



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 PM UTC

PDB ID : 1DO2 / pdb_00001do2
Title : TRIGONAL CRYSTAL FORM OF HEAT SHOCK LOCUS U (HSLU) FROM
ESCHERICHIA COLI
Authors : Bochtler, M.; Hartmann, C.; Song, H.K.; Bourenkov, G.P.; Bartunik, H.D.
Deposited on : 1999-12-18
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

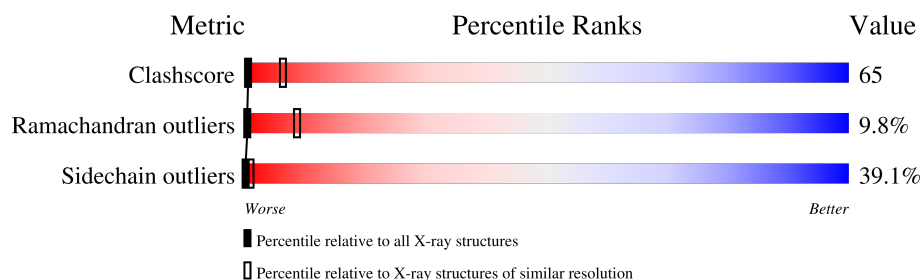
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	442	
1	B	442	
1	C	442	
1	D	442	

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	ANP	A	900	-	-	X	-
2	ANP	C	905	-	-	X	-

2 Entry composition [i](#)

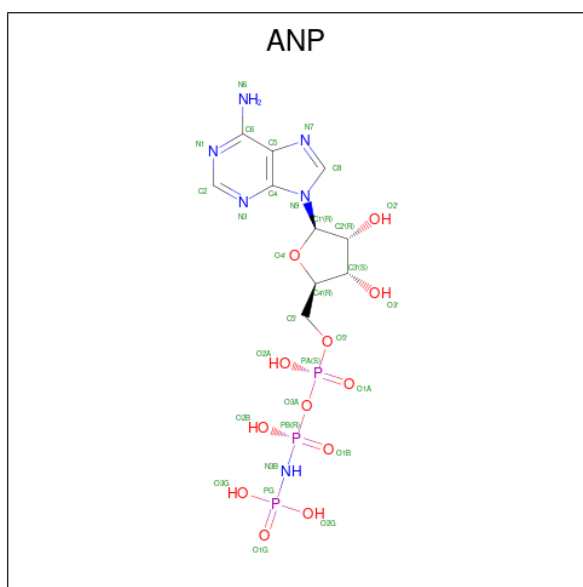
There are 2 unique types of molecules in this entry. The entry contains 12926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEIN (HEAT SHOCK LOCUS U).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	126	0	0
			3216	2008	574	624	10			
1	B	407	Total	C	N	O	S	492	0	0
			3216	2008	574	624	10			
1	C	407	Total	C	N	O	S	103	0	0
			3216	2008	574	624	10			
1	D	407	Total	C	N	O	S	484	0	0
			3216	2008	574	624	10			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



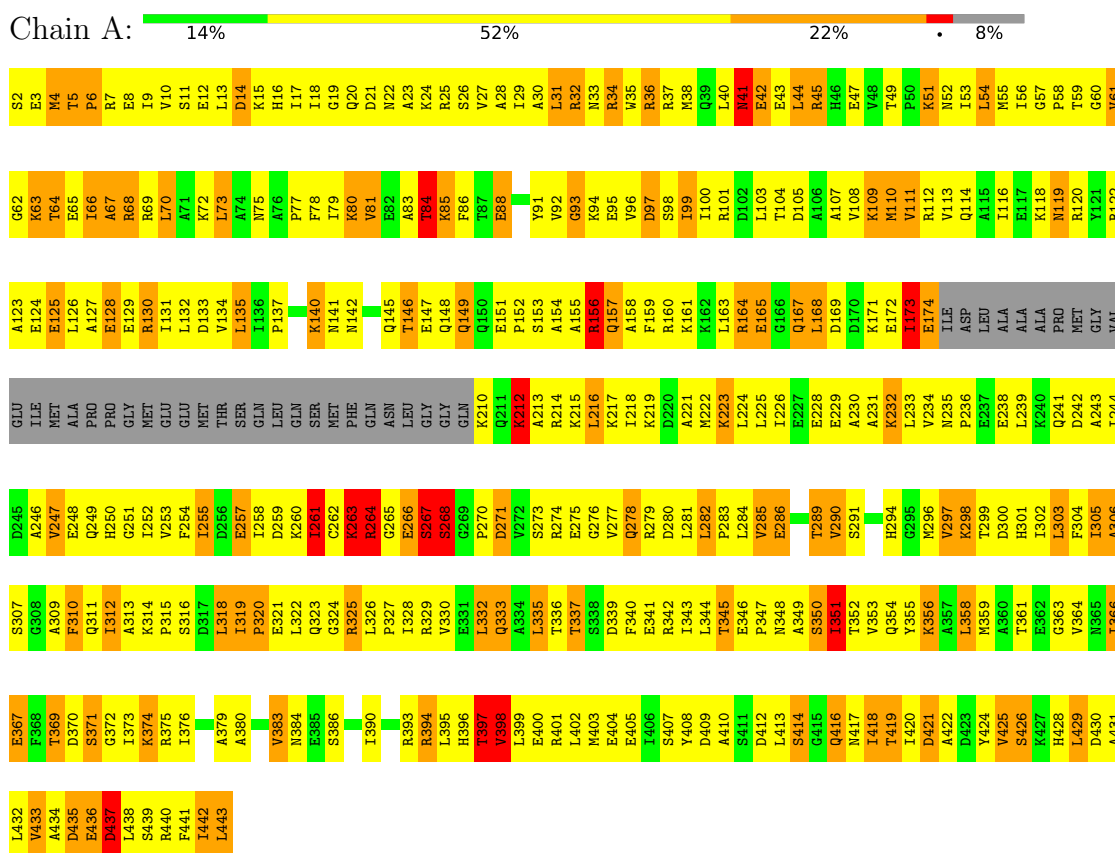
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

3 Residue-property plots

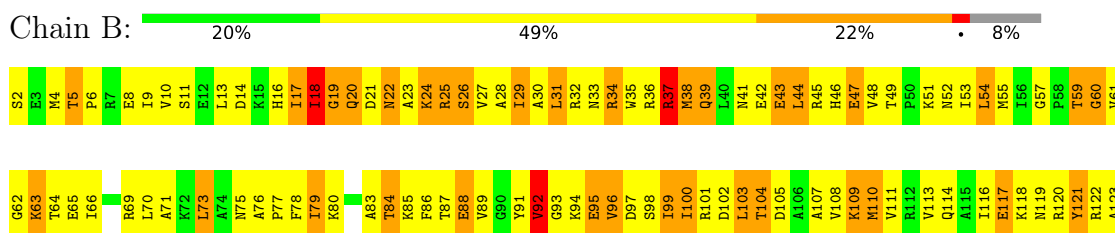
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

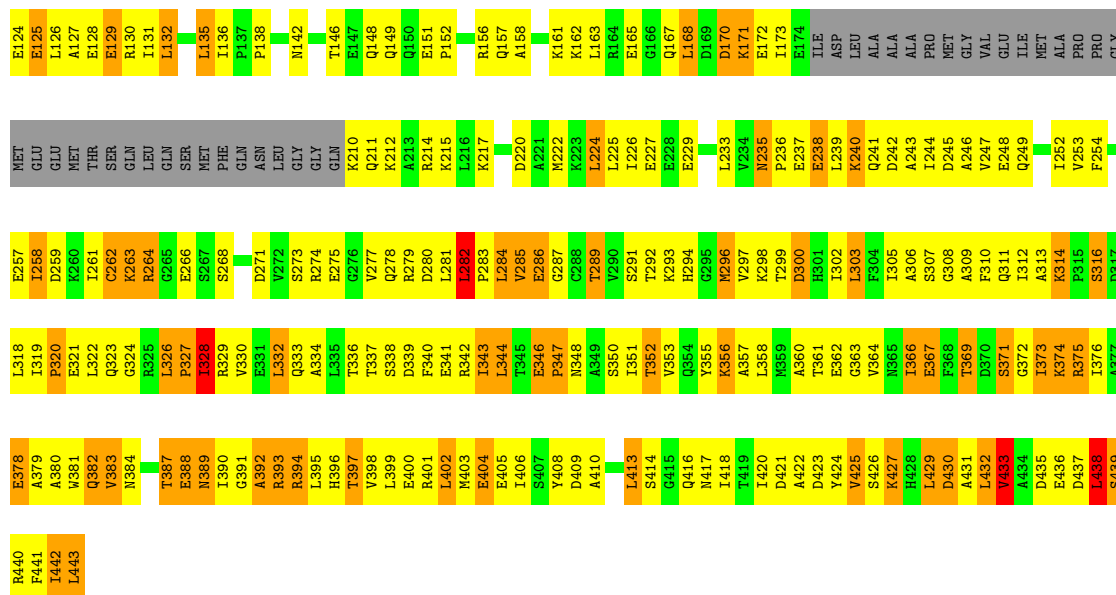
Note EDS was not executed.

- Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)



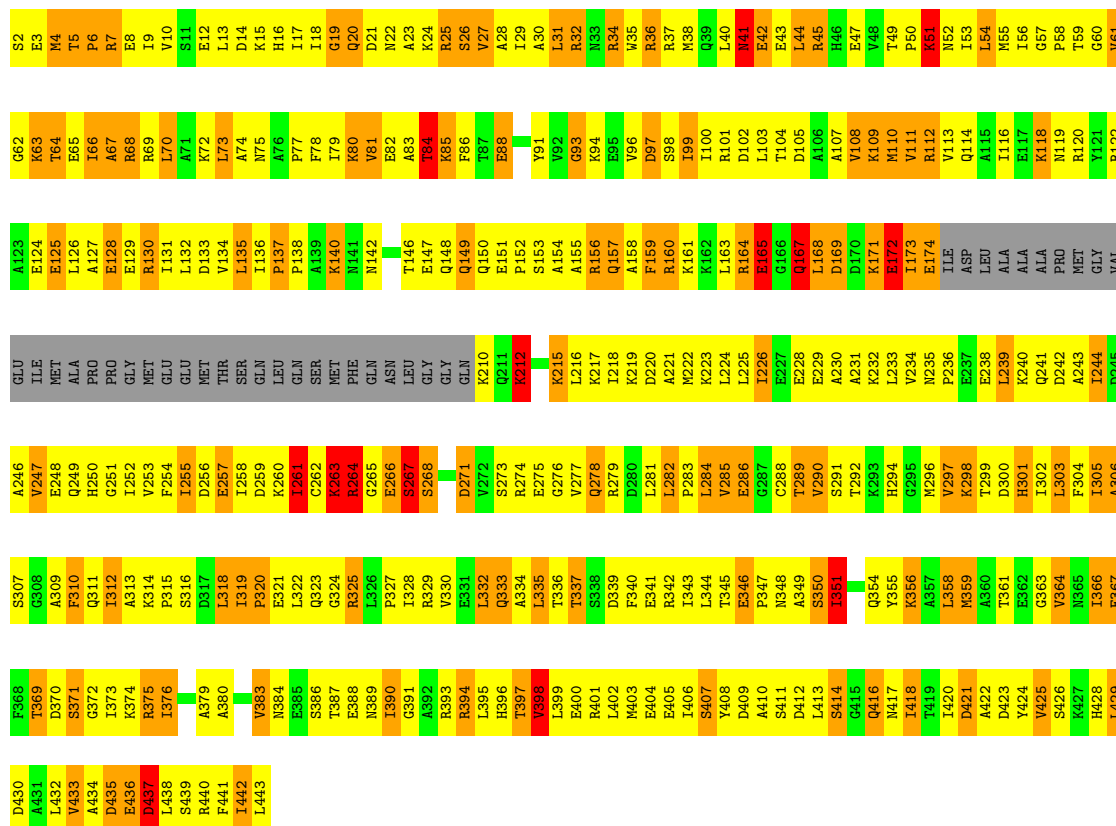
- Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)





• Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)

Chain C: 14% 49% 26% 8%



• Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)

Chain D: 18% 52% 21% 8%

S439	K374	K314	V253	GLU	E124	K63	S2
R440	R375	P315	F254	GLU	E125	E3	E3
F441	I376	S316	T255	MET	L126	M4	M4
T442	A377	D317	D256	THR	A127	T5	T5
L443	E378	L318	E257	SER	E128	P6	P6
	A379	I319	I258	GLN	E129	R69	R7
	A380	P320	D259	LEU	R130	L70	E8
	W381	E321	K260	GLN	I131	A71	I9
	Q382	L322	T261	SER	L132	R72	V10
	V383	Q323	C262	MET	D133	L73	S11
	N384	G324	K263	PHE	V134	A74	
		R325	R264	GLN	L135	N75	D14
		L326	G265	ASN	I136	A76	K15
		P327	E266	LEU	F137	H16	H16
		R328	S267	GLY	P138	I17	I17
		L329	S268	GLN		I18	I18
		V330		GLN	Q145	G19	G19
		E331	D271	K210	T146	Q20	Q20
		L332	V272	Q211	E147	E82	D21
		Q333	S273	K212	Q148	N22	N22
		A334	R274	A213	Q149	T84	A23
		L335	E275	K214	Q150	K85	K24
		T336	G276	K215	E151	F86	R25
		T337	V277	L216		T87	S26
		S338	Q278	K217	R156	E88	V27
		D339	R279	E218	Q157	V89	A28
		F340	D280	K219	A158	G90	I29
		E341	L281	D220		Y91	A30
		R342	P282	A221	K161	V92	L31
		I343	R283	K222	K162	G93	R32
		L344	L284	K223	L163	K94	N33
		T345	V285	L224	R164	E95	R34
		E346	E286	L225	E165	W35	W35
		P347	G287	T226	G166	R36	R36
		N348	C288	E227	Q167	S98	R37
		A349	T289	E228	L168	I99	M38
		S350	V290	E229	D169	I100	G39
		I351	S291	A230	D170	R101	L40
		T352	T292	A231	K171	D102	M41
		V353	K293	K232	E172	L103	E42
		Q354	H294	L233	I173	T104	E43
		Y355	G295	V234	E174	D105	L44
		K356	M296	M235	ILE	A106	R45
		A357	V297	P236	ASP	A107	H46
		L358	K298	E237	LEU	V108	E47
		M359	T299	E238	ALA	K109	V48
		A360	D300	L239	ALA	M110	T49
		T361	H301	K240	ALA	V111	P50
		E362	I302	D241	PRO	R112	K51
		G363	L303	D242	MET	V113	N52
		V364	F304	A243	GLY	Q114	I53
		N365	I305	T244	VAL	A115	L54
		I366	A306	D245	GLU	I116	M55
		E367	S307	A246	ILE	E117	I56
		F368	G308	V247	MET	K118	G57
		T369	A309	E248	ALA	M119	P58
		B370	F310	Q249	PRO	R120	T59
		S371	Q311	H250	PRO	Y121	G60
		G372	I312	G251	GLY	R122	V61
		I373	A313	I252	MET	A123	G62

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.78Å 201.78Å 171.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 4.00	Depositor
% Data completeness (in resolution range)	95.8 (15.00-4.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	10.50	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.229 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12926	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/3255	0.88	9/4385 (0.2%)
1	B	0.35	0/3255	0.82	4/4385 (0.1%)
1	C	0.34	0/3255	0.81	4/4385 (0.1%)
1	D	0.34	0/3255	0.82	6/4385 (0.1%)
All	All	0.35	0/13020	0.83	23/17540 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	CB-CG-CD	13.73	142.87	111.30
1	A	223	LYS	CB-CG-CD	10.09	134.51	111.30
1	B	59	THR	N-CA-C	7.92	122.06	111.30
1	A	263	LYS	N-CA-C	7.25	118.17	108.38
1	D	59	THR	N-CA-C	7.20	121.09	111.30
1	C	263	LYS	N-CA-C	7.09	117.95	108.38
1	A	232	LYS	N-CA-CB	7.08	121.13	110.22
1	D	272	VAL	N-CA-C	-6.79	102.54	112.04
1	A	223	LYS	CG-CD-CE	6.62	126.52	111.30
1	C	93	GLY	N-CA-C	-6.16	106.71	114.16
1	B	168	LEU	CB-CA-C	-5.97	109.68	116.54
1	A	93	GLY	N-CA-C	-5.68	108.42	114.67
1	A	306	ALA	N-CA-C	-5.57	103.56	110.41
1	B	263	LYS	N-CA-C	5.56	115.19	107.73
1	D	266	GLU	N-CA-C	-5.56	108.28	114.62
1	C	306	ALA	N-CA-C	-5.55	103.58	110.41
1	A	91	TYR	N-CA-C	-5.43	105.91	112.54
1	A	173	ILE	N-CA-C	5.42	115.43	108.82
1	D	132	LEU	N-CA-C	-5.35	106.59	113.23
1	B	132	LEU	N-CA-C	-5.34	106.61	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	TYR	N-CA-C	-5.21	105.78	111.82
1	D	127	ALA	N-CA-C	-5.19	106.79	113.23
1	D	376	ILE	N-CA-C	-5.02	105.01	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3216	0	3284	412	0
1	B	3216	0	3284	317	0
1	C	3216	0	3284	464	0
1	D	3216	0	3284	342	0
2	A	31	0	13	9	0
2	C	31	0	13	11	0
All	All	12926	0	13162	1521	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 65.

