



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:53 AM UTC

PDB ID : 5W0S / pdb_00005w0s
EMDB ID : EMD-8750
Title : GroEL using cryoEM
Authors : Roh, S.H.; Chiu, W.
Deposited on : 2017-05-31
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

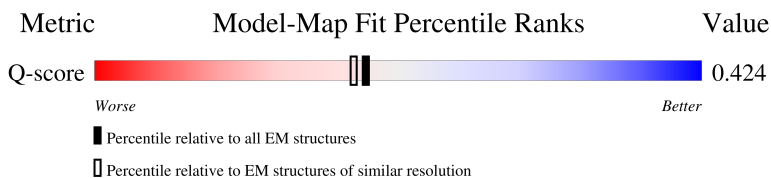
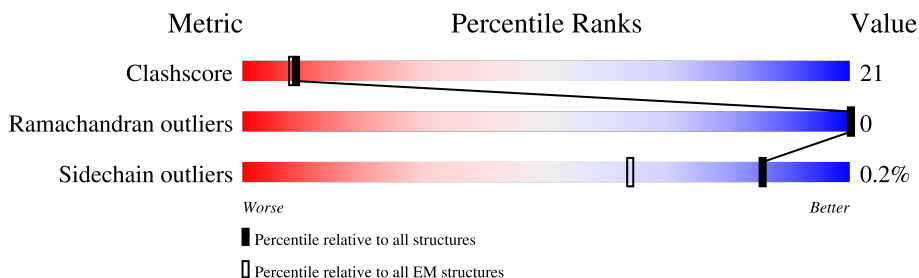
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	1-A	524	15% 81% 19%
1	1-B	524	15% 81% 19%
1	1-C	524	16% 80% 20%
1	1-D	524	15% 80% 20%

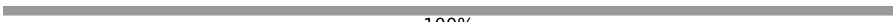
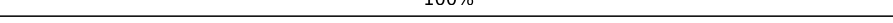
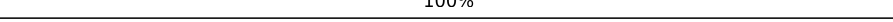
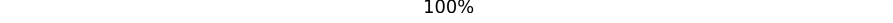
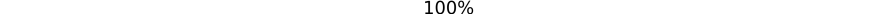
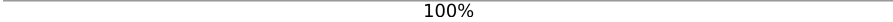
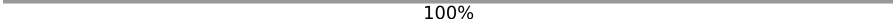
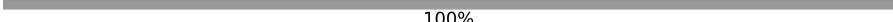
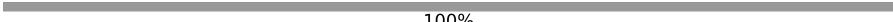
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Mol	Chain	Length	Quality of chain
1	1-E	524	16% 80% 20%
1	1-F	524	16% 81% 19%
1	1-G	524	16% 80% 20%
1	1-H	524	16% 80% 20%
1	1-I	524	15% 81% 19%
1	1-J	524	15% 81% 19%
1	1-K	524	16% 80% 20%
1	1-L	524	15% 80% 20%
1	1-M	524	15% 80% 20%
1	1-N	524	15% 80% 20%
1	2-A	524	50% 50%
1	2-B	524	100%
1	2-C	524	100%
1	2-D	524	100%
1	2-E	524	100%
1	2-F	524	100%
1	2-G	524	100%
1	2-H	524	100%
1	2-I	524	100%
1	2-J	524	100%
1	2-K	524	100%
1	2-L	524	100%
1	2-M	524	100%
1	2-N	524	100%
1	3-A	524	56% 44%

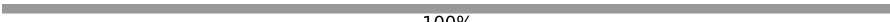
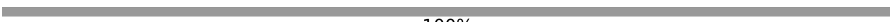
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Mol	Chain	Length	Quality of chain
1	3-B	524	 100%
1	3-C	524	 100%
1	3-D	524	 100%
1	3-E	524	 100%
1	3-F	524	 100%
1	3-G	524	 100%
1	3-H	524	 100%
1	3-I	524	 100%
1	3-J	524	 100%
1	3-K	524	 100%
1	3-L	524	 100%
1	3-M	524	 100%
1	3-N	524	 100%
1	4-A	524	 61% 39%
1	4-B	524	 100%
1	4-C	524	 100%
1	4-D	524	 100%
1	4-E	524	 100%
1	4-F	524	 100%
1	4-G	524	 100%
1	4-H	524	 100%
1	4-I	524	 100%
1	4-J	524	 100%
1	4-K	524	 100%
1	4-L	524	 100%

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Mol	Chain	Length	Quality of chain
1	4-M	524	 100%
1	4-N	524	 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 65574 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	2-A	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	3-A	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	4-A	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-B	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-C	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-D	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-E	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-F	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-G	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-H	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-I	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-J	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-K	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-L	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-M	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		
1	1-N	524	Total	C	N	O	S	0	0
			3851	2395	662	774	20		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	conflict	UNP Q6Q099
B	13	GLY	ARG	conflict	UNP Q6Q099
C	13	GLY	ARG	conflict	UNP Q6Q099
D	13	GLY	ARG	conflict	UNP Q6Q099
E	13	GLY	ARG	conflict	UNP Q6Q099
F	13	GLY	ARG	conflict	UNP Q6Q099
G	13	GLY	ARG	conflict	UNP Q6Q099
H	13	GLY	ARG	conflict	UNP Q6Q099
I	13	GLY	ARG	conflict	UNP Q6Q099
J	13	GLY	ARG	conflict	UNP Q6Q099
K	13	GLY	ARG	conflict	UNP Q6Q099
L	13	GLY	ARG	conflict	UNP Q6Q099
M	13	GLY	ARG	conflict	UNP Q6Q099
N	13	GLY	ARG	conflict	UNP Q6Q099

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	AltConf
2	1-A	19	Total O 19 19	0
2	1-B	12	Total O 12 12	0
2	1-C	14	Total O 14 14	0
2	1-D	14	Total O 14 14	0
2	1-E	10	Total O 10 10	0
2	1-F	6	Total O 6 6	0
2	1-G	13	Total O 13 13	0
2	1-H	1	Total O 1 1	0
2	1-I	3	Total O 3 3	0
2	1-J	5	Total O 5 5	0
2	1-K	1	Total O 1 1	0
2	1-L	2	Total O 2 2	0

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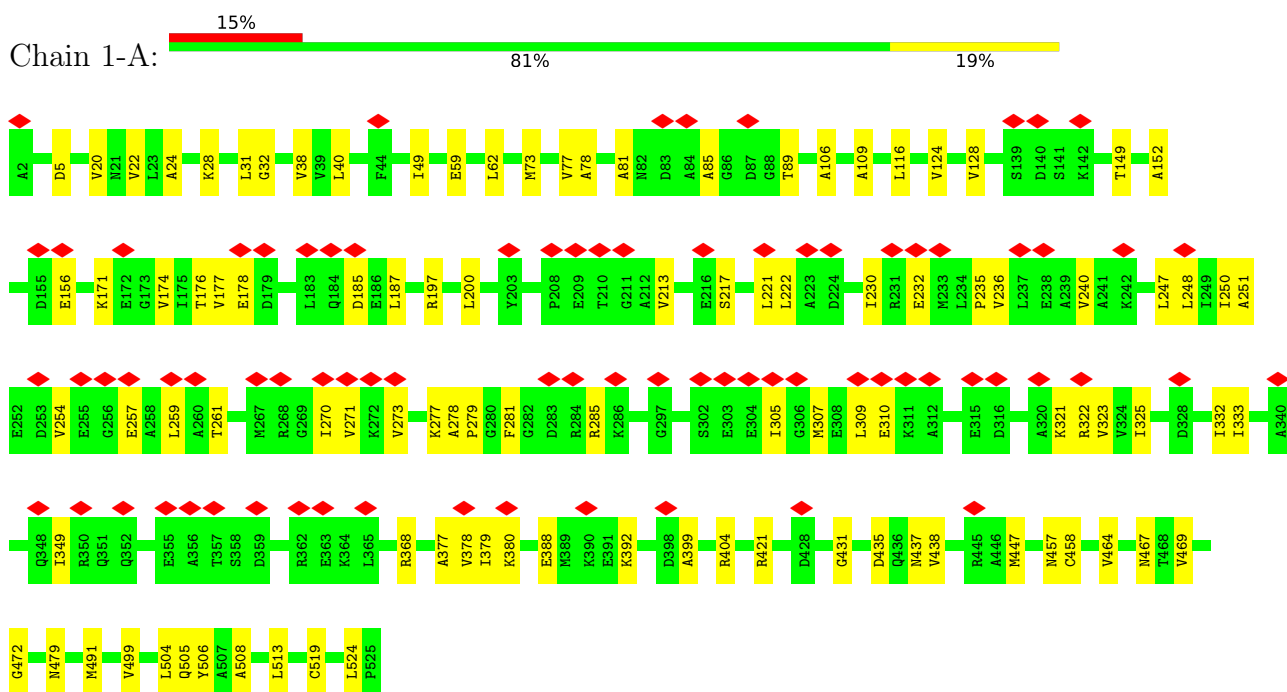
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Mol	Chain	Residues	Atoms		AltConf
2	1-M	5	Total	O	0
			5	5	
2	1-N	2	Total	O	0
			2	2	

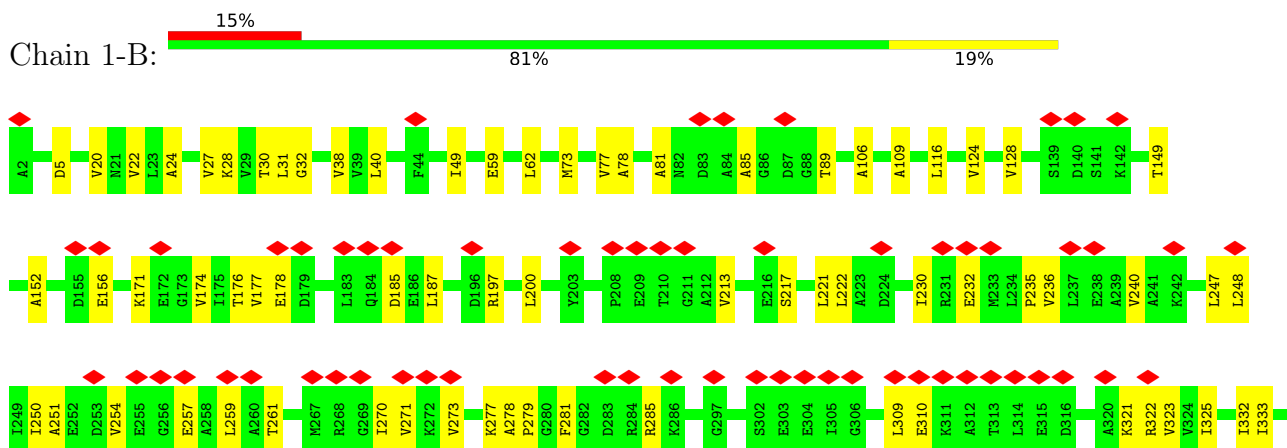
3 Residue-property plots

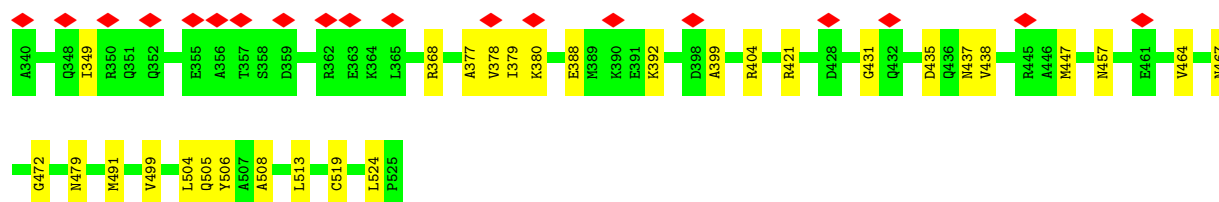
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 60 kDa chaperonin

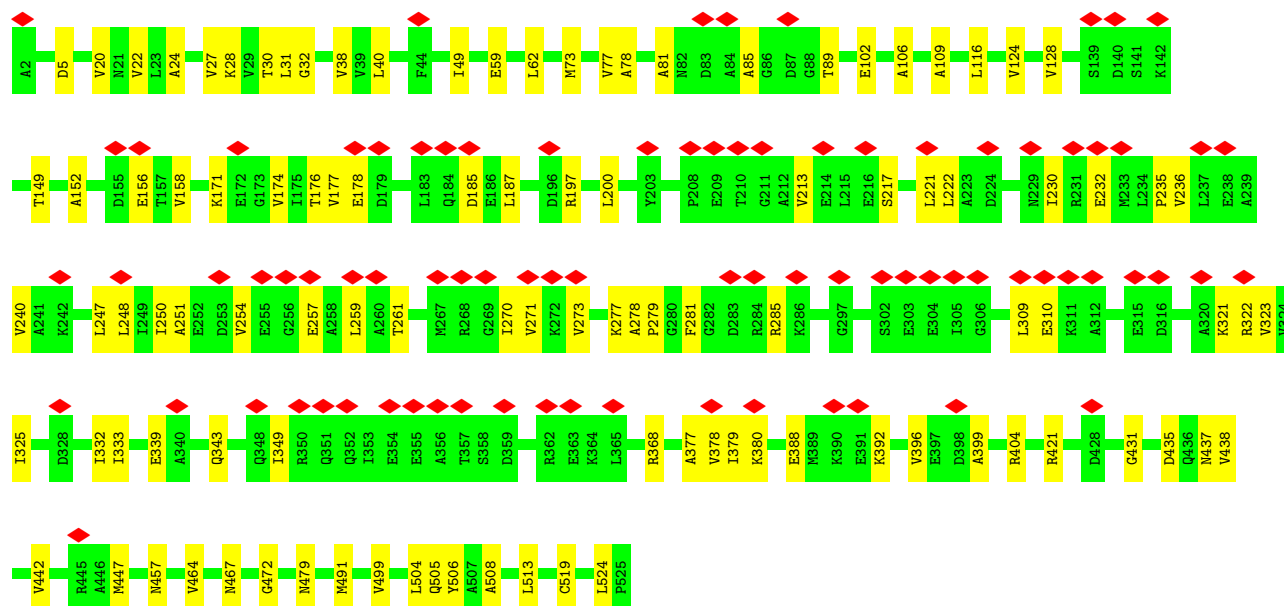
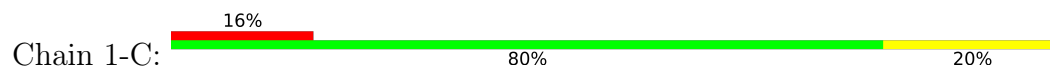


- Molecule 1: 60 kDa chaperonin

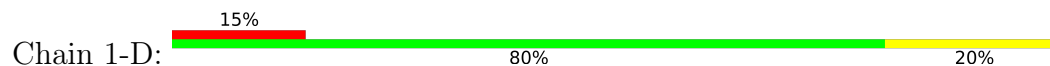




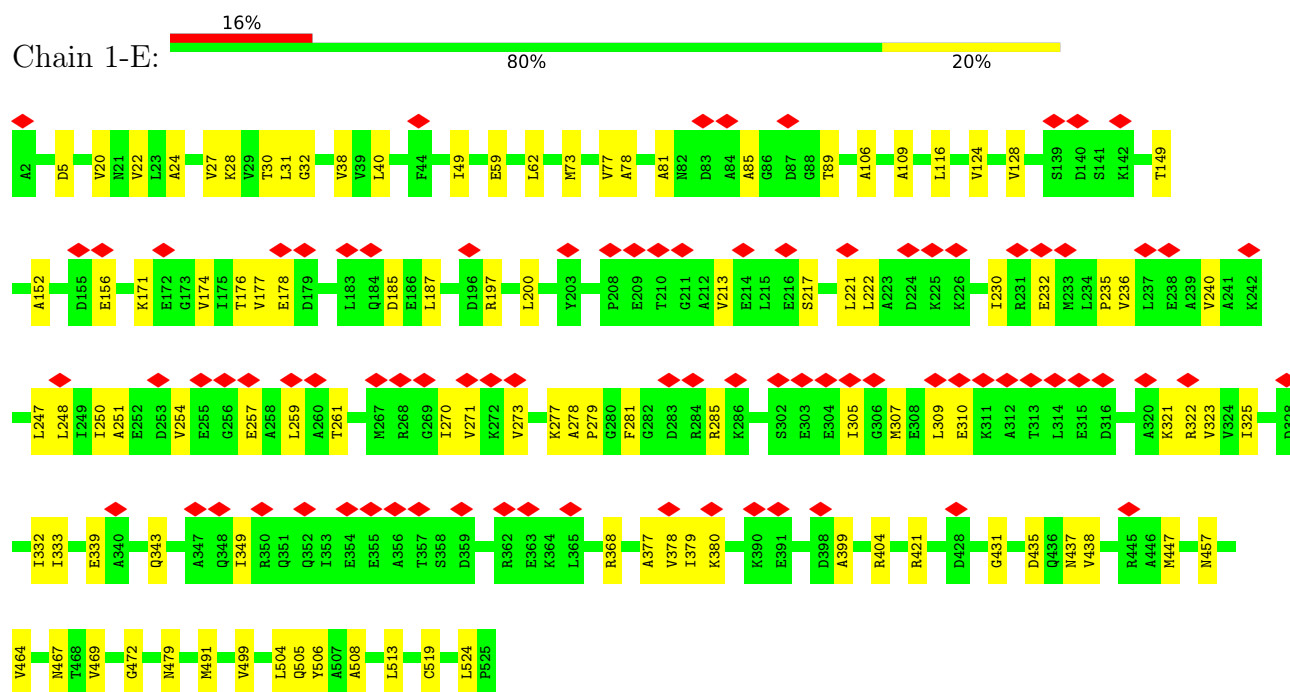
• Molecule 1: 60 kDa chaperonin



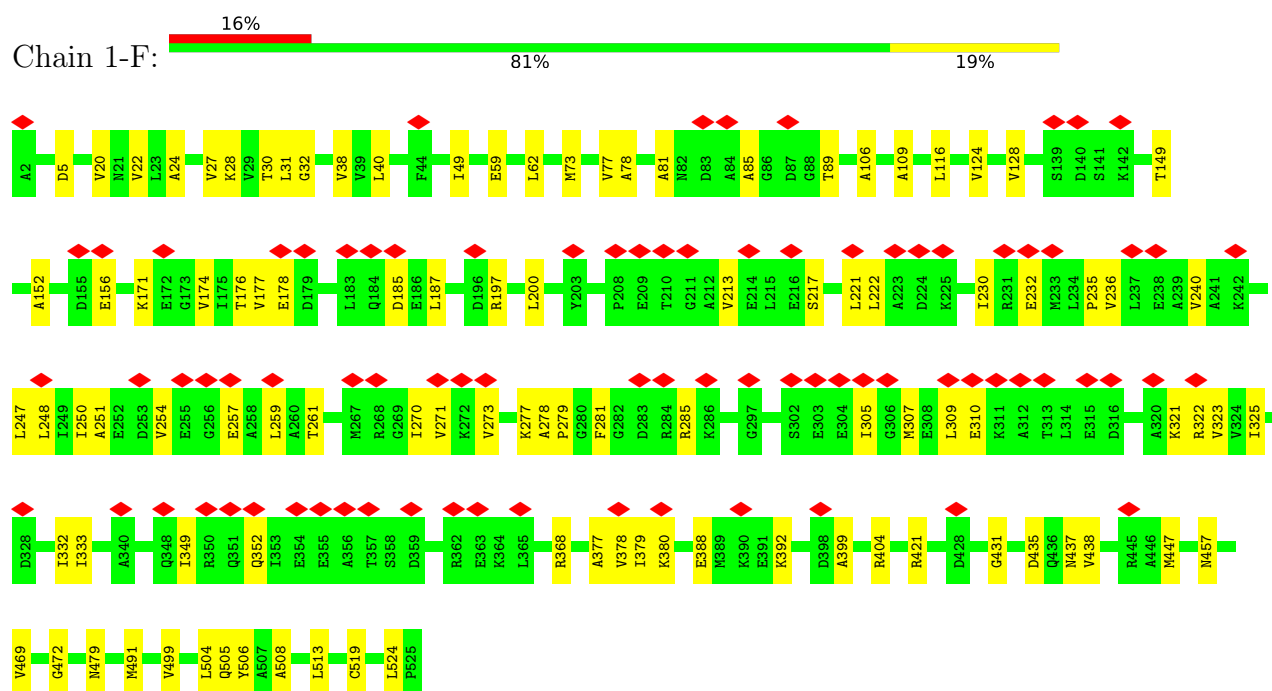
• Molecule 1: 60 kDa chaperonin



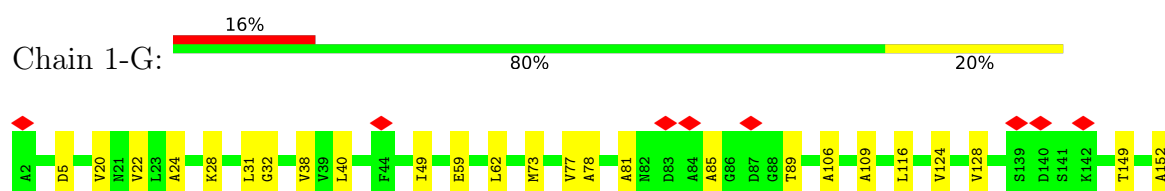
- Molecule 1: 60 kDa chaperonin

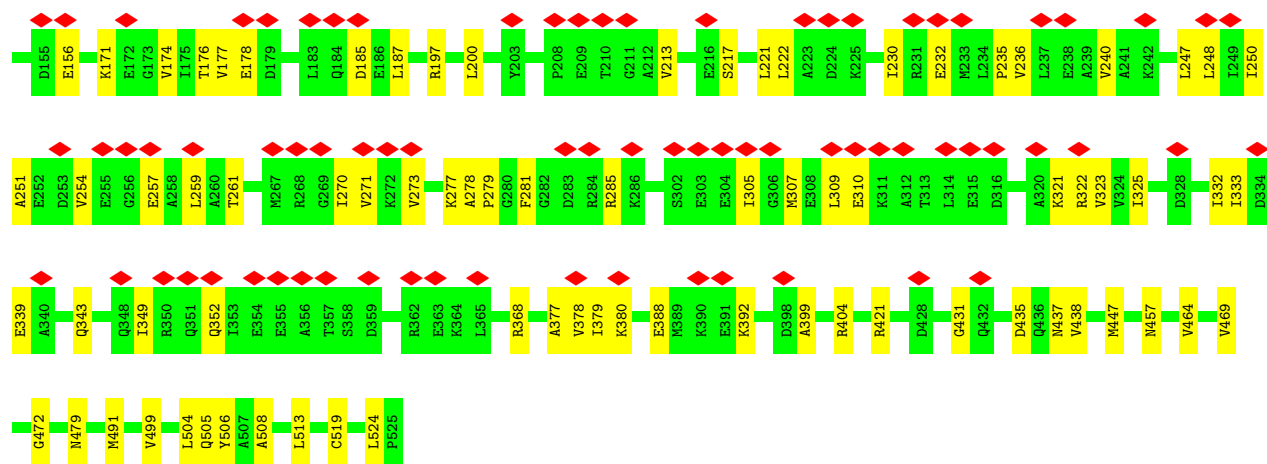


- Molecule 1: 60 kDa chaperonin

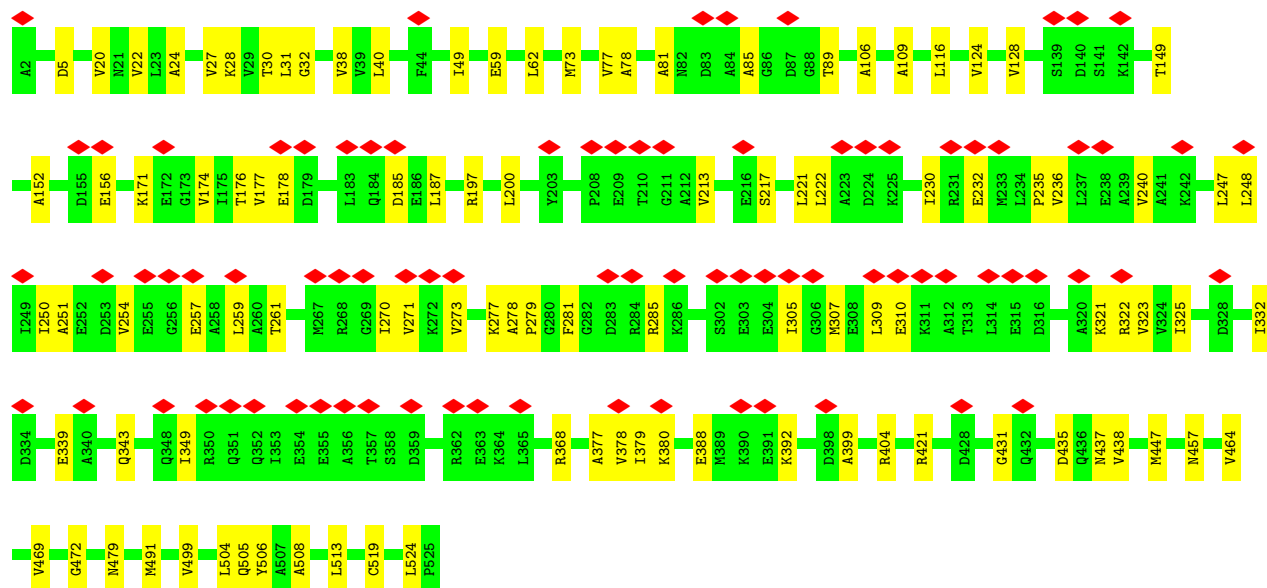
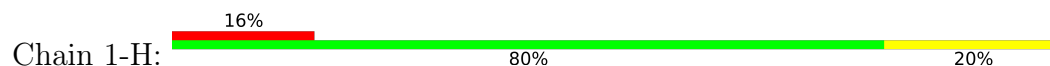


