



Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 05:30 PM EDT

PDB ID : 7LIV
EMDB ID : EMD-23386
Title : Structure of human transfer RNA visualized in the cytomegalovirus, a DNA virus
Authors : Liu, Y.T.; Strugatsky, D.; Liu, W.; Zhou, Z.H.
Deposited on : 2021-01-28
Resolution : 3.60 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

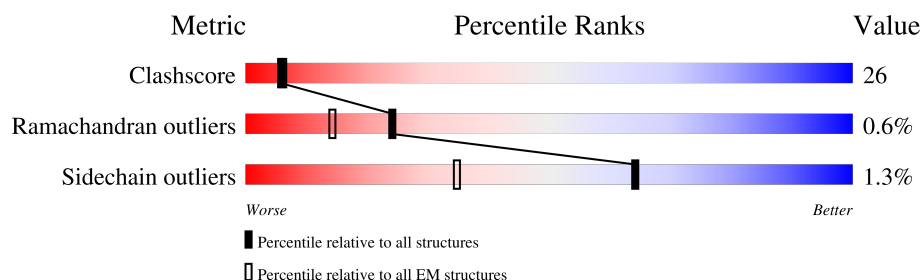
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1370	<div> <div>65%</div> <div>63%</div> <div>33%</div> <div>..</div> </div>
1	C	1370	<div> <div>64%</div> <div>61%</div> <div>37%</div> <div>..</div> </div>
1	J	1370	<div> <div>67%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
2	4	285	<div> <div>94%</div> <div>67%</div> <div>32%</div> <div>.</div> </div>
2	5	285	<div> <div>86%</div> <div>71%</div> <div>29%</div> </div>
2	6	285	<div> <div>80%</div> <div>68%</div> <div>32%</div> </div>
3	D	75	<div> <div>63%</div> <div>47%</div> <div>37%</div> <div>16%</div> </div>
3	E	75	<div> <div>65%</div> <div>59%</div> <div>25%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Z	75	<div><div></div><div>64%</div><div></div><div>56%</div><div>28%</div><div>16%</div></div>
4	p	290	<div><div></div><div>79%</div><div></div><div>98%</div><div></div><div></div></div>
5	q	306	<div><div></div><div>60%</div><div></div><div>78%</div><div></div><div>21%</div></div>
5	r	306	<div><div></div><div>83%</div><div></div><div>99%</div><div></div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47058 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		
1	A	1328	Total	C	N	O	S	0	0
			10526	6706	1827	1934	59		
1	C	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		

- Molecule 2 is a protein called Tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
2	6	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
2	4	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		

- Molecule 3 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	D	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	E	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	p	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

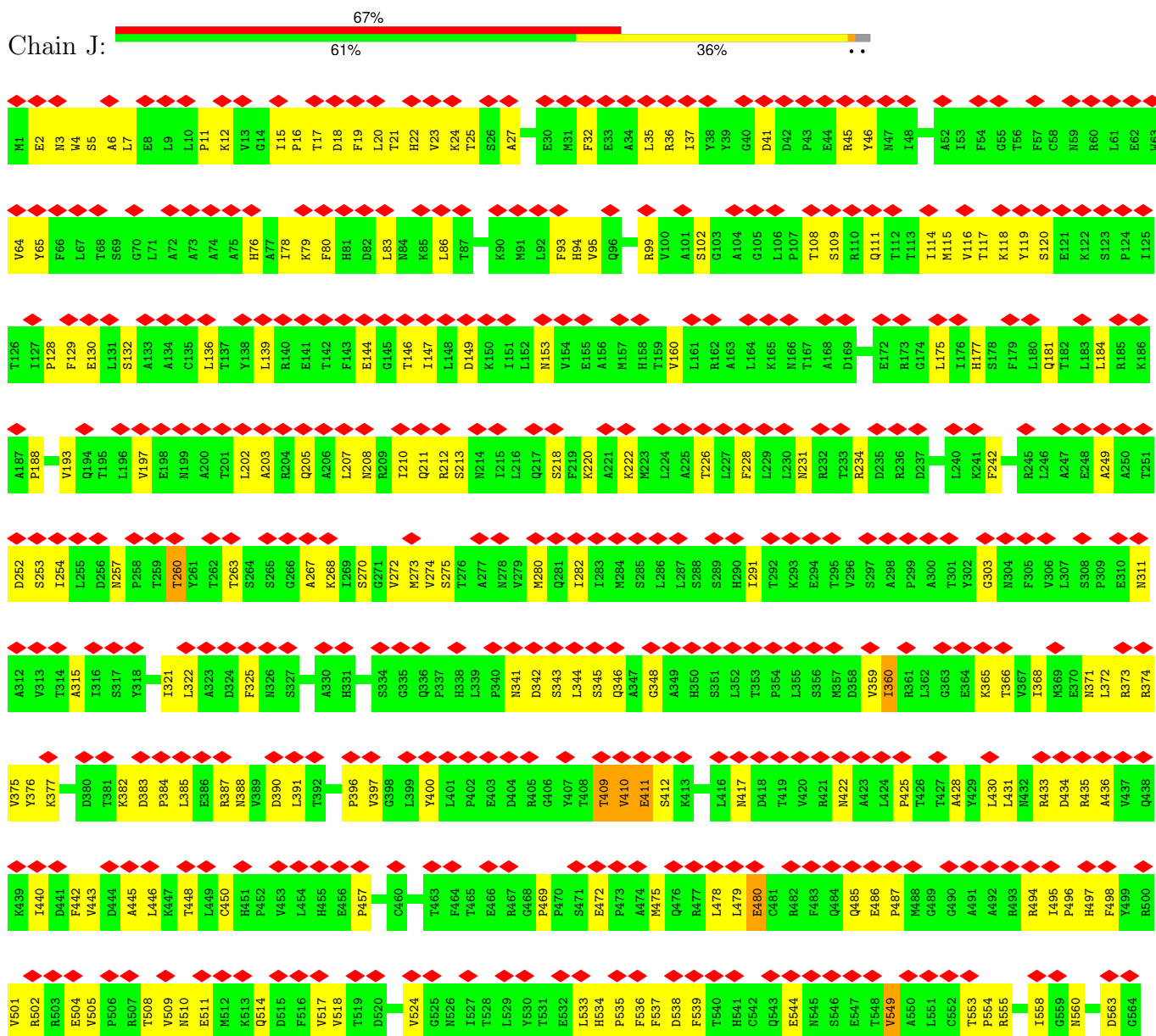
- Molecule 5 is a protein called Triplex capsid protein 2.

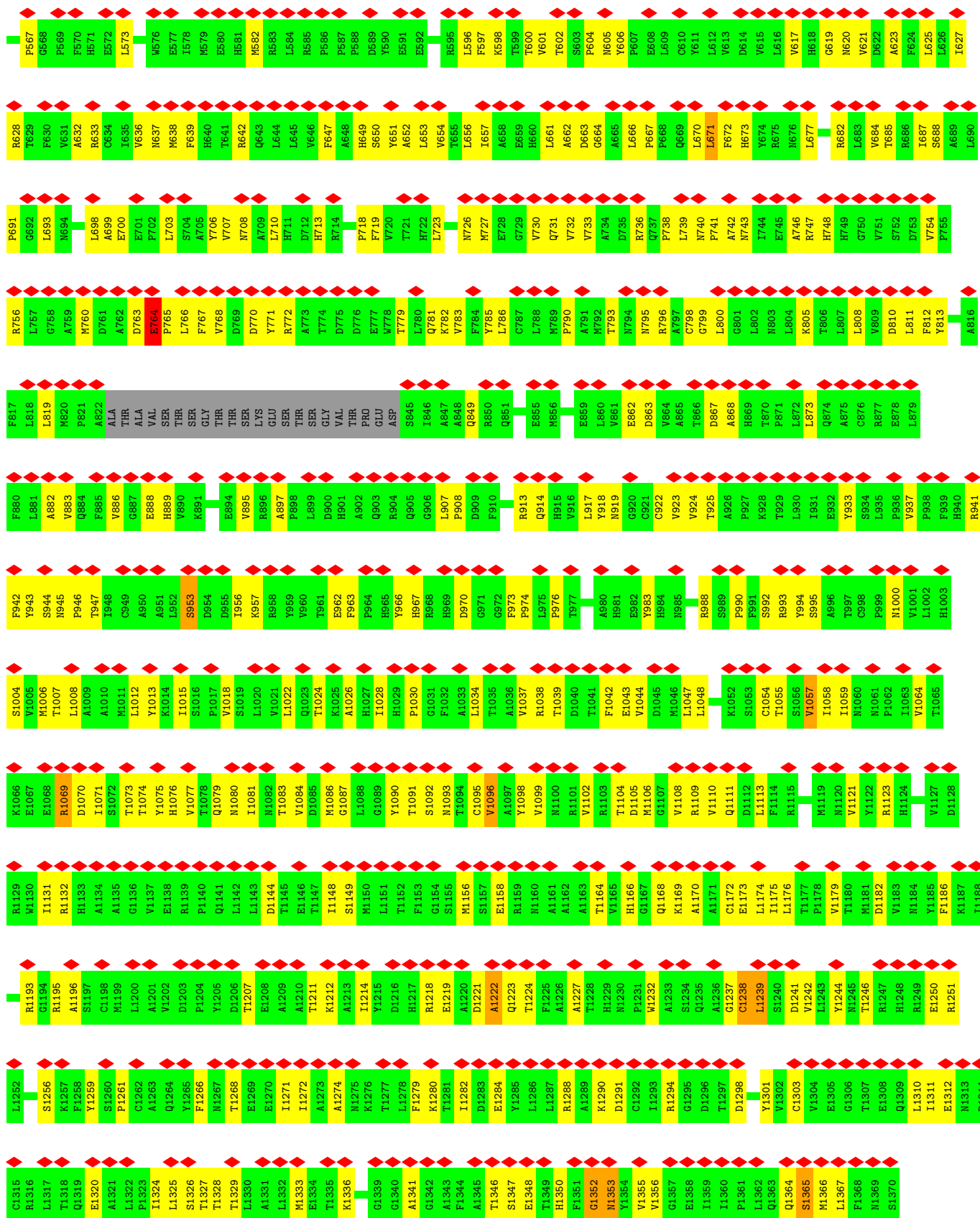
Mol	Chain	Residues	Atoms					AltConf	Trace
5	q	241	Total	C	N	O	S	0	0
			1911	1236	328	331	16		
5	r	304	Total	C	N	O	S	0	0
			2411	1544	420	429	18		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

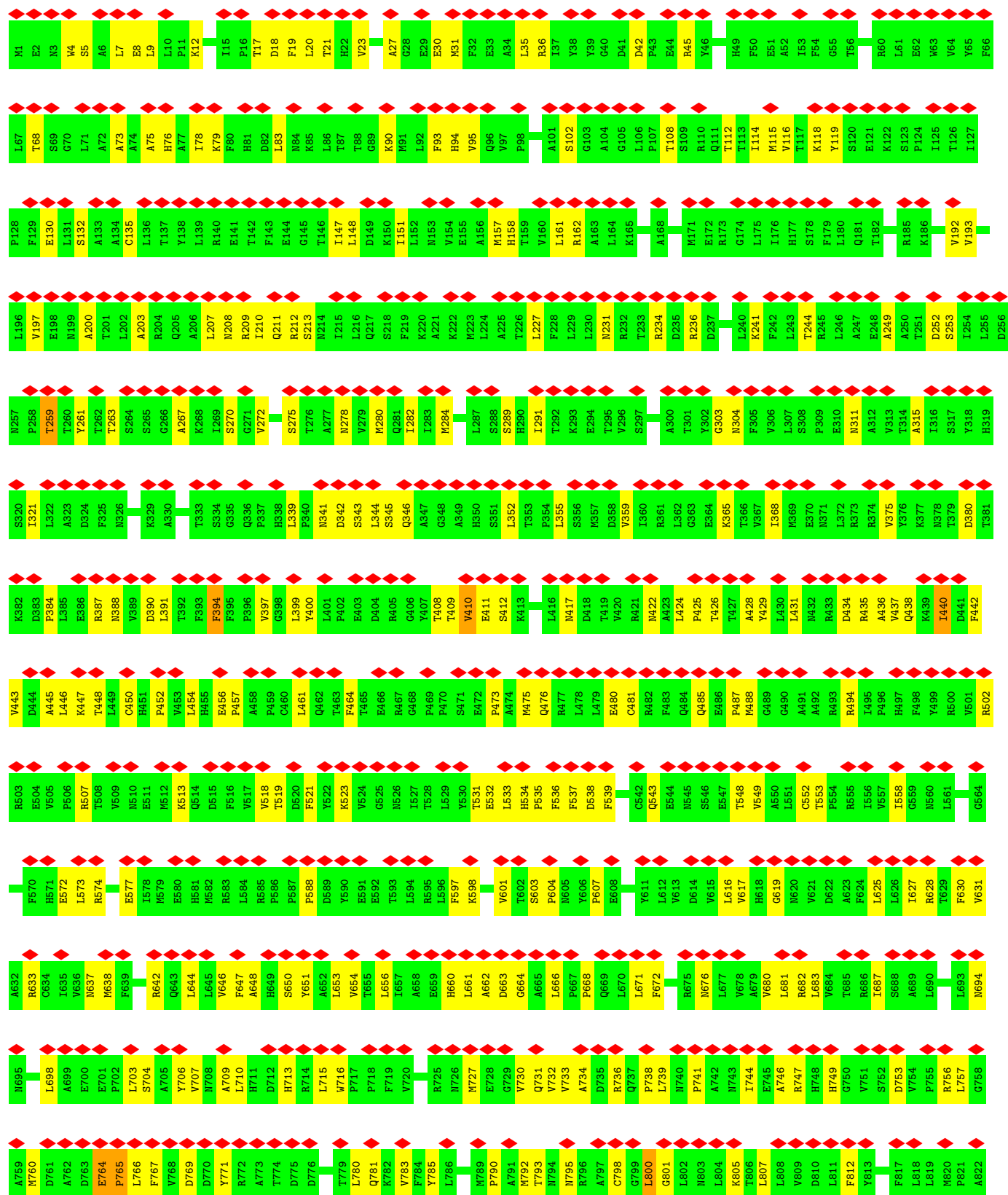
• Molecule 1: Major capsid protein





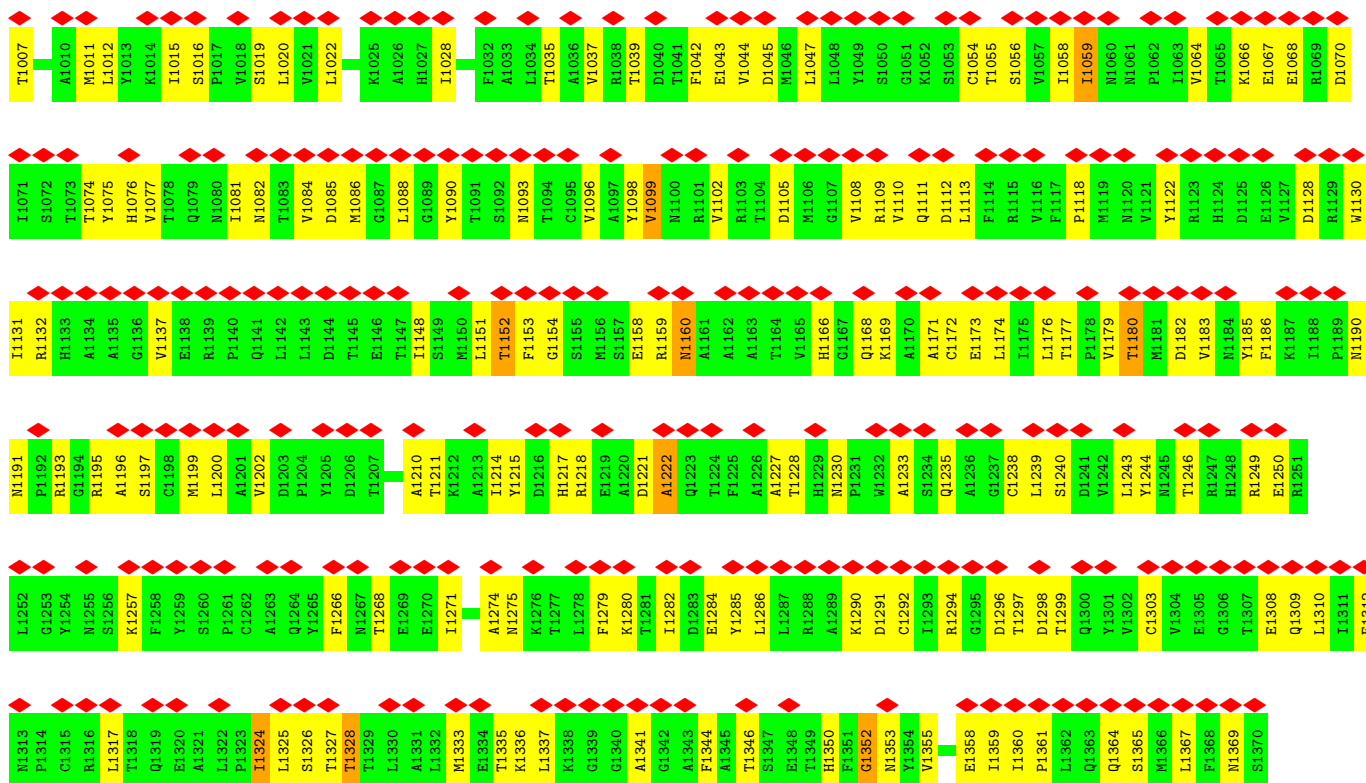
• Molecule 1: Major capsid protein

Chain A:  65% 63% 33% ..

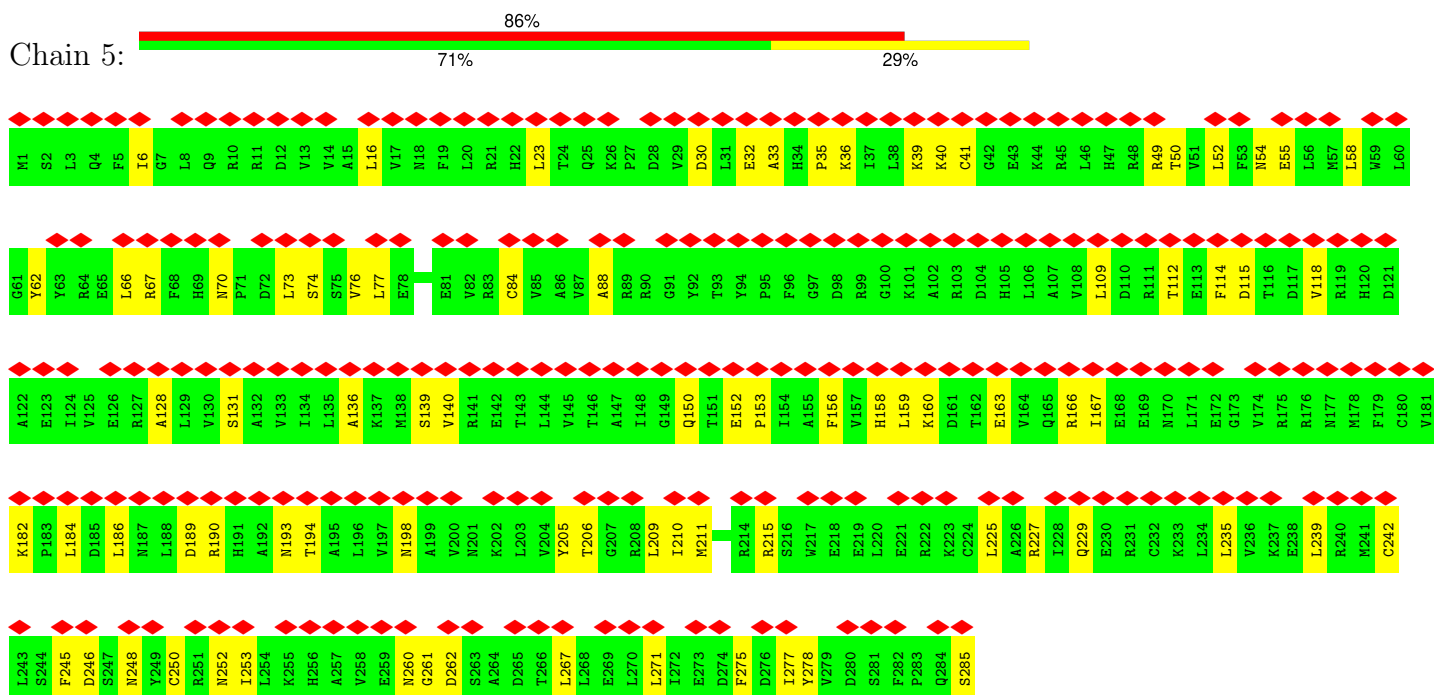




S944	N945	P946	T947	I948	C949	A950	A951	L952	S953	D954	D955	I956	K957	R958	E962	F963	P964	H965	Y966	H967	R968	H969	D970	G971	G972	F973	P974	L975	P976	T977	F979	E982	Y983	H984	N985	V986	L987	S988	S989	P990	F991	S992	Y993	Y994	S995	A996	T997	C998	P999	N1000	V1001	L1002	H1003	S1004	V1005	M1006			
Q884	F885	V886	G887	E888	H889	V890	K891	V892	L893	E894	V895	R896	A897	P898	L899	D900	H901	A902	Q903	R904	Q905	G906	L907	P908	D909	F910	I911	S912	L913	Q914	H915	V916	L917	Y918	N919	G920	C921	C922	V923	Y924	T925	A926	P927	K928	T929	L930	I931	E932	Y933	S934	L935	P936	N937	P938	F939	H940	R941	F942	Y943
ALA	THR	ALA	VAL	SER	THR	SER	GLY	THR	SER	LYS	GLU	SER	THR	SER	GLY	VAL	THR	PRO	GLU	ASP	S845	I846	Q849	R850	Q851	A852	V853	G854	E855	M856	L857	T858	E859	L860	R861	E862	D863	Y864	A865	T866	D867	A868	H869	T870	P871	L872	L873	Q874	A875	C876	R877	E878	L879	F880	L881	A882	W883		
D761	A762	D763	E764	P765	L766	F767	V768	D769	D770	Y771	R772	D775	D776	E777	L780	Q781	K782	W783	F784	Y785	L786	C787	L788	W789	P790	A791	N792	T793	N794	N795	R796	A797	C798	D799	L800	C801	L802	M803	L804	K805	T806	L807	L808	H809	D810	L811	F812	Y813	R814	P815	A816	F817	L818	L819	M820	P821	A822		
G696	Q697	L698	A699	E700	H701	F702	L703	S704	A705	Y706	V707	L710	H711	D712	H713	R714	L715	W716	F717	P718	F719	H722	R725	W726	W727	E728	G729	W730	Q731	W732	W733	A734	D735	R736	Q737	P738	L739	N740	P741	A742	N743	L744	E745	A746	R747	H748	H749	G750	V751	S752	D753	R756	A759	W760					
A632	R633	C634	I635	V636	M637	P638	F639	H640	T641	R642	Q643	L644	L645	V646	F647	A648	Y651	A652	L653	W654	T655	L656	I657	A658	E659	H660	L661	A662	D663	L666	P667	P668	Q669	L670	L671	F672	H673	P674	R675	Y674	N676	A679	V680	L681	R682	L683	R686	I687	S688	A689	L690	P691	G692	L693	N694	N695			
E572	L573	R574	E577	L578	M579	E580	H581	H582	R583	L584	R585	P586	F587	P588	D589	Y590	E591	E592	T593	L594	R595	L596	F597	K598	T599	T600	V601	T602	S603	P604	M605	P606	P607	E608	L609	C610	Y611	L612	V613	D614	V615	L616	V617	H618	G619	N620	V621	D622	A623	F624	L625	L626	I627	R628	T629	F630	V631		
R502	R503	E504	R507	T508	V509	N510	K513	Q514	D515	V518	T519	D520	F521	F522	K523	V524	G525	N526	L529	E532	L533	H534	P535	F536	F537	D538	F539	T540	H541	C542	Q543	E544	N545	S546	E547	T548	V549	A550	L551	C552	T553	P554	R555	T556	V557	T558	L561	P562	D563	L565	A566	P567							
D441	F442	V443	A444	A445	L446	K447	T448	L449	C450	H451	L454	H455	E456	P457	A458	P459	C460	L461	Q462	T463	F464	T465	E466	R467	G468	P469	P470	S471	E472	Q476	R477	L478	L479	E480	C481	R482	F483	Q484	Q485	E486	P487	M488	G489	G490	A491	A492	R493	R494	T495	P496	H497	F498	Y499	R500	V501				
H319	S320	I321	A323	A323	D324	F325	N326	S327	Y328	K329	A330	H331	L332	T333	S334	G335	Q336	P337	H338	L339	P340	N341	D342	S343	L344	S345	Q346	A347	G348	A349	H350	S351	L352	P353	L355	S356	M357	D358	V359	I360	R361	L362	G363	E364	V306	L307	T366	V367	P309	E310	M369	E370	N371	T372	R373	R374	V375	T376	K377
P258	T259	T260	Y261	T262	T263	S264	S265	G266	A267	K268	D269	S270	M273	V274	S275	T276	A277	N278	P279	Q281	K282	I283	M284	S285	L286	L287	S288	S289	H290	I291	T292	K293	E294	T295	V296	S297	A298	P299	A300	T301	Y302	G303	N304	F305	V306	L307	S308	V367	P309	E310	M369	E370	N371	T372	R373	R374	V375	T376	K377
V197	E198	N199	A200	T201	L202	A203	R204	Q205	A206	L207	N208	R209	I210	Q211	R212	I215	L216	Q217	S218	F219	K220	A221	K222	M223	L224	A225	L226	F228	L229	T291	T292	K293	R232	T233	R234	D235	R236	D237	Y238	V239	L240	K241	F242	L243	T244	R245	L246	A247	E248	A249	A250	T251	D252	S253	I254	L255	D256	N257	



• Molecule 2: Tegument protein pp150



• Molecule 2: Tegument protein pp150

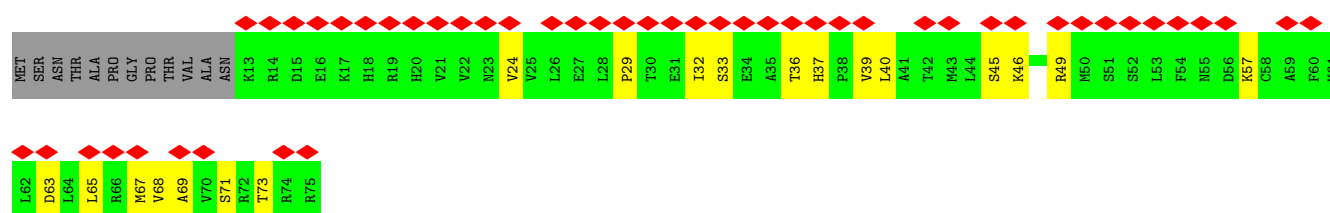
- Molecule 3: Small capsomere-interacting protein

Chain D: 

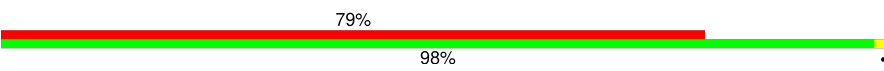


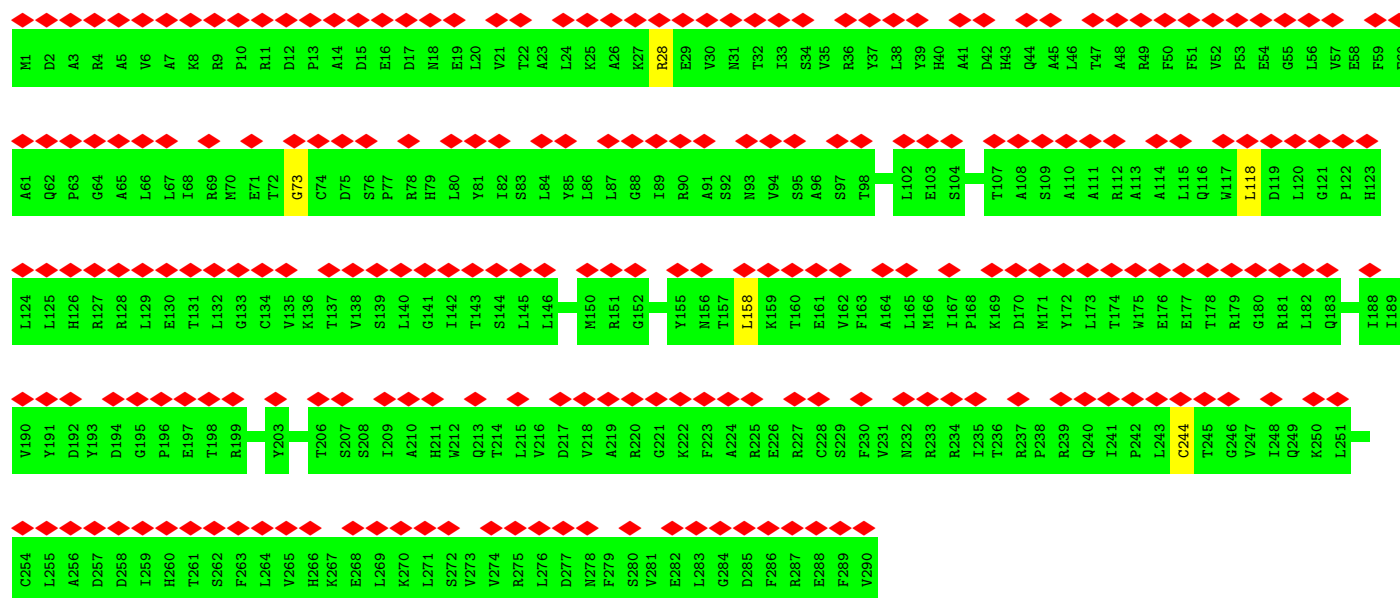
- Molecule 3: Small capsomere-interacting protein

Chain E: 




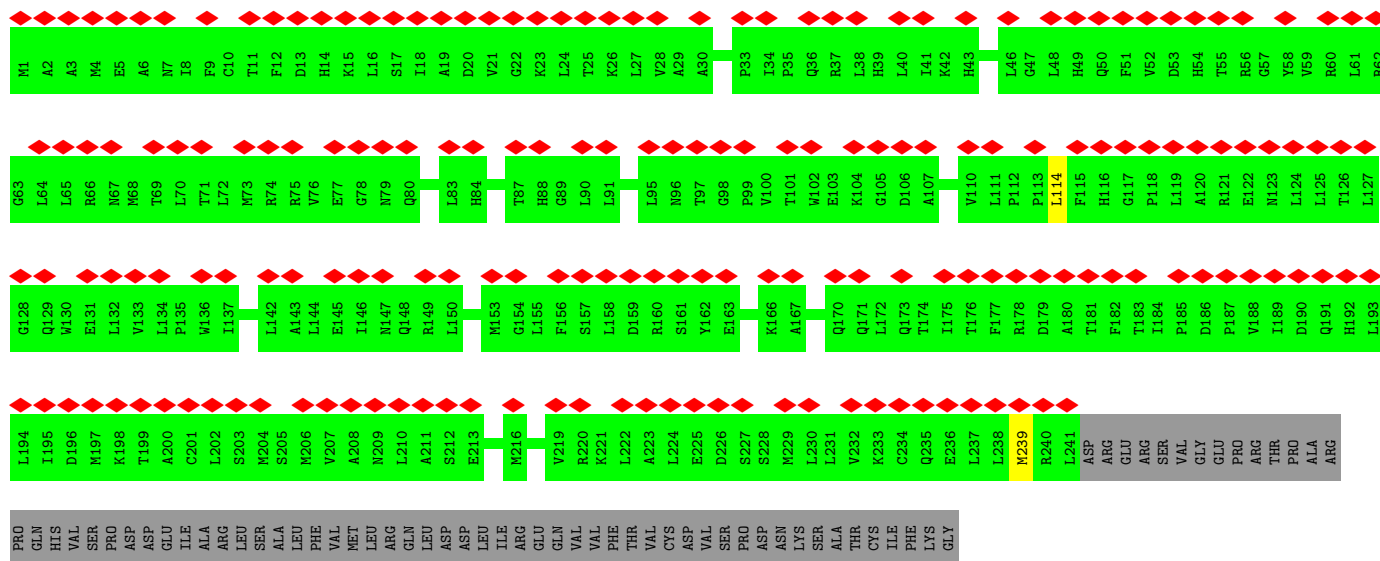
- Molecule 4: Triplex capsid protein 1

Chain p: 

