:HD2	2:D:164:GLU:OE1	1.46	0.93
1:A:254:ARG:NH2	1:A:470:ARG:HH12	1.60	0.92
1:A:448:LEU:HD12	1:A:448:LEU:H	1.33	0.92
1:B:17:PHE:CE1	1:B:98:ILE:HG22	2.04	0.92
1:A:46:ALA:HA	1:A:49:ASN:OD1	1.70	0.92
1:B:375:PHE:CE1	1:B:415:ILE:HD13	2.04	0.92
1:B:201:PHE:CE1	1:B:210:VAL:HG21	2.05	0.92
2:D:30:PRO:O	2:D:98:ALA:HB1	1.68	0.92
1:B:169:LYS:C	1:B:173:ILE:CD1	2.27	0.92
2:C:21:LEU:H	2:C:21:LEU:HD12	1.32	0.92
2:D:199:LYS:HD3	2:D:237:THR:OG1	1.70	0.92
1:A:254:ARG:HH22	1:A:470:ARG:NH1	1.48	0.91
2:C:201:CYS:SG	2:C:237:THR:O	2.28	0.91
1:B:86:TYR:CA	1:B:89:LEU:CD1	2.48	0.91
2:C:66:MET:CE	2:C:95:TYR:CE2	2.53	0.91
2:D:119:ARG:O	2:D:124:LEU:HD12	1.70	0.91
1:A:34:ARG:O	1:A:37:GLN:O	1.88	0.91
1:A:143:PHE:O	1:A:193:HIS:HB2	1.71	0.91
2:C:209:LEU:O	2:C:212:ALA:HB3	1.71	0.91
1:A:91:PRO:HD3	1:A:127:GLN:OE1	1.69	0.91
2:C:175:VAL:HG22	2:D:183:MET:HE2	1.52	0.91
2:D:240:ALA:O	2:D:244:TRP:NE1	2.04	0.91
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.36	0.91
2:D:240:ALA:C	2:D:244:TRP:CD1	2.49	0.91
1:B:68:ILE:C	1:B:69:THR:HG1	1.78	0.91
1:A:100:GLU:O	1:A:104:ASN:OD1	1.87	0.90
1:A:219:THR:C	1:A:220:LEU:CD2	2.41	0.90
2:D:106:PRO:CA	2:D:111:ILE:HD11	2.01	0.90
1:B:77:GLU:O	1:B:80:LEU:HD22	1.71	0.90
2:C:124:LEU:HD13	2:C:328:ILE:N	1.87	0.90
1:B:253:ALA:O	1:B:367:GLY:N	2.03	0.90
1:B:522:LEU:O	1:B:528:ILE:CD1	2.20	0.90
2:D:57:TYR:CE2	2:D:372:ALA:HB2	2.06	0.90
2:D:106:PRO:HB2	2:D:111:ILE:CG1	2.01	0.90
1:A:192:SER:OG	1:A:215:THR:CA	2.17	0.90
2:D:401:LYS:O	2:D:403:LEU:CD1	2.20	0.90
1:A:322:VAL:HG23	4:A:602:ADP:O1B	1.72	0.89
2:C:361:GLU:OE1	5:C:505:HOH:O	1.90	0.89
1:A:229:THR:OG1	1:A:235:PHE:CE1	2.24	0.89
1:B:546:ARG:HH11	1:B:546:ARG:HG3	1.38	0.89
2:D:230:LYS:O	2:D:232:ASN:N	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:384:ILE:O	2:D:387:LYS:N	2.05	0.89
2:C:241:PHE:CD2	2:C:302:MET:HE3	2.07	0.89
1:A:141:LYS:O	1:A:143:PHE:CE1	2.25	0.89
2:C:71:GLY:O	2:C:83:TRP:CZ3	2.26	0.89
2:D:240:ALA:C	2:D:244:TRP:HE1	1.79	0.89
2:D:398:ASP:OD1	2:D:399:GLY:N	2.05	0.89
1:A:482:MET:HE1	1:A:545:TRP:CE3	2.06	0.89
2:C:160:TYR:HB2	2:C:303:ASN:ND2	1.87	0.89
2:D:45:MET:O	2:D:49:VAL:HG23	1.73	0.89
1:A:149:TRP:O	1:A:152:LEU:N	2.06	0.89
1:A:215:THR:OG1	1:A:216:PRO:HD2	1.71	0.89
1:A:361:LYS:NZ	1:A:371:ASP:OD2	2.06	0.88
1:B:300:GLU:O	1:B:303:VAL:CG2	2.20	0.88
2:C:204:GLU:HB3	2:D:190:PHE:CD2	2.08	0.88
1:A:149:TRP:CE3	1:A:152:LEU:CD2	2.56	0.88
1:A:404:LEU:O	1:A:407:GLN:O	1.92	0.88
1:A:7:LEU:CD1	1:A:85:HIS:NE2	2.36	0.88
1:A:311:GLN:NE2	1:A:383:ARG:O	2.07	0.88
2:D:261:GLY:HA3	2:D:263:TRP:HZ3	1.12	0.88
1:A:223:LEU:O	1:A:224:LEU:HD12	1.72	0.88
2:C:268:ASN:OD1	2:C:271:THR:N	1.95	0.88
2:D:273:LYS:HG2	2:D:274:GLU:N	1.89	0.87
2:C:124:LEU:HD12	2:C:327:ASN:HB2	1.52	0.87
1:A:34:ARG:HH21	1:A:258:MET:HE2	1.40	0.87
1:A:461:LYS:C	1:A:462:ASN:HD22	1.81	0.87
1:B:145:PRO:HB3	1:B:149:TRP:CE3	2.09	0.87
2:D:132:ARG:NH1	2:D:133:TYR:O	2.08	0.87
2:D:240:ALA:CB	2:D:244:TRP:HE1	1.88	0.87
1:A:170:SER:N	1:A:173:ILE:CG1	2.14	0.87
1:A:543:ASP:HA	1:A:546:ARG:HD3	1.56	0.87
1:A:192:SER:OG	1:A:215:THR:HA	1.75	0.87
1:A:222:PHE:O	1:A:223:LEU:HD12	1.75	0.87
2:C:221:ASP:O	2:C:273:LYS:NZ	1.95	0.87
2:D:273:LYS:HG2	2:D:274:GLU:H	1.40	0.87
1:B:86:TYR:HA	1:B:89:LEU:CD1	2.03	0.87
1:B:146:ASP:C	1:B:147:HIS:CD2	2.53	0.87
2:D:25:GLU:C	2:D:27:PRO:HD3	2.00	0.87
2:D:203:GLU:CB	2:D:244:TRP:CZ3	2.58	0.86
1:B:7:LEU:CB	1:B:85:HIS:CD2	2.59	0.86
1:B:24:PHE:CZ	1:B:50:ARG:NH2	2.43	0.86
1:A:168:ASN:O	1:A:171:ARG:N	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:GLN:CG	1:B:233:GLU:OE1	2.24	0.86
1:B:229:THR:HG23	1:B:233:GLU:H	1.36	0.86
1:A:525:ASP:C	1:A:528:ILE:HD13	1.92	0.86
1:A:94:PRO:HG3	1:B:26:GLU:CD	1.99	0.86
1:A:403:ASP:C	1:A:404:LEU:HD13	2.01	0.86
1:B:323:MET:HE3	1:B:357:TYR:OH	1.76	0.86
2:C:291:LEU:H	2:C:291:LEU:HD12	1.38	0.86
1:B:462:ASN:HA	1:B:474:TYR:HE1	1.40	0.86
2:D:248:LEU:HD12	2:D:248:LEU:O	1.76	0.86
1:A:180:LEU:HD23	1:A:181:THR:HG23	1.56	0.86
1:B:375:PHE:CD1	1:B:415:ILE:HD12	2.11	0.86
1:A:515:PRO:HA	1:A:518:PHE:CE2	2.10	0.85
2:D:158:ASP:OD1	2:D:159:ILE:N	2.07	0.85
1:A:274:ILE:HG22	1:A:275:LEU:HD23	1.57	0.85
1:B:140:ALA:HB1	1:B:196:VAL:O	1.76	0.85
1:B:222:PHE:C	1:B:223:LEU:HD12	2.01	0.85
1:A:96:PHE:O	1:A:99:ALA:HB3	1.76	0.85
1:B:192:SER:OG	1:B:214:ILE:O	1.90	0.85
2:C:183:MET:HA	2:C:183:MET:HE3	1.56	0.85
1:B:180:LEU:HD12	1:B:180:LEU:H	1.39	0.85
2:C:133:TYR:HA	2:C:317:VAL:CG1	2.06	0.85
2:D:240:ALA:HB1	2:D:244:TRP:NE1	1.91	0.85
1:A:322:VAL:CG2	4:A:602:ADP:O1B	2.24	0.85
1:A:229:THR:O	1:A:232:GLY:CA	2.25	0.85
1:B:312:PHE:CZ	1:B:328:LEU:HD21	2.12	0.85
1:B:346:LYS:HD3	1:B:348:MET:HE3	1.55	0.85
2:C:204:GLU:OE1	2:D:190:PHE:CE2	2.29	0.85
2:D:353:PRO:CG	2:D:405:CYS:SG	2.65	0.85
2:C:262:PRO:O	2:C:264:LEU:HD23	1.77	0.85
2:D:71:GLY:O	2:D:74:SER:N	1.98	0.85
1:A:261:ALA:O	1:A:264:PRO:HD3	1.76	0.84
1:B:522:LEU:O	1:B:528:ILE:HD11	1.74	0.84
2:D:119:ARG:HA	2:D:124:LEU:HD13	1.56	0.84
1:B:178:ARG:C	1:B:182:GLU:OE2	2.20	0.84
2:D:127:CYS:SG	2:D:153:ARG:CD	2.64	0.84
1:A:94:PRO:CG	1:B:26:GLU:OE1	2.25	0.84
1:B:229:THR:HG23	1:B:233:GLU:N	1.90	0.84
1:A:569:PHE:C	1:A:571:VAL:H	1.85	0.84
1:A:287:ILE:HD11	1:A:289:CYS:SG	2.18	0.84
1:B:152:LEU:HD12	1:B:152:LEU:O	1.78	0.84
2:D:235:LYS:O	2:D:239:GLY:CA	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:409:GLY:O	2:D:413:ILE:HG13	1.78	0.84
1:A:172:ASP:HA	1:A:175:TYR:CD2	2.13	0.83
1:B:80:LEU:HD23	1:B:81:ARG:N	1.92	0.83
1:B:201:PHE:CE1	1:B:210:VAL:CG2	2.61	0.83
1:B:327:THR:HG21	1:B:418:ARG:NH2	1.93	0.83
1:A:85:HIS:O	1:A:89:LEU:HD11	1.78	0.83
1:B:60:LEU:HD12	1:B:60:LEU:O	1.78	0.83
1:B:179:HIS:CA	1:B:182:GLU:OE2	2.26	0.83
1:B:8:LEU:HD12	1:B:8:LEU:O	1.78	0.83
2:D:413:ILE:O	2:D:416:MET:HB2	1.77	0.83
1:A:525:ASP:HB3	1:A:528:ILE:HD12	0.85	0.83
1:B:166:TRP:CE2	1:B:234:LEU:HD23	2.13	0.83
1:B:189:LEU:HD12	1:B:189:LEU:O	1.79	0.83
1:A:293:ALA:O	1:A:297:SER:OG	1.97	0.83
2:C:71:GLY:O	2:C:83:TRP:HE3	1.59	0.83
2:C:213:ALA:O	2:C:216:TYR:N	2.12	0.83
2:D:235:LYS:O	2:D:239:GLY:HA3	1.77	0.83
1:A:244:ALA:O	1:A:247:SER:OG	1.95	0.83
1:B:312:PHE:CD1	1:B:328:LEU:CD2	2.61	0.83
2:D:240:ALA:HB1	2:D:244:TRP:CE2	2.13	0.83
1:B:127:GLN:N	1:B:127:GLN:HE21	1.77	0.83
2:C:124:LEU:HD13	2:C:327:ASN:C	2.03	0.83
1:A:535:MET:HB3	1:A:536:HIS:CD2	2.14	0.83
1:B:24:PHE:CE1	1:B:50:ARG:NH2	2.47	0.83
1:B:149:TRP:O	1:B:152:LEU:HB3	1.78	0.83
2:C:153:ARG:HD2	2:C:306:GLY:HA3	1.61	0.83
2:D:392:ASP:O	2:D:396:LEU:HD12	1.79	0.83
2:D:106:PRO:HB3	2:D:111:ILE:HD12	1.57	0.82
1:B:89:LEU:O	1:B:93:TYR:HD1	1.59	0.82
1:A:38:ALA:HA	1:A:40:TRP:CZ3	2.14	0.82
1:A:392:LEU:HD12	1:A:392:LEU:O	1.79	0.82
1:B:346:LYS:HB3	1:B:348:MET:HE3	1.61	0.82
2:C:75:THR:O	2:C:79:GLY:O	1.97	0.82
2:D:99:ILE:HB	2:D:363:MET:CE	2.09	0.82
2:D:322:ILE:O	2:D:358:LEU:HD12	1.78	0.82
1:A:189:LEU:HG	1:A:190:SER:N	1.93	0.82
1:A:257:PHE:HB2	1:A:286:ALA:O	1.80	0.82
2:D:229:HIS:CD2	2:D:242:LYS:HB2	2.14	0.82
1:B:86:TYR:CA	1:B:89:LEU:HD13	2.08	0.82
1:A:565:ARG:O	1:A:568:ARG:HG2	1.79	0.82
1:A:551:ARG:O	1:A:554:GLU:CA	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:CA	1:B:85:HIS:HD2	1.92	0.82
1:B:201:PHE:CD1	1:B:210:VAL:CG2	2.63	0.82
2:C:100:LYS:HG2	2:C:101:GLY:O	1.80	0.82
2:D:92:ILE:CG2	2:D:332:CYS:SG	2.64	0.82
2:D:99:ILE:HB	2:D:363:MET:HE2	1.60	0.82
2:D:169:SER:O	2:D:170:ALA:HB3	1.78	0.82
2:C:128:LEU:HD13	2:C:152:PHE:CE1	2.15	0.82
1:B:212:LYS:CG	1:B:274:ILE:HD11	2.10	0.81
1:B:462:ASN:HA	1:B:474:TYR:CE1	2.14	0.81
2:D:268:ASN:OD1	2:D:271:THR:HG22	1.81	0.81
1:A:39:ASP:HB3	1:A:42:ALA:HB3	1.62	0.81
1:A:46:ALA:CA	1:A:49:ASN:OD1	2.28	0.81
1:B:17:PHE:CE1	1:B:98:ILE:CG2	2.61	0.81
2:D:70:THR:C	2:D:74:SER:OG	2.23	0.81
1:A:229:THR:OG1	1:A:235:PHE:HE1	1.61	0.81
2:C:166:LYS:O	2:C:169:SER:OG	1.97	0.81
1:A:462:ASN:C	1:A:463:PHE:HD1	1.88	0.81
1:B:156:VAL:HG23	1:B:157:ILE:N	1.93	0.81
2:C:158:ASP:HB3	2:C:303:ASN:HB3	1.62	0.81
2:D:127:CYS:SG	2:D:153:ARG:HD3	2.20	0.81
1:A:429:VAL:HG12	1:A:430:GLU:O	1.81	0.81
1:B:365:ARG:HH12	1:B:371:ASP:HB2	1.41	0.81
2:D:154:GLU:O	2:D:303:ASN:ND2	0.66	0.81
1:A:336:LYS:NZ	1:A:416:GLU:OE2	0.66	0.81
1:B:528:ILE:O	1:B:531:LEU:HD12	1.79	0.81
2:C:160:TYR:OH	2:D:230:LYS:NZ	2.13	0.81
1:A:528:ILE:HD13	1:A:528:ILE:H	1.45	0.80
2:D:356:ILE:HD12	2:D:356:ILE:O	1.81	0.80
1:A:141:LYS:O	1:A:143:PHE:HE1	1.62	0.80
1:A:172:ASP:O	1:A:176:ILE:HD13	1.80	0.80
1:B:141:LYS:NZ	1:B:155:ARG:NH1	2.28	0.80
1:B:176:ILE:C	1:B:180:LEU:CD1	2.54	0.80
1:A:26:GLU:O	1:A:29:SER:OG	2.00	0.80
1:A:215:THR:OG1	1:A:216:PRO:CD	2.29	0.80
1:A:107:TYR:CE1	1:A:111:PHE:CD2	2.69	0.80
1:B:23:ARG:NH2	5:B:703:HOH:O	2.14	0.80
1:B:173:ILE:CD1	1:B:173:ILE:H	1.95	0.80
2:C:116:VAL:O	2:C:120:GLN:N	2.11	0.80
1:A:322:VAL:HG21	4:A:602:ADP:O2B	1.81	0.80
2:C:365:ARG:HG2	2:C:365:ARG:HH11	1.45	0.80
2:D:352:ASN:ND2	2:D:392:ASP:OD2	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TRP:HA	1:B:43:VAL:HG23	1.63	0.79
1:B:192:SER:HG	1:B:215:THR:HA	1.16	0.79
2:C:128:LEU:HD13	2:C:152:PHE:CZ	2.17	0.79
1:A:119:GLU:CD	1:A:120:ARG:H	1.90	0.79
1:A:542:ALA:O	1:A:546:ARG:CD	2.28	0.79
1:A:104:ASN:ND2	1:A:122:PHE:O	2.15	0.79
1:B:494:ARG:NH1	1:B:498:ASP:OD1	2.15	0.79
2:D:157:GLU:OE2	2:D:205:GLY:HA3	1.82	0.79
2:D:410:ASP:O	2:D:414:GLU:HG3	1.82	0.79
1:A:66:ARG:O	1:A:69:THR:C	2.09	0.79
2:C:133:TYR:HA	2:C:317:VAL:HG13	1.64	0.79
1:B:229:THR:HG21	1:B:233:GLU:CA	2.06	0.79
2:C:35:ASP:O	2:C:341:THR:HG22	1.83	0.79
2:C:154:GLU:OE1	2:C:157:GLU:CA	2.29	0.79
2:D:119:ARG:CA	2:D:124:LEU:HD12	2.12	0.79
2:D:179:LEU:HA	2:D:183:MET:HB2	1.65	0.79
1:A:60:LEU:HD12	1:A:60:LEU:O	1.82	0.78
2:D:45:MET:HE1	2:D:46:LEU:HD23	1.65	0.78
1:A:229:THR:HG1	1:A:235:PHE:HE1	0.80	0.78
1:A:365:ARG:C	1:A:366:VAL:CG2	2.57	0.78
1:A:39:ASP:O	1:A:42:ALA:N	2.17	0.78
1:B:5:LEU:O	1:B:8:LEU:HB3	1.83	0.78
1:A:7:LEU:O	1:A:11:GLN:CG	2.26	0.78
1:A:394:LEU:HD23	1:A:401:ILE:HD11	1.66	0.78
1:B:146:ASP:C	1:B:147:HIS:CG	2.62	0.78
1:B:201:PHE:CD1	1:B:210:VAL:HG23	2.18	0.78
1:B:229:THR:CG2	1:B:233:GLU:H	1.93	0.78
2:D:257:LEU:HD21	2:D:260:GLY:HA2	1.65	0.78
1:A:189:LEU:HD23	1:A:189:LEU:H	1.49	0.78
1:A:34:ARG:NH2	1:A:258:MET:HE2	1.99	0.78
1:B:515:PRO:O	1:B:540:PHE:HA	1.83	0.78
1:A:321:MET:HB3	1:A:343:ALA:HB2	1.64	0.77
1:B:253:ALA:CB	1:B:367:GLY:HA2	2.14	0.77
1:B:375:PHE:CE1	1:B:415:ILE:CD1	2.63	0.77
1:A:17:PHE:CE1	1:A:98:ILE:CG2	2.66	0.77
1:A:482:MET:CE	1:A:545:TRP:CE3	2.67	0.77
1:B:149:TRP:O	1:B:152:LEU:N	2.16	0.77
2:C:287:GLN:O	2:C:291:LEU:HD13	1.84	0.77
2:D:307:ASP:OD1	2:D:311:ASP:OD2	2.03	0.77
1:A:119:GLU:CG	1:A:120:ARG:HG2	2.13	0.77
1:B:420:VAL:CG1	1:B:465:VAL:HB	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLN:HG3	1:B:291:LYS:N	1.99	0.77
2:C:177:LYS:HE2	2:C:181:GLU:OE1	1.82	0.77
2:D:36:GLY:O	2:D:39:VAL:HG12	1.84	0.77
2:D:402:LEU:C	2:D:403:LEU:HD12	2.09	0.77
1:A:370:ALA:O	1:A:476:TYR:OH	2.03	0.77
2:C:133:TYR:CD1	2:C:134:TYR:O	2.37	0.77
1:B:525:ASP:OD1	1:B:527:ARG:HG3	1.84	0.77
1:B:107:TYR:OH	1:B:120:ARG:NE	2.18	0.77
2:D:222:ARG:HD2	2:D:297:ASP:OD1	1.83	0.77
1:A:322:VAL:CG2	4:A:602:ADP:O2B	2.32	0.77
1:A:365:ARG:C	1:A:366:VAL:HG22	2.08	0.77
1:B:77:GLU:HG3	1:B:78:PHE:H	1.50	0.77
1:A:36:GLU:OE2	1:A:163:ARG:NE	2.18	0.76
1:B:176:ILE:HG22	1:B:180:LEU:CD1	2.04	0.76
2:D:210:VAL:O	2:D:214:ILE:HG13	1.85	0.76
1:A:94:PRO:HG2	1:B:26:GLU:OE1	1.85	0.76
1:A:168:ASN:O	1:A:173:ILE:HD11	1.84	0.76
1:A:525:ASP:HB2	1:A:528:ILE:CD1	2.00	0.76
1:B:32:GLN:O	1:B:36:GLU:HG3	1.83	0.76
2:D:45:MET:CE	2:D:46:LEU:HD23	2.15	0.76
1:B:77:GLU:O	1:B:80:LEU:CD2	2.34	0.76
1:B:215:THR:OG1	1:B:217:SER:OG	1.96	0.76
2:D:240:ALA:HB1	2:D:244:TRP:CZ2	2.20	0.76
2:D:119:ARG:CA	2:D:124:LEU:HD11	1.99	0.76
1:B:229:THR:HG22	1:B:233:GLU:CA	2.13	0.76
1:B:346:LYS:HB3	1:B:348:MET:HE2	1.68	0.76
1:B:474:TYR:HD1	1:B:475:ASP:N	1.82	0.76
1:A:17:PHE:CE1	1:A:98:ILE:HG22	2.20	0.76
1:A:176:ILE:H	1:A:176:ILE:CD1	1.98	0.76
2:D:25:GLU:O	2:D:27:PRO:CD	2.34	0.76
2:D:209:LEU:O	2:D:212:ALA:N	2.19	0.76
1:A:96:PHE:O	1:A:99:ALA:CB	2.33	0.76
2:D:383:ALA:CA	2:D:415:ASN:ND2	2.48	0.76
1:B:79:LEU:O	1:B:82:VAL:HG22	1.86	0.76
2:C:206:THR:HG23	2:C:241:PHE:CD2	2.20	0.76
1:A:40:TRP:CD1	1:A:205:LYS:HG2	2.21	0.75
1:A:180:LEU:HD22	1:A:180:LEU:H	1.51	0.75
1:B:453:ILE:HG23	1:B:479:ILE:HD11	1.69	0.75
1:B:517:GLU:OE2	2:C:107:VAL:CG2	2.27	0.75
2:C:236:PHE:HD2	2:D:164:GLU:CD	1.93	0.75
1:B:254:ARG:HG2	1:B:254:ARG:NH1	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:ASP:OD1	2:C:159:ILE:N	2.17	0.75
2:D:249:ALA:HB3	2:D:264:LEU:HD11	1.68	0.75
2:D:383:ALA:HA	2:D:415:ASN:ND2	2.01	0.75
1:A:20:GLN:NE2	1:A:20:GLN:O	2.19	0.75
1:A:177:ILE:H	1:A:177:ILE:HD13	1.50	0.75
2:D:75:THR:O	2:D:79:GLY:O	2.04	0.75
2:D:268:ASN:CG	2:D:271:THR:HG22	2.11	0.75
1:A:441:TYR:O	1:A:444:ALA:N	2.18	0.75
2:C:21:LEU:HD12	2:C:21:LEU:N	2.02	0.75
2:C:102:PRO:O	2:C:103:LEU:HD23	1.85	0.75
2:C:124:LEU:HD12	2:C:327:ASN:CA	2.16	0.75
2:C:153:ARG:CG	2:C:306:GLY:HA3	2.16	0.75
2:C:29:ILE:CG2	2:C:363:MET:HE1	2.16	0.75
2:C:291:LEU:HD12	2:C:291:LEU:N	2.02	0.75
1:A:419:MET:SD	1:A:472:VAL:CG2	2.74	0.74
1:A:274:ILE:HG22	1:A:275:LEU:HD21	1.66	0.74
2:C:236:PHE:HB2	2:D:164:GLU:OE1	1.86	0.74
1:A:173:ILE:H	1:A:173:ILE:HD12	1.51	0.74
1:A:419:MET:SD	1:A:472:VAL:HG21	2.26	0.74
1:B:550:ASN:O	1:B:554:GLU:HG3	1.88	0.74
1:A:295:THR:HG23	3:A:601:AMP:O3'	1.86	0.74
1:A:322:VAL:CG2	4:A:602:ADP:PB	2.76	0.74
1:A:375:PHE:HE2	1:A:415:ILE:HD12	1.52	0.74
2:C:135:GLN:OE1	2:C:385:ASN:ND2	2.21	0.74
2:C:263:TRP:C	2:C:264:LEU:CD2	2.47	0.74
1:A:375:PHE:CE2	1:A:415:ILE:HD12	2.23	0.74
2:C:124:LEU:HD13	2:C:328:ILE:CA	2.17	0.74
2:D:16:LEU:HD23	2:D:16:LEU:O	1.88	0.74
1:A:163:ARG:C	1:A:164:LEU:HD13	2.13	0.74
1:A:171:ARG:HH12	1:A:175:TYR:HE2	1.32	0.74
1:A:473:PHE:HE2	1:A:479:ILE:CD1	2.00	0.74
1:B:13:ILE:HD12	1:B:13:ILE:H	1.51	0.74
2:C:236:PHE:CE1	2:D:166:LYS:HB2	2.23	0.74
1:A:380:LEU:HD12	1:A:380:LEU:N	2.03	0.74
1:A:359:LEU:HD12	1:A:359:LEU:O	1.88	0.74
2:C:213:ALA:O	2:C:216:TYR:HB3	1.88	0.74
2:D:289:ILE:O	2:D:293:PRO:CG	2.35	0.74
1:A:85:HIS:O	1:A:89:LEU:CD1	2.34	0.73
1:A:212:LYS:HD3	1:A:274:ILE:HD13	1.70	0.73
1:A:238:THR:HB	1:A:568:ARG:HA	1.69	0.73
1:A:368:ARG:CZ	1:A:440:GLU:OE2	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HA	1:B:85:HIS:HD2	1.52	0.73
1:B:361:LYS:CE	1:B:372:THR:O	2.36	0.73
2:C:216:TYR:CE1	2:C:220:ASN:ND2	2.56	0.73
1:A:234:LEU:N	1:A:234:LEU:HD12	2.03	0.73
1:B:312:PHE:CE1	1:B:328:LEU:HD21	2.21	0.73
1:B:327:THR:CG2	1:B:418:ARG:NH2	2.50	0.73
2:C:154:GLU:OE1	2:C:157:GLU:CG	2.36	0.73
2:D:119:ARG:C	2:D:124:LEU:HD12	2.11	0.73
2:C:42:THR:HB	2:C:43:PRO:HD3	1.70	0.73
2:D:45:MET:HE1	2:D:46:LEU:CD2	2.17	0.73
1:A:429:VAL:CG1	1:A:433:GLN:HB2	2.17	0.73
1:B:454:PHE:HB2	1:B:482:MET:HG3	1.68	0.73
1:B:528:ILE:O	1:B:531:LEU:CD1	2.36	0.73
2:D:132:ARG:HG2	2:D:132:ARG:NH1	1.97	0.73
1:B:151:SER:O	1:B:154:MET:HB2	1.87	0.73
1:B:177:ILE:HD13	1:B:177:ILE:N	2.03	0.73
1:B:338:ILE:O	1:B:400:LYS:HE2	1.88	0.73
1:B:546:ARG:HG3	1:B:546:ARG:NH1	1.99	0.73
1:B:192:SER:HG	1:B:214:ILE:C	1.95	0.73
2:C:264:LEU:HD23	2:C:264:LEU:N	2.03	0.73
2:C:326:ALA:HB2	2:C:335:PHE:HD1	1.53	0.73
2:D:189:ARG:CZ	2:D:190:PHE:HE1	2.01	0.73
1:A:253:ALA:O	1:A:365:ARG:HB2	1.89	0.73
1:A:324:LEU:CD2	1:A:393:LEU:HD23	2.18	0.73
1:A:423:ASN:HD22	1:A:461:LYS:HA	1.52	0.73
1:B:89:LEU:HD12	1:B:89:LEU:H	1.53	0.73
1:A:219:THR:O	1:A:220:LEU:CD2	2.35	0.73
1:B:209:LEU:O	1:B:209:LEU:HD23	1.88	0.73
1:B:254:ARG:NH2	1:B:562:ALA:CB	2.51	0.73
1:B:527:ARG:O	1:B:531:LEU:HD11	1.88	0.73
1:A:21:TYR:OH	1:A:264:PRO:HG3	1.87	0.73
2:C:37:ILE:HG21	2:C:342:ALA:HB3	1.70	0.73
1:A:83:LYS:O	1:A:87:THR:N	2.19	0.72
1:A:413:LEU:HD12	1:A:413:LEU:C	2.14	0.72
1:B:17:PHE:CZ	1:B:98:ILE:HB	2.25	0.72
1:B:298:TYR:CE2	3:B:602:AMP:C2	2.74	0.72
2:C:183:MET:HE3	2:C:183:MET:CA	2.19	0.72
2:D:326:ALA:HB2	2:D:335:PHE:CD2	2.24	0.72
2:D:42:THR:HB	2:D:43:PRO:HD3	1.70	0.72
1:B:179:HIS:O	1:B:183:THR:OG1	2.08	0.72
1:B:209:LEU:HD23	1:B:209:LEU:C	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ARG:NH2	1:B:562:ALA:HA	2.05	0.72
2:D:57:TYR:O	2:D:58:LYS:HB2	1.88	0.72
1:B:290:GLN:HG3	1:B:291:LYS:H	1.54	0.72
2:D:240:ALA:CB	2:D:244:TRP:NE1	2.51	0.72
2:D:404:LYS:HB2	2:D:407:GLU:OE1	1.89	0.72
1:B:61:VAL:O	1:B:64:GLN:HB2	1.90	0.72
1:B:117:THR:HG22	1:B:120:ARG:HB2	1.70	0.72
1:B:452:ASN:HD21	1:B:481:TYR:HB3	1.54	0.72
2:C:46:LEU:O	2:C:50:ASP:HB2	1.89	0.72
2:D:214:ILE:O	2:D:218:ILE:CG1	2.31	0.72
1:A:173:ILE:HD12	1:A:173:ILE:N	2.05	0.72
1:B:7:LEU:HB2	1:B:85:HIS:CD2	2.23	0.72
2:C:113:SER:HB3	2:C:116:VAL:HG22	1.72	0.72
2:C:365:ARG:HG2	2:C:365:ARG:NH1	2.01	0.72
1:A:152:LEU:C	1:A:152:LEU:HD12	2.15	0.72
1:A:551:ARG:O	1:A:554:GLU:HB3	1.89	0.71
2:C:285:PHE:CE2	2:C:289:ILE:CG2	2.73	0.71
2:D:16:LEU:HD23	2:D:16:LEU:C	2.15	0.71
1:A:154:MET:O	1:A:158:SER:OG	2.07	0.71
1:A:177:ILE:HG12	1:A:178:ARG:N	2.05	0.71
1:A:209:LEU:HD23	1:A:209:LEU:C	2.14	0.71
1:B:119:GLU:N	1:B:119:GLU:OE2	2.23	0.71
1:B:5:LEU:C	1:B:5:LEU:HD23	2.15	0.71
1:B:42:ALA:O	1:B:46:ALA:N	2.20	0.71
1:B:213:LEU:N	1:B:220:LEU:O	2.23	0.71
1:B:311:GLN:HG2	1:B:384:HIS:O	1.90	0.71
2:C:271:THR:CG2	2:C:273:LYS:HG2	2.20	0.71
2:D:353:PRO:O	2:D:357:ILE:HG13	1.89	0.71
1:A:178:ARG:C	1:A:180:LEU:HD22	2.16	0.71
1:A:117:THR:OG1	1:A:120:ARG:CG	2.38	0.71
1:B:401:ILE:C	1:B:401:ILE:HD12	2.16	0.71
2:C:167:ALA:O	2:C:168:ASP:HB2	1.88	0.71
2:D:313:LEU:O	2:D:316:GLN:HB2	1.90	0.71
2:D:392:ASP:O	2:D:396:LEU:CD1	2.39	0.71
2:C:7:VAL:CG1	2:C:8:PRO:HD2	2.20	0.71
2:C:128:LEU:HD11	2:C:150:VAL:CG1	2.19	0.71
2:D:222:ARG:CD	2:D:297:ASP:OD1	2.39	0.71
2:D:230:LYS:C	2:D:232:ASN:H	1.97	0.71
2:D:100:LYS:HE3	2:D:336:GLU:HB2	1.71	0.71
1:A:201:PHE:CE1	1:A:210:VAL:HG21	2.26	0.71
1:B:78:PHE:HA	1:B:81:ARG:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASP:O	1:B:147:HIS:CG	2.43	0.71
2:D:79:GLY:HA3	2:D:82:VAL:HG12	1.73	0.71
1:A:168:ASN:HD22	1:A:171:ARG:NH1	1.89	0.71
1:A:380:LEU:HD12	1:A:380:LEU:H	1.56	0.71
1:A:546:ARG:NH1	1:A:546:ARG:HG2	2.06	0.71
1:B:133:ARG:HG3	1:B:134:THR:N	2.03	0.71
1:A:285:MET:O	1:A:288:GLY:N	2.23	0.71