- Molecule 1: 60 kDa chaperonin

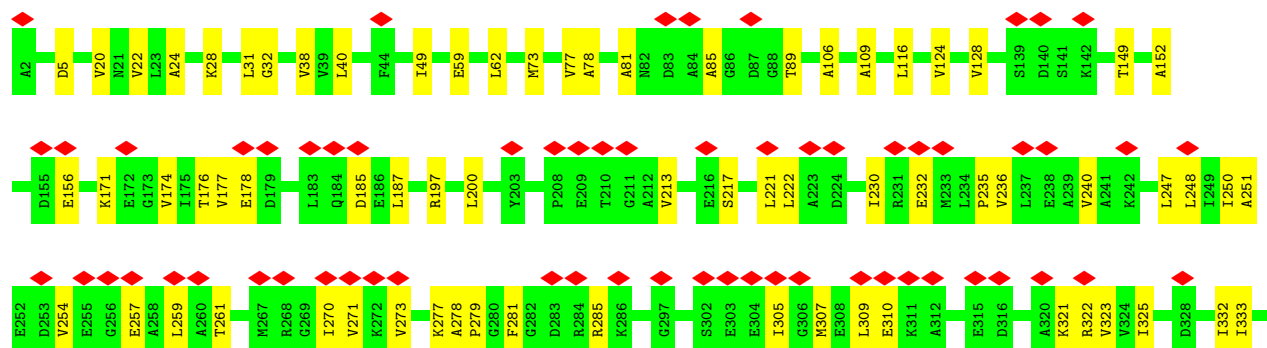
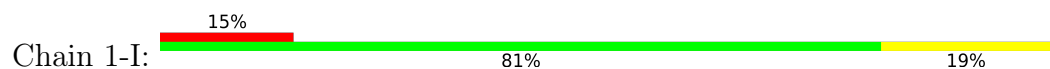


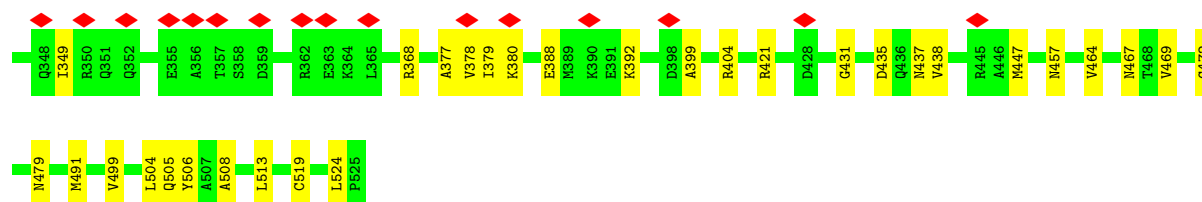


• Molecule 1: 60 kDa chaperonin

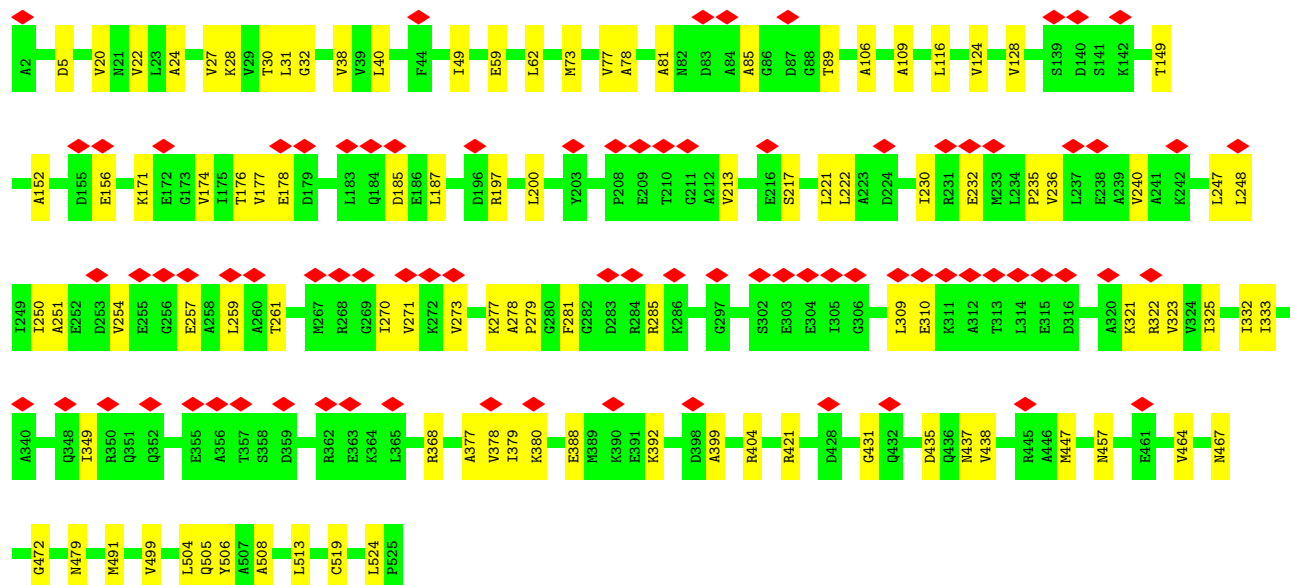
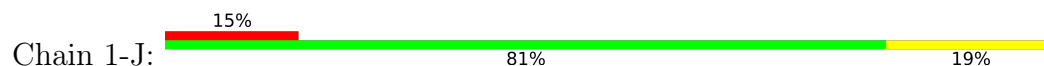


• Molecule 1: 60 kDa chaperonin

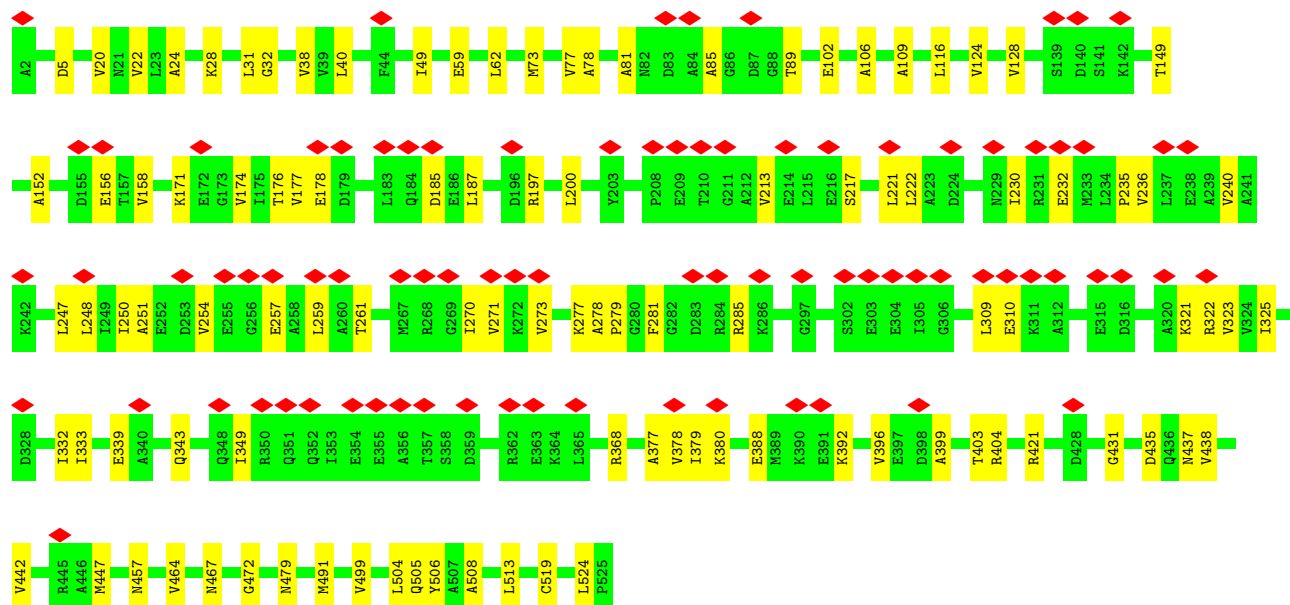
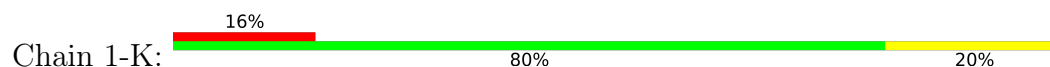




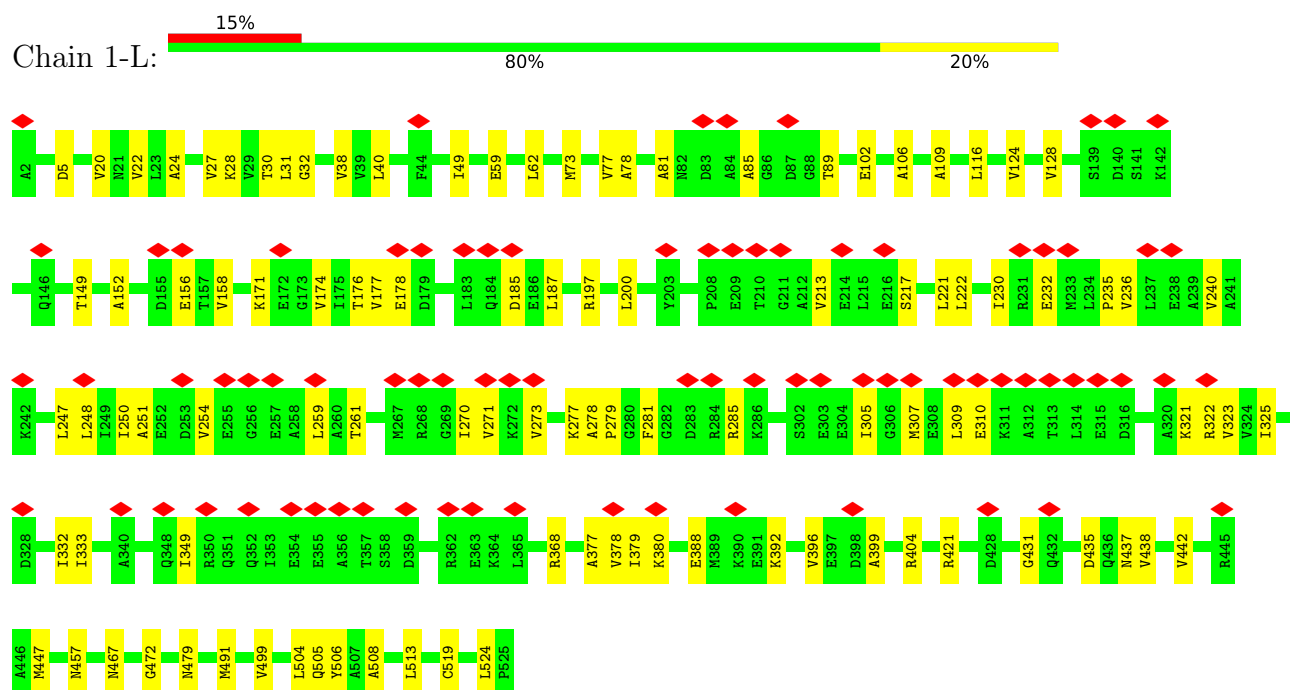
• Molecule 1: 60 kDa chaperonin



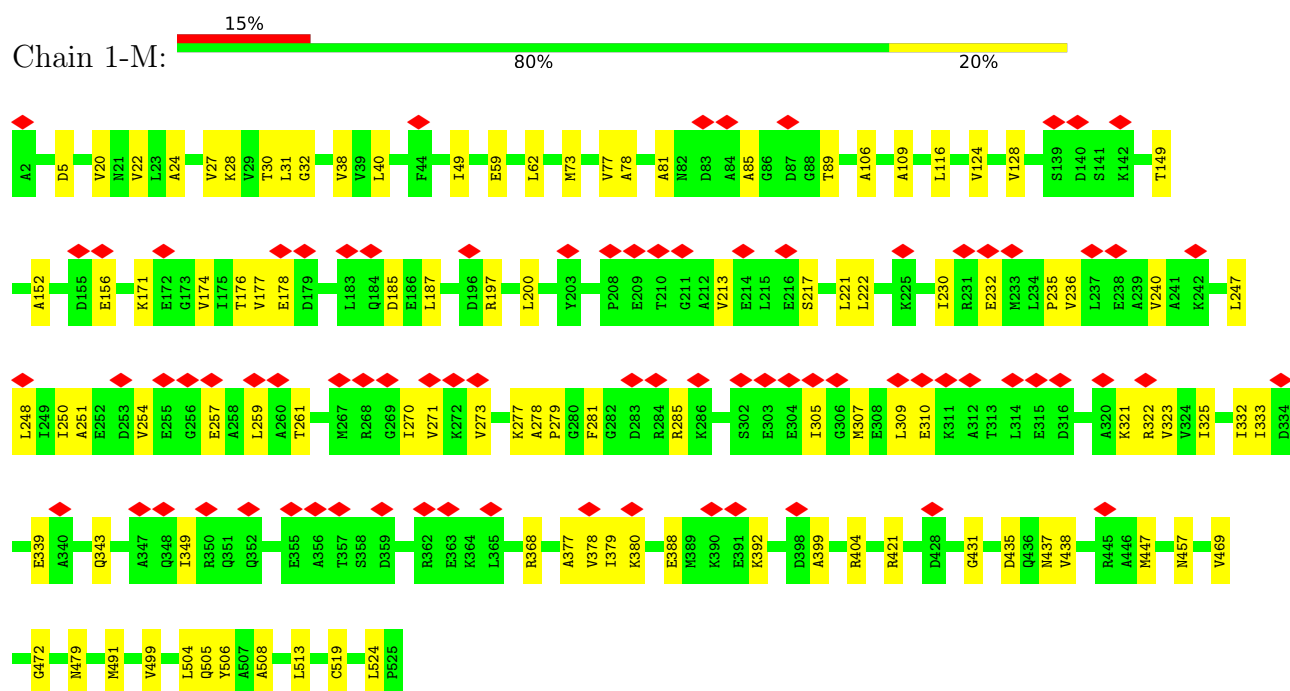
• Molecule 1: 60 kDa chaperonin



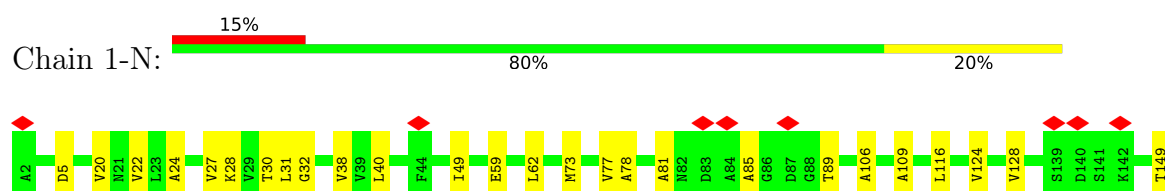
- Molecule 1: 60 kDa chaperonin

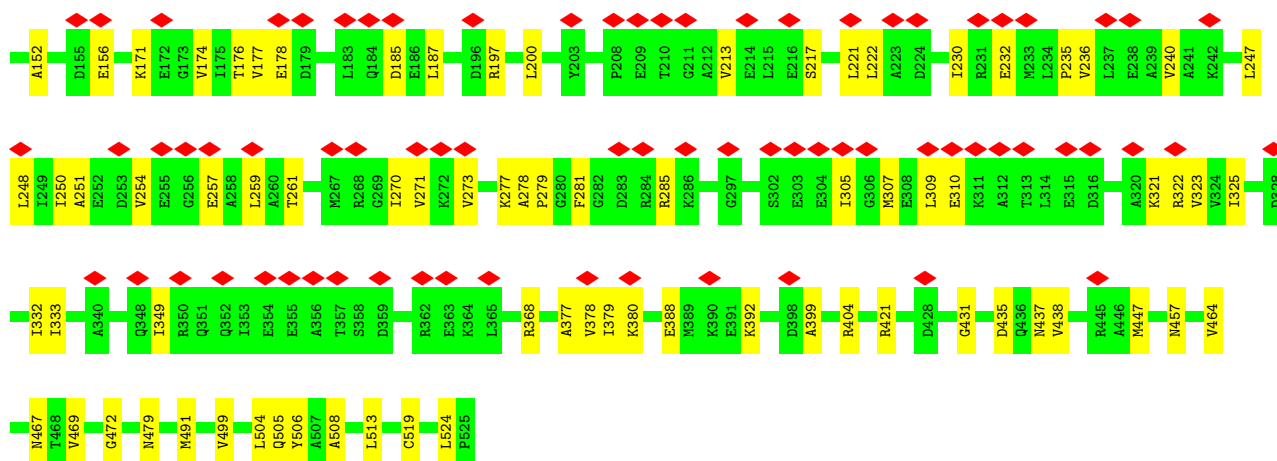


- Molecule 1: 60 kDa chaperonin



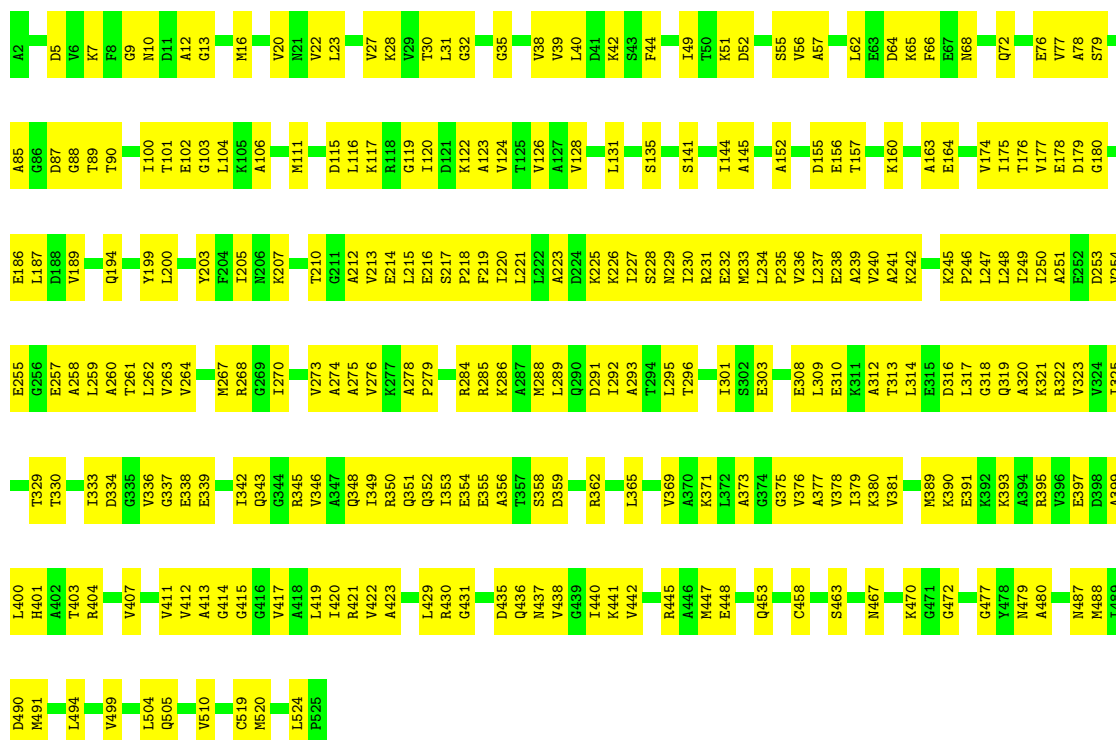
- Molecule 1: 60 kDa chaperonin



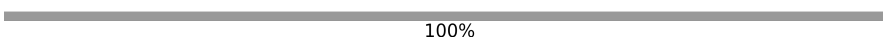


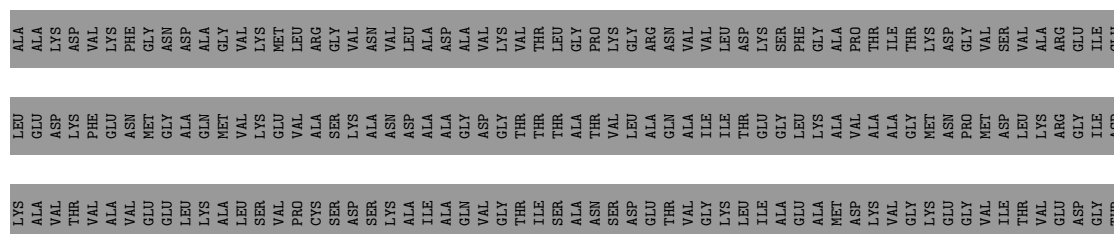
- Molecule 1: 60 kDa chaperonin

Chain 2-A:  50%



- Molecule 1: 60 kDa chaperonin

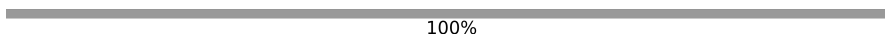
Chain 2-B:  100%



THR	VAL	ARG	SER	LYS	GLY
GLU	ALA	GLU	GLU	ALA	GLY
GLU	SER	LYS	GLU	GLY	GLN
TYR	LEU	LEU	ILE	LYS	GLU
GLY	LEU	GLN	GLY	PRO	GLU
ASN	ALA	GLU	MET	LEU	LEU
MET	ASP	ARG	GLU	LEU	ASP
ILE	LEU	VAL	LEU	ILE	VAL
LEU	ARG	ALA	GLU	ILE	VAL
MET	GLY	ALA	GLU	ALA	GLU
ASP	ASN	LEU	ALA	GLY	GLY
THR	GLN	ALA	THR	ASP	MET
PRO	ASP	GLY	LEU	VAL	GLN
THR	ASN	GLY	LEU	GLU	PHE
GLU	GLN	VAL	GLU	GLY	ARG
GLY	ASP	ALA	GLU	ALA	GLY
ILE	ASN	ILE	GLN	ALA	TYR
VAL	GLY	ILE	ALA	LEU	LEU
THR	ILE	LYS	ALA	ALA	LEU
ARG	LYS	VAL	LYS	THR	SER
SER	VAL	GLY	ARG	LEU	PRO
ALA	ALA	ALA	VAL	VAL	TYR
ALA	LEU	ALA	VAL	VAL	PHE
GLN	ARG	THR	ILE	ASN	ILE
TYR	ALA	GLU	ASN	THR	ASN
ALA	MET	VAL	LYS	MET	LYS
ALA	GLU	GLU	ASP	ARG	PRO
SER	ALA	MET	THR	GLY	GLU
VAL	PRO	LYS	THR	ILE	THR
ALA	LEU	GLU	THR	VAL	GLY
GLY	ARG	LYS	ILE	LYS	ALA
LEU	GLN	LYS	ILE	VAL	VAL
ILE	ILE	ALA	ASP	ALA	GLU
THR	VAL	ARG	GLY	ALA	LEU
THR	LEU	VAL	VAL	VAL	GLU
THR	ASN	GLU	GLY	LYS	SER
GLU	CYS	ASP	GLY	ALA	PRO
CYS	GLY	ALA	GLU	PRO	PHE
MET	GLU	LEU	ALA	GLY	ILE
VAL	VAL	HIS	ALA	PHE	LEU
THR	PRO	ALA	ILE	GLY	LEU
ASP	SER	THR	GLN	ASP	ALA
LEU	VAL	ARG	GLY	ARG	ASP
PRO	VAL	ALA	VAL	LYS	LYS
	ALA	ALA	VAL	LYS	ALA
	ASN	VAL	ALA	ALA	ILE
	THR	GLU	GLN	MET	SER
	VAL	GLU	ILE	LEU	ASN
	LYS	GLY	ARG	GLN	ILE
	GLY	VAL	GLN	ASP	GLU
	ASP	ALA	ILE	GLY	THR
	ASN	GLY	GLU	THR	LEU
	TYR	VAL	ALA	THR	PRO
	GLY	VAL	THR	GLY	VAL
	TYR	ALA	SER	GLY	LEU
	ASN	LEU	ASP	THR	ALA
	ALA	ILE	TYR	VAL	ALA

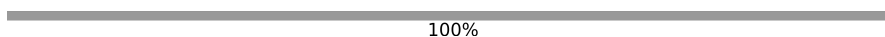
- Molecule 1: 60 kDa chaperonin

Chain 2-C:

[illegible]

- Molecule 1: 60 kDa chaperonin

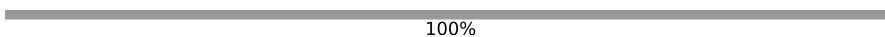
Chain 2-D:

[illegible]

[illegible]

