



## Full wwPDB EM Validation Report ⓘ

Jul 15, 2024 – 02:35 am BST

PDB ID : 8BDA  
EMDB ID : EMD-15980  
Title : IFTA complex in anterograde intraflagellar transport trains (*Chlamydomonas reinhardtii*)  
Authors : Lacey, S.E.; Foster, H.E.; Pigino, G.  
Deposited on : 2022-10-18  
Resolution : 20.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

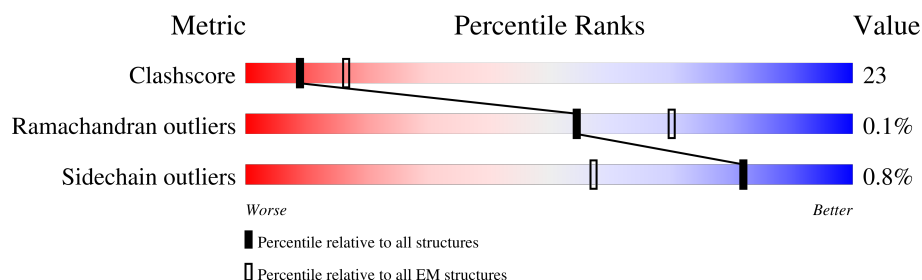
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 20.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	C	1224	<div> <div>8%</div> <div>51%</div> <div>37%</div> <div>12%</div> </div>
2	E	1355	<div> <div>14%</div> <div>60%</div> <div>37%</div> <div>.</div> </div>
3	G	1409	<div> <div>9%</div> <div>50%</div> <div>46%</div> <div>.</div> </div>
4	I	1367	<div> <div>22%</div> <div>53%</div> <div>46%</div> <div>.</div> </div>
5	L	1239	<div> <div>.</div> <div>38%</div> <div>42%</div> <div>20%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 48086 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 Intraflagellar transport protein 121.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1074	Total	C	N	O	S	0	0
			8511	5406	1464	1579	62		

- Molecule 2 is a protein called Intraflagellar transport protein 139.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1325	Total	C	N	O	S	0	0
			10464	6587	1860	1956	61		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	188	GLN	GLU	variant	UNP A9XPA6

- Molecule 3 is a protein called Intraflagellar transport particle protein 140.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	1354	Total	C	N	O	S	0	0
			10600	6657	1867	1998	78		

- Molecule 4 is a protein called Intraflagellar transport protein 144.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	1367	Total	C	N	O	S	0	0
			10579	6654	1857	1998	70		

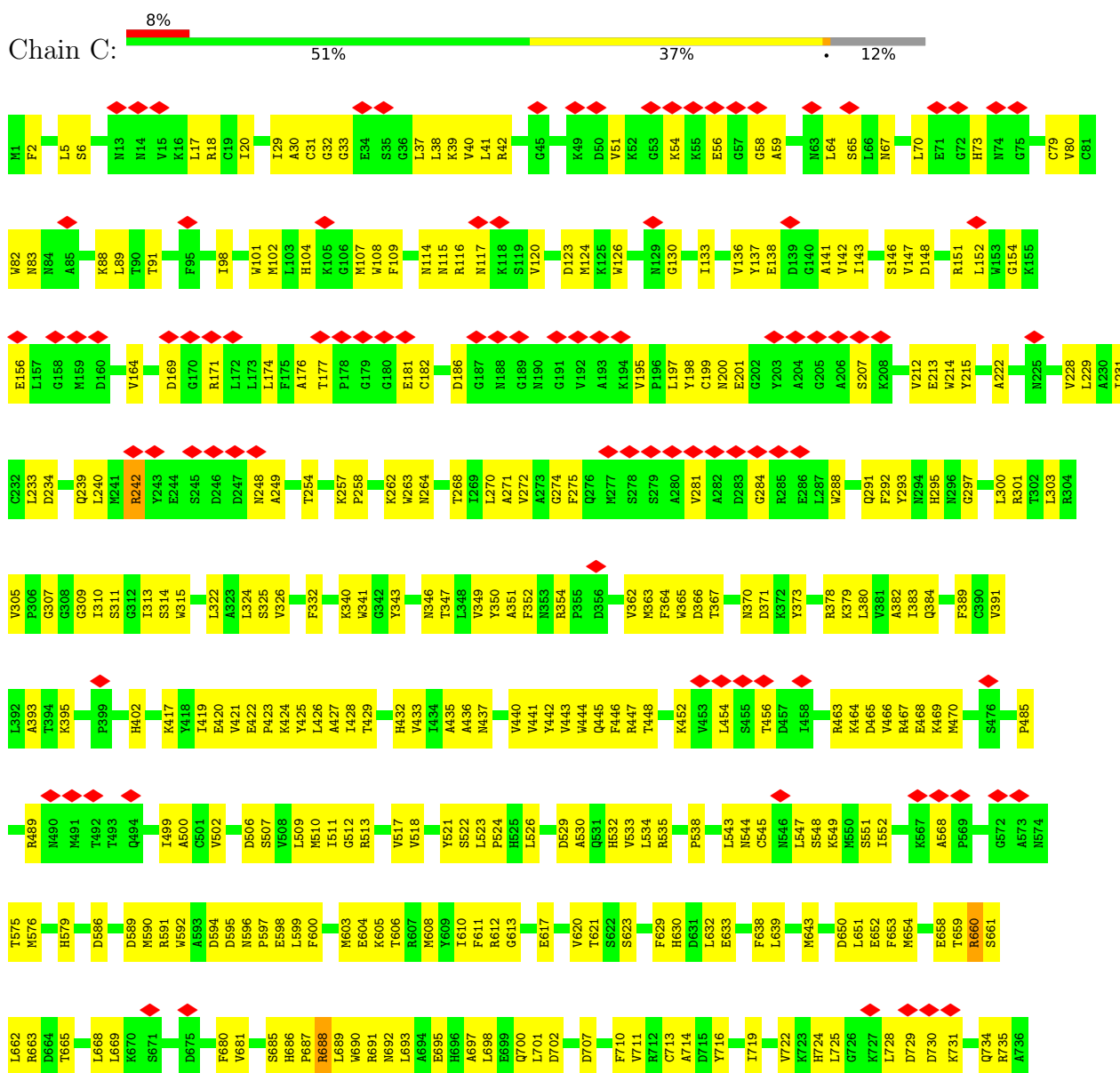
- Molecule 5 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	997	Total	C	N	O	S	0	0
			7932	5064	1373	1455	40		

### 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.

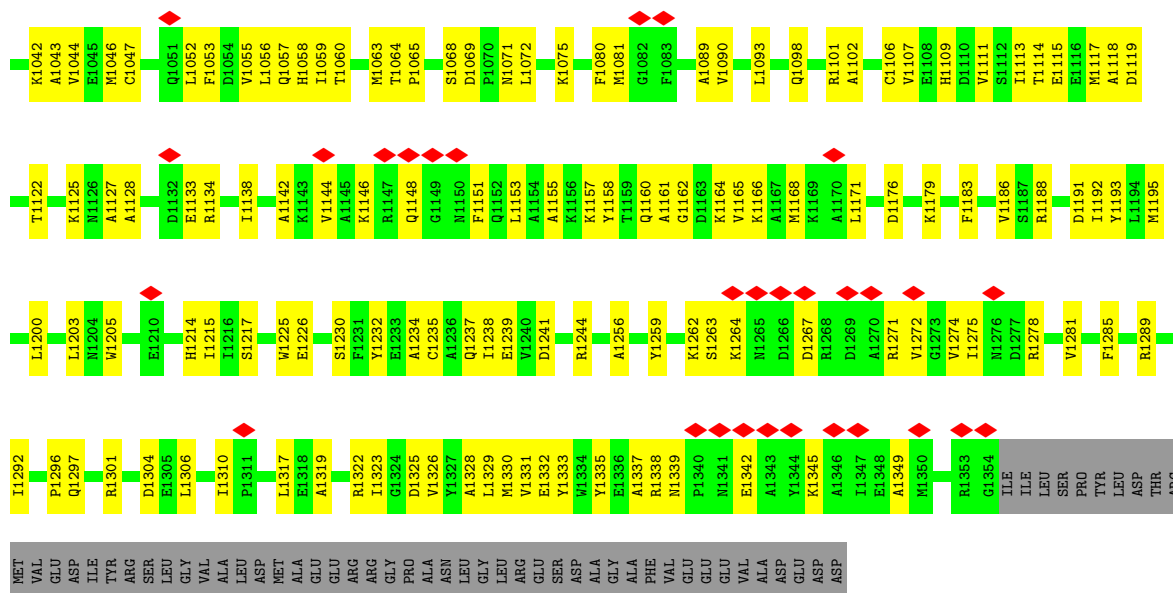
#### • Molecule 1: Intraflagellar transport protein 121



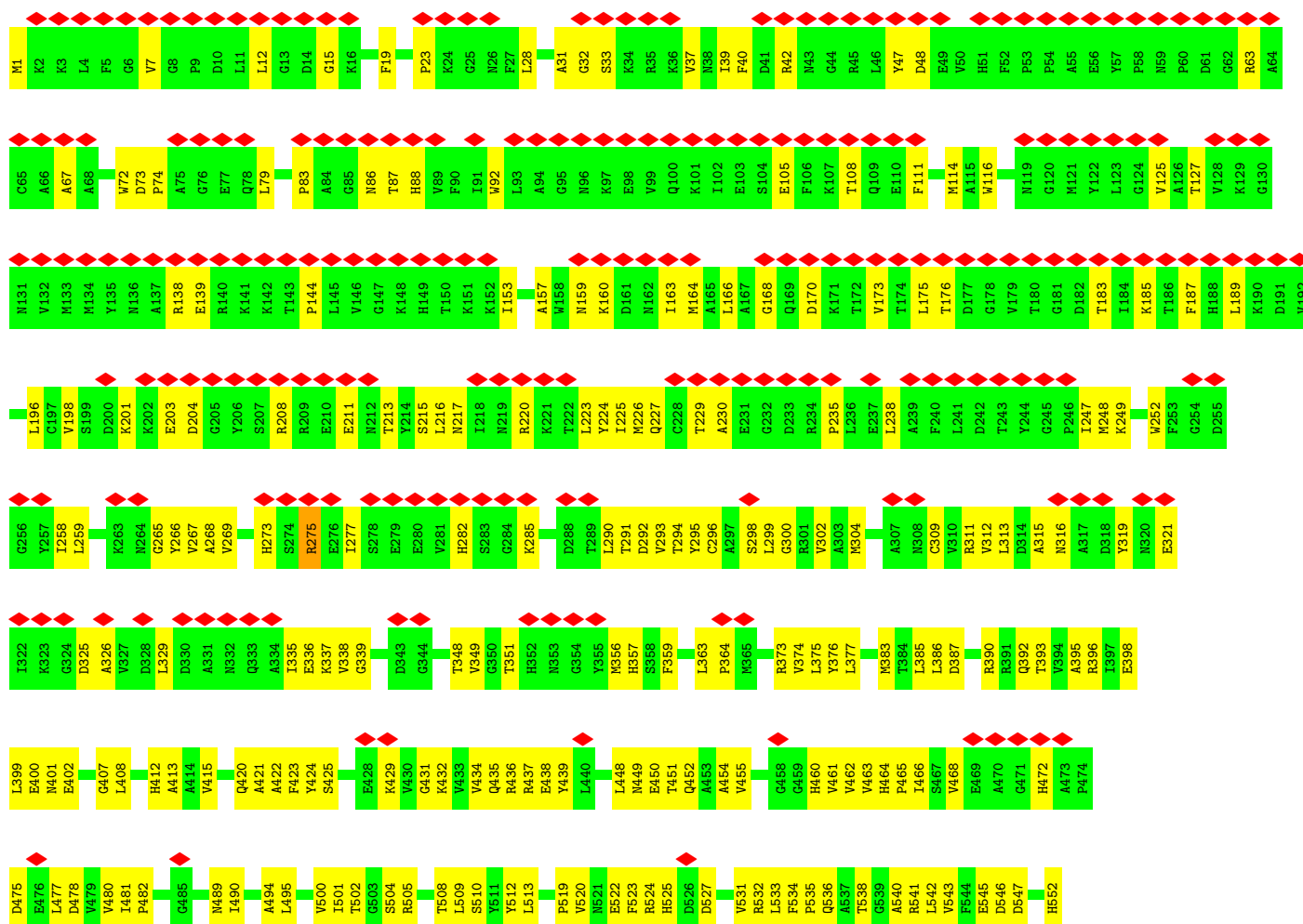


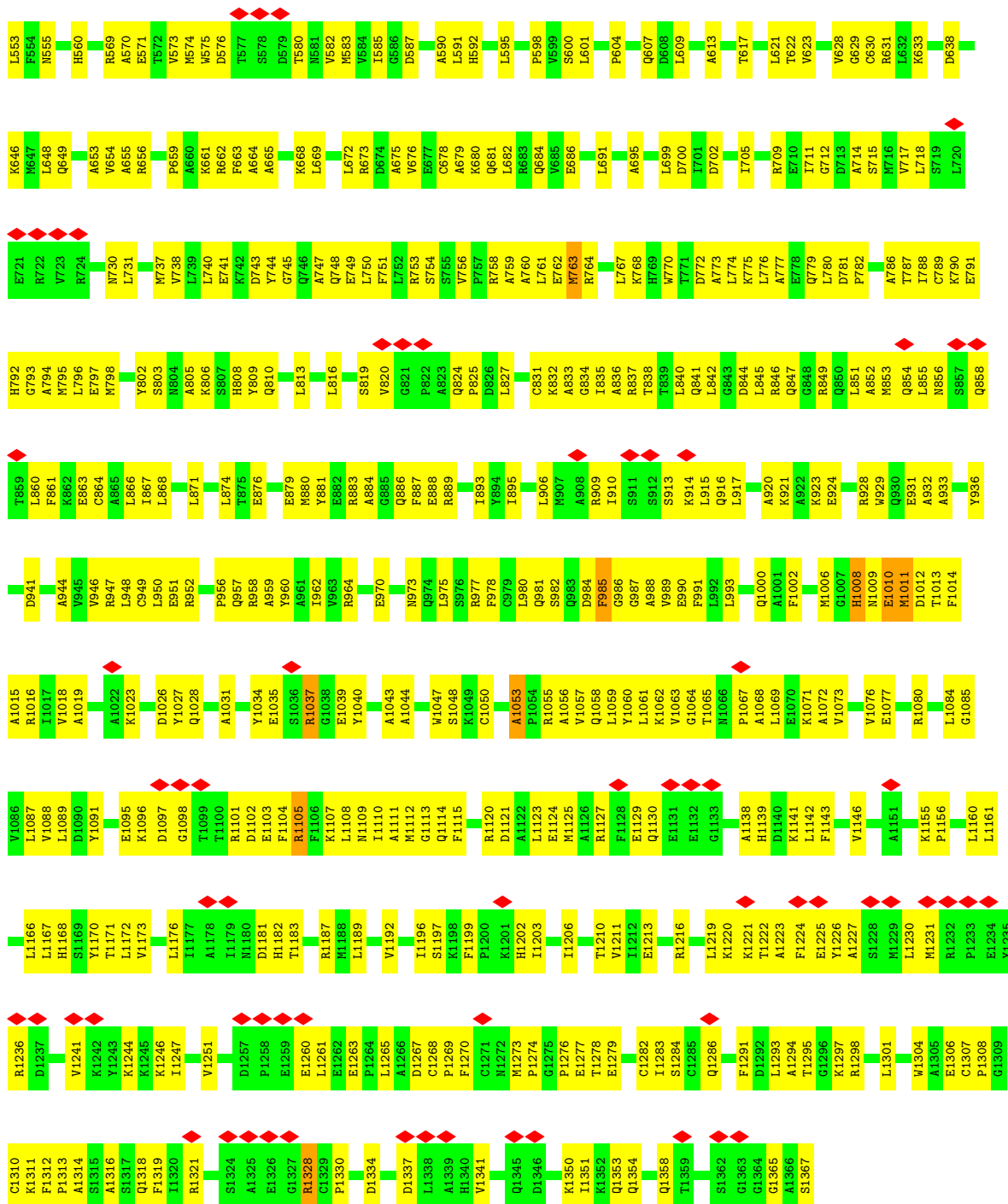


E968	A969	D900	L823	R899	N678	K526	Q458	A397	V321	K241	T165	L75
S970	R761	S901	R825	P610	K679	V527	F459	V398	Y324	T248	N166	L76
G971	L762	R902	A826	K611	P685	A532	T461	D399	N327	G249	S167	I78
R972	D763	E903	C827	L612	G688	K533	S462	R400	L331	E251	V175	G79
P974	V764	L904	G828	L613	F692	P534	R464	V401	N332	A252	A176	W80
E975	H767	I905	K832	V614	T696	H535	C465	L403	E334	T253	A178	K81
A976	C768	L906	A833	Q615	N697	L541	A467	E404	P335	V257	Q179	G82
W978	L769	W908	L834	Q616	N698	P543	L468	N405	V336	T264	E180	A84
Y979	M772	G909	B835	T618	N699	E545	N469	V408	D338	L265	R181	S86
Y980	H774	K910	W836	Q620	N700	E546	M470	P410	L337	A266	A182	I85
T981	A775	L912	E837	F621	W699	K547	Y474	Q411	D339	S267	V184	A90
A983	R776	E913	A837	T622	N701	L546	R475	P413	F339	G414	K185	E92
R984	G777	A702	E623	E623	W703	K654	A476	G415	C342	E270	W186	R93
R985	H778	H704	A624	A624	T705	R555	M479	R416	W343	G194	G194	K94
Y986	R779	W705	V626	V626	S706	N561	K480	Q418	E344	V196	V196	L95
S987	A780	F707	D627	D627	F707	V563	V481	L419	M345	V274	R103	R103
G988	L781	Q708	E628	E628	Q708	A564	E482	Q420	Q346	V275	N104	N104
Y990	H784	G709	R630	R630	W710	A565	V483	D421	P347	Y277	M199	T112
R991	K785	Q711	H631	H631	D712	V567	V484	Q423	A348	N279	S200	A113
L992	S786	D712	B631	B631	P570	V568	M485	L424	G352	D281	E201	S114
A993	E789	D715	H636	H636	E571	G569	T489	L425	V351	L425	G202	G202
K994	A790	K716	V637	V637	P572	E571	K490	L427	G352	D281	V203	V203
D999	D791	T717	V638	V638	A573	E573	K491	L428	N353	D284	L206	L118
L1002	A792	R718	C640	C640	R574	A573	L494	L429	A355	N285	V207	I119
L1005	R793	R719	A641	A641	R574	A573	K495	L430	G361	N286	H208	G121
A1006	A794	A720	T642	T642	A575	A575	F496	G432	P364	N287	Y209	Y209
P1011	A795	L721	T643	T643	V576	V576	D497	G432	R365	N288	P210	D122
A1012	T796	W722	P644	P644	V577	V577	D498	L433	L366	N289	E211	E123
V1013	W797	D723	V645	V645	L578	L578	N499	L434	L366	L290	R312	S128
W1014	A798	F724	D646	D646	V579	V579	H500	L435	V367	D293	Q214	M129
K1015	W799	S725	P647	P647	V580	V580	G501	V436	V369	S294	L215	W130
A1016	H800	L728	D648	D648	W581	W581	S502	N437	N372	V297	L216	K131
T1017	C802	A729	K649	K649	E584	E584	P503	D438	D373	V300	V217	H140
A1018	M803	T730	G650	G650	T585	T585	S505	G439	A374	V301	V218	P147
F1022	I804	D734	L651	L651	V589	V589	N506	E440	I375	C302	L224	G148
A1023	E805	E735	L652	L652	H590	H590	D507	A442	N376	L303	N225	A149
K1024	A807	R738	G654	G654	H591	H591	V508	E443	R379	D306	L227	V150
G1025	K808	W739	V655	V655	D592	D592	R510	V444	L383	D307	T228	I151
Q1026	L810	V740	Q657	Q657	F593	F593	A509	Y445	V309	R308	R229	R152
H1027	B812	K741	P658	P658	T594	T594	R510	K446	N310	V309	D230	V156
E1028	A813	W749	L659	L659	P595	P595	V515	V447	N311	Y309	E231	G157
K1029	C814	E750	H660	H660	E596	E596	W515	T448	L383	N309	D230	L158
A1030	E815	N751	T661	T661	G597	G597	T517	T450	V385	N310	E231	G157
S1031	R816	W752	C667	C667	R598	R598	T517	N451	K386	L311	Q232	P159
T1032	H817	A753	I668	I668	E599	E599	R510	D452	R387	G315	L233	L158
Y1033	D818	H754	G669	G669	P600	P600	N520	M454	D389	T316	L233	P159
M1035	L819	W755	S670	S670	L603	L603	R523	P455	A392	T317	T235	E160
K1039	L820	C756	L675	L675	H604	H604	L524	A456	I393	D318	T236	E161
	N821	T757	L676	L676	F605	F605	L525	S457	M394	R320	T237	M162
	Q822		T677	T677					Q395		T238	P163
									V396		A239	D164

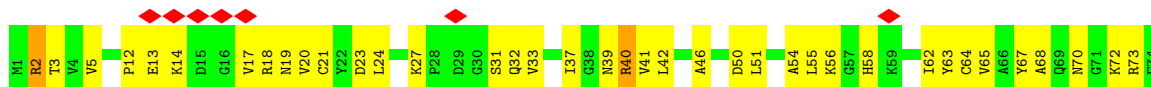
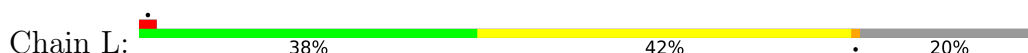


• Molecule 4: Intraflagellar transport protein 144





- Molecule 5: Intraflagellar transport protein 122 homolog



VAL	ASP	ARG	ALA	PHE	T919	T841	L775	L696	K627	Q529	V458	H386	Q309	L155	A75
ASP	ARG	ALA	GLY	SER	A928	R842	K776	R699	E632	A530	R459	V387	M310	L155	S76
ALA	LEU	D778	L844	GLY	Q700	R634	Q777	R699	Q633	L531	L388	C460	T311	L155	G77
LEU	LEU	D779	E845	LEU	L847	E705	D778	R699	L634	F534	L461	L389	T237	L155	A79
ASP	LEU	L847	Q846	LEU	E705	E705	T780	E705	L635	V535	S466	C390	I314	L162	V83
LEU	LEU	L847	R847	LEU	A713	A713	L783	A713	A637	I543	M468	K393	Q316	L162	V83
ASP	ASP	L784	T784	ASP	A637	A637	T784	A637	E638	L546	K469	K394	Q317	L162	V83
PRO	ALA	T784	T784	PRO	E638	E638	T784	E638	L546	M551	A471	L395	L318	L162	V83
VAL	GLY	R785	R785	VAL	M640	M640	T785	M640	L546	M551	A471	L395	L318	L162	V83
THR	THR	R787	R787	THR	A641	A641	T787	A641	M551	M551	A471	L395	L318	L162	V83
TRP	ALA	A720	A720	TRP	F642	F642	T787	A720	M551	M551	A471	L395	L318	L162	V83
ARG	ALA	K721	K721	ARG	F642	F642	T787	K721	M551	M551	A471	L395	L318	L162	V83
CYS	GLY	T722	T722	CYS	F642	F642	T787	T722	M551	M551	A471	L395	L318	L162	V83
THR	THR	T723	T723	THR	F642	F642	T787	T723	M551	M551	A471	L395	L318	L162	V83
THR	THR	T724	T724	THR	F642	F642	T787	T724	M551	M551	A471	L395	L318	L162	V83
ASN	ASN	R725	R725	ASN	F642	F642	T787	R725	M551	M551	A471	L395	L318	L162	V83
PRO	PRO	T726	T726	PRO	F642	F642	T787	T726	M551	M551	A471	L395	L318	L162	V83
LEU	LEU	A796	A796	LEU	F642	F642	T787	A796	M551	M551	A471	L395	L318	L162	V83
ASN	ASN	T797	T797	ASN	F642	F642	T787	T797	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	T798	T798	GLY	F642	F642	T787	T798	M551	M551	A471	L395	L318	L162	V83
ALA	ALA	R799	R799	ALA	F642	F642	T787	R799	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	L800	L800	GLY	F642	F642	T787	L800	M551	M551	A471	L395	L318	L162	V83
LYS	LYS	H801	H801	LYS	F642	F642	T787	H801	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	A871	A871	ASP	F642	F642	T787	A871	M551	M551	A471	L395	L318	L162	V83
TYR	TYR	L872	L872	TYR	F642	F642	T787	L872	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	R873	R873	GLY	F642	F642	T787	R873	M551	M551	A471	L395	L318	L162	V83
ALA	ALA	T874	T874	ALA	F642	F642	T787	T874	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	L875	L875	GLY	F642	F642	T787	L875	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	K876	K876	VAL	F642	F642	T787	K876	M551	M551	A471	L395	L318	L162	V83
MET	MET	A883	A883	MET	F642	F642	T787	A883	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	R887	R887	ASP	F642	F642	T787	R887	M551	M551	A471	L395	L318	L162	V83
GLN	GLN	L987	L987	GLN	F642	F642	T787	L987	M551	M551	A471	L395	L318	L162	V83
LEU	LEU	T988	T988	LEU	F642	F642	T787	T988	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	L988	L988	VAL	F642	F642	T787	L988	M551	M551	A471	L395	L318	L162	V83
PRO	PRO	R889	R889	PRO	F642	F642	T787	R889	M551	M551	A471	L395	L318	L162	V83
LEU	LEU	D747	D747	LEU	F666	F666	T747	D747	M551	M551	A471	L395	L318	L162	V83
GLN	GLN	R813	R813	GLN	F666	F666	T747	R813	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	L891	L891	ASP	F666	F666	T747	L891	M551	M551	A471	L395	L318	L162	V83
PHE	PHE	A971	A971	PHE	F666	F666	T747	A971	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R892	R892	VAL	F666	F666	T747	R892	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	L975	L975	GLY	F666	F666	T747	L975	M551	M551	A471	L395	L318	L162	V83
THR	THR	R893	R893	THR	F666	F666	T747	R893	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	L896	L896	ASP	F666	F666	T747	L896	M551	M551	A471	L395	L318	L162	V83
PHE	PHE	V902	V902	PHE	F666	F666	T747	V902	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	Y903	Y903	VAL	F666	F666	T747	Y903	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	R906	R906	GLY	F666	F666	T747	R906	M551	M551	A471	L395	L318	L162	V83
GLN	GLN	E907	E907	GLN	F666	F666	T747	E907	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	V908	V908	ASP	F666	F666	T747	V908	M551	M551	A471	L395	L318	L162	V83
GLU	GLU	D989	D989	GLU	F666	F666	T747	D989	M551	M551	A471	L395	L318	L162	V83
PHE	PHE	L990	L990	PHE	F666	F666	T747	L990	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	K911	K911	GLY	F666	F666	T747	K911	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	R912	R912	GLY	F666	F666	T747	R912	M551	M551	A471	L395	L318	L162	V83
PRO	PRO	G932	G932	PRO	F666	F666	T747	G932	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	R913	R913	GLY	F666	F666	T747	R913	M551	M551	A471	L395	L318	L162	V83
ALA	ALA	H914	H914	ALA	F666	F666	T747	H914	M551	M551	A471	L395	L318	L162	V83
ASN	ASN	V995	V995	ASN	F666	F666	T747	V995	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R996	R996	VAL	F666	F666	T747	R996	M551	M551	A471	L395	L318	L162	V83
LEU	LEU	S997	S997	LEU	F666	F666	T747	S997	M551	M551	A471	L395	L318	L162	V83
THR	THR	P916	P916	THR	F666	F666	T747	P916	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	S997	S997	GLY	F666	F666	T747	S997	M551	M551	A471	L395	L318	L162	V83
ARG	ARG	L997	L997	ARG	F666	F666	T747	L997	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R918	R918	VAL	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	R918	R918	ASP	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
ARG	ARG	L918	L918	ARG	F666	F666	T747	L918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R918	R918	VAL	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	R918	R918	ASP	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
ARG	ARG	L918	L918	ARG	F666	F666	T747	L918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R918	R918	VAL	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	R918	R918	ASP	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
ARG	ARG	L918	L918	ARG	F666	F666	T747	L918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R918	R918	VAL	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	R918	R918	ASP	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
ARG	ARG	L918	L918	ARG	F666	F666	T747	L918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R918	R918	VAL	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	R918	R918	ASP	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
ARG	ARG	L918	L918	ARG	F666	F666	T747	L918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R918	R918	VAL	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	R918	R918	ASP	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
ARG	ARG	L918	L918	ARG	F666	F666	T747	L918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R918	R918	VAL	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
ASP	ASP	R918	R918	ASP	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
ARG	ARG	L918	L918	ARG	F666	F666	T747	L918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L318	L162	V83
VAL	VAL	R918	R918	VAL	F666	F666	T747	R918	M551	M551	A471	L395	L318	L162	V83
GLY	GLY	PRO	PRO	GLY	F666	F666	T747	PRO	M551	M551	A471	L395	L		

THR	ALA	PRO	PHE	SER	ARG	THR	THR	VAL	ARG	GLY	GLY	GLY	LEU	ALA	PRO	GLY	GLY	ASP	ASP	ALA	GLU	ASP	GLY	GLY	GLY	ASN	LYS	LEU	GLY	GLY	PRO	LEU	GLY	GLY	SER	ALA	ALA	ARG	GLY	PRO	TLE	GLY	GLY	ALA	SER	LYS	ALA	ARG	MET	SER	VAL	PRO	PHE	GLN	GLN	GLY	ARG	PRO	LEU	VAL
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	3897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Warp/Relion/M - CTF Refinement in M	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	104	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.122	Depositor
Minimum map value	-1.291	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	727.2, 727.2, 727.2	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	6.06, 6.06, 6.06	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	C	0.30	0/8701	0.57	0/11769
2	E	0.31	0/10649	0.61	0/14397
3	G	0.33	0/10815	0.63	0/14651
4	I	0.32	0/10781	0.61	0/14601
5	L	0.33	0/8108	0.61	0/10978
All	All	0.32	0/49054	0.61	0/66396

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	C	8511	0	8356	348	0
2	E	10464	0	10515	374	0
3	G	10600	0	10441	569	0
4	I	10579	0	10549	516	0
5	L	7932	0	7900	470	0
All	All	48086	0	47761	2227	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 23.

