



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:00 PM UTC

PDB ID : 3J82 / pdb_00003j82
EMDB ID : EMD-6102
Title : Electron cryo-microscopy of DNCR-1 in complex with F-actin
Authors : Hanc, P.; Fujii, T.; Yamada, Y.; Huotari, J.; Schulz, O.; Ahrens, S.; Kjaer, S.;
Way, M.; Namba, K.; Reis e Sousa, C.
Deposited on : 2014-09-25
Resolution : 7.70 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

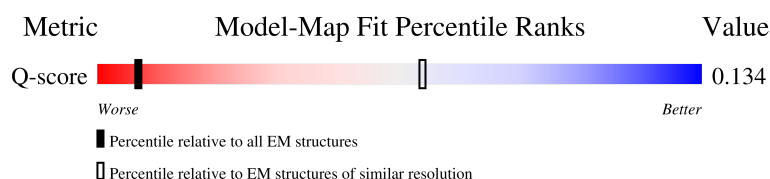
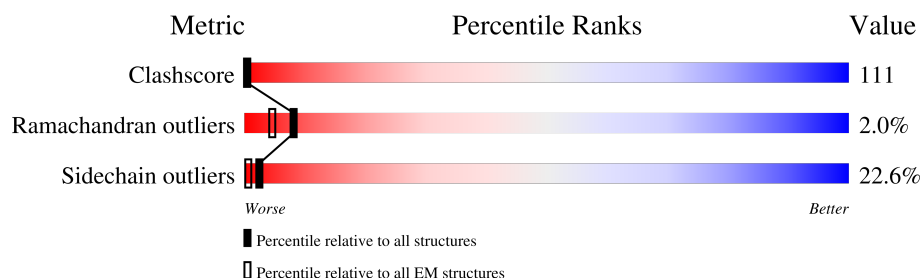
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	384 (7.20 - 8.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	131	58% 29% 53% 16%
2	B	374	7% 17% 55% 25%
2	C	374	7% 18% 55% 24%
2	D	374	8% 18% 58% 21%

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
2	HIC	C	73	-	-	X	-
4	ADP	D	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 C-type lectin domain family 9 member A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	131	Total	C	N	O	S	0	0
			1050	672	171	197	10		

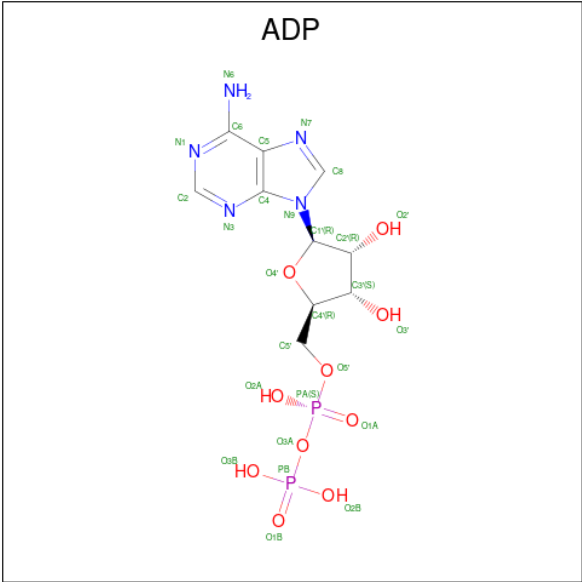
- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	374	Total	C	N	O	S	0	0
			2917	1846	490	559	22		
2	C	374	Total	C	N	O	S	0	0
			2917	1846	490	559	22		
2	D	374	Total	C	N	O	S	0	0
			2918	1846	490	560	22		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	

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

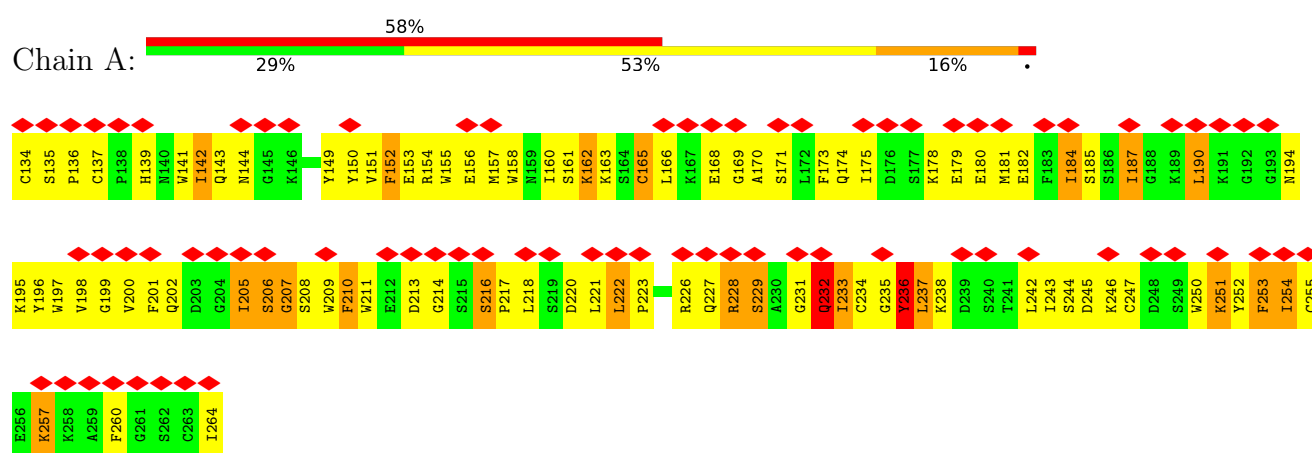


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

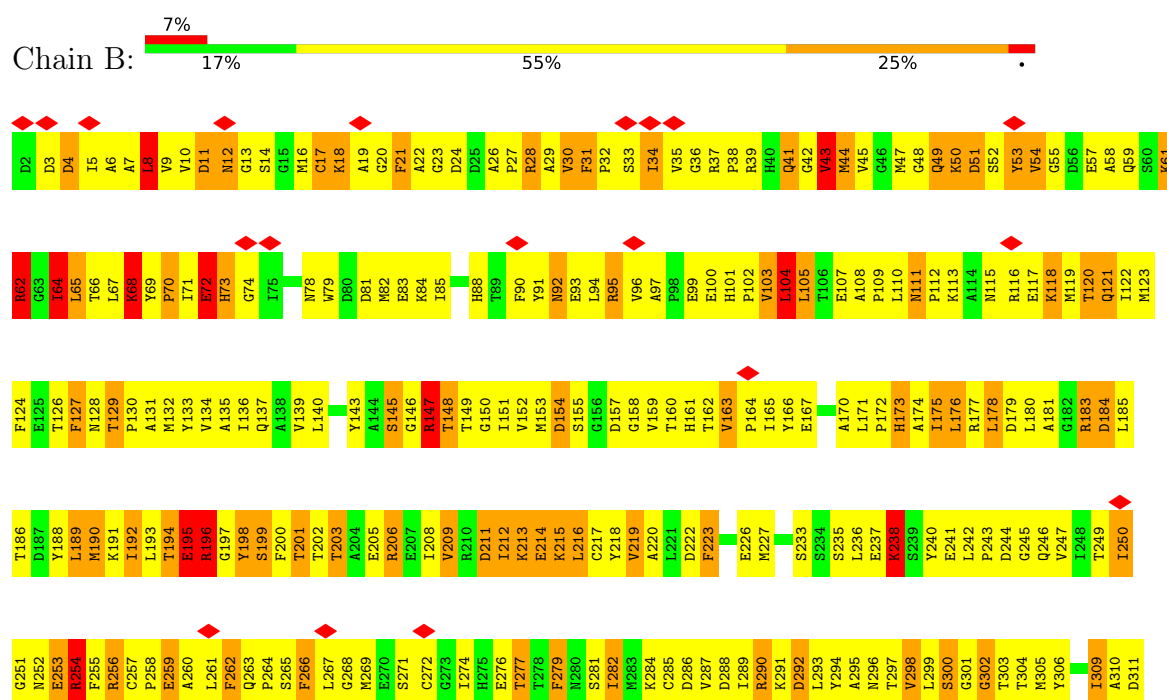
3 Residue-property plots

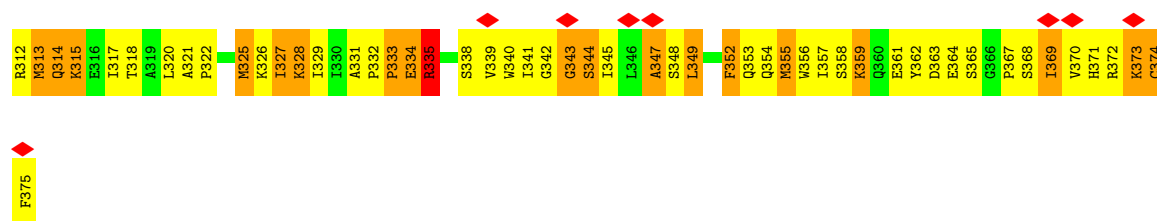
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: C-type lectin domain family 9 member A

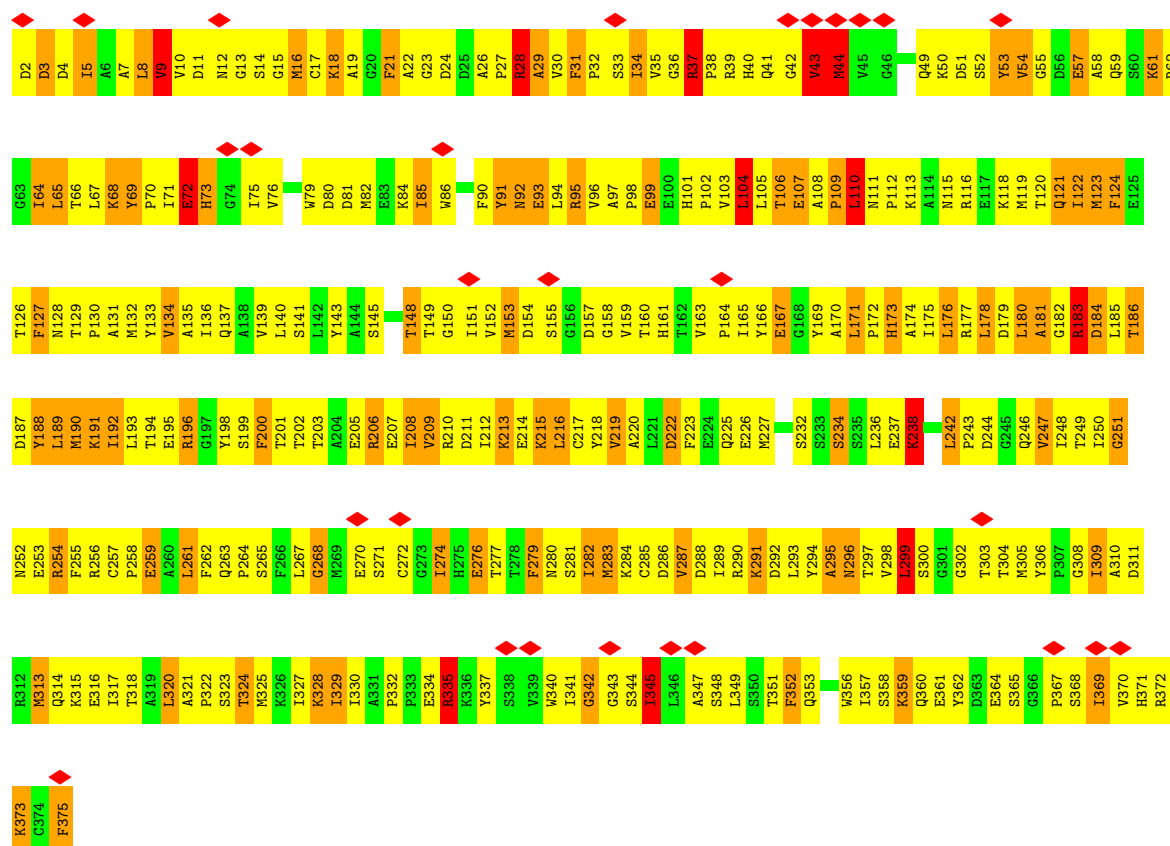
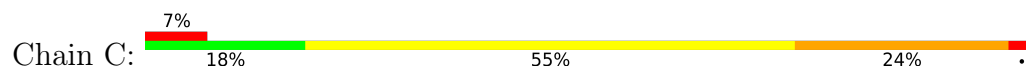


• Molecule 2: Actin, cytoplasmic 1

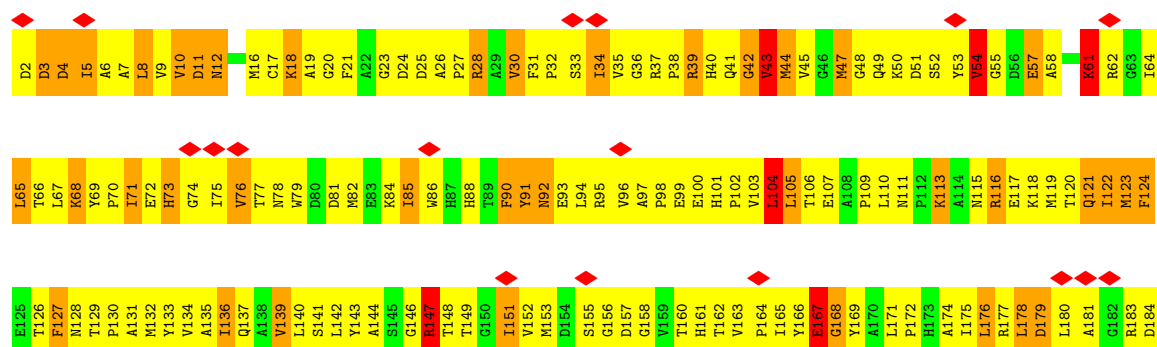


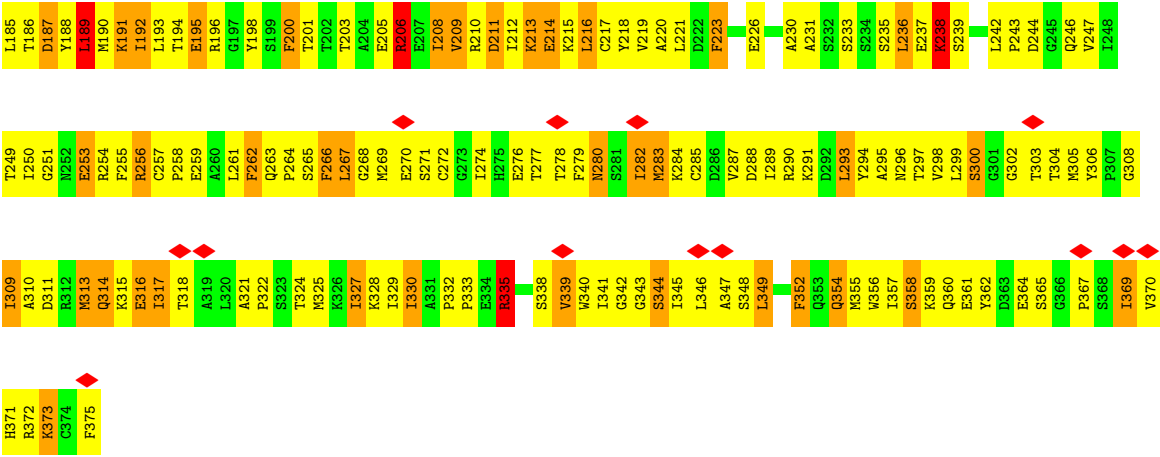


• Molecule 2: Actin, cytoplasmic 1



• Molecule 2: Actin, cytoplasmic 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=166.6°, rise=27.6 Å, axial sym=C1	Depositor
Number of particles used	73608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each Particle	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	109489	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	5.365	Depositor
Minimum map value	-4.137	Depositor
Average map value	0.157	Depositor
Map value standard deviation	0.677	Depositor
Recommended contour level	0.838	Depositor
Map size (Å)	137.0, 137.0, 137.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HIC, CA, 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	1.26	0/1080	1.57	13/1451 (0.9%)
2	B	1.43	2/2967 (0.1%)	1.77	57/4017 (1.4%)
2	C	1.43	3/2967 (0.1%)	1.77	52/4017 (1.3%)
2	D	1.41	2/2968 (0.1%)	1.74	46/4017 (1.1%)
All	All	1.41	7/9982 (0.1%)	1.74	168/13502 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	11
2	C	0	6
2	D	0	3
All	All	0	21

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	343	GLY	CA-C	-5.43	1.46	1.52
2	C	110	LEU	CA-C	-5.33	1.47	1.53
2	C	104	LEU	CA-C	-5.30	1.46	1.52
2	D	54	VAL	CA-CB	-5.26	1.47	1.54
2	C	335	ARG	NE-CZ	5.14	1.38	1.33
2	D	335	ARG	NE-CZ	5.12	1.38	1.33
2	B	335	ARG	NE-CZ	5.08	1.38	1.33

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	262	PHE	CA-CB-CG	-13.47	100.33	113.80
2	B	127	PHE	CA-CB-CG	-11.73	102.07	113.80
2	C	127	PHE	CA-CB-CG	-11.59	102.21	113.80
2	D	127	PHE	CA-CB-CG	-11.05	102.75	113.80
2	C	352	PHE	CA-CB-CG	-10.81	102.99	113.80
2	D	124	PHE	CA-CB-CG	-9.97	103.83	113.80
2	D	352	PHE	CA-CB-CG	-9.46	104.34	113.80
2	C	167	GLU	CB-CG-CD	-9.12	97.09	112.60
2	B	12	ASN	CA-CB-CG	-8.87	103.73	112.60
2	B	352	PHE	CA-CB-CG	-8.85	104.95	113.80
2	D	262	PHE	CA-CB-CG	-8.81	104.99	113.80
2	B	277	THR	CA-CB-CG2	-8.68	95.74	110.50
2	C	124	PHE	CA-CB-CG	-8.66	105.14	113.80
2	D	187	ASP	CA-CB-CG	-8.66	103.94	112.60
2	C	184	ASP	CA-CB-CG	-8.64	103.96	112.60
2	C	262	PHE	CA-CB-CG	-8.47	105.33	113.80
2	B	51	ASP	CA-CB-CG	-8.45	104.15	112.60
2	B	184	ASP	CA-CB-CG	-8.30	104.30	112.60
2	D	12	ASN	CA-CB-CG	-8.08	104.52	112.60
2	D	168	GLY	N-CA-C	-7.97	105.90	114.67
2	B	334	GLU	CA-C-N	7.88	133.87	120.72
2	B	334	GLU	C-N-CA	7.88	133.87	120.72
2	B	333	PRO	CA-C-N	-7.86	109.96	122.76
2	B	333	PRO	C-N-CA	-7.86	109.96	122.76
2	D	25	ASP	CA-CB-CG	-7.83	104.77	112.60
2	B	173	HIS	CA-CB-CG	-7.47	106.33	113.80
2	B	90	PHE	CA-CB-CG	-7.47	106.33	113.80
2	C	109	PRO	CA-C-N	-7.44	112.82	122.79
2	C	109	PRO	C-N-CA	-7.44	112.82	122.79
2	C	295	ALA	CA-C-N	-7.40	112.18	123.14
2	C	295	ALA	C-N-CA	-7.40	112.18	123.14
2	B	154	ASP	CA-CB-CG	-7.33	105.27	112.60
2	C	9	VAL	CA-C-N	7.09	134.73	121.97
2	C	9	VAL	C-N-CA	7.09	134.73	121.97
2	C	173	HIS	CA-CB-CG	-7.04	106.76	113.80
2	B	211	ASP	CA-CB-CG	-6.95	105.65	112.60
2	C	104	LEU	CB-CA-C	-6.93	96.91	109.38
2	C	183	ARG	CB-CA-C	-6.92	100.01	110.88
2	B	334	GLU	CB-CG-CD	-6.92	100.84	112.60
2	D	206	ARG	CB-CA-C	-6.87	100.00	110.92
1	A	253	PHE	CA-CB-CG	-6.84	106.96	113.80
2	B	23	GLY	N-CA-C	-6.77	106.41	115.21
2	C	2	ASP	CA-CB-CG	-6.76	105.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	147	ARG	CA-C-N	6.66	129.50	120.44
2	D	147	ARG	C-N-CA	6.66	129.50	120.44
1	A	169	GLY	N-CA-C	-6.63	105.92	115.27
2	C	268	GLY	N-CA-C	-6.58	106.03	115.64
2	D	90	PHE	CA-CB-CG	-6.58	107.22	113.80
2	B	198	TYR	CA-C-N	-6.57	112.91	122.44
2	B	198	TYR	C-N-CA	-6.57	112.91	122.44
2	D	42	GLY	CA-C-N	6.57	133.53	121.70
2	D	42	GLY	C-N-CA	6.57	133.53	121.70
2	B	91	TYR	CA-CB-CG	-6.54	102.12	113.90
2	C	92	ASN	CA-CB-CG	-6.54	106.06	112.60
2	C	3	ASP	CA-CB-CG	-6.49	106.11	112.60
2	C	252	ASN	N-CA-C	-6.43	104.36	111.82
2	D	167	GLU	CA-C-N	6.35	135.35	121.19
2	D	167	GLU	C-N-CA	6.35	135.35	121.19
2	D	23	GLY	N-CA-C	-6.35	107.14	114.69
2	B	363	ASP	CA-CB-CG	-6.31	106.29	112.60
1	A	260	PHE	CA-CB-CG	-6.26	107.54	113.80
2	C	375	PHE	CA-CB-CG	-6.24	107.56	113.80
2	B	53	TYR	CA-CB-CG	-6.21	102.73	113.90
2	C	296	ASN	CA-CB-CG	-6.21	106.39	112.60
2	C	208	ILE	CB-CA-C	-6.18	104.06	111.97
2	C	188	TYR	N-CA-C	-6.15	104.57	111.28
2	B	223	PHE	CA-CB-CG	-6.15	107.65	113.80
2	C	91	TYR	CA-CB-CG	-6.12	102.88	113.90
2	D	280	ASN	CA-CB-CG	-6.10	106.50	112.60
2	B	364	GLU	CB-CA-C	-6.09	101.51	110.95
2	B	21	PHE	CA-CB-CG	-6.04	107.76	113.80
2	D	211	ASP	CA-CB-CG	-6.01	106.59	112.60
2	C	37	ARG	N-CA-C	-5.99	101.25	108.14
2	B	41	GLN	CB-CA-C	-5.97	109.70	116.63
2	B	246	GLN	CA-C-N	-5.97	115.32	123.14
2	B	246	GLN	C-N-CA	-5.97	115.32	123.14
2	D	91	TYR	CA-CB-CG	-5.95	103.19	113.90
2	B	196	ARG	CD-NE-CZ	-5.93	116.10	124.40
2	D	146	GLY	CA-C-N	-5.92	114.05	122.94
2	D	146	GLY	C-N-CA	-5.92	114.05	122.94
2	D	339	VAL	CB-CA-C	-5.92	104.39	111.97
2	C	106	THR	CA-CB-CG2	-5.89	100.49	110.50
2	B	111	ASN	CA-CB-CG	-5.84	106.76	112.60
2	C	31	PHE	CA-CB-CG	-5.84	107.96	113.80
2	D	296	ASN	CA-CB-CG	-5.82	106.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	GLY	N-CA-C	-5.80	107.24	115.30
2	C	44	MET	N-CA-CB	5.80	120.29	110.49
2	D	168	GLY	CA-C-N	5.80	129.00	120.82
2	D	168	GLY	C-N-CA	5.80	129.00	120.82
2	C	23	GLY	N-CA-C	-5.79	107.80	114.69
1	A	236	TYR	CA-C-N	5.76	132.55	121.54
1	A	236	TYR	C-N-CA	5.76	132.55	121.54
2	C	69	TYR	CB-CA-C	-5.73	105.28	110.44
2	C	279	PHE	CA-CB-CG	-5.73	108.07	113.80
2	C	28	ARG	CB-CA-C	-5.70	102.17	110.96
2	B	104	LEU	CD1-CG-CD2	5.69	123.32	110.80
2	D	122	ILE	CB-CA-C	-5.65	104.73	111.97
1	A	210	PHE	CA-CB-CG	-5.65	108.15	113.80
2	D	104	LEU	CB-CA-C	-5.64	100.93	110.19
2	C	24	ASP	CA-CB-CG	-5.64	106.96	112.60
2	D	267	LEU	N-CA-CB	5.63	120.24	110.39
2	B	179	ASP	CA-CB-CG	-5.55	107.05	112.60
2	B	279	PHE	CA-CB-CG	-5.54	108.25	113.80
2	D	223	PHE	CA-CB-CG	-5.54	108.26	113.80
2	D	267	LEU	CB-CA-C	-5.53	98.89	110.17
2	C	299	LEU	N-CA-C	-5.52	100.88	109.72
2	B	344	SER	N-CA-C	-5.51	105.27	111.28
2	D	3	ASP	CA-CB-CG	-5.50	107.10	112.60
2	C	342	GLY	N-CA-C	-5.49	106.05	113.24
2	C	53	TYR	CA-CB-CG	-5.49	104.02	113.90
2	D	330	ILE	CA-C-N	-5.49	116.22	122.26
2	D	330	ILE	C-N-CA	-5.49	116.22	122.26
1	A	236	TYR	CA-CB-CG	-5.48	104.03	113.90
2	D	101	HIS	CA-C-N	5.48	125.38	119.85
2	D	101	HIS	C-N-CA	5.48	125.38	119.85
2	B	68	LYS	CA-C-N	-5.46	114.12	122.42
2	B	68	LYS	C-N-CA	-5.46	114.12	122.42
1	A	152	PHE	CA-CB-CG	-5.45	108.35	113.80
2	C	99	GLU	N-CA-C	-5.42	105.48	111.71
2	B	266	PHE	N-CA-C	-5.41	105.28	111.07
2	C	234	SER	N-CA-C	-5.40	105.56	111.82
2	C	222	ASP	CA-CB-CG	-5.40	107.20	112.60
2	C	345	ILE	CB-CA-C	-5.39	104.96	112.02
1	A	207	GLY	N-CA-C	-5.36	107.85	115.30
2	C	85	ILE	CB-CA-C	-5.35	105.12	111.97
2	D	266	PHE	N-CA-C	-5.34	105.36	111.07
2	D	200	PHE	CB-CA-C	-5.32	103.57	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	LEU	CA-C-N	-5.31	115.97	122.93
2	B	8	LEU	C-N-CA	-5.31	115.97	122.93
2	C	80	ASP	CA-CB-CG	-5.30	107.30	112.60
2	D	189	LEU	N-CA-C	-5.29	105.51	111.28
2	D	335	ARG	N-CA-C	5.29	118.99	112.54
2	B	335	ARG	N-CA-C	5.28	118.97	112.54
2	D	179	ASP	CA-CB-CG	-5.26	107.34	112.60
2	C	29	ALA	CA-C-N	-5.25	115.15	122.71
2	C	29	ALA	C-N-CA	-5.25	115.15	122.71
2	B	212	ILE	N-CA-C	-5.24	105.27	110.62
2	B	70	PRO	N-CA-C	-5.23	106.25	113.53
2	C	251	GLY	CA-C-N	-5.23	112.36	120.31
2	C	251	GLY	C-N-CA	-5.23	112.36	120.31
2	D	115	ASN	N-CA-CB	5.22	118.38	110.28
2	C	43	VAL	N-CA-CB	5.22	119.85	111.23
2	D	43	VAL	N-CA-C	-5.21	96.42	111.00
2	B	194	THR	N-CA-C	-5.20	106.03	112.38
2	B	31	PHE	CA-CB-CG	-5.20	108.60	113.80
2	C	51	ASP	CA-C-N	-5.16	115.08	122.67
2	C	51	ASP	C-N-CA	-5.16	115.08	122.67
2	B	83	GLU	N-CA-C	-5.16	105.66	111.28
2	B	339	VAL	CB-CA-C	-5.16	105.37	111.97
2	C	21	PHE	CA-CB-CG	-5.16	108.64	113.80
2	B	292	ASP	CA-CB-CG	-5.15	107.45	112.60
2	B	354	GLN	CA-C-N	5.15	127.18	120.28
2	B	354	GLN	C-N-CA	5.15	127.18	120.28
2	B	195	GLU	CA-C-N	-5.13	111.73	121.54
2	B	195	GLU	C-N-CA	-5.13	111.73	121.54
1	A	222	LEU	CA-C-N	5.09	125.09	120.21
1	A	222	LEU	C-N-CA	5.09	125.09	120.21
2	D	24	ASP	CA-CB-CG	-5.08	107.52	112.60
2	C	200	PHE	CB-CA-C	-5.07	104.20	111.70
2	B	104	LEU	CB-CA-C	-5.07	101.44	109.80
1	A	144	ASN	CA-CB-CG	-5.04	107.56	112.60
2	B	104	LEU	N-CA-CB	5.03	118.41	110.56
2	D	51	ASP	CA-C-N	-5.02	115.29	122.67
2	D	51	ASP	C-N-CA	-5.02	115.29	122.67
2	B	302	GLY	CA-C-N	5.01	129.91	121.14
2	B	302	GLY	C-N-CA	5.01	129.91	121.14
2	B	347	ALA	CB-CA-C	-5.01	102.48	110.79
1	A	257	LYS	CB-CA-C	-5.00	99.06	110.07

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	TYR	Peptide
2	B	147	ARG	Sidechain
2	B	183	ARG	Sidechain
2	B	196	ARG	Sidechain
2	B	197	GLY	Peptide
2	B	245	GLY	Peptide
2	B	254	ARG	Sidechain
2	B	301	GLY	Peptide
2	B	335	ARG	Sidechain
2	B	61	LYS	Peptide
2	B	62	ARG	Sidechain
2	B	64	ILE	Peptide
2	C	181	ALA	Peptide
2	C	232	SER	Peptide
2	C	335	ARG	Sidechain
2	C	37	ARG	Sidechain
2	C	61	LYS	Peptide
2	C	9	VAL	Peptide
2	D	167	GLU	Peptide
2	D	335	ARG	Sidechain
2	D	61	LYS	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	1050	0	1002	234	0
2	B	2917	0	2880	692	0
2	C	2917	0	2880	618	0
2	D	2918	0	2880	696	0
3	A	1	0	0	0	0
4	B	27	0	12	8	0
4	C	27	0	12	8	0
4	D	27	0	12	9	0
All	All	9884	0	9678	2181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 111.