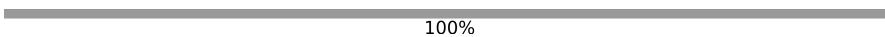
- Molecule 1: 60 kDa chaperonin

Chain 2-E:

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 2-F:

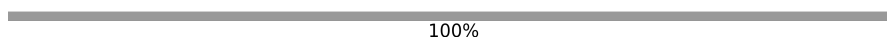


ALA	ALA	LYS	ASP	VAL	LYS	PHE	GLY	ASN	ASP	ALA	GLY	VAL	LYS	VAL	LEU	VAL	LEU	ALA	ASP	ALA	VAL	LYS	VAL	THR	THR	LEU	GLY	PRO	LYS	LYS	GLY	ARG	ASN	VAL	VAL	VAL	LEU	LEU	ASP	LYS	SER	SER	PHE	GLY	ALA	PRO	PRO	THR	THR	ILE	LYS	ASP	GLY	VAL	SER	VAL	ALA	ALA	ARG	ARG	GLU	ILE	THR
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[illegible]

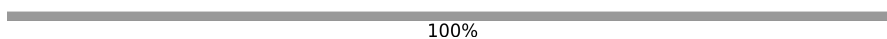
- Molecule 1: 60 kDa chaperonin

Chain 2-G:

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 2-H:





100%

[illegible]

- Molecule 1: 60 kDa chaperonin

100%

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 2-N:

100%

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 3-A:

56%

44%

A436	A437	A438	A439	A440	A441	A445	A448	A452	A458	A459	A460	A469	A472	A476	A477	A478	A479	A485	A486	A487	A488	A491	A492	A493	A494	A495	A496	A508	A511	M514	I515	V521	P525																																																																																																																																																																																																																																																																																																																																																																																																																																																											
A347	A348	A349	A350	A356	A362	A363	A364	A365	A366	A367	A368	A370	A371	A376	I379	A380	A381	A382	A383	A388	A389	A392	A393	A394	A395	A396	L400	A403	A404	A405	A406	A409	A410	A411	A412	A413	A414	A417	A418	A419	A420	A421	A427	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864

- Molecule 1: 60 kDa chaperonin

100%

- Molecule 1: 60 kDa chaperonin

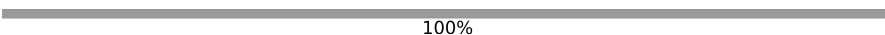
100%

ARG GLU
GLY
LEU
GLN
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ARG
VAL
ALA
LYS
LEU
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VAL
ALA
VAL
TLE
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ALA
ALA
THR
GLU
VAL
GLU
MET
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GLU
LYS
LYS
ALA
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GLU
ASP
LEU
ALA
HIS
ALA
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GLU
GLY
VAL
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GLY
GLY
ALA
LEU
TLE
ARG

[illegible]

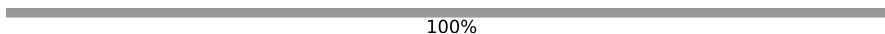
- Molecule 1: 60 kDa chaperonin

Chain 3-F:

[illegible]

- Molecule 1: 60 kDa chaperonin

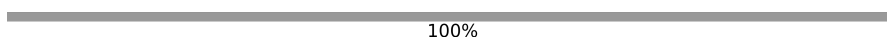
Chain 3-G:

[illegible]

[illegible]

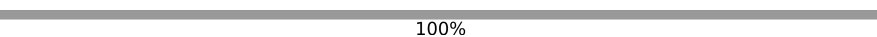
- Molecule 1: 60 kDa chaperonin

Chain 3-H:

[illegible]

- Molecule 1: 60 kDa chaperonin

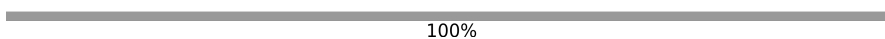
Chain 3-I:

[illegible]

[illegible]

- Molecule 1: 60 kDa chaperonin

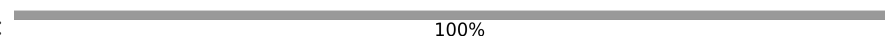
Chain 3-J:



THR	VAL	ARG	SER	LYS	GLY	LEU	ALA	LEU	LYS	LEU	ALA
GLU	ALA	GLU	GLU	ALA	GLY	GLU	GLY	GLN	LEU	GLN	ALA
GLU	SER	LEU	ILE	LYS	GLY	GLU	GLY	LYS	VAL	ASP	LYS
TYR	LEU	GLN	GLY	PRO	LEU	MET	LEU	GLU	VAL	PHE	LYS
ASN	ALA	GLU	MET	LEU	LEU	GLU	ASP	LEU	ALA	ASN	LYS
MET	ASP	ARG	GLU	LEU	ASP	GLU	LEU	VAL	GLU	ASN	PHE
ILE	LEU	VAL	LEU	ILE	ILE	LEU	ILE	VAL	GLU	MET	GLY
ASP	LEU	GLY	LEU	ASP	VAL	LEU	VAL	GLN	LEU	VAL	VAL
PRO	ASP	GLY	GLU	GLY	GLY	ASP	PHE	GLY	SER	LYS	LYS
THR	ASN	ALA	LEU	ALA	GLU	ASN	ARG	GLY	PRO	VAL	MET
VAL	VAL	VAL	GLY	ALA	GLU	GLY	ALA	TYR	CYS	ALA	ARG
THR	GLY	ILE	GLN	LEU	ILE	GLN	ALA	GLY	SER	GLY	GLY
ARG	LYS	LYS	ALA	THR	ALA	ALA	SER	LEU	ASP	LYS	VAL
SER	VAL	GLY	SER	THR	ARG	VAL	LYS	ASN	VAL	ALA	ASN
ALA	ALA	ALA	VAL	VAL	VAL	VAL	VAL	ALA	ALA	ASP	ALA
LEU	LEU	THR	ILE	ASN	ILE	GLU	ASN	PHE	ILE	ALA	ASP
GLN	ARG	THR	ILE	ASN	THR	GLU	ASN	ILE	GLN	GLY	ALA
TYR	ALA	GLU	ASN	THR	ASN	GLU	ASN	ILE	GLN	GLY	ALA
ALA	MET	VAL	ASP	MET	ASP	VAL	LYS	PRO	VAL	ASP	VAL
ALA	GLU	GLU	ASP	ARG	GLY	GLU	PRO	GLY	GLY	GLY	LYS
SER	ALA	MET	THR	GLY	THR	THR	GLU	THR	ILE	THR	THR
VAL	PRO	LYS	THR	ILE	VAL	THR	GLY	THR	ILE	THR	THR
ALA	LEU	GLU	THR	VAL	THR	THR	GLY	SER	SER	LEU	GLY
GLY	ARG	LYS	ILE	LYS	ILE	THR	ALA	ALA	ALA	ALA	LEU
LEU	GLN	LYS	ILE	VAL	VAL	ILE	VAL	ASN	ASN	THR	PRO
MET	ILE	ALA	ASP	ALA	GLY	ALA	GLU	LEU	SER	VAL	LYS
ILE	VAL	ARG	VAL	ALA	VAL	VAL	GLU	GLU	GLY	ALA	GLY
THR	ASN	GLU	GLY	VAL	ILE	GLU	SER	THR	THR	GLN	SER
ASP	SER	THR	GLN	ASP	ILE	ILE	LYS	PRO	THR	LEU	PHE
PRO	VAL	ARG	GLY	ARG	GLY	GLU	ALA	ASP	GLU	LEU	GLY

- Molecule 1: 60 kDa chaperonin

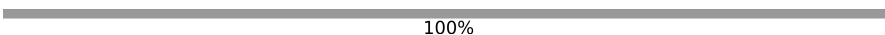
Chain 3-K:

[illegible]

THR	VAL	ARG	SER	LYS
GLU	ALA	GLU	GLU	ALA
GLY	SER	LYS	GLU	LYS
TYR	LYS	LEU	ILE	LYS
GLY	LEU	GLN	GLY	PRO
ASN	ALA	GLU	MET	LEU
MET	ASP	ARG	GLU	LEU
ILE	LEU	VAL	GLU	ILE
ASP	ARG	ALA	GLU	ILE
MET	GLY	LYS	LYS	ALA
ASP	GLN	LEU	ALA	GLU
ILE	ASN	ALA	THR	ASP
LEU	GLU	GLY	LEU	VAL
ASP	ASP	GLY	GLU	GLU
PRO	GLN	VAL	ASP	GLY
THR	ASN	VAL	GLY	ALA
ALA	VAL	VAL	GLN	ALA
ALA	GLY	ILE	ALA	LEU
ARG	LYS	VAL	LYS	ILE
ALA	VAL	GLY	ARG	ALA
SER	ALA	ALA	VAL	VAL
LEU	LEU	ALA	VAL	VAL
GLN	ARG	THR	ILE	ASN
TYR	ALA	GLU	ASN	THR
ALA	MET	VAL	LYS	THR
ALA	GLU	GLU	ASP	MET
SER	ALA	MET	THR	GLY
VAL	PRO	LYS	THR	ILE
ALA	LEU	GLU	THR	VAL
GLY	ARG	LYS	ILE	LYS
LEU	GLN	LYS	ILE	VAL
ILE	VAL	ARG	GLY	ALA
THR	LEU	VAL	VAL	VAL
THR	ASN	GLU	GLY	LYS
GLU	CYS	ASP	GLU	ALA
CYS	GLY	ALA	GLU	PRO
MET	GLU	LEU	ALA	GLY
VAL	GLU	HIS	ALA	PHE
THR	PRO	ALA	ILE	GLY
ASP	SER	THR	GLN	ASP
LEU	VAL	ARG	GLY	ARG
PRO	VAL	ALA	VAL	LYS
	ASN	VAL	ALA	ALA
	THR	GLU	GLN	MET
	VAL	GLY	ILE	LEU
	LYS	VAL	ARG	GLN
	GLY	VAL	GLN	ASP
	ASP	ALA	ILE	ILE
	THR	ALA	GLU	THR
	ASN	GLY	GLU	LEU
	TYR	VAL	ALA	THR
	THR	VAL	THR	GLY
	ASN	ALA	SER	GLY
	ASN	LEU	ASP	THR
	ALA	ILE	TYR	VAL
	ALA	ARG	ASP	ILE

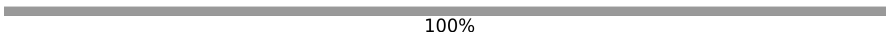
- Molecule 1: 60 kDa chaperonin

Chain 3-L:

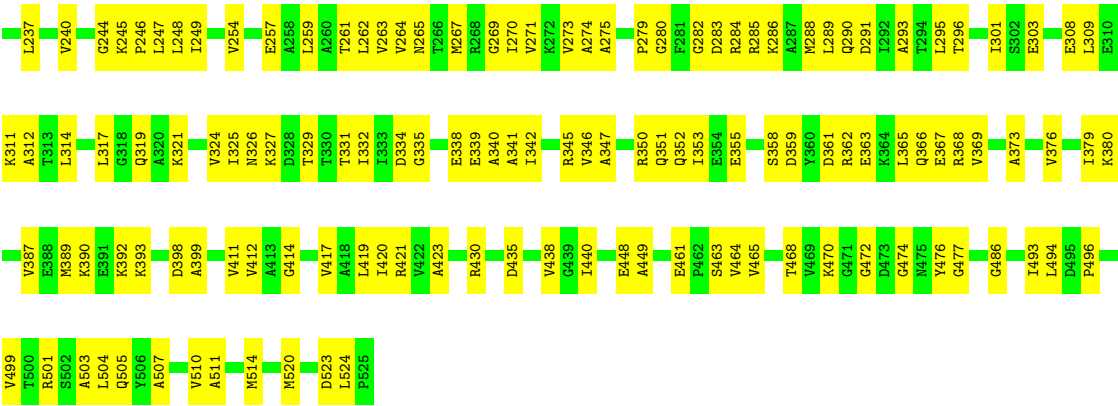
[illegible]

- Molecule 1: 60 kDa chaperonin

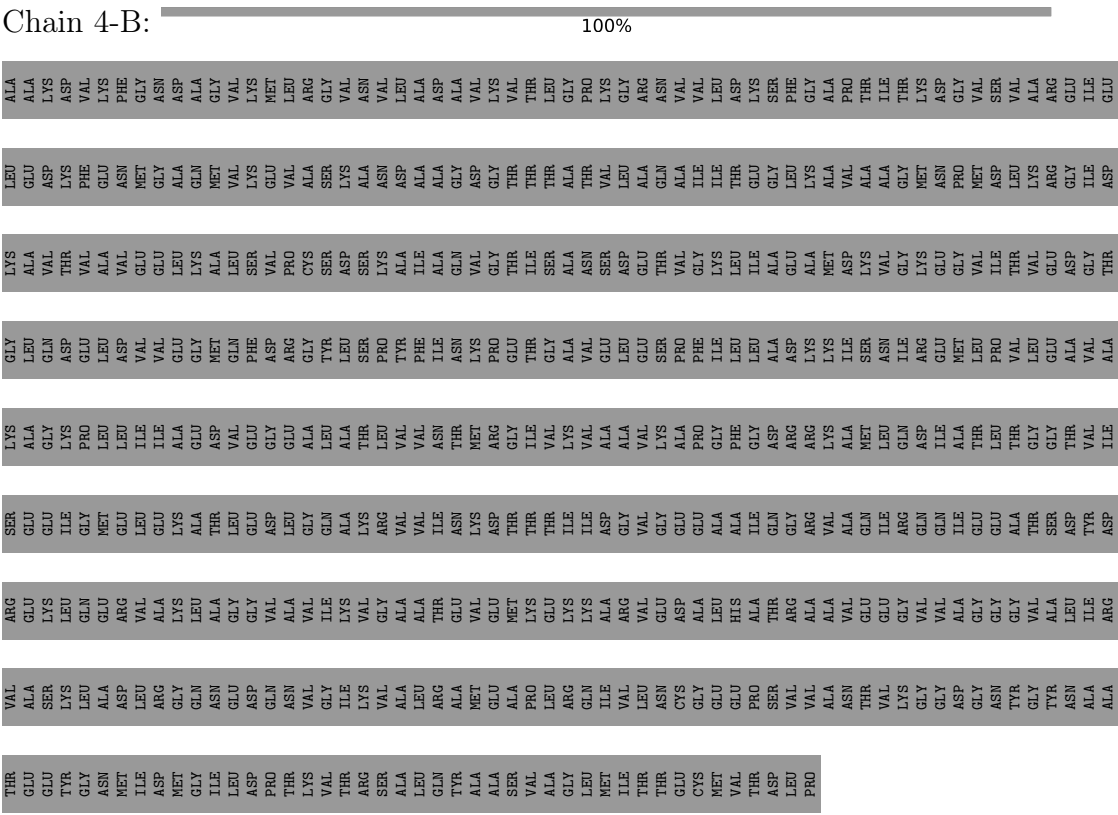
Chain 3-M:

[illegible]

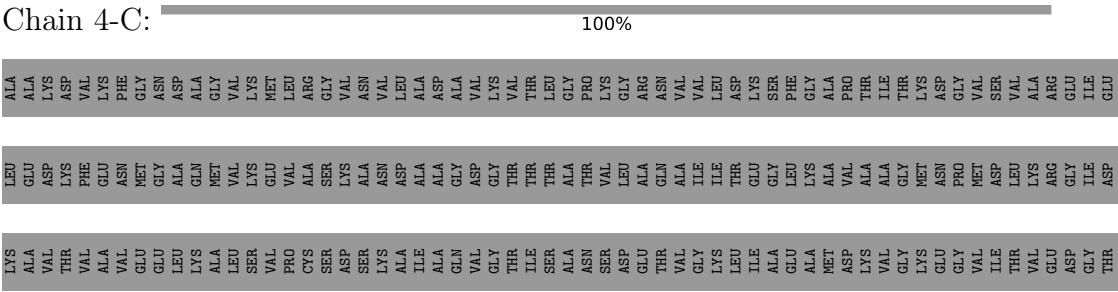




● Molecule 1: 60 kDa chaperonin



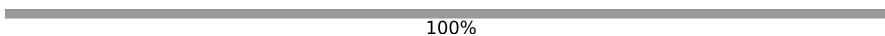
● Molecule 1: 60 kDa chaperonin



THR	VAL	ARG	SER	LYS	GLY
GLU	ALA	GLU	GLU	ALA	GLY
GLU	SER	LYS	GLU	GLY	GLN
TYR	LEU	LEU	ILE	LYS	ASP
GLY	LEU	GLN	GLY	PRO	GLU
ASN	ALA	GLU	MET	LEU	LEU
MET	ASP	ARG	GLU	LEU	ASP
ILE	LEU	VAL	LEU	ILE	VAL
MET	ARG	ALA	GLU	ILE	VAL
ASP	GLY	LYS	ASP	ALA	GLU
ILE	GLN	LEU	ALA	GLY	GLY
LEU	ASN	ALA	THR	ASP	MET
ASP	GLU	GLY	LEU	VAL	GLN
PRO	ASN	GLY	GLU	GLY	PHE
THR	ASN	VAL	ASP	LEU	ARG
VAL	VAL	ALA	GLY	ALA	GLY
THR	ILE	LYS	ALA	LEU	TYR
ARG	LYS	VAL	LYS	ALA	LEU
SER	VAL	GLY	LYS	ALA	SER
ALA	ALA	ALA	VAL	VAL	PRO
LEU	LEU	ALA	VAL	VAL	PHE
GLN	ARG	THR	ILE	ASN	ILE
TYR	ALA	GLU	ASN	THR	ASN
ALA	MET	VAL	LYS	MET	LYS
ALA	GLU	GLU	ASP	ARG	PRO
SER	ALA	MET	THR	GLY	GLU
VAL	PRO	LYS	THR	ILE	THR
ALA	LEU	GLU	THR	VAL	GLY
GLY	ARG	LYS	ILE	LYS	ALA
LEU	GLN	LYS	ILE	VAL	VAL
ILE	ILE	ALA	ASP	ALA	GLU
THR	VAL	ARG	GLY	ALA	LEU
THR	LEU	VAL	VAL	VAL	GLU
THR	ASN	GLU	GLY	LYS	SER
GLU	CYS	ASP	GLY	ALA	PRO
CYS	GLY	ALA	GLU	PRO	PHE
MET	GLU	LEU	ALA	GLY	ILE
VAL	VAL	HIS	ALA	PHE	LEU
THR	PRO	ALA	ILE	GLY	LEU
ASP	SER	THR	GLN	ASP	ALA
LEU	VAL	ARG	GLY	ARG	ASP
PRO	VAL	ALA	VAL	LYS	LYS
	ALA	ALA	ALA	LYS	ARG
	ASN	VAL	ALA	ALA	MET
	THR	GLU	GLN	MET	LEU
	VAL	GLU	ILE	THR	LEU
	LYS	GLY	GLY	THR	PRO
	GLY	ASP	ILE	LEU	VAL
	ASN	GLY	GLU	THR	GLY
	TYR	VAL	THR	GLY	GLU
	GLY	VAL	SER	THR	LEU
	ASN	ALA	ASP	THR	ALA
	ALA	ILE	THR	VAL	ALA
		ARG	ASN	THR	ALA

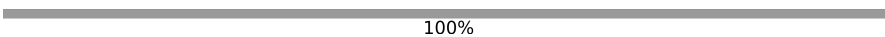
- Molecule 1: 60 kDa chaperonin

Chain 4-D:

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-E:

[illegible]

THR	VAL	ARG	SER	LYS	GLY	LYS	GLY	LYS
THR	VAL	ARG	SER	LYS	GLY	LYS	GLY	LYS
GLU	ALA	GLU	GLU	GLU	LEU	ALA	LEU	ALA
GLU	SER	LYS	GLU	GLU	LEU	GLY	GLN	VAL
TYR	LEU	LEU	ILE	GLY	GLN	PRO	GLU	THR
ASN	ALA	GLU	MET	GLY	LEU	LEU	LEU	ALA
MET	ASP	ARG	GLU	LEU	ASP	LEU	ASP	VAL
ILE	LEU	VAL	LEU	ILE	VAL	ILE	VAL	GLU
ASP	ARG	ALA	GLY	ALA	GLY	ALA	VAL	GLU
MET	ASN	LEU	THR	GLY	ALA	GLU	MET	LYS
LEU	GLU	ILE	LEU	VAL	ASP	VAL	GLN	LEU
PRO	ASP	GLY	GLU	GLU	PHE	GLN	PHE	SER
THR	ASN	ALA	LEU	GLY	GLY	GLY	ARG	PRO
LYS	VAL	VAL	LEU	ALA	VAL	VAL	GLU	CYS
VAL	GLY	ILE	GLN	ILE	GLN	LEU	TYR	SER
THR	ILE	LYS	ALA	LYS	ALA	ALA	LEU	ASP
ARG	LYS	VAL	LYS	THR	THR	THR	SER	SER
SER	VAL	GLY	ARG	LEU	PRO	GLY	PRO	LYS
ALA	ALA	ALA	VAL	VAL	VAL	VAL	TYR	ALA
LEU	LEU	ALA	VAL	VAL	PHE	ILE	PHE	ILE
GLN	ARG	THR	ASN	THR	ASN	THR	ASN	GLN
TYR	ALA	GLU	ASN	THR	ILE	VAL	GLY	VAL
ALA	MET	VAL	LYS	MET	GLY	VAL	PRO	GLY
ALA	GLU	GLU	ASP	ASP	GLY	GLY	GLY	THR
ALA	ALA	MET	THR	THR	THR	ILE	THR	ILE
SER	ALA	THR	THR	THR	THR	VAL	GLY	SER
VAL	PRO	ALA	GLY	LYS	GLY	LYS	GLU	THR
THR	ASN	VAL	GLY	VAL	VAL	VAL	GLU	GLU
THR	LEU	ARG	VAL	VAL	VAL	ALA	SER	THR
GLU	ASN	GLU	GLY	LYS	SER	LYS	PRO	VAL
CYS	GLY	ALA	GLU	PRO	PHE	GLY	PHE	GLY
MET	GLU	LEU	ALA	GLY	ILE	LYS	ILE	LYS
VAL	GLU	HIS	ALA	PHE	ALA	LEU	LEU	LEU
THR	PRO	ALA	ILE	ILE	GLY	LEU	LEU	ILE
ASP	SER	THR	GLN	ASP	ALA	ALA	ALA	ALA
PRO	VAL	ARG	GLY	ARG	ASP	LYS	ASP	GLU
	VAL	ALA	ARG	ARG	ARG	ARG	LYS	ALA
	ALA	ALA	VAL	VAL	ALA	LYS	LYS	MET
	ASN	VAL	VAL	ALA	ALA	ILE	ILE	ASP
	THR	GLU	GLN	MET	SER	SER	SER	LYS
	VAL	GLU	ILE	LEU	ASN	VAL	VAL	GLY
	LYS	GLY	ARG	GLN	GLN	ILE	ILE	GLY
	GLY	VAL	GLN	GLN	GLY	ARG	GLY	LYS
	ASP	ALA	ILE	ILE	ALA	ASP	GLY	GLY
	ASN	GLY	GLU	GLU	THR	LEU	LEU	VAL
	ASN	GLY	GLU	LEU	THR	PRO	VAL	ILE
	TYR	GLY	ALA	THR	VAL	VAL	THR	THR
	GLY	VAL	THR	GLY	GLY	LEU	LEU	VAL
	TYR	ALA	SER	SER	GLY	GLY	GLY	VAL
	ASN	LEU	ASP	THR	THR	ALA	GLU	ASP
	ALA	ILE	TYR	VAL	VAL	VAL	VAL	GLY
	ALA	ASP	ASP	THR	ALA	ALA	ALA	THR

- Molecule 1: 60 kDa chaperonin

Chain 4-F: 100%

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-G: 100%

ALA	ALA	LYS	ASP	VAL	LYS	PHE	GLY	ASN	ASP	ALA	GLY	VAL	LYS	LEU	VAL	LEU	VAL	VAL	THR	THR	LEU	GLY	PRO	PRO	LYS	GLY	LYS	ARG	ASN	VAL	VAL	VAL	LEU	LEU	ASP	LYS	LYS	SER	PHE	GLY	ALA	PRO	PRO	THR	THR	ILE	THR	THR	ASP	LYS	GLY	GLY	VAL	SER	VAL	ALA	ALA	ARG	ARG	GLU	ILE	GLU
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LEU	GLU	ALA	ASP	LYS	PHE	GLU	ASN	MET	GLY	ALA	GLN	MET	VAL	LYS	LYS	THR	ASP
LYS	ALA	VAL	THR	LYS	VAL	GLU	ALA	GLU	GLY	LEU	GLY	ALA	THR	SER	VAL	GLU	THR
GLY	LEU	GLN	ASP	LYS	GLU	LEU	ASP	VAL	ILE	VAL	GLU	MET	GLN	PHE	GLU	GLY	ALA
LYS	ALA	GLY	GLY	PRO	LEU	ILE	ILE	GLU	LYS	ALA	GLU	ASP	THR	GLU	GLY	GLY	ILE
SER	GLU	GLU	ILE	GLY	MET	GLU	LEU	GLU	ALA	THR	GLU	ASP	GLY	GLU	VAL	GLU	ASP
ARG	GLU	LYS	GLY	GLN	GLU	ARG	VAL	VAL	ALA	GLY	VAL	VAL	VAL	GLY	VAL	GLU	ARG
VAL	ALA	SER	LYS	LYS	LEU	ARG	GLY	ASN	GLN	ILE	GLN	VAL	GLY	GLY	GLN	GLY	ALA
THR	GLU	TYR	GLY	ASN	MET	ILE	ASP	PRO	GLY	THR	PRO	THR	THR	GLY	THR	THR	PRO

