



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 09:01 PM UTC

PDB ID : 8ZB7 / pdb_00008zb7
EMDB ID : EMD-39896
Title : Human left ventricle ATM complex
Authors : Li, D.N.; Zhao, Q.Y.; Liu, C.
Deposited on : 2024-04-26
Resolution : 3.19 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

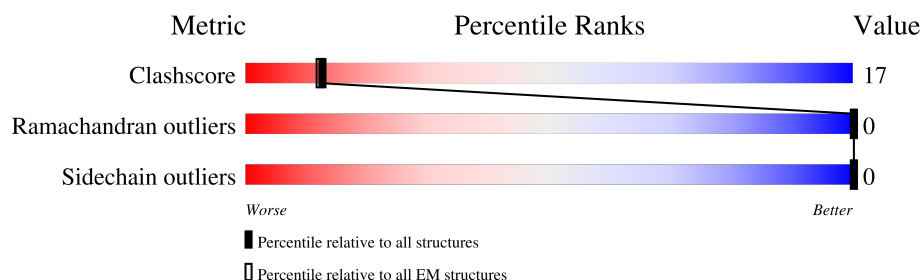
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 Å.

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



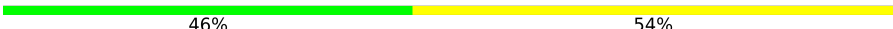
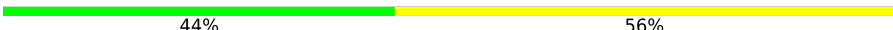
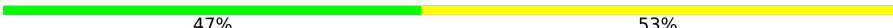
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	G	776	57% 38% .
1	H	776	58% 37% .
1	I	776	57% 39% .
1	J	776	56% 39% .
1	K	776	57% 39% .
1	M	776	58% 38% .
2	A	371	78% 22%
2	B	371	81% 19%
2	C	371	77% 23%

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Mol	Chain	Length	Quality of chain	
2	D	371		
2	E	371		
2	F	371		
3	L	166		
3	N	166		
3	O	166		
3	P	166		

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 58698 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	G	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	H	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	I	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	J	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	K	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		

- Molecule 2 is a protein called Actin, alpha cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	C	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	D	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	E	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	F	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	A	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		

- Molecule 3 is a protein called Tropomyosin alpha-1 chain.

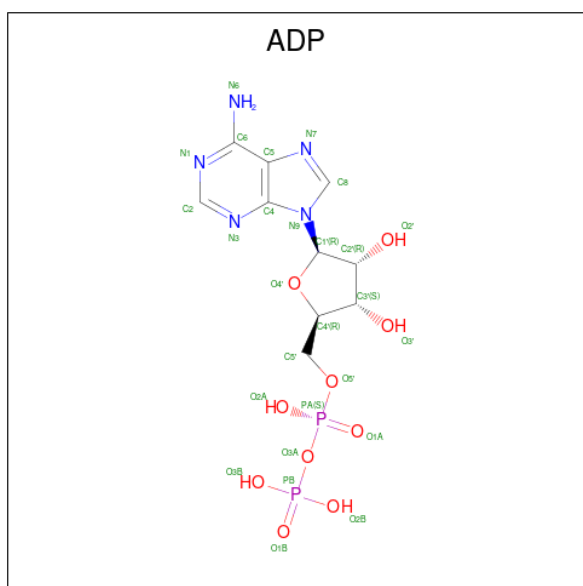
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		
3	L	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		
3	N	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		

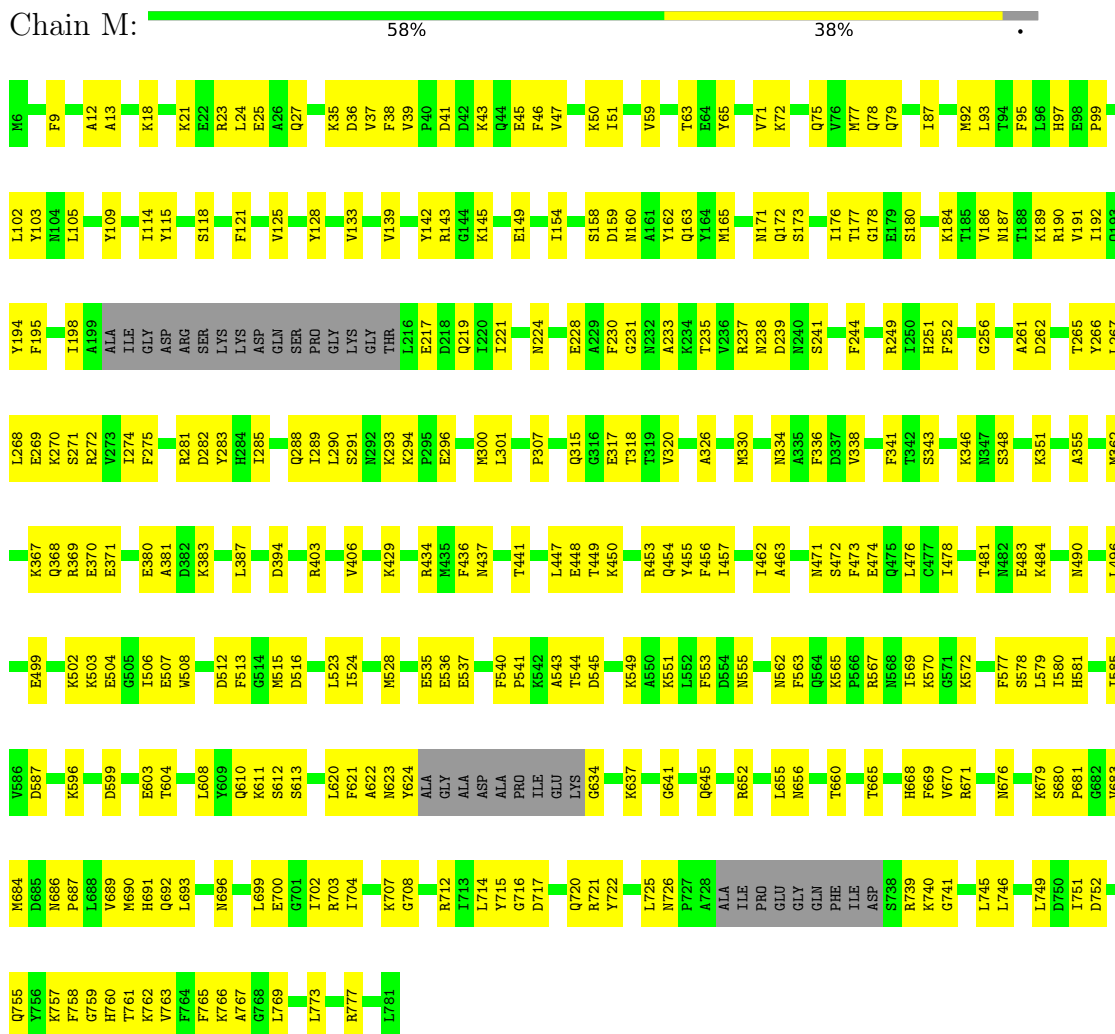
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



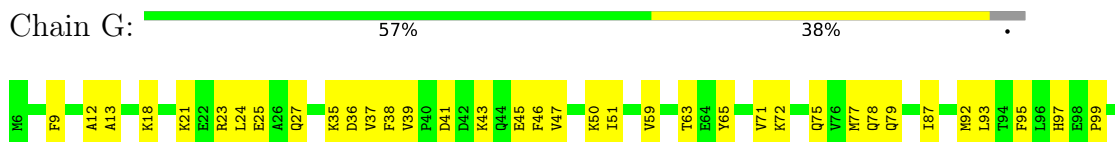
3 Residue-property plots

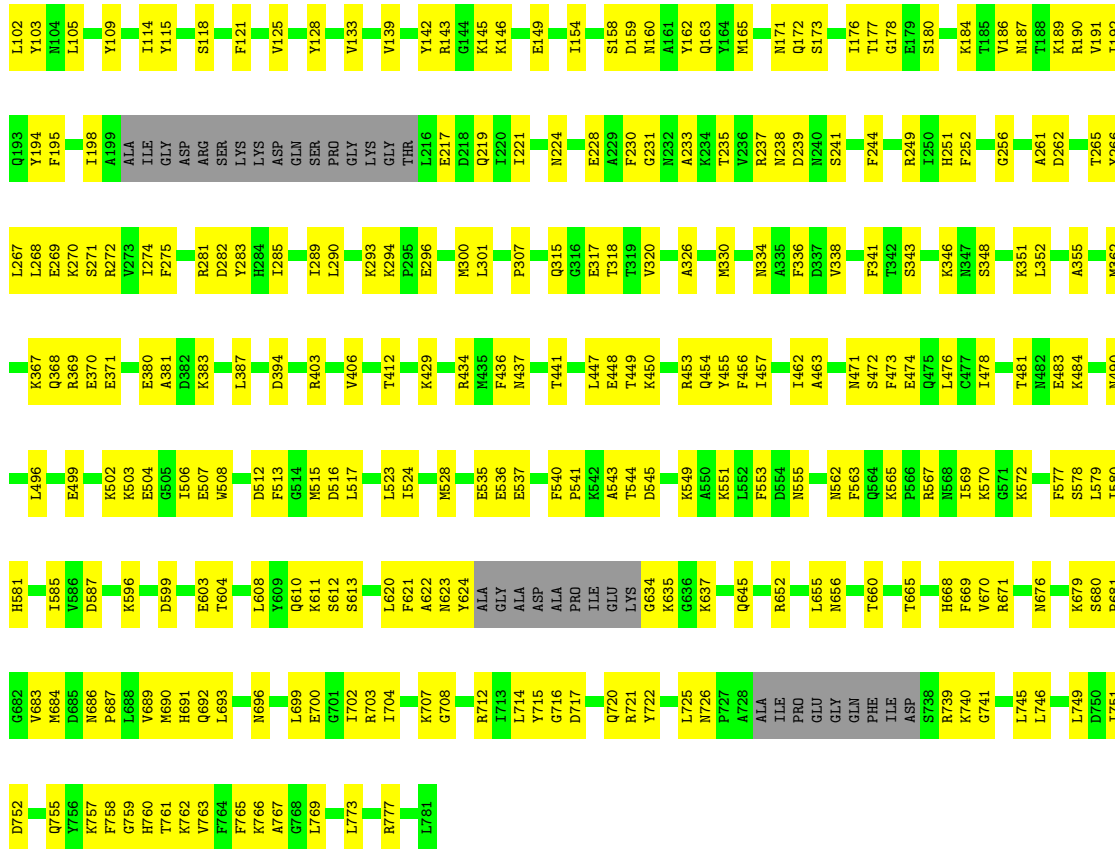
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

• Molecule 1: Myosin-7



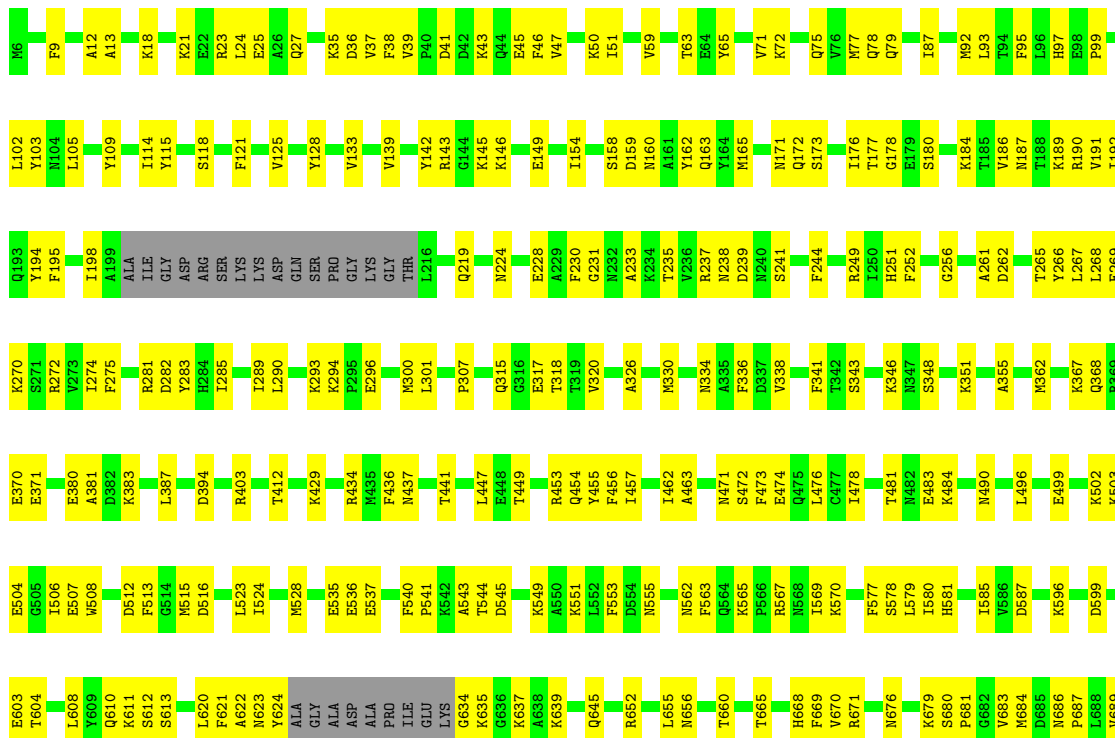
• Molecule 1: Myosin-7



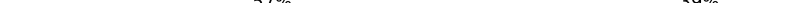


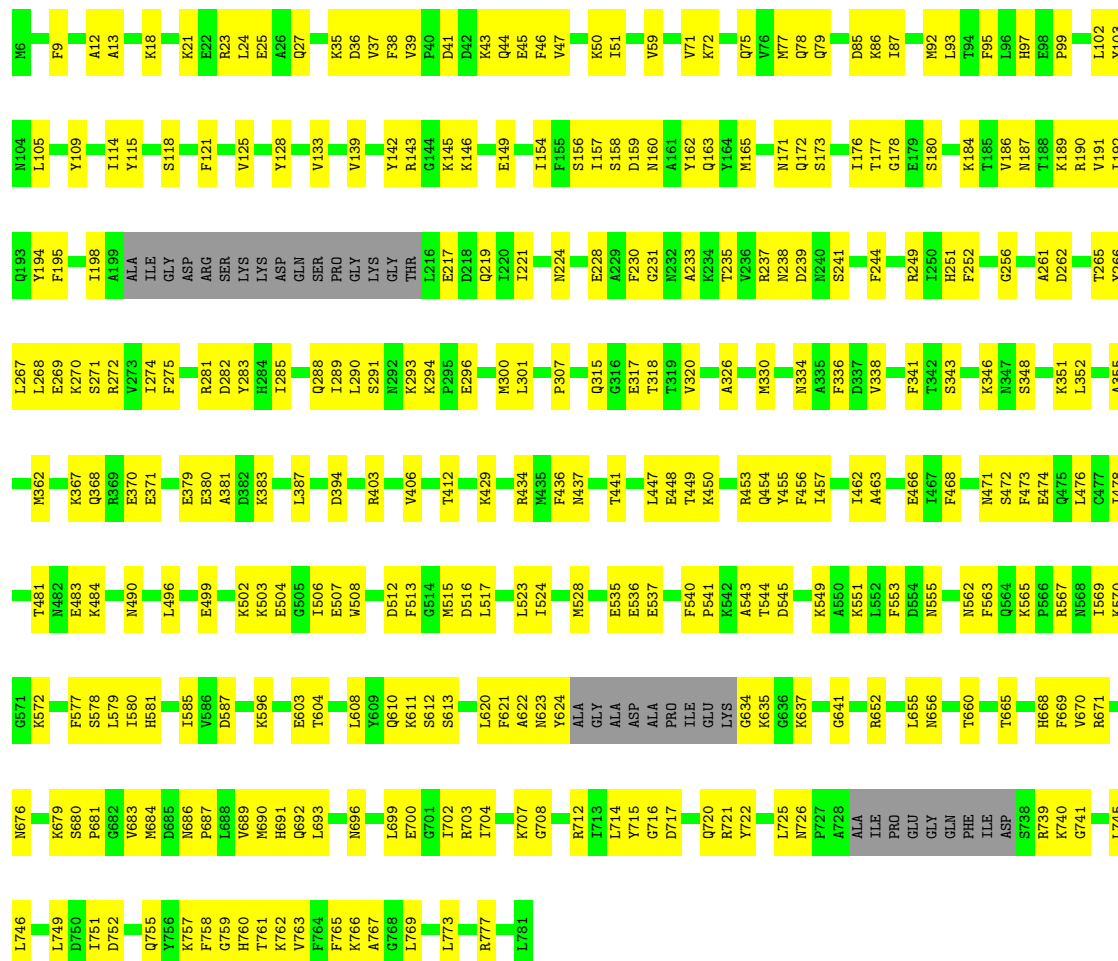
• Molecule 1: Myosin-7

Chain H: 58% 37%

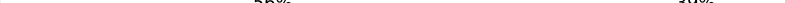


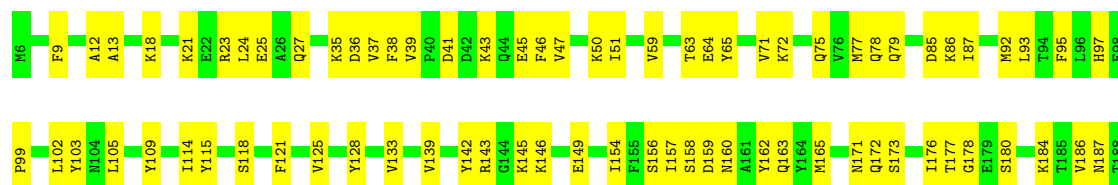
- Molecule 1: Myosin-7

Chain I:  57% 39% .



- Molecule 1: Myosin-7

Chain J:  56% 39% .

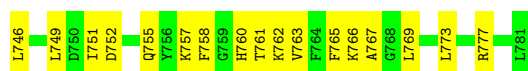


K565	Q475	K351	D262	K189
P566	L476	L352		R190
R669	C477		T265	V191
N668	I478	A355	Y266	I192
I569			L267	Q193
K570	T481	M362	L268	Y194
	K482		E269	F196
F577	K484	K367	K270	
S578	E483	Q368		I198
L579	K484	R369	S271	A199
I580	N490	E370	R272	ALA
H581		E371	V273	ILE
	L496		I274	GLY
		E379	F275	ASP
I585		E380		ARG
V586	E499	D282	R281	SER
D587		A381	Y283	LYS
	K502	D382	H284	LYS
K596	K503	K383	I285	
	E504			
E603	G505	L387		
T604	I506	Q288		
K691	E507	I289		
Q692	E507	D394	L290	GLY
L693	W508		S291	LYS
		R403	N292	
	D512		GLY	
M696	F513	V406	K293	THR
	S611	K294	K294	L216
L699	G612	T412	E217	E217
E700	S613		P295	D218
G701			E296	Q219
I702	L620	K429		I220
R703	F621		M300	I221
I704	A622	R434	L301	
	N623	M435		N224
K707	Y624	F436		
G708		N437	P307	
	ALA			
	GLY			
	ALA		Q315	E228
R712	ASP	T441	G316	A229
I713	ASP		E317	F230
L714	ALA	L447	T318	G231
Y715	PRO	E448	T319	N232
G716	ILE	T449	V320	A233
D717	GLU	K450		K234
	LYS		A326	T236
Q720	G634	R453		V236
R721	K635	Q454	M330	R237
Y722	G636	Y455		N238
	K637	F456	N334	D239
L725	K638	I457	A335	N240
N726	K639		F336	S241
P727	K640	I462	D337	
A728	G641	A463	V338	F244
ALA		K551		
ILE	R652	L552		R249
PRO		F553	F341	I250
GLU	L655	D554	T342	
GLY	N656	N555	S343	H251
GLN				F252
PHE	T660	N471	K346	G256
ILE		S472		
ASP	T665	F473	S348	A261
		F474		

• Molecule 1: Myosin-7

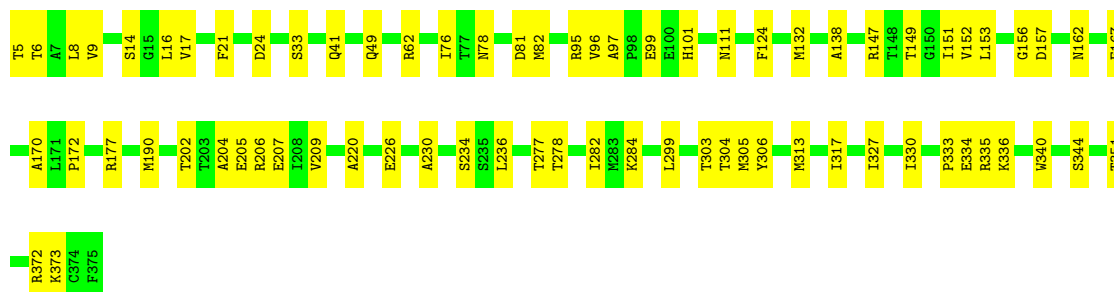
Chain K:  57% 39%

M676	F577	K481	M362	T265	V191	P99	K6
K679	S578	E483	K367	Y266	I192	L102	F9
S680	L579	K484	Q368	L267	Q193	Y103	A12
P681	I580	H581	R369	E269	F195	L105	A13
G682	H581		N490	K270			
V683			E371	S271	I198		
M684	I585	L496	E379	R272	A199	Y109	K18
D685	V586		E379	V273	ALA		
N686	D587	E499	E380	I274	ILE	I114	K21
P687			A381	F275	GLY	Y115	E22
L688	K596	K502	D382		ASP		R23
V689		K503	K383	R281	ARG	S118	L24
M690	E603	E504	L387	D282	LYS	Y121	E25
H691	T604	G505	L387	Y283	LYS		A26
Q692		I506	D394	H284	LYS		Q27
L693	L608	E507		I285	ASP	V125	
	Y609	W508			GLN		K35
N696	Q610		R403	L289	SER	Y128	D36
L699	K611	D512	V406	L290	PRO	V133	V37
E700	S612	F513		K293	GLY		F38
G701	S613	G514	T412	K294	LYS	V139	V39
I702	L620	M515		P295	THR		P40
R703	F621	D516	K429	E296	L216	Y142	D41
I704	A622	L523	R434	M300	E217	R143	D42
K707	N623	I524	M435	L301	D218	G144	K43
G708	Y624	Y636	F436	P307	Q219	K145	E45
	ALA	M528	N437		I220	K146	F46
R712	ALA	E535			I221		V47
I713	ASP	E536	T441	Q315	N224	E149	K50
L714	ALA	E537		G316		I154	I51
Y715	PRO	L715	L447	E317	E228		
G716	ILE	F540	E448	T318	A229	S158	V59
D717	GLU	P541	T449	T319	F230	D159	
	LYS	K542	K450	V320	G231	M160	T63
Q720	G634	A543		A326	N232	A161	E64
R721	K635	T544	R453	K326	A233	Y162	Y65
Y722	G636	D545	Q454	K330	K234	Q163	
	K637		Y455		T235	Y164	V71
L725	K638	K549	F456	K330	V236	M165	K72
N726	K639	K550	I457	N334	R237		
P727	K640	K551		A335	N238	M171	Q75
A728	G641	L552	I462	F336	D239	Q172	V76
		F553	A463	D337	N240	S173	M77
ILE	R652	D554		Y338	S241		Q78
PRO		N555	E466			I176	Q79
GLU	L655		T467	F341	F244	I177	
GLY	N656	N562	F468	T342		G178	D85
GLN		F563		S343	R249	E179	K86
PHE	T660	Q564	N471	K346	H251	S180	I87
ILE		K565	S472	K347	D252		
ASP	T665	P566	F473	S348		K184	M92
		E567			G256	T185	L93
S738	H668	N568	Q475	K351	A261	T187	T94
R739	F669	I569	L476			T188	F95
K740	V670	K570	C477			L96	L96
G741	R671	G571	I478	A355	D262	K189	H97
		K572				P100	E98
L745							



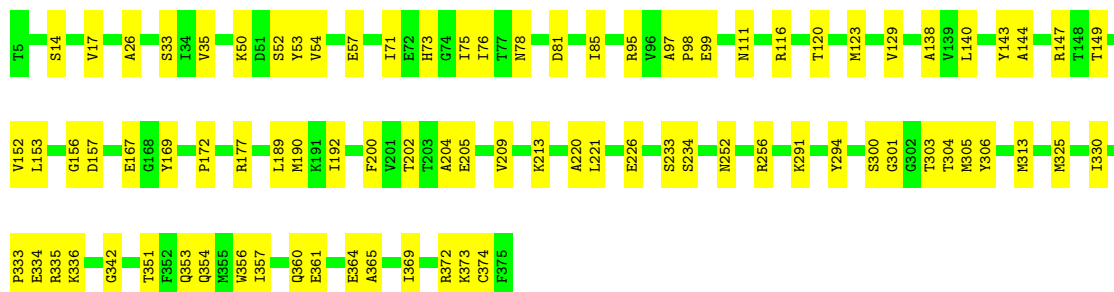
- Molecule 2: Actin, alpha cardiac muscle 1

Chain B: 81% 19%



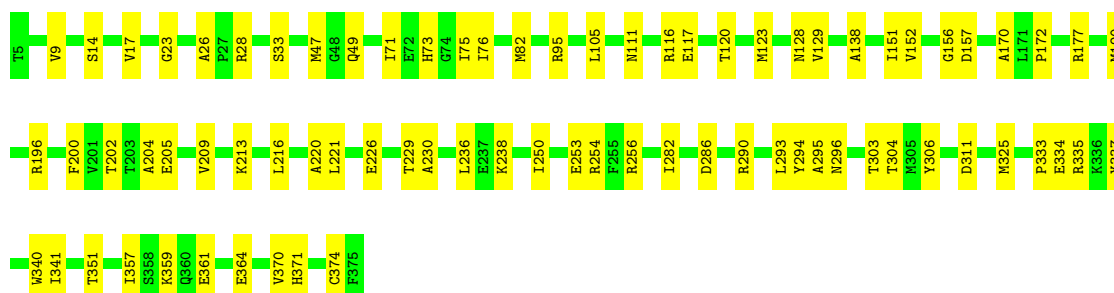
- Molecule 2: Actin, alpha cardiac muscle 1

Chain C: 77% 23%



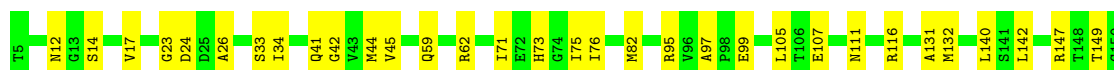
- Molecule 2: Actin, alpha cardiac muscle 1

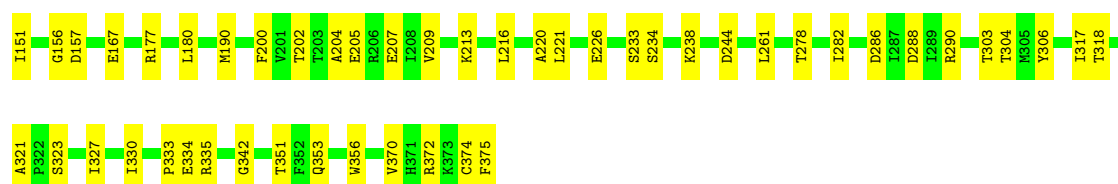
Chain D: 79% 21%



- Molecule 2: Actin, alpha cardiac muscle 1

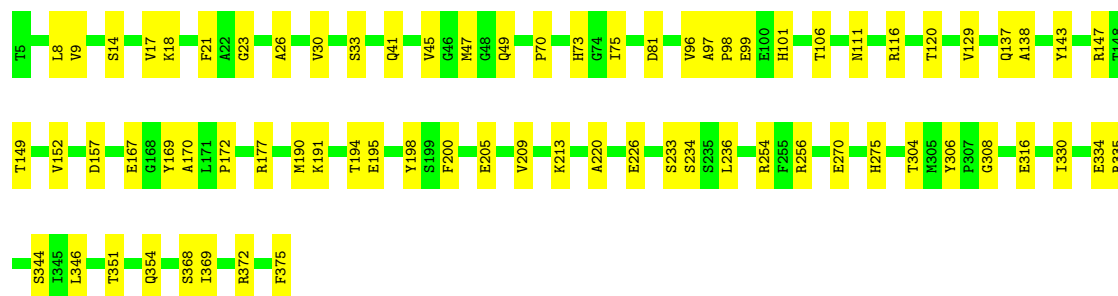
Chain E: 78% 22%





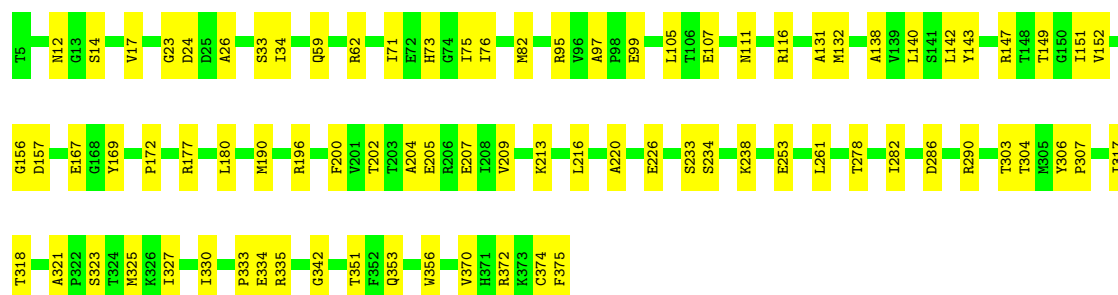
- Molecule 2: Actin, alpha cardiac muscle 1