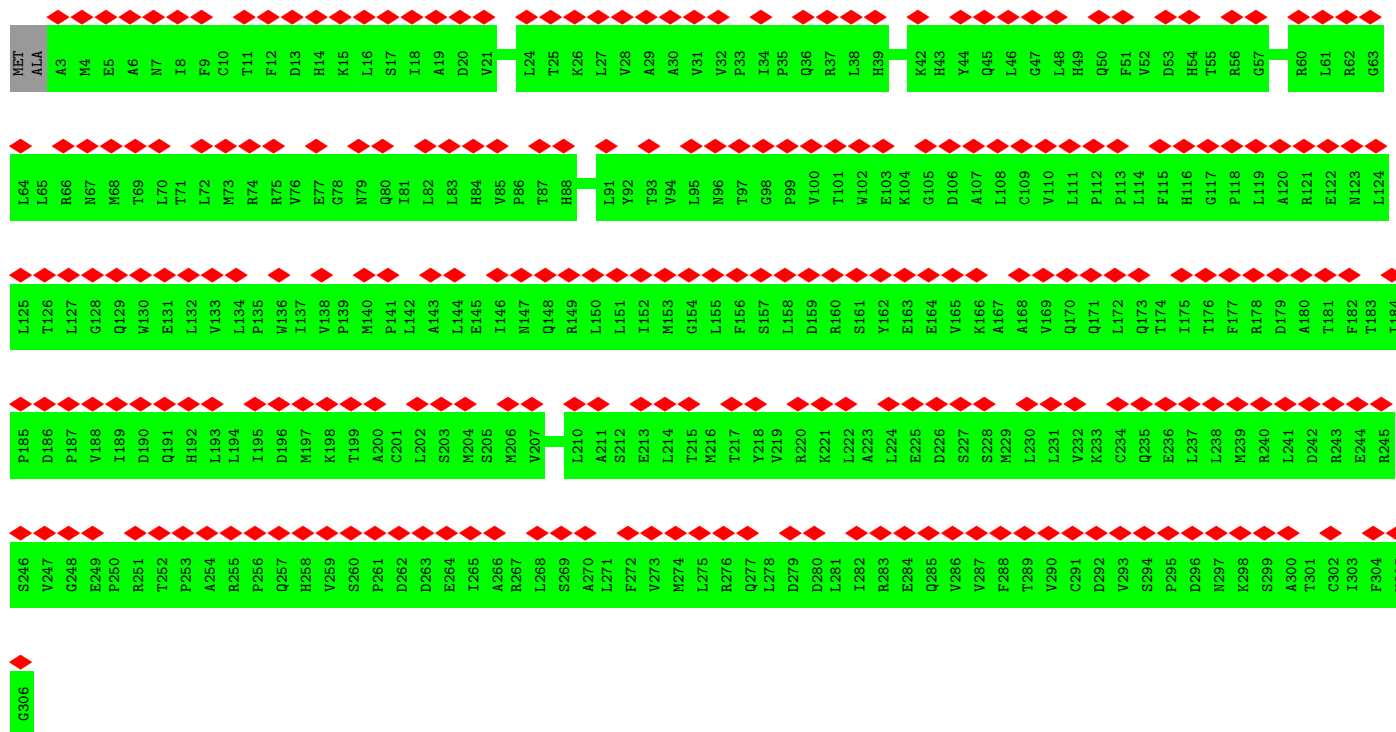
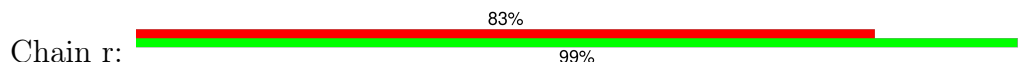


- Molecule 5: Triplex capsid protein 2

Chain q: 



• Molecule 5: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97166	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 ($e^-/\text{\AA}^2$)	18.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	412.16, 412.16, 412.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.61, 1.61, 1.61	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/10779	0.56	0/14684
1	C	0.49	0/10937	0.56	0/14899
1	J	0.48	0/10937	0.56	0/14899
2	4	0.38	0/2366	0.51	0/3192
2	5	0.36	0/2366	0.49	0/3192
2	6	0.40	0/2366	0.51	0/3192
3	D	0.42	0/520	0.50	0/697
3	E	0.41	0/520	0.57	0/697
3	Z	0.41	0/520	0.53	0/697
4	p	0.42	0/2374	0.57	0/3221
5	q	0.39	0/1949	0.55	0/2649
5	r	0.40	0/2458	0.59	0/3339
All	All	0.46	0/48092	0.55	0/65358

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10526	0	10468	605	0
1	C	10681	0	10620	681	0
1	J	10681	0	10618	630	0
2	4	2328	0	2363	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5	2328	0	2363	70	0
2	6	2328	0	2363	81	0
3	D	513	0	539	56	0
3	E	513	0	539	26	0
3	Z	513	0	539	33	0
4	p	2325	0	2362	0	0
5	q	1911	0	2007	0	0
5	r	2411	0	2500	0	0
All	All	47058	0	47281	2125	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 26.