● Molecule 1: 60 kDa chaperonin

Chain 4-H:

100%

ALA	ALA	LYS	ASP	VAL	LYS	PHE	GLY	GLY	ASN	ASP	GLY	ALA	GLN	ASP	LYS	MET	GLU
LEU	GLU	ASP	PHE	GLU	ASN	MET	ILE	ASP	GLY	ALA	GLN	MET	VAL	LYS	GLU	GLY	VAL
LYS	ALA	VAL	THR	VAL	GLU	LEU	LYS	ALA	GLY	THR	VAL	GLY	VAL	SER	VAL	GLU	THR
GLY	LEU	GLN	ASP	LEU	VAL	ASP	VAL	VAL	GLY	THR	GLY	THR	THR	GLY	VAL	GLY	ALA
LYS	ALA	GLY	PRO	LEU	ILE	GLU	GLY	GLY	ALA	THR	GLU	ASP	VAL	VAL	GLY	GLY	ILE
SER	GLU	ILE	GLY	GLY	LYS	THR	GLU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP
ARG	GLU	LYS	GLN	GLY	VAL	ARG	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ARG
VAL	ALA	SER	LYS	LEU	ALA	GLY	ASP	GLY	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA
THR	GLU	TYR	GLY	ASN	MET	ILE	ASP	PRO	GLY	THR	PRO	THR	THR	GLY	THR	THR	PRO

● Molecule 1: 60 kDa chaperonin

Chain 4-I:

100%

[illegible]

- Molecule 1: 60 kDa chaperonin

Chain 4-J: 100%

[illegible]

- Molecule 1: 60 kDa chaperonin

100%

[illegible]

- Molecule 1: 60 kDa chaperonin

100%

[illegible]

THR	GLU	GLU	TYR	GLY	ASN	MET	ILE	ASP	MET	GLY	ILE	LEU	ASP	PRO	THR	LYS	VAL	THR	ARG	SER	ALA	LEU	GLN	TYR	ALA	ALA	SER	VAL	ALA	GLY	LEU	MET	ILE	THR	THR	GLU	CYS	MET	VAL	THR	ASP	LEU	PRO
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	37367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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	1-A	0.21	0/3879	0.24	0/5237
1	1-B	0.35	0/3879	0.62	0/5237
1	1-C	0.35	0/3879	0.62	0/5237
1	1-D	0.35	0/3879	0.62	0/5237
1	1-E	0.35	0/3879	0.62	0/5237
1	1-F	0.35	0/3879	0.62	0/5237
1	1-G	0.35	0/3879	0.62	0/5237
1	1-H	0.35	0/3879	0.62	0/5237
1	1-I	0.35	0/3879	0.62	0/5237
1	1-J	0.35	0/3879	0.62	0/5237
1	1-K	0.35	0/3879	0.62	0/5237
1	1-L	0.35	0/3879	0.62	0/5237
1	1-M	0.35	0/3879	0.62	0/5237
1	1-N	0.35	0/3879	0.62	0/5237
1	2-A	0.21	0/3879	0.24	0/5237
1	3-A	0.21	0/3879	0.24	0/5237
1	4-A	0.21	0/3879	0.24	0/5237
All	All	0.32	0/65943	0.55	0/89029

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	1-B	0	1
1	1-C	0	1
1	1-D	0	1
1	1-E	0	1
1	1-F	0	1
1	1-G	0	1
1	1-H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-I	0	1
1	1-J	0	1
1	1-K	0	1
1	1-L	0	1
1	1-M	0	1
1	1-N	0	1
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	32	GLY	Peptide
1	1-B	32	GLY	Peptide
1	1-C	32	GLY	Peptide
1	1-D	32	GLY	Peptide
1	1-E	32	GLY	Peptide
1	1-F	32	GLY	Peptide
1	1-G	32	GLY	Peptide
1	1-H	32	GLY	Peptide
1	1-I	32	GLY	Peptide
1	1-J	32	GLY	Peptide
1	1-K	32	GLY	Peptide
1	1-L	32	GLY	Peptide
1	1-M	32	GLY	Peptide
1	1-N	32	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3851	0	3970	63	0
1	1-B	3851	0	3970	61	0
1	1-C	3851	0	3970	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-D	3851	0	3970	63	0
1	1-E	3851	0	3970	63	0
1	1-F	3851	0	3970	62	0
1	1-G	3851	0	3970	63	0
1	1-H	3851	0	3970	63	0
1	1-I	3851	0	3970	62	0
1	1-J	3851	0	3970	61	0
1	1-K	3851	0	3970	64	0
1	1-L	3851	0	3970	62	0
1	1-M	3851	0	3970	62	0
1	1-N	3851	0	3970	63	0
1	2-A	3851	0	3970	250	0
1	3-A	3851	0	3970	198	0
1	4-A	3851	0	3970	151	0
2	1-A	19	0	0	1	0
2	1-B	12	0	0	0	0
2	1-C	14	0	0	0	0
2	1-D	14	0	0	0	0
2	1-E	10	0	0	0	0
2	1-F	6	0	0	0	0
2	1-G	13	0	0	0	0
2	1-H	1	0	0	0	0
2	1-I	3	0	0	0	0
2	1-J	5	0	0	0	0
2	1-K	1	0	0	0	0
2	1-L	2	0	0	0	0
2	1-M	5	0	0	0	0
2	1-N	2	0	0	0	0
All	All	65574	0	67490	1416	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 21.