Chain F: 80% 20%



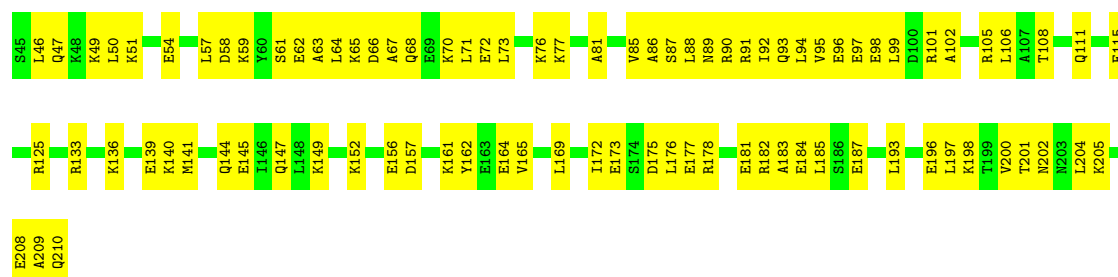
- Molecule 2: Actin, alpha cardiac muscle 1

Chain A: 78% 22%



- Molecule 3: Tropomyosin alpha-1 chain

Chain O: 47% 53%



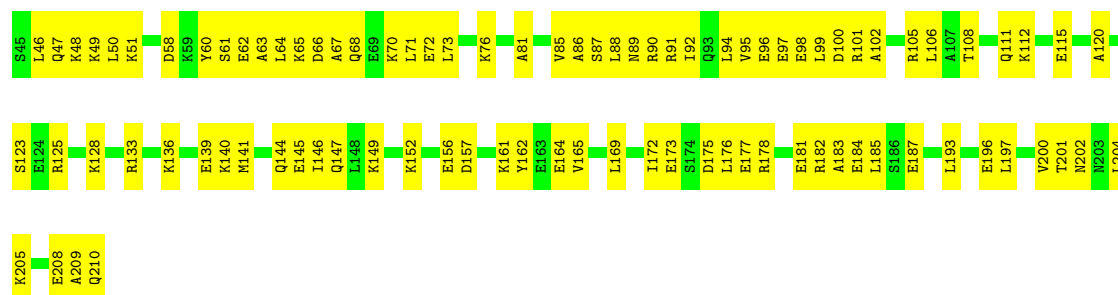
- Molecule 3: Tropomyosin alpha-1 chain

Chain P: 43% 57%



• Molecule 3: Tropomyosin alpha-1 chain

Chain L: 46% 54%



• Molecule 3: Tropomyosin alpha-1 chain

Chain N: 44% 56%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.66°, rise=27.3 Å, axial sym=C1	Depositor
Number of segments used	69013	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	G	0.22	0/6101	0.38	0/8217
1	H	0.22	0/6101	0.38	0/8217
1	I	0.22	0/6101	0.38	0/8217
1	J	0.22	0/6101	0.38	0/8217
1	K	0.22	0/6101	0.38	0/8217
1	M	0.22	0/6101	0.38	0/8217
2	A	0.50	0/2961	0.45	0/4011
2	B	0.46	0/2961	0.43	0/4011
2	C	0.48	0/2961	0.45	0/4011
2	D	0.49	0/2961	0.46	0/4011
2	E	0.50	0/2961	0.45	0/4011
2	F	0.50	0/2961	0.45	0/4011
3	L	0.20	0/1328	0.41	0/1770
3	N	0.19	0/1328	0.43	0/1770
3	O	0.19	0/1328	0.40	0/1770
3	P	0.19	0/1328	0.43	0/1770
All	All	0.32	0/59684	0.41	0/80448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	5974	0	5961	224	0
1	H	5974	0	5961	221	0
1	I	5974	0	5961	232	0
1	J	5974	0	5961	243	0
1	K	5974	0	5961	233	0
1	M	5974	0	5961	213	0
2	A	2898	0	2870	67	0
2	B	2898	0	2871	55	0
2	C	2898	0	2871	62	0
2	D	2898	0	2868	73	0
2	E	2898	0	2871	66	0
2	F	2898	0	2871	55	0
3	L	1326	0	1330	124	0
3	N	1326	0	1332	110	0
3	O	1326	0	1332	91	0
3	P	1326	0	1332	92	0
4	A	27	0	12	3	0
4	B	27	0	12	1	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	3	0
4	F	27	0	12	2	0
All	All	58698	0	58386	1956	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 17.