All (1521) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LYS:HA	1:A:366:ILE:HD11	1.38	1.01
1:C:54:LEU:HD13	1:C:56:ILE:HD11	1.39	1.01
1:A:366:ILE:HD13	1:A:366:ILE:H	1.28	0.98
1:A:54:LEU:HD13	1:A:56:ILE:HD11	1.43	0.97
1:A:282:LEU:HD21	1:A:321:GLU:HB3	1.46	0.97
1:C:426:SER:O	1:C:430:ASP:HB2	1.66	0.96
1:C:299:THR:HA	1:C:302:ILE:HD12	1.47	0.96
1:C:4:MET:HB3	1:C:8:GLU:HB3	1.46	0.96
1:C:366:ILE:HD13	1:C:366:ILE:H	1.30	0.95
1:D:429:LEU:H	1:D:429:LEU:HD22	1.32	0.94
1:C:153:SER:HA	1:C:156:ARG:HB3	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:MET:HB3	1:A:8:GLU:HB3	1.51	0.93
1:A:109:LYS:HG3	1:A:112:ARG:HH21	1.34	0.92
1:C:356:LYS:HA	1:C:366:ILE:HD11	1.50	0.91
1:D:123:ALA:HB1	1:D:226:ILE:HG23	1.52	0.90
1:C:131:ILE:O	1:C:134:VAL:HG12	1.70	0.90
1:A:27:VAL:HG22	1:A:70:LEU:HD13	1.53	0.88
1:A:153:SER:HA	1:A:156:ARG:HB3	1.55	0.87
1:A:18:ILE:H	2:A:900:ANP:HN61	1.23	0.87
1:C:59:THR:HA	2:C:905:ANP:O1G	1.73	0.87
1:C:258:ILE:HG13	1:C:306:ALA:HB1	1.56	0.86
1:C:439:SER:HA	1:C:443:LEU:HD13	1.56	0.85
1:B:83:ALA:HB1	1:B:261:ILE:HD11	1.59	0.84
1:B:235:ASN:HD22	1:B:238:GLU:HG2	1.41	0.84
1:B:356:LYS:HA	1:B:366:ILE:HD11	1.56	0.84
1:C:282:LEU:HD21	1:C:321:GLU:HB3	1.59	0.84
1:A:426:SER:O	1:A:430:ASP:HB2	1.76	0.84
1:D:59:THR:HG21	1:D:390:ILE:HA	1.59	0.84
1:B:429:LEU:H	1:B:429:LEU:HD22	1.43	0.83
1:C:18:ILE:H	2:C:905:ANP:HN61	1.26	0.83
1:D:319:ILE:HG23	1:D:322:LEU:HB3	1.58	0.83
1:C:442:ILE:HG12	1:C:443:LEU:HD12	1.61	0.83
1:D:271:ASP:HA	1:D:274:ARG:HB2	1.60	0.83
1:D:356:LYS:HA	1:D:366:ILE:HD11	1.57	0.83
1:B:319:ILE:HG23	1:B:322:LEU:HB3	1.60	0.82
1:A:42:GLU:HA	1:A:45:ARG:HB2	1.61	0.82
1:A:131:ILE:O	1:A:134:VAL:HG12	1.77	0.82
1:A:59:THR:HA	2:A:900:ANP:O1G	1.79	0.82
1:B:26:SER:HA	1:B:29:ILE:HD12	1.62	0.82
1:C:27:VAL:HG22	1:C:70:LEU:HD13	1.61	0.82
1:A:24:LYS:O	1:A:27:VAL:HG12	1.79	0.82
1:C:369:THR:OG1	1:C:421:ASP:HA	1.80	0.82
1:C:42:GLU:HA	1:C:45:ARG:HB2	1.60	0.82
1:C:319:ILE:HG12	1:C:320:PRO:HD2	1.60	0.82
1:A:113:VAL:HA	1:A:116:ILE:HD12	1.62	0.81
1:A:344:LEU:HA	1:A:351:ILE:HD11	1.62	0.80
1:D:235:ASN:HD22	1:D:238:GLU:HG2	1.47	0.80
1:D:282:LEU:HD21	1:D:321:GLU:HB3	1.63	0.80
1:A:68:ARG:HH11	1:A:68:ARG:HB3	1.45	0.80
1:A:226:ILE:O	1:A:230:ALA:HB2	1.80	0.80
1:B:299:THR:HA	1:B:302:ILE:HG13	1.64	0.79
1:B:432:LEU:HD12	1:B:432:LEU:H	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HA	1:A:302:ILE:HD12	1.65	0.79
1:B:271:ASP:HA	1:B:274:ARG:HB2	1.62	0.79
1:C:113:VAL:HA	1:C:116:ILE:HD12	1.65	0.79
1:D:96:VAL:HG11	1:D:280:ASP:HB3	1.65	0.79
1:C:79:ILE:HG22	1:C:103:LEU:HD13	1.62	0.79
1:A:319:ILE:HG12	1:A:320:PRO:HD2	1.64	0.79
1:B:123:ALA:HB1	1:B:226:ILE:HG23	1.64	0.79
1:C:109:LYS:HG3	1:C:112:ARG:HH21	1.48	0.78
1:D:364:VAL:HG22	1:D:414:SER:HA	1.65	0.78
1:D:299:THR:HA	1:D:302:ILE:HG13	1.66	0.78
1:D:41:ASN:ND2	1:D:43:GLU:HB3	1.98	0.78
1:A:439:SER:HA	1:A:443:LEU:HD13	1.63	0.78
1:C:100:ILE:HD12	1:C:100:ILE:H	1.46	0.78
1:B:364:VAL:HG22	1:B:414:SER:HA	1.64	0.77
1:C:96:VAL:HG12	1:C:284:LEU:HD11	1.65	0.77
1:C:24:LYS:O	1:C:27:VAL:HG12	1.84	0.77
1:C:318:LEU:HD11	1:C:322:LEU:HD23	1.67	0.77
1:B:41:ASN:ND2	1:B:43:GLU:HB3	2.00	0.77
1:C:66:ILE:HD12	1:C:66:ILE:H	1.49	0.77
1:D:432:LEU:HD12	1:D:432:LEU:H	1.50	0.76
1:C:390:ILE:O	1:C:393:ARG:HG3	1.84	0.76
1:B:6:PRO:HA	1:B:9:ILE:HD12	1.67	0.76
1:C:26:SER:HA	1:C:29:ILE:HD12	1.67	0.76
1:C:111:VAL:HG11	1:C:243:ALA:HB2	1.68	0.75
1:C:319:ILE:HD11	1:C:321:GLU:HB2	1.66	0.75
1:A:66:ILE:H	1:A:66:ILE:HD12	1.52	0.75
1:A:390:ILE:HD11	1:A:394:ARG:NE	2.02	0.75
1:D:17:ILE:HG23	1:D:18:ILE:N	2.01	0.75
1:D:355:TYR:OH	1:D:403:MET:HB3	1.86	0.75
1:D:26:SER:HA	1:D:29:ILE:HD12	1.69	0.75
1:B:17:ILE:HG23	1:B:18:ILE:N	1.99	0.74
1:A:100:ILE:HD12	1:A:100:ILE:H	1.52	0.74
1:B:327:PRO:O	1:B:329:ARG:HG2	1.88	0.74
1:A:79:ILE:HG22	1:A:103:LEU:HD13	1.69	0.74
1:B:59:THR:HG21	1:B:390:ILE:HA	1.68	0.74
1:B:61:VAL:O	1:B:61:VAL:HG13	1.87	0.74
1:B:318:LEU:HD21	1:B:322:LEU:HD23	1.69	0.74
1:B:336:THR:HA	1:B:381:TRP:CZ3	2.22	0.74
1:A:442:ILE:HG12	1:A:443:LEU:HD12	1.69	0.73
1:B:263:LYS:HG3	1:B:264:ARG:N	2.02	0.73
1:C:383:VAL:HB	1:C:394:ARG:HH11	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HD11	1:A:394:ARG:HE	1.52	0.73
1:B:91:TYR:HB3	1:B:95:GLU:HB2	1.71	0.73
1:D:426:SER:O	1:D:430:ASP:HB2	1.89	0.73
1:D:83:ALA:HB1	1:D:261:ILE:HD11	1.69	0.73
1:A:361:THR:HG21	1:B:36:ARG:HA	1.70	0.72
1:D:61:VAL:O	1:D:61:VAL:HG13	1.88	0.72
1:B:245:ASP:C	1:B:247:VAL:H	1.98	0.72
1:D:261:ILE:HG22	1:D:278:GLN:HE21	1.55	0.72
1:A:369:THR:OG1	1:A:421:ASP:HA	1.90	0.71
1:C:390:ILE:HD11	1:C:394:ARG:HE	1.55	0.71
1:B:426:SER:O	1:B:430:ASP:HB2	1.89	0.71
1:A:390:ILE:O	1:A:393:ARG:HG3	1.89	0.71
1:B:384:ASN:HD21	1:B:391:GLY:H	1.38	0.71
1:D:397:THR:HG21	1:D:443:LEU:HA	1.72	0.71
1:B:336:THR:HA	1:B:381:TRP:HZ3	1.54	0.71
1:C:226:ILE:O	1:C:230:ALA:HB2	1.90	0.71
1:B:282:LEU:HD21	1:B:321:GLU:HB3	1.73	0.70
1:C:223:LYS:O	1:C:226:ILE:HG22	1.90	0.70
1:C:438:LEU:O	1:C:442:ILE:HD13	1.91	0.70
1:D:245:ASP:C	1:D:247:VAL:H	1.99	0.70
1:A:429:LEU:N	1:A:429:LEU:HD23	2.07	0.70
1:C:234:VAL:HG23	1:C:236:PRO:HD3	1.73	0.70
1:C:289:THR:HG23	1:C:298:LYS:HG2	1.73	0.70
1:D:6:PRO:HA	1:D:9:ILE:HD12	1.74	0.70
1:A:132:LEU:HA	1:A:135:LEU:HD23	1.74	0.70
1:C:61:VAL:HA	1:C:335:LEU:HD11	1.74	0.70
1:C:235:ASN:HB3	1:C:238:GLU:HG2	1.73	0.70
1:B:387:THR:OG1	1:B:388:GLU:N	2.25	0.69
1:A:319:ILE:HD11	1:A:321:GLU:HB2	1.73	0.69
1:C:100:ILE:HD13	1:C:290:VAL:HG21	1.74	0.69
1:C:413:LEU:O	1:C:416:GLN:HB2	1.93	0.69
1:B:397:THR:HG21	1:B:443:LEU:HA	1.75	0.69
1:C:112:ARG:HB3	1:C:239:LEU:HD11	1.75	0.69
1:A:383:VAL:HB	1:A:394:ARG:HH11	1.58	0.69
1:D:23:ALA:HA	1:D:330:VAL:HG21	1.74	0.69
1:D:109:LYS:O	1:D:113:VAL:HG13	1.92	0.69
1:D:43:GLU:O	1:D:47:GLU:HB2	1.92	0.69
1:D:336:THR:HG22	1:D:339:ASP:CG	2.18	0.69
1:D:423:ASP:O	1:D:427:LYS:HB2	1.91	0.69
1:A:278:GLN:HB3	1:A:319:ILE:HG21	1.75	0.69
1:C:70:LEU:HA	1:C:73:LEU:HD22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ASP:O	1:D:249:GLN:HB2	1.93	0.69
1:D:24:LYS:O	1:D:27:VAL:HG22	1.92	0.69
1:A:100:ILE:HD13	1:A:290:VAL:HG21	1.75	0.68
1:A:291:SER:HA	1:A:296:MET:SD	2.33	0.68
1:B:122:ARG:CZ	1:B:126:LEU:HD11	2.24	0.68
1:D:387:THR:OG1	1:D:388:GLU:N	2.23	0.68
1:A:222:MET:O	1:A:226:ILE:HB	1.92	0.68
1:C:86:PHE:HD1	1:C:93:GLY:HA2	1.57	0.68
1:C:277:VAL:HG12	1:C:281:LEU:HD11	1.74	0.68
1:D:117:GLU:HA	1:D:120:ARG:NE	2.08	0.68
1:A:65:GLU:OE2	1:A:69:ARG:HD3	1.93	0.68
1:B:384:ASN:ND2	1:B:391:GLY:H	1.90	0.68
1:A:86:PHE:HD1	1:A:93:GLY:HA2	1.57	0.68
1:C:31:LEU:HD23	1:C:70:LEU:HD11	1.74	0.68
1:A:318:LEU:HD11	1:A:322:LEU:HD23	1.76	0.68
1:B:100:ILE:HG21	1:B:297:VAL:HG21	1.76	0.68
1:C:303:LEU:HD12	1:C:305:ILE:HG12	1.76	0.68
1:A:413:LEU:O	1:A:416:GLN:HB2	1.94	0.67
1:A:4:MET:HE3	1:A:4:MET:H	1.58	0.67
1:A:234:VAL:HG23	1:A:236:PRO:HD3	1.75	0.67
1:C:216:LEU:HD11	1:C:221:ALA:HB2	1.76	0.67
1:A:258:ILE:HG13	1:A:306:ALA:HB1	1.76	0.67
1:C:125:GLU:OE1	1:C:126:LEU:HG	1.95	0.67
1:C:264:ARG:HH11	1:C:264:ARG:HB3	1.58	0.67
1:D:318:LEU:HD23	1:D:319:ILE:N	2.10	0.67
1:D:336:THR:HA	1:D:381:TRP:CZ3	2.29	0.67
1:C:59:THR:HG23	2:C:905:ANP:O3G	1.93	0.67
1:A:422:ALA:O	1:A:425:VAL:HG23	1.95	0.67
1:A:70:LEU:HA	1:A:73:LEU:HD22	1.77	0.67
1:A:96:VAL:HG12	1:A:284:LEU:HD11	1.77	0.67
1:D:394:ARG:O	1:D:398:VAL:HG13	1.95	0.67
1:D:129:GLU:HA	1:D:132:LEU:HB2	1.76	0.67
1:D:282:LEU:O	1:D:286:GLU:N	2.27	0.67
1:A:59:THR:HG23	2:A:900:ANP:O3G	1.94	0.67
1:A:397:THR:HG21	1:A:443:LEU:HA	1.75	0.67
1:C:63:LYS:HB2	2:C:905:ANP:O1B	1.95	0.67
1:C:132:LEU:HD12	1:C:133:ASP:N	2.09	0.67
1:C:278:GLN:HB3	1:C:319:ILE:HG21	1.77	0.67
1:D:327:PRO:O	1:D:329:ARG:HG2	1.94	0.67
1:A:13:LEU:C	1:A:15:LYS:H	2.03	0.67
1:D:127:ALA:O	1:D:131:ILE:HG12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ALA:HB2	1:B:332:LEU:HD11	1.75	0.66
1:B:261:ILE:HG22	1:B:278:GLN:HE21	1.58	0.66
1:C:68:ARG:HH11	1:C:68:ARG:HB3	1.60	0.66
1:B:127:ALA:HA	1:B:225:LEU:HB3	1.77	0.66
1:B:129:GLU:HA	1:B:132:LEU:HB2	1.77	0.66
1:D:5:THR:O	1:D:9:ILE:HG13	1.96	0.66
1:A:223:LYS:O	1:A:226:ILE:HG22	1.94	0.66
1:B:278:GLN:OE1	1:B:319:ILE:HG22	1.95	0.66
1:A:372:GLY:O	1:A:376:ILE:HD12	1.96	0.66
1:A:435:ASP:OD2	1:A:438:LEU:HD23	1.96	0.66
1:B:281:LEU:O	1:B:284:LEU:HG	1.95	0.66
1:C:366:ILE:HD13	1:C:366:ILE:N	2.09	0.66
1:C:390:ILE:HD11	1:C:394:ARG:NE	2.10	0.66
1:A:130:ARG:HA	1:A:133:ASP:HB2	1.78	0.66
1:C:65:GLU:O	1:C:68:ARG:HG2	1.96	0.65
1:C:132:LEU:HA	1:C:135:LEU:HD23	1.76	0.65
1:C:248:GLU:HG3	1:C:297:VAL:HG12	1.78	0.65
1:D:430:ASP:O	1:D:433:VAL:HG23	1.96	0.65
1:B:281:LEU:HD23	1:B:284:LEU:HD11	1.78	0.65
1:A:105:ASP:O	1:A:108:VAL:HB	1.96	0.65
1:A:57:GLY:O	1:A:309:ALA:HB2	1.97	0.65
1:A:132:LEU:HD12	1:A:133:ASP:N	2.11	0.65
1:B:430:ASP:O	1:B:433:VAL:HG23	1.96	0.65
1:D:284:LEU:HA	1:D:299:THR:OG1	1.97	0.65
1:A:31:LEU:HD23	1:A:70:LEU:HD11	1.76	0.65
1:D:281:LEU:O	1:D:284:LEU:HG	1.97	0.65
1:A:344:LEU:HA	1:A:351:ILE:CD1	2.27	0.65
1:B:24:LYS:O	1:B:27:VAL:HG22	1.96	0.65
1:B:383:VAL:HB	1:B:394:ARG:HH11	1.60	0.65
1:A:128:GLU:HA	1:A:131:ILE:HD12	1.79	0.65
1:C:22:ASN:HA	1:C:25:ARG:HG3	1.79	0.65
1:D:318:LEU:HD21	1:D:322:LEU:HD23	1.78	0.65
1:A:327:PRO:HG2	1:A:328:ILE:HD12	1.78	0.64
1:C:128:GLU:HA	1:C:131:ILE:CD1	2.27	0.64
1:C:319:ILE:CD1	1:C:321:GLU:HB2	2.27	0.64
1:D:285:VAL:C	1:D:287:GLY:H	2.05	0.64
1:C:103:LEU:HD23	1:C:247:VAL:HG12	1.79	0.64
1:C:397:THR:HG21	1:C:443:LEU:HA	1.78	0.64
1:B:4:MET:HB3	1:B:8:GLU:HB3	1.80	0.64
1:D:110:MET:O	1:D:113:VAL:HG22	1.98	0.64
1:C:13:LEU:C	1:C:15:LYS:H	2.04	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LEU:HD23	1:D:71:ALA:N	2.13	0.64
1:D:336:THR:HA	1:D:381:TRP:HZ3	1.61	0.64
1:A:153:SER:CA	1:A:156:ARG:HB3	2.25	0.64
1:C:337:THR:O	1:C:340:PHE:HB2	1.97	0.64
1:D:5:THR:HG23	1:D:8:GLU:CD	2.22	0.64
1:D:278:GLN:HA	1:D:281:LEU:HD12	1.80	0.64
1:A:66:ILE:H	1:A:66:ILE:CD1	2.11	0.63
1:D:278:GLN:O	1:D:281:LEU:HB2	1.98	0.63
1:A:61:VAL:HA	1:A:335:LEU:HD11	1.78	0.63
1:B:310:PHE:HB3	1:B:313:ALA:O	1.98	0.63
1:D:235:ASN:O	1:D:239:LEU:HG	1.97	0.63
1:A:277:VAL:HG12	1:A:281:LEU:HD11	1.81	0.63
1:B:83:ALA:HB1	1:B:261:ILE:CD1	2.28	0.63
1:B:395:LEU:HA	1:B:398:VAL:HG22	1.78	0.63
1:C:128:GLU:HA	1:C:131:ILE:HG13	1.80	0.63
1:C:277:VAL:HG12	1:C:281:LEU:CD1	2.29	0.63
1:D:395:LEU:O	1:D:398:VAL:HG22	1.98	0.63
1:A:173:ILE:O	1:A:212:LYS:HB3	1.97	0.63
1:B:254:PHE:HD2	1:B:305:ILE:HB	1.62	0.63
1:A:22:ASN:HA	1:A:25:ARG:HG3	1.80	0.63
1:A:96:VAL:HG11	1:A:281:LEU:HG	1.79	0.63
1:B:245:ASP:O	1:B:249:GLN:HB2	1.98	0.63
1:B:318:LEU:HD23	1:B:319:ILE:N	2.13	0.63
1:B:23:ALA:O	1:B:27:VAL:HG13	1.99	0.63
1:C:222:MET:O	1:C:226:ILE:HB	1.99	0.63
1:A:356:LYS:NZ	1:A:367:GLU:HA	2.13	0.63
1:B:423:ASP:O	1:B:427:LYS:HB2	1.98	0.63
1:D:21:ASP:HA	1:D:24:LYS:HG3	1.80	0.63
1:A:62:GLY:C	1:A:66:ILE:HD13	2.24	0.62
1:A:24:LYS:O	1:A:28:ALA:N	2.31	0.62
1:A:125:GLU:OE1	1:A:126:LEU:HG	1.99	0.62
1:C:23:ALA:HB2	1:C:332:LEU:HD11	1.80	0.62
1:C:128:GLU:HA	1:C:131:ILE:CG1	2.29	0.62
1:A:99:ILE:HG22	1:A:100:ILE:N	2.15	0.62
1:B:121:TYR:O	1:B:125:GLU:HB3	1.99	0.62
1:C:439:SER:HA	1:C:443:LEU:CD1	2.29	0.62
1:D:278:GLN:OE1	1:D:319:ILE:HG22	1.99	0.62
1:D:41:ASN:HD21	1:D:43:GLU:HB3	1.63	0.62
1:A:65:GLU:O	1:A:66:ILE:C	2.42	0.62
1:B:60:GLY:HA2	1:B:63:LYS:CG	2.30	0.62
1:C:20:GLN:HB3	1:C:332:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TRP:CZ3	1:C:36:ARG:HG3	2.33	0.62
1:D:254:PHE:HD2	1:D:305:ILE:HB	1.64	0.62
1:D:383:VAL:HB	1:D:394:ARG:HH11	1.65	0.62
1:D:375:ARG:HA	1:D:378:GLU:HB2	1.82	0.62
1:D:442:ILE:C	1:D:443:LEU:HG	2.23	0.62
1:A:63:LYS:HB2	2:A:900:ANP:O1B	2.00	0.62
1:B:289:THR:HA	1:B:297:VAL:O	2.00	0.62
1:C:363:GLY:O	1:C:414:SER:HA	2.00	0.62
1:C:438:LEU:HB3	1:C:442:ILE:HD11	1.81	0.62
1:D:83:ALA:HB1	1:D:261:ILE:CD1	2.30	0.62
1:D:257:GLU:O	1:D:260:LYS:HB2	2.00	0.62
1:A:129:GLU:O	1:A:132:LEU:HG	2.00	0.62
1:A:265:GLY:O	1:A:266:GLU:HB2	2.00	0.61
1:A:303:LEU:HD12	1:A:305:ILE:HG12	1.81	0.61
1:A:310:PHE:N	1:A:310:PHE:HD2	1.98	0.61
1:A:358:LEU:HD11	1:B:33:ASN:HD22	1.65	0.61
1:B:282:LEU:O	1:B:286:GLU:N	2.33	0.61
1:B:394:ARG:O	1:B:398:VAL:HG13	2.00	0.61
1:C:77:PRO:HA	1:C:110:MET:HE3	1.82	0.61
1:C:128:GLU:HA	1:C:131:ILE:HD12	1.80	0.61
1:B:340:PHE:O	1:B:343:ILE:HG13	2.00	0.61
1:C:312:ILE:HG13	1:C:313:ALA:H	1.65	0.61
1:A:366:ILE:HD13	1:A:366:ILE:N	2.07	0.61
1:C:23:ALA:HA	1:C:330:VAL:HG21	1.83	0.61
1:C:57:GLY:O	1:C:309:ALA:HB2	2.00	0.61
1:D:310:PHE:HB3	1:D:313:ALA:O	2.00	0.61
1:C:97:ASP:HB2	1:C:290:VAL:HG11	1.82	0.61
1:C:105:ASP:O	1:C:108:VAL:HB	2.01	0.61
1:D:271:ASP:HA	1:D:274:ARG:CB	2.29	0.61
1:B:355:TYR:OH	1:B:403:MET:HB3	2.00	0.61
1:A:23:ALA:HA	1:A:330:VAL:HG21	1.83	0.61
1:A:122:ARG:HB3	1:A:126:LEU:HD12	1.81	0.61
1:A:282:LEU:O	1:A:285:VAL:HG23	2.00	0.61
1:B:96:VAL:HG11	1:B:280:ASP:HB3	1.82	0.61
1:C:253:VAL:O	1:C:305:ILE:HG13	2.00	0.61
1:C:255:ILE:O	1:C:306:ALA:HA	2.01	0.61
1:C:265:GLY:O	1:C:266:GLU:HB2	2.00	0.61
1:D:91:TYR:HB3	1:D:95:GLU:HB2	1.82	0.61
1:A:264:ARG:HH11	1:A:264:ARG:HB3	1.65	0.61
1:B:336:THR:HG22	1:B:339:ASP:CG	2.25	0.61
1:A:65:GLU:O	1:A:68:ARG:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:HG23	1:B:8:GLU:CD	2.25	0.61
1:A:312:ILE:HG13	1:A:313:ALA:H	1.66	0.61
1:B:319:ILE:HD12	1:B:320:PRO:HD2	1.83	0.61
1:C:86:PHE:HA	1:C:93:GLY:HA2	1.83	0.61
1:B:235:ASN:O	1:B:239:LEU:HG	2.01	0.61
1:B:284:LEU:HA	1:B:299:THR:OG1	2.01	0.61
1:D:84:THR:C	1:D:86:PHE:H	2.09	0.61
1:C:66:ILE:H	1:C:66:ILE:CD1	2.13	0.60
1:A:62:GLY:O	1:A:63:LYS:C	2.44	0.60
1:A:258:ILE:HA	1:A:261:ILE:HD11	1.82	0.60
1:B:278:GLN:O	1:B:281:LEU:HB2	2.00	0.60
1:C:12:GLU:HG2	1:C:73:LEU:HD12	1.83	0.60
1:D:128:GLU:O	1:D:132:LEU:HB2	2.00	0.60
1:D:263:LYS:HG3	1:D:264:ARG:N	2.16	0.60
1:A:418:ILE:HD13	1:A:418:ILE:N	2.16	0.60
1:A:438:LEU:O	1:A:442:ILE:HD13	2.01	0.60
1:B:438:LEU:CD2	1:B:442:ILE:HD11	2.31	0.60
1:C:281:LEU:O	1:C:284:LEU:HG	2.02	0.60
1:A:5:THR:HB	1:A:6:PRO:HD2	1.84	0.60
1:B:122:ARG:HG3	1:B:233:LEU:HD21	1.81	0.60
1:B:436:GLU:O	1:B:438:LEU:N	2.34	0.60
1:D:27:VAL:HB	1:D:70:LEU:HD13	1.84	0.60
1:A:5:THR:N	1:A:8:GLU:HB2	2.16	0.60
1:B:442:ILE:C	1:B:443:LEU:HG	2.25	0.60
1:C:77:PRO:O	1:C:103:LEU:HD11	2.02	0.60
1:C:212:LYS:HE2	1:C:225:LEU:HD13	1.84	0.60
1:D:44:LEU:HA	1:D:47:GLU:CB	2.31	0.60
1:D:389:ASN:C	1:D:390:ILE:HG13	2.25	0.60
1:A:319:ILE:CD1	1:A:321:GLU:HB2	2.32	0.60
1:C:64:THR:HG22	1:C:68:ARG:HD3	1.83	0.60
1:C:65:GLU:OE2	1:C:69:ARG:HD3	2.02	0.60
1:A:339:ASP:O	1:A:343:ILE:HG13	2.01	0.60
1:D:52:ASN:C	1:D:328:ILE:HD12	2.27	0.60
1:D:100:ILE:HD11	1:D:284:LEU:HB3	1.84	0.60
1:D:223:LYS:HA	1:D:226:ILE:HD12	1.84	0.60
1:D:235:ASN:ND2	1:D:238:GLU:HG2	2.15	0.60
1:C:100:ILE:HG12	1:C:299:THR:CG2	2.31	0.60
1:C:376:ILE:HG13	1:C:425:VAL:HG11	1.83	0.60
1:D:117:GLU:HA	1:D:120:ARG:HG3	1.84	0.60
1:A:275:GLU:O	1:A:278:GLN:HB2	2.02	0.59
1:A:310:PHE:N	1:A:310:PHE:CD2	2.69	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLN:HA	1:B:281:LEU:HD12	1.83	0.59
1:D:340:PHE:O	1:D:343:ILE:HG13	2.02	0.59
1:A:64:THR:O	1:A:67:ALA:HB3	2.02	0.59
1:B:87:THR:O	1:B:88:GLU:HB2	2.01	0.59
1:C:129:GLU:O	1:C:132:LEU:HG	2.02	0.59
1:B:98:SER:O	1:B:99:ILE:C	2.44	0.59
1:C:111:VAL:HG13	1:C:112:ARG:H	1.67	0.59
1:C:163:LEU:C	1:C:165:GLU:H	2.09	0.59
1:C:344:LEU:HA	1:C:351:ILE:HD11	1.82	0.59
1:B:43:GLU:O	1:B:47:GLU:HB2	2.03	0.59
1:B:83:ALA:O	1:B:86:PHE:HD2	1.84	0.59
1:C:340:PHE:O	1:C:344:LEU:HD13	2.01	0.59
1:D:23:ALA:O	1:D:27:VAL:HG13	2.02	0.59
1:B:240:LYS:HG2	1:B:294:HIS:HB3	1.85	0.59
1:C:173:ILE:O	1:C:212:LYS:HB3	2.03	0.59
1:D:4:MET:HB3	1:D:8:GLU:HB3	1.85	0.59
1:D:339:ASP:O	1:D:343:ILE:HG12	2.03	0.59
1:A:108:VAL:HG21	1:A:294:HIS:CE1	2.38	0.59
1:D:57:GLY:C	1:D:309:ALA:HB2	2.28	0.59
1:A:153:SER:HA	1:A:157:GLN:H	1.68	0.59
1:B:397:THR:CG2	1:B:443:LEU:HA	2.33	0.59
1:A:77:PRO:O	1:A:103:LEU:HD11	2.02	0.59
1:D:320:PRO:HA	1:D:323:GLN:HB3	1.84	0.59
1:A:47:GLU:HG3	1:A:47:GLU:O	2.03	0.58
1:A:64:THR:HG22	1:A:68:ARG:HD3	1.83	0.58
1:A:212:LYS:HE2	1:A:225:LEU:HD13	1.85	0.58
1:C:45:ARG:C	1:C:47:GLU:H	2.11	0.58
1:C:151:GLU:N	1:C:152:PRO:HD2	2.19	0.58
1:C:366:ILE:H	1:C:366:ILE:CD1	2.10	0.58
1:C:397:THR:O	1:C:398:VAL:C	2.45	0.58
1:B:91:TYR:HB3	1:B:95:GLU:CB	2.33	0.58
1:B:235:ASN:ND2	1:B:238:GLU:HG2	2.13	0.58
1:D:384:ASN:HD21	1:D:391:GLY:H	1.51	0.58
1:B:57:GLY:C	1:B:309:ALA:HB2	2.27	0.58
1:C:64:THR:C	1:C:68:ARG:HD3	2.28	0.58
1:D:244:ILE:O	1:D:248:GLU:HG2	2.03	0.58
1:D:252:ILE:HD12	1:D:252:ILE:N	2.18	0.58
1:A:5:THR:HA	1:A:32:ARG:NH1	2.18	0.58
1:A:84:THR:C	1:A:86:PHE:H	2.11	0.58
1:B:293:LYS:HE2	1:B:294:HIS:NE2	2.18	0.58
1:D:116:ILE:O	1:D:120:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD12	1:A:44:LEU:H	1.68	0.58
1:A:109:LYS:HA	1:A:112:ARG:NH2	2.19	0.58
1:A:366:ILE:H	1:A:366:ILE:CD1	2.08	0.58
1:A:438:LEU:O	1:A:441:PHE:N	2.35	0.58
1:D:51:LYS:HB2	1:D:328:ILE:HD11	1.84	0.58
1:A:244:ILE:HA	1:A:247:VAL:HG23	1.86	0.58
1:B:128:GLU:O	1:B:132:LEU:HB2	2.03	0.58
1:B:21:ASP:HA	1:B:24:LYS:HG3	1.86	0.58
1:B:110:MET:O	1:B:113:VAL:HG22	2.04	0.58
1:C:5:THR:HB	1:C:6:PRO:HD2	1.85	0.58
1:C:234:VAL:HG23	1:C:235:ASN:H	1.69	0.58
1:C:248:GLU:HG2	1:C:298:LYS:H	1.69	0.58
1:C:383:VAL:HB	1:C:394:ARG:NH1	2.18	0.58
1:A:356:LYS:HZ2	1:A:367:GLU:HA	1.69	0.58
1:B:84:THR:C	1:B:86:PHE:H	2.12	0.58
1:C:339:ASP:O	1:C:343:ILE:HG13	2.04	0.58
1:D:31:LEU:O	1:D:34:ARG:HB2	2.04	0.58
1:D:442:ILE:O	1:D:443:LEU:HG	2.04	0.58
1:C:319:ILE:HD13	1:C:322:LEU:H	1.69	0.57
1:D:70:LEU:O	1:D:73:LEU:HG	2.04	0.57
1:D:127:ALA:HA	1:D:225:LEU:HB3	1.86	0.57
1:D:281:LEU:HD23	1:D:284:LEU:HD11	1.86	0.57
1:A:315:PRO:O	1:A:318:LEU:HB3	2.03	0.57
1:B:339:ASP:O	1:B:343:ILE:HG12	2.05	0.57
1:C:64:THR:O	1:C:67:ALA:HB3	2.04	0.57
1:C:279:ARG:O	1:C:283:PRO:HD2	2.04	0.57
1:C:394:ARG:O	1:C:398:VAL:HG23	2.04	0.57
1:C:422:ALA:O	1:C:425:VAL:HG23	2.05	0.57
1:C:435:ASP:OD2	1:C:438:LEU:HD23	2.04	0.57
1:A:5:THR:HG23	1:A:8:GLU:CD	2.30	0.57
1:C:65:GLU:O	1:C:66:ILE:C	2.47	0.57
1:C:258:ILE:HG13	1:C:306:ALA:CB	2.30	0.57
1:D:17:ILE:C	1:D:18:ILE:HD13	2.29	0.57
1:A:163:LEU:C	1:A:165:GLU:H	2.11	0.57
1:A:356:LYS:CA	1:A:366:ILE:HD11	2.23	0.57
1:B:224:LEU:HA	1:B:227:GLU:OE2	2.04	0.57
1:A:350:SER:OG	1:A:351:ILE:HD12	2.05	0.57
1:A:438:LEU:HB3	1:A:442:ILE:HD11	1.86	0.57
1:B:17:ILE:C	1:B:18:ILE:HD13	2.29	0.57
1:A:323:GLN:HG3	1:A:329:ARG:NH2	2.19	0.57
1:A:337:THR:O	1:A:340:PHE:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:LEU:HD23	1:C:443:LEU:HD11	1.86	0.57
1:A:439:SER:HA	1:A:443:LEU:CD1	2.35	0.57
1:A:66:ILE:HD12	1:A:66:ILE:N	2.18	0.57
1:B:252:ILE:HD12	1:B:252:ILE:N	2.20	0.57
1:C:96:VAL:O	1:C:99:ILE:HD13	2.05	0.57
1:C:402:LEU:CD1	1:C:425:VAL:HA	2.35	0.57
1:C:418:ILE:HD13	1:C:418:ILE:N	2.19	0.57
1:A:397:THR:O	1:A:398:VAL:C	2.46	0.57
1:C:47:GLU:O	1:C:47:GLU:HG3	2.05	0.57
1:C:429:LEU:N	1:C:429:LEU:HD23	2.19	0.57
1:C:84:THR:C	1:C:86:PHE:H	2.13	0.56
1:C:442:ILE:HD13	1:C:442:ILE:H	1.70	0.56
1:B:20:GLN:O	1:B:23:ALA:HB3	2.05	0.56
1:C:12:GLU:O	1:C:12:GLU:HG3	2.04	0.56
1:C:320:PRO:HA	1:C:323:GLN:HB3	1.87	0.56
1:A:212:LYS:O	1:A:213:ALA:HB3	2.04	0.56
1:A:230:ALA:C	1:A:232:LYS:H	2.12	0.56
1:C:66:ILE:HD12	1:C:66:ILE:N	2.19	0.56
1:D:60:GLY:HA2	1:D:63:LYS:CG	2.35	0.56
1:D:84:THR:O	1:D:86:PHE:N	2.39	0.56
1:C:23:ALA:CB	1:C:332:LEU:HD11	2.36	0.56
1:C:403:MET:O	1:C:407:SER:HB2	2.06	0.56
1:C:109:LYS:HA	1:C:112:ARG:NH2	2.21	0.56
1:C:351:ILE:HA	1:C:354:GLN:HE21	1.70	0.56
1:C:355:TYR:OH	1:C:403:MET:HB2	2.06	0.56
1:D:384:ASN:ND2	1:D:391:GLY:H	2.04	0.56
1:A:12:GLU:O	1:A:12:GLU:HG3	2.06	0.56
1:A:69:ARG:HD2	1:A:69:ARG:N	2.20	0.56
1:B:27:VAL:HB	1:B:70:LEU:HD13	1.87	0.56
1:B:281:LEU:O	1:B:282:LEU:C	2.49	0.56
1:C:101:ARG:HA	1:C:292:THR:HG22	1.88	0.56
1:C:122:ARG:HA	1:C:125:GLU:CG	2.36	0.56
1:C:282:LEU:O	1:C:285:VAL:HG23	2.05	0.56
1:A:45:ARG:C	1:A:47:GLU:H	2.13	0.56
1:A:173:ILE:HG22	1:A:174:GLU:H	1.71	0.56
1:A:356:LYS:HA	1:A:366:ILE:CD1	2.25	0.56
1:A:277:VAL:HG12	1:A:281:LEU:CD1	2.35	0.56
1:A:395:LEU:O	1:A:396:HIS:C	2.48	0.56
1:B:41:ASN:HD21	1:B:43:GLU:HB3	1.71	0.56
1:B:245:ASP:O	1:B:247:VAL:N	2.36	0.56
1:C:229:GLU:O	1:C:232:LYS:HE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HA	1:C:351:ILE:CD1	2.36	0.56
1:C:371:SER:HB2	1:C:422:ALA:HB2	1.87	0.56
1:D:41:ASN:O	1:D:45:ARG:HB2	2.05	0.56
1:A:21:ASP:O	1:A:24:LYS:N	2.39	0.56
1:A:367:GLU:HB3	1:A:419:THR:HG22	1.88	0.56
1:B:70:LEU:O	1:B:73:LEU:HG	2.06	0.56
1:B:389:ASN:C	1:B:390:ILE:HG13	2.29	0.56
1:C:262:CYS:O	1:C:263:LYS:HG3	2.06	0.56
1:D:53:ILE:HG12	1:D:328:ILE:HB	1.88	0.56
1:D:281:LEU:O	1:D:282:LEU:C	2.49	0.56
1:A:151:GLU:N	1:A:152:PRO:HD2	2.21	0.55
1:B:100:ILE:O	1:B:101:ARG:C	2.49	0.55
1:A:64:THR:C	1:A:68:ARG:HD3	2.30	0.55
1:B:271:ASP:HA	1:B:274:ARG:CB	2.36	0.55
1:C:174:GLU:HA	1:C:212:LYS:HB3	1.88	0.55
1:C:278:GLN:OE1	1:C:319:ILE:HG22	2.05	0.55
1:B:41:ASN:O	1:B:45:ARG:HB2	2.06	0.55
1:B:70:LEU:HD23	1:B:71:ALA:N	2.21	0.55
1:B:395:LEU:O	1:B:398:VAL:HG22	2.06	0.55
1:B:432:LEU:H	1:B:432:LEU:CD1	2.17	0.55
1:C:4:MET:HE3	1:C:4:MET:H	1.71	0.55
1:C:109:LYS:HG3	1:C:112:ARG:NH2	2.19	0.55
1:C:319:ILE:HD11	1:C:321:GLU:OE2	2.07	0.55
1:A:394:ARG:O	1:A:398:VAL:HG23	2.06	0.55
1:D:59:THR:O	1:D:61:VAL:N	2.40	0.55
1:A:6:PRO:HD3	1:A:32:ARG:HD3	1.87	0.55
1:C:323:GLN:HG3	1:C:329:ARG:NH2	2.22	0.55
1:A:432:LEU:HD23	1:A:443:LEU:HD11	1.88	0.55
1:A:86:PHE:HA	1:A:93:GLY:HA2	1.89	0.55
1:C:275:GLU:O	1:C:278:GLN:HB2	2.06	0.55
1:C:438:LEU:H	1:C:438:LEU:HD22	1.70	0.55
1:C:53:ILE:HG22	1:C:54:LEU:N	2.20	0.55
1:B:10:VAL:HG12	1:B:14:ASP:OD1	2.07	0.55
1:C:399:LEU:O	1:C:403:MET:HG2	2.07	0.55
1:A:77:PRO:HA	1:A:110:MET:HE3	1.88	0.55
1:A:429:LEU:O	1:A:430:ASP:C	2.50	0.55
1:B:125:GLU:HG3	1:B:126:LEU:N	2.18	0.55
1:C:319:ILE:HG23	1:C:322:LEU:CB	2.37	0.55
1:D:402:LEU:HB2	1:D:429:LEU:HD21	1.89	0.55
1:A:351:ILE:HA	1:A:354:GLN:HE21	1.72	0.54