1:A:234:LEU:HD12	1:A:234:LEU:H	1.55	0.70
1:B:177:ILE:HD13	1:B:177:ILE:H	1.56	0.70
1:A:177:ILE:HD13	1:A:177:ILE:N	2.06	0.70
1:A:442:GLY:HA3	1:A:536:HIS:CE1	2.26	0.70
1:A:446:ARG:O	1:A:449:ALA:HB3	1.91	0.70
1:A:546:ARG:O	1:A:550:ASN:CA	2.37	0.70
2:D:133:TYR:HE1	2:D:135:GLN:HA	1.56	0.70
2:D:403:LEU:HD12	2:D:403:LEU:N	2.06	0.70
1:A:546:ARG:HG2	1:A:546:ARG:HH11	1.56	0.70
2:D:157:GLU:OE1	2:D:202:SER:HB3	1.91	0.70
1:B:452:ASN:OD1	1:B:483:THR:HG23	1.91	0.70
2:C:326:ALA:HB2	2:C:362:MET:CE	2.21	0.70
2:D:84:LEU:C	2:D:84:LEU:HD12	2.15	0.70
1:A:253:ALA:HB1	1:A:367:GLY:C	2.16	0.70
2:D:244:TRP:CD1	2:D:244:TRP:H	2.10	0.70
1:A:149:TRP:CD2	1:A:152:LEU:HD23	2.26	0.70
1:A:441:TYR:O	1:A:444:ALA:HB3	1.91	0.70
2:C:16:LEU:HD23	2:C:16:LEU:C	2.16	0.70
1:A:171:ARG:O	1:A:174:HIS:N	2.24	0.70
1:A:462:ASN:O	1:A:463:PHE:CD1	2.45	0.70
1:B:356:CYS:SG	1:B:479:ILE:CG2	2.80	0.70
1:B:461:LYS:C	1:B:462:ASN:HD22	2.00	0.70
1:B:522:LEU:O	1:B:528:ILE:HD12	1.90	0.70
2:C:124:LEU:CD1	2:C:328:ILE:N	2.48	0.70
2:D:248:LEU:HD12	2:D:248:LEU:C	2.15	0.70
1:B:281:ALA:HB2	1:B:300:GLU:OE2	1.91	0.70
1:B:530:PRO:O	1:B:534:GLU:N	2.25	0.70
2:C:352:ASN:CB	2:C:390:THR:HG21	2.21	0.70
2:D:21:LEU:HD12	2:D:21:LEU:O	1.90	0.70
1:A:189:LEU:HD23	1:A:189:LEU:N	2.06	0.69
1:B:212:LYS:HE3	1:B:270:TRP:NE1	2.07	0.69
2:C:133:TYR:CD2	2:C:144:PRO:HB2	2.27	0.69
2:C:158:ASP:CG	2:C:159:ILE:H	1.99	0.69
2:D:102:PRO:O	2:D:103:LEU:HD23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:HD12	1:B:202:TYR:OH	1.92	0.69
1:B:254:ARG:CZ	1:B:562:ALA:HB2	2.22	0.69
1:B:369:MET:HE1	1:B:453:ILE:HG13	1.73	0.69
1:A:570:SER:C	1:A:571:VAL:HG22	2.17	0.69
1:B:97:GLU:HG2	1:B:98:ILE:H	1.57	0.69
1:B:204:ASN:CG	1:B:364:ASP:OD2	2.35	0.69
1:B:568:ARG:HH21	1:B:568:ARG:HG2	1.57	0.69
1:A:94:PRO:HG3	1:B:26:GLU:OE1	1.88	0.69
1:A:422:LEU:CD1	1:A:426:LEU:HD11	2.21	0.69
1:A:528:ILE:CD1	1:A:528:ILE:H	2.05	0.69
1:B:452:ASN:HB2	1:B:552:ILE:HD13	1.73	0.69
1:A:462:ASN:C	1:A:463:PHE:CD1	2.70	0.69
1:B:250:PHE:HB3	1:B:278:LYS:NZ	2.07	0.69
2:D:205:GLY:O	2:D:208:ARG:HB2	1.92	0.69
1:B:40:TRP:HA	1:B:43:VAL:CG2	2.23	0.69
2:C:26:ASN:N	2:C:27:PRO:HD3	2.08	0.69
1:A:60:LEU:HD12	1:A:60:LEU:C	2.18	0.69
2:D:25:GLU:C	2:D:27:PRO:CD	2.65	0.69
2:D:326:ALA:CB	2:D:335:PHE:CD2	2.75	0.69
1:A:180:LEU:HD22	1:A:180:LEU:N	2.07	0.69
1:A:238:THR:HA	1:A:569:PHE:CZ	2.28	0.69
1:A:324:LEU:HD21	1:A:393:LEU:HD23	1.75	0.69
1:B:114:ARG:O	1:B:115:SER:HB2	1.92	0.69
1:B:201:PHE:CD1	1:B:210:VAL:HG21	2.27	0.69
2:C:139:SER:OG	2:C:316:GLN:O	2.10	0.69
2:C:210:VAL:O	2:C:214:ILE:HG13	1.91	0.69
2:D:106:PRO:C	2:D:111:ILE:HD11	2.17	0.69
2:C:148:ASP:OD1	2:C:222:ARG:NH2	2.22	0.69
1:B:222:PHE:C	1:B:223:LEU:CD1	2.65	0.69
2:C:408:PHE:O	2:C:411:ALA:N	2.26	0.69
2:D:326:ALA:HB2	2:D:335:PHE:HD2	1.58	0.69
2:C:99:ILE:HG13	2:C:335:PHE:O	1.93	0.68
2:C:5:VAL:HG23	2:C:67:GLU:O	1.93	0.68
2:D:352:ASN:HB2	2:D:392:ASP:OD2	1.93	0.68
1:A:58:VAL:HG22	1:A:102:PHE:CE1	2.27	0.68
1:A:223:LEU:C	1:A:224:LEU:HD12	2.18	0.68
1:A:303:VAL:O	1:A:306:GLN:CG	2.40	0.68
1:A:561:TYR:HE2	1:A:568:ARG:CZ	2.05	0.68
2:C:21:LEU:H	2:C:21:LEU:CD1	2.06	0.68
1:A:152:LEU:HD12	1:A:152:LEU:O	1.93	0.68
1:B:7:LEU:CB	1:B:85:HIS:HD2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:TRP:CZ2	1:B:234:LEU:HD23	2.29	0.68
1:B:336:LYS:HE2	4:B:601:ADP:C8	2.28	0.68
1:B:442:GLY:HA3	1:B:536:HIS:NE2	2.09	0.68
1:A:220:LEU:HD23	1:A:220:LEU:N	2.03	0.68
1:A:482:MET:CE	1:A:545:TRP:CZ3	2.77	0.68
1:A:551:ARG:C	1:A:554:GLU:H	2.00	0.68
1:B:176:ILE:HD12	1:B:176:ILE:N	2.09	0.68
2:C:133:TYR:HE1	2:C:135:GLN:HA	1.58	0.68
2:C:158:ASP:HB3	2:C:303:ASN:CB	2.24	0.68
2:D:25:GLU:O	2:D:27:PRO:HD2	1.94	0.68
1:A:473:PHE:CE2	1:A:479:ILE:CD1	2.77	0.68
1:A:528:ILE:HD13	1:A:528:ILE:N	2.08	0.68
1:B:368:ARG:NE	1:B:447:GLN:OE1	2.22	0.68
1:B:504:PRO:HG3	2:C:107:VAL:HG13	1.75	0.68
1:A:435:ARG:NH1	1:A:534:GLU:OE2	2.27	0.68
1:B:351:ALA:O	1:B:354:ARG:HB2	1.94	0.68
2:C:26:ASN:N	2:C:27:PRO:CD	2.57	0.68
2:C:175:VAL:HG22	2:D:183:MET:HE3	1.74	0.68
2:C:259:ASP:OD1	2:C:259:ASP:N	2.22	0.68
2:D:203:GLU:HA	2:D:244:TRP:CE3	2.29	0.68
1:A:179:HIS:HD2	1:A:239:CYS:HB3	1.58	0.68
1:A:376:GLU:O	3:A:601:AMP:N6	2.26	0.68
2:D:49:VAL:O	2:D:53:VAL:HG23	1.93	0.68
2:D:57:TYR:HE2	2:D:372:ALA:CB	2.05	0.68
2:D:10:GLN:O	2:D:26:ASN:ND2	2.26	0.67
2:C:271:THR:HB	2:C:273:LYS:CG	2.24	0.67
1:A:254:ARG:HG3	1:A:254:ARG:HH11	1.59	0.67
1:B:89:LEU:O	1:B:93:TYR:HE1	1.77	0.67
1:A:46:ALA:C	1:A:49:ASN:OD1	2.37	0.67
1:A:85:HIS:O	1:A:88:ARG:HG2	1.94	0.67
1:A:171:ARG:HH11	1:A:175:TYR:HE2	1.35	0.67
1:A:543:ASP:HA	1:A:546:ARG:CD	2.24	0.67
1:B:240:LEU:HD22	1:B:245:GLU:HB3	1.76	0.67
2:D:229:HIS:HD2	2:D:242:LYS:HB2	1.58	0.67
1:A:107:TYR:OH	1:A:115:SER:OG	2.10	0.67
1:A:365:ARG:O	1:A:366:VAL:HG23	1.93	0.67
1:B:168:ASN:O	1:B:172:ASP:OD1	2.13	0.67
1:A:229:THR:O	1:A:232:GLY:HA3	1.94	0.67
1:B:141:LYS:HZ2	1:B:155:ARG:HH11	1.42	0.67
2:C:179:LEU:HA	2:C:183:MET:HB2	1.77	0.67
2:C:238:GLU:O	2:C:241:PHE:HB3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:ILE:HD12	2:C:313:LEU:HD23	1.77	0.67
2:D:382:GLY:O	2:D:415:ASN:ND2	2.26	0.67
1:A:17:PHE:HE1	1:A:98:ILE:CG2	2.08	0.67
1:A:274:ILE:C	1:A:275:LEU:HD23	2.19	0.67
1:B:141:LYS:HZ2	1:B:155:ARG:NH1	1.91	0.67
1:B:237:ASP:CG	1:B:568:ARG:CD	2.58	0.67
1:A:54:TYR:O	1:A:58:VAL:HG23	1.95	0.67
1:A:482:MET:HE1	1:A:545:TRP:HE3	1.56	0.67
1:A:570:SER:O	1:A:571:VAL:HG13	1.94	0.67
2:C:172:ALA:O	2:C:176:ILE:HG13	1.95	0.67
2:D:351:VAL:O	2:D:353:PRO:HD3	1.95	0.67
1:A:111:PHE:O	1:A:114:ARG:HG3	1.95	0.67
1:A:404:LEU:HD22	1:A:409:VAL:HG23	1.76	0.67
1:B:148:GLY:HA3	1:B:151:SER:OG	1.94	0.67
1:A:149:TRP:CE3	1:A:152:LEU:HD21	2.30	0.67
1:B:133:ARG:HG3	1:B:134:THR:H	1.59	0.67
1:A:326:PHE:CB	1:A:389:LEU:HD21	2.24	0.66
2:C:42:THR:HB	2:C:43:PRO:CD	2.25	0.66
2:C:258:ILE:HG22	2:C:259:ASP:CG	2.19	0.66
2:D:388:THR:O	2:D:389:VAL:HG13	1.95	0.66
1:A:119:GLU:CD	1:A:120:ARG:HG2	2.20	0.66
1:B:272:ARG:HH22	1:B:280:THR:HG22	1.60	0.66
1:B:419:MET:HE1	1:B:472:VAL:HB	1.77	0.66
2:C:133:TYR:CE1	2:C:134:TYR:C	2.72	0.66
1:A:35:PHE:HE2	1:A:207:ALA:N	1.93	0.66
1:B:40:TRP:CE3	1:B:205:LYS:CE	2.68	0.66
1:A:91:PRO:CD	1:A:127:GLN:OE1	2.43	0.66
1:B:519:ARG:HH21	1:B:533:GLU:CD	2.03	0.66
2:C:287:GLN:O	2:C:291:LEU:CD1	2.44	0.66
2:D:401:LYS:O	2:D:403:LEU:HD12	1.94	0.66
1:A:212:LYS:HD3	1:A:274:ILE:CD1	2.26	0.66
1:B:351:ALA:O	1:B:354:ARG:N	2.28	0.66
2:C:271:THR:HB	2:C:273:LYS:HG2	1.76	0.66
1:A:45:GLN:O	1:A:48:LYS:N	2.29	0.66
1:A:46:ALA:O	1:A:49:ASN:OD1	2.14	0.66
1:A:272:ARG:HH22	1:A:280:THR:HG22	1.61	0.66
2:C:326:ALA:HB2	2:C:362:MET:HE2	1.77	0.66
2:D:274:GLU:HG3	2:D:274:GLU:O	1.94	0.66
2:D:384:ILE:C	2:D:387:LYS:H	2.03	0.66
1:A:222:PHE:C	1:A:223:LEU:CD1	2.69	0.66
1:A:322:VAL:HG22	4:A:602:ADP:PB	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:PHE:C	1:A:571:VAL:N	2.48	0.66
1:B:285:MET:CE	1:B:373:GLN:HE21	2.09	0.66
1:B:365:ARG:HH11	1:B:371:ASP:HB2	0.83	0.66
2:C:41:VAL:HB	2:C:353:PRO:HB3	1.78	0.66
2:C:206:THR:HG23	2:C:241:PHE:CE2	2.30	0.66
2:D:25:GLU:O	2:D:27:PRO:HD3	1.94	0.66
2:D:68:ILE:HD12	2:D:88:THR:HG23	1.77	0.66
2:D:177:LYS:O	2:D:181:GLU:HG2	1.96	0.66
1:A:222:PHE:C	1:A:223:LEU:HD12	2.20	0.65
1:A:298:TYR:CE2	1:A:302:LEU:CD1	2.78	0.65
1:B:77:GLU:HG3	1:B:78:PHE:N	2.11	0.65
2:C:221:ASP:OD2	2:C:271:THR:CG2	2.22	0.65
2:D:203:GLU:HA	2:D:244:TRP:CZ3	2.31	0.65
1:A:404:LEU:HD13	1:A:404:LEU:N	2.11	0.65
2:C:236:PHE:CB	2:D:164:GLU:OE1	2.43	0.65
1:B:327:THR:OG1	1:B:418:ARG:NH2	2.29	0.65
1:B:419:MET:HE1	1:B:472:VAL:CB	2.26	0.65
2:C:248:LEU:CD1	2:C:252:GLU:HG3	2.26	0.65
1:A:117:THR:OG1	1:A:120:ARG:HG2	1.96	0.65
1:A:172:ASP:HA	1:A:175:TYR:HD2	1.60	0.65
1:A:452:ASN:HD21	1:A:481:TYR:HB3	1.61	0.65
1:B:54:TYR:O	1:B:58:VAL:HG23	1.97	0.65
1:B:86:TYR:C	1:B:89:LEU:CD1	2.69	0.65
1:A:215:THR:HG23	1:A:218:GLY:O	1.95	0.65
1:B:494:ARG:HH11	1:B:498:ASP:CG	2.04	0.65
2:C:189:ARG:HH11	2:C:189:ARG:HG3	1.60	0.65
1:A:84:GLU:O	1:A:88:ARG:N	2.27	0.65
1:A:171:ARG:NH1	1:A:171:ARG:HG2	2.10	0.65
1:A:359:LEU:HD21	1:A:481:TYR:CE1	2.31	0.65
1:A:569:PHE:O	1:A:571:VAL:N	2.25	0.65
2:D:171:ASP:O	2:D:174:LYS:HB3	1.95	0.65
1:A:278:LYS:HB3	1:A:282:GLU:HB2	1.78	0.65
1:B:127:GLN:HE21	1:B:127:GLN:CA	2.09	0.65
1:B:152:LEU:HD12	1:B:152:LEU:C	2.22	0.65
2:C:171:ASP:O	2:C:175:VAL:N	2.28	0.65
2:D:189:ARG:HH11	2:D:189:ARG:HG3	1.61	0.65
1:A:381:GLU:OE1	1:A:404:LEU:O	2.13	0.65
1:B:420:VAL:HG13	1:B:465:VAL:HB	1.79	0.65
1:A:117:THR:OG1	1:A:120:ARG:HG3	1.97	0.64
1:A:179:HIS:CD2	1:A:239:CYS:O	2.50	0.64
2:C:16:LEU:HD23	2:C:16:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:226:THR:HA	2:D:278:LYS:O	1.96	0.64
1:A:107:TYR:CD1	1:A:111:PHE:CE2	2.85	0.64
1:A:176:ILE:HD13	1:A:176:ILE:N	2.05	0.64
1:A:323:MET:HE1	1:A:338:ILE:HG13	1.78	0.64
1:B:86:TYR:C	1:B:89:LEU:HD12	2.22	0.64
1:B:134:THR:HG22	1:B:135:ILE:N	2.13	0.64
1:B:419:MET:HE1	1:B:472:VAL:HG11	1.79	0.64
1:A:196:VAL:HG12	1:A:197:ALA:N	2.12	0.64
2:D:265:LYS:O	2:D:265:LYS:HG3	1.96	0.64
1:A:5:LEU:O	1:A:8:LEU:HB3	1.97	0.64
1:B:419:MET:HE1	1:B:472:VAL:CG1	2.27	0.64
1:B:454:PHE:HB2	1:B:482:MET:CG	2.27	0.64
1:A:515:PRO:HA	1:A:518:PHE:CD2	2.32	0.64
1:B:65:LEU:N	1:B:65:LEU:HD12	2.11	0.64
2:C:133:TYR:CA	2:C:317:VAL:HG13	2.27	0.64
2:C:238:GLU:O	2:C:241:PHE:CB	2.46	0.64
2:D:169:SER:OG	2:D:172:ALA:N	2.29	0.64
1:A:94:PRO:CG	1:B:26:GLU:CD	2.67	0.64
1:A:323:MET:HE1	1:A:338:ILE:CG1	2.27	0.64
1:B:13:ILE:HD12	1:B:13:ILE:N	2.11	0.64
1:A:323:MET:CE	1:A:338:ILE:CG1	2.76	0.64
2:C:145:GLU:H	2:C:145:GLU:CD	2.00	0.64
2:C:209:LEU:O	2:C:212:ALA:CB	2.46	0.64
1:A:141:LYS:HG3	1:A:143:PHE:CE1	2.32	0.64
1:A:423:ASN:ND2	1:A:461:LYS:HA	2.12	0.64
1:B:462:ASN:HD22	1:B:462:ASN:N	1.96	0.64
2:C:128:LEU:CD1	2:C:152:PHE:CE1	2.79	0.64
1:B:173:ILE:HD13	1:B:173:ILE:N	2.06	0.64
2:D:37:ILE:CG1	2:D:341:THR:O	2.38	0.64
1:A:450:ALA:O	1:A:552:ILE:HD11	1.99	0.63
1:B:192:SER:CB	1:B:214:ILE:O	2.45	0.63
2:C:291:LEU:H	2:C:291:LEU:CD1	2.09	0.63
1:A:172:ASP:O	1:A:176:ILE:CD1	2.46	0.63
1:B:61:VAL:HG12	1:B:65:LEU:HD13	1.79	0.63
2:D:95:TYR:CZ	5:D:505:HOH:O	2.48	0.63
2:D:189:ARG:HG3	2:D:189:ARG:NH1	2.13	0.63
2:D:297:ASP:O	2:D:299:ILE:CD1	2.46	0.63
1:A:107:TYR:CD2	1:A:121:LEU:HD23	2.33	0.63
1:B:568:ARG:HG2	1:B:568:ARG:NH2	2.11	0.63
2:C:402:LEU:HD12	2:C:403:LEU:H	1.61	0.63
1:A:365:ARG:O	1:A:367:GLY:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:TRP:C	1:B:152:LEU:H	2.06	0.63
2:C:42:THR:O	2:C:46:LEU:HD12	1.97	0.63
2:D:14:ILE:CD1	2:D:23:VAL:HG13	2.29	0.63
2:D:100:LYS:HE3	2:D:336:GLU:CB	2.28	0.63
1:A:171:ARG:O	1:A:174:HIS:CB	2.46	0.63
1:B:141:LYS:HD2	1:B:143:PHE:CE2	2.34	0.63
2:D:104:THR:HG22	2:D:105:THR:O	1.98	0.63
2:D:175:VAL:O	2:D:179:LEU:HD12	1.98	0.63
1:A:201:PHE:CE1	1:A:210:VAL:CG2	2.81	0.63
2:D:89:LEU:O	2:D:93:ARG:HG3	1.99	0.63
1:A:7:LEU:HD12	1:A:85:HIS:NE2	2.05	0.63
1:A:38:ALA:CB	1:A:40:TRP:HZ3	2.12	0.63
1:A:306:GLN:HG3	1:A:307:GLY:N	2.14	0.63
1:B:7:LEU:HA	1:B:85:HIS:CD2	2.33	0.63
1:B:466:THR:OG1	1:B:470:ARG:O	2.16	0.63
1:A:423:ASN:OD1	1:A:424:ILE:N	2.30	0.63
1:B:551:ARG:O	1:B:554:GLU:HB2	1.97	0.63
2:C:116:VAL:HG23	2:C:117:ALA:N	2.14	0.63
1:A:142:ASP:OD1	1:A:142:ASP:N	2.29	0.63
1:A:551:ARG:O	1:A:554:GLU:CB	2.46	0.63
1:B:360:VAL:HG21	1:B:476:TYR:CE2	2.34	0.63
2:C:175:VAL:CG2	2:D:183:MET:CE	2.75	0.63
1:A:140:ALA:HA	1:A:198:ASN:OD1	1.98	0.62
1:A:149:TRP:CA	1:A:152:LEU:HB3	2.28	0.62
1:A:177:ILE:H	1:A:177:ILE:CD1	2.11	0.62
2:C:271:THR:HG22	2:C:273:LYS:HE3	1.76	0.62
1:B:78:PHE:O	1:B:81:ARG:N	2.31	0.62
2:D:169:SER:OG	2:D:172:ALA:CB	2.47	0.62
1:A:456:GLY:HA3	1:A:478:GLU:HB3	1.82	0.62
2:C:39:VAL:HG13	2:C:40:ASP:N	2.14	0.62
2:C:358:LEU:O	2:C:361:GLU:HB3	1.99	0.62
1:A:323:MET:CE	1:A:338:ILE:HG12	2.30	0.62
1:B:310:GLU:HB3	1:B:329:PRO:HG2	1.81	0.62
2:D:95:TYR:O	2:D:96:ARG:HB2	1.98	0.62
1:A:546:ARG:HH11	1:A:546:ARG:CG	2.13	0.62
1:B:121:LEU:C	1:B:121:LEU:HD12	2.24	0.62
1:B:141:LYS:HZ3	1:B:155:ARG:NH1	1.96	0.62
1:B:306:GLN:HG3	1:B:307:GLY:N	2.14	0.62
2:C:392:ASP:OD1	2:C:392:ASP:N	2.31	0.62
2:D:119:ARG:CB	2:D:124:LEU:HD13	2.29	0.62
2:D:393:PHE:HA	2:D:396:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:SER:O	1:A:126:SER:OG	2.12	0.62
1:A:482:MET:CE	1:A:545:TRP:HE3	2.10	0.62
1:B:160:LEU:HD12	1:B:160:LEU:O	1.99	0.62
2:C:326:ALA:CB	2:C:362:MET:HE1	2.29	0.62
2:D:203:GLU:CA	2:D:244:TRP:CZ3	2.82	0.62
1:A:254:ARG:HH21	1:A:470:ARG:HH12	1.30	0.62
2:C:276:VAL:C	2:C:277:ILE:HD13	2.25	0.62
2:C:326:ALA:CB	2:C:362:MET:CE	2.77	0.62
2:D:391:TYR:O	2:D:395:ARG:HG3	2.00	0.62
1:B:338:ILE:O	1:B:400:LYS:CE	2.47	0.62
1:B:102:PHE:O	1:B:106:VAL:HG23	1.99	0.62
1:B:462:ASN:OD1	1:B:475:ASP:CB	2.47	0.62
2:C:7:VAL:HG12	2:C:8:PRO:HD2	1.80	0.62
2:D:158:ASP:C	2:D:160:TYR:H	2.07	0.62
1:A:35:PHE:CD2	1:A:207:ALA:HB2	2.34	0.61
1:B:5:LEU:HD23	1:B:6:GLU:N	2.15	0.61
1:B:267:LEU:HD23	1:B:287:ILE:HG21	1.80	0.61
2:D:209:LEU:CD2	2:D:210:VAL:HG23	2.29	0.61
2:D:389:VAL:N	2:D:403:LEU:HD13	2.14	0.61
1:A:89:LEU:H	1:A:89:LEU:HD12	1.64	0.61
1:A:403:ASP:C	1:A:404:LEU:CD1	2.72	0.61
1:A:481:TYR:HB2	1:A:484:GLU:HG3	1.82	0.61
1:B:168:ASN:O	1:B:171:ARG:HB3	1.99	0.61
2:C:133:TYR:CE1	2:C:135:GLN:HA	2.35	0.61
2:D:39:VAL:O	2:D:43:PRO:HG2	2.00	0.61
1:A:178:ARG:NH2	1:A:182:GLU:OE1	2.34	0.61
2:D:209:LEU:O	2:D:212:ALA:HB3	2.00	0.61
1:A:333:ARG:HH12	1:A:373:GLN:HE22	1.46	0.61
1:B:177:ILE:HA	1:B:180:LEU:HD13	1.81	0.61
1:B:474:TYR:HD1	1:B:475:ASP:H	1.45	0.61
2:C:66:MET:HE1	2:C:95:TYR:HE2	1.57	0.61
2:C:239:GLY:O	2:C:242:LYS:HG2	2.00	0.61
1:A:101:SER:OG	1:A:295:THR:OG1	2.13	0.61
1:B:564:ARG:HH11	1:B:564:ARG:CG	2.13	0.61
2:C:285:PHE:CE2	2:C:289:ILE:HG21	2.35	0.61
2:D:169:SER:O	2:D:171:ASP:N	2.29	0.61
2:D:169:SER:HG	2:D:172:ALA:H	1.46	0.61
2:D:351:VAL:O	2:D:353:PRO:CD	2.49	0.61
2:D:352:ASN:CB	2:D:392:ASP:OD2	2.49	0.61
1:A:368:ARG:NE	1:A:447:GLN:OE1	2.31	0.61
1:B:312:PHE:CE2	1:B:328:LEU:HD21	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:ARG:NH1	2:D:190:PHE:CE1	2.68	0.61
1:A:40:TRP:HE1	1:A:205:LYS:HA	1.66	0.61
1:A:364:ASP:OD1	1:A:364:ASP:N	2.30	0.61
1:B:244:ALA:O	1:B:248:ILE:HG13	2.01	0.61
1:A:96:PHE:O	1:A:99:ALA:CA	2.48	0.61
1:B:62:VAL:HG23	1:B:63:GLU:N	2.14	0.61
1:B:106:VAL:HG12	1:B:110:LEU:HD23	1.83	0.61
2:D:42:THR:HB	2:D:43:PRO:CD	2.31	0.61
2:D:261:GLY:C	2:D:263:TRP:CZ3	2.77	0.61
1:A:509:SER:OG	1:A:512:ASP:OD2	0.62	0.61
1:B:156:VAL:CG2	1:B:157:ILE:H	2.09	0.61
1:B:462:ASN:ND2	4:B:601:ADP:O3B	2.33	0.61
1:B:513:VAL:HG12	1:B:515:PRO:HD3	1.82	0.61
2:D:79:GLY:CA	2:D:82:VAL:HG12	2.30	0.61
1:A:35:PHE:CE2	1:A:207:ALA:N	2.69	0.61
1:A:106:VAL:HG12	1:A:110:LEU:HD12	1.81	0.61
1:A:142:ASP:C	1:A:143:PHE:CD1	2.79	0.61
1:A:179:HIS:O	1:A:183:THR:HG23	2.00	0.61
1:A:287:ILE:CD1	1:A:289:CYS:SG	2.89	0.61
1:A:535:MET:CB	1:A:536:HIS:CD2	2.84	0.61
1:B:474:TYR:HA	1:B:476:TYR:HE1	1.64	0.61
1:A:281:ALA:CB	1:A:300:GLU:OE2	2.48	0.60
1:A:422:LEU:HD12	1:A:426:LEU:HD11	1.82	0.60
1:B:143:PHE:HE1	1:B:155:ARG:HD2	1.66	0.60
1:B:462:ASN:C	1:B:463:PHE:HD1	2.09	0.60
1:B:140:ALA:CB	1:B:196:VAL:O	2.48	0.60
2:C:407:GLU:O	2:C:410:ASP:HB2	2.01	0.60
2:D:242:LYS:HG3	2:D:246:TYR:CE2	2.36	0.60
1:A:114:ARG:O	1:A:115:SER:OG	2.19	0.60
2:C:75:THR:HA	2:C:79:GLY:O	2.01	0.60
2:D:157:GLU:HG2	2:D:157:GLU:O	1.99	0.60
2:D:177:LYS:HE2	2:D:181:GLU:OE2	2.01	0.60
1:B:362:GLU:O	1:B:362:GLU:HG3	2.01	0.60
2:C:158:ASP:CB	2:C:303:ASN:HB3	2.32	0.60
2:D:153:ARG:HH21	2:D:303:ASN:C	2.01	0.60
2:D:199:LYS:CD	2:D:237:THR:OG1	2.48	0.60
1:A:38:ALA:CB	1:A:40:TRP:CZ3	2.85	0.60
1:B:212:LYS:HE3	1:B:270:TRP:CD1	2.36	0.60
2:C:6:VAL:HG23	2:C:6:VAL:O	2.00	0.60
2:C:154:GLU:OE2	2:C:156:SER:OG	2.19	0.60
1:A:189:LEU:H	1:A:189:LEU:CD2	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD12	1:B:60:LEU:C	2.24	0.60
1:B:127:GLN:HG3	1:B:128:PRO:HD2	1.83	0.60
2:D:45:MET:CE	2:D:46:LEU:CD2	2.79	0.60
2:D:382:GLY:C	2:D:415:ASN:HD21	2.05	0.60
2:D:392:ASP:OD1	2:D:392:ASP:N	2.30	0.60
1:A:168:ASN:O	1:A:173:ILE:CD1	2.49	0.60
1:A:171:ARG:HH11	1:A:171:ARG:CG	2.15	0.60
1:A:456:GLY:HA3	1:A:478:GLU:CB	2.31	0.60
1:B:272:ARG:HH22	1:B:280:THR:CG2	2.13	0.60
2:C:133:TYR:CE2	2:C:144:PRO:HG2	2.37	0.60
2:C:366:HIS:ND1	2:C:366:HIS:O	2.34	0.60
1:A:326:PHE:HB3	1:A:389:LEU:HD21	1.83	0.60
1:B:143:PHE:CE1	1:B:155:ARG:HB3	2.36	0.60
1:B:263:LEU:O	1:B:263:LEU:HD23	2.00	0.60
1:B:281:ALA:N	1:B:300:GLU:OE2	2.34	0.60
1:B:332:ASP:N	1:B:332:ASP:OD1	2.34	0.60
2:C:236:PHE:CG	2:D:164:GLU:OE1	2.55	0.60
2:C:388:THR:C	2:C:389:VAL:HG13	2.26	0.60
1:A:119:GLU:CG	1:A:120:ARG:N	2.64	0.60
1:A:166:TRP:CE2	1:A:234:LEU:HD13	2.36	0.60
1:A:441:TYR:O	1:A:444:ALA:CB	2.50	0.60
2:C:268:ASN:HB2	2:C:275:ILE:CD1	2.32	0.60
2:D:169:SER:O	2:D:170:ALA:CB	2.46	0.60
2:D:299:ILE:HD12	2:D:299:ILE:N	2.16	0.60
1:B:39:ASP:O	1:B:43:VAL:HG23	2.01	0.60
2:C:82:VAL:O	2:C:82:VAL:HG13	2.02	0.60
2:C:118:LEU:O	2:C:122:LEU:HD11	1.90	0.60
2:C:326:ALA:HB3	2:C:362:MET:HE1	1.83	0.60
2:D:82:VAL:O	2:D:82:VAL:HG13	2.02	0.60
2:D:283:ASP:OD1	2:D:284:ALA:N	2.35	0.60
2:D:351:VAL:C	2:D:353:PRO:HD3	2.27	0.60
1:B:189:LEU:HD12	1:B:189:LEU:C	2.26	0.59
1:B:568:ARG:O	1:B:571:VAL:HG12	2.02	0.59
2:C:160:TYR:CB	2:C:303:ASN:ND2	2.61	0.59
2:C:263:TRP:O	2:C:264:LEU:CD2	2.42	0.59
2:C:352:ASN:HB3	2:C:390:THR:CB	2.32	0.59
2:D:102:PRO:C	2:D:103:LEU:HD23	2.28	0.59
2:D:127:CYS:SG	2:D:153:ARG:CG	2.90	0.59
2:D:382:GLY:CA	2:D:415:ASN:HD22	2.15	0.59
2:D:404:LYS:N	2:D:407:GLU:OE1	2.32	0.59
1:B:223:LEU:O	1:B:224:LEU:HD23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:LEU:HD12	1:B:531:LEU:H	1.65	0.59
2:C:257:LEU:HD23	2:C:260:GLY:HA2	1.83	0.59
2:D:119:ARG:CB	2:D:124:LEU:CD1	2.80	0.59
1:A:176:ILE:HG12	1:A:177:ILE:N	2.17	0.59
1:A:311:GLN:HE21	1:A:384:HIS:HA	1.66	0.59
1:B:28:THR:O	1:B:28:THR:HG22	2.02	0.59
1:A:328:LEU:HB2	1:A:331:PHE:HB2	1.84	0.59
1:B:192:SER:OG	1:B:214:ILE:C	2.43	0.59
1:B:229:THR:CG2	1:B:233:GLU:CB	2.58	0.59
1:B:254:ARG:NH2	1:B:562:ALA:HB2	2.14	0.59
2:C:154:GLU:O	2:C:303:ASN:OD1	2.20	0.59
1:A:45:GLN:O	1:A:48:LYS:HB2	2.02	0.59
2:C:35:ASP:HB2	2:C:341:THR:HG21	1.83	0.59
1:A:474:TYR:CD1	1:A:475:ASP:N	2.70	0.59