All (2125) 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:C:203:ALA:CB	1:C:207:LEU:HD21	1.30	1.60
1:A:207:LEU:CD1	1:A:212:ARG:HG3	1.38	1.53
1:C:19:PHE:CE1	1:C:23:VAL:N	1.78	1.51
1:J:440:ILE:CD1	1:J:1108:VAL:HG11	1.38	1.50
1:A:207:LEU:HD11	1:A:212:ARG:CG	1.39	1.49
1:C:360:ILE:HD11	1:C:369:MET:SD	1.50	1.49
3:E:37:HIS:HD2	3:E:40:LEU:CB	1.24	1.48
1:J:440:ILE:HD11	1:J:1108:VAL:CG2	1.45	1.47
1:A:21:THR:HG22	1:C:200:ALA:CA	1.44	1.46
1:C:633:ARG:NH2	1:C:870:THR:HG21	1.19	1.44
1:C:186:LYS:NZ	1:C:1055:THR:HG21	1.21	1.43
1:A:521:PHE:CZ	1:A:532:GLU:OE2	1.68	1.43
1:C:764:GLU:HB3	1:C:765:PRO:CD	1.48	1.42
3:Z:37:HIS:HD2	3:Z:40:LEU:CB	1.32	1.42
1:C:687:ILE:HD12	1:C:1006:MET:SD	1.58	1.42
1:A:212:ARG:NH2	1:A:1204:PRO:HD3	1.25	1.41
1:C:1035:THR:CG2	1:C:1176:LEU:CD1	1.96	1.41
1:A:212:ARG:HH22	1:A:1204:PRO:CD	1.34	1.41
3:E:37:HIS:CD2	3:E:40:LEU:HB3	1.57	1.39
1:J:764:GLU:HB3	1:J:765:PRO:CD	1.47	1.38
1:C:489:GLY:CA	1:C:763:ASP:OD2	1.70	1.38
1:C:1285:TYR:CD1	1:C:1317:LEU:HD21	1.58	1.38
1:C:790:PRO:HB3	1:C:942:PHE:CD2	1.56	1.37
1:J:115:MET:O	1:C:35:LEU:CD1	1.71	1.37
2:4:77:LEU:HD11	2:4:114:PHE:CE1	1.59	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1172:CYS:SG	1:J:1261:PRO:HG2	1.65	1.35
1:A:668:PRO:O	1:A:672:PHE:CD2	1.77	1.34
1:A:764:GLU:HB3	1:A:765:PRO:CD	1.55	1.34
1:C:514:GLN:HB2	1:C:993:ARG:NH2	1.37	1.34
1:C:1035:THR:CG2	1:C:1176:LEU:HD12	1.52	1.33
1:C:1285:TYR:CZ	1:C:1317:LEU:HD11	1.61	1.33
2:4:77:LEU:HD11	2:4:114:PHE:CD1	1.63	1.32
1:A:21:THR:CG2	1:C:200:ALA:HA	1.59	1.32
1:C:19:PHE:CZ	1:C:23:VAL:N	1.98	1.32
1:J:35:LEU:CD1	1:A:115:MET:O	1.79	1.31
1:A:790:PRO:HB3	1:A:942:PHE:CD2	1.66	1.31
1:J:440:ILE:CD1	1:J:1108:VAL:CG1	2.06	1.30
1:J:764:GLU:CG	1:J:765:PRO:HD3	1.62	1.30
1:A:630:PHE:CZ	1:A:879:LEU:HD21	1.67	1.30
1:C:203:ALA:CB	1:C:207:LEU:CD2	2.07	1.30
1:C:764:GLU:CG	1:C:765:PRO:HD3	1.61	1.30
2:4:77:LEU:CD1	2:4:114:PHE:CE1	2.15	1.29
1:C:186:LYS:NZ	1:C:1055:THR:CG2	1.95	1.28
1:J:83:LEU:HD22	1:J:1080:ASN:ND2	1.49	1.28
1:J:790:PRO:HB3	1:J:942:PHE:CD2	1.67	1.28
1:C:1035:THR:HG21	1:C:1176:LEU:CD1	1.57	1.27
1:A:1328:THR:HG21	1:A:1353:ASN:OD1	1.35	1.26
1:C:360:ILE:CD1	1:C:369:MET:SD	2.24	1.25
1:J:193:VAL:HG11	1:J:1093:ASN:ND2	1.48	1.25
1:C:203:ALA:HB1	1:C:207:LEU:CD2	1.63	1.25
2:4:248:ASN:OD1	2:4:251:ARG:NH2	1.71	1.24
1:C:1285:TYR:CE1	1:C:1317:LEU:HD11	1.70	1.24
1:C:1285:TYR:CE2	1:C:1317:LEU:HD11	1.71	1.24
1:C:764:GLU:CB	1:C:765:PRO:CD	2.15	1.24
1:C:687:ILE:CD1	1:C:1006:MET:SD	2.25	1.23
1:A:21:THR:HG22	1:C:200:ALA:CB	1.67	1.23
1:J:7:LEU:CD1	1:J:12:LYS:HD3	1.67	1.23
1:C:275:SER:OG	1:C:1047:LEU:HD13	1.32	1.22
1:C:275:SER:OG	1:C:1047:LEU:CD1	1.87	1.21
1:A:795:ASN:OD1	1:A:942:PHE:CE1	1.93	1.21
1:C:733:VAL:CG1	1:C:735:ASP:O	1.87	1.21
1:C:633:ARG:CZ	1:C:870:THR:HG21	1.67	1.21
3:Z:37:HIS:CD2	3:Z:40:LEU:CB	2.23	1.21
1:J:764:GLU:CB	1:J:765:PRO:CD	2.16	1.20
1:A:521:PHE:HZ	1:A:532:GLU:OE2	0.94	1.20
3:E:37:HIS:CD2	3:E:40:LEU:CB	2.15	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:113:GLU:O	2:6:124:ILE:HD13	1.41	1.20
3:Z:37:HIS:CE1	3:Z:39:VAL:CG1	2.25	1.19
1:J:790:PRO:HB2	1:J:942:PHE:CE2	1.76	1.19
1:C:27:ALA:HB1	1:C:35:LEU:HD21	1.21	1.19
1:J:687:ILE:HG21	1:J:1006:MET:HE3	1.21	1.18
1:A:475:MET:SD	1:A:1218:ARG:NH1	2.17	1.18
1:C:7:LEU:CD1	1:C:12:LYS:HD3	1.72	1.18
3:D:47:TYR:CE2	3:D:64:LEU:HD21	1.79	1.17
1:J:1172:CYS:SG	1:J:1261:PRO:CG	2.32	1.17
1:C:19:PHE:CE1	1:C:23:VAL:CA	2.20	1.17
1:C:472:GLU:OE1	1:C:1218:ARG:NH1	1.77	1.16
1:A:19:PHE:CZ	1:C:1088:LEU:HD13	1.54	1.16
1:C:489:GLY:C	1:C:763:ASP:OD2	1.84	1.16
1:C:633:ARG:NH2	1:C:870:THR:CG2	2.08	1.16
3:D:26:LEU:CD1	3:D:64:LEU:CD1	2.24	1.15
1:J:440:ILE:HD13	1:J:1108:VAL:CG1	1.70	1.15
1:J:21:THR:HG22	1:A:200:ALA:CA	1.75	1.15
1:J:35:LEU:HD12	1:A:115:MET:O	0.97	1.15
1:A:90:LYS:HD3	1:A:119:TYR:CE1	1.81	1.15
1:A:800:LEU:CD2	1:A:923:VAL:HG21	1.77	1.15
3:D:47:TYR:HE2	3:D:64:LEU:HD21	0.99	1.15
1:A:800:LEU:HD23	1:A:923:VAL:CG2	1.76	1.15
1:C:1035:THR:HG23	1:C:1176:LEU:CD1	1.66	1.15
1:J:41:ASP:OD1	1:J:45:ARG:NH1	1.80	1.14
1:A:284:MET:SD	1:A:291:ILE:HD13	1.88	1.14
1:C:514:GLN:CB	1:C:993:ARG:NH2	2.10	1.14
1:J:790:PRO:CB	1:J:942:PHE:CE2	2.31	1.14
1:C:790:PRO:CB	1:C:942:PHE:CD2	2.30	1.14
1:J:7:LEU:HD12	1:J:12:LYS:HD3	1.15	1.14
1:C:1285:TYR:CG	1:C:1317:LEU:HD21	1.83	1.14
1:C:203:ALA:HB2	1:C:207:LEU:HD21	1.14	1.13
1:J:440:ILE:CD1	1:J:1108:VAL:HG21	1.77	1.13
1:J:440:ILE:HD11	1:J:1108:VAL:CG1	1.73	1.13
1:J:718:PRO:HD3	1:J:786:LEU:HD21	1.25	1.13
1:C:9:LEU:HD11	1:C:45:ARG:HG2	1.23	1.13
3:Z:37:HIS:CD2	3:Z:40:LEU:HB2	1.81	1.12
3:D:26:LEU:HD11	3:D:64:LEU:CD1	1.77	1.13
1:C:790:PRO:HB2	1:C:942:PHE:CE2	1.83	1.12
2:5:253:ILE:HG21	2:5:271:LEU:HD23	1.28	1.12
1:A:913:ARG:NH1	1:A:981:HIS:CD2	2.17	1.12
1:A:424:LEU:HD23	1:A:577:GLU:OE2	1.46	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:PRO:HB2	1:A:942:PHE:CE2	1.83	1.11
1:J:193:VAL:CG1	1:J:1093:ASN:HD21	1.64	1.11
1:J:207:LEU:HD11	1:J:212:ARG:HG3	1.15	1.11
1:C:1035:THR:CG2	1:C:1176:LEU:HD11	1.78	1.11
1:J:790:PRO:CB	1:J:942:PHE:CD2	2.34	1.11
1:A:431:LEU:HD22	1:A:436:ALA:C	1.71	1.11
1:C:9:LEU:CD1	1:C:45:ARG:CG	2.29	1.11
1:C:1285:TYR:CD1	1:C:1317:LEU:CD2	2.34	1.11
1:J:193:VAL:HG21	1:J:1093:ASN:CG	1.69	1.10
1:A:388:ASN:OD1	1:A:1043:GLU:HA	1.51	1.10
1:A:534:HIS:CE1	1:A:1239:LEU:HD22	1.85	1.10
1:C:489:GLY:HA2	1:C:763:ASP:OD2	1.41	1.10
1:J:115:MET:O	1:C:35:LEU:HD12	0.93	1.10
1:C:795:ASN:OD1	1:C:942:PHE:CD1	2.04	1.10
3:Z:37:HIS:NE2	3:Z:39:VAL:HG13	1.65	1.10
1:J:723:LEU:HB2	1:J:772:ARG:NH2	1.67	1.09
1:C:1285:TYR:CZ	1:C:1317:LEU:CD1	2.34	1.09
1:A:790:PRO:CB	1:A:942:PHE:CE2	2.36	1.09
1:J:35:LEU:HD13	1:A:116:VAL:HG12	1.19	1.09
1:J:440:ILE:HD11	1:J:1108:VAL:CB	1.83	1.08
1:J:534:HIS:CD2	1:J:537:PHE:HD1	1.70	1.08
1:C:1285:TYR:CD1	1:C:1317:LEU:HD11	1.87	1.08
1:J:440:ILE:HD11	1:J:1108:VAL:HG21	1.21	1.08
1:A:193:VAL:HG11	1:A:1093:ASN:HD21	1.15	1.08
1:A:426:THR:CG2	1:A:442:PHE:HE2	1.66	1.08
3:Z:37:HIS:HD2	3:Z:40:LEU:HB2	0.96	1.08
1:J:22:HIS:CG	1:J:23:VAL:H	1.68	1.08
1:A:12:LYS:HE3	1:C:94:HIS:HB3	1.33	1.08
1:A:19:PHE:CZ	1:C:1088:LEU:CD1	2.23	1.07
1:A:1034:LEU:HD22	1:A:1173:GLU:OE2	1.54	1.07
1:C:1160:ASN:ND2	1:C:1298:ASP:H	1.51	1.07
1:A:764:GLU:CB	1:A:765:PRO:CD	2.31	1.07
1:C:9:LEU:HD11	1:C:45:ARG:CG	1.84	1.07
1:C:19:PHE:HE1	1:C:22:HIS:C	1.55	1.07
1:J:764:GLU:HG3	1:J:765:PRO:HD3	1.07	1.07
1:A:942:PHE:CZ	1:A:995:SER:HB3	1.88	1.07
1:C:19:PHE:CE1	1:C:23:VAL:HA	1.80	1.07
1:C:1285:TYR:CE1	1:C:1317:LEU:CD1	2.37	1.07
1:J:80:PHE:CE2	1:J:86:LEU:HD23	1.90	1.06
1:J:117:THR:HG21	1:C:2:GLU:OE2	1.54	1.06
1:A:431:LEU:CD2	1:A:436:ALA:C	2.24	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1285:TYR:CD2	1:C:1317:LEU:HD11	1.88	1.06
2:4:101:LYS:O	2:4:104:ASP:OD1	1.73	1.06
1:J:231:ASN:OD1	1:J:1098:TYR:CD1	2.08	1.06
1:J:598:LYS:HD2	1:J:1000:ASN:CB	1.85	1.06
3:D:26:LEU:HD11	3:D:64:LEU:HD11	1.14	1.06
1:J:538:ASP:OD1	1:J:555:ARG:CZ	2.04	1.06
1:A:790:PRO:CB	1:A:942:PHE:CD2	2.39	1.06
1:A:598:LYS:CD	1:A:792:MET:O	2.04	1.05
1:C:231:ASN:OD1	1:C:1098:TYR:CD1	2.09	1.05
1:J:207:LEU:CD1	1:J:212:ARG:HG3	1.85	1.05
1:C:440:ILE:HD12	1:C:1108:VAL:CG1	1.85	1.05
1:A:521:PHE:HE1	1:A:532:GLU:OE1	1.39	1.05
1:J:687:ILE:HG21	1:J:1006:MET:CE	1.87	1.05
1:A:668:PRO:HB2	1:A:672:PHE:HE2	1.21	1.05
1:C:7:LEU:HD12	1:C:12:LYS:HD3	1.31	1.05
1:J:21:THR:HG22	1:A:200:ALA:HA	1.10	1.04
1:J:41:ASP:OD1	1:J:45:ARG:CZ	2.05	1.04
1:J:723:LEU:HB2	1:J:772:ARG:HH21	1.20	1.04
1:C:508:THR:OG1	1:C:982:GLU:OE1	1.73	1.04
1:C:1341:ALA:O	1:C:1364:GLN:NE2	1.90	1.04
1:C:790:PRO:CB	1:C:942:PHE:CE2	2.39	1.04
1:C:203:ALA:HB2	1:C:207:LEU:CD2	1.81	1.03
1:J:27:ALA:HB1	1:J:35:LEU:HD21	1.37	1.03
1:A:90:LYS:CD	1:A:119:TYR:HE1	1.70	1.03
1:J:440:ILE:CD1	1:J:1108:VAL:CG2	2.34	1.03
1:A:426:THR:CG2	1:A:442:PHE:CE2	2.43	1.02
1:J:83:LEU:CD2	1:J:1080:ASN:ND2	2.22	1.02
1:A:90:LYS:HD3	1:A:119:TYR:HE1	0.90	1.02
1:C:942:PHE:CZ	1:C:995:SER:HB3	1.95	1.02
3:E:37:HIS:CE1	3:E:39:VAL:HG13	1.95	1.02
1:A:1105:ASP:OD2	1:A:1169:LYS:CB	2.07	1.01
1:C:766:LEU:HD22	1:C:891:LYS:HD2	1.37	1.01
1:J:41:ASP:OD1	1:J:45:ARG:NH2	1.93	1.01
1:C:203:ALA:HB1	1:C:207:LEU:HD21	1.04	1.01
1:J:41:ASP:CG	1:J:45:ARG:HH22	1.64	1.01
1:A:668:PRO:HB2	1:A:672:PHE:CE2	1.94	1.01
1:A:942:PHE:HZ	1:A:995:SER:HB3	1.21	1.01
1:A:1034:LEU:CD2	1:A:1173:GLU:OE2	2.08	1.01
1:C:633:ARG:HH22	1:C:870:THR:HG21	1.20	1.01
1:C:795:ASN:OD1	1:C:942:PHE:CE1	2.14	1.01
3:D:25:VAL:O	3:D:57:LYS:CE	2.09	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD11	1:A:12:LYS:HD3	1.43	1.01
1:C:764:GLU:HG3	1:C:765:PRO:HD3	1.01	1.01
1:J:35:LEU:HD13	1:A:116:VAL:CG1	1.90	1.01
1:A:27:ALA:HB1	1:A:35:LEU:CD2	1.91	1.01
1:C:489:GLY:O	1:C:763:ASP:OD1	1.79	1.01
1:J:764:GLU:HB3	1:J:765:PRO:HD2	1.01	1.00
1:C:440:ILE:HD12	1:C:1108:VAL:HG11	1.40	1.00
1:J:718:PRO:HD3	1:J:786:LEU:CD2	1.89	1.00
1:C:19:PHE:HE1	1:C:23:VAL:N	1.28	1.00
1:J:116:VAL:HG12	1:C:35:LEU:HD13	1.43	1.00
1:C:764:GLU:CB	1:C:765:PRO:HD3	1.85	1.00
2:4:77:LEU:HD12	2:4:114:PHE:CE1	1.97	1.00
1:A:7:LEU:CD1	1:A:12:LYS:HD3	1.92	0.99
3:D:25:VAL:O	3:D:57:LYS:HE3	1.62	0.99
1:A:426:THR:HG23	1:A:442:PHE:HE2	1.25	0.99
1:J:119:TYR:OH	1:C:2:GLU:OE2	1.78	0.99
1:J:21:THR:CG2	1:A:200:ALA:HA	1.92	0.99
1:J:116:VAL:CG1	1:C:35:LEU:HD13	1.93	0.99
1:A:193:VAL:HG21	1:A:1093:ASN:CG	1.81	0.99
1:A:630:PHE:CZ	1:A:879:LEU:CD2	2.46	0.99
1:C:514:GLN:HB2	1:C:993:ARG:HH21	1.20	0.99
1:C:942:PHE:CZ	1:C:995:SER:CB	2.45	0.98
1:C:1035:THR:HG21	1:C:1176:LEU:HD11	1.33	0.98
1:J:430:LEU:CD2	1:J:1325:LEU:O	2.11	0.98
1:A:1344:PHE:HB2	1:A:1364:GLN:NE2	1.77	0.98
1:C:27:ALA:CB	1:C:35:LEU:HD21	1.93	0.98
1:J:764:GLU:CB	1:J:765:PRO:HD3	1.82	0.98
1:C:27:ALA:HB1	1:C:35:LEU:CD2	1.93	0.98
1:J:231:ASN:OD1	1:J:1098:TYR:CE1	2.17	0.98
1:A:1102:VAL:HG23	1:A:1366:MET:HE1	1.46	0.98
1:C:231:ASN:ND2	1:C:1099:VAL:H	1.61	0.98
3:Z:37:HIS:HD2	3:Z:40:LEU:HB3	1.27	0.98
1:A:924:VAL:HG12	1:A:925:THR:HG23	1.43	0.97
1:C:275:SER:HG	1:C:1047:LEU:CD1	1.78	0.97
1:A:1328:THR:CG2	1:A:1353:ASN:OD1	2.12	0.97
1:C:1285:TYR:CG	1:C:1317:LEU:HD11	1.99	0.97
1:J:228:PHE:CD1	1:J:1099:VAL:HG23	1.99	0.97
1:A:764:GLU:HB3	1:A:765:PRO:HD3	0.97	0.97
1:C:800:LEU:CD2	1:C:923:VAL:HG21	1.93	0.97
1:J:388:ASN:OD1	1:J:1311:ILE:HG13	1.63	0.97
1:A:795:ASN:OD1	1:A:942:PHE:CD1	2.18	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:113:GLU:O	2:6:124:ILE:CD1	2.12	0.96
1:J:7:LEU:HD12	1:J:12:LYS:CD	1.95	0.96
1:C:9:LEU:CD1	1:C:45:ARG:HG3	1.93	0.96
3:D:26:LEU:HD13	3:D:64:LEU:CD1	1.94	0.96
1:A:1102:VAL:HG23	1:A:1366:MET:CE	1.95	0.96
1:C:764:GLU:HB3	1:C:765:PRO:HD2	0.99	0.96
1:A:668:PRO:O	1:A:672:PHE:HD2	1.36	0.96
1:A:90:LYS:CD	1:A:119:TYR:CE1	2.47	0.96
1:A:888:GLU:O	1:A:919:ASN:ND2	1.98	0.96
1:C:1285:TYR:CE2	1:C:1317:LEU:CD1	2.49	0.96
1:C:231:ASN:HD21	1:C:1099:VAL:N	1.62	0.95
3:E:37:HIS:HD2	3:E:40:LEU:HB2	1.32	0.95
1:J:684:VAL:HG22	1:J:1006:MET:SD	2.07	0.95
1:C:424:LEU:HD23	1:C:577:GLU:OE2	1.67	0.95
1:A:207:LEU:HD11	1:A:212:ARG:HG2	1.45	0.95
1:A:598:LYS:NZ	1:A:792:MET:O	2.00	0.95
1:A:790:PRO:HB3	1:A:942:PHE:HD2	1.25	0.95
1:A:598:LYS:HD3	1:A:792:MET:O	1.65	0.94
1:C:186:LYS:HZ1	1:C:1055:THR:CG2	1.65	0.94
1:J:22:HIS:CD2	1:J:23:VAL:H	1.85	0.94
1:J:604:PRO:HA	1:J:925:THR:HG21	1.50	0.94
1:A:193:VAL:HG21	1:A:1093:ASN:ND2	1.83	0.94
1:C:514:GLN:HB2	1:C:993:ARG:HH22	1.24	0.94
1:J:7:LEU:CD1	1:J:12:LYS:CD	2.46	0.94
1:J:440:ILE:CG1	1:J:1108:VAL:HG21	1.97	0.94
1:A:913:ARG:HH11	1:A:981:HIS:CD2	1.86	0.94
1:A:35:LEU:HD13	1:C:116:VAL:HG13	1.50	0.94
2:5:253:ILE:HG21	2:5:271:LEU:CD2	1.97	0.94
3:Z:37:HIS:CD2	3:Z:40:LEU:HB3	1.95	0.94
3:E:37:HIS:CD2	3:E:40:LEU:HB2	2.02	0.94
1:C:426:THR:O	1:C:442:PHE:CE2	2.21	0.93
1:J:193:VAL:HG11	1:J:1093:ASN:HD21	0.79	0.93
1:C:1160:ASN:OD1	1:C:1298:ASP:HB3	1.68	0.93
1:C:646:VAL:HG12	1:C:647:PHE:CD1	2.04	0.93
1:A:193:VAL:HG11	1:A:1093:ASN:ND2	1.81	0.93
1:J:231:ASN:HD21	1:J:1099:VAL:H	1.05	0.93
1:A:426:THR:HG23	1:A:442:PHE:CE2	2.02	0.93
1:J:1069:ARG:HH11	1:J:1069:ARG:HG3	1.34	0.93
1:A:193:VAL:HG21	1:A:1093:ASN:OD1	1.66	0.93
1:A:766:LEU:HD21	1:A:893:LEU:HD21	1.48	0.93
1:C:489:GLY:O	1:C:763:ASP:CG	2.06	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:CYS:SG	1:A:507:ARG:O	2.25	0.93
1:C:766:LEU:HD22	1:C:891:LYS:CD	1.99	0.93
3:Z:37:HIS:CE1	3:Z:39:VAL:HG12	2.00	0.92
1:A:1056:SER:OG	1:A:1084:VAL:HG22	1.69	0.92
1:A:21:THR:HG22	1:C:200:ALA:HA	0.93	0.92
1:C:231:ASN:OD1	1:C:1098:TYR:HD1	1.47	0.92
1:J:12:LYS:HE3	1:A:94:HIS:HB3	1.49	0.92
1:C:83:LEU:HD12	1:C:1058:ILE:HG22	1.49	0.92
1:C:1056:SER:OG	1:C:1084:VAL:CG2	2.18	0.92
1:C:1285:TYR:CD1	1:C:1317:LEU:CG	2.53	0.92
1:C:175:LEU:CD1	1:C:1081:ILE:HD11	1.99	0.92
1:J:193:VAL:HG21	1:J:1093:ASN:OD1	1.69	0.91
1:A:130:GLU:CD	1:A:1074:THR:HG22	1.90	0.91
1:A:764:GLU:CB	1:A:765:PRO:HD3	1.94	0.91
1:J:231:ASN:ND2	1:J:1099:VAL:H	1.67	0.91
1:C:1160:ASN:HD21	1:C:1298:ASP:H	1.18	0.91
1:A:426:THR:HG22	1:A:442:PHE:CE2	2.04	0.91
1:J:228:PHE:CE1	1:J:1099:VAL:CG2	2.53	0.91
1:C:598:LYS:HD2	1:C:1000:ASN:HD22	1.32	0.91
1:J:37:ILE:HG12	1:A:114:ILE:HG12	1.51	0.91
3:D:25:VAL:HG22	3:D:54:PHE:HE1	1.34	0.91
1:A:630:PHE:CE1	1:A:879:LEU:HD21	2.07	0.90
1:A:942:PHE:CZ	1:A:995:SER:CB	2.53	0.90
1:C:790:PRO:HB3	1:C:942:PHE:HD2	1.09	0.90
3:E:37:HIS:HD2	3:E:40:LEU:HB3	0.75	0.90
1:C:534:HIS:CE1	1:C:1239:LEU:HD22	2.06	0.90
1:C:1285:TYR:CD1	1:C:1317:LEU:CD1	2.55	0.90
1:J:534:HIS:CD2	1:J:537:PHE:CD1	2.60	0.90
1:A:733:VAL:HG22	1:A:738:PRO:HA	1.51	0.90
3:E:69:ALA:O	3:E:73:THR:HG23	1.71	0.90
1:A:744:ILE:O	1:A:765:PRO:HA	1.72	0.89
1:A:1105:ASP:OD2	1:A:1169:LYS:HB2	1.72	0.89
3:D:25:VAL:HG22	3:D:54:PHE:CE1	2.07	0.89
1:A:90:LYS:HG2	1:A:119:TYR:CD1	2.07	0.89
1:J:21:THR:HG22	1:A:200:ALA:CB	2.02	0.89
1:J:22:HIS:CD2	1:J:24:LYS:H	1.89	0.89
1:C:99:ARG:NH1	1:C:111:GLN:HB3	1.86	0.89
1:J:718:PRO:CD	1:J:786:LEU:HD21	2.02	0.89
1:J:732:VAL:HG12	1:J:739:LEU:HD12	1.54	0.89
1:C:7:LEU:HD11	1:C:12:LYS:HD3	1.54	0.89
1:A:207:LEU:HD13	1:A:212:ARG:HG3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:49:ARG:NH2	2:5:242:CYS:SG	2.45	0.89
1:J:723:LEU:CB	1:J:772:ARG:NH2	2.36	0.88
1:J:22:HIS:CG	1:J:23:VAL:N	2.41	0.88
1:C:524:VAL:HG22	1:C:1227:ALA:HB2	1.54	0.88
1:A:598:LYS:HE2	1:A:1000:ASN:ND2	1.86	0.88
1:J:790:PRO:HB3	1:J:942:PHE:HD2	1.32	0.88
1:A:388:ASN:OD1	1:A:1043:GLU:OE1	1.91	0.88
1:A:521:PHE:CE1	1:A:532:GLU:OE1	2.26	0.88
1:A:431:LEU:CD2	1:A:436:ALA:O	2.21	0.88
1:C:752:SER:OG	3:E:46:LYS:NZ	2.07	0.88
1:C:791:ALA:O	1:C:1000:ASN:OD1	1.90	0.88
1:J:1172:CYS:SG	1:J:1261:PRO:CD	2.62	0.87
1:A:1056:SER:OG	1:A:1084:VAL:CG2	2.23	0.87
1:J:7:LEU:O	1:J:12:LYS:NZ	2.07	0.87
3:D:25:VAL:C	3:D:57:LYS:HE3	1.95	0.87
1:J:1172:CYS:SG	1:J:1261:PRO:HD2	2.12	0.87
1:A:521:PHE:CE1	1:A:532:GLU:OE2	2.27	0.87
1:J:45:ARG:NH2	1:J:46:TYR:HE2	1.72	0.87
1:C:275:SER:OG	1:C:1047:LEU:HD12	1.74	0.87
1:C:733:VAL:HG11	1:C:735:ASP:O	1.72	0.87
2:6:166:ARG:HD3	2:6:186:LEU:HD11	1.57	0.87
1:A:130:GLU:OE2	1:A:1074:THR:HG22	1.75	0.86
1:A:913:ARG:NH1	1:A:981:HIS:NE2	2.22	0.86
3:E:37:HIS:CE1	3:E:39:VAL:CG1	2.58	0.86
1:J:1015:ILE:HG22	1:J:1015:ILE:O	1.73	0.86
1:C:1035:THR:HG23	1:C:1176:LEU:HD12	0.87	0.86
1:A:942:PHE:HZ	1:A:995:SER:CB	1.87	0.86
1:C:942:PHE:HZ	1:C:995:SER:CB	1.87	0.86
3:Z:69:ALA:O	3:Z:73:THR:HG23	1.73	0.86
1:J:45:ARG:CZ	1:J:46:TYR:HE2	1.88	0.86
1:C:489:GLY:O	1:C:763:ASP:OD2	1.91	0.86
1:J:430:LEU:HD23	1:J:1325:LEU:O	1.75	0.86
1:A:431:LEU:HD23	1:A:436:ALA:O	1.75	0.86
1:C:790:PRO:HB2	1:C:942:PHE:HE2	1.36	0.86
2:6:246:ASP:CG	2:6:281:SER:HB2	1.96	0.86
1:J:440:ILE:HD13	1:J:1108:VAL:HG11	0.87	0.86
1:A:193:VAL:CG1	1:A:1093:ASN:HD21	1.89	0.86
1:C:83:LEU:CD1	1:C:1058:ILE:HG22	2.05	0.86
1:A:662:ALA:HA	1:A:671:LEU:HD11	1.54	0.85
1:J:118:LYS:HD3	1:C:32:PHE:CE1	2.11	0.85
1:A:687:ILE:HD12	1:A:1006:MET:SD	2.15	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:HD22	1:A:704:SER:HB3	1.40	0.85
1:A:21:THR:CG2	1:C:200:ALA:CB	2.53	0.85
3:Z:37:HIS:CE1	3:Z:39:VAL:HG13	2.02	0.85
1:J:756:ARG:NH2	1:J:886:VAL:O	2.10	0.85
1:J:1069:ARG:O	1:J:1071:ILE:N	2.08	0.85
1:A:270:SER:OG	1:A:365:LYS:HG2	1.76	0.85
1:J:1244:TYR:HB2	1:J:1266:PHE:HD2	1.42	0.85
1:A:749:HIS:NE2	1:A:769:ASP:OD1	2.10	0.85
1:C:756:ARG:NH2	1:C:886:VAL:O	2.10	0.85
1:A:1015:ILE:O	1:A:1015:ILE:HG22	1.77	0.84
1:A:1212:LYS:HG2	1:A:1216:ASP:OD2	1.76	0.84
2:5:140:VAL:O	2:5:140:VAL:HG12	1.74	0.84
3:D:26:LEU:CD1	3:D:64:LEU:HD12	2.05	0.84
2:5:253:ILE:CG2	2:5:271:LEU:HD23	2.08	0.84
2:6:19:PHE:CE2	2:6:26:LYS:NZ	2.45	0.84
1:C:733:VAL:HG22	1:C:738:PRO:HA	1.58	0.84
1:A:536:PHE:CD1	1:A:1015:ILE:HG21	2.13	0.84
1:C:888:GLU:O	1:C:919:ASN:ND2	2.10	0.84
3:E:37:HIS:NE2	3:E:39:VAL:HG13	1.92	0.84
1:A:19:PHE:HZ	1:C:1088:LEU:HD13	1.36	0.84
2:5:253:ILE:CG2	2:5:271:LEU:CD2	2.55	0.84
1:C:231:ASN:HD21	1:C:1099:VAL:H	0.84	0.84
1:J:181:GLN:NE2	1:J:384:PRO:HB3	1.93	0.83
1:A:231:ASN:HD21	1:A:1099:VAL:H	1.26	0.83
1:C:1285:TYR:CG	1:C:1317:LEU:CD2	2.60	0.83
1:C:662:ALA:HA	1:C:671:LEU:HD11	1.61	0.83
1:A:715:LEU:HA	1:A:914:GLN:HE22	1.41	0.83
2:4:239:LEU:O	2:4:251:ARG:NH1	2.11	0.83
1:A:207:LEU:CD1	1:A:212:ARG:CG	2.19	0.83
1:A:388:ASN:ND2	1:A:1043:GLU:OE2	2.12	0.83
1:A:534:HIS:HE1	1:A:1239:LEU:HD22	1.44	0.83
1:J:231:ASN:HD21	1:J:1099:VAL:N	1.75	0.83
1:A:130:GLU:OE2	1:A:1074:THR:CG2	2.26	0.82
1:J:36:ARG:NH2	1:A:115:MET:CE	2.42	0.82
1:J:1327:THR:HG22	1:J:1355:VAL:HG13	1.61	0.82
1:J:440:ILE:HD11	1:J:1108:VAL:HG22	1.61	0.82
1:A:388:ASN:HD21	1:A:1043:GLU:CD	1.83	0.82
1:C:764:GLU:HG3	1:C:765:PRO:CD	1.98	0.82
2:5:140:VAL:HG21	2:5:158:HIS:NE2	1.95	0.82
1:J:723:LEU:CG	1:J:772:ARG:NH2	2.42	0.82
1:C:627:ILE:HD11	1:C:882:ALA:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:448:THR:CG2	1:J:1111:GLN:O	2.27	0.82
1:A:534:HIS:CE1	1:A:1239:LEU:HD13	2.15	0.82
2:5:267:LEU:O	2:5:271:LEU:HG	1.79	0.82
1:J:718:PRO:CD	1:J:786:LEU:CD2	2.58	0.81
1:A:27:ALA:HB1	1:A:35:LEU:HD21	1.62	0.81
1:C:433:ARG:NH1	1:C:1166:HIS:O	2.14	0.81
2:6:49:ARG:HH22	2:6:242:CYS:HB2	1.44	0.81
1:J:344:LEU:HD21	1:J:1086:MET:SD	2.20	0.81
1:J:799:GLY:O	1:J:937:VAL:HG13	1.81	0.81
3:D:26:LEU:CD1	3:D:64:LEU:HD11	1.94	0.81
3:D:47:TYR:HE2	3:D:64:LEU:CD2	1.87	0.81
1:J:2:GLU:OE1	1:A:90:LYS:NZ	2.12	0.81
1:A:668:PRO:O	1:A:672:PHE:CE2	2.33	0.81
1:A:1016:SER:O	1:A:1019:SER:OG	1.97	0.81
1:J:36:ARG:NH2	1:A:115:MET:HE1	1.95	0.81
1:J:228:PHE:CD1	1:J:1099:VAL:CG2	2.64	0.81
1:C:633:ARG:HH22	1:C:870:THR:CG2	1.78	0.81
1:C:1285:TYR:CB	1:C:1317:LEU:HD21	2.11	0.81
1:J:207:LEU:HD11	1:J:212:ARG:CG	2.04	0.80
1:J:181:GLN:HE22	1:J:384:PRO:HB3	1.46	0.80
1:A:207:LEU:HD11	1:A:212:ARG:HG3	0.89	0.80
3:D:26:LEU:HD13	3:D:64:LEU:HD12	1.61	0.80
1:J:193:VAL:HG21	1:J:1093:ASN:ND2	1.96	0.80
1:J:785:TYR:O	1:J:943:TYR:OH	1.97	0.80
1:J:1239:LEU:O	1:J:1239:LEU:HD12	1.82	0.80
3:E:37:HIS:CD2	3:E:40:LEU:H	1.99	0.80
1:C:1285:TYR:HD1	1:C:1317:LEU:HD21	1.41	0.80
1:J:228:PHE:CZ	1:J:1099:VAL:HG21	2.15	0.80
1:C:9:LEU:HD13	1:C:45:ARG:HG3	1.64	0.80
2:6:19:PHE:HE2	2:6:26:LYS:NZ	1.79	0.80
1:A:231:ASN:OD1	1:A:1098:TYR:CD1	2.35	0.80
2:5:156:PHE:HB3	2:5:159:LEU:HD12	1.64	0.80
1:A:130:GLU:CG	1:A:1074:THR:HG22	2.12	0.79
1:A:1092:SER:O	1:A:1093:ASN:OD1	2.00	0.79
3:E:24:VAL:O	3:E:57:LYS:NZ	2.14	0.79
1:A:426:THR:HG22	1:A:442:PHE:CD2	2.17	0.79
1:C:9:LEU:HD12	1:C:45:ARG:HD2	1.63	0.79
1:C:800:LEU:HG	1:C:923:VAL:HG21	1.64	0.79
1:C:1064:VAL:HG22	1:C:1077:VAL:HG12	1.64	0.79
1:J:118:LYS:NZ	1:C:32:PHE:CE1	2.50	0.79
1:A:601:VAL:HG12	1:A:793:THR:HG22	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1067:GLU:OE1	1:C:1076:HIS:NE2	2.15	0.79
1:C:1160:ASN:ND2	1:C:1298:ASP:N	2.29	0.79
1:J:18:ASP:O	1:J:19:PHE:CD1	2.36	0.79
1:J:687:ILE:CG2	1:J:1006:MET:CE	2.60	0.79
1:C:764:GLU:CG	1:C:765:PRO:CD	2.47	0.79
1:C:800:LEU:CG	1:C:923:VAL:HG21	2.13	0.79
1:A:1105:ASP:OD2	1:A:1169:LYS:HB3	1.81	0.78
1:C:1015:ILE:O	1:C:1015:ILE:HG22	1.80	0.78
2:4:181:VAL:HG12	2:4:183:PRO:HD3	1.63	0.78
3:D:43:MET:CE	3:D:67:MET:HG3	2.14	0.78
1:A:9:LEU:CD1	1:A:45:ARG:HG3	2.13	0.78
1:C:275:SER:HG	1:C:1047:LEU:HD13	1.35	0.78
1:A:747:ARG:NE	1:A:749:HIS:HE1	1.80	0.78
1:C:207:LEU:HD22	1:C:211:GLN:OE1	1.84	0.78
1:C:733:VAL:HG12	1:C:735:ASP:O	1.81	0.78
1:J:723:LEU:CB	1:J:772:ARG:HH21	1.96	0.78
1:A:747:ARG:NE	1:A:749:HIS:CE1	2.52	0.78
1:A:212:ARG:CZ	1:A:1204:PRO:HD3	2.12	0.78
1:A:521:PHE:CE1	1:A:532:GLU:CD	2.57	0.78
1:A:800:LEU:HD23	1:A:923:VAL:HG21	0.86	0.78
1:C:472:GLU:OE1	1:C:1218:ARG:CZ	2.31	0.78
1:C:942:PHE:HZ	1:C:995:SER:HB2	1.47	0.78
1:J:601:VAL:HG12	1:J:793:THR:HG22	1.66	0.78
1:A:400:TYR:HE1	1:A:573:LEU:HD12	1.48	0.78
2:5:88:ALA:HB2	2:5:109:LEU:HD22	1.64	0.78
1:C:1285:TYR:CD2	1:C:1317:LEU:CD1	2.67	0.78
1:J:534:HIS:HD2	1:J:537:PHE:HD1	1.27	0.77
2:6:248:ASN:O	2:6:252:ASN:ND2	2.18	0.77
1:J:94:HIS:HB3	1:C:12:LYS:HE3	1.66	0.77
2:4:69:HIS:O	2:4:179:PHE:CE1	2.37	0.77
1:C:1244:TYR:HB2	1:C:1266:PHE:HD2	1.47	0.77
3:D:47:TYR:CE2	3:D:64:LEU:CD2	2.64	0.77
1:A:231:ASN:OD1	1:A:1098:TYR:CE1	2.38	0.77
2:6:166:ARG:HD3	2:6:186:LEU:CD1	2.14	0.77
1:C:186:LYS:HZ2	1:C:1055:THR:HG21	0.87	0.77
1:C:431:LEU:HD23	1:C:437:VAL:HA	1.65	0.77
1:J:45:ARG:CZ	1:J:46:TYR:CE2	2.67	0.77
1:A:668:PRO:C	1:A:672:PHE:CD2	2.58	0.77
1:A:795:ASN:OD1	1:A:942:PHE:CZ	2.37	0.77
1:J:315:ALA:HB2	1:J:321:ILE:HD11	1.66	0.76
1:A:431:LEU:HD23	1:A:437:VAL:HA	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASN:OD1	1:C:1098:TYR:CE1	2.38	0.76
1:J:22:HIS:HD2	1:J:24:LYS:H	1.33	0.76
1:C:203:ALA:HB1	1:C:207:LEU:HD23	1.62	0.76
1:A:130:GLU:HG2	1:A:1074:THR:HA	1.67	0.76
1:J:888:GLU:O	1:J:919:ASN:ND2	2.19	0.76
1:J:1044:VAL:HG11	1:J:1096:VAL:CG1	2.15	0.76
1:C:1044:VAL:HG11	1:C:1096:VAL:HG13	1.66	0.76
1:C:1285:TYR:CE1	1:C:1317:LEU:CG	2.69	0.76
1:A:130:GLU:HG2	1:A:1074:THR:HG22	1.66	0.76
2:4:77:LEU:CD1	2:4:114:PHE:CD1	2.49	0.76
3:D:25:VAL:O	3:D:57:LYS:HE2	1.85	0.75
1:A:790:PRO:HB2	1:A:942:PHE:HE2	1.45	0.75
1:C:175:LEU:CD1	1:C:1081:ILE:CD1	2.63	0.75
1:J:27:ALA:HB1	1:J:35:LEU:CD2	2.16	0.75
1:J:119:TYR:CZ	1:C:2:GLU:OE2	2.40	0.75
1:J:388:ASN:OD1	1:J:1311:ILE:CG1	2.33	0.75
1:J:1092:SER:O	1:J:1093:ASN:OD1	2.05	0.75
1:A:785:TYR:O	1:A:943:TYR:OH	2.04	0.75
1:A:795:ASN:CG	1:A:942:PHE:CE1	2.59	0.75
2:4:69:HIS:O	2:4:179:PHE:HE1	1.67	0.75
1:J:275:SER:HB3	1:J:1047:LEU:HD13	1.68	0.75
1:J:983:TYR:O	1:J:988:ARG:NH2	2.20	0.75
1:J:80:PHE:CE2	1:J:86:LEU:CD2	2.70	0.75
1:J:130:GLU:HB3	1:J:1074:THR:HG22	1.68	0.75
1:C:924:VAL:HG12	1:C:925:THR:HG23	1.69	0.75
1:A:521:PHE:CZ	1:A:532:GLU:CD	2.59	0.74
1:C:1160:ASN:HD21	1:C:1298:ASP:N	1.83	0.74
1:A:448:THR:CG2	1:A:1111:GLN:O	2.35	0.74
1:A:753:ASP:O	1:A:757:LEU:HG	1.87	0.74
1:C:764:GLU:CB	1:C:765:PRO:HD2	1.92	0.74
1:C:942:PHE:HE1	1:C:992:SER:HA	1.52	0.74
1:C:1044:VAL:HG22	1:C:1099:VAL:CG2	2.18	0.74
2:4:77:LEU:HD12	2:4:114:PHE:CZ	2.23	0.74
1:C:186:LYS:HZ3	1:C:1055:THR:HG21	1.50	0.74
1:C:633:ARG:CZ	1:C:870:THR:CG2	2.59	0.74
1:J:344:LEU:CD2	1:J:1086:MET:SD	2.76	0.74
1:A:79:LYS:NZ	1:A:1061:ASN:OD1	2.19	0.74
1:A:424:LEU:HD23	1:A:577:GLU:CD	2.06	0.74
1:A:20:LEU:HD13	1:C:197:VAL:HG22	1.70	0.74
1:A:284:MET:SD	1:A:291:ILE:CD1	2.74	0.74
1:A:388:ASN:ND2	1:A:1043:GLU:CD	2.40	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1160:ASN:CG	1:C:1298:ASP:H	1.89	0.74
2:4:178:MET:HB2	2:4:213:VAL:HG13	1.70	0.74
2:5:253:ILE:HG22	2:5:271:LEU:HD21	1.68	0.73
1:J:118:LYS:NZ	1:C:32:PHE:HE1	1.84	0.73
1:J:1175:ILE:HB	1:J:1239:LEU:HD21	1.69	0.73
1:A:431:LEU:CD2	1:A:437:VAL:HA	2.18	0.73
1:C:1172:CYS:SG	1:C:1173:GLU:N	2.61	0.73
1:C:798:CYS:O	1:C:923:VAL:HB	1.89	0.73
2:6:167:ILE:HG22	2:6:184:LEU:CD1	2.17	0.73
1:C:1195:ARG:NH1	1:C:1227:ALA:O	2.21	0.73
1:A:534:HIS:CE1	1:A:1239:LEU:CD2	2.67	0.73
3:D:25:VAL:CG2	3:D:54:PHE:HE1	2.00	0.73
1:A:1179:VAL:O	1:A:1179:VAL:HG12	1.87	0.73
1:J:193:VAL:CG1	1:J:1093:ASN:ND2	2.32	0.73
1:C:263:THR:HB	1:C:267:ALA:HB3	1.69	0.73
1:J:80:PHE:HE2	1:J:86:LEU:HD23	1.48	0.73
1:A:598:LYS:HZ2	1:A:793:THR:HA	1.52	0.73
1:C:733:VAL:HG13	1:C:735:ASP:O	1.86	0.73
1:C:1056:SER:OG	1:C:1084:VAL:HG23	1.86	0.73
1:J:638:MET:SD	1:J:642:ARG:NH2	2.61	0.72
1:C:388:ASN:OD1	1:C:1043:GLU:OE1	2.06	0.72
1:A:9:LEU:HD11	1:A:45:ARG:HG2	1.70	0.72
1:A:967:HIS:CD2	1:A:967:HIS:O	2.43	0.72
1:J:1069:ARG:HG3	1:J:1069:ARG:NH1	2.00	0.72
3:D:25:VAL:CA	3:D:57:LYS:HE3	2.19	0.72
1:C:8:GLU:HB2	1:C:45:ARG:HD3	1.71	0.72
1:C:231:ASN:ND2	1:C:1099:VAL:HB	2.05	0.72
1:C:1285:TYR:CG	1:C:1317:LEU:CD1	2.72	0.72
1:J:598:LYS:HD2	1:J:1000:ASN:HB3	1.71	0.72
1:A:440:ILE:HB	1:A:1108:VAL:HG11	1.70	0.72
1:J:710:LEU:HD12	1:J:1012:LEU:CD1	2.20	0.72
1:C:800:LEU:HD12	1:C:800:LEU:O	1.90	0.72
1:C:1327:THR:HG22	1:C:1355:VAL:HG13	1.71	0.72
2:6:170:ASN:HD22	2:6:184:LEU:CD2	2.02	0.72
1:J:800:LEU:CD2	1:J:923:VAL:HG21	2.20	0.72
1:J:1174:LEU:O	1:J:1176:LEU:HG	1.90	0.72
1:A:598:LYS:CE	1:A:792:MET:O	2.38	0.72
1:A:668:PRO:C	1:A:672:PHE:CE2	2.64	0.72
1:A:1102:VAL:CG2	1:A:1366:MET:CE	2.68	0.72
3:E:45:SER:O	3:E:49:ARG:NH1	2.23	0.72
1:A:1205:TYR:HE2	1:A:1277:THR:HG23	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:942:PHE:CE1	1:C:992:SER:HA	2.25	0.71
1:C:698:LEU:HB2	1:C:706:TYR:HE2	1.54	0.71
1:C:1148:ILE:O	1:C:1152:THR:OG1	2.06	0.71
1:J:19:PHE:CE2	1:A:1088:LEU:HD22	1.99	0.71
1:J:430:LEU:HD22	1:J:1325:LEU:O	1.89	0.71
1:C:431:LEU:HG	1:C:1333:MET:CE	2.20	0.71
1:C:524:VAL:CG2	1:C:1227:ALA:HB2	2.19	0.71
1:J:727:MET:HB2	1:J:730:VAL:HB	1.73	0.71
1:J:800:LEU:HA	1:J:937:VAL:HG12	1.72	0.71
1:J:1044:VAL:HG11	1:J:1096:VAL:HG12	1.73	0.71
1:A:35:LEU:HD13	1:C:116:VAL:CG1	2.21	0.71
1:A:1034:LEU:HD21	1:A:1173:GLU:OE2	1.91	0.71
1:C:1035:THR:HG21	1:C:1176:LEU:HD13	1.70	0.71
1:J:27:ALA:CB	1:J:35:LEU:HD21	2.18	0.71
1:A:1064:VAL:HG22	1:A:1077:VAL:HG12	1.73	0.71
1:J:231:ASN:OD1	1:J:1098:TYR:HD1	1.73	0.71
1:J:534:HIS:HD2	1:J:537:PHE:CD1	2.06	0.71
1:J:207:LEU:HB2	1:J:211:GLN:HB2	1.72	0.71
1:A:942:PHE:CE1	1:A:992:SER:HA	2.25	0.71
1:C:426:THR:CA	1:C:442:PHE:HE2	2.03	0.70
1:J:116:VAL:HG13	1:C:35:LEU:HD13	1.73	0.70
1:A:7:LEU:O	1:A:12:LYS:NZ	2.24	0.70
1:J:487:PRO:O	1:J:494:ARG:NH2	2.24	0.70
1:A:764:GLU:CB	1:A:765:PRO:HD2	2.20	0.70
1:A:967:HIS:CD2	1:A:969:HIS:HE1	2.09	0.70
3:E:37:HIS:CD2	3:E:40:LEU:N	2.59	0.70
1:J:41:ASP:CG	1:J:45:ARG:HH12	1.95	0.70
1:A:945:ASN:HD22	1:A:948:ILE:HD13	1.56	0.70
1:C:510:ASN:OD1	1:C:982:GLU:OE2	2.09	0.70
2:5:253:ILE:CG2	2:5:271:LEU:HD21	2.21	0.70
1:J:435:ARG:HG3	1:J:1367:LEU:HD13	1.73	0.70
1:A:534:HIS:ND1	1:A:1239:LEU:HD22	2.06	0.70
1:A:601:VAL:CG1	1:A:793:THR:HG22	2.21	0.70
3:Z:37:HIS:CD2	3:Z:40:LEU:N	2.59	0.70
1:J:895:VAL:HB	1:J:914:GLN:HB2	1.74	0.70
1:A:9:LEU:HD11	1:A:45:ARG:CG	2.21	0.70
2:6:156:PHE:HB3	2:6:159:LEU:HD12	1.73	0.70
1:A:942:PHE:HE1	1:A:992:SER:HA	1.56	0.70
1:C:983:TYR:O	1:C:988:ARG:NH2	2.25	0.70
1:J:83:LEU:HD12	1:J:1058:ILE:HG22	1.74	0.70
1:J:146:THR:O	1:J:149:ASP:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:274:VAL:HG11	1:J:372:LEU:HD12	1.74	0.70
1:J:693:LEU:HD11	1:J:1026:ALA:HB2	1.73	0.70
1:C:489:GLY:HA3	1:C:763:ASP:OD2	1.87	0.70
1:C:1336:LYS:NZ	1:C:1346:THR:O	2.25	0.70
1:J:733:VAL:HG22	1:J:738:PRO:HA	1.74	0.70
1:C:27:ALA:CB	1:C:35:LEU:CD2	2.62	0.70
1:C:343:SER:HA	1:C:346:GLN:HB2	1.72	0.70
1:A:380:ASP:OD1	1:A:380:ASP:O	2.10	0.69
2:6:26:LYS:HE2	2:6:34:HIS:NE2	2.05	0.69
1:A:487:PRO:O	1:A:494:ARG:NH2	2.25	0.69
1:A:668:PRO:CB	1:A:672:PHE:HE2	2.03	0.69
1:C:766:LEU:CD2	1:C:891:LYS:CD	2.70	0.69
1:J:45:ARG:NE	1:J:46:TYR:CE2	2.60	0.69
1:J:662:ALA:HA	1:J:671:LEU:HD11	1.73	0.69
1:J:800:LEU:HD21	1:J:923:VAL:HG21	1.73	0.69
1:C:1044:VAL:HG11	1:C:1096:VAL:CG1	2.22	0.69
2:4:101:LYS:O	2:4:104:ASP:CG	2.29	0.69
1:A:9:LEU:CD1	1:A:45:ARG:CG	2.70	0.69
1:A:727:MET:HB2	1:A:730:VAL:HB	1.73	0.69
3:Z:37:HIS:NE2	3:Z:39:VAL:CG1	2.40	0.69
1:A:1102:VAL:HG23	1:A:1366:MET:HE2	1.74	0.69
1:C:737:GLN:HE22	2:4:143:THR:H	1.40	0.69
3:Z:37:HIS:CD2	3:Z:40:LEU:H	2.11	0.69
1:J:628:ARG:HH21	3:Z:75:ARG:HH22	1.41	0.69
3:Z:19:ARG:O	3:Z:23:ASN:HB2	1.93	0.69
1:J:118:LYS:HZ2	1:C:32:PHE:HE1	1.27	0.69
1:A:454:LEU:HD12	1:A:1239:LEU:HD11	1.73	0.69
1:A:798:CYS:O	1:A:923:VAL:HB	1.92	0.69
1:C:447:LYS:HD2	1:C:1112:ASP:HB3	1.73	0.69
1:J:445:ALA:HA	1:J:1110:VAL:HG21	1.73	0.69
1:J:970:ASP:OD2	1:J:993:ARG:NH2	2.24	0.69
1:J:597:PHE:CE1	1:J:601:VAL:HG21	2.28	0.68
1:J:99:ARG:NH1	1:J:111:GLN:HB3	2.07	0.68
1:J:440:ILE:CG1	1:J:1108:VAL:HG11	2.18	0.68
1:A:36:ARG:NH2	1:A:42:ASP:OD2	2.26	0.68
1:A:1344:PHE:H	1:A:1364:GLN:NE2	1.91	0.68
1:C:942:PHE:CZ	1:C:995:SER:HB2	2.22	0.68
1:J:18:ASP:O	1:J:19:PHE:HD1	1.73	0.68
1:J:440:ILE:HG13	1:J:1108:VAL:HG21	1.74	0.68
2:6:26:LYS:HE2	2:6:34:HIS:CE1	2.28	0.68
3:D:43:MET:HE2	3:D:67:MET:HG3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:SER:HB3	1:J:108:THR:HG22	1.75	0.68
1:A:263:THR:HB	1:A:267:ALA:HB3	1.75	0.68
1:J:1034:LEU:HG	1:J:1173:GLU:OE2	1.93	0.68
1:C:718:PRO:HD3	1:C:786:LEU:HD21	1.73	0.68
1:J:601:VAL:CG1	1:J:793:THR:HG22	2.23	0.68
1:J:1244:TYR:HB2	1:J:1266:PHE:CD2	2.28	0.68
1:C:598:LYS:CD	1:C:1000:ASN:HD22	2.06	0.68
1:C:819:LEU:HD11	3:E:32:ILE:HD12	1.74	0.68
1:C:895:VAL:HB	1:C:914:GLN:HB2	1.74	0.68
2:5:73:LEU:HD23	2:5:210:ILE:HD13	1.75	0.68
1:C:440:ILE:HD12	1:C:1108:VAL:HG12	1.72	0.68
1:J:538:ASP:OD1	1:J:555:ARG:NE	2.27	0.68
1:J:723:LEU:CG	1:J:772:ARG:HH22	2.04	0.68
1:J:723:LEU:HD12	1:J:772:ARG:NH2	2.09	0.68
3:E:68:VAL:O	3:E:71:SER:OG	2.07	0.68
1:J:941:ARG:HG3	1:J:992:SER:HB3	1.75	0.68
1:J:1195:ARG:NH1	1:J:1227:ALA:O	2.27	0.68
1:J:118:LYS:HD3	1:C:32:PHE:HE1	1.59	0.67
1:A:647:PHE:HD2	1:A:653:LEU:HD13	1.58	0.67
1:C:601:VAL:HG12	1:C:793:THR:HG22	1.75	0.67
1:C:718:PRO:HD3	1:C:786:LEU:CD2	2.24	0.67
1:C:130:GLU:HB3	1:C:1074:THR:HG22	1.76	0.67
1:J:942:PHE:HE1	1:J:992:SER:HA	1.59	0.67
1:A:21:THR:CG2	1:C:200:ALA:CA	2.35	0.67
1:A:908:PRO:HG3	1:A:1123:ARG:HH12	1.59	0.67
1:C:785:TYR:O	1:C:943:TYR:OH	2.07	0.67
1:C:532:GLU:OE2	1:C:555:ARG:NH1	2.27	0.67
1:J:748:HIS:O	1:J:756:ARG:NH1	2.28	0.67
1:C:536:PHE:CD1	1:C:1015:ILE:HG21	2.30	0.67
3:E:29:PRO:HG2	3:E:32:ILE:HG12	1.74	0.67
1:J:942:PHE:CZ	1:J:995:SER:CB	2.78	0.67
1:A:431:LEU:CD2	1:A:437:VAL:N	2.58	0.67
1:A:741:PRO:HB2	1:A:744:ILE:HG13	1.76	0.67
1:J:115:MET:O	1:C:35:LEU:HD13	1.90	0.67
1:J:790:PRO:HB2	1:J:942:PHE:HE2	1.53	0.67
1:C:999:PRO:O	1:C:1004:SER:OG	2.05	0.67
2:6:167:ILE:HG22	2:6:184:LEU:HD13	1.76	0.67
1:A:231:ASN:ND2	1:A:1099:VAL:H	1.93	0.67
1:C:514:GLN:HB3	1:C:993:ARG:NH2	2.10	0.67
1:J:433:ARG:NH1	1:J:1166:HIS:O	2.28	0.67
1:C:8:GLU:HB2	1:C:45:ARG:CD	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:VAL:HG12	1:C:647:PHE:N	2.10	0.67
1:C:1221:ASP:OD1	1:C:1222:ALA:N	2.27	0.67
2:5:140:VAL:O	2:5:140:VAL:CG1	2.43	0.66
1:A:747:ARG:CD	1:A:749:HIS:CE1	2.77	0.66
2:5:267:LEU:HG	2:5:271:LEU:HD11	1.76	0.66
3:D:39:VAL:O	3:D:43:MET:HG2	1.94	0.66
1:J:35:LEU:CD1	1:A:116:VAL:HG12	2.12	0.66
1:J:118:LYS:CD	1:C:32:PHE:CE1	2.78	0.66
1:C:19:PHE:CE1	1:C:22:HIS:C	2.45	0.66
1:C:1285:TYR:CE1	1:C:1317:LEU:HG	2.31	0.66
1:C:435:ARG:HG3	1:C:1367:LEU:HD13	1.78	0.66
1:C:514:GLN:CB	1:C:993:ARG:HH22	1.90	0.66
2:4:137:LYS:HB3	2:4:142:GLU:HB2	1.78	0.66
1:A:93:PHE:HE1	1:A:118:LYS:HG2	1.60	0.66
1:A:130:GLU:HG2	1:A:1074:THR:CA	2.26	0.66
2:5:267:LEU:HG	2:5:271:LEU:CD1	2.25	0.66
1:C:800:LEU:HD12	1:C:800:LEU:C	2.16	0.66
1:J:1044:VAL:HG22	1:J:1099:VAL:HG22	1.77	0.66
1:A:1048:LEU:HD12	1:A:1094:THR:HG22	1.78	0.66
1:C:812:PHE:HB2	3:E:65:LEU:HD21	1.78	0.66
1:J:207:LEU:HD12	1:J:207:LEU:O	1.96	0.66
1:J:518:VAL:HG11	1:J:567:PRO:HG3	1.76	0.66
1:C:186:LYS:HZ2	1:C:1055:THR:CG2	1.81	0.66
1:J:430:LEU:HD21	1:J:1326:SER:HB2	1.78	0.66
1:J:849:GLN:HB2	1:J:873:LEU:HD13	1.77	0.66
1:A:431:LEU:HD22	1:A:436:ALA:CA	2.26	0.66
1:A:502:ARG:HD3	1:A:962:GLU:HG3	1.78	0.66
1:A:1291:ASP:OD2	1:A:1313:ASN:ND2	2.27	0.66
1:C:782:LYS:O	1:C:786:LEU:HB2	1.96	0.66
1:C:1214:ILE:HD13	1:C:1268:THR:HG23	1.78	0.66
1:J:274:VAL:HG12	1:J:385:LEU:HD11	1.77	0.65
1:J:723:LEU:HG	1:J:772:ARG:NH2	2.10	0.65
1:C:440:ILE:CD1	1:C:1108:VAL:HG11	2.24	0.65
2:4:104:ASP:OD1	2:4:105:HIS:N	2.30	0.65
1:J:647:PHE:HD2	1:J:653:LEU:HD13	1.61	0.65
1:A:212:ARG:HH12	1:A:1204:PRO:HG3	1.60	0.65
1:J:275:SER:HB3	1:J:1047:LEU:CD1	2.25	0.65
1:A:1290:LYS:HB3	1:A:1310:LEU:HB3	1.76	0.65
1:A:311:ASN:HB3	1:A:321:ILE:HD12	1.78	0.65
1:C:598:LYS:HD3	1:C:1000:ASN:CB	2.26	0.65
1:C:687:ILE:HD13	1:C:1006:MET:SD	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:36:ARG:NH2	1:A:115:MET:HE3	2.11	0.65
1:J:710:LEU:HD12	1:J:1012:LEU:HD12	1.76	0.65
1:J:862:GLU:HG3	1:J:863:ASP:H	1.61	0.65
1:J:723:LEU:HG	1:J:772:ARG:HH22	1.61	0.65
1:A:21:THR:HG22	1:C:200:ALA:HB2	1.74	0.65
1:A:388:ASN:OD1	1:A:1043:GLU:CD	2.34	0.65
1:C:1285:TYR:HB2	1:C:1317:LEU:CD2	2.26	0.65
1:A:193:VAL:CG2	1:A:1093:ASN:ND2	2.59	0.65
1:A:800:LEU:HD12	1:A:800:LEU:C	2.17	0.65
1:A:1056:SER:HG	1:A:1084:VAL:HG22	1.60	0.65
1:C:617:VAL:HG12	1:C:619:GLY:H	1.62	0.65
1:A:443:VAL:O	1:A:446:LEU:HB2	1.97	0.64
1:C:508:THR:CB	1:C:982:GLU:OE1	2.45	0.64
1:C:719:PHE:HE1	1:C:939:PHE:HZ	1.43	0.64
1:C:894:GLU:OE2	1:C:915:HIS:NE2	2.31	0.64
1:A:388:ASN:ND2	1:A:1043:GLU:OE1	2.29	0.64
1:A:431:LEU:HD22	1:A:436:ALA:O	1.92	0.64
1:C:411:GLU:HG2	1:C:1350:HIS:HE1	1.61	0.64
1:A:388:ASN:OD1	1:A:1043:GLU:CA	2.38	0.64
1:A:431:LEU:HD22	1:A:436:ALA:N	2.12	0.64
1:A:1174:LEU:HD21	1:A:1266:PHE:HZ	1.63	0.64
1:J:371:ASN:OD1	1:J:372:LEU:N	2.30	0.64
1:A:598:LYS:NZ	1:A:793:THR:HA	2.11	0.64
1:C:7:LEU:HD11	1:C:12:LYS:CD	2.26	0.64
1:J:518:VAL:HB	1:J:1179:VAL:HG11	1.80	0.64
1:A:130:GLU:HG2	1:A:1074:THR:CB	2.27	0.64
1:A:967:HIS:CD2	1:A:969:HIS:CE1	2.86	0.64
1:A:1068:GLU:HG3	1:A:1073:THR:HG22	1.78	0.64
1:A:1113:LEU:HD21	1:A:1243:LEU:HD11	1.79	0.64
1:A:1362:LEU:O	1:A:1366:MET:HG2	1.97	0.64
1:C:207:LEU:CD2	1:C:211:GLN:OE1	2.46	0.64
2:5:70:ASN:ND2	2:6:189:ASP:OD2	2.30	0.64
1:J:45:ARG:NH2	1:J:46:TYR:CE2	2.60	0.64
1:A:19:PHE:HZ	1:C:1088:LEU:HD22	1.60	0.64
2:4:140:VAL:HG11	2:4:158:HIS:HE1	1.63	0.64
1:J:22:HIS:CD2	1:J:23:VAL:N	2.60	0.64
1:J:732:VAL:CG1	1:J:739:LEU:HD12	2.26	0.64
1:A:207:LEU:HD12	1:A:207:LEU:O	1.98	0.64
1:A:650:SER:O	1:A:654:VAL:HG23	1.98	0.64
1:J:687:ILE:CG2	1:J:1006:MET:HE1	2.27	0.64
1:A:983:TYR:O	1:A:988:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:627:ILE:HD11	1:J:882:ALA:HB2	1.80	0.63
1:C:592:GLU:OE2	1:C:595:ARG:NH1	2.31	0.63
1:J:83:LEU:CD2	1:J:1080:ASN:HD21	2.07	0.63
1:J:228:PHE:CE1	1:J:1099:VAL:HG21	2.26	0.63
1:J:617:VAL:HG12	1:J:619:GLY:H	1.64	0.63
1:J:698:LEU:HB2	1:J:706:TYR:HE2	1.62	0.63
1:C:419:THR:HG22	1:C:421:ARG:H	1.62	0.63
1:J:1105:ASP:N	1:J:1168:GLN:O	2.24	0.63
1:A:27:ALA:HB1	1:A:35:LEU:HD22	1.79	0.63
1:C:485:GLN:HE21	1:C:486:GLU:H	1.44	0.63
1:A:280:MET:O	1:A:284:MET:HG2	1.98	0.63
1:C:175:LEU:HD13	1:C:1081:ILE:HD11	1.79	0.63
2:5:49:ARG:NH1	2:5:242:CYS:SG	2.71	0.63
2:5:128:ALA:O	2:5:131:SER:HB3	1.97	0.63
1:J:263:THR:HB	1:J:267:ALA:HB3	1.79	0.63
1:A:315:ALA:HB2	1:A:321:ILE:HD11	1.80	0.63
1:C:360:ILE:HD12	1:C:369:MET:SD	2.35	0.63
1:J:1069:ARG:O	1:J:1071:ILE:HG22	1.98	0.63
1:A:730:VAL:HG13	1:A:895:VAL:HG13	1.81	0.63
1:C:410:VAL:O	1:C:412:SER:N	2.32	0.63
1:J:1069:ARG:C	1:J:1071:ILE:H	2.02	0.63
1:C:770:ASP:OD1	1:C:771:TYR:N	2.32	0.63
1:A:630:PHE:CE1	1:A:879:LEU:CD2	2.76	0.63
1:J:764:GLU:HG3	1:J:765:PRO:CD	2.04	0.62
1:J:448:THR:HG21	1:J:1111:GLN:O	1.98	0.62
1:A:388:ASN:CG	1:A:1043:GLU:OE1	2.38	0.62
1:A:400:TYR:CE1	1:A:573:LEU:HD12	2.31	0.62
1:C:1035:THR:CB	1:C:1176:LEU:HD11	2.28	0.62
1:C:1044:VAL:HG22	1:C:1099:VAL:HG22	1.81	0.62
2:4:140:VAL:HG11	2:4:158:HIS:CE1	2.33	0.62
1:J:700:GLU:HG3	1:J:700:GLU:O	1.99	0.62
1:J:1039:THR:HG21	1:J:1259:TYR:HE2	1.64	0.62
1:A:90:LYS:CG	1:A:119:TYR:CE1	2.82	0.62
1:A:193:VAL:HG21	1:A:1093:ASN:HD21	1.61	0.62
1:A:558:ILE:HD12	1:A:1015:ILE:HD11	1.79	0.62
1:A:862:GLU:HG3	1:A:863:ASP:H	1.64	0.62
1:C:9:LEU:HD12	1:C:45:ARG:CD	2.29	0.62
1:C:194:GLN:OE1	1:C:245:ARG:HD3	2.00	0.62
1:J:867:ASP:OD1	1:J:868:ALA:N	2.32	0.62
1:A:90:LYS:HG2	1:A:119:TYR:CE1	2.34	0.62
1:A:130:GLU:HG2	1:A:1074:THR:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLU:O	1:A:481:CYS:SG	2.57	0.62
2:6:28:ASP:OD1	2:6:176:ARG:NH1	2.28	0.62
2:4:20:LEU:HG	2:4:65:GLU:HG2	1.82	0.62
1:A:12:LYS:HE3	1:C:94:HIS:CB	2.18	0.62
1:A:604:PRO:HA	1:A:925:THR:HG21	1.82	0.62
1:C:790:PRO:CB	1:C:942:PHE:HD2	1.89	0.62
1:C:317:SER:OG	1:C:318:TYR:CD2	2.53	0.62
1:C:534:HIS:CE1	1:C:1239:LEU:HD13	2.35	0.62
1:C:795:ASN:CG	1:C:942:PHE:CD1	2.73	0.62
1:C:1285:TYR:HB2	1:C:1317:LEU:HD21	1.78	0.62
2:5:77:LEU:HD11	2:5:114:PHE:CZ	2.35	0.62
1:J:534:HIS:NE2	1:J:537:PHE:HD1	1.98	0.62
1:A:764:GLU:O	1:A:766:LEU:HD12	2.00	0.62
1:J:633:ARG:O	1:J:637:ASN:ND2	2.25	0.62
1:J:1044:VAL:CG1	1:J:1096:VAL:HG12	2.29	0.62
1:A:710:LEU:HD21	1:A:783:VAL:HG23	1.81	0.62
1:A:1020:LEU:HD21	1:A:1032:PHE:HZ	1.64	0.62
2:6:6:ILE:HB	2:6:50:THR:HG23	1.82	0.62
1:A:259:THR:HG22	1:A:352:LEU:HD11	1.82	0.61
2:5:136:ALA:O	2:5:139:SER:HB3	2.00	0.61
1:J:718:PRO:HD3	1:J:786:LEU:CG	2.31	0.61
1:J:1214:ILE:HD13	1:J:1268:THR:HG23	1.83	0.61
2:4:66:LEU:HB3	2:4:217:TRP:CZ3	2.34	0.61
1:C:1044:VAL:HG22	1:C:1099:VAL:HG23	1.81	0.61
1:C:186:LYS:NZ	1:C:1055:THR:HG23	2.11	0.61
2:4:246:ASP:OD2	2:4:280:ASP:HB2	2.00	0.61
1:J:598:LYS:HD2	1:J:1000:ASN:HB2	1.75	0.61
1:J:812:PHE:HB2	3:Z:65:LEU:HD21	1.82	0.61
1:A:431:LEU:HD23	1:A:437:VAL:CA	2.29	0.61
1:C:800:LEU:HD21	1:C:923:VAL:HG21	1.78	0.61
1:A:1168:GLN:HA	1:A:1298:ASP:O	2.00	0.61
1:C:120:SER:HB3	1:C:1084:VAL:HG12	1.81	0.61
2:4:243:LEU:HD22	3:D:74:ARG:HA	1.82	0.61
2:4:271:LEU:O	2:4:278:TYR:OH	2.19	0.61
1:A:534:HIS:HE1	1:A:1239:LEU:CD2	2.10	0.61
1:C:315:ALA:HB2	1:C:321:ILE:HD11	1.82	0.61
1:C:1328:THR:HG21	1:C:1353:ASN:HD22	1.66	0.61
1:J:1015:ILE:O	1:J:1015:ILE:CG2	2.47	0.61
1:A:1034:LEU:HD22	1:A:1173:GLU:CD	2.19	0.61
1:C:572:GLU:OE2	1:C:994:TYR:OH	2.18	0.61
2:6:164:VAL:HA	2:6:167:ILE:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:ALA:HB3	1:A:1222:ALA:HB3	1.82	0.61
1:C:273:MET:HE2	1:C:1047:LEU:HD11	1.83	0.61
1:C:534:HIS:ND1	1:C:1239:LEU:HB2	2.16	0.61
1:A:7:LEU:HD12	1:A:12:LYS:HD3	1.80	0.61
1:A:417:ASN:O	1:A:422:ASN:ND2	2.27	0.61
1:A:668:PRO:CB	1:A:672:PHE:CE2	2.78	0.61
1:A:941:ARG:HG3	1:A:992:SER:HB3	1.82	0.61
1:C:231:ASN:HD21	1:C:1099:VAL:HB	1.66	0.61
1:C:1016:SER:HB3	1:C:1019:SER:H	1.65	0.61
1:C:1217:HIS:HE2	1:C:1235:GLN:HA	1.66	0.61
1:J:723:LEU:CD1	1:J:772:ARG:HH22	2.14	0.60
1:J:810:ASP:OD2	1:J:933:TYR:OH	2.17	0.60
1:A:1102:VAL:CG2	1:A:1366:MET:HE1	2.28	0.60
1:J:76:HIS:CE1	1:J:78:ILE:HD11	2.35	0.60
1:A:212:ARG:HH22	1:A:1204:PRO:HD3	0.49	0.60
1:A:733:VAL:HG22	1:A:738:PRO:CA	2.26	0.60
1:C:945:ASN:ND2	1:C:947:THR:OG1	2.34	0.60
2:6:170:ASN:HB2	2:6:184:LEU:HD21	1.82	0.60
2:6:260:ASN:O	2:6:262:ASP:N	2.34	0.60
1:J:35:LEU:CD1	1:A:115:MET:C	2.68	0.60
1:J:790:PRO:CB	1:J:942:PHE:HE2	2.06	0.60
1:A:681:LEU:HD22	1:A:783:VAL:HG12	1.83	0.60
1:A:1195:ARG:NH1	1:A:1227:ALA:O	2.34	0.60
1:C:795:ASN:OD1	1:C:942:PHE:CG	2.53	0.60
1:J:41:ASP:CG	1:J:45:ARG:NH2	2.40	0.60
1:J:1109:ARG:HD2	1:J:1169:LYS:CD	2.31	0.60
2:4:166:ARG:HH12	2:4:185:ASP:HA	1.66	0.60
1:A:1105:ASP:CG	1:A:1169:LYS:HA	2.22	0.60
1:C:1160:ASN:CG	1:C:1298:ASP:HB3	2.21	0.60
1:J:431:LEU:HG	1:J:1333:MET:CE	2.31	0.60
1:A:431:LEU:CD2	1:A:437:VAL:CA	2.78	0.60
1:A:1197:SER:HB3	1:A:1214:ILE:HG13	1.84	0.60
3:Z:69:ALA:O	3:Z:73:THR:CG2	2.46	0.60
1:J:1156:MET:SD	1:J:1294:ARG:NH1	2.74	0.60
1:C:1177:THR:O	1:C:1180:THR:OG1	2.20	0.60
1:C:78:ILE:HD12	1:C:344:LEU:HD12	1.84	0.60
2:5:118:VAL:HG12	2:6:90:ARG:HH12	1.67	0.60
2:4:91:GLY:HA3	2:4:106:LEU:HD21	1.84	0.60
1:J:2:GLU:OE1	1:A:90:LYS:HD2	2.02	0.60
1:J:1182:ASP:HB2	1:J:1186:PHE:HB2	1.84	0.59
1:A:597:PHE:O	1:A:601:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:LYS:H	1:A:889:HIS:HE1	1.50	0.59
1:C:426:THR:HB	1:C:442:PHE:HE2	1.66	0.59
2:5:50:THR:HG22	2:5:54:ASN:HD21	1.66	0.59
1:J:19:PHE:CE2	1:A:1088:LEU:CD2	2.51	0.59
1:A:207:LEU:HD11	1:A:212:ARG:CD	2.26	0.59
1:A:435:ARG:HG3	1:A:1367:LEU:HD13	1.83	0.59
1:C:193:VAL:HG12	1:C:249:ALA:HB1	1.84	0.59
1:J:37:ILE:CG1	1:A:114:ILE:HG12	2.29	0.59
1:J:434:ASP:HA	1:J:1367:LEU:HD11	1.83	0.59
1:A:1217:HIS:ND1	1:A:1228:THR:OG1	2.32	0.59
1:J:731:GLN:HB3	1:J:738:PRO:HB3	1.84	0.59
1:A:572:GLU:OE2	1:A:994:TYR:OH	2.21	0.59
1:J:502:ARG:HD2	1:J:962:GLU:HG3	1.84	0.59
1:J:538:ASP:OD1	1:J:555:ARG:NH1	2.36	0.59
1:C:635:ILE:HD11	1:C:657:ILE:HD12	1.85	0.59
1:C:795:ASN:CG	1:C:942:PHE:CE1	2.75	0.59
2:6:170:ASN:HD22	2:6:184:LEU:HG	1.67	0.59
2:4:74:SER:O	2:4:78:GLU:HG2	2.01	0.59
1:A:1221:ASP:OD1	1:A:1222:ALA:N	2.35	0.59
1:J:274:VAL:O	1:J:1047:LEU:HD12	2.03	0.59
1:J:322:LEU:HD12	1:J:322:LEU:O	2.03	0.59
1:A:1328:THR:CG2	1:A:1353:ASN:CG	2.70	0.59
1:C:538:ASP:OD1	1:C:555:ARG:NH1	2.36	0.59
1:C:1152:THR:HB	1:C:1153:PHE:HD1	1.68	0.59
2:4:245:PHE:CZ	2:4:277:ILE:HD11	2.37	0.59
1:J:193:VAL:CG2	1:J:1093:ASN:ND2	2.66	0.59
1:A:391:LEU:HD22	1:A:1042:PHE:HE2	1.67	0.59
1:A:1102:VAL:CG2	1:A:1366:MET:HE2	2.33	0.59
2:5:211:MET:O	2:5:215:ARG:HG2	2.02	0.59
1:J:723:LEU:HD12	1:J:772:ARG:HH22	1.68	0.59
1:A:1344:PHE:HB2	1:A:1364:GLN:HE21	1.64	0.59
1:C:766:LEU:CD2	1:C:891:LYS:HD3	2.32	0.59
1:J:723:LEU:CD1	1:J:772:ARG:NH2	2.66	0.59
1:C:487:PRO:O	1:C:494:ARG:NH2	2.36	0.59
2:6:98:ASP:OD1	2:6:98:ASP:N	2.35	0.59
3:D:22:VAL:HG13	3:D:28:LEU:HD12	1.83	0.59
1:J:1121:VAL:HG12	1:J:1132:ARG:HH12	1.66	0.58
1:A:130:GLU:OE2	1:A:1074:THR:HG21	2.02	0.58
1:A:1034:LEU:CD2	1:A:1175:ILE:HD13	2.32	0.58
1:C:448:THR:CG2	1:C:1111:GLN:O	2.51	0.58
1:A:800:LEU:CD2	1:A:923:VAL:CG2	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:THR:HG21	1:A:1259:TYR:HE2	1.68	0.58
1:J:440:ILE:CD1	1:J:1108:VAL:CB	2.58	0.58
1:J:1109:ARG:HD3	1:J:1169:LYS:HE2	1.85	0.58
1:J:234:ARG:HH22	1:J:282:ILE:HD13	1.67	0.58
1:J:799:GLY:O	1:J:937:VAL:CG1	2.50	0.58
1:A:764:GLU:HB3	1:A:765:PRO:HD2	1.71	0.58
1:C:426:THR:CB	1:C:442:PHE:HE2	2.15	0.58
3:D:33:SER:HB2	3:D:36:THR:HB	1.86	0.58
1:C:84:ASN:N	1:C:84:ASN:OD1	2.36	0.58
1:C:440:ILE:HG23	1:C:440:ILE:O	2.03	0.58
1:C:646:VAL:CG1	1:C:647:PHE:N	2.67	0.58
1:C:713:HIS:H	1:C:713:HIS:CD2	2.22	0.58
3:D:24:VAL:HG12	3:D:54:PHE:HZ	1.69	0.58
3:D:47:TYR:OH	3:D:64:LEU:HD23	2.03	0.58
1:J:311:ASN:HB3	1:J:321:ILE:HD12	1.85	0.58
1:J:478:LEU:HD11	1:J:509:VAL:HG13	1.85	0.58
1:C:443:VAL:O	1:C:446:LEU:HG	2.03	0.58
2:4:245:PHE:CE1	3:D:67:MET:HE1	2.38	0.58
1:J:274:VAL:HG11	1:J:372:LEU:CD1	2.33	0.58
1:A:1034:LEU:HD23	1:A:1175:ILE:HD13	1.84	0.58
1:A:1125:ASP:OD1	1:A:1129:ARG:NH1	2.37	0.58
1:C:489:GLY:HA2	1:C:763:ASP:CG	2.21	0.58
1:C:1160:ASN:HD21	1:C:1297:THR:CA	2.17	0.58
1:A:284:MET:CE	1:A:291:ILE:HG21	2.34	0.58
1:C:763:ASP:O	1:C:764:GLU:O	2.22	0.58
1:C:1035:THR:OG1	1:C:1176:LEU:HD11	2.03	0.58
1:J:242:PHE:HE2	1:J:1095:CYS:HG	1.52	0.58
1:A:630:PHE:CE2	1:A:879:LEU:HG	2.39	0.58
1:A:739:LEU:HG	1:A:739:LEU:O	2.04	0.58
1:C:705:ALA:HB1	1:C:712:ASP:HB3	1.86	0.58
2:5:166:ARG:HD2	2:5:186:LEU:HD11	1.86	0.58
1:J:1109:ARG:CD	1:J:1169:LYS:HD2	2.34	0.57
1:C:426:THR:CA	1:C:442:PHE:CE2	2.86	0.57
1:C:743:ASN:ND2	2:4:158:HIS:O	2.37	0.57
1:A:19:PHE:HZ	1:C:1088:LEU:CD2	2.14	0.57
1:A:598:LYS:HD2	1:A:792:MET:O	2.03	0.57
1:C:9:LEU:CD1	1:C:45:ARG:CD	2.82	0.57
1:J:83:LEU:HD22	1:J:1080:ASN:CG	2.20	0.57
1:J:274:VAL:HG12	1:J:385:LEU:CD1	2.33	0.57
1:A:801:GLY:HA3	1:A:890:VAL:HG11	1.85	0.57
1:C:1160:ASN:HD21	1:C:1297:THR:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1232:TRP:HB3	1:J:1239:LEU:HD23	1.87	0.57
1:C:572:GLU:HB3	1:C:1003:HIS:HE1	1.69	0.57
1:C:741:PRO:HB3	2:4:158:HIS:CG	2.40	0.57
1:J:78:ILE:O	1:J:1058:ILE:HA	2.05	0.57
1:C:534:HIS:HE1	1:C:1239:LEU:HD22	1.64	0.57
1:C:1268:THR:HA	1:C:1271:ILE:HG22	1.87	0.57
1:C:1285:TYR:CZ	1:C:1317:LEU:HD12	2.33	0.57
1:J:730:VAL:HG13	1:J:895:VAL:HG13	1.86	0.57
1:A:448:THR:HG23	1:A:1111:GLN:O	2.03	0.57
1:A:1015:ILE:O	1:A:1015:ILE:CG2	2.51	0.57
2:5:239:LEU:HD13	2:5:250:CYS:HB2	1.87	0.57
2:4:24:THR:HG21	2:4:69:HIS:CD2	2.40	0.57
1:J:1280:LYS:O	1:J:1284:GLU:HG2	2.04	0.57
1:A:756:ARG:NH2	1:A:886:VAL:O	2.37	0.57
1:A:1109:ARG:HH11	1:A:1169:LYS:HD3	1.70	0.57
1:C:431:LEU:CD2	1:C:437:VAL:HA	2.32	0.57
2:6:194:THR:O	2:6:198:ASN:ND2	2.37	0.57
1:J:747:ARG:HG2	1:J:748:HIS:N	2.19	0.57
1:A:845:SER:HB2	1:A:848:ALA:HB3	1.87	0.57
1:A:953:SER:HB2	1:A:956:ILE:HD12	1.85	0.57
1:C:800:LEU:HG	1:C:923:VAL:CG2	2.34	0.57
1:C:849:GLN:HB2	1:C:873:LEU:HD13	1.87	0.57
1:C:1066:LYS:HD2	1:C:1075:TYR:HE1	1.69	0.57
1:J:508:THR:OG1	1:J:511:GLU:HB2	2.04	0.57
1:C:443:VAL:HG13	1:C:446:LEU:HD11	1.87	0.57
1:J:4:TRP:O	1:J:5:SER:OG	2.19	0.56
1:J:7:LEU:HD12	1:J:12:LYS:CE	2.35	0.56
1:C:1190:ASN:OD1	1:C:1191:ASN:N	2.35	0.56
1:J:17:THR:HG21	1:A:95:VAL:HG21	1.87	0.56
1:J:440:ILE:CD1	1:J:1108:VAL:HG13	2.27	0.56
1:J:558:ILE:HD12	1:J:1015:ILE:HD11	1.86	0.56
1:A:212:ARG:NH2	1:A:1204:PRO:CD	2.18	0.56
1:A:853:VAL:CG1	1:A:873:LEU:HD23	2.35	0.56
1:A:1344:PHE:HB2	1:A:1364:GLN:CD	2.26	0.56
1:C:598:LYS:HD3	1:C:1000:ASN:HB2	1.86	0.56
1:C:1085:ASP:OD1	1:C:1086:MET:N	2.39	0.56
1:C:1196:ALA:HB3	1:C:1222:ALA:HB3	1.88	0.56
2:4:35:PRO:O	2:4:39:LYS:HG2	2.05	0.56
2:4:245:PHE:CZ	3:D:67:MET:CE	2.88	0.56
1:J:207:LEU:HD12	1:J:207:LEU:C	2.26	0.56
1:J:431:LEU:HG	1:J:1333:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:536:PHE:CD1	1:J:1015:ILE:HG21	2.40	0.56
1:J:942:PHE:HZ	1:J:995:SER:CB	2.16	0.56
1:J:1109:ARG:CD	1:J:1169:LYS:CD	2.84	0.56
1:A:447:LYS:HD3	1:A:1112:ASP:HB3	1.87	0.56
1:A:1235:GLN:HB2	1:A:1238:CYS:HB3	1.88	0.56
1:J:601:VAL:CG1	1:J:793:THR:CG2	2.83	0.56
1:A:193:VAL:CG1	1:A:1093:ASN:ND2	2.57	0.56
1:C:597:PHE:HE1	1:C:648:ALA:HB1	1.70	0.56
2:6:170:ASN:HD22	2:6:184:LEU:CG	2.18	0.56
1:A:795:ASN:CG	1:A:942:PHE:CD1	2.77	0.56
1:C:739:LEU:CD2	1:C:766:LEU:HD12	2.36	0.56
3:D:29:PRO:HG2	3:D:32:ILE:HG12	1.86	0.56
1:J:118:LYS:CD	1:C:32:PHE:HE1	2.18	0.56
1:J:1365:SER:OG	1:J:1366:MET:N	2.38	0.56
1:C:1176:LEU:HD22	1:C:1230:ASN:CG	2.26	0.56
1:A:598:LYS:HE2	1:A:1000:ASN:HD21	1.71	0.56
1:C:189:PRO:HG3	1:C:1285:TYR:HE2	1.71	0.56
1:J:222:LYS:O	1:J:226:THR:OG1	2.16	0.56
1:A:805:LYS:H	1:A:889:HIS:CE1	2.24	0.56
1:C:534:HIS:CD2	1:C:537:PHE:HD1	2.24	0.56
1:J:117:THR:CG2	1:C:2:GLU:OE2	2.43	0.55
1:A:252:ASP:OD1	1:A:253:SER:N	2.38	0.55
1:C:388:ASN:OD1	1:C:1043:GLU:HA	2.06	0.55
1:C:739:LEU:CD2	1:C:766:LEU:CD1	2.84	0.55
1:C:1168:GLN:NE2	1:C:1294:ARG:O	2.38	0.55
1:C:1182:ASP:HB2	1:C:1186:PHE:HB2	1.88	0.55
1:J:434:ASP:N	1:J:434:ASP:OD1	2.37	0.55
1:J:723:LEU:HG	1:J:768:VAL:HG21	1.88	0.55
1:C:317:SER:OG	1:C:318:TYR:CE2	2.54	0.55
1:C:431:LEU:HG	1:C:1333:MET:HE2	1.86	0.55
1:J:115:MET:C	1:C:35:LEU:CD1	2.65	0.55
1:A:23:VAL:HG12	1:C:114:ILE:HD13	1.87	0.55
1:C:175:LEU:HD12	1:C:1081:ILE:CD1	2.37	0.55
2:4:235:LEU:HD11	2:4:282:PHE:HE1	1.70	0.55
1:A:739:LEU:CD1	1:A:744:ILE:CG2	2.84	0.55
2:5:184:LEU:HD11	2:5:205:TYR:OH	2.06	0.55
1:A:400:TYR:HE1	1:A:573:LEU:CD1	2.18	0.55
1:C:424:LEU:HD23	1:C:577:GLU:CD	2.26	0.55
1:J:718:PRO:CG	1:J:786:LEU:CD2	2.85	0.55
1:J:862:GLU:HG3	1:J:863:ASP:N	2.21	0.55
1:A:236:ARG:HH21	1:A:289:SER:HB3	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:PHE:HD1	1:A:1102:VAL:HG22	1.72	0.55
1:C:719:PHE:HE1	1:C:939:PHE:CZ	2.24	0.55
1:C:1118:PRO:HB2	1:C:1151:LEU:HD23	1.89	0.55
3:D:45:SER:O	3:D:49:ARG:NH1	2.40	0.55
1:J:25:THR:OG1	1:A:203:ALA:O	2.25	0.55
1:J:1246:THR:O	1:J:1250:GLU:HG3	2.07	0.55
1:C:426:THR:HA	1:C:442:PHE:CE2	2.42	0.55
1:C:1132:ARG:HB3	1:C:1137:VAL:O	2.07	0.55
1:A:431:LEU:HD22	1:A:436:ALA:H	1.72	0.55
1:C:78:ILE:CD1	1:C:344:LEU:HD12	2.37	0.55
1:C:698:LEU:O	1:C:699:ALA:HB3	2.06	0.55
2:5:248:ASN:O	2:5:252:ASN:ND2	2.40	0.55
2:6:239:LEU:HD13	2:6:250:CYS:HB2	1.89	0.55
1:J:117:THR:HG21	1:C:2:GLU:CD	2.26	0.55
1:J:1109:ARG:HD2	1:J:1169:LYS:HD2	1.87	0.55
1:A:617:VAL:HG12	1:A:619:GLY:H	1.72	0.55
1:J:95:VAL:HG21	1:C:17:THR:HG21	1.89	0.54
1:J:1290:LYS:HB3	1:J:1310:LEU:HB3	1.90	0.54