All (1416) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:THR:O	1:A:377:ALA:HB3	1.56	1.04
1:A:221:LEU:O	1:A:248:LEU:CB	2.14	0.95
1:A:264:VAL:HA	1:A:267:MET:HG2	1.51	0.92
1:A:197:ARG:HE	1:A:279:PRO:HA	1.35	0.92
1:A:237:LEU:O	1:A:241:ALA:HB2	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:LEU:HA	1:F:378:VAL:O	1.72	0.90
1:N:187:LEU:HA	1:N:378:VAL:O	1.72	0.90
1:M:187:LEU:HA	1:M:378:VAL:O	1.72	0.90
1:E:187:LEU:HA	1:E:378:VAL:O	1.72	0.90
1:G:187:LEU:HA	1:G:378:VAL:O	1.72	0.90
1:H:187:LEU:HA	1:H:378:VAL:O	1.72	0.90
1:A:220:ILE:HB	1:A:318:GLY:O	1.72	0.90
1:I:187:LEU:HA	1:I:378:VAL:O	1.72	0.89
1:A:187:LEU:HA	1:A:378:VAL:O	1.72	0.89
1:D:187:LEU:HA	1:D:378:VAL:O	1.72	0.89
1:J:187:LEU:HA	1:J:378:VAL:O	1.72	0.89
1:A:282:GLY:H	1:A:285:ARG:HH21	1.19	0.89
1:B:187:LEU:HA	1:B:378:VAL:O	1.72	0.89
1:L:187:LEU:HA	1:L:378:VAL:O	1.72	0.89
1:C:187:LEU:HA	1:C:378:VAL:O	1.72	0.88
1:K:187:LEU:HA	1:K:378:VAL:O	1.72	0.88
1:A:220:ILE:HG22	1:A:248:LEU:HB3	1.56	0.88
1:L:185:ASP:HA	1:L:380:LYS:O	1.78	0.83
1:D:185:ASP:HA	1:D:380:LYS:O	1.78	0.83
1:E:185:ASP:HA	1:E:380:LYS:O	1.78	0.83
1:A:427:ALA:O	1:A:441:LYS:NZ	2.11	0.83
1:M:185:ASP:HA	1:M:380:LYS:O	1.78	0.83
1:G:185:ASP:HA	1:G:380:LYS:O	1.78	0.83
1:H:185:ASP:HA	1:H:380:LYS:O	1.78	0.83
1:F:185:ASP:HA	1:F:380:LYS:O	1.78	0.83
1:A:185:ASP:HA	1:A:380:LYS:O	1.78	0.82
1:K:185:ASP:HA	1:K:380:LYS:O	1.78	0.82
1:N:185:ASP:HA	1:N:380:LYS:O	1.78	0.82
1:C:185:ASP:HA	1:C:380:LYS:O	1.78	0.82
1:I:185:ASP:HA	1:I:380:LYS:O	1.78	0.82
1:J:185:ASP:HA	1:J:380:LYS:O	1.78	0.82
1:B:185:ASP:HA	1:B:380:LYS:O	1.78	0.82
1:A:377:ALA:HB1	1:A:379:ILE:HG13	1.62	0.81
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.60	0.81
1:A:284:ARG:NH1	1:A:288:MET:SD	2.53	0.81
1:A:128:VAL:HG21	1:A:505:GLN:HE21	1.46	0.81
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.61	0.80
1:A:325:ILE:HG22	1:A:330:THR:HG23	1.63	0.80
1:A:186:GLU:HB2	1:A:380:LYS:HG3	1.64	0.80
1:A:103:GLY:O	1:A:106:ALA:N	2.13	0.80
1:A:221:LEU:O	1:A:248:LEU:HB3	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:O	1:A:267:MET:N	2.16	0.79
1:A:249:ILE:HB	1:A:275:ALA:HA	1.65	0.79
1:A:285:ARG:O	1:A:288:MET:N	2.15	0.79
1:A:172:GLU:HA	1:A:404:ARG:HH12	1.48	0.78
1:A:421:ARG:NH1	1:A:469:VAL:O	2.17	0.77
1:A:214:GLU:OE2	1:A:322:ARG:NH2	2.17	0.77
1:A:448:GLU:OE2	1:A:470:LYS:NZ	2.16	0.77
1:A:220:ILE:HD11	1:A:296:THR:HG21	1.66	0.76
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.68	0.76
1:A:221:LEU:HD13	1:A:247:LEU:HD11	1.66	0.75
1:A:225:LYS:NZ	1:A:301:ILE:O	2.20	0.75
1:A:81:ALA:O	1:A:85:ALA:HB3	1.87	0.74
1:I:81:ALA:O	1:I:85:ALA:HB3	1.87	0.74
1:G:81:ALA:O	1:G:85:ALA:HB3	1.87	0.74
1:H:81:ALA:O	1:H:85:ALA:HB3	1.87	0.74
1:L:81:ALA:O	1:L:85:ALA:HB3	1.87	0.74
1:D:81:ALA:O	1:D:85:ALA:HB3	1.87	0.74
1:M:81:ALA:O	1:M:85:ALA:HB3	1.87	0.74
1:B:81:ALA:O	1:B:85:ALA:HB3	1.87	0.73
1:E:81:ALA:O	1:E:85:ALA:HB3	1.87	0.73
1:J:81:ALA:O	1:J:85:ALA:HB3	1.87	0.73
1:A:30:THR:OG1	1:A:51:LYS:O	2.06	0.73
1:F:81:ALA:O	1:F:85:ALA:HB3	1.87	0.73
1:N:81:ALA:O	1:N:85:ALA:HB3	1.87	0.73
1:K:81:ALA:O	1:K:85:ALA:HB3	1.87	0.73
1:C:81:ALA:O	1:C:85:ALA:HB3	1.87	0.72
1:A:215:LEU:HD23	1:A:246:PRO:HB2	1.70	0.72
1:A:16:MET:HE2	1:A:514:MET:HE2	1.72	0.72
1:A:226:LYS:HG2	1:A:253:ASP:HB3	1.70	0.72
1:A:291:ASP:OD1	1:A:345:ARG:NH2	2.23	0.72
1:A:356:ALA:O	1:A:362:ARG:NH2	2.23	0.72
1:A:82:ASN:O	1:A:86:GLY:N	2.22	0.71
1:A:281:PHE:HA	1:A:285:ARG:HH21	1.54	0.71
1:A:112:ASN:HB3	1:A:115:ASP:HB2	1.71	0.71
1:A:321:LYS:HG2	1:A:334:ASP:HB2	1.73	0.71
1:A:308:GLU:OE1	1:A:310:GLU:N	2.23	0.71
1:A:291:ASP:OD1	1:A:345:ARG:NH1	2.24	0.71
1:A:194:GLN:O	1:A:371:LYS:NZ	2.21	0.71
1:A:362:ARG:O	1:A:366:GLN:N	2.23	0.71
1:A:349:ILE:HD11	1:A:365:LEU:HD22	1.71	0.70
1:A:85:ALA:HB1	1:A:499:VAL:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:O	1:A:248:LEU:HB2	1.90	0.70
1:A:261:THR:HA	1:A:264:VAL:HG12	1.73	0.70
1:A:189:VAL:HG13	1:A:375:GLY:HA3	1.74	0.70
1:A:322:ARG:O	1:A:333:ILE:HB	1.92	0.70
1:A:193:MET:HE2	1:A:195:PHE:CE1	2.27	0.70
1:A:448:GLU:OE2	1:A:452:ARG:NH1	2.17	0.69
1:A:153:ASN:OD1	1:A:395:ARG:NH1	2.25	0.69
1:A:339:GLU:O	1:A:343:GLN:HB2	1.92	0.69
1:A:383:ALA:HB3	1:A:389:MET:HG3	1.72	0.69
1:A:288:MET:HE3	1:A:368:ARG:HH12	1.57	0.69
1:A:9:GLY:O	1:A:13:GLY:N	2.22	0.69
1:A:219:PHE:HB2	1:A:245:LYS:HZ3	1.57	0.69
1:A:152:ALA:HB2	1:A:399:ALA:HB2	1.75	0.69
1:A:369:VAL:O	1:A:373:ALA:N	2.25	0.69
1:A:128:VAL:HG23	1:A:501:ARG:HG3	1.74	0.69
1:A:432:GLN:N	1:A:436:GLN:OE1	2.20	0.68
1:A:219:PHE:HB2	1:A:245:LYS:HE2	1.75	0.68
1:A:221:LEU:HA	1:A:317:LEU:HD22	1.73	0.68
1:A:411:VAL:HG21	1:A:494:LEU:HD13	1.76	0.68
1:A:232:GLU:HG3	1:A:309:LEU:HB2	1.75	0.68
1:A:232:GLU:HB3	1:A:309:LEU:HD12	1.76	0.68
1:A:460:GLU:N	1:A:460:GLU:OE1	2.27	0.67
1:A:100:ILE:HD11	1:A:511:ALA:HA	1.74	0.67
1:A:179:ASP:O	1:A:380:LYS:HD2	1.94	0.67
1:B:176:THR:O	1:B:377:ALA:HB3	1.95	0.67
1:J:176:THR:O	1:J:377:ALA:HB3	1.95	0.67
1:A:219:PHE:H	1:A:245:LYS:HD3	1.60	0.67
1:A:192:GLY:HA3	1:A:376:VAL:HG23	1.76	0.67
1:A:176:THR:O	1:A:377:ALA:HB3	1.95	0.66
1:K:176:THR:O	1:K:377:ALA:HB3	1.95	0.66
1:A:323:VAL:HG12	1:A:332:ILE:HA	1.76	0.66
1:C:176:THR:O	1:C:377:ALA:HB3	1.95	0.66
1:F:176:THR:O	1:F:377:ALA:HB3	1.95	0.66
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.76	0.66
1:I:176:THR:O	1:I:377:ALA:HB3	1.95	0.66
1:A:378:VAL:HG22	1:A:380:LYS:HD3	1.76	0.66
1:L:176:THR:O	1:L:377:ALA:HB3	1.95	0.66
1:N:176:THR:O	1:N:377:ALA:HB3	1.95	0.66
1:D:176:THR:O	1:D:377:ALA:HB3	1.95	0.66
1:G:176:THR:O	1:G:377:ALA:HB3	1.95	0.66
1:E:176:THR:O	1:E:377:ALA:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:176:THR:O	1:M:377:ALA:HB3	1.95	0.66
1:H:176:THR:O	1:H:377:ALA:HB3	1.95	0.66
1:A:229:ASN:ND2	1:A:232:GLU:OE1	2.30	0.65
1:A:220:ILE:HD11	1:A:296:THR:HG21	1.78	0.65
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.79	0.64
1:A:262:LEU:HD22	1:A:273:VAL:HG11	1.79	0.64
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.79	0.64
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.79	0.64
1:J:247:LEU:HB3	1:J:273:VAL:HG22	1.79	0.64
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.79	0.64
1:H:247:LEU:HB3	1:H:273:VAL:HG22	1.79	0.64
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.79	0.64
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.79	0.64
1:N:247:LEU:HB3	1:N:273:VAL:HG22	1.79	0.64
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.79	0.64
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.79	0.64
1:A:230:ILE:HA	1:A:233:MET:HB3	1.80	0.64
1:K:247:LEU:HB3	1:K:273:VAL:HG22	1.79	0.64
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.79	0.64
1:A:365:LEU:O	1:A:369:VAL:N	2.26	0.64
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.79	0.64
1:A:247:LEU:O	1:A:273:VAL:HA	1.98	0.64
1:A:87:ASP:OD1	1:A:88:GLY:N	2.28	0.63
1:A:119:GLY:HA3	1:A:439:GLY:HA3	1.80	0.63
1:A:280:GLY:HA3	1:A:284:ARG:HH12	1.62	0.63
1:A:479:ASN:OD1	1:A:480:ALA:N	2.31	0.63
1:A:228:SER:HA	1:A:258:ALA:HB2	1.81	0.63
1:A:232:GLU:OE2	1:A:310:GLU:N	2.32	0.63
1:A:61:GLU:OE1	1:A:72:GLN:NE2	2.32	0.62
1:A:197:ARG:HD2	1:A:277:LYS:HB3	1.81	0.62
1:A:76:GLU:O	1:A:79:SER:OG	2.11	0.62
1:D:152:ALA:HB2	1:D:399:ALA:HB2	1.82	0.62
1:L:152:ALA:HB2	1:L:399:ALA:HB2	1.82	0.62
1:A:339:GLU:HA	1:A:342:ILE:HG22	1.81	0.62
1:A:186:GLU:HB3	1:A:380:LYS:HB2	1.82	0.62
1:A:152:ALA:HB2	1:A:399:ALA:HB2	1.82	0.62
1:C:152:ALA:HB2	1:C:399:ALA:HB2	1.82	0.62
1:K:152:ALA:HB2	1:K:399:ALA:HB2	1.82	0.62
1:A:389:MET:O	1:A:393:LYS:N	2.27	0.62
1:B:152:ALA:HB2	1:B:399:ALA:HB2	1.82	0.62
1:E:152:ALA:HB2	1:E:399:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ALA:HB2	1:G:399:ALA:HB2	1.82	0.62
1:I:152:ALA:HB2	1:I:399:ALA:HB2	1.82	0.62
1:M:152:ALA:HB2	1:M:399:ALA:HB2	1.82	0.62
1:A:321:LYS:HB3	1:A:334:ASP:HB2	1.81	0.62
1:C:479:ASN:HD22	1:C:491:MET:HE2	1.65	0.62
1:F:152:ALA:HB2	1:F:399:ALA:HB2	1.82	0.62
1:H:152:ALA:HB2	1:H:399:ALA:HB2	1.82	0.62
1:J:152:ALA:HB2	1:J:399:ALA:HB2	1.82	0.62
1:N:479:ASN:HD22	1:N:491:MET:HE2	1.65	0.62
1:A:237:LEU:O	1:A:241:ALA:CB	2.46	0.62
1:A:479:ASN:HD22	1:A:491:MET:HE2	1.65	0.62
1:F:479:ASN:HD22	1:F:491:MET:HE2	1.65	0.62
1:I:479:ASN:HD22	1:I:491:MET:HE2	1.65	0.62
1:K:479:ASN:HD22	1:K:491:MET:HE2	1.65	0.62
1:N:152:ALA:HB2	1:N:399:ALA:HB2	1.82	0.61
1:A:124:VAL:HG22	1:A:504:LEU:HD21	1.80	0.61
1:A:186:GLU:HB2	1:A:380:LYS:CG	2.28	0.61
1:L:479:ASN:HD22	1:L:491:MET:HE2	1.65	0.61
1:A:104:LEU:HA	1:A:107:VAL:HG12	1.80	0.61
1:D:479:ASN:HD22	1:D:491:MET:HE2	1.65	0.61
1:A:116:LEU:O	1:A:120:ILE:N	2.25	0.61
1:E:479:ASN:HD22	1:E:491:MET:HE2	1.65	0.61
1:A:100:ILE:O	1:A:103:GLY:N	2.34	0.61
1:A:177:VAL:HG22	1:A:379:ILE:HD12	1.81	0.61
1:A:82:ASN:OD1	1:A:89:THR:OG1	2.18	0.61
1:M:479:ASN:HD22	1:M:491:MET:HE2	1.65	0.61
1:A:326:ASN:OD1	1:A:327:LYS:N	2.34	0.61
1:A:376:VAL:HG12	1:A:377:ALA:H	1.66	0.61
1:A:417:VAL:O	1:A:420:ILE:HG22	2.01	0.60
1:A:37:ASN:OD1	1:A:51:LYS:NZ	2.29	0.60
1:A:178:GLU:HB2	1:A:378:VAL:HG23	1.83	0.60
1:A:219:PHE:HB2	1:A:245:LYS:CE	2.31	0.60
1:A:230:ILE:HG23	1:A:257:GLU:HG3	1.82	0.60
1:K:232:GLU:HB3	1:K:309:LEU:HB2	1.84	0.60
1:A:42:LYS:HZ3	1:A:44:PHE:HE1	1.49	0.60
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.84	0.60
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.84	0.60
1:A:199:TYR:HB3	1:A:325:ILE:HD13	1.83	0.60
1:A:5:ASP:OD1	1:A:6:VAL:N	2.33	0.60
1:A:478:TYR:HB2	1:A:485:TYR:HE1	1.66	0.60
1:C:232:GLU:HB3	1:C:309:LEU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:232:GLU:HB3	1:N:309:LEU:HB2	1.84	0.60
1:E:232:GLU:HB3	1:E:309:LEU:HB2	1.84	0.60
1:F:232:GLU:HB3	1:F:309:LEU:HB2	1.84	0.60
1:L:232:GLU:HB3	1:L:309:LEU:HB2	1.84	0.60
1:D:232:GLU:HB3	1:D:309:LEU:HB2	1.84	0.60
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.84	0.60
1:G:479:ASN:HD22	1:G:491:MET:HE2	1.65	0.60
1:M:232:GLU:HB3	1:M:309:LEU:HB2	1.84	0.60
1:J:479:ASN:HD22	1:J:491:MET:HE2	1.65	0.60
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.84	0.60
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.84	0.60
1:B:232:GLU:HB3	1:B:309:LEU:HB2	1.84	0.60
1:B:479:ASN:HD22	1:B:491:MET:HE2	1.65	0.60
1:H:479:ASN:HD22	1:H:491:MET:HE2	1.65	0.60
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.84	0.60
1:A:347:ALA:HA	1:A:350:ARG:HB2	1.83	0.60
1:J:232:GLU:HB3	1:J:309:LEU:HB2	1.84	0.60
1:A:143:ALA:HA	1:A:146:GLN:HG2	1.84	0.60
1:A:145:ALA:HB2	1:A:163:ALA:HB2	1.84	0.59
1:G:232:GLU:HB3	1:G:309:LEU:HB2	1.84	0.59
1:H:177:VAL:HG22	1:H:379:ILE:HD12	1.83	0.59
1:H:232:GLU:HB3	1:H:309:LEU:HB2	1.84	0.59
1:K:177:VAL:HG22	1:K:379:ILE:HD12	1.83	0.59
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.84	0.59
1:A:404:ARG:O	1:A:407:VAL:HG22	2.02	0.59
1:G:177:VAL:HG22	1:G:379:ILE:HD12	1.83	0.59
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.84	0.59
1:A:123:ALA:O	1:A:127:ALA:N	2.26	0.59
1:A:100:ILE:HD11	1:A:511:ALA:HA	1.84	0.59
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.84	0.59
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.84	0.59
1:I:232:GLU:HB3	1:I:309:LEU:HB2	1.84	0.59
1:A:232:GLU:HB3	1:A:309:LEU:HB2	1.84	0.59
1:L:177:VAL:HG22	1:L:379:ILE:HD12	1.83	0.59
1:A:411:VAL:HG21	1:A:494:LEU:HD13	1.85	0.59
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.84	0.59
1:C:177:VAL:HG22	1:C:379:ILE:HD12	1.83	0.59
1:A:296:THR:OG1	1:A:319:GLN:N	2.36	0.59
1:A:177:VAL:HG22	1:A:379:ILE:HD12	1.83	0.59
1:D:177:VAL:HG22	1:D:379:ILE:HD12	1.83	0.59
1:F:177:VAL:HG22	1:F:379:ILE:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.84	0.59
1:I:177:VAL:HG22	1:I:379:ILE:HD12	1.83	0.59
1:N:177:VAL:HG22	1:N:379:ILE:HD12	1.83	0.59
1:J:177:VAL:HG22	1:J:379:ILE:HD12	1.83	0.59
1:A:413:ALA:HB1	1:A:488:MET:HB2	1.83	0.59
1:B:177:VAL:HG22	1:B:379:ILE:HD12	1.83	0.59
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.84	0.59
1:M:177:VAL:HG22	1:M:379:ILE:HD12	1.83	0.58
1:A:120:ILE:O	1:A:123:ALA:N	2.36	0.58
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.84	0.58
1:A:31:LEU:O	1:A:457:ASN:ND2	2.37	0.58
1:E:177:VAL:HG22	1:E:379:ILE:HD12	1.83	0.58
1:I:31:LEU:O	1:I:457:ASN:ND2	2.37	0.58
1:A:131:LEU:O	1:A:135:SER:N	2.35	0.58
1:A:149:THR:HB	1:A:154:SER:HA	1.86	0.58
1:N:31:LEU:O	1:N:457:ASN:ND2	2.37	0.58
1:A:177:VAL:HG13	1:A:379:ILE:HB	1.86	0.58
1:A:166:MET:HE1	1:A:171:LYS:HG2	1.85	0.58
1:A:230:ILE:HD11	1:A:258:ALA:HA	1.84	0.58
1:F:31:LEU:O	1:F:457:ASN:ND2	2.37	0.58
1:A:203:TYR:OH	1:A:267:MET:HA	2.03	0.58
1:A:255:GLU:HA	1:A:259:LEU:HD13	1.85	0.58
1:A:220:ILE:HG23	1:A:248:LEU:HG	1.85	0.58
1:A:282:GLY:O	1:A:285:ARG:NE	2.36	0.58
1:A:463:SER:O	1:A:467:ASN:HB2	2.04	0.58
1:A:523:ASP:OD1	1:A:524:LEU:N	2.37	0.58
1:G:31:LEU:O	1:G:457:ASN:ND2	2.37	0.57
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.85	0.57
1:A:128:VAL:HG21	1:A:505:GLN:HE21	1.70	0.57
1:E:31:LEU:O	1:E:457:ASN:ND2	2.37	0.57
1:H:31:LEU:O	1:H:457:ASN:ND2	2.37	0.57
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.86	0.57
1:A:284:ARG:HG3	1:A:285:ARG:HH22	1.68	0.57
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.86	0.57
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.86	0.57
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.57
1:I:128:VAL:HG21	1:I:505:GLN:HE21	1.70	0.57
1:A:199:TYR:HB3	1:A:325:ILE:HG12	1.85	0.57
1:G:128:VAL:HG21	1:G:505:GLN:HE21	1.70	0.57
1:H:128:VAL:HG21	1:H:505:GLN:HE21	1.70	0.57
1:M:31:LEU:O	1:M:457:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:HE2	1:A:245:LYS:HB3	1.69	0.57
1:L:31:LEU:O	1:L:457:ASN:ND2	2.37	0.57
1:A:353:ILE:HG22	1:A:365:LEU:HB3	1.86	0.57
1:D:31:LEU:O	1:D:457:ASN:ND2	2.37	0.57
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.57
1:L:73:MET:HE3	1:M:49:ILE:HD11	1.87	0.57
1:A:346:VAL:O	1:A:350:ARG:N	2.29	0.57
1:K:31:LEU:O	1:K:457:ASN:ND2	2.37	0.57
1:A:414:GLY:H	1:A:494:LEU:HA	1.69	0.57
1:A:206:ASN:OD1	1:A:213:VAL:HA	2.04	0.57
1:A:477:GLY:C	1:A:488:MET:HE2	2.30	0.57
1:A:511:ALA:O	1:A:515:ILE:N	2.32	0.57
1:B:31:LEU:O	1:B:457:ASN:ND2	2.37	0.57
1:C:31:LEU:O	1:C:457:ASN:ND2	2.37	0.57
1:C:124:VAL:HG21	1:C:508:ALA:HB2	1.87	0.57
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.86	0.57
1:J:128:VAL:HG21	1:J:505:GLN:HE21	1.70	0.57
1:A:219:PHE:O	1:A:245:LYS:NZ	2.37	0.57
1:B:128:VAL:HG21	1:B:505:GLN:HE21	1.70	0.57
1:K:124:VAL:HG21	1:K:508:ALA:HB2	1.87	0.57
1:A:326:ASN:N	1:A:329:THR:O	2.38	0.57
1:D:124:VAL:HG21	1:D:508:ALA:HB2	1.87	0.56
1:J:124:VAL:HG21	1:J:508:ALA:HB2	1.87	0.56
1:L:124:VAL:HG21	1:L:508:ALA:HB2	1.87	0.56
1:M:124:VAL:HG21	1:M:508:ALA:HB2	1.87	0.56
1:A:421:ARG:NH1	1:A:472:GLY:O	2.38	0.56
1:B:124:VAL:HG21	1:B:508:ALA:HB2	1.87	0.56
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.86	0.56
1:E:124:VAL:HG21	1:E:508:ALA:HB2	1.87	0.56
1:J:31:LEU:O	1:J:457:ASN:ND2	2.37	0.56
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.86	0.56
1:A:126:VAL:HG11	1:A:429:LEU:HD22	1.87	0.56
1:A:102:GLU:OE1	1:A:445:ARG:NH2	2.38	0.56
1:A:206:ASN:H	1:A:213:VAL:HG23	1.69	0.56
1:D:128:VAL:HG21	1:D:505:GLN:HE21	1.70	0.56
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.86	0.56
1:L:128:VAL:HG21	1:L:505:GLN:HE21	1.70	0.56
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.86	0.56
1:A:178:GLU:HB2	1:A:378:VAL:HA	1.88	0.56
1:A:305:ILE:HG23	1:A:307:MET:HG2	1.87	0.56
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:VAL:HG21	1:E:505:GLN:HE21	1.70	0.56
1:I:124:VAL:HG21	1:I:508:ALA:HB2	1.87	0.56
1:A:124:VAL:HG21	1:A:508:ALA:HB2	1.87	0.56
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.56
1:A:219:PHE:HB2	1:A:245:LYS:NZ	2.21	0.56
1:A:353:ILE:HA	1:A:356:ALA:HB2	1.88	0.56
1:A:398:ASP:OD1	1:A:399:ALA:N	2.39	0.56
1:A:414:GLY:HA3	1:A:493:ILE:HG22	1.88	0.56
1:M:128:VAL:HG21	1:M:505:GLN:HE21	1.70	0.56
1:N:128:VAL:HG21	1:N:505:GLN:HE21	1.70	0.56
1:A:230:ILE:CD1	1:A:258:ALA:HA	2.35	0.56
1:G:124:VAL:HG21	1:G:508:ALA:HB2	1.87	0.56
1:A:178:GLU:OE2	1:A:333:ILE:HG21	2.05	0.56
1:A:216:GLU:O	1:A:245:LYS:HE2	2.06	0.56
1:A:160:LYS:O	1:A:164:GLU:HG2	2.06	0.56
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.86	0.56
1:F:124:VAL:HG21	1:F:508:ALA:HB2	1.87	0.56
1:F:128:VAL:HG21	1:F:505:GLN:HE21	1.70	0.56
1:H:124:VAL:HG21	1:H:508:ALA:HB2	1.87	0.56
1:N:124:VAL:HG21	1:N:508:ALA:HB2	1.87	0.56
1:K:128:VAL:HG21	1:K:505:GLN:HE21	1.70	0.56
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.56
1:A:199:TYR:CE1	1:A:327:LYS:HA	2.41	0.56
1:A:199:TYR:HA	1:A:276:VAL:HG12	1.88	0.55
1:A:420:ILE:HD11	1:A:448:GLU:HA	1.88	0.55
1:C:128:VAL:HG21	1:C:505:GLN:HE21	1.70	0.55
1:A:279:PRO:O	1:A:285:ARG:NE	2.39	0.55
1:A:199:TYR:CZ	1:A:205:ILE:HD11	2.42	0.55
1:A:116:LEU:O	1:A:119:GLY:N	2.39	0.55
1:A:194:GLN:HA	1:A:330:THR:O	2.06	0.55
1:A:479:ASN:HD22	1:A:491:MET:HE2	1.72	0.55
1:A:219:PHE:CE2	1:A:245:LYS:HB3	2.42	0.55
1:A:122:LYS:NZ	1:A:430:ARG:O	2.34	0.55
1:A:115:ASP:OD2	1:A:436:GLN:N	2.40	0.55
1:A:313:THR:H	1:A:316:ASP:HB2	1.72	0.55
1:B:177:VAL:HG13	1:B:379:ILE:HB	1.89	0.55
1:J:177:VAL:HG13	1:J:379:ILE:HB	1.89	0.55
1:A:175:ILE:HB	1:A:377:ALA:HB2	1.89	0.55
1:A:227:ILE:HD11	1:A:233:MET:HE3	1.89	0.55
1:F:177:VAL:HG13	1:F:379:ILE:HB	1.89	0.55
1:N:177:VAL:HG13	1:N:379:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:OD1	1:A:88:GLY:N	2.36	0.55
1:A:32:GLY:O	1:A:35:GLY:N	2.40	0.54
1:A:128:VAL:HG21	1:A:505:GLN:HE21	1.73	0.54
1:E:177:VAL:HG13	1:E:379:ILE:HB	1.90	0.54
1:M:177:VAL:HG13	1:M:379:ILE:HB	1.90	0.54
1:A:87:ASP:OD1	1:A:88:GLY:N	2.37	0.54
1:A:240:VAL:HG23	1:A:245:LYS:HE3	1.90	0.54
1:A:284:ARG:HG3	1:A:285:ARG:NH2	2.22	0.54
1:A:40:LEU:HD11	1:A:56:VAL:HG22	1.89	0.54
1:A:177:VAL:HG13	1:A:379:ILE:HB	1.90	0.54
1:C:177:VAL:HG13	1:C:379:ILE:HB	1.89	0.54
1:I:177:VAL:HG13	1:I:379:ILE:HB	1.90	0.54
1:A:319:GLN:O	1:A:336:VAL:HG23	2.07	0.54
1:H:177:VAL:HG13	1:H:379:ILE:HB	1.89	0.54
1:K:177:VAL:HG13	1:K:379:ILE:HB	1.90	0.54
1:A:135:SER:HA	1:A:412:VAL:HG12	1.89	0.54
1:A:131:LEU:HG	1:A:422:VAL:HG11	1.89	0.54
1:A:431:GLY:H	1:A:437:ASN:ND2	2.06	0.54
1:A:281:PHE:O	1:A:284:ARG:NH1	2.40	0.54
1:A:353:ILE:HD13	1:A:365:LEU:HG	1.90	0.54
1:D:177:VAL:HG13	1:D:379:ILE:HB	1.90	0.54
1:A:27:VAL:HA	1:A:30:THR:HG22	1.90	0.54
1:A:294:THR:O	1:A:337:GLY:HA3	2.08	0.54
1:G:177:VAL:HG13	1:G:379:ILE:HB	1.90	0.54
1:L:177:VAL:HG13	1:L:379:ILE:HB	1.90	0.54
1:A:19:GLY:HA2	1:A:67:GLU:OE2	2.08	0.54
1:A:7:LYS:CB	1:A:12:ALA:HB2	2.38	0.53
1:A:16:MET:HE2	1:A:520:MET:HE3	1.90	0.53
1:A:195:PHE:CZ	1:A:330:THR:HB	2.43	0.53
1:A:220:ILE:CB	1:A:318:GLY:O	2.52	0.53
1:A:435:ASP:HA	1:A:438:VAL:HG22	1.91	0.53
1:A:123:ALA:HB2	1:A:440:ILE:HG23	1.88	0.53
1:A:293:ALA:O	1:A:296:THR:OG1	2.26	0.53
1:H:49:ILE:HD11	1:N:73:MET:HE3	1.91	0.53
1:A:7:LYS:HB3	1:A:12:ALA:HB2	1.90	0.53
1:A:176:THR:O	1:A:377:ALA:CB	2.45	0.53
1:M:323:VAL:HG12	1:M:332:ILE:HA	1.91	0.53
1:A:348:GLN:O	1:A:351:GLN:HB3	2.09	0.53
1:F:73:MET:HE3	1:G:49:ILE:HD11	1.91	0.53
1:A:16:MET:HE3	1:A:520:MET:SD	2.48	0.53
1:E:323:VAL:HG12	1:E:332:ILE:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:MET:HE3	1:I:49:ILE:HD11	1.91	0.53
1:M:73:MET:HE3	1:N:49:ILE:HD11	1.91	0.53
1:A:401:HIS:O	1:A:404:ARG:HB3	2.09	0.53
1:A:247:LEU:O	1:A:274:ALA:N	2.39	0.53
1:D:73:MET:HE3	1:E:49:ILE:HD11	1.91	0.53
1:A:107:VAL:HG21	1:A:113:PRO:HG3	1.90	0.53
1:A:301:ILE:HG12	1:A:307:MET:HE3	1.91	0.53
1:A:49:ILE:HD11	1:G:73:MET:HE3	1.91	0.53
1:J:323:VAL:HG12	1:J:332:ILE:HA	1.91	0.53
1:N:323:VAL:HG12	1:N:332:ILE:HA	1.91	0.53
1:A:201:SER:H	1:A:204:PHE:HE2	1.54	0.53
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.91	0.53
1:L:323:VAL:HG12	1:L:332:ILE:HA	1.91	0.52
1:A:186:GLU:H	1:A:380:LYS:HB2	1.74	0.52
1:D:323:VAL:HG12	1:D:332:ILE:HA	1.91	0.52
1:F:323:VAL:HG12	1:F:332:ILE:HA	1.91	0.52
1:I:323:VAL:HG12	1:I:332:ILE:HA	1.91	0.52
1:A:219:PHE:CE2	1:A:245:LYS:HB2	2.45	0.52
1:B:323:VAL:HG12	1:B:332:ILE:HA	1.91	0.52
1:C:323:VAL:HG12	1:C:332:ILE:HA	1.91	0.52
1:J:73:MET:HE3	1:K:49:ILE:HD11	1.91	0.52
1:K:323:VAL:HG12	1:K:332:ILE:HA	1.91	0.52
1:A:250:ILE:HA	1:A:276:VAL:O	2.09	0.52
1:A:64:ASP:HB3	1:A:67:GLU:HB3	1.91	0.52
1:H:323:VAL:HG12	1:H:332:ILE:HA	1.91	0.52
1:A:230:ILE:HD12	1:A:231:ARG:N	2.23	0.52
1:A:461:GLU:OE1	1:A:464:VAL:N	2.39	0.52
1:A:323:VAL:HG12	1:A:332:ILE:HA	1.91	0.52
1:E:24:ALA:O	1:E:28:LYS:HB3	2.10	0.52
1:G:323:VAL:HG12	1:G:332:ILE:HA	1.91	0.52
1:M:24:ALA:O	1:M:28:LYS:HB3	2.10	0.52
1:A:219:PHE:CD2	1:A:245:LYS:HE2	2.45	0.52
1:A:113:PRO:C	1:A:115:ASP:H	2.16	0.52
1:A:135:SER:HA	1:A:412:VAL:HG12	1.92	0.52
1:A:421:ARG:NH1	1:A:472:GLY:O	2.42	0.52
1:A:122:LYS:NZ	1:A:430:ARG:O	2.33	0.52
1:A:73:MET:HE3	1:B:49:ILE:HD11	1.92	0.52
1:F:349:ILE:HG12	1:F:368:ARG:HH21	1.75	0.52
1:N:349:ILE:HG12	1:N:368:ARG:HH21	1.75	0.52
1:A:77:VAL:HG21	1:A:510:VAL:CG1	2.40	0.52
1:A:126:VAL:HG11	1:A:429:LEU:CD2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:ALA:O	1:F:28:LYS:HB3	2.10	0.52
1:N:24:ALA:O	1:N:28:LYS:HB3	2.10	0.52
1:A:230:ILE:HD12	1:A:231:ARG:N	2.24	0.52
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.90	0.52
1:B:73:MET:HE3	1:C:49:ILE:HD11	1.91	0.52
1:D:24:ALA:O	1:D:28:LYS:HB3	2.10	0.52
1:D:187:LEU:HD13	1:D:379:ILE:HG12	1.92	0.52
1:A:296:THR:HB	1:A:318:GLY:HA3	1.91	0.52
1:A:363:GLU:HA	1:A:366:GLN:HE21	1.75	0.52
1:E:349:ILE:HG12	1:E:368:ARG:HH21	1.75	0.52
1:H:349:ILE:HG12	1:H:368:ARG:HH21	1.75	0.52
1:L:24:ALA:O	1:L:28:LYS:HB3	2.10	0.52
1:L:187:LEU:HD13	1:L:379:ILE:HG12	1.92	0.52
1:M:349:ILE:HG12	1:M:368:ARG:HH21	1.75	0.52
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.92	0.52
1:A:179:ASP:HB3	1:A:389:MET:HE1	1.91	0.52
1:A:303:GLU:OE1	1:A:303:GLU:N	2.37	0.52
1:I:73:MET:HE3	1:J:49:ILE:HD11	1.92	0.52
1:A:240:VAL:CG2	1:A:245:LYS:HE3	2.40	0.52
1:D:349:ILE:HG12	1:D:368:ARG:HH21	1.75	0.51
1:E:73:MET:HE3	1:F:49:ILE:HD11	1.92	0.51
1:G:349:ILE:HG12	1:G:368:ARG:HH21	1.75	0.51
1:M:187:LEU:HD13	1:M:379:ILE:HG12	1.92	0.51
1:A:162:ILE:HD12	1:A:162:ILE:H	1.75	0.51
1:A:217:SER:O	1:A:245:LYS:NZ	2.38	0.51
1:A:156:GLU:O	1:A:160:LYS:HD3	2.09	0.51
1:A:421:ARG:NH1	1:A:472:GLY:O	2.43	0.51
1:C:187:LEU:HD13	1:C:379:ILE:HG12	1.92	0.51
1:E:187:LEU:HD13	1:E:379:ILE:HG12	1.92	0.51
1:J:187:LEU:HD13	1:J:379:ILE:HG12	1.92	0.51
1:B:24:ALA:O	1:B:28:LYS:HB3	2.10	0.51
1:B:187:LEU:HD13	1:B:379:ILE:HG12	1.92	0.51
1:C:24:ALA:O	1:C:28:LYS:HB3	2.10	0.51
1:G:24:ALA:O	1:G:28:LYS:HB3	2.10	0.51
1:G:171:LYS:O	1:G:404:ARG:NH1	2.44	0.51
1:H:24:ALA:O	1:H:28:LYS:HB3	2.10	0.51
1:H:171:LYS:O	1:H:404:ARG:NH1	2.44	0.51
1:K:24:ALA:O	1:K:28:LYS:HB3	2.10	0.51
1:L:349:ILE:HG12	1:L:368:ARG:HH21	1.75	0.51
1:A:228:SER:C	1:A:257:GLU:HB3	2.35	0.51
1:A:340:ALA:O	1:A:343:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD13	1:A:237:LEU:HD11	1.92	0.51
1:F:171:LYS:O	1:F:404:ARG:NH1	2.44	0.51
1:I:171:LYS:O	1:I:404:ARG:NH1	2.44	0.51
1:I:349:ILE:HG12	1:I:368:ARG:HH21	1.75	0.51
1:J:24:ALA:O	1:J:28:LYS:HB3	2.10	0.51
1:K:187:LEU:HD13	1:K:379:ILE:HG12	1.92	0.51
1:A:31:LEU:HB2	1:A:90:THR:HG21	1.92	0.51
1:A:171:LYS:O	1:A:404:ARG:NH1	2.44	0.51
1:E:171:LYS:O	1:E:404:ARG:NH1	2.44	0.51
1:M:171:LYS:O	1:M:404:ARG:NH1	2.44	0.51
1:N:171:LYS:O	1:N:404:ARG:NH1	2.44	0.51
1:A:219:PHE:HD2	1:A:245:LYS:HE2	1.75	0.51
1:A:254:VAL:HG12	1:A:259:LEU:HD12	1.93	0.51
1:A:213:VAL:O	1:A:324:VAL:HA	2.11	0.51
1:A:504:LEU:O	1:A:507:ALA:N	2.44	0.51
1:C:73:MET:HE3	1:D:49:ILE:HD11	1.92	0.51
1:J:349:ILE:HG12	1:J:368:ARG:HH21	1.75	0.51
1:A:288:MET:HG2	1:A:368:ARG:NH1	2.26	0.51
1:A:349:ILE:HG12	1:A:368:ARG:HH21	1.75	0.51
1:A:187:LEU:HD13	1:A:379:ILE:HG12	1.93	0.51
1:A:234:LEU:HD23	1:A:235:PRO:HD3	1.93	0.51
1:D:257:GLU:O	1:D:261:THR:OG1	2.26	0.51
1:I:24:ALA:O	1:I:28:LYS:HB3	2.10	0.51
1:I:187:LEU:HD13	1:I:379:ILE:HG12	1.92	0.51
1:K:349:ILE:HG12	1:K:368:ARG:HH21	1.75	0.51
1:A:223:ALA:O	1:A:250:ILE:C	2.53	0.51
1:A:165:ALA:HB1	1:A:175:ILE:HD12	1.92	0.51
1:A:24:ALA:O	1:A:28:LYS:HB3	2.10	0.51
1:A:187:LEU:HD13	1:A:379:ILE:HG12	1.92	0.51
1:A:281:PHE:HA	1:A:285:ARG:HE	1.76	0.51
1:B:349:ILE:HG12	1:B:368:ARG:HH21	1.75	0.51
1:I:281:PHE:HA	1:I:285:ARG:HE	1.76	0.51
1:A:122:LYS:HD3	1:A:440:ILE:HD11	1.92	0.51
1:A:223:ALA:HB3	1:A:249:ILE:HG23	1.91	0.51
1:F:187:LEU:HD13	1:F:379:ILE:HG12	1.92	0.51
1:F:281:PHE:HA	1:F:285:ARG:HE	1.76	0.51
1:N:187:LEU:HD13	1:N:379:ILE:HG12	1.92	0.51
1:A:213:VAL:HG22	1:A:325:ILE:HB	1.92	0.51
1:A:224:ASP:O	1:A:225:LYS:HD2	2.11	0.51
1:A:254:VAL:HG23	1:A:259:LEU:HB3	1.92	0.51
1:D:171:LYS:O	1:D:404:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:LYS:O	1:L:404:ARG:NH1	2.44	0.50
1:N:281:PHE:HA	1:N:285:ARG:HE	1.76	0.50
1:A:390:LYS:O	1:A:393:LYS:HB3	2.11	0.50
1:A:388:GLU:O	1:A:392:LYS:N	2.37	0.50
1:A:505:GLN:O	1:A:508:ALA:N	2.44	0.50
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.93	0.50
1:C:349:ILE:HG12	1:C:368:ARG:HH21	1.75	0.50
1:D:421:ARG:NH1	1:D:472:GLY:O	2.45	0.50
1:H:187:LEU:HD13	1:H:379:ILE:HG12	1.92	0.50
1:K:73:MET:HE3	1:L:49:ILE:HD11	1.93	0.50
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.93	0.50
1:G:187:LEU:HD13	1:G:379:ILE:HG12	1.92	0.50
1:J:171:LYS:O	1:J:404:ARG:NH1	2.44	0.50
1:K:281:PHE:HA	1:K:285:ARG:HE	1.76	0.50
1:L:421:ARG:NH1	1:L:472:GLY:O	2.45	0.50
1:A:34:LYS:HG3	1:A:458:CYS:SG	2.50	0.50
1:B:171:LYS:O	1:B:404:ARG:NH1	2.44	0.50
1:C:171:LYS:O	1:C:404:ARG:NH1	2.44	0.50
1:C:281:PHE:HA	1:C:285:ARG:HE	1.76	0.50
1:D:281:PHE:HA	1:D:285:ARG:HE	1.76	0.50
1:E:421:ARG:NH1	1:E:472:GLY:O	2.45	0.50
1:K:171:LYS:O	1:K:404:ARG:NH1	2.44	0.50
1:L:281:PHE:HA	1:L:285:ARG:HE	1.76	0.50
1:M:421:ARG:NH1	1:M:472:GLY:O	2.45	0.50
1:A:389:MET:O	1:A:392:LYS:N	2.43	0.50
1:A:249:ILE:N	1:A:274:ALA:O	2.31	0.50
1:A:421:ARG:NH1	1:A:472:GLY:O	2.45	0.50
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.93	0.50
1:H:421:ARG:NH1	1:H:472:GLY:O	2.45	0.50
1:I:421:ARG:NH1	1:I:472:GLY:O	2.45	0.50
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.93	0.50
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.93	0.50
1:A:288:MET:HA	1:A:291:ASP:OD2	2.12	0.50
1:A:109:ALA:HB2	1:J:109:ALA:HB2	1.94	0.50
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.93	0.50
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.93	0.50
1:G:421:ARG:NH1	1:G:472:GLY:O	2.45	0.50
1:K:421:ARG:NH1	1:K:472:GLY:O	2.45	0.50
1:A:141:SER:O	1:A:144:ILE:HG22	2.12	0.50
1:A:257:GLU:O	1:A:261:THR:HB	2.11	0.50
1:A:295:LEU:O	1:A:337:GLY:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:O	1:A:346:VAL:HG23	2.12	0.50
1:C:421:ARG:NH1	1:C:472:GLY:O	2.45	0.50
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.93	0.50
1:G:281:PHE:HA	1:G:285:ARG:HE	1.76	0.50
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.93	0.50
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.93	0.50
1:F:109:ALA:HB2	1:L:109:ALA:HB2	1.93	0.50
1:H:281:PHE:HA	1:H:285:ARG:HE	1.76	0.50
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.93	0.50
1:A:10:ASN:O	1:A:14:VAL:HG22	2.12	0.50
1:A:23:LEU:HD13	1:A:60:ILE:HD11	1.93	0.50
1:B:109:ALA:HB2	1:I:109:ALA:HB2	1.94	0.50
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.93	0.50
1:A:115:ASP:OD2	1:A:433:ASN:ND2	2.32	0.50
1:A:213:VAL:HG22	1:A:325:ILE:CG2	2.42	0.50
1:A:254:VAL:HG21	1:A:275:ALA:HB1	1.93	0.50
1:F:421:ARG:NH1	1:F:472:GLY:O	2.45	0.49
1:G:109:ALA:HB2	1:K:109:ALA:HB2	1.93	0.49
1:A:155:ASP:OD1	1:A:156:GLU:N	2.40	0.49
1:A:24:ALA:O	1:A:28:LYS:HG2	2.11	0.49
1:A:435:ASP:O	1:A:438:VAL:HG12	2.12	0.49
1:N:247:LEU:O	1:N:273:VAL:HA	2.13	0.49
1:N:421:ARG:NH1	1:N:472:GLY:O	2.45	0.49
1:A:223:ALA:HB3	1:A:227:ILE:HD11	1.93	0.49
1:A:94:VAL:HG12	1:A:449:ALA:HB1	1.95	0.49
1:B:421:ARG:NH1	1:B:472:GLY:O	2.45	0.49
1:D:22:VAL:HG11	1:D:62:LEU:HD21	1.95	0.49
1:E:22:VAL:HG11	1:E:62:LEU:HD21	1.95	0.49
1:E:281:PHE:HA	1:E:285:ARG:HE	1.76	0.49
1:F:247:LEU:O	1:F:273:VAL:HA	2.13	0.49
1:G:247:LEU:O	1:G:273:VAL:HA	2.13	0.49
1:H:247:LEU:O	1:H:273:VAL:HA	2.13	0.49
1:J:281:PHE:HA	1:J:285:ARG:HE	1.76	0.49
1:J:421:ARG:NH1	1:J:472:GLY:O	2.45	0.49
1:L:22:VAL:HG11	1:L:62:LEU:HD21	1.95	0.49
1:M:22:VAL:HG11	1:M:62:LEU:HD21	1.95	0.49
1:A:116:LEU:HD21	1:A:438:VAL:HG23	1.94	0.49
1:A:365:LEU:HA	1:A:368:ARG:HB2	1.93	0.49
1:A:247:LEU:O	1:A:273:VAL:HA	2.13	0.49
1:C:22:VAL:HG11	1:C:62:LEU:HD21	1.94	0.49
1:C:257:GLU:O	1:C:261:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:LEU:O	1:E:273:VAL:HA	2.13	0.49
1:K:257:GLU:O	1:K:261:THR:OG1	2.26	0.49
1:M:281:PHE:HA	1:M:285:ARG:HE	1.76	0.49
1:A:196:ASP:HA	1:A:329:THR:HG23	1.94	0.49
1:B:281:PHE:HA	1:B:285:ARG:HE	1.77	0.49
1:C:109:ALA:HB2	1:H:109:ALA:HB2	1.94	0.49
1:I:247:LEU:O	1:I:273:VAL:HA	2.13	0.49
1:M:247:LEU:O	1:M:273:VAL:HA	2.13	0.49
1:A:39:VAL:HG22	1:A:49:ILE:HG12	1.95	0.49
1:A:350:ARG:O	1:A:353:ILE:HG12	2.12	0.49
1:A:479:ASN:HD22	1:A:491:MET:HE2	1.78	0.49
1:A:326:ASN:HB3	1:A:329:THR:H	1.77	0.49
1:F:22:VAL:HG11	1:F:62:LEU:HD21	1.95	0.49
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.93	0.49
1:N:22:VAL:HG11	1:N:62:LEU:HD21	1.95	0.49
1:A:257:GLU:O	1:A:261:THR:CB	2.61	0.49
1:A:314:LEU:HD22	1:A:317:LEU:HD11	1.95	0.49
1:K:22:VAL:HG11	1:K:62:LEU:HD21	1.95	0.49
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.95	0.49
1:A:441:LYS:O	1:A:445:ARG:HG3	2.13	0.49
1:A:368:ARG:O	1:A:371:LYS:HB3	2.13	0.49
1:A:496:PRO:HD2	1:A:499:VAL:HG11	1.94	0.49
1:A:387:VAL:HG23	1:A:390:LYS:HZ1	1.78	0.49
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.93	0.49
1:B:247:LEU:O	1:B:273:VAL:HA	2.13	0.49
1:A:199:TYR:HA	1:A:276:VAL:HG12	1.93	0.49
1:D:247:LEU:O	1:D:273:VAL:HA	2.13	0.49
1:J:247:LEU:O	1:J:273:VAL:HA	2.13	0.49
1:L:247:LEU:O	1:L:273:VAL:HA	2.13	0.49
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.95	0.49
1:A:420:ILE:CD1	1:A:448:GLU:HA	2.42	0.49
1:D:109:ALA:HB2	1:N:109:ALA:HB2	1.94	0.49
1:A:222:LEU:O	1:A:301:ILE:HG22	2.13	0.49
1:C:247:LEU:O	1:C:273:VAL:HA	2.13	0.48
1:A:219:PHE:CD1	1:A:319:GLN:HB2	2.48	0.48
1:A:213:VAL:H	1:A:325:ILE:HG22	1.78	0.48
1:J:248:LEU:HD22	1:J:323:VAL:HG21	1.95	0.48
1:K:247:LEU:O	1:K:273:VAL:HA	2.13	0.48
1:A:205:ILE:HG23	1:A:212:ALA:O	2.13	0.48
1:A:338:GLU:O	1:A:342:ILE:N	2.33	0.48
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HD22	1:B:323:VAL:HG21	1.95	0.48
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.96	0.48
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.96	0.48
1:E:248:LEU:HD22	1:E:323:VAL:HG21	1.95	0.48
1:A:10:ASN:O	1:A:13:GLY:N	2.46	0.48
1:A:463:SER:O	1:A:467:ASN:CB	2.62	0.48
1:A:135:SER:HA	1:A:412:VAL:HG12	1.95	0.48
1:A:219:PHE:HB3	1:A:317:LEU:HD13	1.94	0.48
1:A:289:LEU:HD12	1:A:290:GLN:N	2.27	0.48
1:A:248:LEU:HD22	1:A:323:VAL:HG21	1.95	0.48
1:F:519:CYS:HB3	1:G:38:VAL:HG22	1.96	0.48
1:H:38:VAL:HG22	1:N:519:CYS:HB3	1.95	0.48
1:K:40:LEU:HD13	1:K:59:GLU:HG3	1.96	0.48
1:L:40:LEU:HD13	1:L:59:GLU:HG3	1.96	0.48
1:M:40:LEU:HD13	1:M:59:GLU:HG3	1.96	0.48
1:M:519:CYS:HB3	1:N:38:VAL:HG22	1.95	0.48
1:A:157:THR:O	1:A:160:LYS:HB3	2.13	0.48
1:A:519:CYS:SG	1:A:520:MET:N	2.86	0.48
1:A:339:GLU:HA	1:A:342:ILE:HG22	1.95	0.48
1:A:487:ASN:O	1:A:491:MET:HG3	2.12	0.48
1:A:169:VAL:HG12	1:A:173:GLY:HA3	1.96	0.48
1:A:421:ARG:NE	1:A:474:GLY:O	2.46	0.48
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.48	0.48
1:A:458:CYS:SG	2:A:602:HOH:O	2.60	0.48
1:B:22:VAL:HG11	1:B:62:LEU:HD21	1.95	0.48
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.96	0.48
1:F:40:LEU:HD13	1:F:59:GLU:HG3	1.96	0.48
1:G:22:VAL:HG11	1:G:62:LEU:HD21	1.95	0.48
1:G:40:LEU:HD13	1:G:59:GLU:HG3	1.96	0.48
1:H:40:LEU:HD13	1:H:59:GLU:HG3	1.96	0.48
1:M:248:LEU:HD22	1:M:323:VAL:HG21	1.95	0.48
1:A:178:GLU:CD	1:A:322:ARG:HD3	2.39	0.48
1:A:253:ASP:OD1	1:A:254:VAL:N	2.45	0.48
1:A:166:MET:O	1:A:170:GLY:N	2.47	0.48
1:A:247:LEU:HD13	1:A:248:LEU:N	2.28	0.48
1:A:194:GLN:HG3	1:A:331:THR:HG22	1.95	0.48
1:A:308:GLU:OE2	1:A:311:LYS:NZ	2.38	0.48
1:H:22:VAL:HG11	1:H:62:LEU:HD21	1.95	0.48
1:I:248:LEU:HD22	1:I:323:VAL:HG21	1.95	0.48
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.95	0.48
1:N:40:LEU:HD13	1:N:59:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:THR:O	1:A:264:VAL:HB	2.12	0.48
1:A:289:LEU:HA	1:A:292:ILE:HG22	1.95	0.48
1:A:16:MET:O	1:A:19:GLY:N	2.45	0.48
1:F:248:LEU:HD22	1:F:323:VAL:HG21	1.95	0.48
1:H:519:CYS:HB3	1:I:38:VAL:HG22	1.96	0.48
1:N:248:LEU:HD22	1:N:323:VAL:HG21	1.95	0.48
1:A:220:ILE:H	1:A:319:GLN:HA	1.78	0.48
1:A:260:ALA:O	1:A:264:VAL:HG23	2.14	0.48
1:A:358:SER:O	1:A:362:ARG:HG3	2.14	0.48
1:A:232:GLU:OE2	1:A:308:GLU:HG3	2.13	0.48
1:B:257:GLU:O	1:B:261:THR:OG1	2.26	0.48
1:F:257:GLU:O	1:F:261:THR:OG1	2.26	0.48
1:I:40:LEU:HD13	1:I:59:GLU:HG3	1.96	0.48
1:L:519:CYS:HB3	1:M:38:VAL:HG22	1.94	0.48
1:A:308:GLU:CD	1:A:309:LEU:N	2.72	0.48
1:A:362:ARG:O	1:A:366:GLN:NE2	2.47	0.48
1:C:248:LEU:HD22	1:C:323:VAL:HG21	1.95	0.48
1:H:77:VAL:HG12	1:H:506:TYR:HB3	1.96	0.48
1:K:248:LEU:HD22	1:K:323:VAL:HG21	1.95	0.48
1:A:221:LEU:O	1:A:248:LEU:O	2.32	0.48
1:A:121:ASP:O	1:A:125:THR:HG22	2.14	0.48
1:A:240:VAL:O	1:A:244:GLY:N	2.45	0.48
1:A:38:VAL:HG22	1:G:519:CYS:HB3	1.96	0.48
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.96	0.48
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.96	0.48
1:B:447:MET:HE2	1:B:504:LEU:HD11	1.96	0.48