All (1956) 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:I:368:GLN:HE22	3:N:142:GLU:CB	1.15	1.57
1:J:368:GLN:HE22	3:L:100:ASP:CA	1.21	1.49
1:I:368:GLN:HE22	3:N:142:GLU:CA	1.21	1.48
1:I:368:GLN:NE2	3:N:142:GLU:HB3	1.30	1.45
1:J:368:GLN:NE2	3:L:100:ASP:CA	1.78	1.45
1:K:368:GLN:NE2	3:N:61:SER:HB3	1.28	1.43
2:D:254:ARG:HH12	3:L:128:LYS:NZ	1.13	1.42
1:K:368:GLN:NE2	3:N:61:SER:CB	1.80	1.41
3:O:173:GLU:CG	1:H:368:GLN:HE21	1.36	1.39
1:J:368:GLN:HG2	3:L:99:LEU:CD1	1.52	1.38
1:I:368:GLN:NE2	3:N:142:GLU:CA	1.92	1.33
1:J:368:GLN:NE2	3:L:100:ASP:HA	1.32	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:368:GLN:HE22	3:N:61:SER:CB	1.42	1.20
1:J:368:GLN:HE22	3:L:100:ASP:CB	1.52	1.19
1:J:368:GLN:HG2	3:L:99:LEU:HD12	1.27	1.17
1:K:368:GLN:HE22	3:N:61:SER:CA	1.56	1.16
1:J:368:GLN:NE2	3:L:100:ASP:CB	2.10	1.15
2:D:221:LEU:HD21	3:L:136:LYS:HZ3	1.13	1.13
2:D:254:ARG:NH1	3:L:128:LYS:NZ	1.99	1.11
3:O:173:GLU:HG2	1:H:368:GLN:NE2	1.63	1.11
2:D:311:ASP:HB3	3:L:136:LYS:HE2	1.23	1.11
2:D:221:LEU:CD2	3:L:136:LYS:HZ3	1.65	1.08
1:I:368:GLN:NE2	3:N:142:GLU:CB	1.88	1.06
3:O:173:GLU:CG	1:H:368:GLN:NE2	2.19	1.04
2:D:238:LYS:NZ	3:L:125:ARG:CD	2.18	1.03
2:D:221:LEU:HD21	3:L:136:LYS:NZ	1.73	1.02
3:O:173:GLU:HG2	1:H:368:GLN:HE21	0.86	1.01
2:D:238:LYS:HZ1	3:L:125:ARG:HG2	1.24	0.98
1:I:368:GLN:NE2	3:N:142:GLU:HA	1.81	0.95
1:I:368:GLN:HE22	3:N:142:GLU:HA	1.31	0.95
1:K:368:GLN:HE22	3:N:61:SER:HA	1.29	0.95
2:D:238:LYS:NZ	3:L:125:ARG:HD2	1.82	0.94
1:J:368:GLN:HG2	3:L:99:LEU:HD11	1.48	0.94
2:D:221:LEU:HD11	3:L:136:LYS:NZ	1.81	0.94
1:J:368:GLN:NE2	3:L:100:ASP:HB2	1.80	0.94
1:J:368:GLN:CG	3:L:99:LEU:CD1	2.45	0.94
1:I:368:GLN:NE2	3:N:142:GLU:N	2.13	0.94
2:D:254:ARG:HH12	3:L:128:LYS:HZ1	1.05	0.92
1:K:368:GLN:NE2	3:N:61:SER:CA	2.25	0.91
2:A:149:THR:HG22	2:A:167:GLU:H	1.35	0.91
3:O:96:GLU:HG3	1:G:368:GLN:OE1	1.69	0.91
2:D:254:ARG:HH12	3:L:128:LYS:HZ2	1.20	0.90
1:J:368:GLN:HE22	3:L:100:ASP:HA	0.86	0.90
2:E:41:GLN:HE21	2:A:172:PRO:HG3	1.37	0.89
2:E:149:THR:HG22	2:E:167:GLU:H	1.35	0.89
1:J:142:TYR:HA	1:J:145:LYS:HE2	1.55	0.88
2:E:147:ARG:HH21	2:E:330:ILE:HG12	1.38	0.88
1:K:142:TYR:HA	1:K:145:LYS:HE2	1.55	0.88
1:I:142:TYR:HA	1:I:145:LYS:HE2	1.55	0.87
1:K:368:GLN:HE21	3:N:61:SER:HB3	1.12	0.87
2:A:147:ARG:HH21	2:A:330:ILE:HG12	1.38	0.87
1:M:142:TYR:HA	1:M:145:LYS:HE2	1.55	0.87
2:B:149:THR:HG22	2:B:167:GLU:H	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:THR:HG22	2:F:167:GLU:H	1.39	0.86
1:K:369:ARG:CB	3:L:60:TYR:OH	2.24	0.86
1:G:142:TYR:HA	1:G:145:LYS:HE2	1.55	0.85
1:H:142:TYR:HA	1:H:145:LYS:HE2	1.55	0.85
2:D:221:LEU:HD11	3:L:136:LYS:HZ1	1.40	0.85
1:J:368:GLN:NE2	3:L:100:ASP:N	2.25	0.84
1:K:369:ARG:HB2	3:L:60:TYR:OH	1.78	0.83
1:J:368:GLN:CG	3:L:99:LEU:HD12	2.07	0.83
2:D:254:ARG:NH1	3:L:128:LYS:HZ1	1.68	0.83
2:D:238:LYS:HZ1	3:L:125:ARG:CG	1.91	0.82
2:E:351:THR:OG1	1:J:536:GLU:OE2	1.96	0.82
1:H:230:PHE:HA	1:H:285:ILE:HD11	1.61	0.82
1:G:230:PHE:HA	1:G:285:ILE:HD11	1.61	0.82
2:F:47:MET:HB3	1:G:540:PHE:CZ	2.14	0.82
1:I:293:LYS:HE2	1:I:326:ALA:HB1	1.62	0.81
1:G:293:LYS:HE2	1:G:326:ALA:HB1	1.62	0.81
1:J:230:PHE:HA	1:J:285:ILE:HD11	1.61	0.81
1:K:368:GLN:NE2	3:N:61:SER:HA	1.89	0.81
3:L:73:LEU:HA	3:L:76:LYS:HD3	1.62	0.81
1:M:293:LYS:HE2	1:M:326:ALA:HB1	1.62	0.81
1:J:293:LYS:HE2	1:J:326:ALA:HB1	1.62	0.81
1:K:230:PHE:HA	1:K:285:ILE:HD11	1.61	0.81
1:K:293:LYS:HE2	1:K:326:ALA:HB1	1.62	0.81
1:M:230:PHE:HA	1:M:285:ILE:HD11	1.61	0.81
1:I:230:PHE:HA	1:I:285:ILE:HD11	1.61	0.80
1:H:293:LYS:HE2	1:H:326:ALA:HB1	1.62	0.80
2:C:149:THR:HG22	2:C:167:GLU:H	1.46	0.80
2:D:238:LYS:NZ	3:L:125:ARG:CG	2.45	0.80
2:C:351:THR:OG1	1:G:536:GLU:OE2	1.99	0.80
1:K:536:GLU:OE2	2:A:351:THR:OG1	1.98	0.80
1:H:528:MET:SD	1:H:555:ASN:ND2	2.55	0.80
2:B:351:THR:HG23	1:H:536:GLU:OE1	1.81	0.79
2:D:238:LYS:NZ	3:L:125:ARG:HG2	1.98	0.79
3:O:73:LEU:HA	3:O:76:LYS:HD3	1.62	0.79
1:K:528:MET:SD	1:K:555:ASN:ND2	2.55	0.79
2:D:351:THR:OG1	1:I:536:GLU:OE2	1.99	0.79
3:P:91:ARG:HE	1:G:369:ARG:HH21	1.28	0.79
1:G:528:MET:SD	1:G:555:ASN:ND2	2.55	0.79
1:M:528:MET:SD	1:M:555:ASN:ND2	2.55	0.79
2:C:147:ARG:HH21	2:C:330:ILE:HG12	1.46	0.79
2:D:202:THR:HG22	2:D:204:ALA:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:105:ARG:HG3	3:P:106:LEU:HD11	1.65	0.79
3:L:105:ARG:HG3	3:N:106:LEU:HD11	1.64	0.79
1:I:528:MET:SD	1:I:555:ASN:ND2	2.55	0.79
2:D:254:ARG:HH12	3:L:128:LYS:HZ3	1.31	0.78
1:J:528:MET:SD	1:J:555:ASN:ND2	2.55	0.78
3:P:165:VAL:HA	3:P:168:LYS:HD2	1.67	0.77
1:K:368:GLN:NE2	3:N:61:SER:HB2	1.96	0.77
3:N:165:VAL:HA	3:N:168:LYS:HD2	1.67	0.77
3:O:96:GLU:HG3	1:G:368:GLN:CD	2.09	0.76
3:L:71:LEU:HD22	3:N:70:LYS:HD2	1.68	0.75
2:C:35:VAL:HG21	2:C:81:ASP:HB2	1.69	0.75
3:P:91:ARG:HE	1:G:369:ARG:NH2	1.85	0.75
1:J:368:GLN:CD	3:L:100:ASP:HA	2.11	0.75
2:B:351:THR:HG23	1:H:536:GLU:CD	2.12	0.74
2:B:24:ASP:OD1	1:H:639:LYS:O	2.06	0.73
1:I:128:TYR:HB2	1:I:681:PRO:HG3	1.70	0.73
3:O:173:GLU:CB	1:H:368:GLN:NE2	2.51	0.73
3:O:71:LEU:HD22	3:P:70:LYS:HD2	1.68	0.73
1:K:281:ARG:NH2	1:K:318:THR:O	2.22	0.73
1:K:128:TYR:HB2	1:K:681:PRO:HG3	1.69	0.73
1:M:281:ARG:NH2	1:M:318:THR:O	2.22	0.73
1:I:512:ASP:HB3	1:I:515:MET:HE1	1.71	0.73
3:L:71:LEU:HD21	3:N:71:LEU:HA	1.70	0.73
1:G:281:ARG:NH2	1:G:318:THR:O	2.22	0.72
1:M:128:TYR:HB2	1:M:681:PRO:HG3	1.69	0.72
1:G:512:ASP:HB3	1:G:515:MET:HE1	1.70	0.72
1:G:536:GLU:OE2	1:G:551:LYS:NZ	2.22	0.72
2:F:106:THR:HG22	2:F:137:GLN:HG2	1.69	0.72
1:G:45:GLU:HG2	1:G:46:PHE:HD2	1.54	0.72
1:J:281:ARG:NH2	1:J:318:THR:O	2.22	0.72
3:O:173:GLU:CD	1:H:368:GLN:HE21	1.98	0.72
1:J:128:TYR:HB2	1:J:681:PRO:HG3	1.70	0.72
1:J:512:ASP:HB3	1:J:515:MET:HE1	1.70	0.72
1:K:92:MET:HE1	1:K:712:ARG:H	1.54	0.72
1:M:536:GLU:OE2	1:M:551:LYS:NZ	2.22	0.72
1:G:490:ASN:ND2	1:G:513:PHE:O	2.23	0.72
1:I:92:MET:HE1	1:I:712:ARG:H	1.54	0.72
1:I:281:ARG:NH2	1:I:318:THR:O	2.22	0.72
1:M:512:ASP:HB3	1:M:515:MET:HE1	1.71	0.72
1:H:281:ARG:NH2	1:H:318:THR:O	2.22	0.72
1:H:490:ASN:ND2	1:H:513:PHE:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:294:LYS:HG3	1:M:330:MET:HE1	1.72	0.72
1:H:128:TYR:HB2	1:H:681:PRO:HG3	1.70	0.72
1:G:128:TYR:HB2	1:G:681:PRO:HG3	1.69	0.72
1:I:294:LYS:HG3	1:I:330:MET:HE1	1.72	0.72
1:J:490:ASN:ND2	1:J:513:PHE:O	2.23	0.72
1:H:294:LYS:HG3	1:H:330:MET:HE1	1.72	0.72
1:H:536:GLU:OE2	1:H:551:LYS:NZ	2.22	0.72
1:I:490:ASN:ND2	1:I:513:PHE:O	2.23	0.72
1:I:536:GLU:OE2	1:I:551:LYS:NZ	2.22	0.72
1:H:45:GLU:HG2	1:H:46:PHE:HD2	1.54	0.71
1:K:294:LYS:HG3	1:K:330:MET:HE1	1.72	0.71
3:O:71:LEU:HD21	3:P:71:LEU:HA	1.70	0.71
1:H:92:MET:HE1	1:H:712:ARG:H	1.54	0.71
1:K:536:GLU:OE2	1:K:551:LYS:NZ	2.22	0.71
1:I:45:GLU:HG2	1:I:46:PHE:HD2	1.54	0.71
1:J:294:LYS:HG3	1:J:330:MET:HE1	1.72	0.71
1:J:536:GLU:OE2	1:J:551:LYS:NZ	2.22	0.71
2:C:202:THR:HG22	2:C:204:ALA:H	1.56	0.71
1:G:294:LYS:HG3	1:G:330:MET:HE1	1.72	0.71
1:H:512:ASP:HB3	1:H:515:MET:HE1	1.70	0.71
1:K:45:GLU:HG2	1:K:46:PHE:HD2	1.54	0.71
1:M:45:GLU:HG2	1:M:46:PHE:HD2	1.54	0.71
2:D:221:LEU:CD1	3:L:136:LYS:NZ	2.54	0.71
1:H:739:ARG:NH2	1:H:760:HIS:O	2.24	0.71
1:J:92:MET:HE1	1:J:712:ARG:H	1.54	0.71
1:J:739:ARG:NH2	1:J:760:HIS:O	2.24	0.71
1:K:490:ASN:ND2	1:K:513:PHE:O	2.23	0.71
1:K:739:ARG:NH2	1:K:760:HIS:O	2.24	0.71
2:A:307:PRO:CB	3:L:48:LYS:HE2	2.21	0.71
1:H:512:ASP:OD1	1:H:513:PHE:N	2.24	0.71
1:H:755:GLN:HB3	1:H:769:LEU:HD11	1.73	0.71
1:K:512:ASP:HB3	1:K:515:MET:HE1	1.71	0.71
1:M:739:ARG:NH2	1:M:760:HIS:O	2.24	0.70
1:K:512:ASP:OD1	1:K:513:PHE:N	2.24	0.70
1:M:490:ASN:ND2	1:M:513:PHE:O	2.23	0.70
1:M:755:GLN:HB3	1:M:769:LEU:HD11	1.73	0.70
3:P:138:GLU:HA	3:P:141:MET:HG2	1.74	0.70
1:J:45:GLU:HG2	1:J:46:PHE:HD2	1.54	0.70
1:G:512:ASP:OD1	1:G:513:PHE:N	2.24	0.70
1:G:755:GLN:HB3	1:G:769:LEU:HD11	1.73	0.70
1:I:512:ASP:OD1	1:I:513:PHE:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:739:ARG:NH2	1:I:760:HIS:O	2.24	0.70
1:M:92:MET:HE1	1:M:712:ARG:H	1.54	0.70
2:E:244:ASP:O	2:A:325:MET:CE	2.39	0.70
3:O:133:ARG:NH2	3:P:138:GLU:OE2	2.25	0.70
1:G:92:MET:HE1	1:G:712:ARG:H	1.54	0.70
2:B:351:THR:HG21	1:H:551:LYS:HZ1	1.57	0.70
1:J:512:ASP:OD1	1:J:513:PHE:N	2.24	0.70
3:N:102:ALA:O	3:N:105:ARG:NH1	2.25	0.70
1:M:512:ASP:OD1	1:M:513:PHE:N	2.24	0.70
2:A:317:ILE:HG22	2:A:327:ILE:HD13	1.74	0.69
1:G:739:ARG:NH2	1:G:760:HIS:O	2.24	0.69
3:L:133:ARG:NH2	3:N:138:GLU:OE2	2.25	0.69
2:D:221:LEU:CD1	3:L:136:LYS:HZ3	2.04	0.69
1:K:639:LYS:O	2:A:24:ASP:OD1	2.11	0.69
1:K:755:GLN:HB3	1:K:769:LEU:HD11	1.73	0.69
3:N:138:GLU:HA	3:N:141:MET:HG2	1.74	0.69
1:J:18:LYS:O	1:J:23:ARG:NH1	2.26	0.69
3:P:102:ALA:O	3:P:105:ARG:NH1	2.25	0.69
1:G:523:LEU:HD21	1:G:563:PHE:HB2	1.74	0.69
2:C:291:LYS:HG2	2:C:325:MET:HE1	1.74	0.69
2:D:17:VAL:HG23	2:D:33:SER:HB3	1.74	0.69
1:G:18:LYS:O	1:G:23:ARG:NH1	2.26	0.69
1:I:18:LYS:O	1:I:23:ARG:NH1	2.26	0.69
1:I:523:LEU:HD21	1:I:563:PHE:HB2	1.74	0.69
1:K:18:LYS:O	1:K:23:ARG:NH1	2.26	0.69
1:H:18:LYS:O	1:H:23:ARG:NH1	2.26	0.68
1:J:755:GLN:HB3	1:J:769:LEU:HD11	1.73	0.68
3:O:97:GLU:HB3	3:O:101:ARG:HH12	1.59	0.68
1:J:523:LEU:HD21	1:J:563:PHE:HB2	1.74	0.68
1:G:355:ALA:HB2	1:G:387:LEU:HD22	1.76	0.68
1:M:523:LEU:HD21	1:M:563:PHE:HB2	1.74	0.68
3:O:157:ASP:O	3:O:161:LYS:HG2	1.93	0.68
1:H:523:LEU:HD21	1:H:563:PHE:HB2	1.74	0.68
3:L:157:ASP:O	3:L:161:LYS:HG2	1.93	0.68
1:J:355:ALA:HB2	1:J:387:LEU:HD22	1.76	0.68
1:K:355:ALA:HB2	1:K:387:LEU:HD22	1.76	0.68
1:M:355:ALA:HB2	1:M:387:LEU:HD22	1.76	0.68
1:H:355:ALA:HB2	1:H:387:LEU:HD22	1.76	0.68
1:I:755:GLN:HB3	1:I:769:LEU:HD11	1.73	0.68
1:M:18:LYS:O	1:M:23:ARG:NH1	2.26	0.68
1:I:355:ALA:HB2	1:I:387:LEU:HD22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:523:LEU:HD21	1:K:563:PHE:HB2	1.74	0.68
3:L:67:ALA:HA	3:L:70:LYS:HD2	1.76	0.67
2:B:41:GLN:HE22	2:F:172:PRO:HG3	1.57	0.67
2:E:317:ILE:HG22	2:E:327:ILE:HD13	1.74	0.67
3:N:140:LYS:O	3:N:144:GLN:NE2	2.27	0.67
2:B:17:VAL:HG23	2:B:33:SER:HB3	1.76	0.67
3:P:140:LYS:O	3:P:144:GLN:NE2	2.27	0.67
2:C:213:LYS:NZ	4:C:401:ADP:O2'	2.26	0.67
2:D:200:PHE:HB3	2:D:205:GLU:HB3	1.76	0.67
3:O:67:ALA:HA	3:O:70:LYS:HD2	1.76	0.67
2:A:156:GLY:O	2:A:303:THR:OG1	2.11	0.67
2:E:156:GLY:O	2:E:303:THR:OG1	2.11	0.67
1:K:368:GLN:HE22	3:N:61:SER:HB2	1.50	0.67
3:L:97:GLU:HB3	3:L:101:ARG:HH12	1.59	0.66
1:M:348:SER:HA	1:M:351:LYS:HG2	1.78	0.66
2:E:351:THR:OG1	1:J:536:GLU:CD	2.38	0.66
2:F:200:PHE:HB3	2:F:205:GLU:HB3	1.77	0.66
3:O:193:LEU:HD21	3:P:197:LEU:HD22	1.76	0.66
1:H:348:SER:HA	1:H:351:LYS:HG2	1.78	0.66
3:O:62:GLU:HA	3:O:65:LYS:HD2	1.78	0.66
3:P:102:ALA:O	3:P:106:LEU:HB2	1.95	0.65
3:O:182:ARG:NH2	3:P:186:SER:OG	2.29	0.65
1:G:274:ILE:O	1:G:315:GLN:NE2	2.30	0.65
1:I:348:SER:HA	1:I:351:LYS:HG2	1.78	0.65
1:J:348:SER:HA	1:J:351:LYS:HG2	1.78	0.65
2:E:24:ASP:OD1	1:J:639:LYS:O	2.13	0.65
1:G:37:VAL:HG12	1:G:78:GLN:HA	1.77	0.65
1:I:37:VAL:HG12	1:I:78:GLN:HA	1.77	0.65
1:K:536:GLU:CD	2:A:351:THR:OG1	2.39	0.65
3:N:102:ALA:O	3:N:106:LEU:HB2	1.95	0.65
3:L:62:GLU:HA	3:L:65:LYS:HD2	1.78	0.65
3:L:182:ARG:NH2	3:N:186:SER:OG	2.29	0.65
3:L:193:LEU:HD21	3:N:197:LEU:HD22	1.76	0.65
2:B:351:THR:HG21	1:H:551:LYS:NZ	2.12	0.65
2:F:213:LYS:NZ	4:F:401:ADP:O2'	2.27	0.65
1:I:274:ILE:O	1:I:315:GLN:NE2	2.30	0.65
1:K:274:ILE:O	1:K:315:GLN:NE2	2.30	0.65
1:H:37:VAL:HG12	1:H:78:GLN:HA	1.77	0.65
1:M:37:VAL:HG12	1:M:78:GLN:HA	1.77	0.65
1:M:274:ILE:O	1:M:315:GLN:NE2	2.30	0.65
1:H:274:ILE:O	1:H:315:GLN:NE2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:351:THR:OG1	1:G:536:GLU:CD	2.40	0.64
1:G:348:SER:HA	1:G:351:LYS:HG2	1.78	0.64
1:K:610:GLN:NE2	1:K:621:PHE:O	2.30	0.64
3:O:93:GLN:HA	1:G:368:GLN:HE22	1.62	0.64
1:K:37:VAL:HG12	1:K:78:GLN:HA	1.77	0.64
1:K:252:PHE:O	1:K:454:GLN:N	2.28	0.64
1:K:348:SER:HA	1:K:351:LYS:HG2	1.78	0.64
1:H:610:GLN:NE2	1:H:621:PHE:O	2.30	0.64
1:H:252:PHE:O	1:H:454:GLN:N	2.28	0.64
2:C:156:GLY:O	2:C:303:THR:OG1	2.15	0.64
1:J:37:VAL:HG12	1:J:78:GLN:HA	1.77	0.64
1:M:265:THR:HG21	1:M:436:PHE:HE2	1.63	0.64
1:J:274:ILE:O	1:J:315:GLN:NE2	2.30	0.64
2:E:41:GLN:NE2	2:A:172:PRO:HG3	2.12	0.64
1:I:610:GLN:NE2	1:I:621:PHE:O	2.30	0.64
1:J:610:GLN:NE2	1:J:621:PHE:O	2.30	0.64
2:A:307:PRO:HB3	3:L:48:LYS:HE2	1.80	0.64
1:K:162:TYR:OH	1:K:256:GLY:O	2.16	0.64
1:G:265:THR:HG21	1:G:436:PHE:HE2	1.63	0.63
2:C:220:ALA:HB1	2:C:226:GLU:HG3	1.79	0.63
1:G:610:GLN:NE2	1:G:621:PHE:O	2.30	0.63
1:H:265:THR:HG21	1:H:436:PHE:HE2	1.63	0.63
2:B:351:THR:HG23	1:H:536:GLU:OE2	1.98	0.63
1:M:162:TYR:OH	1:M:256:GLY:O	2.16	0.63
2:B:202:THR:HG22	2:B:204:ALA:H	1.63	0.63
1:J:265:THR:HG21	1:J:436:PHE:HE2	1.63	0.63
2:D:351:THR:OG1	1:I:536:GLU:CD	2.41	0.63
1:K:265:THR:HG21	1:K:436:PHE:HE2	1.63	0.63
2:A:220:ALA:HB1	2:A:226:GLU:HG3	1.81	0.63
1:I:700:GLU:O	1:I:704:ILE:HG12	1.99	0.63
1:J:252:PHE:O	1:J:454:GLN:N	2.28	0.63
2:D:190:MET:HG2	2:D:209:VAL:HG21	1.81	0.63
1:I:265:THR:HG21	1:I:436:PHE:HE2	1.63	0.63
1:J:516:ASP:N	1:J:516:ASP:OD1	2.30	0.63
2:E:220:ALA:HB1	2:E:226:GLU:HG3	1.81	0.62
1:M:610:GLN:NE2	1:M:621:PHE:O	2.30	0.62
2:C:14:SER:O	2:C:157:ASP:HB3	2.00	0.62
2:D:304:THR:O	2:D:335:ARG:NH1	2.32	0.62
1:G:700:GLU:O	1:G:704:ILE:HG12	1.99	0.62
1:I:506:ILE:HD11	1:I:757:LYS:HG2	1.82	0.62
1:K:700:GLU:O	1:K:704:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:144:GLN:NE2	3:P:144:GLN:HB3	2.15	0.62
1:K:506:ILE:HD11	1:K:757:LYS:HG2	1.82	0.62
3:L:144:GLN:NE2	3:N:144:GLN:HB3	2.15	0.62
1:H:516:ASP:N	1:H:516:ASP:OD1	2.30	0.62
2:A:286:ASP:O	2:A:290:ARG:NE	2.33	0.62
1:M:252:PHE:O	1:M:454:GLN:N	2.28	0.62
1:M:549:LYS:HE3	1:M:553:PHE:HE2	1.65	0.62
3:O:102:ALA:HA	3:O:105:ARG:HE	1.65	0.62
1:H:700:GLU:O	1:H:704:ILE:HG12	1.99	0.62
1:M:700:GLU:O	1:M:704:ILE:HG12	1.99	0.62
2:E:286:ASP:O	2:E:290:ARG:NE	2.33	0.62
1:I:162:TYR:OH	1:I:256:GLY:O	2.16	0.62
2:A:334:GLU:OE1	2:A:334:GLU:N	2.29	0.62
1:H:549:LYS:HE3	1:H:553:PHE:HE2	1.65	0.62
1:G:549:LYS:HE3	1:G:553:PHE:HE2	1.65	0.61
1:J:700:GLU:O	1:J:704:ILE:HG12	1.99	0.61
3:L:102:ALA:HA	3:L:105:ARG:HE	1.65	0.61
1:H:506:ILE:HD11	1:H:757:LYS:HG2	1.82	0.61
1:J:506:ILE:HD11	1:J:757:LYS:HG2	1.82	0.61
2:C:351:THR:O	2:C:354:GLN:NE2	2.33	0.61
1:G:285:ILE:O	1:G:289:ILE:HG12	2.01	0.61
2:B:8:LEU:HD13	2:B:101:HIS:HB3	1.83	0.61
2:F:116:ARG:NH2	2:F:375:PHE:O	2.33	0.61
3:P:89:ASN:HA	3:P:92:ILE:HD12	1.82	0.61
1:J:187:ASN:O	1:J:191:VAL:HG23	2.00	0.61
1:K:549:LYS:HE3	1:K:553:PHE:HE2	1.65	0.61
1:M:285:ILE:O	1:M:289:ILE:HG12	2.01	0.61
2:D:334:GLU:OE1	2:D:334:GLU:N	2.30	0.61
1:H:380:GLU:HA	1:H:383:LYS:HG2	1.83	0.61
1:J:368:GLN:HE21	3:L:100:ASP:N	1.94	0.61
1:I:187:ASN:O	1:I:191:VAL:HG23	2.00	0.61
1:I:285:ILE:O	1:I:289:ILE:HG12	2.01	0.61
1:K:187:ASN:O	1:K:191:VAL:HG23	2.00	0.61
1:M:506:ILE:HD11	1:M:757:LYS:HG2	1.82	0.61
2:B:351:THR:CG2	1:H:536:GLU:OE2	2.49	0.61
2:F:8:LEU:HD13	2:F:101:HIS:HB3	1.83	0.61
1:J:549:LYS:HE3	1:J:553:PHE:HE2	1.65	0.61
1:K:285:ILE:O	1:K:289:ILE:HG12	2.01	0.61
2:E:111:ASN:OD1	2:E:177:ARG:NH1	2.33	0.60
1:I:294:LYS:NZ	1:I:296:GLU:OE2	2.30	0.60
1:J:162:TYR:OH	1:J:256:GLY:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:89:ASN:HA	3:N:92:ILE:HD12	1.82	0.60
3:P:91:ARG:NE	1:G:369:ARG:NH2	2.49	0.60
1:G:187:ASN:O	1:G:191:VAL:HG23	2.00	0.60
1:H:285:ILE:O	1:H:289:ILE:HG12	2.01	0.60
1:J:285:ILE:O	1:J:289:ILE:HG12	2.01	0.60
1:K:380:GLU:HA	1:K:383:LYS:HG2	1.83	0.60
1:K:516:ASP:N	1:K:516:ASP:OD1	2.30	0.60
3:P:175:ASP:O	3:P:178:ARG:NH1	2.35	0.60
1:G:516:ASP:OD1	1:G:516:ASP:N	2.30	0.60
1:I:549:LYS:HE3	1:I:553:PHE:HE2	1.65	0.60
1:J:380:GLU:HA	1:J:383:LYS:HG2	1.82	0.60
1:K:294:LYS:NZ	1:K:296:GLU:OE2	2.30	0.60
3:N:175:ASP:O	3:N:178:ARG:NH1	2.35	0.60
1:H:187:ASN:O	1:H:191:VAL:HG23	2.00	0.60
1:I:380:GLU:HA	1:I:383:LYS:HG2	1.83	0.60
1:M:516:ASP:N	1:M:516:ASP:OD1	2.30	0.60
1:H:162:TYR:OH	1:H:256:GLY:O	2.16	0.60
1:I:472:SER:OG	1:I:473:PHE:N	2.35	0.60
1:J:233:ALA:O	1:J:241:SER:OG	2.20	0.60
2:A:202:THR:HG22	2:A:204:ALA:H	1.66	0.60
1:M:252:PHE:HE1	1:M:457:ILE:HD12	1.67	0.60
2:C:111:ASN:OD1	2:C:177:ARG:NH1	2.35	0.60
1:K:252:PHE:HE1	1:K:457:ILE:HD12	1.67	0.60
1:M:187:ASN:O	1:M:191:VAL:HG23	2.00	0.60
2:F:143:TYR:HE2	2:F:346:LEU:HD13	1.66	0.60
1:G:380:GLU:HA	1:G:383:LYS:HG2	1.82	0.60
1:I:39:VAL:HG23	1:I:71:VAL:HG21	1.84	0.60
1:I:233:ALA:O	1:I:241:SER:OG	2.20	0.60
1:G:506:ILE:HD11	1:G:757:LYS:HG2	1.82	0.60
1:J:294:LYS:NZ	1:J:296:GLU:OE2	2.30	0.60
3:O:173:GLU:HB3	1:H:368:GLN:NE2	2.17	0.60
1:G:252:PHE:HE1	1:G:457:ILE:HD12	1.67	0.60
1:G:708:GLY:O	1:G:766:LYS:NZ	2.28	0.60
1:H:165:MET:HE1	1:H:252:PHE:HB2	1.84	0.60
1:J:39:VAL:HG23	1:J:71:VAL:HG21	1.84	0.60
1:K:472:SER:OG	1:K:473:PHE:N	2.35	0.60
1:M:656:ASN:O	1:M:660:THR:HG23	2.02	0.59
1:M:676:ASN:ND2	1:M:683:VAL:O	2.36	0.59
2:B:334:GLU:OE1	2:B:334:GLU:N	2.31	0.59
2:F:334:GLU:OE1	2:F:334:GLU:N	2.29	0.59
1:G:165:MET:HE1	1:G:252:PHE:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:656:ASN:O	1:I:660:THR:HG23	2.02	0.59
1:J:656:ASN:O	1:J:660:THR:HG23	2.02	0.59
1:M:380:GLU:HA	1:M:383:LYS:HG2	1.83	0.59
2:E:334:GLU:OE1	2:E:334:GLU:N	2.29	0.59
1:I:165:MET:HE1	1:I:252:PHE:HB2	1.84	0.59
1:J:252:PHE:HE1	1:J:457:ILE:HD12	1.67	0.59
1:K:656:ASN:O	1:K:660:THR:HG23	2.02	0.59
1:M:165:MET:HE1	1:M:252:PHE:HB2	1.84	0.59
2:E:318:THR:HA	2:E:327:ILE:HD12	1.84	0.59
1:H:233:ALA:O	1:H:241:SER:OG	2.20	0.59
1:H:252:PHE:HE1	1:H:457:ILE:HD12	1.67	0.59
1:I:516:ASP:OD1	1:I:516:ASP:N	2.30	0.59
1:I:676:ASN:ND2	1:I:683:VAL:O	2.36	0.59
1:J:437:ASN:O	1:J:441:THR:HG23	2.02	0.59
1:J:676:ASN:ND2	1:J:683:VAL:O	2.35	0.59
1:K:165:MET:HE1	1:K:252:PHE:HB2	1.84	0.59
1:H:143:ARG:NH1	1:H:159:ASP:OD2	2.36	0.59
1:H:656:ASN:O	1:H:660:THR:HG23	2.02	0.59
1:H:676:ASN:ND2	1:H:683:VAL:O	2.36	0.59
1:I:143:ARG:NH1	1:I:159:ASP:OD2	2.36	0.59
1:K:437:ASN:O	1:K:441:THR:HG23	2.02	0.59
1:K:676:ASN:ND2	1:K:683:VAL:O	2.36	0.59
2:A:318:THR:HA	2:A:327:ILE:HD12	1.84	0.59
3:O:88:LEU:O	3:O:92:ILE:HG23	2.03	0.59
1:G:676:ASN:ND2	1:G:683:VAL:O	2.36	0.59
1:I:437:ASN:O	1:I:441:THR:HG23	2.02	0.59
1:J:165:MET:HE1	1:J:252:PHE:HB2	1.84	0.59
3:N:189:LYS:O	3:N:193:LEU:HG	2.02	0.59
2:E:202:THR:HG22	2:E:204:ALA:H	1.66	0.59
1:G:39:VAL:HG23	1:G:71:VAL:HG21	1.84	0.59
1:G:143:ARG:NH1	1:G:159:ASP:OD2	2.36	0.59
1:K:233:ALA:O	1:K:241:SER:OG	2.20	0.59
1:M:437:ASN:O	1:M:441:THR:HG23	2.02	0.59
2:B:21:PHE:HZ	2:B:96:VAL:HG11	1.67	0.59
1:G:233:ALA:O	1:G:241:SER:OG	2.20	0.59
1:K:39:VAL:HG23	1:K:71:VAL:HG21	1.84	0.59
2:D:213:LYS:NZ	4:D:401:ADP:O2'	2.28	0.59
1:G:437:ASN:O	1:G:441:THR:HG23	2.02	0.59
1:M:472:SER:OG	1:M:473:PHE:N	2.35	0.59
1:H:437:ASN:O	1:H:441:THR:HG23	2.02	0.59
1:K:143:ARG:NH1	1:K:159:ASP:OD2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:111:ASN:OD1	2:A:177:ARG:NH1	2.33	0.59
1:M:143:ARG:NH1	1:M:159:ASP:OD2	2.36	0.58
1:M:39:VAL:HG23	1:M:71:VAL:HG21	1.84	0.58
2:E:213:LYS:NZ	4:E:401:ADP:O2'	2.28	0.58
1:J:143:ARG:NH1	1:J:159:ASP:OD2	2.36	0.58
1:G:656:ASN:O	1:G:660:THR:HG23	2.02	0.58
3:L:144:GLN:O	3:L:147:GLN:NE2	2.35	0.58
1:M:233:ALA:O	1:M:241:SER:OG	2.20	0.58
1:M:746:LEU:HG	1:M:751:ILE:HD12	1.86	0.58
2:B:111:ASN:OD1	2:B:177:ARG:NH1	2.32	0.58
1:H:746:LEU:HG	1:H:751:ILE:HD12	1.86	0.58
2:A:200:PHE:HB3	2:A:205:GLU:HB3	1.86	0.58
3:L:105:ARG:HE	3:N:106:LEU:HD21	1.68	0.58
3:P:189:LYS:O	3:P:193:LEU:HG	2.02	0.58
1:G:162:TYR:OH	1:G:256:GLY:O	2.16	0.58
1:G:746:LEU:HG	1:G:751:ILE:HD12	1.86	0.58
1:H:39:VAL:HG23	1:H:71:VAL:HG21	1.84	0.58
2:E:200:PHE:HB3	2:E:205:GLU:HB3	1.86	0.58
1:I:252:PHE:HE1	1:I:457:ILE:HD12	1.67	0.58
1:I:676:ASN:ND2	1:I:680:SER:O	2.28	0.58
1:K:72:LYS:H	1:K:75:GLN:HE21	1.52	0.58
1:K:536:GLU:CD	2:A:351:THR:HG1	2.10	0.58
3:L:88:LEU:O	3:L:92:ILE:HG23	2.03	0.58
2:F:111:ASN:OD1	2:F:177:ARG:NH1	2.35	0.58
1:I:72:LYS:H	1:I:75:GLN:HE21	1.52	0.58
1:J:72:LYS:H	1:J:75:GLN:HE21	1.52	0.58
3:L:144:GLN:HA	3:L:147:GLN:HG3	1.84	0.58
1:H:270:LYS:HB3	1:H:429:LYS:HD2	1.86	0.58
2:F:47:MET:HB3	1:G:540:PHE:HZ	1.65	0.58
3:L:141:MET:O	3:L:145:GLU:HG2	2.04	0.58
3:O:144:GLN:HA	3:O:147:GLN:HG3	1.84	0.57
1:I:746:LEU:HG	1:I:751:ILE:HD12	1.86	0.57
1:M:270:LYS:HB3	1:M:429:LYS:HD2	1.86	0.57
2:B:351:THR:HG22	1:H:528:MET:HE1	1.85	0.57
1:G:472:SER:OG	1:G:473:PHE:N	2.35	0.57
1:J:725:LEU:O	1:J:726:ASN:ND2	2.37	0.57
1:K:109:TYR:HD2	1:K:684:MET:HE2	1.70	0.57
1:K:269:GLU:HG3	1:K:272:ARG:HG2	1.86	0.57
1:K:478:ILE:O	1:K:481:THR:OG1	2.22	0.57
1:G:72:LYS:H	1:G:75:GLN:HE21	1.52	0.57
1:G:269:GLU:HG3	1:G:272:ARG:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:PHE:O	1:I:454:GLN:N	2.28	0.57
1:J:269:GLU:HG3	1:J:272:ARG:HG2	1.86	0.57
1:J:109:TYR:HD2	1:J:684:MET:HE2	1.70	0.57
1:J:761:THR:HG23	1:J:762:LYS:HG3	1.86	0.57
2:C:189:LEU:HA	2:C:192:ILE:HG22	1.86	0.57
2:D:156:GLY:O	2:D:303:THR:OG1	2.19	0.57
3:O:141:MET:O	3:O:145:GLU:HG2	2.04	0.57
1:I:269:GLU:HG3	1:I:272:ARG:HG2	1.86	0.57
1:I:368:GLN:HG2	3:N:141:MET:HG3	1.87	0.57
2:D:111:ASN:OD1	2:D:177:ARG:NH1	2.31	0.57
1:I:270:LYS:HB3	1:I:429:LYS:HD2	1.86	0.57
1:M:269:GLU:HG3	1:M:272:ARG:HG2	1.86	0.57
1:I:725:LEU:O	1:I:726:ASN:ND2	2.37	0.57
1:K:368:GLN:HG3	3:L:60:TYR:HE2	1.68	0.57
1:G:270:LYS:HB3	1:G:429:LYS:HD2	1.86	0.57
1:G:294:LYS:NZ	1:G:296:GLU:OE2	2.30	0.57
1:G:474:GLU:OE2	1:G:596:LYS:NZ	2.38	0.57
1:H:269:GLU:HG3	1:H:272:ARG:HG2	1.86	0.57
1:J:270:LYS:HB3	1:J:429:LYS:HD2	1.86	0.57
1:K:536:GLU:OE1	2:A:351:THR:OG1	2.23	0.57
1:G:109:TYR:HD2	1:G:684:MET:HE2	1.70	0.57
1:I:761:THR:HG23	1:I:762:LYS:HG3	1.86	0.57
1:M:725:LEU:O	1:M:726:ASN:ND2	2.37	0.56
2:B:190:MET:HG3	2:B:209:VAL:HG11	1.87	0.56
2:E:351:THR:OG1	1:J:536:GLU:OE1	2.23	0.56
2:F:116:ARG:O	2:F:120:THR:HG23	2.05	0.56
1:G:252:PHE:O	1:G:454:GLN:N	2.28	0.56
1:H:761:THR:HG23	1:H:762:LYS:HG3	1.86	0.56
1:M:109:TYR:HD2	1:M:684:MET:HE2	1.70	0.56
1:M:478:ILE:O	1:M:481:THR:OG1	2.22	0.56
1:H:109:TYR:HD2	1:H:684:MET:HE2	1.70	0.56
1:H:676:ASN:ND2	1:H:680:SER:O	2.28	0.56
1:I:368:GLN:CD	3:N:142:GLU:HA	2.30	0.56
2:C:192:ILE:HD11	2:C:256:ARG:CZ	2.36	0.56
2:D:351:THR:HG1	1:I:536:GLU:CD	2.12	0.56