1:C:136:ILE:HD12	1:C:156:ARG:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:PRO:O	1:C:318:LEU:HB3	2.07	0.54
1:A:254:PHE:CD2	1:A:305:ILE:HB	2.42	0.54
1:C:18:ILE:HD13	1:C:343:ILE:HG12	1.88	0.54
1:C:99:ILE:HG22	1:C:100:ILE:N	2.21	0.54
1:D:237:GLU:C	1:D:239:LEU:H	2.13	0.54
1:A:145:GLN:HA	1:A:145:GLN:OE1	2.07	0.54
1:B:318:LEU:HD21	1:B:322:LEU:CD2	2.37	0.54
1:B:375:ARG:HA	1:B:378:GLU:HB2	1.89	0.54
1:C:320:PRO:O	1:C:321:GLU:C	2.49	0.54
1:A:132:LEU:HA	1:A:135:LEU:HB2	1.89	0.54
1:C:261:ILE:HG22	1:C:274:ARG:HB3	1.89	0.54
1:D:229:GLU:HA	1:D:232:LYS:HD2	1.89	0.54
1:C:60:GLY:H	2:C:905:ANP:PG	2.31	0.54
1:C:62:GLY:O	1:C:63:LYS:C	2.51	0.54
1:A:127:ALA:HB2	1:A:226:ILE:HA	1.90	0.54
1:B:31:LEU:O	1:B:34:ARG:HB2	2.07	0.54
1:C:114:GLN:O	1:C:118:LYS:HB2	2.07	0.54
1:C:402:LEU:HD13	1:C:425:VAL:HA	1.88	0.54
1:A:100:ILE:HD11	1:A:284:LEU:HD22	1.90	0.54
1:B:59:THR:O	1:B:61:VAL:N	2.41	0.54
1:C:229:GLU:HB3	1:C:232:LYS:NZ	2.23	0.54
1:C:322:LEU:O	1:C:325:ARG:N	2.41	0.54
1:D:224:LEU:HA	1:D:227:GLU:OE2	2.08	0.54
1:C:298:LYS:C	1:C:300:ASP:H	2.14	0.54
1:A:358:LEU:HD11	1:B:33:ASN:ND2	2.22	0.54
1:B:28:ALA:O	1:B:29:ILE:C	2.51	0.54
1:B:104:THR:O	1:B:107:ALA:HB3	2.07	0.54
1:B:245:ASP:C	1:B:247:VAL:N	2.65	0.54
1:B:285:VAL:C	1:B:287:GLY:H	2.16	0.54
1:C:26:SER:CA	1:C:29:ILE:HD12	2.38	0.54
1:C:69:ARG:HD2	1:C:69:ARG:N	2.22	0.54
1:D:98:SER:O	1:D:99:ILE:C	2.50	0.54
1:A:278:GLN:OE1	1:A:319:ILE:HG22	2.08	0.54
1:C:288:CYS:O	1:C:298:LYS:HD3	2.07	0.54
1:A:109:LYS:O	1:A:112:ARG:HB3	2.07	0.53
1:B:127:ALA:O	1:B:131:ILE:HG12	2.08	0.53
1:C:413:LEU:O	1:C:414:SER:C	2.51	0.53
1:D:236:PRO:O	1:D:240:LYS:HB2	2.08	0.53
1:A:399:LEU:O	1:A:402:LEU:HB3	2.09	0.53
1:A:413:LEU:O	1:A:414:SER:C	2.51	0.53
1:C:291:SER:HA	1:C:296:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LEU:HD11	1:D:33:ASN:HD22	1.73	0.53
1:A:367:GLU:O	1:A:420:ILE:N	2.41	0.53
1:B:275:GLU:O	1:B:278:GLN:HB2	2.08	0.53
1:C:310:PHE:HD2	1:C:310:PHE:N	2.06	0.53
1:D:289:THR:HA	1:D:297:VAL:O	2.07	0.53
1:D:340:PHE:HA	1:D:343:ILE:HD11	1.90	0.53
1:A:21:ASP:O	1:A:22:ASN:C	2.52	0.53
1:A:53:ILE:HG22	1:A:54:LEU:N	2.23	0.53
1:A:155:ALA:O	1:A:158:ALA:HB3	2.08	0.53
1:C:271:ASP:C	1:C:273:SER:H	2.16	0.53
1:A:20:GLN:HB3	1:A:332:LEU:HD12	1.91	0.53
1:C:254:PHE:CD2	1:C:305:ILE:HB	2.44	0.53
1:A:55:MET:O	1:A:307:SER:HA	2.09	0.53
1:A:100:ILE:HG12	1:A:299:THR:CG2	2.38	0.53
1:B:51:LYS:HB2	1:B:328:ILE:HD11	1.91	0.53
1:B:109:LYS:O	1:B:113:VAL:HG13	2.08	0.53
1:C:112:ARG:HH11	1:C:112:ARG:HG2	1.74	0.53
1:D:104:THR:O	1:D:107:ALA:HB3	2.09	0.53
1:A:322:LEU:O	1:A:325:ARG:N	2.41	0.53
1:B:100:ILE:CG2	1:B:297:VAL:HG21	2.39	0.53
1:D:52:ASN:O	1:D:327:PRO:HD2	2.08	0.53
1:D:235:ASN:HD22	1:D:235:ASN:H	1.57	0.53
1:A:234:VAL:HG23	1:A:235:ASN:H	1.73	0.53
1:A:383:VAL:HB	1:A:394:ARG:NH1	2.23	0.53
1:A:432:LEU:O	1:A:434:ALA:N	2.42	0.53
1:B:375:ARG:HA	1:B:375:ARG:HE	1.74	0.53
1:C:140:LYS:H	1:C:140:LYS:HD3	1.72	0.53
1:A:109:LYS:HE2	1:B:289:THR:HB	1.91	0.53
1:A:271:ASP:C	1:A:273:SER:H	2.16	0.53
1:A:325:ARG:O	1:A:327:PRO:HD3	2.08	0.53
1:B:44:LEU:O	1:B:45:ARG:C	2.52	0.53
1:D:243:ALA:O	1:D:247:VAL:HG23	2.09	0.53
1:D:285:VAL:C	1:D:287:GLY:N	2.65	0.53
1:D:355:TYR:CZ	1:D:403:MET:HB3	2.43	0.53
1:D:397:THR:CG2	1:D:443:LEU:HA	2.38	0.53
1:B:299:THR:HA	1:B:302:ILE:CG1	2.35	0.52
1:C:44:LEU:HD12	1:C:44:LEU:H	1.73	0.52
1:C:234:VAL:HG23	1:C:235:ASN:N	2.24	0.52
1:C:240:LYS:C	1:C:242:ASP:H	2.16	0.52
1:C:310:PHE:N	1:C:310:PHE:CD2	2.76	0.52
1:C:361:THR:C	1:C:363:GLY:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ALA:O	1:D:86:PHE:HD2	1.91	0.52
1:D:356:LYS:CA	1:D:366:ILE:HD11	2.36	0.52
1:A:18:ILE:N	2:A:900:ANP:HN61	2.01	0.52
1:A:279:ARG:O	1:A:283:PRO:HD2	2.10	0.52
1:B:429:LEU:O	1:B:430:ASP:C	2.52	0.52
1:A:248:GLU:HG3	1:A:297:VAL:HG12	1.90	0.52
1:B:84:THR:O	1:B:86:PHE:N	2.43	0.52
1:B:100:ILE:HD11	1:B:284:LEU:HB3	1.91	0.52
1:B:379:ALA:O	1:B:380:ALA:C	2.52	0.52
1:C:9:ILE:HG23	1:C:73:LEU:HD11	1.91	0.52
1:D:248:GLU:HA	1:D:302:ILE:HD11	1.91	0.52
1:A:23:ALA:HB2	1:A:332:LEU:HD11	1.90	0.52
1:C:65:GLU:HA	1:C:68:ARG:CG	2.40	0.52
1:C:319:ILE:HG12	1:C:320:PRO:CD	2.37	0.52
1:D:78:PHE:CE1	1:D:254:PHE:HB2	2.45	0.52
1:D:240:LYS:CG	1:D:294:HIS:HB3	2.40	0.52
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.75	0.52
1:A:371:SER:HB2	1:A:422:ALA:HB2	1.91	0.52
1:B:340:PHE:HA	1:B:343:ILE:HG13	1.92	0.52
1:D:44:LEU:HA	1:D:47:GLU:HB2	1.90	0.52
1:A:320:PRO:HA	1:A:323:GLN:HB3	1.92	0.52
1:D:123:ALA:O	1:D:127:ALA:HB2	2.10	0.52
1:D:387:THR:C	1:D:388:GLU:HG2	2.35	0.52
1:A:216:LEU:HD11	1:A:221:ALA:HB2	1.91	0.52
1:B:367:GLU:HG2	1:B:417:ASN:HD21	1.75	0.52
1:C:13:LEU:C	1:C:15:LYS:N	2.67	0.52
1:C:432:LEU:O	1:C:434:ALA:N	2.43	0.52
1:D:22:ASN:ND2	1:D:22:ASN:H	2.06	0.52
1:D:271:ASP:CA	1:D:274:ARG:HB2	2.37	0.52
1:D:375:ARG:HA	1:D:375:ARG:HE	1.75	0.52
1:B:340:PHE:HA	1:B:343:ILE:HD11	1.91	0.52
1:C:6:PRO:HD3	1:C:32:ARG:HD3	1.90	0.52
1:A:9:ILE:HG23	1:A:73:LEU:HD11	1.92	0.52
1:B:402:LEU:HB2	1:B:429:LEU:HD21	1.92	0.52
1:C:107:ALA:HB1	1:C:247:VAL:HG22	1.91	0.52
1:C:231:ALA:O	1:C:234:VAL:HG22	2.10	0.52
1:D:235:ASN:ND2	1:D:235:ASN:N	2.57	0.52
1:D:319:ILE:HD12	1:D:320:PRO:HD2	1.91	0.52
1:A:128:GLU:O	1:A:131:ILE:HB	2.10	0.52
1:C:239:LEU:HD23	1:C:240:LYS:N	2.25	0.52
1:C:327:PRO:HG2	1:C:328:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ILE:HD13	1:C:418:ILE:H	1.75	0.52
1:A:68:ARG:HB3	1:A:68:ARG:NH1	2.19	0.51
1:C:127:ALA:HB2	1:C:226:ILE:HA	1.92	0.51
1:C:135:LEU:O	1:C:137:PRO:HD3	2.09	0.51
1:D:59:THR:CG2	1:D:390:ILE:HA	2.37	0.51
1:A:12:GLU:HG2	1:A:73:LEU:HD12	1.92	0.51
1:A:320:PRO:O	1:A:321:GLU:C	2.52	0.51
1:B:344:LEU:HD21	1:B:376:ILE:CG2	2.40	0.51
1:B:387:THR:C	1:B:388:GLU:HG2	2.35	0.51
1:C:442:ILE:HG12	1:C:443:LEU:CD1	2.38	0.51
1:A:80:LYS:HA	1:A:254:PHE:HB3	1.92	0.51
1:B:52:ASN:C	1:B:328:ILE:HD12	2.35	0.51
1:B:438:LEU:HD13	1:B:438:LEU:C	2.35	0.51
1:C:5:THR:N	1:C:8:GLU:HB2	2.24	0.51
1:C:5:THR:HA	1:C:32:ARG:NH1	2.24	0.51
1:D:35:TRP:CE3	1:D:36:ARG:HG2	2.45	0.51
1:D:429:LEU:O	1:D:430:ASP:C	2.52	0.51
1:D:432:LEU:H	1:D:432:LEU:CD1	2.20	0.51
1:A:104:THR:O	1:A:107:ALA:HB3	2.09	0.51
1:A:436:GLU:O	1:A:437:ASP:C	2.53	0.51
1:B:5:THR:O	1:B:9:ILE:HG13	2.10	0.51
1:C:21:ASP:O	1:C:22:ASN:C	2.53	0.51
1:C:55:MET:O	1:C:307:SER:HA	2.10	0.51
1:C:65:GLU:C	1:C:69:ARG:HG2	2.35	0.51
1:D:87:THR:O	1:D:88:GLU:HB2	2.10	0.51
1:A:277:VAL:O	1:A:278:GLN:C	2.53	0.51
1:C:21:ASP:O	1:C:24:LYS:N	2.44	0.51
1:C:107:ALA:HB2	1:C:247:VAL:HG13	1.93	0.51
1:D:25:ARG:O	1:D:28:ALA:HB3	2.10	0.51
1:A:103:LEU:HD23	1:A:247:VAL:HG12	1.92	0.51
1:A:127:ALA:O	1:A:225:LEU:HD23	2.11	0.51
1:A:275:GLU:O	1:A:276:GLY:C	2.54	0.51
1:B:237:GLU:CD	1:B:237:GLU:N	2.68	0.51
1:C:100:ILE:HG12	1:C:299:THR:HG22	1.92	0.51
1:C:130:ARG:HB2	1:C:225:LEU:HD21	1.92	0.51
1:C:258:ILE:HA	1:C:261:ILE:HD11	1.92	0.51
1:C:282:LEU:O	1:C:286:GLU:HB2	2.11	0.51
1:C:319:ILE:HG23	1:C:322:LEU:HB2	1.93	0.51
1:C:436:GLU:O	1:C:437:ASP:C	2.52	0.51
1:D:44:LEU:HA	1:D:47:GLU:HB3	1.92	0.51
1:D:351:ILE:CD1	1:D:399:LEU:HD13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:PHE:O	1:A:343:ILE:HB	2.11	0.51
1:D:86:PHE:CE1	1:D:96:VAL:HA	2.46	0.51
1:D:224:LEU:C	1:D:226:ILE:H	2.18	0.51
1:D:391:GLY:O	1:D:392:ALA:C	2.53	0.51
1:A:128:GLU:HA	1:A:131:ILE:CD1	2.40	0.51
1:A:252:ILE:HG23	1:A:303:LEU:HB3	1.92	0.51
1:A:442:ILE:HD13	1:A:442:ILE:H	1.76	0.51
1:A:140:LYS:H	1:A:140:LYS:HD3	1.76	0.51
1:A:248:GLU:HG2	1:A:298:LYS:H	1.76	0.51
1:B:55:MET:O	1:B:307:SER:HA	2.11	0.51
1:B:126:LEU:HB2	1:B:229:GLU:HG3	1.93	0.51
1:C:135:LEU:HB3	1:C:159:PHE:CD1	2.46	0.51
1:C:244:ILE:HA	1:C:247:VAL:HG23	1.92	0.51
1:C:421:ASP:OD1	1:C:423:ASP:HB2	2.11	0.51
1:C:438:LEU:O	1:C:441:PHE:N	2.39	0.51
1:D:100:ILE:O	1:D:101:ARG:C	2.54	0.51
1:D:371:SER:O	1:D:422:ALA:HB2	2.11	0.51
1:A:375:ARG:O	1:A:376:ILE:C	2.53	0.50
1:B:61:VAL:O	1:B:61:VAL:CG1	2.59	0.50
1:B:285:VAL:C	1:B:287:GLY:N	2.68	0.50
1:B:420:ILE:N	1:B:420:ILE:HD12	2.26	0.50
1:C:53:ILE:HG12	1:C:328:ILE:HB	1.93	0.50
1:D:285:VAL:O	1:D:287:GLY:N	2.44	0.50
1:D:354:GLN:O	1:D:357:ALA:HB3	2.11	0.50
1:A:86:PHE:CD1	1:A:93:GLY:HA2	2.43	0.50
1:C:18:ILE:N	2:C:905:ANP:N6	2.48	0.50
1:C:104:THR:HA	1:C:247:VAL:HG11	1.93	0.50
1:C:310:PHE:HB3	1:C:313:ALA:O	2.11	0.50
1:D:105:ASP:O	1:D:108:VAL:HG12	2.11	0.50
1:A:131:ILE:HD11	1:A:222:MET:HA	1.92	0.50
1:B:65:GLU:O	1:B:66:ILE:C	2.54	0.50
1:B:429:LEU:O	1:B:431:ALA:N	2.45	0.50
1:C:31:LEU:O	1:C:34:ARG:HB2	2.11	0.50
1:C:64:THR:HG22	1:C:68:ARG:CD	2.41	0.50
1:C:344:LEU:HD11	1:C:395:LEU:HD13	1.94	0.50
1:B:105:ASP:O	1:B:108:VAL:HG12	2.12	0.50
1:B:374:LYS:O	1:B:378:GLU:HB2	2.11	0.50
1:B:383:VAL:HB	1:B:394:ARG:NH1	2.24	0.50
1:C:127:ALA:O	1:C:131:ILE:HG13	2.11	0.50
1:C:254:PHE:HD2	1:C:305:ILE:HB	1.77	0.50
1:D:235:ASN:ND2	1:D:235:ASN:H	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:SER:O	1:A:351:ILE:C	2.54	0.50
1:B:98:SER:O	1:B:101:ARG:N	2.45	0.50
1:B:105:ASP:C	1:B:107:ALA:H	2.20	0.50
1:C:299:THR:HA	1:C:302:ILE:CD1	2.31	0.50
1:D:125:GLU:O	1:D:128:GLU:HG2	2.11	0.50
1:D:356:LYS:HA	1:D:366:ILE:CD1	2.37	0.50
1:D:395:LEU:HA	1:D:398:VAL:HG22	1.92	0.50
1:A:64:THR:HG22	1:A:68:ARG:CD	2.42	0.50
1:A:96:VAL:O	1:A:99:ILE:HD13	2.12	0.50
1:B:285:VAL:O	1:B:287:GLY:N	2.45	0.50
1:C:24:LYS:O	1:C:28:ALA:N	2.41	0.50
1:C:346:GLU:N	1:C:347:PRO:HD2	2.26	0.50
1:C:429:LEU:O	1:C:430:ASP:C	2.54	0.50
1:D:27:VAL:HB	1:D:70:LEU:CD1	2.42	0.50
1:D:237:GLU:C	1:D:239:LEU:N	2.69	0.50
1:A:5:THR:CB	1:A:6:PRO:HD2	2.41	0.50
1:A:24:LYS:HA	1:A:27:VAL:HG12	1.93	0.50
1:B:35:TRP:CE3	1:B:36:ARG:HG2	2.47	0.50
1:B:240:LYS:HE2	1:B:294:HIS:HD2	1.77	0.50
1:C:25:ARG:O	1:C:28:ALA:HB3	2.12	0.50
1:C:174:GLU:HA	1:C:212:LYS:CB	2.41	0.50
1:C:372:GLY:O	1:C:376:ILE:HD12	2.12	0.50
1:D:44:LEU:O	1:D:45:ARG:C	2.55	0.50
1:D:255:ILE:HG21	1:D:258:ILE:HD11	1.94	0.50
1:B:340:PHE:HA	1:B:343:ILE:CG1	2.42	0.50
1:B:405:GLU:O	1:B:408:TYR:N	2.45	0.50
1:C:396:HIS:CD2	1:C:396:HIS:H	2.28	0.50
1:C:155:ALA:O	1:C:158:ALA:HB3	2.12	0.49
1:D:245:ASP:O	1:D:247:VAL:N	2.44	0.49
1:B:23:ALA:HA	1:B:330:VAL:HG21	1.94	0.49
1:B:439:SER:HA	1:B:443:LEU:HD12	1.94	0.49
1:C:31:LEU:HD23	1:C:70:LEU:CD1	2.42	0.49
1:C:153:SER:O	1:C:154:ALA:C	2.55	0.49
1:C:375:ARG:O	1:C:376:ILE:C	2.54	0.49
1:D:350:SER:CB	1:D:353:VAL:HG23	2.42	0.49
1:A:21:ASP:HA	1:A:24:LYS:HD2	1.93	0.49
1:A:298:LYS:C	1:A:300:ASP:H	2.19	0.49
1:C:79:ILE:HG22	1:C:103:LEU:CD1	2.38	0.49
1:C:83:ALA:O	1:C:84:THR:C	2.54	0.49
1:C:420:ILE:HG23	1:C:424:TYR:CD1	2.47	0.49
1:B:53:ILE:O	1:B:305:ILE:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:PHE:CD1	1:C:93:GLY:HA2	2.42	0.49
1:D:84:THR:C	1:D:86:PHE:N	2.70	0.49
1:D:111:VAL:HG21	1:D:243:ALA:HA	1.93	0.49
1:D:275:GLU:O	1:D:278:GLN:HB2	2.11	0.49
1:A:346:GLU:N	1:A:347:PRO:HD2	2.25	0.49
1:B:113:VAL:HG23	1:B:114:GLN:HG3	1.93	0.49
1:B:243:ALA:O	1:B:247:VAL:HG23	2.11	0.49
1:C:225:LEU:HG	1:C:229:GLU:HG3	1.95	0.49
1:C:244:ILE:O	1:C:248:GLU:HB2	2.12	0.49
1:C:347:PRO:HG2	1:C:350:SER:HB2	1.95	0.49
1:D:366:ILE:HB	1:D:420:ILE:HD11	1.95	0.49
1:A:145:GLN:C	1:A:146:THR:HG23	2.36	0.49
1:B:421:ASP:OD2	1:B:423:ASP:HB2	2.13	0.49
1:C:102:ASP:O	1:C:105:ASP:HB2	2.11	0.49
1:C:420:ILE:HG23	1:C:424:TYR:HD1	1.77	0.49
1:D:344:LEU:HD21	1:D:376:ILE:CG2	2.41	0.49
1:A:25:ARG:O	1:A:28:ALA:HB3	2.13	0.49
1:A:438:LEU:H	1:A:438:LEU:HD22	1.77	0.49
1:B:238:GLU:O	1:B:242:ASP:HB2	2.13	0.49
1:D:340:PHE:HA	1:D:343:ILE:CG1	2.43	0.49
1:D:428:HIS:HB2	1:D:429:LEU:HD22	1.95	0.49
1:A:310:PHE:HB3	1:A:313:ALA:O	2.13	0.49
1:B:54:LEU:HB2	1:B:326:LEU:HG	1.95	0.49
1:B:391:GLY:O	1:B:392:ALA:C	2.56	0.49
1:C:27:VAL:HG13	1:C:70:LEU:HD13	1.94	0.49
1:C:275:GLU:O	1:C:276:GLY:C	2.54	0.49
1:C:395:LEU:O	1:C:396:HIS:C	2.55	0.49
1:D:318:LEU:HD22	1:D:323:GLN:CA	2.42	0.49
1:D:421:ASP:OD2	1:D:423:ASP:HB2	2.12	0.49
1:A:26:SER:HA	1:A:29:ILE:HD12	1.94	0.49
1:A:124:GLU:O	1:A:127:ALA:HB3	2.13	0.49
1:B:86:PHE:HB2	1:B:277:VAL:HG13	1.93	0.49
1:B:438:LEU:HD22	1:B:442:ILE:HD11	1.94	0.49
1:C:62:GLY:O	1:C:64:THR:N	2.46	0.49
1:C:74:ALA:O	1:C:75:ASN:HB3	2.13	0.49
1:C:96:VAL:HG11	1:C:281:LEU:HG	1.94	0.49
1:D:105:ASP:C	1:D:107:ALA:N	2.70	0.49
1:A:153:SER:HA	1:A:156:ARG:CB	2.38	0.49
1:B:111:VAL:HG11	1:B:243:ALA:HB2	1.95	0.49
1:C:107:ALA:CB	1:C:247:VAL:HG22	2.43	0.49
1:C:108:VAL:O	1:C:111:VAL:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ILE:HG23	1:C:303:LEU:HB3	1.94	0.49
1:D:20:GLN:O	1:D:23:ALA:HB3	2.12	0.49
1:A:13:LEU:C	1:A:15:LYS:N	2.65	0.48
1:A:83:ALA:O	1:A:85:LYS:N	2.46	0.48
1:A:235:ASN:OD1	1:A:238:GLU:HB3	2.13	0.48
1:D:405:GLU:O	1:D:408:TYR:N	2.46	0.48
1:D:438:LEU:CD2	1:D:442:ILE:HD11	2.43	0.48
1:A:75:ASN:HD21	1:A:114:GLN:HE22	1.59	0.48
1:A:355:TYR:OH	1:A:403:MET:HB2	2.13	0.48
1:B:438:LEU:HD21	1:B:442:ILE:HD11	1.95	0.48
1:C:65:GLU:HA	1:C:68:ARG:HG2	1.96	0.48
1:C:103:LEU:CD2	1:C:247:VAL:HG12	2.43	0.48
1:D:271:ASP:C	1:D:273:SER:N	2.71	0.48
1:D:362:GLU:C	1:D:364:VAL:H	2.21	0.48
1:A:18:ILE:HD13	1:A:343:ILE:HG12	1.94	0.48
1:A:361:THR:C	1:A:363:GLY:H	2.20	0.48
1:B:84:THR:C	1:B:86:PHE:N	2.72	0.48
1:C:54:LEU:HD23	1:C:306:ALA:C	2.39	0.48
1:A:319:ILE:HG12	1:A:320:PRO:CD	2.40	0.48
1:B:25:ARG:O	1:B:28:ALA:HB3	2.13	0.48
1:B:432:LEU:O	1:B:433:VAL:C	2.56	0.48
1:C:5:THR:CB	1:C:6:PRO:HD2	2.42	0.48
1:D:379:ALA:O	1:D:380:ALA:C	2.56	0.48
1:A:52:ASN:O	1:A:327:PRO:HD2	2.13	0.48
1:A:68:ARG:O	1:A:69:ARG:C	2.57	0.48
1:A:316:SER:HA	1:A:323:GLN:HE22	1.79	0.48
1:B:319:ILE:HD12	1:B:320:PRO:CD	2.43	0.48
1:D:240:LYS:HE2	1:D:294:HIS:HD2	1.78	0.48
1:D:288:CYS:O	1:D:299:THR:N	2.41	0.48
1:D:432:LEU:HD12	1:D:432:LEU:N	2.25	0.48
1:A:21:ASP:HA	1:A:24:LYS:HG3	1.96	0.48
1:B:44:LEU:HA	1:B:47:GLU:CB	2.43	0.48
1:B:282:LEU:O	1:B:283:PRO:C	2.56	0.48
1:C:80:LYS:HG3	1:C:81:VAL:N	2.27	0.48
1:C:259:ASP:HB3	1:C:310:PHE:CE2	2.49	0.48
1:C:359:MET:HE2	1:C:406:ILE:HG22	1.95	0.48
1:D:54:LEU:HD23	1:D:329:ARG:HD3	1.95	0.48
1:A:83:ALA:O	1:A:84:THR:C	2.56	0.48
1:A:92:VAL:O	1:A:95:GLU:HB2	2.13	0.48
1:A:327:PRO:HG2	1:A:328:ILE:CD1	2.43	0.48
1:A:367:GLU:CB	1:A:419:THR:HG22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:HD22	1:A:394:ARG:NH1	2.11	0.48
1:C:64:THR:O	1:C:68:ARG:HD3	2.14	0.48
1:A:6:PRO:HA	1:A:9:ILE:HD12	1.95	0.48
1:A:69:ARG:O	1:A:73:LEU:HB3	2.14	0.48
1:A:437:ASP:O	1:A:440:ARG:N	2.47	0.48
1:C:240:LYS:C	1:C:242:ASP:N	2.69	0.48
1:D:23:ALA:HB2	1:D:332:LEU:HD11	1.96	0.48
1:A:55:MET:HE3	1:A:254:PHE:HE2	1.78	0.48
1:C:32:ARG:HG2	1:C:36:ARG:NE	2.29	0.48
1:C:69:ARG:O	1:C:73:LEU:HB3	2.14	0.48
1:C:239:LEU:O	1:C:242:ASP:HB2	2.12	0.48
1:C:278:GLN:HG2	1:C:322:LEU:CD2	2.43	0.48
1:C:320:PRO:O	1:C:323:GLN:N	2.47	0.48
1:C:432:LEU:O	1:C:433:VAL:C	2.56	0.48
1:D:229:GLU:OE1	1:D:232:LYS:HD2	2.14	0.48
1:A:10:VAL:O	1:A:13:LEU:N	2.42	0.48
1:A:152:PRO:C	1:A:154:ALA:N	2.72	0.48
1:A:282:LEU:HA	1:A:285:VAL:HG23	1.96	0.48
1:C:322:LEU:C	1:C:324:GLY:N	2.72	0.48
1:C:325:ARG:HA	1:C:325:ARG:HD3	1.55	0.48
1:D:62:GLY:O	1:D:63:LYS:C	2.56	0.48
1:D:398:VAL:HG23	1:D:399:LEU:N	2.29	0.48
1:A:379:ALA:O	1:A:380:ALA:C	2.56	0.47
1:B:247:VAL:C	1:B:249:GLN:H	2.22	0.47
1:C:384:ASN:ND2	1:C:394:ARG:HG2	2.29	0.47
1:D:62:GLY:O	1:D:65:GLU:N	2.47	0.47
1:D:383:VAL:HB	1:D:394:ARG:NH1	2.29	0.47
1:A:27:VAL:CG2	1:A:70:LEU:HD13	2.34	0.47
1:A:98:SER:O	1:A:101:ARG:HB3	2.14	0.47
1:A:244:ILE:O	1:A:248:GLU:HB2	2.14	0.47
1:A:363:GLY:O	1:A:414:SER:HA	2.15	0.47
1:C:13:LEU:HD23	1:C:24:LYS:HB3	1.96	0.47
1:C:131:ILE:HD11	1:C:222:MET:HA	1.96	0.47
1:C:277:VAL:C	1:C:281:LEU:HD12	2.39	0.47
1:B:372:GLY:O	1:B:375:ARG:N	2.47	0.47
1:C:169:ASP:H	1:C:218:ILE:HG22	1.79	0.47
1:C:241:GLN:HA	1:C:244:ILE:HD11	1.97	0.47
1:C:298:LYS:C	1:C:300:ASP:N	2.73	0.47
1:C:379:ALA:O	1:C:380:ALA:C	2.57	0.47
1:C:390:ILE:HG22	1:D:320:PRO:HB3	1.97	0.47
1:D:100:ILE:HG21	1:D:297:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LEU:C	1:D:226:ILE:N	2.72	0.47
1:D:374:LYS:O	1:D:378:GLU:HB2	2.15	0.47
1:A:54:LEU:HD23	1:A:306:ALA:C	2.39	0.47
1:A:254:PHE:HD2	1:A:305:ILE:HB	1.78	0.47
1:B:54:LEU:O	1:B:54:LEU:HG	2.14	0.47
1:B:405:GLU:O	1:B:406:ILE:C	2.57	0.47
1:C:62:GLY:C	1:C:66:ILE:HD13	2.39	0.47
1:A:111:VAL:HG13	1:A:112:ARG:N	2.28	0.47
1:A:396:HIS:CD2	1:A:396:HIS:H	2.31	0.47
1:B:105:ASP:C	1:B:107:ALA:N	2.68	0.47
1:B:381:TRP:CD1	1:B:381:TRP:C	2.92	0.47
1:C:289:THR:HA	1:C:297:VAL:O	2.15	0.47
1:D:288:CYS:O	1:D:298:LYS:HA	2.14	0.47
1:A:7:ARG:HA	1:A:10:VAL:HB	1.97	0.47
1:C:18:ILE:N	2:C:905:ANP:HN61	2.02	0.47
1:C:77:PRO:HD2	1:C:250:HIS:O	2.14	0.47
1:C:127:ALA:O	1:C:225:LEU:HD23	2.15	0.47
1:C:151:GLU:H	1:C:152:PRO:HD2	1.78	0.47
1:C:340:PHE:O	1:C:341:GLU:C	2.57	0.47
1:D:340:PHE:O	1:D:341:GLU:C	2.57	0.47
1:A:168:LEU:N	1:A:218:ILE:CG2	2.78	0.47
1:A:214:ARG:CZ	1:B:233:LEU:HG	2.45	0.47
1:A:402:LEU:CD1	1:A:425:VAL:HA	2.45	0.47
1:C:267:SER:O	1:C:268:SER:C	2.57	0.47
1:C:350:SER:O	1:C:351:ILE:C	2.58	0.47
1:D:107:ALA:O	1:D:110:MET:N	2.47	0.47
1:D:356:LYS:HD3	1:D:366:ILE:O	2.15	0.47
1:A:42:GLU:O	1:A:43:GLU:C	2.57	0.47
1:A:110:MET:O	1:A:111:VAL:C	2.58	0.47
1:C:10:VAL:O	1:C:13:LEU:N	2.47	0.47
1:C:124:GLU:O	1:C:127:ALA:HB3	2.14	0.47
1:C:333:GLN:CD	1:C:333:GLN:H	2.23	0.47
1:D:113:VAL:HG23	1:D:114:GLN:HG3	1.97	0.47
1:D:131:ILE:HD11	1:D:222:MET:SD	2.55	0.47
1:A:55:MET:HE3	1:A:305:ILE:HG21	1.96	0.47
1:A:319:ILE:HD13	1:A:322:LEU:H	1.80	0.47
1:B:17:ILE:HG23	1:B:18:ILE:H	1.77	0.47
1:C:20:GLN:HB3	1:C:332:LEU:CD1	2.45	0.47
1:C:173:ILE:HG22	1:C:174:GLU:H	1.79	0.47
1:D:21:ASP:CA	1:D:24:LYS:HG3	2.45	0.47
1:D:244:ILE:HD11	1:D:296:MET:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CZ3	1:A:36:ARG:HG3	2.50	0.47
1:A:316:SER:HA	1:A:323:GLN:OE1	2.14	0.47
1:B:29:ILE:O	1:B:30:ALA:C	2.59	0.47
1:B:307:SER:OG	1:B:308:GLY:N	2.47	0.47
1:C:52:ASN:O	1:C:328:ILE:HD12	2.14	0.47
1:A:437:ASP:O	1:A:438:LEU:C	2.58	0.46
1:B:23:ALA:HB2	1:B:332:LEU:CD1	2.42	0.46
1:C:135:LEU:C	1:C:137:PRO:HD3	2.40	0.46
1:C:316:SER:HA	1:C:323:GLN:OE1	2.15	0.46
1:D:298:LYS:HB3	1:D:300:ASP:OD2	2.15	0.46
1:D:365:ASN:O	1:D:418:ILE:HG12	2.15	0.46
1:A:18:ILE:N	1:A:18:ILE:HD12	2.29	0.46
1:C:64:THR:HG22	1:C:68:ARG:NE	2.30	0.46
1:C:325:ARG:C	1:C:327:PRO:HD3	2.41	0.46
1:C:399:LEU:HD23	1:C:400:GLU:N	2.30	0.46
1:D:439:SER:C	1:D:441:PHE:H	2.23	0.46
1:A:132:LEU:O	1:A:135:LEU:HB2	2.15	0.46
1:B:27:VAL:HG23	1:B:70:LEU:HD12	1.97	0.46
1:C:277:VAL:O	1:C:278:GLN:C	2.57	0.46
1:B:244:ILE:CG2	1:B:245:ASP:N	2.78	0.46
1:B:406:ILE:HD11	1:B:424:TYR:OH	2.15	0.46
1:C:111:VAL:HG13	1:C:112:ARG:N	2.29	0.46
1:C:112:ARG:HD2	1:C:113:VAL:N	2.31	0.46
1:D:254:PHE:CZ	1:D:307:SER:HB2	2.51	0.46
1:B:86:PHE:HE1	1:B:95:GLU:O	1.98	0.46
1:C:55:MET:HE3	1:C:254:PHE:HE2	1.81	0.46
1:C:163:LEU:C	1:C:165:GLU:N	2.74	0.46
1:C:257:GLU:O	1:C:258:ILE:C	2.56	0.46
1:C:344:LEU:CD1	1:C:395:LEU:HD13	2.46	0.46
1:D:320:PRO:O	1:D:321:GLU:C	2.57	0.46
1:D:360:ALA:HA	1:D:364:VAL:O	2.15	0.46
1:A:376:ILE:HG13	1:A:425:VAL:HG11	1.97	0.46
1:B:27:VAL:HG23	1:B:28:ALA:N	2.29	0.46
1:B:371:SER:O	1:B:422:ALA:HB2	2.16	0.46
1:B:372:GLY:O	1:B:373:ILE:C	2.57	0.46
1:B:395:LEU:O	1:B:396:HIS:C	2.58	0.46
1:B:432:LEU:HD12	1:B:432:LEU:N	2.23	0.46
1:C:82:GLU:O	1:C:85:LYS:HG2	2.15	0.46
1:C:261:ILE:H	1:C:261:ILE:HG13	1.29	0.46
1:C:442:ILE:O	1:C:443:LEU:HG	2.15	0.46
1:A:23:ALA:CB	1:A:332:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LYS:O	1:A:64:THR:C	2.58	0.46
1:A:140:LYS:HE3	1:A:140:LYS:HB2	1.69	0.46
1:A:285:VAL:HB	1:A:325:ARG:HG3	1.97	0.46
1:A:432:LEU:C	1:A:434:ALA:N	2.71	0.46
1:D:236:PRO:HA	1:D:239:LEU:HD12	1.98	0.46
1:A:65:GLU:HA	1:A:68:ARG:CG	2.46	0.46
1:A:130:ARG:O	1:A:133:ASP:HB2	2.15	0.46
1:A:153:SER:O	1:A:154:ALA:C	2.58	0.46
1:A:270:PRO:O	1:A:274:ARG:HG3	2.15	0.46
1:C:108:VAL:O	1:C:109:LYS:C	2.59	0.46
1:C:285:VAL:HB	1:C:325:ARG:HG3	1.96	0.46
1:C:319:ILE:HD13	1:C:321:GLU:N	2.29	0.46
1:C:432:LEU:N	1:C:432:LEU:HD12	2.31	0.46
1:D:116:ILE:HD11	1:D:230:ALA:HB1	1.97	0.46
1:D:247:VAL:C	1:D:249:GLN:H	2.22	0.46
1:D:439:SER:HA	1:D:443:LEU:CD1	2.46	0.46
1:B:328:ILE:H	1:B:328:ILE:HG13	1.36	0.46
1:C:319:ILE:CD1	1:C:322:LEU:H	2.28	0.46
1:C:376:ILE:O	1:C:379:ALA:HB3	2.16	0.46
1:D:65:GLU:O	1:D:66:ILE:C	2.56	0.46
1:D:105:ASP:C	1:D:107:ALA:H	2.23	0.46
1:D:340:PHE:HA	1:D:343:ILE:HG13	1.97	0.46
1:D:436:GLU:O	1:D:438:LEU:N	2.42	0.46
1:A:80:LYS:HG3	1:A:81:VAL:N	2.29	0.46
1:A:333:GLN:N	1:A:333:GLN:CD	2.74	0.46
1:B:340:PHE:HA	1:B:343:ILE:CD1	2.46	0.46
1:B:344:LEU:HD21	1:B:376:ILE:HG22	1.98	0.46
1:C:29:ILE:O	1:C:30:ALA:C	2.59	0.46
1:C:156:ARG:O	1:C:157:GLN:C	2.58	0.46
1:D:271:ASP:C	1:D:274:ARG:H	2.23	0.46
1:D:438:LEU:HD22	1:D:442:ILE:HD11	1.98	0.46
1:A:22:ASN:O	1:A:25:ARG:HB2	2.16	0.45
1:A:62:GLY:O	1:A:64:THR:N	2.49	0.45
1:B:125:GLU:O	1:B:128:GLU:HG2	2.16	0.45
1:B:362:GLU:OE1	1:B:410:ALA:HB3	2.16	0.45
1:C:98:SER:O	1:C:101:ARG:HB3	2.16	0.45
1:D:235:ASN:HB2	1:D:238:GLU:HB3	1.98	0.45
1:D:345:THR:C	1:D:347:PRO:HD2	2.40	0.45
1:A:230:ALA:C	1:A:232:LYS:N	2.72	0.45
1:A:347:PRO:HG2	1:A:350:SER:HB2	1.97	0.45
1:B:14:ASP:HA	1:B:24:LYS:HZ2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HB3	1:C:159:PHE:HD1	1.80	0.45
1:C:335:LEU:HD21	2:C:905:ANP:N1	2.31	0.45
1:D:17:ILE:HG13	1:D:18:ILE:H	1.80	0.45
1:D:44:LEU:O	1:D:47:GLU:N	2.45	0.45
1:A:261:ILE:HG22	1:A:274:ARG:HB3	1.98	0.45
1:A:402:LEU:HD13	1:A:425:VAL:HA	1.97	0.45
1:B:362:GLU:C	1:B:364:VAL:H	2.24	0.45
1:C:172:GLU:HB3	1:C:215:LYS:HA	1.97	0.45
1:C:438:LEU:H	1:C:438:LEU:CD2	2.29	0.45
1:D:33:ASN:HA	1:D:36:ARG:HG3	1.99	0.45
1:D:63:LYS:HB3	1:D:332:LEU:CD2	2.46	0.45
1:D:366:ILE:HB	1:D:420:ILE:CD1	2.46	0.45
1:A:109:LYS:O	1:A:110:MET:C	2.60	0.45
1:A:399:LEU:HD23	1:A:400:GLU:N	2.31	0.45
1:B:340:PHE:O	1:B:344:LEU:HB2	2.16	0.45
1:C:366:ILE:N	1:C:366:ILE:CD1	2.74	0.45
1:D:128:GLU:HB3	1:D:222:MET:SD	2.56	0.45
1:D:293:LYS:HE2	1:D:294:HIS:NE2	2.31	0.45
1:D:439:SER:HA	1:D:443:LEU:HD12	1.97	0.45