All (2227) 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)
5:L:796:ALA:HB1	5:L:800:LEU:HG	1.44	0.98
3:G:1028:GLU:HA	3:G:1052:LEU:HD11	1.45	0.98
2:E:1144:ALA:O	2:E:1148:LEU:HB2	1.65	0.96
5:L:907:GLU:O	5:L:911:LYS:HB2	1.70	0.91
1:C:445:GLN:HE22	1:C:524:PRO:HB3	1.38	0.89
3:G:1006:ALA:HB1	3:G:1033:LEU:HD11	1.52	0.89
5:L:815:ALA:O	5:L:819:SER:HB3	1.74	0.85
5:L:799:LEU:HD12	5:L:802:ALA:HB2	1.62	0.81
1:C:879:ASP:O	1:C:883:LEU:HB2	1.81	0.80
1:C:902:ILE:O	1:C:906:LEU:HB2	1.81	0.79
5:L:808:GLN:HA	5:L:834:GLY:HA2	1.65	0.79
4:I:748:GLN:HB2	4:I:760:ALA:HB1	1.63	0.79
5:L:640:MET:HG3	5:L:649:ALA:HB2	1.66	0.78
3:G:1022:PHE:HZ	3:G:1034:TYR:HE2	1.30	0.78
5:L:471:ALA:H	5:L:501:TRP:HE1	1.30	0.78
4:I:302:VAL:HB	4:I:313:LEU:HB2	1.65	0.78
3:G:638:VAL:HG12	3:G:659:ILE:HD13	1.66	0.78
3:G:1043:ALA:HA	3:G:1046:MET:HG2	1.66	0.77
2:E:1350:ARG:HH12	5:L:183:TRP:H	1.31	0.77
1:C:697:ALA:HA	1:C:700:GLN:HG2	1.67	0.76
3:G:520:ASN:HB3	3:G:541:LEU:HB3	1.68	0.76
3:G:1030:ALA:HB3	3:G:1046:MET:HE1	1.68	0.75
4:I:695:ALA:HB1	4:I:700:ASP:HB2	1.69	0.75
1:C:17:LEU:HA	1:C:33:GLY:HA2	1.67	0.75
3:G:838:GLU:HB2	3:G:845:LEU:HD12	1.68	0.75
2:E:677:ASP:HB2	2:E:712:ARG:HD2	1.68	0.75
2:E:554:ALA:HA	2:E:557:ILE:HD12	1.69	0.74
5:L:155:LEU:HD12	5:L:165:ARG:HD2	1.69	0.74
3:G:1115:GLU:O	3:G:1119:ASP:HB2	1.87	0.74
5:L:942:VAL:HG12	5:L:944:LEU:H	1.50	0.74
5:L:534:PHE:HB2	5:L:546:LEU:HB3	1.70	0.74
2:E:1043:ILE:HD12	2:E:1055:VAL:HG13	1.69	0.73
2:E:1002:GLU:O	2:E:1006:ILE:HB	1.89	0.73
2:E:1280:MET:HG3	2:E:1289:ALA:HB2	1.69	0.73
5:L:587:TRP:HA	5:L:590:LEU:HD12	1.70	0.73
4:I:1048:SER:HA	4:I:1056:ALA:HB1	1.70	0.73
4:I:1073:VAL:HG11	4:I:1107:LYS:HG3	1.70	0.73
3:G:577:ARG:HD3	3:G:590:VAL:HG13	1.70	0.72
2:E:1083:ASN:HB2	2:E:1092:ALA:HB2	1.72	0.72
3:G:546:LEU:HB3	3:G:567:VAL:HG21	1.72	0.72
2:E:278:GLN:O	2:E:282:LEU:HB2	1.89	0.72
1:C:215:TYR:HB3	1:C:228:VAL:HB	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:979:TYR:HA	3:G:982:LEU:HB2	1.72	0.71
5:L:124:LEU:HB2	5:L:133:ALA:HB3	1.72	0.71
3:G:1127:ALA:H	3:G:1157:LYS:HZ1	1.37	0.71
4:I:856:ASN:HB3	4:I:860:LEU:HB3	1.72	0.71
3:G:786:SER:HB3	3:G:806:ASP:HB2	1.72	0.71
4:I:481:ILE:HG21	4:I:502:THR:HG21	1.72	0.71
2:E:340:ALA:HB2	2:E:355:ARG:HB2	1.71	0.71
5:L:154:ALA:HA	5:L:164:ILE:HA	1.72	0.71
2:E:1199:LEU:HD13	2:E:1221:ARG:HG3	1.72	0.70
4:I:655:ALA:HB1	4:I:662:ARG:HB2	1.72	0.70
2:E:702:THR:HB	2:E:721:LYS:HG3	1.73	0.70
3:G:473:VAL:N	3:G:484:VAL:O	2.23	0.70
3:G:721:LEU:HD22	3:G:755:MET:HG2	1.73	0.70
4:I:461:VAL:HB	4:I:481:ILE:HB	1.74	0.70
3:G:718:ARG:O	3:G:722:LEU:HB2	1.90	0.70
3:G:741:LYS:HB2	4:I:798:MET:HG2	1.72	0.70
3:G:808:LYS:NZ	3:G:827:CYS:SG	2.65	0.70
5:L:787:TYR:CE2	5:L:799:LEU:HD23	2.27	0.70
1:C:448:THR:HG23	1:C:467:ARG:HH11	1.56	0.70
3:G:508:VAL:HA	3:G:513:LEU:HA	1.74	0.70
5:L:682:PHE:O	5:L:690:GLN:NE2	2.23	0.70
1:C:788:LEU:O	1:C:792:HIS:ND1	2.23	0.70
1:C:822:VAL:HG13	1:C:834:LEU:HG	1.74	0.69
1:C:234:ASP:HA	1:C:258:PRO:HD2	1.75	0.69
3:G:481:VAL:HB	3:G:494:LEU:HB2	1.75	0.69
5:L:471:ALA:HA	5:L:481:VAL:HA	1.73	0.69
5:L:748:LYS:NZ	5:L:777:MET:SD	2.65	0.69
4:I:764:ARG:HB3	4:I:773:ALA:HB2	1.74	0.69
4:I:1308:PRO:HG3	4:I:1341:VAL:HA	1.74	0.69
5:L:63:TYR:H	5:L:78:GLY:HA2	1.58	0.69
5:L:345:GLN:HE21	5:L:376:ASP:HA	1.56	0.69
5:L:395:LEU:HB2	5:L:408:TRP:HB2	1.75	0.69
5:L:787:TYR:HE2	5:L:799:LEU:HD23	1.57	0.69
4:I:153:ILE:HA	4:I:168:GLY:HA2	1.75	0.69
4:I:490:ILE:HA	4:I:504:SER:HA	1.75	0.69
5:L:417:ILE:HD11	5:L:429:LEU:HB3	1.74	0.69
5:L:586:ASP:O	5:L:590:LEU:HG	1.92	0.69
5:L:679:ALA:HB1	5:L:696:LEU:HB3	1.75	0.69
3:G:843:ILE:HG13	5:L:824:PHE:HD2	1.58	0.68
4:I:571:GLU:H	4:I:587:ASP:HA	1.57	0.68
2:E:22:GLN:HA	2:E:42:ARG:HH12	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:693:GLU:HG2	2:E:701:VAL:HG13	1.75	0.68
3:G:564:ALA:HA	3:G:580:VAL:HA	1.75	0.68
4:I:949:CYS:SG	4:I:958:ARG:NE	2.66	0.68
1:C:213:GLU:HG2	1:C:262:LYS:HA	1.73	0.68
3:G:427:LEU:HB2	3:G:434:LEU:HD11	1.76	0.68
5:L:936:LEU:HD22	5:L:955:LEU:HD13	1.76	0.68
3:G:410:PRO:HB3	3:G:696:THR:HG22	1.75	0.68
5:L:264:TRP:HB2	5:L:282:GLU:HB2	1.76	0.68
5:L:460:CYS:HB2	5:L:473:VAL:HB	1.75	0.68
2:E:964:HIS:HB3	2:E:967:HIS:HB2	1.76	0.67
4:I:1058:GLN:NE2	4:I:1087:LEU:O	2.27	0.67
5:L:571:PHE:HA	5:L:574:ALA:HB3	1.75	0.67
2:E:736:ARG:HH12	2:E:759:ASP:HB3	1.59	0.67
3:G:615:VAL:HB	3:G:641:ALA:HB3	1.77	0.67
4:I:376:TYR:HE1	4:I:386:LEU:HB3	1.59	0.67
4:I:779:GLN:HG3	4:I:780:LEU:HG	1.75	0.67
5:L:780:THR:HG1	5:L:803:HIS:HE2	1.40	0.67
1:C:384:GLN:HG3	1:C:428:ILE:HG22	1.76	0.67
2:E:821:ILE:HB	2:E:846:LEU:HD13	1.76	0.67
4:I:374:VAL:HG21	4:I:621:LEU:HB3	1.76	0.67
4:I:385:LEU:HB3	4:I:395:ALA:HB3	1.75	0.67
5:L:742:VAL:HA	5:L:745:GLN:HB2	1.75	0.67
2:E:874:THR:OG1	2:E:917:LYS:NZ	2.26	0.67
4:I:852:ALA:O	4:I:856:ASN:ND2	2.26	0.67
5:L:458:VAL:HG11	5:L:461:LEU:HD23	1.76	0.67
3:G:975:GLU:HA	3:G:978:ARG:HE	1.60	0.67
2:E:911:GLN:HE22	2:E:936:ILE:HG13	1.60	0.67
3:G:738:ARG:HE	4:I:866:LEU:HD22	1.60	0.67
2:E:1352:GLY:HA2	2:E:1355:PRO:HB3	1.78	0.66
3:G:1022:PHE:CZ	3:G:1034:TYR:HE2	2.12	0.66
3:G:710:MET:HE1	3:G:721:LEU:HB2	1.78	0.66
4:I:1196:ILE:HD11	4:I:1199:PHE:HB2	1.77	0.66
1:C:176:ALA:HA	1:C:182:CYS:HA	1.77	0.66
3:G:644:PHE:HB2	3:G:729:ALA:HB3	1.77	0.66
3:G:799:VAL:HG11	4:I:718:LEU:HD22	1.76	0.66
3:G:858:ARG:HE	4:I:705:ILE:HG21	1.59	0.66
5:L:218:ARG:HG3	5:L:252:GLY:HA3	1.78	0.66
1:C:691:ARG:NH1	1:C:713:CYS:SG	2.69	0.66
2:E:1163:VAL:HG21	2:E:1198:VAL:HG12	1.78	0.66
3:G:555:ARG:HB3	3:G:564:ALA:HB3	1.77	0.66
3:G:616:GLN:HB2	3:G:667:CYS:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:604:TYR:HA	2:E:607:VAL:HG22	1.76	0.66
2:E:902:GLN:OE1	2:E:906:ARG:NH2	2.29	0.66
1:C:469:LYS:HA	1:C:485:PRO:HA	1.78	0.66
3:G:49:ASP:O	3:G:55:ASN:ND2	2.28	0.66
4:I:400:GLU:HB2	4:I:436:ARG:HH22	1.60	0.66
3:G:1106:CYS:SG	3:G:1107:VAL:N	2.69	0.66
5:L:824:PHE:HA	5:L:827:ALA:HB3	1.77	0.66
3:G:215:LEU:HB3	3:G:227:LEU:HB2	1.78	0.66
3:G:468:ILE:HA	3:G:473:VAL:HA	1.76	0.66
4:I:1098:GLY:HA2	4:I:1101:ARG:HE	1.61	0.65
1:C:762:ILE:O	1:C:766:MET:HB3	1.96	0.65
1:C:843:ASP:HA	1:C:848:LEU:HD11	1.78	0.65
5:L:753:CYS:O	5:L:757:CYS:HB2	1.96	0.65
5:L:345:GLN:HE22	5:L:350:VAL:HG22	1.61	0.65
3:G:446:LYS:HB2	3:G:456:ALA:HB2	1.79	0.65
4:I:48:ASP:OD2	4:I:92:TRP:NE1	2.29	0.65
4:I:1166:LEU:HD11	4:I:1197:SER:H	1.62	0.65
1:C:510:MET:HG3	1:C:518:VAL:HG11	1.79	0.65
2:E:881:VAL:HG22	2:E:910:LEU:HB3	1.76	0.65
1:C:1110:MET:SD	2:E:849:ARG:NH2	2.70	0.65
4:I:215:SER:HB2	4:I:223:LEU:HD11	1.79	0.65
1:C:762:ILE:O	1:C:766:MET:CB	2.44	0.65
3:G:432:GLY:HA2	3:G:447:VAL:HB	1.78	0.65
2:E:231:LEU:O	2:E:239:GLN:NE2	2.29	0.65
2:E:1196:VAL:O	2:E:1200:LEU:HB2	1.96	0.65
3:G:721:LEU:HD11	3:G:754:HIS:H	1.61	0.65
3:G:847:SER:HA	5:L:842:ARG:HH21	1.61	0.65
3:G:439:GLY:HA2	3:G:464:ARG:HA	1.79	0.64
3:G:942:ARG:NH1	3:G:975:GLU:OE1	2.30	0.64
4:I:585:ILE:HB	4:I:592:HIS:HB2	1.79	0.64
5:L:304:TYR:HD2	5:L:316:GLN:HE21	1.45	0.64
5:L:870:GLU:O	5:L:874:SER:N	2.28	0.64
4:I:1058:GLN:HG2	4:I:1087:LEU:HD12	1.79	0.64
4:I:1065:THR:H	4:I:1068:ALA:HB3	1.60	0.64
1:C:239:GLN:HB2	1:C:249:ALA:HB1	1.78	0.64
5:L:736:TRP:HB3	5:L:761:PHE:HE1	1.61	0.64
2:E:1231:GLU:HB3	2:E:1234:GLU:HB2	1.78	0.64
5:L:14:LYS:HG2	5:L:40:ARG:HH11	1.61	0.64
5:L:854:GLU:HG3	5:L:856:ARG:HB2	1.79	0.64
4:I:509:LEU:HB3	4:I:523:PHE:HB3	1.78	0.64
4:I:1009:ASN:O	4:I:1011:MET:HE3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:114:LEU:HB3	5:L:125:TRP:HB3	1.78	0.64
5:L:298:GLY:HA3	5:L:336:ALA:HA	1.79	0.64
1:C:54:LYS:HB3	1:C:58:GLY:HA3	1.78	0.64
2:E:877:LEU:HD23	2:E:917:LYS:HE3	1.78	0.64
3:G:970:SER:OG	3:G:972:ARG:NH2	2.31	0.64
4:I:782:PRO:HB2	4:I:819:SER:HA	1.79	0.64
5:L:908:VAL:HG22	5:L:918:ARG:HA	1.80	0.64
3:G:1035:MET:HG2	3:G:1059:ILE:HG13	1.79	0.64
4:I:1231:MET:SD	4:I:1236:ARG:NH2	2.70	0.64
5:L:757:CYS:HA	5:L:760:HIS:HB2	1.78	0.64
1:C:518:VAL:HB	1:C:532:HIS:HB2	1.80	0.64
1:C:697:ALA:HB1	1:C:702:ASP:HB2	1.78	0.64
3:G:863:GLU:OE1	3:G:866:ARG:NH2	2.31	0.64
4:I:731:LEU:HB2	4:I:754:SER:HB2	1.79	0.64
4:I:748:GLN:HG2	4:I:764:ARG:HH21	1.62	0.64
4:I:1293:LEU:HD21	4:I:1330:PRO:HD2	1.80	0.64
3:G:1128:ALA:HB2	3:G:1138:ILE:HG21	1.80	0.64
3:G:443:GLU:HA	3:G:458:GLN:HA	1.79	0.63
1:C:765:ARG:O	1:C:773:LYS:NZ	2.31	0.63
4:I:504:SER:OG	4:I:508:THR:N	2.31	0.63
5:L:588:LYS:NZ	5:L:612:ASP:OD2	2.31	0.63
1:C:463:ARG:HB3	1:C:466:VAL:HB	1.80	0.63
5:L:101:ALA:O	5:L:103:GLN:NE2	2.31	0.63
5:L:676:LYS:HG2	5:L:700:GLN:HG2	1.80	0.63
2:E:612:LEU:HD13	2:E:620:ASP:HB3	1.80	0.63
1:C:305:VAL:HG12	1:C:307:GLY:H	1.64	0.63
1:C:366:ASP:HB2	1:C:371:ASP:HB2	1.80	0.63
3:G:496:PHE:HB2	3:G:503:PRO:HG3	1.79	0.63
3:G:1200:LEU:HD12	3:G:1215:ILE:HD11	1.81	0.63
5:L:197:ALA:HB3	5:L:205:LYS:HB2	1.81	0.63
5:L:762:ARG:NH1	5:L:789:GLU:O	2.29	0.63
1:C:725:LEU:O	1:C:734:GLN:NE2	2.31	0.63
2:E:371:ALA:HA	2:E:439:LEU:HD22	1.80	0.63
4:I:437:ARG:NH2	4:I:475:ASP:OD1	2.31	0.63
4:I:853:MET:SD	4:I:883:ARG:NH2	2.72	0.63
5:L:13:GLU:HB2	5:L:19:ASN:HD21	1.63	0.63
2:E:132:ARG:HA	2:E:135:ARG:HG2	1.81	0.63
2:E:1196:VAL:HG11	2:E:1234:GLU:HB3	1.81	0.63
5:L:498:SER:OG	5:L:535:VAL:N	2.32	0.63
4:I:217:ASN:ND2	4:I:247:ILE:O	2.28	0.62
4:I:748:GLN:NE2	4:I:749:GLU:OE2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:946:ARG:O	2:E:948:ARG:NH1	2.32	0.62
4:I:1265:LEU:HD22	4:I:1276:PRO:HA	1.80	0.62
5:L:334:LYS:H	5:L:345:GLN:HB2	1.64	0.62
1:C:367:THR:HB	1:C:654:MET:HG3	1.79	0.62
2:E:702:THR:HG21	2:E:724:ARG:HB3	1.79	0.62
2:E:1185:LEU:O	2:E:1189:ALA:N	2.29	0.62
5:L:41:VAL:HB	5:L:55:LEU:HB2	1.81	0.62
2:E:509:PRO:HG3	2:E:806:ARG:HH22	1.64	0.62
1:C:878:ILE:HD12	1:C:899:PHE:HD2	1.64	0.62
4:I:387:ASP:HB3	4:I:390:ARG:HG2	1.80	0.62
1:C:264:ASN:ND2	1:C:268:THR:OG1	2.32	0.62
1:C:610:ILE:HD13	1:C:659:THR:HG22	1.81	0.62
3:G:321:VAL:HG21	3:G:369:VAL:HG11	1.82	0.62
5:L:650:ALA:HB1	5:L:659:VAL:HG13	1.80	0.62
5:L:807:ARG:HA	5:L:810:VAL:HG22	1.80	0.62
3:G:906:LEU:HD21	3:G:930:ASP:HB3	1.82	0.62
1:C:545:CYS:HB3	1:C:594:ASP:HA	1.81	0.62
1:C:865:VAL:HG13	1:C:877:ALA:HB1	1.81	0.62
2:E:19:ARG:HH21	2:E:253:GLN:HB2	1.64	0.62
2:E:538:ALA:HB2	2:E:553:LYS:HB3	1.82	0.62
5:L:122:VAL:HG21	5:L:155:LEU:HD22	1.82	0.62
5:L:517:LEU:HG	5:L:519:ILE:HD11	1.81	0.62
1:C:207:SER:HB3	1:C:233:LEU:HD13	1.82	0.62
4:I:659:PRO:HB3	4:I:662:ARG:HH21	1.65	0.62
4:I:944:ALA:HB1	4:I:947:ARG:HH21	1.63	0.62
4:I:1060:TYR:HE2	4:I:1071:LYS:HB3	1.65	0.62
3:G:525:LEU:HA	3:G:534:PRO:HA	1.82	0.61
3:G:780:ALA:O	3:G:784:ALA:HB2	2.00	0.61
1:C:687:PRO:HB3	1:C:690:TRP:HD1	1.66	0.61
1:C:713:CYS:SG	1:C:714:ALA:N	2.70	0.61
2:E:382:GLU:HB3	2:E:385:GLU:HB2	1.82	0.61
4:I:390:ARG:HG3	4:I:392:GLN:H	1.64	0.61
4:I:1222:THR:HA	4:I:1225:GLU:HG3	1.82	0.61
5:L:314:ILE:HG12	5:L:325:ARG:HB3	1.81	0.61
1:C:89:LEU:HB3	1:C:101:TRP:HB2	1.81	0.61
5:L:787:TYR:CD2	5:L:799:LEU:HB2	2.36	0.61
1:C:764:MET:SD	1:C:767:ARG:NH2	2.69	0.61
3:G:866:ARG:NH1	3:G:884:PHE:O	2.28	0.61
3:G:1011:PRO:HA	3:G:1014:MET:HB3	1.81	0.61
4:I:672:LEU:O	4:I:676:VAL:N	2.33	0.61
4:I:679:ALA:HA	4:I:682:LEU:HG	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:22:GLN:OE1	2:E:42:ARG:NH2	2.34	0.61
2:E:978:HIS:HB3	2:E:983:ASP:HB2	1.82	0.61
2:E:1350:ARG:NH1	5:L:181:PRO:O	2.33	0.61
5:L:614:ARG:NH2	5:L:642:PHE:O	2.32	0.61
4:I:759:ALA:O	4:I:763:MET:HG3	2.00	0.61
1:C:463:ARG:HH11	1:C:466:VAL:HG21	1.65	0.61
1:C:891:VAL:O	1:C:895:GLN:NE2	2.34	0.61
2:E:301:ALA:O	2:E:305:GLY:N	2.31	0.61
3:G:793:ARG:NH1	3:G:796:THR:OG1	2.33	0.61
4:I:424:TYR:HB3	4:I:431:GLY:HA2	1.81	0.61
4:I:508:THR:OG1	4:I:524:ARG:NH2	2.34	0.61
5:L:342:LEU:HB3	5:L:353:TYR:HB2	1.83	0.61
5:L:774:LEU:HB2	5:L:786:LEU:HD22	1.81	0.61
5:L:783:LEU:O	5:L:786:LEU:N	2.34	0.61
2:E:244:LEU:HD22	2:E:257:ALA:HA	1.80	0.61
2:E:1297:TRP:HB2	2:E:1304:SER:HB3	1.83	0.61
4:I:662:ARG:NE	4:I:678:CYS:SG	2.74	0.61
5:L:459:ARG:NH1	5:L:497:ASN:O	2.33	0.61
1:C:454:LEU:HB3	1:C:456:THR:HG23	1.83	0.61
1:C:650:ASP:HB3	1:C:652:GLU:HG2	1.81	0.61
3:G:264:THR:HA	3:G:279:ASN:HA	1.83	0.61
3:G:351:VAL:O	3:G:376:ASN:ND2	2.34	0.61
1:C:340:LYS:HB2	1:C:351:ALA:HB3	1.82	0.61
1:C:422:GLU:HG2	1:C:424:LYS:HG3	1.82	0.61
2:E:1240:LEU:HD11	2:E:1262:CYS:HB2	1.82	0.61
3:G:78:ILE:HB	3:G:86:SER:HB2	1.81	0.61
5:L:408:TRP:HE1	5:L:446:PRO:HA	1.64	0.61
3:G:494:LEU:HD13	3:G:525:LEU:HD22	1.83	0.60
4:I:494:ALA:HB3	4:I:501:ILE:HB	1.83	0.60
1:C:604:GLU:HG2	1:C:605:LYS:H	1.66	0.60
3:G:778:ALA:HA	3:G:781:LEU:HB3	1.82	0.60
1:C:771:TRP:HA	1:C:774:VAL:HB	1.82	0.60
3:G:542:CYS:HA	3:G:579:VAL:HG11	1.82	0.60
3:G:961:PHE:HB2	3:G:985:ARG:HD2	1.83	0.60
4:I:311:ARG:HE	4:I:326:ALA:HB1	1.67	0.60
4:I:1076:VAL:HG21	4:I:1108:LEU:HD11	1.82	0.60
5:L:124:LEU:O	5:L:129:GLN:NE2	2.33	0.60
1:C:80:VAL:HA	1:C:91:THR:HG22	1.82	0.60
1:C:530:ALA:HB1	1:C:576:MET:HG2	1.83	0.60
2:E:15:GLU:OE2	2:E:299:ARG:NH1	2.34	0.60
2:E:584:ALA:HB1	2:E:611:VAL:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:810:GLN:HA	4:I:813:LEU:HD12	1.81	0.60
5:L:394:LYS:HG2	5:L:409:VAL:HG22	1.84	0.60
5:L:991:ALA:HA	5:L:994:VAL:HB	1.82	0.60
1:C:73:HIS:NE2	1:C:91:THR:OG1	2.30	0.60
3:G:275:VAL:HB	3:G:288:LEU:HB2	1.83	0.60
3:G:794:VAL:O	3:G:798:ALA:HB2	2.00	0.60
4:I:813:LEU:HD22	4:I:832:LYS:HG3	1.84	0.60
1:C:512:GLY:HA2	1:C:518:VAL:HG22	1.82	0.60
1:C:854:LYS:NZ	5:L:466:SER:OG	2.34	0.60
2:E:693:GLU:HA	2:E:701:VAL:HG22	1.82	0.60
2:E:828:ILE:HD12	2:E:839:LEU:HD21	1.83	0.60
5:L:682:PHE:HA	5:L:686:GLY:HA2	1.84	0.60
2:E:703:VAL:HG13	2:E:735:ALA:HB2	1.84	0.60
3:G:640:CYS:N	3:G:657:GLN:O	2.29	0.60
4:I:630:CYS:N	4:I:638:ASP:O	2.34	0.60
1:C:927:ARG:HH11	1:C:938:LEU:HD22	1.67	0.60
2:E:235:GLY:HA2	2:E:474:PRO:HD2	1.84	0.60
2:E:1341:ILE:HG23	2:E:1342:ARG:HD2	1.83	0.60
5:L:33:VAL:HB	5:L:46:ALA:HB2	1.83	0.60
5:L:415:ARG:HH12	5:L:475:GLU:HB3	1.67	0.60
5:L:679:ALA:HA	5:L:696:LEU:HD13	1.83	0.60
2:E:886:MET:HA	2:E:889:LYS:HB2	1.84	0.60
2:E:1048:ARG:NH1	2:E:1230:ASP:O	2.35	0.60
3:G:621:PHE:HE2	3:G:629:ARG:HB3	1.66	0.60
4:I:67:ALA:HA	4:I:83:PRO:HA	1.84	0.60
4:I:536:GLN:NE2	4:I:580:THR:OG1	2.35	0.60
5:L:818:LEU:HG	5:L:823:ARG:HD2	1.82	0.60
2:E:1036:TYR:HB3	2:E:1074:GLY:HA3	1.83	0.60
3:G:39:GLY:HA2	3:G:55:ASN:HB3	1.82	0.60
3:G:883:LEU:HD21	3:G:886:ALA:HB2	1.84	0.60
5:L:659:VAL:HB	5:L:682:PHE:HZ	1.67	0.60
1:C:855:PHE:HB3	1:C:860:LEU:HB2	1.83	0.59
2:E:804:ILE:HD11	2:E:826:LYS:HB3	1.83	0.59
2:E:1158:THR:H	2:E:1161:TYR:HB3	1.66	0.59
2:E:478:LEU:O	2:E:482:LEU:N	2.31	0.59
2:E:878:GLN:OE1	2:E:917:LYS:NZ	2.35	0.59
4:I:159:ASN:HD21	4:I:163:ILE:HB	1.67	0.59
4:I:423:PHE:HD2	4:I:435:GLN:HB2	1.68	0.59
4:I:738:VAL:HG21	4:I:763:MET:HG2	1.84	0.59
2:E:1170:MET:CE	2:E:1185:LEU:HD11	2.32	0.59
4:I:1:MET:HG3	4:I:325:ASP:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1105:ARG:NH2	4:I:1124:GLU:OE2	2.35	0.59
5:L:842:ARG:NH1	5:L:846:GLN:OE1	2.36	0.59
1:C:151:ARG:HE	1:C:154:GLY:HA3	1.66	0.59
2:E:307:LEU:HA	2:E:485:ALA:HB2	1.83	0.59
5:L:108:ASN:HB2	5:L:113:GLN:HB3	1.84	0.59
5:L:730:LEU:HD22	5:L:738:LYS:HB3	1.83	0.59
5:L:773:THR:HA	5:L:776:LYS:HD2	1.84	0.59
3:G:74:PRO:HB2	3:G:90:ALA:HB3	1.84	0.59
3:G:215:LEU:HD23	3:G:227:LEU:HD12	1.83	0.59
3:G:769:LEU:O	3:G:773:GLU:N	2.35	0.59
3:G:1032:THR:O	3:G:1035:MET:HE2	2.02	0.59
3:G:1133:GLU:HG2	3:G:1138:ILE:HG12	1.84	0.59
2:E:1100:ARG:NH2	2:E:1113:MET:SD	2.76	0.59
3:G:738:ARG:HH12	4:I:863:GLU:HA	1.67	0.59
3:G:1155:ALA:HA	3:G:1158:TYR:HB2	1.84	0.59
4:I:1105:ARG:O	4:I:1109:ASN:ND2	2.36	0.59
5:L:578:ALA:HA	5:L:582:VAL:HG22	1.84	0.59
5:L:723:TYR:HE2	5:L:745:GLN:HB3	1.68	0.59
5:L:723:TYR:O	5:L:727:ILE:HB	2.03	0.59
3:G:1044:VAL:HG11	3:G:1069:ASP:HB2	1.85	0.59
4:I:758:ARG:HH12	4:I:781:ASP:HB2	1.68	0.59
4:I:916:GLN:NE2	4:I:931:GLU:OE2	2.36	0.59
5:L:761:PHE:HA	5:L:764:ALA:HB3	1.84	0.59
4:I:802:TYR:HA	4:I:805:ALA:HB3	1.85	0.59
5:L:109:PRO:HD2	5:L:150:GLY:HA2	1.85	0.59
1:C:1099:ASN:HA	1:C:1102:ARG:HB3	1.84	0.59
3:G:1183:PHE:HA	3:G:1186:VAL:HG12	1.85	0.59
3:G:82:ASP:N	3:G:82:ASP:OD1	2.33	0.59
4:I:86:ASN:ND2	4:I:88:HIS:O	2.36	0.59
4:I:1354:GLN:OE1	4:I:1358:GLN:NE2	2.35	0.59
5:L:14:LYS:HD2	5:L:56:LYS:HD2	1.85	0.59
1:C:83:ASN:ND2	1:C:130:GLY:O	2.36	0.58
2:E:238:GLU:OE2	2:E:268:ARG:NH2	2.36	0.58
3:G:387:PHE:HA	3:G:392:ALA:HA	1.84	0.58
4:I:837:ARG:NH1	4:I:863:GLU:OE2	2.36	0.58
1:C:300:LEU:O	1:C:301:ARG:NE	2.32	0.58
3:G:643:ILE:HG21	3:G:651:ILE:HG23	1.85	0.58
3:G:705:THR:O	3:G:708:GLN:NE2	2.28	0.58
3:G:804:ILE:HB	4:I:715:SER:HB3	1.84	0.58
4:I:220:ARG:NH1	4:I:248:MET:O	2.37	0.58
4:I:1009:ASN:O	4:I:1011:MET:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:261:ARG:NH1	5:L:279:VAL:O	2.36	0.58
1:C:660:ARG:HA	1:C:663:ARG:HB2	1.85	0.58
2:E:658:ARG:NH2	2:E:691:GLU:OE1	2.36	0.58
3:G:613:LEU:N	3:G:643:ILE:O	2.36	0.58
3:G:900:ASP:HA	5:L:914:HIS:HA	1.85	0.58
4:I:946:VAL:HG13	4:I:959:ALA:HB1	1.84	0.58
4:I:947:ARG:O	4:I:951:GLU:HB2	2.03	0.58
5:L:351:VAL:HA	5:L:370:LYS:HG2	1.85	0.58
5:L:980:LEU:H	5:L:988:VAL:HG11	1.69	0.58
2:E:255:ILE:HG23	2:E:282:LEU:HD11	1.86	0.58
3:G:1026:GLN:HB3	3:G:1029:LYS:HB2	1.84	0.58
4:I:1139:HIS:CD2	4:I:1167:LEU:HD22	2.38	0.58
5:L:156:GLY:HA2	5:L:162:ILE:HA	1.85	0.58
2:E:1029:LEU:HD11	2:E:1039:LEU:HA	1.84	0.58
4:I:866:LEU:HD21	4:I:889:ARG:HH12	1.68	0.58
5:L:783:LEU:O	5:L:784:ILE:C	2.42	0.58
5:L:854:GLU:HB2	5:L:856:ARG:HH11	1.68	0.58
5:L:867:LEU:HB3	5:L:896:LEU:HD13	1.86	0.58
1:C:310:ILE:HG12	1:C:326:VAL:HG22	1.84	0.58
2:E:303:PRO:HB2	2:E:476:LEU:HG	1.85	0.58
3:G:1134:ARG:HB3	3:G:1161:ALA:HB3	1.85	0.58
4:I:1129:GLU:HG3	4:I:1138:ALA:HB2	1.85	0.58
5:L:600:LEU:HD12	5:L:626:ARG:HD2	1.84	0.58
5:L:928:ALA:HB1	5:L:932:LEU:HD22	1.86	0.58
4:I:1199:PHE:HB3	4:I:1202:HIS:HB2	1.86	0.58
5:L:303:ARG:HB2	5:L:337:VAL:HG11	1.84	0.58
5:L:775:LEU:HG	5:L:783:LEU:HD11	1.85	0.58
1:C:79:CYS:HB3	1:C:124:MET:HB3	1.86	0.58
2:E:1104:ARG:NH1	2:E:1104:ARG:O	2.36	0.58
3:G:175:VAL:HA	3:G:184:VAL:HA	1.85	0.58
3:G:734:ASP:HA	3:G:738:ARG:HB3	1.86	0.58
5:L:20:VAL:HG13	5:L:282:GLU:HA	1.85	0.58
5:L:27:LYS:HE2	5:L:32:GLN:HB2	1.85	0.58
5:L:737:ASP:OD1	5:L:738:LYS:N	2.37	0.58
5:L:960:VAL:HA	5:L:968:ALA:HA	1.85	0.58
1:C:446:PHE:O	1:C:467:ARG:NH2	2.37	0.58
1:C:695:GLU:HA	1:C:698:LEU:HB3	1.85	0.58
3:G:385:TYR:HB3	3:G:668:ILE:HG22	1.86	0.58
3:G:420:GLN:O	3:G:441:ARG:NH2	2.37	0.58
3:G:1339:ASN:ND2	3:G:1342:GLU:OE1	2.37	0.58
4:I:412:HIS:HD2	4:I:434:VAL:HG21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:780:THR:OG1	5:L:803:HIS:NE2	2.26	0.58
1:C:801:ASP:O	1:C:802:ARG:NH1	2.37	0.58
1:C:878:ILE:HD11	1:C:897:HIS:HB2	1.86	0.58
2:E:736:ARG:NH2	2:E:759:ASP:OD1	2.36	0.58
5:L:73:ARG:HD3	5:L:112:GLN:HG2	1.86	0.58
1:C:730:ASP:O	1:C:734:GLN:N	2.37	0.57
2:E:74:ALA:HB1	2:E:117:TYR:HE2	1.69	0.57
3:G:397:ALA:HB3	3:G:400:ARG:HB3	1.85	0.57
3:G:435:LEU:HD11	3:G:442:ALA:HB1	1.86	0.57
3:G:563:VAL:O	3:G:581:TRP:N	2.35	0.57
3:G:752:MET:CG	3:G:768:CYS:HB2	2.34	0.57
3:G:1241:ASP:O	3:G:1244:ARG:NH1	2.37	0.57
1:C:902:ILE:HG13	1:C:903:GLU:HG2	1.86	0.57
1:C:1080:PHE:O	1:C:1084:CYS:N	2.30	0.57
2:E:1174:ASP:O	2:E:1178:ILE:N	2.31	0.57
1:C:594:ASP:HB2	1:C:630:HIS:HB2	1.85	0.57
2:E:88:HIS:HA	2:E:91:ILE:HD12	1.87	0.57
2:E:272:ASN:O	2:E:276:ALA:N	2.35	0.57
2:E:1167:TYR:HE1	2:E:1201:ALA:HB2	1.68	0.57
4:I:300:GLY:O	4:I:315:ALA:N	2.36	0.57
1:C:275:PHE:HA	1:C:288:TRP:HA	1.87	0.57
1:C:365:TRP:NE1	1:C:370:ASN:OD1	2.38	0.57
1:C:1033:TRP:HB2	1:C:1055:LEU:HD21	1.86	0.57
2:E:864:LEU:HB3	2:E:883:ALA:HB3	1.87	0.57
4:I:1211:VAL:HG11	4:I:1230:LEU:HD11	1.86	0.57
3:G:215:LEU:N	3:G:227:LEU:O	2.32	0.57
3:G:467:ALA:O	3:G:474:TYR:N	2.38	0.57
3:G:555:ARG:NE	3:G:604:MET:HA	2.19	0.57
4:I:19:PHE:H	4:I:337:LYS:HD3	1.69	0.57
4:I:802:TYR:HD2	4:I:838:THR:HA	1.68	0.57
5:L:949:VAL:HG12	5:L:996:ARG:HD2	1.85	0.57
1:C:772:PHE:HB3	1:C:776:ARG:HH12	1.69	0.57
1:C:789:LEU:HD22	1:C:815:ALA:HA	1.87	0.57
2:E:94:LEU:HD13	2:E:97:LYS:HD3	1.85	0.57
3:G:17:ALA:HB1	3:G:29:LEU:HD11	1.86	0.57