2:D:357:ILE:HG12	2:D:374:CYS:HB3	1.86	0.56
3:P:108:THR:HA	3:P:111:GLN:HG2	1.86	0.56
3:P:159:ASP:O	3:P:163:GLU:HG2	2.06	0.56
1:G:761:THR:HG23	1:G:762:LYS:HG3	1.86	0.56
1:H:725:LEU:O	1:H:726:ASN:ND2	2.37	0.56
1:I:474:GLU:OE2	1:I:596:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:746:LEU:HG	1:J:751:ILE:HD12	1.86	0.56
1:K:270:LYS:HB3	1:K:429:LYS:HD2	1.86	0.56
1:K:725:LEU:O	1:K:726:ASN:ND2	2.37	0.56
1:M:610:GLN:HG2	1:M:620:LEU:O	2.05	0.56
1:H:471:ASN:ND2	1:H:587:ASP:O	2.36	0.56
1:H:610:GLN:HG2	1:H:620:LEU:O	2.05	0.56
1:I:109:TYR:HD2	1:I:684:MET:HE2	1.69	0.56
1:K:610:GLN:HG2	1:K:620:LEU:O	2.05	0.56
1:M:761:THR:HG23	1:M:762:LYS:HG3	1.86	0.56
1:H:72:LYS:H	1:H:75:GLN:HE21	1.52	0.56
1:H:294:LYS:NZ	1:H:296:GLU:OE2	2.30	0.56
1:K:746:LEU:HG	1:K:751:ILE:HD12	1.86	0.56
1:M:72:LYS:H	1:M:75:GLN:HE21	1.52	0.56
2:C:351:THR:OG1	1:G:536:GLU:OE1	2.23	0.56
2:F:14:SER:O	2:F:157:ASP:HB3	2.06	0.56
1:G:610:GLN:HG2	1:G:620:LEU:O	2.05	0.56
1:I:504:GLU:OE2	1:I:761:THR:HG22	2.06	0.56
3:N:108:THR:HA	3:N:111:GLN:HG2	1.86	0.56
1:K:761:THR:HG23	1:K:762:LYS:HG3	1.86	0.56
2:A:14:SER:O	2:A:157:ASP:HB3	2.06	0.56
2:D:221:LEU:CG	3:L:136:LYS:HZ3	2.17	0.56
2:E:14:SER:O	2:E:157:ASP:HB3	2.06	0.56
2:E:41:GLN:HE21	2:A:172:PRO:CG	2.14	0.56
1:G:504:GLU:OE2	1:G:761:THR:HG22	2.06	0.56
1:I:478:ILE:O	1:I:481:THR:OG1	2.22	0.56
3:O:105:ARG:HE	3:P:106:LEU:HD21	1.68	0.56
1:J:471:ASN:ND2	1:J:587:ASP:O	2.36	0.56
1:M:504:GLU:OE2	1:M:761:THR:HG22	2.06	0.56
2:D:220:ALA:HB1	2:D:226:GLU:HG3	1.88	0.56
1:G:725:LEU:O	1:G:726:ASN:ND2	2.37	0.56
1:M:474:GLU:OE2	1:M:596:LYS:NZ	2.38	0.55
2:B:317:ILE:HG23	2:B:327:ILE:HG21	1.88	0.55
1:I:721:ARG:O	1:I:777:ARG:HD3	2.06	0.55
1:K:504:GLU:OE2	1:K:761:THR:HG22	2.06	0.55
1:H:472:SER:OG	1:H:473:PHE:N	2.35	0.55
1:H:474:GLU:OE2	1:H:596:LYS:NZ	2.38	0.55
1:H:504:GLU:OE2	1:H:761:THR:HG22	2.06	0.55
1:H:535:GLU:OE2	1:H:652:ARG:NH2	2.39	0.55
1:I:535:GLU:OE2	1:I:652:ARG:NH2	2.39	0.55
1:J:504:GLU:OE2	1:J:761:THR:HG22	2.06	0.55
1:J:535:GLU:OE2	1:J:652:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:535:GLU:OE2	1:K:652:ARG:NH2	2.39	0.55
1:H:721:ARG:O	1:H:777:ARG:HD3	2.06	0.55
1:I:610:GLN:HG2	1:I:620:LEU:O	2.05	0.55
1:M:721:ARG:O	1:M:777:ARG:HD3	2.06	0.55
1:J:610:GLN:HG2	1:J:620:LEU:O	2.05	0.55
3:N:159:ASP:O	3:N:163:GLU:HG2	2.06	0.55
2:B:95:ARG:O	1:H:635:LYS:HA	2.05	0.55
1:H:478:ILE:O	1:H:481:THR:OG1	2.22	0.55
1:H:506:ILE:HG13	1:H:508:TRP:CZ3	2.42	0.55
1:J:24:LEU:HA	1:J:27:GLN:HG2	1.89	0.55
1:K:24:LEU:HA	1:K:27:GLN:HG2	1.89	0.55
1:K:281:ARG:HG2	1:K:317:GLU:HB2	1.88	0.55
1:K:721:ARG:O	1:K:777:ARG:HD3	2.06	0.55
2:C:369:ILE:HG12	2:C:374:CYS:SG	2.46	0.55
2:D:351:THR:OG1	1:I:536:GLU:OE1	2.25	0.55
1:J:721:ARG:O	1:J:777:ARG:HD3	2.07	0.55
2:A:213:LYS:NZ	4:A:401:ADP:O2'	2.28	0.55
1:M:24:LEU:HA	1:M:27:GLN:HG2	1.89	0.55
2:B:202:THR:HB	2:B:205:GLU:HG3	1.88	0.55
1:K:474:GLU:OE2	1:K:596:LYS:NZ	2.38	0.55
3:N:82:GLU:HA	3:N:85:VAL:HG12	1.88	0.55
1:M:506:ILE:HG13	1:M:508:TRP:CZ3	2.42	0.55
3:P:47:GLN:OE1	3:P:47:GLN:N	2.39	0.55
1:G:24:LEU:HA	1:G:27:GLN:HG2	1.89	0.55
1:G:535:GLU:OE2	1:G:652:ARG:NH2	2.39	0.55
1:H:24:LEU:HA	1:H:27:GLN:HG2	1.89	0.55
3:P:82:GLU:HA	3:P:85:VAL:HG12	1.88	0.55
1:G:173:SER:O	1:G:668:HIS:N	2.39	0.55
1:H:281:ARG:HG2	1:H:317:GLU:HB2	1.88	0.55
1:I:24:LEU:HA	1:I:27:GLN:HG2	1.89	0.55
1:I:471:ASN:ND2	1:I:587:ASP:O	2.36	0.55
1:J:281:ARG:HG2	1:J:317:GLU:HB2	1.88	0.55
1:J:474:GLU:OE2	1:J:596:LYS:NZ	2.38	0.55
1:K:708:GLY:O	1:K:766:LYS:NZ	2.28	0.55
1:M:281:ARG:HG2	1:M:317:GLU:HB2	1.88	0.54
1:M:535:GLU:OE2	1:M:652:ARG:NH2	2.39	0.54
2:F:369:ILE:HD12	2:F:372:ARG:HG3	1.88	0.54
3:O:144:GLN:O	3:O:147:GLN:NE2	2.35	0.54
1:G:471:ASN:ND2	1:G:587:ASP:O	2.36	0.54
1:G:478:ILE:O	1:G:481:THR:OG1	2.22	0.54
1:M:173:SER:O	1:M:668:HIS:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ARG:O	2:D:120:THR:HG23	2.07	0.54
2:F:147:ARG:HH22	2:F:330:ILE:HG12	1.73	0.54
3:P:98:GLU:OE2	3:P:99:LEU:HD12	2.08	0.54
1:G:721:ARG:O	1:G:777:ARG:HD3	2.07	0.54
2:A:321:ALA:HB3	2:A:327:ILE:HD11	1.89	0.54
3:N:173:GLU:O	3:N:177:GLU:HG2	2.07	0.54
3:O:61:SER:O	3:O:65:LYS:HG3	2.07	0.54
3:O:105:ARG:NE	3:P:106:LEU:HD21	2.22	0.54
1:J:478:ILE:O	1:J:481:THR:OG1	2.22	0.54
1:J:708:GLY:O	1:J:766:LYS:NZ	2.28	0.54
3:P:173:GLU:O	3:P:177:GLU:HG2	2.07	0.54
1:G:281:ARG:HG2	1:G:317:GLU:HB2	1.88	0.54
1:G:506:ILE:HG13	1:G:508:TRP:CZ3	2.42	0.54
1:G:676:ASN:ND2	1:G:680:SER:O	2.28	0.54
3:L:201:THR:HA	3:L:204:LEU:HG	1.89	0.54
1:J:368:GLN:HE21	3:L:100:ASP:HB2	1.70	0.54
1:M:294:LYS:NZ	1:M:296:GLU:OE2	2.30	0.54
2:E:321:ALA:HB3	2:E:327:ILE:HD11	1.89	0.54
1:I:281:ARG:HG2	1:I:317:GLU:HB2	1.88	0.54
1:M:676:ASN:ND2	1:M:680:SER:O	2.28	0.54
3:P:197:LEU:HD23	3:P:198:LYS:HZ2	1.73	0.54
1:K:471:ASN:ND2	1:K:587:ASP:O	2.36	0.54
1:H:173:SER:O	1:H:668:HIS:N	2.39	0.54
1:J:434:ARG:HH22	1:J:623:ASN:CG	2.16	0.54
1:K:506:ILE:HG13	1:K:508:TRP:CZ3	2.42	0.54
2:B:220:ALA:HB1	2:B:226:GLU:HG3	1.90	0.54
1:I:434:ARG:HH22	1:I:623:ASN:CG	2.16	0.54
1:K:368:GLN:HG3	3:L:60:TYR:CE2	2.43	0.54
1:M:562:ASN:HD22	1:M:580:ILE:HD11	1.73	0.54
3:O:161:LYS:O	3:O:165:VAL:HG23	2.08	0.54
3:P:75:GLU:O	3:P:79:THR:HG23	2.08	0.54
1:G:434:ARG:HH22	1:G:623:ASN:CG	2.16	0.54
1:G:562:ASN:HD22	1:G:580:ILE:HD11	1.73	0.54
1:I:562:ASN:HD22	1:I:580:ILE:HD11	1.73	0.54
3:L:105:ARG:NE	3:N:106:LEU:HD21	2.22	0.54
3:N:98:GLU:OE2	3:N:99:LEU:HD12	2.08	0.54
1:J:562:ASN:HD22	1:J:580:ILE:HD11	1.73	0.53
1:J:687:PRO:HA	1:J:690:MET:HE3	1.91	0.53
1:K:173:SER:O	1:K:668:HIS:N	2.39	0.53
1:K:434:ARG:HH22	1:K:623:ASN:CG	2.16	0.53
3:L:61:SER:O	3:L:65:LYS:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:75:GLU:O	3:N:79:THR:HG23	2.08	0.53
2:D:286:ASP:O	2:D:290:ARG:NE	2.40	0.53
2:F:304:THR:O	2:F:335:ARG:NH1	2.42	0.53
3:P:124:GLU:O	3:P:128:LYS:HG2	2.08	0.53
1:I:244:PHE:HB3	1:I:268:LEU:HD13	1.91	0.53
1:I:687:PRO:HA	1:I:690:MET:HE3	1.91	0.53
2:B:151:ILE:HG21	2:B:282:ILE:HD11	1.89	0.53
3:O:68:GLN:O	3:O:72:GLU:HG2	2.09	0.53
3:O:201:THR:HA	3:O:204:LEU:HG	1.89	0.53
1:H:244:PHE:HB3	1:H:268:LEU:HD13	1.91	0.53
1:I:506:ILE:HG13	1:I:508:TRP:CZ3	2.42	0.53
3:L:161:LYS:O	3:L:165:VAL:HG23	2.08	0.53
1:J:244:PHE:HB3	1:J:268:LEU:HD13	1.91	0.53
1:M:434:ARG:HH22	1:M:623:ASN:CG	2.16	0.53
3:N:197:LEU:HD23	3:N:198:LYS:NZ	2.24	0.53
1:M:244:PHE:HB3	1:M:268:LEU:HD13	1.91	0.53
1:M:334:ASN:O	1:M:338:VAL:HG22	2.09	0.53
1:G:334:ASN:O	1:G:338:VAL:HG22	2.09	0.53
1:J:173:SER:O	1:J:668:HIS:N	2.39	0.53
3:N:124:GLU:O	3:N:128:LYS:HG2	2.08	0.53
2:C:153:LEU:HD22	2:C:313:MET:HE1	1.91	0.53
2:E:244:ASP:O	2:A:325:MET:HE2	2.08	0.53
1:H:334:ASN:O	1:H:338:VAL:HG22	2.09	0.53
1:I:173:SER:O	1:I:668:HIS:N	2.39	0.53
1:I:580:ILE:HG22	1:I:585:ILE:HG12	1.90	0.53
1:K:244:PHE:HB3	1:K:268:LEU:HD13	1.91	0.53
1:K:565:LYS:O	1:K:578:SER:OG	2.25	0.53
1:K:687:PRO:HA	1:K:690:MET:HE3	1.91	0.53
2:C:116:ARG:O	2:C:120:THR:HG23	2.07	0.53
2:C:172:PRO:HG3	2:F:41:GLN:HE21	1.73	0.53
2:C:233:SER:OG	2:C:234:SER:N	2.41	0.53
1:J:235:THR:HG23	1:J:241:SER:OG	2.09	0.53
1:J:506:ILE:HG13	1:J:508:TRP:CZ3	2.42	0.53
3:L:141:MET:HE1	3:N:144:GLN:HB2	1.91	0.53
3:N:73:LEU:O	3:N:77:LYS:NZ	2.42	0.53
2:D:120:THR:HG21	2:D:370:VAL:HG21	1.90	0.53
1:H:580:ILE:HG22	1:H:585:ILE:HG12	1.90	0.53
1:M:249:ARG:HB2	1:M:262:ASP:HB2	1.91	0.53
1:M:692:GLN:O	1:M:696:ASN:HB2	2.09	0.53
2:B:306:TYR:CE1	4:B:401:ADP:H2	2.27	0.53
1:H:434:ARG:HH22	1:H:623:ASN:CG	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:692:GLN:O	1:I:696:ASN:HB2	2.09	0.53
1:K:235:THR:HG23	1:K:241:SER:OG	2.09	0.53
1:K:562:ASN:HD22	1:K:580:ILE:HD11	1.73	0.53
2:E:26:ALA:HB1	1:J:406:VAL:HG12	1.91	0.52
2:F:220:ALA:HB1	2:F:226:GLU:HG3	1.91	0.52
3:P:197:LEU:HD23	3:P:198:LYS:NZ	2.24	0.52
1:G:244:PHE:HB3	1:G:268:LEU:HD13	1.91	0.52
1:H:249:ARG:HB2	1:H:262:ASP:HB2	1.91	0.52
1:I:235:THR:HG23	1:I:241:SER:OG	2.09	0.52
1:I:708:GLY:O	1:I:766:LYS:NZ	2.28	0.52
1:J:334:ASN:O	1:J:338:VAL:HG22	2.09	0.52
1:J:565:LYS:O	1:J:578:SER:OG	2.25	0.52
1:J:580:ILE:HG22	1:J:585:ILE:HG12	1.90	0.52
2:B:153:LEU:HD22	2:B:313:MET:HE1	1.91	0.52
3:O:91:ARG:O	3:O:95:VAL:HG23	2.10	0.52
1:H:562:ASN:HD22	1:H:580:ILE:HD11	1.73	0.52
1:H:565:LYS:O	1:H:578:SER:OG	2.25	0.52
3:O:81:ALA:O	3:O:85:VAL:HG13	2.09	0.52
1:G:580:ILE:HG22	1:G:585:ILE:HG12	1.90	0.52
1:H:722:TYR:CE2	1:H:773:LEU:HB3	2.44	0.52
1:I:334:ASN:O	1:I:338:VAL:HG22	2.09	0.52
1:M:471:ASN:ND2	1:M:587:ASP:O	2.36	0.52
1:G:235:THR:HG23	1:G:241:SER:OG	2.09	0.52
1:G:249:ARG:HB2	1:G:262:ASP:HB2	1.91	0.52
1:K:692:GLN:O	1:K:696:ASN:HB2	2.09	0.52
1:K:722:TYR:CE2	1:K:773:LEU:HB3	2.44	0.52
1:M:687:PRO:HA	1:M:690:MET:HE3	1.91	0.52
1:G:687:PRO:HA	1:G:690:MET:HE3	1.91	0.52
1:K:249:ARG:HB2	1:K:262:ASP:HB2	1.91	0.52
3:L:81:ALA:O	3:L:85:VAL:HG13	2.10	0.52
1:I:249:ARG:N	1:I:262:ASP:O	2.41	0.52
1:M:235:THR:HG23	1:M:241:SER:OG	2.09	0.52
1:J:154:ILE:HD11	1:J:190:ARG:HG3	1.92	0.52
1:K:334:ASN:O	1:K:338:VAL:HG22	2.09	0.52
3:L:68:GLN:O	3:L:72:GLU:HG2	2.09	0.52
3:L:91:ARG:O	3:L:95:VAL:HG23	2.10	0.52
1:M:722:TYR:CE2	1:M:773:LEU:HB3	2.44	0.52
3:P:181:GLU:O	3:P:185:LEU:HG	2.10	0.52
1:H:687:PRO:HA	1:H:690:MET:HE3	1.91	0.52
1:I:565:LYS:O	1:I:578:SER:OG	2.25	0.52
1:J:249:ARG:HB2	1:J:262:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:TYR:CE2	4:D:401:ADP:H2	2.28	0.52
2:E:62:ARG:HH11	2:E:207:GLU:HB2	1.75	0.52
3:O:173:GLU:CD	1:H:368:GLN:NE2	2.64	0.52
1:J:472:SER:OG	1:J:473:PHE:N	2.35	0.52
1:J:692:GLN:O	1:J:696:ASN:HB2	2.09	0.52
1:J:722:TYR:CE2	1:J:773:LEU:HB3	2.44	0.52
3:N:181:GLU:O	3:N:185:LEU:HG	2.10	0.52
1:M:565:LYS:O	1:M:578:SER:OG	2.25	0.52
2:F:21:PHE:HZ	2:F:96:VAL:HG11	1.75	0.52
1:I:154:ILE:HD11	1:I:190:ARG:HG3	1.92	0.52
1:I:249:ARG:HB2	1:I:262:ASP:HB2	1.91	0.52
1:K:154:ILE:HD11	1:K:190:ARG:HG3	1.92	0.52
1:K:580:ILE:HG22	1:K:585:ILE:HG12	1.90	0.52
2:E:233:SER:OG	2:E:234:SER:N	2.43	0.51
1:G:537:GLU:HG3	1:G:543:ALA:HB1	1.92	0.51
1:H:235:THR:HG23	1:H:241:SER:OG	2.09	0.51
1:M:537:GLU:HG3	1:M:543:ALA:HB1	1.92	0.51
2:F:233:SER:OG	2:F:234:SER:N	2.43	0.51
1:I:265:THR:HG21	1:I:436:PHE:CE2	2.44	0.51
1:I:269:GLU:OE1	1:I:270:LYS:N	2.44	0.51
2:A:233:SER:OG	2:A:234:SER:N	2.43	0.51
3:L:145:GLU:O	3:L:149:LYS:HG2	2.11	0.51
1:M:265:THR:HG21	1:M:436:PHE:CE2	2.44	0.51
1:G:265:THR:HG21	1:G:436:PHE:CE2	2.44	0.51
1:G:722:TYR:CE2	1:G:773:LEU:HB3	2.44	0.51
1:H:269:GLU:OE1	1:H:270:LYS:N	2.44	0.51
1:H:692:GLN:O	1:H:696:ASN:HB2	2.09	0.51
1:H:708:GLY:O	1:H:766:LYS:NZ	2.28	0.51
1:J:676:ASN:ND2	1:J:680:SER:O	2.28	0.51
2:B:147:ARG:HH12	2:B:330:ILE:HG13	1.75	0.51
1:J:269:GLU:OE1	1:J:270:LYS:N	2.44	0.51
1:M:580:ILE:HG22	1:M:585:ILE:HG12	1.90	0.51
2:C:365:ALA:HB3	2:C:369:ILE:HD12	1.92	0.51
1:G:249:ARG:N	1:G:262:ASP:O	2.41	0.51
1:H:51:ILE:HD12	1:H:59:VAL:HB	1.92	0.51
1:H:265:THR:HG21	1:H:436:PHE:CE2	2.44	0.51
1:J:265:THR:HG21	1:J:436:PHE:CE2	2.44	0.51
1:H:537:GLU:HG3	1:H:543:ALA:HB1	1.92	0.51
1:I:722:TYR:CE2	1:I:773:LEU:HB3	2.44	0.51
2:A:62:ARG:HH11	2:A:207:GLU:HB2	1.75	0.51
1:M:51:ILE:HD12	1:M:59:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:603:GLU:OE2	1:M:624:TYR:HA	2.11	0.51
1:G:449:THR:O	1:G:453:ARG:NH2	2.44	0.51
1:H:449:THR:O	1:H:453:ARG:NH2	2.44	0.51
1:M:269:GLU:OE1	1:M:270:LYS:N	2.44	0.51
1:M:686:ASN:O	1:M:690:MET:HG3	2.11	0.51
3:O:182:ARG:NH2	3:O:183:ALA:HA	2.26	0.51
1:G:603:GLU:OE2	1:G:624:TYR:HA	2.11	0.51
1:G:686:ASN:O	1:G:690:MET:HG3	2.11	0.51
1:G:692:GLN:O	1:G:696:ASN:HB2	2.09	0.51
1:H:230:PHE:CD1	1:H:285:ILE:HG12	2.46	0.51
1:I:449:THR:O	1:I:453:ARG:NH2	2.44	0.51
2:C:200:PHE:HB3	2:C:205:GLU:HB3	1.93	0.51
3:O:141:MET:HE1	3:P:144:GLN:HB2	1.91	0.51
3:P:136:LYS:HG2	3:P:140:LYS:HE2	1.93	0.51
1:H:603:GLU:OE2	1:H:624:TYR:HA	2.11	0.51
1:H:686:ASN:O	1:H:690:MET:HG3	2.11	0.51
1:I:603:GLU:OE2	1:I:624:TYR:HA	2.11	0.51
1:J:537:GLU:HG3	1:J:543:ALA:HB1	1.92	0.51
1:K:449:THR:O	1:K:453:ARG:NH2	2.44	0.51
1:K:537:GLU:HG3	1:K:543:ALA:HB1	1.92	0.51
2:A:17:VAL:HG23	2:A:33:SER:HB2	1.92	0.51
1:M:708:GLY:O	1:M:766:LYS:NZ	2.28	0.51
2:C:190:MET:HG3	2:C:209:VAL:HG11	1.92	0.51
1:G:51:ILE:HD12	1:G:59:VAL:HB	1.92	0.51
1:K:265:THR:HG21	1:K:436:PHE:CE2	2.44	0.51
1:K:269:GLU:OE1	1:K:270:LYS:N	2.44	0.51
1:K:474:GLU:H	1:K:474:GLU:CD	2.18	0.51
1:K:603:GLU:OE2	1:K:624:TYR:HA	2.11	0.51
1:K:676:ASN:HB3	1:K:684:MET:HA	1.93	0.51
2:B:21:PHE:CZ	2:B:96:VAL:HG11	2.46	0.50
3:P:72:GLU:O	3:P:76:LYS:HG3	2.12	0.50
1:G:154:ILE:HD11	1:G:190:ARG:HG3	1.92	0.50
1:G:230:PHE:CD1	1:G:285:ILE:HG12	2.46	0.50
1:G:565:LYS:O	1:G:578:SER:OG	2.25	0.50
1:J:449:THR:O	1:J:453:ARG:NH2	2.44	0.50
1:K:51:ILE:HD12	1:K:59:VAL:HB	1.92	0.50
1:K:230:PHE:CD1	1:K:285:ILE:HG12	2.46	0.50
3:O:145:GLU:O	3:O:149:LYS:HG2	2.11	0.50
1:I:537:GLU:HG3	1:I:543:ALA:HB1	1.92	0.50
1:J:230:PHE:CD1	1:J:285:ILE:HG12	2.46	0.50
1:K:676:ASN:ND2	1:K:680:SER:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:686:ASN:O	1:K:690:MET:HG3	2.11	0.50
3:L:182:ARG:NH2	3:L:183:ALA:HA	2.26	0.50
1:M:154:ILE:HD11	1:M:190:ARG:HG3	1.92	0.50
1:M:249:ARG:N	1:M:262:ASP:O	2.41	0.50
2:E:17:VAL:HG23	2:E:33:SER:HB2	1.92	0.50
1:I:230:PHE:CD1	1:I:285:ILE:HG12	2.46	0.50
1:I:752:ASP:HB2	1:I:755:GLN:HG3	1.94	0.50
1:J:676:ASN:HB3	1:J:684:MET:HA	1.93	0.50
1:J:686:ASN:O	1:J:690:MET:HG3	2.11	0.50
1:M:230:PHE:CD1	1:M:285:ILE:HG12	2.46	0.50
1:M:449:THR:O	1:M:453:ARG:NH2	2.44	0.50
2:E:304:THR:O	2:E:335:ARG:NH1	2.45	0.50
1:H:154:ILE:HD11	1:H:190:ARG:HG3	1.92	0.50
1:J:474:GLU:H	1:J:474:GLU:CD	2.18	0.50
2:C:17:VAL:HG23	2:C:33:SER:HB3	1.94	0.50
3:P:73:LEU:O	3:P:77:LYS:NZ	2.42	0.50
3:P:204:LEU:O	3:P:208:GLU:HB2	2.12	0.50
1:G:269:GLU:OE1	1:G:270:LYS:N	2.44	0.50
1:I:676:ASN:HB3	1:I:684:MET:HA	1.93	0.50
1:J:51:ILE:HD12	1:J:59:VAL:HB	1.92	0.50
2:A:180:LEU:HD22	2:A:261:LEU:HD23	1.94	0.50
2:B:304:THR:O	2:B:335:ARG:NH1	2.45	0.50
2:D:23:GLY:O	1:I:641:GLY:N	2.40	0.50
1:I:51:ILE:HD12	1:I:59:VAL:HB	1.92	0.50
1:J:603:GLU:OE2	1:J:624:TYR:HA	2.11	0.50
1:J:745:LEU:HG	1:J:749:LEU:HD13	1.94	0.50
1:K:369:ARG:HB3	3:L:60:TYR:OH	2.11	0.50
2:A:304:THR:O	2:A:335:ARG:NH1	2.45	0.50
2:E:180:LEU:HD22	2:E:261:LEU:HD23	1.94	0.50
1:I:189:LYS:O	1:I:192:ILE:HG12	2.12	0.50
3:N:47:GLN:OE1	3:N:47:GLN:N	2.39	0.50
3:N:204:LEU:O	3:N:208:GLU:HB2	2.12	0.50
1:H:189:LYS:O	1:H:192:ILE:HG12	2.12	0.50
1:J:752:ASP:HB2	1:J:755:GLN:HG3	1.94	0.50
3:L:47:GLN:O	3:L:51:LYS:HG2	2.11	0.50
2:B:124:PHE:CZ	2:B:132:MET:HG2	2.47	0.49
1:G:171:ASN:OD1	1:G:456:PHE:N	2.40	0.49
1:G:290:LEU:HD13	1:G:307:PRO:HB3	1.94	0.49
1:J:115:TYR:HE2	1:J:154:ILE:HG23	1.77	0.49
1:K:219:GLN:OE1	1:K:219:GLN:N	2.42	0.49
2:A:306:TYR:CE2	4:A:401:ADP:H2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:189:LYS:O	1:M:192:ILE:HG12	2.12	0.49
2:C:147:ARG:NH2	2:C:330:ILE:HG12	2.21	0.49
2:E:190:MET:HG2	2:E:209:VAL:HG21	1.93	0.49
1:J:189:LYS:O	1:J:192:ILE:HG12	2.12	0.49
2:A:73:HIS:C	2:A:75:ILE:H	2.21	0.49
3:N:136:LYS:HG2	3:N:140:LYS:HE2	1.93	0.49
1:M:745:LEU:HG	1:M:749:LEU:HD13	1.94	0.49
2:D:337:TYR:O	2:D:341:ILE:HG12	2.12	0.49
1:H:281:ARG:HD2	1:H:320:VAL:HG22	1.94	0.49
1:J:219:GLN:OE1	1:J:219:GLN:N	2.42	0.49
1:K:406:VAL:HG12	2:A:26:ALA:HB1	1.94	0.49
1:M:371:GLU:OE1	2:F:147:ARG:NH2	2.44	0.49
2:E:73:HIS:C	2:E:75:ILE:H	2.21	0.49
1:H:249:ARG:N	1:H:262:ASP:O	2.41	0.49
1:I:171:ASN:OD1	1:I:456:PHE:N	2.40	0.49
1:J:370:GLU:HG2	1:J:371:GLU:H	1.78	0.49
1:M:281:ARG:HD2	1:M:320:VAL:HG22	1.94	0.49
1:M:290:LEU:HD13	1:M:307:PRO:HB3	1.94	0.49
1:M:714:LEU:HA	1:M:762:LYS:HA	1.95	0.49
1:M:752:ASP:HB2	1:M:755:GLN:HG3	1.94	0.49
2:C:143:TYR:OH	2:F:45:VAL:O	2.27	0.49
2:E:306:TYR:CE2	4:E:401:ADP:H2	2.30	0.49
3:O:47:GLN:O	3:O:51:LYS:HG2	2.11	0.49
1:G:281:ARG:HD2	1:G:320:VAL:HG22	1.95	0.49
1:G:714:LEU:HA	1:G:762:LYS:HA	1.95	0.49
1:H:370:GLU:HG2	1:H:371:GLU:H	1.78	0.49
1:I:115:TYR:CE2	1:I:154:ILE:HG23	2.48	0.49
1:J:281:ARG:HD2	1:J:320:VAL:HG22	1.94	0.49
1:J:714:LEU:HA	1:J:762:LYS:HA	1.95	0.49
3:L:71:LEU:HD21	3:N:71:LEU:CA	2.42	0.49
3:N:58:ASP:O	3:N:62:GLU:HG2	2.12	0.49
1:M:506:ILE:HG13	1:M:508:TRP:HZ3	1.78	0.49
2:B:14:SER:O	2:B:157:ASP:HB3	2.12	0.49
1:G:370:GLU:HG2	1:G:371:GLU:H	1.78	0.49
1:G:752:ASP:HB2	1:G:755:GLN:HG3	1.94	0.49
1:H:506:ILE:HG13	1:H:508:TRP:HZ3	1.78	0.49
1:H:752:ASP:HB2	1:H:755:GLN:HG3	1.93	0.49
1:I:290:LEU:HD13	1:I:307:PRO:HB3	1.94	0.49
1:J:716:GLY:O	1:J:720:GLN:HG2	2.13	0.49
1:K:281:ARG:HD2	1:K:320:VAL:HG22	1.94	0.49
1:K:506:ILE:HG13	1:K:508:TRP:HZ3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:714:LEU:HA	1:K:762:LYS:HA	1.95	0.49
1:K:745:LEU:HG	1:K:749:LEU:HD13	1.94	0.49
1:K:752:ASP:HB2	1:K:755:GLN:HG3	1.94	0.49
3:N:72:GLU:O	3:N:76:LYS:HG3	2.12	0.49
1:M:115:TYR:HE2	1:M:154:ILE:HG23	1.77	0.49
2:F:18:LYS:HG2	2:F:30:VAL:HG22	1.94	0.49
2:F:306:TYR:CE2	4:F:401:ADP:H2	2.30	0.49
3:O:202:ASN:O	3:O:205:LYS:HG3	2.13	0.49
3:P:58:ASP:O	3:P:62:GLU:HG2	2.12	0.49
1:H:115:TYR:HE2	1:H:154:ILE:HG23	1.77	0.49
1:H:745:LEU:HG	1:H:749:LEU:HD13	1.94	0.49
1:I:686:ASN:O	1:I:690:MET:HG3	2.11	0.49
1:J:506:ILE:HG13	1:J:508:TRP:HZ3	1.78	0.49
1:J:763:VAL:HG13	1:J:765:PHE:CE2	2.48	0.49
1:K:716:GLY:O	1:K:720:GLN:HG2	2.13	0.49
1:M:716:GLY:O	1:M:720:GLN:HG2	2.13	0.49
2:F:368:SER:HB2	2:F:372:ARG:HH12	1.77	0.49
1:H:714:LEU:HA	1:H:762:LYS:HA	1.95	0.49
1:I:714:LEU:HA	1:I:762:LYS:HA	1.95	0.49
1:I:716:GLY:O	1:I:720:GLN:HG2	2.13	0.49
2:A:190:MET:HG2	2:A:209:VAL:HG21	1.93	0.49
1:M:676:ASN:HB3	1:M:684:MET:HA	1.93	0.49
3:O:106:LEU:HD22	3:P:105:ARG:CZ	2.43	0.49
1:G:35:LYS:HD2	1:G:51:ILE:HB	1.94	0.49
1:G:115:TYR:CE2	1:G:154:ILE:HG23	2.48	0.49
1:G:139:VAL:HG13	1:G:194:TYR:HD1	1.78	0.49
1:G:676:ASN:HB3	1:G:684:MET:HA	1.93	0.49
1:G:716:GLY:O	1:G:720:GLN:HG2	2.13	0.49
1:H:716:GLY:O	1:H:720:GLN:HG2	2.13	0.49
1:I:281:ARG:HD2	1:I:320:VAL:HG22	1.94	0.49
1:K:473:PHE:HB3	1:K:596:LYS:HD2	1.94	0.49
1:K:763:VAL:HG13	1:K:765:PHE:CE2	2.48	0.49
1:M:35:LYS:HD2	1:M:51:ILE:HB	1.94	0.49
1:M:115:TYR:CE2	1:M:154:ILE:HG23	2.48	0.49
1:M:370:GLU:HG2	1:M:371:GLU:H	1.78	0.49
2:E:107:GLU:HG2	2:E:111:ASN:HD22	1.78	0.49
1:I:21:LYS:O	1:I:25:GLU:HG2	2.13	0.49
1:I:219:GLN:OE1	1:I:219:GLN:N	2.42	0.49
1:J:699:LEU:HA	1:J:702:ILE:HG12	1.95	0.49
3:L:111:GLN:O	3:L:115:GLU:HG2	2.13	0.49
2:B:156:GLY:O	2:B:303:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:LYS:O	1:G:192:ILE:HG12	2.12	0.48
1:G:474:GLU:H	1:G:474:GLU:CD	2.18	0.48
1:G:506:ILE:HG13	1:G:508:TRP:HZ3	1.78	0.48
1:H:35:LYS:HD2	1:H:51:ILE:HB	1.94	0.48
1:H:676:ASN:HB3	1:H:684:MET:HA	1.93	0.48
1:I:370:GLU:HG2	1:I:371:GLU:H	1.78	0.48
1:I:473:PHE:HB3	1:I:596:LYS:HD2	1.94	0.48
1:I:474:GLU:H	1:I:474:GLU:CD	2.18	0.48
1:I:506:ILE:HG13	1:I:508:TRP:HZ3	1.78	0.48
1:I:763:VAL:HG13	1:I:765:PHE:CE2	2.48	0.48
1:J:115:TYR:CE2	1:J:154:ILE:HG23	2.48	0.48
1:J:473:PHE:HB3	1:J:596:LYS:HD2	1.94	0.48
1:K:115:TYR:CE2	1:K:154:ILE:HG23	2.48	0.48
1:K:699:LEU:HA	1:K:702:ILE:HG12	1.95	0.48
3:L:108:THR:O	3:L:111:GLN:HG3	2.13	0.48
3:L:202:ASN:O	3:L:205:LYS:HG3	2.13	0.48
1:M:473:PHE:HB3	1:M:596:LYS:HD2	1.94	0.48
1:G:95:PHE:HB3	1:G:97:HIS:NE2	2.29	0.48
1:I:699:LEU:HA	1:I:702:ILE:HG12	1.95	0.48
1:J:290:LEU:HD13	1:J:307:PRO:HB3	1.94	0.48
1:J:499:GLU:HA	1:J:502:LYS:HG2	1.95	0.48
1:K:370:GLU:HG2	1:K:371:GLU:H	1.78	0.48
2:D:230:ALA:HB2	2:D:236:LEU:HD12	1.96	0.48
3:O:96:GLU:OE2	3:P:95:VAL:HG11	2.13	0.48
3:P:201:THR:O	3:P:205:LYS:HG2	2.13	0.48
1:G:473:PHE:HB3	1:G:596:LYS:HD2	1.94	0.48
1:I:139:VAL:HG13	1:I:194:TYR:HD1	1.78	0.48
1:I:499:GLU:HA	1:I:502:LYS:HG2	1.95	0.48
1:K:189:LYS:O	1:K:192:ILE:HG12	2.12	0.48
2:A:107:GLU:HG2	2:A:111:ASN:HD22	1.78	0.48
1:M:21:LYS:O	1:M:25:GLU:HG2	2.13	0.48
1:G:699:LEU:HA	1:G:702:ILE:HG12	1.95	0.48
1:H:21:LYS:O	1:H:25:GLU:HG2	2.13	0.48
1:H:95:PHE:HB3	1:H:97:HIS:NE2	2.29	0.48
1:H:115:TYR:CE2	1:H:154:ILE:HG23	2.48	0.48
1:H:290:LEU:HD13	1:H:307:PRO:HB3	1.94	0.48
1:H:473:PHE:HB3	1:H:596:LYS:HD2	1.94	0.48
1:H:715:TYR:OH	1:H:759:GLY:O	2.26	0.48
1:I:9:PHE:HB2	1:I:13:ALA:HB2	1.96	0.48
1:I:115:TYR:HE2	1:I:154:ILE:HG23	1.77	0.48
1:I:715:TYR:OH	1:I:759:GLY:O	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:745:LEU:HG	1:I:749:LEU:HD13	1.94	0.48
1:J:21:LYS:O	1:J:25:GLU:HG2	2.13	0.48
1:K:499:GLU:HA	1:K:502:LYS:HG2	1.95	0.48
1:K:611:LYS:HE2	1:K:611:LYS:HB3	1.61	0.48
1:M:139:VAL:HG13	1:M:194:TYR:HD1	1.78	0.48
2:D:71:ILE:HG12	2:D:76:ILE:HG12	1.95	0.48
2:F:73:HIS:C	2:F:75:ILE:H	2.22	0.48
1:J:95:PHE:HB3	1:J:97:HIS:NE2	2.29	0.48
1:J:496:LEU:HA	1:J:499:GLU:OE1	2.14	0.48
1:K:95:PHE:HB3	1:K:97:HIS:NE2	2.29	0.48
1:K:115:TYR:HE2	1:K:154:ILE:HG23	1.78	0.48
1:M:699:LEU:HA	1:M:702:ILE:HG12	1.95	0.48
3:O:111:GLN:O	3:O:115:GLU:HG2	2.13	0.48
3:O:202:ASN:OD1	3:O:205:LYS:HE3	2.14	0.48
1:G:172:GLN:HB2	1:G:457:ILE:HG23	1.96	0.48
1:G:187:ASN:O	1:G:190:ARG:HG2	2.14	0.48
1:G:611:LYS:HB3	1:G:611:LYS:HE2	1.61	0.48
1:G:634:GLY:O	1:G:637:LYS:HG2	2.14	0.48
1:I:634:GLY:O	1:I:637:LYS:HG2	2.14	0.48
1:J:139:VAL:HG13	1:J:194:TYR:HD1	1.78	0.48
1:K:9:PHE:HB2	1:K:13:ALA:HB2	1.96	0.48
2:E:76:ILE:HD13	2:E:82:MET:HG2	1.95	0.48
1:H:699:LEU:HA	1:H:702:ILE:HG12	1.95	0.48
1:I:95:PHE:HB3	1:I:97:HIS:NE2	2.29	0.48
1:I:496:LEU:HA	1:I:499:GLU:OE1	2.14	0.48
1:J:368:GLN:HG2	3:L:99:LEU:HD13	1.76	0.48
1:J:368:GLN:HE21	3:L:100:ASP:CA	2.01	0.48
1:K:35:LYS:HD2	1:K:51:ILE:HB	1.94	0.48
1:K:290:LEU:HD13	1:K:307:PRO:HB3	1.94	0.48
2:A:76:ILE:HD13	2:A:82:MET:HG2	1.95	0.48
1:M:187:ASN:O	1:M:190:ARG:HG2	2.14	0.48
3:O:70:LYS:HA	3:O:73:LEU:HG	1.96	0.48
3:O:108:THR:O	3:O:111:GLN:HG3	2.13	0.48
1:G:745:LEU:HG	1:G:749:LEU:HD13	1.94	0.48
1:G:763:VAL:HG13	1:G:765:PHE:CE2	2.48	0.48
1:H:562:ASN:HB3	1:H:580:ILE:HG12	1.95	0.48
1:J:634:GLY:O	1:J:637:LYS:HG2	2.14	0.48
1:K:21:LYS:O	1:K:25:GLU:HG2	2.13	0.48
3:L:106:LEU:HD22	3:N:105:ARG:CZ	2.43	0.48
1:M:763:VAL:HG13	1:M:765:PHE:CE2	2.48	0.48
2:D:226:GLU:HA	2:D:229:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:PHE:HB2	1:M:13:ALA:HB2	1.96	0.48
1:M:172:GLN:HB2	1:M:457:ILE:HG23	1.96	0.48