1:A:450:CYS:O	1:A:1122:TYR:OH	2.22	0.54
1:A:1042:PHE:CD1	1:A:1102:VAL:HG22	2.42	0.54
2:6:7:GLY:HA3	2:6:46:LEU:HD13	1.89	0.54
1:J:1037:VAL:HG22	1:J:1172:CYS:HB2	1.89	0.54
1:A:79:LYS:N	1:A:303:GLY:O	2.33	0.54
1:A:1214:ILE:HG21	1:A:1272:ILE:HD11	1.89	0.54
1:C:146:THR:O	1:C:149:ASP:N	2.36	0.54
1:C:186:LYS:HZ1	1:C:1055:THR:HG23	1.64	0.54
1:C:730:VAL:HG13	1:C:895:VAL:HG13	1.88	0.54
1:A:388:ASN:CG	1:A:1043:GLU:CD	2.65	0.54
1:A:715:LEU:HA	1:A:914:GLN:NE2	2.18	0.54
1:C:193:VAL:HG21	1:C:1093:ASN:HB3	1.90	0.54
1:C:597:PHE:CE1	1:C:648:ALA:HB1	2.43	0.54
1:C:1285:TYR:CD1	1:C:1317:LEU:HG	2.42	0.54
2:6:118:VAL:O	2:6:214:ARG:NH1	2.40	0.54
2:6:259:GLU:O	2:6:263:SER:HB2	2.06	0.54
1:J:93:PHE:HE1	1:J:118:LYS:HG2	1.72	0.54
1:J:760:MET:HA	1:J:888:GLU:OE1	2.08	0.54
1:J:942:PHE:CZ	1:J:995:SER:HB3	2.43	0.54
1:A:867:ASP:OD1	1:A:868:ALA:N	2.40	0.54
1:C:78:ILE:HD12	1:C:344:LEU:CD1	2.37	0.54
1:C:413:LYS:HD3	1:C:1335:THR:HG21	1.89	0.54
2:4:245:PHE:CZ	3:D:67:MET:HE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:245:PHE:HZ	3:D:67:MET:CE	2.21	0.54
1:C:966:TYR:HB3	1:C:973:PHE:HB2	1.88	0.54
2:5:33:ALA:O	2:5:35:PRO:HD3	2.08	0.54
1:A:193:VAL:HG12	1:A:249:ALA:HB1	1.88	0.54
1:A:707:VAL:HG22	1:A:1022:LEU:HD23	1.90	0.54
1:C:270:SER:OG	1:C:365:LYS:HG2	2.07	0.54
1:C:360:ILE:CG1	1:C:369:MET:SD	2.96	0.54
1:C:524:VAL:HG22	1:C:1227:ALA:CB	2.32	0.54
2:4:118:VAL:HB	2:4:214:ARG:CZ	2.37	0.54
2:4:245:PHE:HZ	2:4:277:ILE:HD11	1.72	0.54
3:E:63:ASP:O	3:E:67:MET:HG2	2.07	0.54
1:J:193:VAL:CB	1:J:1093:ASN:ND2	2.70	0.54
1:J:193:VAL:HG12	1:J:249:ALA:HB1	1.89	0.54
1:A:76:HIS:HE1	1:A:344:LEU:O	1.91	0.54
1:A:193:VAL:CB	1:A:1093:ASN:ND2	2.71	0.54
3:D:62:LEU:O	3:D:66:ARG:HG2	2.06	0.54
1:J:228:PHE:CE2	1:J:1099:VAL:HG21	2.43	0.54
1:A:1179:VAL:O	1:A:1179:VAL:CG1	2.53	0.54
1:C:19:PHE:CD1	1:C:21:THR:O	2.61	0.54
1:C:426:THR:HA	1:C:442:PHE:HE2	1.70	0.54
1:C:710:LEU:HB2	1:C:1012:LEU:HD23	1.88	0.54
3:E:37:HIS:CD2	3:E:40:LEU:CA	2.89	0.54
1:J:597:PHE:CE1	1:J:601:VAL:CG2	2.90	0.54
1:J:994:TYR:OH	1:J:1007:THR:HG21	2.07	0.54
1:A:90:LYS:HG2	1:A:119:TYR:HD1	1.69	0.54
1:A:1195:ARG:NH2	1:A:1216:ASP:O	2.41	0.54
2:5:260:ASN:O	2:5:262:ASP:N	2.41	0.54
1:J:41:ASP:OD2	1:J:45:ARG:NH2	2.34	0.54
1:A:157:MET:O	1:A:161:LEU:HG	2.08	0.54
1:A:429:TYR:HA	1:A:438:GLN:O	2.08	0.54
2:5:49:ARG:CZ	2:5:242:CYS:SG	2.96	0.54
1:J:448:THR:HG22	1:J:1113:LEU:HD13	1.90	0.53
1:A:552:CYS:SG	1:A:907:LEU:HD11	2.48	0.53
1:C:175:LEU:HD11	1:C:1081:ILE:HD11	1.89	0.53
1:C:710:LEU:HD21	1:C:783:VAL:HG23	1.90	0.53
1:J:36:ARG:HH22	1:A:115:MET:HE1	1.69	0.53
1:J:1271:ILE:HD12	1:J:1274:ALA:HB3	1.88	0.53
1:A:630:PHE:HZ	1:A:879:LEU:HD21	1.57	0.53
1:C:278:ASN:O	1:C:282:ILE:HG13	2.08	0.53
2:5:163:GLU:OE2	2:5:186:LEU:HD22	2.08	0.53
3:D:26:LEU:HD13	3:D:64:LEU:HD13	1.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:246:ASP:N	2:5:246:ASP:OD1	2.40	0.53
2:6:246:ASP:OD2	2:6:281:SER:N	2.42	0.53
1:J:517:VAL:HG12	1:J:518:VAL:N	2.24	0.53
1:J:707:VAL:HG22	1:J:1022:LEU:HD23	1.89	0.53
1:C:1056:SER:OG	1:C:1084:VAL:HG22	2.07	0.53
1:C:1280:LYS:O	1:C:1284:GLU:HG3	2.08	0.53
1:J:409:THR:O	1:J:411:GLU:N	2.40	0.53
1:J:533:LEU:HB2	1:J:539:PHE:CE2	2.43	0.53
1:C:545:ASN:N	1:C:545:ASN:OD1	2.41	0.53
1:C:1043:GLU:C	1:C:1044:VAL:HG23	2.29	0.53
1:J:231:ASN:ND2	1:J:1099:VAL:HB	2.24	0.53
1:J:485:GLN:HE21	1:J:486:GLU:H	1.56	0.53
1:C:93:PHE:HB2	1:C:116:VAL:HG23	1.91	0.53
1:J:275:SER:OG	1:J:280:MET:HG2	2.09	0.53
1:J:558:ILE:HD13	1:J:1015:ILE:HG12	1.91	0.53
1:A:536:PHE:CE1	1:A:1015:ILE:HG21	2.44	0.53
1:A:1325:LEU:HD22	1:A:1344:PHE:CE2	2.43	0.53
3:Z:37:HIS:CD2	3:Z:40:LEU:CA	2.89	0.53
1:J:435:ARG:H	1:J:1367:LEU:HD11	1.74	0.53
2:4:227:ARG:O	2:4:231:ARG:HG2	2.07	0.53
1:J:743:ASN:HD21	2:6:160:LYS:HA	1.73	0.53
1:A:284:MET:HA	1:A:291:ILE:CD1	2.38	0.53
1:A:698:LEU:HD23	1:A:1127:VAL:HG22	1.91	0.53
1:C:801:GLY:HA3	1:C:890:VAL:HB	1.91	0.53
2:6:249:TYR:CE2	3:E:67:MET:HE1	2.43	0.53
1:C:311:ASN:HB3	1:C:321:ILE:HD12	1.91	0.53
2:4:167:ILE:HG13	2:4:185:ASP:OD2	2.09	0.53
1:J:12:LYS:HE3	1:A:94:HIS:CB	2.32	0.52
1:A:21:THR:HG22	1:C:200:ALA:HB1	1.82	0.52
1:A:343:SER:HA	1:A:346:GLN:HB2	1.90	0.52
1:A:633:ARG:O	1:A:637:ASN:ND2	2.39	0.52
1:C:209:ARG:HA	1:C:212:ARG:NH1	2.24	0.52
1:J:188:PRO:HG2	1:J:1093:ASN:OD1	2.09	0.52
1:A:197:VAL:O	1:A:197:VAL:HG12	2.09	0.52
1:C:269:ILE:HD13	1:C:368:ILE:HD11	1.91	0.52
3:Z:37:HIS:HE1	3:Z:39:VAL:CG1	2.14	0.52
1:A:473:PRO:HA	1:A:476:GLN:HG2	1.91	0.52
1:A:534:HIS:CE1	1:A:1239:LEU:CD1	2.90	0.52
1:A:760:MET:HB3	1:A:889:HIS:CD2	2.45	0.52
1:A:1271:ILE:HD12	1:A:1274:ALA:HB3	1.90	0.52
1:J:193:VAL:CG2	1:J:1093:ASN:OD1	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:430:LEU:HD23	1:J:1326:SER:HA	1.92	0.52
1:J:495:ILE:HG22	1:J:496:PRO:HD3	1.90	0.52
1:J:1193:ARG:NH2	1:J:1195:ARG:O	2.41	0.52
1:A:1034:LEU:CD2	1:A:1175:ILE:CD1	2.87	0.52
1:C:15:ILE:HD12	1:C:16:PRO:HD2	1.91	0.52
1:C:687:ILE:CD1	1:C:1006:MET:CE	2.86	0.52
1:C:719:PHE:CE1	1:C:939:PHE:HZ	2.24	0.52
2:5:245:PHE:CZ	2:5:277:ILE:HD11	2.44	0.52
1:J:7:LEU:CD1	1:J:12:LYS:CE	2.88	0.52
1:J:620:ASN:HB2	1:J:623:ALA:HB3	1.92	0.52
1:C:259:THR:HG22	1:C:352:LEU:HD11	1.90	0.52
2:6:245:PHE:CZ	2:6:277:ILE:HD11	2.45	0.52
1:J:718:PRO:CG	1:J:786:LEU:HD21	2.40	0.52
1:J:1290:LYS:HE3	1:J:1312:GLU:HB3	1.92	0.52
1:A:1193:ARG:NH2	1:A:1195:ARG:O	2.43	0.52
1:C:193:VAL:O	1:C:197:VAL:HG23	2.09	0.52
1:C:426:THR:HB	1:C:442:PHE:CE2	2.45	0.52
1:A:8:GLU:OE1	1:A:45:ARG:HB2	2.09	0.52
1:A:1048:LEU:HD12	1:A:1094:THR:CG2	2.40	0.52
1:C:598:LYS:HB2	1:C:792:MET:HE3	1.92	0.52
1:A:20:LEU:CD1	1:C:197:VAL:HG22	2.38	0.52
1:A:21:THR:HG21	1:C:200:ALA:HA	1.79	0.52
1:A:212:ARG:HH12	1:A:1204:PRO:CG	2.22	0.52
1:A:341:ASN:OD1	1:A:345:SER:HB3	2.09	0.52
1:A:426:THR:CG2	1:A:442:PHE:CD2	2.85	0.52
1:A:790:PRO:CB	1:A:942:PHE:HE2	2.03	0.52
1:C:203:ALA:CB	1:C:207:LEU:HD23	2.23	0.52
2:6:29:VAL:HG11	2:6:179:PHE:HE2	1.74	0.52
1:J:344:LEU:HD23	1:J:1086:MET:SD	2.49	0.52
1:J:374:ARG:NH1	1:J:374:ARG:HB3	2.25	0.52
1:J:782:LYS:O	1:J:786:LEU:HB2	2.10	0.52
2:6:246:ASP:HB2	2:6:278:TYR:HA	1.92	0.52
1:J:322:LEU:HD21	1:J:325:PHE:HD1	1.73	0.52
1:A:1318:THR:OG1	1:A:1320:GLU:OE2	2.18	0.52
1:C:68:THR:HA	1:C:355:LEU:CD1	2.40	0.52
1:C:869:HIS:CD2	1:C:870:THR:HG23	2.44	0.52
3:D:25:VAL:HA	3:D:57:LYS:HE3	1.90	0.52
1:J:1064:VAL:HG13	1:J:1077:VAL:HG22	1.91	0.51
1:A:359:VAL:HG12	1:A:368:ILE:HD13	1.93	0.51
1:A:1292:CYS:HB2	1:A:1310:LEU:HD23	1.92	0.51
1:C:74:ALA:HB1	1:C:1054:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:601:VAL:HG11	1:J:793:THR:CG2	2.41	0.51
1:J:1268:THR:HA	1:J:1271:ILE:HG22	1.92	0.51
1:A:192:VAL:HG11	1:A:1282:ILE:HD12	1.92	0.51
2:5:30:ASP:HB3	2:5:33:ALA:HB2	1.93	0.51
2:5:267:LEU:CG	2:5:271:LEU:HD11	2.38	0.51
2:6:259:GLU:HG3	2:6:260:ASN:N	2.26	0.51
1:A:19:PHE:CZ	1:C:1088:LEU:HD22	2.43	0.51
1:C:122:LYS:HG2	1:C:1082:ASN:ND2	2.25	0.51
2:5:140:VAL:HG21	2:5:158:HIS:CD2	2.45	0.51
2:4:31:LEU:HD23	2:4:59:TRP:CZ2	2.46	0.51
1:A:410:VAL:O	1:A:412:SER:N	2.43	0.51
1:C:601:VAL:CG1	1:C:793:THR:HG22	2.40	0.51
1:C:1182:ASP:OD1	1:C:1183:VAL:N	2.43	0.51
3:D:20:HIS:CD2	3:D:24:VAL:HG21	2.45	0.51
1:J:698:LEU:HB2	1:J:706:TYR:CE2	2.44	0.51
1:J:795:ASN:OD1	1:J:942:PHE:CE1	2.63	0.51
1:J:1057:VAL:HG12	1:J:1083:THR:HG22	1.93	0.51
1:A:212:ARG:NH1	1:A:1204:PRO:HG3	2.25	0.51
1:C:457:PRO:HG3	1:C:537:PHE:CD2	2.46	0.51
1:C:633:ARG:NH1	1:C:870:THR:CB	2.73	0.51
1:C:800:LEU:HD23	1:C:923:VAL:HG21	1.85	0.51
2:4:31:LEU:HD11	2:4:58:LEU:HD21	1.93	0.51
1:J:2:GLU:OE1	1:A:90:LYS:CE	2.58	0.51
1:J:1038:ARG:HG3	1:J:1170:ALA:O	2.10	0.51
1:A:193:VAL:CG2	1:A:1093:ASN:HD21	2.21	0.51
1:C:392:THR:HA	1:C:1039:THR:HA	1.93	0.51
1:C:966:TYR:O	1:C:973:PHE:HB3	2.11	0.51
3:D:43:MET:SD	3:D:67:MET:CE	2.99	0.51
1:J:924:VAL:O	1:J:925:THR:CG2	2.58	0.51
1:A:90:LYS:CG	1:A:119:TYR:CD1	2.87	0.51
1:A:858:THR:O	1:A:862:GLU:HG2	2.11	0.51
1:C:80:PHE:CE1	1:C:305:PHE:HD2	2.28	0.51
1:C:1176:LEU:CD2	1:C:1230:ASN:CG	2.79	0.51
2:6:245:PHE:HZ	2:6:277:ILE:HD11	1.76	0.51
1:A:79:LYS:O	1:A:304:ASN:HA	2.10	0.51
1:A:706:TYR:CD1	1:A:900:ASP:OD2	2.64	0.51
1:C:375:VAL:O	1:C:375:VAL:HG12	2.11	0.51
2:4:74:SER:HA	2:4:77:LEU:HB3	1.93	0.51
1:J:83:LEU:HD22	1:J:1080:ASN:HD22	1.59	0.51
1:J:628:ARG:HG3	1:J:661:LEU:HD11	1.93	0.51
1:J:1104:THR:HG22	1:J:1106:MET:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:HB3	1:A:108:THR:HG22	1.93	0.51
1:A:731:GLN:HB3	1:A:738:PRO:HB3	1.91	0.51
1:A:733:VAL:CG2	1:A:738:PRO:HA	2.34	0.51
1:A:753:ASP:O	1:A:757:LEU:CG	2.58	0.51
1:A:898:PRO:HG3	1:A:911:ILE:HG12	1.93	0.51
1:C:514:GLN:C	1:C:993:ARG:HH22	2.14	0.51
1:C:739:LEU:HD21	1:C:766:LEU:HG	1.93	0.51
1:C:1290:LYS:HB3	1:C:1310:LEU:HB3	1.92	0.51
2:6:32:GLU:HG3	2:6:59:TRP:HH2	1.76	0.51
2:4:245:PHE:HB2	3:D:71:SER:HA	1.93	0.51
1:J:205:GLN:HG3	1:C:24:LYS:HE2	1.92	0.51
1:A:1336:LYS:NZ	1:A:1346:THR:O	2.32	0.51
2:6:137:LYS:NZ	2:6:152:GLU:OE1	2.44	0.51
1:J:383:ASP:OD1	1:J:384:PRO:HD2	2.10	0.50
1:J:684:VAL:O	1:J:687:ILE:HG22	2.12	0.50
1:J:713:HIS:CD2	1:J:726:ASN:HD21	2.29	0.50
1:A:1292:CYS:HB2	1:A:1310:LEU:CD2	2.40	0.50
1:J:908:PRO:HG3	1:J:1123:ARG:HH12	1.76	0.50
1:J:1336:LYS:HE2	1:J:1355:VAL:HG11	1.94	0.50
1:A:231:ASN:HD21	1:A:1099:VAL:N	2.01	0.50
1:A:448:THR:HG21	1:A:1111:GLN:O	2.09	0.50
1:A:747:ARG:HD3	1:A:749:HIS:CE1	2.45	0.50
1:J:79:LYS:N	1:J:303:GLY:O	2.36	0.50
1:J:1054:CYS:SG	1:J:1055:THR:HG22	2.51	0.50
1:A:431:LEU:HD23	1:A:436:ALA:C	2.12	0.50
1:A:732:VAL:O	1:A:739:LEU:N	2.29	0.50
1:A:1359:ILE:HG23	1:A:1360:ILE:HG13	1.92	0.50
2:4:109:LEU:O	2:4:112:THR:HG22	2.12	0.50
1:J:514:GLN:HE22	1:J:563:ASP:H	1.58	0.50
1:J:524:VAL:HA	1:J:1227:ALA:HB2	1.92	0.50
1:A:443:VAL:HG22	1:A:1024:THR:HG22	1.93	0.50
1:A:588:PRO:HG2	1:A:683:LEU:HD11	1.94	0.50
1:A:862:GLU:HG3	1:A:863:ASP:N	2.26	0.50
1:J:19:PHE:CE2	1:J:32:PHE:HZ	2.30	0.50
1:J:653:LEU:O	1:J:657:ILE:HG12	2.12	0.50
1:A:445:ALA:HA	1:A:1110:VAL:HG21	1.94	0.50
1:C:707:VAL:HG22	1:C:1022:LEU:HD23	1.93	0.50
1:C:945:ASN:HD22	1:C:948:ILE:HD13	1.77	0.50
1:J:7:LEU:HD11	1:J:12:LYS:CD	2.38	0.50
1:J:341:ASN:HD21	1:J:345:SER:HB3	1.76	0.50
1:J:534:HIS:NE2	1:J:537:PHE:CD1	2.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1221:ASP:HB3	1:J:1224:THR:O	2.10	0.50
1:A:4:TRP:O	1:A:5:SER:OG	2.29	0.50
1:A:853:VAL:HG13	1:A:873:LEU:CD2	2.42	0.50
1:C:188:PRO:HA	1:C:1286:LEU:HD21	1.93	0.50
1:C:384:PRO:O	1:C:387:ARG:HD3	2.11	0.50
1:C:1308:GLU:OE1	1:C:1308:GLU:N	2.44	0.50
2:5:16:LEU:HD13	2:5:58:LEU:HD21	1.94	0.50
2:4:250:CYS:SG	2:4:278:TYR:HB2	2.51	0.50
1:C:120:SER:HB3	1:C:1084:VAL:CG1	2.41	0.50
1:C:733:VAL:HG22	1:C:738:PRO:CA	2.36	0.50
1:C:801:GLY:HA3	1:C:890:VAL:CB	2.41	0.50
1:C:1055:THR:HG22	1:C:1085:ASP:HA	1.94	0.50
1:C:1193:ARG:HG3	1:C:1266:PHE:CE1	2.47	0.50
1:C:1296:ASP:OD1	1:C:1297:THR:N	2.45	0.50
1:J:144:GLU:O	1:J:146:THR:HG23	2.12	0.50
1:J:457:PRO:HG3	1:J:537:PHE:CD2	2.47	0.50
1:A:78:ILE:O	1:A:1058:ILE:HA	2.10	0.50
1:A:574:ARG:NH2	1:A:1010:ALA:O	2.43	0.50
1:A:601:VAL:CG1	1:A:793:THR:CG2	2.88	0.50
1:C:431:LEU:CG	1:C:1333:MET:CE	2.89	0.50
1:C:954:ASP:O	1:C:958:ARG:HG2	2.12	0.50
1:C:1168:GLN:HA	1:C:1298:ASP:O	2.12	0.50
3:D:47:TYR:OH	3:D:64:LEU:CD2	2.60	0.50
1:J:663:ASP:OD1	1:J:664:GLY:N	2.45	0.50
1:J:946:PRO:HG3	1:J:973:PHE:CD1	2.47	0.50
1:A:764:GLU:HB2	1:A:765:PRO:HD2	1.94	0.50
1:C:633:ARG:NH1	1:C:870:THR:HG21	2.19	0.50
1:C:1152:THR:HB	1:C:1153:PHE:CD1	2.47	0.50
2:6:249:TYR:HE2	3:E:67:MET:HE1	1.74	0.50
1:J:443:VAL:O	1:J:446:LEU:HG	2.11	0.49
1:J:1212:LYS:HB3	1:J:1219:GLU:OE1	2.12	0.49
1:A:207:LEU:HD12	1:A:207:LEU:C	2.33	0.49
2:4:243:LEU:HB3	3:D:74:ARG:HH11	1.77	0.49
1:J:118:LYS:CD	1:C:32:PHE:CD1	2.95	0.49
1:J:1121:VAL:HG12	1:J:1132:ARG:NH1	2.27	0.49
1:J:388:ASN:CG	1:J:1311:ILE:HG13	2.30	0.49
1:J:763:ASP:O	1:J:764:GLU:O	2.29	0.49
1:A:17:THR:HG21	1:C:95:VAL:HG21	1.94	0.49
1:A:343:SER:HA	1:A:346:GLN:CB	2.43	0.49
1:A:638:MET:HE3	1:A:642:ARG:HD2	1.92	0.49
1:A:1020:LEU:HD21	1:A:1032:PHE:CZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:ASP:HB3	1:A:1316:ARG:NH2	2.27	0.49
1:A:687:ILE:CD1	1:A:1006:MET:SD	2.95	0.49
1:A:1327:THR:HG22	1:A:1355:VAL:HG13	1.94	0.49
1:C:535:PRO:O	1:C:555:ARG:NH2	2.44	0.49
2:5:55:GLU:HA	2:5:58:LEU:HD12	1.95	0.49
1:J:400:TYR:HE1	1:J:573:LEU:HD12	1.76	0.49
1:J:800:LEU:C	1:J:800:LEU:HD12	2.32	0.49
1:C:227:LEU:O	1:C:1096:VAL:HB	2.13	0.49
1:C:397:VAL:HG22	1:C:428:ALA:CB	2.43	0.49
1:C:647:PHE:HD2	1:C:653:LEU:HD13	1.78	0.49
1:J:270:SER:OG	1:J:365:LYS:HG3	2.13	0.49
1:J:790:PRO:CG	1:J:942:PHE:CE2	2.93	0.49
1:A:231:ASN:HD21	1:A:1099:VAL:HB	1.77	0.49
1:A:812:PHE:HB2	3:D:65:LEU:HD21	1.93	0.49
1:C:1244:TYR:HB2	1:C:1266:PHE:CD2	2.38	0.49
1:J:15:ILE:HD12	1:J:16:PRO:HD2	1.95	0.49
1:J:485:GLN:OE1	1:J:913:ARG:NH2	2.46	0.49
1:J:651:TYR:CE2	1:J:781:GLN:HG2	2.48	0.49
1:A:538:ASP:OD1	1:A:539:PHE:N	2.46	0.49
1:A:1328:THR:HG22	1:A:1353:ASN:CG	2.33	0.49
1:J:129:PHE:CZ	1:J:1075:TYR:HD2	2.30	0.49
1:J:132:SER:O	1:J:136:LEU:HD12	2.13	0.49
1:J:397:VAL:HG22	1:J:428:ALA:CB	2.42	0.49
1:J:924:VAL:O	1:J:925:THR:HG23	2.12	0.49
1:A:967:HIS:NE2	1:A:969:HIS:HE1	2.11	0.49
1:C:710:LEU:O	1:C:782:LYS:NZ	2.33	0.49
1:C:748:HIS:O	1:C:756:ARG:NH1	2.46	0.49
1:C:1056:SER:HG	1:C:1084:VAL:CG2	2.23	0.49
1:C:1185:TYR:OH	1:C:1191:ASN:O	2.23	0.49
1:J:177:HIS:ND1	1:J:376:TYR:OH	2.27	0.49
1:A:638:MET:HB2	1:A:646:VAL:HG21	1.95	0.49
1:C:22:HIS:O	1:C:23:VAL:C	2.51	0.49
1:C:371:ASN:OD1	1:C:372:LEU:N	2.45	0.49
1:C:524:VAL:HG11	1:C:1218:ARG:O	2.12	0.49
1:C:565:LEU:HD22	1:C:1177:THR:HB	1.94	0.49
1:C:1154:GLY:HA2	1:C:1257:LYS:HD3	1.93	0.49
1:C:1291:ASP:OD1	1:C:1291:ASP:N	2.45	0.49
2:5:41:CYS:SG	2:5:55:GLU:HG3	2.52	0.49
1:J:448:THR:HG23	1:J:1111:GLN:O	2.10	0.49
1:J:698:LEU:O	1:J:699:ALA:HB3	2.12	0.49
1:A:1278:LEU:O	1:A:1282:ILE:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:THR:HG23	1:C:910:PHE:CE1	2.48	0.49
1:C:994:TYR:OH	1:C:1007:THR:HG21	2.13	0.49
2:5:150:GLN:HG2	2:5:150:GLN:O	2.12	0.49
2:5:225:LEU:O	2:5:229:GLN:NE2	2.45	0.49
2:6:121:ASP:HB3	2:6:214:ARG:HH12	1.77	0.49
1:A:158:HIS:O	1:A:162:ARG:HG3	2.12	0.48
1:A:603:SER:OG	1:A:644:LEU:HD22	2.13	0.48
1:A:976:PRO:HD2	1:A:979:PHE:HD2	1.77	0.48
1:A:1044:VAL:HG23	1:A:1099:VAL:HA	1.95	0.48
1:C:853:VAL:HB	1:C:857:LEU:HD23	1.94	0.48
1:J:924:VAL:HG12	1:J:925:THR:HG23	1.94	0.48
1:C:273:MET:CE	1:C:1047:LEU:HD21	2.44	0.48
1:C:362:LEU:HD22	1:C:367:VAL:HG21	1.94	0.48
1:C:534:HIS:ND1	1:C:1239:LEU:HD22	2.25	0.48
1:C:646:VAL:HG12	1:C:647:PHE:HD1	1.70	0.48
1:J:7:LEU:HD13	1:J:12:LYS:HD3	1.83	0.48
1:J:768:VAL:HG23	1:J:918:TYR:OH	2.13	0.48
1:J:941:ARG:CG	1:J:992:SER:HB3	2.40	0.48
1:J:1173:GLU:O	1:J:1244:TYR:OH	2.20	0.48
1:A:93:PHE:CE1	1:A:118:LYS:HG2	2.45	0.48
1:C:646:VAL:CG1	1:C:647:PHE:CD1	2.86	0.48
1:C:718:PRO:HD3	1:C:786:LEU:CG	2.42	0.48
1:C:867:ASP:OD1	1:C:868:ALA:N	2.46	0.48
1:C:1122:TYR:HB2	1:C:1128:ASP:HB2	1.94	0.48
2:6:217:TRP:NE1	2:6:221:GLU:OE1	2.46	0.48
2:4:115:ASP:OD1	2:4:116:THR:N	2.46	0.48
1:J:1168:GLN:NE2	1:J:1294:ARG:O	2.42	0.48
1:A:9:LEU:HD13	1:A:45:ARG:HG3	1.90	0.48
1:C:382:LYS:HD3	1:C:1309:GLN:HG3	1.94	0.48
2:4:108:VAL:HA	2:4:111:ARG:HG3	1.95	0.48
1:J:184:LEU:HD23	1:J:1048:LEU:HD13	1.96	0.48
1:A:231:ASN:ND2	1:A:1099:VAL:HB	2.28	0.48
1:A:663:ASP:OD1	1:A:664:GLY:N	2.46	0.48
1:J:231:ASN:HD21	1:J:1099:VAL:CA	2.27	0.48
1:J:535:PRO:HB3	1:J:1232:TRP:CH2	2.48	0.48
1:C:83:LEU:HD11	1:C:1058:ILE:HG22	1.89	0.48
2:6:206:THR:O	2:6:210:ILE:HG12	2.14	0.48
2:4:60:LEU:HB3	2:4:268:LEU:HD22	1.94	0.48
1:J:80:PHE:HB3	1:J:1058:ILE:CG2	2.43	0.48
1:J:397:VAL:HG22	1:J:428:ALA:HB2	1.95	0.48
1:A:397:VAL:HG22	1:A:428:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LYS:HZ3	1:C:1055:THR:CG2	2.14	0.48
1:C:1068:GLU:HG2	1:C:1070:ASP:H	1.79	0.48
1:J:76:HIS:HE1	1:J:78:ILE:HD11	1.79	0.48
1:C:440:ILE:HB	1:C:1108:VAL:HG11	1.96	0.48
1:C:448:THR:HG22	1:C:1113:LEU:HB2	1.95	0.48
1:C:633:ARG:HH12	1:C:870:THR:HB	1.78	0.48
1:C:681:LEU:HD22	1:C:783:VAL:HG12	1.96	0.48
1:C:1211:THR:O	1:C:1215:TYR:HB2	2.14	0.48
1:C:1271:ILE:HD12	1:C:1274:ALA:HB3	1.95	0.48
2:5:84:CYS:O	2:5:109:LEU:HD21	2.14	0.48
2:4:208:ARG:O	2:4:212:ASN:HB2	2.14	0.48
1:J:120:SER:HB3	1:J:1084:VAL:HG12	1.94	0.48
1:C:739:LEU:C	1:C:741:PRO:HD2	2.35	0.48
1:C:1160:ASN:CG	1:C:1298:ASP:CB	2.81	0.48
2:5:245:PHE:CE2	2:5:277:ILE:HD11	2.48	0.48
3:D:43:MET:SD	3:D:67:MET:HE2	2.53	0.48
1:J:228:PHE:CG	1:J:1099:VAL:HG23	2.45	0.48
1:J:924:VAL:C	1:J:925:THR:HG23	2.35	0.48
1:A:425:PRO:HB3	1:A:1328:THR:CG2	2.43	0.48
1:A:895:VAL:HB	1:A:914:GLN:HB2	1.96	0.48
1:A:1123:ARG:HE	1:A:1123:ARG:HB2	1.38	0.48
1:C:102:SER:OG	1:C:103:GLY:N	2.46	0.48
1:C:794:ASN:ND2	1:C:1000:ASN:HD21	2.12	0.48
1:C:1326:SER:O	1:C:1355:VAL:HA	2.13	0.48
3:Z:47:TYR:OH	3:Z:63:ASP:OD1	2.21	0.48
1:J:114:ILE:HG22	1:C:35:LEU:HD11	1.96	0.47
1:J:1004:SER:HA	1:J:1007:THR:HG22	1.95	0.47
1:A:597:PHE:CE1	1:A:648:ALA:HB1	2.49	0.47
1:C:287:LEU:O	1:C:291:ILE:HG13	2.13	0.47
3:Z:68:VAL:O	3:Z:71:SER:OG	2.27	0.47
1:J:21:THR:H	1:A:200:ALA:HB1	1.78	0.47
1:J:410:VAL:O	1:J:412:SER:N	2.47	0.47
1:J:598:LYS:CD	1:J:1000:ASN:CB	2.74	0.47
1:J:1221:ASP:OD1	1:J:1222:ALA:N	2.46	0.47
1:A:741:PRO:HG3	2:5:160:LYS:HE2	1.96	0.47
2:4:50:THR:OG1	2:4:283:PRO:O	2.27	0.47
1:J:2:GLU:OE1	1:A:90:LYS:CD	2.63	0.47
1:J:220:LYS:NZ	1:J:1320:GLU:OE2	2.27	0.47
1:J:431:LEU:CG	1:J:1333:MET:CE	2.92	0.47
1:A:21:THR:CG2	1:C:200:ALA:HB2	2.39	0.47
1:A:941:ARG:CG	1:A:992:SER:HB3	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:VAL:HG23	1:C:361:ARG:HH12	1.80	0.47
1:J:210:ILE:O	1:J:213:SER:OG	2.26	0.47
1:J:431:LEU:HA	1:J:436:ALA:O	2.15	0.47
1:J:1214:ILE:HG21	1:J:1272:ILE:HD11	1.96	0.47
1:C:801:GLY:HA3	1:C:890:VAL:HG11	1.97	0.47
2:6:88:ALA:HA	2:6:106:LEU:HD22	1.96	0.47
3:Z:29:PRO:HG2	3:Z:32:ILE:HG12	1.96	0.47
1:J:703:LEU:HA	1:J:703:LEU:HD12	1.72	0.47
1:A:970:ASP:OD1	1:A:993:ARG:HA	2.15	0.47
1:C:177:HIS:CE1	1:C:384:PRO:HD3	2.49	0.47
1:C:344:LEU:HD21	1:C:1086:MET:SD	2.54	0.47
2:6:136:ALA:O	2:6:140:VAL:HG23	2.14	0.47
2:4:164:VAL:HA	2:4:167:ILE:HG22	1.96	0.47
1:C:408:THR:HG23	1:C:1350:HIS:HA	1.97	0.47
1:C:601:VAL:HG12	1:C:601:VAL:O	2.13	0.47
1:C:734:ALA:HB2	1:C:766:LEU:HD11	1.96	0.47
1:J:83:LEU:HD23	1:J:1080:ASN:HD21	1.79	0.47
1:J:400:TYR:CE1	1:J:573:LEU:HD12	2.50	0.47
1:J:796:ARG:O	1:J:945:ASN:ND2	2.41	0.47
1:J:1196:ALA:HB3	1:J:1222:ALA:HB3	1.97	0.47
1:A:682:ARG:HD3	1:A:682:ARG:HA	1.69	0.47
1:A:967:HIS:NE2	1:A:969:HIS:CE1	2.83	0.47
1:C:8:GLU:CB	1:C:45:ARG:HD3	2.43	0.47
1:C:19:PHE:HZ	1:C:23:VAL:H	1.27	0.47
1:C:78:ILE:O	1:C:1058:ILE:HA	2.14	0.47
1:C:426:THR:C	1:C:442:PHE:CE2	2.87	0.47
1:C:431:LEU:HD11	1:C:1337:LEU:HD21	1.97	0.47
1:C:514:GLN:CB	1:C:993:ARG:HH21	1.98	0.47
1:C:694:ASN:HD22	1:C:704:SER:HB3	1.78	0.47
1:C:1004:SER:HA	1:C:1007:THR:HG22	1.95	0.47
2:6:246:ASP:OD2	2:6:281:SER:HB2	2.12	0.47
1:J:667:PRO:HD2	1:J:670:LEU:HD12	1.97	0.47
1:J:718:PRO:CG	1:J:786:LEU:HD23	2.45	0.47
1:J:718:PRO:HG2	1:J:943:TYR:HE2	1.80	0.47
1:A:390:ASP:O	1:A:391:LEU:HD12	2.15	0.47
1:A:434:ASP:HA	1:A:1367:LEU:HD11	1.96	0.47
1:A:1212:LYS:HB3	1:A:1219:GLU:OE1	2.15	0.47
1:A:1244:TYR:HB2	1:A:1266:PHE:CD2	2.49	0.47
2:4:276:ASP:OD2	3:D:49:ARG:NH2	2.48	0.47
1:J:177:HIS:O	1:J:181:GLN:HG2	2.14	0.47
1:J:1069:ARG:NH1	1:J:1069:ARG:CG	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:THR:HG23	1:A:1350:HIS:HA	1.97	0.47
1:A:734:ALA:CB	1:A:766:LEU:HD11	2.44	0.47
1:A:1105:ASP:N	1:A:1168:GLN:O	2.45	0.47
1:C:192:VAL:O	1:C:196:LEU:HG	2.14	0.47
1:C:1233:ALA:HA	1:C:1238:CYS:SG	2.55	0.47
1:C:1325:LEU:HD22	1:C:1344:PHE:CD2	2.49	0.47
1:J:425:PRO:HB3	1:J:1328:THR:HG21	1.97	0.47
1:A:452:PRO:HG3	1:A:1122:TYR:CE1	2.50	0.47
1:A:1109:ARG:HD2	1:A:1169:LYS:HD2	1.95	0.47
1:A:1365:SER:OG	1:A:1366:MET:N	2.48	0.47
1:C:19:PHE:CE1	1:C:21:THR:O	2.68	0.47
1:C:175:LEU:HD11	1:C:1081:ILE:CD1	2.43	0.47
1:C:504:GLU:HG2	1:C:966:TYR:OH	2.15	0.47
2:4:24:THR:HG21	2:4:69:HIS:CG	2.49	0.47
3:D:33:SER:HB2	3:D:36:THR:CB	2.45	0.47
1:J:119:TYR:HH	1:C:2:GLU:CD	2.12	0.46
1:A:739:LEU:CD1	1:A:744:ILE:HG21	2.44	0.46
1:C:880:PHE:HE1	3:E:65:LEU:HG	1.80	0.46
1:C:1290:LYS:HD3	1:C:1312:GLU:HG2	1.97	0.46
1:J:83:LEU:HD23	1:J:1080:ASN:ND2	2.23	0.46
1:J:252:ASP:OD1	1:J:253:SER:N	2.48	0.46
1:J:322:LEU:HD21	1:J:325:PHE:CD1	2.51	0.46
1:J:371:ASN:HD21	1:J:373:ARG:HB3	1.80	0.46
1:J:710:LEU:HD21	1:J:783:VAL:HG22	1.97	0.46
1:J:740:ASN:N	1:J:741:PRO:HD2	2.31	0.46
1:J:819:LEU:HD11	3:Z:32:ILE:CD1	2.45	0.46
1:J:1043:GLU:C	1:J:1044:VAL:HG23	2.34	0.46
1:J:1083:THR:O	1:J:1083:THR:OG1	2.30	0.46
1:A:853:VAL:HG13	1:A:873:LEU:HD21	1.96	0.46
1:C:94:HIS:ND1	1:C:94:HIS:O	2.48	0.46
2:6:19:PHE:HE2	2:6:26:LYS:HZ3	1.50	0.46
2:6:41:CYS:SG	2:6:55:GLU:HG3	2.55	0.46
1:J:27:ALA:CB	1:J:35:LEU:CD2	2.88	0.46
1:J:231:ASN:OD1	1:J:1098:TYR:HE1	1.90	0.46
1:J:682:ARG:HA	1:J:685:THR:HG22	1.96	0.46
1:J:764:GLU:CG	1:J:765:PRO:CD	2.50	0.46
1:J:942:PHE:HZ	1:J:995:SER:HB2	1.79	0.46
1:J:1109:ARG:HD3	1:J:1169:LYS:CE	2.45	0.46
1:A:147:ILE:O	1:A:151:ILE:HG12	2.15	0.46
1:A:342:ASP:OD1	1:A:342:ASP:N	2.47	0.46
1:A:1057:VAL:HG12	1:A:1083:THR:HG22	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:VAL:O	1:C:197:VAL:HG12	2.14	0.46
1:C:510:ASN:OD1	1:C:982:GLU:CD	2.53	0.46
1:C:1015:ILE:O	1:C:1015:ILE:CG2	2.54	0.46
1:J:3:ASN:HD21	1:J:6:ALA:HB2	1.79	0.46
1:J:80:PHE:CB	1:J:1058:ILE:CG2	2.93	0.46
1:J:184:LEU:HD23	1:J:184:LEU:HA	1.81	0.46
1:J:275:SER:CB	1:J:1047:LEU:HD13	2.40	0.46
1:J:450:CYS:SG	1:J:1131:ILE:HD12	2.55	0.46
1:A:1344:PHE:H	1:A:1364:GLN:HE22	1.60	0.46
1:C:7:LEU:CD1	1:C:12:LYS:CD	2.65	0.46
1:C:475:MET:SD	1:C:1218:ARG:NH1	2.88	0.46
1:C:518:VAL:HB	1:C:1179:VAL:HG11	1.97	0.46
1:C:805:LYS:H	1:C:889:HIS:HE1	1.63	0.46
2:6:246:ASP:OD1	2:6:247:SER:N	2.48	0.46
1:J:254:ILE:HD12	1:J:1086:MET:HA	1.97	0.46
1:J:1193:ARG:HB2	1:J:1266:PHE:HE1	1.80	0.46
1:A:207:LEU:HD13	1:A:212:ARG:N	2.30	0.46
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.68	0.46
2:5:35:PRO:O	2:5:39:LYS:HG2	2.16	0.46
2:5:115:ASP:HA	2:6:93:THR:HG21	1.97	0.46
2:4:6:ILE:HG22	2:4:284:GLN:HB3	1.97	0.46
2:4:73:LEU:HD21	2:4:213:VAL:HG11	1.98	0.46
1:J:621:VAL:O	1:J:625:LEU:HG	2.16	0.46
1:A:913:ARG:HH12	1:A:981:HIS:CD2	2.09	0.46
1:A:1058:ILE:HG13	1:A:1082:ASN:HB2	1.96	0.46
1:C:21:THR:O	1:C:22:HIS:C	2.53	0.46
1:C:504:GLU:HB2	1:C:963:PHE:HE2	1.81	0.46
1:C:666:LEU:HD12	1:C:666:LEU:HA	1.84	0.46
1:J:560:ASN:HA	1:J:990:PRO:HG2	1.96	0.46
1:J:808:LEU:CD2	1:J:886:VAL:HG21	2.46	0.46
1:A:464:PHE:CD1	1:A:533:LEU:HD11	2.49	0.46
1:C:408:THR:HG22	1:C:411:GLU:HB2	1.98	0.46
2:6:117:ASP:OD2	2:6:119:ARG:NH2	2.49	0.46
2:4:2:SER:OG	2:4:272:ILE:HG21	2.16	0.46
1:J:382:LYS:HG3	1:J:383:ASP:N	2.31	0.46
1:A:434:ASP:OD1	1:A:434:ASP:N	2.48	0.46
1:A:461:LEU:HD13	1:A:552:CYS:HB2	1.98	0.46
1:A:1021:VAL:O	1:A:1025:LYS:HD3	2.16	0.46
1:C:269:ILE:HD11	1:C:296:VAL:HG22	1.98	0.46
1:C:1044:VAL:HG12	1:C:1045:ASP:N	2.31	0.46
1:J:139:LEU:HD22	1:J:160:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:303:GLY:CA	1:J:348:GLY:HA3	2.46	0.46
1:J:431:LEU:HD21	1:J:1333:MET:HE2	1.97	0.46
1:C:147:ILE:O	1:C:151:ILE:HG12	2.16	0.46
1:C:795:ASN:ND2	1:C:942:PHE:CE1	2.83	0.46
2:5:206:THR:O	2:5:210:ILE:HG12	2.16	0.46
2:4:10:ARG:O	2:4:14:VAL:HG23	2.16	0.46
1:J:118:LYS:HD3	1:C:32:PHE:CD1	2.50	0.46
1:A:698:LEU:HB2	1:A:706:TYR:HE2	1.80	0.46
1:A:949:CYS:SG	1:A:956:ILE:HG21	2.55	0.46
1:C:242:PHE:HD2	1:C:243:LEU:HD23	1.81	0.46
1:C:1043:GLU:O	1:C:1044:VAL:HG23	2.16	0.46
1:J:390:ASP:O	1:J:391:LEU:HD12	2.15	0.45
1:J:682:ARG:HA	1:J:682:ARG:HD3	1.79	0.45
1:J:798:CYS:SG	1:J:799:GLY:N	2.89	0.45
1:A:18:ASP:O	1:A:19:PHE:HD1	1.98	0.45
1:A:543:GLN:OE1	1:A:548:THR:HG22	2.16	0.45
1:A:607:PRO:HG3	1:A:638:MET:HE2	1.99	0.45
1:A:766:LEU:HD21	1:A:893:LEU:CD2	2.34	0.45
1:C:341:ASN:OD1	1:C:345:SER:HB3	2.15	0.45
1:C:698:LEU:HD11	1:C:1130:TRP:CD1	2.52	0.45
1:C:1158:GLU:OE1	1:C:1299:THR:HG21	2.16	0.45
1:J:118:LYS:CE	1:C:32:PHE:HE1	2.29	0.45
1:A:795:ASN:ND2	1:A:942:PHE:CE1	2.83	0.45
1:C:360:ILE:HG22	1:C:362:LEU:CD1	2.46	0.45
1:C:1043:GLU:O	1:C:1044:VAL:CG2	2.65	0.45
2:5:67:ARG:O	2:5:70:ASN:HB2	2.16	0.45
2:6:246:ASP:OD2	2:6:281:SER:CA	2.64	0.45
1:J:597:PHE:CZ	1:J:601:VAL:HG21	2.51	0.45
1:J:601:VAL:HG12	1:J:601:VAL:O	2.16	0.45
1:A:625:LEU:HD23	3:D:75:ARG:NH1	2.31	0.45
1:A:1347:SER:O	1:A:1348:GLU:HG3	2.15	0.45
1:A:1350:HIS:O	1:A:1352:GLY:N	2.38	0.45
1:C:515:ASP:OD1	1:C:515:ASP:N	2.49	0.45
1:C:740:ASN:N	1:C:741:PRO:HD2	2.31	0.45
1:C:891:LYS:HE2	1:C:891:LYS:HB3	1.76	0.45
1:C:1042:PHE:CD1	1:C:1102:VAL:HG22	2.50	0.45
1:C:1217:HIS:CE1	1:C:1228:THR:HG1	2.32	0.45
2:5:23:LEU:HD21	2:5:62:TYR:HE1	1.81	0.45
2:5:36:LYS:HE3	2:5:40:LYS:HE2	1.97	0.45
2:6:145:VAL:HG22	2:6:152:GLU:HG2	1.99	0.45
2:4:243:LEU:HD13	3:D:74:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:HIS:O	1:J:78:ILE:HG13	2.17	0.45
1:J:207:LEU:HD13	1:J:212:ARG:HG3	1.90	0.45
1:A:651:TYR:CD2	1:A:781:GLN:HG2	2.51	0.45
1:C:578:ILE:HG12	1:C:1028:ILE:HD12	1.99	0.45
2:5:194:THR:O	2:5:198:ASN:ND2	2.50	0.45
1:J:341:ASN:OD1	1:J:345:SER:HB3	2.16	0.45
1:A:703:LEU:HA	1:A:703:LEU:HD12	1.69	0.45
1:A:883:VAL:O	1:A:886:VAL:HG23	2.17	0.45
1:C:22:HIS:O	1:C:25:THR:N	2.47	0.45
1:C:293:LYS:HB2	1:C:293:LYS:HE3	1.82	0.45
1:C:574:ARG:O	1:C:577:GLU:HB2	2.16	0.45
2:6:274:ASP:O	2:6:277:ILE:HG22	2.16	0.45
1:J:35:LEU:CD1	1:A:116:VAL:CG1	2.79	0.45
1:J:498:PHE:O	1:J:501:VAL:HG22	2.17	0.45
1:J:628:ARG:NH2	3:Z:75:ARG:HH12	2.14	0.45
1:J:805:LYS:H	1:J:889:HIS:HE1	1.64	0.45
1:J:1237:GLY:O	1:J:1238:CYS:O	2.33	0.45
1:J:1271:ILE:HD12	1:J:1271:ILE:HA	1.81	0.45
1:A:431:LEU:HG	1:A:1333:MET:CE	2.46	0.45
1:C:534:HIS:CD2	1:C:537:PHE:CD1	3.04	0.45
1:C:1285:TYR:CB	1:C:1317:LEU:CD2	2.84	0.45
2:5:32:GLU:OE2	2:5:227:ARG:CZ	2.65	0.45
1:J:486:GLU:HG2	1:J:487:PRO:HD2	1.98	0.45
1:J:1168:GLN:HA	1:J:1298:ASP:O	2.16	0.45
1:A:21:THR:H	1:C:200:ALA:HB1	1.82	0.45
1:A:30:GLU:HB3	1:C:1280:LYS:HD3	1.98	0.45
1:C:122:LYS:HG2	1:C:1082:ASN:HD21	1.81	0.45
1:C:247:ALA:HB1	1:C:365:LYS:HD3	1.98	0.45
1:C:731:GLN:HB3	1:C:738:PRO:HB3	1.97	0.45
1:C:941:ARG:HE	1:C:941:ARG:HB2	1.61	0.45
1:J:273:MET:CE	1:J:1047:LEU:HD21	2.47	0.45
1:J:495:ILE:HD13	1:J:937:VAL:HA	1.99	0.45
1:J:746:ALA:O	1:J:767:PHE:HA	2.17	0.45
1:A:749:HIS:CD2	1:A:769:ASP:OD1	2.69	0.45
1:A:853:VAL:CG1	1:A:873:LEU:CD2	2.94	0.45
1:C:202:LEU:HD12	1:C:203:ALA:N	2.31	0.45
2:4:66:LEU:HB3	2:4:217:TRP:HZ3	1.78	0.45
2:4:211:MET:O	2:4:215:ARG:HG2	2.16	0.45
1:J:647:PHE:O	1:J:654:VAL:CG2	2.65	0.45
1:J:953:SER:HB2	1:J:956:ILE:HD12	1.99	0.45
1:J:1218:ARG:HA	1:J:1218:ARG:HD2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HB	1:A:1058:ILE:HG22	1.99	0.45
1:A:681:LEU:HB3	1:A:780:LEU:HD22	1.99	0.45
1:A:746:ALA:O	1:A:767:PHE:HA	2.17	0.45
1:C:2:GLU:OE1	1:C:34:ALA:HB3	2.17	0.45
1:C:344:LEU:CD2	1:C:1086:MET:SD	3.05	0.45
1:C:651:TYR:CD2	1:C:781:GLN:HG2	2.52	0.45
1:C:1296:ASP:OD1	1:C:1297:THR:HG23	2.17	0.45
2:6:107:ALA:O	2:6:111:ARG:HG3	2.17	0.45
2:4:136:ALA:HB2	2:4:200:VAL:HG11	1.99	0.45
1:J:94:HIS:CB	1:C:12:LYS:HE3	2.43	0.45
1:A:132:SER:OG	1:A:135:CYS:SG	2.72	0.45
1:C:5:SER:HA	1:C:8:GLU:HG3	1.99	0.45
1:C:633:ARG:NH1	1:C:870:THR:HB	2.32	0.45
1:C:862:GLU:HG3	1:C:863:ASP:N	2.32	0.45
1:C:1105:ASP:N	1:C:1168:GLN:O	2.34	0.45
1:J:1044:VAL:CG1	1:J:1096:VAL:CG1	2.90	0.44
1:A:18:ASP:O	1:A:19:PHE:CD1	2.70	0.44
1:C:294:GLU:OE1	1:C:359:VAL:HG21	2.17	0.44
1:C:598:LYS:HD3	1:C:1000:ASN:HB3	1.96	0.44
2:6:60:LEU:HA	2:6:60:LEU:HD23	1.75	0.44
2:4:170:ASN:ND2	2:4:182:LYS:O	2.43	0.44
1:J:21:THR:CG2	1:A:200:ALA:CB	2.86	0.44
1:C:79:LYS:O	1:C:304:ASN:HA	2.17	0.44
1:C:1290:LYS:CB	1:C:1310:LEU:HB3	2.47	0.44
1:J:303:GLY:HA2	1:J:348:GLY:HA3	1.98	0.44
1:J:435:ARG:N	1:J:1367:LEU:HD11	2.32	0.44
1:J:650:SER:O	1:J:654:VAL:HG23	2.17	0.44
1:A:68:THR:HG23	1:A:355:LEU:HD13	1.99	0.44
1:A:945:ASN:HD22	1:A:948:ILE:CD1	2.26	0.44
1:C:1130:TRP:CE3	1:C:1131:ILE:HD13	2.52	0.44
1:C:1239:LEU:O	1:C:1243:LEU:HB2	2.17	0.44
2:4:243:LEU:HD22	3:D:74:ARG:HD3	1.99	0.44
3:D:24:VAL:CG1	3:D:54:PHE:HZ	2.30	0.44
1:J:37:ILE:HD11	1:A:114:ILE:HD13	2.00	0.44
1:J:341:ASN:HD21	1:J:345:SER:CB	2.30	0.44
1:J:1038:ARG:NH2	1:J:1324:ILE:HD13	2.32	0.44
1:J:1341:ALA:O	1:J:1364:GLN:NE2	2.50	0.44
1:A:35:LEU:HG	1:A:36:ARG:N	2.31	0.44
1:A:999:PRO:O	1:A:1004:SER:OG	2.36	0.44
1:C:645:LEU:HD11	1:C:674:TYR:CE2	2.52	0.44
1:C:718:PRO:HD3	1:C:786:LEU:HG	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:PRO:HB3	2:4:158:HIS:CD2	2.53	0.44
2:5:267:LEU:O	2:5:271:LEU:CG	2.58	0.44
3:D:37:HIS:CD2	3:D:40:LEU:H	2.35	0.44
1:J:941:ARG:HE	1:J:941:ARG:HB2	1.44	0.44
1:A:148:LEU:HD12	1:A:148:LEU:HA	1.84	0.44
1:A:275:SER:OG	1:A:280:MET:HG2	2.18	0.44
1:A:713:HIS:H	1:A:713:HIS:CD2	2.35	0.44
1:A:1240:SER:HG	1:A:1266:PHE:HE2	1.64	0.44
1:C:22:HIS:O	1:C:24:LYS:N	2.51	0.44
1:C:633:ARG:HH22	1:C:870:THR:HG22	1.72	0.44
1:C:1044:VAL:CG1	1:C:1096:VAL:HG13	2.44	0.44
2:6:92:TYR:CE1	2:6:106:LEU:HD13	2.53	0.44
1:J:205:GLN:HG3	1:C:24:LYS:CE	2.47	0.44
1:J:472:GLU:HB2	1:J:475:MET:HG2	1.99	0.44
1:J:1059:ILE:HD12	1:J:1079:GLN:HE22	1.82	0.44
1:A:31:MET:CE	1:C:1279:PHE:CE1	3.00	0.44
1:A:272:VAL:HG23	1:A:368:ILE:HB	1.98	0.44
1:A:1064:VAL:HA	1:A:1076:HIS:O	2.18	0.44
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.74	0.44
1:C:611:TYR:O	1:C:615:VAL:HG23	2.18	0.44
1:C:646:VAL:CG1	1:C:647:PHE:H	2.29	0.44
2:6:244:SER:O	2:6:248:ASN:HB2	2.17	0.44
1:J:94:HIS:HD2	1:J:115:MET:HE3	1.82	0.44
1:J:1042:PHE:CD1	1:J:1102:VAL:HG22	2.53	0.44
1:J:1266:PHE:O	1:J:1268:THR:N	2.49	0.44
1:A:321:ILE:HD13	1:A:321:ILE:HA	1.71	0.44
1:A:1020:LEU:HD12	1:A:1020:LEU:HA	1.70	0.44
1:C:274:VAL:O	1:C:1047:LEU:HD12	2.18	0.44
1:C:425:PRO:HB3	1:C:1328:THR:CG2	2.48	0.44
1:C:504:GLU:HB2	1:C:963:PHE:CE2	2.53	0.44
1:C:790:PRO:O	1:C:995:SER:OG	2.36	0.44
2:5:52:LEU:HB2	2:5:235:LEU:HD13	1.98	0.44
2:6:171:LEU:O	2:6:212:ASN:ND2	2.50	0.44
1:J:128:PRO:HB3	1:J:1076:HIS:ND1	2.33	0.44
1:J:1042:PHE:O	1:J:1044:VAL:HG23	2.17	0.44
1:J:1102:VAL:HG23	1:J:1366:MET:SD	2.58	0.44
1:J:1158:GLU:HB3	1:J:1301:TYR:OH	2.17	0.44
1:A:656:LEU:HB3	1:A:660:HIS:HD2	1.82	0.44
1:C:716:TRP:CZ2	1:C:730:VAL:HG11	2.53	0.44
1:J:396:PRO:O	1:J:397:VAL:HG23	2.17	0.44
1:J:790:PRO:CG	1:J:942:PHE:HE2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1223:GLN:HE21	1:J:1223:GLN:HB3	1.52	0.44
1:A:278:ASN:ND2	1:A:1045:ASP:OD2	2.48	0.44
1:A:518:VAL:HB	1:A:1179:VAL:HG11	2.00	0.44
1:A:625:LEU:HD23	3:D:75:ARG:HH12	1.83	0.44
1:A:716:TRP:HZ2	1:A:730:VAL:HG11	1.83	0.44
1:C:80:PHE:HB3	1:C:1058:ILE:CG2	2.48	0.44
1:C:1217:HIS:CE1	1:C:1228:THR:OG1	2.71	0.44
2:6:26:LYS:CE	2:6:34:HIS:CE1	2.99	0.44
2:6:90:ARG:HD3	2:6:90:ARG:HA	1.40	0.44
2:4:1:MET:N	2:4:64:ARG:HH11	2.16	0.44
1:J:64:VAL:HG12	1:J:65:TYR:N	2.33	0.43
1:A:241:LYS:HA	1:A:244:THR:HG22	1.99	0.43
1:A:1307:THR:OG1	1:A:1308:GLU:OE1	2.29	0.43
1:C:307:LEU:HD23	1:C:307:LEU:HA	1.76	0.43
1:C:689:ALA:HB2	1:C:711:HIS:NE2	2.33	0.43
1:C:737:GLN:NE2	2:4:143:THR:H	2.13	0.43
1:C:1325:LEU:HD22	1:C:1344:PHE:CE2	2.53	0.43
2:5:41:CYS:SG	2:5:54:ASN:HB2	2.58	0.43
2:5:76:VAL:HG11	2:5:209:LEU:HD23	2.00	0.43
2:5:275:PHE:HA	2:5:278:TYR:CE2	2.53	0.43
1:J:268:LYS:O	1:J:366:THR:OG1	2.35	0.43
1:J:639:PHE:CG	1:J:670:LEU:HD21	2.54	0.43
1:J:754:VAL:HB	3:Z:50:MET:HE1	1.99	0.43
1:A:601:VAL:HG12	1:A:601:VAL:O	2.16	0.43
1:A:1063:ILE:O	1:A:1077:VAL:HA	2.17	0.43
1:A:1172:CYS:SG	1:A:1173:GLU:N	2.89	0.43
1:C:1109:ARG:CD	1:C:1169:LYS:HD2	2.47	0.43
2:6:267:LEU:O	2:6:271:LEU:HB2	2.18	0.43
2:4:175:ARG:HB2	2:4:212:ASN:ND2	2.32	0.43
3:D:43:MET:HE2	3:D:47:TYR:OH	2.18	0.43
1:J:37:ILE:HG12	1:A:114:ILE:CG1	2.35	0.43
1:J:86:LEU:O	1:J:86:LEU:HD12	2.18	0.43
1:J:188:PRO:HG3	1:J:1090:TYR:CG	2.53	0.43
1:J:469:PRO:HB3	1:J:479:LEU:HD11	2.00	0.43
1:J:495:ILE:HG13	1:J:976:PRO:HG2	2.01	0.43
1:J:779:THR:O	1:J:783:VAL:HG23	2.18	0.43
1:A:384:PRO:O	1:A:387:ARG:HD3	2.18	0.43
1:A:533:LEU:HB2	1:A:539:PHE:CE2	2.53	0.43
1:A:764:GLU:O	1:A:766:LEU:N	2.52	0.43
1:A:967:HIS:O	1:A:967:HIS:CG	2.71	0.43
1:C:76:HIS:CE1	1:C:78:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:VAL:HG12	1:C:368:ILE:HD13	2.01	0.43
2:5:118:VAL:CG1	2:6:90:ARG:HH12	2.32	0.43
2:4:161:ASP:O	2:4:165:GLN:HG2	2.18	0.43
1:J:431:LEU:HD11	1:J:1333:MET:CE	2.48	0.43
1:J:1018:VAL:HG12	1:J:1131:ILE:HD11	2.00	0.43
1:J:1109:ARG:HD2	1:J:1169:LYS:HD3	2.00	0.43
1:J:1109:ARG:HD3	1:J:1169:LYS:CD	2.47	0.43
1:A:425:PRO:HB3	1:A:1328:THR:HG21	2.00	0.43
1:A:431:LEU:HD21	1:A:437:VAL:HA	1.96	0.43
1:C:564:GLY:O	1:C:1179:VAL:HG21	2.18	0.43
1:C:1110:VAL:HA	1:C:1171:ALA:HB3	1.99	0.43
1:C:1290:LYS:H	1:C:1290:LYS:HG2	1.63	0.43
1:J:208:ASN:N	1:J:211:GLN:HG3	2.33	0.43
1:J:563:ASP:OD2	1:J:993:ARG:HG2	2.18	0.43
1:J:596:LEU:O	1:J:600:THR:HG22	2.17	0.43
1:J:1026:ALA:HB3	1:J:1028:ILE:HG12	2.01	0.43
1:C:396:PRO:HB3	1:C:1186:PHE:CZ	2.54	0.43
1:C:719:PHE:N	1:C:719:PHE:CD1	2.86	0.43
1:C:1197:SER:HB3	1:C:1214:ILE:HG13	1.99	0.43
1:J:21:THR:HG22	1:A:200:ALA:HB2	1.92	0.43
1:J:79:LYS:HB2	1:J:303:GLY:O	2.19	0.43
1:J:83:LEU:CD1	1:J:1058:ILE:HG22	2.48	0.43
1:J:558:ILE:HD12	1:J:558:ILE:HA	1.80	0.43
1:J:760:MET:SD	1:J:805:LYS:HB2	2.59	0.43
1:J:966:TYR:O	1:J:973:PHE:HB3	2.19	0.43
1:J:983:TYR:HA	1:J:988:ARG:HE	1.84	0.43
1:J:1144:ASP:O	1:J:1148:ILE:HG12	2.17	0.43
1:A:7:LEU:HD11	1:A:12:LYS:CD	2.30	0.43
1:C:529:LEU:O	1:C:1235:GLN:NE2	2.52	0.43
1:C:1257:LYS:HD2	1:C:1257:LYS:N	2.34	0.43
2:5:66:LEU:HD23	2:5:66:LEU:HA	1.71	0.43
2:5:74:SER:OG	2:6:89:ARG:NH2	2.51	0.43
1:J:535:PRO:O	1:J:555:ARG:HD2	2.18	0.43
1:J:628:ARG:NH2	3:Z:75:ARG:HH22	2.10	0.43
1:A:21:THR:N	1:C:200:ALA:HB1	2.34	0.43
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.84	0.43
1:A:485:GLN:HB2	1:A:913:ARG:HH22	1.84	0.43
1:A:534:HIS:ND1	1:A:535:PRO:HD2	2.34	0.43
1:A:1034:LEU:HD23	1:A:1175:ILE:CD1	2.46	0.43
1:A:1285:TYR:O	1:A:1289:ALA:HB3	2.19	0.43
1:C:195:THR:HB	1:C:219:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:ASN:OD1	1:C:438:GLN:NE2	2.51	0.43
2:4:31:LEU:HD23	2:4:59:TRP:CH2	2.54	0.43
1:J:257:ASN:HB2	1:J:260:THR:HG23	2.00	0.43
1:J:597:PHE:HA	1:J:600:THR:HG22	1.99	0.43
1:J:944:SER:O	1:J:944:SER:OG	2.29	0.43
1:A:193:VAL:CB	1:A:1093:ASN:HD21	2.28	0.43
1:A:698:LEU:HB2	1:A:706:TYR:CE2	2.54	0.43
1:A:1022:LEU:HD12	1:A:1022:LEU:HA	1.69	0.43
1:C:228:PHE:O	1:C:232:ARG:HG3	2.18	0.43
1:C:383:ASP:OD1	1:C:384:PRO:HD2	2.18	0.43
1:C:610:CYS:SG	1:C:647:PHE:HA	2.59	0.43
2:6:170:ASN:HD22	2:6:184:LEU:HD21	1.79	0.43
2:4:274:ASP:OD1	2:4:274:ASP:N	2.52	0.43
1:J:475:MET:O	1:J:478:LEU:HB3	2.18	0.43
1:J:485:GLN:OE1	1:J:913:ARG:CZ	2.67	0.43
1:A:616:LEU:HD23	1:A:616:LEU:HA	1.78	0.43
1:A:1202:VAL:HG11	1:A:1210:ALA:HA	2.01	0.43
1:C:395:PHE:CD2	1:C:1324:ILE:HD11	2.54	0.43
3:D:65:LEU:HD12	3:D:65:LEU:HA	1.87	0.43
1:J:730:VAL:HG22	1:J:897:ALA:HB2	2.01	0.43
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.75	0.43
1:C:19:PHE:HD1	1:C:21:THR:O	2.02	0.43
1:C:292:THR:O	1:C:359:VAL:HG22	2.19	0.43
1:C:601:VAL:CG1	1:C:793:THR:CG2	2.97	0.43
1:C:795:ASN:OD1	1:C:942:PHE:CZ	2.67	0.43
1:C:940:HIS:HB3	1:C:942:PHE:O	2.19	0.43
2:5:6:ILE:HB	2:5:50:THR:HG23	2.00	0.43
3:E:33:SER:HB2	3:E:36:THR:OG1	2.18	0.43
1:J:197:VAL:HA	1:C:20:LEU:HD13	2.00	0.42
1:J:377:LYS:HA	1:J:377:LYS:HD2	1.78	0.42
1:J:505:VAL:HG21	1:J:974:PRO:HG3	2.01	0.42
1:J:582:MET:HE1	1:J:691:PRO:HD2	2.01	0.42
1:J:1328:THR:HB	1:J:1353:ASN:HB3	2.01	0.42
1:A:464:PHE:HD1	1:A:533:LEU:HD11	1.84	0.42
1:A:647:PHE:CD2	1:A:653:LEU:HD13	2.48	0.42
1:A:765:PRO:O	1:A:767:PHE:CD2	2.72	0.42
1:C:280:MET:O	1:C:284:MET:HG2	2.19	0.42
1:C:359:VAL:CG2	1:C:361:ARG:HH12	2.32	0.42
1:C:780:LEU:HD23	1:C:780:LEU:HA	1.85	0.42
2:4:7:GLY:HA3	2:4:46:LEU:HD22	2.00	0.42
3:Z:37:HIS:CE1	3:Z:39:VAL:HG11	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:504:GLU:HB2	1:J:963:PHE:CE2	2.54	0.42
1:J:1207:THR:O	1:J:1211:THR:HG22	2.19	0.42
1:A:73:ALA:HA	1:A:261:TYR:CZ	2.54	0.42
1:A:1012:LEU:HD12	1:A:1012:LEU:HA	1.70	0.42
1:C:186:LYS:HB2	1:C:186:LYS:HE2	1.60	0.42
1:C:277:ALA:HB2	1:C:371:ASN:HD21	1.84	0.42
1:C:1246:THR:O	1:C:1250:GLU:HG3	2.19	0.42
1:C:1336:LYS:NZ	1:C:1346:THR:HG23	2.34	0.42
2:6:64:ARG:NH1	2:6:268:LEU:HD23	2.34	0.42
1:J:149:ASP:OD2	1:J:153:ASN:ND2	2.53	0.42
1:J:231:ASN:HD21	1:J:1099:VAL:HB	1.85	0.42
1:J:446:LEU:HD21	1:J:1024:THR:HG21	2.00	0.42
1:J:554:PRO:HD3	1:J:907:LEU:HD12	2.02	0.42
1:J:598:LYS:O	1:J:602:THR:HG23	2.20	0.42
1:J:813:TYR:H	3:Z:65:LEU:HD11	1.82	0.42
1:A:452:PRO:O	1:A:456:GLU:HG2	2.19	0.42
1:A:480:GLU:O	1:A:480:GLU:HG3	2.19	0.42
1:A:1131:ILE:HD13	1:A:1131:ILE:HA	1.77	0.42
1:C:273:MET:CE	1:C:1047:LEU:HD11	2.46	0.42
1:C:443:VAL:HG13	1:C:446:LEU:CD1	2.48	0.42
1:C:1007:THR:O	1:C:1011:MET:HG3	2.19	0.42
3:Z:22:VAL:HG13	3:Z:28:LEU:HD12	2.02	0.42
1:J:342:ASP:OD1	1:J:342:ASP:N	2.45	0.42
1:J:947:THR:HG22	1:J:967:HIS:NE2	2.33	0.42
1:A:710:LEU:HB2	1:A:1012:LEU:HD23	2.01	0.42
1:C:431:LEU:HD22	1:C:436:ALA:C	2.40	0.42
1:C:544:GLU:O	1:C:546:SER:N	2.52	0.42
1:C:1044:VAL:CG2	1:C:1099:VAL:CG2	2.95	0.42
1:C:1336:LYS:HE3	1:C:1355:VAL:HG11	2.00	0.42
1:J:80:PHE:CD2	1:J:86:LEU:CD2	3.02	0.42
1:A:627:ILE:O	1:A:631:VAL:HG12	2.19	0.42
1:C:270:SER:OG	1:C:365:LYS:CG	2.67	0.42
1:C:360:ILE:O	1:C:366:THR:HA	2.20	0.42
1:C:1090:TYR:HE2	1:C:1282:ILE:HD11	1.84	0.42
2:5:84:CYS:SG	2:5:112:THR:HG21	2.59	0.42
2:6:175:ARG:HG3	2:6:216:SER:OG	2.20	0.42
1:J:431:LEU:HG	1:J:1333:MET:HE2	2.00	0.42
1:J:598:LYS:CD	1:J:1000:ASN:HB2	2.46	0.42
1:J:742:ALA:HB3	2:6:192:ALA:HB1	2.00	0.42
1:J:808:LEU:HD23	1:J:883:VAL:HG13	2.01	0.42
1:A:208:ASN:OD1	1:A:209:ARG:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:OD1	1:A:694:ASN:N	2.52	0.42
1:A:1105:ASP:OD1	1:A:1169:LYS:HA	2.19	0.42
1:C:445:ALA:HA	1:C:1110:VAL:HG21	2.01	0.42
2:6:260:ASN:O	2:6:263:SER:N	2.38	0.42
1:J:99:ARG:HD2	1:J:109:SER:O	2.19	0.42
1:J:175:LEU:HD13	1:J:1081:ILE:HD11	2.02	0.42
1:J:443:VAL:HG13	1:J:446:LEU:CD1	2.49	0.42
1:J:596:LEU:HD23	1:J:673:HIS:CD2	2.55	0.42
1:J:661:LEU:HD23	1:J:666:LEU:HD13	2.01	0.42
1:A:234:ARG:HH12	1:A:282:ILE:HD13	1.85	0.42
1:A:601:VAL:HG11	1:A:793:THR:CG2	2.50	0.42
1:A:1124:HIS:HE1	1:A:1126:GLU:HB3	1.84	0.42
1:C:157:MET:O	1:C:161:LEU:HG	2.20	0.42
1:C:447:LYS:HB2	1:C:447:LYS:HE3	1.78	0.42
2:6:160:LYS:HE3	2:6:160:LYS:HB2	1.83	0.42
2:4:235:LEU:HD23	2:4:254:LEU:HD21	2.02	0.42
1:J:343:SER:HA	1:J:346:GLN:CB	2.50	0.42
1:J:1008:LEU:O	1:J:1012:LEU:HG	2.20	0.42
1:J:1239:LEU:HD12	1:J:1239:LEU:C	2.38	0.42
1:J:1291:ASP:N	1:J:1291:ASP:OD1	2.51	0.42
1:A:958:ARG:HA	1:A:961:THR:HG22	2.02	0.42
1:C:639:PHE:CG	1:C:670:LEU:HD21	2.54	0.42
1:C:746:ALA:O	1:C:767:PHE:HD1	2.03	0.42
1:C:894:GLU:HG2	1:C:915:HIS:CD2	2.55	0.42
2:4:66:LEU:HB3	2:4:217:TRP:CH2	2.54	0.42
1:J:372:LEU:O	1:J:375:VAL:HG22	2.19	0.42
1:J:514:GLN:NE2	1:J:563:ASP:H	2.17	0.42
1:J:517:VAL:CG1	1:J:518:VAL:N	2.82	0.42
1:J:770:ASP:OD1	1:J:771:TYR:N	2.52	0.42
1:J:1073:THR:O	1:J:1073:THR:OG1	2.38	0.42
1:A:210:ILE:O	1:A:213:SER:OG	2.18	0.42
1:A:426:THR:O	1:A:442:PHE:CE2	2.73	0.42
1:A:638:MET:SD	1:A:642:ARG:NH2	2.93	0.42
1:A:1054:CYS:HB2	1:A:1091:THR:OG1	2.19	0.42
1:C:698:LEU:HB2	1:C:706:TYR:CE2	2.44	0.42
1:C:1202:VAL:HG11	1:C:1210:ALA:HB2	2.02	0.42
1:C:1358:GLU:OE2	1:C:1361:PRO:HA	2.20	0.42
1:A:676:ASN:O	1:A:680:VAL:HG23	2.20	0.42
1:A:709:ALA:HB2	1:A:1014:LYS:HG2	2.01	0.42
1:A:1291:ASP:OD1	1:A:1291:ASP:N	2.52	0.42
1:C:1193:ARG:HG3	1:C:1266:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1200:LEU:HA	1:C:1200:LEU:HD23	1.84	0.42
1:J:396:PRO:HD3	1:J:1186:PHE:CD2	2.55	0.41
1:J:417:ASN:O	1:J:422:ASN:ND2	2.42	0.41
1:J:582:MET:SD	1:J:691:PRO:HD2	2.60	0.41
1:J:1087:GLY:HA3	1:J:1091:THR:HG21	2.02	0.41
1:A:628:ARG:HG3	1:A:661:LEU:HD11	2.03	0.41
1:A:710:LEU:HD12	1:A:1012:LEU:HD23	2.02	0.41
1:A:1268:THR:O	1:A:1272:ILE:HG12	2.20	0.41
1:C:91:MET:O	1:C:117:THR:HA	2.20	0.41
1:C:651:TYR:HA	1:C:654:VAL:HG12	2.02	0.41
1:C:719:PHE:HE2	1:C:922:CYS:CA	2.33	0.41
1:C:801:GLY:HA3	1:C:890:VAL:CG1	2.49	0.41
2:5:285:SER:O	2:5:285:SER:OG	2.36	0.41
1:J:218:SER:O	1:J:222:LYS:HG2	2.20	0.41
1:J:343:SER:HA	1:J:346:GLN:HB3	2.02	0.41
1:J:558:ILE:N	1:J:1013:TYR:O	2.49	0.41
1:J:1123:ARG:HE	1:J:1123:ARG:HB2	1.58	0.41
1:J:1336:LYS:NZ	1:J:1346:THR:O	2.45	0.41
1:A:457:PRO:HD3	1:A:537:PHE:CZ	2.55	0.41
1:A:553:THR:HG23	1:A:910:PHE:CE1	2.56	0.41
1:C:687:ILE:HD12	1:C:1006:MET:CE	2.39	0.41
2:6:170:ASN:CB	2:6:184:LEU:HD21	2.49	0.41
2:4:56:LEU:HD21	2:4:232:CYS:SG	2.60	0.41
3:D:47:TYR:CZ	3:D:64:LEU:CD2	3.02	0.41
1:J:632:ALA:O	1:J:636:VAL:HG12	2.20	0.41
1:A:435:ARG:HH21	1:A:1364:GLN:HA	1.85	0.41
1:C:424:LEU:HD12	1:C:425:PRO:HD2	2.02	0.41
1:C:1131:ILE:HD13	1:C:1131:ILE:HA	1.82	0.41
1:C:1350:HIS:C	1:C:1352:GLY:H	2.22	0.41
3:Z:20:HIS:O	3:Z:24:VAL:N	2.45	0.41
1:J:37:ILE:CG2	1:A:112:THR:CG2	2.98	0.41
1:J:442:PHE:CE2	1:J:1030:PRO:HD2	2.55	0.41
1:J:1251:ARG:H	1:J:1251:ARG:HD2	1.84	0.41
1:J:1347:SER:C	1:J:1348:GLU:HG3	2.41	0.41
1:A:438:GLN:HE22	1:A:1107:GLY:HA2	1.84	0.41
1:A:513:LYS:HZ1	1:A:531:THR:HG22	1.86	0.41
1:A:661:LEU:HD23	1:A:666:LEU:HD13	2.02	0.41
1:C:79:LYS:HA	1:C:1059:ILE:O	2.21	0.41
1:C:396:PRO:HD3	1:C:1186:PHE:CD1	2.55	0.41
1:C:449:LEU:HB3	1:C:1020:LEU:HD23	2.02	0.41
1:C:458:ALA:HB3	1:C:459:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:MET:CE	1:C:642:ARG:HD2	2.50	0.41
1:C:1160:ASN:OD1	1:C:1298:ASP:CB	2.55	0.41
1:A:207:LEU:HD11	1:A:212:ARG:NE	2.35	0.41
1:A:867:ASP:HB3	1:A:870:THR:HG23	2.01	0.41
1:A:1110:VAL:HA	1:A:1171:ALA:HB3	2.03	0.41
1:C:291:ILE:HG12	1:C:360:ILE:HG12	2.03	0.41
1:C:343:SER:HA	1:C:346:GLN:CB	2.45	0.41
1:C:463:THR:O	1:C:467:ARG:NH1	2.53	0.41
1:C:598:LYS:CD	1:C:1000:ASN:HB2	2.50	0.41
1:C:727:MET:HB2	1:C:730:VAL:HB	2.02	0.41
2:5:235:LEU:O	2:5:239:LEU:HG	2.21	0.41
1:J:604:PRO:C	1:J:606:TYR:H	2.24	0.41
1:A:536:PHE:CD1	1:A:1015:ILE:CG2	2.97	0.41
2:6:234:LEU:O	2:6:238:GLU:HG2	2.21	0.41
1:J:274:VAL:CG1	1:J:385:LEU:HD11	2.45	0.41
1:J:544:GLU:CD	1:J:549:VAL:HG21	2.41	0.41
1:J:677:LEU:HD23	1:J:677:LEU:HA	1.88	0.41
1:A:75:ALA:HB1	1:A:1057:VAL:HG22	2.03	0.41
1:C:80:PHE:O	1:C:83:LEU:HB2	2.20	0.41
1:C:276:THR:OG1	1:C:1045:ASP:OD2	2.39	0.41
1:C:746:ALA:O	1:C:767:PHE:HA	2.21	0.41
1:C:989:SER:N	1:C:990:PRO:HD2	2.36	0.41
1:C:1109:ARG:HD2	1:C:1169:LYS:HD2	2.02	0.41
1:C:1174:LEU:O	1:C:1176:LEU:HG	2.20	0.41
2:6:71:PRO:HD3	2:6:179:PHE:HE1	1.86	0.41
2:4:41:CYS:SG	2:4:55:GLU:HG3	2.61	0.41
3:Z:44:LEU:HD23	3:Z:44:LEU:HA	1.93	0.41
1:J:272:VAL:HG23	1:J:368:ILE:HB	2.01	0.41
1:J:322:LEU:HD11	1:J:325:PHE:HA	2.01	0.41
1:J:384:PRO:O	1:J:387:ARG:HD3	2.20	0.41
1:J:1232:TRP:CD1	1:J:1232:TRP:N	2.88	0.41
1:A:207:LEU:HB2	1:A:211:GLN:HB2	2.03	0.41
1:A:457:PRO:HG3	1:A:537:PHE:CD2	2.56	0.41
1:A:1132:ARG:HD3	1:A:1132:ARG:HA	1.90	0.41
1:C:227:LEU:HD12	1:C:227:LEU:HA	1.71	0.41
1:C:540:THR:OG1	1:C:541:HIS:N	2.54	0.41
1:C:995:SER:HA	1:C:998:CYS:SG	2.61	0.41
2:5:189:ASP:OD1	2:5:198:ASN:HB3	2.21	0.41
2:6:171:LEU:HD23	2:6:171:LEU:HA	1.93	0.41
1:J:291:ILE:HA	1:J:359:VAL:O	2.21	0.41
1:J:291:ILE:HG12	1:J:360:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:652:ALA:O	1:J:656:LEU:HG	2.21	0.41
1:J:1131:ILE:HD13	1:J:1131:ILE:HA	1.78	0.41
1:J:1279:PHE:HA	1:J:1282:ILE:HG12	2.02	0.41
1:J:1280:LYS:HA	1:J:1280:LYS:HD2	1.94	0.41
1:A:23:VAL:HG12	1:C:114:ILE:CD1	2.51	0.41
1:A:193:VAL:CG2	1:A:1093:ASN:OD1	2.54	0.41
1:A:630:PHE:CZ	1:A:879:LEU:CG	3.02	0.41
1:A:633:ARG:NH1	1:A:870:THR:HG21	2.36	0.41
1:A:716:TRP:CZ2	1:A:730:VAL:HG11	2.56	0.41
1:A:747:ARG:CZ	1:A:749:HIS:HE1	2.33	0.41
1:A:760:MET:HB3	1:A:889:HIS:HD2	1.86	0.41
1:A:780:LEU:HD23	1:A:780:LEU:HA	1.85	0.41
1:A:1109:ARG:HH11	1:A:1169:LYS:CD	2.33	0.41
1:A:1132:ARG:HB3	1:A:1137:VAL:O	2.20	0.41
1:C:79:LYS:HB2	1:C:303:GLY:O	2.21	0.41
1:C:495:ILE:HD13	1:C:937:VAL:HA	2.02	0.41
1:C:941:ARG:HG3	1:C:992:SER:HB3	2.03	0.41
1:C:1359:ILE:HG23	1:C:1360:ILE:HG13	2.03	0.41
2:5:152:GLU:O	2:5:153:PRO:C	2.55	0.41
2:6:17:VAL:O	2:6:21:ARG:HG3	2.20	0.41
3:E:69:ALA:O	3:E:73:THR:CG2	2.57	0.41
1:J:431:LEU:CD2	1:J:1333:MET:HE2	2.50	0.41
1:J:549:VAL:H	1:J:549:VAL:HG22	1.61	0.41
1:J:957:LYS:HE3	1:J:957:LYS:HB2	1.76	0.41
1:A:21:THR:CA	1:C:200:ALA:HB1	2.51	0.41
1:A:488:MET:SD	1:A:894:GLU:HB2	2.61	0.41
1:A:1344:PHE:CB	1:A:1364:GLN:NE2	2.67	0.41
1:C:4:TRP:O	1:C:7:LEU:HB3	2.21	0.41
1:C:855:GLU:O	1:C:859:GLU:HG2	2.21	0.41
1:C:945:ASN:HD22	1:C:948:ILE:CD1	2.34	0.41
1:J:448:THR:CG2	1:J:1113:LEU:HD13	2.50	0.40
1:J:480:GLU:H	1:J:480:GLU:HG3	1.67	0.40
1:J:672:PHE:HD1	1:J:672:PHE:HA	1.69	0.40
1:J:741:PRO:HB3	2:6:158:HIS:ND1	2.35	0.40
1:J:813:TYR:OH	3:Z:28:LEU:HD23	2.21	0.40
1:J:1268:THR:O	1:J:1272:ILE:HG12	2.21	0.40
1:A:7:LEU:HD23	1:C:115:MET:SD	2.60	0.40
1:A:20:LEU:HD13	1:C:197:VAL:CG2	2.47	0.40
2:6:81:GLU:OE2	2:6:113:GLU:HA	2.21	0.40
2:4:225:LEU:HA	2:4:225:LEU:HD23	1.71	0.40
2:4:271:LEU:O	2:4:271:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:66:ARG:O	3:D:70:VAL:HG23	2.22	0.40
1:J:1288:ARG:O	1:J:1290:LYS:N	2.54	0.40
1:J:1350:HIS:C	1:J:1352:GLY:H	2.23	0.40
1:A:394:PHE:HB2	1:A:1037:VAL:HG12	2.03	0.40
1:A:706:TYR:HD1	1:A:900:ASP:OD2	2.04	0.40
1:A:807:LEU:HD13	1:A:933:TYR:CD2	2.57	0.40
1:C:734:ALA:CB	1:C:766:LEU:HD21	2.51	0.40
1:J:11:PRO:HB2	1:A:339:LEU:HD13	2.03	0.40
1:J:649:HIS:HD2	1:J:922:CYS:O	2.04	0.40
1:J:688:SER:CB	1:J:708:ASN:HD22	2.34	0.40
1:J:1038:ARG:NH1	1:J:1106:MET:O	2.54	0.40
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.76	0.40
1:A:519:THR:O	1:A:523:LYS:NZ	2.54	0.40
1:C:533:LEU:HB2	1:C:539:PHE:CE2	2.56	0.40
1:C:947:THR:HG22	1:C:967:HIS:CE1	2.56	0.40
1:C:1112:ASP:OD1	1:C:1112:ASP:N	2.52	0.40
2:5:167:ILE:HD11	2:5:205:TYR:CD1	2.56	0.40
2:6:19:PHE:CE2	2:6:37:ILE:HG13	2.56	0.40
2:6:71:PRO:HD3	2:6:179:PHE:CE1	2.55	0.40
2:6:121:ASP:OD2	2:6:214:ARG:NH2	2.54	0.40
1:J:114:ILE:CG2	1:C:35:LEU:HD11	2.52	0.40
1:J:396:PRO:O	1:J:397:VAL:CG2	2.70	0.40
1:J:719:PHE:HD1	1:J:917:LEU:HD23	1.86	0.40
1:J:1175:ILE:HD13	1:J:1175:ILE:HA	1.91	0.40
1:J:1238:CYS:SG	1:J:1241:ASP:HB2	2.61	0.40
1:J:1325:LEU:HA	1:J:1356:VAL:O	2.21	0.40
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.52	0.40
1:A:703:LEU:HG	1:A:1022:LEU:HD21	2.03	0.40
1:A:860:LEU:O	1:A:864:VAL:HB	2.22	0.40
1:A:1266:PHE:HD1	1:A:1266:PHE:N	2.20	0.40
1:C:354:PRO:O	1:C:355:LEU:HG	2.21	0.40
1:C:508:THR:CG2	1:C:982:GLU:OE1	2.70	0.40
1:C:1199:MET:HB3	1:C:1275:ASN:HB3	2.04	0.40
2:5:190:ARG:HB2	2:5:193:ASN:ND2	2.37	0.40
1:J:202:LEU:HD12	1:J:203:ALA:N	2.36	0.40
1:J:411:GLU:O	1:J:411:GLU:HG2	2.20	0.40
1:J:647:PHE:CD2	1:J:653:LEU:HD13	2.50	0.40
1:J:1279:PHE:HD1	1:J:1282:ILE:HD11	1.86	0.40
1:A:450:CYS:SG	1:A:1131:ILE:HD12	2.61	0.40
1:A:487:PRO:HB3	1:A:736:ARG:HG3	2.04	0.40
1:A:1251:ARG:HD2	1:A:1251:ARG:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:THR:HG22	1:C:264:SER:O	2.21	0.40
1:C:388:ASN:OD1	1:C:1043:GLU:CD	2.60	0.40
1:C:435:ARG:H	1:C:1367:LEU:HD11	1.85	0.40
1:C:739:LEU:HD21	1:C:766:LEU:CD1	2.52	0.40
1:C:1037:VAL:HG22	1:C:1172:CYS:HB3	2.03	0.40
1:C:1365:SER:O	1:C:1369:ASN:CB	2.69	0.40
2:5:159:LEU:HD23	2:5:159:LEU:HA	1.91	0.40
2:4:42:GLY:HA2	2:4:45:ARG:NH2	2.36	0.40
3:D:26:LEU:HD23	3:D:26:LEU:HA	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1322/1370 (96%)	1242 (94%)	73 (6%)	7 (0%)	25	59
1	C	1344/1370 (98%)	1255 (93%)	78 (6%)	11 (1%)	16	51
1	J	1344/1370 (98%)	1262 (94%)	71 (5%)	11 (1%)	16	51
2	4	283/285 (99%)	273 (96%)	10 (4%)	0	100	100
2	5	283/285 (99%)	271 (96%)	11 (4%)	1 (0%)	30	63
2	6	283/285 (99%)	274 (97%)	8 (3%)	1 (0%)	30	63
3	D	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
3	E	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
3	Z	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
4	p	288/290 (99%)	273 (95%)	13 (4%)	2 (1%)	19	53
5	q	239/306 (78%)	231 (97%)	7 (3%)	1 (0%)	30	63
5	r	302/306 (99%)	288 (95%)	14 (5%)	0	100	100
All	All	5871/6092 (96%)	5548 (94%)	289 (5%)	34 (1%)	24	55