4:I:111:PHE:HA	4:I:127:THR:HA	1.85	0.57
4:I:888:GLU:OE2	4:I:909:ARG:NH1	2.38	0.57
1:C:136:VAL:HG21	1:C:164:VAL:HG11	1.85	0.57
2:E:801:VAL:HG13	2:E:827:ALA:HB1	1.86	0.57
2:E:1342:ARG:HA	2:E:1346:LEU:HD23	1.85	0.57
3:G:67:ILE:HB	3:G:76:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:297:VAL:O	3:G:317:THR:OG1	2.22	0.57
4:I:204:ASP:H	4:I:275:ARG:HH12	1.51	0.57
4:I:543:VAL:HG21	4:I:583:MET:HG3	1.86	0.57
3:G:442:ALA:N	3:G:459:PHE:O	2.37	0.57
3:G:979:TYR:O	3:G:983:ALA:N	2.37	0.57
3:G:1044:VAL:HG22	3:G:1056:LEU:HD11	1.86	0.57
5:L:565:TYR:HB3	5:L:574:ALA:HB2	1.87	0.57
3:G:445:TYR:HA	3:G:455:PRO:HA	1.87	0.57
3:G:981:THR:HA	3:G:1005:LEU:HD11	1.87	0.57
4:I:747:ALA:HB3	4:I:763:MET:HE1	1.87	0.57
4:I:793:GLY:HA2	4:I:805:ALA:HA	1.87	0.57
4:I:816:LEU:HD22	4:I:824:GLN:HB3	1.86	0.57
4:I:1108:LEU:O	4:I:1112:MET:N	2.33	0.57
4:I:1268:CYS:SG	4:I:1284:SER:OG	2.62	0.57
5:L:474:ASP:OD2	5:L:478:LYS:NZ	2.35	0.57
5:L:730:LEU:HD23	5:L:735:TRP:HE3	1.70	0.57
1:C:861:CYS:HA	1:C:884:LEU:HD12	1.86	0.57
3:G:70:HIS:HB2	3:G:75:LEU:HB3	1.86	0.57
3:G:1301:ARG:NH1	3:G:1304:ASP:OD2	2.38	0.57
4:I:738:VAL:CG2	4:I:763:MET:HG2	2.35	0.57
4:I:884:ALA:O	4:I:886:GLN:NE2	2.37	0.57
4:I:1011:MET:SD	4:I:1012:ASP:N	2.78	0.57
5:L:985:GLN:NE2	5:L:989:ASP:OD1	2.38	0.57
5:L:663:MET:O	5:L:699:ARG:NH1	2.38	0.56
1:C:701:LEU:HD21	1:C:735:ARG:HH12	1.69	0.56
2:E:286:MET:SD	2:E:289:GLN:NE2	2.78	0.56
2:E:1308:GLY:HA2	2:E:1311:LEU:HD12	1.87	0.56
3:G:1014:MET:HG3	3:G:1033:LEU:O	2.04	0.56
4:I:429:LYS:HB3	4:I:432:LYS:HB3	1.87	0.56
4:I:538:THR:HG23	4:I:540:ALA:H	1.70	0.56
4:I:1105:ARG:HA	4:I:1108:LEU:HB3	1.87	0.56
5:L:909:VAL:HB	5:L:951:VAL:HG22	1.88	0.56
1:C:234:ASP:HB2	1:C:257:LYS:HD2	1.88	0.56
2:E:10:HIS:HA	2:E:118:LEU:HD21	1.86	0.56
2:E:29:LEU:HA	2:E:38:LEU:HD13	1.87	0.56
3:G:123:GLU:HA	3:G:150:VAL:HG13	1.87	0.56
4:I:844:ASP:HB3	4:I:847:GLN:HB3	1.87	0.56
4:I:1170:TYR:HB2	4:I:1192:VAL:HG21	1.87	0.56
5:L:96:TYR:HD2	5:L:132:VAL:HG22	1.70	0.56
5:L:692:SER:HB2	5:L:695:GLU:HB3	1.88	0.56
5:L:739:LEU:HD21	5:L:760:HIS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:774:LEU:HD22	5:L:786:LEU:HB2	1.88	0.56
1:C:64:LEU:HD11	1:C:67:ASN:HB2	1.88	0.56
2:E:333:ALA:O	2:E:337:VAL:HB	2.05	0.56
2:E:687:ASP:OD1	2:E:690:ARG:NH2	2.39	0.56
3:G:639:ASP:HA	3:G:658:PRO:HA	1.86	0.56
3:G:906:LEU:HG	3:G:928:ALA:HB1	1.87	0.56
4:I:1053:ALA:HB1	4:I:1084:LEU:HD22	1.87	0.56
1:C:632:LEU:HB2	1:C:662:LEU:HD13	1.88	0.56
2:E:522:LEU:HD22	2:E:832:ARG:HH21	1.70	0.56
3:G:185:LYS:HA	3:G:196:VAL:H	1.71	0.56
3:G:404:GLU:OE2	3:G:698:ASN:ND2	2.38	0.56
3:G:1235:CYS:O	3:G:1239:GLU:HB2	2.05	0.56
4:I:895:ILE:HG21	4:I:915:LEU:HD22	1.87	0.56
4:I:1196:ILE:HG12	4:I:1203:ILE:HD13	1.86	0.56
5:L:68:ALA:HB3	5:L:72:LYS:H	1.70	0.56
5:L:966:LYS:HA	5:L:969:ARG:HE	1.69	0.56
2:E:554:ALA:HB2	2:E:570:LEU:HD23	1.87	0.56
3:G:440:GLU:OE2	3:G:441:ARG:NH1	2.39	0.56
3:G:670:SER:HA	3:G:675:LEU:HA	1.87	0.56
3:G:944:TRP:HB3	3:G:982:LEU:HD23	1.88	0.56
4:I:509:LEU:HD11	4:I:533:LEU:HD21	1.88	0.56
4:I:1294:ALA:HB1	4:I:1318:GLN:HB2	1.88	0.56
1:C:612:ARG:NH2	1:C:661:SER:OG	2.28	0.56
2:E:1029:LEU:HD12	2:E:1042:LEU:HD23	1.88	0.56
2:E:1148:LEU:HB3	2:E:1149:LYS:NZ	2.20	0.56
3:G:591:HIS:HB2	3:G:651:ILE:HB	1.86	0.56
1:C:1024:TRP:HD1	1:C:1027:ALA:HB3	1.70	0.56
2:E:677:ASP:OD2	2:E:712:ARG:NH1	2.39	0.56
3:G:88:TRP:HB2	3:G:95:LEU:HD12	1.87	0.56
3:G:576:VAL:N	3:G:594:THR:OG1	2.36	0.56
3:G:1018:ALA:HB2	3:G:1033:LEU:HB3	1.88	0.56
3:G:1043:ALA:HB1	3:G:1059:ILE:HD13	1.87	0.56
3:G:1306:LEU:HD13	3:G:1326:VAL:HG22	1.86	0.56
4:I:435:GLN:NE2	4:I:466:ILE:O	2.38	0.56
4:I:758:ARG:O	4:I:762:GLU:HG3	2.06	0.56
4:I:1269:PRO:HA	4:I:1301:LEU:HD21	1.87	0.56
5:L:673:ASP:OD1	5:L:674:GLU:N	2.39	0.56
1:C:146:SER:OG	1:C:148:ASP:OD1	2.23	0.56
1:C:711:VAL:HG22	5:L:668:ASP:HB2	1.87	0.56
2:E:736:ARG:HG3	2:E:760:LEU:HD13	1.87	0.56
3:G:446:LYS:N	3:G:454:MET:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:749:TRP:HE3	3:G:752:MET:HA	1.71	0.56
3:G:804:ILE:HG22	4:I:714:ALA:HB1	1.87	0.56
3:G:811:TYR:HE2	3:G:823:LEU:HD12	1.70	0.56
4:I:760:ALA:HA	4:I:763:MET:SD	2.46	0.56
4:I:1008:HIS:CE1	4:I:1010:GLU:HG3	2.40	0.56
1:C:262:LYS:HG2	1:C:314:SER:HA	1.88	0.56
3:G:1114:THR:H	3:G:1117:MET:HB3	1.70	0.56
4:I:225:ILE:HD12	4:I:277:ILE:HD11	1.88	0.56
4:I:1202:HIS:O	4:I:1206:ILE:N	2.36	0.56
1:C:891:VAL:HG22	1:C:902:ILE:HD12	1.87	0.55
2:E:292:LYS:HB3	2:E:328:LEU:HD22	1.87	0.55
4:I:407:GLY:HA3	4:I:448:LEU:HD13	1.88	0.55
4:I:950:LEU:HD13	4:I:978:PHE:HB2	1.89	0.55
4:I:1307:CYS:O	4:I:1311:LYS:N	2.36	0.55
3:G:293:ASP:OD2	3:G:320:ARG:NH2	2.40	0.55
4:I:1091:TYR:O	4:I:1095:GLU:HB2	2.06	0.55
5:L:255:LEU:HD22	5:L:310:MET:HG3	1.87	0.55
2:E:331:GLU:HG3	2:E:362:LEU:HD11	1.88	0.55
3:G:399:ASP:HB3	3:G:419:LEU:H	1.71	0.55
3:G:800:HIS:ND1	4:I:741:GLU:OE2	2.38	0.55
3:G:1151:PHE:HD2	3:G:1179:LYS:HG2	1.69	0.55
4:I:189:LEU:HD11	4:I:216:LEU:HD22	1.89	0.55
4:I:532:ARG:NE	4:I:545:GLU:OE1	2.34	0.55
4:I:591:LEU:HD22	4:I:628:VAL:HG21	1.87	0.55
4:I:813:LEU:HD23	4:I:831:CYS:HB2	1.87	0.55
5:L:573:SER:OG	5:L:576:ARG:NH2	2.39	0.55
5:L:675:ALA:O	5:L:679:ALA:CB	2.53	0.55
1:C:638:PHE:HB2	1:C:653:PHE:HB3	1.88	0.55
2:E:289:GLN:NE2	2:E:290:GLU:O	2.39	0.55
4:I:532:ARG:NH1	4:I:570:ALA:O	2.40	0.55
4:I:1283:ILE:HG12	4:I:1298:ARG:HH22	1.71	0.55
1:C:608:MET:H	1:C:621:THR:HA	1.71	0.55
2:E:337:VAL:HG11	2:E:368:GLU:HB3	1.88	0.55
2:E:1077:TYR:HB2	2:E:1109:ALA:HB2	1.89	0.55
2:E:1311:LEU:HB3	2:E:1327:VAL:HG21	1.89	0.55
3:G:327:ASN:ND2	3:G:342:CYS:O	2.39	0.55
3:G:1226:GLU:HG3	3:G:1263:SER:HB3	1.87	0.55
4:I:1035:GLU:HG2	4:I:1040:TYR:HD1	1.72	0.55
5:L:225:LEU:H	5:L:240:GLY:HA2	1.72	0.55
1:C:98:ILE:HB	1:C:114:ASN:HB3	1.88	0.55
1:C:878:ILE:HG21	1:C:899:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:819:LEU:HA	3:G:822:GLN:HG3	1.88	0.55
3:G:935:VAL:HA	3:G:939:CYS:HB2	1.88	0.55
4:I:439:TYR:OH	4:I:464:HIS:NE2	2.40	0.55
4:I:678:CYS:HA	4:I:681:GLN:HG3	1.88	0.55
4:I:749:GLU:OE1	4:I:753:ARG:NH1	2.33	0.55
4:I:1096:LYS:HB2	4:I:1101:ARG:HB3	1.89	0.55
4:I:1328:ARG:HH12	4:I:1330:PRO:HB3	1.71	0.55
1:C:533:VAL:O	1:C:535:ARG:NH1	2.40	0.55
2:E:944:SER:HB2	2:E:949:GLN:HG3	1.89	0.55
4:I:977:ARG:O	4:I:981:GLN:HG3	2.07	0.55
5:L:13:GLU:OE1	5:L:19:ASN:ND2	2.39	0.55
5:L:230:PHE:HB3	5:L:235:TYR:HB2	1.89	0.55
5:L:303:ARG:HA	5:L:317:HIS:HA	1.89	0.55
1:C:445:GLN:HG2	1:C:467:ARG:HD2	1.88	0.55
1:C:910:ALA:HB2	1:C:925:LEU:HD11	1.89	0.55
2:E:71:ALA:HA	2:E:113:LEU:HD13	1.89	0.55
2:E:349:THR:HA	2:E:352:ALA:HB3	1.89	0.55
2:E:771:CYS:SG	2:E:806:ARG:NH1	2.80	0.55
3:G:308:ARG:NH2	3:G:361:GLY:O	2.37	0.55
3:G:707:PHE:O	3:G:711:GLN:NE2	2.40	0.55
4:I:849:ARG:HG3	4:I:876:GLU:HB3	1.88	0.55
4:I:864:CYS:HA	4:I:867:ILE:HB	1.88	0.55
4:I:1084:LEU:O	4:I:1088:VAL:N	2.39	0.55
4:I:1102:ASP:OD1	4:I:1105:ARG:NH1	2.40	0.55
5:L:731:ALA:O	5:L:763:ARG:NH2	2.40	0.55
1:C:378:ARG:HG3	1:C:379:LYS:HG3	1.89	0.55
1:C:752:TYR:HB2	1:C:761:ALA:HB2	1.89	0.55
2:E:190:LEU:HB3	2:E:213:ILE:HG21	1.89	0.55
3:G:845:LEU:HG	3:G:849:HIS:CE1	2.42	0.55
4:I:15:GLY:HA2	4:I:63:ARG:HA	1.87	0.55
1:C:1055:LEU:HA	1:C:1058:TYR:HB2	1.89	0.55
3:G:513:LEU:N	3:G:525:LEU:O	2.37	0.55
4:I:1044:ALA:HB1	4:I:1059:LEU:HB3	1.89	0.55
5:L:412:SER:HB3	5:L:433:LEU:HD13	1.88	0.55
1:C:59:ALA:HA	1:C:606:THR:HG21	1.88	0.54
3:G:175:VAL:HG22	3:G:184:VAL:HG22	1.88	0.54
3:G:311:LEU:HD12	3:G:364:PRO:HB2	1.90	0.54
3:G:704:MET:HE1	3:G:718:ARG:HH12	1.72	0.54
5:L:659:VAL:H	5:L:691:ARG:HH12	1.55	0.54
1:C:270:LEU:HD23	1:C:293:TYR:HB2	1.90	0.54
3:G:507:ASP:O	3:G:514:ALA:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:566:LEU:HG	3:G:603:LEU:HD11	1.87	0.54
3:G:755:MET:HA	3:G:780:ALA:HB1	1.89	0.54
3:G:1035:MET:SD	3:G:1058:HIS:HB2	2.47	0.54
4:I:796:LEU:CB	4:I:805:ALA:HB2	2.37	0.54
5:L:379:LEU:HB2	5:L:390:CYS:HB3	1.88	0.54
1:C:20:ILE:HB	1:C:325:SER:HB2	1.89	0.54
2:E:173:LEU:HG	2:E:196:ILE:HD13	1.89	0.54
2:E:1005:SER:HB3	2:E:1024:HIS:CD2	2.42	0.54
3:G:752:MET:HG2	3:G:768:CYS:SG	2.47	0.54
4:I:309:CYS:SG	4:I:311:ARG:NH1	2.80	0.54
4:I:420:GLN:HA	4:I:438:GLU:HA	1.89	0.54
4:I:957:GLN:OE1	4:I:964:ARG:NH2	2.40	0.54
1:C:669:LEU:HD22	1:C:693:LEU:HB2	1.88	0.54
3:G:718:ARG:HH21	3:G:722:LEU:HD11	1.72	0.54
3:G:741:LYS:O	4:I:802:TYR:OH	2.21	0.54
4:I:335:ILE:HA	4:I:351:THR:HA	1.89	0.54
4:I:600:SER:OG	4:I:601:LEU:N	2.40	0.54
4:I:653:ALA:HA	4:I:656:ARG:HB2	1.89	0.54
5:L:481:VAL:HB	5:L:491:PHE:HB3	1.89	0.54
5:L:847:LEU:HB2	5:L:863:TYR:HE2	1.72	0.54
1:C:568:ALA:HA	1:C:575:THR:HB	1.90	0.54
1:C:771:TRP:HB3	1:C:792:HIS:CE1	2.43	0.54
1:C:1074:ALA:O	1:C:1078:ASN:ND2	2.41	0.54
2:E:59:LEU:HD11	2:E:68:LEU:HD22	1.89	0.54
3:G:402:VAL:HG12	3:G:404:GLU:HG3	1.88	0.54
3:G:473:VAL:O	3:G:484:VAL:N	2.40	0.54
4:I:1059:LEU:HD23	4:I:1062:LYS:HD2	1.90	0.54
5:L:351:VAL:HG22	5:L:370:LYS:HE3	1.89	0.54
5:L:502:ASN:HB2	5:L:508:MET:HB3	1.90	0.54
5:L:651:ARG:HA	5:L:654:THR:HG23	1.89	0.54
2:E:538:ALA:HB1	2:E:570:LEU:HD21	1.88	0.54
3:G:968:GLU:OE1	3:G:980:TYR:OH	2.24	0.54
4:I:153:ILE:HD13	4:I:166:LEU:HD22	1.90	0.54
4:I:399:LEU:HD22	4:I:415:VAL:HG21	1.88	0.54
5:L:112:GLN:H	5:L:127:PRO:HG3	1.71	0.54
5:L:857:TYR:HB3	5:L:903:TYR:HD1	1.72	0.54
2:E:9:VAL:HA	2:E:20:HIS:HE1	1.72	0.54
2:E:707:GLU:HA	2:E:710:ILE:HD12	1.89	0.54
4:I:663:PHE:HA	4:I:675:ALA:HA	1.88	0.54
1:C:533:VAL:HB	1:C:575:THR:HG23	1.90	0.54
3:G:594:THR:HG21	3:G:622:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:304:MET:HB2	4:I:311:ARG:H	1.72	0.54
4:I:813:LEU:CD2	4:I:832:LYS:HG3	2.38	0.54
4:I:1011:MET:HE2	4:I:1039:GLU:OE2	2.08	0.54
2:E:293:ASN:HB3	2:E:296:LEU:HB3	1.90	0.54
2:E:736:ARG:NH1	2:E:756:CYS:O	2.41	0.54
3:G:543:PRO:O	3:G:547:LYS:N	2.41	0.54
3:G:834:LEU:HD23	3:G:848:THR:HG22	1.89	0.54
4:I:840:LEU:HD21	4:I:868:LEU:HG	1.89	0.54
1:C:222:ALA:HB2	1:C:268:THR:HG22	1.90	0.54
1:C:275:PHE:HB3	1:C:288:TRP:CE2	2.42	0.54
2:E:65:ASN:O	2:E:69:GLU:N	2.31	0.54
3:G:616:GLN:OE1	3:G:667:CYS:N	2.41	0.54
3:G:804:ILE:HD11	3:G:823:LEU:HB3	1.90	0.54
3:G:834:LEU:HB3	3:G:849:HIS:NE2	2.23	0.54
3:G:1296:PRO:HG3	3:G:1337:ALA:HB1	1.90	0.54
4:I:512:TYR:HA	4:I:519:PRO:HA	1.89	0.54
4:I:959:ALA:HA	4:I:962:ILE:HG22	1.90	0.54
4:I:1105:ARG:HA	4:I:1108:LEU:CB	2.38	0.54
4:I:1124:GLU:HA	4:I:1127:ARG:HG2	1.90	0.54
5:L:318:LEU:HD11	5:L:551:MET:HG3	1.89	0.54
5:L:771:LYS:NZ	5:L:772:GLU:OE2	2.39	0.54
1:C:518:VAL:N	1:C:532:HIS:O	2.41	0.53
2:E:1010:GLU:HA	2:E:1013:PHE:HB3	1.90	0.53
3:G:160:GLU:OE2	3:G:229:ARG:NH2	2.41	0.53
3:G:555:ARG:HE	3:G:604:MET:HA	1.72	0.53
1:C:464:LYS:O	1:C:467:ARG:NE	2.41	0.53
1:C:591:ARG:NH1	1:C:592:TRP:O	2.41	0.53
2:E:1189:ALA:HA	2:E:1198:VAL:HB	1.91	0.53
3:G:841:ASP:HB2	3:G:844:HIS:H	1.73	0.53
3:G:1109:HIS:HB3	3:G:1111:VAL:HG22	1.90	0.53
5:L:194:VAL:HA	5:L:208:MET:HE2	1.90	0.53
5:L:350:VAL:HB	5:L:371:ILE:HB	1.89	0.53
1:C:137:TYR:HB2	1:C:141:ALA:HB3	1.90	0.53
1:C:763:ASP:HA	1:C:766:MET:HB3	1.90	0.53
2:E:347:ASP:HB3	2:E:643:ARG:HB3	1.90	0.53
3:G:447:VAL:HG13	3:G:453:ILE:HG13	1.90	0.53
4:I:768:LYS:HE2	4:I:791:GLU:HG3	1.91	0.53
4:I:1034:TYR:HB2	4:I:1043:ALA:HB2	1.88	0.53
4:I:1080:ARG:NH1	4:I:1110:ILE:O	2.40	0.53
4:I:1183:THR:OG1	4:I:1261:LEU:O	2.24	0.53
4:I:1263:GLU:HG3	4:I:1277:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:247:LEU:HD13	5:L:258:ILE:HD11	1.88	0.53
5:L:577:VAL:HA	5:L:580:LEU:HD12	1.90	0.53
1:C:51:VAL:HA	1:C:54:LYS:HB2	1.91	0.53
1:C:902:ILE:O	1:C:906:LEU:CB	2.54	0.53
3:G:794:VAL:O	3:G:798:ALA:CB	2.56	0.53
3:G:821:ASN:O	3:G:825:ARG:NH1	2.42	0.53
3:G:886:ALA:O	3:G:890:THR:N	2.30	0.53
4:I:1073:VAL:HG13	4:I:1108:LEU:HD13	1.91	0.53
5:L:230:PHE:HB2	5:L:237:THR:HG23	1.90	0.53
5:L:350:VAL:HG21	5:L:371:ILE:HD12	1.91	0.53
5:L:793:TRP:HB2	5:L:814:TYR:HE1	1.74	0.53
1:C:966:GLU:HA	1:C:969:LYS:HE2	1.91	0.53
2:E:743:TYR:HA	2:E:747:ARG:HB2	1.91	0.53
2:E:811:LEU:HD13	2:E:819:ARG:HB3	1.90	0.53
3:G:465:CYS:SG	3:G:466:MET:N	2.81	0.53
3:G:805:GLU:OE1	3:G:808:LYS:NZ	2.40	0.53
4:I:1161:LEU:HD13	4:I:1291:PHE:HE2	1.73	0.53
4:I:1316:ALA:HA	4:I:1319:PHE:HB3	1.91	0.53
5:L:73:ARG:HG3	5:L:87:THR:HA	1.90	0.53
5:L:295:THR:O	5:L:297:HIS:ND1	2.37	0.53
5:L:342:LEU:N	5:L:353:TYR:O	2.41	0.53
5:L:787:TYR:CE2	5:L:798:LEU:HB3	2.42	0.53
5:L:832:GLN:HA	5:L:837:PRO:HD3	1.91	0.53
1:C:568:ALA:HB2	1:C:575:THR:H	1.73	0.53
1:C:774:VAL:HA	1:C:777:LEU:HD12	1.90	0.53
1:C:856:GLN:OE1	1:C:876:ARG:NH2	2.41	0.53
3:G:808:LYS:HG2	3:G:820:LEU:HA	1.88	0.53
3:G:1281:VAL:HG11	3:G:1306:LEU:HD11	1.90	0.53
4:I:238:LEU:HD21	4:I:277:ILE:HG13	1.89	0.53
4:I:1182:HIS:ND1	4:I:1213:GLU:OE1	2.42	0.53
5:L:394:LYS:HA	5:L:409:VAL:HA	1.89	0.53
3:G:19:TRP:HE1	3:G:368:VAL:N	2.07	0.53
3:G:568:VAL:HA	3:G:576:VAL:HA	1.89	0.53
3:G:598:ARG:NH2	3:G:639:ASP:OD2	2.42	0.53
3:G:667:CYS:HA	3:G:677:THR:HA	1.90	0.53
4:I:294:THR:HG21	4:I:339:GLY:HA2	1.89	0.53
4:I:684:GLN:HG3	4:I:686:GLU:HG3	1.90	0.53
4:I:796:LEU:HB3	4:I:805:ALA:HB2	1.91	0.53
5:L:40:ARG:HG3	5:L:56:LYS:HG3	1.90	0.53
5:L:779:ASP:O	5:L:783:LEU:N	2.42	0.53
1:C:17:LEU:O	1:C:311:SER:OG	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASN:HB3	1:C:88:LYS:H	1.74	0.53
3:G:286:TYR:CZ	3:G:339:PHE:HB2	2.44	0.53
3:G:799:VAL:HG22	3:G:804:ILE:HG13	1.89	0.53
3:G:820:LEU:O	3:G:824:TYR:HB2	2.08	0.53
4:I:840:LEU:HD12	4:I:845:LEU:HA	1.91	0.53
2:E:1076:HIS:ND1	2:E:1095:GLU:OE1	2.41	0.53
3:G:394:MET:O	3:G:402:VAL:N	2.40	0.53
4:I:816:LEU:HD21	4:I:827:LEU:HD23	1.91	0.53
1:C:262:LYS:HB3	1:C:313:ILE:HG13	1.91	0.53
2:E:883:ALA:O	2:E:887:LEU:HB2	2.08	0.53
3:G:182:ALA:HB2	3:G:202:GLY:HA2	1.91	0.53
3:G:265:LEU:HB3	3:G:278:TYR:HB3	1.91	0.53
3:G:669:GLY:N	3:G:676:LEU:O	2.41	0.53
3:G:927:LYS:NZ	5:L:915:SER:O	2.42	0.53
1:C:352:PHE:HE2	1:C:354:ARG:HG2	1.74	0.52
1:C:784:ASP:HB3	1:C:788:LEU:HD23	1.90	0.52
2:E:918:LEU:HB3	2:E:929:GLN:HG3	1.89	0.52
3:G:756:CYS:HB3	3:G:761:ARG:HG3	1.92	0.52
4:I:299:LEU:O	4:I:316:ASN:ND2	2.42	0.52
1:C:382:ALA:H	1:C:393:ALA:HB3	1.74	0.52
1:C:822:VAL:O	1:C:826:TYR:HB2	2.09	0.52
2:E:303:PRO:HA	2:E:480:ALA:HB2	1.91	0.52
2:E:1239:TRP:HB3	2:E:1258:LEU:HD22	1.91	0.52
3:G:654:GLN:HB2	3:G:729:ALA:HB2	1.90	0.52
3:G:789:GLU:HB3	3:G:810:LEU:HB2	1.90	0.52
4:I:1097:ASP:OD1	4:I:1097:ASP:N	2.42	0.52
4:I:1108:LEU:HD12	4:I:1111:ALA:HB3	1.91	0.52
5:L:345:GLN:HG2	5:L:380:LEU:HD22	1.90	0.52
5:L:505:PHE:HB3	5:L:508:MET:HB2	1.91	0.52
1:C:116:ARG:NH2	1:C:156:GLU:OE2	2.43	0.52
2:E:619:ASP:OD1	2:E:619:ASP:N	2.42	0.52
2:E:1315:TYR:O	2:E:1348:LYS:NZ	2.39	0.52
3:G:496:PHE:CE2	3:G:523:ARG:HB3	2.44	0.52
3:G:580:VAL:HG11	3:G:645:VAL:HG11	1.91	0.52
3:G:1017:THR:HB	3:G:1033:LEU:HG	1.92	0.52
3:G:1176:ASP:HA	3:G:1203:LEU:HD22	1.91	0.52
5:L:55:LEU:HD11	5:L:90:ALA:HB1	1.90	0.52
5:L:171:GLU:OE2	5:L:174:ARG:NH1	2.42	0.52
5:L:483:ASN:O	5:L:487:LYS:N	2.41	0.52
1:C:42:ARG:HH21	1:C:65:SER:HB2	1.75	0.52
2:E:896:GLU:O	2:E:900:TYR:N	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1026:GLN:NE2	2:E:1027:GLN:OE1	2.43	0.52
3:G:612:LEU:HD11	3:G:642:ILE:HG23	1.91	0.52
4:I:1130:GLN:HE21	4:I:1167:LEU:HD12	1.74	0.52
5:L:110:VAL:HG12	5:L:111:THR:HG23	1.91	0.52
2:E:551:LEU:HG	2:E:574:VAL:HG11	1.90	0.52
2:E:1167:TYR:HA	2:E:1170:MET:SD	2.49	0.52
3:G:182:ALA:HB3	3:G:199:MET:HG3	1.91	0.52
3:G:569:GLY:N	3:G:575:ALA:O	2.43	0.52
3:G:825:ARG:HD3	3:G:833:ALA:HA	1.91	0.52
5:L:302:ASP:O	5:L:318:LEU:N	2.37	0.52
5:L:618:LEU:HD13	5:L:642:PHE:HB2	1.91	0.52
5:L:721:LYS:HD3	5:L:723:TYR:HE1	1.73	0.52
1:C:697:ALA:O	1:C:702:ASP:N	2.42	0.52
1:C:728:LEU:HD23	1:C:734:GLN:HA	1.91	0.52
1:C:1030:TYR:HD1	1:C:1062:LEU:HD11	1.74	0.52
2:E:285:SER:O	2:E:288:ARG:NH1	2.42	0.52
3:G:821:ASN:O	3:G:825:ARG:HG2	2.08	0.52
5:L:801:HIS:HB2	5:L:811:TYR:OH	2.10	0.52
2:E:959:GLU:HG2	2:E:963:HIS:CE1	2.44	0.52
3:G:599:GLN:HB2	3:G:620:VAL:HB	1.90	0.52
3:G:898:ALA:HB2	5:L:855:THR:HG21	1.91	0.52
3:G:1237:GLN:NE2	3:G:1322:ARG:O	2.43	0.52
4:I:1002:PHE:HZ	4:I:1037:ARG:HH22	1.58	0.52
5:L:18:ARG:NH2	5:L:282:GLU:OE2	2.41	0.52
5:L:906:TYR:O	5:L:910:HIS:HB3	2.10	0.52
1:C:212:VAL:HG13	1:C:231:ILE:HG12	1.92	0.52
3:G:642:ILE:HD11	3:G:675:LEU:HD11	1.92	0.52
5:L:388:ILE:HD11	5:L:443:VAL:HG22	1.92	0.52
5:L:775:LEU:CG	5:L:783:LEU:HD11	2.40	0.52
1:C:1089:ILE:HD12	2:E:783:PRO:HG3	1.92	0.52
3:G:58:ASN:HD22	3:G:62:THR:H	1.57	0.52
3:G:405:ASN:HB3	3:G:408:VAL:HG23	1.92	0.52
3:G:842:ARG:NH1	5:L:822:ASP:OD2	2.42	0.52
5:L:317:HIS:O	5:L:321:GLU:N	2.33	0.52
5:L:980:LEU:HD21	5:L:996:ARG:HH22	1.75	0.52
1:C:762:ILE:HG13	1:C:765:ARG:HH21	1.74	0.52
2:E:850:LEU:HB3	2:E:852:GLN:HE22	1.74	0.52
2:E:985:ASP:N	2:E:985:ASP:OD1	2.43	0.52
3:G:720:ALA:CB	3:G:752:MET:O	2.58	0.52
4:I:1146:VAL:HA	4:I:1156:PRO:HD2	1.91	0.52
5:L:96:TYR:CZ	5:L:125:TRP:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:343:ALA:HA	5:L:352:ILE:HA	1.92	0.52
5:L:725:ARG:HH22	5:L:732:LYS:HZ2	1.57	0.52
5:L:793:TRP:HB3	5:L:817:TRP:HB3	1.91	0.52
1:C:610:ILE:HB	1:C:617:GLU:HB2	1.91	0.51
2:E:1294:GLU:HB3	2:E:1311:LEU:HD21	1.92	0.51
3:G:526:LYS:N	3:G:533:LYS:O	2.42	0.51
4:I:1143:PHE:HE2	4:I:1310:CYS:HB2	1.74	0.51
2:E:927:ALA:HA	2:E:930:ARG:HE	1.74	0.51
2:E:1221:ARG:HA	2:E:1224:LYS:HB2	1.92	0.51
3:G:707:PHE:HA	3:G:755:MET:SD	2.51	0.51
4:I:437:ARG:NH1	4:I:439:TYR:OH	2.43	0.51
4:I:590:ALA:HA	4:I:613:ALA:HA	1.92	0.51
4:I:803:SER:HA	4:I:842:LEU:HD11	1.93	0.51
4:I:854:GLN:HG3	4:I:855:LEU:HG	1.91	0.51
5:L:228:SER:OG	5:L:237:THR:OG1	2.27	0.51
5:L:637:ALA:HB2	5:L:652:LEU:HB2	1.92	0.51
3:G:913:GLU:HA	3:G:921:ALA:HB2	1.92	0.51
3:G:1028:GLU:HA	3:G:1052:LEU:CD1	2.29	0.51
4:I:138:ARG:HG3	4:I:139:GLU:HG3	1.92	0.51
4:I:920:ALA:HB1	4:I:932:ALA:HA	1.92	0.51
4:I:1227:ALA:HB1	4:I:1247:ILE:HG23	1.91	0.51
4:I:1337:ASP:N	4:I:1337:ASP:OD1	2.44	0.51
5:L:24:LEU:HD22	5:L:278:ALA:HB1	1.92	0.51
5:L:188:ASN:HB3	5:L:191:GLU:HB2	1.91	0.51
5:L:412:SER:OG	5:L:413:VAL:N	2.42	0.51
2:E:134:LEU:HD13	2:E:140:MET:HB3	1.92	0.51
3:G:469:ASN:HB2	3:G:474:TYR:CE2	2.45	0.51
3:G:1237:GLN:HE22	3:G:1325:ASP:H	1.59	0.51
4:I:1139:HIS:HD2	4:I:1167:LEU:HD22	1.74	0.51
5:L:512:SER:HB2	5:L:531:LEU:HB3	1.92	0.51
5:L:525:PRO:HG2	5:L:564:ARG:HG3	1.92	0.51
5:L:780:THR:HB	5:L:799:LEU:CD1	2.40	0.51
2:E:319:TYR:HE1	2:E:355:ARG:HD2	1.75	0.51
2:E:337:VAL:HG13	2:E:356:PHE:HE1	1.75	0.51
3:G:874:CYS:HB3	5:L:842:ARG:NH1	2.26	0.51
3:G:1296:PRO:HG2	3:G:1338:ARG:HE	1.76	0.51
4:I:400:GLU:OE1	4:I:436:ARG:NH2	2.44	0.51
4:I:622:THR:O	4:I:629:GLY:N	2.44	0.51
4:I:795:MET:SD	4:I:796:LEU:HG	2.50	0.51
4:I:1112:MET:O	4:I:1114:GLN:NE2	2.43	0.51
4:I:1123:LEU:HB2	4:I:1160:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:964:ALA:O	5:L:967:LEU:N	2.42	0.51
1:C:288:TRP:CD1	1:C:309:GLY:HA2	2.45	0.51
1:C:608:MET:HB3	1:C:620:VAL:O	2.11	0.51
1:C:971:LYS:O	1:C:975:LEU:N	2.37	0.51
2:E:1173:LYS:HD3	2:E:1178:ILE:HD11	1.93	0.51
4:I:248:MET:SD	4:I:249:LYS:N	2.84	0.51
4:I:452:GLN:HB2	4:I:495:LEU:HD21	1.92	0.51
5:L:535:VAL:HG13	5:L:543:ILE:HG23	1.93	0.51
2:E:844:GLY:HA2	2:E:847:LEU:HD12	1.92	0.51
4:I:15:GLY:HA3	4:I:33:SER:HB3	1.91	0.51
4:I:576:ASP:HA	4:I:623:VAL:HG13	1.93	0.51
4:I:1108:LEU:O	4:I:1111:ALA:HB3	2.10	0.51
5:L:309:GLN:OE1	5:L:325:ARG:NH1	2.42	0.51
5:L:454:HIS:CE1	5:L:474:ASP:HB3	2.45	0.51
1:C:70:LEU:HD11	1:C:108:TRP:HB2	1.91	0.51
1:C:841:LEU:HD22	1:C:847:LEU:HD13	1.92	0.51
2:E:1252:TYR:HB3	2:E:1279:ILE:HG23	1.92	0.51
3:G:621:PHE:HB3	3:G:625:ASN:HB2	1.93	0.51
3:G:1274:VAL:HG22	3:G:1317:LEU:HB3	1.92	0.51
4:I:415:VAL:O	4:I:422:ALA:N	2.33	0.51
5:L:682:PHE:CD1	5:L:691:ARG:HB2	2.45	0.51
5:L:799:LEU:HD12	5:L:802:ALA:CB	2.38	0.51
1:C:198:TYR:HA	1:C:201:GLU:HB2	1.93	0.51
2:E:904:GLN:HG3	2:E:936:ILE:HG23	1.93	0.51
3:G:216:LEU:HB3	3:G:224:LEU:HD11	1.93	0.51
3:G:265:LEU:O	3:G:278:TYR:N	2.42	0.51
3:G:724:PHE:HZ	3:G:758:ARG:HB2	1.76	0.51
3:G:925:TYR:O	3:G:929:GLY:N	2.44	0.51
3:G:1237:GLN:HG2	3:G:1322:ARG:HB2	1.93	0.51
4:I:1044:ALA:HA	4:I:1047:TRP:HB2	1.93	0.51