1:A:156:ARG:O	1:A:157:GLN:C	2.59	0.45
1:B:369:THR:HG23	1:B:420:ILE:O	2.17	0.45
1:B:396:HIS:O	1:B:400:GLU:HB2	2.16	0.45
1:C:102:ASP:O	1:C:105:ASP:N	2.49	0.45
1:C:128:GLU:O	1:C:131:ILE:HB	2.16	0.45
1:C:136:ILE:O	1:C:138:PRO:HD3	2.16	0.45
1:C:255:ILE:CG2	1:C:258:ILE:HD11	2.46	0.45
1:C:366:ILE:HG22	1:C:418:ILE:HD11	1.98	0.45
1:C:405:GLU:O	1:C:408:TYR:N	2.47	0.45
1:D:29:ILE:O	1:D:30:ALA:C	2.58	0.45
1:A:156:ARG:O	1:A:159:PHE:N	2.50	0.45
1:A:325:ARG:HA	1:A:325:ARG:HD3	1.55	0.45
1:A:402:LEU:HB2	1:A:429:LEU:HD21	1.99	0.45
1:B:21:ASP:O	1:B:22:ASN:C	2.58	0.45
1:B:44:LEU:HA	1:B:47:GLU:HB2	1.98	0.45
1:C:264:ARG:HB3	1:C:264:ARG:NH1	2.29	0.45
1:D:10:VAL:HG12	1:D:14:ASP:OD1	2.17	0.45
1:D:41:ASN:C	1:D:45:ARG:HB2	2.41	0.45
1:D:54:LEU:HA	1:D:306:ALA:HB3	1.99	0.45
1:D:126:LEU:HB2	1:D:229:GLU:HG3	1.99	0.45
1:D:340:PHE:O	1:D:344:LEU:HB2	2.17	0.45
1:A:257:GLU:O	1:A:258:ILE:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PRO:O	1:B:321:GLU:C	2.59	0.45
1:C:97:ASP:HB2	1:C:290:VAL:CG1	2.46	0.45
1:C:153:SER:CA	1:C:156:ARG:HB3	2.34	0.45
1:C:333:GLN:CD	1:C:333:GLN:N	2.75	0.45
1:D:33:ASN:O	1:D:34:ARG:C	2.60	0.45
1:A:34:ARG:NH2	1:A:250:HIS:HA	2.32	0.45
1:B:27:VAL:HA	1:B:53:ILE:CD1	2.47	0.45
1:B:346:GLU:O	1:B:347:PRO:C	2.59	0.45
1:C:7:ARG:HG2	1:C:8:GLU:N	2.32	0.45
1:C:34:ARG:HH22	1:C:251:GLY:H	1.65	0.45
1:C:44:LEU:HA	1:C:47:GLU:HB3	1.99	0.45
1:C:52:ASN:HB3	1:C:304:PHE:O	2.16	0.45
1:C:257:GLU:HG2	1:C:260:LYS:CG	2.47	0.45
1:C:350:SER:OG	1:C:351:ILE:HD12	2.17	0.45
1:A:44:LEU:HD12	1:A:44:LEU:N	2.30	0.45
1:A:100:ILE:HG12	1:A:299:THR:HG22	1.99	0.45
1:A:234:VAL:HG23	1:A:235:ASN:N	2.32	0.45
1:B:318:LEU:HD21	1:B:322:LEU:CG	2.47	0.45
1:B:442:ILE:O	1:B:443:LEU:HG	2.17	0.45
1:C:34:ARG:NH2	1:C:251:GLY:H	2.15	0.45
1:C:63:LYS:O	1:C:64:THR:C	2.59	0.45
1:C:122:ARG:HB3	1:C:126:LEU:HD12	1.98	0.45
1:C:389:ASN:C	1:C:391:GLY:H	2.25	0.45
1:D:54:LEU:O	1:D:54:LEU:HG	2.16	0.45
1:D:59:THR:O	1:D:60:GLY:C	2.59	0.45
1:D:79:ILE:HG12	1:D:81:VAL:HG23	1.99	0.45
1:D:350:SER:O	1:D:353:VAL:HB	2.16	0.45
1:A:277:VAL:O	1:A:280:ASP:N	2.50	0.45
1:B:322:LEU:C	1:B:324:GLY:N	2.74	0.45
1:C:18:ILE:N	1:C:18:ILE:HD12	2.31	0.45
1:C:84:THR:O	1:C:86:PHE:N	2.47	0.45
1:C:101:ARG:HA	1:C:292:THR:CG2	2.47	0.45
1:C:259:ASP:HB3	1:C:310:PHE:CD2	2.52	0.45
1:C:335:LEU:HD11	2:C:905:ANP:H2	1.99	0.45
1:D:47:GLU:OE1	1:D:47:GLU:O	2.34	0.45
1:D:100:ILE:HG12	1:D:299:THR:CG2	2.47	0.45
1:D:344:LEU:HD21	1:D:376:ILE:HG22	1.99	0.45
1:A:31:LEU:HD23	1:A:70:LEU:CD1	2.45	0.44
1:A:54:LEU:O	1:A:56:ILE:HD12	2.17	0.44
1:A:429:LEU:O	1:A:432:LEU:N	2.50	0.44
1:A:432:LEU:O	1:A:433:VAL:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ASN:ND2	1:B:22:ASN:H	2.15	0.44
1:B:117:GLU:HA	1:B:120:ARG:NE	2.31	0.44
1:B:248:GLU:HA	1:B:302:ILE:HD11	1.99	0.44
1:C:61:VAL:HG12	1:C:335:LEU:HG	2.00	0.44
1:C:78:PHE:CG	1:C:79:ILE:N	2.84	0.44
1:C:437:ASP:O	1:C:438:LEU:C	2.60	0.44
1:C:442:ILE:HG22	1:D:329:ARG:CB	2.47	0.44
1:A:32:ARG:HG2	1:A:36:ARG:NE	2.33	0.44
1:A:98:SER:O	1:A:99:ILE:C	2.59	0.44
1:A:174:GLU:HA	1:A:212:LYS:HB3	1.99	0.44
1:B:29:ILE:O	1:B:32:ARG:N	2.49	0.44
1:B:59:THR:C	1:B:61:VAL:N	2.73	0.44
1:C:98:SER:O	1:C:99:ILE:C	2.59	0.44
1:D:92:VAL:HB	1:D:93:GLY:H	1.53	0.44
1:D:318:LEU:HD22	1:D:323:GLN:N	2.33	0.44
1:D:357:ALA:O	1:D:360:ALA:HB3	2.18	0.44
1:D:381:TRP:CD1	1:D:381:TRP:C	2.94	0.44
1:D:421:ASP:OD1	1:D:424:TYR:HB2	2.18	0.44
1:A:31:LEU:O	1:A:34:ARG:HB2	2.18	0.44
1:A:109:LYS:HA	1:A:112:ARG:HH21	1.82	0.44
1:A:257:GLU:HG2	1:A:260:LYS:CG	2.47	0.44
1:A:408:TYR:O	1:A:410:ALA:N	2.50	0.44
1:B:53:ILE:HG12	1:B:328:ILE:HB	1.99	0.44
1:B:233:LEU:HD12	1:B:233:LEU:N	2.32	0.44
1:B:244:ILE:HD11	1:B:296:MET:O	2.17	0.44
1:B:259:ASP:O	1:B:262:CYS:HB2	2.17	0.44
1:C:42:GLU:O	1:C:43:GLU:C	2.61	0.44
1:C:319:ILE:HG23	1:C:322:LEU:HB3	1.99	0.44
1:D:282:LEU:O	1:D:283:PRO:C	2.60	0.44
1:D:282:LEU:CB	1:D:283:PRO:HD3	2.47	0.44
1:A:60:GLY:H	2:A:900:ANP:PG	2.40	0.44
1:A:78:PHE:CG	1:A:79:ILE:N	2.85	0.44
1:B:235:ASN:ND2	1:B:235:ASN:H	2.15	0.44
1:B:252:ILE:HA	1:B:303:LEU:O	2.17	0.44
1:B:356:LYS:CA	1:B:366:ILE:HD11	2.37	0.44
1:D:59:THR:C	1:D:61:VAL:N	2.75	0.44
1:D:284:LEU:HG	1:D:284:LEU:H	1.53	0.44
1:D:360:ALA:O	1:D:363:GLY:N	2.48	0.44
1:A:316:SER:HA	1:A:323:GLN:NE2	2.33	0.44
1:B:20:GLN:O	1:B:21:ASP:C	2.59	0.44
1:B:360:ALA:O	1:B:363:GLY:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ARG:NH1	1:B:426:SER:HB3	2.33	0.44
1:D:27:VAL:HA	1:D:53:ILE:CD1	2.48	0.44
1:D:274:ARG:O	1:D:277:VAL:N	2.50	0.44
1:A:120:ARG:HA	1:A:123:ALA:CB	2.48	0.44
1:A:231:ALA:O	1:A:234:VAL:HG22	2.18	0.44
1:B:44:LEU:O	1:B:47:GLU:N	2.49	0.44
1:C:230:ALA:C	1:C:232:LYS:H	2.26	0.44
1:C:318:LEU:HG	1:C:319:ILE:N	2.32	0.44
1:C:367:GLU:O	1:C:420:ILE:N	2.45	0.44
1:A:21:ASP:HA	1:A:24:LYS:CG	2.48	0.44
1:A:34:ARG:NH2	1:A:251:GLY:H	2.15	0.44
1:A:97:ASP:O	1:A:98:SER:C	2.60	0.44
1:A:119:ASN:HD22	1:A:119:ASN:HA	1.52	0.44
1:A:132:LEU:HD12	1:A:132:LEU:C	2.42	0.44
1:B:298:LYS:HB3	1:B:300:ASP:OD2	2.18	0.44
1:C:125:GLU:HG3	1:C:126:LEU:H	1.82	0.44
1:C:369:THR:C	1:C:371:SER:N	2.74	0.44
1:C:372:GLY:O	1:C:375:ARG:HB2	2.17	0.44
1:C:432:LEU:C	1:C:434:ALA:N	2.75	0.44
1:D:128:GLU:O	1:D:132:LEU:N	2.50	0.44
1:D:284:LEU:O	1:D:299:THR:HB	2.18	0.44
1:D:287:GLY:HA2	1:D:299:THR:C	2.43	0.44
1:D:421:ASP:O	1:D:425:VAL:HG23	2.18	0.44
1:B:351:ILE:CD1	1:B:399:LEU:HD13	2.48	0.44
1:C:387:THR:HA	1:C:440:ARG:NH2	2.32	0.44
1:D:78:PHE:CZ	1:D:254:PHE:HB2	2.53	0.44
1:D:237:GLU:CD	1:D:237:GLU:N	2.76	0.44
1:D:375:ARG:HG3	1:D:422:ALA:HA	2.00	0.44
1:A:65:GLU:C	1:A:69:ARG:HG2	2.43	0.44
1:A:267:SER:O	1:A:268:SER:C	2.60	0.44
1:A:350:SER:HB3	1:A:353:VAL:HG23	2.00	0.44
1:B:33:ASN:O	1:B:34:ARG:C	2.61	0.44
1:B:355:TYR:CZ	1:B:403:MET:HB3	2.53	0.44
1:C:21:ASP:HA	1:C:24:LYS:HD2	1.99	0.44
1:C:65:GLU:O	1:C:69:ARG:HG2	2.17	0.44
1:C:220:ASP:O	1:C:223:LYS:N	2.50	0.44
1:D:125:GLU:HG3	1:D:126:LEU:N	2.32	0.44
1:D:340:PHE:HA	1:D:343:ILE:CD1	2.48	0.44
1:C:68:ARG:O	1:C:69:ARG:C	2.60	0.43
1:C:86:PHE:HA	1:C:93:GLY:CA	2.44	0.43
1:C:132:LEU:HD12	1:C:132:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ILE:HD13	1:C:319:ILE:C	2.43	0.43
1:C:399:LEU:O	1:C:402:LEU:HB3	2.18	0.43
1:D:100:ILE:N	1:D:100:ILE:HD12	2.33	0.43
1:D:246:ALA:HA	1:D:250:HIS:ND1	2.32	0.43
1:D:282:LEU:HD23	1:D:286:GLU:CD	2.43	0.43
1:A:11:SER:HA	1:A:14:ASP:OD1	2.18	0.43
1:A:61:VAL:HG11	1:A:333:GLN:O	2.19	0.43
1:A:348:ASN:O	1:A:349:ALA:HB3	2.19	0.43
1:B:69:ARG:HG3	1:B:73:LEU:HD23	1.99	0.43
1:B:91:TYR:C	1:B:95:GLU:HB3	2.43	0.43
1:B:116:ILE:O	1:B:120:ARG:HG3	2.17	0.43
1:B:123:ALA:O	1:B:127:ALA:HB2	2.18	0.43
1:B:356:LYS:HA	1:B:366:ILE:CD1	2.36	0.43
1:B:375:ARG:HG3	1:B:422:ALA:HA	1.99	0.43
1:C:276:GLY:O	1:C:277:VAL:C	2.60	0.43
1:C:299:THR:O	1:C:300:ASP:C	2.61	0.43
1:A:24:LYS:O	1:A:25:ARG:C	2.60	0.43
1:A:130:ARG:CA	1:A:133:ASP:HB2	2.46	0.43
1:A:149:GLN:C	1:A:152:PRO:HD2	2.44	0.43
1:B:379:ALA:O	1:B:383:VAL:HG23	2.17	0.43
1:C:21:ASP:CG	1:C:22:ASN:N	2.76	0.43
1:C:168:LEU:N	1:C:218:ILE:CG2	2.81	0.43
1:C:278:GLN:HG2	1:C:322:LEU:HD22	2.00	0.43
1:C:292:THR:C	1:C:294:HIS:N	2.76	0.43
1:D:346:GLU:O	1:D:347:PRO:C	2.61	0.43
1:A:18:ILE:N	2:A:900:ANP:N6	2.47	0.43
1:A:67:ALA:O	1:A:68:ARG:C	2.61	0.43
1:A:399:LEU:O	1:A:402:LEU:N	2.51	0.43
1:B:92:VAL:HB	1:B:93:GLY:H	1.54	0.43
1:B:257:GLU:O	1:B:258:ILE:C	2.61	0.43
1:B:318:LEU:HD22	1:B:323:GLN:CA	2.48	0.43
1:B:361:THR:C	1:B:363:GLY:H	2.26	0.43
1:B:381:TRP:O	1:B:382:GLN:C	2.61	0.43
1:C:28:ALA:O	1:C:29:ILE:C	2.61	0.43
1:C:281:LEU:O	1:C:282:LEU:C	2.62	0.43
1:D:117:GLU:HA	1:D:120:ARG:CZ	2.48	0.43
1:D:343:ILE:O	1:D:347:PRO:HG2	2.19	0.43
1:A:253:VAL:O	1:A:305:ILE:HG13	2.19	0.43
1:C:6:PRO:HA	1:C:9:ILE:HD12	1.99	0.43
1:C:424:TYR:O	1:C:425:VAL:C	2.60	0.43
1:C:437:ASP:O	1:C:440:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:GLY:HA3	1:D:302:ILE:HG23	2.00	0.43
1:D:398:VAL:CG2	1:D:399:LEU:N	2.81	0.43
1:A:24:LYS:C	1:A:27:VAL:HG12	2.41	0.43
1:A:157:GLN:O	1:A:158:ALA:C	2.61	0.43
1:A:223:LYS:HA	1:A:226:ILE:HB	2.01	0.43
1:A:342:ARG:O	1:A:347:PRO:HD2	2.18	0.43
1:B:236:PRO:O	1:B:240:LYS:HB2	2.18	0.43
1:B:247:VAL:C	1:B:249:GLN:N	2.76	0.43
1:B:271:ASP:C	1:B:274:ARG:H	2.27	0.43
1:B:383:VAL:O	1:B:387:THR:HG23	2.18	0.43
1:C:369:THR:HB	1:C:372:GLY:H	1.84	0.43
1:D:22:ASN:ND2	1:D:22:ASN:N	2.67	0.43
1:D:32:ARG:O	1:D:33:ASN:C	2.62	0.43
1:D:240:LYS:HG2	1:D:294:HIS:HB3	2.00	0.43
1:D:438:LEU:HD13	1:D:438:LEU:C	2.43	0.43
1:A:255:ILE:N	1:A:255:ILE:HD13	2.34	0.43
1:B:62:GLY:O	1:B:63:LYS:C	2.60	0.43
1:B:119:ASN:C	1:B:121:TYR:H	2.26	0.43
1:D:53:ILE:O	1:D:305:ILE:HA	2.18	0.43
1:D:86:PHE:HB2	1:D:277:VAL:HG13	2.00	0.43
1:D:310:PHE:N	1:D:310:PHE:CD2	2.87	0.43
1:D:319:ILE:HG23	1:D:319:ILE:O	2.19	0.43
1:D:350:SER:HB3	1:D:353:VAL:HG23	1.99	0.43
1:A:41:ASN:O	1:A:42:GLU:C	2.61	0.43
1:A:64:THR:HG22	1:A:68:ARG:NE	2.33	0.43
1:A:276:GLY:O	1:A:277:VAL:C	2.59	0.43
1:A:366:ILE:HA	1:A:418:ILE:O	2.19	0.43
1:B:31:LEU:O	1:B:31:LEU:HD22	2.18	0.43
1:B:398:VAL:HG23	1:B:399:LEU:N	2.33	0.43
1:C:384:ASN:HD22	1:C:394:ARG:NH1	2.17	0.43
1:D:252:ILE:HA	1:D:303:LEU:O	2.19	0.43
1:A:64:THR:O	1:A:65:GLU:C	2.62	0.43
1:A:258:ILE:HD13	1:A:261:ILE:HD11	2.00	0.43
1:A:372:GLY:O	1:A:375:ARG:HB2	2.19	0.43
1:A:373:ILE:O	1:A:374:LYS:C	2.62	0.43
1:A:405:GLU:O	1:A:408:TYR:N	2.51	0.43
1:A:409:ASP:O	1:A:413:LEU:HD23	2.18	0.43
1:B:117:GLU:HA	1:B:120:ARG:HG3	1.99	0.43
1:B:282:LEU:CB	1:B:283:PRO:HD3	2.49	0.43
1:B:340:PHE:O	1:B:341:GLU:C	2.62	0.43
1:B:357:ALA:O	1:B:360:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLY:O	1:B:393:ARG:N	2.52	0.43
1:C:77:PRO:CD	1:C:246:ALA:HB1	2.49	0.43
1:C:216:LEU:HD11	1:C:221:ALA:CB	2.45	0.43
1:C:255:ILE:HD13	1:C:255:ILE:N	2.33	0.43
1:C:342:ARG:O	1:C:347:PRO:HD2	2.19	0.43
1:D:76:ALA:CB	1:D:252:ILE:HD11	2.49	0.43
1:D:307:SER:OG	1:D:308:GLY:N	2.52	0.43
1:D:310:PHE:CD1	1:D:314:LYS:HA	2.53	0.43
1:A:5:THR:HG23	1:A:8:GLU:OE2	2.19	0.43
1:A:340:PHE:O	1:A:341:GLU:C	2.62	0.43
1:A:351:ILE:HD12	1:A:352:THR:H	1.84	0.43
1:A:440:ARG:HB3	1:B:316:SER:CB	2.49	0.43
1:B:54:LEU:HD13	1:B:306:ALA:HB3	2.00	0.43
1:B:103:LEU:HD21	1:B:247:VAL:HG13	2.01	0.43
1:B:274:ARG:O	1:B:277:VAL:N	2.51	0.43
1:C:12:GLU:CG	1:C:73:LEU:HD12	2.47	0.43
1:C:104:THR:O	1:C:107:ALA:HB3	2.19	0.43
1:C:168:LEU:N	1:C:218:ILE:HG22	2.33	0.43
1:C:169:ASP:H	1:C:218:ILE:CG2	2.32	0.43
1:C:171:LYS:O	1:C:172:GLU:HB3	2.19	0.43
1:C:366:ILE:HA	1:C:418:ILE:O	2.19	0.43
1:C:405:GLU:O	1:C:406:ILE:C	2.60	0.43
1:C:439:SER:O	1:C:443:LEU:HB2	2.18	0.43
1:D:111:VAL:HG21	1:D:243:ALA:CA	2.49	0.43
1:D:123:ALA:CB	1:D:226:ILE:HG23	2.36	0.43
1:D:351:ILE:HG13	1:D:352:THR:N	2.34	0.43
1:D:405:GLU:O	1:D:406:ILE:C	2.61	0.43
1:A:53:ILE:HG12	1:A:328:ILE:HB	2.00	0.42
1:A:168:LEU:N	1:A:218:ILE:HG22	2.34	0.42
1:B:129:GLU:HA	1:B:132:LEU:CB	2.45	0.42
1:B:236:PRO:HA	1:B:239:LEU:HD12	2.00	0.42
1:B:384:ASN:HD21	1:B:391:GLY:N	2.10	0.42
1:C:235:ASN:OD1	1:C:238:GLU:HB3	2.18	0.42
1:D:69:ARG:O	1:D:73:LEU:HD23	2.19	0.42
1:D:103:LEU:HD23	1:D:104:THR:N	2.34	0.42
1:A:52:ASN:O	1:A:328:ILE:HD12	2.18	0.42
1:A:107:ALA:HB1	1:A:247:VAL:HG22	2.01	0.42
1:A:259:ASP:HB3	1:A:310:PHE:CE2	2.54	0.42
1:A:361:THR:HG21	1:B:36:ARG:CA	2.45	0.42
1:B:13:LEU:CD1	1:B:73:LEU:HD21	2.49	0.42
1:B:100:ILE:N	1:B:100:ILE:HD12	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ILE:O	1:B:320:PRO:C	2.62	0.42
1:B:439:SER:HA	1:B:443:LEU:CD1	2.49	0.42
1:D:240:LYS:C	1:D:242:ASP:N	2.76	0.42
1:D:245:ASP:C	1:D:247:VAL:N	2.67	0.42
1:A:5:THR:O	1:A:8:GLU:HB2	2.19	0.42
1:A:65:GLU:HA	1:A:68:ARG:HG2	2.01	0.42
1:A:131:ILE:CG2	1:A:218:ILE:HD11	2.50	0.42
1:A:299:THR:O	1:A:300:ASP:C	2.62	0.42
1:A:319:ILE:HG23	1:A:322:LEU:CB	2.49	0.42
1:A:325:ARG:C	1:A:327:PRO:HD3	2.44	0.42
1:A:420:ILE:HG23	1:A:424:TYR:HD1	1.83	0.42
1:B:38:MET:HE1	1:B:46:HIS:NE2	2.34	0.42
1:B:78:PHE:CG	1:B:79:ILE:N	2.86	0.42
1:B:263:LYS:HG3	1:B:264:ARG:H	1.79	0.42
1:B:351:ILE:HG13	1:B:352:THR:N	2.32	0.42
1:B:404:GLU:HB3	1:B:405:GLU:H	1.69	0.42
1:C:27:VAL:CG2	1:C:70:LEU:HD13	2.39	0.42
1:C:216:LEU:HD11	1:C:221:ALA:CA	2.49	0.42
1:C:271:ASP:C	1:C:273:SER:N	2.76	0.42
1:D:38:MET:HE1	1:D:46:HIS:NE2	2.35	0.42
1:D:320:PRO:CA	1:D:323:GLN:HB3	2.49	0.42
1:D:381:TRP:CD1	1:D:382:GLN:N	2.87	0.42
1:A:44:LEU:HA	1:A:47:GLU:HB3	2.02	0.42
1:A:135:LEU:HD13	1:A:135:LEU:HA	1.88	0.42
1:A:319:ILE:HG23	1:A:322:LEU:HB2	2.01	0.42
1:B:243:ALA:O	1:B:244:ILE:C	2.63	0.42
1:C:34:ARG:NH2	1:C:250:HIS:HA	2.34	0.42
1:C:68:ARG:HB3	1:C:68:ARG:NH1	2.31	0.42
1:A:424:TYR:CZ	1:A:428:HIS:NE2	2.87	0.42
1:A:432:LEU:N	1:A:432:LEU:HD12	2.35	0.42
1:B:27:VAL:CG2	1:B:28:ALA:N	2.81	0.42
1:B:101:ARG:O	1:B:102:ASP:C	2.62	0.42
1:C:112:ARG:HG2	1:C:112:ARG:NH1	2.32	0.42
1:C:167:GLN:HB2	1:C:218:ILE:CG2	2.49	0.42
1:C:358:LEU:HD11	1:D:33:ASN:ND2	2.33	0.42
1:C:380:ALA:HB2	1:C:398:VAL:HG21	2.01	0.42
1:D:432:LEU:O	1:D:433:VAL:C	2.61	0.42
1:A:246:ALA:O	1:A:247:VAL:C	2.62	0.42
1:A:282:LEU:O	1:A:286:GLU:HB2	2.20	0.42
1:A:351:ILE:H	1:A:351:ILE:HG13	1.57	0.42
1:B:235:ASN:ND2	1:B:235:ASN:N	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:PRO:O	1:B:328:ILE:C	2.62	0.42
1:C:104:THR:HG21	1:C:297:VAL:HG21	2.01	0.42
1:C:256:ASP:OD1	1:C:257:GLU:N	2.53	0.42
1:D:117:GLU:O	1:D:120:ARG:HB2	2.20	0.42
1:D:129:GLU:HA	1:D:132:LEU:CB	2.48	0.42
1:D:325:ARG:O	1:D:327:PRO:HD3	2.20	0.42
1:D:404:GLU:O	1:D:405:GLU:C	2.63	0.42
1:A:64:THR:O	1:A:68:ARG:HD3	2.20	0.42
1:A:167:GLN:HB2	1:A:168:LEU:H	1.46	0.42
1:A:212:LYS:O	1:A:213:ALA:CB	2.66	0.42
1:A:262:CYS:O	1:A:263:LYS:HG3	2.20	0.42
1:A:442:ILE:O	1:A:443:LEU:HG	2.19	0.42
1:B:59:THR:O	1:B:60:GLY:C	2.61	0.42
1:B:237:GLU:C	1:B:239:LEU:N	2.75	0.42
1:C:41:ASN:O	1:C:42:GLU:C	2.63	0.42
1:C:45:ARG:C	1:C:47:GLU:N	2.77	0.42
1:C:322:LEU:HD12	1:C:322:LEU:HA	1.89	0.42
1:D:253:VAL:HG21	1:D:304:PHE:CE2	2.55	0.42
1:D:330:VAL:O	1:D:330:VAL:HG13	2.19	0.42
1:D:359:MET:HE2	1:D:359:MET:HA	2.02	0.42
1:D:361:THR:C	1:D:363:GLY:H	2.28	0.42
1:D:395:LEU:O	1:D:396:HIS:C	2.62	0.42
1:A:29:ILE:O	1:A:30:ALA:C	2.62	0.42
1:A:366:ILE:N	1:A:366:ILE:CD1	2.73	0.42
1:B:271:ASP:C	1:B:273:SER:N	2.77	0.42
1:C:100:ILE:O	1:C:104:THR:HG23	2.20	0.42
1:C:288:CYS:C	1:C:298:LYS:HD3	2.45	0.42
1:C:340:PHE:O	1:C:343:ILE:N	2.53	0.42
1:C:344:LEU:HD11	1:C:395:LEU:CD1	2.49	0.42
1:D:31:LEU:O	1:D:31:LEU:HD22	2.20	0.42
1:D:274:ARG:O	1:D:275:GLU:C	2.62	0.42
1:D:302:ILE:HG22	1:D:303:LEU:N	2.34	0.42
1:A:120:ARG:HA	1:A:123:ALA:HB3	2.02	0.42
1:A:241:GLN:HA	1:A:244:ILE:HD11	2.00	0.42
1:A:322:LEU:C	1:A:324:GLY:N	2.76	0.42
1:B:36:ARG:O	1:B:37:ARG:C	2.63	0.42
1:B:103:LEU:HD21	1:B:247:VAL:CG1	2.50	0.42
1:C:350:SER:O	1:C:354:GLN:HG3	2.20	0.42
1:D:131:ILE:HD11	1:D:222:MET:HG2	2.02	0.42
1:D:238:GLU:O	1:D:242:ASP:HB2	2.20	0.42
1:D:393:ARG:O	1:D:394:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:HG23	2:A:900:ANP:N6	2.35	0.42
1:B:37:ARG:NH2	1:B:45:ARG:O	2.52	0.42
1:B:284:LEU:HG	1:B:284:LEU:H	1.61	0.42
1:C:375:ARG:HD3	1:C:375:ARG:HA	1.94	0.42
1:C:379:ALA:O	1:C:383:VAL:HG23	2.20	0.42
1:D:124:GLU:HA	1:D:127:ALA:HB3	2.02	0.42
1:D:442:ILE:HD13	1:D:442:ILE:N	2.35	0.42
1:A:340:PHE:O	1:A:344:LEU:HD13	2.19	0.41
1:C:130:ARG:HA	1:C:133:ASP:HB2	2.01	0.41
1:C:172:GLU:O	1:C:172:GLU:HG3	2.19	0.41
1:D:69:ARG:HG3	1:D:73:LEU:CD2	2.50	0.41
1:D:292:THR:CG2	1:D:297:VAL:HG22	2.49	0.41
1:D:429:LEU:O	1:D:431:ALA:N	2.53	0.41
1:A:163:LEU:C	1:A:165:GLU:N	2.74	0.41
1:A:289:THR:HA	1:A:297:VAL:O	2.19	0.41
1:A:344:LEU:HD11	1:A:395:LEU:HD22	2.02	0.41
1:B:27:VAL:HB	1:B:70:LEU:CD1	2.50	0.41
1:B:86:PHE:CE1	1:B:96:VAL:HA	2.55	0.41
1:B:302:ILE:HG22	1:B:303:LEU:N	2.34	0.41
1:B:439:SER:C	1:B:441:PHE:H	2.28	0.41
1:C:29:ILE:O	1:C:32:ARG:N	2.53	0.41
1:C:167:GLN:HB2	1:C:218:ILE:HG23	2.02	0.41
1:C:282:LEU:HA	1:C:285:VAL:HG23	2.03	0.41
1:D:76:ALA:HB1	1:D:252:ILE:HD11	2.02	0.41
1:D:122:ARG:HD3	1:D:233:LEU:HD21	2.02	0.41
1:D:271:ASP:HA	1:D:274:ARG:CG	2.49	0.41
1:D:318:LEU:HD21	1:D:322:LEU:CD2	2.47	0.41
1:D:369:THR:HG23	1:D:420:ILE:O	2.20	0.41
1:A:258:ILE:HG13	1:A:306:ALA:CB	2.48	0.41
1:A:298:LYS:C	1:A:300:ASP:N	2.78	0.41
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.84	0.41
1:A:340:PHE:O	1:A:343:ILE:N	2.53	0.41
1:A:345:THR:C	1:A:347:PRO:HD2	2.45	0.41
1:A:431:ALA:O	1:A:434:ALA:HB3	2.20	0.41
1:B:431:ALA:O	1:B:432:LEU:C	2.63	0.41
1:C:17:ILE:HA	2:C:905:ANP:HN61	1.84	0.41
1:C:98:SER:O	1:C:101:ARG:N	2.52	0.41
1:C:108:VAL:HG12	1:C:109:LYS:N	2.34	0.41
1:C:442:ILE:HD13	1:C:442:ILE:N	2.35	0.41
1:D:54:LEU:HD23	1:D:329:ARG:CD	2.50	0.41
1:D:134:VAL:O	1:D:134:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ILE:N	1:D:255:ILE:HD13	2.34	0.41
1:A:21:ASP:O	1:A:24:LYS:HB2	2.21	0.41
1:A:33:ASN:HA	1:A:36:ARG:HD3	2.02	0.41
1:A:63:LYS:O	1:A:66:ILE:HB	2.19	0.41
1:A:70:LEU:O	1:A:73:LEU:HD23	2.21	0.41
1:A:108:VAL:HG12	1:A:109:LYS:N	2.36	0.41
1:A:109:LYS:NZ	1:B:298:LYS:HG2	2.35	0.41
1:A:259:ASP:HB3	1:A:310:PHE:CD2	2.54	0.41
1:A:436:GLU:O	1:A:438:LEU:N	2.53	0.41
1:B:76:ALA:HB1	1:B:77:PRO:HD2	2.01	0.41
1:C:83:ALA:O	1:C:85:LYS:N	2.53	0.41
1:C:278:GLN:HA	1:C:281:LEU:HD12	2.00	0.41
1:C:344:LEU:HD11	1:C:395:LEU:HD22	2.01	0.41
1:C:375:ARG:HB2	1:C:425:VAL:HG21	2.03	0.41
1:D:27:VAL:HG23	1:D:70:LEU:HD12	2.01	0.41
1:A:255:ILE:O	1:A:306:ALA:HA	2.21	0.41
1:A:442:ILE:HA	1:B:329:ARG:HG3	2.02	0.41
1:B:19:GLY:O	1:B:24:LYS:HE2	2.20	0.41
1:B:107:ALA:O	1:B:110:MET:N	2.53	0.41
1:C:109:LYS:HA	1:C:112:ARG:CZ	2.50	0.41
1:C:149:GLN:C	1:C:152:PRO:HD2	2.45	0.41
1:C:348:ASN:O	1:C:349:ALA:HB3	2.21	0.41
1:D:336:THR:HG22	1:D:339:ASP:OD2	2.19	0.41
1:A:84:THR:O	1:A:86:PHE:N	2.51	0.41
1:A:111:VAL:HG11	1:A:243:ALA:HB2	2.03	0.41
1:A:127:ALA:CB	1:A:226:ILE:HA	2.50	0.41
1:B:409:ASP:O	1:B:413:LEU:HD11	2.20	0.41
1:C:140:LYS:HD3	1:C:140:LYS:N	2.35	0.41
1:C:156:ARG:O	1:C:159:PHE:N	2.54	0.41
1:D:20:GLN:O	1:D:21:ASP:C	2.63	0.41
1:D:337:THR:O	1:D:341:GLU:HG3	2.20	0.41
1:D:399:LEU:O	1:D:402:LEU:HD23	2.21	0.41
1:B:274:ARG:O	1:B:275:GLU:C	2.62	0.41
1:B:394:ARG:HA	1:B:394:ARG:HD3	1.76	0.41
1:B:432:LEU:O	1:B:435:ASP:N	2.53	0.41
1:C:50:PRO:C	1:C:51:LYS:HG2	2.45	0.41
1:C:301:HIS:O	1:C:302:ILE:HG13	2.21	0.41
1:C:424:TYR:CZ	1:C:428:HIS:NE2	2.89	0.41
1:A:64:THR:HB	2:A:900:ANP:O1A	2.20	0.41
1:A:274:ARG:O	1:A:275:GLU:C	2.61	0.41
1:A:384:ASN:ND2	1:A:394:ARG:NH1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LEU:CB	1:B:283:PRO:CD	2.99	0.41
1:B:310:PHE:CD1	1:B:314:LYS:HA	2.56	0.41
1:B:338:SER:O	1:B:339:ASP:C	2.63	0.41
1:B:425:VAL:O	1:B:426:SER:C	2.62	0.41
1:C:61:VAL:HG11	1:C:334:ALA:HA	2.03	0.41
1:C:75:ASN:O	1:C:75:ASN:CG	2.63	0.41
1:C:278:GLN:O	1:C:281:LEU:HB2	2.21	0.41
1:C:410:ALA:O	1:C:413:LEU:N	2.54	0.41
1:D:18:ILE:N	1:D:18:ILE:HD13	2.36	0.41
1:D:28:ALA:O	1:D:29:ILE:C	2.63	0.41
1:A:56:ILE:HD12	1:A:56:ILE:N	2.36	0.41
1:A:255:ILE:HD11	1:A:304:PHE:HB3	2.03	0.41
1:A:333:GLN:CD	1:A:333:GLN:H	2.29	0.41
1:B:54:LEU:HD23	1:B:329:ARG:HD3	2.03	0.41
1:B:127:ALA:CA	1:B:225:LEU:HB3	2.49	0.41
1:B:336:THR:HG23	1:B:338:SER:HB3	2.03	0.41
1:C:157:GLN:HA	1:C:160:ARG:HB3	2.02	0.41
1:C:344:LEU:HD12	1:C:344:LEU:N	2.36	0.41
1:C:429:LEU:O	1:C:432:LEU:N	2.54	0.41
1:D:70:LEU:HD23	1:D:70:LEU:C	2.45	0.41
1:D:107:ALA:O	1:D:110:MET:HB2	2.20	0.41
1:D:240:LYS:HE2	1:D:294:HIS:CD2	2.55	0.41
1:C:7:ARG:HA	1:C:10:VAL:HB	2.03	0.41
1:C:22:ASN:O	1:C:25:ARG:HB2	2.21	0.41
1:C:355:TYR:CZ	1:C:403:MET:HB2	2.56	0.41
1:C:430:ASP:O	1:C:433:VAL:HG22	2.21	0.41
1:B:271:ASP:CA	1:B:274:ARG:HB2	2.41	0.40
1:C:151:GLU:N	1:C:152:PRO:CD	2.84	0.40
1:C:288:CYS:HA	1:C:298:LYS:HZ2	1.86	0.40
1:C:405:GLU:O	1:C:409:ASP:N	2.52	0.40
1:D:100:ILE:CG2	1:D:297:VAL:HG21	2.51	0.40
1:D:110:MET:C	1:D:112:ARG:N	2.77	0.40
1:D:381:TRP:O	1:D:382:GLN:C	2.64	0.40
1:A:278:GLN:HG2	1:A:322:LEU:CD2	2.52	0.40
1:A:320:PRO:O	1:A:323:GLN:N	2.53	0.40
1:A:438:LEU:O	1:A:441:PHE:HB2	2.21	0.40
1:B:6:PRO:HD3	1:B:32:ARG:HD3	2.04	0.40
1:B:318:LEU:HD22	1:B:323:GLN:N	2.36	0.40
1:C:102:ASP:C	1:C:104:THR:N	2.79	0.40
1:C:136:ILE:O	1:C:136:ILE:HG22	2.22	0.40
1:C:252:ILE:HG22	1:C:253:VAL:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ILE:HA	1:D:329:ARG:HG3	2.03	0.40
1:D:32:ARG:O	1:D:35:TRP:N	2.53	0.40
1:D:39:GLN:O	1:D:40:LEU:HD23	2.20	0.40
1:D:271:ASP:HA	1:D:274:ARG:HG3	2.03	0.40
1:A:86:PHE:HA	1:A:93:GLY:CA	2.50	0.40
1:A:271:ASP:C	1:A:273:SER:N	2.77	0.40
1:A:398:VAL:HG12	1:A:429:LEU:CD1	2.52	0.40
1:C:64:THR:HB	2:C:905:ANP:O1A	2.21	0.40
1:C:279:ARG:O	1:C:282:LEU:HB2	2.21	0.40
1:D:51:LYS:CB	1:D:328:ILE:HD11	2.50	0.40
1:D:261:ILE:HG22	1:D:261:ILE:O	2.21	0.40
1:A:17:ILE:HD11	1:A:69:ARG:CG	2.52	0.40
1:A:252:ILE:HG23	1:A:303:LEU:O	2.21	0.40
1:B:32:ARG:O	1:B:33:ASN:C	2.64	0.40
1:B:98:SER:OG	1:B:99:ILE:N	2.55	0.40
1:C:19:GLY:O	1:C:24:LYS:HE3	2.21	0.40
1:C:80:LYS:HA	1:C:254:PHE:HB3	2.03	0.40
1:C:375:ARG:CB	1:C:425:VAL:HG21	2.52	0.40
1:C:438:LEU:HD22	1:C:438:LEU:N	2.37	0.40
1:D:69:ARG:O	1:D:70:LEU:C	2.65	0.40
1:D:86:PHE:HE1	1:D:95:GLU:O	2.04	0.40
1:D:328:ILE:H	1:D:328:ILE:HG13	1.35	0.40
1:A:153:SER:O	1:A:157:GLN:HB2	2.22	0.40
1:A:424:TYR:O	1:A:428:HIS:CD2	2.74	0.40
1:B:96:VAL:CG1	1:B:97:ASP:N	2.85	0.40
1:B:103:LEU:HD23	1:B:104:THR:N	2.37	0.40
1:B:119:ASN:OD1	1:B:233:LEU:HD23	2.20	0.40
1:B:237:GLU:C	1:B:239:LEU:H	2.29	0.40
1:B:399:LEU:O	1:B:402:LEU:HD23	2.22	0.40
1:B:404:GLU:O	1:B:405:GLU:C	2.64	0.40
1:B:439:SER:O	1:B:443:LEU:HD12	2.20	0.40
1:D:247:VAL:C	1:D:249:GLN:N	2.78	0.40
1:D:282:LEU:CB	1:D:283:PRO:CD	2.99	0.40
1:D:439:SER:O	1:D:443:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/442 (91%)	262 (65%)	102 (25%)	39 (10%)	0	9
1	B	403/442 (91%)	251 (62%)	111 (28%)	41 (10%)	0	8
1	C	403/442 (91%)	258 (64%)	104 (26%)	41 (10%)	0	8
1	D	403/442 (91%)	251 (62%)	115 (28%)	37 (9%)	0	10
All	All	1612/1768 (91%)	1022 (63%)	432 (27%)	158 (10%)	0	9