All (2181) 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:C:73:HIC:HD2	2:C:183:ARG:NH1	1.50	1.26
2:D:300:SER:HA	2:D:335:ARG:HD3	1.25	1.18
2:B:61:LYS:HD2	2:B:64:ILE:HG21	1.26	1.17
2:D:178:LEU:HD12	2:D:180:LEU:H	1.12	1.14
2:C:189:LEU:HD12	2:C:209:VAL:HG22	1.28	1.14
2:B:216:LEU:HD21	2:B:254:ARG:HG2	1.27	1.14
2:C:8:LEU:HB2	2:C:103:VAL:HG22	1.26	1.13
2:B:253:GLU:HA	2:B:256:ARG:HG2	1.31	1.13
2:C:140:LEU:HD23	2:C:343:GLY:HA2	1.26	1.12
2:D:11:ASP:HB2	2:D:18:LYS:HD3	1.31	1.12
2:C:7:ALA:HB1	2:C:104:LEU:HD21	1.31	1.11
2:C:163:VAL:HG12	2:C:175:ILE:HG13	1.20	1.11
2:C:35:VAL:HG12	2:C:68:LYS:HB3	1.18	1.11
2:C:9:VAL:HG22	2:C:104:LEU:HD23	1.13	1.11
2:C:135:ALA:HB1	2:C:140:LEU:HD11	1.16	1.10
1:A:142:ILE:HD11	1:A:149:TYR:HB2	1.33	1.10
2:C:34:ILE:HG12	2:C:54:VAL:HG11	1.34	1.10
2:C:191:LYS:HE3	2:C:191:LYS:HA	1.30	1.10
2:B:34:ILE:HG13	2:B:67:LEU:HD22	1.22	1.08
2:C:190:MET:HE3	2:C:209:VAL:HG11	1.33	1.08
2:B:149:THR:HG22	2:B:166:TYR:HA	1.35	1.08
2:B:251:GLY:HA2	2:B:254:ARG:HD3	1.29	1.08
2:D:7:ALA:HB1	2:D:104:LEU:HD21	1.36	1.08
2:C:34:ILE:HG13	2:C:67:LEU:HD22	1.18	1.07
2:C:37:ARG:HG2	2:C:38:PRO:HD2	1.31	1.07
2:C:251:GLY:HA2	2:C:254:ARG:HD3	1.09	1.07
2:D:176:LEU:HD21	2:D:277:THR:HG23	1.30	1.07
2:C:216:LEU:HD11	2:C:250:ILE:HG21	1.07	1.07
2:C:290:ARG:HD2	2:D:244:ASP:HB2	1.37	1.06
2:B:305:MET:HG3	4:B:401:ADP:C6	1.91	1.06
2:C:285:CYS:HB3	2:C:289:ILE:HD11	1.37	1.05
2:C:35:VAL:HG22	2:C:52:SER:HB3	1.35	1.05
2:D:8:LEU:HB2	2:D:103:VAL:HG22	1.32	1.05
2:D:285:CYS:HB3	2:D:289:ILE:HD11	1.33	1.05
2:C:305:MET:HG3	4:C:401:ADP:C6	1.91	1.05
2:B:176:LEU:HD11	2:B:277:THR:HG22	1.38	1.05
2:D:305:MET:HG3	4:D:401:ADP:C6	1.91	1.04
2:C:216:LEU:HD23	2:C:254:ARG:HG3	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:272:CYS:HB3	2:C:276:GLU:HG2	1.40	1.03
2:D:116:ARG:HD2	2:D:134:VAL:HG11	1.08	1.03
2:D:120:THR:HG23	2:D:132:MET:HE2	1.40	1.03
2:B:216:LEU:HD11	2:B:250:ILE:HG12	1.36	1.03
2:B:220:ALA:HB1	2:B:226:GLU:HG3	1.39	1.02
2:B:8:LEU:HB3	2:B:103:VAL:HG13	1.40	1.00
2:B:7:ALA:HB1	2:B:104:LEU:HD21	1.43	1.00
2:C:153:MET:HG3	2:C:299:LEU:HA	1.43	1.00
2:C:61:LYS:HG3	2:C:64:ILE:HG22	1.44	0.99
2:B:195:GLU:HA	2:C:110:LEU:HD11	1.42	0.99
2:B:35:VAL:HG12	2:B:68:LYS:HB2	1.44	0.99
2:B:250:ILE:HD12	2:B:253:GLU:HG2	1.44	0.99
2:D:349:LEU:HD22	2:D:352:PHE:HD1	1.27	0.98
2:B:332:PRO:HG2	2:B:335:ARG:HH21	1.24	0.98
2:D:139:VAL:HG12	2:D:140:LEU:HD12	1.45	0.98
2:D:106:THR:HG22	2:D:135:ALA:HB3	1.41	0.98
2:C:11:ASP:HB2	2:C:18:LYS:HG2	1.45	0.98
2:C:39:ARG:HH22	2:C:203:THR:HG21	1.27	0.97
2:C:332:PRO:HG2	2:C:335:ARG:HH21	1.26	0.97
2:B:282:ILE:HD11	2:B:293:LEU:HD13	1.47	0.97
2:B:148:THR:HG22	2:B:149:THR:HG23	1.43	0.97
2:B:152:VAL:HG23	2:B:298:VAL:HG12	1.43	0.96
1:A:181:MET:HE1	1:A:242:LEU:HD12	1.44	0.96
2:B:73:HIC:HD2	2:B:183:ARG:NH1	1.80	0.96
2:B:189:LEU:HA	2:B:192:ILE:HD11	1.47	0.96
2:D:61:LYS:HB3	2:D:65:LEU:HD22	1.46	0.96
2:D:349:LEU:HD22	2:D:352:PHE:CD1	2.01	0.96
2:B:285:CYS:HB3	2:B:289:ILE:HD11	1.45	0.96
2:C:11:ASP:HB3	2:C:18:LYS:HE2	1.46	0.96
2:D:35:VAL:HG22	2:D:52:SER:HB3	1.47	0.96
2:B:176:LEU:HD21	2:B:277:THR:HG21	1.48	0.96
2:D:166:TYR:HD2	2:D:167:GLU:HG2	1.32	0.95
2:D:54:VAL:HA	2:D:58:ALA:HB2	1.49	0.95
2:C:35:VAL:HA	2:C:54:VAL:HG21	1.48	0.95
2:B:82:MET:HE3	2:B:82:MET:HA	1.47	0.94
2:B:37:ARG:HG3	2:B:38:PRO:HD2	1.48	0.94
2:B:73:HIC:HD2	2:B:183:ARG:HH12	1.30	0.94
2:D:61:LYS:HE2	2:D:64:ILE:HG21	1.48	0.94
2:D:357:ILE:HG12	2:D:370:VAL:HG23	1.47	0.94
2:B:36:GLY:H	2:B:52:SER:HB3	1.30	0.94
2:C:216:LEU:HD11	2:C:250:ILE:CG2	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ALA:CB	2:D:347:ALA:HB1	1.98	0.94
2:C:34:ILE:HG12	2:C:54:VAL:CG1	1.97	0.94
2:B:34:ILE:HG12	2:B:54:VAL:CG1	1.98	0.93
2:D:134:VAL:HG23	2:D:370:VAL:HG21	1.49	0.93
2:C:140:LEU:HD23	2:C:343:GLY:CA	1.98	0.93
2:D:71:ILE:HG23	2:D:75:ILE:C	1.93	0.93
1:A:181:MET:O	1:A:184:ILE:HD13	1.68	0.93
1:A:154:ARG:CZ	2:D:231:ALA:HB1	1.98	0.93
2:D:152:VAL:HG23	2:D:298:VAL:HB	1.50	0.93
2:D:282:ILE:HG23	2:D:290:ARG:HD3	1.49	0.93
2:C:251:GLY:CA	2:C:254:ARG:HD3	1.99	0.93
2:B:190:MET:HE2	2:B:209:VAL:CG1	1.99	0.93
2:D:34:ILE:HG12	2:D:54:VAL:HG11	1.49	0.92
2:D:11:ASP:HB2	2:D:18:LYS:CD	1.99	0.92
2:C:282:ILE:HG13	2:C:294:TYR:CE2	2.04	0.92
2:C:7:ALA:CB	2:C:347:ALA:HB1	1.99	0.92
2:C:43:VAL:HG13	2:C:44:MET:H	1.32	0.92
2:D:285:CYS:CB	2:D:289:ILE:HD11	1.98	0.92
1:A:181:MET:HA	1:A:184:ILE:HD13	1.52	0.92
2:B:140:LEU:HD23	2:B:343:GLY:CA	1.99	0.92
2:D:9:VAL:HG21	2:D:344:SER:HA	1.51	0.92
1:A:181:MET:C	1:A:184:ILE:HD13	1.94	0.91
2:B:8:LEU:CB	2:B:103:VAL:HG13	1.99	0.91
2:B:294:TYR:HD1	2:B:327:ILE:HD11	1.34	0.91
2:B:9:VAL:HG22	2:B:104:LEU:HD23	1.53	0.91
2:D:41:GLN:HG3	2:D:42:GLY:H	1.33	0.91
2:C:120:THR:HB	2:C:367:PRO:HB3	1.53	0.91
2:B:285:CYS:CB	2:B:289:ILE:HD11	2.01	0.90
1:A:173:PHE:CZ	1:A:198:VAL:HG12	2.07	0.90
2:D:152:VAL:HG23	2:D:298:VAL:CB	2.02	0.90
2:D:166:TYR:CD2	2:D:167:GLU:HG2	2.07	0.90
2:D:278:THR:HG21	2:D:313:MET:HE1	1.53	0.90
2:B:193:LEU:HD21	2:B:253:GLU:HG3	1.52	0.89
2:D:37:ARG:H	2:D:66:THR:HG22	1.37	0.89
1:A:173:PHE:CZ	1:A:237:LEU:HD12	2.08	0.89
1:A:181:MET:HA	1:A:184:ILE:CD1	2.03	0.89
2:C:187:ASP:HA	2:C:190:MET:SD	2.13	0.89
2:D:140:LEU:HD23	2:D:343:GLY:CA	2.03	0.89
2:D:116:ARG:CD	2:D:134:VAL:HG11	2.01	0.88
2:B:349:LEU:HD22	2:B:352:PHE:CD1	2.08	0.88
2:C:73:HIC:HD2	2:C:183:ARG:HH12	1.23	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ILE:CG1	2:C:67:LEU:HD22	2.04	0.88
1:A:151:VAL:HG22	1:A:254:ILE:HD13	1.53	0.88
1:A:181:MET:CA	1:A:184:ILE:HD13	2.03	0.88
2:B:195:GLU:HA	2:C:110:LEU:CD1	2.02	0.88
2:B:251:GLY:HA2	2:B:254:ARG:CD	2.03	0.88
2:C:190:MET:HE2	2:C:206:ARG:HB2	1.55	0.88
2:D:148:THR:CG2	2:D:167:GLU:HA	2.04	0.88
1:A:155:TRP:HE3	1:A:250:TRP:HB2	1.36	0.87
2:B:110:LEU:CD1	2:D:195:GLU:HA	2.04	0.87
2:C:104:LEU:HD21	2:C:347:ALA:HB1	1.55	0.87
2:C:190:MET:HE3	2:C:209:VAL:CG1	2.04	0.87
2:D:52:SER:HB2	2:D:84:LYS:HZ1	1.38	0.87
2:B:35:VAL:HG12	2:B:68:LYS:CB	2.04	0.87
2:D:7:ALA:HB3	2:D:347:ALA:HB1	1.56	0.87
2:C:34:ILE:HG13	2:C:67:LEU:CD2	2.03	0.87
2:B:257:CYS:HB3	2:B:258:PRO:HD3	1.54	0.87
2:C:9:VAL:HG22	2:C:104:LEU:CD2	2.03	0.87
2:B:151:ILE:CG2	2:B:297:THR:HG22	2.05	0.87
2:B:190:MET:HE1	2:B:206:ARG:HA	1.57	0.87
2:C:216:LEU:CD2	2:C:254:ARG:HG3	2.03	0.87
2:D:208:ILE:HG21	2:D:242:LEU:CD1	2.05	0.86
2:B:136:ILE:HG23	2:B:139:VAL:H	1.40	0.86
2:C:7:ALA:HB1	2:C:104:LEU:CD2	2.05	0.86
2:C:58:ALA:HB1	2:C:65:LEU:CD1	2.05	0.86
2:C:281:SER:HA	2:C:284:LYS:HD2	1.57	0.86
2:D:133:TYR:CZ	2:D:375:PHE:HB2	2.11	0.86
2:C:287:VAL:HG23	2:D:244:ASP:CB	2.05	0.86
2:D:8:LEU:CB	2:D:103:VAL:HG22	2.06	0.86
2:D:216:LEU:HD11	2:D:250:ILE:HG21	1.57	0.86
2:B:236:LEU:HD12	2:B:237:GLU:N	1.91	0.86
2:C:163:VAL:HG12	2:C:175:ILE:CG1	2.03	0.86
2:C:257:CYS:HB3	2:C:258:PRO:HD3	1.58	0.86
2:B:34:ILE:HG12	2:B:54:VAL:HG11	1.57	0.86
2:C:54:VAL:HA	2:C:58:ALA:HB2	1.56	0.86
2:C:61:LYS:HG3	2:C:64:ILE:CG2	2.06	0.86
2:B:176:LEU:HD21	2:B:277:THR:CG2	2.05	0.85
2:B:35:VAL:HG22	2:B:52:SER:CB	2.06	0.85
2:B:317:ILE:HD11	2:B:329:ILE:HD11	1.59	0.85
2:C:272:CYS:CB	2:C:276:GLU:HG2	2.06	0.85
2:D:34:ILE:CG1	2:D:54:VAL:HG11	2.05	0.85
1:A:202:GLN:HB2	1:A:209:TRP:CZ3	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:ILE:HD12	2:D:256:ARG:HD2	1.58	0.85
1:A:153:GLU:OE1	2:D:236:LEU:HD11	1.77	0.85
2:C:106:THR:HB	2:C:137:GLN:HG2	1.58	0.85
2:D:253:GLU:HA	2:D:256:ARG:HG3	1.58	0.85
1:A:195:LYS:HB3	1:A:236:TYR:CD1	2.12	0.85
2:D:300:SER:CA	2:D:335:ARG:HD3	2.07	0.85
2:D:253:GLU:HA	2:D:256:ARG:CG	2.06	0.85
2:B:190:MET:HE2	2:B:209:VAL:HG11	1.58	0.85
2:B:208:ILE:HD11	2:B:243:PRO:HG2	1.59	0.84
2:D:148:THR:HG23	2:D:167:GLU:HA	1.59	0.84
1:A:197:TRP:CE2	1:A:251:LYS:HB2	2.11	0.84
2:C:285:CYS:HB3	2:C:289:ILE:CD1	2.06	0.84
2:D:50:LYS:HB3	2:D:53:TYR:CD1	2.12	0.84
2:D:61:LYS:HG3	2:D:64:ILE:CG2	2.07	0.84
2:D:104:LEU:HD21	2:D:347:ALA:HB1	1.56	0.84
1:A:142:ILE:CD1	1:A:149:TYR:HB2	2.07	0.84
2:C:216:LEU:CD1	2:C:250:ILE:HG21	2.01	0.84
2:B:121:GLN:NE2	2:B:122:ILE:HD12	1.93	0.84
2:B:50:LYS:HB3	2:B:53:TYR:CE1	2.11	0.84
2:D:250:ILE:HG13	2:D:253:GLU:CG	2.06	0.84
2:C:8:LEU:CB	2:C:103:VAL:HG22	2.07	0.84
2:D:140:LEU:HD23	2:D:343:GLY:HA2	1.57	0.84
2:D:211:ASP:HA	2:D:214:GLU:OE2	1.78	0.84
2:B:143:TYR:CE1	2:B:345:ILE:HG21	2.13	0.84
2:C:153:MET:HG3	2:C:299:LEU:CA	2.08	0.84
2:C:290:ARG:HA	2:C:293:LEU:CD1	2.08	0.84
1:A:233:ILE:HG13	1:A:245:ASP:O	1.78	0.84
2:B:113:LYS:HG2	2:B:371:HIS:NE2	1.92	0.83
2:C:188:TYR:O	2:C:192:ILE:HG13	1.78	0.83
2:D:346:LEU:HA	2:D:349:LEU:HD12	1.59	0.83
1:A:173:PHE:CD1	1:A:254:ILE:HB	2.13	0.83
2:D:140:LEU:O	2:D:342:GLY:HA3	1.77	0.83
2:D:86:TRP:CE2	2:D:123:MET:HE1	2.12	0.83
2:D:43:VAL:HG22	2:D:44:MET:H	1.42	0.83
2:D:105:LEU:HD11	2:D:123:MET:HE2	1.60	0.83
1:A:173:PHE:CE1	1:A:254:ILE:HB	2.13	0.83
1:A:233:ILE:HG12	1:A:247:CYS:N	1.93	0.83
2:B:200:PHE:HA	2:B:205:GLU:OE2	1.79	0.83
2:C:39:ARG:NH2	2:C:203:THR:HG21	1.94	0.83
2:C:176:LEU:HD11	2:C:277:THR:CG2	2.09	0.83
2:C:189:LEU:HD12	2:C:209:VAL:CG2	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:THR:O	2:D:206:ARG:HB2	1.78	0.83
2:D:341:ILE:O	2:D:345:ILE:HD12	1.78	0.83
2:C:61:LYS:HE3	2:C:64:ILE:HG21	1.60	0.83
2:D:300:SER:H	2:D:304:THR:HG21	1.44	0.82
2:B:180:LEU:HD12	2:B:184:ASP:HB2	1.59	0.82
2:D:250:ILE:HG13	2:D:253:GLU:HG2	1.59	0.82
1:A:243:ILE:HG22	1:A:244:SER:H	1.42	0.82
2:C:290:ARG:HD2	2:D:244:ASP:CB	2.10	0.82
2:B:59:GLN:O	2:B:62:ARG:HG2	1.78	0.82
2:B:216:LEU:CD1	2:B:250:ILE:HG12	2.10	0.82
2:B:250:ILE:HG13	2:B:251:GLY:N	1.95	0.82
2:C:136:ILE:O	2:C:139:VAL:HG12	1.79	0.82
2:C:211:ASP:OD1	2:C:215:LYS:HE2	1.80	0.82
2:D:7:ALA:HB1	2:D:104:LEU:CD2	2.08	0.82
2:D:176:LEU:HD21	2:D:277:THR:CG2	2.10	0.82
2:C:153:MET:SD	2:C:299:LEU:HG	2.19	0.82
2:D:278:THR:HG21	2:D:313:MET:CE	2.10	0.82
2:C:143:TYR:CE2	2:D:45:VAL:HG11	2.15	0.81
2:C:68:LYS:HD3	2:C:69:TYR:N	1.96	0.81
2:C:302:GLY:O	2:C:305:MET:HG2	1.79	0.81
2:D:302:GLY:O	2:D:305:MET:HG2	1.80	0.81
2:D:61:LYS:O	2:D:64:ILE:HG22	1.79	0.81
2:C:118:LYS:HE3	2:C:122:ILE:HD11	1.63	0.81
2:C:36:GLY:O	2:C:52:SER:HA	1.81	0.81
2:C:164:PRO:O	2:C:165:ILE:HD13	1.81	0.81
2:C:176:LEU:HD21	2:C:277:THR:CG2	2.11	0.81
2:C:237:GLU:O	2:C:249:THR:HG23	1.80	0.81
2:B:136:ILE:O	2:B:139:VAL:HG12	1.81	0.81
2:C:57:GLU:O	2:C:61:LYS:HB2	1.79	0.81
2:B:133:TYR:OH	2:B:375:PHE:HB2	1.81	0.81
2:B:36:GLY:N	2:B:52:SER:HB3	1.95	0.80
2:B:135:ALA:HB3	2:B:140:LEU:HD11	1.63	0.80
2:C:11:ASP:OD2	2:C:340:TRP:HA	1.81	0.80
2:C:176:LEU:HD11	2:C:277:THR:HG23	1.60	0.80
2:B:250:ILE:HD12	2:B:253:GLU:CG	2.11	0.80
2:D:180:LEU:CD1	2:D:184:ASP:HB2	2.11	0.80
2:C:367:PRO:O	2:C:370:VAL:HG12	1.80	0.80
2:D:164:PRO:HG2	2:D:174:ALA:HB1	1.63	0.80
2:B:189:LEU:HA	2:B:192:ILE:CD1	2.11	0.80
2:D:180:LEU:HD11	2:D:185:LEU:CD2	2.11	0.80
1:A:200:VAL:O	1:A:234:CYS:HB2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:ARG:HG3	2:D:38:PRO:HD2	1.64	0.80
2:B:216:LEU:HD21	2:B:254:ARG:CG	2.11	0.80
1:A:157:MET:HG2	1:A:160:ILE:HB	1.62	0.80
2:B:8:LEU:HD11	2:B:94:LEU:CD1	2.11	0.80
2:B:12:ASN:HD21	2:B:105:LEU:HD12	1.46	0.80
2:B:272:CYS:HB3	2:B:276:GLU:CG	2.12	0.80
2:C:10:VAL:CG2	2:C:105:LEU:HD13	2.12	0.80
1:A:155:TRP:CE3	1:A:250:TRP:HB2	2.16	0.80
2:D:58:ALA:HA	2:D:61:LYS:HB2	1.62	0.80
2:B:35:VAL:HG22	2:B:52:SER:HB3	1.64	0.80
2:C:37:ARG:HG2	2:C:38:PRO:CD	2.10	0.80
2:D:28:ARG:NH1	2:D:28:ARG:HB3	1.97	0.80
2:D:86:TRP:CZ2	2:D:123:MET:HE1	2.17	0.80
2:B:16:MET:HG2	2:B:30:VAL:HG22	1.62	0.79
2:C:71:ILE:HD11	2:C:85:ILE:CD1	2.12	0.79
2:C:59:GLN:O	2:C:62:ARG:HG3	1.82	0.79
2:D:237:GLU:O	2:D:249:THR:HG23	1.81	0.79
2:B:110:LEU:HD21	2:D:195:GLU:HB2	1.62	0.79
2:B:358:SER:H	2:B:361:GLU:HG2	1.47	0.79
2:C:206:ARG:O	2:C:209:VAL:HG12	1.83	0.79
2:B:272:CYS:HB3	2:B:276:GLU:CB	2.13	0.79
2:B:174:ALA:HA	2:B:284:LYS:HD2	1.63	0.79
2:B:190:MET:CE	2:B:206:ARG:HA	2.12	0.79
2:D:121:GLN:HE21	2:D:122:ILE:HD12	1.46	0.79
2:B:113:LYS:HG2	2:B:371:HIS:CD2	2.18	0.79
2:B:262:PHE:CZ	2:B:312:ARG:HD3	2.18	0.79
2:C:35:VAL:CG2	2:C:52:SER:HB3	2.10	0.79
2:D:358:SER:O	2:D:361:GLU:HG2	1.82	0.79
2:B:10:VAL:HG23	2:B:105:LEU:HD13	1.65	0.79
2:C:73:HIC:HD2	2:C:183:ARG:HH11	1.39	0.79
2:D:121:GLN:NE2	2:D:122:ILE:HD12	1.97	0.79
2:D:190:MET:HE2	2:D:209:VAL:CG1	2.13	0.79
1:A:184:ILE:HD12	1:A:184:ILE:H	1.48	0.79
2:B:104:LEU:HD21	2:B:347:ALA:HB1	1.64	0.79
2:B:107:GLU:O	2:B:137:GLN:HG3	1.83	0.79
2:C:143:TYR:HE2	2:D:45:VAL:HG21	1.46	0.79
2:D:35:VAL:HG12	2:D:68:LYS:CB	2.12	0.79
2:D:61:LYS:HG3	2:D:64:ILE:HG21	1.65	0.79
2:D:242:LEU:HG	2:D:243:PRO:HD2	1.64	0.78
2:C:196:ARG:NH2	2:C:250:ILE:HA	1.98	0.78
2:D:106:THR:HG22	2:D:135:ALA:CB	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ILE:CG1	2:B:67:LEU:HD22	2.10	0.78
2:B:216:LEU:HD11	2:B:250:ILE:HG21	1.65	0.78
2:B:250:ILE:CD1	2:B:253:GLU:HG2	2.14	0.78
2:D:282:ILE:CD1	2:D:293:LEU:HD22	2.14	0.78
2:D:306:TYR:O	2:D:309:ILE:HG23	1.83	0.78
2:C:35:VAL:HG12	2:C:68:LYS:CB	2.08	0.78
2:C:135:ALA:HB1	2:C:140:LEU:CD1	2.08	0.78
2:B:35:VAL:CA	2:B:54:VAL:HG21	2.13	0.78
2:B:180:LEU:HD13	2:B:267:LEU:HD12	1.66	0.78
2:C:238:LYS:O	2:C:250:ILE:HG22	1.84	0.78
2:D:257:CYS:HB3	2:D:258:PRO:HD3	1.66	0.78
2:B:148:THR:CG2	2:B:149:THR:HG23	2.13	0.78
2:B:176:LEU:HD11	2:B:277:THR:CG2	2.14	0.78
2:C:143:TYR:CD2	2:D:45:VAL:HG11	2.18	0.78
2:C:238:LYS:HE2	2:C:254:ARG:CZ	2.14	0.78
2:D:132:MET:O	2:D:357:ILE:HB	1.84	0.78
1:A:157:MET:HG2	1:A:160:ILE:CB	2.14	0.77
1:A:173:PHE:HZ	1:A:237:LEU:HD12	1.47	0.77
1:A:195:LYS:HD3	1:A:251:LYS:HE3	1.65	0.77
2:B:54:VAL:HA	2:B:58:ALA:HB2	1.66	0.77
2:D:97:ALA:HB3	2:D:100:GLU:OE1	1.84	0.77
2:B:65:LEU:HD11	2:B:67:LEU:CD2	2.14	0.77
2:C:164:PRO:HB3	2:C:293:LEU:CD2	2.14	0.77
2:C:178:LEU:HD12	2:C:180:LEU:H	1.49	0.77
2:C:236:LEU:HD12	2:C:237:GLU:N	1.99	0.77
2:D:136:ILE:HG22	2:D:139:VAL:HB	1.67	0.77
1:A:158:TRP:CG	1:A:234:CYS:HG	2.02	0.77
2:B:36:GLY:O	2:B:52:SER:HA	1.83	0.77
2:B:203:THR:O	2:B:206:ARG:HG2	1.83	0.77
2:B:61:LYS:HD2	2:B:64:ILE:CG2	2.10	0.77
2:B:317:ILE:HD12	2:B:327:ILE:HG12	1.64	0.77
2:C:50:LYS:HB3	2:C:53:TYR:CD1	2.19	0.77
2:C:299:LEU:HD21	2:C:309:ILE:HG13	1.67	0.77
1:A:154:ARG:HD3	2:D:231:ALA:O	1.84	0.77
2:B:294:TYR:CD1	2:B:327:ILE:HD11	2.17	0.77
2:B:133:TYR:CZ	2:B:375:PHE:HB2	2.20	0.77
2:B:178:LEU:HD12	2:B:180:LEU:H	1.49	0.77
2:B:211:ASP:HA	2:B:214:GLU:OE2	1.84	0.77
1:A:211:TRP:HB2	1:A:213:ASP:OD1	1.84	0.76
2:B:14:SER:HA	2:B:71:ILE:HG22	1.67	0.76
2:C:190:MET:CE	2:C:206:ARG:HB2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:190:MET:HE1	2:C:206:ARG:NH2	2.00	0.76
2:D:61:LYS:HE2	2:D:64:ILE:CG2	2.14	0.76
2:B:242:LEU:HG	2:B:243:PRO:HD2	1.67	0.76
2:C:192:ILE:HD12	2:C:193:LEU:N	2.00	0.76
2:C:309:ILE:HG12	2:C:310:ALA:N	1.99	0.76
2:B:82:MET:CE	2:B:85:ILE:HB	2.15	0.76
2:B:293:LEU:H	2:B:293:LEU:HD12	1.50	0.76
2:C:133:TYR:OH	2:C:375:PHE:HB2	1.84	0.76
2:C:290:ARG:HA	2:C:293:LEU:HD13	1.67	0.76
2:B:65:LEU:HD12	2:B:66:THR:O	1.85	0.76
2:B:237:GLU:O	2:B:249:THR:HG23	1.86	0.76
2:C:134:VAL:O	2:C:375:PHE:HB3	1.84	0.76
2:B:208:ILE:HD13	2:B:242:LEU:HD11	1.67	0.76
2:C:242:LEU:HB3	2:C:244:ASP:OD1	1.84	0.76
2:D:220:ALA:CB	2:D:226:GLU:HG3	2.16	0.76
2:D:35:VAL:CA	2:D:54:VAL:HG21	2.15	0.76
2:C:35:VAL:CA	2:C:54:VAL:HG21	2.16	0.76
2:C:288:ASP:OD2	2:D:62:ARG:HD2	1.86	0.76
2:D:236:LEU:O	2:D:251:GLY:HA2	1.85	0.76
2:D:8:LEU:HD12	2:D:90:PHE:HE1	1.51	0.76
2:B:361:GLU:OE1	2:B:369:ILE:HD12	1.84	0.76
2:C:7:ALA:HB3	2:C:22:ALA:HB2	1.67	0.76
2:C:279:PHE:O	2:C:282:ILE:HG22	1.86	0.76
2:D:133:TYR:OH	2:D:375:PHE:HB2	1.83	0.76
2:B:286:ASP:O	2:B:290:ARG:HG2	1.85	0.76
2:B:50:LYS:HB3	2:B:53:TYR:CD1	2.21	0.75
2:D:105:LEU:HD11	2:D:123:MET:CE	2.14	0.75
2:D:300:SER:HA	2:D:335:ARG:CD	2.13	0.75
2:B:135:ALA:CB	2:B:140:LEU:HD11	2.16	0.75
2:B:164:PRO:HG2	2:B:174:ALA:CB	2.16	0.75
2:B:367:PRO:O	2:B:370:VAL:HG12	1.86	0.75
2:D:35:VAL:CG2	2:D:52:SER:HB3	2.15	0.75
2:B:7:ALA:CB	2:B:347:ALA:HB1	2.16	0.75
2:B:110:LEU:HD13	2:D:195:GLU:HA	1.68	0.75
2:B:196:ARG:NH2	2:B:250:ILE:HA	2.01	0.75
2:B:314:GLN:HG3	2:B:315:LYS:N	2.01	0.75
2:B:345:ILE:O	2:B:349:LEU:HD12	1.85	0.75
2:B:369:ILE:O	2:B:369:ILE:HD13	1.86	0.75
2:D:309:ILE:HG12	2:D:310:ALA:N	2.00	0.75
2:B:92:ASN:O	2:B:95:ARG:HD3	1.87	0.75
2:C:14:SER:HA	2:C:71:ILE:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG22	1:A:235:GLY:O	1.86	0.75
2:B:110:LEU:HD21	2:D:195:GLU:CB	2.16	0.75
2:B:118:LYS:O	2:B:122:ILE:HD13	1.87	0.75
2:B:68:LYS:HD2	2:B:69:TYR:N	2.02	0.75
2:C:337:TYR:O	2:C:341:ILE:HG12	1.87	0.75
1:A:195:LYS:HD3	1:A:251:LYS:CE	2.15	0.75
2:B:250:ILE:CG1	2:B:254:ARG:HG2	2.16	0.75
2:C:8:LEU:HB2	2:C:103:VAL:CG2	2.10	0.74
2:D:153:MET:CE	2:D:274:ILE:HD13	2.17	0.74
2:D:220:ALA:HB1	2:D:226:GLU:HG3	1.67	0.74
1:A:238:LYS:HB3	1:A:243:ILE:HD11	1.68	0.74
2:B:235:SER:O	2:B:238:LYS:HE2	1.87	0.74
2:C:7:ALA:HB3	2:C:347:ALA:HB1	1.67	0.74
2:C:12:ASN:HD21	2:C:105:LEU:HD12	1.51	0.74
2:D:122:ILE:HG23	2:D:126:THR:CG2	2.17	0.74
2:C:133:TYR:CZ	2:C:375:PHE:HB2	2.21	0.74
2:C:341:ILE:O	2:C:345:ILE:HD13	1.86	0.74
2:D:233:SER:HB2	2:D:236:LEU:HG	1.68	0.74
2:B:71:ILE:H	2:B:71:ILE:HD12	1.53	0.74
2:C:79:TRP:CE2	2:C:118:LYS:HG2	2.22	0.74
2:D:36:GLY:HA2	2:D:66:THR:HG23	1.70	0.74
2:D:261:LEU:HD21	2:D:303:THR:CG2	2.16	0.74
2:C:196:ARG:HH22	2:C:250:ILE:HA	1.52	0.74
2:C:287:VAL:HG21	2:D:242:LEU:HG	1.69	0.74
2:D:7:ALA:CB	2:D:104:LEU:HD21	2.16	0.74
2:B:192:ILE:O	2:B:195:GLU:HB3	1.88	0.74
2:D:58:ALA:HB1	2:D:65:LEU:HD13	1.69	0.74
2:D:116:ARG:HD2	2:D:134:VAL:CG1	2.03	0.74
1:A:154:ARG:HD2	2:D:231:ALA:HA	1.69	0.74
2:C:153:MET:HG3	2:C:299:LEU:CB	2.17	0.74
1:A:157:MET:CG	1:A:160:ILE:H	2.00	0.74
2:B:7:ALA:HB1	2:B:104:LEU:CD2	2.15	0.74
2:B:10:VAL:CG2	2:B:105:LEU:HD13	2.17	0.74
2:B:152:VAL:HG12	2:B:163:VAL:HG23	1.70	0.74
2:D:164:PRO:HG2	2:D:174:ALA:CB	2.17	0.74
2:D:216:LEU:CD1	2:D:250:ILE:HG21	2.17	0.74
2:D:113:LYS:HE2	2:D:371:HIS:NE2	2.03	0.74
1:A:174:GLN:HB3	1:A:211:TRP:CD2	2.22	0.74
2:B:154:ASP:OD1	2:B:300:SER:HB3	1.88	0.74
2:B:272:CYS:HB3	2:B:276:GLU:HB3	1.69	0.74
2:C:178:LEU:CD1	2:C:180:LEU:H	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:ILE:HD11	2:C:243:PRO:HG2	1.70	0.74
2:D:36:GLY:O	2:D:52:SER:HA	1.87	0.74
2:B:104:LEU:HG	2:B:347:ALA:HB2	1.69	0.73
2:B:82:MET:HE3	2:B:85:ILE:HB	1.70	0.73
2:B:314:GLN:O	2:B:318:THR:HG23	1.87	0.73
2:D:106:THR:CG2	2:D:140:LEU:HD22	2.18	0.73
2:C:113:LYS:HG2	2:C:371:HIS:CD2	2.23	0.73
2:D:52:SER:HB2	2:D:84:LYS:NZ	2.03	0.73
2:D:61:LYS:CE	2:D:64:ILE:HG21	2.17	0.73
2:C:68:LYS:HD3	2:C:68:LYS:C	2.13	0.73
2:B:27:PRO:HG3	2:B:340:TRP:CG	2.23	0.73
2:B:151:ILE:HG23	2:B:297:THR:HG22	1.70	0.73
2:D:20:GLY:HA2	2:D:28:ARG:CD	2.18	0.73
1:A:156:GLU:OE1	1:A:161:SER:HA	1.88	0.73
2:B:152:VAL:HG23	2:B:298:VAL:CG1	2.16	0.73
2:C:256:ARG:O	2:C:259:GLU:HB2	1.89	0.73
1:A:221:LEU:O	1:A:242:LEU:HD22	1.87	0.73
2:B:151:ILE:O	2:B:297:THR:HA	1.87	0.73
2:D:70:PRO:HB3	2:D:78:ASN:ND2	2.04	0.73
2:C:171:LEU:HD23	2:C:174:ALA:H	1.54	0.73
2:D:293:LEU:HD12	2:D:293:LEU:H	1.53	0.73
2:B:9:VAL:CG2	2:B:104:LEU:HD23	2.17	0.73
2:B:302:GLY:O	2:B:305:MET:HG2	1.86	0.73
1:A:142:ILE:H	1:A:142:ILE:HD13	1.54	0.73
2:B:161:HIS:NE2	2:B:177:ARG:HD2	2.04	0.73
2:C:369:ILE:O	2:C:369:ILE:HD13	1.88	0.73