5:L:247:LEU:HG	5:L:255:LEU:HD12	1.93	0.51
1:C:825:PHE:HB3	1:C:830:ASP:HB2	1.92	0.51
1:C:1100:ASP:OD1	1:C:1100:ASP:N	2.44	0.51
2:E:192:GLY:HA2	2:E:195:LYS:HE3	1.93	0.51
2:E:709:ALA:O	2:E:714:ASP:N	2.44	0.51
3:G:751:ASN:HD21	3:G:774:HIS:CE1	2.29	0.51
3:G:1281:VAL:O	3:G:1285:PHE:N	2.41	0.51
4:I:573:VAL:HG22	4:I:585:ILE:HG12	1.93	0.51
4:I:773:ALA:O	4:I:777:ALA:HB2	2.11	0.51
4:I:833:ALA:HB1	4:I:860:LEU:HD13	1.93	0.51
5:L:675:ALA:O	5:L:679:ALA:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LYS:HA	1:C:402:HIS:HA	1.92	0.50
1:C:507:SER:HA	1:C:523:LEU:HB2	1.93	0.50
2:E:458:GLU:HA	2:E:461:ILE:HG12	1.92	0.50
2:E:1035:HIS:O	2:E:1039:LEU:N	2.36	0.50
3:G:104:ASN:HB3	3:G:122:ASP:HB2	1.92	0.50
3:G:484:VAL:HA	3:G:490:VAL:HA	1.93	0.50
3:G:1052:LEU:HB3	3:G:1055:VAL:HB	1.94	0.50
4:I:265:GLY:HA2	4:I:290:LEU:HB2	1.92	0.50
4:I:374:VAL:HG11	4:I:621:LEU:HD13	1.93	0.50
4:I:455:VAL:N	4:I:462:VAL:O	2.43	0.50
5:L:665:MET:SD	5:L:669:LEU:HD12	2.51	0.50
5:L:933:LEU:HA	5:L:955:LEU:HD21	1.94	0.50
1:C:596:ASN:HB3	1:C:599:LEU:HD12	1.93	0.50
2:E:596:PHE:HZ	2:E:623:ARG:HH12	1.59	0.50
3:G:577:ARG:HA	3:G:592:ASP:HA	1.93	0.50
3:G:659:ILE:O	3:G:661:THR:N	2.44	0.50
4:I:87:THR:HG21	4:I:108:THR:HA	1.93	0.50
4:I:164:MET:N	4:I:176:THR:O	2.44	0.50
4:I:259:LEU:HD21	4:I:302:VAL:HG13	1.93	0.50
5:L:871:ALA:HA	5:L:892:ARG:HH21	1.75	0.50
1:C:115:ASN:OD1	1:C:117:ASN:ND2	2.39	0.50
1:C:801:ASP:HB3	5:L:580:LEU:HD23	1.93	0.50
1:C:906:LEU:HG	1:C:925:LEU:HD13	1.93	0.50
2:E:113:LEU:O	2:E:117:TYR:N	2.33	0.50
2:E:655:LEU:HB3	2:E:692:PHE:HD1	1.75	0.50
2:E:874:THR:HG23	2:E:878:GLN:HE22	1.76	0.50
2:E:1009:ALA:HB1	2:E:1021:ALA:HA	1.94	0.50
3:G:176:ALA:HB3	3:G:183:VAL:HB	1.93	0.50
3:G:643:ILE:HG12	3:G:653:LEU:HA	1.93	0.50
3:G:805:GLU:HA	3:G:808:LYS:HE3	1.92	0.50
3:G:1039:LYS:HG3	3:G:1042:LYS:HB2	1.94	0.50
3:G:1200:LEU:HA	3:G:1203:LEU:HG	1.91	0.50
3:G:1296:PRO:HB2	3:G:1338:ARG:HH21	1.77	0.50
4:I:338:VAL:HG23	4:I:349:VAL:HG22	1.93	0.50
4:I:623:VAL:HA	4:I:628:VAL:HA	1.91	0.50
4:I:663:PHE:HE1	4:I:691:LEU:HD23	1.76	0.50
1:C:207:SER:OG	1:C:234:ASP:OD1	2.29	0.50
3:G:710:MET:HA	3:G:717:THR:HG21	1.93	0.50
3:G:1330:MET:HA	3:G:1333:TYR:CZ	2.46	0.50
4:I:510:SER:HA	4:I:522:GLU:HG2	1.93	0.50
5:L:558:GLN:O	5:L:562:MET:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:772:GLU:O	5:L:776:LYS:N	2.44	0.50
3:G:286:TYR:OH	3:G:343:TRP:NE1	2.45	0.50
3:G:306:ASP:O	3:G:310:ASN:N	2.42	0.50
3:G:434:LEU:O	3:G:445:TYR:N	2.38	0.50
4:I:198:VAL:HG12	4:I:211:GLU:HB3	1.93	0.50
4:I:978:PHE:O	4:I:982:SER:N	2.43	0.50
5:L:632:GLU:HG2	5:L:635:LEU:HD12	1.93	0.50
5:L:637:ALA:O	5:L:641:ALA:HB2	2.12	0.50
5:L:748:LYS:HG2	5:L:754:LEU:HD11	1.93	0.50
5:L:828:ARG:HE	5:L:840:ALA:HB1	1.75	0.50
1:C:347:THR:HA	1:C:366:ASP:HA	1.94	0.50
1:C:543:LEU:HB3	1:C:547:LEU:HG	1.93	0.50
1:C:774:VAL:HG12	1:C:792:HIS:HE1	1.76	0.50
2:E:40:PHE:CE2	2:E:71:ALA:HB1	2.47	0.50
2:E:339:ALA:HA	2:E:342:GLN:HG3	1.94	0.50
2:E:580:LYS:HD2	2:E:583:LEU:HD12	1.94	0.50
2:E:965:ASP:OD1	2:E:965:ASP:N	2.42	0.50
3:G:88:TRP:HZ2	3:G:93:ARG:HD3	1.76	0.50
3:G:184:VAL:HB	3:G:197:VAL:HG12	1.93	0.50
1:C:598:GLU:HB3	1:C:613:GLY:HA2	1.92	0.50
2:E:310:SER:HA	2:E:532:GLU:HB3	1.94	0.50
3:G:206:LEU:HD12	3:G:217:VAL:HG22	1.94	0.50
3:G:834:LEU:HB3	3:G:849:HIS:CE1	2.46	0.50
3:G:1234:ALA:HA	3:G:1278:ARG:HH12	1.75	0.50
4:I:295:TYR:HD1	4:I:302:VAL:HG22	1.77	0.50
5:L:784:ILE:HG12	5:L:810:VAL:HA	1.94	0.50
5:L:883:ALA:O	5:L:887:ARG:N	2.27	0.50
5:L:949:VAL:HG22	5:L:978:LEU:HB3	1.94	0.50
1:C:258:PRO:HA	1:C:274:GLY:HA3	1.92	0.50
1:C:687:PRO:HB3	1:C:690:TRP:CD1	2.47	0.50
2:E:266:LEU:HD13	2:E:314:LEU:HA	1.93	0.50
4:I:936:TYR:O	4:I:941:ASP:N	2.43	0.50
5:L:480:LEU:HG	5:L:492:GLU:HG3	1.92	0.50
1:C:739:ALA:HA	1:C:744:ARG:HE	1.77	0.50
1:C:837:LEU:HD23	1:C:840:ALA:HB3	1.93	0.50
2:E:1148:LEU:HB3	2:E:1149:LYS:HZ2	1.77	0.50
3:G:589:HIS:HB3	3:G:651:ILE:HD12	1.94	0.50
4:I:375:LEU:HD13	4:I:408:LEU:HD13	1.93	0.50
1:C:685:SER:OG	1:C:686:HIS:N	2.44	0.49
2:E:925:ALA:HA	2:E:928:LEU:HB3	1.94	0.49
3:G:379:ARG:HH22	3:G:423:GLN:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:842:ARG:HD3	5:L:822:ASP:HB2	1.93	0.49
3:G:980:TYR:HB3	3:G:985:ARG:HB2	1.93	0.49
3:G:1011:PRO:HA	3:G:1014:MET:CB	2.41	0.49
3:G:1017:THR:HB	3:G:1033:LEU:CD1	2.42	0.49
4:I:525:HIS:CE1	4:I:527:ASP:HB2	2.47	0.49
4:I:547:ASP:OD1	4:I:547:ASP:N	2.45	0.49
4:I:790:LYS:HD3	4:I:831:CYS:SG	2.52	0.49
5:L:436:GLY:HA2	5:L:458:VAL:HG23	1.93	0.49
5:L:507:ASP:HB3	5:L:522:GLY:HA2	1.94	0.49
1:C:432:HIS:HB3	1:C:443:VAL:HG13	1.93	0.49
1:C:795:ILE:HA	1:C:798:TYR:HB3	1.93	0.49
2:E:387:ALA:HB2	2:E:443:LEU:HD11	1.93	0.49
2:E:938:PHE:HZ	2:E:970:SER:HA	1.77	0.49
2:E:1295:ASN:HA	2:E:1298:LYS:HD2	1.94	0.49
5:L:3:THR:HG21	5:L:258:ILE:HA	1.94	0.49
1:C:313:ILE:HB	1:C:322:LEU:HD11	1.93	0.49
1:C:592:TRP:CE3	1:C:600:PHE:HB3	2.47	0.49
2:E:19:ARG:HH12	2:E:289:GLN:HB3	1.77	0.49
2:E:703:VAL:HA	2:E:706:CYS:HB2	1.93	0.49
2:E:1086:ILE:HG22	2:E:1086:ILE:O	2.12	0.49
3:G:935:VAL:O	3:G:940:PHE:N	2.46	0.49
3:G:1053:PHE:HA	3:G:1056:LEU:HB3	1.94	0.49
4:I:772:ASP:HA	4:I:775:LYS:HB2	1.94	0.49
4:I:845:LEU:O	4:I:849:ARG:HB2	2.12	0.49
4:I:1125:MET:SD	4:I:1141:LYS:NZ	2.77	0.49
1:C:421:VAL:HA	1:C:437:ASN:HD21	1.78	0.49
1:C:882:VAL:HG11	1:C:901:GLN:HG2	1.94	0.49
2:E:557:ILE:HA	2:E:560:MET:HG3	1.94	0.49
2:E:564:GLU:HG3	2:E:567:ALA:H	1.78	0.49
3:G:543:PRO:HD2	3:G:546:LEU:HB2	1.94	0.49
3:G:712:ASP:O	3:G:776:ARG:NE	2.38	0.49
3:G:811:TYR:CE2	3:G:823:LEU:HD12	2.47	0.49
3:G:927:LYS:HE2	5:L:856:ARG:HG2	1.94	0.49
3:G:1225:TRP:HD1	3:G:1263:SER:HA	1.77	0.49
4:I:413:ALA:O	4:I:424:TYR:N	2.42	0.49
4:I:879:GLU:OE1	4:I:883:ARG:NH1	2.45	0.49
5:L:23:ASP:HB3	5:L:65:VAL:HG22	1.93	0.49
1:C:182:CYS:HB3	1:C:195:VAL:HB	1.94	0.49
1:C:402:HIS:N	1:C:419:ILE:O	2.41	0.49
1:C:441:VAL:HG21	1:C:511:ILE:HD13	1.93	0.49
1:C:724:HIS:O	1:C:728:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:349:THR:O	2:E:350:THR:C	2.51	0.49
2:E:1012:MET:O	2:E:1017:HIS:ND1	2.45	0.49
3:G:270:GLU:HG2	3:G:301:VAL:HA	1.93	0.49
3:G:483:VAL:O	3:G:491:LYS:N	2.45	0.49
3:G:842:ARG:HB3	5:L:822:ASP:HB2	1.94	0.49
4:I:7:VAL:H	4:I:356:MET:HB3	1.76	0.49
4:I:170:ASP:OD1	4:I:170:ASP:N	2.43	0.49
5:L:114:LEU:O	5:L:125:TRP:N	2.38	0.49
5:L:270:PRO:HA	5:L:277:VAL:HA	1.93	0.49
1:C:604:GLU:HG2	1:C:605:LYS:HD3	1.95	0.49
1:C:843:ASP:N	1:C:843:ASP:OD1	2.42	0.49
3:G:429:LEU:HA	3:G:434:LEU:HA	1.94	0.49
3:G:675:LEU:O	3:G:702:ALA:N	2.36	0.49
3:G:1056:LEU:HD12	3:G:1059:ILE:HB	1.93	0.49
4:I:880:MET:HA	4:I:883:ARG:HG2	1.93	0.49
5:L:126:SER:H	5:L:129:GLN:NE2	2.11	0.49
5:L:389:LEU:HB2	5:L:396:GLN:HB2	1.94	0.49
1:C:352:PHE:HE1	1:C:363:MET:HB2	1.77	0.49
1:C:518:VAL:O	1:C:532:HIS:N	2.46	0.49
1:C:548:SER:OG	1:C:549:LYS:N	2.45	0.49
1:C:668:LEU:HD11	1:C:680:PHE:HB3	1.95	0.49
2:E:47:LEU:HG	2:E:52:THR:HA	1.95	0.49
2:E:1087:ASN:O	2:E:1301:ASN:ND2	2.42	0.49
3:G:117:ARG:HA	3:G:131:LYS:HA	1.95	0.49
3:G:277:MET:HB2	3:G:286:TYR:CZ	2.48	0.49
3:G:279:ASN:HB3	3:G:284:ASP:HB2	1.94	0.49
3:G:403:LEU:HD13	3:G:453:ILE:HG12	1.94	0.49
3:G:516:VAL:HG13	3:G:520:ASN:HA	1.94	0.49
4:I:754:SER:OG	4:I:756:VAL:O	2.31	0.49
5:L:845:GLU:HA	5:L:848:CYS:HB2	1.94	0.49
1:C:292:PHE:HE2	1:C:303:LEU:HB2	1.78	0.49
1:C:654:MET:N	1:C:654:MET:SD	2.85	0.49
1:C:1033:TRP:HZ2	1:C:1066:GLU:HG3	1.77	0.49
2:E:491:VAL:HG22	2:E:516:VAL:HG13	1.95	0.49
2:E:538:ALA:CB	2:E:570:LEU:HD21	2.43	0.49
3:G:119:ILE:HG13	3:G:129:MET:HG3	1.95	0.49
3:G:425:LEU:HD12	3:G:464:ARG:HB3	1.94	0.49
3:G:513:LEU:HB3	3:G:525:LEU:HB2	1.93	0.49
3:G:523:ARG:HE	3:G:525:LEU:HD11	1.76	0.49
3:G:1191:ASP:N	3:G:1191:ASP:OD1	2.45	0.49
4:I:676:VAL:HG22	4:I:691:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:874:LEU:HD11	4:I:893:ILE:HG21	1.93	0.49
4:I:933:ALA:HB2	4:I:948:LEU:HD12	1.94	0.49
5:L:37:ILE:HB	5:L:42:LEU:HD12	1.95	0.49
5:L:50:ASP:OD1	5:L:50:ASP:N	2.46	0.49
5:L:338:TYR:OH	5:L:427:GLU:OE2	2.29	0.49
5:L:980:LEU:HG	5:L:996:ARG:HH12	1.77	0.49
2:E:19:ARG:HE	2:E:253:GLN:HB2	1.77	0.49
2:E:65:ASN:HB3	2:E:68:LEU:HG	1.95	0.49
2:E:1202:MET:HB3	2:E:1218:GLN:HG3	1.93	0.49
5:L:800:LEU:HB3	5:L:814:TYR:HB2	1.95	0.49
1:C:2:PHE:HA	1:C:301:ARG:HD2	1.94	0.49
1:C:1093:SER:C	1:C:1094:MET:HG3	2.33	0.49
3:G:318:ASP:OD2	3:G:320:ARG:NH2	2.45	0.49
4:I:678:CYS:O	4:I:681:GLN:NE2	2.45	0.49
5:L:328:CYS:HB3	5:L:346:LEU:HD11	1.93	0.49
5:L:375:LEU:HD11	5:L:389:LEU:HD11	1.95	0.49
5:L:796:ALA:O	5:L:800:LEU:HD23	2.13	0.49
2:E:538:ALA:HA	2:E:541:LEU:HD12	1.94	0.48
2:E:599:ARG:HA	2:E:604:TYR:HD2	1.78	0.48
2:E:810:ALA:HA	2:E:813:THR:HG22	1.95	0.48
2:E:878:GLN:HG2	2:E:918:LEU:HD22	1.96	0.48
3:G:1142:ALA:HB2	3:G:1157:LYS:HB2	1.95	0.48
4:I:229:THR:OG1	4:I:230:ALA:N	2.46	0.48
4:I:452:GLN:HA	4:I:465:PRO:HA	1.95	0.48
4:I:546:ASP:HB3	4:I:552:HIS:CD2	2.48	0.48
4:I:986:GLY:HA2	4:I:989:VAL:HG12	1.95	0.48
4:I:1279:GLU:OE2	4:I:1298:ARG:NH2	2.43	0.48
5:L:987:GLU:HG2	5:L:988:VAL:HG23	1.94	0.48
2:E:943:GLN:O	2:E:947:ALA:N	2.45	0.48
3:G:20:SER:HB2	3:G:27:SER:HA	1.93	0.48
3:G:37:ALA:HB2	3:G:57:LYS:HG3	1.94	0.48
3:G:324:TYR:HB3	3:G:343:TRP:CE3	2.49	0.48
3:G:1289:ARG:NH2	3:G:1332:GLU:OE2	2.36	0.48
4:I:924:GLU:HG3	4:I:929:TRP:CD2	2.48	0.48
4:I:1023:LYS:HG3	4:I:1026:ASP:H	1.78	0.48
4:I:1268:CYS:HB3	4:I:1273:MET:H	1.78	0.48
5:L:473:VAL:HG23	5:L:499:VAL:HG12	1.95	0.48
5:L:980:LEU:HB2	5:L:988:VAL:HG21	1.95	0.48
1:C:88:LYS:HG2	1:C:102:MET:HE1	1.95	0.48
2:E:1290:ALA:HB2	2:E:1314:ASN:HB2	1.95	0.48
3:G:217:VAL:O	3:G:225:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1068:SER:OG	3:G:1069:ASP:N	2.46	0.48
4:I:393:THR:OG1	4:I:396:ARG:NH2	2.46	0.48
4:I:646:LYS:HA	4:I:649:GLN:HG2	1.95	0.48
1:C:432:HIS:CE1	1:C:523:LEU:HD13	2.48	0.48
1:C:538:PRO:HB3	1:C:552:ILE:HG23	1.95	0.48
2:E:17:TYR:HH	2:E:256:MET:H	1.62	0.48
2:E:1219:LEU:HD21	2:E:1241:LEU:HD23	1.96	0.48
3:G:33:LEU:HD12	3:G:37:ALA:HB3	1.96	0.48
3:G:415:GLY:HA2	3:G:451:ASN:HB3	1.96	0.48
3:G:752:MET:HG3	3:G:768:CYS:HB2	1.95	0.48
4:I:730:ASN:ND2	4:I:750:LEU:O	2.40	0.48
4:I:764:ARG:NE	4:I:772:ASP:HB2	2.28	0.48
4:I:813:LEU:CD2	4:I:831:CYS:HB2	2.43	0.48
5:L:744:ARG:HE	5:L:776:LYS:NZ	2.11	0.48
5:L:910:HIS:HA	5:L:950:ASN:HB2	1.95	0.48
1:C:391:VAL:HG21	1:C:433:VAL:HG11	1.95	0.48
2:E:736:ARG:NH1	2:E:759:ASP:HB3	2.27	0.48
2:E:737:MET:HB3	2:E:772:MET:SD	2.53	0.48
3:G:896:ILE:HG13	3:G:904:LEU:HB2	1.95	0.48
4:I:159:ASN:HB3	4:I:198:VAL:HG11	1.95	0.48
4:I:292:ASP:OD2	4:I:337:LYS:HG3	2.14	0.48
4:I:364:PRO:HG2	4:I:377:LEU:HD22	1.96	0.48
5:L:662:ALA:HB1	5:L:666:PHE:CE2	2.49	0.48
5:L:725:ARG:NH1	5:L:729:ILE:HG13	2.29	0.48
1:C:544:ASN:ND2	1:C:597:PRO:O	2.38	0.48
1:C:939:LEU:HD13	1:C:962:LEU:HB3	1.95	0.48
1:C:947:ALA:HB1	1:C:1062:LEU:HD23	1.94	0.48
2:E:823:TYR:O	2:E:827:ALA:N	2.42	0.48
3:G:908:TRP:O	3:G:920:LYS:HE2	2.13	0.48
3:G:990:VAL:HG21	3:G:1013:VAL:HB	1.96	0.48
3:G:1125:LYS:O	3:G:1157:LYS:NZ	2.46	0.48
4:I:267:VAL:HG21	4:I:313:LEU:HD11	1.95	0.48
4:I:794:ALA:C	4:I:796:LEU:H	2.17	0.48
4:I:923:LYS:O	4:I:928:ARG:N	2.46	0.48
5:L:518:SER:HB3	5:L:526:LEU:HD21	1.95	0.48
5:L:908:VAL:HG22	5:L:919:THR:H	1.78	0.48
1:C:442:TYR:HB2	1:C:470:MET:HG2	1.95	0.48
2:E:236:ASP:N	2:E:236:ASP:OD1	2.46	0.48
3:G:31:VAL:O	3:G:39:GLY:N	2.33	0.48
3:G:70:HIS:N	3:G:75:LEU:O	2.45	0.48
3:G:120:THR:OG1	3:G:128:SER:O	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:324:TYR:HB3	3:G:343:TRP:HE3	1.77	0.48
3:G:336:VAL:HG22	3:G:338:ASP:H	1.78	0.48
3:G:591:HIS:NE2	3:G:596:GLU:OE1	2.47	0.48
3:G:769:LEU:HD22	3:G:774:HIS:HB3	1.95	0.48
3:G:939:CYS:HB3	3:G:963:LEU:HD13	1.95	0.48
5:L:388:ILE:HG21	5:L:429:LEU:HD11	1.96	0.48
1:C:104:HIS:N	1:C:107:MET:O	2.47	0.48
3:G:80:TRP:HB2	3:G:84:ALA:HB3	1.95	0.48
3:G:598:ARG:HH21	3:G:637:VAL:HG13	1.79	0.48
3:G:942:ARG:NH2	3:G:967:TYR:OH	2.46	0.48
4:I:582:VAL:HA	4:I:595:LEU:HA	1.96	0.48
4:I:860:LEU:HA	4:I:863:GLU:HB3	1.96	0.48
5:L:110:VAL:HG23	5:L:150:GLY:HA3	1.96	0.48
5:L:672:PHE:HA	5:L:675:ALA:HB3	1.95	0.48
1:C:310:ILE:HD13	1:C:324:LEU:HD23	1.95	0.48
2:E:12:TYR:OH	2:E:254:ASN:ND2	2.46	0.48
2:E:884:TRP:HD1	2:E:907:ALA:HB2	1.78	0.48
3:G:828:GLY:HA3	4:I:711:ILE:HD12	1.94	0.48
4:I:1109:ASN:ND2	4:I:1121:ASP:OD2	2.47	0.48
5:L:304:TYR:HB2	5:L:318:LEU:HD11	1.96	0.48
1:C:731:LYS:HD3	1:C:731:LYS:HA	1.72	0.48
1:C:778:ILE:HG12	1:C:785:ASP:HA	1.96	0.48
2:E:251:ASP:OD1	2:E:251:ASP:N	2.46	0.48
2:E:1004:ALA:O	2:E:1008:LEU:HB2	2.14	0.48
3:G:31:VAL:HG22	3:G:375:ILE:HG21	1.96	0.48
3:G:60:ARG:HD3	3:G:84:ALA:HB2	1.96	0.48
3:G:545:GLU:HG2	3:G:546:LEU:HG	1.95	0.48
3:G:1138:ILE:HG22	3:G:1157:LYS:HB3	1.96	0.48
4:I:157:ALA:H	4:I:196:LEU:HD23	1.79	0.48
4:I:373:ARG:HB3	4:I:385:LEU:HD11	1.96	0.48
4:I:412:HIS:CD2	4:I:434:VAL:HG21	2.48	0.48
4:I:764:ARG:HE	4:I:772:ASP:HB2	1.78	0.48
4:I:1142:LEU:HD22	4:I:1160:LEU:HG	1.95	0.48
5:L:600:LEU:HB3	5:L:619:VAL:HG13	1.96	0.48
1:C:639:LEU:O	1:C:643:MET:N	2.45	0.47
1:C:1071:LEU:O	1:C:1075:ALA:HB3	2.14	0.47
2:E:547:LEU:HB3	2:E:574:VAL:HG13	1.96	0.47
2:E:635:ARG:O	2:E:658:ARG:NH2	2.46	0.47
2:E:919:ARG:HH21	2:E:929:GLN:HB2	1.79	0.47
2:E:1006:ILE:HD13	2:E:1024:HIS:HB3	1.96	0.47
3:G:578:LEU:HD23	3:G:651:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:790:ALA:H	3:G:794:VAL:HG23	1.78	0.47
3:G:1053:PHE:O	3:G:1057:GLN:N	2.46	0.47
3:G:1072:LEU:HA	3:G:1075:LYS:HE3	1.96	0.47
4:I:437:ARG:NH1	4:I:478:ASP:OD1	2.35	0.47
4:I:450:GLU:HG2	4:I:451:THR:HG23	1.95	0.47
4:I:846:ARG:NH1	4:I:876:GLU:OE2	2.47	0.47
5:L:85:ILE:HG21	5:L:125:TRP:CH2	2.49	0.47
5:L:236:ILE:N	5:L:248:TYR:O	2.45	0.47
5:L:724:ASP:N	5:L:724:ASP:OD1	2.45	0.47
1:C:143:ILE:HG23	1:C:151:ARG:HG3	1.96	0.47
1:C:805:TRP:CE3	1:C:824:CYS:HA	2.49	0.47
1:C:1021:ASP:N	1:C:1021:ASP:OD1	2.47	0.47
2:E:842:GLU:O	2:E:846:LEU:HG	2.14	0.47
3:G:431:LYS:HA	3:G:431:LYS:HD2	1.66	0.47
3:G:621:PHE:HB2	3:G:629:ARG:HH21	1.78	0.47
3:G:751:ASN:HD22	3:G:769:LEU:HD21	1.79	0.47
4:I:175:LEU:HD12	4:I:185:LYS:HB2	1.95	0.47
5:L:523:ASP:N	5:L:523:ASP:OD1	2.46	0.47
1:C:30:ALA:HA	1:C:40:VAL:HA	1.96	0.47
2:E:565:SER:OG	2:E:595:ASN:OD1	2.25	0.47
2:E:968:VAL:HG22	2:E:994:LEU:HD11	1.94	0.47
3:G:403:LEU:HD22	3:G:447:VAL:HG11	1.96	0.47
4:I:494:ALA:HB2	4:I:533:LEU:HB3	1.97	0.47
4:I:648:LEU:HD21	4:I:665:ALA:HB3	1.96	0.47
4:I:676:VAL:O	4:I:680:LYS:HG2	2.13	0.47
5:L:587:TRP:HA	5:L:590:LEU:CD1	2.40	0.47
1:C:254:THR:HB	1:C:291:GLN:HE22	1.80	0.47
2:E:44:TYR:HB2	2:E:116:PHE:HD1	1.79	0.47
4:I:208:ARG:H	4:I:229:THR:HB	1.79	0.47
4:I:290:LEU:HD21	4:I:293:VAL:HB	1.95	0.47
4:I:1189:LEU:HD13	4:I:1210:THR:HA	1.97	0.47
5:L:328:CYS:SG	5:L:353:TYR:OH	2.66	0.47
5:L:383:THR:OG1	5:L:386:HIS:N	2.44	0.47
5:L:429:LEU:N	5:L:441:ILE:O	2.42	0.47
1:C:148:ASP:OD1	1:C:148:ASP:N	2.45	0.47
1:C:532:HIS:HA	1:C:576:MET:H	1.80	0.47
1:C:651:LEU:HA	1:C:654:MET:HG2	1.94	0.47
1:C:691:ARG:HH21	1:C:710:PHE:HA	1.79	0.47
1:C:691:ARG:HH12	1:C:714:ALA:N	2.12	0.47
2:E:1259:CYS:HB3	2:E:1276:MET:HE2	1.96	0.47
2:E:1273:TRP:HZ3	2:E:1299:HIS:HD1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:275:VAL:H	3:G:288:LEU:H	1.61	0.47
3:G:484:VAL:HG12	3:G:490:VAL:HG22	1.96	0.47
3:G:949:ASP:HB2	3:G:957:ASN:HA	1.97	0.47
3:G:1232:TYR:HD2	3:G:1256:ALA:HA	1.79	0.47
4:I:913:SER:O	4:I:917:LEU:HB3	2.15	0.47
5:L:647:GLN:HE22	5:L:678:TRP:HD1	1.60	0.47
1:C:432:HIS:CD2	1:C:523:LEU:HD22	2.49	0.47
1:C:681:VAL:HG11	1:C:690:TRP:CG	2.50	0.47
1:C:804:LYS:HD3	1:C:804:LYS:HA	1.71	0.47
2:E:263:MET:HB3	2:E:476:LEU:HD11	1.96	0.47
2:E:638:LEU:HG	2:E:653:PRO:HD3	1.95	0.47
2:E:685:ILE:HG13	2:E:708:LEU:HD22	1.96	0.47
2:E:994:LEU:HD21	2:E:1001:ASN:HD22	1.79	0.47
3:G:1128:ALA:HB1	3:G:1134:ARG:HG2	1.96	0.47
3:G:1200:LEU:HD22	3:G:1203:LEU:HD11	1.97	0.47
4:I:203:GLU:OE2	4:I:227:GLN:NE2	2.48	0.47
4:I:792:HIS:HA	4:I:795:MET:HG3	1.96	0.47
4:I:881:TYR:O	4:I:886:GLN:N	2.44	0.47
5:L:807:ARG:HH22	5:L:876:LYS:HE2	1.80	0.47
1:C:37:LEU:HD21	1:C:39:LYS:HE2	1.96	0.47
1:C:56:GLU:HA	1:C:621:THR:H	1.79	0.47
1:C:716:TYR:HE2	5:L:665:MET:HG3	1.80	0.47
1:C:1097:ILE:HG23	1:C:1101:LYS:HE2	1.96	0.47
2:E:495:LEU:HG	2:E:543:LEU:HD12	1.96	0.47
2:E:974:VAL:O	2:E:978:HIS:ND1	2.48	0.47
2:E:1110:ILE:O	2:E:1114:VAL:HG22	2.14	0.47
2:E:1128:GLU:HB2	2:E:1247:ILE:HG22	1.97	0.47
2:E:1247:ILE:HD13	2:E:1252:TYR:HA	1.96	0.47
2:E:1322:VAL:HG22	2:E:1353:LEU:H	1.79	0.47
3:G:19:TRP:CZ3	3:G:29:LEU:HB2	2.50	0.47
3:G:526:LYS:HB2	3:G:535:HIS:HB2	1.96	0.47
3:G:902:ARG:HH11	5:L:916:PRO:HD3	1.78	0.47
3:G:974:PRO:HA	3:G:977:ILE:HG12	1.97	0.47
3:G:1164:LYS:O	3:G:1166:LYS:N	2.48	0.47
4:I:513:LEU:HB2	4:I:520:VAL:HG22	1.96	0.47
4:I:851:LEU:HA	4:I:854:GLN:HG2	1.96	0.47
4:I:1127:ARG:HA	4:I:1130:GLN:HB2	1.95	0.47
4:I:1306:GLU:OE2	4:I:1311:LYS:NZ	2.44	0.47
5:L:21:CYS:HA	5:L:37:ILE:HG12	1.97	0.47
5:L:230:PHE:N	5:L:235:TYR:O	2.47	0.47
5:L:793:TRP:HB2	5:L:814:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:933:LEU:HB3	5:L:967:LEU:HD11	1.96	0.47
1:C:688:ARG:NH1	1:C:692:ASN:OD1	2.47	0.47
3:G:218:VAL:HG21	3:G:257:VAL:HG21	1.97	0.47
3:G:315:GLY:HA2	3:G:321:VAL:HG22	1.97	0.47
3:G:720:ALA:HB1	3:G:752:MET:O	2.14	0.47
3:G:977:ILE:HA	3:G:980:TYR:CD2	2.49	0.47
3:G:988:HIS:O	3:G:993:ALA:N	2.48	0.47
4:I:28:LEU:O	4:I:40:PHE:N	2.43	0.47
4:I:500:VAL:HB	4:I:512:TYR:HD2	1.79	0.47
4:I:761:LEU:HB2	4:I:776:LEU:HD22	1.97	0.47
4:I:786:ALA:HB1	4:I:816:LEU:HG	1.96	0.47
4:I:1282:CYS:O	4:I:1286:GLN:N	2.48	0.47
5:L:350:VAL:HG11	5:L:387:VAL:HG11	1.97	0.47
5:L:622:THR:HG21	5:L:639:ILE:HG13	1.97	0.47
5:L:659:VAL:HG21	5:L:687:ARG:HG3	1.96	0.47
5:L:862:PHE:HA	5:L:865:TYR:HB3	1.97	0.47
5:L:934:MET:O	5:L:940:ARG:NH1	2.48	0.47
1:C:240:LEU:HD21	1:C:270:LEU:HD22	1.97	0.47
1:C:384:GLN:HG2	1:C:427:ALA:HA	1.97	0.47
1:C:941:ASP:HA	1:C:944:LYS:HE2	1.97	0.47
2:E:588:LEU:HD21	2:E:608:GLN:HG3	1.97	0.47
2:E:1023:TYR:O	2:E:1026:GLN:HG3	2.14	0.47
3:G:520:ASN:O	3:G:541:LEU:N	2.40	0.47
3:G:808:LYS:HA	3:G:811:TYR:CD2	2.50	0.47
4:I:731:LEU:HD12	4:I:751:PHE:CE1	2.50	0.47
4:I:797:GLU:OE2	4:I:834:GLY:HA2	2.15	0.47
1:C:18:ARG:N	1:C:32:GLY:O	2.48	0.47
1:C:263:TRP:HZ3	1:C:295:HIS:HA	1.79	0.47
3:G:968:GLU:HG3	3:G:973:ILE:HG12	1.97	0.47
3:G:1146:LYS:HG3	3:G:1171:LEU:HG	1.96	0.47
3:G:1158:TYR:HA	3:G:1162:GLY:HA3	1.97	0.47
3:G:1289:ARG:NH2	3:G:1292:ILE:HG21	2.30	0.47
4:I:248:MET:HE1	4:I:292:ASP:HA	1.95	0.47
4:I:437:ARG:HH11	4:I:464:HIS:CE1	2.32	0.47
5:L:875:ILE:HD12	5:L:889:ALA:HB1	1.96	0.47
2:E:18:PHE:O	2:E:22:GLN:NE2	2.48	0.46
2:E:500:GLY:O	2:E:542:TYR:OH	2.31	0.46
2:E:588:LEU:HD11	2:E:608:GLN:HG3	1.97	0.46
2:E:1123:ASP:H	2:E:1237:ARG:HD2	1.80	0.46
3:G:275:VAL:HG22	3:G:300:VAL:HG21	1.97	0.46
3:G:520:ASN:OD1	3:G:547:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:863:GLU:HA	3:G:866:ARG:HE	1.80	0.46
3:G:1272:VAL:HA	3:G:1275:ILE:HB	1.96	0.46
4:I:23:PRO:HG3	4:I:74:PRO:HA	1.97	0.46
4:I:413:ALA:N	4:I:424:TYR:O	2.49	0.46
4:I:465:PRO:HD2	4:I:477:LEU:HG	1.96	0.46
4:I:802:TYR:O	4:I:806:LYS:HB2	2.15	0.46
5:L:349:LYS:HD2	5:L:370:LYS:HE2	1.96	0.46
5:L:654:THR:HG22	5:L:687:ARG:HB2	1.97	0.46
1:C:234:ASP:OD1	1:C:234:ASP:N	2.42	0.46
1:C:591:ARG:HA	1:C:591:ARG:HD2	1.71	0.46
1:C:762:ILE:O	1:C:766:MET:HB2	2.14	0.46
1:C:968:GLU:HB2	1:C:1024:TRP:HB3	1.98	0.46
2:E:1034:ASN:HD21	2:E:1075:TYR:HB2	1.79	0.46
3:G:738:ARG:HH22	4:I:863:GLU:HA	1.79	0.46
3:G:819:LEU:HD22	3:G:822:GLN:HE21	1.80	0.46
3:G:1310:ILE:HD13	3:G:1323:ILE:HD11	1.97	0.46
4:I:436:ARG:HD3	4:I:436:ARG:HA	1.72	0.46
4:I:482:PRO:HG3	4:I:490:ILE:HD12	1.97	0.46
4:I:595:LEU:N	4:I:607:GLN:O	2.47	0.46
4:I:760:ALA:O	4:I:764:ARG:HG2	2.14	0.46
4:I:840:LEU:HD23	4:I:867:ILE:HG22	1.97	0.46
4:I:868:LEU:HD13	4:I:876:GLU:HB2	1.98	0.46
4:I:1173:VAL:HG21	4:I:1189:LEU:HG	1.95	0.46
4:I:1211:VAL:HG12	4:I:1226:TYR:HB3	1.98	0.46
4:I:1273:MET:HG3	4:I:1284:SER:HB3	1.96	0.46
5:L:307:ARG:HD3	5:L:332:VAL:HB	1.96	0.46
5:L:957:LYS:HZ3	5:L:975:LEU:HD11	1.80	0.46
1:C:32:GLY:HA3	1:C:80:VAL:HG21	1.97	0.46