1:B:21:TYR:HE1	1:B:25:LEU:HD21	1.68	0.59
1:B:90:LEU:N	1:B:91:PRO:HD3	2.18	0.59
1:B:200:LEU:HD12	1:B:202:TYR:CZ	2.37	0.59
2:C:26:ASN:N	2:C:26:ASN:OD1	2.36	0.59
2:D:236:PHE:O	2:D:240:ALA:HB2	2.03	0.59
1:A:85:HIS:C	1:A:89:LEU:HD11	2.25	0.59
1:A:560:VAL:HG13	1:A:560:VAL:O	2.03	0.59
1:B:54:TYR:CE1	1:B:58:VAL:HG21	2.38	0.59
1:B:242:THR:OG1	1:B:245:GLU:OE2	0.59	0.59
2:C:29:ILE:HG21	2:C:363:MET:CE	2.20	0.59
2:C:149:MET:CE	2:C:299:ILE:HD11	2.33	0.59
2:D:292:ARG:N	2:D:293:PRO:HD3	2.18	0.59
1:A:57:HIS:O	1:A:60:LEU:HB3	2.03	0.59
1:A:107:TYR:CD1	1:A:111:PHE:HE2	2.19	0.59
1:B:143:PHE:CE1	1:B:155:ARG:HD2	2.37	0.59
1:B:272:ARG:O	1:B:276:PRO:HD3	2.03	0.59
1:B:462:ASN:OD1	1:B:475:ASP:HB2	2.03	0.59
2:D:345:TYR:O	2:D:348:GLN:HB2	2.03	0.59
1:A:171:ARG:HH11	1:A:171:ARG:HG2	1.66	0.59
1:B:508:VAL:HG23	1:B:508:VAL:O	2.02	0.59
1:A:116:LEU:O	1:A:117:THR:HG23	2.03	0.58
1:A:168:ASN:CB	1:A:171:ARG:NE	2.59	0.58
1:A:365:ARG:O	1:A:366:VAL:CG2	2.48	0.58
1:A:444:ALA:C	1:A:448:LEU:HD11	2.23	0.58
1:B:281:ALA:HB2	1:B:300:GLU:CD	2.28	0.58
1:B:439:GLU:HA	1:B:535:MET:HE3	1.85	0.58
2:C:5:VAL:HG21	2:C:68:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:ASP:CB	2:C:303:ASN:CB	2.81	0.58
2:C:171:ASP:O	2:C:174:LYS:HB3	2.02	0.58
1:A:38:ALA:CA	1:A:40:TRP:CZ3	2.85	0.58
1:A:119:GLU:CG	1:A:120:ARG:H	2.15	0.58
2:C:49:VAL:O	2:C:53:VAL:HG23	2.03	0.58
2:C:154:GLU:OE2	2:C:156:SER:CA	2.51	0.58
2:D:241:PHE:HD2	2:D:302:MET:HE3	1.68	0.58
2:D:261:GLY:C	2:D:263:TRP:CE3	2.81	0.58
1:A:17:PHE:CE1	1:A:98:ILE:HG21	2.38	0.58
1:A:107:TYR:HE1	1:A:111:PHE:HE2	1.43	0.58
1:A:473:PHE:CE2	1:A:479:ILE:HD12	2.38	0.58
1:B:327:THR:HG1	1:B:418:ARG:NH2	2.01	0.58
1:B:546:ARG:HH11	1:B:546:ARG:CG	2.12	0.58
1:A:5:LEU:N	1:A:6:GLU:OE1	2.36	0.58
1:A:551:ARG:HA	1:A:554:GLU:HB3	1.85	0.58
1:B:246:ALA:HA	1:B:249:VAL:HG12	1.84	0.58
2:C:84:LEU:C	2:C:84:LEU:HD12	2.29	0.58
2:C:349:ASP:OD1	2:C:405:CYS:HB3	2.02	0.58
2:D:285:PHE:CE1	2:D:289:ILE:CG2	2.86	0.58
1:B:107:TYR:CE1	1:B:111:PHE:CD2	2.92	0.58
1:B:117:THR:OG1	1:B:118:PRO:HD2	2.03	0.58
1:B:275:LEU:N	1:B:276:PRO:HD3	2.19	0.58
1:B:495:TYR:HB3	1:B:496:PRO:HD2	1.84	0.58
2:C:25:GLU:OE1	2:C:61:ARG:HG2	2.03	0.58
2:C:271:THR:CB	2:C:273:LYS:HG2	2.34	0.58
2:D:189:ARG:HG3	2:D:190:PHE:CD1	2.39	0.58
1:A:296:GLU:O	1:A:300:GLU:HG3	2.03	0.58
1:A:420:VAL:O	1:A:420:VAL:HG13	2.03	0.58
1:A:473:PHE:HE2	1:A:479:ILE:HD12	1.67	0.58
1:B:135:ILE:HD12	1:B:266:ALA:HB2	1.86	0.58
1:B:254:ARG:NH2	1:B:562:ALA:CA	2.67	0.58
2:C:288:GLN:HE22	2:C:292:ARG:HH11	1.51	0.58
2:D:5:VAL:HG23	2:D:5:VAL:O	2.04	0.58
1:A:13:ILE:O	1:A:16:GLY:N	2.35	0.58
1:A:333:ARG:HH22	1:A:373:GLN:HE22	1.50	0.58
1:B:186:PRO:CD	1:B:187:GLU:OE1	2.51	0.58
2:D:57:TYR:OH	2:D:369:TRP:HB3	2.04	0.58
1:B:192:SER:HG	1:B:215:THR:CA	1.91	0.58
2:C:66:MET:HG3	2:C:66:MET:O	2.04	0.58
2:C:326:ALA:HB2	2:C:335:PHE:CD1	2.38	0.58
1:A:106:VAL:HG12	1:A:110:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:HD12	1:A:426:LEU:H	1.68	0.57
1:B:42:ALA:HA	1:B:45:GLN:HB3	1.84	0.57
2:C:24:PRO:O	2:C:27:PRO:HD3	2.04	0.57
2:C:149:MET:HE3	2:C:299:ILE:HD11	1.84	0.57
2:D:201:CYS:SG	2:D:206:THR:OG1	2.62	0.57
1:A:375:PHE:CE2	1:A:415:ILE:CD1	2.87	0.57
1:B:89:LEU:HD12	1:B:89:LEU:N	2.17	0.57
2:C:23:VAL:O	2:C:23:VAL:HG13	2.04	0.57
2:C:124:LEU:CD1	2:C:327:ASN:HB2	2.31	0.57
1:A:368:ARG:NH1	1:A:440:GLU:OE2	2.37	0.57
1:A:404:LEU:O	1:A:407:GLN:N	2.38	0.57
1:A:80:LEU:N	1:A:80:LEU:HD12	2.18	0.57
1:A:86:TYR:OH	1:A:99:ALA:O	2.22	0.57
1:B:117:THR:HG23	1:B:120:ARG:H	1.68	0.57
1:B:366:VAL:HG12	1:B:366:VAL:O	2.04	0.57
1:B:375:PHE:HD1	1:B:415:ILE:HD12	1.64	0.57
2:D:127:CYS:SG	2:D:129:ARG:NH1	2.78	0.57
1:A:167:GLN:HG2	1:A:233:GLU:HB3	1.86	0.57
1:A:451:ALA:O	1:A:452:ASN:HB3	2.02	0.57
1:A:506:TYR:N	1:A:506:TYR:CD1	2.73	0.57
1:B:107:TYR:CG	1:B:121:LEU:HD23	2.39	0.57
1:B:147:HIS:CD2	1:B:147:HIS:N	2.72	0.57
1:B:271:LEU:O	1:B:274:ILE:HB	2.05	0.57
2:C:35:ASP:O	2:C:341:THR:CG2	2.53	0.57
2:C:317:VAL:O	2:C:317:VAL:HG12	2.05	0.57
2:D:12:LYS:HG3	2:D:13:LYS:N	2.19	0.57
1:A:168:ASN:HB2	1:A:171:ARG:NE	1.87	0.57
1:A:192:SER:OG	1:A:215:THR:CB	2.52	0.57
1:B:172:ASP:O	1:B:176:ILE:HD13	2.04	0.57
2:D:307:ASP:OD1	2:D:311:ASP:CG	2.48	0.57
1:A:118:PRO:C	1:A:119:GLU:OE2	2.48	0.57
1:A:333:ARG:HH12	1:A:373:GLN:NE2	2.03	0.57
1:B:271:LEU:O	1:B:274:ILE:N	2.38	0.57
2:C:5:VAL:HG13	2:C:5:VAL:O	2.04	0.57
1:A:83:LYS:HD3	1:A:87:THR:OG1	2.05	0.57
1:A:88:ARG:CB	1:A:88:ARG:HH11	2.18	0.57
1:A:189:LEU:CG	1:A:190:SER:N	2.68	0.57
1:A:342:PHE:HD1	1:A:342:PHE:N	2.02	0.57
1:A:561:TYR:N	1:A:561:TYR:HD1	2.02	0.57
1:B:462:ASN:C	1:B:463:PHE:CD1	2.83	0.57
1:B:494:ARG:C	1:B:495:TYR:CD1	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:OG	1:A:215:THR:HB	2.03	0.57
1:A:254:ARG:HH11	1:A:254:ARG:CG	2.17	0.57
1:B:275:LEU:N	1:B:276:PRO:CD	2.68	0.57
1:B:332:ASP:O	1:B:417:ARG:HD3	2.05	0.57
1:B:517:GLU:CD	2:C:107:VAL:HG23	2.24	0.57
2:C:133:TYR:CA	2:C:317:VAL:CG1	2.83	0.57
2:D:125:TYR:CD1	2:D:125:TYR:N	2.73	0.57
2:D:158:ASP:CG	2:D:159:ILE:H	2.08	0.57
1:A:141:LYS:O	1:A:143:PHE:CD1	2.57	0.56
2:D:23:VAL:HG11	2:D:367:MET:HE2	1.87	0.56
1:A:149:TRP:C	1:A:152:LEU:H	2.13	0.56
1:A:335:PHE:N	1:A:335:PHE:CD1	2.73	0.56
1:B:139:LEU:HD12	1:B:139:LEU:H	1.71	0.56
1:B:212:LYS:CE	1:B:270:TRP:NE1	2.68	0.56
1:B:506:TYR:N	1:B:506:TYR:CD1	2.73	0.56
2:C:133:TYR:CD1	2:C:134:TYR:N	2.72	0.56
2:C:248:LEU:HD12	2:C:248:LEU:O	2.04	0.56
2:D:169:SER:C	2:D:171:ASP:N	2.62	0.56
1:A:293:ALA:O	1:A:297:SER:N	2.37	0.56
1:A:499:GLU:HB2	1:A:500:LEU:HD12	1.86	0.56
1:A:509:SER:CA	1:A:512:ASP:OD2	2.53	0.56
1:A:536:HIS:CD2	1:A:536:HIS:N	2.73	0.56
1:A:546:ARG:O	1:A:550:ASN:N	2.39	0.56
1:A:554:GLU:HG2	1:A:554:GLU:O	2.05	0.56
1:B:32:GLN:NE2	1:B:162:LEU:HA	2.20	0.56
1:B:157:ILE:O	1:B:160:LEU:CD1	2.54	0.56
1:B:335:PHE:N	1:B:335:PHE:CD1	2.72	0.56
1:B:528:ILE:C	1:B:531:LEU:HD12	2.29	0.56
2:C:157:GLU:OE2	2:C:201:CYS:HA	2.05	0.56
2:C:171:ASP:N	2:C:171:ASP:OD1	2.36	0.56
2:D:57:TYR:OH	2:D:369:TRP:CA	2.53	0.56
2:D:202:SER:OG	2:D:204:GLU:N	2.38	0.56
2:D:284:ALA:O	2:D:287:GLN:HB2	2.05	0.56
2:D:363:MET:O	2:D:367:MET:HG3	2.04	0.56
1:B:82:VAL:HG23	1:B:83:LYS:N	2.20	0.56
1:B:107:TYR:HH	1:B:120:ARG:HE	1.51	0.56
1:B:301:TYR:CE1	1:B:305:LEU:CD2	2.88	0.56
2:C:213:ALA:O	2:C:216:TYR:CB	2.53	0.56
2:D:134:TYR:O	2:D:137:THR:OG1	2.19	0.56
1:A:168:ASN:ND2	1:A:171:ARG:NH1	2.54	0.56
1:B:256:TYR:OH	1:B:361:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:271:THR:CG2	2:C:273:LYS:CG	2.83	0.56
2:D:148:ASP:OD1	2:D:222:ARG:NH1	2.38	0.56
1:A:458:MET:HE1	1:A:545:TRP:HH2	1.70	0.56
1:B:13:ILE:H	1:B:13:ILE:CD1	2.19	0.56
1:B:86:TYR:CD2	1:B:103:PHE:HD2	2.24	0.56
1:B:442:GLY:HA3	1:B:536:HIS:CD2	2.41	0.56
2:C:171:ASP:HA	2:C:174:LYS:HB3	1.87	0.56
2:D:189:ARG:CZ	2:D:190:PHE:CE1	2.87	0.56
1:A:327:THR:OG1	1:A:328:LEU:N	2.37	0.56
1:A:369:MET:HE1	1:A:453:ILE:HG13	1.88	0.56
2:C:25:GLU:OE1	2:C:61:ARG:NE	2.36	0.56
2:C:365:ARG:NH2	2:C:374:ASP:OD1	2.35	0.56
2:D:80:GLN:O	2:D:80:GLN:HG3	2.04	0.56
2:D:196:ILE:HG22	2:D:197:GLY:N	2.21	0.56
1:A:252:PHE:CD1	1:A:253:ALA:N	2.74	0.56
1:B:61:VAL:HG12	1:B:65:LEU:CD1	2.35	0.56
1:B:253:ALA:HB1	1:B:367:GLY:HA2	1.87	0.56
2:C:402:LEU:HD12	2:C:402:LEU:C	2.31	0.56
2:D:289:ILE:HD12	2:D:313:LEU:HD23	1.87	0.56
1:B:172:ASP:O	1:B:176:ILE:CD1	2.53	0.56
1:B:274:ILE:HG22	1:B:275:LEU:HG	1.88	0.56
1:A:32:GLN:HA	1:A:202:TYR:CZ	2.42	0.55
1:A:88:ARG:HH11	1:A:88:ARG:HB2	1.71	0.55
1:A:97:GLU:HG2	1:A:98:ILE:H	1.70	0.55
1:A:143:PHE:CD1	1:A:143:PHE:N	2.73	0.55
1:B:173:ILE:HG12	1:B:174:HIS:N	2.21	0.55
1:B:176:ILE:C	1:B:180:LEU:HD12	2.12	0.55
2:C:37:ILE:CG2	2:C:342:ALA:HB3	2.36	0.55
2:D:158:ASP:C	2:D:160:TYR:N	2.60	0.55
2:D:354:GLY:O	2:D:358:LEU:HG	2.06	0.55
1:A:179:HIS:CD2	1:A:239:CYS:HB3	2.39	0.55
1:A:332:ASP:N	1:A:332:ASP:OD1	2.39	0.55
1:B:172:ASP:O	1:B:175:TYR:HB2	2.06	0.55
2:C:78:TYR:HB3	2:C:82:VAL:HG11	1.86	0.55
1:A:78:PHE:CD1	1:A:79:LEU:N	2.70	0.55
1:A:459:LEU:HD12	1:A:461:LYS:HE3	1.87	0.55
1:B:7:LEU:CA	1:B:85:HIS:CD2	2.79	0.55
1:B:145:PRO:CB	1:B:149:TRP:CE3	2.86	0.55
1:B:176:ILE:HD12	1:B:176:ILE:H	1.69	0.55
1:A:101:SER:HG	1:A:295:THR:HG1	1.47	0.55
1:A:208:TRP:CE2	1:A:225:PRO:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:PRO:CD	1:A:345:GLN:H	2.19	0.55
1:B:39:ASP:O	1:B:43:VAL:CG2	2.54	0.55
2:D:106:PRO:CA	2:D:111:ILE:CD1	2.74	0.55
2:D:415:ASN:C	2:D:416:MET:OXT	2.44	0.55
1:B:35:PHE:CD1	1:B:35:PHE:C	2.85	0.55
1:B:8:LEU:HD12	1:B:8:LEU:C	2.25	0.55
1:B:544:TYR:CE1	1:B:548:LEU:HD21	2.42	0.55
2:C:348:GLN:O	2:C:349:ASP:CB	2.55	0.55
2:D:106:PRO:HB2	2:D:111:ILE:HG13	1.84	0.55
2:D:234:MET:HB2	2:D:237:THR:HG23	1.88	0.55
2:D:331:GLU:OE1	2:D:331:GLU:N	2.39	0.55
1:B:201:PHE:O	1:B:208:TRP:HB2	2.07	0.55
1:B:441:TYR:CD1	1:B:441:TYR:C	2.85	0.55
1:A:6:GLU:O	1:A:9:ILE:N	2.39	0.55
1:A:35:PHE:CD1	1:A:35:PHE:C	2.85	0.55
1:A:56:HIS:C	1:A:56:HIS:CD2	2.85	0.55
1:B:90:LEU:N	1:B:91:PRO:CD	2.69	0.55
2:C:8:PRO:CG	2:C:28:ILE:HG23	2.31	0.55
2:C:116:VAL:O	2:C:120:GLN:HB2	2.07	0.55
2:C:216:TYR:CZ	2:C:220:ASN:ND2	2.75	0.55
2:C:229:HIS:ND1	2:C:229:HIS:O	2.40	0.55
2:D:175:VAL:HG12	2:D:179:LEU:CD1	2.37	0.55
1:A:31:ALA:CB	1:A:202:TYR:CD2	2.90	0.55
1:A:238:THR:OG1	1:A:239:CYS:N	2.39	0.55
1:B:31:ALA:O	1:B:34:ARG:N	2.39	0.55
2:C:178:PHE:CD1	2:C:178:PHE:C	2.85	0.55
1:A:34:ARG:NH2	1:A:258:MET:CE	2.69	0.55
1:A:104:ASN:OD1	1:A:104:ASN:N	2.37	0.55
1:A:365:ARG:C	1:A:367:GLY:H	2.14	0.55
1:B:564:ARG:HH11	1:B:564:ARG:HG3	1.72	0.55
2:C:258:ILE:O	2:C:259:ASP:OD1	2.22	0.55
1:A:324:LEU:HD23	1:A:393:LEU:HD23	1.89	0.54
2:C:112:ARG:HG2	2:C:113:SER:N	2.20	0.54
2:C:229:HIS:O	2:C:281:ILE:HA	2.07	0.54
2:D:209:LEU:HD23	2:D:210:VAL:HG23	1.89	0.54
1:A:193:HIS:C	1:A:194:LEU:HD12	2.31	0.54
1:B:7:LEU:HB3	1:B:85:HIS:CD2	2.38	0.54
1:B:97:GLU:HG2	1:B:98:ILE:N	2.23	0.54
2:C:133:TYR:CD1	2:C:133:TYR:C	2.85	0.54
2:C:206:THR:O	2:C:210:VAL:HG23	2.06	0.54
2:C:271:THR:HB	2:C:273:LYS:H	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:TYR:C	2:D:133:TYR:CD1	2.85	0.54
1:A:561:TYR:N	1:A:561:TYR:CD1	2.73	0.54
1:B:176:ILE:C	1:B:180:LEU:HD11	2.27	0.54
1:B:235:PHE:CD1	1:B:235:PHE:C	2.85	0.54
2:D:235:LYS:O	2:D:239:GLY:N	2.40	0.54
1:A:38:ALA:HA	1:A:40:TRP:CE3	2.42	0.54
1:A:342:PHE:N	1:A:342:PHE:CD1	2.73	0.54
2:C:8:PRO:HG3	2:C:28:ILE:CG2	2.30	0.54
2:C:133:TYR:CD1	2:C:134:TYR:C	2.85	0.54
2:D:356:ILE:HG23	2:D:357:ILE:N	2.22	0.54
1:A:116:LEU:HD12	1:A:116:LEU:N	2.23	0.54
1:B:149:TRP:C	1:B:149:TRP:CD1	2.86	0.54
1:B:522:LEU:HD12	1:B:522:LEU:N	2.22	0.54
2:D:66:MET:HE1	5:D:505:HOH:O	2.06	0.54
2:D:119:ARG:O	2:D:124:LEU:CD1	2.52	0.54
1:A:17:PHE:HE1	1:A:98:ILE:HG21	1.72	0.54
1:A:66:ARG:O	1:A:69:THR:N	2.18	0.54
1:A:189:LEU:HG	1:A:190:SER:H	1.72	0.54
1:B:54:TYR:CD1	1:B:54:TYR:C	2.85	0.54
1:B:528:ILE:C	1:B:531:LEU:CD1	2.80	0.54
1:A:17:PHE:CZ	1:A:98:ILE:HB	2.43	0.54
1:A:462:ASN:HD22	1:A:462:ASN:N	1.99	0.54
1:B:254:ARG:CZ	1:B:562:ALA:CB	2.86	0.54
2:D:203:GLU:O	2:D:207:LYS:HG3	2.07	0.54
1:A:441:TYR:C	1:A:441:TYR:CD1	2.85	0.54
2:D:31:TYR:HA	2:D:99:ILE:O	2.07	0.54
2:D:95:TYR:O	2:D:96:ARG:CB	2.56	0.54
1:A:528:ILE:HG12	1:A:529:GLY:N	2.23	0.54
1:B:37:GLN:O	1:B:38:ALA:HB3	2.06	0.54
1:B:178:ARG:O	1:B:182:GLU:CD	2.51	0.54
2:C:151:ILE:HD13	2:C:299:ILE:HG13	1.89	0.54
2:C:236:PHE:CD2	2:D:164:GLU:CD	2.79	0.54
2:D:45:MET:O	2:D:49:VAL:CG2	2.51	0.54
2:D:285:PHE:CD1	2:D:285:PHE:C	2.85	0.54
1:A:323:MET:CE	1:A:338:ILE:HG13	2.37	0.54
1:B:323:MET:HE1	1:B:357:TYR:CE1	2.43	0.54
1:B:531:LEU:O	1:B:534:GLU:N	2.41	0.54
2:C:133:TYR:CZ	2:C:134:TYR:O	2.56	0.54
2:C:154:GLU:OE1	2:C:157:GLU:HG2	2.08	0.54
2:D:179:LEU:O	2:D:184:GLY:N	2.41	0.54
1:A:54:TYR:CD1	1:A:54:TYR:C	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:NZ	3:B:602:AMP:O3P	2.39	0.53
2:C:133:TYR:HD2	2:C:144:PRO:HB2	1.71	0.53
2:C:135:GLN:HG3	2:C:381:GLU:HG2	1.90	0.53
1:A:305:LEU:HD12	1:A:306:GLN:N	2.22	0.53
1:B:515:PRO:O	1:B:540:PHE:CA	2.56	0.53
2:C:178:PHE:C	2:C:178:PHE:HD1	2.16	0.53
2:C:326:ALA:CB	2:C:335:PHE:CD1	2.91	0.53
2:D:132:ARG:HH11	2:D:132:ARG:CG	2.10	0.53
1:B:107:TYR:CD1	1:B:107:TYR:C	2.85	0.53
2:C:71:GLY:O	2:C:83:TRP:HZ3	1.87	0.53
2:D:224:SER:HB2	2:D:276:VAL:O	2.09	0.53
1:A:312:PHE:O	1:A:386:SER:OG	2.27	0.53
1:A:359:LEU:HD12	1:A:359:LEU:C	2.32	0.53
1:B:187:GLU:H	1:B:187:GLU:CD	1.94	0.53
2:C:153:ARG:CD	2:C:306:GLY:CA	2.41	0.53
2:D:131:VAL:HG21	2:D:313:LEU:HD13	1.90	0.53
1:A:379:VAL:HG13	1:A:379:VAL:O	2.08	0.53
1:B:312:PHE:CD1	1:B:328:LEU:HD23	2.36	0.53
1:B:325:VAL:HA	1:B:335:PHE:O	2.07	0.53
1:B:440:GLU:HG2	1:B:471:VAL:HG23	1.89	0.53
1:B:485:VAL:HG21	1:B:513:VAL:HG21	1.90	0.53
2:C:7:VAL:HG13	2:C:8:PRO:HD2	1.88	0.53
2:C:160:TYR:CE1	2:C:304:LEU:CD1	2.91	0.53
2:D:169:SER:C	2:D:171:ASP:H	2.13	0.53
1:A:229:THR:O	1:A:232:GLY:N	2.41	0.53
1:B:59:GLY:O	1:B:62:VAL:HG22	2.09	0.53
1:B:237:ASP:CB	1:B:569:PHE:HE1	1.83	0.53
2:C:37:ILE:O	2:C:40:ASP:HB2	2.09	0.53
1:B:13:ILE:O	1:B:16:GLY:N	2.41	0.53
2:C:69:TYR:N	2:C:69:TYR:CD1	2.77	0.53
2:D:37:ILE:O	2:D:40:ASP:HB2	2.09	0.53
2:D:130:PRO:HG3	2:D:362:MET:SD	2.49	0.53
1:A:482:MET:HE1	1:A:545:TRP:CZ3	2.41	0.53
1:B:149:TRP:O	1:B:152:LEU:CB	2.54	0.53
1:B:176:ILE:CD1	1:B:176:ILE:H	2.21	0.53
1:B:257:PHE:HB2	1:B:286:ALA:O	2.08	0.53
1:B:443:ASN:O	1:B:447:GLN:HG3	2.08	0.53
2:C:183:MET:CA	2:C:183:MET:CE	2.85	0.53
2:C:225:VAL:HB	2:C:277:ILE:HD12	1.91	0.53
2:D:240:ALA:CA	2:D:244:TRP:HE1	2.20	0.53
1:A:14:LEU:HD11	1:A:93:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:TYR:CE1	1:B:25:LEU:HD21	2.44	0.53
1:B:281:ALA:CB	1:B:300:GLU:OE2	2.56	0.53
2:C:271:THR:HG21	2:C:273:LYS:CG	2.39	0.53
2:D:116:VAL:O	2:D:119:ARG:HG3	2.09	0.53
1:A:215:THR:CG2	1:A:218:GLY:O	2.57	0.53
1:B:253:ALA:CA	1:B:367:GLY:HA2	2.39	0.53
2:C:78:TYR:CB	2:C:82:VAL:HG11	2.39	0.53
2:D:128:LEU:HD13	2:D:152:PHE:CE1	2.44	0.53
2:D:261:GLY:CA	2:D:263:TRP:CH2	2.73	0.53
1:A:31:ALA:CB	1:A:202:TYR:HD2	2.22	0.52
1:A:324:LEU:HB3	1:A:337:VAL:HG13	1.90	0.52
1:A:431:GLY:O	1:A:435:ARG:N	2.39	0.52
2:D:161:ALA:CB	2:D:163:ILE:HG13	2.38	0.52
2:D:189:ARG:NH1	2:D:190:PHE:HE1	2.06	0.52
2:D:196:ILE:CG2	2:D:197:GLY:N	2.72	0.52
1:A:77:GLU:OE2	1:A:78:PHE:HB2	2.09	0.52
1:A:107:TYR:HE1	1:A:111:PHE:CE2	2.17	0.52
1:A:281:ALA:HB3	1:A:300:GLU:OE2	2.09	0.52
1:B:100:GLU:O	1:B:103:PHE:HB3	2.10	0.52
1:B:134:THR:CG2	1:B:135:ILE:N	2.72	0.52
2:C:183:MET:HA	2:C:183:MET:CE	2.34	0.52
1:A:404:LEU:CD2	1:A:409:VAL:CG2	2.87	0.52
1:A:474:TYR:HD1	1:A:475:ASP:N	2.07	0.52
1:A:561:TYR:CE2	1:A:568:ARG:CZ	2.90	0.52
1:B:148:GLY:C	1:B:151:SER:OG	2.52	0.52
1:B:434:LEU:C	1:B:436:ASP:N	2.66	0.52
1:A:254:ARG:CG	1:A:254:ARG:NH1	2.73	0.52
1:B:148:GLY:CA	1:B:151:SER:OG	2.58	0.52
1:B:156:VAL:HG23	1:B:157:ILE:HG13	1.91	0.52
1:B:303:VAL:O	1:B:306:GLN:HG3	2.10	0.52
2:D:227:LEU:CD1	2:D:227:LEU:N	2.73	0.52
1:A:96:PHE:CD1	1:A:96:PHE:N	2.73	0.52
1:B:223:LEU:C	1:B:224:LEU:HD23	2.35	0.52
1:B:335:PHE:HA	1:B:414:TYR:O	2.08	0.52
2:D:384:ILE:O	2:D:387:LYS:CA	2.56	0.52
1:B:176:ILE:N	1:B:176:ILE:CD1	2.73	0.52
1:B:524:ALA:O	2:C:76:GLN:NE2	2.43	0.52
2:C:352:ASN:CB	2:C:390:THR:OG1	2.58	0.52
1:A:87:THR:HG23	1:A:122:PHE:CZ	2.44	0.52
1:A:171:ARG:NH1	1:A:171:ARG:CG	2.73	0.52
1:A:460:PHE:C	1:A:462:ASN:N	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:HB3	1:A:551:ARG:HH11	1.74	0.52
2:C:352:ASN:HB2	2:C:390:THR:OG1	2.09	0.52
1:A:195:GLN:HG2	1:A:270:TRP:HZ2	1.74	0.52
1:A:509:SER:N	1:A:512:ASP:OD2	2.42	0.52
1:B:41:HIS:O	1:B:45:GLN:HB3	2.09	0.52
1:B:117:THR:CG2	1:B:120:ARG:HB2	2.40	0.52
1:B:285:MET:CE	1:B:373:GLN:NE2	2.73	0.52
2:C:45:MET:HE2	2:C:99:ILE:HD13	1.92	0.52
2:C:51:ALA:CB	2:C:413:ILE:CD1	2.88	0.52
2:C:204:GLU:O	2:C:208:ARG:HB2	2.10	0.52
2:D:119:ARG:C	2:D:124:LEU:CD1	2.74	0.52
2:D:249:ALA:CB	2:D:264:LEU:HD11	2.37	0.52
2:D:299:ILE:CD1	2:D:299:ILE:N	2.72	0.52
2:D:403:LEU:CD1	2:D:403:LEU:N	2.73	0.52
1:A:223:LEU:CD1	1:A:223:LEU:N	2.73	0.52
1:A:239:CYS:C	1:A:240:LEU:HD12	2.35	0.52
1:A:240:LEU:N	1:A:240:LEU:CD1	2.73	0.52
1:B:253:ALA:CB	1:B:367:GLY:CA	2.87	0.52
1:B:323:MET:CE	1:B:357:TYR:OH	2.55	0.52
2:C:25:GLU:HB3	2:C:61:ARG:HG2	1.90	0.52
2:C:158:ASP:HB2	2:C:303:ASN:HB2	1.92	0.52
2:C:289:ILE:HD12	2:C:313:LEU:CD2	2.40	0.52
2:D:45:MET:HG2	2:D:49:VAL:CG2	2.40	0.52
2:D:75:THR:HG23	2:D:80:GLN:HA	1.90	0.52
1:A:88:ARG:CB	1:A:88:ARG:NH1	2.73	0.52
1:A:201:PHE:CD2	1:A:259:VAL:HB	2.44	0.52
1:B:88:ARG:O	1:B:88:ARG:HG2	2.10	0.52
1:B:473:PHE:CZ	1:B:475:ASP:O	2.63	0.52
1:B:567:GLN:O	1:B:568:ARG:C	2.50	0.52
2:D:45:MET:CE	2:D:46:LEU:N	2.73	0.52
2:D:261:GLY:CA	2:D:263:TRP:HZ3	1.88	0.52
1:A:109:ARG:CG	1:A:109:ARG:HH11	2.22	0.51
1:A:181:THR:O	1:A:184:LEU:O	2.28	0.51
1:B:146:ASP:CB	1:B:147:HIS:CD2	2.91	0.51
1:B:356:CYS:SG	1:B:479:ILE:HG21	2.50	0.51
2:C:158:ASP:CG	2:C:159:ILE:N	2.68	0.51
1:A:21:TYR:O	1:A:24:PHE:HB3	2.09	0.51
1:A:77:GLU:CG	1:A:78:PHE:N	2.74	0.51
1:A:357:TYR:CE1	1:A:476:TYR:HD2	2.27	0.51
1:A:404:LEU:N	1:A:404:LEU:CD1	2.73	0.51
1:B:68:ILE:O	1:B:69:THR:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:HD2	1:B:130:ARG:O	2.10	0.51
2:C:183:MET:HE3	2:C:183:MET:O	2.11	0.51
1:A:80:LEU:N	1:A:80:LEU:CD1	2.73	0.51
2:C:45:MET:SD	2:C:45:MET:C	2.93	0.51
2:D:166:LYS:O	2:D:169:SER:HB3	2.10	0.51
1:A:116:LEU:N	1:A:116:LEU:CD1	2.73	0.51
1:A:213:LEU:N	1:A:220:LEU:O	2.43	0.51
1:A:481:TYR:HB2	1:A:484:GLU:CG	2.41	0.51
1:A:570:SER:O	1:A:571:VAL:HG22	2.10	0.51
1:B:80:LEU:CD2	1:B:80:LEU:N	2.73	0.51
1:B:453:ILE:CG2	1:B:479:ILE:HD11	2.40	0.51
2:C:190:PHE:N	2:C:191:PRO:CD	2.73	0.51
2:D:78:TYR:HB3	2:D:82:VAL:HG11	1.91	0.51
1:A:229:THR:O	1:A:232:GLY:HA2	2.09	0.51
1:A:290:GLN:HG3	1:A:291:LYS:N	2.25	0.51
1:B:130:ARG:O	1:B:131:ARG:C	2.53	0.51
1:B:522:LEU:N	1:B:522:LEU:CD1	2.73	0.51
2:C:160:TYR:CZ	2:C:304:LEU:HD12	2.45	0.51
1:A:97:GLU:HA	1:A:100:GLU:OE1	2.11	0.51
1:A:141:LYS:O	1:A:141:LYS:HG3	2.10	0.51
1:A:201:PHE:CD1	1:A:210:VAL:CG2	2.94	0.51
1:A:422:LEU:HG	1:A:426:LEU:HD11	1.93	0.51
1:B:20:GLN:HG3	1:B:21:TYR:N	2.25	0.51
1:B:80:LEU:HD23	1:B:80:LEU:N	2.26	0.51
1:B:204:ASN:HD21	1:B:364:ASP:CG	2.01	0.51