2:B:358:SER:H	2:B:361:GLU:CG	2.01	0.72
2:C:65:LEU:HG	2:C:66:THR:O	1.89	0.72
2:C:192:ILE:HB	2:C:256:ARG:NH2	2.04	0.72
2:D:58:ALA:HB1	2:D:65:LEU:CD1	2.19	0.72
2:D:152:VAL:HG23	2:D:298:VAL:CG1	2.19	0.72
1:A:135:SER:HB2	1:A:136:PRO:HD2	1.71	0.72
1:A:174:GLN:HA	1:A:211:TRP:CZ3	2.24	0.72
2:C:140:LEU:O	2:C:342:GLY:HA3	1.89	0.72
2:B:176:LEU:H	2:B:176:LEU:HD13	1.52	0.72
2:D:290:ARG:HA	2:D:293:LEU:HD13	1.71	0.72
1:A:157:MET:HG2	1:A:160:ILE:CG2	2.20	0.72
2:B:7:ALA:HB1	2:B:356:TRP:CH2	2.25	0.72
2:B:140:LEU:O	2:B:342:GLY:HA3	1.90	0.72
2:C:65:LEU:O	2:C:65:LEU:HD23	1.90	0.72
2:C:118:LYS:HD2	2:C:121:GLN:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:PHE:CZ	2:B:96:VAL:HG11	2.24	0.72
2:C:35:VAL:HA	2:C:54:VAL:CG2	2.18	0.72
2:C:202:THR:OG1	2:C:205:GLU:HG3	1.90	0.72
2:D:7:ALA:HB1	2:D:356:TRP:HH2	1.55	0.72
2:D:134:VAL:HB	2:D:375:PHE:OXT	1.89	0.72
1:A:195:LYS:CD	1:A:251:LYS:HE3	2.19	0.72
2:D:172:PRO:O	2:D:175:ILE:HG22	1.88	0.72
2:B:164:PRO:HG2	2:B:174:ALA:HB1	1.71	0.72
2:C:143:TYR:CE1	2:C:345:ILE:HG21	2.24	0.72
2:C:285:CYS:CB	2:C:289:ILE:HD11	2.18	0.72
2:D:357:ILE:HD11	2:D:375:PHE:O	1.88	0.72
2:B:190:MET:HE1	2:B:206:ARG:CA	2.19	0.71
2:D:208:ILE:HG21	2:D:242:LEU:HD11	1.71	0.71
2:C:10:VAL:HG23	2:C:105:LEU:HD13	1.72	0.71
2:C:7:ALA:CB	2:C:104:LEU:HD21	2.17	0.71
2:C:8:LEU:O	2:C:103:VAL:HG13	1.91	0.71
2:D:157:ASP:H	4:D:401:ADP:PB	2.14	0.71
2:B:136:ILE:CG2	2:B:139:VAL:HB	2.20	0.71
2:D:104:LEU:HD21	2:D:347:ALA:CB	2.19	0.71
2:D:190:MET:HE2	2:D:209:VAL:HG11	1.73	0.71
1:A:200:VAL:HG13	1:A:235:GLY:H	1.55	0.71
1:A:233:ILE:HD12	1:A:234:CYS:O	1.90	0.71
2:C:38:PRO:HB3	2:C:64:ILE:HD11	1.72	0.71
2:C:157:ASP:H	4:C:401:ADP:PB	2.14	0.71
2:D:258:PRO:O	2:D:261:LEU:HD13	1.90	0.71
2:B:164:PRO:HB3	2:B:293:LEU:CD2	2.21	0.71
2:C:39:ARG:HG2	2:C:66:THR:HB	1.72	0.71
2:C:61:LYS:CE	2:C:64:ILE:HG21	2.20	0.71
2:C:104:LEU:HD21	2:C:347:ALA:CB	2.20	0.71
2:D:18:LYS:H	2:D:18:LYS:HD2	1.54	0.71
2:B:20:GLY:HA2	2:B:28:ARG:HD2	1.72	0.71
2:B:131:ALA:HB1	2:B:357:ILE:O	1.91	0.71
2:C:121:GLN:HG3	2:C:122:ILE:N	2.02	0.71
1:A:196:TYR:HA	1:A:252:TYR:O	1.90	0.71
1:A:155:TRP:CH2	2:B:117:GLU:HB2	2.26	0.71
2:C:71:ILE:H	2:C:71:ILE:HD12	1.56	0.71
2:B:157:ASP:H	4:B:401:ADP:PB	2.14	0.70
2:C:321:ALA:HB1	2:C:322:PRO:HD2	1.72	0.70
2:D:32:PRO:HB3	2:D:34:ILE:HD11	1.74	0.70
2:D:134:VAL:HG23	2:D:370:VAL:CG2	2.20	0.70
2:D:143:TYR:CE1	2:D:345:ILE:HG21	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PRO:HB3	2:B:293:LEU:HD21	1.72	0.70
2:B:282:ILE:HD12	2:B:290:ARG:HB3	1.71	0.70
2:C:50:LYS:HB3	2:C:53:TYR:CE1	2.26	0.70
2:B:34:ILE:HG22	2:B:68:LYS:O	1.92	0.70
2:D:196:ARG:HH22	2:D:250:ILE:HA	1.57	0.70
2:C:97:ALA:HB1	2:C:99:GLU:OE1	1.91	0.70
2:D:71:ILE:HG22	2:D:74:GLY:C	2.17	0.70
2:B:104:LEU:HD22	2:B:104:LEU:N	2.07	0.70
2:C:305:MET:HE2	4:C:401:ADP:N6	2.07	0.70
2:B:242:LEU:CD1	2:B:243:PRO:HD2	2.22	0.70
2:C:190:MET:HE2	2:C:206:ARG:CB	2.21	0.70
1:A:150:TYR:O	1:A:254:ILE:HG23	1.91	0.70
2:B:61:LYS:CD	2:B:64:ILE:HG21	2.15	0.70
2:B:180:LEU:CD1	2:B:184:ASP:HB2	2.22	0.70
2:C:41:GLN:HG3	2:C:42:GLY:H	1.56	0.70
2:D:216:LEU:HD11	2:D:250:ILE:CG2	2.21	0.70
1:A:156:GLU:HB3	1:A:160:ILE:HG23	1.74	0.69
2:D:137:GLN:HB3	2:D:339:VAL:HG11	1.72	0.69
2:D:185:LEU:HD11	2:D:258:PRO:HA	1.73	0.69
1:A:155:TRP:HE3	1:A:250:TRP:CB	2.04	0.69
1:A:156:GLU:HG3	1:A:253:PHE:CE1	2.28	0.69
2:B:242:LEU:CG	2:B:243:PRO:HD2	2.21	0.69
2:C:157:ASP:O	2:C:182:GLY:HA3	1.91	0.69
2:D:142:LEU:HD12	2:D:142:LEU:O	1.91	0.69
2:B:192:ILE:H	2:B:192:ILE:HD13	1.56	0.69
2:C:192:ILE:HD12	2:C:193:LEU:H	1.57	0.69
1:A:162:LYS:O	1:A:166:LEU:HG	1.91	0.69
2:B:7:ALA:CB	2:B:104:LEU:HD21	2.18	0.69
2:C:189:LEU:HA	2:C:192:ILE:HD11	1.75	0.69
2:D:107:GLU:OE2	2:D:111:ASN:HB3	1.92	0.69
2:D:216:LEU:CD2	2:D:254:ARG:HG2	2.21	0.69
2:D:305:MET:HE2	4:D:401:ADP:N6	2.07	0.69
1:A:236:TYR:CE2	1:A:245:ASP:HB2	2.28	0.69
2:B:39:ARG:NH2	2:B:66:THR:HA	2.08	0.69
2:B:171:LEU:HD23	2:B:174:ALA:HB2	1.75	0.69
2:C:158:GLY:HA3	2:C:183:ARG:NH2	2.08	0.69
2:D:131:ALA:HB1	2:D:357:ILE:O	1.92	0.69
1:A:157:MET:O	1:A:160:ILE:HG22	1.93	0.69
2:B:149:THR:CG2	2:B:167:GLU:H	2.06	0.69
2:B:251:GLY:CA	2:B:254:ARG:HG3	2.22	0.69
2:B:372:ARG:NE	2:B:372:ARG:HA	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:166:TYR:HD2	2:C:167:GLU:HG2	1.57	0.69
2:C:194:THR:HA	2:C:198:TYR:O	1.91	0.69
2:D:221:LEU:H	2:D:221:LEU:HD22	1.57	0.69
2:B:206:ARG:CZ	2:B:206:ARG:HB2	2.21	0.69
2:B:216:LEU:CD1	2:B:250:ILE:HG21	2.23	0.69
2:D:149:THR:HA	2:D:165:ILE:O	1.92	0.69
2:D:194:THR:HA	2:D:198:TYR:O	1.92	0.69
2:B:193:LEU:CD2	2:B:253:GLU:HG3	2.23	0.69
2:B:294:TYR:HD1	2:B:327:ILE:CD1	2.03	0.69
2:B:305:MET:HE2	4:B:401:ADP:N6	2.07	0.69
2:B:357:ILE:HD11	2:B:375:PHE:O	1.93	0.69
2:C:104:LEU:HD13	2:C:133:TYR:HB3	1.73	0.69
2:C:132:MET:O	2:C:357:ILE:HB	1.93	0.69
2:C:176:LEU:HD21	2:C:277:THR:HG23	1.75	0.69
2:D:35:VAL:HA	2:D:54:VAL:HG21	1.73	0.69
2:D:361:GLU:HG3	2:D:369:ILE:HG21	1.75	0.69
1:A:187:ILE:O	1:A:190:LEU:HB3	1.93	0.68
2:C:15:GLY:O	2:C:32:PRO:HA	1.93	0.68
2:B:104:LEU:HD21	2:B:347:ALA:CB	2.22	0.68
2:B:120:THR:CG2	2:B:367:PRO:HB3	2.23	0.68
2:C:287:VAL:HG23	2:D:244:ASP:CG	2.17	0.68
2:D:34:ILE:HG22	2:D:68:LYS:O	1.93	0.68
2:D:35:VAL:HG12	2:D:68:LYS:HB2	1.75	0.68
1:A:184:ILE:CD1	1:A:184:ILE:H	2.07	0.68
2:C:191:LYS:HE3	2:C:191:LYS:CA	2.16	0.68
2:B:208:ILE:HG21	2:B:242:LEU:HD11	1.74	0.68
2:C:157:ASP:N	4:C:401:ADP:O3A	2.27	0.68
2:C:299:LEU:CD2	2:C:309:ILE:HG13	2.23	0.68
2:D:148:THR:O	2:D:165:ILE:HG22	1.94	0.68
2:B:140:LEU:HD23	2:B:343:GLY:HA3	1.75	0.68
2:B:145:SER:HB3	2:B:147:ARG:HG2	1.75	0.68
2:B:216:LEU:HD11	2:B:250:ILE:CG1	2.18	0.68
2:D:158:GLY:HA3	2:D:183:ARG:NH2	2.08	0.68
2:B:174:ALA:CA	2:B:284:LYS:HD2	2.22	0.68
1:A:200:VAL:HA	1:A:210:PHE:O	1.93	0.68
2:B:261:LEU:HB3	2:B:274:ILE:HD11	1.75	0.68
2:B:290:ARG:HA	2:B:293:LEU:HD13	1.76	0.68
2:C:11:ASP:OD1	2:C:106:THR:HG21	1.94	0.68
2:B:208:ILE:HG21	2:B:242:LEU:CD1	2.24	0.68
2:D:208:ILE:HG21	2:D:242:LEU:HD12	1.76	0.67
2:B:216:LEU:HD11	2:B:250:ILE:CG2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:VAL:HG23	2:C:105:LEU:HA	1.75	0.67
2:C:90:PHE:CG	2:C:98:PRO:HG3	2.29	0.67
2:D:187:ASP:O	2:D:191:LYS:HG2	1.95	0.67
1:A:142:ILE:HD13	1:A:149:TYR:O	1.95	0.67
2:B:7:ALA:HB1	2:B:356:TRP:HH2	1.57	0.67
2:B:54:VAL:HG12	2:B:55:GLY:N	2.10	0.67
2:B:99:GLU:HG2	2:B:100:GLU:OE1	1.93	0.67
2:D:39:ARG:HE	2:D:66:THR:HA	1.59	0.67
2:B:65:LEU:HD11	2:B:67:LEU:HD21	1.76	0.67
2:B:122:ILE:O	2:B:126:THR:HG22	1.94	0.67
2:B:332:PRO:HG2	2:B:335:ARG:NH2	2.05	0.67
2:D:97:ALA:HB1	2:D:99:GLU:CD	2.19	0.67
1:A:181:MET:HE1	1:A:242:LEU:CD1	2.23	0.67
2:B:34:ILE:HA	2:B:68:LYS:O	1.93	0.67
2:B:71:ILE:HD11	2:B:85:ILE:CD1	2.25	0.67
2:B:261:LEU:HB3	2:B:274:ILE:CD1	2.24	0.67
2:D:282:ILE:HD13	2:D:293:LEU:HD22	1.75	0.67
1:A:155:TRP:HH2	2:B:117:GLU:HB2	1.60	0.67
1:A:190:LEU:HD11	1:A:194:ASN:ND2	2.08	0.67
2:C:34:ILE:O	2:C:54:VAL:HG21	1.95	0.67
2:D:149:THR:HG22	2:D:166:TYR:HA	1.75	0.67
2:D:313:MET:HB3	2:D:329:ILE:HD13	1.76	0.67
1:A:157:MET:HG3	1:A:160:ILE:H	1.59	0.67
2:B:43:VAL:HG22	2:B:44:MET:H	1.57	0.67
2:B:50:LYS:HD3	2:B:50:LYS:N	2.09	0.67
2:B:157:ASP:N	4:B:401:ADP:O3A	2.27	0.67
2:B:300:SER:HA	2:B:335:ARG:HD3	1.76	0.67
2:C:104:LEU:HD22	2:C:104:LEU:N	2.10	0.67
2:C:190:MET:CE	2:C:209:VAL:HG11	2.19	0.67
2:D:306:TYR:HB2	2:D:309:ILE:CG2	2.25	0.67
1:A:184:ILE:HD12	1:A:184:ILE:N	2.08	0.67
2:B:190:MET:HE1	2:B:206:ARG:HB2	1.77	0.67
2:C:68:LYS:O	2:C:70:PRO:HD3	1.94	0.67
2:D:107:GLU:O	2:D:137:GLN:HG3	1.95	0.67
2:D:242:LEU:HB3	2:D:244:ASP:OD1	1.95	0.67
2:B:9:VAL:HG22	2:B:104:LEU:CD2	2.24	0.67
2:B:152:VAL:CG2	2:B:298:VAL:HG12	2.22	0.67
2:B:176:LEU:C	2:B:176:LEU:HD22	2.20	0.67
2:C:73:HIC:CD2	2:C:183:ARG:HH12	2.03	0.67
2:C:120:THR:HA	2:C:132:MET:SD	2.35	0.67
2:C:133:TYR:HD1	2:C:357:ILE:HD12	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:CYS:HB3	2:D:289:ILE:CD1	2.18	0.67
2:B:42:GLY:O	2:B:43:VAL:HG12	1.95	0.67
2:C:35:VAL:CG1	2:C:68:LYS:HB3	2.12	0.67
2:D:153:MET:HE1	2:D:274:ILE:HD13	1.76	0.67
2:D:157:ASP:N	4:D:401:ADP:O3A	2.27	0.67
1:A:137:CYS:SG	1:A:143:GLN:HB2	2.35	0.66
2:C:176:LEU:HD21	2:C:277:THR:HG21	1.75	0.66
2:B:34:ILE:HG12	2:B:54:VAL:HG13	1.77	0.66
2:B:190:MET:HE2	2:B:209:VAL:HG12	1.77	0.66
2:B:35:VAL:HA	2:B:54:VAL:HG21	1.76	0.66
2:B:242:LEU:HD12	2:B:243:PRO:HD2	1.76	0.66
2:C:190:MET:HE1	2:C:206:ARG:CZ	2.24	0.66
2:D:294:TYR:HD1	2:D:327:ILE:CD1	2.06	0.66
2:D:299:LEU:CD2	2:D:309:ILE:HG13	2.26	0.66
2:B:321:ALA:HB1	2:B:322:PRO:HD2	1.77	0.66
2:C:120:THR:HG23	2:C:132:MET:SD	2.36	0.66
2:C:299:LEU:HD21	2:C:309:ILE:CG1	2.25	0.66
1:A:154:ARG:NH1	2:D:231:ALA:HB1	2.09	0.66
2:B:54:VAL:HG12	2:B:55:GLY:H	1.59	0.66
2:C:244:ASP:OD2	2:C:246:GLN:HG3	1.96	0.66
2:D:69:TYR:HB2	2:D:72:GLU:HG3	1.76	0.66
2:D:105:LEU:CD1	2:D:123:MET:HE2	2.25	0.66
1:A:161:SER:HB2	1:A:253:PHE:CG	2.29	0.66
2:B:143:TYR:OH	2:B:349:LEU:HD11	1.96	0.66
2:B:341:ILE:O	2:B:345:ILE:HD12	1.96	0.66
2:C:287:VAL:HG23	2:D:244:ASP:HB3	1.77	0.66
2:D:294:TYR:HD1	2:D:327:ILE:HD13	1.61	0.66
1:A:157:MET:HG2	1:A:160:ILE:HG22	1.76	0.66
2:B:32:PRO:HD2	2:B:55:GLY:HA2	1.77	0.66
2:B:195:GLU:HG2	2:C:110:LEU:HD21	1.76	0.66
2:B:285:CYS:HB3	2:B:289:ILE:CD1	2.23	0.66
2:C:218:TYR:HE2	2:C:254:ARG:CZ	2.08	0.66
2:D:157:ASP:O	2:D:181:ALA:HB3	1.96	0.66
2:D:178:LEU:HD12	2:D:180:LEU:N	1.98	0.66
2:B:149:THR:HG22	2:B:166:TYR:CA	2.19	0.66
2:C:11:ASP:HA	2:C:106:THR:OG1	1.96	0.66
2:C:287:VAL:HG23	2:D:244:ASP:N	2.11	0.66
2:D:65:LEU:HD11	2:D:67:LEU:CD2	2.26	0.66
2:D:86:TRP:CD2	2:D:123:MET:HE1	2.30	0.66
1:A:202:GLN:HB2	1:A:209:TRP:CH2	2.31	0.66
2:B:152:VAL:CG1	2:B:163:VAL:HG23	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:ALA:CB	2:C:140:LEU:HD11	2.10	0.66
2:C:373:LYS:HD2	2:C:373:LYS:O	1.95	0.66
2:D:120:THR:CG2	2:D:132:MET:HE2	2.23	0.66
2:D:163:VAL:CG1	2:D:175:ILE:HG13	2.26	0.66
1:A:158:TRP:CD1	1:A:234:CYS:HG	2.14	0.65
2:B:71:ILE:O	2:B:72:GLU:C	2.39	0.65
2:B:136:ILE:HG22	2:B:139:VAL:HB	1.76	0.65
2:D:71:ILE:HG23	2:D:76:VAL:N	2.11	0.65
2:C:42:GLY:O	2:C:43:VAL:HG12	1.96	0.65
2:C:140:LEU:CD2	2:C:343:GLY:HA2	2.16	0.65
1:A:156:GLU:HB3	1:A:160:ILE:CG2	2.26	0.65
1:A:208:SER:HG	1:A:210:PHE:HE2	1.43	0.65
2:C:361:GLU:HG3	2:C:369:ILE:HG21	1.78	0.65
2:B:134:VAL:O	2:B:375:PHE:HB3	1.97	0.65
2:B:174:ALA:O	2:B:284:LYS:HD2	1.97	0.65
2:B:236:LEU:HD12	2:B:237:GLU:CA	2.27	0.65
2:C:58:ALA:HB1	2:C:65:LEU:HD13	1.78	0.65
2:C:335:ARG:HH11	2:C:335:ARG:HB2	1.61	0.65
2:D:190:MET:O	2:D:194:THR:HG23	1.96	0.65
2:B:174:ALA:HA	2:B:284:LYS:CD	2.27	0.65
2:B:191:LYS:HA	2:B:191:LYS:HE2	1.79	0.65
2:C:7:ALA:HB1	2:C:347:ALA:HB1	1.78	0.65
2:D:196:ARG:NH2	2:D:250:ILE:HA	2.11	0.65
2:B:300:SER:HA	2:B:335:ARG:NH1	2.11	0.65
2:C:192:ILE:HB	2:C:256:ARG:HH21	1.61	0.65
2:C:365:SER:CB	2:C:369:ILE:HB	2.26	0.65
2:D:36:GLY:HA2	2:D:66:THR:CG2	2.27	0.65
2:D:140:LEU:HD23	2:D:343:GLY:HA3	1.77	0.65
2:D:152:VAL:HG23	2:D:298:VAL:HG12	1.78	0.65
2:B:37:ARG:O	2:B:66:THR:HG22	1.95	0.65
1:A:165:CYS:HB2	1:A:255:CYS:SG	2.37	0.65
2:B:335:ARG:HB2	2:B:335:ARG:HH11	1.62	0.65
2:D:189:LEU:HA	2:D:192:ILE:CD1	2.27	0.65
1:A:243:ILE:HG22	1:A:244:SER:N	2.12	0.65
2:B:21:PHE:HZ	2:B:96:VAL:HG11	1.61	0.65
2:B:97:ALA:HB3	2:B:100:GLU:OE1	1.96	0.65
2:B:180:LEU:CD1	2:B:267:LEU:HD12	2.27	0.65
1:A:180:GLU:O	1:A:184:ILE:CD1	2.44	0.65
2:C:213:LYS:HA	2:C:217:CYS:SG	2.36	0.65
2:C:357:ILE:HD11	2:C:375:PHE:O	1.97	0.65
2:D:34:ILE:HG23	2:D:69:TYR:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:VAL:HG22	2:B:52:SER:HB2	1.78	0.64
2:B:103:VAL:C	2:B:356:TRP:HZ3	2.04	0.64
2:C:91:TYR:O	2:C:95:ARG:HA	1.96	0.64
2:D:58:ALA:CA	2:D:61:LYS:HB2	2.27	0.64
2:C:190:MET:HE2	2:C:206:ARG:HA	1.79	0.64
2:D:7:ALA:HB1	2:D:356:TRP:CH2	2.31	0.64
1:A:151:VAL:HG22	1:A:254:ILE:CD1	2.27	0.64
2:B:121:GLN:HE21	2:B:121:GLN:C	2.05	0.64
2:B:189:LEU:HD12	2:B:189:LEU:O	1.95	0.64
2:C:86:TRP:CE2	2:C:123:MET:HE1	2.32	0.64
2:C:107:GLU:OE2	2:C:111:ASN:HB3	1.98	0.64
2:C:250:ILE:HD11	2:C:253:GLU:HB2	1.80	0.64
2:C:112:PRO:CD	2:C:115:ASN:HD21	2.10	0.64
2:C:216:LEU:CD2	2:C:250:ILE:HG12	2.26	0.64
2:D:106:THR:HG21	2:D:140:LEU:HD22	1.80	0.64
2:B:73:HIC:CD2	2:B:183:ARG:HH12	2.09	0.64
2:B:112:PRO:HD2	2:B:115:ASN:HD21	1.63	0.64
2:B:132:MET:CE	2:B:134:VAL:HG23	2.28	0.64
2:B:194:THR:HG22	2:B:199:SER:HA	1.80	0.64
2:C:133:TYR:HD1	2:C:357:ILE:CD1	2.11	0.64
2:D:180:LEU:HD12	2:D:184:ASP:HB2	1.78	0.64
2:D:261:LEU:HD21	2:D:303:THR:HG21	1.79	0.64
2:B:132:MET:O	2:B:357:ILE:HB	1.97	0.64
2:D:37:ARG:CG	2:D:38:PRO:HD2	2.27	0.64
2:D:136:ILE:O	2:D:140:LEU:HD13	1.98	0.64
2:D:335:ARG:HB2	2:D:335:ARG:HH11	1.62	0.64
2:C:158:GLY:HA2	2:C:183:ARG:NE	2.12	0.64
2:B:194:THR:HA	2:B:198:TYR:O	1.98	0.64
2:B:272:CYS:CB	2:B:276:GLU:HB3	2.27	0.64
2:C:71:ILE:HD11	2:C:85:ILE:HD11	1.80	0.64
2:D:109:PRO:HA	2:D:136:ILE:HD11	1.79	0.64
2:D:171:LEU:HD23	2:D:285:CYS:SG	2.37	0.64
2:D:190:MET:HE1	2:D:206:ARG:HA	1.78	0.64
2:B:34:ILE:HG13	2:B:67:LEU:CD2	2.14	0.64
2:B:104:LEU:HD22	2:B:104:LEU:H	1.63	0.64
2:B:158:GLY:HA2	2:B:183:ARG:NE	2.13	0.64
2:C:27:PRO:HG3	2:C:340:TRP:CG	2.33	0.64
2:C:300:SER:HA	2:C:335:ARG:HD3	1.79	0.64
2:D:120:THR:HA	2:D:132:MET:CE	2.28	0.64
2:D:156:GLY:O	2:D:181:ALA:HB1	1.97	0.64
2:D:235:SER:O	2:D:238:LYS:HE3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TRP:HB3	1:A:250:TRP:HB3	1.79	0.64
2:D:357:ILE:HG23	2:D:361:GLU:CD	2.22	0.64
2:C:71:ILE:O	2:C:72:GLU:C	2.40	0.63
2:C:254:ARG:HG2	2:C:254:ARG:HH11	1.63	0.63
2:B:238:LYS:HE3	2:B:254:ARG:HH22	1.63	0.63
2:B:300:SER:H	2:B:304:THR:HG21	1.63	0.63
2:C:298:VAL:HA	2:C:330:ILE:O	1.98	0.63
2:D:91:TYR:O	2:D:95:ARG:HG2	1.98	0.63
2:C:250:ILE:CD1	2:C:253:GLU:HB2	2.28	0.63
2:C:288:ASP:OD1	2:D:243:PRO:HG2	1.99	0.63
2:D:104:LEU:HD22	2:D:104:LEU:N	2.12	0.63
2:B:174:ALA:C	2:B:284:LYS:HD2	2.23	0.63
2:C:104:LEU:HD22	2:C:356:TRP:HH2	1.62	0.63
2:C:164:PRO:HB3	2:C:293:LEU:HD23	1.79	0.63
2:D:64:ILE:HG23	2:D:65:LEU:N	2.14	0.63
2:B:201:THR:HG22	2:B:202:THR:HG23	1.79	0.63
2:C:54:VAL:HG12	2:C:55:GLY:N	2.14	0.63
2:C:139:VAL:CG1	2:C:140:LEU:HD12	2.28	0.63
2:D:321:ALA:HB1	2:D:322:PRO:HD2	1.81	0.63
2:B:189:LEU:HD12	2:B:189:LEU:C	2.24	0.63
2:D:236:LEU:HD12	2:D:237:GLU:N	2.14	0.63
2:B:140:LEU:HD23	2:B:343:GLY:HA2	1.78	0.63
2:B:289:ILE:HD12	2:B:293:LEU:HD11	1.81	0.63
2:C:202:THR:HG23	2:C:205:GLU:OE1	1.99	0.63
2:C:290:ARG:HA	2:C:293:LEU:HD12	1.80	0.63
2:D:65:LEU:HD11	2:D:67:LEU:HD21	1.81	0.63
2:B:12:ASN:HD21	2:B:105:LEU:CD1	2.11	0.63
2:B:111:ASN:OD1	2:B:112:PRO:HD2	1.99	0.63
2:B:7:ALA:HB3	2:B:347:ALA:HB1	1.80	0.63
2:C:288:ASP:HA	2:D:243:PRO:HB2	1.81	0.63
2:B:58:ALA:HB1	2:B:65:LEU:HD13	1.81	0.62
2:C:65:LEU:HD11	2:C:67:LEU:HD21	1.81	0.62
2:C:358:SER:O	2:C:361:GLU:HG2	1.99	0.62
2:D:250:ILE:HG13	2:D:253:GLU:HG3	1.80	0.62
2:D:253:GLU:CA	2:D:256:ARG:HG3	2.28	0.62
2:B:21:PHE:HZ	2:B:96:VAL:CG1	2.12	0.62
2:B:154:ASP:CG	2:B:300:SER:HB3	2.24	0.62
2:C:153:MET:HG3	2:C:299:LEU:HB3	1.81	0.62
2:C:334:GLU:HA	2:C:334:GLU:OE1	1.99	0.62
2:C:250:ILE:HG13	2:C:251:GLY:N	2.14	0.62
1:A:174:GLN:HB3	1:A:211:TRP:CE3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:LEU:CD2	2:D:343:GLY:HA2	2.27	0.62
2:D:278:THR:CG2	2:D:313:MET:HE1	2.26	0.62
2:C:131:ALA:HB1	2:C:357:ILE:O	2.00	0.62
2:C:185:LEU:HD21	2:C:261:LEU:HD11	1.82	0.62
2:D:152:VAL:CG2	2:D:298:VAL:HB	2.27	0.62
2:D:165:ILE:HG23	2:D:168:GLY:O	1.98	0.62
1:A:162:LYS:HZ2	1:A:166:LEU:HD21	1.64	0.62
2:B:220:ALA:CB	2:B:226:GLU:HG3	2.23	0.62
2:B:272:CYS:HB3	2:B:276:GLU:HG3	1.81	0.62
2:C:71:ILE:HD12	2:C:71:ILE:N	2.14	0.62
2:D:7:ALA:HB2	2:D:356:TRP:CZ2	2.35	0.62
2:D:86:TRP:CH2	2:D:123:MET:HE1	2.34	0.62
2:C:10:VAL:HG22	2:C:104:LEU:O	2.00	0.62
2:C:211:ASP:O	2:C:214:GLU:HG2	2.00	0.62
2:D:9:VAL:O	2:D:19:ALA:HA	1.99	0.62
2:D:35:VAL:HG12	2:D:68:LYS:HB3	1.79	0.62
1:A:209:TRP:CE2	1:A:223:PRO:HG2	2.35	0.62
2:B:370:VAL:HG13	2:B:371:HIS:N	2.14	0.62
2:D:120:THR:HG23	2:D:132:MET:CE	2.25	0.62
2:D:192:ILE:HG12	2:D:193:LEU:N	2.13	0.62
2:B:268:GLY:HA3	2:C:173:HIS:CE1	2.34	0.62
2:C:191:LYS:HA	2:C:191:LYS:CE	2.17	0.62
2:C:226:GLU:OE1	2:C:226:GLU:HA	1.98	0.62
2:B:34:ILE:C	2:B:54:VAL:HG21	2.25	0.61
2:B:43:VAL:HG13	2:B:44:MET:N	2.15	0.61
2:B:161:HIS:CD2	2:B:175:ILE:HD11	2.35	0.61
2:D:280:ASN:O	2:D:284:LYS:HG3	1.99	0.61
2:C:208:ILE:O	2:C:212:ILE:HD12	2.00	0.61
2:D:54:VAL:HG13	2:D:58:ALA:CB	2.29	0.61
2:D:209:VAL:HA	2:D:212:ILE:HD12	1.82	0.61
1:A:173:PHE:CE2	1:A:237:LEU:HD12	2.35	0.61
2:C:279:PHE:HZ	2:C:283:MET:HE3	1.66	0.61
2:D:8:LEU:HD12	2:D:90:PHE:CE1	2.35	0.61
2:D:120:THR:HB	2:D:367:PRO:HB3	1.82	0.61
2:C:124:PHE:O	2:C:128:ASN:HA	2.00	0.61
2:C:157:ASP:O	2:C:181:ALA:HB3	2.00	0.61
2:C:250:ILE:HD11	2:C:253:GLU:CB	2.30	0.61
2:D:11:ASP:HA	2:D:106:THR:OG1	2.00	0.61
1:A:162:LYS:NZ	1:A:166:LEU:HD11	2.16	0.61
2:B:71:ILE:HD12	2:B:71:ILE:N	2.14	0.61
2:B:150:GLY:HA2	2:B:296:ASN:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:ILE:HA	2:B:361:GLU:OE2	2.00	0.61
2:C:165:ILE:CD1	2:C:170:ALA:HA	2.31	0.61
2:C:180:LEU:HA	2:C:184:ASP:OD2	1.99	0.61
2:C:287:VAL:HG23	2:D:244:ASP:H	1.65	0.61
2:D:104:LEU:HD11	2:D:347:ALA:HA	1.81	0.61
2:D:295:ALA:O	2:D:328:LYS:HB3	2.00	0.61
2:D:299:LEU:HD13	2:D:330:ILE:O	2.00	0.61
2:C:9:VAL:HG11	2:C:343:GLY:HA3	1.81	0.61
2:D:58:ALA:CB	2:D:65:LEU:HD13	2.30	0.61
2:D:71:ILE:HG22	2:D:75:ILE:N	2.16	0.61
2:D:299:LEU:HD23	2:D:309:ILE:HG13	1.83	0.61
2:B:250:ILE:HG13	2:B:254:ARG:HG2	1.80	0.61
2:C:92:ASN:O	2:C:95:ARG:HD2	2.01	0.61
2:D:50:LYS:HG2	2:D:53:TYR:CE2	2.35	0.61
2:D:106:THR:HG22	2:D:140:LEU:HD22	1.81	0.61
2:D:218:TYR:CE1	2:D:255:PHE:HB3	2.35	0.61
1:A:173:PHE:CE1	1:A:198:VAL:HG12	2.35	0.61
1:A:180:GLU:O	1:A:184:ILE:HD12	2.01	0.61
1:A:197:TRP:CZ2	1:A:251:LYS:HB2	2.35	0.61
2:B:70:PRO:HB3	2:B:78:ASN:ND2	2.15	0.61
2:C:90:PHE:CD1	2:C:98:PRO:HG3	2.36	0.61
2:C:216:LEU:HD21	2:C:250:ILE:CG1	2.30	0.61
2:C:220:ALA:CB	2:C:226:GLU:HG3	2.31	0.61
2:C:351:THR:HG1	2:C:352:PHE:HD1	1.47	0.61
2:D:163:VAL:HG12	2:D:175:ILE:HG13	1.82	0.61
2:D:369:ILE:HD13	2:D:369:ILE:O	2.01	0.61
2:B:357:ILE:HG23	2:B:361:GLU:CG	2.31	0.61
2:C:166:TYR:CD2	2:C:167:GLU:HG2	2.35	0.61
2:D:191:LYS:HA	2:D:191:LYS:HE3	1.83	0.61
2:B:32:PRO:HD2	2:B:55:GLY:C	2.26	0.60
2:B:39:ARG:HH22	2:B:203:THR:HG21	1.64	0.60
2:B:216:LEU:HD21	2:B:250:ILE:CG1	2.31	0.60
2:C:34:ILE:HB	2:C:68:LYS:H	1.65	0.60
2:C:352:PHE:CE2	2:D:45:VAL:HG23	2.36	0.60
2:C:357:ILE:HG23	2:C:361:GLU:OE1	2.00	0.60
2:B:123:MET:O	2:B:127:PHE:HB2	2.01	0.60
2:B:216:LEU:HD21	2:B:250:ILE:HG12	1.82	0.60
2:C:26:ALA:HB1	2:C:27:PRO:HD2	1.82	0.60
2:C:176:LEU:HD22	2:C:176:LEU:C	2.26	0.60
1:A:157:MET:HE2	1:A:247:CYS:SG	2.42	0.60
2:B:159:VAL:HG22	2:B:160:THR:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:ILE:HG22	2:B:349:LEU:CD1	2.32	0.60
2:C:17:CYC:HB3	2:C:31:PHE:CE1	2.36	0.60
2:C:178:LEU:HD13	2:C:179:ASP:N	2.16	0.60
2:C:291:LYS:HA	2:C:325:MET:SD	2.42	0.60
2:C:314:GLN:HB3	2:C:329:ILE:HD13	1.83	0.60
2:D:82:MET:CE	2:D:85:ILE:HB	2.31	0.60
2:D:308:GLY:HA2	2:D:311:ASP:OD1	2.00	0.60
2:B:160:THR:HB	2:B:178:LEU:HB3	1.83	0.60
2:B:190:MET:HE1	2:B:206:ARG:CB	2.32	0.60
2:C:329:ILE:HD12	2:C:329:ILE:N	2.15	0.60