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	409	THR
1	J	410	VAL
1	J	764	GLU
1	J	1070	ASP
1	J	1238	CYS
1	A	764	GLU
1	A	1222	ALA
1	C	409	THR
1	C	764	GLU
1	C	1222	ALA
1	J	1222	ALA
1	A	409	THR
1	A	410	VAL
1	A	411	GLU
1	C	410	VAL
1	C	411	GLU
1	C	1159	ARG
1	C	1160	ASN
2	5	261	GLY
2	6	261	GLY
4	p	73	GLY
1	J	411	GLU
1	J	1352	GLY
1	C	545	ASN
1	C	970	ASP
1	C	1352	GLY
5	q	239	MET
1	J	605	ASN
1	J	736	ARG
1	A	1352	GLY
4	p	244	CYS
1	C	23	VAL
1	J	147	ILE
1	A	765	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1155/1192 (97%)	1137 (98%)	18 (2%)	58	76
1	C	1174/1192 (98%)	1156 (98%)	18 (2%)	60	78
1	J	1174/1192 (98%)	1149 (98%)	25 (2%)	48	71
2	4	256/257 (100%)	254 (99%)	2 (1%)	79	88
2	5	256/257 (100%)	255 (100%)	1 (0%)	89	95
2	6	256/257 (100%)	256 (100%)	0	100	100
3	D	59/68 (87%)	59 (100%)	0	100	100
3	E	59/68 (87%)	59 (100%)	0	100	100
3	Z	59/68 (87%)	59 (100%)	0	100	100
4	p	252/252 (100%)	249 (99%)	3 (1%)	67	82
5	q	214/273 (78%)	213 (100%)	1 (0%)	86	93
5	r	272/273 (100%)	272 (100%)	0	100	100
All	All	5186/5349 (97%)	5118 (99%)	68 (1%)	64	81