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	63	LYS
1	A	110	MET
1	A	268	SER
1	A	398	VAL
1	A	436	GLU
1	A	437	ASP
1	B	17	ILE
1	B	99	ILE
1	B	135	LEU
1	B	171	LYS
1	B	262	CYS
1	B	392	ALA
1	B	404	GLU
1	B	430	ASP
1	B	437	ASP
1	C	45	ARG
1	C	63	LYS
1	C	110	MET
1	C	111	VAL
1	C	172	GLU
1	C	212	LYS

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Mol	Chain	Res	Type
1	C	268	SER
1	C	398	VAL
1	C	436	GLU
1	C	437	ASP
1	D	17	ILE
1	D	135	LEU
1	D	171	LYS
1	D	262	CYS
1	D	327	PRO
1	D	392	ALA
1	D	404	GLU
1	D	430	ASP
1	A	41	ASN
1	A	67	ALA
1	A	84	THR
1	A	99	ILE
1	A	165	GLU
1	A	212	LYS
1	A	264	ARG
1	A	397	THR
1	A	404	GLU
1	A	414	SER
1	A	433	VAL
1	B	18	ILE
1	B	39	GLN
1	B	60	GLY
1	B	85	LYS
1	B	89	VAL
1	B	138	PRO
1	B	246	ALA
1	B	327	PRO
1	B	328	ILE
1	B	334	ALA
1	B	353	VAL
1	B	416	GLN
1	B	425	VAL
1	B	438	LEU
1	C	19	GLY
1	C	42	GLU
1	C	99	ILE
1	C	165	GLU
1	C	264	ARG