1:B:222:PHE:C	1:B:222:PHE:CD1	2.88	0.51
1:B:304:TYR:OH	1:B:330:GLY:HA3	2.09	0.51
2:C:29:ILE:HD12	2:C:363:MET:HE3	1.92	0.51
2:C:146:LEU:O	2:C:293:PRO:HG2	2.10	0.51
1:B:65:LEU:N	1:B:65:LEU:CD1	2.73	0.51
1:B:186:PRO:N	1:B:187:GLU:OE1	2.44	0.51
1:B:401:ILE:HD12	1:B:401:ILE:O	2.09	0.51
2:D:79:GLY:HA3	2:D:82:VAL:CG1	2.40	0.51
1:B:41:HIS:O	1:B:45:GLN:CB	2.59	0.51
2:C:256:GLU:O	2:C:265:LYS:HG2	2.11	0.51
2:D:26:ASN:N	2:D:27:PRO:CD	2.73	0.51
2:D:238:GLU:OE2	2:D:302:MET:SD	2.69	0.51
1:A:88:ARG:NH1	1:A:88:ARG:HB3	2.25	0.51
1:A:103:PHE:CD2	1:A:122:PHE:HD2	2.29	0.51
1:B:132:PHE:CD1	1:B:132:PHE:C	2.88	0.51
2:D:219:ALA:HB3	2:D:220:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASN:O	1:A:52:HIS:N	2.40	0.51
1:A:177:ILE:O	1:A:181:THR:N	2.30	0.51
1:A:281:ALA:HB2	1:A:300:GLU:OE2	2.10	0.51
1:A:515:PRO:O	1:A:518:PHE:CD2	2.64	0.51
1:B:143:PHE:O	1:B:193:HIS:HB2	2.11	0.51
1:B:144:HIS:HB3	1:B:145:PRO:HD2	1.93	0.51
2:C:214:ILE:HG22	2:C:218:ILE:HD11	1.93	0.51
2:D:57:TYR:CG	2:D:61:ARG:HD2	2.46	0.51
1:A:32:GLN:HB2	1:A:202:TYR:OH	2.11	0.50
1:A:142:ASP:C	1:A:143:PHE:HD1	2.18	0.50
1:A:223:LEU:C	1:A:224:LEU:CD1	2.83	0.50
1:B:254:ARG:HH22	1:B:562:ALA:HA	1.76	0.50
2:D:222:ARG:HB3	2:D:297:ASP:OD1	2.11	0.50
2:D:230:LYS:H	2:D:238:GLU:CG	2.10	0.50
2:D:230:LYS:N	2:D:238:GLU:HG2	2.08	0.50
2:D:383:ALA:HA	2:D:415:ASN:HD21	1.75	0.50
2:D:415:ASN:O	2:D:416:MET:OXT	2.30	0.50
1:A:35:PHE:CE2	1:A:207:ALA:HB2	2.46	0.50
1:A:118:PRO:HD2	1:A:119:GLU:H	1.76	0.50
1:A:239:CYS:C	1:A:240:LEU:CD1	2.84	0.50
1:A:460:PHE:O	1:A:462:ASN:N	2.44	0.50
1:B:5:LEU:HD23	1:B:6:GLU:CA	2.41	0.50
1:A:31:ALA:HB3	1:A:202:TYR:CD2	2.46	0.50
1:A:100:GLU:O	1:A:103:PHE:HB3	2.11	0.50
1:A:141:LYS:HE2	1:A:143:PHE:CZ	2.46	0.50
1:A:448:LEU:HD12	1:A:448:LEU:N	2.15	0.50
1:B:529:GLY:N	1:B:530:PRO:HD2	2.26	0.50
2:C:118:LEU:C	2:C:122:LEU:CD1	2.70	0.50
2:D:159:ILE:HG12	2:D:199:LYS:HB2	1.93	0.50
2:D:189:ARG:NH1	2:D:190:PHE:CD1	2.80	0.50
2:D:209:LEU:CD2	2:D:210:VAL:N	2.66	0.50
1:A:173:ILE:H	1:A:173:ILE:CD1	2.15	0.50
1:A:180:LEU:N	1:A:180:LEU:CD2	2.73	0.50
1:A:463:PHE:CE1	1:A:473:PHE:CD1	3.00	0.50
1:B:160:LEU:HB2	1:B:161:PRO:HD2	1.93	0.50
1:B:168:ASN:HB2	1:B:171:ARG:HB2	1.93	0.50
2:D:234:MET:HG3	2:D:238:GLU:CB	2.41	0.50
1:A:531:LEU:O	1:A:534:GLU:N	2.44	0.50
1:B:173:ILE:HG12	1:B:174:HIS:H	1.75	0.50
1:B:179:HIS:HD1	1:B:179:HIS:C	2.20	0.50
1:B:332:ASP:C	1:B:333:ARG:HG3	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LYS:NZ	1:B:405:GLY:O	2.31	0.50
2:C:48:VAL:HA	2:C:413:ILE:HD11	1.93	0.50
2:D:7:VAL:HG13	5:D:505:HOH:O	2.12	0.50
2:D:12:LYS:O	2:D:28:ILE:HG13	2.11	0.50
1:A:94:PRO:HG3	1:B:26:GLU:OE2	2.12	0.50
1:A:222:PHE:C	1:A:223:LEU:HD13	2.37	0.50
1:A:450:ALA:O	1:A:552:ILE:CD1	2.59	0.50
1:A:452:ASN:ND2	1:A:482:MET:H	2.10	0.50
1:B:208:TRP:CE3	1:B:225:PRO:HB3	2.47	0.50
1:B:485:VAL:CG2	1:B:513:VAL:HG23	2.42	0.50
2:C:119:ARG:CG	2:C:119:ARG:HH11	2.24	0.50
2:C:158:ASP:CB	2:C:303:ASN:HB2	2.41	0.50
2:D:150:VAL:HG11	2:D:216:TYR:CE2	2.46	0.50
1:B:97:GLU:O	1:B:100:GLU:HG3	2.12	0.50
1:B:111:PHE:CE2	1:B:120:ARG:NH2	2.79	0.50
1:B:333:ARG:HB3	1:B:416:GLU:O	2.11	0.50
1:B:548:LEU:O	1:B:552:ILE:HG13	2.11	0.50
2:D:141:VAL:HG23	2:D:144:PRO:HB3	1.94	0.50
2:D:388:THR:C	2:D:389:VAL:HG13	2.37	0.50
1:A:177:ILE:CG1	1:A:178:ARG:N	2.75	0.50
1:B:108:CYS:O	1:B:112:ASP:N	2.44	0.50
1:B:357:TYR:CD2	1:B:414:TYR:CE2	3.00	0.50
1:A:230:ASP:O	1:A:231:ASP:C	2.54	0.50
1:A:312:PHE:CE1	1:A:328:LEU:HG	2.47	0.50
1:A:404:LEU:CD2	1:A:409:VAL:HG23	2.41	0.50
2:C:357:ILE:O	2:C:360:ALA:HB3	2.11	0.50
2:D:266:VAL:CG2	2:D:277:ILE:CD1	2.90	0.50
1:A:28:THR:HG23	1:A:258:MET:HG3	1.93	0.49
1:A:168:ASN:HD22	1:A:171:ARG:CZ	2.25	0.49
1:A:451:ALA:O	1:A:452:ASN:CB	2.60	0.49
1:B:301:TYR:CE2	1:B:302:LEU:HD12	2.47	0.49
1:B:336:LYS:HE2	4:B:601:ADP:H8	1.76	0.49
1:B:525:ASP:HB3	1:B:528:ILE:HG12	1.94	0.49
2:C:386:ALA:O	2:C:387:LYS:HB2	2.11	0.49
2:D:45:MET:HE2	2:D:46:LEU:N	2.27	0.49
1:A:77:GLU:HG2	1:A:78:PHE:N	2.27	0.49
1:A:220:LEU:HB3	1:A:221:PRO:HD2	1.94	0.49
2:C:209:LEU:O	2:C:212:ALA:N	2.45	0.49
2:C:326:ALA:CB	2:C:335:PHE:HD1	2.24	0.49
2:D:401:LYS:O	2:D:403:LEU:HD11	2.08	0.49
1:A:36:GLU:OE2	1:A:163:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:HH22	1:A:373:GLN:NE2	2.10	0.49
1:B:117:THR:HG22	1:B:120:ARG:HD3	1.94	0.49
1:B:132:PHE:CD1	1:B:134:THR:HA	2.48	0.49
1:B:323:MET:CE	1:B:357:TYR:CE1	2.96	0.49
2:D:209:LEU:HD21	2:D:210:VAL:HG23	1.94	0.49
1:A:28:THR:HA	1:A:258:MET:HE3	1.94	0.49
1:A:31:ALA:HB3	1:A:202:TYR:HD2	1.77	0.49
1:A:141:LYS:HE2	1:A:143:PHE:HZ	1.77	0.49
1:A:225:PRO:HG2	1:A:225:PRO:O	2.13	0.49
1:A:321:MET:O	1:A:339:LYS:HE2	2.13	0.49
2:C:328:ILE:HG22	2:C:329:GLY:N	2.27	0.49
1:A:56:HIS:O	1:A:60:LEU:N	2.45	0.49
1:A:107:TYR:CD2	1:A:121:LEU:CD2	2.95	0.49
1:A:458:MET:HE1	1:A:545:TRP:CH2	2.46	0.49
1:A:565:ARG:O	1:A:568:ARG:CG	2.54	0.49
1:B:160:LEU:CD1	1:B:160:LEU:C	2.86	0.49
1:B:213:LEU:O	1:B:220:LEU:N	2.28	0.49
1:B:272:ARG:O	1:B:275:LEU:N	2.44	0.49
2:C:154:GLU:CD	2:C:157:GLU:N	2.47	0.49
2:C:178:PHE:HD1	2:C:178:PHE:O	1.96	0.49
2:C:271:THR:HB	2:C:273:LYS:HG3	1.93	0.49
1:A:78:PHE:C	1:A:80:LEU:N	2.67	0.49
1:A:90:LEU:HB2	1:A:91:PRO:HD3	1.93	0.49
1:A:176:ILE:CD1	1:A:176:ILE:N	2.73	0.49
1:A:227:HIS:O	1:A:234:LEU:HA	2.12	0.49
1:A:473:PHE:HE2	1:A:479:ILE:HD13	1.75	0.49
1:B:176:ILE:O	1:B:180:LEU:HD11	2.03	0.49
2:C:39:VAL:O	2:C:43:PRO:HG2	2.13	0.49
2:D:189:ARG:NH1	2:D:189:ARG:O	2.44	0.49
1:A:185:GLY:O	1:A:188:ASN:HB2	2.13	0.49
1:A:192:SER:CB	1:A:215:THR:HB	2.43	0.49
1:A:382:LYS:NZ	1:A:405:GLY:O	2.33	0.49
2:C:28:ILE:HA	2:C:64:SER:O	2.13	0.49
2:C:241:PHE:HD2	2:C:302:MET:HE3	1.71	0.49
2:C:360:ALA:O	2:C:363:MET:HB3	2.11	0.49
2:D:30:PRO:HD2	2:D:97:VAL:O	2.13	0.49
2:D:234:MET:HG3	2:D:238:GLU:HB3	1.95	0.49
2:D:407:GLU:HA	2:D:410:ASP:OD2	2.12	0.49
1:A:441:TYR:C	1:A:444:ALA:H	2.21	0.49
2:C:189:ARG:HG3	2:C:189:ARG:NH1	2.27	0.49
2:D:220:ASN:ND2	2:D:220:ASN:N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TRP:NE1	1:A:205:LYS:HA	2.27	0.49
1:A:274:ILE:CG2	1:A:275:LEU:HD23	2.38	0.49
1:B:304:TYR:OH	1:B:330:GLY:C	2.56	0.49
1:B:525:ASP:HA	2:C:76:GLN:HE22	1.77	0.49
1:B:528:ILE:HA	1:B:531:LEU:CD1	2.42	0.49
2:D:82:VAL:O	2:D:82:VAL:HG22	2.12	0.49
1:A:77:GLU:CD	1:A:78:PHE:HB2	2.38	0.49
1:A:196:VAL:CG1	1:A:197:ALA:N	2.76	0.49
1:A:346:LYS:HD3	1:A:348:MET:HE3	1.94	0.49
1:B:17:PHE:CE1	1:B:98:ILE:HB	2.47	0.49
1:B:50:ARG:HD2	1:B:258:MET:CE	2.20	0.49
1:B:103:PHE:C	1:B:103:PHE:CD1	2.91	0.49
1:A:298:TYR:O	1:A:301:TYR:HB3	2.13	0.48
1:B:97:GLU:OE2	1:B:265:ALA:HB2	2.13	0.48
1:B:509:SER:N	1:B:512:ASP:OD2	2.45	0.48
2:C:229:HIS:ND1	2:C:231:GLY:N	2.59	0.48
2:D:45:MET:HE3	2:D:46:LEU:HA	1.95	0.48
1:A:153:LEU:O	1:A:157:ILE:HG12	2.13	0.48
1:B:17:PHE:CD2	1:B:17:PHE:C	2.91	0.48
2:D:133:TYR:CD2	2:D:144:PRO:HB2	2.48	0.48
2:D:353:PRO:HG2	2:D:405:CYS:SG	2.52	0.48
1:A:551:ARG:O	1:A:554:GLU:C	2.56	0.48
1:B:223:LEU:CD1	1:B:223:LEU:N	2.76	0.48
1:B:224:LEU:CD2	1:B:239:CYS:HA	2.44	0.48
1:B:249:VAL:O	1:B:249:VAL:HG22	2.12	0.48
1:B:332:ASP:C	1:B:418:ARG:HB3	2.39	0.48
2:C:166:LYS:HG2	2:C:167:ALA:N	2.27	0.48
2:C:357:ILE:O	2:C:360:ALA:N	2.46	0.48
2:D:14:ILE:HD13	2:D:24:PRO:HD2	1.96	0.48
2:D:266:VAL:HG23	2:D:277:ILE:HD12	1.95	0.48
1:A:121:LEU:CD1	1:A:121:LEU:C	2.86	0.48
1:A:271:LEU:O	1:A:274:ILE:N	2.46	0.48
1:B:5:LEU:HD23	1:B:6:GLU:HA	1.94	0.48
1:B:327:THR:CG2	1:B:418:ARG:HH21	2.26	0.48
2:C:271:THR:CB	2:C:273:LYS:CG	2.90	0.48
2:C:352:ASN:HB3	2:C:390:THR:HG21	1.94	0.48
2:D:45:MET:HG2	2:D:49:VAL:HG23	1.94	0.48
2:D:125:TYR:H	2:D:125:TYR:HD1	1.60	0.48
1:A:423:ASN:OD1	1:A:424:ILE:HG13	2.13	0.48
1:B:200:LEU:HB3	1:B:208:TRP:O	2.13	0.48
1:B:208:TRP:HA	1:B:225:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ARG:HB3	1:B:369:MET:HB2	1.95	0.48
1:B:485:VAL:HG21	1:B:513:VAL:CG2	2.44	0.48
2:C:307:ASP:O	2:C:311:ASP:HB2	2.13	0.48
2:D:229:HIS:HD1	2:D:229:HIS:C	2.20	0.48
1:A:109:ARG:CG	1:A:109:ARG:NH1	2.77	0.48
1:A:179:HIS:HD2	1:A:239:CYS:CB	2.24	0.48
1:A:230:ASP:OD1	1:A:230:ASP:N	2.46	0.48
1:A:234:LEU:H	1:A:234:LEU:CD1	2.18	0.48
1:A:531:LEU:O	1:A:535:MET:N	2.41	0.48
1:B:17:PHE:CE1	1:B:98:ILE:CB	2.97	0.48
1:B:121:LEU:C	1:B:121:LEU:CD1	2.85	0.48
1:B:240:LEU:HD22	1:B:245:GLU:CB	2.43	0.48
1:B:372:THR:HG1	1:B:414:TYR:HD2	1.62	0.48
1:B:552:ILE:O	1:B:555:GLY:N	2.46	0.48
1:A:107:TYR:HB3	1:A:121:LEU:HD23	1.94	0.48
1:A:299:ARG:O	1:A:302:LEU:N	2.46	0.48
1:B:117:THR:OG1	1:B:118:PRO:CD	2.62	0.48
1:B:422:LEU:N	1:B:463:PHE:O	2.44	0.48
2:D:263:TRP:HB3	2:D:277:ILE:O	2.13	0.48
1:A:107:TYR:CZ	1:A:111:PHE:CD2	3.02	0.48
1:A:334:VAL:O	1:A:334:VAL:HG23	2.13	0.48
1:A:422:LEU:CG	1:A:426:LEU:HD11	2.43	0.48
1:B:127:GLN:CG	1:B:128:PRO:HD2	2.43	0.48
1:B:133:ARG:O	1:B:134:THR:OG1	2.26	0.48
1:B:333:ARG:NH1	1:B:415:ILE:HG21	2.27	0.48
1:B:476:TYR:CD1	1:B:476:TYR:N	2.81	0.48
2:C:133:TYR:CE2	2:C:144:PRO:CG	2.97	0.48
2:C:230:LYS:HE2	2:C:232:ASN:OD1	2.14	0.48
2:D:352:ASN:HA	2:D:353:PRO:HD2	1.37	0.48
1:A:20:GLN:NE2	1:A:20:GLN:C	2.72	0.48
1:A:149:TRP:CZ3	1:A:152:LEU:HD21	2.48	0.48
1:A:191:LYS:HD2	1:A:191:LYS:HA	1.60	0.48
1:A:256:TYR:OH	1:A:371:ASP:OD2	2.28	0.48
1:A:352:HIS:HD1	1:A:352:HIS:C	2.21	0.48
1:B:84:GLU:O	1:B:87:THR:CB	2.61	0.48
1:B:135:ILE:HD12	1:B:266:ALA:CB	2.43	0.48
1:B:145:PRO:CB	1:B:149:TRP:HE3	2.26	0.48
2:C:39:VAL:CG1	2:C:40:ASP:N	2.77	0.48
2:C:160:TYR:CD1	2:D:233:ILE:HG21	2.48	0.48
2:C:257:LEU:CD2	2:C:260:GLY:HA2	2.42	0.48
2:D:372:ALA:O	2:D:375:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:VAL:O	1:A:64:GLN:N	2.47	0.48
1:A:168:ASN:C	1:A:171:ARG:N	2.72	0.48
1:A:293:ALA:O	1:A:297:SER:CB	2.62	0.48
2:D:229:HIS:C	2:D:229:HIS:ND1	2.72	0.48
2:D:328:ILE:HG22	2:D:329:GLY:N	2.28	0.48
1:A:396:GLU:OE1	1:A:396:GLU:HA	2.13	0.47
2:C:116:VAL:CG2	2:C:117:ALA:N	2.77	0.47
2:C:245:GLY:O	2:C:248:LEU:HB3	2.14	0.47
2:C:365:ARG:HH11	2:C:365:ARG:CG	2.15	0.47
1:A:460:PHE:C	1:A:462:ASN:H	2.21	0.47
1:B:179:HIS:N	1:B:182:GLU:OE2	2.46	0.47
1:B:192:SER:OG	1:B:215:THR:CB	2.60	0.47
1:B:299:ARG:O	1:B:302:LEU:N	2.47	0.47
1:B:303:VAL:HG23	1:B:304:TYR:N	2.27	0.47
1:B:334:VAL:HG13	1:B:418:ARG:HB2	1.96	0.47
2:C:30:PRO:HA	2:C:66:MET:O	2.14	0.47
1:A:344:PRO:HD2	1:A:345:GLN:H	1.79	0.47
1:B:62:VAL:CG2	1:B:63:GLU:N	2.76	0.47
1:B:80:LEU:CD2	1:B:81:ARG:HG2	2.44	0.47
2:C:133:TYR:CB	2:C:317:VAL:HG13	2.45	0.47
2:D:157:GLU:OE1	2:D:202:SER:CB	2.61	0.47
1:A:31:ALA:HB1	1:A:202:TYR:CD2	2.49	0.47
1:A:229:THR:OG1	1:A:235:PHE:CD1	2.65	0.47
1:B:201:PHE:CE1	1:B:210:VAL:HG23	2.42	0.47
1:B:474:TYR:CD1	1:B:475:ASP:N	2.73	0.47
2:D:167:ALA:O	2:D:168:ASP:HB2	2.14	0.47
1:B:208:TRP:CZ3	1:B:225:PRO:HB3	2.49	0.47
1:A:40:TRP:HA	1:A:43:VAL:CG2	2.45	0.47
1:A:321:MET:HB3	1:A:343:ALA:CB	2.39	0.47
1:B:80:LEU:CD2	1:B:80:LEU:H	2.27	0.47
1:B:329:PRO:O	1:B:418:ARG:NH1	2.48	0.47
1:B:425:TRP:CE2	1:B:429:VAL:HG11	2.50	0.47
2:C:258:ILE:CA	2:C:259:ASP:OD1	2.60	0.47
1:A:219:THR:N	1:A:220:LEU:HD23	2.29	0.47
1:A:274:ILE:O	1:A:275:LEU:HD23	2.14	0.47
1:A:293:ALA:C	1:A:297:SER:OG	2.57	0.47
1:A:333:ARG:NH1	1:A:373:GLN:HE22	2.12	0.47
1:A:420:VAL:CG1	1:A:465:VAL:HB	2.44	0.47
1:B:96:PHE:O	1:B:99:ALA:HB3	2.14	0.47
1:B:135:ILE:CD1	1:B:266:ALA:HB2	2.45	0.47
1:B:160:LEU:HD12	1:B:160:LEU:C	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:HIS:ND1	2:C:366:HIS:C	2.73	0.47
2:D:388:THR:O	2:D:389:VAL:CG1	2.62	0.47
1:A:143:PHE:N	1:A:143:PHE:HD1	2.11	0.47
1:A:322:VAL:HG22	4:A:602:ADP:O1B	2.08	0.47
1:B:254:ARG:HG3	1:B:367:GLY:HA3	1.96	0.47
1:B:368:ARG:HB2	1:B:448:LEU:HD21	1.96	0.47
1:B:550:ASN:O	1:B:554:GLU:CG	2.60	0.47
2:C:285:PHE:HE2	2:C:289:ILE:HG21	1.80	0.47
2:C:352:ASN:CA	2:C:390:THR:HG21	2.45	0.47
2:D:11:GLY:HA3	2:D:28:ILE:HG12	1.97	0.47
1:A:201:PHE:CD1	1:A:210:VAL:HG23	2.50	0.47
1:A:453:ILE:HG23	1:A:479:ILE:CG1	2.44	0.47
1:A:482:MET:CE	1:A:545:TRP:HZ3	2.28	0.47
1:B:178:ARG:O	1:B:182:GLU:HG3	2.15	0.47
1:B:354:ARG:HH21	1:B:412:HIS:CE1	2.33	0.47
1:B:520:HIS:C	1:B:520:HIS:ND1	2.72	0.47
2:C:229:HIS:ND1	2:C:229:HIS:C	2.73	0.47
2:D:41:VAL:HG23	2:D:42:THR:N	2.29	0.47
2:D:341:THR:O	2:D:342:ALA:C	2.57	0.47
1:A:104:ASN:ND2	1:A:122:PHE:C	2.73	0.47
1:A:179:HIS:ND1	1:A:179:HIS:C	2.73	0.47
1:A:238:THR:HA	1:A:569:PHE:CE2	2.50	0.47
1:A:403:ASP:O	1:A:404:LEU:CD1	2.63	0.47
1:B:105:SER:OG	3:B:602:AMP:H5'2	2.15	0.47
1:B:360:VAL:HG21	1:B:476:TYR:CD2	2.50	0.47
1:B:274:ILE:C	1:B:276:PRO:HD3	2.39	0.46
2:C:271:THR:HG21	2:C:273:LYS:CD	2.43	0.46
2:D:161:ALA:HB3	2:D:163:ILE:HG13	1.96	0.46
2:D:185:VAL:HG23	2:D:185:VAL:O	2.14	0.46
1:B:61:VAL:O	1:B:65:LEU:HD13	2.16	0.46
1:B:346:LYS:CB	1:B:348:MET:CE	2.81	0.46
2:C:57:TYR:CD1	2:C:61:ARG:CD	2.99	0.46
2:C:75:THR:CA	2:C:79:GLY:O	2.62	0.46
1:A:23:ARG:HH21	1:A:23:ARG:CG	2.27	0.46
1:A:253:ALA:HB1	1:A:367:GLY:O	2.15	0.46
1:A:323:MET:HE1	1:A:338:ILE:HG12	1.95	0.46
1:B:42:ALA:CA	1:B:45:GLN:HB3	2.45	0.46
1:B:86:TYR:O	1:B:89:LEU:HD12	2.15	0.46
1:B:208:TRP:CD2	1:B:225:PRO:HB3	2.50	0.46
1:B:327:THR:HG21	1:B:418:ARG:HH21	1.74	0.46
1:B:462:ASN:O	1:B:463:PHE:CD1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:TYR:HB2	2:C:317:VAL:HG13	1.97	0.46
2:D:229:HIS:NE2	2:D:242:LYS:HD3	2.29	0.46
1:A:313:ILE:O	1:A:327:THR:HG22	2.15	0.46
1:B:97:GLU:CG	1:B:98:ILE:N	2.78	0.46
1:B:254:ARG:HG3	1:B:367:GLY:CA	2.45	0.46
2:D:158:ASP:O	2:D:160:TYR:N	2.48	0.46
2:D:177:LYS:O	2:D:181:GLU:CG	2.63	0.46
2:D:220:ASN:N	2:D:220:ASN:HD22	2.13	0.46
1:A:238:THR:HA	1:A:569:PHE:CE1	2.49	0.46
1:A:254:ARG:NH2	1:A:470:ARG:CZ	2.41	0.46
1:A:301:TYR:CE1	1:A:305:LEU:HD23	2.50	0.46
1:A:323:MET:HE2	1:A:338:ILE:HA	1.98	0.46
1:A:466:THR:HG22	1:A:470:ARG:O	2.16	0.46
1:A:516:GLU:H	1:A:516:GLU:HG2	1.47	0.46
1:B:145:PRO:HB3	1:B:149:TRP:CZ3	2.50	0.46
1:B:209:LEU:C	1:B:209:LEU:CD2	2.85	0.46
1:B:422:LEU:HD12	1:B:422:LEU:O	2.16	0.46
2:C:204:GLU:OE1	2:D:190:PHE:CE1	2.66	0.46
2:C:292:ARG:HB3	2:C:295:GLU:HG3	1.97	0.46
1:A:45:GLN:O	1:A:49:ASN:OD1	2.32	0.46
1:A:149:TRP:HZ2	1:A:189:LEU:O	1.98	0.46
1:A:173:ILE:HA	1:A:176:ILE:HD12	1.28	0.46
1:A:179:HIS:NE2	1:A:239:CYS:O	2.48	0.46
1:A:209:LEU:C	1:A:209:LEU:CD2	2.85	0.46
1:B:160:LEU:CB	1:B:161:PRO:HD2	2.45	0.46
1:B:253:ALA:HB1	1:B:367:GLY:C	2.40	0.46
1:B:259:VAL:O	1:B:259:VAL:HG13	2.14	0.46
1:B:284:TYR:HA	1:B:287:ILE:HD11	1.97	0.46
1:B:531:LEU:C	1:B:534:GLU:H	2.24	0.46
2:C:354:GLY:O	2:C:358:LEU:HG	2.16	0.46
1:A:219:THR:CA	1:A:220:LEU:HD23	2.34	0.46
1:A:413:LEU:HD12	1:A:414:TYR:CA	2.46	0.46
1:B:107:TYR:CE1	1:B:111:PHE:HD2	2.32	0.46
2:C:112:ARG:CD	5:C:503:HOH:O	2.62	0.46
2:C:166:LYS:CG	2:C:167:ALA:N	2.79	0.46
2:D:37:ILE:O	2:D:40:ASP:N	2.48	0.46
2:D:99:ILE:CB	2:D:363:MET:CE	2.90	0.46
2:D:257:LEU:CD2	2:D:260:GLY:HA2	2.40	0.46
2:D:266:VAL:HG21	2:D:277:ILE:CD1	2.45	0.46
1:A:35:PHE:CE2	1:A:207:ALA:CB	2.98	0.46
1:A:166:TRP:HB2	1:A:169:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:TYR:OH	1:A:330:GLY:HA3	2.15	0.46
1:A:389:LEU:HD12	1:A:389:LEU:HA	1.85	0.46
1:A:118:PRO:CD	1:A:119:GLU:H	2.28	0.46
1:A:303:VAL:HG23	1:A:304:TYR:N	2.31	0.46
1:A:403:ASP:O	1:A:404:LEU:HD12	2.16	0.46
1:A:570:SER:C	1:A:571:VAL:CG2	2.85	0.46
2:C:328:ILE:HG22	2:C:329:GLY:H	1.81	0.46
2:D:351:VAL:O	2:D:405:CYS:HB2	2.16	0.46
1:A:172:ASP:O	1:A:175:TYR:N	2.48	0.46
1:A:287:ILE:CG1	1:A:289:CYS:SG	3.04	0.46
1:B:173:ILE:O	1:B:177:ILE:CG1	2.63	0.46
2:D:338:THR:HG22	2:D:355:SER:OG	2.16	0.46
1:A:119:GLU:HG2	1:A:120:ARG:N	2.30	0.45
1:A:303:VAL:C	1:A:306:GLN:HG2	2.36	0.45
1:A:522:LEU:HD12	1:A:540:PHE:CE1	2.51	0.45
1:B:54:TYR:HE1	1:B:58:VAL:HG21	1.78	0.45
1:B:78:PHE:H	1:B:78:PHE:HD1	1.64	0.45
1:B:495:TYR:O	1:B:498:ASP:HB2	2.16	0.45
2:C:132:ARG:HG2	2:C:133:TYR:O	2.16	0.45
2:C:160:TYR:CE1	2:C:304:LEU:HD12	2.51	0.45
2:D:82:VAL:HG22	2:D:85:PRO:HD3	1.97	0.45
2:D:408:PHE:O	2:D:412:ILE:HG12	2.15	0.45
1:A:121:LEU:C	1:A:121:LEU:HD12	2.42	0.45
1:A:229:THR:HG22	1:A:230:ASP:N	2.30	0.45
1:A:378:PHE:O	1:A:409:VAL:HA	2.15	0.45
1:A:453:ILE:HG23	1:A:479:ILE:HG13	1.97	0.45
1:B:100:GLU:O	1:B:101:SER:C	2.58	0.45
1:B:426:LEU:HD23	1:B:426:LEU:HA	1.72	0.45
2:C:285:PHE:C	2:C:285:PHE:CD2	2.94	0.45
1:A:77:GLU:N	1:A:77:GLU:OE1	2.48	0.45
1:A:94:PRO:CG	1:B:26:GLU:OE2	2.65	0.45
1:A:441:TYR:O	1:A:442:GLY:C	2.59	0.45
2:C:388:THR:C	2:C:389:VAL:CG1	2.90	0.45
2:D:31:TYR:CD1	2:D:66:MET:O	2.69	0.45
1:A:123:ILE:HG13	1:A:124:PHE:CD2	2.51	0.45
1:A:322:VAL:HG21	1:A:477:ALA:HB2	1.98	0.45
1:B:21:TYR:OH	1:B:264:PRO:CG	2.64	0.45
1:B:61:VAL:O	1:B:64:GLN:N	2.49	0.45
1:B:141:LYS:HD2	1:B:143:PHE:CZ	2.51	0.45
1:B:312:PHE:CZ	1:B:328:LEU:CD2	2.82	0.45
1:B:513:VAL:C	1:B:515:PRO:HD3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:VAL:O	2:C:43:PRO:HD2	2.16	0.45
2:D:68:ILE:HG22	2:D:91:LEU:HD13	1.97	0.45
2:D:297:ASP:O	2:D:299:ILE:HD13	2.13	0.45
1:A:80:LEU:O	1:A:81:ARG:C	2.59	0.45
1:A:226:ILE:HG22	1:A:227:HIS:N	2.32	0.45
1:B:106:VAL:O	1:B:110:LEU:HD23	2.16	0.45
2:C:75:THR:C	2:C:79:GLY:O	2.59	0.45
2:C:217:ALA:O	2:C:221:ASP:N	2.50	0.45
2:D:106:PRO:HG3	2:D:113:SER:CB	2.47	0.45
1:A:101:SER:O	1:A:105:SER:OG	2.31	0.45
1:A:142:ASP:HA	1:A:195:GLN:HA	1.99	0.45
1:B:174:HIS:HD1	1:B:174:HIS:C	2.24	0.45
1:B:401:ILE:C	1:B:401:ILE:CD1	2.85	0.45
1:B:547:ALA:O	1:B:550:ASN:N	2.49	0.45
2:C:130:PRO:CD	2:C:362:MET:SD	3.05	0.45
2:D:292:ARG:N	2:D:293:PRO:CD	2.78	0.45
1:A:213:LEU:HB3	1:A:220:LEU:O	2.17	0.45
1:B:78:PHE:CA	1:B:81:ARG:HG3	2.44	0.45
1:B:327:THR:CB	1:B:418:ARG:HH21	2.30	0.45
1:B:494:ARG:HB3	1:B:495:TYR:CE1	2.52	0.45
1:B:528:ILE:HG13	1:B:529:GLY:N	2.31	0.45
2:C:190:PHE:CD1	2:D:204:GLU:CB	3.00	0.45
2:C:238:GLU:OE1	2:C:302:MET:HG3	2.03	0.45
2:D:29:ILE:HA	2:D:30:PRO:HD3	1.68	0.45
1:A:172:ASP:O	1:A:175:TYR:HB2	2.17	0.45
1:B:118:PRO:HB2	1:B:119:GLU:OE2	2.16	0.45
1:B:253:ALA:HB1	1:B:367:GLY:CA	2.47	0.45
1:B:514:PHE:HA	1:B:515:PRO:HD2	1.67	0.45
2:C:146:LEU:O	2:C:293:PRO:CG	2.65	0.45
2:D:57:TYR:OH	2:D:369:TRP:CB	2.65	0.45
1:B:132:PHE:CD1	1:B:132:PHE:O	2.70	0.45
1:B:482:MET:O	1:B:549:GLN:NE2	2.49	0.45
2:C:16:LEU:C	2:C:16:LEU:CD2	2.85	0.45
2:C:160:TYR:CE1	2:C:304:LEU:HD13	2.50	0.45