1:C:447:MET:HE2	1:C:504:LEU:HD11	1.96	0.48
1:J:40:LEU:HD13	1:J:59:GLU:HG3	1.96	0.48
1:J:217:SER:N	1:J:321:LYS:O	2.46	0.48
1:J:270:ILE:HG22	1:J:271:VAL:HG23	1.96	0.48
1:J:447:MET:HE2	1:J:504:LEU:HD11	1.96	0.48
1:A:167:ASP:OD1	1:A:168:LYS:N	2.46	0.48
1:B:40:LEU:HD13	1:B:59:GLU:HG3	1.96	0.47
1:B:217:SER:N	1:B:321:LYS:O	2.46	0.47
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.96	0.47
1:G:77:VAL:HG12	1:G:506:TYR:HB3	1.96	0.47
1:G:447:MET:HE2	1:G:504:LEU:HD11	1.96	0.47
1:H:447:MET:HE2	1:H:504:LEU:HD11	1.96	0.47
1:I:77:VAL:HG12	1:I:506:TYR:HB3	1.96	0.47
1:J:257:GLU:O	1:J:261:THR:OG1	2.26	0.47
1:L:270:ILE:HG22	1:L:271:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:217:SER:N	1:M:321:LYS:O	2.46	0.47
1:M:270:ILE:HG22	1:M:271:VAL:HG23	1.96	0.47
1:A:219:PHE:HA	1:A:319:GLN:HA	1.95	0.47
1:A:230:ILE:HG23	1:A:257:GLU:CG	2.43	0.47
1:A:303:GLU:OE1	1:A:303:GLU:N	2.44	0.47
1:A:177:VAL:HG12	1:A:393:LYS:NZ	2.29	0.47
1:A:200:LEU:HG	1:A:276:VAL:HA	1.96	0.47
1:A:221:LEU:HD22	1:A:236:VAL:HG11	1.97	0.47
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.96	0.47
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.96	0.47
1:F:77:VAL:HG12	1:F:506:TYR:HB3	1.96	0.47
1:I:447:MET:HE2	1:I:504:LEU:HD11	1.96	0.47
1:K:447:MET:HE2	1:K:504:LEU:HD11	1.96	0.47
1:N:77:VAL:HG12	1:N:506:TYR:HB3	1.96	0.47
1:N:257:GLU:O	1:N:261:THR:OG1	2.26	0.47
1:A:288:MET:O	1:A:291:ASP:N	2.48	0.47
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.96	0.47
1:D:221:LEU:HD22	1:D:236:VAL:HG11	1.97	0.47
1:D:248:LEU:HD22	1:D:323:VAL:HG21	1.95	0.47
1:E:217:SER:N	1:E:321:LYS:O	2.46	0.47
1:F:447:MET:HE2	1:F:504:LEU:HD11	1.96	0.47
1:I:221:LEU:HD22	1:I:236:VAL:HG11	1.97	0.47
1:K:270:ILE:HG22	1:K:271:VAL:HG23	1.96	0.47
1:A:115:ASP:OD2	1:A:436:GLN:HG3	2.14	0.47
1:A:194:GLN:HE21	1:A:329:THR:HG21	1.79	0.47
1:A:237:LEU:HD21	1:A:247:LEU:HG	1.96	0.47
1:A:213:VAL:N	1:A:325:ILE:HG22	2.29	0.47
1:A:225:LYS:HE3	1:A:227:ILE:HG12	1.96	0.47
1:A:22:VAL:HG11	1:A:62:LEU:HD21	1.95	0.47
1:A:447:MET:HE2	1:A:504:LEU:HD11	1.96	0.47
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.96	0.47
1:B:221:LEU:HD22	1:B:236:VAL:HG11	1.97	0.47
1:C:221:LEU:HD22	1:C:236:VAL:HG11	1.97	0.47
1:D:447:MET:HE2	1:D:504:LEU:HD11	1.96	0.47
1:I:270:ILE:HG22	1:I:271:VAL:HG23	1.96	0.47
1:J:77:VAL:HG12	1:J:506:TYR:HB3	1.96	0.47
1:K:221:LEU:HD22	1:K:236:VAL:HG11	1.97	0.47
1:L:221:LEU:HD22	1:L:236:VAL:HG11	1.97	0.47
1:L:248:LEU:HD22	1:L:323:VAL:HG21	1.95	0.47
1:N:447:MET:HE2	1:N:504:LEU:HD11	1.96	0.47
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:VAL:HG11	1:I:62:LEU:HD21	1.95	0.47
1:J:221:LEU:HD22	1:J:236:VAL:HG11	1.97	0.47
1:K:254:VAL:HG12	1:K:259:LEU:HB2	1.97	0.47
1:L:447:MET:HE2	1:L:504:LEU:HD11	1.96	0.47
1:A:77:VAL:HG21	1:A:510:VAL:HG13	1.97	0.47
1:A:155:ASP:HB2	1:A:395:ARG:HH12	1.79	0.47
1:A:296:THR:O	1:A:336:VAL:HB	2.15	0.47
1:A:352:GLN:HA	1:A:355:GLU:OE2	2.15	0.47
1:A:519:CYS:HB3	1:B:38:VAL:HG22	1.96	0.47
1:C:254:VAL:HG12	1:C:259:LEU:HB2	1.97	0.47
1:G:221:LEU:HD22	1:G:236:VAL:HG11	1.97	0.47
1:L:254:VAL:HG12	1:L:259:LEU:HB2	1.97	0.47
1:M:221:LEU:HD22	1:M:236:VAL:HG11	1.97	0.47
1:A:339:GLU:O	1:A:343:GLN:CB	2.60	0.47
1:A:197:ARG:NE	1:A:278:ALA:O	2.48	0.47
1:A:403:THR:HA	1:A:406:ALA:HB3	1.96	0.47
1:A:478:TYR:HB2	1:A:485:TYR:CE1	2.49	0.47
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.97	0.47
1:D:254:VAL:HG12	1:D:259:LEU:HB2	1.97	0.47
1:E:109:ALA:HB2	1:M:109:ALA:HB2	1.96	0.47
1:E:221:LEU:HD22	1:E:236:VAL:HG11	1.97	0.47
1:E:447:MET:HE2	1:E:504:LEU:HD11	1.96	0.47
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.96	0.47
1:G:248:LEU:HD22	1:G:323:VAL:HG21	1.95	0.47
1:H:221:LEU:HD22	1:H:236:VAL:HG11	1.97	0.47
1:I:519:CYS:HB3	1:J:38:VAL:HG22	1.96	0.47
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.97	0.47
1:J:519:CYS:HB3	1:K:38:VAL:HG22	1.95	0.47
1:M:447:MET:HE2	1:M:504:LEU:HD11	1.96	0.47
1:N:270:ILE:HG22	1:N:271:VAL:HG23	1.96	0.47
1:A:391:GLU:OE2	1:A:395:ARG:NE	2.27	0.47
1:A:419:LEU:HD22	1:A:504:LEU:HD12	1.95	0.47
1:A:461:GLU:OE1	1:A:463:SER:N	2.48	0.47
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.96	0.47
1:H:248:LEU:HD22	1:H:323:VAL:HG21	1.95	0.47
1:H:270:ILE:HG22	1:H:271:VAL:HG23	1.96	0.47
1:M:254:VAL:HG12	1:M:259:LEU:HB2	1.97	0.47
1:N:221:LEU:HD22	1:N:236:VAL:HG11	1.97	0.47
1:A:356:ALA:O	1:A:362:ARG:NH2	2.48	0.47
1:A:174:VAL:HG21	1:A:194:GLN:CD	2.39	0.47
1:A:361:ASP:O	1:A:365:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.97	0.47
1:F:221:LEU:HD22	1:F:236:VAL:HG11	1.97	0.47
1:M:513:LEU:HB3	1:N:49:ILE:HD13	1.97	0.47
1:A:389:MET:O	1:A:392:LYS:N	2.48	0.47
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.96	0.47
1:E:77:VAL:HG12	1:E:506:TYR:HB3	1.96	0.47
1:E:435:ASP:HA	1:E:438:VAL:HG22	1.97	0.47
1:E:519:CYS:HB3	1:F:38:VAL:HG22	1.96	0.47
1:H:217:SER:N	1:H:321:LYS:O	2.46	0.47
1:K:77:VAL:HG12	1:K:506:TYR:HB3	1.96	0.47
1:A:193:MET:HE3	1:A:292:ILE:HG21	1.97	0.47
1:B:519:CYS:HB3	1:C:38:VAL:HG22	1.96	0.46
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.96	0.46
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.97	0.46
1:M:435:ASP:HA	1:M:438:VAL:HG22	1.97	0.46
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.97	0.46
1:A:7:LYS:HB3	1:A:12:ALA:HB2	1.95	0.46
1:A:245:LYS:HD2	1:A:245:LYS:C	2.40	0.46
1:A:115:ASP:OD2	1:A:435:ASP:HB2	2.15	0.46
1:A:129:GLU:O	1:A:132:LYS:N	2.48	0.46
1:A:149:THR:HG21	1:A:156:GLU:HA	1.97	0.46
1:A:193:MET:SD	1:A:332:ILE:HD13	2.55	0.46
1:A:230:ILE:O	1:A:234:LEU:N	2.42	0.46
1:A:364:LYS:O	1:A:367:GLU:HB2	2.15	0.46
1:D:519:CYS:HB3	1:E:38:VAL:HG22	1.96	0.46
1:G:217:SER:N	1:G:321:LYS:O	2.46	0.46
1:L:77:VAL:HG12	1:L:506:TYR:HB3	1.96	0.46
1:M:27:VAL:O	1:M:30:THR:OG1	2.33	0.46
1:M:77:VAL:HG12	1:M:506:TYR:HB3	1.96	0.46
1:A:28:LYS:HD3	1:A:453:GLN:NE2	2.30	0.46
1:A:226:LYS:HD3	1:A:255:GLU:OE2	2.15	0.46
1:A:194:GLN:HE21	1:A:329:THR:HG21	1.79	0.46
1:A:496:PRO:O	1:A:499:VAL:HG12	2.15	0.46
1:D:435:ASP:HA	1:D:438:VAL:HG22	1.97	0.46
1:F:435:ASP:HA	1:F:438:VAL:HG22	1.97	0.46
1:L:435:ASP:HA	1:L:438:VAL:HG22	1.97	0.46
1:N:435:ASP:HA	1:N:438:VAL:HG22	1.97	0.46
1:A:236:VAL:HG22	1:A:312:ALA:O	2.15	0.46
1:A:124:VAL:O	1:A:127:ALA:N	2.48	0.46
1:G:254:VAL:HG12	1:G:259:LEU:HB2	1.97	0.46
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:CG	1:A:88:GLY:H	2.23	0.46
1:A:265:ASN:O	1:A:269:GLY:N	2.48	0.46
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.97	0.46
1:A:251:ALA:O	1:A:278:ALA:N	2.30	0.46
1:A:219:PHE:HB2	1:A:247:LEU:HD23	1.98	0.46
1:B:27:VAL:O	1:B:30:THR:OG1	2.33	0.46
1:G:435:ASP:HA	1:G:438:VAL:HG22	1.97	0.46
1:I:254:VAL:HG12	1:I:259:LEU:HB2	1.97	0.46
1:A:203:TYR:CD2	1:A:263:VAL:HG13	2.51	0.46
1:A:369:VAL:O	1:A:373:ALA:N	2.40	0.46
1:A:16:MET:SD	1:A:514:MET:HG3	2.56	0.46
1:A:199:TYR:CE1	1:A:327:LYS:HA	2.50	0.46
1:J:27:VAL:O	1:J:30:THR:OG1	2.33	0.46
1:A:230:ILE:O	1:A:234:LEU:HG	2.16	0.46
1:A:257:GLU:O	1:A:261:THR:OG1	2.26	0.46
1:A:200:LEU:H	1:A:200:LEU:HD23	1.81	0.46
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.97	0.46
1:A:78:ALA:HB1	1:A:89:THR:HG23	1.97	0.46
1:A:197:ARG:HE	1:A:279:PRO:HA	1.81	0.46
1:H:435:ASP:HA	1:H:438:VAL:HG22	1.97	0.46
1:L:78:ALA:HB1	1:L:89:THR:HG23	1.97	0.46
1:L:217:SER:N	1:L:321:LYS:O	2.46	0.46
1:A:20:VAL:O	1:A:23:LEU:N	2.49	0.46
1:A:144:ILE:HA	1:A:147:VAL:HG12	1.97	0.46
1:A:259:LEU:O	1:A:263:VAL:HG23	2.16	0.46
1:G:78:ALA:HB1	1:G:89:THR:HG23	1.97	0.46
1:I:197:ARG:HE	1:I:279:PRO:HA	1.81	0.46
1:K:78:ALA:HB1	1:K:89:THR:HG23	1.97	0.46
1:A:180:GLY:H	1:A:389:MET:CE	2.29	0.46
1:A:185:ASP:CA	1:A:382:GLY:H	2.29	0.46
1:A:510:VAL:O	1:A:514:MET:N	2.44	0.46
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.96	0.45
1:D:78:ALA:HB1	1:D:89:THR:HG23	1.97	0.45
1:D:213:VAL:HB	1:D:325:ILE:HB	1.99	0.45
1:H:197:ARG:HE	1:H:279:PRO:HA	1.81	0.45
1:I:78:ALA:HB1	1:I:89:THR:HG23	1.97	0.45
1:I:257:GLU:O	1:I:261:THR:OG1	2.26	0.45
1:K:197:ARG:HE	1:K:279:PRO:HA	1.81	0.45
1:L:213:VAL:HB	1:L:325:ILE:HB	1.99	0.45
1:A:232:GLU:O	1:A:233:MET:HE2	2.16	0.45
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLU:O	1:A:261:THR:N	2.49	0.45
1:A:359:ASP:HA	1:A:362:ARG:HE	1.80	0.45
1:B:197:ARG:HE	1:B:279:PRO:HA	1.81	0.45
1:C:78:ALA:HB1	1:C:89:THR:HG23	1.97	0.45
1:C:197:ARG:HE	1:C:279:PRO:HA	1.81	0.45
1:D:217:SER:N	1:D:321:LYS:O	2.46	0.45
1:G:197:ARG:HE	1:G:279:PRO:HA	1.81	0.45
1:H:78:ALA:HB1	1:H:89:THR:HG23	1.97	0.45
1:A:239:ALA:O	1:A:242:LYS:HG3	2.16	0.45
1:A:85:ALA:HB1	1:A:499:VAL:HG23	1.99	0.45
1:A:197:ARG:O	1:A:330:THR:OG1	2.24	0.45
1:A:19:GLY:HA2	1:A:67:GLU:OE2	2.17	0.45
1:A:363:GLU:O	1:A:367:GLU:HG3	2.17	0.45
1:B:78:ALA:HB1	1:B:89:THR:HG23	1.97	0.45
1:C:213:VAL:HB	1:C:325:ILE:HB	1.99	0.45
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.99	0.45
1:J:197:ARG:HE	1:J:279:PRO:HA	1.81	0.45
1:J:213:VAL:HB	1:J:325:ILE:HB	1.99	0.45
1:K:213:VAL:HB	1:K:325:ILE:HB	1.99	0.45
1:K:519:CYS:HB3	1:L:38:VAL:HG22	1.97	0.45
1:A:487:ASN:HB3	1:A:490:ASP:HB2	1.97	0.45
1:A:100:ILE:O	1:A:103:GLY:N	2.45	0.45
1:A:343:GLN:O	1:A:347:ALA:N	2.32	0.45
1:A:213:VAL:HB	1:A:325:ILE:HB	1.99	0.45
1:A:435:ASP:HA	1:A:438:VAL:HG22	1.97	0.45
1:B:213:VAL:HB	1:B:325:ILE:HB	1.99	0.45
1:B:435:ASP:HA	1:B:438:VAL:HG22	1.97	0.45
1:I:213:VAL:HB	1:I:325:ILE:HB	1.99	0.45
1:I:217:SER:N	1:I:321:LYS:O	2.46	0.45
1:J:78:ALA:HB1	1:J:89:THR:HG23	1.97	0.45
1:J:435:ASP:HA	1:J:438:VAL:HG22	1.97	0.45
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.99	0.45
1:A:194:GLN:HG2	1:A:331:THR:HB	1.98	0.45
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.99	0.45
1:E:213:VAL:HB	1:E:325:ILE:HB	1.99	0.45
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.99	0.45
1:K:435:ASP:HA	1:K:438:VAL:HG22	1.97	0.45
1:M:213:VAL:HB	1:M:325:ILE:HB	1.99	0.45
1:N:197:ARG:HE	1:N:279:PRO:HA	1.81	0.45
1:A:193:MET:HB3	1:A:332:ILE:HB	1.97	0.45
1:A:232:GLU:OE2	1:A:310:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:O	1:A:164:GLU:HB2	2.16	0.45
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.99	0.45
1:C:435:ASP:HA	1:C:438:VAL:HG22	1.97	0.45
1:I:435:ASP:HA	1:I:438:VAL:HG22	1.97	0.45
1:A:221:LEU:O	1:A:248:LEU:C	2.60	0.45
1:A:320:ALA:HA	1:A:334:ASP:O	2.17	0.45
1:A:414:GLY:N	1:A:494:LEU:HA	2.31	0.45
1:A:217:SER:N	1:A:321:LYS:O	2.46	0.45
1:E:78:ALA:HB1	1:E:89:THR:HG23	1.97	0.45
1:F:197:ARG:HE	1:F:279:PRO:HA	1.81	0.45
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.99	0.45
1:H:27:VAL:O	1:H:30:THR:OG1	2.33	0.45
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.99	0.45
1:M:78:ALA:HB1	1:M:89:THR:HG23	1.97	0.45
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.99	0.45
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.99	0.45
1:A:176:THR:H	1:A:376:VAL:HG12	1.81	0.45
1:A:397:GLU:O	1:A:400:LEU:HB3	2.17	0.45
1:A:191:GLU:OE1	1:A:335:GLY:N	2.47	0.45
1:A:293:ALA:HA	1:A:296:THR:HG22	1.98	0.45
1:A:353:ILE:HA	1:A:365:LEU:HD11	1.97	0.45
1:D:197:ARG:HE	1:D:279:PRO:HA	1.81	0.45
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.99	0.45
1:F:78:ALA:HB1	1:F:89:THR:HG23	1.97	0.45
1:L:197:ARG:HE	1:L:279:PRO:HA	1.81	0.45
1:A:5:ASP:HB2	1:A:524:LEU:HD22	1.97	0.45
1:A:215:LEU:HB2	1:A:323:VAL:CG2	2.47	0.45
1:A:346:VAL:O	1:A:350:ARG:HG2	2.17	0.45
1:A:311:LYS:N	1:A:311:LYS:HD2	2.31	0.45
1:A:42:LYS:HZ3	1:A:44:PHE:HB3	1.82	0.45
1:A:265:ASN:OD1	1:A:270:ILE:HB	2.17	0.45
1:C:235:PRO:HG3	1:C:310:GLU:HA	1.99	0.45
1:F:513:LEU:HB3	1:G:49:ILE:HD13	1.99	0.45
1:G:213:VAL:HB	1:G:325:ILE:HB	1.99	0.45
1:H:49:ILE:HD13	1:N:513:LEU:HB3	1.99	0.45
1:H:213:VAL:HB	1:H:325:ILE:HB	1.99	0.45
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.99	0.45
1:N:78:ALA:HB1	1:N:89:THR:HG23	1.97	0.45
1:A:214:GLU:C	1:A:215:LEU:HD22	2.41	0.45
1:A:217:SER:HA	1:A:321:LYS:HA	1.99	0.45
1:A:186:GLU:OE1	1:A:187:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:SER:OG	1:A:255:GLU:O	2.29	0.45
1:A:346:VAL:HA	1:A:349:ILE:HG22	1.98	0.45
1:A:128:VAL:HG21	1:A:505:GLN:NE2	2.31	0.45
1:M:197:ARG:HE	1:M:279:PRO:HA	1.81	0.44
1:A:252:GLU:HB2	1:A:285:ARG:NH1	2.32	0.44
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.98	0.44
1:A:233:MET:O	1:A:237:LEU:HD12	2.18	0.44
1:A:346:VAL:O	1:A:349:ILE:HG22	2.18	0.44
1:A:264:VAL:HA	1:A:267:MET:HB3	1.98	0.44
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.99	0.44
1:D:222:LEU:HD23	1:D:250:ILE:HB	1.99	0.44
1:E:197:ARG:HE	1:E:279:PRO:HA	1.81	0.44
1:F:213:VAL:HB	1:F:325:ILE:HB	1.99	0.44
1:K:222:LEU:HD23	1:K:250:ILE:HB	1.99	0.44
1:L:222:LEU:HD23	1:L:250:ILE:HB	1.99	0.44
1:M:149:THR:HG22	1:M:156:GLU:HA	1.99	0.44
1:D:149:THR:HG22	1:D:156:GLU:HA	1.99	0.44
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.99	0.44
1:L:149:THR:HG22	1:L:156:GLU:HA	1.99	0.44
1:N:106:ALA:HB3	1:N:116:LEU:HD21	1.99	0.44
1:N:213:VAL:HB	1:N:325:ILE:HB	1.99	0.44
1:A:245:LYS:HD2	1:A:246:PRO:O	2.17	0.44
1:A:359:ASP:OD1	1:A:362:ARG:NH1	2.50	0.44
1:A:107:VAL:CG2	1:A:113:PRO:HG3	2.47	0.44
1:A:406:ALA:HA	1:A:496:PRO:HB3	1.98	0.44
1:C:222:LEU:HD23	1:C:250:ILE:HB	2.00	0.44
1:F:106:ALA:HB3	1:F:116:LEU:HD21	1.99	0.44
1:A:233:MET:SD	1:A:237:LEU:HD23	2.57	0.44
1:A:419:LEU:O	1:A:423:ALA:N	2.41	0.44
1:D:27:VAL:O	1:D:30:THR:OG1	2.33	0.44
1:E:106:ALA:HB3	1:E:116:LEU:HD21	1.99	0.44
1:J:513:LEU:HB3	1:K:49:ILE:HD13	1.99	0.44
1:M:106:ALA:HB3	1:M:116:LEU:HD21	1.99	0.44
1:N:149:THR:HG22	1:N:156:GLU:HA	1.99	0.44
1:A:30:THR:HB	1:A:51:LYS:O	2.17	0.44
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.99	0.44
1:A:111:MET:SD	1:A:438:VAL:HG21	2.58	0.44
1:A:228:SER:HA	1:A:258:ALA:CB	2.46	0.44
1:A:174:VAL:HG11	1:A:376:VAL:HG22	2.00	0.44
1:A:205:ILE:HG12	1:A:211:GLY:O	2.18	0.44
1:A:295:LEU:HD12	1:A:296:THR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:HA	1:A:366:GLN:HB3	2.00	0.44
1:A:513:LEU:HB3	1:B:49:ILE:HD13	1.99	0.44
1:E:149:THR:HG22	1:E:156:GLU:HA	1.99	0.44
1:G:222:LEU:HD23	1:G:250:ILE:HB	1.99	0.44
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.99	0.44
1:I:513:LEU:HB3	1:J:49:ILE:HD13	1.99	0.44
1:A:268:ARG:NH1	1:A:270:ILE:HG21	2.33	0.44
1:A:396:VAL:O	1:A:400:LEU:N	2.50	0.44
1:B:513:LEU:HB3	1:C:49:ILE:HD13	1.99	0.44
1:C:149:THR:HG22	1:C:156:GLU:HA	1.99	0.44
1:F:149:THR:HG22	1:F:156:GLU:HA	1.99	0.44
1:K:149:THR:HG22	1:K:156:GLU:HA	1.99	0.44
1:A:245:LYS:NZ	1:A:246:PRO:O	2.39	0.44
1:A:286:LYS:HD3	1:A:286:LYS:H	1.83	0.44
1:A:294:THR:HG21	1:A:342:ILE:HA	1.99	0.44
1:A:344:GLY:O	1:A:348:GLN:N	2.35	0.44
1:A:213:VAL:HG12	1:A:325:ILE:HB	1.99	0.44
1:A:301:ILE:HD13	1:A:309:LEU:HA	2.00	0.44
1:A:339:GLU:HA	1:A:342:ILE:HB	1.99	0.44
1:A:411:VAL:HG21	1:A:494:LEU:HB3	2.00	0.44
1:H:513:LEU:HB3	1:I:49:ILE:HD13	1.99	0.44
1:L:106:ALA:HB3	1:L:116:LEU:HD21	1.99	0.44
1:A:149:THR:CG2	1:A:156:GLU:HA	2.48	0.44
1:A:222:LEU:HD22	1:A:289:LEU:HD12	2.00	0.44
1:A:197:ARG:HH21	1:A:280:GLY:N	2.16	0.44
1:D:106:ALA:HB3	1:D:116:LEU:HD21	1.99	0.43
1:G:106:ALA:HB3	1:G:116:LEU:HD21	1.99	0.43
1:H:106:ALA:HB3	1:H:116:LEU:HD21	1.99	0.43
1:H:149:THR:HG22	1:H:156:GLU:HA	1.99	0.43
1:L:27:VAL:O	1:L:30:THR:OG1	2.33	0.43
1:L:513:LEU:HB3	1:M:49:ILE:HD13	1.99	0.43
1:A:38:VAL:HG11	1:A:56:VAL:HG11	2.00	0.43
1:A:365:LEU:O	1:A:369:VAL:HG12	2.17	0.43
1:A:209:GLU:OE1	1:A:209:GLU:N	2.37	0.43
1:A:226:LYS:HD3	1:A:226:LYS:H	1.83	0.43
1:D:513:LEU:HB3	1:E:49:ILE:HD13	1.99	0.43
1:E:222:LEU:HD23	1:E:250:ILE:HB	1.99	0.43
1:G:149:THR:HG22	1:G:156:GLU:HA	1.99	0.43
1:M:222:LEU:HD23	1:M:250:ILE:HB	1.99	0.43
1:A:268:ARG:HB2	1:A:270:ILE:HG13	2.00	0.43
1:A:378:VAL:CG2	1:A:380:LYS:HD3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:VAL:HG11	1:A:393:LYS:N	2.34	0.43
1:A:49:ILE:HD13	1:G:513:LEU:HB3	1.99	0.43
1:B:222:LEU:HD23	1:B:250:ILE:HB	2.00	0.43
1:J:222:LEU:HD23	1:J:250:ILE:HB	2.00	0.43
1:K:513:LEU:HB3	1:L:49:ILE:HD13	1.99	0.43
1:A:221:LEU:HD12	1:A:236:VAL:HG11	1.99	0.43
1:A:225:LYS:O	1:A:251:ALA:HB1	2.17	0.43
1:A:190:VAL:HG11	1:A:333:ILE:HG23	2.01	0.43
1:A:230:ILE:O	1:A:233:MET:N	2.50	0.43
1:A:285:ARG:O	1:A:288:MET:N	2.51	0.43
1:I:149:THR:HG22	1:I:156:GLU:HA	1.99	0.43
1:A:222:LEU:O	1:A:301:ILE:N	2.51	0.43
1:A:245:LYS:HG3	1:A:246:PRO:HD2	1.99	0.43
1:B:106:ALA:HB3	1:B:116:LEU:HD21	1.99	0.43
1:E:513:LEU:HB3	1:F:49:ILE:HD13	2.01	0.43
1:J:106:ALA:HB3	1:J:116:LEU:HD21	1.99	0.43
1:A:10:ASN:C	1:A:12:ALA:N	2.77	0.43
1:A:389:MET:O	1:A:393:LYS:HG2	2.18	0.43
1:B:149:THR:HG22	1:B:156:GLU:HA	1.99	0.43
1:J:149:THR:HG22	1:J:156:GLU:HA	2.00	0.43
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.75	0.43
1:A:216:GLU:OE2	1:A:322:ARG:NE	2.25	0.43
1:A:403:THR:O	1:A:407:VAL:HG13	2.18	0.43
1:A:177:VAL:HG12	1:A:393:LYS:HE2	2.00	0.43
1:A:149:THR:HG22	1:A:156:GLU:HA	1.99	0.43
1:C:431:GLY:H	1:C:437:ASN:ND2	2.17	0.43
1:D:20:VAL:O	1:D:24:ALA:HB3	2.18	0.43
1:I:322:ARG:O	1:I:333:ILE:HB	2.19	0.43
1:J:20:VAL:O	1:J:24:ALA:HB3	2.18	0.43
1:K:106:ALA:HB3	1:K:116:LEU:HD21	1.99	0.43
1:L:20:VAL:O	1:L:24:ALA:HB3	2.19	0.43
1:A:100:ILE:O	1:A:101:THR:C	2.61	0.43
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.79	0.43
1:A:255:GLU:N	1:A:255:GLU:OE1	2.51	0.43
1:A:283:ASP:O	1:A:286:LYS:HG2	2.19	0.43
1:A:322:ARG:O	1:A:333:ILE:HB	2.19	0.43
1:B:20:VAL:O	1:B:24:ALA:HB3	2.18	0.43
1:B:431:GLY:H	1:B:437:ASN:ND2	2.17	0.43
1:C:106:ALA:HB3	1:C:116:LEU:HD21	1.99	0.43
1:J:322:ARG:O	1:J:333:ILE:HB	2.19	0.43
1:J:431:GLY:H	1:J:437:ASN:ND2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:431:GLY:H	1:K:437:ASN:ND2	2.17	0.43
1:A:31:LEU:HD12	1:A:32:GLY:H	1.83	0.43
1:A:144:ILE:HG13	1:A:403:THR:HG23	2.01	0.43
1:A:265:ASN:O	1:A:270:ILE:HG13	2.19	0.43
1:A:278:ALA:HB1	1:A:289:LEU:HD21	2.00	0.43
1:A:431:GLY:H	1:A:437:ASN:ND2	2.17	0.43
1:C:513:LEU:HB3	1:D:49:ILE:HD13	2.00	0.43
1:F:431:GLY:H	1:F:437:ASN:ND2	2.17	0.43
1:G:322:ARG:O	1:G:333:ILE:HB	2.19	0.43
1:H:322:ARG:O	1:H:333:ILE:HB	2.19	0.43
1:I:431:GLY:H	1:I:437:ASN:ND2	2.17	0.43
1:A:68:ASN:O	1:A:72:GLN:HG2	2.19	0.43
1:A:237:LEU:HA	1:A:240:VAL:CG1	2.49	0.43
1:A:448:GLU:OE2	1:A:470:LYS:NZ	2.25	0.43
1:A:363:GLU:O	1:A:367:GLU:HG3	2.19	0.43
1:A:124:VAL:O	1:A:128:VAL:HG12	2.18	0.43
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.99	0.43
1:B:322:ARG:O	1:B:333:ILE:HB	2.19	0.43
1:I:20:VAL:O	1:I:24:ALA:HB3	2.18	0.43
1:I:106:ALA:HB3	1:I:116:LEU:HD21	1.99	0.43
1:K:20:VAL:O	1:K:24:ALA:HB3	2.19	0.43
1:L:431:GLY:H	1:L:437:ASN:ND2	2.17	0.43
1:M:20:VAL:O	1:M:24:ALA:HB3	2.18	0.43
1:N:431:GLY:H	1:N:437:ASN:ND2	2.17	0.43
1:A:87:ASP:HB3	1:A:499:VAL:HG21	2.01	0.43
1:A:421:ARG:NH2	1:A:476:TYR:O	2.52	0.43
1:A:161:LEU:HD11	1:A:379:ILE:HG23	2.00	0.43
1:A:249:ILE:O	1:A:275:ALA:HA	2.19	0.43
1:C:20:VAL:O	1:C:24:ALA:HB3	2.19	0.42
1:D:431:GLY:H	1:D:437:ASN:ND2	2.17	0.42
1:E:20:VAL:O	1:E:24:ALA:HB3	2.18	0.42
1:F:322:ARG:O	1:F:333:ILE:HB	2.19	0.42
1:N:322:ARG:O	1:N:333:ILE:HB	2.19	0.42
1:A:144:ILE:HA	1:A:147:VAL:HG12	2.01	0.42
1:A:22:VAL:HG11	1:A:62:LEU:HD21	2.00	0.42
1:A:215:LEU:HB3	1:A:218:PRO:HB3	2.00	0.42
1:K:178:GLU:HG2	1:K:322:ARG:HH11	1.85	0.42
1:M:431:GLY:H	1:M:437:ASN:ND2	2.17	0.42
1:A:20:VAL:O	1:A:24:ALA:HB3	2.19	0.42
1:A:222:LEU:HD23	1:A:250:ILE:HB	1.99	0.42
1:C:178:GLU:HG2	1:C:322:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:VAL:HG21	1:E:247:LEU:HD22	2.02	0.42
1:F:27:VAL:O	1:F:30:THR:OG1	2.33	0.42
1:M:240:VAL:HG21	1:M:247:LEU:HD22	2.02	0.42
1:A:247:LEU:HD13	1:A:248:LEU:N	2.34	0.42
1:B:178:GLU:HG2	1:B:322:ARG:HH11	1.85	0.42
1:D:240:VAL:HG21	1:D:247:LEU:HD22	2.02	0.42
1:E:431:GLY:H	1:E:437:ASN:ND2	2.17	0.42
1:F:20:VAL:O	1:F:24:ALA:HB3	2.18	0.42
1:F:222:LEU:HD23	1:F:250:ILE:HB	1.99	0.42
1:G:20:VAL:O	1:G:24:ALA:HB3	2.18	0.42
1:J:178:GLU:HG2	1:J:322:ARG:HH11	1.85	0.42
1:A:359:ASP:O	1:A:362:ARG:HB2	2.19	0.42
1:A:81:ALA:O	1:A:85:ALA:N	2.52	0.42
1:A:219:PHE:CD1	1:A:319:GLN:HG3	2.54	0.42
1:D:178:GLU:HG2	1:D:322:ARG:HH11	1.84	0.42
1:F:240:VAL:HG21	1:F:247:LEU:HD22	2.02	0.42
1:H:431:GLY:H	1:H:437:ASN:ND2	2.17	0.42
1:I:222:LEU:HD23	1:I:250:ILE:HB	1.99	0.42
1:L:178:GLU:HG2	1:L:322:ARG:HH11	1.85	0.42
1:L:240:VAL:HG21	1:L:247:LEU:HD22	2.02	0.42
1:N:20:VAL:O	1:N:24:ALA:HB3	2.18	0.42
1:N:222:LEU:HD23	1:N:250:ILE:HB	2.00	0.42
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.69	0.42
1:A:4:LYS:HD2	1:A:521:VAL:HG12	2.01	0.42
1:A:177:VAL:HG11	1:A:393:LYS:HG3	2.00	0.42
1:A:204:PHE:CE2	1:A:213:VAL:HG21	2.54	0.42
1:A:262:LEU:HD12	1:A:273:VAL:O	2.19	0.42
1:A:358:SER:HB3	1:A:361:ASP:OD2	2.20	0.42
1:G:431:GLY:H	1:G:437:ASN:ND2	2.17	0.42
1:H:5:ASP:HB2	1:H:524:LEU:HD23	2.02	0.42
1:H:20:VAL:O	1:H:24:ALA:HB3	2.18	0.42
1:K:217:SER:N	1:K:321:LYS:O	2.46	0.42
1:K:322:ARG:O	1:K:333:ILE:HB	2.19	0.42
1:N:5:ASP:HB2	1:N:524:LEU:HD23	2.02	0.42
1:N:217:SER:N	1:N:321:LYS:O	2.46	0.42
1:N:240:VAL:HG21	1:N:247:LEU:HD22	2.02	0.42
1:A:193:MET:HE2	1:A:195:PHE:CD1	2.53	0.42
1:A:205:ILE:HA	1:A:213:VAL:HB	2.01	0.42
1:A:178:GLU:HG2	1:A:322:ARG:HH11	1.85	0.42
1:B:251:ALA:O	1:B:278:ALA:N	2.53	0.42
1:C:322:ARG:O	1:C:333:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ASP:HB2	1:F:524:LEU:HD23	2.02	0.42
1:F:251:ALA:O	1:F:278:ALA:N	2.53	0.42
1:N:27:VAL:O	1:N:30:THR:OG1	2.33	0.42
1:N:178:GLU:HG2	1:N:322:ARG:HH11	1.85	0.42
1:N:251:ALA:O	1:N:278:ALA:N	2.53	0.42
1:A:235:PRO:O	1:A:238:GLU:HB2	2.20	0.42
1:A:419:LEU:HA	1:A:419:LEU:HD23	1.82	0.42
1:A:19:GLY:HA2	1:A:67:GLU:CD	2.44	0.42
1:A:383:ALA:HB1	1:A:388:GLU:CG	2.50	0.42
1:A:61:GLU:OE2	1:A:75:LYS:NZ	2.53	0.42
1:A:359:ASP:HA	1:A:362:ARG:NE	2.35	0.42
1:A:251:ALA:O	1:A:278:ALA:N	2.53	0.42
1:D:251:ALA:O	1:D:278:ALA:N	2.53	0.42
1:E:251:ALA:O	1:E:278:ALA:N	2.53	0.42
1:E:322:ARG:O	1:E:333:ILE:HB	2.19	0.42
1:G:5:ASP:HB2	1:G:524:LEU:HD23	2.02	0.42
1:H:178:GLU:HG2	1:H:322:ARG:HH11	1.85	0.42
1:H:257:GLU:O	1:H:261:THR:OG1	2.26	0.42
1:I:178:GLU:HG2	1:I:322:ARG:HH11	1.85	0.42
1:J:251:ALA:O	1:J:278:ALA:N	2.53	0.42
1:K:399:ALA:O	1:K:403:THR:OG1	2.31	0.42
1:L:251:ALA:O	1:L:278:ALA:N	2.53	0.42
1:M:178:GLU:HG2	1:M:322:ARG:HH11	1.85	0.42
1:M:251:ALA:O	1:M:278:ALA:N	2.53	0.42
1:A:175:ILE:HD12	1:A:175:ILE:O	2.19	0.42
1:A:350:ARG:O	1:A:354:GLU:HG2	2.20	0.42
1:A:209:GLU:HG2	1:A:210:THR:N	2.34	0.42
1:E:178:GLU:HG2	1:E:322:ARG:HH11	1.85	0.42
1:F:217:SER:N	1:F:321:LYS:O	2.46	0.42
1:G:20:VAL:O	1:G:24:ALA:CB	2.68	0.42
1:G:178:GLU:HG2	1:G:322:ARG:HH11	1.85	0.42
1:G:251:ALA:O	1:G:278:ALA:N	2.53	0.42
1:G:257:GLU:O	1:G:261:THR:OG1	2.26	0.42
1:G:421:ARG:NH2	1:G:469:VAL:O	2.53	0.42
1:H:20:VAL:O	1:H:24:ALA:CB	2.68	0.42
1:H:240:VAL:HG21	1:H:247:LEU:HD22	2.02	0.42
1:M:322:ARG:O	1:M:333:ILE:HB	2.19	0.42
1:A:52:ASP:HB3	1:A:55:SER:HB2	2.02	0.42
1:A:365:LEU:HD13	1:A:365:LEU:HA	1.75	0.42
1:A:132:LYS:HE2	1:A:409:GLU:OE1	2.20	0.42
1:A:252:GLU:O	1:A:277:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG13	1:A:90:THR:HG22	2.01	0.42
1:A:152:ALA:HB2	1:A:399:ALA:HB2	2.00	0.42
1:C:217:SER:N	1:C:321:LYS:O	2.46	0.42
1:C:240:VAL:HG21	1:C:247:LEU:HD22	2.02	0.42
1:E:464:VAL:HG11	1:N:467:ASN:HD22	1.85	0.42
1:F:20:VAL:O	1:F:24:ALA:CB	2.68	0.42
1:F:178:GLU:HG2	1:F:322:ARG:HH11	1.85	0.42
1:G:240:VAL:HG21	1:G:247:LEU:HD22	2.02	0.42
1:H:251:ALA:O	1:H:278:ALA:N	2.53	0.42
1:H:421:ARG:NH2	1:H:469:VAL:O	2.53	0.42
1:I:5:ASP:HB2	1:I:524:LEU:HD23	2.02	0.42
1:I:251:ALA:O	1:I:278:ALA:N	2.53	0.42
1:K:240:VAL:HG21	1:K:247:LEU:HD22	2.02	0.42
1:N:20:VAL:O	1:N:24:ALA:CB	2.68	0.42
1:A:27:VAL:HG21	1:A:57:ALA:HB2	2.02	0.42
1:A:390:LYS:HD3	1:A:393:LYS:HD3	2.01	0.42
1:A:64:ASP:HB3	1:A:67:GLU:CB	2.50	0.42
1:A:214:GLU:C	1:A:215:LEU:HD12	2.45	0.42
1:A:247:LEU:HD13	1:A:248:LEU:N	2.35	0.42
1:A:341:ALA:O	1:A:345:ARG:N	2.51	0.42
1:E:5:ASP:HB2	1:E:524:LEU:HD23	2.02	0.41
1:M:5:ASP:HB2	1:M:524:LEU:HD23	2.02	0.41
1:A:285:ARG:NE	1:A:285:ARG:HA	2.34	0.41
1:A:195:PHE:HB2	1:A:279:PRO:HB3	2.02	0.41
1:A:213:VAL:HG22	1:A:325:ILE:CB	2.50	0.41
1:A:233:MET:C	1:A:235:PRO:HD2	2.45	0.41
1:A:239:ALA:HA	1:A:242:LYS:HE3	2.01	0.41
1:A:350:ARG:HE	1:A:369:VAL:HG21	1.84	0.41
1:A:87:ASP:CG	1:A:88:GLY:H	2.26	0.41
1:A:226:LYS:HG2	1:A:226:LYS:O	2.20	0.41
1:A:338:GLU:HG3	1:A:340:ALA:H	1.84	0.41
1:A:5:ASP:HB2	1:A:524:LEU:HD23	2.02	0.41
1:D:322:ARG:O	1:D:333:ILE:HB	2.19	0.41
1:A:116:LEU:O	1:A:117:LYS:C	2.61	0.41
1:A:247:LEU:O	1:A:274:ALA:HB3	2.20	0.41
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.83	0.41
1:A:301:ILE:HG23	1:A:307:MET:HG3	2.02	0.41
1:A:325:ILE:HG13	1:A:326:ASN:O	2.19	0.41
1:A:15:LYS:O	1:A:67:GLU:HA	2.20	0.41
1:A:295:LEU:HD13	1:A:332:ILE:HD13	2.02	0.41
1:A:465:VAL:O	1:A:468:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:O	1:A:24:ALA:CB	2.68	0.41
1:E:421:ARG:NH2	1:E:469:VAL:O	2.53	0.41
1:I:20:VAL:O	1:I:24:ALA:CB	2.68	0.41
1:L:322:ARG:O	1:L:333:ILE:HB	2.19	0.41
1:M:421:ARG:NH2	1:M:469:VAL:O	2.53	0.41
1:A:66:PHE:HD1	1:A:520:MET:HE2	1.85	0.41
1:A:178:GLU:HG2	1:A:322:ARG:HH11	1.85	0.41
1:A:221:LEU:O	1:A:248:LEU:CA	2.67	0.41
1:A:242:LYS:NZ	1:A:314:LEU:HD11	2.35	0.41
1:A:162:ILE:HD11	1:A:396:VAL:HG23	2.03	0.41
1:A:240:VAL:HG21	1:A:247:LEU:HD22	2.02	0.41
1:A:464:VAL:HG11	1:K:467:ASN:HD22	1.86	0.41
1:A:22:VAL:HG11	1:A:62:LEU:HD21	2.03	0.41
1:A:64:ASP:O	1:A:65:LYS:C	2.62	0.41
1:A:265:ASN:OD1	1:A:270:ILE:HD11	2.20	0.41
1:A:346:VAL:O	1:A:350:ARG:HG2	2.20	0.41
1:A:99:ILE:O	1:A:103:GLY:N	2.54	0.41
1:A:262:LEU:HD11	1:A:275:ALA:HB2	2.02	0.41
1:A:352:GLN:OE1	1:A:365:LEU:HD13	2.20	0.41
1:B:240:VAL:HG21	1:B:247:LEU:HD22	2.02	0.41
1:C:251:ALA:O	1:C:278:ALA:N	2.53	0.41
1:C:467:ASN:HD22	1:I:464:VAL:HG11	1.86	0.41
1:E:20:VAL:O	1:E:24:ALA:CB	2.68	0.41
1:A:247:LEU:C	1:A:248:LEU:HD22	2.46	0.41
1:A:116:LEU:HD23	1:A:439:GLY:HA2	2.03	0.41
1:A:177:VAL:HG22	1:A:379:ILE:CG2	2.50	0.41
1:A:169:VAL:CG1	1:A:173:GLY:HA3	2.50	0.41
1:A:476:TYR:HA	1:A:486:GLY:O	2.20	0.41
1:A:467:ASN:HD22	1:K:464:VAL:HG11	1.86	0.41
1:J:240:VAL:HG21	1:J:247:LEU:HD22	2.02	0.41
1:K:251:ALA:O	1:K:278:ALA:N	2.53	0.41
1:M:20:VAL:O	1:M:24:ALA:CB	2.68	0.41
1:A:113:PRO:C	1:A:115:ASP:N	2.79	0.41
1:A:92:ALA:HB2	1:A:503:ALA:HA	2.01	0.41
1:G:388:GLU:O	1:G:392:LYS:CB	2.69	0.41
1:H:388:GLU:O	1:H:392:LYS:CB	2.69	0.41
1:I:240:VAL:HG21	1:I:247:LEU:HD22	2.02	0.41
1:A:169:VAL:HG22	1:A:173:GLY:HA3	2.03	0.41
1:A:266:THR:C	1:A:269:GLY:H	2.28	0.41
1:A:352:GLN:HA	1:A:355:GLU:OE2	2.20	0.41
1:B:5:ASP:HB2	1:B:524:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:GLU:O	1:C:392:LYS:CB	2.69	0.41
1:C:464:VAL:HG11	1:I:467:ASN:HD22	1.86	0.41
1:J:5:ASP:HB2	1:J:524:LEU:HD23	2.02	0.41
1:K:20:VAL:O	1:K:24:ALA:CB	2.68	0.41
1:K:388:GLU:O	1:K:392:LYS:CB	2.69	0.41
1:L:5:ASP:HB2	1:L:524:LEU:HD23	2.02	0.41
1:N:388:GLU:O	1:N:392:LYS:CB	2.69	0.41
1:A:175:ILE:HB	1:A:377:ALA:CB	2.50	0.41
1:A:213:VAL:HB	1:A:325:ILE:HG13	2.03	0.41
1:A:415:GLY:C	1:A:417:VAL:H	2.29	0.41
1:A:205:ILE:H	1:A:205:ILE:HD12	1.85	0.41
1:A:309:LEU:O	1:A:312:ALA:N	2.45	0.41
1:A:421:ARG:NH2	1:A:469:VAL:O	2.53	0.41
1:B:20:VAL:O	1:B:24:ALA:CB	2.68	0.41
1:B:464:VAL:HG11	1:J:467:ASN:HD22	1.86	0.41
1:C:5:ASP:HB2	1:C:524:LEU:HD23	2.02	0.41
1:C:20:VAL:O	1:C:24:ALA:CB	2.68	0.41
1:D:5:ASP:HB2	1:D:524:LEU:HD23	2.02	0.41
1:D:20:VAL:O	1:D:24:ALA:CB	2.68	0.41
1:E:27:VAL:O	1:E:30:THR:OG1	2.33	0.41
1:E:257:GLU:O	1:E:261:THR:OG1	2.26	0.41
1:E:305:ILE:HG21	1:E:307:MET:HE2	2.03	0.41
1:E:467:ASN:HD22	1:N:464:VAL:HG11	1.86	0.41
1:F:305:ILE:HG21	1:F:307:MET:HE2	2.03	0.41
1:F:388:GLU:O	1:F:392:LYS:CB	2.69	0.41
1:J:20:VAL:O	1:J:24:ALA:CB	2.68	0.41
1:K:5:ASP:HB2	1:K:524:LEU:HD23	2.02	0.41
1:L:20:VAL:O	1:L:24:ALA:CB	2.68	0.41
1:A:22:VAL:CG1	1:A:62:LEU:HD11	2.51	0.41
1:A:248:LEU:HD13	1:A:248:LEU:HA	1.87	0.41
1:A:376:VAL:HG12	1:A:377:ALA:N	2.33	0.41
1:A:423:ALA:HB2	1:A:447:MET:HB2	2.03	0.41
1:A:40:LEU:HD21	1:A:56:VAL:HA	2.02	0.41
1:A:321:LYS:HG2	1:A:322:ARG:HH11	1.86	0.41
1:A:411:VAL:HG23	1:A:495:ASP:O	2.21	0.41
1:A:488:MET:SD	1:A:493:ILE:HD11	2.61	0.41
1:A:283:ASP:O	1:A:285:ARG:N	2.54	0.41
1:A:388:GLU:O	1:A:392:LYS:CB	2.69	0.41
1:B:467:ASN:HD22	1:J:464:VAL:HG11	1.86	0.41
1:F:352:GLN:OE1	1:F:368:ARG:NH2	2.53	0.41
1:I:421:ARG:NH2	1:I:469:VAL:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:257:GLU:O	1:M:261:THR:OG1	2.26	0.41
1:M:305:ILE:HG21	1:M:307:MET:HE2	2.03	0.41
1:N:305:ILE:HG21	1:N:307:MET:HE2	2.03	0.41
1:D:388:GLU:O	1:D:392:LYS:CB	2.69	0.40
1:G:305:ILE:HG21	1:G:307:MET:HE2	2.03	0.40
1:H:305:ILE:HG21	1:H:307:MET:HE2	2.03	0.40
1:I:388:GLU:O	1:I:392:LYS:CB	2.69	0.40
1:K:339:GLU:O	1:K:343:GLN:CB	2.70	0.40
1:A:42:LYS:NZ	1:A:44:PHE:HB3	2.36	0.40
1:A:207:LYS:HE3	1:A:210:THR:OG1	2.20	0.40
1:A:263:VAL:O	1:A:267:MET:HB3	2.22	0.40
1:A:188:ASP:OD1	1:A:188:ASP:N	2.50	0.40
1:A:224:ASP:C	1:A:225:LYS:HD2	2.46	0.40
1:A:347:ALA:O	1:A:351:GLN:HG2	2.21	0.40
1:B:388:GLU:O	1:B:392:LYS:CB	2.69	0.40
1:C:27:VAL:O	1:C:30:THR:OG1	2.33	0.40
1:C:339:GLU:O	1:C:343:GLN:CB	2.70	0.40
1:J:388:GLU:O	1:J:392:LYS:CB	2.69	0.40
1:L:388:GLU:O	1:L:392:LYS:CB	2.69	0.40
1:A:301:ILE:HD13	1:A:301:ILE:HA	1.96	0.40
1:A:193:MET:HG3	1:A:371:LYS:NZ	2.36	0.40
1:A:252:GLU:HB2	1:A:285:ARG:HH11	1.86	0.40
1:A:232:GLU:O	1:A:309:LEU:HD12	2.20	0.40
1:A:305:ILE:HG21	1:A:307:MET:HE2	2.03	0.40
1:C:102:GLU:HB2	1:C:442:VAL:HG13	2.04	0.40
1:D:467:ASN:HD22	1:H:464:VAL:HG11	1.86	0.40
1:G:464:VAL:HG11	1:L:467:ASN:HD22	1.86	0.40
1:H:339:GLU:O	1:H:343:GLN:CB	2.70	0.40
1:K:102:GLU:HB2	1:K:442:VAL:HG13	2.04	0.40
1:A:349:ILE:O	1:A:353:ILE:HG23	2.20	0.40
1:A:64:ASP:O	1:A:67:GLU:HB3	2.21	0.40
1:A:320:ALA:HB1	1:A:333:ILE:O	2.21	0.40
1:A:18:ARG:HG3	1:A:67:GLU:HG2	2.03	0.40
1:A:324:VAL:HG22	1:A:331:THR:OG1	2.21	0.40
1:D:305:ILE:HG21	1:D:307:MET:HE2	2.03	0.40
1:F:421:ARG:NH2	1:F:469:VAL:O	2.53	0.40
1:G:339:GLU:O	1:G:343:GLN:CB	2.70	0.40
1:G:352:GLN:OE1	1:G:368:ARG:NH2	2.53	0.40
1:I:305:ILE:HG21	1:I:307:MET:HE2	2.03	0.40
1:K:158:VAL:HG13	1:K:396:VAL:HG22	2.04	0.40
1:L:102:GLU:HB2	1:L:442:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:158:VAL:HG13	1:L:396:VAL:HG22	2.04	0.40
1:L:305:ILE:HG21	1:L:307:MET:HE2	2.03	0.40
1:M:339:GLU:O	1:M:343:GLN:CB	2.70	0.40
1:M:388:GLU:O	1:M:392:LYS:CB	2.69	0.40
1:A:254:VAL:HG13	1:A:258:ALA:CB	2.52	0.40
1:A:447:MET:HE2	1:A:504:LEU:HD11	2.04	0.40
1:C:158:VAL:HG13	1:C:396:VAL:HG22	2.04	0.40
1:D:102:GLU:HB2	1:D:442:VAL:HG13	2.04	0.40
1:D:158:VAL:HG13	1:D:396:VAL:HG22	2.04	0.40
1:E:339:GLU:O	1:E:343:GLN:CB	2.70	0.40
1:N:421:ARG:NH2	1:N:469:VAL:O	2.53	0.40
1:A:78:ALA:HB1	1:A:89:THR:HG23	2.03	0.40
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.77	0.40
1:A:333:ILE:HG22	1:A:334:ASP:CG	2.46	0.40
1:A:131:LEU:HA	1:A:131:LEU:HD23	1.79	0.40
1:A:220:ILE:HG22	1:A:248:LEU:HG	2.03	0.40
1:A:228:SER:OG	1:A:255:GLU:O	2.38	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	1-A	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-B	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-C	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-D	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-E	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-F	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-G	522/524 (100%)	506 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-H	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-I	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-J	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-K	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-L	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-M	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	1-N	522/524 (100%)	506 (97%)	16 (3%)	0	100	100
1	2-A	522/524 (100%)	445 (85%)	77 (15%)	0	100	100
1	3-A	522/524 (100%)	452 (87%)	70 (13%)	0	100	100
1	4-A	522/524 (100%)	468 (90%)	54 (10%)	0	100	100
All	All	8874/8908 (100%)	8449 (95%)	425 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-B	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-C	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-D	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-E	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-F	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-G	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-H	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-I	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-J	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-K	404/404 (100%)	403 (100%)	1 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-L	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-M	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	1-N	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	2-A	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	3-A	404/404 (100%)	403 (100%)	1 (0%)	87	85
1	4-A	404/404 (100%)	403 (100%)	1 (0%)	87	85
All	All	6868/6868 (100%)	6851 (100%)	17 (0%)	85	85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	174	VAL
1	1-B	174	VAL
1	1-C	174	VAL
1	1-D	174	VAL
1	1-E	174	VAL
1	1-F	174	VAL
1	1-G	174	VAL
1	1-H	174	VAL
1	1-I	174	VAL
1	1-J	174	VAL
1	1-K	174	VAL
1	1-L	174	VAL
1	1-M	174	VAL
1	1-N	174	VAL
1	2-A	174	VAL
1	3-A	174	VAL
1	4-A	174	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	37	ASN
1	1-A	479	ASN
1	1-A	505	GLN
1	1-B	37	ASN
1	1-B	479	ASN
1	1-B	505	GLN
1	1-C	37	ASN