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	20	LEU
1	J	260	THR
1	J	360	ILE
1	J	480	GLU
1	J	497	HIS
1	J	510	ASN
1	J	549	VAL
1	J	553	THR
1	J	671	LEU
1	J	764	GLU
1	J	766	LEU
1	J	811	LEU
1	J	953	SER
1	J	1057	VAL
1	J	1069	ARG
1	J	1096	VAL
1	J	1149	SER
1	J	1164	THR
1	J	1239	LEU
1	J	1242	VAL

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Mol	Chain	Res	Type
1	J	1256	SER
1	J	1303	CYS
1	J	1329	THR
1	J	1353	ASN
1	J	1365	SER
1	A	83	LEU
1	A	259	THR
1	A	375	VAL
1	A	394	PHE
1	A	440	ILE
1	A	549	VAL
1	A	771	TYR
1	A	800	LEU
1	A	949	CYS
1	A	1077	VAL
1	A	1095	CYS
1	A	1099	VAL
1	A	1282	ILE
1	A	1320	GLU
1	A	1324	ILE
1	A	1328	THR
1	A	1362	LEU
1	A	1365	SER
1	C	405	ARG
1	C	480	GLU
1	C	654	VAL
1	C	727	MET
1	C	764	GLU
1	C	772	ARG
1	C	798	CYS
1	C	1002	LEU
1	C	1059	ILE
1	C	1099	VAL
1	C	1152	THR
1	C	1180	THR
1	C	1240	SER
1	C	1249	ARG
1	C	1292	CYS
1	C	1303	CYS
1	C	1324	ILE
1	C	1328	THR
2	5	182	LYS