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Mol	Chain	Res	Type
1	C	267	SER
1	C	414	SER
1	C	433	VAL
1	D	18	ILE
1	D	19	GLY
1	D	39	GLN
1	D	60	GLY
1	D	75	ASN
1	D	85	LYS
1	D	89	VAL
1	D	99	ILE
1	D	138	PRO
1	D	151	GLU
1	D	246	ALA
1	D	286	GLU
1	D	334	ALA
1	D	353	VAL
1	D	425	VAL
1	D	438	LEU
1	A	42	GLU
1	A	58	PRO
1	A	141	ASN
1	A	156	ARG
1	A	386	SER
1	B	37	ARG
1	B	151	GLU
1	B	158	ALA
1	B	286	GLU
1	C	40	LEU
1	C	41	ASN
1	C	58	PRO
1	C	84	THR
1	C	85	LYS
1	C	88	GLU
1	C	386	SER
1	C	404	GLU
1	D	150	GLN
1	D	169	ASP
1	D	264	ARG
1	D	416	GLN
1	D	437	ASP
1	A	6	PRO

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Mol	Chain	Res	Type
1	A	85	LYS
1	A	88	GLU
1	A	164	ARG
1	A	261	ILE
1	A	267	SER
1	B	75	ASN
1	B	347	PRO
1	B	432	LEU
1	C	67	ALA
1	C	261	ILE
1	C	397	THR
1	D	37	ARG
1	D	240	LYS
1	A	40	LEU
1	A	51	LYS
1	A	64	THR
1	B	170	ASP
1	C	6	PRO
1	C	51	LYS
1	C	164	ARG
1	D	158	ALA
1	A	19	GLY
1	A	426	SER
1	B	29	ILE
1	B	79	ILE
1	B	285	VAL
1	C	64	THR
1	C	137	PRO
1	C	167	GLN
1	D	328	ILE
1	D	408	TYR
1	A	137	PRO
1	B	92	VAL
1	B	433	VAL
1	C	351	ILE
1	C	376	ILE
1	D	92	VAL
1	D	347	PRO
1	B	19	GLY
1	B	100	ILE
1	B	152	PRO
1	B	320	PRO