1:M:715:TYR:OH	1:M:759:GLY:O	2.26	0.48
2:D:123:MET:O	2:D:129:VAL:HG22	2.14	0.48
1:G:21:LYS:O	1:G:25:GLU:HG2	2.13	0.48
1:G:143:ARG:NH1	1:G:143:ARG:HA	2.29	0.48
1:G:177:THR:OG1	1:G:671:ARG:NH1	2.47	0.48
1:G:275:PHE:HA	1:G:315:GLN:NE2	2.29	0.48
1:G:621:PHE:CG	1:G:622:ALA:N	2.82	0.48
1:H:172:GLN:HB2	1:H:457:ILE:HG23	1.96	0.48
1:H:634:GLY:O	1:H:637:LYS:HG2	2.14	0.48
1:H:763:VAL:HG13	1:H:765:PHE:CE2	2.48	0.48
1:I:160:ASN:HA	1:I:163:GLN:HE21	1.79	0.48
1:K:160:ASN:HA	1:K:163:GLN:HE21	1.79	0.48
1:K:171:ASN:OD1	1:K:456:PHE:N	2.40	0.48
1:M:275:PHE:HA	1:M:315:GLN:NE2	2.29	0.47
1:M:462:ILE:HG23	1:M:463:ALA:O	2.14	0.47
1:G:115:TYR:HE2	1:G:154:ILE:HG23	1.77	0.47
1:H:187:ASN:O	1:H:190:ARG:HG2	2.14	0.47
1:H:462:ILE:HG23	1:H:463:ALA:O	2.14	0.47
1:I:403:ARG:H	1:I:604:THR:HG21	1.79	0.47
1:J:562:ASN:HB3	1:J:580:ILE:HG12	1.95	0.47
1:K:139:VAL:HG13	1:K:194:TYR:HD1	1.78	0.47
1:K:187:ASN:O	1:K:190:ARG:HG2	2.14	0.47
1:K:496:LEU:HA	1:K:499:GLU:OE1	2.14	0.47
1:M:237:ARG:HH12	1:M:691:HIS:CD2	2.33	0.47
1:M:496:LEU:HA	1:M:499:GLU:OE1	2.14	0.47
2:B:162:ASN:ND2	2:B:277:THR:HG22	2.29	0.47
3:O:58:ASP:O	3:O:62:GLU:HG2	2.14	0.47
1:G:237:ARG:HH12	1:G:691:HIS:CD2	2.33	0.47
1:G:499:GLU:HA	1:G:502:LYS:HG2	1.95	0.47
1:G:567:ARG:HH21	1:G:585:ILE:HG22	1.79	0.47
1:I:368:GLN:HE21	3:N:142:GLU:N	2.05	0.47
1:J:35:LYS:HD2	1:J:51:ILE:HB	1.94	0.47
1:J:160:ASN:HA	1:J:163:GLN:HE21	1.79	0.47
1:J:187:ASN:O	1:J:190:ARG:HG2	2.14	0.47
1:J:462:ILE:HG23	1:J:463:ALA:O	2.14	0.47
1:K:634:GLY:O	1:K:637:LYS:HG2	2.14	0.47
3:L:202:ASN:OD1	3:L:205:LYS:HE3	2.14	0.47
3:N:194:GLU:O	3:N:198:LYS:HG2	2.14	0.47
1:M:177:THR:OG1	1:M:671:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:73:LEU:O	3:P:77:LYS:HG2	2.14	0.47
3:P:200:VAL:HA	3:P:203:ASN:HD22	1.79	0.47
1:H:296:GLU:O	1:H:300:MET:HG2	2.15	0.47
1:I:187:ASN:O	1:I:190:ARG:HG2	2.14	0.47
1:I:368:GLN:CD	3:N:142:GLU:HB3	2.25	0.47
1:I:611:LYS:HB3	1:I:611:LYS:HE2	1.61	0.47
1:J:343:SER:HA	1:J:346:LYS:HE2	1.97	0.47
1:K:249:ARG:N	1:K:262:ASP:O	2.41	0.47
2:A:372:ARG:O	2:A:375:PHE:HB2	2.14	0.47
1:M:143:ARG:NH1	1:M:143:ARG:HA	2.29	0.47
1:M:296:GLU:O	1:M:300:MET:HG2	2.15	0.47
1:M:499:GLU:HA	1:M:502:LYS:HG2	1.95	0.47
2:B:62:ARG:HH11	2:B:207:GLU:HB2	1.78	0.47
2:E:23:GLY:O	1:J:641:GLY:N	2.43	0.47
3:P:194:GLU:O	3:P:198:LYS:HG2	2.14	0.47
1:H:139:VAL:HG13	1:H:194:TYR:HD1	1.78	0.47
1:I:35:LYS:HD2	1:I:51:ILE:HB	1.94	0.47
1:K:343:SER:HA	1:K:346:LYS:HE2	1.97	0.47
3:N:201:THR:O	3:N:205:LYS:HG2	2.13	0.47
1:M:95:PHE:HB3	1:M:97:HIS:NE2	2.29	0.47
1:M:567:ARG:HH21	1:M:585:ILE:HG22	1.79	0.47
2:D:196:ARG:HD2	2:D:253:GLU:OE2	2.14	0.47
3:P:88:LEU:O	3:P:92:ILE:HG13	2.15	0.47
1:G:367:LYS:HE2	1:G:367:LYS:HB3	1.63	0.47
1:H:177:THR:OG1	1:H:671:ARG:NH1	2.47	0.47
1:J:143:ARG:NH1	1:J:143:ARG:HA	2.29	0.47
1:K:143:ARG:NH1	1:K:143:ARG:HA	2.29	0.47
1:K:717:ASP:CG	1:K:721:ARG:HE	2.23	0.47
3:L:58:ASP:O	3:L:62:GLU:HG2	2.14	0.47
3:N:106:LEU:O	3:N:110:LEU:HG	2.15	0.47
1:M:766:LYS:H	1:M:769:LEU:HD13	1.80	0.47
1:G:562:ASN:HB3	1:G:580:ILE:HG12	1.95	0.47
1:H:143:ARG:NH1	1:H:143:ARG:HA	2.29	0.47
1:H:237:ARG:HH12	1:H:691:HIS:CD2	2.33	0.47
1:I:577:PHE:HE2	1:I:579:LEU:HD13	1.80	0.47
1:I:766:LYS:H	1:I:769:LEU:HD13	1.80	0.47
1:J:403:ARG:H	1:J:604:THR:HG21	1.79	0.47
1:J:621:PHE:CG	1:J:622:ALA:N	2.82	0.47
1:K:296:GLU:O	1:K:300:MET:HG2	2.15	0.47
1:M:368:GLN:NE2	3:P:138:GLU:OE1	2.48	0.47
1:M:474:GLU:H	1:M:474:GLU:CD	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:634:GLY:O	1:M:637:LYS:HG2	2.14	0.47
2:B:230:ALA:HB2	2:B:236:LEU:HD12	1.96	0.47
2:C:221:LEU:HD22	3:P:90:ARG:HB3	1.96	0.47
2:E:147:ARG:NH2	1:J:371:GLU:OE1	2.47	0.47
2:E:213:LYS:HZ1	4:E:401:ADP:HO2'	1.55	0.47
2:E:372:ARG:O	2:E:375:PHE:HB2	2.14	0.47
2:F:21:PHE:CZ	2:F:96:VAL:HG11	2.49	0.47
3:O:177:GLU:O	3:O:181:GLU:HG2	2.15	0.47
3:P:65:LYS:HA	3:P:68:GLN:OE1	2.15	0.47
1:H:9:PHE:HB2	1:H:13:ALA:HB2	1.96	0.47
1:H:275:PHE:HA	1:H:315:GLN:NE2	2.29	0.47
1:H:499:GLU:HA	1:H:502:LYS:HG2	1.95	0.47
1:I:143:ARG:NH1	1:I:143:ARG:HA	2.29	0.47
1:I:343:SER:HA	1:I:346:LYS:HE2	1.97	0.47
1:I:476:LEU:HD11	1:I:524:ILE:HD12	1.97	0.47
1:I:621:PHE:CG	1:I:622:ALA:N	2.82	0.47
1:J:9:PHE:HB2	1:J:13:ALA:HB2	1.96	0.47
1:J:237:ARG:HH12	1:J:691:HIS:CD2	2.33	0.47
1:J:368:GLN:NE2	3:L:99:LEU:HD12	2.29	0.47
1:J:476:LEU:HD11	1:J:524:ILE:HD12	1.97	0.47
1:J:577:PHE:HE2	1:J:579:LEU:HD13	1.80	0.47
1:K:172:GLN:HB2	1:K:457:ILE:HG23	1.96	0.47
1:K:177:THR:OG1	1:K:671:ARG:NH1	2.47	0.47
1:K:476:LEU:HD11	1:K:524:ILE:HD12	1.97	0.47
1:K:567:ARG:HH21	1:K:585:ILE:HG22	1.79	0.47
1:K:641:GLY:N	2:A:23:GLY:O	2.43	0.47
1:M:621:PHE:CG	1:M:622:ALA:N	2.82	0.47
2:E:45:VAL:O	2:A:143:TYR:OH	2.29	0.47
2:F:47:MET:HB3	1:G:540:PHE:CE2	2.50	0.47
1:G:766:LYS:H	1:G:769:LEU:HD13	1.80	0.47
1:H:496:LEU:HA	1:H:499:GLU:OE1	2.14	0.47
1:H:621:PHE:CG	1:H:622:ALA:N	2.82	0.47
1:I:237:ARG:HH12	1:I:691:HIS:CD2	2.33	0.47
1:I:462:ILE:HG23	1:I:463:ALA:O	2.14	0.47
1:I:562:ASN:HB3	1:I:580:ILE:HG12	1.95	0.47
1:K:562:ASN:HB3	1:K:580:ILE:HG12	1.95	0.47
3:L:70:LYS:HA	3:L:73:LEU:HG	1.96	0.47
2:B:5:THR:OG1	2:B:6:THR:N	2.46	0.47
2:E:151:ILE:HG21	2:E:282:ILE:HD11	1.97	0.47
2:F:17:VAL:HG23	2:F:33:SER:HB3	1.97	0.47
1:G:9:PHE:HB2	1:G:13:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ALA:HB3	1:G:447:LEU:HD21	1.97	0.47
1:H:160:ASN:HA	1:H:163:GLN:HE21	1.79	0.47
1:H:766:LYS:H	1:H:769:LEU:HD13	1.80	0.47
1:I:178:GLY:C	1:I:184:LYS:HD3	2.40	0.47
1:J:275:PHE:HA	1:J:315:GLN:NE2	2.29	0.47
1:K:577:PHE:HE2	1:K:579:LEU:HD13	1.80	0.47
1:K:635:LYS:HA	2:A:95:ARG:O	2.14	0.47
3:N:65:LYS:HA	3:N:68:GLN:OE1	2.15	0.47
3:N:73:LEU:O	3:N:77:LYS:HG2	2.14	0.47
1:M:160:ASN:HA	1:M:163:GLN:HE21	1.79	0.47
1:M:562:ASN:HB3	1:M:580:ILE:HG12	1.95	0.47
2:B:76:ILE:HD13	2:B:82:MET:HG2	1.96	0.47
2:C:73:HIS:C	2:C:75:ILE:H	2.23	0.47
1:H:343:SER:HA	1:H:346:LYS:HE2	1.97	0.47
1:I:177:THR:OG1	1:I:671:ARG:NH1	2.47	0.47
1:I:717:ASP:CG	1:I:721:ARG:HE	2.22	0.47
1:J:172:GLN:HB2	1:J:457:ILE:HG23	1.96	0.47
1:K:38:PHE:N	1:K:77:MET:O	2.47	0.47
1:K:261:ALA:HB3	1:K:447:LEU:HD21	1.97	0.47
1:K:462:ILE:HG23	1:K:463:ALA:O	2.14	0.47
1:K:621:PHE:CG	1:K:622:ALA:N	2.82	0.47
3:N:124:GLU:O	3:N:127:MET:HG2	2.15	0.47
3:N:200:VAL:HA	3:N:203:ASN:HD22	1.79	0.47
2:B:162:ASN:HD22	2:B:277:THR:HG22	1.81	0.46
2:D:73:HIS:C	2:D:75:ILE:H	2.23	0.46
2:E:95:ARG:O	1:J:635:LYS:HA	2.15	0.46
2:F:190:MET:HG3	2:F:209:VAL:HG11	1.96	0.46
1:G:476:LEU:HD11	1:G:524:ILE:HD12	1.97	0.46
1:I:567:ARG:HH21	1:I:585:ILE:HG22	1.79	0.46
1:K:371:GLU:OE1	2:A:147:ARG:NH2	2.49	0.46
3:L:49:LYS:HZ1	3:N:50:LEU:HD22	1.79	0.46
3:L:50:LEU:HD11	3:N:53:THR:HG21	1.98	0.46
2:F:195:GLU:OE2	2:F:256:ARG:NH2	2.49	0.46
3:O:94:LEU:O	3:O:98:GLU:HG3	2.15	0.46
1:G:403:ARG:H	1:G:604:THR:HG21	1.79	0.46
1:G:462:ILE:HG23	1:G:463:ALA:O	2.14	0.46
1:G:496:LEU:HA	1:G:499:GLU:OE1	2.14	0.46
1:G:715:TYR:OH	1:G:759:GLY:O	2.26	0.46
1:J:766:LYS:H	1:J:769:LEU:HD13	1.80	0.46
1:K:237:ARG:HH12	1:K:691:HIS:CD2	2.33	0.46
1:K:679:LYS:HD3	1:K:679:LYS:HA	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:188:GLY:O	3:N:192:GLU:HG2	2.15	0.46
1:M:261:ALA:HB3	1:M:447:LEU:HD21	1.97	0.46
3:P:106:LEU:O	3:P:110:LEU:HG	2.15	0.46
3:P:124:GLU:O	3:P:127:MET:HG2	2.15	0.46
1:G:717:ASP:CG	1:G:721:ARG:HE	2.22	0.46
1:H:484:LYS:HG3	1:H:655:LEU:HD21	1.98	0.46
1:H:717:ASP:CG	1:H:721:ARG:HE	2.22	0.46
1:I:275:PHE:HA	1:I:315:GLN:NE2	2.29	0.46
1:J:283:TYR:HB3	1:J:285:ILE:HD12	1.98	0.46
1:J:368:GLN:HE21	3:L:99:LEU:HD12	1.80	0.46
1:K:572:LYS:HB3	1:K:572:LYS:HE2	1.69	0.46
3:L:136:LYS:HA	3:L:139:GLU:HG2	1.97	0.46
3:L:177:GLU:O	3:L:181:GLU:HG2	2.15	0.46
3:N:144:GLN:O	3:N:147:GLN:HG3	2.15	0.46
2:C:334:GLU:OE1	2:C:334:GLU:N	2.37	0.46
2:D:216:LEU:HD22	2:D:238:LYS:HD3	1.96	0.46
2:F:97:ALA:HB1	2:F:99:GLU:OE1	2.15	0.46
3:P:153:HIS:O	3:P:156:GLU:HG3	2.15	0.46
1:G:484:LYS:HG3	1:G:655:LEU:HD21	1.98	0.46
1:H:47:VAL:HA	1:H:103:TYR:OH	2.16	0.46
1:H:219:GLN:OE1	1:H:219:GLN:N	2.42	0.46
1:H:567:ARG:HH21	1:H:585:ILE:HG22	1.79	0.46
1:H:637:LYS:HD3	1:H:637:LYS:HA	1.75	0.46
1:I:172:GLN:HB2	1:I:457:ILE:HG23	1.96	0.46
1:J:171:ASN:OD1	1:J:456:PHE:N	2.40	0.46
1:J:177:THR:OG1	1:J:671:ARG:NH1	2.47	0.46
1:J:261:ALA:HB3	1:J:447:LEU:HD21	1.97	0.46
1:J:703:ARG:O	1:J:707:LYS:HE2	2.16	0.46
3:N:88:LEU:O	3:N:92:ILE:HG13	2.15	0.46
1:M:38:PHE:N	1:M:77:MET:O	2.47	0.46
1:M:47:VAL:HA	1:M:103:TYR:OH	2.16	0.46
1:M:343:SER:HA	1:M:346:LYS:HE2	1.97	0.46
1:M:476:LEU:HD11	1:M:524:ILE:HD12	1.97	0.46
1:G:160:ASN:HA	1:G:163:GLN:HE21	1.79	0.46
1:G:178:GLY:C	1:G:184:LYS:HD3	2.40	0.46
1:G:296:GLU:O	1:G:300:MET:HG2	2.14	0.46
1:H:261:ALA:HB3	1:H:447:LEU:HD21	1.97	0.46
3:L:161:LYS:O	3:L:164:GLU:HG2	2.16	0.46
3:L:196:GLU:O	3:L:200:VAL:HG22	2.14	0.46
1:M:186:VAL:HG13	1:M:190:ARG:HH21	1.81	0.46
1:M:219:GLN:OE1	1:M:219:GLN:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:483:GLU:OE2	1:M:581:HIS:HB3	2.16	0.46
1:M:484:LYS:HG3	1:M:655:LEU:HD21	1.98	0.46
1:M:717:ASP:CG	1:M:721:ARG:HE	2.23	0.46
2:C:301:GLY:O	2:C:304:THR:OG1	2.32	0.46
3:O:165:VAL:O	3:O:169:LEU:HB2	2.16	0.46
3:O:173:GLU:HB3	1:H:368:GLN:HE22	1.80	0.46
1:G:186:VAL:HG13	1:G:190:ARG:HH21	1.81	0.46
1:I:283:TYR:HB3	1:I:285:ILE:HD12	1.98	0.46
1:J:296:GLU:O	1:J:300:MET:HG2	2.15	0.46
1:J:717:ASP:CG	1:J:721:ARG:HE	2.23	0.46
1:K:403:ARG:H	1:K:604:THR:HG21	1.79	0.46
1:K:766:LYS:H	1:K:769:LEU:HD13	1.80	0.46
3:L:94:LEU:O	3:L:98:GLU:HG3	2.15	0.46
3:N:197:LEU:HD23	3:N:198:LYS:HZ2	1.80	0.46
2:C:252:ASN:HB3	2:C:256:ARG:HD3	1.97	0.46
1:H:178:GLY:C	1:H:184:LYS:HD3	2.40	0.46
1:H:403:ARG:H	1:H:604:THR:HG21	1.79	0.46
1:H:569:ILE:O	1:H:570:LYS:HG2	2.16	0.46
1:K:275:PHE:HA	1:K:315:GLN:NE2	2.29	0.46
1:K:569:ILE:O	1:K:570:LYS:HG2	2.16	0.46
2:A:151:ILE:HG21	2:A:282:ILE:HD11	1.97	0.46
1:M:171:ASN:OD1	1:M:456:PHE:N	2.40	0.46
3:O:87:SER:O	3:O:91:ARG:HG2	2.16	0.46
3:O:196:GLU:O	3:O:200:VAL:HG22	2.15	0.46
1:G:343:SER:HA	1:G:346:LYS:HE2	1.97	0.46
1:I:483:GLU:OE2	1:I:581:HIS:HB3	2.16	0.46
1:K:282:ASP:OD1	1:K:283:TYR:N	2.45	0.46
3:L:87:SER:O	3:L:91:ARG:HG2	2.16	0.46
1:M:92:MET:HE1	1:M:712:ARG:N	2.28	0.46
1:M:703:ARG:O	1:M:707:LYS:HE2	2.16	0.46
2:C:361:GLU:O	2:C:364:GLU:HG3	2.16	0.46
2:E:116:ARG:HG2	2:E:370:VAL:HG11	1.98	0.46
2:F:70:PRO:HB3	2:F:81:ASP:HB3	1.98	0.46
3:P:144:GLN:O	3:P:147:GLN:HG3	2.15	0.46
1:H:186:VAL:HG13	1:H:190:ARG:HH21	1.81	0.46
1:H:282:ASP:OD1	1:H:283:TYR:N	2.45	0.46
1:I:296:GLU:O	1:I:300:MET:HG2	2.15	0.46
1:I:703:ARG:O	1:I:707:LYS:HE2	2.16	0.46
1:K:231:GLY:HA3	1:K:244:PHE:CD1	2.51	0.46
1:K:283:TYR:HB3	1:K:285:ILE:HD12	1.98	0.46
1:K:703:ARG:O	1:K:707:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:116:ARG:HG2	2:A:370:VAL:HG11	1.98	0.46
3:N:162:TYR:HA	3:N:165:VAL:HG12	1.97	0.46
3:N:199:THR:HG22	3:N:203:ASN:HD21	1.81	0.46
1:M:178:GLY:C	1:M:184:LYS:HD3	2.40	0.46
1:M:577:PHE:HE2	1:M:579:LEU:HD13	1.80	0.46
3:O:71:LEU:HD21	3:P:71:LEU:CA	2.42	0.46
3:O:161:LYS:O	3:O:164:GLU:HG2	2.16	0.46
3:P:188:GLY:O	3:P:192:GLU:HG2	2.15	0.46
1:G:38:PHE:N	1:G:77:MET:O	2.47	0.46
1:G:569:ILE:O	1:G:570:LYS:HG2	2.16	0.46
1:H:476:LEU:HD11	1:H:524:ILE:HD12	1.97	0.46
1:H:766:LYS:HG3	1:H:767:ALA:H	1.81	0.46
1:I:114:ILE:HG23	1:I:125:VAL:O	2.16	0.46
1:I:231:GLY:HA3	1:I:244:PHE:CD1	2.51	0.46
1:I:766:LYS:HG3	1:I:767:ALA:H	1.81	0.46
1:J:567:ARG:HH21	1:J:585:ILE:HG22	1.79	0.46
1:J:739:ARG:HD2	1:J:758:PHE:CZ	2.51	0.46
1:J:766:LYS:HG3	1:J:767:ALA:H	1.81	0.46
1:K:178:GLY:C	1:K:184:LYS:HD3	2.40	0.46
3:P:162:TYR:HA	3:P:165:VAL:HG12	1.97	0.45
1:G:158:SER:HB3	1:G:195:PHE:CE1	2.51	0.45
1:H:577:PHE:HE2	1:H:579:LEU:HD13	1.80	0.45
1:J:47:VAL:HA	1:J:103:TYR:OH	2.16	0.45
1:J:114:ILE:HG23	1:J:125:VAL:O	2.16	0.45
1:K:47:VAL:HA	1:K:103:TYR:OH	2.16	0.45
1:M:403:ARG:H	1:M:604:THR:HG21	1.79	0.45
2:C:71:ILE:HG12	2:C:76:ILE:HG12	1.98	0.45
2:C:306:TYR:CE1	4:C:401:ADP:H2	2.34	0.45
2:C:333:PRO:HB2	1:G:412:THR:O	2.16	0.45
3:O:50:LEU:HD11	3:P:53:THR:HG21	1.98	0.45
3:O:63:ALA:HA	3:O:66:ASP:OD2	2.16	0.45
3:P:167:ARG:O	3:P:171:ILE:HG12	2.17	0.45
3:P:199:THR:HG22	3:P:203:ASN:HD21	1.81	0.45
1:G:47:VAL:HA	1:G:103:TYR:OH	2.16	0.45
1:G:739:ARG:HD2	1:G:758:PHE:CZ	2.52	0.45
1:G:766:LYS:HG3	1:G:767:ALA:H	1.81	0.45
1:J:178:GLY:C	1:J:184:LYS:HD3	2.40	0.45
1:J:231:GLY:HA3	1:J:244:PHE:CD1	2.51	0.45
1:J:569:ILE:O	1:J:570:LYS:HG2	2.16	0.45
1:K:114:ILE:HG23	1:K:125:VAL:O	2.16	0.45
3:L:184:GLU:O	3:L:187:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:105:ARG:HA	3:N:108:THR:OG1	2.17	0.45
3:N:153:HIS:O	3:N:156:GLU:HG3	2.15	0.45
1:M:38:PHE:CE2	1:M:79:GLN:HA	2.52	0.45
1:M:739:ARG:HD2	1:M:758:PHE:CZ	2.52	0.45
3:O:175:ASP:O	3:O:178:ARG:HG3	2.16	0.45
1:G:577:PHE:HE2	1:G:579:LEU:HD13	1.80	0.45
1:H:38:PHE:N	1:H:77:MET:O	2.47	0.45
1:H:483:GLU:OE2	1:H:581:HIS:HB3	2.16	0.45
1:I:38:PHE:N	1:I:77:MET:O	2.47	0.45
1:I:186:VAL:HG13	1:I:190:ARG:HH21	1.81	0.45
1:I:569:ILE:O	1:I:570:LYS:HG2	2.16	0.45
1:J:671:ARG:HB3	1:J:696:ASN:HD21	1.81	0.45
1:K:186:VAL:HG13	1:K:190:ARG:HH21	1.81	0.45
1:K:671:ARG:HB3	1:K:696:ASN:HD21	1.82	0.45
1:M:766:LYS:HG3	1:M:767:ALA:H	1.81	0.45
2:B:9:VAL:O	2:B:340:TRP:NE1	2.45	0.45
2:F:170:ALA:O	2:F:172:PRO:HD3	2.15	0.45
1:G:283:TYR:HB3	1:G:285:ILE:HD12	1.98	0.45
1:H:38:PHE:CE2	1:H:79:GLN:HA	2.52	0.45
1:H:611:LYS:HE2	1:H:611:LYS:HB3	1.61	0.45
1:I:47:VAL:HA	1:I:103:TYR:OH	2.16	0.45
1:I:474:GLU:OE1	1:I:474:GLU:N	2.32	0.45
1:M:158:SER:HB3	1:M:195:PHE:CE1	2.51	0.45
2:F:98:PRO:O	2:F:129:VAL:HA	2.16	0.45
3:O:136:LYS:HA	3:O:139:GLU:HG2	1.97	0.45
1:G:483:GLU:OE2	1:G:581:HIS:HB3	2.16	0.45
1:H:671:ARG:HB3	1:H:696:ASN:HD21	1.81	0.45
1:I:671:ARG:HB3	1:I:696:ASN:HD21	1.82	0.45
1:K:38:PHE:CE2	1:K:79:GLN:HA	2.52	0.45
3:L:165:VAL:O	3:L:169:LEU:HB2	2.16	0.45
3:L:175:ASP:O	3:L:178:ARG:HG3	2.16	0.45
1:M:569:ILE:O	1:M:570:LYS:HG2	2.16	0.45
1:H:114:ILE:HG23	1:H:125:VAL:O	2.17	0.45
1:H:474:GLU:H	1:H:474:GLU:CD	2.18	0.45
1:K:484:LYS:HG3	1:K:655:LEU:HD21	1.98	0.45
1:K:766:LYS:HG3	1:K:767:ALA:H	1.81	0.45
3:L:63:ALA:HA	3:L:66:ASP:OD2	2.16	0.45
2:C:50:LYS:HE2	2:C:52:SER:O	2.17	0.45
2:C:305:MET:HA	2:C:335:ARG:NH1	2.32	0.45
3:O:184:GLU:O	3:O:187:GLU:HG3	2.16	0.45
1:G:38:PHE:CE2	1:G:79:GLN:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:739:ARG:HD2	1:H:758:PHE:CZ	2.51	0.45
1:J:483:GLU:OE2	1:J:581:HIS:HB3	2.16	0.45
1:K:293:LYS:HE3	1:K:330:MET:HE3	1.99	0.45
1:K:483:GLU:OE2	1:K:581:HIS:HB3	2.16	0.45
2:A:307:PRO:HB2	3:L:48:LYS:HE2	1.98	0.45
1:M:114:ILE:HG23	1:M:125:VAL:O	2.16	0.45
1:M:369:ARG:HE	3:O:133:ARG:NH1	2.14	0.45
1:M:671:ARG:HB3	1:M:696:ASN:HD21	1.81	0.45
2:C:294:TYR:HD2	2:C:325:MET:HE2	1.82	0.45
1:G:703:ARG:O	1:G:707:LYS:HE2	2.16	0.45
1:H:283:TYR:HB3	1:H:285:ILE:HD12	1.98	0.45
1:H:703:ARG:O	1:H:707:LYS:HE2	2.16	0.45
1:I:261:ALA:HB3	1:I:447:LEU:HD21	1.97	0.45
1:J:186:VAL:HG13	1:J:190:ARG:HH21	1.81	0.45
1:K:158:SER:HB3	1:K:195:PHE:CE1	2.51	0.45
2:B:206:ARG:HE	2:B:206:ARG:HB2	1.54	0.45
2:E:34:ILE:HD11	2:E:59:GLN:HG2	1.98	0.45
2:F:194:THR:HA	2:F:198:TYR:O	2.17	0.45
3:O:173:GLU:O	3:O:176:LEU:HG	2.17	0.45
1:H:92:MET:HE1	1:H:712:ARG:N	2.28	0.45
1:J:282:ASP:OD1	1:J:283:TYR:N	2.45	0.45
1:J:293:LYS:HE3	1:J:330:MET:HE3	1.99	0.45
1:K:367:LYS:HE2	1:K:367:LYS:HB3	1.63	0.45
3:L:102:ALA:HA	3:L:105:ARG:NE	2.31	0.45
3:N:139:GLU:O	3:N:142:GLU:HG3	2.17	0.45
1:M:283:TYR:HB3	1:M:285:ILE:HD12	1.98	0.45
1:M:641:GLY:N	2:F:23:GLY:O	2.42	0.45
2:D:117:GLU:OE2	2:D:371:HIS:NE2	2.46	0.45
2:D:151:ILE:HG21	2:D:282:ILE:HD11	1.98	0.45
2:F:47:MET:SD	2:F:49:GLN:NE2	2.90	0.45
3:P:135:GLN:O	3:P:139:GLU:HG2	2.16	0.45
1:H:231:GLY:HA3	1:H:244:PHE:CD1	2.51	0.45
1:H:752:ASP:OD1	1:H:755:GLN:NE2	2.50	0.45
1:J:38:PHE:CE2	1:J:79:GLN:HA	2.52	0.45
1:J:158:SER:HB3	1:J:195:PHE:CE1	2.51	0.45
1:K:739:ARG:HD2	1:K:758:PHE:CZ	2.52	0.45
3:N:167:ARG:O	3:N:171:ILE:HG12	2.17	0.45
1:M:231:GLY:HA3	1:M:244:PHE:CD1	2.51	0.44
1:M:572:LYS:HB3	1:M:572:LYS:HE2	1.69	0.44
2:C:54:VAL:HG13	2:C:85:ILE:HD13	1.98	0.44
2:E:216:LEU:HD22	2:E:238:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:139:GLU:O	3:P:142:GLU:HG3	2.17	0.44
1:H:251:HIS:NE2	1:H:262:ASP:OD2	2.51	0.44
1:I:38:PHE:CE2	1:I:79:GLN:HA	2.52	0.44
1:I:484:LYS:HG3	1:I:655:LEU:HD21	1.98	0.44
1:I:544:THR:HG22	1:I:545:ASP:H	1.82	0.44
1:I:739:ARG:HD2	1:I:758:PHE:CZ	2.51	0.44
1:J:484:LYS:HG3	1:J:655:LEU:HD21	1.98	0.44
3:N:135:GLN:O	3:N:139:GLU:HG2	2.16	0.44
1:M:43:LYS:HB3	1:M:43:LYS:HE3	1.85	0.44
1:M:752:ASP:OD1	1:M:755:GLN:NE2	2.50	0.44
2:C:53:TYR:HB3	2:C:57:GLU:OE1	2.16	0.44
2:F:190:MET:HG2	2:F:209:VAL:HG21	1.98	0.44
3:O:102:ALA:HA	3:O:105:ARG:NE	2.31	0.44
1:G:114:ILE:HG23	1:G:125:VAL:O	2.17	0.44
1:G:251:HIS:NE2	1:G:262:ASP:OD2	2.51	0.44
1:H:158:SER:HB3	1:H:195:PHE:CE1	2.51	0.44
1:H:293:LYS:HE3	1:H:330:MET:HE3	1.99	0.44
1:I:293:LYS:HE3	1:I:330:MET:HE3	1.99	0.44
1:K:637:LYS:HD3	1:K:637:LYS:HA	1.75	0.44
1:M:282:ASP:OD1	1:M:283:TYR:N	2.45	0.44
2:B:147:ARG:NH2	1:H:371:GLU:OE1	2.49	0.44
2:B:284:LYS:HE3	2:B:284:LYS:HB2	1.84	0.44
2:D:253:GLU:HA	2:D:256:ARG:HB2	1.99	0.44
2:F:143:TYR:CE2	2:F:346:LEU:HD13	2.49	0.44
3:O:71:LEU:HD23	3:O:71:LEU:HA	1.67	0.44
1:G:544:THR:HG22	1:G:545:ASP:H	1.82	0.44
1:J:249:ARG:N	1:J:262:ASP:O	2.41	0.44
1:J:503:LYS:HD2	1:J:503:LYS:C	2.43	0.44
2:B:138:ALA:HB1	2:B:152:VAL:HG11	2.00	0.44
2:E:42:GLY:HA2	2:A:169:TYR:HA	2.00	0.44
1:H:544:THR:HG22	1:H:545:ASP:H	1.82	0.44
1:J:679:LYS:HD3	1:J:679:LYS:HA	1.74	0.44
2:A:216:LEU:HD22	2:A:238:LYS:HD3	2.00	0.44
3:N:89:ASN:O	3:N:93:GLN:NE2	2.51	0.44
1:M:45:GLU:HG2	1:M:46:PHE:CD2	2.44	0.44
2:B:9:VAL:HG21	2:B:344:SER:HA	2.00	0.44
2:E:140:LEU:O	2:E:342:GLY:HA3	2.18	0.44
2:F:149:THR:HG22	2:F:167:GLU:N	2.19	0.44
3:P:178:ARG:HA	3:P:181:GLU:CD	2.43	0.44
1:G:102:LEU:HD21	1:G:686:ASN:HD22	1.83	0.44
1:G:231:GLY:HA3	1:G:244:PHE:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:671:ARG:HB3	1:G:696:ASN:HD21	1.81	0.44
1:H:149:GLU:OE1	1:H:149:GLU:N	2.51	0.44
1:I:158:SER:HB3	1:I:195:PHE:CE1	2.51	0.44
1:I:752:ASP:OD1	1:I:755:GLN:NE2	2.50	0.44
3:L:197:LEU:HD12	3:N:200:VAL:HG11	2.00	0.44
2:E:323:SER:O	2:E:323:SER:OG	2.36	0.44
2:F:191:LYS:O	2:F:194:THR:HG22	2.17	0.44
1:G:219:GLN:OE1	1:G:219:GLN:N	2.42	0.44
1:H:341:PHE:CE2	1:H:346:LYS:HG2	2.53	0.44
1:J:194:TYR:CE2	1:J:198:ILE:HD13	2.53	0.44
1:K:46:PHE:O	1:K:103:TYR:OH	2.27	0.44
1:K:544:THR:HG22	1:K:545:ASP:H	1.82	0.44
3:N:121:ASP:O	3:N:124:GLU:HG3	2.18	0.44
1:M:149:GLU:OE1	1:M:149:GLU:N	2.51	0.44
1:M:251:HIS:NE2	1:M:262:ASP:OD2	2.51	0.44
2:B:333:PRO:HB2	1:H:412:THR:O	2.18	0.44
2:C:305:MET:HE2	2:C:336:LYS:H	1.83	0.44
1:H:336:PHE:CG	1:H:341:PHE:HZ	2.36	0.44
1:I:149:GLU:N	1:I:149:GLU:OE1	2.51	0.44
1:J:540:PHE:CG	1:J:541:PRO:HD2	2.53	0.44
1:J:637:LYS:HD3	1:J:637:LYS:HA	1.75	0.44
1:K:149:GLU:OE1	1:K:149:GLU:N	2.51	0.44
1:K:194:TYR:CE2	1:K:198:ILE:HD13	2.53	0.44
1:K:341:PHE:CE2	1:K:346:LYS:HG2	2.53	0.44
1:K:503:LYS:C	1:K:503:LYS:HD2	2.43	0.44
1:M:194:TYR:CE2	1:M:198:ILE:HD13	2.53	0.44
1:M:224:ASN:O	1:M:228:GLU:HG2	2.18	0.44
1:M:341:PHE:CE2	1:M:346:LYS:HG2	2.53	0.44
1:G:149:GLU:OE1	1:G:149:GLU:N	2.51	0.44
1:H:224:ASN:O	1:H:228:GLU:HG2	2.18	0.44
1:H:503:LYS:HD2	1:H:503:LYS:C	2.43	0.44
1:H:540:PHE:CG	1:H:541:PRO:HD2	2.53	0.44
1:J:43:LYS:HB3	1:J:43:LYS:HE3	1.85	0.44
1:J:544:THR:HG22	1:J:545:ASP:H	1.82	0.44
1:K:224:ASN:O	1:K:228:GLU:HG2	2.18	0.44
1:K:336:PHE:CG	1:K:341:PHE:HZ	2.36	0.44
1:K:752:ASP:OD1	1:K:755:GLN:NE2	2.51	0.44
1:M:503:LYS:HD2	1:M:503:LYS:C	2.43	0.44
2:D:95:ARG:O	1:I:635:LYS:HA	2.17	0.44
3:P:89:ASN:O	3:P:93:GLN:NE2	2.51	0.44
3:P:105:ARG:HA	3:P:108:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:128:LYS:O	3:P:131:GLU:HG3	2.18	0.44
3:P:190:CYS:HA	3:P:193:LEU:HD12	2.00	0.44
1:G:224:ASN:O	1:G:228:GLU:HG2	2.18	0.44
1:G:544:THR:HG22	1:G:545:ASP:N	2.33	0.44
1:G:637:LYS:HD3	1:G:637:LYS:HA	1.75	0.44
1:I:102:LEU:HD21	1:I:686:ASN:HD22	1.83	0.44
1:I:336:PHE:CG	1:I:341:PHE:HZ	2.36	0.44
1:J:336:PHE:CG	1:J:341:PHE:HZ	2.36	0.44
1:J:752:ASP:OD1	1:J:755:GLN:NE2	2.50	0.44
1:K:102:LEU:HD21	1:K:686:ASN:HD22	1.83	0.44
2:A:34:ILE:HD11	2:A:59:GLN:HG2	1.98	0.44
1:M:102:LEU:HD21	1:M:686:ASN:HD22	1.83	0.43
2:E:288:ASP:OD1	2:E:288:ASP:N	2.43	0.43
3:O:193:LEU:HA	3:O:193:LEU:HD23	1.73	0.43
3:P:175:ASP:O	3:P:178:ARG:HD3	2.18	0.43
3:P:189:LYS:HB3	3:P:189:LYS:HE2	1.87	0.43
1:G:92:MET:HE1	1:G:712:ARG:N	2.28	0.43
1:G:171:ASN:HB2	1:G:665:THR:HG22	2.00	0.43
1:H:176:ILE:HA	1:H:670:VAL:HB	2.01	0.43
1:I:224:ASN:O	1:I:228:GLU:HG2	2.18	0.43
1:I:503:LYS:HD2	1:I:503:LYS:C	2.43	0.43
1:J:149:GLU:OE1	1:J:149:GLU:N	2.51	0.43
1:J:224:ASN:O	1:J:228:GLU:HG2	2.18	0.43
1:J:341:PHE:CE2	1:J:346:LYS:HG2	2.53	0.43
1:K:251:HIS:NE2	1:K:262:ASP:OD2	2.51	0.43
3:L:173:GLU:O	3:L:176:LEU:HG	2.17	0.43
3:N:178:ARG:HA	3:N:181:GLU:CD	2.43	0.43
1:M:176:ILE:HA	1:M:670:VAL:HB	2.00	0.43
1:M:293:LYS:HE3	1:M:330:MET:HE3	1.99	0.43
1:M:336:PHE:CG	1:M:341:PHE:HZ	2.36	0.43
1:M:544:THR:HG22	1:M:545:ASP:H	1.82	0.43
2:E:221:LEU:HD22	3:N:97:GLU:CD	2.43	0.43
1:G:503:LYS:HD2	1:G:503:LYS:C	2.43	0.43
1:H:194:TYR:CE2	1:H:198:ILE:HD13	2.53	0.43
1:I:176:ILE:HA	1:I:670:VAL:HB	2.01	0.43
1:I:341:PHE:CE2	1:I:346:LYS:HG2	2.53	0.43
1:I:367:LYS:HE2	1:I:367:LYS:HB3	1.63	0.43
1:J:102:LEU:HD21	1:J:686:ASN:HD22	1.83	0.43
1:J:251:HIS:NE2	1:J:262:ASP:OD2	2.51	0.43
1:K:146:LYS:HA	1:K:146:LYS:HD2	1.76	0.43
1:K:412:THR:O	2:A:333:PRO:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:46:LEU:HD12	3:N:46:LEU:HD11	2.00	0.43
1:M:506:ILE:CD1	1:M:757:LYS:HG2	2.48	0.43
1:M:544:THR:HG22	1:M:545:ASP:N	2.33	0.43
2:C:140:LEU:O	2:C:342:GLY:HA3	2.18	0.43
2:D:14:SER:O	2:D:157:ASP:HB3	2.19	0.43
1:G:341:PHE:CE2	1:G:346:LYS:HG2	2.53	0.43
1:H:544:THR:HG22	1:H:545:ASP:N	2.33	0.43
1:I:171:ASN:HB2	1:I:665:THR:HG22	2.00	0.43
1:M:612:SER:OG	1:M:613:SER:N	2.52	0.43
2:D:26:ALA:HB1	1:I:406:VAL:HG12	2.00	0.43
2:D:138:ALA:HB1	2:D:152:VAL:CG1	2.49	0.43
2:D:282:ILE:HD12	2:D:293:LEU:HB3	1.99	0.43