2:C:202:SER:OG	2:C:205:GLY:N	2.48	0.45
2:C:373:ALA:O	2:C:377:VAL:HG23	2.16	0.45
2:D:130:PRO:HA	2:D:150:VAL:HA	1.98	0.45
2:D:356:ILE:HD12	2:D:356:ILE:C	2.36	0.45
2:D:383:ALA:O	2:D:386:ALA:HB3	2.17	0.45
1:A:526:PRO:O	1:A:530:PRO:HD2	2.16	0.45
1:B:80:LEU:CD2	1:B:81:ARG:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LYS:HG2	1:B:274:ILE:HD11	1.95	0.45
1:B:222:PHE:O	1:B:222:PHE:CD1	2.70	0.45
1:B:254:ARG:NH1	1:B:254:ARG:CG	2.73	0.45
2:C:242:LYS:CG	2:C:243:ASP:N	2.80	0.45
2:D:26:ASN:N	2:D:27:PRO:HD3	2.31	0.45
1:A:392:LEU:HD12	1:A:392:LEU:C	2.37	0.44
1:B:246:ALA:HA	1:B:249:VAL:CG1	2.46	0.44
2:C:154:GLU:OE1	2:C:157:GLU:HG3	2.13	0.44
2:C:154:GLU:CD	2:C:156:SER:HG	2.22	0.44
2:D:45:MET:HE3	2:D:46:LEU:HD23	1.98	0.44
2:D:114:LEU:HD12	2:D:114:LEU:HA	1.78	0.44
2:D:159:ILE:O	2:D:159:ILE:HG22	2.16	0.44
2:D:352:ASN:HD22	2:D:392:ASP:CG	2.19	0.44
1:A:77:GLU:CD	1:A:77:GLU:C	2.85	0.44
1:B:14:LEU:HD12	1:B:14:LEU:O	2.17	0.44
1:B:200:LEU:H	1:B:200:LEU:HG	1.57	0.44
1:B:320:GLY:HA3	4:B:601:ADP:O2A	2.16	0.44
1:B:346:LYS:CD	1:B:348:MET:HE1	2.28	0.44
1:B:457:ASP:O	1:B:458:MET:CB	2.65	0.44
2:C:286:LEU:O	2:C:289:ILE:HG12	2.17	0.44
2:D:328:ILE:CG2	2:D:329:GLY:N	2.80	0.44
1:A:525:ASP:N	1:A:528:ILE:CD1	2.60	0.44
1:B:230:ASP:OD1	1:B:230:ASP:N	2.50	0.44
1:B:312:PHE:CD1	1:B:328:LEU:HD22	2.50	0.44
2:C:276:VAL:O	2:C:277:ILE:HD13	2.17	0.44
2:C:352:ASN:CB	2:C:390:THR:CG2	2.94	0.44
2:D:319:GLY:O	2:D:320:ILE:C	2.60	0.44
1:A:456:GLY:HA3	1:A:478:GLU:HB2	1.99	0.44
1:A:538:ASP:OD1	1:A:538:ASP:N	2.50	0.44
1:B:116:LEU:H	1:B:116:LEU:HG	1.57	0.44
1:B:145:PRO:HB3	1:B:149:TRP:HE3	1.73	0.44
1:B:295:THR:OG1	3:B:602:AMP:O3'	1.84	0.44
2:C:113:SER:HB3	2:C:116:VAL:CG2	2.43	0.44
2:C:154:GLU:O	2:C:303:ASN:CG	2.60	0.44
2:C:353:PRO:HG2	2:C:357:ILE:HD11	1.99	0.44
2:D:133:TYR:CE2	2:D:144:PRO:HG2	2.52	0.44
2:D:169:SER:HG	2:D:172:ALA:N	2.12	0.44
2:D:209:LEU:C	2:D:212:ALA:H	2.25	0.44
1:A:394:LEU:CD2	1:A:401:ILE:HD11	2.43	0.44
1:B:35:PHE:CD2	1:B:207:ALA:HB2	2.53	0.44
1:B:143:PHE:HB3	1:B:152:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:N	1:B:274:ILE:CD1	2.81	0.44
1:B:466:THR:OG1	1:B:470:ARG:HB2	2.17	0.44
1:B:552:ILE:C	1:B:555:GLY:H	2.25	0.44
2:D:307:ASP:O	2:D:311:ASP:HB2	2.18	0.44
1:A:78:PHE:HA	1:A:81:ARG:HG3	2.00	0.44
1:A:561:TYR:CE2	1:A:568:ARG:NH1	2.85	0.44
1:B:260:TYR:CD2	1:B:262:PRO:HD3	2.53	0.44
1:B:272:ARG:O	1:B:275:LEU:C	2.60	0.44
1:B:274:ILE:C	1:B:276:PRO:CD	2.91	0.44
2:C:114:LEU:HD12	2:C:114:LEU:HA	1.84	0.44
1:A:117:THR:HB	1:A:118:PRO:CD	2.48	0.44
1:A:287:ILE:HG13	1:A:289:CYS:SG	2.58	0.44
1:A:365:ARG:CZ	1:A:371:ASP:HB2	2.47	0.44
1:A:452:ASN:HD21	1:A:481:TYR:CB	2.27	0.44
1:A:103:PHE:CD2	1:A:122:PHE:CD2	3.06	0.44
1:A:176:ILE:HG12	1:A:177:ILE:H	1.83	0.44
1:B:116:LEU:HD12	1:B:116:LEU:O	2.17	0.44
1:B:127:GLN:CB	1:B:128:PRO:HD2	2.47	0.44
1:B:177:ILE:CD1	1:B:177:ILE:H	2.19	0.44
1:B:369:MET:CE	1:B:453:ILE:HG13	2.46	0.44
2:C:25:GLU:C	2:C:27:PRO:CD	2.90	0.44
2:D:357:ILE:O	2:D:360:ALA:HB3	2.18	0.44
1:A:260:TYR:CE2	1:A:262:PRO:HG3	2.52	0.44
1:A:356:CYS:SG	1:A:479:ILE:HG22	2.58	0.44
2:C:23:VAL:HG21	2:C:367:MET:HE2	1.99	0.44
2:C:308:TYR:O	2:C:312:ALA:HB2	2.18	0.44
2:C:348:GLN:O	2:C:349:ASP:HB2	2.18	0.44
2:C:407:GLU:O	2:C:410:ASP:CB	2.66	0.44
2:D:3:SER:OG	2:D:78:TYR:OH	2.30	0.44
2:D:137:THR:HG22	2:D:138:PRO:N	2.32	0.44
1:A:24:PHE:O	1:A:27:VAL:HG12	2.17	0.43
1:A:60:LEU:C	1:A:60:LEU:CD1	2.88	0.43
1:A:139:LEU:H	1:A:139:LEU:HG	1.56	0.43
1:A:142:ASP:HA	1:A:194:LEU:O	2.18	0.43
1:A:280:THR:OG1	1:A:281:ALA:N	2.51	0.43
1:B:5:LEU:C	1:B:5:LEU:CD2	2.85	0.43
1:B:23:ARG:HD2	1:B:23:ARG:HA	1.78	0.43
1:B:456:GLY:HA3	1:B:478:GLU:O	2.18	0.43
1:B:477:ALA:O	1:B:478:GLU:C	2.56	0.43
1:B:543:ASP:O	1:B:546:ARG:HB2	2.18	0.43
2:C:341:THR:O	2:C:342:ALA:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:361:GLU:OE2	2:C:365:ARG:HD2	2.18	0.43
2:C:407:GLU:O	2:C:410:ASP:N	2.51	0.43
2:D:127:CYS:SG	2:D:153:ARG:HD2	2.54	0.43
2:D:154:GLU:HG3	2:D:303:ASN:HD22	1.83	0.43
1:A:238:THR:CA	1:A:569:PHE:CZ	3.00	0.43
1:A:292:HIS:O	1:A:295:THR:N	2.51	0.43
1:A:359:LEU:HD21	1:A:481:TYR:HE1	1.81	0.43
1:A:422:LEU:CD2	1:A:441:TYR:HD2	2.31	0.43
1:B:474:TYR:CD1	1:B:474:TYR:C	2.96	0.43
2:D:31:TYR:HD1	2:D:66:MET:O	2.01	0.43
2:D:133:TYR:CE1	2:D:135:GLN:HA	2.44	0.43
1:A:5:LEU:HD22	1:A:5:LEU:HA	1.86	0.43
1:A:78:PHE:CG	1:A:79:LEU:N	2.85	0.43
1:A:196:VAL:HG12	1:A:197:ALA:H	1.81	0.43
1:A:561:TYR:HD2	1:A:563:TYR:CE1	2.36	0.43
1:B:177:ILE:HA	1:B:180:LEU:CD1	2.46	0.43
1:B:420:VAL:HG12	1:B:465:VAL:HB	1.97	0.43
1:B:425:TRP:NE1	1:B:429:VAL:HG11	2.33	0.43
1:B:565:ARG:HD2	1:B:565:ARG:HA	1.81	0.43
2:C:159:ILE:HD12	2:C:199:LYS:HB2	1.99	0.43
1:A:39:ASP:O	1:A:41:HIS:N	2.51	0.43
1:A:167:GLN:HG2	1:A:233:GLU:CB	2.37	0.43
1:A:429:VAL:CG1	1:A:430:GLU:O	2.60	0.43
1:A:446:ARG:HH21	1:A:536:HIS:HB3	1.83	0.43
1:B:56:HIS:O	1:B:60:LEU:N	2.40	0.43
1:B:100:GLU:H	1:B:100:GLU:HG2	1.58	0.43
1:B:453:ILE:HA	1:B:453:ILE:HD13	1.75	0.43
1:B:517:GLU:O	1:B:521:TRP:CZ3	2.72	0.43
1:B:567:GLN:C	1:B:568:ARG:O	2.56	0.43
2:C:206:THR:CG2	2:C:241:PHE:CD2	2.98	0.43
2:C:305:ASN:O	2:C:309:ILE:HG12	2.18	0.43
1:A:174:HIS:HA	1:A:177:ILE:HD12	1.85	0.43
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.83	0.43
1:A:327:THR:OG1	1:A:418:ARG:NH2	2.51	0.43
1:A:548:LEU:C	1:A:550:ASN:N	2.75	0.43
1:B:420:VAL:HG13	1:B:420:VAL:O	2.17	0.43
1:B:461:LYS:NZ	4:B:601:ADP:PB	2.92	0.43
1:B:526:PRO:HD3	2:C:76:GLN:HE22	1.84	0.43
2:C:227:LEU:O	2:C:279:ASP:HA	2.18	0.43
2:C:232:ASN:OD1	2:C:232:ASN:N	2.51	0.43
2:D:17:GLN:O	2:D:18:ASN:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:PRO:O	2:D:106:PRO:HG2	2.18	0.43
2:D:151:ILE:HG21	2:D:310:SER:OG	2.18	0.43
2:D:227:LEU:N	2:D:227:LEU:HD13	2.33	0.43
1:A:35:PHE:HE2	1:A:207:ALA:H	1.63	0.43
2:C:125:TYR:CE1	2:C:208:ARG:HG2	2.53	0.43
2:D:42:THR:N	2:D:43:PRO:HD2	2.34	0.43
1:A:168:ASN:O	1:A:171:ARG:HB3	2.05	0.43
1:A:548:LEU:C	1:A:550:ASN:H	2.25	0.43
1:B:284:TYR:O	1:B:287:ILE:HG13	2.19	0.43
2:C:119:ARG:CG	2:C:119:ARG:NH1	2.81	0.43
2:C:149:MET:HA	2:C:297:ASP:O	2.18	0.43
2:C:353:PRO:O	2:C:357:ILE:HD13	2.03	0.43
2:C:380:MET:HE3	2:C:380:MET:HB3	1.79	0.43
2:D:97:VAL:O	2:D:97:VAL:HG13	2.19	0.43
2:D:280:VAL:CG2	2:D:285:PHE:HD2	2.32	0.43
2:D:326:ALA:HB1	2:D:335:PHE:CD2	2.54	0.43
1:A:107:TYR:CZ	1:A:111:PHE:HD2	2.36	0.43
1:A:201:PHE:CD1	1:A:210:VAL:HG21	2.53	0.43
1:B:104:ASN:OD1	1:B:122:PHE:HB2	2.18	0.43
1:B:222:PHE:O	1:B:222:PHE:HD1	2.01	0.43
1:B:442:GLY:HA3	1:B:536:HIS:CE1	2.54	0.43
2:C:388:THR:O	2:C:389:VAL:HG13	2.19	0.43
2:D:37:ILE:HD11	2:D:340:GLY:O	2.19	0.43
2:D:45:MET:HE3	2:D:46:LEU:CA	2.48	0.43
2:D:240:ALA:CA	2:D:244:TRP:NE1	2.79	0.43
1:A:179:HIS:N	1:A:180:LEU:HD22	2.33	0.43
1:A:294:LYS:O	1:A:297:SER:CB	2.62	0.43
1:A:522:LEU:HD12	1:A:540:PHE:HE1	1.82	0.43
1:A:539:LEU:HD23	1:A:539:LEU:HA	1.80	0.43
1:B:168:ASN:HB2	1:B:171:ARG:CB	2.49	0.43
1:B:320:GLY:CA	4:B:601:ADP:O2A	2.67	0.43
1:B:413:LEU:HD21	1:B:415:ILE:HG13	2.00	0.43
1:B:462:ASN:OD1	1:B:475:ASP:HB3	2.17	0.43
2:C:133:TYR:HA	2:C:317:VAL:HG11	1.98	0.43
2:C:371:GLU:O	2:C:374:ASP:HB2	2.19	0.43
2:C:410:ASP:O	2:C:413:ILE:N	2.52	0.43
2:D:45:MET:HE2	2:D:46:LEU:HG	1.99	0.43
2:D:289:ILE:O	2:D:293:PRO:CD	2.66	0.43
1:A:460:PHE:O	1:A:461:LYS:C	2.62	0.43
1:B:44:GLN:O	1:B:47:MET:HB3	2.18	0.43
1:B:458:MET:HE1	1:B:545:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:GLU:OE1	2:C:157:GLU:CB	2.66	0.43
2:C:191:PRO:O	2:C:194:CYS:HB3	2.19	0.43
2:C:265:LYS:HG2	2:C:265:LYS:H	1.65	0.43
1:A:211:GLY:O	1:A:222:PHE:O	2.37	0.42
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.75	0.42
1:A:551:ARG:CA	1:A:554:GLU:HB3	2.48	0.42
1:B:45:GLN:CD	1:B:45:GLN:C	2.87	0.42
1:B:237:ASP:HB3	1:B:569:PHE:HE1	1.74	0.42
1:A:248:ILE:HG22	1:A:254:ARG:NH1	2.34	0.42
1:A:463:PHE:CD1	1:A:463:PHE:N	2.82	0.42
1:A:535:MET:HB3	1:A:536:HIS:NE2	2.34	0.42
2:C:26:ASN:HA	2:C:62:LYS:O	2.19	0.42
2:C:170:ALA:O	2:C:174:LYS:N	2.48	0.42
2:C:248:LEU:HD12	2:C:252:GLU:HG3	1.99	0.42
2:C:388:THR:O	2:C:389:VAL:CG1	2.67	0.42
2:D:57:TYR:OH	2:D:369:TRP:C	2.62	0.42
2:D:169:SER:OG	2:D:172:ALA:HB2	2.18	0.42
2:D:192:GLU:O	2:D:193:HIS:HB2	2.18	0.42
2:D:393:PHE:O	2:D:396:LEU:N	2.52	0.42
1:A:148:GLY:C	1:A:150:GLU:N	2.77	0.42
1:A:171:ARG:O	1:A:174:HIS:HB2	2.17	0.42
1:A:240:LEU:N	1:A:240:LEU:HD13	2.34	0.42
1:A:543:ASP:CA	1:A:546:ARG:CD	2.96	0.42
1:B:304:TYR:OH	1:B:330:GLY:CA	2.67	0.42
1:B:568:ARG:HH21	1:B:568:ARG:CG	2.23	0.42
2:C:79:GLY:N	2:C:82:VAL:CG1	2.83	0.42
2:C:166:LYS:C	2:C:169:SER:HG	2.23	0.42
2:C:308:TYR:O	2:C:312:ALA:CB	2.67	0.42
2:C:408:PHE:O	2:C:411:ALA:HB3	2.19	0.42
2:D:384:ILE:O	2:D:387:LYS:HA	2.19	0.42
1:A:466:THR:CG2	1:A:470:ARG:HB2	2.48	0.42
2:C:190:PHE:HB3	2:D:202:SER:HB2	2.00	0.42
1:A:17:PHE:CZ	1:A:98:ILE:CG2	3.02	0.42
1:A:30:GLY:O	1:A:31:ALA:C	2.61	0.42
1:A:65:LEU:HB3	1:A:69:THR:HG22	1.99	0.42
1:B:82:VAL:CG2	1:B:83:LYS:N	2.83	0.42
1:B:111:PHE:O	1:B:114:ARG:HG2	2.19	0.42
1:B:166:TRP:CE2	1:B:234:LEU:CD2	2.95	0.42
2:C:226:THR:HA	2:C:278:LYS:O	2.20	0.42
2:D:21:LEU:HD12	2:D:21:LEU:C	2.44	0.42
2:D:141:VAL:CG2	2:D:144:PRO:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:LEU:O	2:D:212:ALA:CB	2.65	0.42
2:D:259:ASP:C	2:D:261:GLY:H	2.27	0.42
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.88	0.42
1:A:87:THR:HG23	1:A:122:PHE:HZ	1.82	0.42
1:A:229:THR:HB	1:A:232:GLY:HA2	2.00	0.42
1:B:9:ILE:O	1:B:13:ILE:HD12	2.20	0.42
1:B:238:THR:OG1	1:B:239:CYS:N	2.43	0.42
1:B:380:LEU:O	1:B:407:GLN:HA	2.19	0.42
2:C:388:THR:O	2:C:388:THR:OG1	2.38	0.42
2:D:30:PRO:O	2:D:98:ALA:CB	2.53	0.42
2:D:99:ILE:CG2	2:D:363:MET:HE1	2.49	0.42
1:A:54:TYR:CE1	1:A:58:VAL:HG21	2.55	0.42
1:A:91:PRO:O	1:A:92:ASP:CB	2.67	0.42
1:A:338:ILE:HG22	1:A:339:LYS:O	2.19	0.42
1:B:204:ASN:OD1	1:B:364:ASP:OD2	2.38	0.42
1:B:301:TYR:CE1	1:B:305:LEU:HD23	2.53	0.42
1:A:96:PHE:H	1:A:96:PHE:HD1	1.58	0.42
1:A:176:ILE:HB	1:A:180:LEU:HD12	1.81	0.42
1:A:213:LEU:HB2	1:A:222:PHE:HB2	2.02	0.42
1:B:356:CYS:SG	1:B:479:ILE:HG22	2.59	0.42
1:B:528:ILE:O	1:B:531:LEU:HD13	2.19	0.42
2:C:149:MET:HE2	2:C:149:MET:HB3	1.80	0.42
2:C:175:VAL:CG2	2:D:183:MET:HE3	2.44	0.42
2:C:239:GLY:C	2:C:241:PHE:N	2.74	0.42
2:D:230:LYS:C	2:D:232:ASN:N	2.59	0.42
2:D:268:ASN:CG	2:D:271:THR:CG2	2.88	0.42
2:D:375:LEU:HD12	2:D:375:LEU:HA	1.78	0.42
1:A:143:PHE:CE2	1:A:156:VAL:HG22	2.55	0.42
1:A:365:ARG:NH1	1:A:371:ASP:HB3	2.35	0.42
1:B:326:PHE:CD1	1:B:326:PHE:N	2.88	0.42
1:B:365:ARG:C	1:B:366:VAL:HG23	2.43	0.42
1:B:425:TRP:O	1:B:429:VAL:HG13	2.19	0.42
1:B:544:TYR:CZ	1:B:548:LEU:HD11	2.55	0.42
2:C:323:ALA:HA	2:C:324:PRO:HD3	1.74	0.42
2:D:192:GLU:O	2:D:193:HIS:C	2.62	0.42
1:A:344:PRO:CG	1:A:345:GLN:N	2.83	0.42
1:A:514:PHE:O	1:A:517:GLU:HG2	2.19	0.42
1:A:531:LEU:O	1:A:534:GLU:HB3	2.20	0.42
1:B:461:LYS:HZ1	4:B:601:ADP:PB	2.42	0.42
2:C:377:VAL:O	2:C:381:GLU:HB2	2.20	0.42
2:D:212:ALA:O	2:D:213:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:C	1:A:54:TYR:HD1	2.26	0.41
1:A:147:HIS:O	1:A:148:GLY:C	2.63	0.41
1:A:414:TYR:N	1:A:414:TYR:CD1	2.88	0.41
1:A:462:ASN:OD1	1:A:475:ASP:CB	2.67	0.41
1:B:295:THR:HG1	3:B:602:AMP:C3'	2.23	0.41
1:B:564:ARG:CG	1:B:564:ARG:NH1	2.73	0.41
2:C:11:GLY:HA3	2:C:28:ILE:HG12	2.02	0.41
2:C:23:VAL:HG21	2:C:367:MET:CE	2.49	0.41
2:D:79:GLY:N	2:D:82:VAL:CG1	2.83	0.41
2:D:409:GLY:O	2:D:412:ILE:HB	2.21	0.41
1:A:39:ASP:C	1:A:41:HIS:N	2.76	0.41
1:A:237:ASP:OD2	1:A:561:TYR:CE2	2.73	0.41
1:A:490:ILE:O	1:A:490:ILE:HG23	2.20	0.41
1:B:298:TYR:CZ	3:B:602:AMP:H2	2.30	0.41
1:B:320:GLY:O	1:B:339:LYS:NZ	2.45	0.41
2:C:286:LEU:HD21	2:C:309:ILE:HD13	2.01	0.41
2:C:337:ALA:HB1	2:C:339:HIS:NE2	2.35	0.41
2:D:38:GLY:HA2	2:D:41:VAL:HG22	2.02	0.41
1:A:119:GLU:OE2	1:A:120:ARG:N	2.51	0.41
1:A:271:LEU:O	1:A:272:ARG:C	2.64	0.41
1:A:344:PRO:CD	1:A:345:GLN:N	2.83	0.41
1:B:186:PRO:HD2	1:B:187:GLU:OE1	2.18	0.41
1:B:411:ARG:HE	1:B:411:ARG:HB2	1.64	0.41
2:D:169:SER:OG	2:D:172:ALA:HB3	2.20	0.41
2:D:291:LEU:H	2:D:291:LEU:CD1	2.09	0.41
1:A:186:PRO:HA	1:A:189:LEU:HD22	1.13	0.41
1:A:404:LEU:HD21	1:A:409:VAL:HG21	2.02	0.41
1:B:53:LEU:HA	1:B:53:LEU:HD12	1.81	0.41
1:B:107:TYR:CZ	1:B:111:PHE:CD2	3.08	0.41
1:B:273:GLU:O	1:B:276:PRO:HD3	2.20	0.41
1:B:368:ARG:HD3	1:B:368:ARG:HA	1.91	0.41
1:B:458:MET:HE1	1:B:545:TRP:HH2	1.86	0.41
2:C:201:CYS:HB2	2:C:237:THR:HG22	2.02	0.41
2:C:229:HIS:CD2	2:C:242:LYS:HB3	2.56	0.41
2:D:39:VAL:O	2:D:43:PRO:HD2	2.20	0.41
2:D:57:TYR:OH	2:D:369:TRP:HA	2.19	0.41
1:A:119:GLU:CD	1:A:119:GLU:H	2.25	0.41
1:A:561:TYR:HE2	1:A:568:ARG:NE	2.18	0.41
1:B:24:PHE:HA	1:B:53:LEU:HD23	2.03	0.41
1:B:78:PHE:O	1:B:81:ARG:CB	2.67	0.41
1:B:101:SER:O	1:B:102:PHE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:HD13	1:B:110:LEU:HA	1.85	0.41
1:B:462:ASN:CA	1:B:474:TYR:CE1	2.97	0.41
2:C:236:PHE:HE1	2:D:166:LYS:HB2	1.79	0.41
2:C:352:ASN:CB	2:C:390:THR:CB	2.98	0.41
2:D:79:GLY:CA	2:D:82:VAL:CG1	2.96	0.41
2:D:131:VAL:HG21	2:D:313:LEU:CD1	2.49	0.41
2:D:202:SER:OG	2:D:204:GLU:C	2.51	0.41
2:D:241:PHE:CD2	2:D:302:MET:HE3	2.52	0.41
2:D:398:ASP:CG	2:D:399:GLY:N	2.77	0.41
1:A:17:PHE:O	1:A:18:ASP:C	2.60	0.41
1:A:45:GLN:C	1:A:48:LYS:H	2.28	0.41
1:A:47:MET:O	1:A:47:MET:SD	2.79	0.41
1:A:89:LEU:CD1	1:A:89:LEU:H	2.28	0.41
1:A:175:TYR:C	1:A:177:ILE:HD13	2.45	0.41
1:A:245:GLU:OE2	1:A:567:GLN:NE2	2.53	0.41
1:A:281:ALA:HB2	1:A:296:GLU:HB3	2.02	0.41
1:A:404:LEU:HD22	1:A:409:VAL:CG2	2.45	0.41
1:A:463:PHE:CE1	1:A:473:PHE:HD1	2.36	0.41
1:A:559:ASP:OD1	1:A:559:ASP:N	2.52	0.41
1:B:172:ASP:OD1	1:B:172:ASP:N	2.44	0.41
2:C:213:ALA:C	2:C:216:TYR:H	2.24	0.41
2:D:141:VAL:HG22	2:D:316:GLN:O	2.20	0.41
1:A:179:HIS:CD2	1:A:239:CYS:CB	3.01	0.41
1:A:322:VAL:HG11	1:A:477:ALA:HB1	2.03	0.41
1:A:333:ARG:NH2	1:A:373:GLN:HE22	2.15	0.41
1:A:490:ILE:HA	1:A:491:PRO:HD3	1.94	0.41
1:B:166:TRP:NE1	1:B:234:LEU:CD2	2.83	0.41
1:B:174:HIS:C	1:B:174:HIS:ND1	2.77	0.41
1:B:359:LEU:HD13	1:B:481:TYR:OH	2.21	0.41
2:C:144:PRO:C	2:C:146:LEU:N	2.75	0.41
2:C:144:PRO:O	2:C:146:LEU:N	2.54	0.41
2:C:166:LYS:HB3	2:C:166:LYS:HE3	1.76	0.41
2:C:248:LEU:HD12	2:C:248:LEU:C	2.43	0.41
2:D:23:VAL:HG11	2:D:367:MET:CE	2.49	0.41
2:D:161:ALA:HB1	2:D:163:ILE:HG13	2.02	0.41
1:A:19:ALA:O	1:A:20:GLN:C	2.60	0.41
1:A:168:ASN:O	1:A:169:LYS:C	2.58	0.41
1:B:186:PRO:HA	1:B:189:LEU:HB3	2.02	0.41
2:C:183:MET:HE3	2:C:183:MET:C	2.46	0.41
2:D:80:GLN:C	2:D:81:ASP:OD1	2.55	0.41
1:A:97:GLU:HG2	1:A:98:ILE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ARG:O	1:A:545:TRP:HD1	2.04	0.41
1:A:548:LEU:O	1:A:552:ILE:HG13	2.20	0.41
1:B:17:PHE:O	1:B:18:ASP:C	2.63	0.41
1:B:31:ALA:O	1:B:32:GLN:C	2.61	0.41
1:B:54:TYR:C	1:B:54:TYR:HD1	2.28	0.41
1:B:84:GLU:O	1:B:87:THR:HB	2.20	0.41
1:B:157:ILE:C	1:B:159:ASP:N	2.74	0.41
1:B:274:ILE:N	1:B:274:ILE:HD12	2.36	0.41
1:B:356:CYS:HB3	1:B:479:ILE:HG21	2.02	0.41
1:B:432:GLN:O	1:B:432:GLN:HG3	2.20	0.41
1:B:452:ASN:ND2	1:B:481:TYR:HD1	2.18	0.41
1:B:485:VAL:CG2	1:B:513:VAL:CG2	2.98	0.41
2:C:25:GLU:C	2:C:27:PRO:HD3	2.46	0.41
2:C:124:LEU:HD13	2:C:328:ILE:C	2.46	0.41
2:C:171:ASP:C	2:C:175:VAL:HG23	2.41	0.41
2:C:337:ALA:HB2	2:C:356:ILE:HD12	2.03	0.41
2:D:119:ARG:HB3	2:D:124:LEU:HD13	2.03	0.41
2:D:127:CYS:SG	2:D:127:CYS:O	2.79	0.41
2:D:266:VAL:HG23	2:D:277:ILE:CD1	2.51	0.41
2:D:281:ILE:O	2:D:285:PHE:HB2	2.21	0.41
2:D:289:ILE:CG1	2:D:290:LEU:N	2.84	0.41
2:D:391:TYR:O	2:D:395:ARG:CG	2.67	0.41
1:A:23:ARG:NH2	1:A:23:ARG:CG	2.81	0.41
1:B:94:PRO:HG2	1:B:95:ARG:HG3	2.03	0.41
2:C:361:GLU:HG2	2:C:373:ALA:HB1	2.02	0.41
2:D:116:VAL:O	2:D:117:ALA:C	2.62	0.41
2:D:377:VAL:O	2:D:381:GLU:HG2	2.21	0.41
1:A:107:TYR:CE1	1:A:111:PHE:HD2	2.29	0.40
1:A:152:LEU:C	1:A:152:LEU:CD1	2.85	0.40
1:A:171:ARG:C	1:A:174:HIS:H	2.28	0.40
1:A:390:MET:O	1:A:390:MET:SD	2.79	0.40
1:A:546:ARG:HA	1:A:549:GLN:HG2	2.02	0.40
1:B:365:ARG:C	1:B:367:GLY:N	2.78	0.40
1:B:518:PHE:O	1:B:519:ARG:C	2.64	0.40
1:B:519:ARG:NE	1:B:533:GLU:OE2	2.51	0.40
1:B:535:MET:H	1:B:535:MET:HG2	1.72	0.40
2:C:286:LEU:CD2	2:C:309:ILE:HD13	2.51	0.40
1:A:165:HIS:O	1:A:233:GLU:HA	2.20	0.40
1:A:223:LEU:N	1:A:223:LEU:HD13	2.37	0.40
1:A:381:GLU:HG3	1:A:407:GLN:HG3	0.88	0.40
1:A:457:ASP:C	1:A:459:LEU:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ASN:OD1	1:A:475:ASP:HB2	2.21	0.40
1:B:47:MET:SD	1:B:47:MET:O	2.79	0.40
1:B:127:GLN:HG3	1:B:128:PRO:CD	2.51	0.40
1:B:172:ASP:N	1:B:173:ILE:HD13	2.35	0.40
1:B:472:VAL:HG12	1:B:473:PHE:N	2.36	0.40
2:C:151:ILE:HD13	2:C:299:ILE:HB	2.02	0.40
2:C:380:MET:O	2:C:384:ILE:HG13	2.21	0.40
2:D:14:ILE:HD13	2:D:23:VAL:HG13	2.01	0.40
2:D:189:ARG:HH11	2:D:189:ARG:CG	2.29	0.40
1:A:179:HIS:O	1:A:179:HIS:ND1	2.54	0.40
1:A:272:ARG:O	1:A:273:GLU:C	2.62	0.40
1:A:448:LEU:CD1	1:A:448:LEU:H	2.10	0.40
1:B:179:HIS:C	1:B:179:HIS:ND1	2.77	0.40
1:B:372:THR:OG1	1:B:414:TYR:HD2	2.04	0.40
2:D:268:ASN:HA	2:D:269:PRO:HD2	1.84	0.40
1:A:35:PHE:O	1:A:36:GLU:C	2.61	0.40
1:A:208:TRP:CD2	1:A:225:PRO:HB3	2.56	0.40
1:A:224:LEU:CD1	1:A:224:LEU:N	2.85	0.40
1:A:324:LEU:HD21	1:A:393:LEU:CD2	2.47	0.40
1:A:529:GLY:N	1:A:530:PRO:HD2	2.36	0.40
1:B:69:THR:O	1:B:70:ASN:ND2	2.54	0.40
1:B:170:SER:HA	1:B:173:ILE:HG13	1.80	0.40
1:B:192:SER:HG	1:B:215:THR:N	2.16	0.40
1:B:460:PHE:C	1:B:462:ASN:N	2.79	0.40
1:B:473:PHE:CE1	1:B:475:ASP:O	2.74	0.40
2:C:57:TYR:CG	2:C:61:ARG:HD3	2.56	0.40
2:C:154:GLU:OE2	2:C:156:SER:CB	2.70	0.40
2:D:41:VAL:CG2	2:D:42:THR:N	2.84	0.40
2:D:45:MET:HE3	2:D:46:LEU:N	2.36	0.40
2:D:288:GLN:HA	2:D:291:LEU:HD13	2.03	0.40
2:D:360:ALA:O	2:D:361:GLU:C	2.63	0.40
1:A:353:VAL:O	1:A:356:CYS:HB2	2.21	0.40
1:A:413:LEU:HD12	1:A:414:TYR:C	2.47	0.40
1:A:440:GLU:O	1:A:441:TYR:C	2.62	0.40
1:A:514:PHE:CD1	1:A:514:PHE:N	2.89	0.40
1:B:35:PHE:CE2	1:B:207:ALA:HB2	2.56	0.40
1:B:351:ALA:O	1:B:352:HIS:C	2.65	0.40
1:B:381:GLU:O	1:B:382:LYS:C	2.65	0.40
2:C:67:GLU:OE2	2:C:73:LYS:NZ	2.54	0.40
2:C:116:VAL:O	2:C:117:ALA:C	2.62	0.40
2:C:190:PHE:CE1	2:D:204:GLU:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:236:PHE:CD1	2:D:166:LYS:HB2	2.56	0.40
2:D:356:ILE:HG23	2:D:357:ILE:H	1.87	0.40