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Mol	Chain	Res	Type
2	4	178	MET
2	4	212	ASN
4	p	28	ARG
4	p	118	LEU
4	p	158	LEU
5	q	114	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	3	ASN
1	J	22	HIS
1	J	76	HIS
1	J	94	HIS
1	J	181	GLN
1	J	231	ASN
1	J	514	GLN
1	J	649	HIS
1	J	713	HIS
1	J	722	HIS
1	J	889	HIS
1	J	901	HIS
1	J	903	GLN
1	J	985	ASN
1	J	1029	HIS
1	J	1080	ASN
1	J	1093	ASN
1	J	1111	GLN
1	J	1141	GLN
1	J	1166	HIS
1	J	1223	GLN
1	A	76	HIS
1	A	181	GLN
1	A	205	GLN
1	A	231	ASN
1	A	438	GLN
1	A	649	HIS
1	A	713	HIS
1	A	722	HIS
1	A	794	ASN
1	A	889	HIS
1	A	901	HIS

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Mol	Chain	Res	Type
1	A	903	GLN
1	A	914	GLN
1	A	915	HIS
1	A	945	ASN
1	A	969	HIS
1	A	985	ASN
1	A	1000	ASN
1	A	1093	ASN
1	A	1111	GLN
1	A	1364	GLN
1	C	3	ASN
1	C	181	GLN
1	C	205	GLN
1	C	231	ASN
1	C	311	ASN
1	C	438	GLN
1	C	485	GLN
1	C	534	HIS
1	C	673	HIS
1	C	713	HIS
1	C	722	HIS
1	C	737	GLN
1	C	794	ASN
1	C	869	HIS
1	C	889	HIS
1	C	901	HIS
1	C	903	GLN
1	C	914	GLN
1	C	985	ASN
1	C	1000	ASN
1	C	1003	HIS
1	C	1029	HIS
1	C	1141	GLN
1	C	1160	ASN
1	C	1223	GLN
1	C	1350	HIS
1	C	1353	ASN
1	C	1364	GLN
2	5	22	HIS
2	5	34	HIS
2	5	54	ASN
2	5	229	GLN

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Mol	Chain	Res	Type
2	5	252	ASN
2	6	170	ASN
2	6	252	ASN
2	6	260	ASN
2	4	158	HIS
2	4	252	ASN
3	Z	37	HIS
3	D	20	HIS
3	E	37	HIS
4	p	183	GLN
4	p	266	HIS
5	q	39	HIS
5	q	50	GLN
5	q	54	HIS
5	q	147	ASN
5	q	192	HIS
5	q	235	GLN
5	r	50	GLN
5	r	191	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

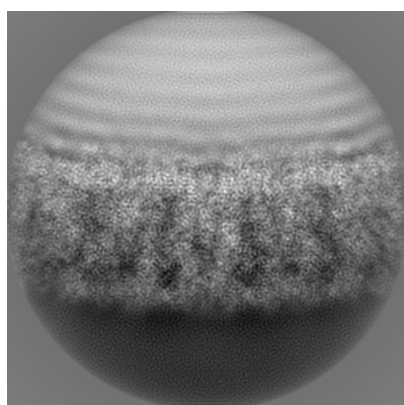
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23386. These allow visual inspection of the internal detail of the map and identification of artifacts.