2:B:155:SER:HB3	2:B:303:THR:HB	1.84	0.60
2:B:317:ILE:CD1	2:B:329:ILE:HD11	2.32	0.60
2:D:216:LEU:HD23	2:D:254:ARG:HG2	1.82	0.60
2:D:20:GLY:HA2	2:D:28:ARG:HD3	1.84	0.60
2:D:39:ARG:NE	2:D:66:THR:HA	2.16	0.60
2:D:189:LEU:HA	2:D:192:ILE:HD11	1.82	0.60
2:D:242:LEU:CG	2:D:243:PRO:HD2	2.31	0.60
2:D:257:CYC:CB	2:D:258:PRO:HD3	2.30	0.60
2:B:124:PHE:O	2:B:128:ASN:HA	2.02	0.60
2:B:358:SER:H	2:B:361:GLU:CD	2.10	0.60
2:C:155:SER:HB3	2:C:303:THR:HB	1.84	0.60
2:D:304:THR:O	2:D:309:ILE:HD12	2.02	0.60
2:C:12:ASN:ND2	2:C:105:LEU:HD12	2.17	0.60
2:B:317:ILE:HD11	2:B:327:ILE:CG2	2.32	0.60
2:C:167:GLU:OE2	2:D:64:ILE:HG12	2.02	0.60
2:C:178:LEU:HD12	2:C:180:LEU:N	2.16	0.60
2:C:261:LEU:HB3	2:C:274:ILE:HD11	1.83	0.60
2:C:279:PHE:CZ	2:C:283:MET:HE3	2.37	0.60
2:D:133:TYR:HD1	2:D:357:ILE:CD1	2.15	0.60
2:D:293:LEU:HD12	2:D:293:LEU:N	2.17	0.60
1:A:190:LEU:C	1:A:190:LEU:HD13	2.27	0.59
2:B:192:ILE:HG13	2:B:256:ARG:NE	2.16	0.59
2:C:345:ILE:O	2:C:349:LEU:HD12	2.02	0.59
2:D:73:HIC:HA	2:D:183:ARG:HH12	1.67	0.59
2:D:153:MET:CE	2:D:274:ILE:HG21	2.31	0.59
2:D:194:THR:HG22	2:D:200:PHE:H	1.67	0.59
1:A:181:MET:HA	1:A:184:ILE:HD11	1.83	0.59
1:A:190:LEU:HD11	1:A:194:ASN:HD22	1.66	0.59
2:B:71:ILE:HG22	2:B:71:ILE:O	2.01	0.59
1:A:156:GLU:HG3	1:A:253:PHE:HE1	1.66	0.59
2:D:332:PRO:HG2	2:D:335:ARG:HH21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:CG	1:A:238:LYS:HD2	2.33	0.59
2:C:41:GLN:CG	2:C:42:GLY:H	2.16	0.59
2:C:295:ALA:O	2:C:328:LYS:HB2	2.02	0.59
2:C:314:GLN:HA	2:C:329:ILE:HD11	1.84	0.59
2:D:31:PHE:HB2	2:D:32:PRO:HD2	1.84	0.59
2:D:264:PRO:CB	2:D:269:MET:HB2	2.32	0.59
2:B:349:LEU:HD22	2:B:352:PHE:CE1	2.37	0.59
2:C:71:ILE:HG22	2:C:71:ILE:O	2.01	0.59
2:C:220:ALA:HB2	2:C:226:GLU:HG3	1.85	0.59
2:B:49:GLN:HG2	2:B:50:LYS:H	1.68	0.59
2:B:238:LYS:HE3	2:B:254:ARG:NH2	2.18	0.59
2:C:73:HIC:CD2	2:C:183:ARG:NH1	2.45	0.59
2:D:18:LYS:HD2	2:D:18:LYS:N	2.17	0.59
2:D:34:ILE:HG23	2:D:69:TYR:CD2	2.37	0.59
2:D:136:ILE:HG23	2:D:139:VAL:H	1.68	0.59
1:A:210:PHE:HB3	1:A:214:GLY:HA2	1.83	0.59
1:A:236:TYR:HE2	1:A:245:ASP:HB2	1.64	0.59
2:B:34:ILE:CG1	2:B:54:VAL:HG11	2.29	0.59
2:B:194:THR:HG22	2:B:200:PHE:H	1.67	0.59
2:B:357:ILE:HG13	2:B:361:GLU:OE1	2.03	0.59
2:D:5:ILE:HD13	2:D:5:ILE:N	2.18	0.59
2:C:104:LEU:CD1	2:C:133:TYR:HB3	2.32	0.59
2:D:97:ALA:HB1	2:D:99:GLU:OE2	2.03	0.59
2:D:251:GLY:O	2:D:254:ARG:HG3	2.02	0.59
2:B:8:LEU:HB2	2:B:103:VAL:HG13	1.85	0.59
2:C:34:ILE:C	2:C:54:VAL:HG21	2.28	0.59
2:C:225:GLN:HA	2:C:225:GLN:OE1	2.02	0.59
2:D:218:TYR:HE2	2:D:254:ARG:CZ	2.15	0.59
2:B:49:GLN:HG2	2:B:50:LYS:N	2.18	0.58
2:C:104:LEU:CD2	2:C:356:TRP:HH2	2.15	0.58
2:C:176:LEU:CD1	2:C:277:THR:HG23	2.30	0.58
2:D:28:ARG:HB3	2:D:28:ARG:CZ	2.32	0.58
2:D:272:CYS:HB3	2:D:276:GLU:HB3	1.84	0.58
2:B:32:PRO:HG2	2:B:55:GLY:O	2.02	0.58
2:B:218:TYR:HD1	2:B:219:VAL:O	1.85	0.58
2:C:357:ILE:HG23	2:C:361:GLU:CG	2.33	0.58
2:C:357:ILE:HA	2:C:361:GLU:OE1	2.03	0.58
2:D:97:ALA:HB1	2:D:99:GLU:OE1	2.02	0.58
2:D:134:VAL:O	2:D:375:PHE:HB3	2.03	0.58
2:D:189:LEU:O	2:D:189:LEU:HD13	2.04	0.58
1:A:175:ILE:HD12	1:A:175:ILE:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ALA:HB1	2:D:27:PRO:HD2	1.84	0.58
2:C:133:TYR:HH	2:C:375:PHE:HB2	1.68	0.58
2:D:70:PRO:HB3	2:D:78:ASN:HD21	1.66	0.58
2:D:261:LEU:H	2:D:261:LEU:HD12	1.68	0.58
1:A:201:PHE:HD1	1:A:234:CYS:HB3	1.67	0.58
2:B:16:MET:CG	2:B:30:VAL:HG22	2.32	0.58
2:B:28:ARG:HD3	2:B:94:LEU:CD2	2.33	0.58
2:C:324:THR:HG23	2:C:325:MET:N	2.19	0.58
2:C:372:ARG:NE	2:C:372:ARG:HA	2.19	0.58
2:D:16:MET:HG2	2:D:30:VAL:HG22	1.84	0.58
2:B:39:ARG:CZ	2:B:66:THR:HA	2.34	0.58
2:B:107:GLU:HG3	2:B:111:ASN:ND2	2.19	0.58
2:C:39:ARG:NH2	2:C:66:THR:HA	2.18	0.58
2:C:281:SER:HA	2:C:284:LYS:CD	2.31	0.58
2:D:106:THR:CG2	2:D:135:ALA:HB3	2.25	0.58
2:B:22:ALA:HB1	2:B:348:SER:HB3	1.86	0.58
2:B:263:GLN:HB2	2:B:266:PHE:CE1	2.38	0.58
2:C:357:ILE:HG23	2:C:361:GLU:HG3	1.85	0.58
2:D:50:LYS:HG3	2:D:53:TYR:CZ	2.38	0.58
2:C:11:ASP:CB	2:C:18:LYS:HG2	2.26	0.58
2:D:216:LEU:HD23	2:D:254:ARG:CG	2.34	0.58
2:B:28:ARG:HG2	2:B:28:ARG:HH11	1.66	0.58
2:B:264:PRO:HB2	2:B:269:MET:HB3	1.86	0.58
2:C:116:ARG:HD2	2:C:371:HIS:ND1	2.18	0.58
2:D:282:ILE:CG2	2:D:290:ARG:HD3	2.28	0.58
2:B:39:ARG:NH2	2:B:203:THR:HG21	2.19	0.57
2:B:269:MET:HG3	2:B:271:SER:OG	2.04	0.57
2:D:316:GLU:HA	2:D:316:GLU:OE2	2.03	0.57
2:D:362:TYR:CE1	2:D:367:PRO:HG3	2.38	0.57
2:B:120:THR:HG22	2:B:362:TYR:CE1	2.39	0.57
2:B:251:GLY:HA2	2:B:254:ARG:CG	2.34	0.57
2:B:255:PHE:O	2:B:258:PRO:HD2	2.03	0.57
2:C:314:GLN:HG3	2:C:315:LYS:N	2.19	0.57
2:B:170:ALA:O	2:B:172:PRO:HD3	2.04	0.57
2:C:39:ARG:HH22	2:C:203:THR:CG2	2.09	0.57
2:C:86:TRP:CZ3	2:C:122:ILE:HG21	2.39	0.57
2:C:164:PRO:HG3	2:C:281:SER:OG	2.04	0.57
2:D:7:ALA:HB2	2:D:356:TRP:HZ2	1.68	0.57
2:D:330:ILE:HG22	2:D:332:PRO:HD3	1.87	0.57
2:B:32:PRO:HD2	2:B:55:GLY:CA	2.34	0.57
2:B:250:ILE:HG13	2:B:254:ARG:CG	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:HIS:CD2	2:B:372:ARG:HH21	2.22	0.57
2:D:250:ILE:HG23	2:D:250:ILE:O	2.04	0.57
2:D:261:LEU:HD12	2:D:261:LEU:N	2.19	0.57
2:B:104:LEU:CD2	2:B:356:TRP:HH2	2.17	0.57
2:B:157:ASP:O	2:B:183:ARG:HG2	2.05	0.57
2:B:300:SER:HA	2:B:335:ARG:HH11	1.69	0.57
2:C:369:ILE:HD13	2:C:369:ILE:C	2.29	0.57
2:B:306:TYR:O	2:B:309:ILE:HG23	2.05	0.57
2:C:34:ILE:HG23	2:C:69:TYR:CE2	2.39	0.57
2:C:139:VAL:HG13	2:C:140:LEU:HD12	1.84	0.57
2:C:174:ALA:O	2:C:284:LYS:HD3	2.04	0.57
2:D:236:LEU:HD13	2:D:251:GLY:HA3	1.87	0.57
2:C:314:GLN:HE21	2:C:315:LYS:HA	1.68	0.57
2:B:103:VAL:O	2:B:356:TRP:HZ3	1.87	0.57
2:C:316:GLU:HA	2:C:316:GLU:OE2	2.05	0.57
2:B:11:ASP:HB3	2:B:18:LYS:HG2	1.86	0.57
2:B:335:ARG:NH1	2:B:335:ARG:HB2	2.20	0.57
2:C:208:ILE:HD11	2:C:243:PRO:CG	2.35	0.57
2:C:270:GLU:OE1	2:C:270:GLU:HA	2.04	0.57
1:A:162:LYS:HZ2	1:A:166:LEU:HD11	1.69	0.57
2:B:34:ILE:HG23	2:B:69:TYR:CE2	2.40	0.57
2:B:357:ILE:HG23	2:B:361:GLU:HG3	1.87	0.57
2:D:54:VAL:CA	2:D:58:ALA:HB2	2.31	0.57
2:D:180:LEU:HD11	2:D:185:LEU:HD23	1.85	0.57
1:A:199:GLY:HA3	1:A:211:TRP:HE3	1.68	0.56
1:A:233:ILE:HG12	1:A:247:CYS:H	1.70	0.56
2:D:104:LEU:CD2	2:D:356:TRP:HH2	2.18	0.56
2:B:12:ASN:ND2	2:B:105:LEU:HD12	2.19	0.56
2:C:16:MET:SD	2:C:30:VAL:HG22	2.45	0.56
2:D:282:ILE:HG22	2:D:283:MET:N	2.21	0.56
2:D:335:ARG:HB2	2:D:335:ARG:NH1	2.20	0.56
1:A:205:ILE:HG23	1:A:206:SER:H	1.70	0.56
2:B:39:ARG:HG2	2:B:66:THR:HB	1.86	0.56
2:B:65:LEU:HD11	2:B:67:LEU:HD23	1.86	0.56
2:B:208:ILE:HD13	2:B:242:LEU:CD1	2.35	0.56
2:C:5:ILE:HD13	2:C:5:ILE:N	2.20	0.56
2:C:10:VAL:HG21	2:C:105:LEU:HD13	1.86	0.56
2:C:122:ILE:HG23	2:C:126:THR:CG2	2.36	0.56
2:C:308:GLY:HA2	2:C:311:ASP:OD1	2.05	0.56
2:D:35:VAL:HA	2:D:54:VAL:CG2	2.35	0.56
2:D:37:ARG:N	2:D:66:THR:HG22	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:GLN:HG3	2:D:42:GLY:N	2.13	0.56
2:D:57:GLU:H	2:D:57:GLU:CD	2.12	0.56
2:D:70:PRO:CB	2:D:78:ASN:HD21	2.18	0.56
2:D:139:VAL:CG1	2:D:140:LEU:HD12	2.27	0.56
1:A:181:MET:CA	1:A:184:ILE:CD1	2.74	0.56
2:D:61:LYS:HB3	2:D:65:LEU:CD2	2.29	0.56
2:D:153:MET:HE1	2:D:274:ILE:HG21	1.87	0.56
2:B:180:LEU:HD12	2:B:184:ASP:CB	2.35	0.56
2:B:192:ILE:HD13	2:B:192:ILE:N	2.19	0.56
2:B:256:ARG:HG3	2:B:257:CYS:N	2.19	0.56
2:B:357:ILE:HA	2:B:361:GLU:CD	2.30	0.56
2:B:373:LYS:HD2	2:B:373:LYS:O	2.04	0.56
2:C:112:PRO:HD2	2:C:115:ASN:HD21	1.71	0.56
2:B:253:GLU:CA	2:B:256:ARG:HG2	2.21	0.56
2:D:176:LEU:CD2	2:D:277:THR:HG23	2.19	0.56
2:B:150:GLY:CA	2:B:296:ASN:HB2	2.35	0.56
2:B:305:MET:HE2	4:B:401:ADP:HN61	1.71	0.56
2:C:54:VAL:HG12	2:C:55:GLY:H	1.69	0.56
2:D:32:PRO:HG2	2:D:55:GLY:O	2.06	0.56
2:D:253:GLU:H	2:D:253:GLU:CD	2.13	0.56
2:D:305:MET:HE2	4:D:401:ADP:HN61	1.71	0.56
2:B:68:LYS:HD2	2:B:69:TYR:H	1.68	0.56
2:C:254:ARG:HG2	2:C:254:ARG:NH1	2.19	0.56
2:C:305:MET:HE2	4:C:401:ADP:HN61	1.71	0.56
2:C:335:ARG:HB2	2:C:335:ARG:NH1	2.20	0.56
2:B:161:HIS:HD2	2:B:175:ILE:HD11	1.71	0.56
2:C:216:LEU:HD21	2:C:250:ILE:HG12	1.88	0.56
1:A:187:ILE:HD11	1:A:254:ILE:CD1	2.36	0.56
2:B:32:PRO:HB2	2:B:34:ILE:CD1	2.36	0.56
2:C:300:SER:HA	2:C:335:ARG:NH1	2.21	0.56
2:D:11:ASP:OD2	2:D:340:TRP:HA	2.06	0.56
2:D:185:LEU:CD1	2:D:258:PRO:HA	2.35	0.56
2:D:233:SER:CB	2:D:236:LEU:HG	2.34	0.56
1:A:175:ILE:HA	1:A:180:GLU:OE1	2.06	0.55
2:B:192:ILE:CD1	2:B:192:ILE:H	2.18	0.55
2:C:313:MET:O	2:C:317:ILE:HG12	2.05	0.55
2:D:103:VAL:O	2:D:132:MET:HA	2.06	0.55
2:D:209:VAL:HG12	2:D:210:ARG:N	2.21	0.55
2:D:300:SER:HB3	2:D:335:ARG:NH1	2.20	0.55
2:B:261:LEU:HD21	2:B:303:THR:CG2	2.36	0.55
2:C:259:GLU:OE1	2:C:259:GLU:HA	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ARG:HH11	2:B:28:ARG:CG	2.20	0.55
2:B:70:PRO:HB3	2:B:78:ASN:HD21	1.71	0.55
2:C:357:ILE:HD13	2:C:370:VAL:HG23	1.89	0.55
2:D:122:ILE:HG23	2:D:126:THR:HG22	1.89	0.55
2:D:357:ILE:HD12	2:D:357:ILE:N	2.21	0.55
1:A:151:VAL:HG22	1:A:187:ILE:HD11	1.88	0.55
2:B:3:ASP:CG	2:B:4:ASP:H	2.14	0.55
2:B:27:PRO:HG3	2:B:340:TRP:CD2	2.41	0.55
2:B:362:TYR:CE1	2:B:367:PRO:HG3	2.42	0.55
2:C:163:VAL:CG1	2:C:175:ILE:HG13	2.14	0.55
2:D:76:VAL:HG11	2:D:79:TRP:CZ3	2.42	0.55
2:D:81:ASP:O	2:D:84:LYS:HB2	2.07	0.55
1:A:195:LYS:HE2	1:A:236:TYR:CE1	2.41	0.55
2:B:37:ARG:HG3	2:B:38:PRO:CD	2.31	0.55
2:B:97:ALA:HB1	2:B:99:GLU:OE1	2.07	0.55
2:D:185:LEU:HD21	2:D:261:LEU:HD11	1.88	0.55
2:D:220:ALA:HB1	2:D:226:GLU:CG	2.34	0.55
1:A:154:ARG:HD3	2:D:231:ALA:C	2.32	0.55
1:A:184:ILE:O	1:A:187:ILE:N	2.32	0.55
2:B:151:ILE:HB	2:B:293:LEU:HD23	1.89	0.55
2:D:158:GLY:HA3	2:D:183:ARG:CZ	2.37	0.55
2:D:167:GLU:C	2:D:169:TYR:H	2.13	0.55
2:D:176:LEU:O	2:D:176:LEU:HD22	2.06	0.55
2:B:317:ILE:HD11	2:B:327:ILE:HG21	1.88	0.55
2:B:317:ILE:HD12	2:B:327:ILE:CG1	2.35	0.55
2:D:133:TYR:HA	2:D:357:ILE:HD13	1.88	0.55
1:A:218:LEU:CD1	1:A:221:LEU:HD22	2.37	0.55
1:A:233:ILE:HG12	1:A:246:LYS:C	2.32	0.55
2:C:43:VAL:HG13	2:C:44:MET:N	2.14	0.55
2:C:222:ASP:HB2	2:C:225:GLN:HB3	1.89	0.55
2:C:314:GLN:NE2	2:C:315:LYS:HA	2.21	0.55
2:B:29:ALA:HB1	2:B:93:GLU:OE1	2.07	0.55
2:C:41:GLN:HG3	2:C:42:GLY:N	2.22	0.55
1:A:170:ALA:HB1	1:A:255:CYS:HB3	1.89	0.55
2:B:196:ARG:HH21	2:B:250:ILE:HA	1.71	0.55
2:D:216:LEU:HD22	2:D:250:ILE:HD13	1.89	0.55
1:A:195:LYS:HD3	1:A:251:LYS:HE2	1.88	0.54
1:A:222:LEU:HB3	1:A:223:PRO:HD2	1.89	0.54
2:B:110:LEU:CD2	2:D:195:GLU:HA	2.36	0.54
2:B:251:GLY:HA2	2:B:254:ARG:HG3	1.89	0.54
2:D:357:ILE:HG23	2:D:361:GLU:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:ALA:O	2:C:111:ASN:HB2	2.07	0.54
2:C:304:THR:O	2:C:309:ILE:HD12	2.07	0.54
2:C:314:GLN:HE21	2:C:315:LYS:CA	2.19	0.54
2:D:28:ARG:HB3	2:D:28:ARG:HH11	1.70	0.54
2:D:107:GLU:CD	2:D:111:ASN:HB3	2.32	0.54
2:D:151:ILE:HG23	2:D:297:THR:HG22	1.89	0.54
2:D:176:LEU:HD22	2:D:176:LEU:C	2.32	0.54
2:D:287:VAL:HG13	2:D:288:ASP:N	2.22	0.54
2:B:79:TRP:CE2	2:B:118:LYS:HG3	2.43	0.54
2:B:236:LEU:HD12	2:B:236:LEU:C	2.32	0.54
2:C:328:LYS:C	2:C:329:ILE:HD12	2.31	0.54
2:C:353:GLN:HA	2:C:356:TRP:HD1	1.72	0.54
2:D:57:GLU:O	2:D:61:LYS:HB2	2.07	0.54
2:D:123:MET:HB2	2:D:132:MET:SD	2.47	0.54
2:D:274:ILE:O	2:D:278:THR:HG23	2.07	0.54
2:D:314:GLN:HG3	2:D:315:LYS:N	2.22	0.54
2:B:104:LEU:HD22	2:B:356:TRP:HH2	1.72	0.54
2:C:104:LEU:HD11	2:C:347:ALA:HA	1.89	0.54
2:C:108:ALA:HB1	2:C:109:PRO:HD2	1.89	0.54
2:C:306:TYR:O	2:C:309:ILE:HG23	2.07	0.54
2:D:43:VAL:HG22	2:D:44:MET:N	2.14	0.54
1:A:196:TYR:O	1:A:236:TYR:HB2	2.07	0.54
2:B:241:GLU:HA	2:B:247:VAL:HA	1.89	0.54
2:C:38:PRO:HB3	2:C:64:ILE:CD1	2.37	0.54
2:D:35:VAL:CG1	2:D:68:LYS:HB2	2.37	0.54
2:D:70:PRO:HB3	2:D:78:ASN:CG	2.33	0.54
2:D:118:LYS:O	2:D:121:GLN:HG3	2.08	0.54
2:B:35:VAL:HG12	2:B:68:LYS:HB3	1.88	0.54
2:C:43:VAL:CG1	2:C:44:MET:H	2.09	0.54
2:C:120:THR:HG22	2:C:362:TYR:CD1	2.42	0.54
1:A:135:SER:HB2	1:A:136:PRO:CD	2.37	0.54
2:C:174:ALA:HA	2:C:284:LYS:HD3	1.90	0.54
2:D:106:THR:HA	2:D:135:ALA:HB3	1.89	0.54
2:D:121:GLN:HE21	2:D:122:ILE:N	2.06	0.54
2:D:152:VAL:HG23	2:D:298:VAL:C	2.33	0.54
1:A:178:LYS:HG3	1:A:179:GLU:N	2.23	0.54
2:C:318:THR:HG22	2:C:327:ILE:HG13	1.89	0.54
2:D:151:ILE:HG23	2:D:151:ILE:O	2.06	0.54
2:D:367:PRO:O	2:D:370:VAL:HG12	2.07	0.54
2:B:208:ILE:CD1	2:B:243:PRO:HG2	2.35	0.54
2:B:238:LYS:O	2:B:250:ILE:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:LEU:O	2:C:96:VAL:HG13	2.08	0.54
2:C:190:MET:HE2	2:C:206:ARG:CA	2.37	0.54
2:D:7:ALA:HB1	2:D:347:ALA:HB1	1.87	0.54
2:D:104:LEU:HD13	2:D:356:TRP:CZ3	2.43	0.54
2:D:293:LEU:H	2:D:293:LEU:CD1	2.20	0.54
2:B:369:ILE:HD13	2:B:369:ILE:C	2.33	0.54
2:C:370:VAL:HG13	2:C:371:HIS:N	2.23	0.54
2:D:8:LEU:HB2	2:D:103:VAL:CG2	2.22	0.54
1:A:245:ASP:CG	1:A:246:LYS:H	2.15	0.53
2:B:250:ILE:HG12	2:B:254:ARG:HG2	1.90	0.53
2:B:299:LEU:HD22	2:B:331:ALA:HB2	1.90	0.53
2:B:345:ILE:HG22	2:B:349:LEU:HD12	1.90	0.53
2:C:38:PRO:HD3	2:C:49:GLN:OE1	2.08	0.53
2:C:321:ALA:HB1	2:C:322:PRO:CD	2.38	0.53
2:C:335:ARG:CZ	2:C:335:ARG:HB3	2.34	0.53
2:C:349:LEU:HD23	2:C:352:PHE:CD1	2.43	0.53
2:D:8:LEU:CG	2:D:103:VAL:HG22	2.38	0.53
2:D:82:MET:HE3	2:D:85:ILE:HB	1.90	0.53
2:D:180:LEU:HD12	2:D:181:ALA:H	1.72	0.53
2:B:117:GLU:CD	2:B:368:SER:HB3	2.33	0.53
2:B:162:THR:O	2:B:175:ILE:HG13	2.07	0.53
2:D:39:ARG:HE	2:D:66:THR:CA	2.21	0.53
2:D:210:ARG:HD2	2:D:214:GLU:OE1	2.08	0.53
1:A:200:VAL:CG2	1:A:209:TRP:HB3	2.38	0.53
2:B:155:SER:OG	2:B:160:THR:HG23	2.08	0.53
2:B:192:ILE:HB	2:B:256:ARG:NH2	2.22	0.53
2:D:120:THR:HA	2:D:132:MET:HE1	1.91	0.53
2:D:192:ILE:HG21	2:D:256:ARG:CD	2.39	0.53
2:C:39:ARG:CZ	2:C:66:THR:HA	2.38	0.53
2:C:151:ILE:HG23	2:C:151:ILE:O	2.08	0.53
2:B:105:LEU:O	2:B:134:VAL:HA	2.09	0.53
2:B:357:ILE:HG23	2:B:361:GLU:CD	2.34	0.53
2:C:172:PRO:O	2:C:175:ILE:HG22	2.09	0.53
2:C:190:MET:HG3	2:C:209:VAL:HG21	1.90	0.53
2:D:6:ALA:O	2:D:102:PRO:HD2	2.09	0.53
2:D:230:ALA:HA	2:D:233:SER:OG	2.08	0.53
1:A:152:PHE:HD2	1:A:154:ARG:H	1.55	0.53
1:A:154:ARG:NE	2:D:231:ALA:HB1	2.24	0.53
2:D:50:LYS:HB3	2:D:53:TYR:CE1	2.43	0.53
2:D:54:VAL:O	2:D:57:GLU:HG2	2.09	0.53
2:B:104:LEU:CD2	2:B:356:TRP:CH2	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:GLU:HG3	2:B:111:ASN:HD22	1.73	0.53
2:B:195:GLU:CA	2:C:110:LEU:HD11	2.25	0.53
2:B:217:CYS:HB3	2:B:258:PRO:HG3	1.89	0.53
2:B:335:ARG:CZ	2:B:335:ARG:HB3	2.35	0.53
2:C:133:TYR:HA	2:C:357:ILE:CD1	2.39	0.53
2:B:7:ALA:CB	2:B:356:TRP:CZ2	2.92	0.53
2:C:238:LYS:HE2	2:C:254:ARG:NH1	2.23	0.53
2:C:357:ILE:CD1	2:C:370:VAL:HG23	2.39	0.53
2:D:140:LEU:HB3	2:D:343:GLY:N	2.24	0.53
2:D:157:ASP:O	2:D:183:ARG:HB2	2.09	0.53
2:D:360:GLN:OE1	2:D:360:GLN:HA	2.07	0.53
1:A:157:MET:HG2	1:A:160:ILE:H	1.74	0.53
1:A:195:LYS:HG2	1:A:238:LYS:HD2	1.91	0.53
2:B:108:ALA:HB1	2:B:109:PRO:HD2	1.91	0.53
2:B:120:THR:HG22	2:B:367:PRO:HB3	1.90	0.53
2:B:217:CYS:HB2	2:B:306:TYR:HE2	1.73	0.53
2:C:287:VAL:CG2	2:D:244:ASP:H	2.22	0.53
2:D:45:VAL:O	2:D:45:VAL:HG13	2.09	0.53
1:A:154:ARG:CD	2:D:231:ALA:HA	2.39	0.53
1:A:227:GLN:O	1:A:228:ARG:HB2	2.09	0.53
2:B:109:PRO:HA	2:B:136:ILE:HD11	1.90	0.53
2:B:126:THR:HG23	2:B:127:PHE:CD2	2.43	0.53
2:C:10:VAL:HG23	2:C:10:VAL:O	2.07	0.53
2:C:38:PRO:HG2	2:C:49:GLN:HE22	1.73	0.53
2:C:223:PHE:O	2:C:227:MET:HG2	2.09	0.53
2:D:274:ILE:O	2:D:277:THR:HB	2.09	0.53
2:B:104:LEU:HD11	2:B:347:ALA:HA	1.91	0.52
2:B:293:LEU:HD12	2:B:293:LEU:N	2.23	0.52
2:C:9:VAL:HG11	2:C:343:GLY:CA	2.39	0.52
2:C:38:PRO:CG	2:C:49:GLN:HE22	2.22	0.52
2:C:65:LEU:HD23	2:C:65:LEU:C	2.33	0.52
2:D:104:LEU:CD1	2:D:356:TRP:CH2	2.92	0.52
2:B:216:LEU:CD2	2:B:250:ILE:HD11	2.39	0.52
2:C:49:GLN:HG2	2:C:50:LYS:N	2.24	0.52
2:C:287:VAL:O	2:C:290:ARG:HG3	2.09	0.52
2:D:75:ILE:O	2:D:77:THR:N	2.41	0.52
2:D:158:GLY:HA2	2:D:183:ARG:NE	2.24	0.52
1:A:238:LYS:HB3	1:A:243:ILE:CD1	2.36	0.52
2:C:21:PHE:HZ	2:C:96:VAL:HG11	1.75	0.52
2:C:34:ILE:HA	2:C:68:LYS:O	2.09	0.52
2:C:158:GLY:HA2	2:C:183:ARG:HE	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:373:LYS:O	2:D:373:LYS:HD2	2.08	0.52
1:A:184:ILE:O	1:A:187:ILE:HB	2.10	0.52
2:B:219:VAL:HG13	2:B:220:ALA:N	2.23	0.52
2:C:7:ALA:HB3	2:C:22:ALA:CB	2.38	0.52
2:D:242:LEU:HD12	2:D:243:PRO:CD	2.40	0.52
2:D:365:SER:OG	2:D:369:ILE:HB	2.10	0.52
1:A:198:VAL:HG22	1:A:235:GLY:C	2.34	0.52
2:B:118:LYS:HD2	2:B:122:ILE:CD1	2.39	0.52
2:B:136:ILE:HG22	2:B:139:VAL:CG1	2.40	0.52
2:B:176:LEU:HD13	2:B:176:LEU:N	2.24	0.52
2:B:259:GLU:OE1	2:B:259:GLU:HA	2.09	0.52
2:B:287:VAL:HA	2:B:290:ARG:CG	2.39	0.52
2:C:104:LEU:CD1	2:C:356:TRP:CH2	2.93	0.52
2:C:213:LYS:HD3	2:C:214:GLU:N	2.24	0.52
2:D:99:GLU:O	2:D:130:PRO:HG3	2.09	0.52
2:D:180:LEU:HD13	2:D:267:LEU:HD11	1.92	0.52
2:D:291:LYS:HA	2:D:325:MET:SD	2.49	0.52
2:B:104:LEU:CD1	2:B:356:TRP:CH2	2.92	0.52
2:C:287:VAL:HA	2:D:244:ASP:HB3	1.92	0.52
2:B:82:MET:HE3	2:B:82:MET:CA	2.29	0.52
2:B:216:LEU:HD21	2:B:250:ILE:HD11	1.92	0.52
2:B:236:LEU:HD12	2:B:237:GLU:HA	1.91	0.52
2:C:10:VAL:HA	2:C:19:ALA:HB2	1.90	0.52
2:C:99:GLU:O	2:C:130:PRO:HD3	2.09	0.52
2:C:311:ASP:O	2:C:314:GLN:HG3	2.10	0.52
2:C:361:GLU:OE1	2:C:369:ILE:HD12	2.10	0.52
2:D:263:GLN:HB2	2:D:266:PHE:CE1	2.44	0.52
1:A:198:VAL:HG23	1:A:200:VAL:HG12	1.91	0.52
2:B:70:PRO:HG3	2:B:81:ASP:CB	2.39	0.52
2:C:287:VAL:HG23	2:D:244:ASP:CA	2.39	0.52
2:D:49:GLN:HG2	2:D:50:LYS:N	2.25	0.52
2:D:155:SER:HB3	2:D:303:THR:HB	1.91	0.52
2:D:104:LEU:CD2	2:D:356:TRP:CH2	2.93	0.51
1:A:152:PHE:CD1	1:A:253:PHE:CZ	2.98	0.51
2:B:11:ASP:CB	2:B:18:LYS:HG2	2.39	0.51
2:C:81:ASP:HA	2:C:84:LYS:HD3	1.92	0.51
2:C:90:PHE:O	2:C:94:LEU:HB2	2.10	0.51
2:C:361:GLU:HA	2:C:364:GLU:HG2	1.92	0.51
2:C:365:SER:HB2	2:C:369:ILE:HB	1.92	0.51
2:D:71:ILE:CG2	2:D:75:ILE:N	2.73	0.51
2:D:118:LYS:HE3	2:D:122:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ALA:O	2:B:102:PRO:HD2	2.09	0.51
2:B:152:VAL:HG23	2:B:298:VAL:C	2.35	0.51
2:D:166:TYR:HD2	2:D:167:GLU:CG	2.14	0.51
2:D:250:ILE:CG1	2:D:253:GLU:HG2	2.35	0.51
2:B:189:LEU:O	2:B:192:ILE:HD13	2.10	0.51
2:C:104:LEU:CD2	2:C:356:TRP:CH2	2.93	0.51
2:D:26:ALA:HB1	2:D:27:PRO:CD	2.41	0.51
2:D:139:VAL:HG12	2:D:140:LEU:N	2.22	0.51
2:D:171:LEU:HD12	2:D:172:PRO:HD2	1.93	0.51
1:A:151:VAL:CG2	1:A:187:ILE:HD11	2.41	0.51
1:A:157:MET:N	1:A:160:ILE:HG22	2.25	0.51
1:A:202:GLN:HE22	1:A:232:GLN:HG3	1.75	0.51
2:B:261:LEU:HD23	2:B:274:ILE:HD11	1.91	0.51
2:B:358:SER:N	2:B:361:GLU:HG2	2.22	0.51
2:C:212:ILE:HG23	2:C:216:LEU:HD13	1.92	0.51
2:C:216:LEU:HD21	2:C:250:ILE:HG13	1.91	0.51
2:D:314:GLN:CA	2:D:329:ILE:HD11	2.40	0.51
2:B:34:ILE:CG2	2:B:69:TYR:CZ	2.94	0.51
2:C:176:LEU:HD11	2:C:277:THR:HG22	1.92	0.51
2:C:189:LEU:O	2:C:189:LEU:HD13	2.11	0.51
2:D:259:GLU:OE1	2:D:262:PHE:HB2	2.10	0.51
2:B:151:ILE:HG23	2:B:151:ILE:O	2.10	0.51
2:B:317:ILE:CD1	2:B:327:ILE:HG12	2.35	0.51
2:C:79:TRP:CG	2:C:118:LYS:HE2	2.45	0.51
2:C:186:THR:O	2:C:189:LEU:HB3	2.10	0.51
2:B:263:GLN:HB2	2:B:266:PHE:CD1	2.46	0.51
2:B:361:GLU:O	2:B:365:SER:HB2	2.11	0.51
2:C:40:HIS:O	2:C:41:GLN:HB3	2.10	0.51
2:C:165:ILE:HD12	2:C:170:ALA:HA	1.93	0.51
2:D:213:LYS:NZ	4:D:401:ADP:O2'	2.36	0.51
1:A:151:VAL:HG13	1:A:196:TYR:CE2	2.46	0.51
2:B:24:ASP:HB2	2:B:340:TRP:HH2	1.75	0.51
2:B:113:LYS:HG2	2:B:371:HIS:CE1	2.46	0.51
2:B:152:VAL:HG23	2:B:298:VAL:O	2.11	0.51
2:B:180:LEU:HD13	2:B:267:LEU:CD1	2.39	0.51
2:B:282:ILE:HG13	2:B:294:TYR:CE2	2.46	0.51
2:C:34:ILE:CG2	2:C:69:TYR:CZ	2.94	0.51
2:C:332:PRO:HG2	2:C:335:ARG:NH2	2.10	0.51