1:G:752:ASP:OD1	1:G:755:GLN:NE2	2.51	0.43
1:I:118:SER:OG	1:I:121:PHE:HB2	2.18	0.43
1:I:251:HIS:NE2	1:I:262:ASP:OD2	2.51	0.43
1:I:506:ILE:CD1	1:I:757:LYS:HG2	2.48	0.43
1:J:176:ILE:HA	1:J:670:VAL:HB	2.00	0.43
1:K:45:GLU:HG2	1:K:46:PHE:CD2	2.44	0.43
1:K:85:ASP:OD1	1:K:86:LYS:N	2.48	0.43
1:M:118:SER:OG	1:M:121:PHE:HB2	2.18	0.43
1:M:180:SER:HB3	1:M:238:ASN:ND2	2.34	0.43
2:B:97:ALA:HB1	2:B:99:GLU:OE2	2.19	0.43
2:B:153:LEU:HD23	2:B:299:LEU:HD22	2.01	0.43
2:F:9:VAL:HG21	2:F:344:SER:HA	2.00	0.43
3:O:92:ILE:HG13	1:G:368:GLN:HE21	1.84	0.43
3:O:209:ALA:O	3:O:210:GLN:HG3	2.19	0.43
1:G:118:SER:OG	1:G:121:PHE:HB2	2.18	0.43
1:G:612:SER:OG	1:G:613:SER:N	2.52	0.43
1:H:171:ASN:HB2	1:H:665:THR:HG22	2.00	0.43
1:H:394:ASP:OD2	1:H:608:LEU:HD21	2.19	0.43
1:I:165:MET:HE3	1:I:455:TYR:HB2	2.01	0.43
1:K:540:PHE:CG	1:K:541:PRO:HD2	2.53	0.43
1:K:544:THR:HG22	1:K:545:ASP:N	2.33	0.43
2:A:140:LEU:O	2:A:342:GLY:HA3	2.18	0.43
3:N:175:ASP:O	3:N:178:ARG:HD3	2.18	0.43
1:M:611:LYS:HB3	1:M:611:LYS:HE2	1.61	0.43
2:D:254:ARG:CZ	3:L:128:LYS:HZ1	2.29	0.43
3:O:96:GLU:O	3:O:99:LEU:HG	2.18	0.43
3:O:197:LEU:HD12	3:P:200:VAL:HG11	2.00	0.43
3:P:121:ASP:O	3:P:124:GLU:HG3	2.18	0.43
3:P:140:LYS:O	3:P:143:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:LYS:HB3	1:G:43:LYS:HE3	1.85	0.43
1:G:194:TYR:CE2	1:G:198:ILE:HD13	2.53	0.43
1:G:336:PHE:CG	1:G:341:PHE:HZ	2.36	0.43
1:G:572:LYS:HE2	1:G:572:LYS:HB3	1.69	0.43
1:H:367:LYS:HE2	1:H:367:LYS:HB3	1.63	0.43
1:I:540:PHE:CG	1:I:541:PRO:HD2	2.53	0.43
1:I:572:LYS:HB3	1:I:572:LYS:HE2	1.69	0.43
1:I:637:LYS:HD3	1:I:637:LYS:HA	1.75	0.43
1:J:118:SER:OG	1:J:121:PHE:HB2	2.18	0.43
1:J:165:MET:HE3	1:J:455:TYR:HB2	2.01	0.43
1:J:544:THR:HG22	1:J:545:ASP:N	2.33	0.43
1:J:611:LYS:HE2	1:J:611:LYS:HB3	1.61	0.43
1:K:118:SER:OG	1:K:121:PHE:HB2	2.18	0.43
1:M:165:MET:HE3	1:M:455:TYR:HB2	2.01	0.43
1:M:171:ASN:HB2	1:M:665:THR:HG22	2.00	0.43
1:M:394:ASP:OD2	1:M:608:LEU:HD21	2.19	0.43
1:M:679:LYS:HD3	1:M:679:LYS:HA	1.74	0.43
2:B:49:GLN:HG2	2:F:169:TYR:CZ	2.53	0.43
2:C:26:ALA:HB1	1:G:406:VAL:HG12	2.00	0.43
2:E:334:GLU:H	2:E:334:GLU:CD	2.25	0.43
3:O:49:LYS:HZ1	3:P:50:LEU:HD13	1.83	0.43
1:G:176:ILE:HA	1:G:670:VAL:HB	2.00	0.43
1:G:269:GLU:OE1	1:G:271:SER:N	2.31	0.43
1:G:540:PHE:CG	1:G:541:PRO:HD2	2.53	0.43
1:H:165:MET:HE3	1:H:455:TYR:HB2	2.01	0.43
1:I:41:ASP:OD2	1:I:43:LYS:N	2.52	0.43
1:I:394:ASP:OD2	1:I:608:LEU:HD21	2.19	0.43
1:J:41:ASP:OD2	1:J:43:LYS:N	2.52	0.43
1:J:85:ASP:OD1	1:J:86:LYS:N	2.48	0.43
1:K:41:ASP:OD2	1:K:43:LYS:N	2.52	0.43
1:K:362:MET:HE1	1:K:381:ALA:HA	2.01	0.43
2:C:95:ARG:O	1:G:635:LYS:HA	2.19	0.43
2:C:300:SER:HA	2:C:335:ARG:HG2	2.00	0.43
2:F:275:HIS:CD2	2:F:316:GLU:HB3	2.53	0.43
3:O:66:ASP:HB2	3:O:70:LYS:NZ	2.34	0.43
1:H:118:SER:OG	1:H:121:PHE:HB2	2.19	0.43
1:H:180:SER:HB3	1:H:238:ASN:ND2	2.34	0.43
1:I:544:THR:HG22	1:I:545:ASP:N	2.33	0.43
1:I:679:LYS:HD3	1:I:679:LYS:HA	1.74	0.43
1:J:171:ASN:HB2	1:J:665:THR:HG22	2.00	0.43
1:J:367:LYS:HB3	1:J:367:LYS:HE2	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:434:ARG:HH22	1:J:623:ASN:ND2	2.17	0.43
1:K:394:ASP:OD2	1:K:608:LEU:HD21	2.19	0.43
1:K:434:ARG:HH22	1:K:623:ASN:ND2	2.17	0.43
2:A:97:ALA:HB1	2:A:99:GLU:OE2	2.18	0.43
2:A:213:LYS:HZ1	4:A:401:ADP:HO2'	1.60	0.43
2:A:353:GLN:NE2	2:A:356:TRP:HE1	2.16	0.43
3:L:120:ALA:O	3:L:123:SER:OG	2.31	0.43
2:C:357:ILE:HG12	2:C:374:CYS:HB2	2.00	0.43
2:E:132:MET:HE2	2:E:132:MET:HB2	1.96	0.43
3:O:205:LYS:O	3:O:208:GLU:HG2	2.19	0.43
1:G:165:MET:HE3	1:G:455:TYR:HB2	2.01	0.43
1:G:293:LYS:HE3	1:G:330:MET:HE3	1.99	0.43
1:G:394:ASP:OD2	1:G:608:LEU:HD21	2.19	0.43
1:I:269:GLU:OE1	1:I:271:SER:N	2.31	0.43
1:I:282:ASP:OD1	1:I:283:TYR:N	2.45	0.43
1:J:180:SER:HB3	1:J:238:ASN:ND2	2.34	0.43
1:J:352:LEU:HD12	1:J:352:LEU:HA	1.88	0.43
1:K:165:MET:HE3	1:K:455:TYR:HB2	2.01	0.43
1:K:176:ILE:HA	1:K:670:VAL:HB	2.01	0.43
3:L:172:ILE:HB	3:N:172:ILE:HD12	2.01	0.43
3:N:48:LYS:HE2	3:N:48:LYS:HB2	1.87	0.43
3:N:128:LYS:O	3:N:131:GLU:HG3	2.18	0.43
3:N:190:CYS:HA	3:N:193:LEU:HD12	2.00	0.43
1:M:540:PHE:CG	1:M:541:PRO:HD2	2.53	0.43
2:E:97:ALA:HB1	2:E:99:GLU:OE2	2.18	0.43
2:E:147:ARG:NH2	2:E:330:ILE:HG12	2.19	0.43
1:H:102:LEU:HD21	1:H:686:ASN:HD22	1.83	0.43
1:H:434:ARG:HH22	1:H:623:ASN:ND2	2.17	0.43
1:I:194:TYR:CE2	1:I:198:ILE:HD13	2.53	0.43
1:I:715:TYR:CZ	1:I:763:VAL:HB	2.54	0.43
1:J:394:ASP:OD2	1:J:608:LEU:HD21	2.19	0.43
1:K:180:SER:HB3	1:K:238:ASN:ND2	2.34	0.43
1:K:715:TYR:CZ	1:K:763:VAL:HB	2.54	0.43
2:A:12:ASN:HD21	2:A:105:LEU:HD12	1.84	0.43
2:A:323:SER:O	2:A:323:SER:OG	2.36	0.43
1:M:102:LEU:O	1:M:105:LEU:HG	2.19	0.42
1:M:369:ARG:HE	3:O:133:ARG:CZ	2.31	0.42
1:M:434:ARG:HH22	1:M:623:ASN:ND2	2.17	0.42
2:C:98:PRO:O	2:C:129:VAL:HA	2.18	0.42
2:D:250:ILE:HG23	2:D:253:GLU:HG2	2.01	0.42
1:G:180:SER:HB3	1:G:238:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:502:LYS:HA	1:G:507:GLU:OE1	2.19	0.42
1:H:102:LEU:O	1:H:105:LEU:HG	2.19	0.42
1:H:679:LYS:HD3	1:H:679:LYS:HA	1.74	0.42
1:I:45:GLU:HG2	1:I:46:PHE:CD2	2.44	0.42
1:J:715:TYR:CZ	1:J:763:VAL:HB	2.54	0.42
2:A:147:ARG:NH2	2:A:330:ILE:HG12	2.19	0.42
3:L:152:LYS:O	3:L:156:GLU:HG2	2.19	0.42
3:L:209:ALA:O	3:L:210:GLN:HG3	2.19	0.42
3:N:169:LEU:HA	3:N:172:ILE:HG12	2.01	0.42
1:M:77:MET:HB2	1:M:97:HIS:CE1	2.54	0.42
2:C:291:LYS:CG	2:C:325:MET:HE1	2.47	0.42
1:G:77:MET:HB2	1:G:97:HIS:CE1	2.54	0.42
1:G:102:LEU:O	1:G:105:LEU:HG	2.19	0.42
1:H:77:MET:HB2	1:H:97:HIS:CE1	2.54	0.42
1:J:38:PHE:N	1:J:77:MET:O	2.47	0.42
1:K:171:ASN:HB2	1:K:665:THR:HG22	2.00	0.42
3:L:66:ASP:HB2	3:L:70:LYS:NZ	2.34	0.42
2:C:144:ALA:HB2	2:C:342:GLY:N	2.34	0.42
2:D:47:MET:HB3	2:D:49:GLN:OE1	2.19	0.42
2:D:295:ALA:O	2:D:296:ASN:ND2	2.53	0.42
2:E:71:ILE:HG12	2:E:76:ILE:HG12	2.01	0.42
2:F:138:ALA:HB1	2:F:152:VAL:HG11	2.01	0.42
2:F:334:GLU:H	2:F:334:GLU:CD	2.25	0.42
3:O:46:LEU:HD12	3:P:46:LEU:HD11	2.00	0.42
3:O:152:LYS:O	3:O:156:GLU:HG2	2.19	0.42
3:P:172:ILE:HG13	3:P:173:GLU:N	2.34	0.42
1:G:282:ASP:OD1	1:G:283:TYR:N	2.45	0.42
1:I:92:MET:HE1	1:I:712:ARG:N	2.28	0.42
1:J:362:MET:HE1	1:J:381:ALA:HA	2.01	0.42
1:J:368:GLN:HE22	3:L:100:ASP:CG	2.20	0.42
1:K:612:SER:OG	1:K:613:SER:N	2.52	0.42
2:B:170:ALA:O	2:B:172:PRO:HD3	2.20	0.42
2:C:353:GLN:NE2	2:C:356:TRP:HE1	2.17	0.42
2:C:369:ILE:HA	2:C:372:ARG:HD3	2.02	0.42
2:E:353:GLN:NE2	2:E:356:TRP:HE1	2.16	0.42
3:O:71:LEU:CD2	3:P:70:LYS:HD2	2.46	0.42
3:P:169:LEU:HA	3:P:172:ILE:HG12	2.02	0.42
1:I:434:ARG:HH22	1:I:623:ASN:ND2	2.17	0.42
1:I:502:LYS:HA	1:I:507:GLU:OE1	2.19	0.42
1:J:502:LYS:HA	1:J:507:GLU:OE1	2.19	0.42
1:J:506:ILE:CD1	1:J:757:LYS:HG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:71:LEU:CD2	3:N:70:LYS:HD2	2.46	0.42
3:L:96:GLU:O	3:L:99:LEU:HG	2.18	0.42
3:O:86:ALA:HA	3:O:89:ASN:ND2	2.35	0.42
1:G:434:ARG:HH22	1:G:623:ASN:ND2	2.17	0.42
1:G:506:ILE:CD1	1:G:757:LYS:HG2	2.48	0.42
1:G:679:LYS:HD3	1:G:679:LYS:HA	1.74	0.42
1:H:41:ASP:OD2	1:H:43:LYS:N	2.52	0.42
1:H:301:LEU:HD22	1:H:387:LEU:HD11	2.02	0.42
1:H:715:TYR:CZ	1:H:763:VAL:HB	2.54	0.42
2:A:71:ILE:HG12	2:A:76:ILE:HG12	2.01	0.42
3:N:102:ALA:HA	3:N:105:ARG:NE	2.34	0.42
3:N:140:LYS:O	3:N:143:ILE:HG22	2.19	0.42
3:N:172:ILE:HG13	3:N:173:GLU:N	2.34	0.42
1:M:301:LEU:HD22	1:M:387:LEU:HD11	2.02	0.42
1:M:474:GLU:OE1	1:M:474:GLU:N	2.32	0.42
2:C:360:GLN:H	2:C:360:GLN:CD	2.28	0.42
2:D:170:ALA:O	2:D:172:PRO:HD3	2.20	0.42
2:F:351:THR:O	2:F:354:GLN:NE2	2.53	0.42
1:I:612:SER:OG	1:I:613:SER:N	2.52	0.42
1:J:266:TYR:HB3	1:J:267:LEU:HG	2.02	0.42
1:J:612:SER:OG	1:J:613:SER:N	2.52	0.42
3:L:182:ARG:O	3:L:185:LEU:HG	2.19	0.42
3:L:193:LEU:HD23	3:L:193:LEU:HA	1.73	0.42
3:N:166:ALA:O	3:N:170:VAL:HG23	2.20	0.42
1:M:266:TYR:HB3	1:M:267:LEU:HG	2.02	0.42
2:D:202:THR:HG23	2:F:270:GLU:OE1	2.18	0.42
1:G:352:LEU:HD12	1:G:352:LEU:HA	1.88	0.42
1:H:612:SER:OG	1:H:613:SER:N	2.52	0.42
1:I:85:ASP:OD1	1:I:86:LYS:N	2.48	0.42
1:I:362:MET:HE1	1:I:381:ALA:HA	2.01	0.42
1:I:758:PHE:HA	1:I:763:VAL:HG23	2.01	0.42
1:K:102:LEU:O	1:K:105:LEU:HG	2.19	0.42
3:L:205:LYS:O	3:L:208:GLU:HG2	2.19	0.42
1:M:41:ASP:OD2	1:M:43:LYS:N	2.52	0.42
1:M:367:LYS:HB3	1:M:367:LYS:HE2	1.63	0.42
1:M:502:LYS:HA	1:M:507:GLU:OE1	2.19	0.42
1:M:669:PHE:HB3	1:M:671:ARG:CZ	2.50	0.42
2:C:138:ALA:HB1	2:C:152:VAL:CG1	2.49	0.42
2:C:192:ILE:HD13	2:C:192:ILE:HG21	1.79	0.42
2:E:12:ASN:HD21	2:E:105:LEU:HD12	1.84	0.42
3:O:64:LEU:HG	3:P:64:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:102:ALA:HA	3:P:105:ARG:NE	2.34	0.42
1:G:41:ASP:OD2	1:G:43:LYS:N	2.52	0.42
1:G:301:LEU:HD22	1:G:387:LEU:HD11	2.02	0.42
1:H:266:TYR:HB3	1:H:267:LEU:HG	2.02	0.42
1:I:77:MET:HB2	1:I:97:HIS:CE1	2.54	0.42
1:I:180:SER:HB3	1:I:238:ASN:ND2	2.34	0.42
1:K:474:GLU:OE1	1:K:474:GLU:N	2.32	0.42
1:K:502:LYS:HA	1:K:507:GLU:OE1	2.19	0.42
3:L:64:LEU:HG	3:N:64:LEU:HD12	2.01	0.42
1:M:406:VAL:HG12	2:F:26:ALA:HB1	2.02	0.42
2:B:278:THR:O	2:B:282:ILE:HG12	2.19	0.42
2:E:44:MET:HE3	2:A:142:LEU:HD23	2.01	0.42
2:E:190:MET:HG3	2:E:209:VAL:HG11	2.02	0.42
2:E:221:LEU:CD2	3:N:97:GLU:OE1	2.68	0.42
3:O:182:ARG:O	3:O:185:LEU:HG	2.19	0.42
1:H:502:LYS:HA	1:H:507:GLU:OE1	2.19	0.42
1:H:758:PHE:HA	1:H:763:VAL:HG23	2.02	0.42
1:I:102:LEU:O	1:I:105:LEU:HG	2.19	0.42
1:I:266:TYR:HB3	1:I:267:LEU:HG	2.02	0.42
1:K:266:TYR:HB3	1:K:267:LEU:HG	2.02	0.42
1:K:301:LEU:HD22	1:K:387:LEU:HD11	2.02	0.42
1:K:669:PHE:HB3	1:K:671:ARG:CZ	2.50	0.42
1:M:36:ASP:CG	1:M:50:LYS:HG3	2.45	0.42
1:M:715:TYR:CZ	1:M:763:VAL:HB	2.54	0.42
1:M:758:PHE:HA	1:M:763:VAL:HG23	2.02	0.42
2:B:149:THR:HG22	2:B:167:GLU:N	2.21	0.42
2:D:76:ILE:HD13	2:D:82:MET:HG2	2.02	0.42
3:P:126:GLY:O	3:P:130:ILE:HG12	2.20	0.42
1:G:266:TYR:HB3	1:G:267:LEU:HG	2.02	0.42
1:G:362:MET:HE1	1:G:381:ALA:HA	2.01	0.42
1:J:740:LYS:HG3	1:J:741:GLY:N	2.35	0.42
2:A:132:MET:HE2	2:A:132:MET:HB2	1.96	0.42
2:B:138:ALA:HB1	2:B:152:VAL:CG1	2.49	0.41
2:E:142:LEU:HD12	2:E:142:LEU:HA	1.88	0.41
1:G:36:ASP:CG	1:G:50:LYS:HG3	2.46	0.41
1:H:36:ASP:CG	1:H:50:LYS:HG3	2.45	0.41
1:J:63:THR:HG1	1:J:64:GLU:H	1.67	0.41
3:N:175:ASP:HA	3:N:178:ARG:NE	2.35	0.41
2:B:305:MET:HE1	2:B:336:LYS:H	1.84	0.41
2:C:305:MET:SD	2:C:335:ARG:NH1	2.93	0.41
1:H:669:PHE:HB3	1:H:671:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:740:LYS:HG3	1:I:741:GLY:N	2.35	0.41
1:K:740:LYS:HG3	1:K:741:GLY:N	2.35	0.41
3:L:86:ALA:HA	3:L:89:ASN:ND2	2.34	0.41
1:M:362:MET:HE1	1:M:381:ALA:HA	2.01	0.41
1:M:447:LEU:O	1:M:447:LEU:HD23	2.21	0.41
3:O:172:ILE:HB	3:P:172:ILE:HD12	2.01	0.41
3:P:147:GLN:HA	3:P:150:GLU:OE1	2.21	0.41
1:J:36:ASP:CG	1:J:50:LYS:HG3	2.46	0.41
1:J:758:PHE:HA	1:J:763:VAL:HG23	2.02	0.41
1:K:36:ASP:CG	1:K:50:LYS:HG3	2.46	0.41
3:N:136:LYS:HE3	3:N:136:LYS:HB3	1.68	0.41
1:M:740:LYS:HG3	1:M:741:GLY:N	2.35	0.41
2:C:373:LYS:HD2	2:C:373:LYS:C	2.46	0.41
2:D:116:ARG:HG2	2:D:370:VAL:HG11	2.02	0.41
2:D:128:ASN:OD1	2:D:359:LYS:NZ	2.42	0.41
1:G:293:LYS:HG2	1:G:330:MET:HE3	2.03	0.41
1:I:41:ASP:OD2	1:I:44:GLN:N	2.35	0.41
1:J:102:LEU:O	1:J:105:LEU:HG	2.19	0.41
1:J:301:LEU:HD22	1:J:387:LEU:HD11	2.02	0.41
1:J:526:LYS:HA	1:J:526:LYS:HD3	1.90	0.41
2:A:190:MET:HG3	2:A:209:VAL:HG11	2.02	0.41
3:N:199:THR:O	3:N:203:ASN:ND2	2.53	0.41
2:B:234:SER:O	2:B:234:SER:OG	2.38	0.41
1:G:447:LEU:HD23	1:G:447:LEU:O	2.21	0.41
1:G:474:GLU:OE1	1:G:474:GLU:N	2.32	0.41
1:G:669:PHE:HB3	1:G:671:ARG:CZ	2.50	0.41
1:H:362:MET:HE1	1:H:381:ALA:HA	2.01	0.41
1:I:669:PHE:HB3	1:I:671:ARG:CZ	2.50	0.41
1:J:146:LYS:HA	1:J:146:LYS:HD2	1.76	0.41
1:J:671:ARG:HB3	1:J:696:ASN:ND2	2.36	0.41
1:K:87:ILE:HG21	1:K:93:LEU:HG	2.03	0.41
3:N:126:GLY:O	3:N:130:ILE:HG12	2.20	0.41
3:N:170:VAL:O	3:N:173:GLU:HG3	2.21	0.41
2:B:16:LEU:HD23	2:B:16:LEU:HA	1.88	0.41
3:P:152:LYS:HG3	3:P:153:HIS:N	2.36	0.41
1:I:217:GLU:O	1:I:221:ILE:HG12	2.21	0.41
1:J:301:LEU:HA	1:J:301:LEU:HD23	1.75	0.41
1:K:77:MET:HB2	1:K:97:HIS:CE1	2.54	0.41
1:K:506:ILE:CD1	1:K:757:LYS:HG2	2.48	0.41
2:A:196:ARG:HD2	2:A:253:GLU:OE2	2.21	0.41
2:A:278:THR:O	2:A:282:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:269:GLU:OE1	1:M:271:SER:N	2.31	0.41
1:M:293:LYS:HG2	1:M:330:MET:HE3	2.03	0.41
1:M:599:ASP:O	1:M:645:GLN:HB2	2.21	0.41
1:M:769:LEU:H	1:M:769:LEU:HD12	1.86	0.41
2:C:169:TYR:CZ	2:F:49:GLN:HG2	2.55	0.41
2:D:28:ARG:HH12	1:I:637:LYS:CG	2.33	0.41
2:D:361:GLU:O	2:D:364:GLU:HG3	2.21	0.41
2:F:138:ALA:HB1	2:F:152:VAL:CG1	2.50	0.41
3:P:166:ALA:O	3:P:170:VAL:HG23	2.20	0.41
3:P:199:THR:O	3:P:203:ASN:ND2	2.54	0.41
1:G:517:LEU:HA	1:G:517:LEU:HD12	1.84	0.41
1:H:146:LYS:HA	1:H:146:LYS:HD2	1.76	0.41
1:H:447:LEU:O	1:H:447:LEU:HD23	2.20	0.41
1:H:599:ASP:O	1:H:645:GLN:HB2	2.21	0.41
1:H:671:ARG:HB3	1:H:696:ASN:ND2	2.36	0.41
1:I:301:LEU:HD22	1:I:387:LEU:HD11	2.02	0.41
1:J:217:GLU:O	1:J:221:ILE:HG12	2.21	0.41
1:J:669:PHE:HB3	1:J:671:ARG:CZ	2.50	0.41
1:K:447:LEU:O	1:K:447:LEU:HD23	2.21	0.41
1:K:758:PHE:HA	1:K:763:VAL:HG23	2.02	0.41
3:N:197:LEU:O	3:N:201:THR:HG23	2.21	0.41
1:M:671:ARG:HB3	1:M:696:ASN:ND2	2.36	0.41
2:B:78:ASN:HB3	2:B:81:ASP:HB2	2.02	0.41
2:C:78:ASN:HB3	2:C:81:ASP:OD1	2.21	0.41
2:C:138:ALA:HB1	2:C:152:VAL:HG11	2.03	0.41
3:O:57:LEU:HD21	3:P:57:LEU:HG	2.03	0.41
3:P:175:ASP:HA	3:P:178:ARG:NE	2.35	0.41
1:G:599:ASP:O	1:G:645:GLN:HB2	2.21	0.41
1:G:671:ARG:HB3	1:G:696:ASN:ND2	2.36	0.41
1:G:715:TYR:CZ	1:G:763:VAL:HB	2.54	0.41
1:H:238:ASN:OD1	1:H:239:ASP:N	2.54	0.41
1:J:87:ILE:HG21	1:J:93:LEU:HG	2.03	0.41
1:J:92:MET:HE1	1:J:712:ARG:N	2.28	0.41
1:J:156:SER:OG	1:J:157:ILE:N	2.54	0.41
1:M:23:ARG:O	1:M:27:GLN:HG2	2.21	0.41
2:D:105:LEU:HD11	2:D:123:MET:HE3	2.03	0.41
2:D:294:TYR:CD2	2:D:325:MET:HG2	2.56	0.41
2:D:333:PRO:HB2	1:I:412:THR:O	2.21	0.41
2:E:333:PRO:HB2	1:J:412:THR:O	2.21	0.41
3:P:94:LEU:O	3:P:97:GLU:HG3	2.21	0.41
1:G:46:PHE:CG	1:G:99:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:238:ASN:OD1	1:G:239:ASP:N	2.54	0.41
1:H:45:GLU:HG2	1:H:46:PHE:CD2	2.44	0.41
1:H:63:THR:HG23	1:H:65:TYR:H	1.86	0.41
1:H:293:LYS:HG2	1:H:330:MET:HE3	2.03	0.41
1:H:740:LYS:HG3	1:H:741:GLY:N	2.35	0.41
1:I:23:ARG:O	1:I:27:GLN:HG2	2.21	0.41
1:I:36:ASP:CG	1:I:50:LYS:HG3	2.45	0.41
1:I:146:LYS:HA	1:I:146:LYS:HD2	1.76	0.41
1:I:238:ASN:OD1	1:I:239:ASP:N	2.54	0.41
1:I:481:THR:HG22	1:I:655:LEU:HD22	2.03	0.41
1:I:671:ARG:HB3	1:I:696:ASN:ND2	2.36	0.41
1:I:689:VAL:O	1:I:693:LEU:HD23	2.21	0.41
1:J:63:THR:HG23	1:J:65:TYR:H	1.86	0.41
1:J:77:MET:HB2	1:J:97:HIS:CE1	2.54	0.41
1:J:301:LEU:HD21	1:J:351:LYS:HA	2.03	0.41
1:J:517:LEU:HD12	1:J:517:LEU:HA	1.84	0.41
1:J:689:VAL:O	1:J:693:LEU:HD23	2.21	0.41
1:K:43:LYS:HB3	1:K:43:LYS:HE3	1.85	0.41
1:K:238:ASN:OD1	1:K:239:ASP:N	2.54	0.41
1:K:379:GLU:H	1:K:379:GLU:CD	2.27	0.41
1:K:689:VAL:O	1:K:693:LEU:HD23	2.21	0.41
2:A:131:ALA:HB1	2:A:356:TRP:HB3	2.03	0.41
3:L:86:ALA:HB1	3:L:90:ARG:HH12	1.86	0.41
3:L:139:GLU:HG3	3:L:140:LYS:N	2.36	0.41
3:L:146:ILE:HD13	3:L:146:ILE:HA	1.94	0.41
3:N:94:LEU:O	3:N:97:GLU:HG3	2.21	0.41
3:N:152:LYS:HG3	3:N:153:HIS:N	2.36	0.41
1:M:87:ILE:HG21	1:M:93:LEU:HG	2.03	0.41
2:F:236:LEU:O	2:F:254:ARG:NH1	2.49	0.41
1:G:63:THR:HG23	1:G:65:TYR:H	1.86	0.41
1:G:146:LYS:HB3	1:G:149:GLU:OE1	2.21	0.41
1:G:740:LYS:HG3	1:G:741:GLY:N	2.35	0.41
1:H:87:ILE:HG21	1:H:93:LEU:HG	2.03	0.41
1:H:171:ASN:OD1	1:H:456:PHE:N	2.40	0.41
1:I:46:PHE:CG	1:I:99:PRO:HG3	2.56	0.41
1:I:146:LYS:HB3	1:I:149:GLU:OE1	2.21	0.41
1:J:23:ARG:O	1:J:27:GLN:HG2	2.21	0.41
1:J:146:LYS:HB3	1:J:149:GLU:OE1	2.21	0.41
3:N:50:LEU:O	3:N:54:GLU:HG3	2.21	0.41
1:M:506:ILE:O	1:M:506:ILE:HG23	2.22	0.40
2:C:97:ALA:HB1	2:C:99:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:131:ALA:HB1	2:E:356:TRP:HB3	2.03	0.40
2:E:278:THR:O	2:E:282:ILE:HG12	2.20	0.40
3:O:77:LYS:HB3	3:O:77:LYS:HE2	1.91	0.40
1:G:12:ALA:HB1	1:G:133:VAL:HG12	2.04	0.40
1:G:290:LEU:HD23	1:G:290:LEU:HA	1.92	0.40
1:G:448:GLU:OE1	1:G:450:LYS:HD2	2.22	0.40
1:H:689:VAL:O	1:H:693:LEU:HD23	2.21	0.40
1:H:769:LEU:H	1:H:769:LEU:HD12	1.86	0.40
1:I:156:SER:OG	1:I:157:ILE:N	2.54	0.40
1:I:447:LEU:HD23	1:I:447:LEU:O	2.21	0.40
1:J:447:LEU:HD23	1:J:447:LEU:O	2.21	0.40
1:K:23:ARG:O	1:K:27:GLN:HG2	2.21	0.40
1:K:146:LYS:HB3	1:K:149:GLU:OE1	2.21	0.40
1:K:217:GLU:O	1:K:221:ILE:HG12	2.21	0.40
1:K:301:LEU:HD21	1:K:351:LYS:HA	2.03	0.40
1:K:481:THR:HG22	1:K:655:LEU:HD22	2.03	0.40
3:L:205:LYS:HA	3:L:208:GLU:CD	2.46	0.40
1:M:12:ALA:HB1	1:M:133:VAL:HG12	2.04	0.40
2:C:123:MET:O	2:C:129:VAL:HG22	2.21	0.40
2:E:372:ARG:O	2:E:374:CYS:N	2.55	0.40
3:O:162:TYR:CD1	3:P:161:LYS:HD3	2.56	0.40
3:O:205:LYS:HA	3:O:208:GLU:CD	2.46	0.40
3:P:48:LYS:HB2	3:P:48:LYS:HE2	1.87	0.40
3:P:50:LEU:O	3:P:54:GLU:HG3	2.21	0.40
1:G:23:ARG:O	1:G:27:GLN:HG2	2.21	0.40
1:G:87:ILE:HG21	1:G:93:LEU:HG	2.03	0.40
1:H:285:ILE:HD12	1:H:285:ILE:H	1.87	0.40
1:I:12:ALA:HB1	1:I:133:VAL:HG12	2.04	0.40
1:I:301:LEU:HD21	1:I:351:LYS:HA	2.03	0.40
1:J:12:ALA:HB1	1:J:133:VAL:HG12	2.04	0.40
1:J:46:PHE:CG	1:J:99:PRO:HG3	2.56	0.40
1:J:238:ASN:OD1	1:J:239:ASP:N	2.54	0.40
1:J:481:THR:HG22	1:J:655:LEU:HD22	2.03	0.40
1:K:46:PHE:CG	1:K:99:PRO:HG3	2.56	0.40
1:K:269:GLU:OE1	1:K:271:SER:N	2.31	0.40
2:A:138:ALA:HB1	2:A:152:VAL:CG1	2.52	0.40
2:A:372:ARG:O	2:A:374:CYS:N	2.54	0.40
3:L:112:LYS:HA	3:L:112:LYS:HD2	1.83	0.40
1:M:46:PHE:CG	1:M:99:PRO:HG3	2.56	0.40
1:M:63:THR:HG23	1:M:65:TYR:H	1.86	0.40
1:M:238:ASN:OD1	1:M:239:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:689:VAL:O	1:M:693:LEU:HD23	2.21	0.40
2:E:244:ASP:O	2:A:325:MET:HE1	2.19	0.40
3:O:86:ALA:HB1	3:O:90:ARG:HH12	1.86	0.40
3:O:198:LYS:O	3:O:201:THR:HG22	2.21	0.40
3:P:105:ARG:HH12	3:P:106:LEU:HD13	1.86	0.40
3:P:124:GLU:HA	3:P:127:MET:HG2	2.04	0.40
1:G:285:ILE:HD12	1:G:285:ILE:H	1.87	0.40
1:G:549:LYS:HE3	1:G:553:PHE:CE2	2.52	0.40
1:G:769:LEU:H	1:G:769:LEU:HD12	1.86	0.40
1:I:87:ILE:HG21	1:I:93:LEU:HG	2.03	0.40
1:I:288:GLN:O	1:I:291:SER:HB3	2.22	0.40
1:I:352:LEU:HD12	1:I:352:LEU:HA	1.88	0.40
1:I:379:GLU:H	1:I:379:GLU:CD	2.27	0.40
1:I:517:LEU:HD12	1:I:517:LEU:HA	1.84	0.40
1:J:506:ILE:O	1:J:506:ILE:HG23	2.22	0.40
1:K:63:THR:HG23	1:K:65:TYR:H	1.86	0.40
3:L:67:ALA:O	3:L:71:LEU:HG	2.22	0.40
3:N:64:LEU:O	3:N:68:GLN:HG3	2.21	0.40
3:N:147:GLN:HA	3:N:150:GLU:OE1	2.21	0.40
1:M:448:GLU:OE1	1:M:450:LYS:HD2	2.22	0.40
1:M:637:LYS:HA	1:M:637:LYS:HD3	1.75	0.40
2:B:372:ARG:HG2	2:B:373:LYS:H	1.86	0.40
2:D:138:ALA:HB1	2:D:152:VAL:HG11	2.04	0.40
3:O:50:LEU:O	3:O:54:GLU:HG3	2.22	0.40
3:P:91:ARG:O	3:P:95:VAL:HG22	2.22	0.40
3:P:197:LEU:O	3:P:201:THR:HG23	2.21	0.40
1:G:217:GLU:O	1:G:221:ILE:HG12	2.21	0.40
1:G:689:VAL:O	1:G:693:LEU:HD23	2.21	0.40
1:H:23:ARG:O	1:H:27:GLN:HG2	2.21	0.40
1:I:448:GLU:OE1	1:I:450:LYS:HD2	2.21	0.40
1:I:466:GLU:HB2	1:I:468:PHE:CE2	2.57	0.40
1:J:288:GLN:O	1:J:291:SER:HB3	2.22	0.40
1:J:448:GLU:OE1	1:J:450:LYS:HD2	2.22	0.40
1:J:466:GLU:HB2	1:J:468:PHE:CE2	2.57	0.40
1:K:466:GLU:HB2	1:K:468:PHE:CE2	2.57	0.40
1:K:506:ILE:O	1:K:506:ILE:HG23	2.22	0.40
3:L:47:GLN:HA	3:L:51:LYS:HZ3	1.86	0.40
3:N:91:ARG:O	3:N:95:VAL:HG22	2.22	0.40
1:M:217:GLU:O	1:M:221:ILE:HG12	2.21	0.40
1:M:288:GLN:O	1:M:291:SER:HB3	2.22	0.40
1:M:301:LEU:HD21	1:M:351:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:VAL:O	2:D:340:TRP:NE1	2.48	0.40
2:E:44:MET:CE	2:A:142:LEU:HD23	2.52	0.40
2:F:308:GLY:HA3	3:O:125:ARG:HH21	1.87	0.40
3:O:59:LYS:HA	3:O:62:GLU:HG2	2.04	0.40
3:O:139:GLU:HG3	3:O:140:LYS:N	2.36	0.40
1:H:12:ALA:HB1	1:H:133:VAL:HG12	2.04	0.40
1:H:46:PHE:CG	1:H:99:PRO:HG3	2.56	0.40
1:H:506:ILE:CD1	1:H:757:LYS:HG2	2.48	0.40
1:H:776:MET:O	1:H:779:GLU:HG3	2.22	0.40
1:J:46:PHE:O	1:J:103:TYR:OH	2.27	0.40
1:J:379:GLU:H	1:J:379:GLU:CD	2.27	0.40
1:J:769:LEU:H	1:J:769:LEU:HD12	1.86	0.40
1:K:12:ALA:HB1	1:K:133:VAL:HG12	2.04	0.40
1:K:290:LEU:HD23	1:K:290:LEU:HA	1.92	0.40
1:K:448:GLU:OE1	1:K:450:LYS:HD2	2.22	0.40
3:L:162:TYR:CD1	3:N:161:LYS:HD3	2.56	0.40
3:N:124:GLU:HA	3:N:127:MET:HG2	2.04	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	H	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	I	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	J	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	K	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	M	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
2	A	369/371 (100%)	347 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	369/371 (100%)	349 (95%)	20 (5%)	0	100	100
2	C	369/371 (100%)	352 (95%)	17 (5%)	0	100	100
2	D	369/371 (100%)	344 (93%)	25 (7%)	0	100	100
2	E	369/371 (100%)	347 (94%)	22 (6%)	0	100	100
2	F	369/371 (100%)	348 (94%)	21 (6%)	0	100	100
3	L	164/166 (99%)	164 (100%)	0	0	100	100
3	N	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
3	O	164/166 (99%)	164 (100%)	0	0	100	100
3	P	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
All	All	7274/7546 (96%)	6917 (95%)	357 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	644/668 (96%)	644 (100%)	0	100	100
1	H	644/668 (96%)	644 (100%)	0	100	100
1	I	644/668 (96%)	644 (100%)	0	100	100
1	J	644/668 (96%)	644 (100%)	0	100	100
1	K	644/668 (96%)	644 (100%)	0	100	100
1	M	644/668 (96%)	644 (100%)	0	100	100
2	A	314/314 (100%)	314 (100%)	0	100	100
2	B	314/314 (100%)	314 (100%)	0	100	100
2	C	314/314 (100%)	314 (100%)	0	100	100
2	D	314/314 (100%)	314 (100%)	0	100	100
2	E	314/314 (100%)	314 (100%)	0	100	100
2	F	314/314 (100%)	314 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	141/141 (100%)	141 (100%)	0	100	100
3	N	141/141 (100%)	141 (100%)	0	100	100
3	O	141/141 (100%)	141 (100%)	0	100	100
3	P	141/141 (100%)	141 (100%)	0	100	100
All	All	6312/6456 (98%)	6312 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	75	GLN
1	M	79	GLN
1	M	80	ASN
1	M	163	GLN
1	M	222	GLN
1	M	224	ASN
1	M	284	HIS
1	M	358	HIS
1	M	418	GLN
1	M	490	ASN
1	M	562	ASN
1	M	623	ASN
1	M	661	ASN
1	M	691	HIS
2	B	73	HIS
2	B	88	HIS
2	B	92	ASN
2	B	115	ASN
2	B	162	ASN
2	B	173	HIS
2	B	252	ASN
2	C	173	HIS
2	C	275	HIS
2	C	280	ASN
2	C	353	GLN
2	D	87	HIS
2	D	88	HIS
2	D	92	ASN
2	D	115	ASN