1:C:364:PHE:N	1:C:373:TYR:O	2.48	0.46
2:E:111:LEU:HD12	2:E:130:VAL:HG12	1.97	0.46
2:E:229:ARG:HD3	2:E:229:ARG:H	1.80	0.46
2:E:346:MET:HB2	2:E:648:ARG:HB2	1.97	0.46
3:G:209:TYR:HB3	3:G:214:GLN:HB2	1.95	0.46
3:G:503:PRO:HA	3:G:517:THR:HA	1.97	0.46
3:G:927:LYS:HZ3	5:L:917:PHE:HB2	1.80	0.46
3:G:1034:TYR:CG	3:G:1039:LYS:HB3	2.50	0.46
4:I:224:TYR:HB3	4:I:235:PRO:HB3	1.98	0.46
5:L:501:TRP:HZ3	5:L:507:ASP:HA	1.80	0.46
5:L:844:LEU:HG	5:L:863:TYR:HB3	1.97	0.46
1:C:56:GLU:HG3	1:C:620:VAL:HA	1.96	0.46
1:C:123:ASP:HB3	1:C:164:VAL:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:ILE:HG12	1:C:893:LEU:HD23	1.97	0.46
1:C:914:LEU:HD23	1:C:919:VAL:HG22	1.96	0.46
2:E:203:LEU:HD21	2:E:234:LEU:HA	1.98	0.46
3:G:229:ARG:HG3	3:G:236:TRP:CE2	2.50	0.46
3:G:712:ASP:OD1	3:G:779:ARG:NH2	2.49	0.46
3:G:738:ARG:HH21	4:I:866:LEU:HD13	1.79	0.46
3:G:749:TRP:CE3	3:G:752:MET:SD	3.09	0.46
4:I:203:GLU:HG2	4:I:273:HIS:HA	1.97	0.46
5:L:104:CYS:SG	5:L:144:ILE:HG12	2.56	0.46
5:L:378:ASN:ND2	5:L:392:GLU:OE2	2.48	0.46
5:L:410:LEU:HD12	5:L:414:ILE:HD11	1.98	0.46
1:C:20:ILE:HG13	1:C:31:CYS:HA	1.96	0.46
1:C:586:ASP:HB2	1:C:605:LYS:HD2	1.97	0.46
2:E:238:GLU:O	2:E:241:THR:OG1	2.25	0.46
2:E:492:ARG:HD3	2:E:648:ARG:HH22	1.81	0.46
2:E:1198:VAL:HG23	2:E:1199:LEU:HG	1.98	0.46
3:G:164:ASP:N	3:G:164:ASP:OD1	2.49	0.46
3:G:274:VAL:HB	3:G:287:VAL:HB	1.98	0.46
3:G:516:VAL:HG21	3:G:541:LEU:HD22	1.96	0.46
3:G:1134:ARG:HH21	3:G:1160:GLN:HG2	1.81	0.46
4:I:12:LEU:HB3	4:I:32:GLY:HA3	1.97	0.46
4:I:31:ALA:HB2	4:I:37:VAL:HG22	1.97	0.46
4:I:114:MET:HB3	4:I:125:VAL:HG13	1.97	0.46
4:I:449:ASN:ND2	4:I:450:GLU:OE1	2.48	0.46
4:I:460:HIS:HB3	4:I:480:VAL:HG13	1.98	0.46
4:I:836:ALA:O	4:I:840:LEU:HB2	2.16	0.46
4:I:1080:ARG:HA	4:I:1080:ARG:HD3	1.82	0.46
5:L:235:TYR:HB3	5:L:247:LEU:HD11	1.97	0.46
5:L:241:THR:HA	5:L:264:TRP:CD1	2.51	0.46
5:L:414:ILE:HG23	5:L:431:VAL:HG13	1.97	0.46
5:L:930:ARG:HG3	5:L:964:ALA:HB2	1.98	0.46
1:C:420:GLU:HB2	1:C:489:ARG:HH21	1.79	0.46
1:C:749:GLU:HG3	1:C:761:ALA:HB1	1.97	0.46
2:E:904:GLN:HB3	2:E:940:LEU:HD21	1.97	0.46
2:E:937:CYS:HB2	2:E:956:LEU:HD23	1.98	0.46
3:G:757:ILE:HG21	3:G:784:ALA:HA	1.97	0.46
3:G:951:VAL:HA	3:G:955:ALA:HA	1.98	0.46
3:G:1093:LEU:O	3:G:1098:GLN:N	2.39	0.46
3:G:1235:CYS:O	3:G:1239:GLU:CB	2.63	0.46
4:I:1101:ARG:HA	4:I:1104:PHE:HB2	1.96	0.46
4:I:1120:ARG:NH1	4:I:1124:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1270:PHE:HE1	4:I:1351:ILE:HA	1.79	0.46
5:L:121:ASP:HB2	5:L:134:LYS:HB3	1.97	0.46
5:L:342:LEU:O	5:L:353:TYR:N	2.40	0.46
5:L:566:LEU:HD22	5:L:589:GLN:HB3	1.98	0.46
5:L:752:ARG:O	5:L:756:MET:HG3	2.16	0.46
3:G:468:ILE:HG12	3:G:470:ASN:H	1.80	0.46
3:G:612:LEU:HB2	3:G:644:PHE:CE1	2.51	0.46
3:G:613:LEU:HG	3:G:615:VAL:HG22	1.96	0.46
3:G:717:THR:HG23	3:G:721:LEU:HD12	1.97	0.46
3:G:763:ASP:O	3:G:767:HIS:ND1	2.47	0.46
3:G:801:LEU:H	3:G:803:MET:HG3	1.81	0.46
4:I:72:TRP:CE2	4:I:79:LEU:HD13	2.51	0.46
4:I:398:GLU:OE2	4:I:429:LYS:NZ	2.48	0.46
5:L:799:LEU:CD1	5:L:802:ALA:HB2	2.41	0.46
2:E:345:MET:HG3	2:E:485:ALA:HB1	1.97	0.46
3:G:735:GLU:O	3:G:739:SER:OG	2.31	0.46
3:G:883:LEU:HG	3:G:885:GLU:H	1.80	0.46
3:G:887:GLU:CD	3:G:887:GLU:H	2.19	0.46
5:L:27:LYS:HG3	5:L:67:TYR:CZ	2.50	0.46
5:L:94:LEU:HG	5:L:125:TRP:HE1	1.81	0.46
5:L:143:SER:HB2	5:L:185:ILE:HG12	1.97	0.46
5:L:294:SER:O	5:L:307:ARG:NH2	2.48	0.46
5:L:663:MET:HE3	5:L:678:TRP:HB3	1.98	0.46
5:L:724:ASP:H	5:L:752:ARG:HH21	1.62	0.46
5:L:787:TYR:CD2	5:L:798:LEU:HB3	2.50	0.46
1:C:425:TYR:HB2	1:C:436:ALA:HB3	1.98	0.46
2:E:1047:ARG:HH11	2:E:1052:LEU:HD21	1.81	0.46
3:G:152:ARG:NH2	3:G:177:ASP:O	2.49	0.46
3:G:212:ARG:HH21	3:G:280:PHE:HB3	1.81	0.46
3:G:279:ASN:HD21	3:G:281:ASP:HB3	1.80	0.46
3:G:555:ARG:CZ	3:G:605:PHE:H	2.29	0.46
3:G:605:PHE:HA	3:G:613:LEU:HA	1.97	0.46
3:G:724:PHE:CD2	3:G:755:MET:HG3	2.51	0.46
3:G:749:TRP:H	3:G:752:MET:HE1	1.81	0.46
3:G:1113:ILE:HB	3:G:1118:ALA:HB2	1.96	0.46
4:I:1077:GLU:O	4:I:1080:ARG:NE	2.48	0.46
5:L:387:VAL:HG23	5:L:400:PHE:HD1	1.80	0.46
5:L:910:HIS:NE2	5:L:947:SER:OG	2.46	0.46
1:C:534:LEU:HB3	1:C:552:ILE:HD13	1.98	0.46
2:E:1086:ILE:HD12	2:E:1086:ILE:N	2.30	0.46
3:G:704:MET:HG3	3:G:707:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1043:ALA:HA	3:G:1046:MET:CG	2.41	0.46
4:I:105:GLU:HB2	4:I:144:PRO:HB3	1.98	0.46
4:I:654:VAL:HG12	4:I:661:LYS:HD2	1.98	0.46
5:L:250:ARG:NH1	5:L:251:ASP:OD1	2.49	0.46
5:L:428:GLY:HA2	5:L:442:PHE:HA	1.98	0.46
5:L:430:LEU:HD12	5:L:430:LEU:HA	1.81	0.46
5:L:902:VAL:HG11	5:L:942:VAL:HG22	1.98	0.46
1:C:197:LEU:HB3	1:C:200:ASN:HB2	1.99	0.45
1:C:214:TRP:HE1	1:C:228:VAL:HG23	1.81	0.45
1:C:891:VAL:HA	1:C:902:ILE:HG21	1.98	0.45
2:E:1231:GLU:O	2:E:1235:PHE:N	2.40	0.45
3:G:412:ARG:NH1	3:G:449:GLU:O	2.49	0.45
4:I:745:GLY:O	4:I:748:GLN:HG3	2.16	0.45
4:I:1113:GLY:HA3	4:I:1367:SER:HB3	1.98	0.45
5:L:229:TYR:HB3	5:L:233:GLY:HA2	1.97	0.45
5:L:633:GLN:HB2	5:L:652:LEU:HD22	1.97	0.45
5:L:669:LEU:HD23	5:L:669:LEU:HA	1.82	0.45
5:L:856:ARG:O	5:L:858:ALA:N	2.47	0.45
5:L:909:VAL:HG12	5:L:950:ASN:HB3	1.98	0.45
1:C:509:LEU:HB3	1:C:521:TYR:HB2	1.97	0.45
1:C:1076:PHE:O	1:C:1079:GLN:NE2	2.49	0.45
2:E:10:HIS:HE1	2:E:150:ILE:HD11	1.81	0.45
2:E:461:ILE:HG22	2:E:487:ILE:HA	1.98	0.45
2:E:653:PRO:HB2	2:E:658:ARG:HD2	1.98	0.45
2:E:767:TYR:HD2	2:E:803:LEU:HD22	1.81	0.45
3:G:627:ASP:OD1	3:G:627:ASP:N	2.48	0.45
3:G:1071:ASN:OD1	3:G:1072:LEU:N	2.50	0.45
3:G:1345:LYS:O	3:G:1349:ALA:N	2.41	0.45
4:I:291:THR:OG1	4:I:336:GLU:HA	2.16	0.45
4:I:738:VAL:HA	4:I:744:TYR:CE1	2.52	0.45
4:I:924:GLU:HB2	4:I:932:ALA:HB2	1.98	0.45
1:C:136:VAL:HG22	1:C:142:VAL:HA	1.98	0.45
1:C:417:LYS:NZ	1:C:465:ASP:OD2	2.46	0.45
2:E:151:ILE:HG13	2:E:172:ALA:HB2	1.98	0.45
2:E:689:ILE:HG13	2:E:704:ALA:HB3	1.97	0.45
2:E:1170:MET:HE3	2:E:1185:LEU:HD11	1.98	0.45
3:G:58:ASN:ND2	3:G:62:THR:H	2.13	0.45
3:G:527:VAL:HG12	3:G:532:ALA:HA	1.98	0.45
3:G:609:GLU:OE1	3:G:722:LEU:HB3	2.16	0.45
3:G:989:GLY:O	3:G:1002:LEU:HA	2.16	0.45
3:G:1259:TYR:HA	3:G:1262:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:390:CYS:HA	5:L:395:LEU:HD23	1.98	0.45
5:L:393:LYS:NZ	5:L:411:ASP:O	2.48	0.45
5:L:397:LEU:HD23	5:L:405:GLU:HB2	1.97	0.45
5:L:418:LYS:HZ2	5:L:420:VAL:HA	1.80	0.45
1:C:445:GLN:NE2	1:C:524:PRO:HB3	2.19	0.45
2:E:336:VAL:HA	2:E:355:ARG:HH21	1.79	0.45
2:E:709:ALA:HB1	2:E:714:ASP:HB3	1.98	0.45
3:G:463:SER:H	3:G:475:ARG:HD3	1.81	0.45
3:G:894:ASN:HB3	5:L:854:GLU:HA	1.98	0.45
4:I:296:CYS:SG	4:I:298:SER:OG	2.74	0.45
4:I:329:LEU:HD21	4:I:359:PHE:HZ	1.82	0.45
4:I:489:ASN:O	4:I:505:ARG:N	2.42	0.45
4:I:1103:GLU:O	4:I:1107:LYS:HG2	2.17	0.45
4:I:1189:LEU:HA	4:I:1192:VAL:HG12	1.98	0.45
5:L:135:HIS:CD2	5:L:155:LEU:HD11	2.50	0.45
5:L:155:LEU:O	5:L:163:SER:OG	2.35	0.45
1:C:968:GLU:HA	1:C:1023:ALA:HB1	1.99	0.45
4:I:921:LYS:HA	4:I:921:LYS:HD2	1.78	0.45
4:I:944:ALA:HA	4:I:947:ARG:HB3	1.98	0.45
4:I:1241:VAL:HG23	4:I:1244:LYS:HD3	1.98	0.45
5:L:929:SER:HA	5:L:958:GLN:HG3	1.97	0.45
1:C:270:LEU:N	1:C:293:TYR:O	2.49	0.45
1:C:362:VAL:HG22	1:C:380:LEU:HD22	1.99	0.45
3:G:750:GLU:OE2	3:G:774:HIS:NE2	2.49	0.45
3:G:802:GLY:HA2	4:I:714:ALA:HB3	1.98	0.45
3:G:825:ARG:NH1	3:G:836:VAL:HG11	2.32	0.45
3:G:872:ALA:O	3:G:876:LEU:N	2.47	0.45
3:G:874:CYS:HB3	5:L:842:ARG:HH12	1.82	0.45
3:G:1030:ALA:CB	3:G:1046:MET:HE1	2.43	0.45
4:I:909:ARG:HG3	4:I:910:ILE:HD12	1.97	0.45
4:I:956:PRO:HG3	4:I:978:PHE:CZ	2.51	0.45
4:I:1168:HIS:CE1	4:I:1172:LEU:HD22	2.51	0.45
4:I:1220:LYS:HA	4:I:1223:ALA:HB3	1.98	0.45
1:C:445:GLN:NE2	1:C:448:THR:HA	2.32	0.45
1:C:775:GLU:OE2	1:C:779:ARG:NE	2.50	0.45
2:E:27:GLU:O	2:E:31:LYS:HG2	2.16	0.45
2:E:279:LEU:HD11	2:E:317:ILE:HB	1.99	0.45
3:G:967:TYR:O	3:G:972:ARG:N	2.50	0.45
3:G:1192:ILE:HA	3:G:1195:MET:HG3	1.99	0.45
4:I:114:MET:HA	4:I:125:VAL:HA	1.99	0.45
4:I:468:VAL:HG13	4:I:472:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:601:LEU:HD22	4:I:699:LEU:HG	1.99	0.45
4:I:809:TYR:O	4:I:813:LEU:HG	2.17	0.45
4:I:842:LEU:HA	4:I:842:LEU:HD23	1.76	0.45
4:I:858:GLN:NE2	4:I:884:ALA:O	2.44	0.45
5:L:783:LEU:HD12	5:L:799:LEU:HG	1.99	0.45
5:L:912:SER:HB3	5:L:918:ARG:HH21	1.80	0.45
1:C:17:LEU:O	1:C:325:SER:OG	2.35	0.45
2:E:37:VAL:HG23	2:E:112:HIS:ND1	2.32	0.45
2:E:359:ALA:O	2:E:363:ASP:N	2.48	0.45
2:E:1107:SER:OG	2:E:1152:ARG:O	2.35	0.45
3:G:273:ASN:HB2	3:G:290:LEU:HB2	1.98	0.45
3:G:611:LYS:HB2	3:G:611:LYS:HE3	1.67	0.45
3:G:810:LEU:HA	3:G:813:ALA:HB3	1.98	0.45
4:I:421:ALA:HB3	4:I:437:ARG:HB2	1.99	0.45
4:I:709:ARG:NE	4:I:717:VAL:HG12	2.31	0.45
5:L:501:TRP:CE3	5:L:509:PHE:HB3	2.52	0.45
5:L:749:THR:OG1	5:L:750:ASP:N	2.50	0.45
1:C:595:ASP:OD2	1:C:632:LEU:N	2.47	0.45
1:C:739:ALA:HB1	1:C:744:ARG:HB2	1.99	0.45
2:E:378:ILE:HB	2:E:446:LYS:HG3	1.99	0.45
2:E:929:GLN:O	2:E:933:THR:HG22	2.17	0.45
2:E:1322:VAL:HG22	2:E:1353:LEU:N	2.32	0.45
3:G:182:ALA:HB1	3:G:203:VAL:HG23	1.98	0.45
3:G:186:TRP:N	3:G:194:GLY:O	2.39	0.45
3:G:578:LEU:HB2	3:G:593:PHE:HE2	1.82	0.45
3:G:652:LEU:HD22	3:G:730:THR:HA	1.98	0.45
3:G:973:ILE:O	3:G:977:ILE:HG12	2.17	0.45
4:I:373:ARG:HH11	4:I:385:LEU:HD21	1.82	0.45
4:I:541:ARG:HG3	4:I:555:ASN:HA	1.97	0.45
5:L:345:GLN:NE2	5:L:350:VAL:HG22	2.30	0.45
5:L:458:VAL:HG13	5:L:472:VAL:HG13	1.99	0.45
5:L:772:GLU:HA	5:L:775:LEU:HB2	1.99	0.45
1:C:199:CYS:HB3	1:C:239:GLN:HG2	1.98	0.45
2:E:282:LEU:O	2:E:286:MET:HG2	2.17	0.45
2:E:913:GLN:O	2:E:917:LYS:N	2.37	0.45
3:G:513:LEU:O	3:G:525:LEU:N	2.37	0.45
3:G:797:VAL:HA	3:G:800:HIS:CE1	2.51	0.45
4:I:412:HIS:HA	4:I:425:SER:HA	1.98	0.45
5:L:134:LYS:HB2	5:L:136:LYS:HZ2	1.82	0.45
5:L:243:LYS:HD3	5:L:263:SER:HA	1.99	0.45
5:L:271:ARG:HB3	5:L:274:HIS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:THR:HG21	1:C:689:LEU:HD13	1.98	0.44
2:E:491:VAL:O	2:E:495:LEU:HD13	2.17	0.44
2:E:705:ASP:OD1	2:E:705:ASP:N	2.50	0.44
2:E:1350:ARG:HH21	2:E:1353:LEU:HD13	1.82	0.44
3:G:571:GLU:OE2	3:G:574:ARG:NH2	2.48	0.44
3:G:945:LYS:HZ3	3:G:982:LEU:HG	1.81	0.44
4:I:1:MET:HE3	4:I:312:VAL:HG21	1.99	0.44
4:I:1027:TYR:O	4:I:1031:ALA:CB	2.65	0.44
4:I:1267:ASP:HA	4:I:1274:PRO:HA	1.99	0.44
5:L:184:SER:OG	5:L:198:GLY:O	2.35	0.44
5:L:725:ARG:NH1	5:L:725:ARG:O	2.50	0.44
5:L:783:LEU:O	5:L:787:TYR:N	2.48	0.44
1:C:6:SER:OG	1:C:332:PHE:O	2.29	0.44
1:C:589:ASP:H	1:C:603:MET:HB2	1.83	0.44
1:C:594:ASP:N	1:C:629:PHE:O	2.36	0.44
1:C:728:LEU:HB3	1:C:734:GLN:HG2	1.99	0.44
2:E:103:ARG:HH22	2:E:125:ARG:HH12	1.65	0.44
2:E:234:LEU:HD22	2:E:239:GLN:HE22	1.83	0.44
2:E:722:LEU:HD22	2:E:739:MET:HE2	2.00	0.44
2:E:1043:ILE:HG23	2:E:1055:VAL:HG13	1.98	0.44
3:G:817:TYR:O	3:G:820:LEU:HB3	2.18	0.44
3:G:901:SER:HB2	3:G:903:GLU:OE1	2.17	0.44
4:I:39:ILE:HG22	4:I:47:TYR:HB3	1.98	0.44
5:L:175:ILE:HG23	5:L:211:GLY:HA2	1.99	0.44
1:C:104:HIS:HB3	1:C:109:PHE:HD2	1.82	0.44
1:C:181:GLU:HG2	1:C:197:LEU:HD11	1.99	0.44
1:C:437:ASN:HB2	1:C:440:VAL:HB	1.99	0.44
1:C:589:ASP:HB3	1:C:603:MET:HG3	1.98	0.44
3:G:618:THR:HB	3:G:636:HIS:HD2	1.82	0.44
3:G:679:LYS:HE2	3:G:700:SER:HB3	1.99	0.44
4:I:495:LEU:HD13	4:I:500:VAL:HG13	2.00	0.44
4:I:861:PHE:HB3	4:I:884:ALA:HB2	1.98	0.44
4:I:960:TYR:HD1	4:I:991:PHE:HE2	1.63	0.44
4:I:1224:PHE:HE1	4:I:1251:VAL:HA	1.82	0.44
5:L:23:ASP:HB2	5:L:64:CYS:HA	1.98	0.44
5:L:77:GLY:HA2	5:L:83:VAL:HG22	2.00	0.44
5:L:117:ALA:HA	5:L:122:VAL:HA	2.00	0.44
5:L:638:GLU:HA	5:L:641:ALA:HB3	1.99	0.44
5:L:988:VAL:HA	5:L:991:ALA:HB3	1.99	0.44
1:C:293:TYR:HB3	1:C:297:GLY:HA2	2.00	0.44
1:C:931:HIS:O	1:C:935:ALA:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:258:GLN:HB2	2:E:282:LEU:HD22	1.99	0.44
2:E:1192:ASP:OD1	2:E:1192:ASP:N	2.51	0.44
2:E:1199:LEU:HD22	2:E:1218:GLN:HE21	1.81	0.44
3:G:267:SER:OG	3:G:276:ARG:O	2.28	0.44
3:G:286:TYR:HH	3:G:343:TRP:HE1	1.61	0.44
3:G:721:LEU:HA	3:G:724:PHE:HB3	1.98	0.44
3:G:874:CYS:O	3:G:877:VAL:HG22	2.17	0.44
3:G:1015:ILE:HA	3:G:1018:ALA:HB3	1.99	0.44
4:I:383:MET:HB3	4:I:399:LEU:HD11	2.00	0.44
4:I:1183:THR:HB	4:I:1261:LEU:HD23	2.00	0.44
5:L:653:PHE:CD1	5:L:657:GLY:HA3	2.52	0.44
1:C:349:VAL:HG12	1:C:383:ILE:HD13	1.98	0.44
2:E:343:LYS:HE2	2:E:351:ASN:HB2	1.99	0.44
2:E:457:LEU:HD13	2:E:490:VAL:HG22	1.99	0.44
2:E:1007:MET:HA	2:E:1010:GLU:HG3	1.99	0.44
2:E:1009:ALA:HA	2:E:1012:MET:SD	2.57	0.44
2:E:1216:ARG:HH21	2:E:1246:HIS:HA	1.82	0.44
3:G:13:ALA:HB1	3:G:375:ILE:HG12	1.98	0.44
3:G:843:ILE:HG12	5:L:822:ASP:HA	2.00	0.44
3:G:1188:ARG:NH1	3:G:1193:TYR:OH	2.51	0.44
4:I:73:ASP:HB3	4:I:116:TRP:CD2	2.52	0.44
4:I:269:VAL:HG21	4:I:319:TYR:CZ	2.53	0.44
4:I:1307:CYS:N	4:I:1312:PHE:O	2.49	0.44
5:L:107:TYR:CZ	5:L:114:LEU:HB2	2.53	0.44
5:L:511:TYR:CE2	5:L:518:SER:HB2	2.53	0.44
5:L:559:SER:HA	5:L:562:MET:HB2	1.98	0.44
5:L:995:ILE:HG23	5:L:996:ARG:HG3	1.99	0.44
1:C:177:THR:N	1:C:181:GLU:O	2.49	0.44
1:C:1071:LEU:O	1:C:1075:ALA:CB	2.66	0.44
2:E:700:ARG:HG2	2:E:704:ALA:N	2.32	0.44
2:E:877:LEU:O	2:E:881:VAL:HG23	2.17	0.44
3:G:883:LEU:HD12	3:G:912:LEU:HD12	1.99	0.44
3:G:1093:LEU:HB3	3:G:1098:GLN:HB2	2.00	0.44
3:G:1267:ASP:OD2	3:G:1271:ARG:NH2	2.50	0.44
4:I:648:LEU:O	4:I:656:ARG:NH2	2.37	0.44
4:I:980:LEU:HD21	4:I:1000:GLN:CG	2.48	0.44
1:C:729:ASP:N	1:C:729:ASP:OD1	2.51	0.44
1:C:775:GLU:HG2	1:C:814:GLN:HG2	2.00	0.44
2:E:197:MET:HG3	2:E:206:CYS:HB2	2.00	0.44
3:G:413:PRO:HA	3:G:414:PRO:HD3	1.92	0.44
3:G:653:LEU:HD11	3:G:656:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:725:SER:HA	3:G:728:LEU:HB2	2.00	0.44
3:G:952:THR:OG1	3:G:956:ASP:OD2	2.29	0.44
4:I:816:LEU:HD11	4:I:827:LEU:HG	1.99	0.44
4:I:1213:GLU:OE2	4:I:1216:ARG:NH2	2.50	0.44
5:L:143:SER:O	5:L:156:GLY:N	2.50	0.44
5:L:304:TYR:CZ	5:L:306:TYR:HB3	2.52	0.44
5:L:386:HIS:CD2	5:L:425:ARG:HD3	2.52	0.44
5:L:717:TYR:HA	5:L:720:ALA:HB3	1.99	0.44
1:C:445:GLN:HE21	1:C:448:THR:HA	1.83	0.44
3:G:589:HIS:CG	3:G:650:GLY:HA2	2.53	0.44
3:G:716:LYS:HD2	3:G:719:ARG:HH21	1.83	0.44
4:I:793:GLY:O	4:I:797:GLU:N	2.51	0.44
4:I:871:LEU:HD23	4:I:871:LEU:HA	1.81	0.44
4:I:1076:VAL:HG22	4:I:1084:LEU:HG	1.99	0.44
4:I:1156:PRO:HB3	4:I:1160:LEU:HD13	2.00	0.44
5:L:334:LYS:HD2	5:L:334:LYS:HA	1.81	0.44
5:L:468:ASN:HA	5:L:484:LEU:HD12	2.00	0.44
5:L:518:SER:HB3	5:L:526:LEU:HD11	1.99	0.44
5:L:966:LYS:HA	5:L:969:ARG:HH21	1.82	0.44
1:C:944:LYS:HG2	1:C:1061:LEU:HA	1.99	0.44
2:E:896:GLU:HB3	2:E:899:GLY:HA3	2.00	0.44
3:G:267:SER:H	3:G:277:MET:HE2	1.83	0.44
3:G:403:LEU:HD11	3:G:429:LEU:HD13	2.00	0.44
3:G:1080:PHE:HB3	3:G:1089:ALA:HB2	2.00	0.44
4:I:787:THR:O	4:I:790:LYS:N	2.50	0.44
4:I:950:LEU:HD22	4:I:978:PHE:CG	2.53	0.44
5:L:632:GLU:HA	5:L:635:LEU:HD12	2.00	0.44
1:C:240:LEU:HD11	1:C:270:LEU:HD22	2.00	0.43
1:C:599:LEU:HA	1:C:611:PHE:O	2.18	0.43
1:C:822:VAL:HG11	1:C:851:ILE:HG12	2.00	0.43
2:E:121:LYS:HA	2:E:121:LYS:HD2	1.73	0.43
2:E:811:LEU:HB3	2:E:816:ASP:O	2.18	0.43
3:G:417:LEU:HB2	3:G:453:ILE:HB	1.99	0.43
3:G:603:LEU:HD23	3:G:615:VAL:HG13	2.00	0.43
3:G:723:ASP:HB3	3:G:735:GLU:HB3	2.00	0.43
3:G:1060:THR:HG22	3:G:1063:MET:HE3	1.99	0.43
3:G:1205:TRP:CZ3	3:G:1238:ILE:HG13	2.53	0.43
3:G:1267:ASP:O	3:G:1271:ARG:HG2	2.17	0.43
3:G:1297:GLN:HG2	3:G:1338:ARG:HH22	1.83	0.43
4:I:853:MET:HG3	4:I:861:PHE:HE1	1.81	0.43
4:I:1072:ALA:O	4:I:1076:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:162:ILE:HG21	5:L:195:LEU:HD21	2.00	0.43
5:L:370:LYS:O	5:L:372:GLN:NE2	2.50	0.43
5:L:386:HIS:HA	5:L:399:ASN:HA	2.00	0.43
5:L:452:ILE:HD13	5:L:452:ILE:HA	1.91	0.43
5:L:600:LEU:HD22	5:L:619:VAL:HA	1.99	0.43
5:L:847:LEU:HA	5:L:850:ASN:HB2	2.00	0.43
5:L:888:SER:HA	5:L:891:GLU:HB2	1.99	0.43
1:C:40:VAL:HG11	1:C:108:TRP:NE1	2.33	0.43
1:C:88:LYS:HE3	1:C:147:VAL:HG22	1.99	0.43
1:C:116:ARG:HD2	1:C:143:ILE:HD11	2.00	0.43
1:C:768:LEU:HB2	5:L:611:ARG:NE	2.33	0.43
2:E:1026:GLN:HB2	2:E:1058:TYR:CZ	2.54	0.43
3:G:1013:VAL:HA	3:G:1016:ASP:HB3	1.99	0.43
4:I:176:THR:HA	4:I:183:THR:HA	2.00	0.43
4:I:259:LEU:HD22	4:I:295:TYR:HB2	2.00	0.43
4:I:730:ASN:HB2	4:I:750:LEU:HB3	2.00	0.43
5:L:793:TRP:HE3	5:L:817:TRP:HB3	1.83	0.43
5:L:814:TYR:HE2	5:L:830:ALA:HB2	1.83	0.43
1:C:737:GLU:HA	1:C:740:VAL:HG12	2.00	0.43
2:E:213:ILE:HA	2:E:216:ARG:HD2	1.99	0.43
2:E:881:VAL:HG22	2:E:910:LEU:HD23	2.00	0.43
2:E:892:LYS:HB2	2:E:900:TYR:CD1	2.52	0.43
3:G:505:SER:HB3	3:G:516:VAL:HB	2.01	0.43
3:G:945:LYS:HZ2	3:G:982:LEU:HA	1.83	0.43
3:G:987:SER:HA	3:G:1013:VAL:HG11	1.99	0.43
3:G:1144:VAL:O	3:G:1148:GLN:N	2.51	0.43
3:G:1158:TYR:CD2	3:G:1168:MET:HE1	2.54	0.43
4:I:42:ARG:HH21	4:I:402:GLU:HG2	1.83	0.43
4:I:923:LYS:HE3	4:I:928:ARG:HH21	1.83	0.43
4:I:1109:ASN:HB3	4:I:1114:GLN:O	2.18	0.43
4:I:1318:GLN:HA	4:I:1321:ARG:HG3	1.99	0.43
5:L:5:VAL:HG22	5:L:289:PHE:CE1	2.53	0.43
5:L:112:GLN:N	5:L:127:PRO:HG3	2.33	0.43
5:L:224:PRO:HA	5:L:240:GLY:HA3	2.00	0.43
5:L:247:LEU:HD22	5:L:291:LEU:HD23	2.00	0.43
5:L:454:HIS:ND1	5:L:456:ALA:O	2.52	0.43
5:L:646:TYR:HB3	5:L:661:ARG:HH12	1.83	0.43
5:L:743:VAL:HG22	5:L:753:CYS:HB3	2.00	0.43
1:C:606:THR:HG23	1:C:623:SER:HB2	1.99	0.43
2:E:343:LYS:HA	2:E:343:LYS:HD2	1.86	0.43
2:E:884:TRP:NE1	2:E:903:ALA:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:497:ASP:O	3:G:501:GLY:N	2.45	0.43
3:G:1033:LEU:HD13	3:G:1033:LEU:HA	1.81	0.43
3:G:1237:GLN:NE2	3:G:1325:ASP:H	2.17	0.43
4:I:454:ALA:HB2	4:I:495:LEU:HB2	1.99	0.43
4:I:837:ARG:HB3	4:I:867:ILE:HD13	2.01	0.43
4:I:923:LYS:HD3	4:I:923:LYS:HA	1.83	0.43
3:G:387:PHE:N	3:G:668:ILE:O	2.51	0.43
3:G:474:TYR:HD1	3:G:483:VAL:HG22	1.83	0.43
3:G:685:PRO:HA	3:G:692:PHE:HA	1.99	0.43
3:G:1064:THR:HA	3:G:1065:PRO:HD3	1.86	0.43
3:G:1292:ILE:HG12	3:G:1329:LEU:HD11	2.00	0.43
4:I:946:VAL:HA	4:I:949:CYS:HB2	2.01	0.43
4:I:970:GLU:HA	4:I:973:ASN:HB3	2.00	0.43
4:I:985:PHE:O	4:I:988:ALA:N	2.52	0.43
5:L:122:VAL:H	5:L:135:HIS:H	1.65	0.43
5:L:421:GLY:O	5:L:467:ARG:NH1	2.52	0.43
5:L:729:ILE:HA	5:L:732:LYS:NZ	2.34	0.43
1:C:389:PHE:HB2	1:C:428:ILE:HD11	2.00	0.43
1:C:444:TRP:CE2	1:C:446:PHE:HB3	2.53	0.43
2:E:576:VAL:HG13	2:E:610:LYS:HE2	2.00	0.43
2:E:1148:LEU:HG	2:E:1161:TYR:CZ	2.53	0.43
3:G:441:ARG:HA	3:G:460:GLU:HA	2.00	0.43
3:G:561:ASN:ND2	3:G:584:GLU:HG3	2.33	0.43
4:I:269:VAL:HB	4:I:282:HIS:HB3	2.00	0.43
4:I:717:VAL:HG23	4:I:718:LEU:HD12	2.01	0.43
4:I:1048:SER:HB3	4:I:1057:VAL:HG12	2.00	0.43
4:I:1246:LYS:HA	4:I:1246:LYS:HD3	1.65	0.43
5:L:334:LYS:NZ	5:L:335:ILE:O	2.51	0.43
5:L:625:GLY:HA3	5:L:635:LEU:HD22	2.00	0.43
1:C:146:SER:HB3	1:C:152:LEU:HD11	2.00	0.43
1:C:423:PRO:HB2	1:C:426:LEU:HD22	2.01	0.43
1:C:447:ARG:HE	1:C:452:LYS:HD3	1.84	0.43
1:C:500:ALA:H	1:C:513:ARG:HA	1.83	0.43
2:E:40:PHE:HE1	2:E:55:ALA:HB1	1.84	0.43
2:E:321:MET:HA	2:E:324:ARG:HB2	2.00	0.43
2:E:1039:LEU:O	2:E:1043:ILE:HG12	2.18	0.43
3:G:621:PHE:CE2	3:G:629:ARG:HB3	2.51	0.43
3:G:808:LYS:HB3	3:G:820:LEU:HD12	2.00	0.43
3:G:842:ARG:HB3	5:L:822:ASP:N	2.34	0.43
3:G:991:ARG:NH1	3:G:994:LYS:HZ2	2.17	0.43
3:G:1259:TYR:O	3:G:1263:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1047:TRP:HZ3	4:I:1055:ARG:HH12	1.65	0.43
4:I:1314:ALA:HB1	4:I:1319:PHE:CG	2.53	0.43
5:L:258:ILE:HG23	5:L:291:LEU:HD11	2.01	0.43
5:L:676:LYS:NZ	5:L:700:GLN:HB3	2.33	0.43
1:C:169:ASP:N	1:C:169:ASP:OD1	2.45	0.43
1:C:522:SER:HB3	1:C:529:ASP:OD2	2.18	0.43
2:E:228:THR:HA	2:E:240:VAL:HG13	2.01	0.43
2:E:457:LEU:HD22	2:E:490:VAL:HG22	2.01	0.43
2:E:484:PRO:O	2:E:488:THR:OG1	2.27	0.43
3:G:446:LYS:NZ	3:G:447:VAL:O	2.50	0.43
3:G:715:ASP:HA	3:G:718:ARG:HG2	2.01	0.43
3:G:721:LEU:HB3	3:G:755:MET:SD	2.59	0.43
3:G:1345:LYS:HD2	3:G:1345:LYS:HA	1.82	0.43
4:I:311:ARG:HB3	4:I:321:GLU:HG2	2.00	0.43
4:I:802:TYR:CD2	4:I:838:THR:HA	2.51	0.43
4:I:1350:LYS:HD2	4:I:1353:GLN:HB3	2.00	0.43
5:L:347:GLN:HA	5:L:374:LYS:HE2	2.01	0.43
5:L:546:LEU:HB2	5:L:551:MET:HE1	2.01	0.43
5:L:679:ALA:HB2	5:L:699:ARG:HH21	1.83	0.43
5:L:746:LEU:HD12	5:L:746:LEU:HA	1.89	0.43
5:L:796:ALA:C	5:L:800:LEU:HB2	2.39	0.43
1:C:771:TRP:CD1	1:C:792:HIS:HA	2.54	0.43
1:C:794:LYS:HE2	5:L:609:ARG:HD2	2.01	0.43
2:E:957:TYR:HB3	2:E:974:VAL:HG12	1.99	0.43