All (5) 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:A:499:GLU:OE1	2:D:345:TYR:OH[3_555]	1.57	0.63
1:A:507:SER:OG	2:C:279:ASP:OD1[3_555]	1.61	0.59
2:D:295:GLU:OE2	2:D:398:ASP:OD1[2_455]	1.84	0.36
1:A:520:HIS:NE2	2:D:104:THR:OG1[3_555]	2.09	0.11
2:C:135:GLN:NE2	2:C:401:LYS:N[3_445]	2.18	0.02

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	548/568 (96%)	528 (96%)	15 (3%)	5 (1%)	14	43
1	B	557/568 (98%)	548 (98%)	7 (1%)	2 (0%)	30	60
2	C	413/415 (100%)	398 (96%)	13 (3%)	2 (0%)	24	55
2	D	413/415 (100%)	391 (95%)	14 (3%)	8 (2%)	6	28
All	All	1931/1966 (98%)	1865 (97%)	49 (2%)	17 (1%)	14	43

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	200	PRO
2	D	200	PRO
1	A	69	THR
1	A	570	SER

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Mol	Chain	Res	Type
2	D	231	GLY
1	B	366	VAL
2	C	324	PRO
2	D	106	PRO
1	A	225	PRO
1	A	366	VAL
1	B	225	PRO
2	D	130	PRO
2	D	324	PRO
2	D	26	ASN
1	A	138	PRO
2	D	138	PRO
2	D	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/498 (97%)	366 (76%)	119 (24%)	1	3
1	B	494/498 (99%)	385 (78%)	109 (22%)	1	5
2	C	337/337 (100%)	261 (77%)	76 (23%)	1	5
2	D	337/337 (100%)	258 (77%)	79 (23%)	1	4
All	All	1653/1670 (99%)	1270 (77%)	383 (23%)	1	4