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Mol	Chain	Res	Type
2	D	121	GLN
2	D	225	ASN
2	D	275	HIS
2	D	296	ASN
2	D	353	GLN
2	E	41	GLN
2	E	49	GLN
2	E	92	ASN
2	E	161	HIS
2	E	162	ASN
2	E	173	HIS
2	E	353	GLN
2	F	41	GLN
2	F	88	HIS
2	F	92	ASN
2	F	225	ASN
2	F	275	HIS
2	F	371	HIS
3	O	93	GLN
3	O	144	GLN
3	O	203	ASN
3	P	202	ASN
3	P	203	ASN
1	G	75	GLN
1	G	79	GLN
1	G	80	ASN
1	G	163	GLN
1	G	222	GLN
1	G	224	ASN
1	G	284	HIS
1	G	358	HIS
1	G	368	GLN
1	G	418	GLN
1	G	490	ASN
1	G	562	ASN
1	G	623	ASN
1	G	661	ASN
1	G	691	HIS
1	H	75	GLN
1	H	79	GLN
1	H	80	ASN
1	H	163	GLN

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Mol	Chain	Res	Type
1	H	222	GLN
1	H	224	ASN
1	H	284	HIS
1	H	358	HIS
1	H	368	GLN
1	H	418	GLN
1	H	490	ASN
1	H	562	ASN
1	H	623	ASN
1	H	661	ASN
1	H	691	HIS
1	I	75	GLN
1	I	79	GLN
1	I	80	ASN
1	I	163	GLN
1	I	222	GLN
1	I	224	ASN
1	I	284	HIS
1	I	358	HIS
1	I	368	GLN
1	I	418	GLN
1	I	490	ASN
1	I	562	ASN
1	I	623	ASN
1	I	661	ASN
1	I	691	HIS
1	I	755	GLN
1	J	75	GLN
1	J	79	GLN
1	J	80	ASN
1	J	163	GLN
1	J	222	GLN
1	J	224	ASN
1	J	284	HIS
1	J	358	HIS
1	J	368	GLN
1	J	418	GLN
1	J	490	ASN
1	J	562	ASN
1	J	623	ASN
1	J	661	ASN
1	J	691	HIS