3:G:386:LYS:HA	3:G:386:LYS:HD2	1.79	0.43
3:G:447:VAL:HG22	3:G:453:ILE:HG23	2.00	0.43
3:G:1214:HIS:O	3:G:1217:SER:OG	2.23	0.43
3:G:1281:VAL:HG21	3:G:1306:LEU:HD21	2.00	0.43
4:I:914:LYS:HG3	4:I:915:LEU:HD23	2.00	0.43
4:I:1048:SER:OG	4:I:1060:TYR:HB2	2.19	0.43
4:I:1063:VAL:HG23	4:I:1064:GLY:H	1.84	0.43
1:C:120:VAL:HB	1:C:138:GLU:HB2	2.01	0.43
1:C:771:TRP:O	1:C:792:HIS:NE2	2.51	0.43
1:C:878:ILE:HD13	1:C:894:ALA:HA	2.01	0.43
1:C:1068:TYR:HB3	1:C:1090:LYS:HZ3	1.83	0.43
2:E:9:VAL:HA	2:E:20:HIS:CE1	2.52	0.43
2:E:158:ASP:HB3	2:E:302:ARG:HE	1.84	0.43
2:E:301:ALA:HB1	2:E:318:THR:HG22	2.01	0.43
2:E:1043:ILE:HG22	2:E:1085:TYR:HE2	1.84	0.43
3:G:43:GLU:HB2	3:G:366:LEU:HD11	1.99	0.43
3:G:462:THR:H	3:G:475:ARG:NH1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:960:TYR:HD1	4:I:991:PHE:CE2	2.37	0.43
4:I:1065:THR:HB	4:I:1067:PRO:HD2	1.99	0.43
5:L:682:PHE:CE1	5:L:687:ARG:HD2	2.54	0.43
1:C:522:SER:HB3	1:C:529:ASP:OD1	2.19	0.42
1:C:665:THR:O	1:C:669:LEU:HG	2.19	0.42
2:E:263:MET:SD	2:E:301:ALA:HA	2.59	0.42
2:E:365:LEU:HB3	2:E:396:MET:SD	2.59	0.42
2:E:703:VAL:HG21	2:E:731:HIS:HB2	2.00	0.42
2:E:1304:SER:H	2:E:1334:ALA:HB1	1.83	0.42
3:G:764:VAL:HG23	4:I:798:MET:HE2	2.00	0.42
3:G:809:LYS:HA	3:G:812:ILE:HD12	1.99	0.42
3:G:867:LYS:O	3:G:871:ALA:N	2.49	0.42
3:G:1106:CYS:SG	3:G:1122:THR:OG1	2.52	0.42
4:I:173:VAL:HB	4:I:187:PHE:HB2	1.99	0.42
4:I:673:ARG:HA	4:I:673:ARG:HD3	1.68	0.42
4:I:841:GLN:NE2	4:I:867:ILE:O	2.52	0.42
5:L:27:LYS:NZ	5:L:67:TYR:OH	2.33	0.42
5:L:117:ALA:HA	5:L:122:VAL:HG22	2.00	0.42
5:L:705:GLU:HG3	5:L:717:TYR:OH	2.19	0.42
5:L:793:TRP:HB3	5:L:817:TRP:CB	2.49	0.42
2:E:863:ALA:HB1	2:E:866:ARG:NH2	2.33	0.42
2:E:933:THR:HG23	2:E:963:HIS:CG	2.54	0.42
3:G:279:ASN:HB2	3:G:286:TYR:HE2	1.84	0.42
3:G:975:GLU:HA	3:G:978:ARG:NE	2.30	0.42
3:G:1330:MET:HA	3:G:1333:TYR:CE2	2.54	0.42
5:L:70:ASN:ND2	5:L:112:GLN:OE1	2.52	0.42
5:L:350:VAL:HG11	5:L:387:VAL:HG21	2.01	0.42
5:L:619:VAL:O	5:L:623:GLU:HB2	2.19	0.42
5:L:659:VAL:HB	5:L:682:PHE:CZ	2.52	0.42
5:L:724:ASP:N	5:L:752:ARG:HH21	2.17	0.42
1:C:288:TRP:CG	1:C:309:GLY:HA2	2.54	0.42
2:E:41:TRP:CH2	2:E:115:SER:HB2	2.53	0.42
2:E:237:TRP:HZ2	2:E:268:ARG:HB3	1.83	0.42
3:G:912:LEU:HD22	3:G:915:LEU:HD22	1.99	0.42
3:G:1014:MET:O	3:G:1033:LEU:HD12	2.20	0.42
4:I:160:LYS:HD2	4:I:211:GLU:HG3	2.01	0.42
4:I:339:GLY:N	4:I:348:THR:O	2.41	0.42
4:I:774:LEU:HG	4:I:788:ILE:HD13	2.01	0.42
4:I:906:LEU:HD23	4:I:906:LEU:HA	1.85	0.42
4:I:921:LYS:NZ	4:I:936:TYR:OH	2.33	0.42
4:I:1028:GLN:HG3	4:I:1050:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1076:VAL:HA	4:I:1084:LEU:HD23	2.00	0.42
4:I:1155:LYS:NZ	4:I:1156:PRO:O	2.49	0.42
5:L:51:LEU:HD21	5:L:54:ALA:HB2	2.02	0.42
1:C:174:LEU:HD11	1:C:214:TRP:CE3	2.54	0.42
1:C:429:THR:HB	1:C:506:ASP:HA	2.01	0.42
1:C:887:TRP:HZ2	1:C:909:TYR:HB2	1.83	0.42
2:E:742:ILE:O	2:E:746:HIS:HB3	2.20	0.42
2:E:1015:LYS:HB2	2:E:1017:HIS:CE1	2.55	0.42
2:E:1026:GLN:HB2	2:E:1058:TYR:CE2	2.55	0.42
3:G:207:VAL:O	3:G:216:LEU:N	2.52	0.42
3:G:485:ASN:N	3:G:489:THR:O	2.51	0.42
3:G:1039:LYS:HE3	3:G:1039:LYS:HB2	1.73	0.42
4:I:401:ASN:OD1	4:I:436:ARG:NH1	2.51	0.42
4:I:920:ALA:HA	4:I:931:GLU:HG3	2.01	0.42
5:L:255:LEU:HD21	5:L:311:THR:HG23	2.01	0.42
5:L:472:VAL:O	5:L:480:LEU:N	2.45	0.42
1:C:29:ILE:HG23	1:C:41:LEU:HB2	2.00	0.42
1:C:126:TRP:CE2	1:C:133:ILE:HD12	2.54	0.42
1:C:856:GLN:HE21	1:C:880:CYS:HB2	1.84	0.42
1:C:887:TRP:HA	1:C:890:ALA:HB3	2.02	0.42
2:E:689:ILE:O	2:E:693:GLU:HG3	2.19	0.42
2:E:1100:ARG:HH22	2:E:1147:LEU:HD11	1.84	0.42
2:E:1353:LEU:HG	5:L:225:LEU:HA	2.01	0.42
3:G:47:PRO:HG2	3:G:50:PRO:HG3	2.02	0.42
3:G:238:THR:HG21	3:G:241:LYS:HE3	2.02	0.42
3:G:401:VAL:HB	3:G:417:LEU:HD23	2.02	0.42
3:G:403:LEU:HD12	3:G:434:LEU:HD22	2.01	0.42
3:G:752:MET:HG2	3:G:768:CYS:HB2	2.02	0.42
3:G:843:ILE:HG13	5:L:824:PHE:CD2	2.47	0.42
3:G:1230:SER:HB3	3:G:1271:ARG:NE	2.33	0.42
4:I:225:ILE:HD11	4:I:258:ILE:HD11	2.01	0.42
4:I:226:MET:SD	4:I:226:MET:N	2.87	0.42
4:I:790:LYS:HD2	4:I:809:TYR:HE1	1.83	0.42
4:I:824:GLN:HA	4:I:825:PRO:HD3	1.88	0.42
4:I:1176:LEU:HB3	4:I:1181:ASP:HB3	2.02	0.42
5:L:202:GLY:HA2	5:L:224:PRO:HD3	2.00	0.42
5:L:517:LEU:HB3	5:L:529:GLN:HB3	2.00	0.42
1:C:442:TYR:OH	1:C:468:GLU:OE1	2.28	0.42
1:C:502:VAL:HG22	1:C:511:ILE:HA	2.01	0.42
2:E:12:TYR:HB2	2:E:20:HIS:CE1	2.55	0.42
2:E:176:PHE:CD1	2:E:189:ALA:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:342:GLN:HA	2:E:345:MET:HG2	2.02	0.42
2:E:509:PRO:HG2	2:E:767:TYR:HE2	1.85	0.42
2:E:722:LEU:HD12	2:E:722:LEU:HA	1.84	0.42
2:E:1110:ILE:HA	2:E:1113:MET:HG2	2.02	0.42
3:G:383:LEU:HB3	3:G:395:GLN:HB3	2.00	0.42
3:G:716:LYS:HG2	3:G:749:TRP:HB3	2.01	0.42
3:G:1146:LYS:HA	3:G:1171:LEU:HD21	2.00	0.42
5:L:218:ARG:NH1	5:L:252:GLY:O	2.53	0.42
5:L:276:PHE:HA	5:L:289:PHE:O	2.19	0.42
5:L:426:ARG:HH11	5:L:444:ASP:HB2	1.85	0.42
5:L:683:ALA:HA	5:L:693:VAL:HA	2.02	0.42
1:C:341:TRP:HZ3	1:C:343:TYR:HB2	1.84	0.42
1:C:468:GLU:HG3	1:C:485:PRO:HB3	2.02	0.42
1:C:912:HIS:CE1	5:L:448:PRO:HD2	2.55	0.42
1:C:940:GLN:HG2	1:C:1025:ARG:HH22	1.84	0.42
3:G:122:ASP:N	3:G:122:ASP:OD1	2.52	0.42
3:G:268:ALA:HB2	3:G:275:VAL:HG13	2.02	0.42
3:G:333:LEU:HB3	3:G:626:VAL:HG11	2.00	0.42
3:G:423:GLN:HB2	3:G:438:ASP:HB2	2.01	0.42
3:G:429:LEU:HB2	3:G:434:LEU:HD13	2.01	0.42
3:G:468:ILE:HG12	3:G:470:ASN:N	2.34	0.42
3:G:786:SER:OG	3:G:807:ALA:N	2.53	0.42
3:G:801:LEU:HD13	4:I:740:LEU:HD23	2.02	0.42
3:G:1153:LEU:HD11	3:G:1157:LYS:HE2	2.01	0.42
4:I:86:ASN:HD22	4:I:88:HIS:CE1	2.37	0.42
4:I:543:VAL:HA	4:I:553:LEU:HA	2.02	0.42
4:I:574:MET:HG2	4:I:623:VAL:HG12	2.01	0.42
5:L:58:HIS:NE2	5:L:76:SER:O	2.34	0.42
5:L:578:ALA:HB1	5:L:587:TRP:NE1	2.35	0.42
1:C:499:ILE:HA	1:C:513:ARG:HA	2.01	0.42
1:C:1091:LEU:O	1:C:1102:ARG:HG2	2.19	0.42
2:E:222:PRO:HA	2:E:225:VAL:HG12	2.01	0.42
2:E:282:LEU:HA	2:E:282:LEU:HD12	1.74	0.42
3:G:19:TRP:CD2	3:G:29:LEU:HD13	2.54	0.42
4:I:363:LEU:HB2	4:I:631:ARG:NH2	2.35	0.42
4:I:424:TYR:OH	4:I:436:ARG:NH2	2.53	0.42
4:I:534:PHE:CG	4:I:573:VAL:HB	2.54	0.42
4:I:832:LYS:O	4:I:835:ILE:HG22	2.19	0.42
5:L:31:SER:OG	5:L:32:GLN:N	2.51	0.42
5:L:62:ILE:HD13	5:L:76:SER:HB2	2.00	0.42
5:L:819:SER:HA	5:L:827:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:VAL:HG23	1:C:284:GLY:H	1.84	0.42
1:C:350:TYR:CZ	1:C:363:MET:HG2	2.54	0.42
1:C:895:GLN:HE22	1:C:902:ILE:HD13	1.85	0.42
2:E:977:LEU:O	2:E:981:ASN:ND2	2.53	0.42
3:G:883:LEU:HB2	3:G:917:GLU:OE1	2.20	0.42
3:G:961:PHE:CZ	3:G:965:ARG:HB3	2.55	0.42
4:I:705:ILE:HA	4:I:709:ARG:HD3	2.02	0.42
4:I:803:SER:HB3	4:I:842:LEU:HD21	2.02	0.42
4:I:960:TYR:CE1	4:I:984:ASP:HB2	2.55	0.42
5:L:39:ASN:HA	5:L:62:ILE:H	1.85	0.42
5:L:277:VAL:O	5:L:288:MET:HA	2.20	0.42
5:L:760:HIS:ND1	5:L:763:ARG:HD3	2.35	0.42
5:L:787:TYR:HD2	5:L:799:LEU:H	1.68	0.42
5:L:837:PRO:HD2	5:L:874:SER:HB2	2.01	0.42
1:C:271:ALA:HB2	1:C:315:TRP:HZ2	1.84	0.42
2:E:345:MET:HA	2:E:492:ARG:HH22	1.85	0.42
2:E:438:TYR:O	2:E:442:LEU:HB2	2.20	0.42
2:E:911:GLN:NE2	2:E:936:ILE:HG13	2.32	0.42
3:G:112:THR:HG21	3:G:117:ARG:HB2	2.02	0.42
4:I:204:ASP:H	4:I:275:ARG:NH1	2.16	0.42
4:I:375:LEU:HB2	4:I:408:LEU:HD22	2.02	0.42
4:I:759:ALA:HA	4:I:762:GLU:CD	2.40	0.42
4:I:1085:GLY:O	4:I:1089:LEU:HB3	2.20	0.42
4:I:1167:LEU:HD23	4:I:1171:THR:OG1	2.19	0.42
5:L:12:PRO:HG2	5:L:51:LEU:HD22	2.01	0.42
5:L:157:CYS:SG	5:L:163:SER:OG	2.60	0.42
5:L:330:ASP:OD1	5:L:331:TYR:N	2.53	0.42
5:L:598:LEU:O	5:L:626:ARG:NE	2.53	0.42
5:L:831:TYR:HA	5:L:834:GLY:O	2.20	0.42
5:L:906:TYR:HA	5:L:951:VAL:HG21	2.01	0.42
5:L:931:PHE:HA	5:L:967:LEU:HD22	2.02	0.42
2:E:539:ARG:HA	2:E:539:ARG:HD2	1.82	0.41
3:G:185:LYS:HE2	3:G:185:LYS:HB3	1.82	0.41
3:G:417:LEU:HD22	3:G:453:ILE:HG21	2.02	0.41
3:G:476:ALA:HB1	3:G:504:THR:HA	2.02	0.41
3:G:576:VAL:HG11	3:G:600:PRO:HD2	2.02	0.41
3:G:1301:ARG:HA	3:G:1301:ARG:HD3	1.71	0.41
4:I:292:ASP:HB2	4:I:336:GLU:O	2.20	0.41
4:I:664:ALA:O	4:I:668:LYS:HG2	2.19	0.41
4:I:797:GLU:OE2	4:I:837:ARG:HB2	2.20	0.41
5:L:79:ALA:HA	5:L:101:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:587:TRP:HB3	5:L:610:ILE:HD11	2.02	0.41
5:L:637:ALA:O	5:L:641:ALA:CB	2.68	0.41
5:L:723:TYR:CE2	5:L:745:GLN:HB3	2.52	0.41
1:C:719:ILE:HD12	1:C:722:VAL:HB	2.02	0.41
1:C:766:MET:HG3	1:C:788:LEU:HG	2.01	0.41
1:C:855:PHE:HD2	1:C:864:GLY:HA2	1.85	0.41
2:E:40:PHE:CD1	2:E:59:LEU:HB2	2.55	0.41
2:E:1054:ASP:OD1	2:E:1054:ASP:N	2.44	0.41
3:G:724:PHE:CE1	3:G:756:CYS:HA	2.55	0.41
4:I:266:TYR:HD1	4:I:285:LYS:HD2	1.84	0.41
4:I:535:PRO:HA	4:I:542:LEU:HB3	2.01	0.41
5:L:158:PHE:HA	5:L:181:PRO:HB3	2.01	0.41
5:L:495:ASN:HB3	5:L:516:MET:HB3	2.02	0.41
5:L:508:MET:SD	5:L:521:THR:HG23	2.60	0.41
5:L:725:ARG:HH22	5:L:732:LYS:NZ	2.18	0.41
5:L:857:TYR:N	5:L:907:GLU:OE1	2.52	0.41
1:C:199:CYS:HB2	1:C:233:LEU:HG	2.02	0.41
1:C:1109:ALA:HB1	2:E:815:HIS:CD2	2.54	0.41
2:E:154:GLN:NE2	2:E:168:GLU:OE1	2.53	0.41
2:E:1207:MET:HE1	2:E:1241:LEU:HD11	2.01	0.41
2:E:1273:TRP:O	2:E:1276:MET:HG2	2.21	0.41
3:G:387:PHE:HD1	3:G:392:ALA:HB2	1.85	0.41
3:G:828:GLY:HA3	4:I:712:GLY:H	1.85	0.41
3:G:980:TYR:HA	3:G:985:ARG:HG3	2.02	0.41
4:I:79:LEU:HB3	4:I:92:TRP:HE3	1.86	0.41
4:I:609:LEU:HD22	4:I:669:LEU:HA	2.02	0.41
4:I:949:CYS:SG	4:I:958:ARG:NH2	2.89	0.41
5:L:627:LYS:HB2	5:L:627:LYS:HE2	1.86	0.41
1:C:30:ALA:HB1	1:C:38:LEU:HG	2.02	0.41
1:C:33:GLY:HA3	1:C:37:LEU:HB3	2.03	0.41
2:E:107:ASP:HB3	2:E:133:VAL:HG13	2.01	0.41
2:E:944:SER:HA	2:E:947:ALA:HB3	2.02	0.41
2:E:1036:TYR:HB2	2:E:1105:TRP:CE2	2.55	0.41
2:E:1104:ARG:HD2	2:E:1104:ARG:HA	1.82	0.41
2:E:1321:TYR:HA	2:E:1348:LYS:HD2	2.01	0.41
3:G:266:ALA:HB1	3:G:303:LEU:HD13	2.02	0.41
3:G:389:ASP:HB3	3:G:431:LYS:HG2	2.02	0.41
3:G:494:LEU:HB3	3:G:523:ARG:HH22	1.85	0.41
4:I:266:TYR:HE2	4:I:268:ALA:HB2	1.86	0.41
4:I:376:TYR:CE1	4:I:386:LEU:HB3	2.48	0.41
4:I:960:TYR:HA	4:I:991:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1018:VAL:HG13	4:I:1019:ALA:H	1.85	0.41
4:I:1115:PHE:CD2	4:I:1365:GLY:HA3	2.54	0.41
5:L:89:LYS:HB2	5:L:89:LYS:HE2	1.84	0.41
5:L:324:VAL:HG11	5:L:364:HIS:CD2	2.54	0.41
5:L:724:ASP:O	5:L:727:ILE:HG22	2.19	0.41
1:C:517:VAL:HG22	1:C:533:VAL:HG22	2.02	0.41
1:C:707:ASP:O	1:C:711:VAL:HG23	2.20	0.41
1:C:923:ILE:HD13	1:C:923:ILE:HA	1.93	0.41
2:E:304:PHE:HB2	2:E:476:LEU:HD11	2.02	0.41
2:E:306:ARG:NH1	2:E:338:GLU:HG2	2.35	0.41
2:E:315:LEU:HD21	2:E:343:LYS:HZ2	1.85	0.41
3:G:717:THR:OG1	3:G:751:ASN:OD1	2.37	0.41
3:G:1081:MET:HG3	3:G:1101:ARG:HH21	1.85	0.41
4:I:481:ILE:HD12	4:I:512:TYR:CE2	2.55	0.41
4:I:509:LEU:HD12	4:I:509:LEU:HA	1.97	0.41
4:I:617:THR:HG22	4:I:633:LYS:HE3	2.03	0.41
4:I:656:ARG:CZ	4:I:662:ARG:HD3	2.50	0.41
4:I:950:LEU:HD22	4:I:978:PHE:CD1	2.54	0.41
5:L:245:VAL:H	5:L:259:ALA:HB3	1.85	0.41
5:L:872:LEU:HB2	5:L:893:PHE:CG	2.54	0.41
1:C:970:PHE:O	1:C:973:ARG:HG2	2.21	0.41
1:C:1040:LEU:HD12	1:C:1040:LEU:HA	1.92	0.41
2:E:195:LYS:HB3	2:E:230:MET:SD	2.60	0.41
2:E:259:ALA:O	2:E:263:MET:HG2	2.20	0.41
3:G:5:TYR:CZ	3:G:398:VAL:HG13	2.56	0.41
3:G:385:TYR:HE2	3:G:678:ASN:HD22	1.69	0.41
3:G:1056:LEU:HD12	3:G:1056:LEU:HA	1.77	0.41
3:G:1310:ILE:HG13	3:G:1319:ALA:HB3	2.02	0.41
4:I:782:PRO:HD2	4:I:820:VAL:HG22	2.03	0.41
4:I:789:CYS:O	4:I:808:HIS:HB3	2.19	0.41
4:I:868:LEU:HA	4:I:868:LEU:HD23	1.75	0.41
4:I:1069:LEU:HD21	4:I:1091:TYR:HD1	1.85	0.41
4:I:1143:PHE:CE2	4:I:1310:CYS:HB2	2.56	0.41
4:I:1219:LEU:HA	4:I:1260:GLU:HA	2.02	0.41
5:L:75:ALA:HA	5:L:85:ILE:HA	2.02	0.41
5:L:278:ALA:HA	5:L:288:MET:HE1	2.02	0.41
1:C:171:ARG:HH21	1:C:186:ASP:HB2	1.84	0.41
1:C:600:PHE:CZ	1:C:611:PHE:HB2	2.55	0.41
1:C:868:PHE:HB3	1:C:873:ASP:HB3	2.03	0.41
2:E:552:ARG:HA	2:E:552:ARG:HD2	1.87	0.41
2:E:611:VAL:O	2:E:615:ASN:N	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:678:ALA:H	2:E:681:ALA:HB3	1.85	0.41
2:E:1258:LEU:HD23	2:E:1258:LEU:HA	1.93	0.41
3:G:9:ILE:HB	3:G:375:ILE:HB	2.03	0.41
3:G:841:ASP:O	3:G:845:LEU:N	2.47	0.41
3:G:1337:ALA:O	3:G:1338:ARG:HG2	2.20	0.41
4:I:673:ARG:HH22	4:I:702:ASP:HB3	1.86	0.41
4:I:737:MET:SD	4:I:743:ASP:HB3	2.61	0.41
4:I:987:GLY:O	4:I:990:GLU:HB2	2.20	0.41
4:I:1057:VAL:O	4:I:1061:LEU:HG	2.21	0.41
4:I:1167:LEU:HA	4:I:1199:PHE:CE2	2.56	0.41
5:L:2:ARG:NH1	5:L:294:SER:HB3	2.36	0.41
5:L:65:VAL:HG12	5:L:76:SER:HA	2.03	0.41
5:L:72:LYS:HB3	5:L:73:ARG:HD2	2.02	0.41
5:L:125:TRP:HA	5:L:129:GLN:HE21	1.85	0.41
5:L:618:LEU:HD11	5:L:639:ILE:HA	2.03	0.41
5:L:705:GLU:HG2	5:L:713:ALA:HB1	2.02	0.41
1:C:242:ARG:HH22	1:C:248:ASN:HB3	1.86	0.41
1:C:347:THR:OG1	1:C:366:ASP:OD1	2.22	0.41
2:E:173:LEU:HG	2:E:196:ILE:HG21	2.03	0.41
2:E:383:LEU:HD11	2:E:640:VAL:HG21	2.02	0.41
2:E:618:LEU:O	2:E:622:LYS:HB2	2.21	0.41
2:E:979:LEU:HD12	2:E:979:LEU:HA	1.95	0.41
3:G:9:ILE:HD12	3:G:29:LEU:HD23	2.03	0.41
3:G:422:MET:HE2	3:G:436:VAL:HG23	2.02	0.41
3:G:780:ALA:O	3:G:784:ALA:CB	2.68	0.41
4:I:770:TRP:HH2	4:I:795:MET:HG2	1.85	0.41
4:I:924:GLU:O	4:I:929:TRP:NE1	2.53	0.41
4:I:1060:TYR:CE2	4:I:1068:ALA:HA	2.55	0.41
5:L:295:THR:HB	5:L:306:TYR:HB2	2.02	0.41
5:L:723:TYR:CG	5:L:746:LEU:HD13	2.55	0.41
1:C:214:TRP:CE2	1:C:229:LEU:HB2	2.55	0.41
1:C:272:VAL:O	1:C:291:GLN:N	2.46	0.41
1:C:535:ARG:HB2	1:C:579:HIS:CE1	2.56	0.41
1:C:868:PHE:HB3	1:C:873:ASP:O	2.21	0.41
1:C:882:VAL:HG22	1:C:890:ALA:HB1	2.03	0.41
1:C:940:GLN:O	1:C:944:LYS:HG3	2.21	0.41
1:C:1110:MET:HG2	2:E:817:TYR:CE1	2.55	0.41
2:E:12:TYR:O	2:E:16:GLY:N	2.54	0.41
2:E:156:GLN:HG3	2:E:229:ARG:HG2	2.02	0.41
2:E:298:PHE:CE1	2:E:325:ALA:HB1	2.56	0.41
2:E:310:SER:OG	2:E:311:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:811:LEU:HA	2:E:811:LEU:HD23	1.93	0.41
2:E:1165:GLU:O	2:E:1169:ILE:HG13	2.20	0.41
2:E:1272:ALA:O	2:E:1276:MET:HE2	2.21	0.41
3:G:130:TRP:CE2	3:G:140:HIS:HB2	2.56	0.41
3:G:315:GLY:HA3	3:G:355:ALA:HB3	2.03	0.41
3:G:392:ALA:HB3	3:G:699:VAL:HG21	2.02	0.41
3:G:668:ILE:HD11	3:G:699:VAL:HG13	2.03	0.41
3:G:676:LEU:HD23	3:G:701:LYS:HG2	2.03	0.41
3:G:677:THR:OG1	3:G:700:SER:OG	2.30	0.41
3:G:959:ALA:HB1	3:G:983:ALA:HB1	2.03	0.41
3:G:1035:MET:HG2	3:G:1059:ILE:CG1	2.47	0.41
3:G:1325:ASP:HA	3:G:1328:ALA:HB3	2.02	0.41
4:I:12:LEU:HD11	4:I:356:MET:HB2	2.03	0.41
4:I:252:TRP:NE1	4:I:258:ILE:HG12	2.35	0.41
4:I:531:VAL:HG23	4:I:547:ASP:HA	2.03	0.41
4:I:598:PRO:HA	4:I:604:PRO:HA	2.02	0.41
4:I:744:TYR:CE2	4:I:767:LEU:HD12	2.56	0.41
4:I:993:LEU:HD11	4:I:1014:PHE:HA	2.03	0.41
4:I:1015:ALA:HA	4:I:1018:VAL:HG12	2.02	0.41
4:I:1155:LYS:HE2	4:I:1155:LYS:HB2	1.92	0.41
4:I:1187:ARG:NH1	4:I:1278:THR:OG1	2.54	0.41
5:L:247:LEU:HD12	5:L:247:LEU:HA	1.89	0.41
5:L:303:ARG:HH21	5:L:360:ASP:HA	1.85	0.41
5:L:371:ILE:HD13	5:L:375:LEU:HD23	2.02	0.41
5:L:469:LYS:O	5:L:501:TRP:NE1	2.53	0.41
5:L:739:LEU:O	5:L:743:VAL:HG23	2.20	0.41
5:L:799:LEU:C	5:L:801:HIS:H	2.23	0.41
2:E:874:THR:O	2:E:878:GLN:NE2	2.54	0.41
2:E:967:HIS:CE1	2:E:969:PRO:HG2	2.56	0.41
2:E:1029:LEU:HD13	2:E:1039:LEU:HD12	2.02	0.41
2:E:1304:SER:HA	2:E:1307:VAL:HB	2.03	0.41
2:E:1333:LYS:HD3	2:E:1333:LYS:HA	1.77	0.41
3:G:85:ILE:HD13	3:G:120:THR:HG21	2.02	0.41
3:G:479:ASN:OD1	3:G:479:ASN:N	2.53	0.41
3:G:721:LEU:HA	3:G:721:LEU:HD23	1.81	0.41
3:G:1127:ALA:H	3:G:1157:LYS:NZ	2.13	0.41
5:L:748:LYS:HZ3	5:L:776:LYS:HB3	1.85	0.41
5:L:812:LEU:HB3	5:L:816:LYS:NZ	2.36	0.41
1:C:5:LEU:HD11	1:C:305:VAL:HG22	2.03	0.40
1:C:82:TRP:CZ3	1:C:89:LEU:HB2	2.55	0.40
1:C:522:SER:O	1:C:526:LEU:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:263:MET:SD	2:E:304:PHE:HB3	2.61	0.40
2:E:496:GLN:HB2	2:E:654:THR:HB	2.03	0.40
3:G:846:LYS:HE3	5:L:842:ARG:HD2	2.02	0.40
3:G:967:TYR:CE2	3:G:979:TYR:HE2	2.39	0.40
3:G:986:TYR:O	3:G:1013:VAL:HG21	2.21	0.40
3:G:999:ASP:HA	3:G:1002:LEU:HB3	2.03	0.40
3:G:1329:LEU:HA	3:G:1329:LEU:HD12	1.83	0.40
4:I:543:VAL:HG23	4:I:575:TRP:CH2	2.56	0.40
4:I:545:GLU:OE1	4:I:569:ARG:NH1	2.54	0.40
4:I:764:ARG:HA	4:I:764:ARG:HD3	1.91	0.40
4:I:975:LEU:HD13	4:I:991:PHE:CD2	2.55	0.40
4:I:1013:THR:HA	4:I:1016:ARG:HB3	2.03	0.40
5:L:197:ALA:N	5:L:205:LYS:O	2.49	0.40
5:L:305:ALA:HA	5:L:315:ILE:HA	2.03	0.40
5:L:474:ASP:OD1	5:L:474:ASP:N	2.51	0.40
5:L:847:LEU:HB2	5:L:863:TYR:CE2	2.55	0.40
5:L:911:LYS:HB3	5:L:915:SER:O	2.20	0.40
1:C:30:ALA:HB2	1:C:40:VAL:HG22	2.03	0.40
1:C:551:SER:CB	1:C:590:MET:HG3	2.51	0.40
1:C:711:VAL:HG13	5:L:668:ASP:HA	2.03	0.40
1:C:846:PRO:HA	1:C:871:ALA:HB1	2.04	0.40
2:E:539:ARG:NH1	2:E:570:LEU:HA	2.36	0.40
2:E:602:PRO:HA	2:E:605:HIS:HB2	2.03	0.40
2:E:900:TYR:OH	2:E:939:ASP:OD2	2.37	0.40
2:E:1141:VAL:HG23	2:E:1168:ALA:HB1	2.02	0.40
2:E:1323:GLU:HA	5:L:264:TRP:CZ3	2.56	0.40
3:G:70:HIS:CD2	3:G:75:LEU:HD23	2.56	0.40
3:G:435:LEU:HD21	3:G:466:MET:SD	2.62	0.40
3:G:462:THR:OG1	3:G:482:GLU:OE1	2.34	0.40
3:G:696:THR:OG1	3:G:697:SER:N	2.54	0.40
4:I:201:LYS:HB2	4:I:213:THR:HG21	2.04	0.40
4:I:357:HIS:HB3	4:I:359:PHE:CE2	2.56	0.40
4:I:560:HIS:CG	4:I:604:PRO:HG2	2.56	0.40
4:I:856:ASN:HD22	4:I:861:PHE:N	2.19	0.40
4:I:1304:TRP:CZ3	4:I:1313:PRO:HA	2.56	0.40
5:L:39:ASN:HA	5:L:62:ILE:HG13	2.02	0.40
5:L:276:PHE:HB3	5:L:288:MET:HB3	2.04	0.40
5:L:762:ARG:NH2	5:L:767:PHE:HA	2.36	0.40
1:C:20:ILE:HG12	1:C:29:ILE:HD11	2.03	0.40
1:C:346:ASN:O	1:C:367:THR:N	2.42	0.40
2:E:32:ARG:HD3	2:E:32:ARG:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:290:GLU:OE2	2:E:293:ASN:ND2	2.54	0.40
2:E:617:LYS:HB3	2:E:620:ASP:HB2	2.02	0.40
2:E:770:TYR:HA	2:E:773:LEU:HG	2.02	0.40
3:G:64:CYS:SG	3:G:67:ILE:HG23	2.62	0.40
3:G:229:ARG:HG2	3:G:235:THR:HA	2.04	0.40
3:G:753:ALA:HB3	3:G:764:VAL:HG21	2.03	0.40
3:G:849:HIS:HB3	3:G:868:HIS:O	2.21	0.40
3:G:910:LYS:NZ	3:G:913:GLU:OE1	2.42	0.40
3:G:1090:VAL:HG22	3:G:1102:ALA:HB1	2.04	0.40
4:I:461:VAL:HG12	4:I:463:VAL:HG23	2.04	0.40
4:I:776:LEU:O	4:I:780:LEU:HB2	2.21	0.40
4:I:887:PHE:HD2	4:I:906:LEU:HD21	1.86	0.40
4:I:929:TRP:CE3	4:I:952:ARG:HG2	2.57	0.40
4:I:949:CYS:SG	4:I:959:ALA:HB2	2.61	0.40
4:I:1002:PHE:O	4:I:1006:MET:HG2	2.21	0.40
4:I:1098:GLY:HA2	4:I:1101:ARG:NE	2.34	0.40
4:I:1293:LEU:HD23	4:I:1319:PHE:HE1	1.86	0.40
5:L:17:VAL:HG11	5:L:39:ASN:H	1.86	0.40
5:L:565:TYR:CE2	5:L:577:VAL:HG21	2.57	0.40
5:L:855:THR:HA	5:L:857:TYR:CE1	2.57	0.40
5:L:951:VAL:O	5:L:955:LEU:HB3	2.21	0.40
1:C:435:ALA:N	1:C:442:TYR:O	2.55	0.40
2:E:919:ARG:NH1	2:E:926:VAL:O	2.55	0.40
2:E:979:LEU:HA	2:E:983:ASP:H	1.86	0.40
2:E:1081:ILE:HG22	2:E:1112:HIS:CE1	2.56	0.40
2:E:1137:SER:HB2	2:E:1140:ALA:HB3	2.02	0.40
3:G:1047:CYS:SG	3:G:1056:LEU:HD13	2.62	0.40
4:I:481:ILE:HD13	4:I:481:ILE:HA	1.94	0.40
4:I:1084:LEU:HA	4:I:1084:LEU:HD12	1.79	0.40
4:I:1295:THR:HG22	4:I:1297:LYS:HD2	2.02	0.40
4:I:1334:ASP:OD1	4:I:1334:ASP:N	2.47	0.40
5:L:386:HIS:HD2	5:L:425:ARG:HD3	1.86	0.40
5:L:454:HIS:CD2	5:L:480:LEU:HD22	2.56	0.40
5:L:960:VAL:HG23	5:L:971:ALA:HB3	2.04	0.40
1:C:633:GLU:HG3	1:C:658:GLU:HG2	2.04	0.40
1:C:759:ASP:HA	1:C:762:ILE:HB	2.03	0.40
2:E:315:LEU:HD21	2:E:343:LYS:NZ	2.37	0.40
2:E:574:VAL:O	2:E:578:GLN:N	2.46	0.40
2:E:815:HIS:HA	2:E:817:TYR:CZ	2.57	0.40
3:G:3:ILE:HB	3:G:383:LEU:HD11	2.04	0.40
3:G:443:GLU:HG3	3:G:445:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:444:VAL:N	3:G:457:SER:O	2.44	0.40
3:G:593:PHE:CZ	3:G:615:VAL:HG11	2.56	0.40
3:G:774:HIS:CE1	3:G:776:ARG:HB2	2.56	0.40
3:G:852:TYR:HA	3:G:855:PHE:HB3	2.03	0.40
3:G:1289:ARG:HH21	3:G:1292:ILE:HG21	1.87	0.40
3:G:1331:VAL:HG12	3:G:1335:TYR:HE2	1.86	0.40
4:I:201:LYS:NZ	4:I:227:GLN:HE21	2.19	0.40
4:I:329:LEU:HD11	4:I:349:VAL:HG11	2.04	0.40
4:I:501:ILE:HG21	4:I:542:LEU:HD21	2.02	0.40
4:I:1350:LYS:HD2	4:I:1350:LYS:HA	1.83	0.40
5:L:723:TYR:HB2	5:L:746:LEU:HD22	2.02	0.40
5:L:773:THR:HG22	5:L:776:LYS:HZ2	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1070/1224 (87%)	974 (91%)	96 (9%)	0	100	100
2	E	1321/1355 (98%)	1229 (93%)	91 (7%)	1 (0%)	51	86
3	G	1352/1409 (96%)	1191 (88%)	160 (12%)	1 (0%)	51	86
4	I	1365/1367 (100%)	1245 (91%)	116 (8%)	4 (0%)	41	77
5	L	995/1239 (80%)	872 (88%)	121 (12%)	2 (0%)	47	81
All	All	6103/6594 (93%)	5511 (90%)	584 (10%)	8 (0%)	54	86