2:D:217:CYS:HA	2:D:254:ARG:HB3	1.92	0.51
1:A:155:TRP:CD1	1:A:252:TYR:CZ	2.99	0.50
2:B:37:ARG:HB2	2:B:51:ASP:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LEU:CD2	2:B:277:THR:CG2	2.86	0.50
2:B:192:ILE:HB	2:B:256:ARG:CZ	2.40	0.50
2:B:317:ILE:HD11	2:B:329:ILE:CD1	2.38	0.50
2:C:14:SER:HA	2:C:71:ILE:CG2	2.39	0.50
2:C:143:TYR:CE2	2:D:45:VAL:HG21	2.37	0.50
2:C:238:LYS:HE2	2:C:254:ARG:NH2	2.26	0.50
2:D:7:ALA:CB	2:D:356:TRP:CZ2	2.94	0.50
2:D:242:LEU:HD12	2:D:243:PRO:HD3	1.92	0.50
2:D:329:ILE:C	2:D:330:ILE:HG13	2.36	0.50
1:A:174:GLN:C	1:A:175:ILE:HD12	2.36	0.50
2:B:88:HIS:NE2	2:B:93:GLU:HG3	2.26	0.50
2:B:167:GLU:HG3	2:B:167:GLU:O	2.11	0.50
2:B:328:LYS:C	2:B:329:ILE:HD12	2.37	0.50
2:C:5:ILE:HD13	2:C:5:ILE:H	1.76	0.50
2:C:176:LEU:CG	2:C:277:THR:HG23	2.42	0.50
2:D:34:ILE:CG2	2:D:69:TYR:CZ	2.94	0.50
1:A:187:ILE:HD11	1:A:254:ILE:HD11	1.92	0.50
2:B:126:THR:HG23	2:B:127:PHE:N	2.27	0.50
2:B:158:GLY:HA2	2:B:183:ARG:CD	2.42	0.50
2:B:223:PHE:CD1	2:B:259:GLU:HG2	2.46	0.50
2:C:122:ILE:O	2:C:126:THR:HG22	2.10	0.50
2:C:332:PRO:CG	2:C:335:ARG:HH21	2.12	0.50
2:D:54:VAL:HG12	2:D:55:GLY:N	2.26	0.50
2:D:104:LEU:HD22	2:D:356:TRP:HH2	1.77	0.50
1:A:155:TRP:CH2	2:B:117:GLU:CB	2.95	0.50
2:B:123:MET:HA	2:B:127:PHE:HD2	1.76	0.50
2:B:300:SER:CA	2:B:335:ARG:HD3	2.40	0.50
2:C:34:ILE:HG12	2:C:54:VAL:HG13	1.91	0.50
2:C:34:ILE:CG2	2:C:69:TYR:CE2	2.95	0.50
2:C:149:THR:HG22	2:C:166:TYR:HA	1.94	0.50
2:D:7:ALA:CB	2:D:356:TRP:CH2	2.93	0.50
2:D:70:PRO:CB	2:D:78:ASN:ND2	2.73	0.50
2:B:36:GLY:HA2	2:B:66:THR:HG23	1.94	0.50
2:B:45:VAL:HG13	2:B:45:VAL:O	2.11	0.50
2:B:236:LEU:CD1	2:B:237:GLU:HG2	2.41	0.50
2:D:43:VAL:O	2:D:44:MET:HB3	2.10	0.50
2:D:53:TYR:N	2:D:53:TYR:HD1	2.09	0.50
2:D:314:GLN:N	2:D:329:ILE:HD11	2.26	0.50
1:A:163:LYS:O	1:A:166:LEU:HB2	2.11	0.50
1:A:195:LYS:HG3	1:A:238:LYS:HD2	1.92	0.50
2:B:11:ASP:OD2	2:B:340:TRP:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:MET:CG	2:D:30:VAL:HG22	2.41	0.50
2:D:50:LYS:HG2	2:D:53:TYR:CD2	2.47	0.50
1:A:156:GLU:CD	1:A:253:PHE:CE1	2.90	0.50
1:A:226:ARG:HG3	1:A:227:GLN:H	1.76	0.50
2:B:133:TYR:CE1	2:B:355:MET:CG	2.94	0.50
2:B:133:TYR:HH	2:B:375:PHE:HB2	1.74	0.50
2:B:216:LEU:CD2	2:B:254:ARG:HA	2.41	0.50
2:C:294:TYR:CD2	2:C:325:MET:HE1	2.47	0.50
2:D:65:LEU:HD12	2:D:66:THR:O	2.12	0.50
2:D:134:VAL:CG2	2:D:370:VAL:HG21	2.32	0.50
2:D:180:LEU:HG	2:D:181:ALA:N	2.27	0.50
2:D:261:LEU:H	2:D:261:LEU:CD1	2.23	0.50
2:D:317:ILE:CD1	2:D:327:ILE:HG21	2.42	0.50
2:B:37:ARG:H	2:B:66:THR:CG2	2.24	0.50
2:C:79:TRP:CD2	2:C:118:LYS:HG2	2.46	0.50
2:C:107:GLU:O	2:C:137:GLN:HG3	2.11	0.50
2:C:176:LEU:CD2	2:C:277:THR:HG23	2.41	0.50
2:D:34:ILE:CG2	2:D:69:TYR:CE1	2.95	0.50
2:D:193:LEU:HD13	2:D:200:PHE:CE1	2.47	0.50
2:D:218:TYR:CE2	2:D:254:ARG:CZ	2.95	0.50
2:D:305:MET:HG3	4:D:401:ADP:C5	2.45	0.50
2:B:305:MET:HG3	4:B:401:ADP:C5	2.45	0.50
2:D:34:ILE:HA	2:D:68:LYS:O	2.12	0.50
2:D:294:TYR:CE2	2:D:325:MET:HE1	2.47	0.50
1:A:153:GLU:CD	2:D:236:LEU:HD11	2.36	0.49
1:A:195:LYS:HG2	1:A:238:LYS:CD	2.42	0.49
2:B:332:PRO:HD2	2:B:335:ARG:NE	2.27	0.49
2:C:3:ASP:HB3	2:C:4:ASP:OD1	2.12	0.49
2:C:54:VAL:O	2:C:57:GLU:HG2	2.11	0.49
2:C:180:LEU:HD12	2:C:184:ASP:HB2	1.94	0.49
2:D:104:LEU:HG	2:D:347:ALA:HB2	1.94	0.49
2:D:216:LEU:HD21	2:D:254:ARG:HG2	1.92	0.49
2:B:265:SER:HA	2:B:269:MET:O	2.12	0.49
2:C:58:ALA:O	2:C:61:LYS:HB3	2.11	0.49
2:C:120:THR:CG2	2:C:362:TYR:CD1	2.95	0.49
2:D:148:THR:HG22	2:D:149:THR:HG23	1.94	0.49
2:D:335:ARG:CZ	2:D:335:ARG:HB3	2.35	0.49
1:A:195:LYS:CG	1:A:236:TYR:CE1	2.96	0.49
2:B:223:PHE:CE1	2:B:259:GLU:HG2	2.47	0.49
2:B:242:LEU:HD12	2:B:243:PRO:CD	2.41	0.49
2:B:249:THR:HG22	2:B:250:ILE:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:ILE:HG13	2:B:290:ARG:N	2.26	0.49
2:D:88:HIS:O	2:D:92:ASN:HB2	2.12	0.49
1:A:154:ARG:CD	2:D:231:ALA:CA	2.91	0.49
2:B:92:ASN:HD22	2:B:92:ASN:N	2.10	0.49
2:B:358:SER:O	2:B:361:GLU:HG2	2.11	0.49
2:C:192:ILE:O	2:C:195:GLU:HG3	2.13	0.49
2:C:305:MET:HG3	4:C:401:ADP:N6	2.26	0.49
2:D:140:LEU:HD12	2:D:140:LEU:N	2.27	0.49
2:D:313:MET:O	2:D:317:ILE:HG12	2.12	0.49
2:B:120:THR:HG22	2:B:362:TYR:HE1	1.77	0.49
2:D:3:ASP:CG	2:D:4:ASP:H	2.20	0.49
2:D:40:HIS:O	2:D:41:GLN:HB3	2.12	0.49
2:D:50:LYS:CG	2:D:53:TYR:CZ	2.95	0.49
2:B:41:GLN:CG	2:B:42:GLY:H	2.25	0.49
2:B:54:VAL:HA	2:B:58:ALA:CB	2.41	0.49
2:C:349:LEU:CD2	2:C:352:PHE:CD1	2.95	0.49
2:D:34:ILE:HG21	2:D:69:TYR:CZ	2.47	0.49
2:D:70:PRO:O	2:D:77:THR:N	2.42	0.49
2:D:105:LEU:CG	2:D:123:MET:HE2	2.43	0.49
2:B:7:ALA:HB2	2:B:356:TRP:CZ2	2.47	0.49
2:B:94:LEU:HB3	2:B:96:VAL:HG13	1.94	0.49
2:B:214:GLU:HG2	2:B:215:LYS:N	2.27	0.49
2:B:216:LEU:CD2	2:B:250:ILE:HG12	2.42	0.49
2:B:259:GLU:HG3	2:B:266:PHE:CZ	2.47	0.49
2:B:299:LEU:HD12	2:B:299:LEU:N	2.28	0.49
2:C:282:ILE:HD12	2:C:290:ARG:HD3	1.95	0.49
2:C:341:ILE:HG22	2:C:345:ILE:CD1	2.43	0.49
2:D:72:GLU:C	2:D:74:GLY:H	2.21	0.49
1:A:155:TRP:NE1	1:A:252:TYR:CZ	2.81	0.49
2:B:104:LEU:CD2	2:B:347:ALA:CB	2.91	0.49
2:D:8:LEU:HD23	2:D:8:LEU:N	2.28	0.49
2:D:92:ASN:HD22	2:D:92:ASN:N	2.10	0.49
1:A:150:TYR:CE2	1:A:152:PHE:HA	2.47	0.49
2:B:14:SER:HA	2:B:71:ILE:CG2	2.39	0.49
2:B:28:ARG:HB3	2:B:28:ARG:NH1	2.28	0.49
2:B:35:VAL:N	2:B:54:VAL:HG21	2.27	0.49
2:C:82:MET:HE2	2:C:86:TRP:CE2	2.48	0.49
2:C:104:LEU:HD13	2:C:356:TRP:CH2	2.47	0.49
2:C:192:ILE:HB	2:C:256:ARG:CZ	2.43	0.49
1:A:173:PHE:HD1	1:A:254:ILE:O	1.96	0.49
2:B:41:GLN:HG3	2:B:42:GLY:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:MET:HG3	2:B:45:VAL:N	2.27	0.49
2:B:71:ILE:H	2:B:71:ILE:CD1	2.23	0.49
2:C:169:TYR:OH	2:D:40:HIS:HB3	2.12	0.49
1:A:218:LEU:CD1	1:A:220:ASP:H	2.25	0.48
2:B:32:PRO:HB2	2:B:34:ILE:HD13	1.94	0.48
2:C:305:MET:HG3	4:C:401:ADP:C5	2.45	0.48
2:B:148:THR:HG23	2:B:167:GLU:HA	1.94	0.48
2:B:184:ASP:HB3	2:B:267:LEU:HD13	1.94	0.48
2:B:251:GLY:C	2:B:254:ARG:HG3	2.38	0.48
2:C:9:VAL:CG2	2:C:104:LEU:HD23	2.08	0.48
2:C:12:ASN:OD1	2:C:82:MET:HE1	2.13	0.48
2:C:358:SER:H	2:C:361:GLU:CD	2.21	0.48
1:A:171:SER:O	1:A:255:CYS:HA	2.13	0.48
2:B:329:ILE:HD12	2:B:329:ILE:N	2.28	0.48
2:C:196:ARG:HH22	2:C:250:ILE:CA	2.22	0.48
2:C:285:CYS:HB3	2:C:289:ILE:CG1	2.43	0.48
2:C:286:ASP:O	2:C:289:ILE:HG12	2.12	0.48
2:D:133:TYR:CD1	2:D:357:ILE:CD1	2.95	0.48
2:B:129:THR:HG23	2:B:131:ALA:N	2.29	0.48
2:B:190:MET:SD	2:B:206:ARG:HA	2.52	0.48
2:B:264:PRO:HG2	2:B:271:SER:O	2.13	0.48
2:C:353:GLN:HA	2:C:356:TRP:CD1	2.48	0.48
2:D:34:ILE:HG21	2:D:69:TYR:CE1	2.49	0.48
2:D:152:VAL:CG2	2:D:298:VAL:HG12	2.44	0.48
2:D:162:THR:HG23	2:D:277:THR:HG21	1.94	0.48
2:D:180:LEU:HD12	2:D:181:ALA:N	2.28	0.48
2:B:17:CYS:HB3	2:B:31:PHE:CE1	2.49	0.48
2:B:104:LEU:CD2	2:B:347:ALA:HB2	2.43	0.48
2:C:11:ASP:HB3	2:C:18:LYS:CE	2.31	0.48
2:C:208:ILE:HG22	2:C:212:ILE:CD1	2.43	0.48
2:C:351:THR:OG1	2:C:352:PHE:HD1	1.96	0.48
2:D:264:PRO:HG2	2:D:271:SER:O	2.13	0.48
2:B:53:TYR:N	2:B:53:TYR:HD1	2.12	0.48
2:B:133:TYR:CE1	2:B:355:MET:HG2	2.48	0.48
2:B:21:PHE:N	2:B:21:PHE:CD1	2.82	0.48
2:B:163:VAL:CG1	2:B:175:ILE:HD12	2.43	0.48
2:B:216:LEU:HD21	2:B:250:ILE:CD1	2.43	0.48
2:C:8:LEU:H	2:C:103:VAL:HA	1.79	0.48
2:C:104:LEU:HD13	2:C:133:TYR:CB	2.43	0.48
2:C:289:ILE:O	2:C:293:LEU:HD12	2.14	0.48
2:D:279:PHE:CZ	2:D:283:MET:CE	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:CG	1:A:253:PHE:CE1	2.96	0.48
2:B:129:THR:HG23	2:B:131:ALA:H	1.77	0.48
2:B:148:THR:HG22	2:B:149:THR:N	2.26	0.48
2:D:299:LEU:C	2:D:335:ARG:HD3	2.39	0.48
2:B:240:TYR:O	2:B:247:VAL:HG23	2.14	0.48
2:B:362:TYR:CD1	2:B:367:PRO:HA	2.49	0.48
2:C:193:LEU:HD13	2:C:200:PHE:CE1	2.48	0.48
2:C:332:PRO:HD2	2:C:335:ARG:NE	2.28	0.48
2:C:349:LEU:HB3	2:C:352:PHE:HB2	1.95	0.48
2:D:120:THR:HA	2:D:132:MET:SD	2.54	0.48
2:D:189:LEU:HA	2:D:192:ILE:HD13	1.95	0.48
2:B:211:ASP:O	2:B:215:LYS:HG3	2.13	0.48
2:C:299:LEU:N	2:C:299:LEU:HD12	2.28	0.48
2:D:163:VAL:HG23	2:D:163:VAL:O	2.14	0.48
2:D:180:LEU:HD11	2:D:185:LEU:HD22	1.93	0.48
2:B:35:VAL:CG1	2:B:68:LYS:HB2	2.31	0.47
2:B:136:ILE:HG22	2:B:139:VAL:CB	2.44	0.47
2:C:27:PRO:HG3	2:C:340:TRP:CB	2.43	0.47
2:C:198:TYR:CE1	2:C:248:ILE:HG22	2.49	0.47
2:C:294:TYR:CG	2:C:325:MET:CE	2.97	0.47
2:D:86:TRP:CE3	2:D:122:ILE:HG21	2.48	0.47
2:D:126:THR:HG23	2:D:127:PHE:CD2	2.49	0.47
2:D:148:THR:HG22	2:D:167:GLU:HA	1.90	0.47
2:D:185:LEU:HD21	2:D:261:LEU:CD1	2.44	0.47
2:D:244:ASP:OD2	2:D:246:GLN:HG3	2.14	0.47
2:D:305:MET:HG3	4:D:401:ADP:N6	2.26	0.47
2:B:121:GLN:HE21	2:B:122:ILE:N	2.12	0.47
2:B:39:ARG:HH22	2:B:203:THR:CG2	2.26	0.47
2:B:103:VAL:O	2:B:132:MET:HA	2.13	0.47
2:B:294:TYR:CG	2:B:325:MET:HE2	2.49	0.47
2:C:81:ASP:O	2:C:84:LYS:HB2	2.13	0.47
2:C:176:LEU:HD13	2:C:176:LEU:N	2.29	0.47
2:C:335:ARG:CZ	2:C:335:ARG:CB	2.91	0.47
2:D:43:VAL:HG13	2:D:44:MET:N	2.29	0.47
2:D:137:GLN:HB3	2:D:339:VAL:CG1	2.40	0.47
1:A:173:PHE:CE2	1:A:237:LEU:CD1	2.96	0.47
2:B:365:SER:CB	2:B:369:ILE:HB	2.44	0.47
2:C:34:ILE:HG22	2:C:69:TYR:CG	2.49	0.47
2:C:153:MET:O	2:C:299:LEU:HA	2.14	0.47
2:C:358:SER:H	2:C:361:GLU:HG2	1.78	0.47
2:D:8:LEU:O	2:D:104:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:VAL:HG12	2:D:175:ILE:CG1	2.43	0.47
2:D:211:ASP:OD1	2:D:215:LYS:HD2	2.14	0.47
2:B:31:PHE:N	2:B:31:PHE:CD1	2.82	0.47
2:B:61:LYS:HB3	2:B:64:ILE:HG22	1.97	0.47
2:B:69:TYR:N	2:B:69:TYR:CD1	2.83	0.47
2:B:159:VAL:HG22	2:B:160:THR:H	1.77	0.47
2:B:181:ALA:O	2:B:185:LEU:HD23	2.15	0.47
2:B:309:ILE:HG12	2:B:310:ALA:N	2.30	0.47
2:C:148:THR:HG22	2:C:167:GLU:HA	1.97	0.47
2:D:122:ILE:HG22	2:D:123:MET:N	2.28	0.47
2:B:26:ALA:HB1	2:B:27:PRO:HD2	1.97	0.47
2:B:34:ILE:HD13	2:B:34:ILE:N	2.30	0.47
2:B:212:ILE:HG23	2:B:216:LEU:HD13	1.96	0.47
2:B:369:ILE:HG23	2:B:370:VAL:N	2.29	0.47
2:C:362:TYR:CE1	2:C:367:PRO:HG3	2.50	0.47
2:D:53:TYR:CD1	2:D:53:TYR:N	2.81	0.47
2:D:104:LEU:CD2	2:D:347:ALA:CB	2.92	0.47
2:D:110:LEU:HD23	2:D:110:LEU:C	2.40	0.47
2:D:152:VAL:HA	2:D:298:VAL:H	1.78	0.47
2:D:263:GLN:O	2:D:266:PHE:HD1	1.96	0.47
1:A:195:LYS:HG2	1:A:236:TYR:CE1	2.50	0.47
2:B:39:ARG:HH21	2:B:66:THR:HA	1.79	0.47
2:B:104:LEU:HD13	2:B:356:TRP:CZ3	2.50	0.47
2:B:163:VAL:HG12	2:B:175:ILE:HD12	1.95	0.47
2:B:209:VAL:O	2:B:212:ILE:HB	2.14	0.47
2:B:287:VAL:HG13	2:B:288:ASP:N	2.28	0.47
2:B:305:MET:HG3	4:B:401:ADP:N6	2.26	0.47
2:C:73:HIC:HA	2:C:183:ARG:HH12	1.78	0.47
2:C:94:LEU:O	2:C:95:ARG:HB2	2.14	0.47
2:C:303:THR:O	2:C:303:THR:HG22	2.15	0.47
2:C:359:LYS:HE2	2:C:359:LYS:HB2	1.50	0.47
2:D:65:LEU:CD1	2:D:67:LEU:HD23	2.44	0.47
2:D:71:ILE:CG2	2:D:74:GLY:C	2.87	0.47
2:B:16:MET:HG3	2:B:31:PHE:O	2.14	0.47
2:B:120:THR:HA	2:B:132:MET:SD	2.55	0.47
2:C:104:LEU:HG	2:C:347:ALA:HB2	1.96	0.47
2:C:264:PRO:HG2	2:C:271:SER:O	2.15	0.47
2:C:345:ILE:HG22	2:C:349:LEU:CD1	2.44	0.47
2:D:120:THR:HG22	2:D:124:PHE:CD2	2.50	0.47
2:D:190:MET:HE1	2:D:206:ARG:CA	2.45	0.47
1:A:231:GLY:O	1:A:232:GLN:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:TYR:CD1	2:B:53:TYR:N	2.83	0.47
2:B:104:LEU:CG	2:B:347:ALA:HB2	2.42	0.47
2:B:176:LEU:HD23	2:B:177:ARG:O	2.14	0.47
2:B:264:PRO:CB	2:B:269:MET:HB3	2.45	0.47
2:C:8:LEU:HD23	2:C:101:HIS:HB3	1.96	0.47
2:C:13:GLY:HA3	2:C:18:LYS:NZ	2.29	0.47
2:C:163:VAL:O	2:C:163:VAL:HG23	2.15	0.47
2:C:164:PRO:HB3	2:C:293:LEU:HD21	1.95	0.47
2:C:206:ARG:HG3	2:C:207:GLU:N	2.30	0.47
2:D:303:THR:O	2:D:303:THR:HG22	2.15	0.47
1:A:197:TRP:CE2	1:A:251:LYS:CB	2.94	0.47
2:B:120:THR:HG21	2:B:367:PRO:HB3	1.96	0.47
1:A:195:LYS:HD2	1:A:251:LYS:HE3	1.93	0.46
2:B:190:MET:O	2:B:194:THR:HG23	2.15	0.46
2:C:129:THR:OG1	2:C:130:PRO:HD2	2.15	0.46
2:C:176:LEU:HD13	2:C:176:LEU:H	1.79	0.46
2:D:79:TRP:CE2	2:D:118:LYS:HG2	2.50	0.46
2:D:166:TYR:O	2:D:167:GLU:HG3	2.15	0.46
2:D:192:ILE:O	2:D:195:GLU:HG3	2.15	0.46
2:D:264:PRO:HB2	2:D:269:MET:HB2	1.96	0.46
1:A:156:GLU:CG	1:A:253:PHE:HE1	2.29	0.46
1:A:158:TRP:CG	1:A:234:CYS:SG	3.06	0.46
1:A:195:LYS:HG2	1:A:236:TYR:HE1	1.81	0.46
1:A:195:LYS:NZ	2:B:118:LYS:HZ1	2.13	0.46
1:A:218:LEU:HD12	1:A:221:LEU:HD22	1.96	0.46
1:A:238:LYS:HB2	1:A:243:ILE:HD12	1.97	0.46
2:B:152:VAL:HA	2:B:298:VAL:O	2.16	0.46
2:C:184:ASP:HB3	2:C:267:LEU:CD1	2.46	0.46
2:C:219:VAL:HG22	2:C:220:ALA:N	2.30	0.46
2:C:242:LEU:HD12	2:C:242:LEU:HA	1.72	0.46
2:D:94:LEU:HB3	2:D:96:VAL:HG13	1.98	0.46
2:D:190:MET:HG2	2:D:209:VAL:HG21	1.96	0.46
2:B:79:TRP:CD2	2:B:118:LYS:HG3	2.49	0.46
2:B:149:THR:HG22	2:B:167:GLU:H	1.80	0.46
2:B:206:ARG:HH11	2:B:206:ARG:HG3	1.81	0.46
2:B:370:VAL:HG13	2:B:371:HIS:H	1.81	0.46
2:C:280:ASN:O	2:C:284:LYS:HG3	2.16	0.46
2:D:122:ILE:O	2:D:126:THR:HG22	2.16	0.46
2:D:160:THR:HB	2:D:178:LEU:HB3	1.98	0.46
2:D:205:GLU:HA	2:D:208:ILE:HG13	1.97	0.46
2:D:282:ILE:HG23	2:D:290:ARG:CD	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:294:TYR:CD1	2:D:327:ILE:CD1	2.94	0.46
2:B:36:GLY:H	2:B:52:SER:CB	2.15	0.46
2:B:133:TYR:HE2	2:B:135:ALA:HB2	1.81	0.46
2:B:216:LEU:CD2	2:B:254:ARG:HG2	2.20	0.46
2:B:299:LEU:HD11	2:B:329:ILE:HG23	1.96	0.46
2:C:58:ALA:HB1	2:C:65:LEU:HD12	1.94	0.46
2:C:86:TRP:CD2	2:C:123:MET:HE1	2.51	0.46
2:D:265:SER:C	2:D:268:GLY:H	2.23	0.46
1:A:233:ILE:HG13	1:A:245:ASP:C	2.39	0.46
2:B:184:ASP:HB3	2:B:267:LEU:CD1	2.45	0.46
2:C:113:LYS:CG	2:C:371:HIS:CD2	2.97	0.46
2:C:143:TYR:CD1	2:C:143:TYR:C	2.94	0.46
2:D:113:LYS:HB2	2:D:371:HIS:CD2	2.51	0.46
2:D:133:TYR:HD1	2:D:357:ILE:HD13	1.81	0.46
2:D:242:LEU:CD1	2:D:243:PRO:HD2	2.45	0.46
2:D:272:CYS:HB3	2:D:276:GLU:CB	2.46	0.46
2:D:290:ARG:CA	2:D:293:LEU:HD13	2.44	0.46
2:B:8:LEU:HD23	2:B:101:HIS:HB2	1.98	0.46
2:B:82:MET:HA	2:B:82:MET:CE	2.33	0.46
2:B:152:VAL:CG1	2:B:163:VAL:CG2	2.94	0.46
2:C:18:LYS:N	2:C:18:LYS:HD3	2.30	0.46
2:C:120:THR:HG22	2:C:362:TYR:CE1	2.50	0.46
2:C:152:VAL:HG23	2:C:298:VAL:HB	1.97	0.46
2:C:287:VAL:CG2	2:D:244:ASP:N	2.76	0.46
2:B:176:LEU:HD21	2:B:277:THR:HG23	1.95	0.46
2:C:362:TYR:HE1	2:C:367:PRO:CG	2.29	0.46
2:D:5:ILE:HD13	2:D:5:ILE:H	1.78	0.46
2:D:78:ASN:ND2	2:D:81:ASP:OD2	2.49	0.46
2:D:86:TRP:CZ3	2:D:123:MET:HE1	2.50	0.46
2:D:158:GLY:CA	2:D:183:ARG:CZ	2.94	0.46
2:D:185:LEU:HD11	2:D:261:LEU:CD1	2.46	0.46
2:B:53:TYR:O	2:B:54:VAL:HB	2.16	0.46
2:B:70:PRO:HG3	2:B:81:ASP:HB2	1.97	0.46
2:B:148:THR:O	2:B:165:ILE:HG22	2.16	0.46
2:B:186:THR:HG22	2:B:213:LYS:HZ2	1.81	0.46
2:B:194:THR:O	2:C:110:LEU:HD13	2.16	0.46
2:B:216:LEU:CD2	2:B:250:ILE:CD1	2.94	0.46
2:D:321:ALA:HB1	2:D:322:PRO:CD	2.45	0.46
1:A:156:GLU:HB2	1:A:161:SER:HB3	1.98	0.46
1:A:202:GLN:HG2	1:A:207:GLY:HA2	1.98	0.46
2:B:7:ALA:HB2	2:B:356:TRP:HZ2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:73:HIC:C	2:C:75:ILE:H	2.28	0.46
2:C:361:GLU:CG	2:C:369:ILE:HG21	2.44	0.46
1:A:158:TRP:CD1	1:A:234:CYS:SG	3.09	0.46
1:A:199:GLY:HA3	1:A:211:TRP:CE3	2.49	0.46
2:B:107:GLU:OE1	2:B:116:ARG:HD3	2.16	0.46
2:B:117:GLU:OE2	2:B:368:SER:HB3	2.16	0.46
2:B:140:LEU:CD2	2:B:343:GLY:HA2	2.46	0.46
2:C:3:ASP:CG	2:C:4:ASP:H	2.24	0.46
2:C:153:MET:HE2	2:C:299:LEU:HB3	1.97	0.46
2:C:247:VAL:HG13	2:C:248:ILE:N	2.30	0.46
2:D:136:ILE:CG2	2:D:139:VAL:HB	2.39	0.46
2:D:180:LEU:CD2	2:D:261:LEU:HA	2.46	0.46
2:D:349:LEU:HD22	2:D:352:PHE:CE1	2.48	0.46
2:B:8:LEU:CD1	2:B:94:LEU:CD1	2.89	0.45
2:B:50:LYS:HG2	2:B:53:TYR:CZ	2.51	0.45
2:B:139:VAL:HG12	2:B:140:LEU:HD12	1.97	0.45
2:B:303:THR:O	2:B:303:THR:HG22	2.15	0.45
2:C:253:GLU:HA	2:C:256:ARG:HG2	1.97	0.45
2:C:314:GLN:CB	2:C:329:ILE:CD1	2.95	0.45
2:D:58:ALA:HB1	2:D:65:LEU:HD11	1.96	0.45
2:D:118:LYS:HD2	2:D:121:GLN:CG	2.46	0.45
2:D:129:THR:OG1	2:D:130:PRO:HD2	2.16	0.45
2:D:143:TYR:HE1	2:D:345:ILE:HG21	1.79	0.45
2:D:185:LEU:HD11	2:D:261:LEU:HD11	1.98	0.45
2:D:279:PHE:HZ	2:D:283:MET:HE1	1.81	0.45
2:B:81:ASP:O	2:B:84:LYS:HB2	2.15	0.45
2:B:335:ARG:CZ	2:B:335:ARG:CB	2.91	0.45
2:C:10:VAL:HG21	2:C:105:LEU:CD1	2.46	0.45
2:C:104:LEU:CD2	2:C:347:ALA:CB	2.91	0.45
2:C:286:ASP:H	2:C:289:ILE:HD11	1.81	0.45
2:D:34:ILE:C	2:D:54:VAL:HG21	2.41	0.45
2:D:299:LEU:CD2	2:D:309:ILE:CG1	2.95	0.45
2:B:31:PHE:HB2	2:B:32:PRO:HD2	1.97	0.45
2:D:11:ASP:CB	2:D:18:LYS:HD3	2.21	0.45
2:D:126:THR:HG23	2:D:127:PHE:N	2.32	0.45
2:D:186:THR:CG2	2:D:213:LYS:HZ1	2.29	0.45
1:A:152:PHE:CG	1:A:253:PHE:CE1	3.04	0.45
1:A:162:LYS:HD3	1:A:166:LEU:HD21	1.98	0.45
2:B:313:MET:O	2:B:317:ILE:HG12	2.16	0.45
2:C:299:LEU:N	2:C:299:LEU:CD1	2.80	0.45
2:C:317:ILE:O	2:C:320:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:THR:OG1	2:D:370:VAL:HG11	2.16	0.45
2:D:314:GLN:HA	2:D:329:ILE:HD11	1.99	0.45
1:A:195:LYS:CD	1:A:236:TYR:CE1	2.99	0.45
1:A:202:GLN:HE22	1:A:232:GLN:HE21	1.64	0.45
2:B:173:HIS:CE1	2:D:268:GLY:HA3	2.52	0.45
2:B:257:CYS:HB3	2:B:258:PRO:CD	2.37	0.45
2:B:293:LEU:H	2:B:293:LEU:CD1	2.27	0.45
2:C:50:LYS:HG2	2:C:53:TYR:CZ	2.52	0.45
2:C:190:MET:O	2:C:194:THR:HG23	2.17	0.45
2:B:41:GLN:HG3	2:B:42:GLY:H	1.81	0.45
2:B:218:TYR:CD1	2:B:218:TYR:C	2.95	0.45
2:B:238:LYS:HD2	2:B:254:ARG:NH1	2.32	0.45
2:C:13:GLY:HA3	2:C:16:MET:O	2.17	0.45
2:C:218:TYR:O	2:C:255:PHE:HA	2.17	0.45
2:C:223:PHE:CD1	2:C:259:GLU:HG3	2.51	0.45
2:C:290:ARG:CA	2:C:293:LEU:HD12	2.45	0.45
2:C:341:ILE:HG22	2:C:345:ILE:HD11	1.97	0.45
2:C:362:TYR:HE1	2:C:367:PRO:CB	2.28	0.45
2:D:34:ILE:HG13	2:D:67:LEU:HD22	1.98	0.45
2:D:144:ALA:HB2	2:D:341:ILE:HG22	1.99	0.45
2:D:162:THR:CG2	2:D:277:THR:CG2	2.95	0.45
2:D:190:MET:HE2	2:D:209:VAL:HB	1.99	0.45
1:A:195:LYS:CG	1:A:238:LYS:CD	2.94	0.45
2:B:28:ARG:CD	2:B:94:LEU:CD2	2.94	0.45
2:B:189:LEU:CD1	2:B:193:LEU:CD1	2.95	0.45
2:B:201:THR:CG2	2:B:202:THR:CG2	2.95	0.45
2:D:113:LYS:HB2	2:D:371:HIS:CG	2.52	0.45
2:D:335:ARG:CZ	2:D:335:ARG:CB	2.91	0.45
1:A:158:TRP:HD1	1:A:197:TRP:HB3	1.81	0.45
1:A:198:VAL:HG11	1:A:237:LEU:HG	1.98	0.45
1:A:202:GLN:NE2	1:A:232:GLN:HG3	2.32	0.45
1:A:218:LEU:CD1	1:A:221:LEU:CD2	2.95	0.45
2:B:34:ILE:HG22	2:B:68:LYS:C	2.42	0.45
2:B:133:TYR:CE1	2:B:355:MET:HG3	2.52	0.45
2:B:321:ALA:HB1	2:B:322:PRO:CD	2.44	0.45
2:C:104:LEU:CD2	2:C:104:LEU:N	2.80	0.45
2:C:107:GLU:CG	2:C:111:ASN:HD22	2.30	0.45
2:D:335:ARG:O	2:D:338:SER:HB3	2.17	0.45
1:A:152:PHE:CE2	1:A:154:ARG:HB2	2.52	0.45
1:A:155:TRP:CZ3	2:B:117:GLU:OE1	2.69	0.45
1:A:232:GLN:O	1:A:233:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:CB	1:A:243:ILE:CD1	2.95	0.45
2:B:236:LEU:HD12	2:B:237:GLU:HG2	1.99	0.45
2:C:133:TYR:CD1	2:C:357:ILE:CD1	2.95	0.45
2:D:54:VAL:CG1	2:D:58:ALA:CB	2.94	0.45
2:D:106:THR:CG2	2:D:140:LEU:CD2	2.93	0.45
2:D:151:ILE:O	2:D:297:THR:HA	2.16	0.45
2:D:203:THR:HA	2:D:206:ARG:HG3	1.99	0.45
2:D:279:PHE:CZ	2:D:283:MET:HE1	2.52	0.45
1:A:197:TRP:NE1	1:A:251:LYS:HB2	2.30	0.45
1:A:200:VAL:HG22	1:A:209:TRP:HE3	1.82	0.45
2:B:7:ALA:HB1	2:B:356:TRP:CZ2	2.51	0.45
2:B:82:MET:HE3	2:B:85:ILE:HD12	1.98	0.45
2:B:124:PHE:CE2	2:B:132:MET:HG2	2.52	0.45
2:B:370:VAL:HG23	2:B:375:PHE:C	2.41	0.45
2:C:5:ILE:HG13	2:C:102:PRO:HG2	1.99	0.45
2:C:104:LEU:HD22	2:C:356:TRP:CH2	2.48	0.45
2:C:359:LYS:HG3	2:C:360:GLN:N	2.31	0.45
2:D:86:TRP:CE3	2:D:123:MET:HE1	2.51	0.45
2:D:103:VAL:CG1	2:D:105:LEU:CD2	2.95	0.45
2:D:193:LEU:HA	2:D:193:LEU:HD23	1.74	0.45
2:D:371:HIS:HD2	2:D:372:ARG:NE	2.15	0.45
1:A:195:LYS:CE	2:B:118:LYS:HZ1	2.30	0.44
2:B:13:GLY:O	2:B:71:ILE:HG21	2.17	0.44
2:B:175:ILE:HG23	2:B:175:ILE:O	2.16	0.44
2:C:29:ALA:HB1	2:C:93:GLU:HG2	1.99	0.44
2:C:79:TRP:CD1	2:C:118:LYS:HE2	2.51	0.44
2:C:99:GLU:HA	2:C:128:ASN:O	2.17	0.44