All (383) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	GLU
1	A	7	LEU
1	A	12	THR
1	A	20	GLN
1	A	23	ARG
1	A	29	SER
1	A	49	ASN

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Mol	Chain	Res	Type
1	A	53	LEU
1	A	54	TYR
1	A	60	LEU
1	A	66	ARG
1	A	77	GLU
1	A	79	LEU
1	A	81	ARG
1	A	82	VAL
1	A	83	LYS
1	A	84	GLU
1	A	87	THR
1	A	89	LEU
1	A	96	PHE
1	A	97	GLU
1	A	101	SER
1	A	104	ASN
1	A	109	ARG
1	A	110	LEU
1	A	117	THR
1	A	119	GLU
1	A	121	LEU
1	A	127	GLN
1	A	139	LEU
1	A	142	ASP
1	A	143	PHE
1	A	152	LEU
1	A	158	SER
1	A	167	GLN
1	A	169	LYS
1	A	170	SER
1	A	171	ARG
1	A	172	ASP
1	A	173	ILE
1	A	176	ILE
1	A	177	ILE
1	A	179	HIS
1	A	180	LEU
1	A	181	THR
1	A	191	LYS
1	A	192	SER
1	A	204	ASN
1	A	209	LEU

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Mol	Chain	Res	Type
1	A	215	THR
1	A	220	LEU
1	A	223	LEU
1	A	230	ASP
1	A	231	ASP
1	A	234	LEU
1	A	240	LEU
1	A	242	THR
1	A	247	SER
1	A	254	ARG
1	A	255	SER
1	A	258	MET
1	A	272	ARG
1	A	282	GLU
1	A	295	THR
1	A	297	SER
1	A	311	GLN
1	A	323	MET
1	A	331	PHE
1	A	332	ASP
1	A	335	PHE
1	A	345	GLN
1	A	347	GLU
1	A	349	SER
1	A	356	CYS
1	A	366	VAL
1	A	371	ASP
1	A	380	LEU
1	A	382	LYS
1	A	386	SER
1	A	390	MET
1	A	392	LEU
1	A	396	GLU
1	A	403	ASP
1	A	404	LEU
1	A	406	GLU
1	A	411	ARG
1	A	413	LEU
1	A	430	GLU
1	A	434	LEU
1	A	435	ARG
1	A	441	TYR

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Mol	Chain	Res	Type
1	A	448	LEU
1	A	452	ASN
1	A	461	LYS
1	A	462	ASN
1	A	470	ARG
1	A	475	ASP
1	A	479	ILE
1	A	480	CYS
1	A	482	MET
1	A	484	GLU
1	A	506	TYR
1	A	507	SER
1	A	509	SER
1	A	516	GLU
1	A	525	ASP
1	A	527	ARG
1	A	528	ILE
1	A	535	MET
1	A	536	HIS
1	A	546	ARG
1	A	549	GLN
1	A	550	ASN
1	A	551	ARG
1	A	561	TYR
1	A	567	GLN
1	A	568	ARG
1	A	571	VAL
1	B	5	LEU
1	B	6	GLU
1	B	7	LEU
1	B	8	LEU
1	B	11	GLN
1	B	20	GLN
1	B	34	ARG
1	B	54	TYR
1	B	60	LEU
1	B	80	LEU
1	B	87	THR
1	B	89	LEU
1	B	97	GLU
1	B	100	GLU
1	B	107	TYR

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Mol	Chain	Res	Type
1	B	109	ARG
1	B	110	LEU
1	B	115	SER
1	B	116	LEU
1	B	119	GLU
1	B	125	SER
1	B	127	GLN
1	B	130	ARG
1	B	131	ARG
1	B	139	LEU
1	B	146	ASP
1	B	147	HIS
1	B	152	LEU
1	B	155	ARG
1	B	158	SER
1	B	159	ASP
1	B	160	LEU
1	B	164	LEU
1	B	168	ASN
1	B	172	ASP
1	B	173	ILE
1	B	174	HIS
1	B	177	ILE
1	B	180	LEU
1	B	181	THR
1	B	182	GLU
1	B	183	THR
1	B	187	GLU
1	B	189	LEU
1	B	192	SER
1	B	194	LEU
1	B	200	LEU
1	B	209	LEU
1	B	213	LEU
1	B	220	LEU
1	B	222	PHE
1	B	229	THR
1	B	230	ASP
1	B	234	LEU
1	B	242	THR
1	B	254	ARG
1	B	255	SER

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Mol	Chain	Res	Type
1	B	257	PHE
1	B	263	LEU
1	B	287	ILE
1	B	294	LYS
1	B	297	SER
1	B	301	TYR
1	B	302	LEU
1	B	305	LEU
1	B	306	GLN
1	B	309	ASN
1	B	314	GLU
1	B	328	LEU
1	B	332	ASP
1	B	335	PHE
1	B	346	LYS
1	B	347	GLU
1	B	348	MET
1	B	354	ARG
1	B	361	LYS
1	B	371	ASP
1	B	374	GLU
1	B	389	LEU
1	B	396	GLU
1	B	401	ILE
1	B	404	LEU
1	B	418	ARG
1	B	419	MET
1	B	428	GLN
1	B	435	ARG
1	B	436	ASP
1	B	441	TYR
1	B	452	ASN
1	B	458	MET
1	B	461	LYS
1	B	462	ASN
1	B	466	THR
1	B	474	TYR
1	B	475	ASP
1	B	506	TYR
1	B	509	SER
1	B	516	GLU
1	B	519	ARG

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Mol	Chain	Res	Type
1	B	527	ARG
1	B	531	LEU
1	B	532	PHE
1	B	546	ARG
1	B	549	GLN
1	B	564	ARG
1	B	565	ARG
1	B	566	ARG
1	B	568	ARG
1	B	569	PHE
2	C	3	SER
2	C	16	LEU
2	C	17	GLN
2	C	26	ASN
2	C	35	ASP
2	C	41	VAL
2	C	45	MET
2	C	46	LEU
2	C	50	ASP
2	C	55	LYS
2	C	61	ARG
2	C	62	LYS
2	C	66	MET
2	C	69	TYR
2	C	74	SER
2	C	81	ASP
2	C	84	LEU
2	C	107	VAL
2	C	111	ILE
2	C	112	ARG
2	C	114	LEU
2	C	119	ARG
2	C	122	LEU
2	C	124	LEU
2	C	127	CYS
2	C	139	SER
2	C	145	GLU
2	C	154	GLU
2	C	164	GLU
2	C	171	ASP
2	C	173	GLU
2	C	177	LYS

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Mol	Chain	Res	Type
2	C	178	PHE
2	C	179	LEU
2	C	180	ARG
2	C	182	GLU
2	C	183	MET
2	C	187	LYS
2	C	194	CYS
2	C	204	GLU
2	C	209	LEU
2	C	222	ARG
2	C	230	LYS
2	C	237	THR
2	C	242	LYS
2	C	247	GLN
2	C	248	LEU
2	C	257	LEU
2	C	259	ASP
2	C	264	LEU
2	C	265	LYS
2	C	267	LYS
2	C	268	ASN
2	C	271	THR
2	C	273	LYS
2	C	295	GLU
2	C	297	ASP
2	C	299	ILE
2	C	302	MET
2	C	310	SER
2	C	320	ILE
2	C	334	LEU
2	C	341	THR
2	C	344	LYS
2	C	352	ASN
2	C	366	HIS
2	C	377	VAL
2	C	390	THR
2	C	394	GLU
2	C	397	MET
2	C	401	LYS
2	C	402	LEU
2	C	406	SER
2	C	410	ASP

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Mol	Chain	Res	Type
2	C	413	ILE
2	C	414	GLU
2	D	3	SER
2	D	13	LYS
2	D	15	THR
2	D	16	LEU
2	D	17	GLN
2	D	20	LYS
2	D	25	GLU
2	D	33	GLU
2	D	37	ILE
2	D	39	VAL
2	D	41	VAL
2	D	45	MET
2	D	55	LYS
2	D	60	GLU
2	D	61	ARG
2	D	74	SER
2	D	84	LEU
2	D	112	ARG
2	D	114	LEU
2	D	119	ARG
2	D	122	LEU
2	D	124	LEU
2	D	125	TYR
2	D	127	CYS
2	D	128	LEU
2	D	129	ARG
2	D	132	ARG
2	D	145	GLU
2	D	153	ARG
2	D	154	GLU
2	D	164	GLU
2	D	179	LEU
2	D	182	GLU
2	D	183	MET
2	D	194	CYS
2	D	199	LYS
2	D	202	SER
2	D	204	GLU
2	D	208	ARG
2	D	209	LEU

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Mol	Chain	Res	Type
2	D	215	GLU
2	D	218	ILE
2	D	220	ASN
2	D	227	LEU
2	D	233	ILE
2	D	237	THR
2	D	238	GLU
2	D	242	LYS
2	D	244	TRP
2	D	248	LEU
2	D	250	ARG
2	D	257	LEU
2	D	263	TRP
2	D	264	LEU
2	D	265	LYS
2	D	267	LYS
2	D	273	LYS
2	D	277	ILE
2	D	290	LEU
2	D	291	LEU
2	D	297	ASP
2	D	299	ILE
2	D	303	ASN
2	D	317	VAL
2	D	330	ASP
2	D	331	GLU
2	D	341	THR
2	D	351	VAL
2	D	355	SER
2	D	356	ILE
2	D	362	MET
2	D	367	MET
2	D	370	THR
2	D	371	GLU
2	D	384	ILE
2	D	387	LYS
2	D	392	ASP
2	D	397	MET
2	D	412	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	56	HIS
1	A	57	HIS
1	A	64	GLN
1	A	85	HIS
1	A	204	ASN
1	A	311	GLN
1	A	373	GLN
1	A	452	ASN
1	A	462	ASN
1	A	468	HIS
1	A	536	HIS
1	A	549	GLN
1	A	556	HIS
1	A	567	GLN
1	B	70	ASN
1	B	85	HIS
1	B	127	GLN
1	B	227	HIS
1	B	228	GLN
1	B	373	GLN
1	B	412	HIS
1	B	462	ASN
1	B	549	GLN
2	C	76	GLN
2	C	80	GLN
2	C	143	HIS
2	C	287	GLN
2	C	288	GLN
2	C	303	ASN
2	D	143	HIS
2	D	247	GLN
2	D	288	GLN
2	D	303	ASN
2	D	339	HIS
2	D	415	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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$
4	ADP	A	602	-	28,29,29	1.76	4 (14%)	43,45,45	1.89	13 (30%)
3	AMP	B	602	-	25,25,25	1.42	5 (20%)	37,38,38	1.83	10 (27%)
4	ADP	B	601	-	28,29,29	1.97	6 (21%)	43,45,45	2.62	21 (48%)
3	AMP	A	601	-	25,25,25	1.34	4 (16%)	37,38,38	2.04	8 (21%)