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Mol	Chain	Res	Type
1	J	726	ASN
1	K	75	GLN
1	K	79	GLN
1	K	80	ASN
1	K	163	GLN
1	K	222	GLN
1	K	224	ASN
1	K	284	HIS
1	K	358	HIS
1	K	368	GLN
1	K	418	GLN
1	K	490	ASN
1	K	562	ASN
1	K	623	ASN
1	K	661	ASN
1	K	691	HIS
1	K	755	GLN
2	A	92	ASN
2	A	161	HIS
2	A	162	ASN
2	A	297	ASN
2	A	353	GLN
3	L	93	GLN
3	L	144	GLN
3	L	203	ASN
3	N	202	ASN
3	N	203	ASN

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

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	D	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.76	9 (20%)
4	ADP	B	401	-	28,29,29	1.40	5 (17%)	43,45,45	1.76	9 (20%)
4	ADP	F	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.76	9 (20%)
4	ADP	A	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.76	9 (20%)
4	ADP	C	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.80	9 (20%)
4	ADP	E	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.76	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	401	-	-	5/16/32/32	0/3/3/3
4	ADP	B	401	-	-	4/16/32/32	0/3/3/3
4	ADP	F	401	-	-	5/16/32/32	0/3/3/3
4	ADP	A	401	-	-	4/16/32/32	0/3/3/3
4	ADP	C	401	-	-	3/16/32/32	0/3/3/3
4	ADP	E	401	-	-	4/16/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	ADP	C5-C4	4.41	1.47	1.39
4	B	401	ADP	C5-C4	4.37	1.46	1.39
4	F	401	ADP	C5-C4	4.35	1.46	1.39
4	D	401	ADP	C5-C4	4.34	1.46	1.39
4	A	401	ADP	C5-C4	4.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	ADP	C5-C4	4.31	1.46	1.39
4	D	401	ADP	C5-N7	-2.62	1.34	1.39
4	B	401	ADP	C5-N7	-2.60	1.34	1.39
4	E	401	ADP	C5-N7	-2.57	1.34	1.39
4	F	401	ADP	C5-N7	-2.56	1.34	1.39
4	A	401	ADP	C5-N7	-2.55	1.34	1.39
4	C	401	ADP	C5-N7	-2.50	1.34	1.39
4	B	401	ADP	C5-C6	2.43	1.47	1.41
4	C	401	ADP	C5-C6	2.43	1.47	1.41
4	F	401	ADP	C5-C6	2.40	1.47	1.41
4	A	401	ADP	C5-C6	2.40	1.47	1.41
4	E	401	ADP	C5-C6	2.40	1.47	1.41
4	D	401	ADP	C5-C6	2.37	1.47	1.41
4	D	401	ADP	C4-N9	-2.29	1.32	1.37
4	E	401	ADP	C4-N9	-2.29	1.32	1.37
4	A	401	ADP	C4-N9	-2.29	1.32	1.37
4	C	401	ADP	C4-N9	-2.28	1.32	1.37
4	F	401	ADP	C4-N9	-2.27	1.33	1.37
4	B	401	ADP	C8-N7	2.25	1.36	1.31
4	B	401	ADP	C4-N9	-2.25	1.33	1.37
4	A	401	ADP	C8-N7	2.25	1.36	1.31
4	C	401	ADP	C8-N7	2.24	1.36	1.31
4	E	401	ADP	C8-N7	2.24	1.36	1.31
4	D	401	ADP	C8-N7	2.23	1.36	1.31
4	F	401	ADP	C8-N7	2.19	1.35	1.31

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ADP	C5-C4-N3	-5.70	118.86	126.72
4	C	401	ADP	C5-C4-N3	-5.57	119.05	126.72
4	D	401	ADP	C5-C4-N3	-5.56	119.06	126.72
4	F	401	ADP	C5-C4-N3	-5.55	119.07	126.72
4	E	401	ADP	C5-C4-N3	-5.55	119.08	126.72
4	A	401	ADP	C5-C4-N3	-5.54	119.09	126.72
4	B	401	ADP	N3-C4-N9	4.40	134.65	127.17
4	C	401	ADP	N3-C4-N9	4.39	134.63	127.17
4	D	401	ADP	N3-C4-N9	4.35	134.56	127.17
4	F	401	ADP	N3-C4-N9	4.33	134.53	127.17
4	A	401	ADP	N3-C4-N9	4.28	134.44	127.17
4	E	401	ADP	N3-C4-N9	4.27	134.43	127.17
4	C	401	ADP	C2-N3-C4	3.60	120.61	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	ADP	C2-N3-C4	3.57	120.55	111.83
4	E	401	ADP	C2-N3-C4	3.57	120.54	111.83
4	F	401	ADP	C2-N3-C4	3.56	120.53	111.83
4	B	401	ADP	C2-N3-C4	3.49	120.36	111.83
4	D	401	ADP	C2-N3-C4	3.48	120.34	111.83
4	B	401	ADP	C4-C5-N7	-3.38	106.72	110.58
4	E	401	ADP	C4-C5-N7	-3.36	106.74	110.58
4	A	401	ADP	C4-C5-N7	-3.34	106.77	110.58
4	F	401	ADP	C4-C5-N7	-3.33	106.78	110.58
4	D	401	ADP	C4-C5-N7	-3.32	106.79	110.58
4	C	401	ADP	C4-C5-N7	-3.29	106.82	110.58
4	C	401	ADP	N3-C2-N1	-3.16	123.80	128.58
4	F	401	ADP	N3-C2-N1	-3.12	123.86	128.58
4	A	401	ADP	N3-C2-N1	-3.12	123.86	128.58
4	E	401	ADP	N3-C2-N1	-3.11	123.87	128.58
4	D	401	ADP	N3-C2-N1	-2.95	124.12	128.58
4	B	401	ADP	N3-C2-N1	-2.85	124.28	128.58
4	C	401	ADP	C4-N9-C8	2.71	108.58	105.74
4	D	401	ADP	C4-N9-C8	2.62	108.49	105.74
4	F	401	ADP	C4-N9-C8	2.58	108.45	105.74
4	A	401	ADP	C4-N9-C8	2.56	108.43	105.74
4	E	401	ADP	C4-N9-C8	2.55	108.41	105.74
4	B	401	ADP	C4-N9-C8	2.50	108.36	105.74
4	B	401	ADP	C5-N7-C8	2.32	107.10	103.45
4	E	401	ADP	C5-N7-C8	2.31	107.08	103.45
4	D	401	ADP	C5-N7-C8	2.30	107.07	103.45
4	F	401	ADP	C5-N7-C8	2.30	107.07	103.45
4	C	401	ADP	C5-N7-C8	2.30	107.06	103.45
4	A	401	ADP	C5-N7-C8	2.29	107.05	103.45
4	A	401	ADP	C6-C5-N7	2.24	136.41	132.09
4	E	401	ADP	C6-C5-N7	2.24	136.40	132.09
4	F	401	ADP	C6-C5-N7	2.19	136.31	132.09
4	C	401	ADP	C6-C5-N7	2.17	136.27	132.09
4	C	401	ADP	C3'-C2'-C1'	2.16	105.54	101.46
4	D	401	ADP	C3'-C2'-C1'	2.15	105.53	101.46
4	B	401	ADP	C3'-C2'-C1'	2.12	105.47	101.46
4	D	401	ADP	C6-C5-N7	2.10	136.14	132.09
4	B	401	ADP	C6-C5-N7	2.06	136.07	132.09
4	A	401	ADP	C3'-C2'-C1'	2.03	105.31	101.46
4	E	401	ADP	C3'-C2'-C1'	2.03	105.30	101.46
4	F	401	ADP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	ADP	C5'-O5'-PA-O2A
4	B	401	ADP	C5'-O5'-PA-O3A
4	C	401	ADP	C5'-O5'-PA-O2A
4	D	401	ADP	C5'-O5'-PA-O2A
4	D	401	ADP	C5'-O5'-PA-O3A
4	E	401	ADP	C5'-O5'-PA-O2A
4	F	401	ADP	C5'-O5'-PA-O2A
4	F	401	ADP	C5'-O5'-PA-O3A
4	A	401	ADP	C5'-O5'-PA-O2A
4	B	401	ADP	C5'-O5'-PA-O1A
4	D	401	ADP	C5'-O5'-PA-O1A
4	E	401	ADP	C5'-O5'-PA-O1A
4	E	401	ADP	C5'-O5'-PA-O3A
4	F	401	ADP	C5'-O5'-PA-O1A
4	A	401	ADP	C5'-O5'-PA-O1A
4	A	401	ADP	C5'-O5'-PA-O3A
4	E	401	ADP	PB-O3A-PA-O2A
4	A	401	ADP	PB-O3A-PA-O2A
4	B	401	ADP	PB-O3A-PA-O2A
4	D	401	ADP	PB-O3A-PA-O1A
4	F	401	ADP	PB-O3A-PA-O1A
4	F	401	ADP	PB-O3A-PA-O2A
4	C	401	ADP	PB-O3A-PA-O1A
4	C	401	ADP	PB-O3A-PA-O2A
4	D	401	ADP	PB-O3A-PA-O2A

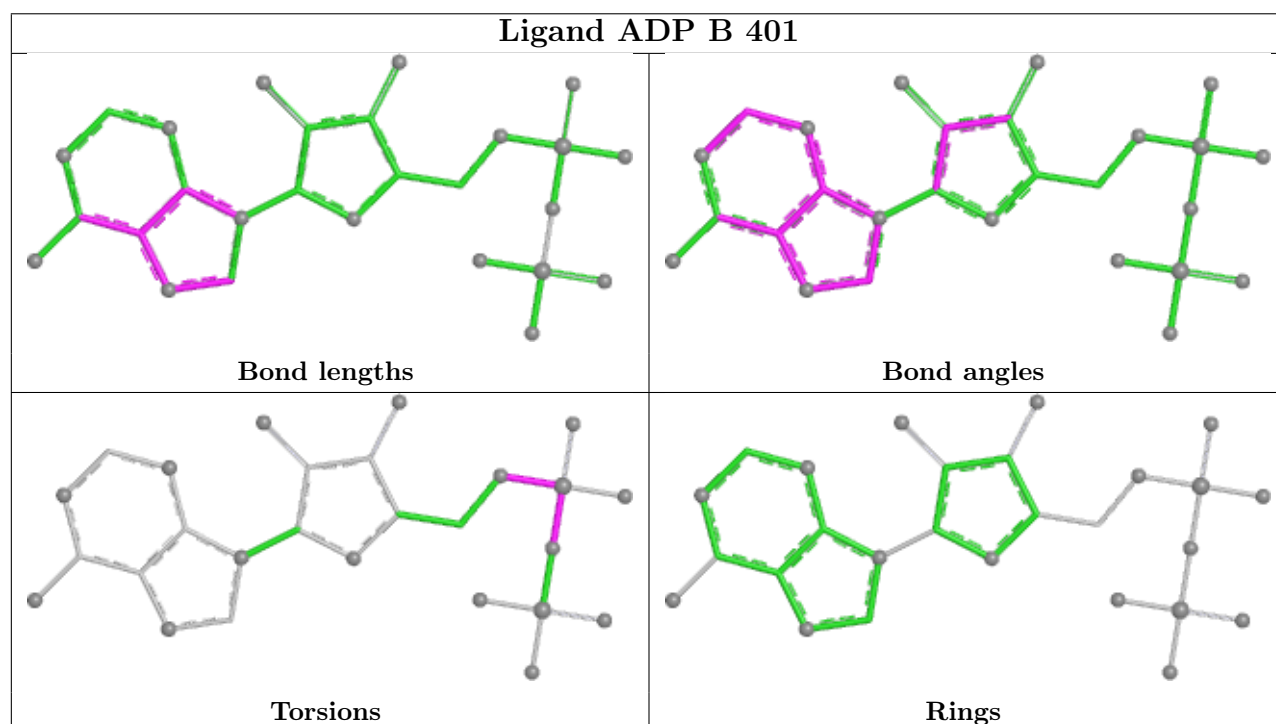
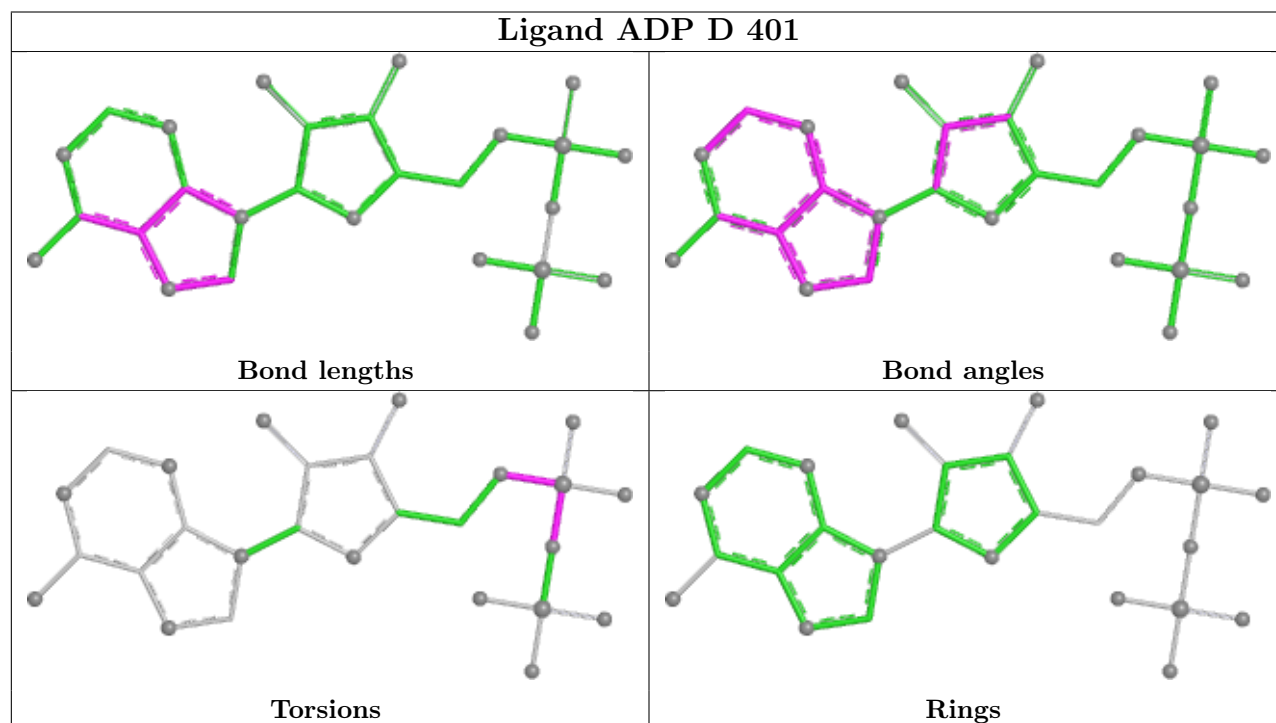
There are no ring outliers.

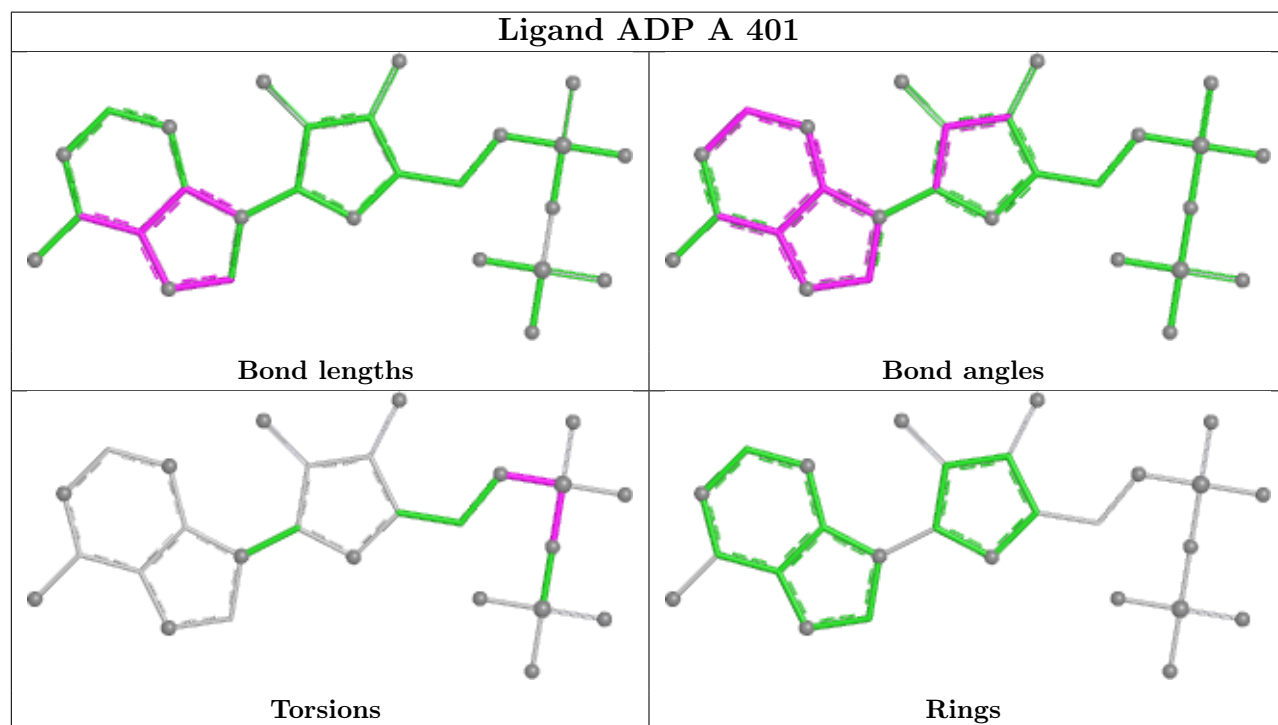
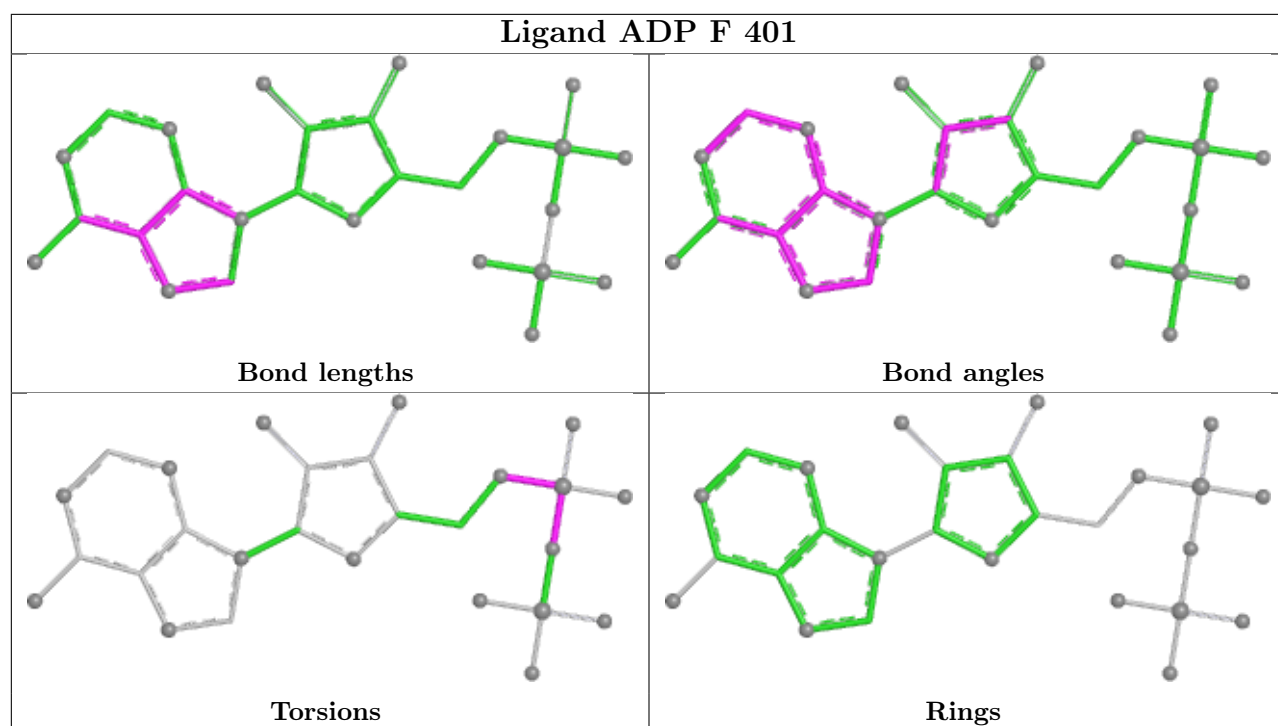
6 monomers are involved in 13 short contacts:

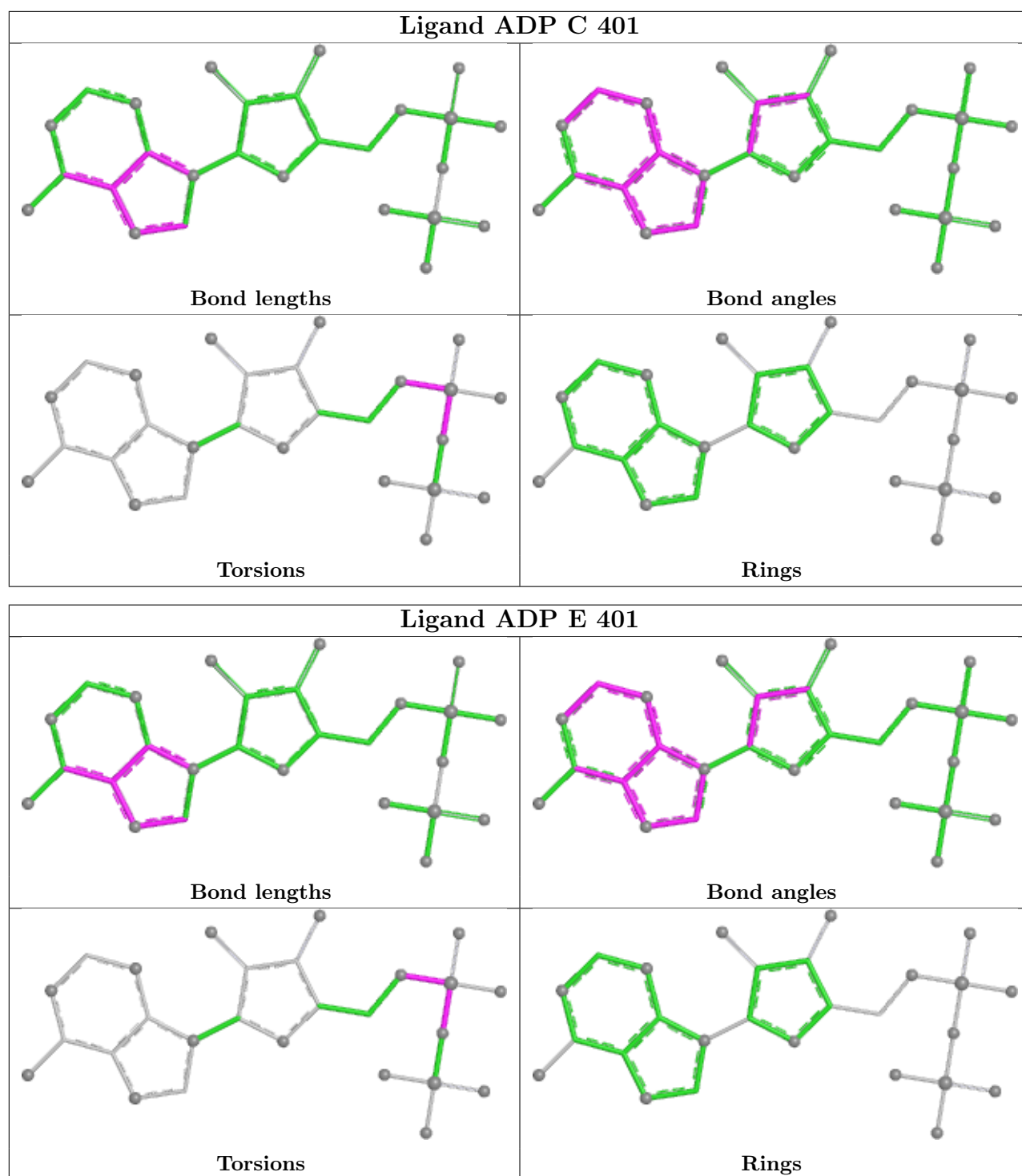
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	ADP	2	0
4	B	401	ADP	1	0
4	F	401	ADP	2	0
4	A	401	ADP	3	0
4	C	401	ADP	2	0
4	E	401	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39896. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.