2:C:154:ASP:HA	2:C:300:SER:HB2	1.98	0.44
2:C:178:LEU:HD21	2:C:271:SER:OG	2.17	0.44
2:C:236:LEU:HD12	2:C:236:LEU:C	2.42	0.44
2:D:155:SER:CB	2:D:303:THR:HB	2.47	0.44
2:D:332:PRO:HA	2:D:333:PRO:HD3	1.51	0.44
1:A:218:LEU:CD1	1:A:220:ASP:CB	2.95	0.44
1:A:237:LEU:HA	1:A:237:LEU:HD23	1.64	0.44
2:B:94:LEU:HD23	2:B:94:LEU:HA	1.66	0.44
2:B:110:LEU:CD2	2:D:195:GLU:CA	2.95	0.44
2:B:180:LEU:CD1	2:B:267:LEU:CD1	2.93	0.44
2:B:189:LEU:HD11	2:B:193:LEU:CD1	2.47	0.44
2:C:13:GLY:O	2:C:71:ILE:HG21	2.17	0.44
2:C:71:ILE:CD1	2:C:85:ILE:HD11	2.46	0.44
2:C:249:THR:HG22	2:C:250:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:PHE:HD1	2:D:28:ARG:NE	2.15	0.44
2:B:37:ARG:H	2:B:66:THR:HG22	1.81	0.44
2:C:53:TYR:CD1	2:C:53:TYR:N	2.85	0.44
2:C:61:LYS:HE3	2:C:64:ILE:CG2	2.41	0.44
2:C:64:ILE:O	2:C:64:ILE:HD13	2.18	0.44
2:C:218:TYR:CE2	2:C:254:ARG:CZ	2.94	0.44
2:D:223:PHE:HB2	2:D:259:GLU:OE2	2.17	0.44
2:D:247:VAL:HG13	2:D:247:VAL:O	2.16	0.44
2:B:32:PRO:HB2	2:B:34:ILE:HD11	2.00	0.44
2:C:140:LEU:C	2:C:342:GLY:HA3	2.42	0.44
2:C:218:TYR:CD1	2:C:218:TYR:C	2.96	0.44
2:D:216:LEU:HD22	2:D:250:ILE:CD1	2.47	0.44
2:D:221:LEU:HD22	2:D:221:LEU:N	2.27	0.44
2:D:264:PRO:HB3	2:D:269:MET:HB2	1.99	0.44
2:D:349:LEU:HB3	2:D:352:PHE:HB2	1.99	0.44
2:B:58:ALA:HB1	2:B:65:LEU:CD1	2.45	0.44
2:B:135:ALA:HB1	2:B:140:LEU:HD11	1.95	0.44
2:C:193:LEU:HA	2:C:193:LEU:HD23	1.67	0.44
2:D:8:LEU:HG	2:D:103:VAL:HG22	1.99	0.44
2:D:70:PRO:C	2:D:71:ILE:HG13	2.42	0.44
2:D:82:MET:HE3	2:D:85:ILE:HG13	1.98	0.44
2:D:120:THR:HG22	2:D:124:PHE:CE2	2.53	0.44
2:D:290:ARG:O	2:D:294:TYR:HD2	2.00	0.44
2:D:306:TYR:O	2:D:309:ILE:HD13	2.18	0.44
2:D:362:TYR:HE1	2:D:367:PRO:HG3	1.78	0.44
2:C:26:ALA:HB1	2:C:27:PRO:CD	2.47	0.44
2:C:218:TYR:O	2:C:258:PRO:HG2	2.17	0.44
2:C:305:MET:CG	4:C:401:ADP:C6	2.83	0.44
2:D:68:LYS:HD3	2:D:69:TYR:N	2.32	0.44
2:D:151:ILE:CG2	2:D:297:THR:HG22	2.47	0.44
2:D:306:TYR:HB2	2:D:309:ILE:HG23	1.99	0.44
1:A:195:LYS:HE2	1:A:236:TYR:OH	2.16	0.44
2:B:20:GLY:HA2	2:B:28:ARG:CD	2.46	0.44
2:B:110:LEU:CD2	2:D:195:GLU:HB2	2.43	0.44
2:C:86:TRP:CE3	2:C:122:ILE:HG21	2.51	0.44
2:C:151:ILE:O	2:C:297:THR:HA	2.17	0.44
2:C:169:TYR:CZ	2:D:40:HIS:HB3	2.52	0.44
1:A:150:TYR:HE2	1:A:152:PHE:HA	1.83	0.44
1:A:152:PHE:HE2	1:A:154:ARG:HB2	1.82	0.44
1:A:157:MET:H	1:A:160:ILE:CG2	2.30	0.44
1:A:181:MET:CE	1:A:242:LEU:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLY:HA2	2:B:66:THR:O	2.18	0.44
2:B:104:LEU:HD13	2:B:356:TRP:CH2	2.52	0.44
2:C:121:GLN:HG3	2:C:122:ILE:H	1.78	0.44
2:D:36:GLY:N	2:D:54:VAL:CG2	2.81	0.44
2:D:143:TYR:OH	2:D:349:LEU:HD11	2.17	0.44
2:D:294:TYR:CD1	2:D:327:ILE:HD11	2.53	0.44
2:D:357:ILE:HA	2:D:361:GLU:OE2	2.18	0.44
2:D:364:GLU:CG	2:D:365:SER:N	2.81	0.44
1:A:151:VAL:HG21	1:A:187:ILE:CD1	2.47	0.44
1:A:155:TRP:CD1	1:A:155:TRP:N	2.85	0.44
1:A:200:VAL:HG23	1:A:210:PHE:O	2.17	0.44
2:B:99:GLU:O	2:B:130:PRO:HG3	2.18	0.44
2:B:132:MET:HE3	2:B:132:MET:HB2	1.90	0.44
2:D:2:ASP:HB3	2:D:3:ASP:H	1.44	0.44
2:D:99:GLU:HG3	2:D:128:ASN:OD1	2.17	0.44
1:A:226:ARG:HG3	1:A:227:GLN:N	2.33	0.43
2:B:7:ALA:CB	2:B:356:TRP:CH2	2.98	0.43
2:B:287:VAL:HA	2:B:290:ARG:HG3	2.00	0.43
2:C:220:ALA:HB1	2:C:226:GLU:CG	2.48	0.43
2:D:103:VAL:HG12	2:D:105:LEU:HD23	2.00	0.43
2:D:317:ILE:CD1	2:D:327:ILE:CG2	2.96	0.43
2:B:43:VAL:O	2:B:44:MET:HB3	2.18	0.43
2:B:140:LEU:C	2:B:342:GLY:HA3	2.42	0.43
2:B:152:VAL:HG23	2:B:298:VAL:CB	2.49	0.43
2:B:345:ILE:HG22	2:B:349:LEU:HD11	1.99	0.43
2:C:113:LYS:CG	2:C:371:HIS:NE2	2.81	0.43
2:C:236:LEU:HD12	2:C:237:GLU:CA	2.48	0.43
2:C:362:TYR:HE1	2:C:367:PRO:HG3	1.83	0.43
2:D:44:MET:HG3	2:D:45:VAL:C	2.42	0.43
2:D:62:ARG:O	2:D:65:LEU:HD23	2.18	0.43
2:D:191:LYS:HA	2:D:191:LYS:CE	2.49	0.43
1:A:170:ALA:HA	1:A:257:LYS:HG2	2.00	0.43
2:B:149:THR:HG23	2:B:167:GLU:H	1.80	0.43
2:B:176:LEU:CD2	2:B:277:THR:HG21	2.33	0.43
2:B:194:THR:CG2	2:B:200:PHE:H	2.30	0.43
2:B:279:PHE:O	2:B:282:ILE:HG22	2.19	0.43
2:B:357:ILE:HD12	2:B:357:ILE:N	2.32	0.43
2:C:34:ILE:HG21	2:C:69:TYR:CZ	2.54	0.43
2:C:112:PRO:CG	2:C:115:ASN:HD21	2.31	0.43
2:C:358:SER:H	2:C:361:GLU:CG	2.31	0.43
2:D:107:GLU:HG2	2:D:111:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:HIS:NE2	2:D:177:ARG:CD	2.81	0.43
2:D:190:MET:HE2	2:D:209:VAL:CB	2.47	0.43
2:D:346:LEU:HA	2:D:349:LEU:CD1	2.41	0.43
1:A:165:CYS:HA	1:A:168:GLU:OE1	2.17	0.43
2:B:36:GLY:N	2:B:54:VAL:CG2	2.81	0.43
2:B:311:ASP:O	2:B:314:GLN:HG3	2.18	0.43
2:C:7:ALA:HB2	2:C:356:TRP:HZ2	1.83	0.43
2:D:39:ARG:HE	2:D:66:THR:CB	2.32	0.43
2:D:208:ILE:HD13	2:D:243:PRO:CD	2.48	0.43
1:A:182:GLU:C	1:A:182:GLU:CD	2.86	0.43
1:A:202:GLN:OE1	1:A:207:GLY:HA2	2.19	0.43
2:B:50:LYS:HG2	2:B:53:TYR:CE2	2.53	0.43
2:B:64:ILE:CG2	2:B:65:LEU:N	2.81	0.43
2:B:104:LEU:HD13	2:B:133:TYR:HB3	1.99	0.43
2:D:270:GLU:HA	2:D:270:GLU:OE1	2.18	0.43
2:D:324:THR:CG2	2:D:325:MET:N	2.82	0.43
2:D:369:ILE:CG2	2:D:370:VAL:N	2.81	0.43
1:A:139:HIS:O	1:A:141:TRP:HD1	2.02	0.43
1:A:154:ARG:CD	2:D:231:ALA:HB1	2.49	0.43
2:B:16:MET:SD	2:B:30:VAL:CG2	3.07	0.43
2:B:126:THR:CG2	2:B:127:PHE:CD2	3.01	0.43
2:B:172:PRO:O	2:B:175:ILE:HG22	2.19	0.43
2:B:317:ILE:HD11	2:B:327:ILE:HG23	1.99	0.43
2:C:297:THR:OG1	2:C:329:ILE:HA	2.18	0.43
2:C:300:SER:HA	2:C:335:ARG:HH11	1.83	0.43
2:D:8:LEU:HD13	2:D:94:LEU:HD13	2.01	0.43
2:D:65:LEU:CD1	2:D:67:LEU:CD2	2.95	0.43
2:D:92:ASN:HD22	2:D:92:ASN:H	1.67	0.43
2:D:218:TYR:CD1	2:D:218:TYR:C	2.97	0.43
2:D:282:ILE:HD11	2:D:293:LEU:HB2	2.01	0.43
2:D:294:TYR:CD2	2:D:325:MET:CE	3.01	0.43
1:A:165:CYS:SG	1:A:171:SER:HA	2.59	0.43
1:A:202:GLN:HG2	1:A:207:GLY:C	2.43	0.43
2:B:190:MET:HG2	2:B:209:VAL:HG11	1.99	0.43
2:B:285:CYS:SG	2:B:289:ILE:HD11	2.59	0.43
2:C:21:PHE:CD1	2:C:28:ARG:NE	2.86	0.43
2:C:54:VAL:CG1	2:C:55:GLY:H	2.30	0.43
2:C:104:LEU:HD22	2:C:104:LEU:H	1.82	0.43
2:C:161:HIS:NE2	2:C:177:ARG:CD	2.82	0.43
2:C:166:TYR:O	2:C:167:GLU:HG3	2.19	0.43
2:C:261:LEU:HD21	2:C:303:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LYS:CB	2:B:53:TYR:CE1	2.95	0.43
2:B:105:LEU:CB	2:B:134:VAL:HG22	2.49	0.43
2:B:315:LYS:HB2	2:B:315:LYS:HE2	1.88	0.43
2:C:140:LEU:HD12	2:C:140:LEU:N	2.34	0.43
2:C:257:CYS:HB3	2:C:258:PRO:CD	2.38	0.43
2:C:299:LEU:O	2:C:335:ARG:HD3	2.19	0.43
2:C:370:VAL:CG1	2:C:371:HIS:N	2.82	0.43
2:D:20:GLY:HA2	2:D:28:ARG:CG	2.48	0.43
2:D:21:PHE:CD1	2:D:28:ARG:NE	2.87	0.43
2:D:81:ASP:HA	2:D:84:LYS:HD3	2.01	0.43
2:D:151:ILE:CG2	2:D:293:LEU:HB3	2.48	0.43
2:D:300:SER:O	2:D:304:THR:HG23	2.18	0.43
2:D:354:GLN:HG3	2:D:355:MET:N	2.33	0.43
1:A:236:TYR:CD2	1:A:236:TYR:N	2.81	0.43
1:A:236:TYR:O	1:A:236:TYR:CG	2.71	0.43
2:B:120:THR:OG1	2:B:370:VAL:HG11	2.18	0.43
2:B:255:PHE:C	2:B:258:PRO:HD2	2.43	0.43
2:C:5:ILE:N	2:C:5:ILE:CD1	2.82	0.43
2:C:64:ILE:CG2	2:C:65:LEU:N	2.82	0.43
2:D:35:VAL:CG2	2:D:52:SER:CB	2.94	0.43
2:D:300:SER:N	2:D:335:ARG:HD3	2.33	0.43
2:B:332:PRO:HA	2:B:333:PRO:HD3	1.62	0.43
2:C:10:VAL:CG2	2:C:105:LEU:HA	2.46	0.43
2:C:139:VAL:HG12	2:C:140:LEU:HD12	1.99	0.43
2:C:139:VAL:HG13	2:C:140:LEU:N	2.33	0.43
2:C:163:VAL:HG12	2:C:175:ILE:CD1	2.48	0.43
2:C:261:LEU:N	2:C:261:LEU:CD1	2.82	0.43
2:D:106:THR:HB	2:D:137:GLN:HG2	2.00	0.43
2:D:140:LEU:N	2:D:140:LEU:CD1	2.82	0.43
2:D:178:LEU:HD13	2:D:179:ASP:H	1.83	0.43
2:D:346:LEU:CA	2:D:349:LEU:HD12	2.41	0.43
1:A:157:MET:CG	1:A:160:ILE:HB	2.42	0.42
1:A:181:MET:CE	1:A:242:LEU:CD1	2.96	0.42
2:B:31:PHE:HB3	2:B:93:GLU:OE2	2.18	0.42
2:B:41:GLN:CG	2:B:42:GLY:N	2.82	0.42
2:B:122:ILE:HG23	2:B:126:THR:HG22	2.01	0.42
2:B:188:TYR:HB2	2:B:267:LEU:HD21	1.99	0.42
2:C:220:ALA:HB1	2:C:226:GLU:HG3	2.01	0.42
2:D:21:PHE:CZ	2:D:96:VAL:CG1	3.02	0.42
2:D:49:GLN:HG2	2:D:50:LYS:H	1.84	0.42
2:D:73:HIC:O	2:D:75:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:LEU:CB	2:D:352:PHE:HB2	2.49	0.42
1:A:195:LYS:CB	1:A:236:TYR:CD1	2.95	0.42
2:B:153:MET:HG3	2:B:153:MET:O	2.19	0.42
2:C:76:VAL:HG22	2:C:82:MET:SD	2.59	0.42
2:C:150:GLY:HA2	2:C:296:ASN:HB2	2.01	0.42
2:C:198:TYR:HB3	2:C:200:PHE:CE1	2.54	0.42
2:C:282:ILE:CG2	2:C:283:MET:N	2.81	0.42
2:C:314:GLN:CG	2:C:315:LYS:N	2.82	0.42
2:D:8:LEU:HD13	2:D:94:LEU:CD1	2.49	0.42
2:D:38:PRO:HB3	2:D:41:GLN:H	1.83	0.42
2:D:180:LEU:CG	2:D:181:ALA:N	2.82	0.42
1:A:156:GLU:HG3	1:A:253:PHE:CD1	2.53	0.42
1:A:160:ILE:CG2	1:A:161:SER:N	2.82	0.42
2:B:35:VAL:HA	2:B:54:VAL:CG2	2.45	0.42
2:B:136:ILE:O	2:B:140:LEU:HD12	2.19	0.42
2:C:9:VAL:HG11	2:C:343:GLY:C	2.44	0.42
2:C:76:VAL:CG2	2:C:82:MET:SD	3.08	0.42
2:C:101:HIS:O	2:C:103:VAL:HG23	2.19	0.42
2:C:189:LEU:O	2:C:192:ILE:HD12	2.19	0.42
2:C:345:ILE:CD1	2:C:345:ILE:N	2.82	0.42
2:D:35:VAL:C	2:D:54:VAL:HG21	2.44	0.42
2:D:66:THR:O	2:D:67:LEU:HD23	2.18	0.42
2:D:103:VAL:CG1	2:D:104:LEU:N	2.82	0.42
2:D:314:GLN:HA	2:D:317:ILE:HD11	2.00	0.42
1:A:157:MET:N	1:A:160:ILE:CG2	2.82	0.42
1:A:200:VAL:HG21	1:A:209:TRP:HB3	2.01	0.42
2:B:33:SER:O	2:B:34:ILE:HG23	2.19	0.42
2:B:189:LEU:HB2	2:B:257:CYS:SG	2.59	0.42
2:B:370:VAL:CG1	2:B:371:HIS:N	2.83	0.42
2:C:149:THR:HB	2:C:292:ASP:OD2	2.19	0.42
2:C:283:MET:HA	2:C:290:ARG:NH2	2.33	0.42
2:D:20:GLY:HA2	2:D:28:ARG:HG2	2.01	0.42
2:D:34:ILE:CG2	2:D:69:TYR:CE2	3.01	0.42
2:D:147:ARG:HE	2:D:147:ARG:HB3	1.72	0.42
2:D:282:ILE:CG1	2:D:293:LEU:HD22	2.49	0.42
2:D:299:LEU:HD21	2:D:309:ILE:HG13	2.00	0.42
1:A:195:LYS:HE2	1:A:236:TYR:HE1	1.83	0.42
1:A:196:TYR:C	1:A:236:TYR:HB2	2.44	0.42
1:A:228:ARG:CG	1:A:229:SER:N	2.82	0.42
2:B:345:ILE:HA	2:B:348:SER:OG	2.19	0.42
2:C:190:MET:HG3	2:C:209:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:VAL:HG12	2:D:55:GLY:H	1.84	0.42
2:D:174:ALA:O	2:D:284:LYS:HD2	2.19	0.42
2:D:189:LEU:HD12	2:D:209:VAL:HG22	2.01	0.42
2:D:362:TYR:CE1	2:D:367:PRO:CG	3.03	0.42
2:B:35:VAL:C	2:B:54:VAL:HG21	2.45	0.42
2:B:107:GLU:HG2	2:B:111:ASN:HB2	2.01	0.42
2:B:139:VAL:CG1	2:B:140:LEU:N	2.83	0.42
2:B:327:ILE:O	2:B:327:ILE:HG22	2.19	0.42
2:C:16:MET:SD	2:C:30:VAL:CG2	3.07	0.42
2:C:107:GLU:HG3	2:C:111:ASN:HD22	1.85	0.42
2:C:314:GLN:HB3	2:C:329:ILE:CD1	2.47	0.42
2:D:21:PHE:CZ	2:D:96:VAL:HG11	2.55	0.42
2:D:27:PRO:HG3	2:D:340:TRP:CG	2.54	0.42
1:A:194:ASN:HB2	1:A:196:TYR:CE1	2.55	0.42
2:B:71:ILE:HD11	2:B:85:ILE:HD13	1.98	0.42
2:B:152:VAL:HA	2:B:298:VAL:H	1.84	0.42
2:B:298:VAL:HG12	2:B:299:LEU:O	2.20	0.42
2:C:53:TYR:N	2:C:53:TYR:HD1	2.18	0.42
2:C:103:VAL:O	2:C:356:TRP:HZ3	2.02	0.42
2:C:110:LEU:O	2:C:112:PRO:HD3	2.19	0.42
2:D:58:ALA:HA	2:D:61:LYS:CB	2.43	0.42
2:D:102:PRO:HA	2:D:131:ALA:O	2.20	0.42
2:D:157:ASP:C	2:D:181:ALA:HB3	2.44	0.42
1:A:196:TYR:CD2	1:A:252:TYR:HB2	2.55	0.42
2:B:17:CYS:SG	2:B:31:PHE:HE1	2.42	0.42
2:B:21:PHE:O	2:B:24:ASP:HB2	2.20	0.42
2:B:105:LEU:HB2	2:B:134:VAL:HG22	2.00	0.42
2:B:110:LEU:CD2	2:D:195:GLU:CB	2.93	0.42
2:B:223:PHE:O	2:B:227:MET:HG2	2.19	0.42
2:B:295:ALA:O	2:B:328:LYS:HB3	2.20	0.42
2:C:39:ARG:HE	2:C:66:THR:CB	2.33	0.42
2:C:65:LEU:HD11	2:C:67:LEU:CD2	2.48	0.42
2:C:126:THR:HG23	2:C:127:PHE:CD2	2.55	0.42
2:C:133:TYR:HA	2:C:357:ILE:HD12	2.00	0.42
2:C:250:ILE:CG1	2:C:251:GLY:N	2.82	0.42
2:C:349:LEU:CB	2:C:352:PHE:HB2	2.49	0.42
2:D:152:VAL:HA	2:D:298:VAL:O	2.19	0.42
2:D:163:VAL:HG13	2:D:175:ILE:HG13	1.98	0.42
2:D:220:ALA:HB2	2:D:226:GLU:HG3	1.98	0.42
2:D:256:ARG:O	2:D:259:GLU:HB3	2.20	0.42
2:D:314:GLN:N	2:D:329:ILE:CD1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HG23	1:A:161:SER:N	2.34	0.42
1:A:200:VAL:N	1:A:211:TRP:CE3	2.88	0.42
2:B:189:LEU:HG	2:B:209:VAL:HG22	2.00	0.42
2:B:195:GLU:O	2:C:110:LEU:HD22	2.20	0.42
2:B:362:TYR:CE1	2:B:367:PRO:CG	3.03	0.42
2:C:49:GLN:CG	2:C:50:LYS:N	2.82	0.42
2:C:107:GLU:HG3	2:C:111:ASN:HB2	2.01	0.42
2:C:188:TYR:CZ	2:C:192:ILE:HG21	2.55	0.42
2:C:219:VAL:CG2	2:C:220:ALA:N	2.83	0.42
2:C:314:GLN:CB	2:C:329:ILE:HD13	2.47	0.42
2:D:31:PHE:N	2:D:31:PHE:CD1	2.87	0.42
2:D:50:LYS:CG	2:D:53:TYR:CE2	3.01	0.42
2:D:107:GLU:CG	2:D:111:ASN:CB	2.98	0.42
2:D:261:LEU:CD2	2:D:303:THR:CG2	2.94	0.42
1:A:222:LEU:HB3	1:A:223:PRO:CD	2.50	0.42
2:B:71:ILE:HG23	2:B:74:GLY:O	2.20	0.42
2:B:164:PRO:HG2	2:B:174:ALA:HB3	1.98	0.42
2:B:193:LEU:HD23	2:B:193:LEU:HA	1.78	0.42
2:B:250:ILE:HG13	2:B:251:GLY:H	1.80	0.42
2:C:22:ALA:HB1	2:C:348:SER:HB3	2.00	0.42
2:C:34:ILE:HG22	2:C:69:TYR:CD1	2.55	0.42
2:C:71:ILE:H	2:C:71:ILE:CD1	2.25	0.42
2:C:362:TYR:CD1	2:C:367:PRO:HA	2.55	0.42
2:D:47:MET:HB2	2:D:48:GLY:H	1.38	0.42
2:D:104:LEU:HD13	2:D:356:TRP:CH2	2.53	0.42
2:D:187:ASP:HA	2:D:190:MET:HG3	2.01	0.42
1:A:161:SER:HB2	1:A:253:PHE:CD2	2.55	0.41
1:A:218:LEU:HD13	1:A:220:ASP:H	1.84	0.41
2:B:50:LYS:CB	2:B:53:TYR:CD1	2.98	0.41
2:B:110:LEU:HD11	2:D:195:GLU:HA	1.94	0.41
2:B:166:TYR:HE1	2:B:292:ASP:OD2	2.03	0.41
2:B:357:ILE:CG2	2:B:358:SER:N	2.83	0.41
2:C:43:VAL:CG1	2:C:44:MET:N	2.80	0.41
2:C:118:LYS:HD2	2:C:121:GLN:CG	2.45	0.41
2:C:282:ILE:HG13	2:C:294:TYR:HE2	1.75	0.41
2:D:97:ALA:HA	2:D:98:PRO:HD3	1.76	0.41
2:D:133:TYR:CE1	2:D:355:MET:CG	3.03	0.41
2:D:178:LEU:CD1	2:D:179:ASP:N	2.83	0.41
2:D:180:LEU:HD21	2:D:261:LEU:HG	2.01	0.41
2:D:357:ILE:CD1	2:D:357:ILE:N	2.83	0.41
1:A:156:GLU:CD	1:A:253:PHE:HE1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:SER:CB	1:A:253:PHE:CG	3.00	0.41
2:B:240:TYR:C	2:B:247:VAL:HG23	2.44	0.41
2:C:361:GLU:HB2	2:C:369:ILE:HG21	2.01	0.41
2:D:32:PRO:CB	2:D:34:ILE:HD11	2.44	0.41
2:D:37:ARG:O	2:D:65:LEU:HA	2.21	0.41
2:D:218:TYR:O	2:D:255:PHE:HA	2.19	0.41
1:A:201:PHE:CG	1:A:202:GLN:N	2.89	0.41
2:B:201:THR:HG22	2:B:202:THR:CG2	2.48	0.41
2:B:247:VAL:O	2:B:247:VAL:HG13	2.20	0.41
2:B:263:GLN:CD	2:B:266:PHE:HE1	2.28	0.41
2:D:118:LYS:O	2:D:122:ILE:HD13	2.19	0.41
1:A:163:LYS:HD3	1:A:166:LEU:HD12	2.02	0.41
2:B:39:ARG:NE	2:B:66:THR:HA	2.34	0.41
2:B:101:HIS:HA	2:B:102:PRO:HD3	1.86	0.41
2:B:122:ILE:HG23	2:B:126:THR:CG2	2.51	0.41
2:B:126:THR:CG2	2:B:127:PHE:N	2.82	0.41
2:C:38:PRO:HA	2:C:64:ILE:HD13	2.02	0.41
2:C:53:TYR:O	2:C:54:VAL:HB	2.19	0.41
2:C:165:ILE:HD13	2:C:170:ALA:HA	2.03	0.41
2:C:169:TYR:CE1	2:D:42:GLY:O	2.73	0.41
2:C:362:TYR:CE1	2:C:367:PRO:CG	3.03	0.41
2:D:144:ALA:HB1	2:D:341:ILE:HG21	2.02	0.41
2:D:188:TYR:CZ	2:D:192:ILE:CG2	3.03	0.41
1:A:142:ILE:HD11	1:A:149:TYR:CB	2.25	0.41
2:B:155:SER:CB	2:B:303:THR:HB	2.49	0.41
2:B:159:VAL:CG2	2:B:160:THR:N	2.83	0.41
2:B:176:LEU:CD1	2:B:277:THR:CG2	2.92	0.41
2:B:218:TYR:HE2	2:B:254:ARG:HE	1.68	0.41
2:C:122:ILE:HG23	2:C:126:THR:HG21	2.02	0.41
2:C:216:LEU:HD22	2:C:250:ILE:HG12	2.00	0.41
2:D:18:LYS:CD	2:D:18:LYS:N	2.82	0.41
2:D:211:ASP:HA	2:D:214:GLU:CD	2.43	0.41
2:D:213:LYS:HA	2:D:217:CYS:SG	2.61	0.41
1:A:201:PHE:O	1:A:209:TRP:HA	2.21	0.41
1:A:216:SER:HA	1:A:217:PRO:HD3	1.86	0.41
2:B:267:LEU:HD23	2:B:267:LEU:HA	1.86	0.41
2:B:306:TYR:O	2:B:309:ILE:HD12	2.20	0.41
2:C:54:VAL:CA	2:C:58:ALA:HB2	2.37	0.41
2:C:329:ILE:N	2:C:329:ILE:CD1	2.82	0.41
2:D:104:LEU:HD22	2:D:356:TRP:CH2	2.55	0.41
2:D:191:LYS:HE3	2:D:191:LYS:CA	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:HG3	1:A:229:SER:H	1.85	0.41
2:B:8:LEU:HD11	2:B:94:LEU:HD12	1.95	0.41
2:B:18:LYS:HA	2:B:30:VAL:HG23	2.02	0.41
2:B:249:THR:CG2	2:B:250:ILE:N	2.84	0.41
2:B:317:ILE:CD1	2:B:327:ILE:CG2	2.99	0.41
2:D:31:PHE:CE1	2:D:93:GLU:OE1	2.73	0.41
2:D:133:TYR:CE1	2:D:355:MET:HG2	2.56	0.41
2:B:332:PRO:CD	2:B:335:ARG:HE	2.33	0.41
2:B:345:ILE:CG2	2:B:349:LEU:HD11	2.51	0.41
2:B:361:GLU:HG3	2:B:369:ILE:HG21	2.03	0.41
2:C:10:VAL:H	2:C:10:VAL:HG13	1.38	0.41
2:C:155:SER:CB	2:C:303:THR:HB	2.49	0.41
2:C:158:GLY:HA3	2:C:183:ARG:HH21	1.80	0.41
2:C:340:TRP:CH2	2:C:344:SER:HB3	2.55	0.41
1:A:153:GLU:O	1:A:252:TYR:HE2	2.04	0.41
1:A:154:ARG:HD2	2:D:231:ALA:CA	2.41	0.41
2:B:34:ILE:CG2	2:B:69:TYR:CE1	3.04	0.41
2:B:34:ILE:HG21	2:B:69:TYR:CZ	2.56	0.41
2:B:54:VAL:CG1	2:B:55:GLY:N	2.78	0.41
2:B:119:MET:HB3	2:B:119:MET:HE3	1.88	0.41
2:B:124:PHE:CE1	2:B:359:LYS:HA	2.56	0.41
2:B:129:THR:OG1	2:B:130:PRO:HD2	2.20	0.41
2:B:180:LEU:CD1	2:B:184:ASP:CB	2.96	0.41
2:B:359:LYS:O	2:B:362:TYR:HB3	2.20	0.41
2:C:279:PHE:HB2	2:C:320:LEU:HD12	2.01	0.41
2:D:16:MET:HE3	2:D:16:MET:HB2	1.84	0.41
2:D:21:PHE:HZ	2:D:96:VAL:CG1	2.34	0.41
2:D:64:ILE:CG2	2:D:65:LEU:N	2.83	0.41
2:D:104:LEU:CD2	2:D:104:LEU:N	2.81	0.41
2:D:116:ARG:NH1	2:D:134:VAL:HG12	2.35	0.41
2:D:164:PRO:HB3	2:D:293:LEU:HD21	2.03	0.41
2:D:208:ILE:HD13	2:D:243:PRO:HD2	2.03	0.41
2:D:314:GLN:O	2:D:318:THR:HG23	2.21	0.41
2:D:361:GLU:CG	2:D:369:ILE:HG21	2.48	0.41
1:A:175:ILE:HG21	1:A:181:MET:HB2	2.02	0.41
2:B:19:ALA:O	2:B:28:ARG:HG3	2.21	0.41
2:B:71:ILE:CD1	2:B:85:ILE:CD1	2.96	0.41
2:B:152:VAL:O	2:B:152:VAL:HG13	2.20	0.41
2:B:259:GLU:HG3	2:B:266:PHE:CE1	2.55	0.41
2:B:320:LEU:HD23	2:B:320:LEU:HA	1.87	0.41
2:B:365:SER:HB2	2:B:369:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:GLN:CG	2:C:42:GLY:N	2.81	0.41
2:D:124:PHE:O	2:D:128:ASN:HA	2.20	0.41
2:B:211:ASP:OD1	2:B:215:LYS:HD2	2.20	0.40
2:B:353:GLN:O	2:B:356:TRP:HD1	2.04	0.40
2:C:21:PHE:CD1	2:C:21:PHE:N	2.89	0.40
2:C:94:LEU:HD23	2:C:94:LEU:HA	1.87	0.40
2:D:18:LYS:HG2	2:D:340:TRP:HD1	1.85	0.40
2:D:34:ILE:CG2	2:D:69:TYR:CD1	3.04	0.40
2:D:73:HIC:HD2	2:D:183:ARG:NH1	2.36	0.40
2:D:305:MET:CG	4:D:401:ADP:C6	2.83	0.40
2:B:124:PHE:CZ	2:B:132:MET:HG2	2.57	0.40
2:B:302:GLY:HA3	4:B:401:ADP:O5'	2.21	0.40
2:C:254:ARG:O	2:C:258:PRO:HD2	2.21	0.40
2:D:8:LEU:HD11	2:D:96:VAL:HG21	2.01	0.40
2:D:10:VAL:HG23	2:D:12:ASN:OD1	2.20	0.40
2:D:31:PHE:CD1	2:D:93:GLU:OE1	2.74	0.40
2:D:54:VAL:HG13	2:D:58:ALA:HB2	2.01	0.40
2:D:103:VAL:HG11	2:D:105:LEU:CD2	2.52	0.40
2:D:162:THR:HG21	2:D:277:THR:CG2	2.51	0.40
2:D:208:ILE:HD13	2:D:243:PRO:HG2	2.03	0.40
2:D:358:SER:H	2:D:361:GLU:HG2	1.85	0.40
1:A:199:GLY:CA	1:A:211:TRP:HE3	2.33	0.40
2:B:47:MET:HB2	2:B:48:GLY:H	1.27	0.40
2:B:58:ALA:O	2:B:65:LEU:HD22	2.21	0.40
2:B:64:ILE:HG23	2:B:65:LEU:N	2.36	0.40
2:B:153:MET:SD	2:B:313:MET:SD	3.19	0.40
2:B:260:ALA:HA	2:B:263:GLN:O	2.20	0.40
2:B:297:THR:OG1	2:B:329:ILE:HA	2.21	0.40
2:C:68:LYS:HZ2	2:C:68:LYS:HG2	1.77	0.40
2:C:203:THR:O	2:C:206:ARG:HG2	2.21	0.40
2:C:209:VAL:CG1	2:C:210:ARG:N	2.82	0.40
2:D:31:PHE:HB2	2:D:32:PRO:CD	2.50	0.40
2:D:133:TYR:CD1	2:D:357:ILE:HD13	2.54	0.40
1:A:208:SER:OG	1:A:210:PHE:HE2	2.02	0.40
2:B:189:LEU:C	2:B:189:LEU:CD1	2.94	0.40
2:B:206:ARG:HH11	2:B:206:ARG:CG	2.35	0.40
2:B:252:ASN:HA	2:B:255:PHE:CE2	2.56	0.40
2:B:261:LEU:HD21	2:B:303:THR:HG21	2.01	0.40
2:C:34:ILE:CG2	2:C:69:TYR:CE1	3.05	0.40
2:C:152:VAL:HG23	2:C:298:VAL:O	2.21	0.40
2:C:218:TYR:HE2	2:C:254:ARG:NH2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:LEU:CD2	2:D:176:LEU:C	2.94	0.40
2:D:192:ILE:CG2	2:D:256:ARG:CZ	3.00	0.40
2:D:299:LEU:HD12	2:D:299:LEU:N	2.36	0.40
1:A:196:TYR:O	1:A:198:VAL:HG13	2.22	0.40
2:B:10:VAL:CG2	2:B:105:LEU:CD1	2.94	0.40
2:B:349:LEU:HB3	2:B:352:PHE:HB2	2.02	0.40
2:B:374:CYS:HB2	2:B:375:PHE:H	1.75	0.40
2:C:104:LEU:HD13	2:C:356:TRP:CZ3	2.56	0.40
2:C:265:SER:C	2:C:268:GLY:H	2.29	0.40
2:D:117:GLU:HA	2:D:367:PRO:HB2	2.02	0.40
2:D:212:ILE:O	2:D:216:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	129/131 (98%)	117 (91%)	7 (5%)	5 (4%)	2	19
2	B	371/374 (99%)	347 (94%)	16 (4%)	8 (2%)	5	29
2	C	371/374 (99%)	343 (92%)	22 (6%)	6 (2%)	7	38
2	D	371/374 (99%)	342 (92%)	23 (6%)	6 (2%)	7	38
All	All	1242/1253 (99%)	1149 (92%)	68 (6%)	25 (2%)	8	31