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	730	PRO
3	G	1165	VAL

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Mol	Chain	Res	Type
4	I	1053	ALA
5	L	778	ASP
4	I	1008	HIS
4	I	1010	GLU
5	L	784	ILE
4	I	985	PHE

### 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	C	904/1005 (90%)	897 (99%)	7 (1%)	81	89
2	E	1092/1114 (98%)	1082 (99%)	10 (1%)	78	87
3	G	1117/1162 (96%)	1107 (99%)	10 (1%)	78	87
4	I	1119/1119 (100%)	1112 (99%)	7 (1%)	86	92
5	L	840/1035 (81%)	834 (99%)	6 (1%)	84	90
All	All	5072/5435 (93%)	5032 (99%)	40 (1%)	82	89

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	242	ARG
1	C	660	ARG
1	C	688	ARG
1	C	773	LYS
1	C	1025	ARG
1	C	1094	MET
1	C	1102	ARG
2	E	127	ARG
2	E	229	ARG
2	E	277	LYS
2	E	288	ARG
2	E	459	ARG
2	E	712	ARG

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Mol	Chain	Res	Type
2	E	720	LYS
2	E	948	ARG
2	E	976	LYS
2	E	1343	LYS
3	G	103	ARG
3	G	212	ARG
3	G	365	ARG
3	G	469	ASN
3	G	554	MET
3	G	793	ARG
3	G	832	LYS
3	G	866	ARG
3	G	902	ARG
3	G	1264	LYS
4	I	275	ARG
4	I	763	MET
4	I	1011	MET
4	I	1037	ARG
4	I	1105	ARG
4	I	1221	LYS
4	I	1328	ARG
5	L	2	ARG
5	L	40	ARG
5	L	250	ARG
5	L	418	LYS
5	L	467	ARG
5	L	687	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	445	GLN
1	C	814	GLN
1	C	895	GLN
2	E	20	HIS
2	E	239	GLN
2	E	254	ASN
2	E	289	GLN
3	G	58	ASN
3	G	376	ASN
3	G	698	ASN
3	G	751	ASN

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Mol	Chain	Res	Type
3	G	822	GLN
3	G	1284	GLN
4	I	88	HIS
4	I	227	GLN
4	I	536	GLN
4	I	792	HIS
4	I	811	GLN
4	I	1052	GLN
4	I	1058	GLN
5	L	19	ASN
5	L	129	GLN
5	L	345	GLN
5	L	733	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15980. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X