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Mol	Chain	Res	Type
1	1-C	479	ASN
1	1-C	505	GLN
1	1-D	37	ASN
1	1-D	467	ASN
1	1-D	479	ASN
1	1-D	505	GLN
1	1-E	37	ASN
1	1-E	467	ASN
1	1-E	479	ASN
1	1-E	505	GLN
1	1-F	37	ASN
1	1-F	479	ASN
1	1-F	505	GLN
1	1-G	37	ASN
1	1-G	479	ASN
1	1-G	505	GLN
1	1-H	37	ASN
1	1-H	479	ASN
1	1-H	505	GLN
1	1-I	37	ASN
1	1-I	479	ASN
1	1-I	505	GLN
1	1-J	37	ASN
1	1-J	479	ASN
1	1-J	505	GLN
1	1-K	37	ASN
1	1-K	479	ASN
1	1-K	505	GLN
1	1-L	37	ASN
1	1-L	290	GLN
1	1-L	467	ASN
1	1-L	479	ASN
1	1-L	505	GLN
1	1-M	37	ASN
1	1-M	467	ASN
1	1-M	479	ASN
1	1-M	505	GLN
1	1-N	37	ASN
1	1-N	479	ASN
1	1-N	505	GLN
1	2-A	82	ASN
1	2-A	146	GLN