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	43	VAL
2	B	72	GLU
2	B	244	ASP
2	B	374	CYS

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Mol	Chain	Res	Type
2	C	43	VAL
2	C	44	MET
2	C	72	GLU
2	C	323	SER
2	D	76	VAL
1	A	237	LEU
2	B	44	MET
2	B	54	VAL
2	B	238	LYS
2	C	54	VAL
2	C	238	LYS
2	D	4	ASP
2	D	43	VAL
2	D	167	GLU
2	D	238	LYS
1	A	228	ARG
2	B	4	ASP
1	A	232	GLN
2	D	54	VAL
1	A	229	SER
1	A	233	ILE

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 PDB entries followed by that with respect to all EM entries.

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	115/115 (100%)	100 (87%)	15 (13%)	4	15
2	B	316/316 (100%)	238 (75%)	78 (25%)	1	4
2	C	316/316 (100%)	240 (76%)	76 (24%)	1	4
2	D	316/316 (100%)	245 (78%)	71 (22%)	1	6
All	All	1063/1063 (100%)	823 (77%)	240 (23%)	2	6

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

Mol	Chain	Res	Type
1	A	134	CYS
1	A	142	ILE
1	A	162	LYS
1	A	165	CYS
1	A	184	ILE
1	A	185	SER
1	A	187	ILE
1	A	190	LEU
1	A	205	ILE
1	A	206	SER
1	A	216	SER
1	A	232	GLN
1	A	251	LYS
1	A	254	ILE
1	A	264	ILE
2	B	5	ILE
2	B	8	LEU
2	B	11	ASP
2	B	17	CYS
2	B	18	LYS
2	B	28	ARG
2	B	30	VAL
2	B	34	ILE
2	B	43	VAL
2	B	49	GLN
2	B	50	LYS
2	B	57	GLU
2	B	62	ARG
2	B	64	ILE
2	B	65	LEU
2	B	68	LYS
2	B	72	GLU
2	B	92	ASN
2	B	95	ARG
2	B	103	VAL
2	B	104	LEU
2	B	105	LEU
2	B	118	LYS
2	B	120	THR
2	B	121	GLN
2	B	129	THR
2	B	145	SER
2	B	147	ARG

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Mol	Chain	Res	Type
2	B	148	THR
2	B	163	VAL
2	B	175	ILE
2	B	176	LEU
2	B	178	LEU
2	B	189	LEU
2	B	190	MET
2	B	192	ILE
2	B	195	GLU
2	B	199	SER
2	B	201	THR
2	B	203	THR
2	B	206	ARG
2	B	209	VAL
2	B	213	LYS
2	B	214	GLU
2	B	215	LYS
2	B	216	LEU
2	B	219	VAL
2	B	222	ASP
2	B	233	SER
2	B	238	LYS
2	B	250	ILE
2	B	253	GLU
2	B	254	ARG
2	B	256	ARG
2	B	259	GLU
2	B	281	SER
2	B	282	ILE
2	B	290	ARG
2	B	291	LYS
2	B	298	VAL
2	B	300	SER
2	B	309	ILE
2	B	313	MET
2	B	314	GLN
2	B	315	LYS
2	B	325	MET
2	B	326	LYS
2	B	327	ILE
2	B	328	LYS
2	B	334	GLU

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Mol	Chain	Res	Type
2	B	335	ARG
2	B	338	SER
2	B	344	SER
2	B	349	LEU
2	B	355	MET
2	B	359	LYS
2	B	369	ILE
2	B	373	LYS
2	C	5	ILE
2	C	8	LEU
2	C	16	MET
2	C	18	LYS
2	C	28	ARG
2	C	33	SER
2	C	34	ILE
2	C	37	ARG
2	C	44	MET
2	C	57	GLU
2	C	64	ILE
2	C	65	LEU
2	C	68	LYS
2	C	72	GLU
2	C	93	GLU
2	C	95	ARG
2	C	104	LEU
2	C	107	GLU
2	C	110	LEU
2	C	119	MET
2	C	121	GLN
2	C	122	ILE
2	C	123	MET
2	C	134	VAL
2	C	141	SER
2	C	145	SER
2	C	148	THR
2	C	153	MET
2	C	159	VAL
2	C	160	THR
2	C	171	LEU
2	C	176	LEU
2	C	178	LEU
2	C	180	LEU

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Mol	Chain	Res	Type
2	C	183	ARG
2	C	186	THR
2	C	189	LEU
2	C	190	MET
2	C	191	LYS
2	C	192	ILE
2	C	196	ARG
2	C	199	SER
2	C	201	THR
2	C	206	ARG
2	C	209	VAL
2	C	213	LYS
2	C	215	LYS
2	C	216	LEU
2	C	219	VAL
2	C	234	SER
2	C	238	LYS
2	C	242	LEU
2	C	247	VAL
2	C	254	ARG
2	C	259	GLU
2	C	261	LEU
2	C	263	GLN
2	C	274	ILE
2	C	276	GLU
2	C	282	ILE
2	C	283	MET
2	C	287	VAL
2	C	291	LYS
2	C	299	LEU
2	C	309	ILE
2	C	313	MET
2	C	320	LEU
2	C	324	THR
2	C	328	LYS
2	C	329	ILE
2	C	335	ARG
2	C	345	ILE
2	C	359	LYS
2	C	368	SER
2	C	369	ILE
2	C	373	LYS

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Mol	Chain	Res	Type
2	D	5	ILE
2	D	8	LEU
2	D	10	VAL
2	D	11	ASP
2	D	17	CYS
2	D	18	LYS
2	D	28	ARG
2	D	30	VAL
2	D	33	SER
2	D	34	ILE
2	D	39	ARG
2	D	44	MET
2	D	47	MET
2	D	57	GLU
2	D	61	LYS
2	D	65	LEU
2	D	68	LYS
2	D	71	ILE
2	D	85	ILE
2	D	92	ASN
2	D	104	LEU
2	D	105	LEU
2	D	113	LYS
2	D	116	ARG
2	D	119	MET
2	D	121	GLN
2	D	123	MET
2	D	136	ILE
2	D	139	VAL
2	D	141	SER
2	D	147	ARG
2	D	151	ILE
2	D	167	GLU
2	D	176	LEU
2	D	178	LEU
2	D	189	LEU
2	D	191	LYS
2	D	192	ILE
2	D	195	GLU
2	D	201	THR
2	D	206	ARG
2	D	208	ILE

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Mol	Chain	Res	Type
2	D	209	VAL
2	D	213	LYS
2	D	214	GLU
2	D	216	LEU
2	D	219	VAL
2	D	236	LEU
2	D	238	LYS
2	D	239	SER
2	D	253	GLU
2	D	256	ARG
2	D	282	ILE
2	D	283	MET
2	D	293	LEU
2	D	300	SER
2	D	309	ILE
2	D	313	MET
2	D	314	GLN
2	D	316	GLU
2	D	317	ILE
2	D	327	ILE
2	D	335	ARG
2	D	344	SER
2	D	348	SER
2	D	349	LEU
2	D	354	GLN
2	D	358	SER
2	D	359	LYS
2	D	369	ILE
2	D	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	194	ASN
1	A	232	GLN
2	B	12	ASN
2	B	92	ASN
2	B	121	GLN
2	B	280	ASN
2	B	353	GLN
2	C	92	ASN

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Mol	Chain	Res	Type
2	C	115	ASN
2	C	121	GLN
2	C	314	GLN
2	C	353	GLN
2	D	59	GLN
2	D	87	HIS
2	D	111	ASN
2	D	121	GLN
2	D	137	GLN
2	D	252	ASN
2	D	353	GLN
2	D	371	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HIC	B	73	2	10,11,12	1.15	1 (10%)	9,14,16	3.77	2 (22%)
2	HIC	D	73	2	10,11,12	1.15	1 (10%)	9,14,16	3.76	2 (22%)
2	HIC	C	73	2	10,11,12	1.15	1 (10%)	9,14,16	3.77	2 (22%)

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
2	HIC	B	73	2	-	2/5/6/8	0/1/1/1
2	HIC	D	73	2	-	2/5/6/8	0/1/1/1
2	HIC	C	73	2	-	2/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	HIC	CD2-NE2	-2.06	1.34	1.37
2	D	73	HIC	CD2-NE2	-2.03	1.34	1.37
2	C	73	HIC	CD2-NE2	-2.00	1.34	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	73	HIC	NE2-CE1-ND1	-9.85	108.89	112.66
2	D	73	HIC	NE2-CE1-ND1	-9.84	108.90	112.66
2	B	73	HIC	NE2-CE1-ND1	-9.82	108.90	112.66
2	B	73	HIC	CD2-NE2-CE1	4.56	108.51	106.71
2	C	73	HIC	CD2-NE2-CE1	4.53	108.50	106.71
2	D	73	HIC	CD2-NE2-CE1	4.47	108.47	106.71

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	73	HIC	CA-CB-CG-CD2
2	D	73	HIC	CA-CB-CG-ND1
2	B	73	HIC	CA-CB-CG-CD2
2	C	73	HIC	CA-CB-CG-CD2
2	C	73	HIC	CA-CB-CG-ND1
2	B	73	HIC	CA-CB-CG-ND1

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	73	HIC	3	0
2	D	73	HIC	3	0
2	C	73	HIC	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	D	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
4	ADP	B	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
4	ADP	C	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	401	-	-	0/16/32/32	0/3/3/3
4	ADP	B	401	-	-	0/16/32/32	0/3/3/3
4	ADP	C	401	-	-	0/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	ADP	C5-C4	4.74	1.47	1.39
4	B	401	ADP	C5-C4	4.74	1.47	1.39
4	D	401	ADP	C5-C4	4.74	1.47	1.39
4	D	401	ADP	C5-C6	2.77	1.48	1.41
4	C	401	ADP	C5-C6	2.77	1.48	1.41
4	B	401	ADP	C5-C6	2.74	1.48	1.41
4	D	401	ADP	C8-N7	2.38	1.36	1.31
4	C	401	ADP	C8-N7	2.36	1.36	1.31
4	B	401	ADP	C8-N7	2.33	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ADP	C5-N7	-2.26	1.35	1.39
4	C	401	ADP	C5-N7	-2.23	1.35	1.39
4	B	401	ADP	C5-N7	-2.18	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	ADP	C5-C4-N3	-5.85	118.67	126.72
4	B	401	ADP	C5-C4-N3	-5.83	118.68	126.72
4	D	401	ADP	C5-C4-N3	-5.82	118.70	126.72
4	C	401	ADP	N3-C4-N9	4.62	135.03	127.17
4	B	401	ADP	N3-C4-N9	4.61	135.01	127.17
4	D	401	ADP	N3-C4-N9	4.58	134.95	127.17
4	C	401	ADP	C2-N3-C4	3.72	120.91	111.83
4	D	401	ADP	C2-N3-C4	3.69	120.85	111.83
4	B	401	ADP	C2-N3-C4	3.69	120.85	111.83
4	B	401	ADP	C4-C5-N7	-3.50	106.58	110.58
4	D	401	ADP	C4-C5-N7	-3.46	106.63	110.58
4	C	401	ADP	C4-C5-N7	-3.45	106.63	110.58
4	C	401	ADP	N3-C2-N1	-3.24	123.68	128.58
4	D	401	ADP	N3-C2-N1	-3.20	123.74	128.58
4	B	401	ADP	N3-C2-N1	-3.19	123.75	128.58
4	B	401	ADP	C4-N9-C8	2.60	108.47	105.74
4	C	401	ADP	C4-N9-C8	2.59	108.46	105.74
4	B	401	ADP	C5-N7-C8	2.56	107.47	103.45
4	D	401	ADP	C3'-C2'-C1'	2.55	106.28	101.46
4	D	401	ADP	C4-N9-C8	2.54	108.41	105.74
4	C	401	ADP	C3'-C2'-C1'	2.54	106.28	101.46
4	D	401	ADP	C5-N7-C8	2.54	107.44	103.45
4	B	401	ADP	C3'-C2'-C1'	2.54	106.27	101.46
4	C	401	ADP	C5-N7-C8	2.53	107.43	103.45
4	B	401	ADP	C6-C5-N7	2.09	136.11	132.09
4	D	401	ADP	C6-C5-N7	2.08	136.10	132.09
4	C	401	ADP	C6-C5-N7	2.06	136.07	132.09

There are no chirality outliers.

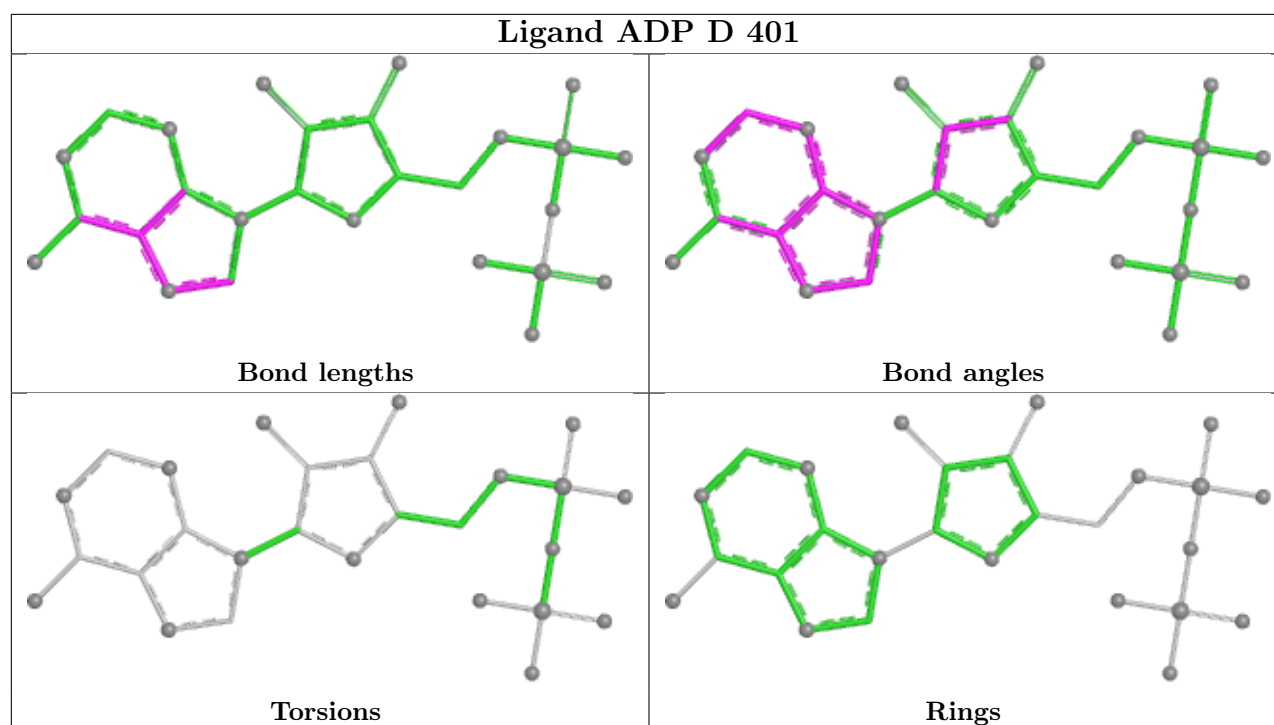
There are no torsion outliers.