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Mol	Chain	Res	Type
1	C	320	PRO
1	D	282	LEU
1	C	66	ILE
1	A	111	VAL
1	A	320	PRO
1	A	351	ILE
1	B	282	LEU
1	C	364	VAL
1	C	390	ILE
1	A	66	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/376 (93%)	218 (62%)	131 (38%)	0	1
1	B	349/376 (93%)	215 (62%)	134 (38%)	0	1
1	C	349/376 (93%)	207 (59%)	142 (41%)	0	0
1	D	349/376 (93%)	210 (60%)	139 (40%)	0	1
All	All	1396/1504 (93%)	850 (61%)	546 (39%)	0	1

All (546) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	GLU
1	A	4	MET
1	A	5	THR
1	A	14	ASP
1	A	16	HIS
1	A	31	LEU
1	A	32	ARG
1	A	34	ARG
1	A	36	ARG
1	A	37	ARG

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Mol	Chain	Res	Type
1	A	38	MET
1	A	41	ASN
1	A	44	LEU
1	A	49	THR
1	A	51	LYS
1	A	54	LEU
1	A	61	VAL
1	A	68	ARG
1	A	70	LEU
1	A	72	LYS
1	A	73	LEU
1	A	80	LYS
1	A	81	VAL
1	A	84	THR
1	A	88	GLU
1	A	94	LYS
1	A	97	ASP
1	A	109	LYS
1	A	118	LYS
1	A	119	ASN
1	A	125	GLU
1	A	128	GLU
1	A	130	ARG
1	A	135	LEU
1	A	140	LYS
1	A	142	ASN
1	A	146	THR
1	A	147	GLU
1	A	148	GLN
1	A	149	GLN
1	A	156	ARG
1	A	157	GLN
1	A	160	ARG
1	A	161	LYS
1	A	164	ARG
1	A	167	GLN
1	A	168	LEU
1	A	169	ASP
1	A	171	LYS
1	A	172	GLU
1	A	173	ILE
1	A	174	GLU

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Mol	Chain	Res	Type
1	A	210	LYS
1	A	212	LYS
1	A	215	LYS
1	A	216	LEU
1	A	217	LYS
1	A	219	LYS
1	A	224	LEU
1	A	228	GLU
1	A	229	GLU
1	A	233	LEU
1	A	239	LEU
1	A	242	ASP
1	A	247	VAL
1	A	249	GLN
1	A	255	ILE
1	A	257	GLU
1	A	261	ILE
1	A	263	LYS
1	A	264	ARG
1	A	266	GLU
1	A	267	SER
1	A	268	SER
1	A	271	ASP
1	A	278	GLN
1	A	282	LEU
1	A	285	VAL
1	A	286	GLU
1	A	289	THR
1	A	290	VAL
1	A	297	VAL
1	A	298	LYS
1	A	301	HIS
1	A	303	LEU
1	A	305	ILE
1	A	310	PHE
1	A	311	GLN
1	A	312	ILE
1	A	314	LYS
1	A	318	LEU
1	A	319	ILE
1	A	325	ARG
1	A	326	LEU

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Mol	Chain	Res	Type
1	A	332	LEU
1	A	333	GLN
1	A	335	LEU
1	A	336	THR
1	A	337	THR
1	A	345	THR
1	A	350	SER
1	A	351	ILE
1	A	356	LYS
1	A	358	LEU
1	A	359	MET
1	A	364	VAL
1	A	366	ILE
1	A	367	GLU
1	A	369	THR
1	A	370	ASP
1	A	371	SER
1	A	374	LYS
1	A	383	VAL
1	A	394	ARG
1	A	397	THR
1	A	398	VAL
1	A	401	ARG
1	A	407	SER
1	A	412	ASP
1	A	416	GLN
1	A	417	ASN
1	A	418	ILE
1	A	419	THR
1	A	421	ASP
1	A	425	VAL
1	A	429	LEU
1	A	435	ASP
1	A	437	ASP
1	A	442	ILE
1	A	443	LEU
1	B	2	SER
1	B	5	THR
1	B	11	SER
1	B	16	HIS
1	B	18	ILE
1	B	20	GLN