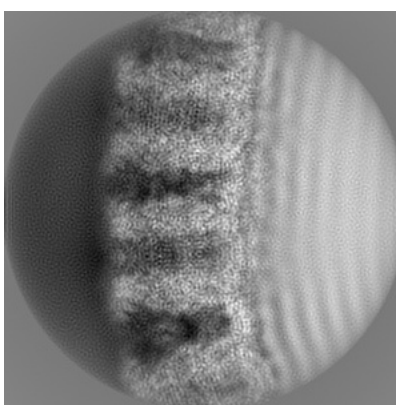
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

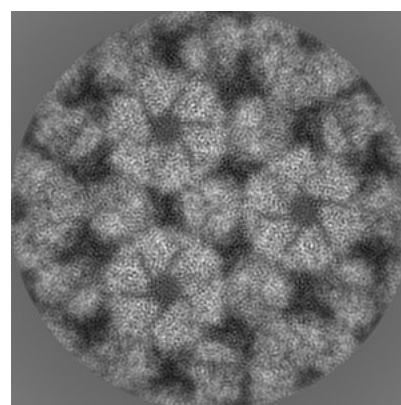
6.1.1 Primary map



X



Y

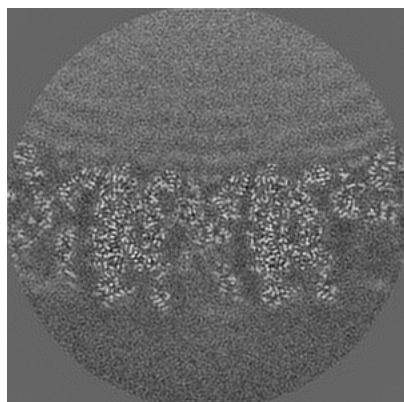


Z

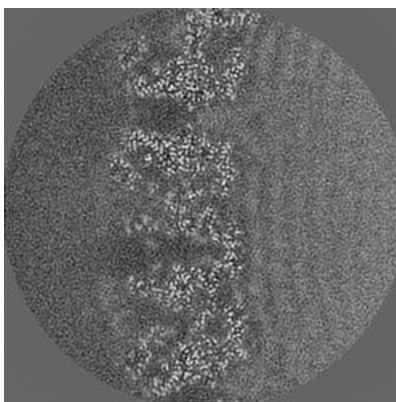
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

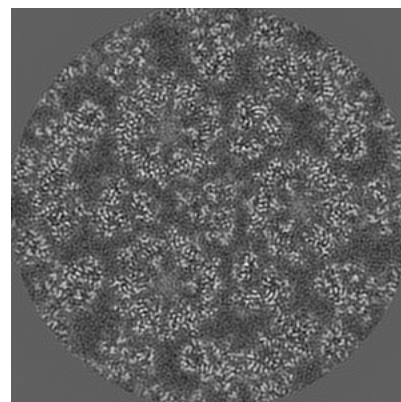
6.2.1 Primary map



X Index: 128



Y Index: 128

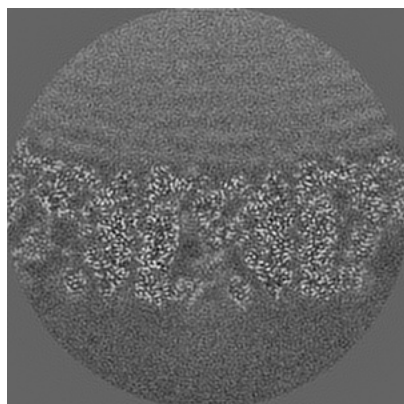


Z Index: 128

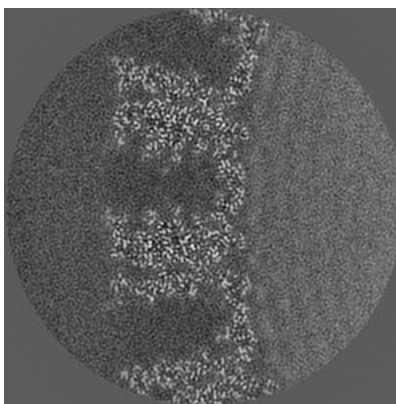
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

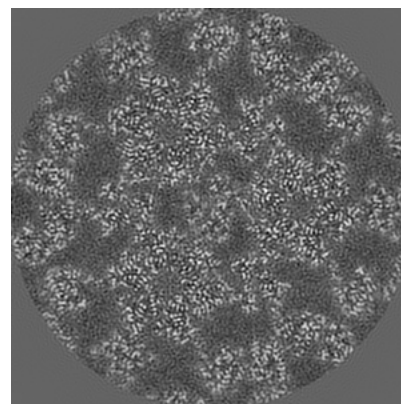
6.3.1 Primary map



X Index: 119



Y Index: 153

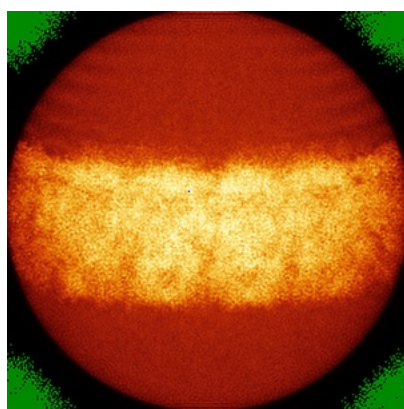


Z Index: 121

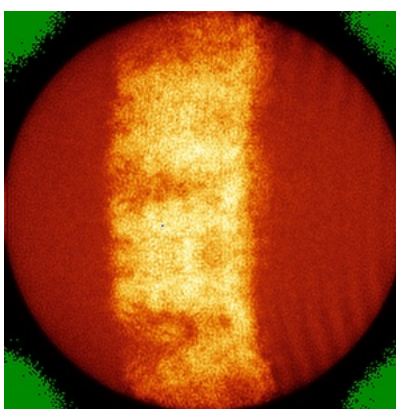
The images above show the largest variance slices of the map in three orthogonal directions.

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

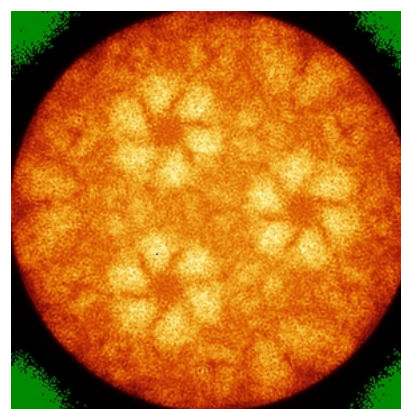
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

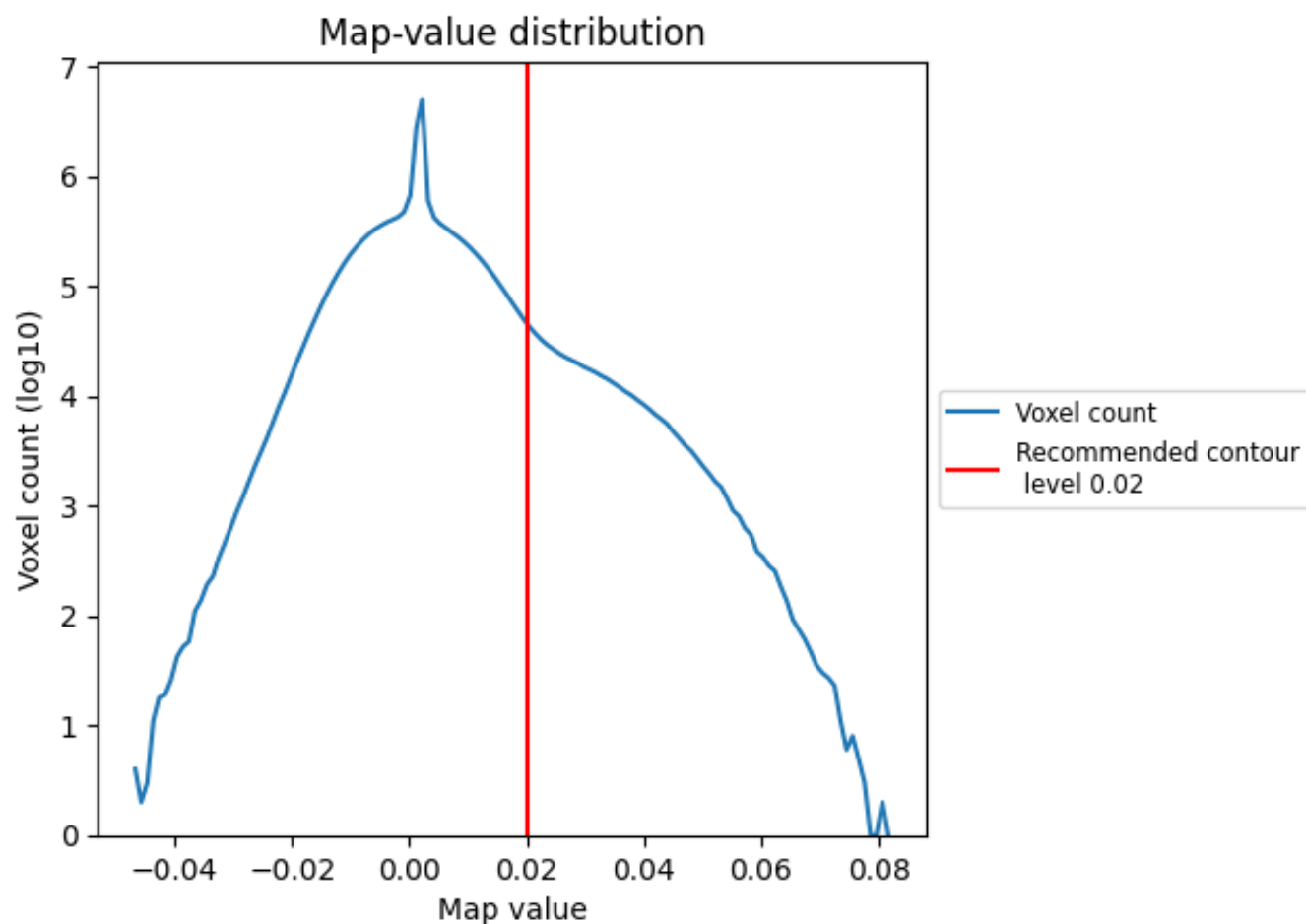
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

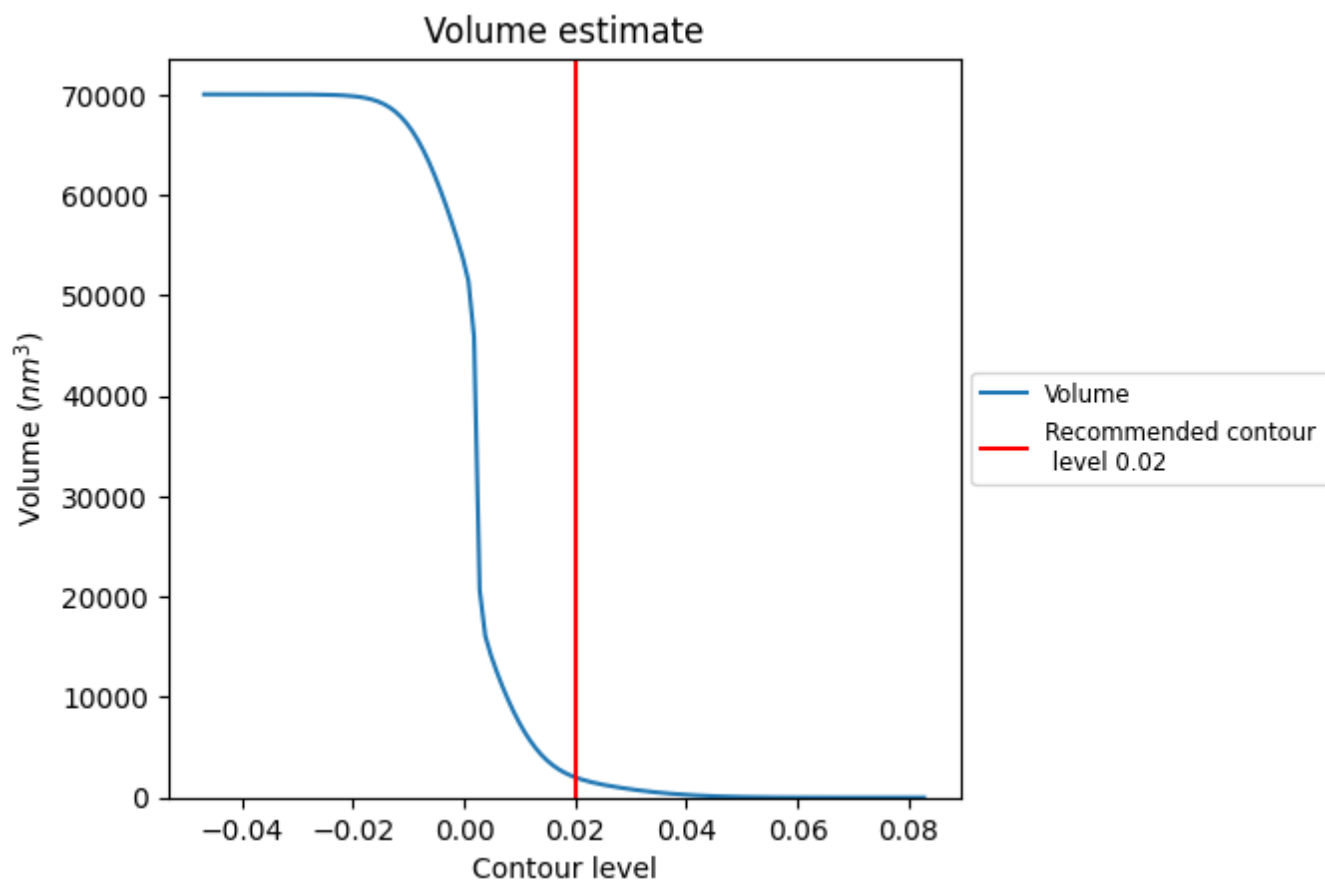
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

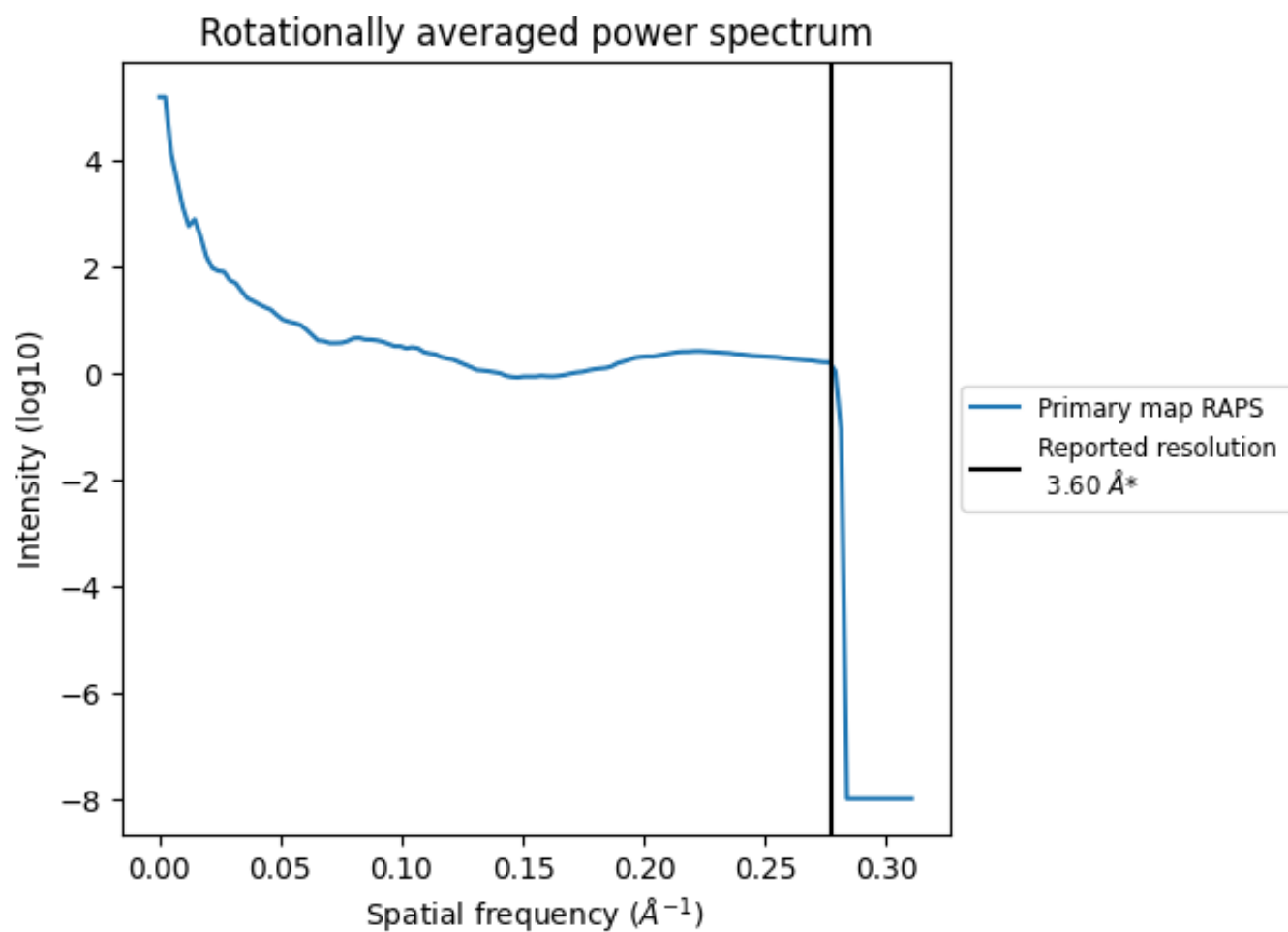
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2015 nm³; this corresponds to an approximate mass of 1820 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

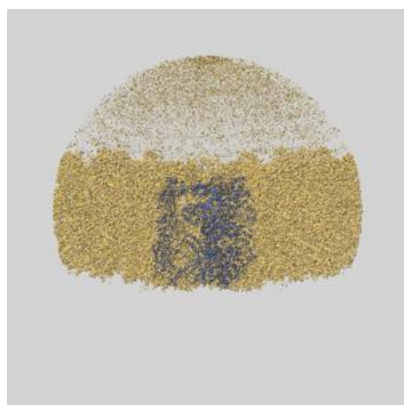
8 Fourier-Shell correlation

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

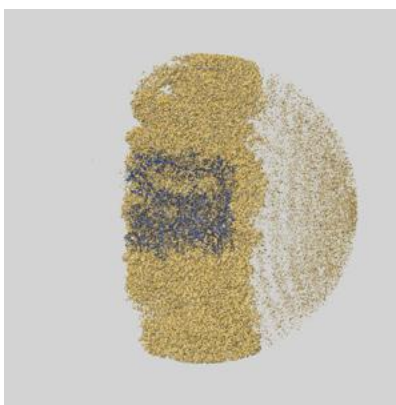
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23386 and PDB model 7LIV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

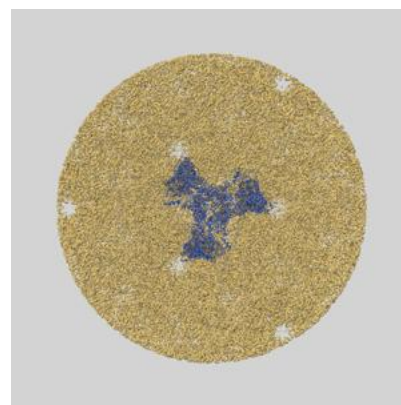
9.1 Map-model overlay [i](#)



X



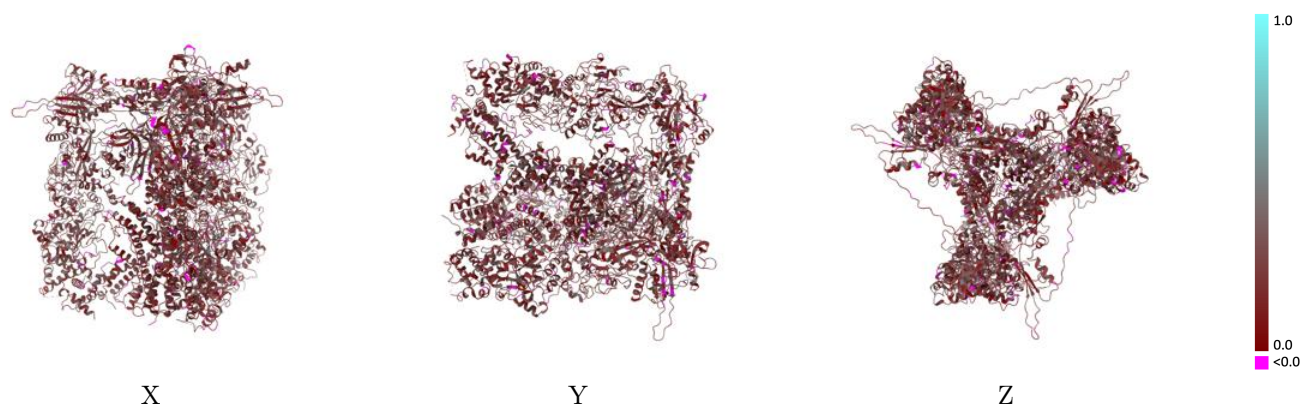
Y



Z

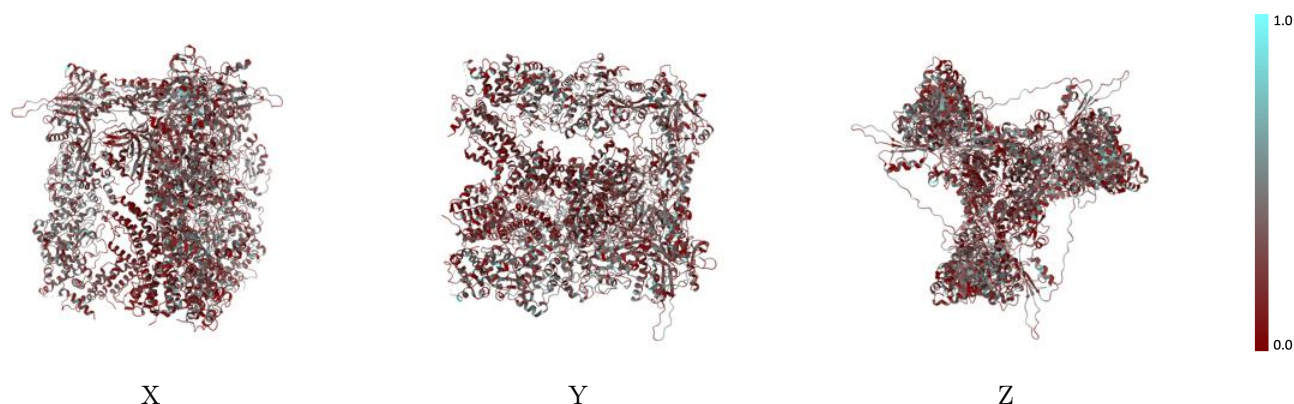
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



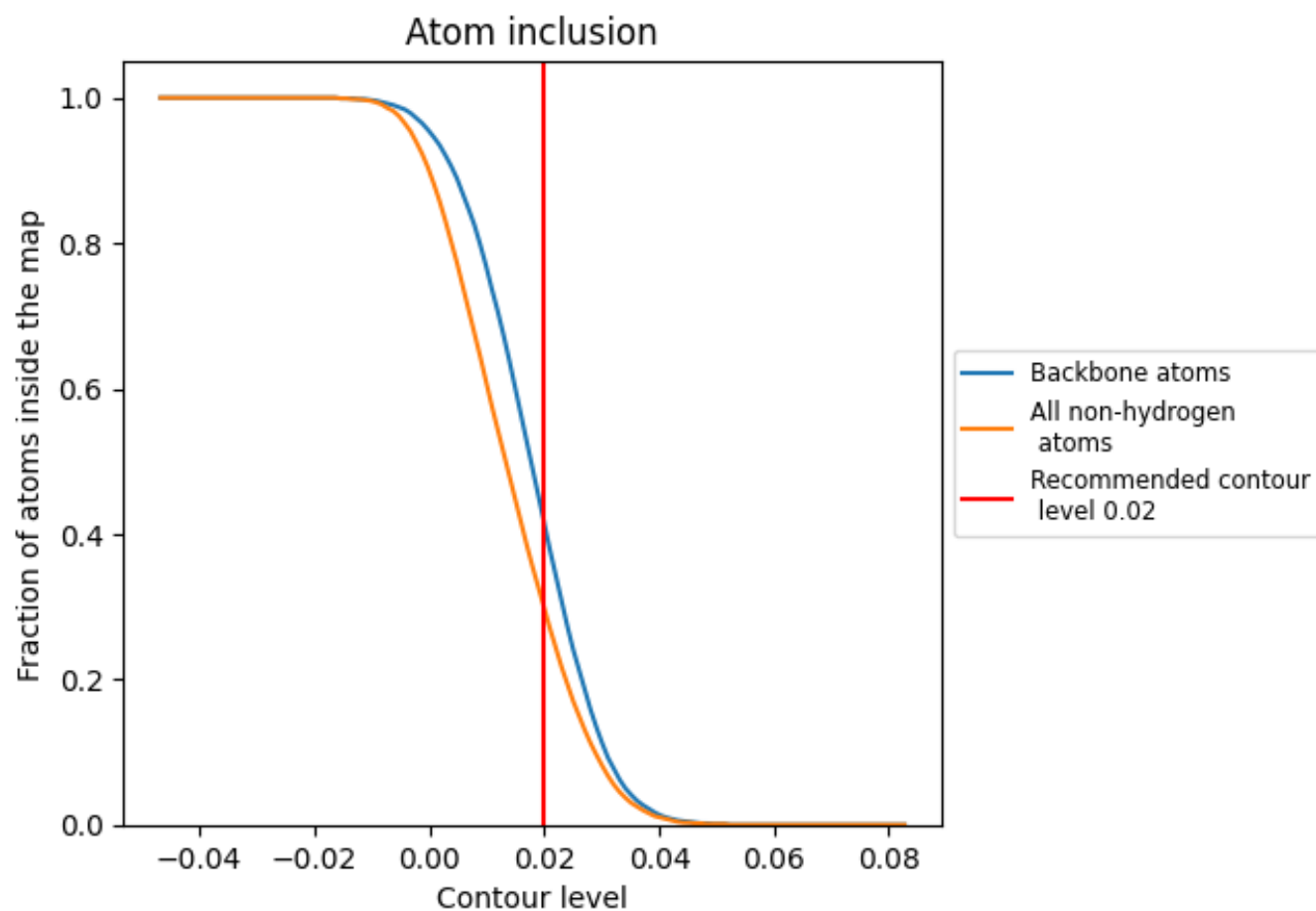
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 42% of all backbone atoms, 30% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2980	<div></div> 0.2310
4	<div></div> 0.1420	<div></div> 0.2040
5	<div></div> 0.1790	<div></div> 0.2130
6	<div></div> 0.2370	<div></div> 0.2360
A	<div></div> 0.3340	<div></div> 0.2400
C	<div></div> 0.3420	<div></div> 0.2380
D	<div></div> 0.2550	<div></div> 0.2280
E	<div></div> 0.2710	<div></div> 0.2290
J	<div></div> 0.3310	<div></div> 0.2290
Z	<div></div> 0.2570	<div></div> 0.2250
p	<div></div> 0.2280	<div></div> 0.2260
q	<div></div> 0.2700	<div></div> 0.2350
r	<div></div> 0.2320	<div></div> 0.2150

1.0

0.0

<0.0