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
4	ADP	A	602	-	-	6/16/32/32	0/3/3/3
3	AMP	B	602	-	-	4/10/26/26	0/3/3/3
4	ADP	B	601	-	-	6/16/32/32	0/3/3/3
3	AMP	A	601	-	-	0/10/26/26	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	ADP	PA-O3A	5.52	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	ADP	PA-O3A	5.37	1.65	1.59
4	B	601	ADP	C5-C4	4.91	1.47	1.39
3	B	602	AMP	C5-C4	4.29	1.46	1.39
4	A	602	ADP	C5-C4	4.24	1.46	1.39
4	B	601	ADP	C5-N7	-3.76	1.32	1.39
3	A	601	AMP	C5-C4	3.44	1.45	1.39
3	A	601	AMP	C5-N7	-3.27	1.33	1.39
4	A	602	ADP	C5-N7	-3.12	1.33	1.39
3	B	602	AMP	C4-N9	-2.74	1.32	1.37
3	B	602	AMP	C5-N7	-2.58	1.34	1.39
4	B	601	ADP	C8-N9	-2.44	1.33	1.37
4	B	601	ADP	C8-N7	2.38	1.36	1.31
4	B	601	ADP	C5-C6	2.34	1.47	1.41
4	A	602	ADP	C4-N9	-2.28	1.32	1.37
3	A	601	AMP	C4-N9	-2.26	1.33	1.37
3	B	602	AMP	C5-C6	2.25	1.47	1.41
3	B	602	AMP	C8-N7	2.18	1.35	1.31
3	A	601	AMP	C8-N7	2.08	1.35	1.31

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	ADP	C5-C4-N3	-7.78	116.00	126.72
4	B	601	ADP	N3-C4-N9	5.92	137.24	127.17
3	A	601	AMP	C5-C4-N3	-5.86	118.64	126.72
4	B	601	ADP	O3B-PB-O3A	-5.50	86.18	104.64
4	A	602	ADP	C5-C4-N3	-4.69	120.26	126.72
4	A	602	ADP	N3-C4-N9	4.54	134.89	127.17
3	B	602	AMP	C5-C4-N3	-4.53	120.48	126.72
3	A	601	AMP	N3-C4-N9	4.35	134.57	127.17
3	A	601	AMP	C2-N3-C4	4.04	121.69	111.83
3	B	602	AMP	N3-C4-N9	4.01	133.99	127.17
4	B	601	ADP	C2-N3-C4	3.99	121.58	111.83
3	A	601	AMP	N3-C2-N1	-3.97	122.57	128.58
4	B	601	ADP	C4-C5-N7	-3.87	106.15	110.58
4	B	601	ADP	O3A-PA-O1A	-3.66	99.69	110.70
4	A	602	ADP	C4-N9-C8	3.59	109.51	105.74
3	B	602	AMP	C4-N9-C8	3.53	109.45	105.74
4	B	601	ADP	O3B-PB-O1B	3.49	124.42	110.83
4	A	602	ADP	O3B-PB-O1B	3.38	124.00	110.83
3	A	601	AMP	O4'-C1'-N9	3.31	114.44	108.09
4	B	601	ADP	N3-C2-N1	-3.15	123.81	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	AMP	C2-N3-C4	3.09	119.37	111.83
4	B	601	ADP	C2'-C1'-N9	-3.02	105.80	113.30
4	B	601	ADP	C2'-C3'-C4'	3.02	108.44	102.61
4	A	602	ADP	N3-C2-N1	-3.00	124.04	128.58
4	B	601	ADP	C5-N7-C8	2.90	108.00	103.45
4	B	601	ADP	O5'-C5'-C4'	2.86	118.73	108.99
3	A	601	AMP	C4-C5-N7	-2.85	107.33	110.58
3	B	602	AMP	N3-C2-N1	-2.84	124.28	128.58
4	A	602	ADP	C2-N3-C4	2.74	118.53	111.83
4	B	601	ADP	C1'-N9-C8	-2.68	121.14	127.09
4	A	602	ADP	N6-C6-N1	2.58	124.13	118.38
3	B	602	AMP	C4-C5-N7	-2.56	107.66	110.58
3	B	602	AMP	O3P-P-O2P	2.54	117.34	107.80
4	B	601	ADP	C6-C5-C4	2.45	120.52	117.18
4	B	601	ADP	O2B-PB-O3A	2.42	112.74	104.64
4	A	602	ADP	O4'-C1'-N9	2.40	112.69	108.09
4	A	602	ADP	C4-C5-N7	-2.31	107.94	110.58
4	B	601	ADP	C4'-O4'-C1'	2.30	114.55	109.47
4	A	602	ADP	N9-C8-N7	-2.30	110.67	113.94
3	A	601	AMP	C5-N7-C8	2.29	107.06	103.45
4	A	602	ADP	C2-N1-C6	2.28	122.48	118.73
4	B	601	ADP	O2B-PB-O1B	-2.28	101.96	110.83
4	A	602	ADP	C5-N7-C8	2.28	107.03	103.45
3	B	602	AMP	N9-C8-N7	-2.26	110.72	113.94
3	A	601	AMP	C2'-C1'-N9	-2.26	107.68	113.30
4	B	601	ADP	N6-C6-N1	2.24	123.36	118.38
4	A	602	ADP	O5'-PA-O1A	-2.20	100.20	108.94
3	B	602	AMP	O3P-P-O5'	-2.19	100.96	106.67
4	B	601	ADP	O4'-C4'-C5'	2.16	116.26	109.33
4	B	601	ADP	C4-N9-C1'	2.15	131.66	126.63
4	B	601	ADP	C3'-C2'-C1'	2.03	105.31	101.46
3	B	602	AMP	C5-N7-C8	2.02	106.62	103.45

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	AMP	C5'-O5'-P-O2P
3	B	602	AMP	C5'-O5'-P-O3P
4	A	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	O4'-C4'-C5'-O5'
4	B	601	ADP	PA-O3A-PB-O2B

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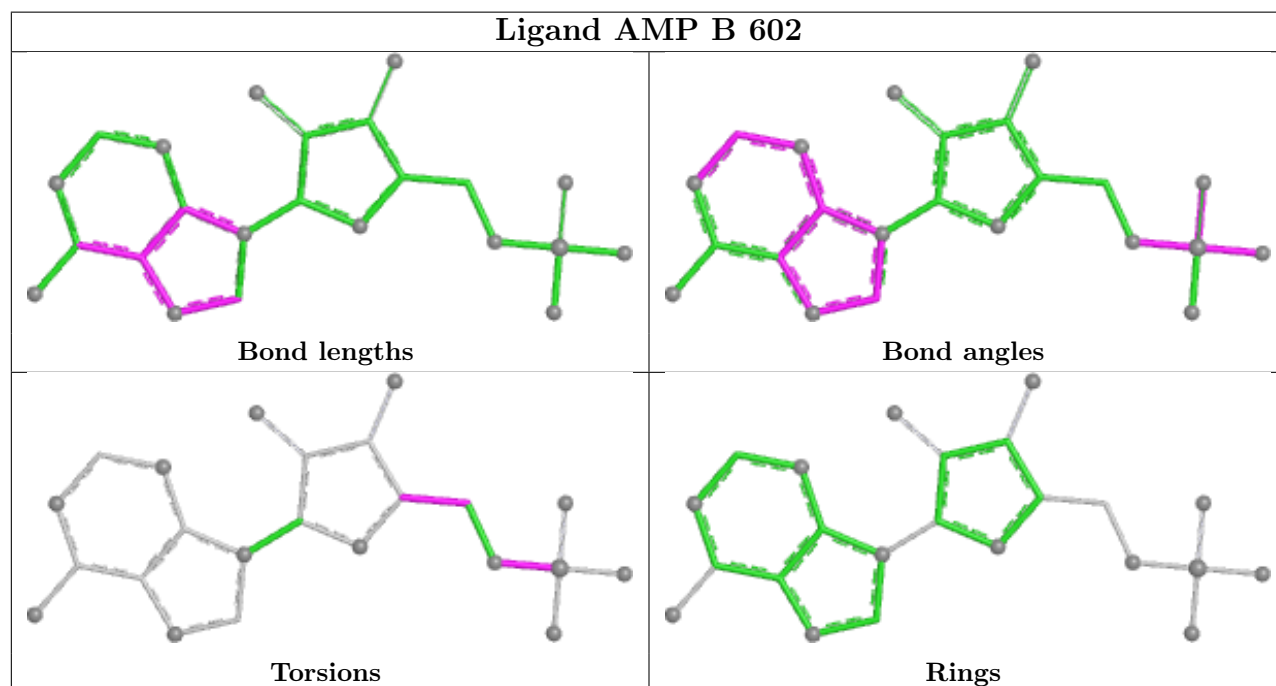
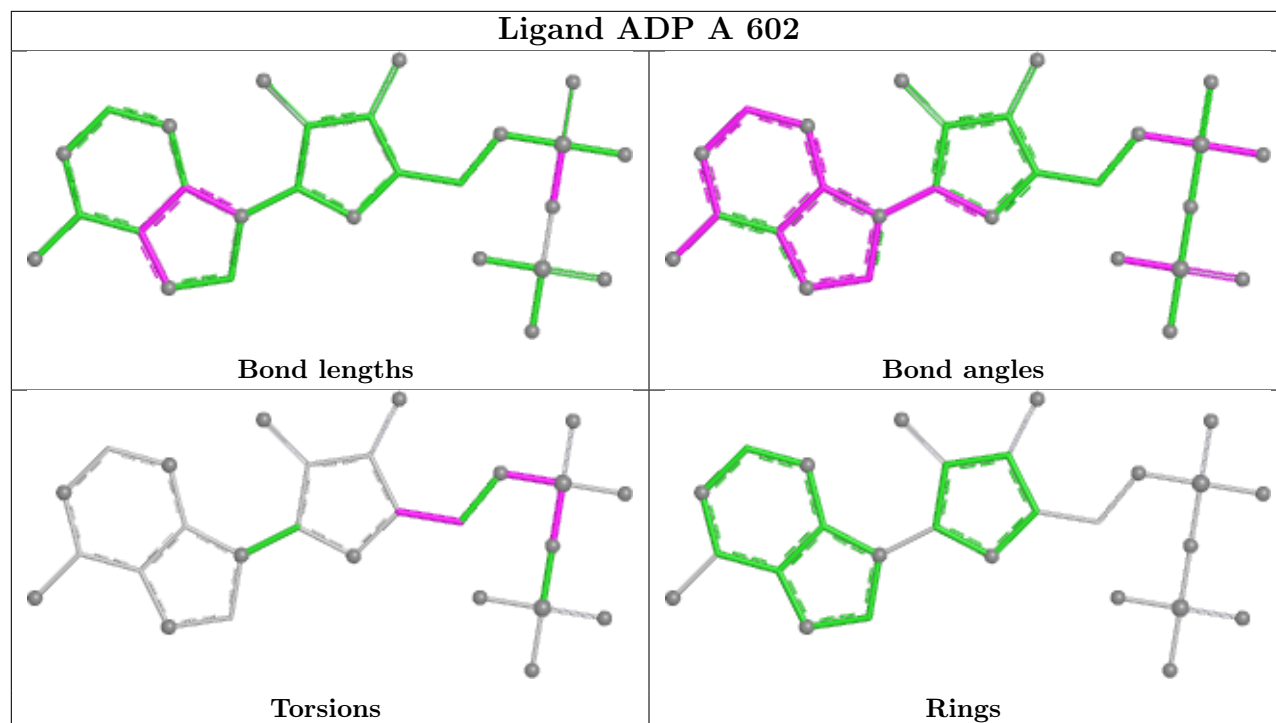
Mol	Chain	Res	Type	Atoms
4	A	602	ADP	C3'-C4'-C5'-O5'
4	B	601	ADP	C4'-C5'-O5'-PA
4	B	601	ADP	C3'-C4'-C5'-O5'
4	A	602	ADP	C5'-O5'-PA-O2A
4	A	602	ADP	C5'-O5'-PA-O3A
3	B	602	AMP	O4'-C4'-C5'-O5'
4	B	601	ADP	PB-O3A-PA-O1A
3	B	602	AMP	C5'-O5'-P-O1P
4	B	601	ADP	PA-O3A-PB-O1B
4	A	602	ADP	PB-O3A-PA-O2A
4	B	601	ADP	PB-O3A-PA-O2A

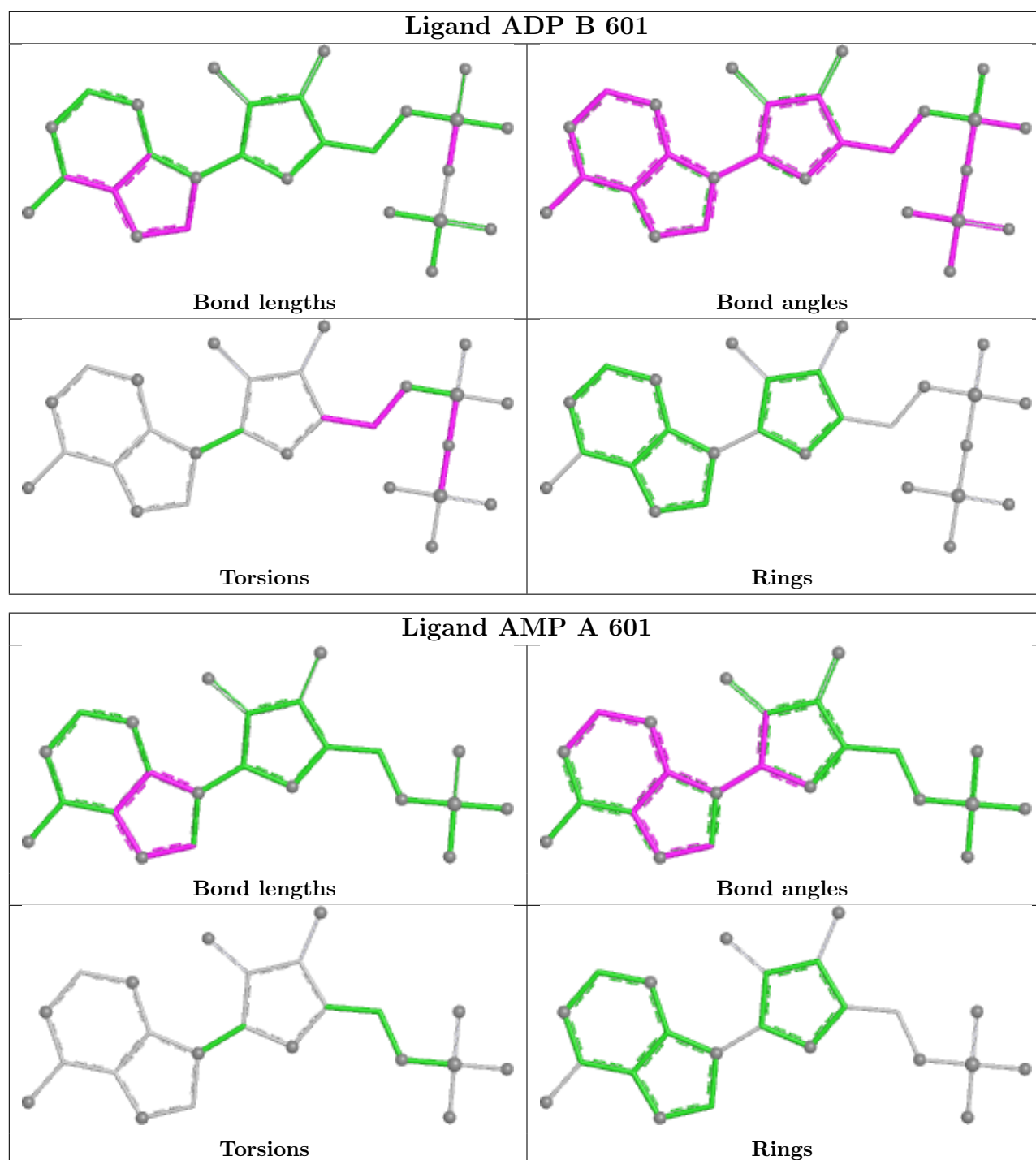
There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ADP	7	0
3	B	602	AMP	7	0
4	B	601	ADP	7	0
3	A	601	AMP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	554/568 (97%)	0.39	11 (1%) 65 46	56, 86, 119, 145	0
1	B	561/568 (98%)	0.34	12 (2%) 63 44	58, 83, 117, 151	0
2	C	415/415 (100%)	0.18	1 (0%) 91 86	46, 69, 97, 123	0
2	D	415/415 (100%)	0.23	5 (1%) 76 58	56, 76, 99, 123	0
All	All	1945/1966 (98%)	0.30	29 (1%) 72 53	46, 80, 111, 151	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	GLY	3.4
1	B	477	ALA	3.4
1	B	93	TYR	3.3
1	A	279	THR	3.0
1	A	381	GLU	2.9
1	A	229	THR	2.8
1	B	238	THR	2.6
1	B	569	PHE	2.6
1	A	38	ALA	2.5
1	A	69	THR	2.5
1	B	217	SER	2.4
2	D	178	PHE	2.3
1	B	156	VAL	2.3
2	D	154	GLU	2.3
1	B	227	HIS	2.2
1	A	170	SER	2.2
2	D	21	LEU	2.2
1	A	169	LYS	2.2
2	C	71	GLY	2.2
1	A	322	VAL	2.2
2	D	296	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	87	THR	2.1
2	D	125	TYR	2.1
1	A	475	ASP	2.1
1	B	237	ASP	2.1
1	B	457	ASP	2.1
1	A	469	GLY	2.1
1	B	556	HIS	2.0
1	A	189	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

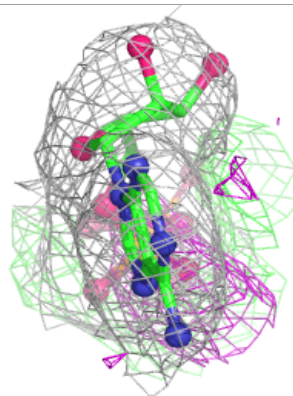
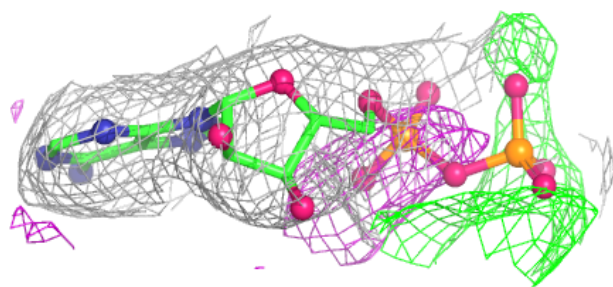
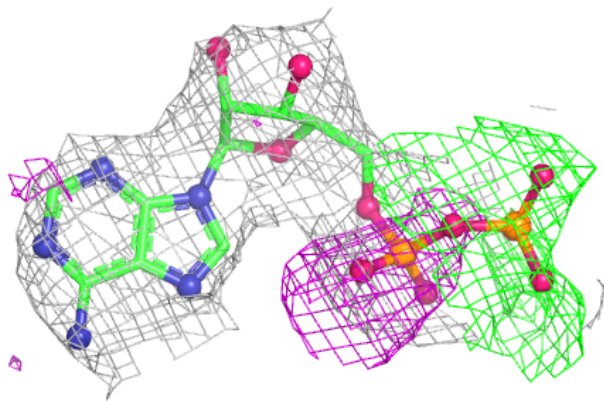
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	A	602	27/27	0.87	0.13	57,78,84,96	0
4	ADP	B	601	27/27	0.91	0.11	63,69,79,93	0
3	AMP	A	601	23/23	0.96	0.10	71,82,87,88	0
3	AMP	B	602	23/23	0.97	0.08	68,76,81,85	0

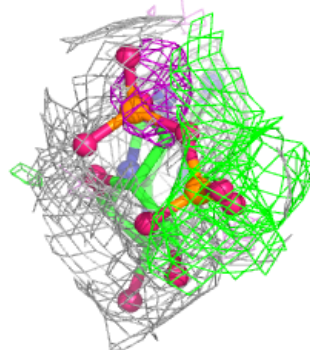
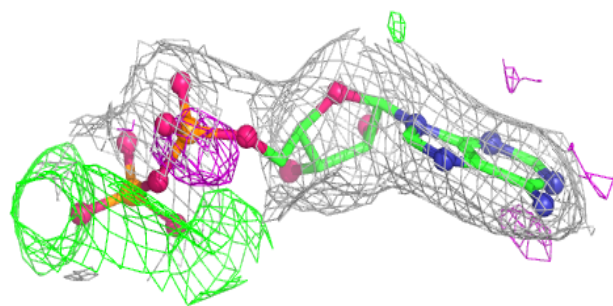
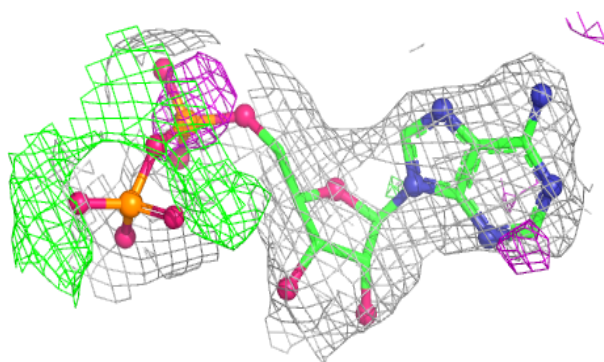
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 602:

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

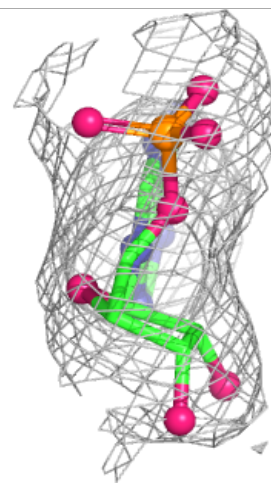
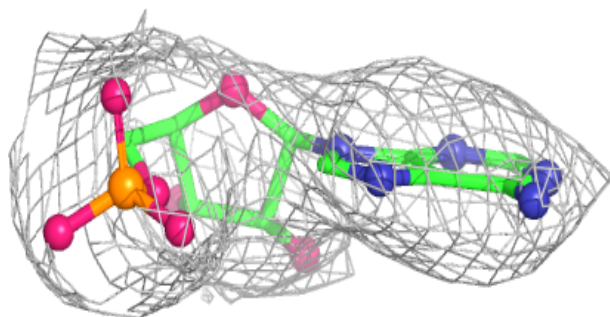
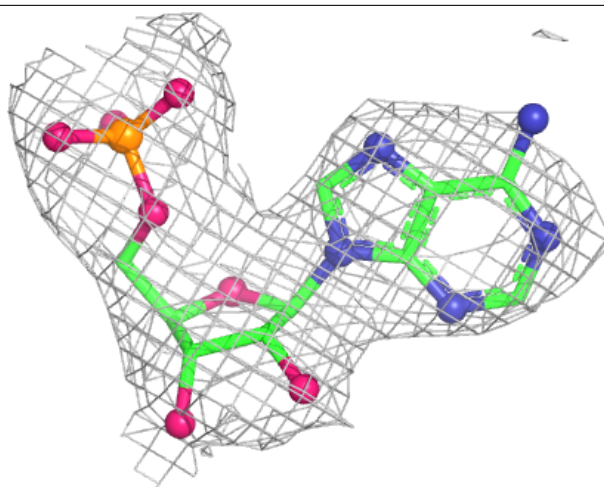
**Electron density around ADP B 601:**

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



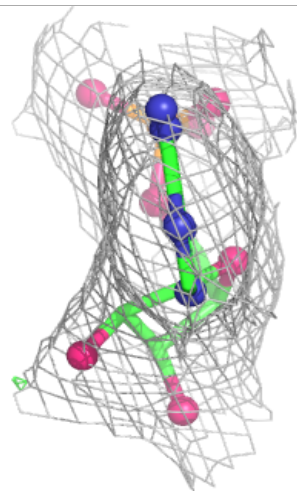
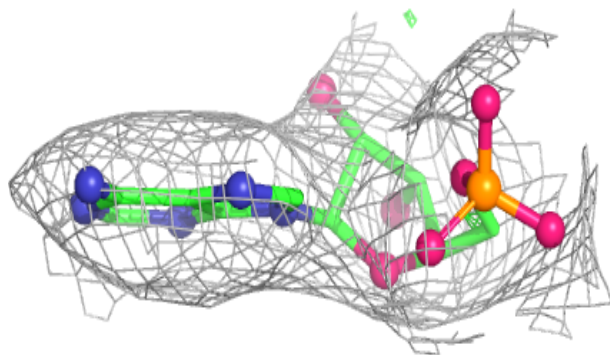
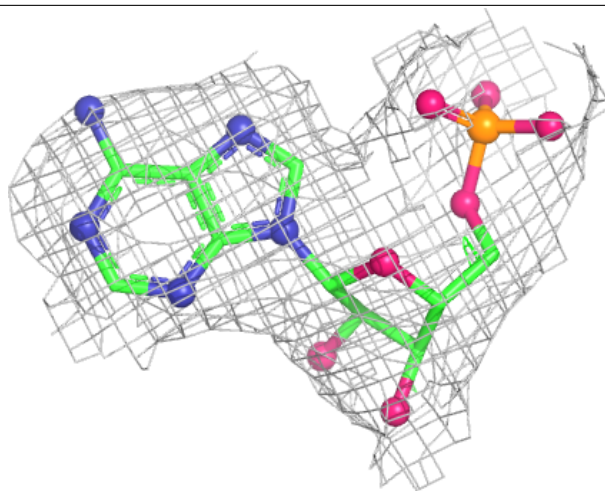
Electron density around AMP A 601:

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



Electron density around AMP B 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.