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Mol	Chain	Res	Type
1	B	22	ASN
1	B	24	LYS
1	B	25	ARG
1	B	26	SER
1	B	31	LEU
1	B	34	ARG
1	B	37	ARG
1	B	38	MET
1	B	39	GLN
1	B	42	GLU
1	B	43	GLU
1	B	44	LEU
1	B	47	GLU
1	B	48	VAL
1	B	49	THR
1	B	54	LEU
1	B	63	LYS
1	B	64	THR
1	B	73	LEU
1	B	80	LYS
1	B	84	THR
1	B	88	GLU
1	B	92	VAL
1	B	94	LYS
1	B	95	GLU
1	B	96	VAL
1	B	103	LEU
1	B	104	THR
1	B	109	LYS
1	B	110	MET
1	B	117	GLU
1	B	118	LYS
1	B	121	TYR
1	B	124	GLU
1	B	125	GLU
1	B	129	GLU
1	B	130	ARG
1	B	135	LEU
1	B	136	ILE
1	B	142	ASN
1	B	146	THR
1	B	148	GLN

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Mol	Chain	Res	Type
1	B	149	GLN
1	B	156	ARG
1	B	157	GLN
1	B	161	LYS
1	B	162	LYS
1	B	163	LEU
1	B	165	GLU
1	B	167	GLN
1	B	168	LEU
1	B	170	ASP
1	B	171	LYS
1	B	172	GLU
1	B	173	ILE
1	B	210	LYS
1	B	211	GLN
1	B	212	LYS
1	B	214	ARG
1	B	215	LYS
1	B	217	LYS
1	B	220	ASP
1	B	222	MET
1	B	224	LEU
1	B	235	ASN
1	B	238	GLU
1	B	240	LYS
1	B	241	GLN
1	B	253	VAL
1	B	258	ILE
1	B	264	ARG
1	B	266	GLU
1	B	268	SER
1	B	279	ARG
1	B	282	LEU
1	B	284	LEU
1	B	289	THR
1	B	291	SER
1	B	292	THR
1	B	296	MET
1	B	300	ASP
1	B	303	LEU
1	B	311	GLN
1	B	312	ILE

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Mol	Chain	Res	Type
1	B	314	LYS
1	B	316	SER
1	B	326	LEU
1	B	328	ILE
1	B	332	LEU
1	B	333	GLN
1	B	337	THR
1	B	342	ARG
1	B	343	ILE
1	B	344	LEU
1	B	346	GLU
1	B	348	ASN
1	B	350	SER
1	B	352	THR
1	B	356	LYS
1	B	358	LEU
1	B	366	ILE
1	B	367	GLU
1	B	369	THR
1	B	371	SER
1	B	373	ILE
1	B	374	LYS
1	B	375	ARG
1	B	378	GLU
1	B	382	GLN
1	B	383	VAL
1	B	387	THR
1	B	388	GLU
1	B	389	ASN
1	B	393	ARG
1	B	394	ARG
1	B	397	THR
1	B	401	ARG
1	B	402	LEU
1	B	413	LEU
1	B	418	ILE
1	B	427	LYS
1	B	429	LEU
1	B	433	VAL
1	B	438	LEU
1	B	439	SER
1	B	440	ARG

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Mol	Chain	Res	Type
1	B	442	ILE
1	B	443	LEU
1	C	2	SER
1	C	3	GLU
1	C	4	MET
1	C	5	THR
1	C	7	ARG
1	C	14	ASP
1	C	16	HIS
1	C	20	GLN
1	C	25	ARG
1	C	26	SER
1	C	27	VAL
1	C	31	LEU
1	C	32	ARG
1	C	34	ARG
1	C	36	ARG
1	C	37	ARG
1	C	38	MET
1	C	41	ASN
1	C	44	LEU
1	C	49	THR
1	C	51	LYS
1	C	54	LEU
1	C	61	VAL
1	C	68	ARG
1	C	70	LEU
1	C	72	LYS
1	C	73	LEU
1	C	80	LYS
1	C	81	VAL
1	C	84	THR
1	C	88	GLU
1	C	94	LYS
1	C	97	ASP
1	C	108	VAL
1	C	109	LYS
1	C	112	ARG
1	C	118	LYS
1	C	119	ASN
1	C	120	ARG
1	C	125	GLU

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Mol	Chain	Res	Type
1	C	128	GLU
1	C	130	ARG
1	C	135	LEU
1	C	140	LYS
1	C	142	ASN
1	C	146	THR
1	C	147	GLU
1	C	148	GLN
1	C	149	GLN
1	C	150	GLN
1	C	156	ARG
1	C	157	GLN
1	C	159	PHE
1	C	160	ARG
1	C	161	LYS
1	C	164	ARG
1	C	165	GLU
1	C	167	GLN
1	C	168	LEU
1	C	169	ASP
1	C	171	LYS
1	C	172	GLU
1	C	173	ILE
1	C	174	GLU
1	C	210	LYS
1	C	212	LYS
1	C	215	LYS
1	C	217	LYS
1	C	219	LYS
1	C	224	LEU
1	C	226	ILE
1	C	228	GLU
1	C	233	LEU
1	C	239	LEU
1	C	244	ILE
1	C	247	VAL
1	C	249	GLN
1	C	255	ILE
1	C	257	GLU
1	C	261	ILE
1	C	263	LYS
1	C	264	ARG

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Mol	Chain	Res	Type
1	C	266	GLU
1	C	267	SER
1	C	271	ASP
1	C	278	GLN
1	C	282	LEU
1	C	284	LEU
1	C	285	VAL
1	C	286	GLU
1	C	289	THR
1	C	290	VAL
1	C	297	VAL
1	C	298	LYS
1	C	301	HIS
1	C	303	LEU
1	C	305	ILE
1	C	310	PHE
1	C	311	GLN
1	C	312	ILE
1	C	314	LYS
1	C	318	LEU
1	C	319	ILE
1	C	325	ARG
1	C	332	LEU
1	C	333	GLN
1	C	335	LEU
1	C	336	THR
1	C	337	THR
1	C	345	THR
1	C	346	GLU
1	C	350	SER
1	C	351	ILE
1	C	356	LYS
1	C	358	LEU
1	C	359	MET
1	C	364	VAL
1	C	366	ILE
1	C	367	GLU
1	C	369	THR
1	C	370	ASP
1	C	371	SER
1	C	373	ILE
1	C	374	LYS

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Mol	Chain	Res	Type
1	C	375	ARG
1	C	383	VAL
1	C	388	GLU
1	C	394	ARG
1	C	398	VAL
1	C	401	ARG
1	C	407	SER
1	C	411	SER
1	C	412	ASP
1	C	416	GLN
1	C	417	ASN
1	C	418	ILE
1	C	421	ASP
1	C	425	VAL
1	C	429	LEU
1	C	435	ASP
1	C	437	ASP
1	C	442	ILE
1	D	2	SER
1	D	5	THR
1	D	8	GLU
1	D	11	SER
1	D	16	HIS
1	D	18	ILE
1	D	20	GLN
1	D	22	ASN
1	D	24	LYS
1	D	25	ARG
1	D	31	LEU
1	D	34	ARG
1	D	37	ARG
1	D	38	MET
1	D	39	GLN
1	D	42	GLU
1	D	43	GLU
1	D	44	LEU
1	D	47	GLU
1	D	48	VAL
1	D	49	THR
1	D	55	MET
1	D	63	LYS
1	D	64	THR

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Mol	Chain	Res	Type
1	D	73	LEU
1	D	80	LYS
1	D	82	GLU
1	D	84	THR
1	D	88	GLU
1	D	92	VAL
1	D	94	LYS
1	D	96	VAL
1	D	103	LEU
1	D	104	THR
1	D	109	LYS
1	D	110	MET
1	D	111	VAL
1	D	118	LYS
1	D	121	TYR
1	D	122	ARG
1	D	124	GLU
1	D	125	GLU
1	D	130	ARG
1	D	135	LEU
1	D	136	ILE
1	D	145	GLN
1	D	146	THR
1	D	147	GLU
1	D	148	GLN
1	D	149	GLN
1	D	156	ARG
1	D	157	GLN
1	D	161	LYS
1	D	162	LYS
1	D	163	LEU
1	D	165	GLU
1	D	167	GLN
1	D	168	LEU
1	D	169	ASP
1	D	170	ASP
1	D	171	LYS
1	D	172	GLU
1	D	173	ILE
1	D	210	LYS
1	D	211	GLN
1	D	212	LYS

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Mol	Chain	Res	Type
1	D	214	ARG
1	D	215	LYS
1	D	217	LYS
1	D	219	LYS
1	D	220	ASP
1	D	224	LEU
1	D	235	ASN
1	D	238	GLU
1	D	239	LEU
1	D	240	LYS
1	D	253	VAL
1	D	258	ILE
1	D	260	LYS
1	D	264	ARG
1	D	266	GLU
1	D	268	SER
1	D	279	ARG
1	D	282	LEU
1	D	284	LEU
1	D	289	THR
1	D	291	SER
1	D	292	THR
1	D	296	MET
1	D	300	ASP
1	D	303	LEU
1	D	311	GLN
1	D	312	ILE
1	D	314	LYS
1	D	316	SER
1	D	326	LEU
1	D	328	ILE
1	D	332	LEU
1	D	333	GLN
1	D	337	THR
1	D	342	ARG
1	D	343	ILE
1	D	344	LEU
1	D	346	GLU
1	D	348	ASN
1	D	350	SER
1	D	352	THR
1	D	356	LYS

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Mol	Chain	Res	Type
1	D	358	LEU
1	D	365	ASN
1	D	366	ILE
1	D	367	GLU
1	D	369	THR
1	D	371	SER
1	D	373	ILE
1	D	374	LYS
1	D	375	ARG
1	D	378	GLU
1	D	382	GLN
1	D	383	VAL
1	D	387	THR
1	D	388	GLU
1	D	390	ILE
1	D	393	ARG
1	D	394	ARG
1	D	396	HIS
1	D	397	THR
1	D	401	ARG
1	D	402	LEU
1	D	413	LEU
1	D	418	ILE
1	D	427	LYS
1	D	429	LEU
1	D	433	VAL
1	D	438	LEU
1	D	439	SER
1	D	440	ARG
1	D	442	ILE
1	D	443	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	75	ASN
1	A	119	ASN
1	A	149	GLN
1	A	250	HIS
1	A	294	HIS
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	365	ASN
1	A	384	ASN
1	A	396	HIS
1	A	417	ASN
1	B	16	HIS
1	B	22	ASN
1	B	33	ASN
1	B	235	ASN
1	B	323	GLN
1	B	354	GLN
1	B	382	GLN
1	B	417	ASN
1	C	39	GLN
1	C	41	ASN
1	C	114	GLN
1	C	119	ASN
1	C	149	GLN
1	C	250	HIS
1	C	294	HIS
1	C	354	GLN
1	C	365	ASN
1	C	384	ASN
1	C	396	HIS
1	C	417	ASN
1	D	16	HIS
1	D	22	ASN
1	D	41	ASN
1	D	46	HIS
1	D	323	GLN
1	D	354	GLN
1	D	382	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ANP	A	900	-	33,33,33	1.13	4 (12%)	45,52,52	1.19	2 (4%)
2	ANP	C	905	-	33,33,33	1.11	4 (12%)	45,52,52	1.18	2 (4%)

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	ANP	A	900	-	-	8/18/38/38	0/3/3/3
2	ANP	C	905	-	-	8/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ANP	PG-O1G	2.92	1.50	1.46
2	C	905	ANP	PG-O1G	2.68	1.50	1.46
2	A	900	ANP	PG-O2G	-2.64	1.49	1.56
2	C	905	ANP	PG-O2G	-2.63	1.49	1.56
2	C	905	ANP	PB-O1B	2.43	1.49	1.46
2	A	900	ANP	PB-O2B	-2.41	1.50	1.56
2	C	905	ANP	PB-O2B	-2.40	1.50	1.56
2	A	900	ANP	PB-O1B	2.00	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ANP	O2B-PB-O1B	4.79	120.14	109.87
2	C	905	ANP	O2B-PB-O1B	4.79	120.14	109.87
2	A	900	ANP	O1G-PG-N3B	-4.23	105.55	111.77
2	C	905	ANP	O1G-PG-N3B	-4.19	105.61	111.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	ANP	PB-N3B-PG-O1G
2	A	900	ANP	PG-N3B-PB-O1B
2	A	900	ANP	PG-N3B-PB-O3A
2	A	900	ANP	O4'-C1'-N9-C8
2	A	900	ANP	O4'-C1'-N9-C4
2	C	905	ANP	PB-N3B-PG-O1G
2	C	905	ANP	PG-N3B-PB-O1B
2	C	905	ANP	PG-N3B-PB-O3A
2	C	905	ANP	O4'-C1'-N9-C8
2	C	905	ANP	O4'-C1'-N9-C4
2	A	900	ANP	PB-O3A-PA-O2A
2	C	905	ANP	PB-O3A-PA-O2A
2	A	900	ANP	C4'-C5'-O5'-PA
2	C	905	ANP	C4'-C5'-O5'-PA
2	A	900	ANP	PB-O3A-PA-O1A
2	C	905	ANP	PB-O3A-PA-O1A

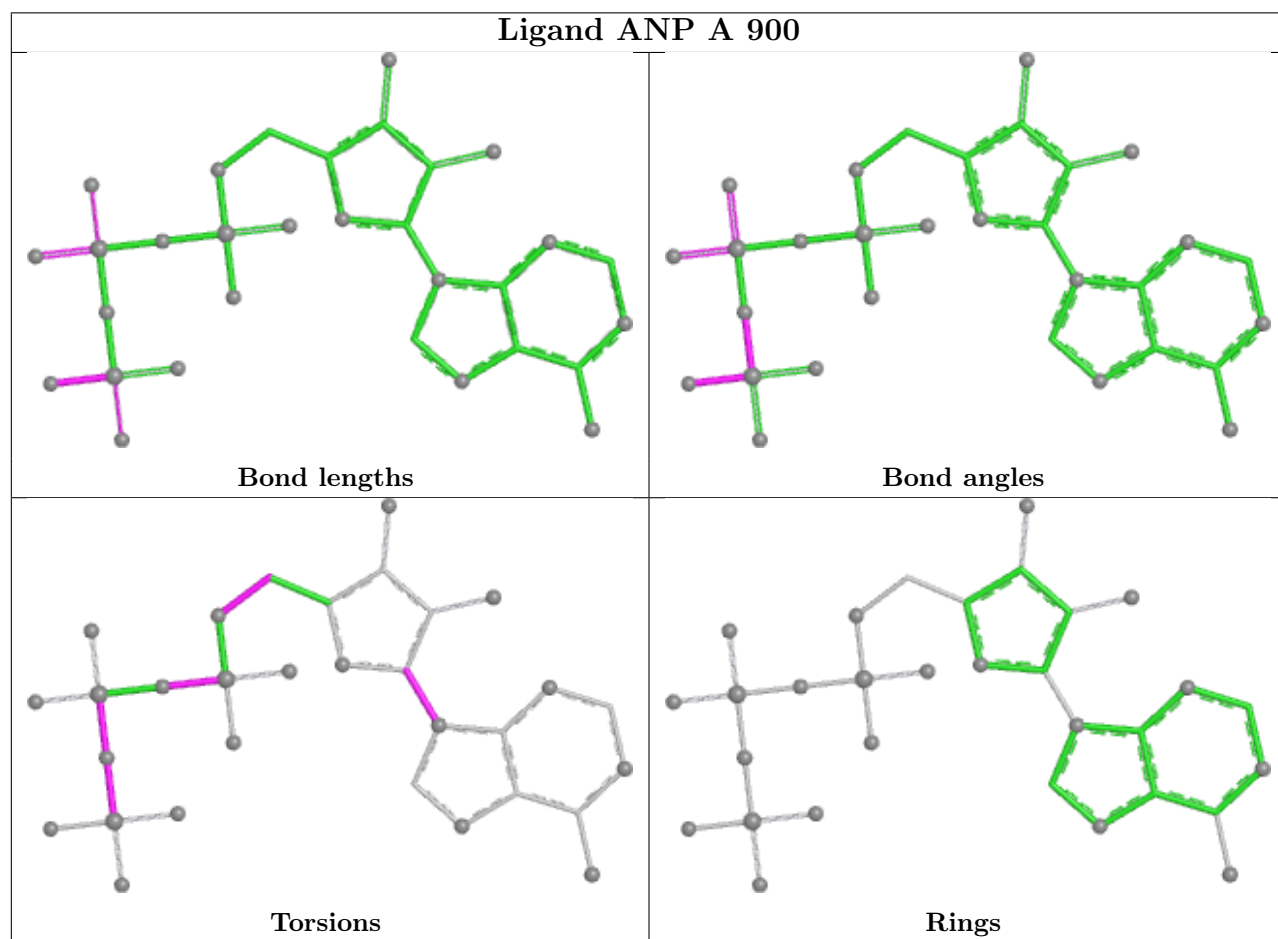
There are no ring outliers.

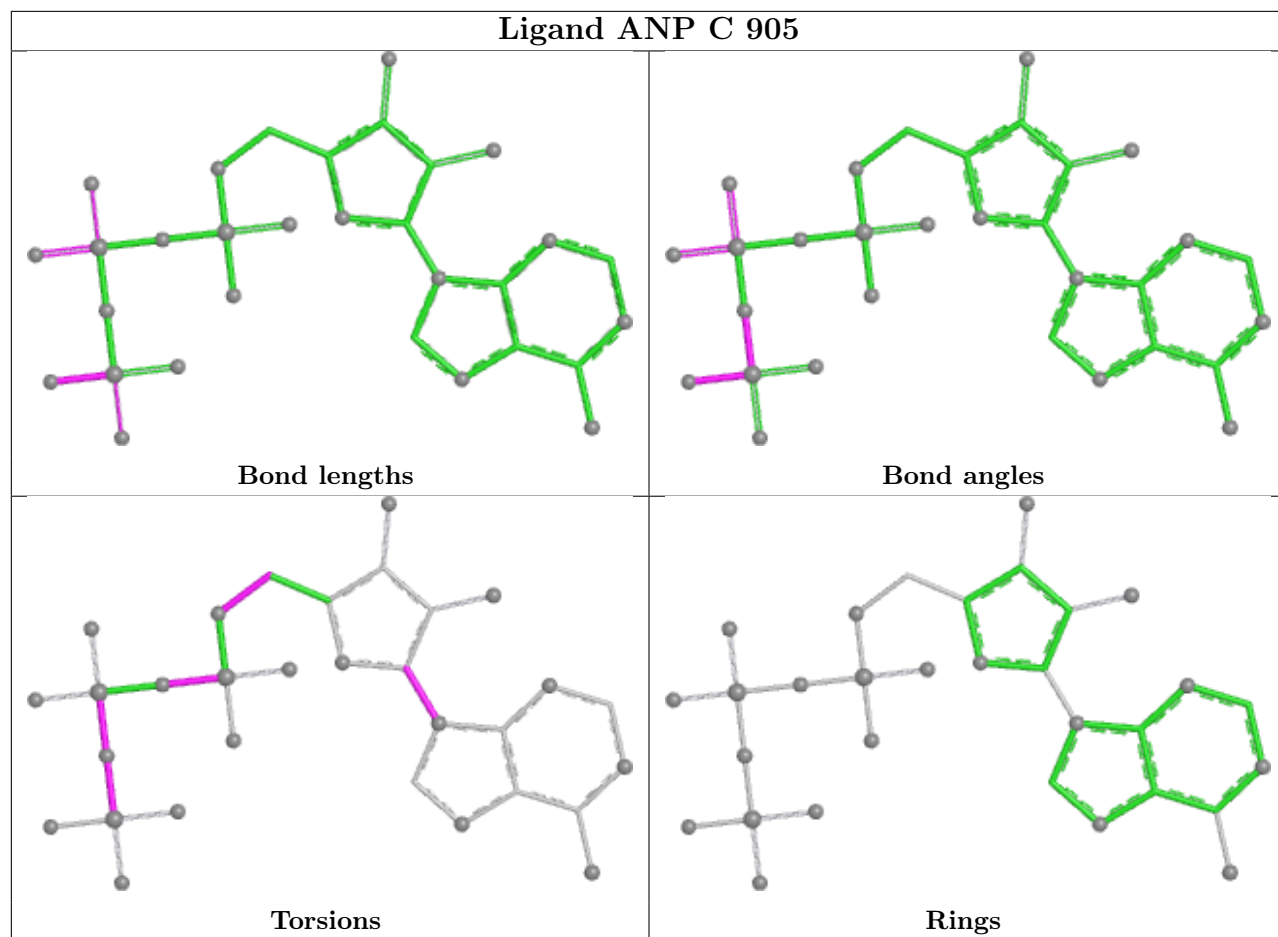
2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	ANP	9	0
2	C	905	ANP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.