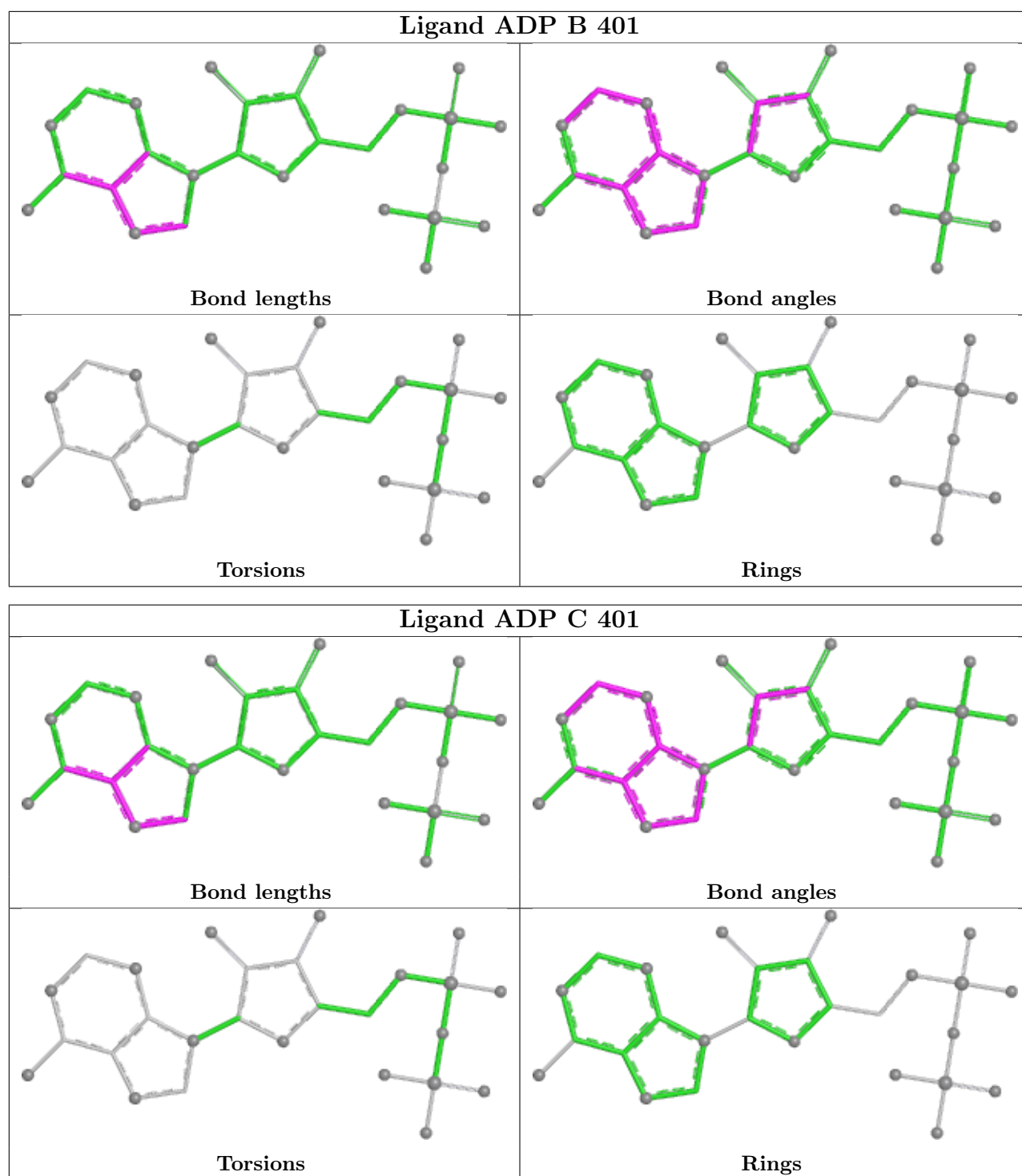
There are no ring outliers.

3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	ADP	9	0
4	B	401	ADP	8	0
4	C	401	ADP	8	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6102. These allow visual inspection of the internal detail of the map and identification of artifacts.

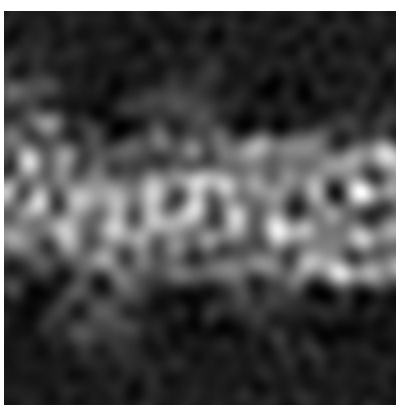
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

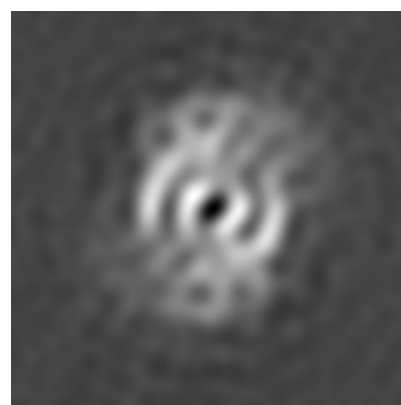
6.1.1 Primary map



X



Y

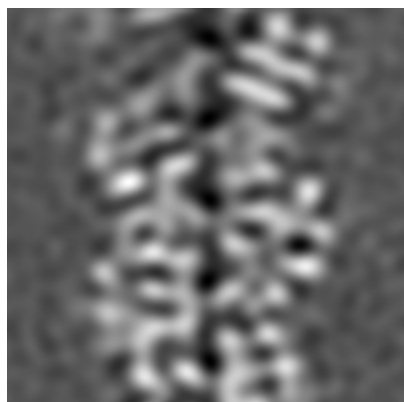


Z

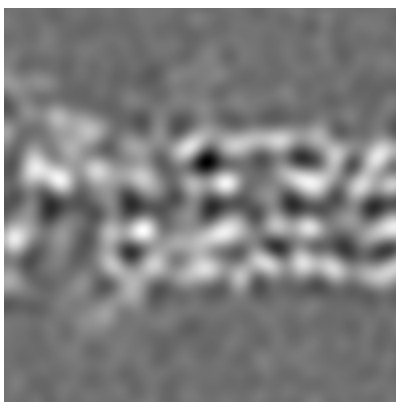
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

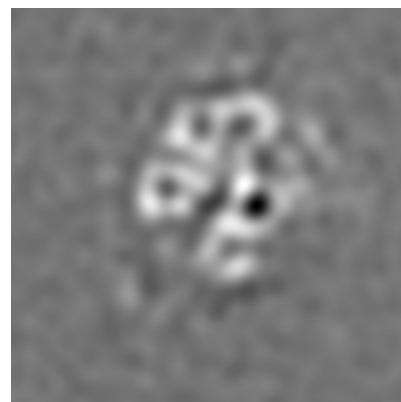
6.2.1 Primary map



X Index: 50



Y Index: 50



Z Index: 50

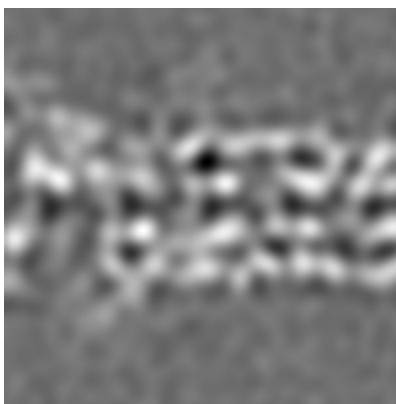
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

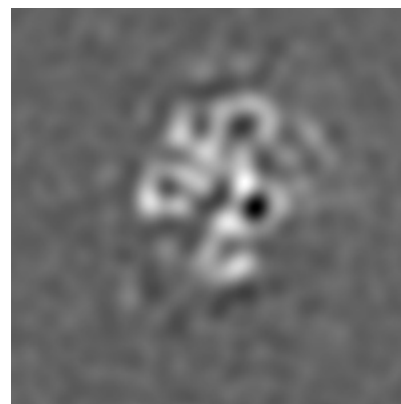
6.3.1 Primary map



X Index: 44



Y Index: 50

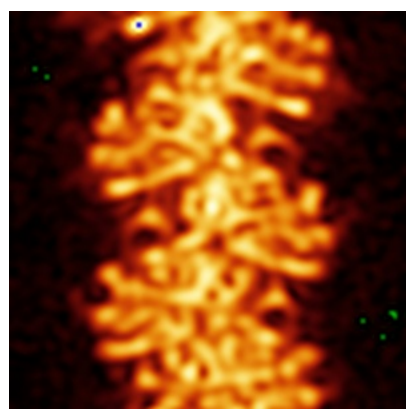


Z Index: 49

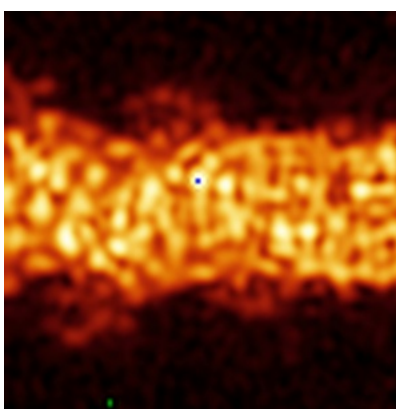
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

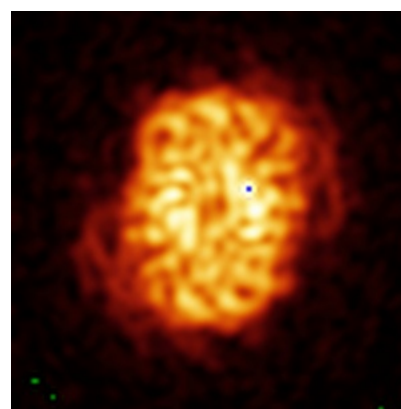
6.4.1 Primary map



X



Y

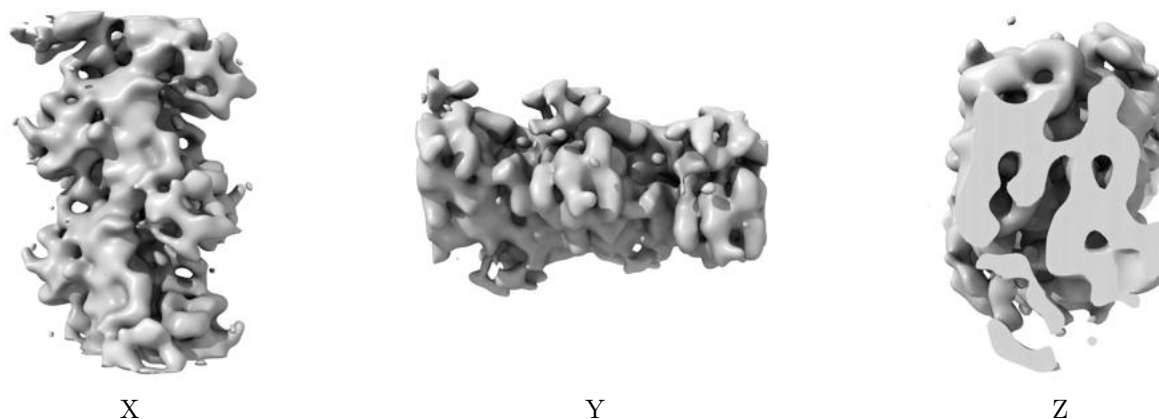


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.838. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

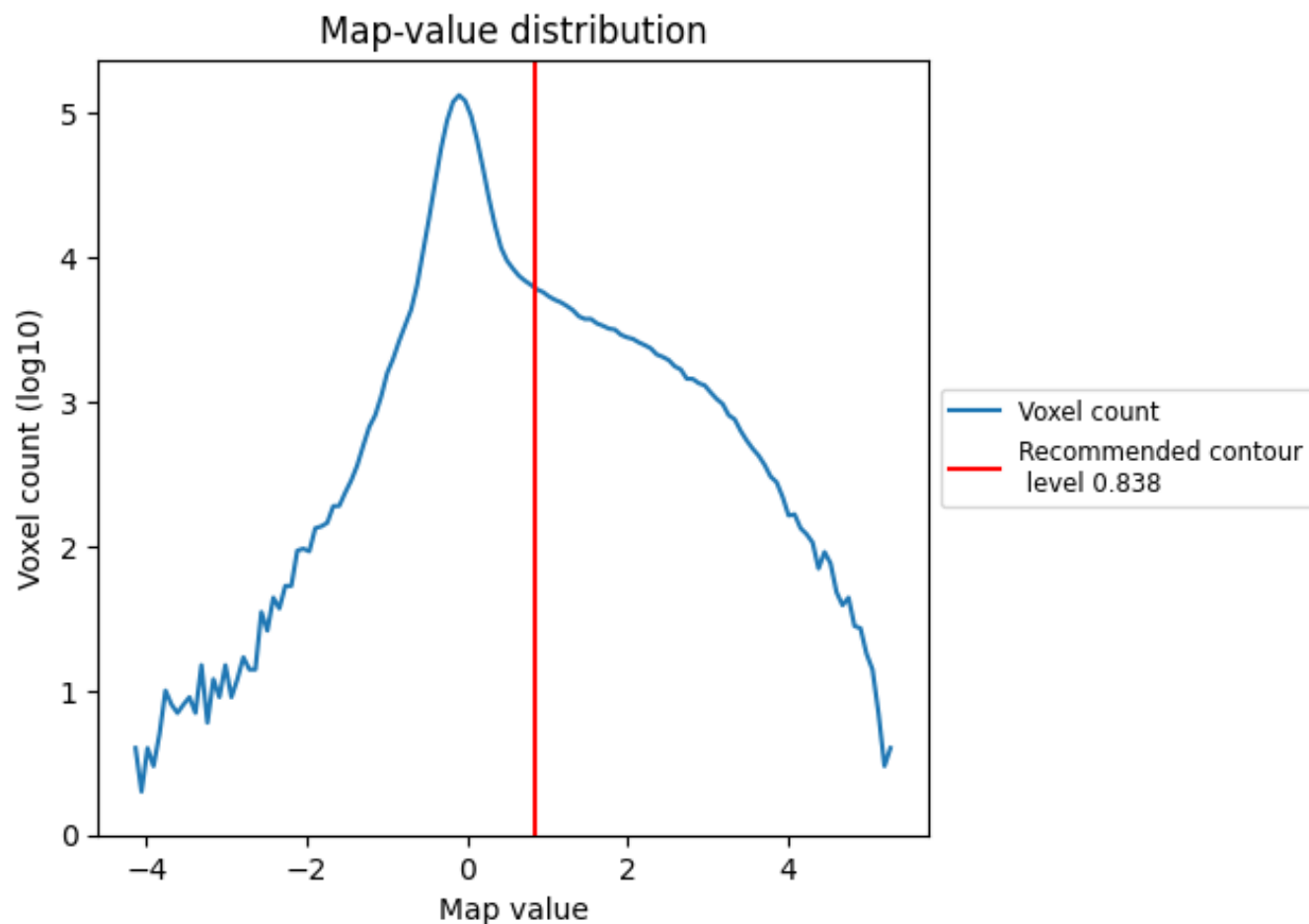
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

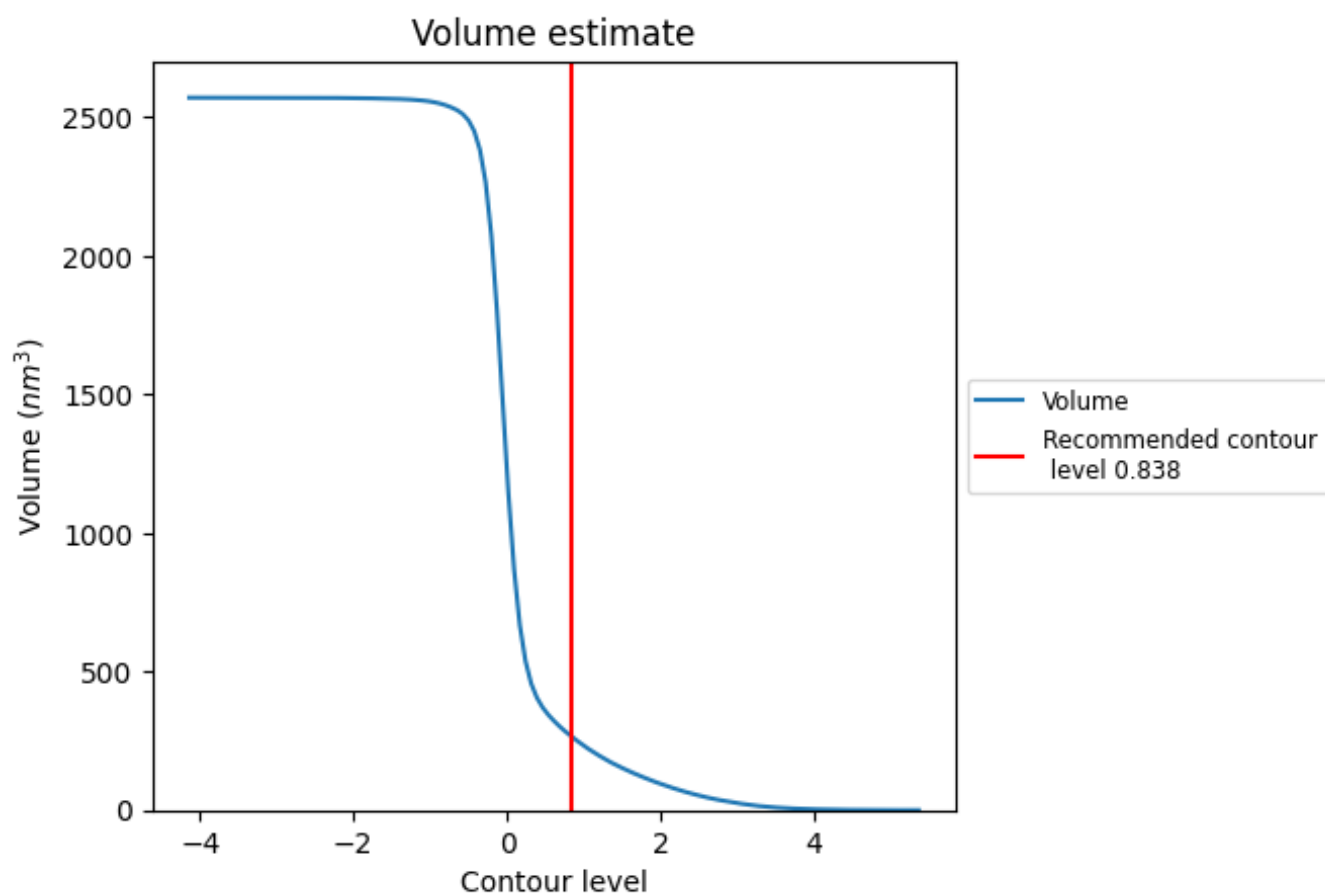
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

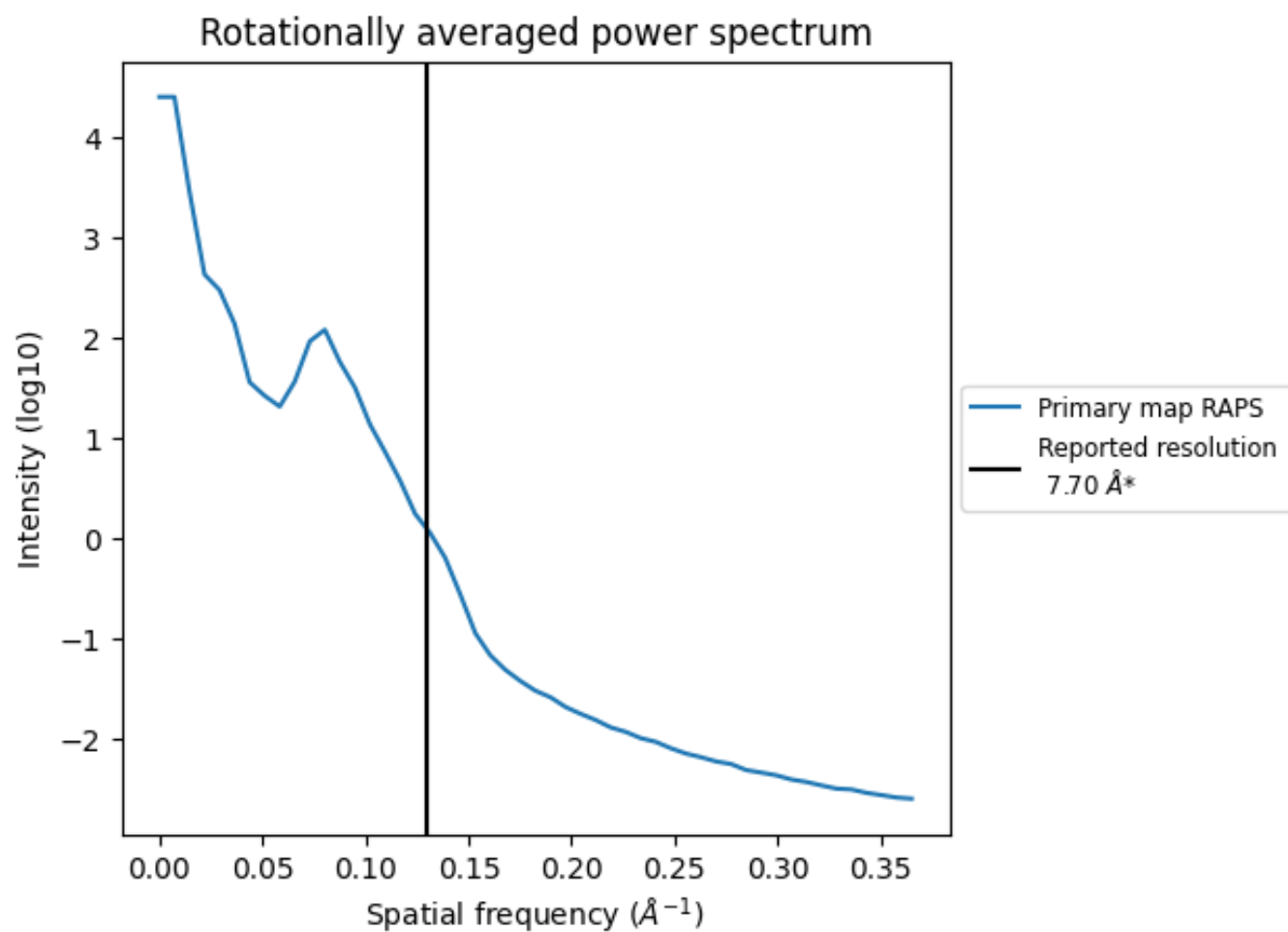
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 267 nm³; this corresponds to an approximate mass of 241 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.130 Å⁻¹

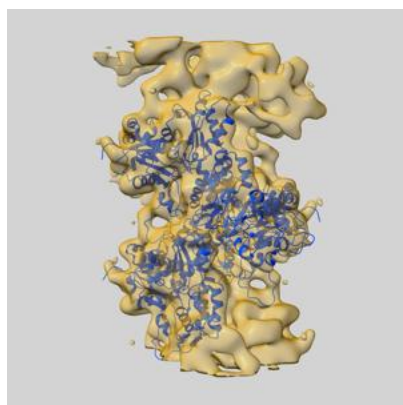
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

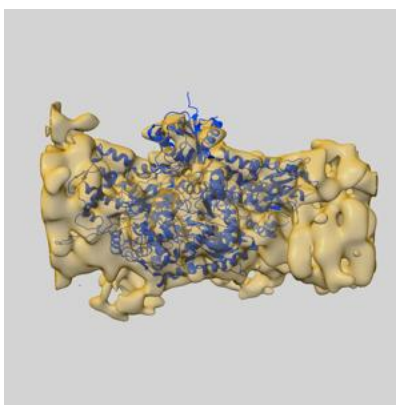
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6102 and PDB model 3J82. Per-residue inclusion information can be found in section [3](#) on page [6](#).

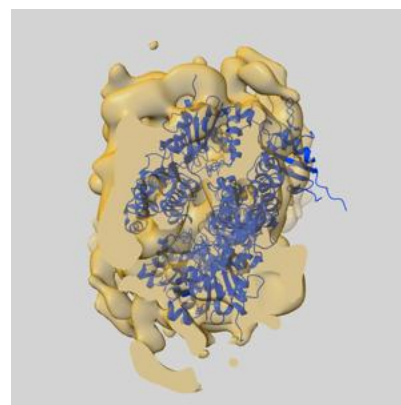
9.1 Map-model overlay [i](#)



X



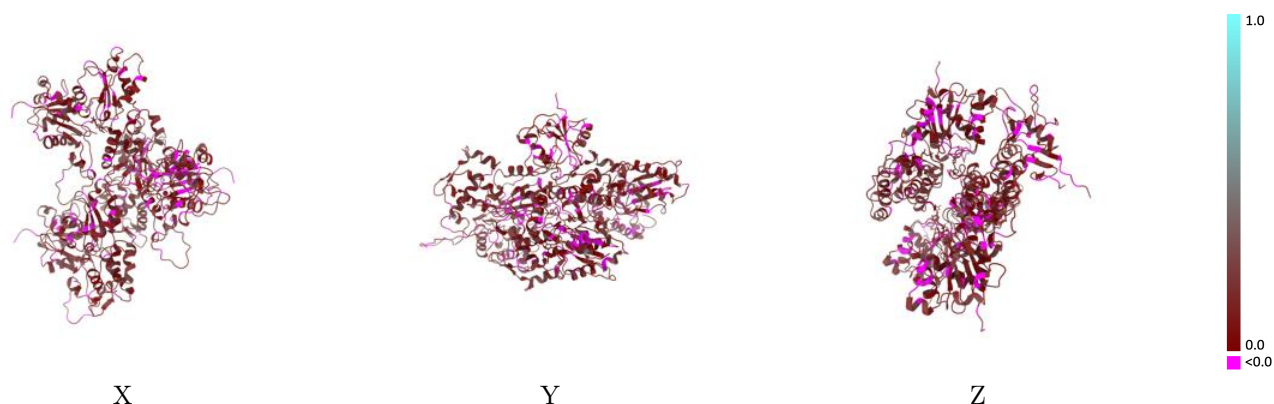
Y



Z

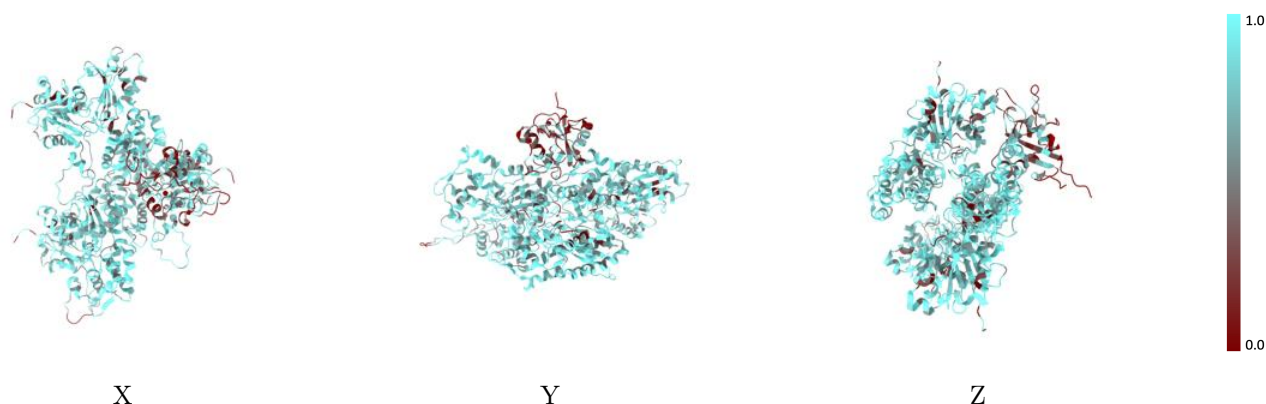
The images above show the 3D surface view of the map at the recommended contour level 0.838 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



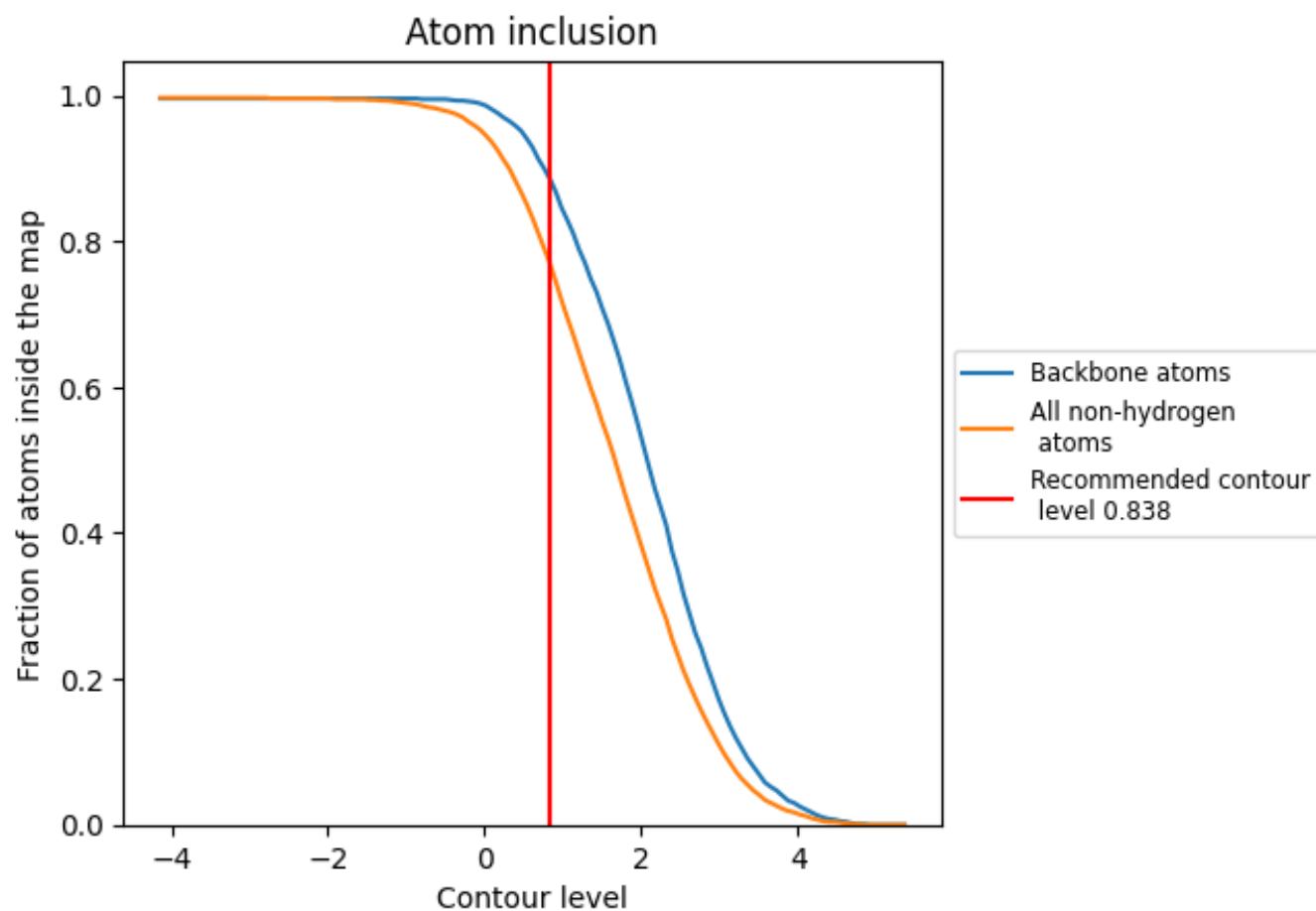
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.838).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.838) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.1340
A	0.3930	0.1000
B	0.8140	0.1380
C	0.8100	0.1360
D	0.8170	0.1410