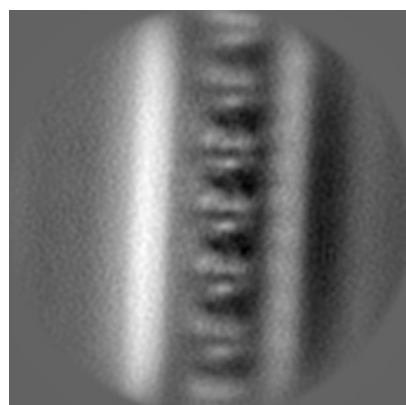


Y

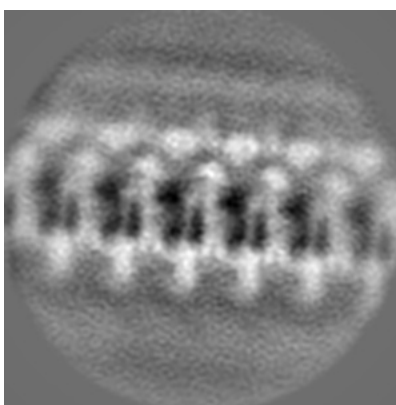


Z

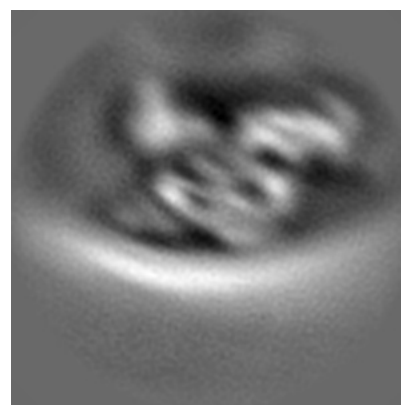
#### 6.1.2 Raw map



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: 60

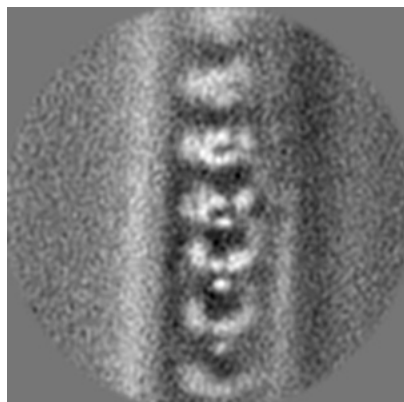


Y Index: 60

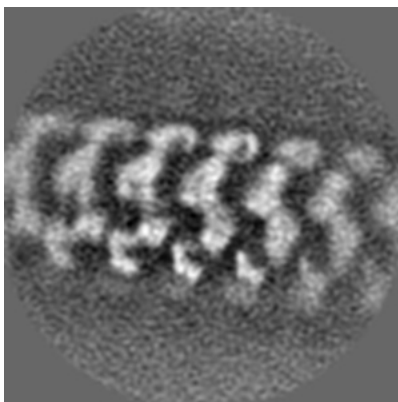


Z Index: 60

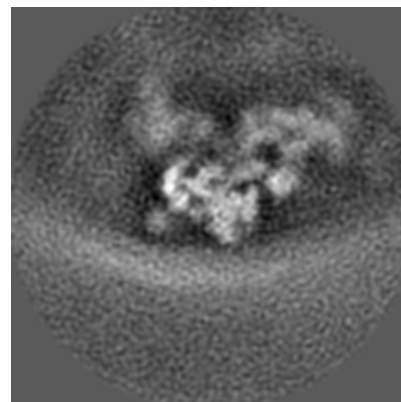
### 6.2.2 Raw map



X Index: 60



Y Index: 60



Z Index: 60

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: 48

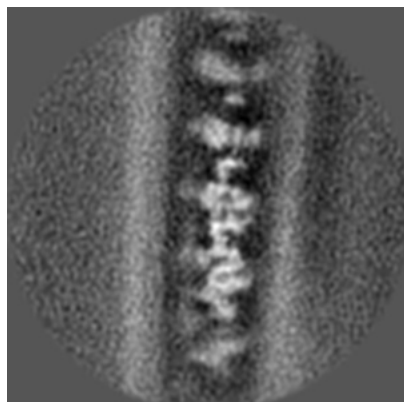


Y Index: 63

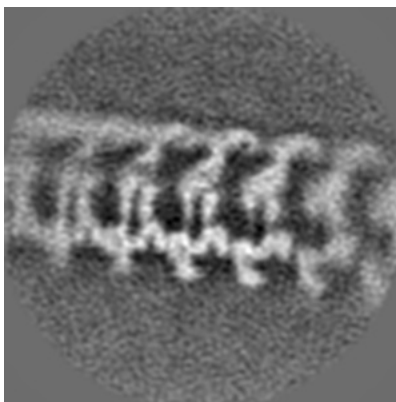


Z Index: 61

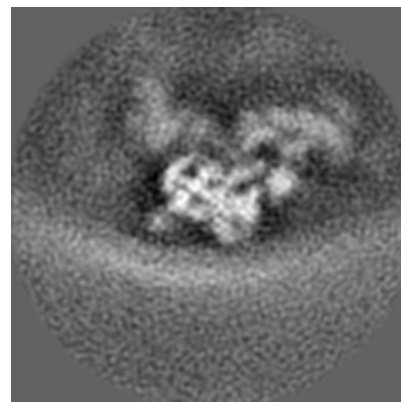
### 6.3.2 Raw map



X Index: 49



Y Index: 63



Z Index: 61

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

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

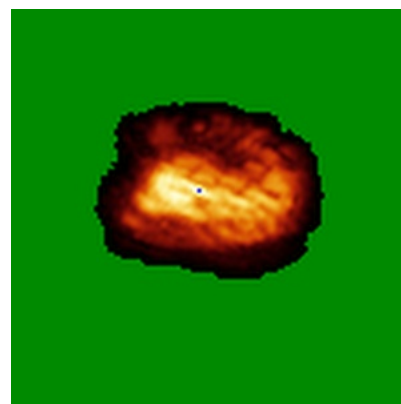
### 6.4.1 Primary map



X

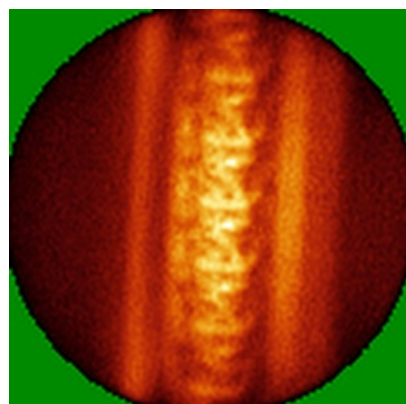


Y

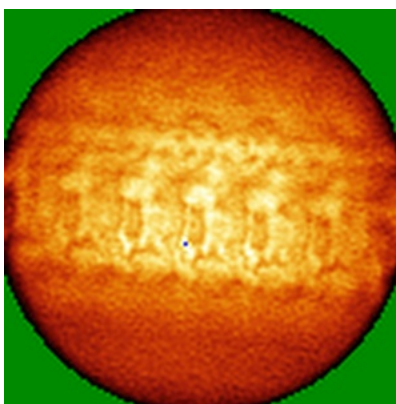


Z

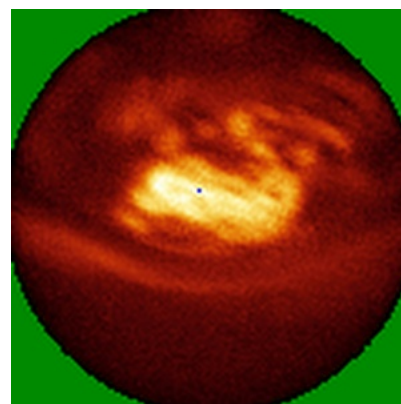
### 6.4.2 Raw map



X



Y



Z

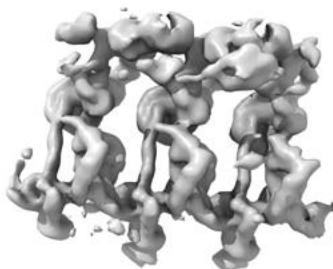
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

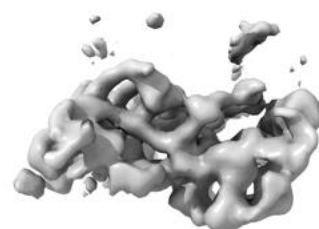
### 6.5.1 Primary map



X



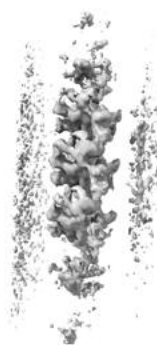
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

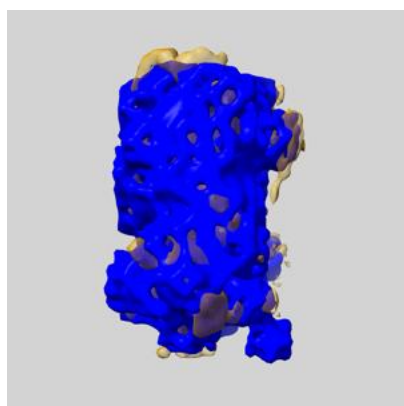
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

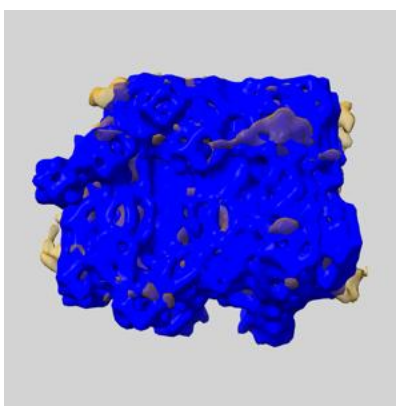
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

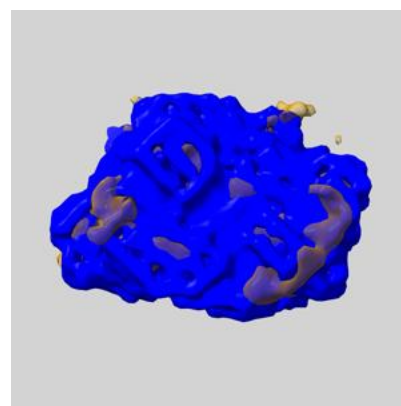
### 6.6.1 emd\_15980\_msk\_1.map [i](#)



X



Y

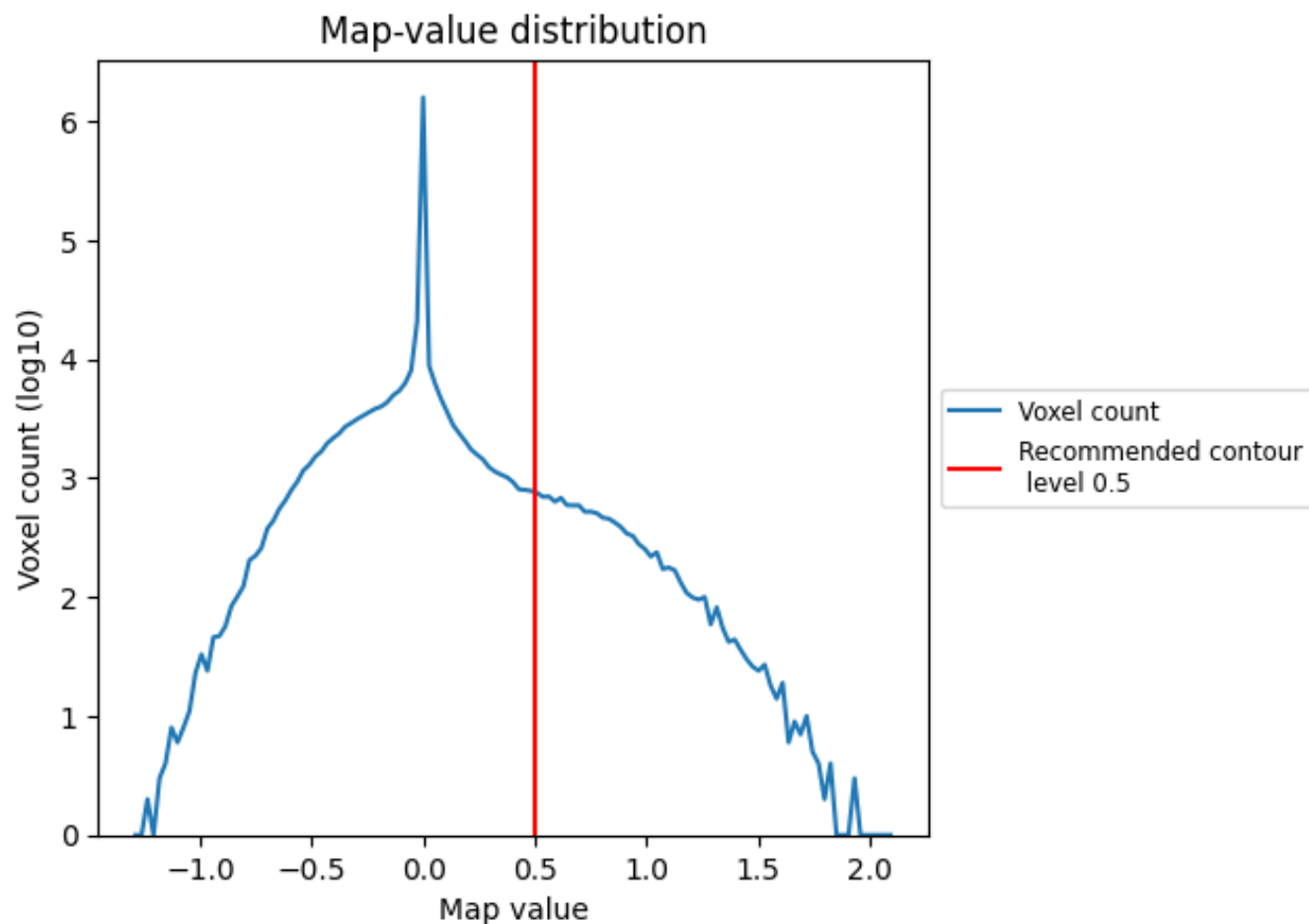


Z

## 7 Map analysis [i](#)

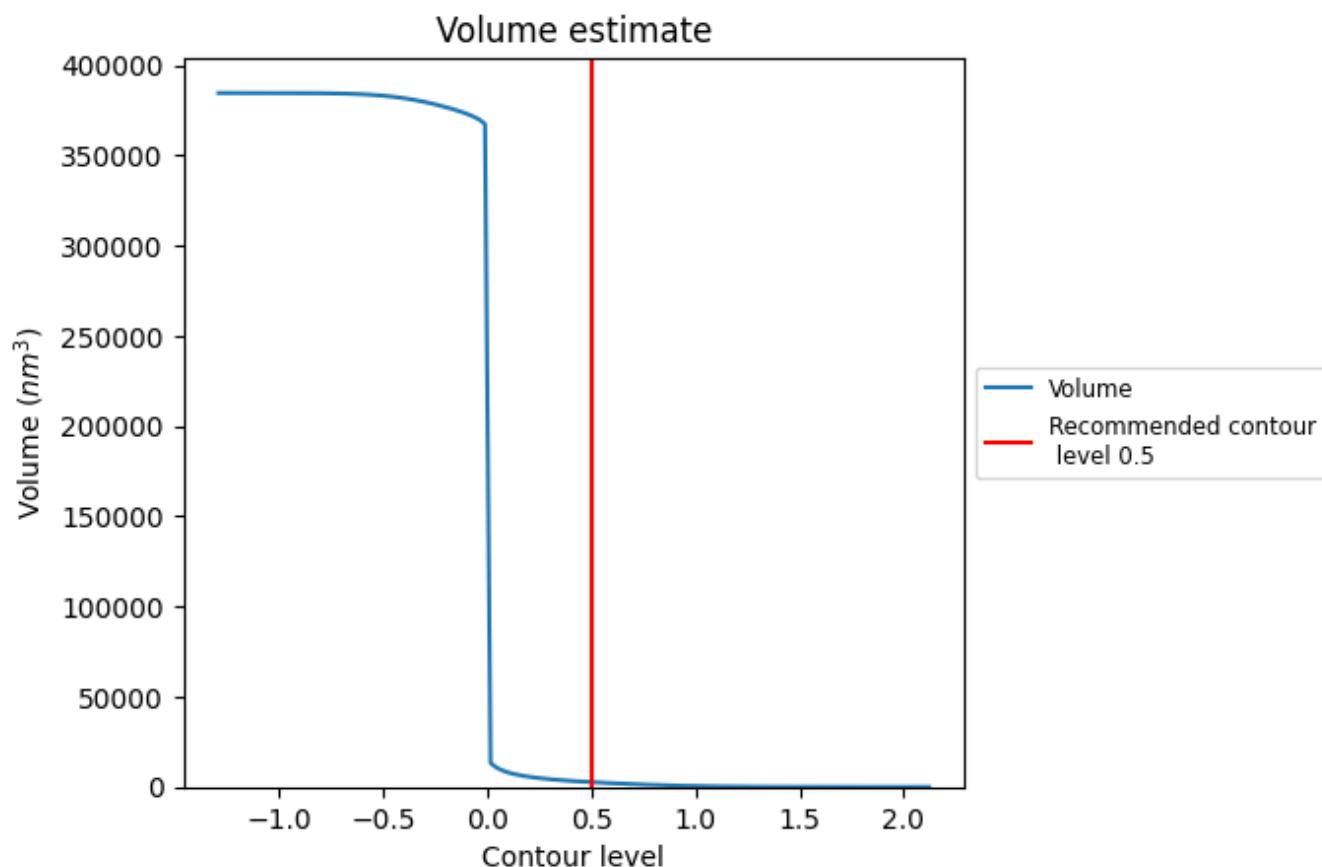
This section contains the results of statistical analysis of the map.

### 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.

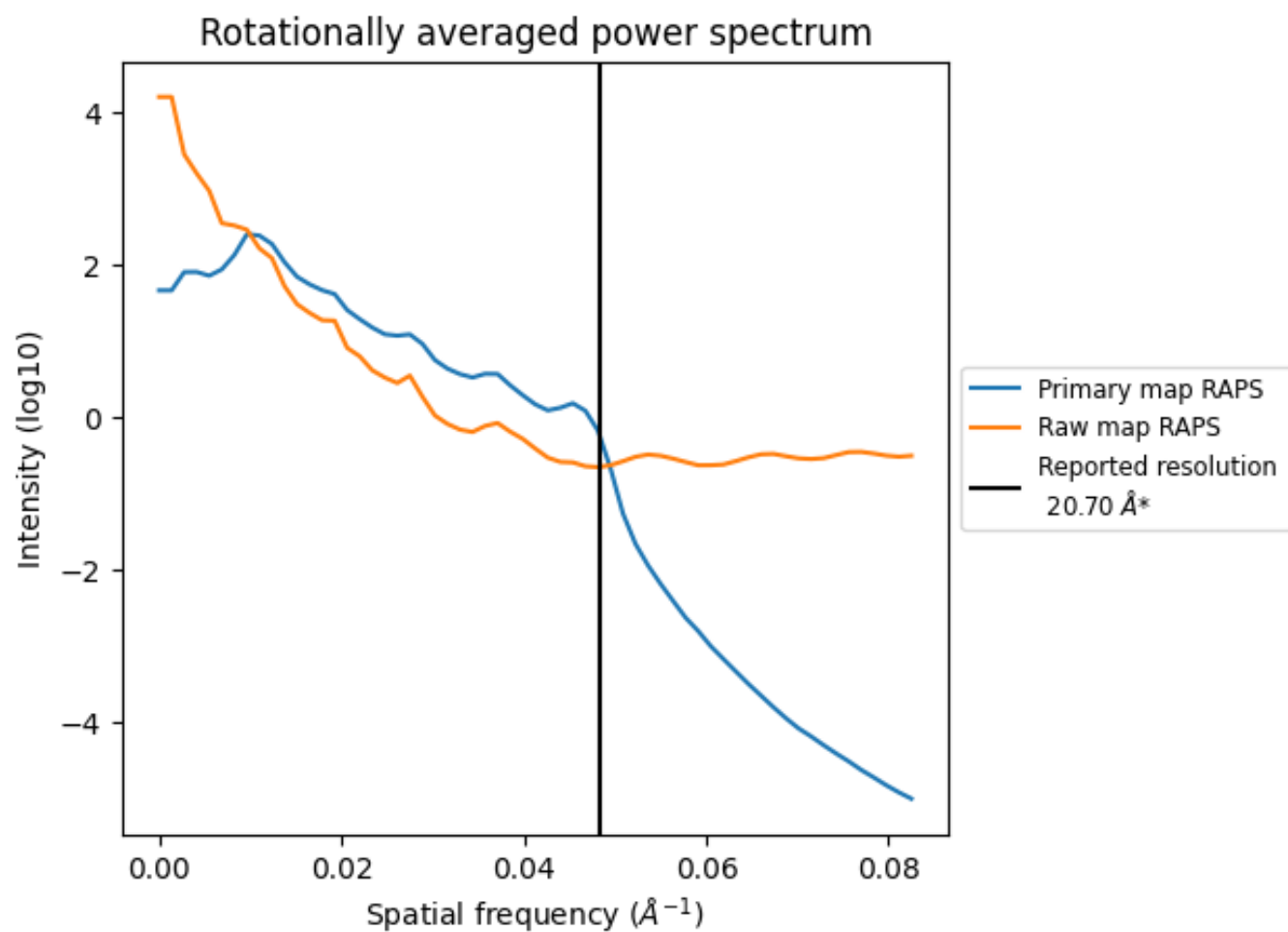
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2681 nm<sup>3</sup>; this corresponds to an approximate mass of 2422 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 ⓘ

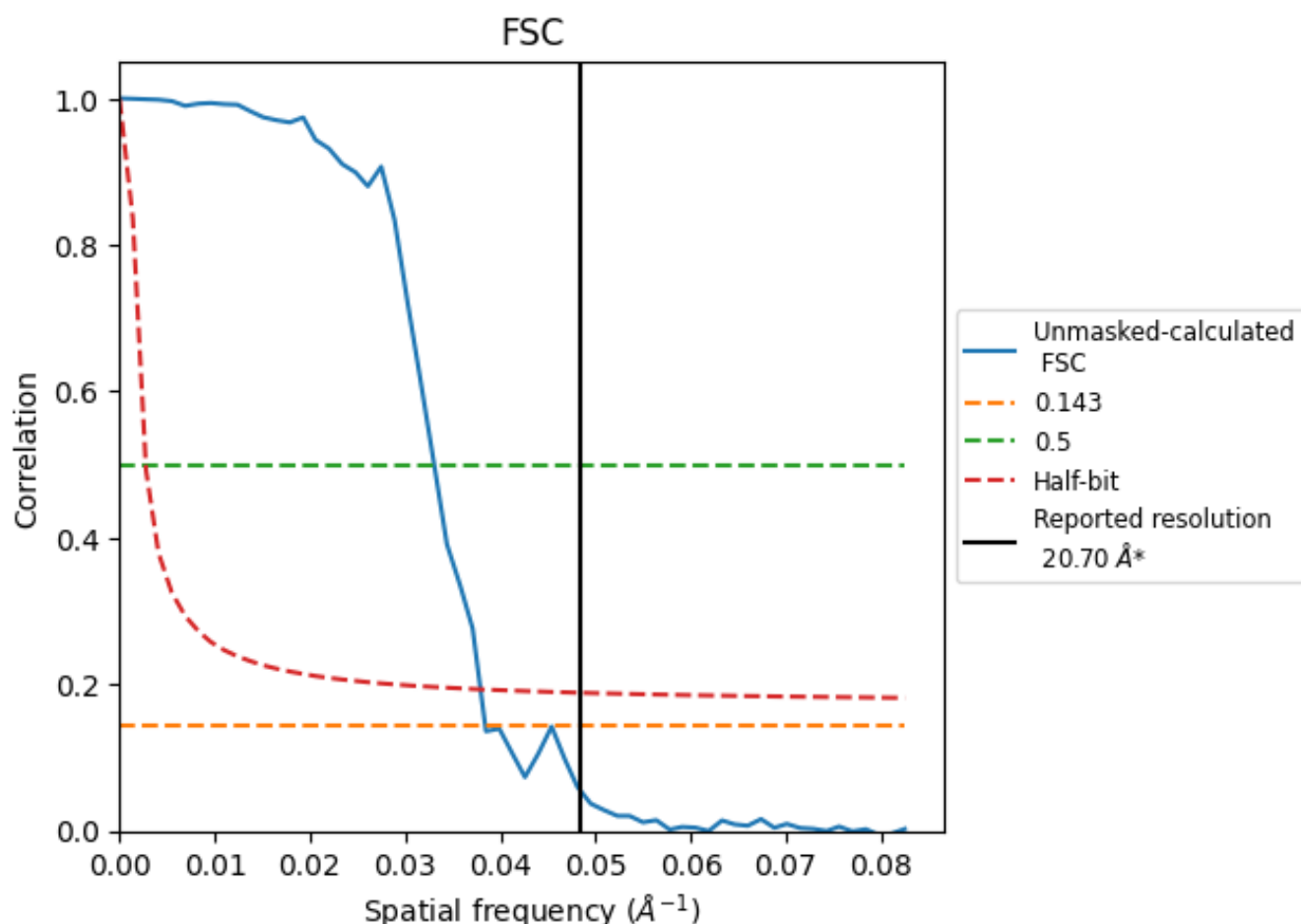


\*Reported resolution corresponds to spatial frequency of 0.048 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.048  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

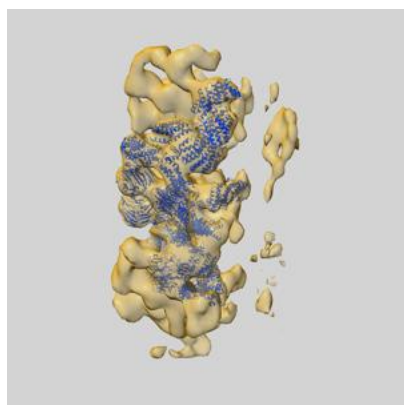
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	20.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	26.04	30.21	26.39

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 26.04 differs from the reported value 20.7 by more than 10 %

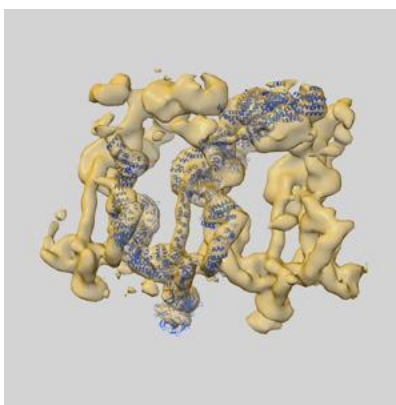
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15980 and PDB model 8BDA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

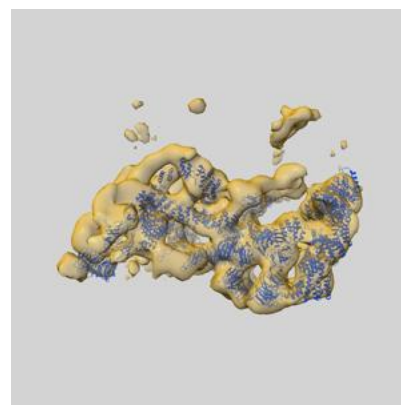
### 9.1 Map-model overlay [i](#)



X



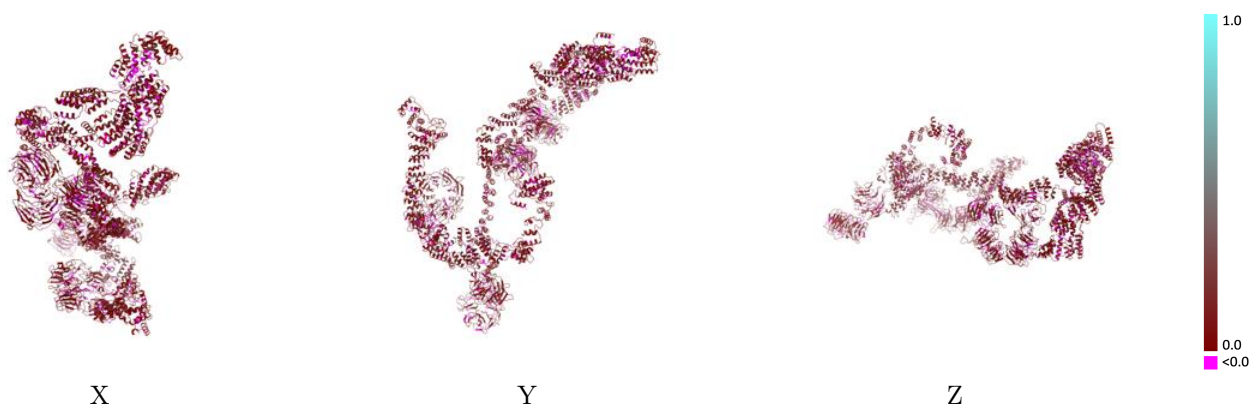
Y



Z

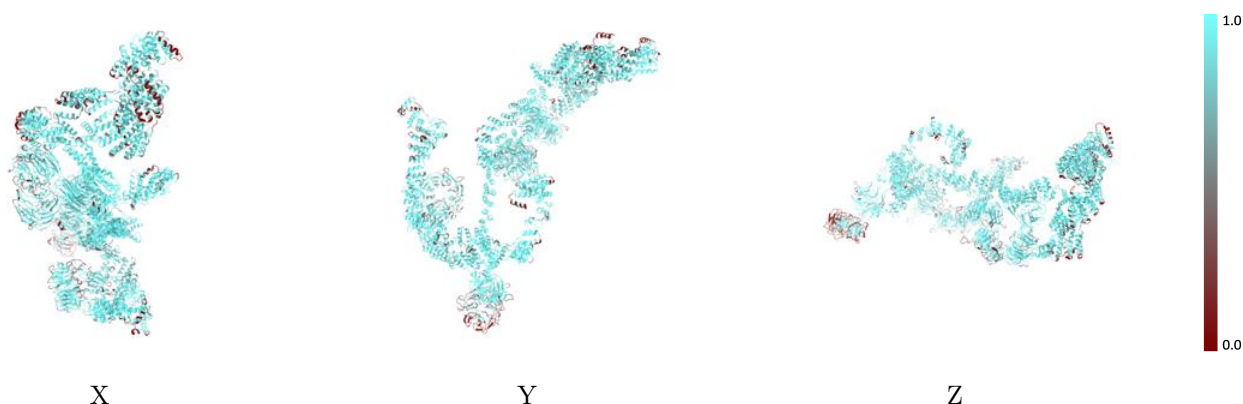
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



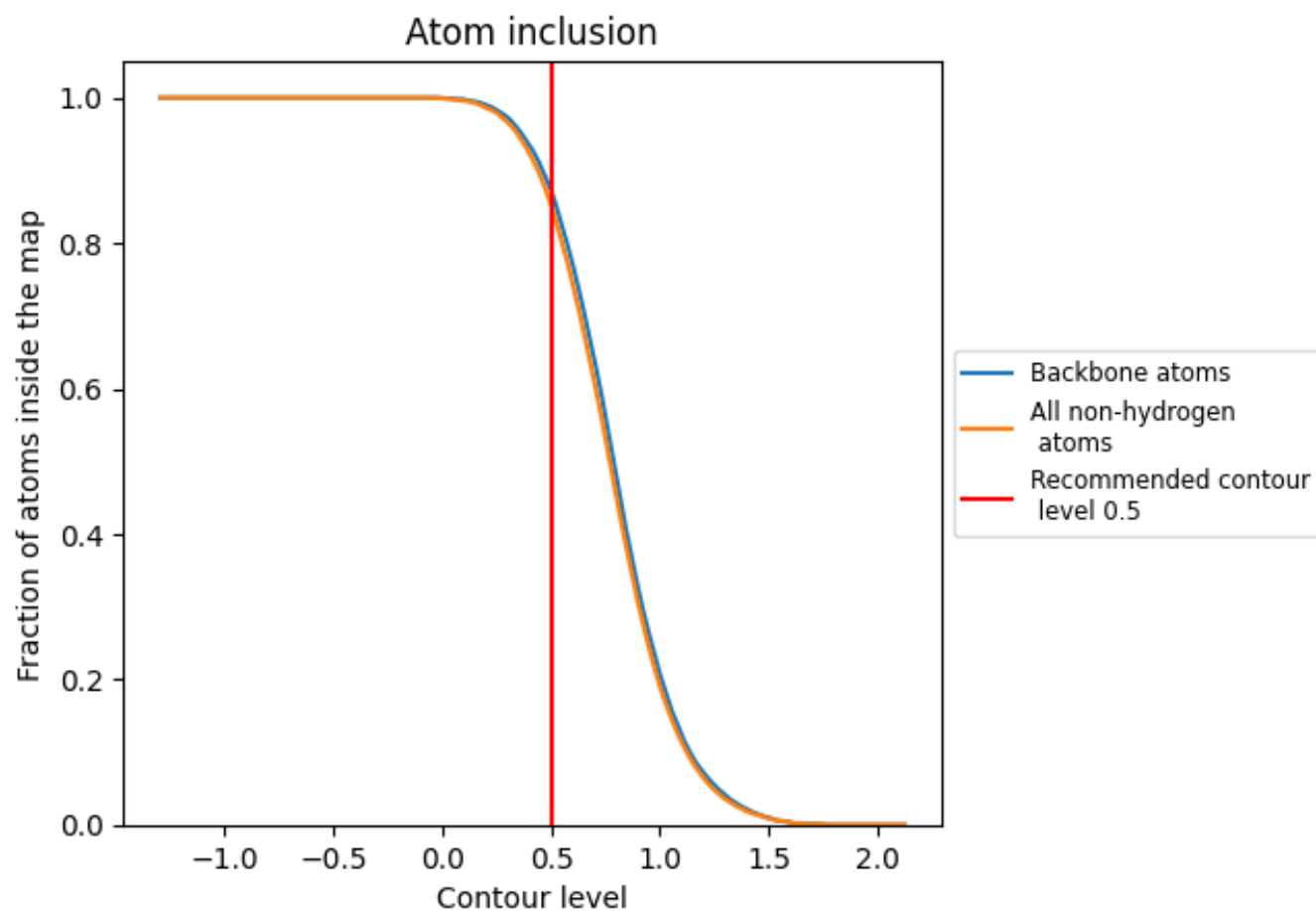
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8530	<div></div> 0.0800
C	<div></div> 0.8840	<div></div> 0.0780
E	<div></div> 0.8250	<div></div> 0.0740
G	<div></div> 0.8790	<div></div> 0.0840
I	<div></div> 0.7550	<div></div> 0.0810
L	<div></div> 0.9510	<div></div> 0.0840