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Mol	Chain	Res	Type
1	2-A	290	GLN
1	2-A	453	GLN
1	2-A	505	GLN
1	3-A	453	GLN
1	3-A	467	ASN
1	3-A	479	ASN
1	3-A	505	GLN
1	4-A	37	ASN
1	4-A	72	GLN
1	4-A	453	GLN
1	4-A	505	GLN

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 oligosaccharides 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.

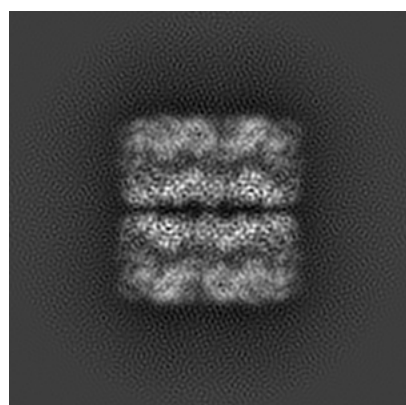
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8750. These allow visual inspection of the internal detail of the map and identification of artifacts.

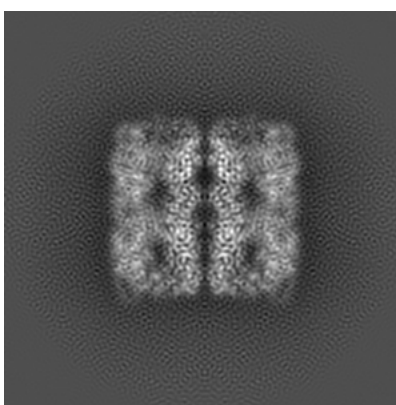
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

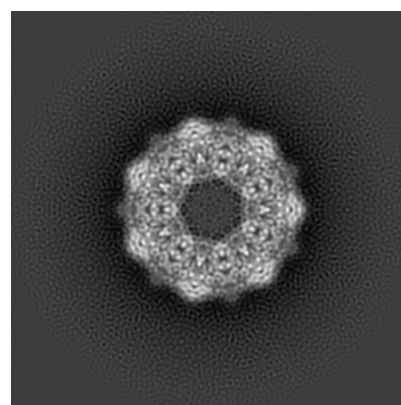
6.1.1 Primary map



X



Y

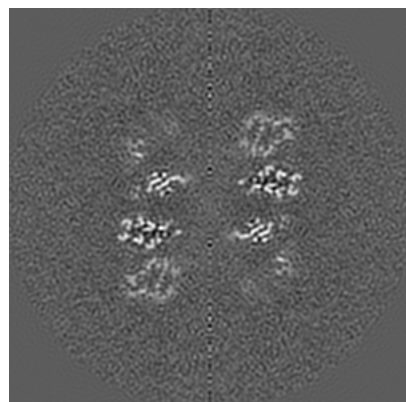


Z

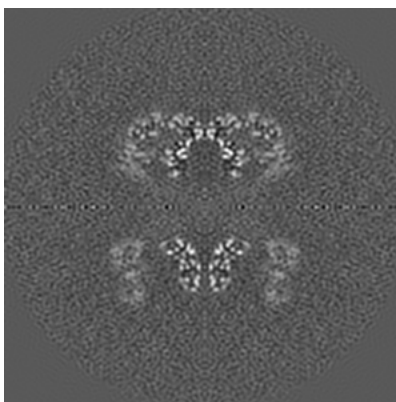
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

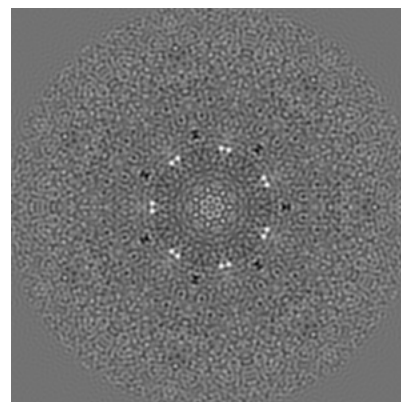
6.2.1 Primary map



X Index: 120



Y Index: 120

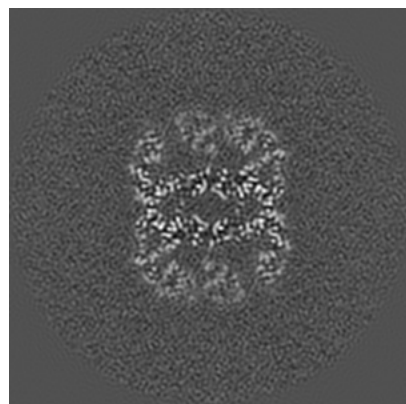


Z Index: 120

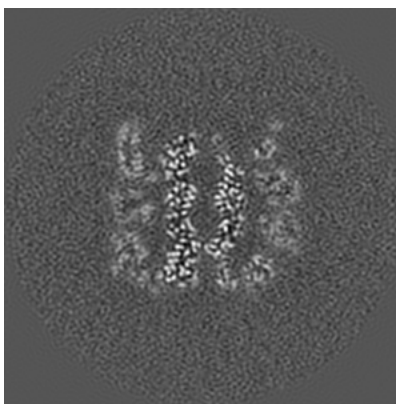
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

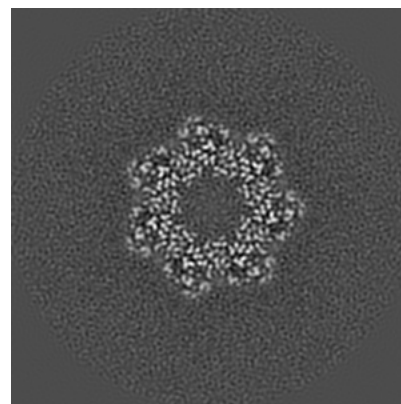
6.3.1 Primary map



X Index: 148



Y Index: 94

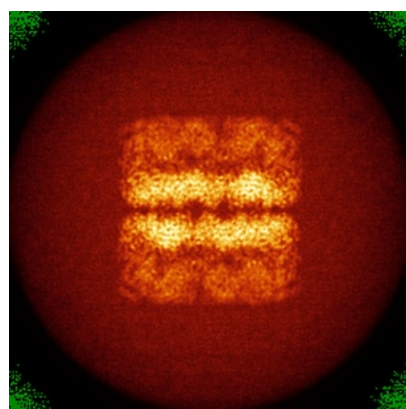


Z Index: 133

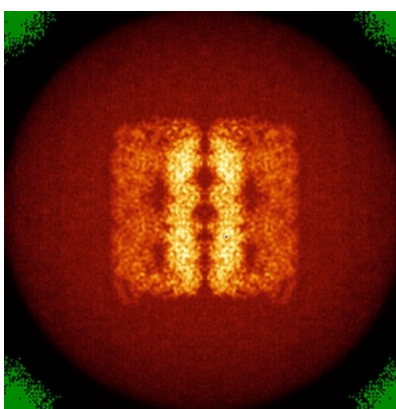
The images above show the largest variance slices of the map in three orthogonal directions.

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

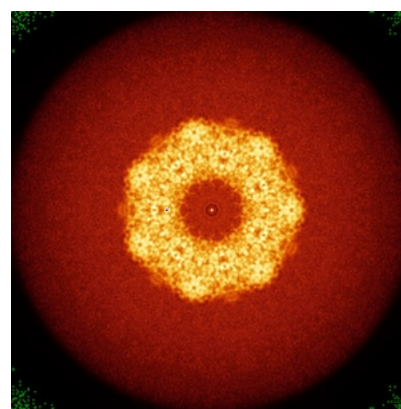
6.4.1 Primary map



X



Y

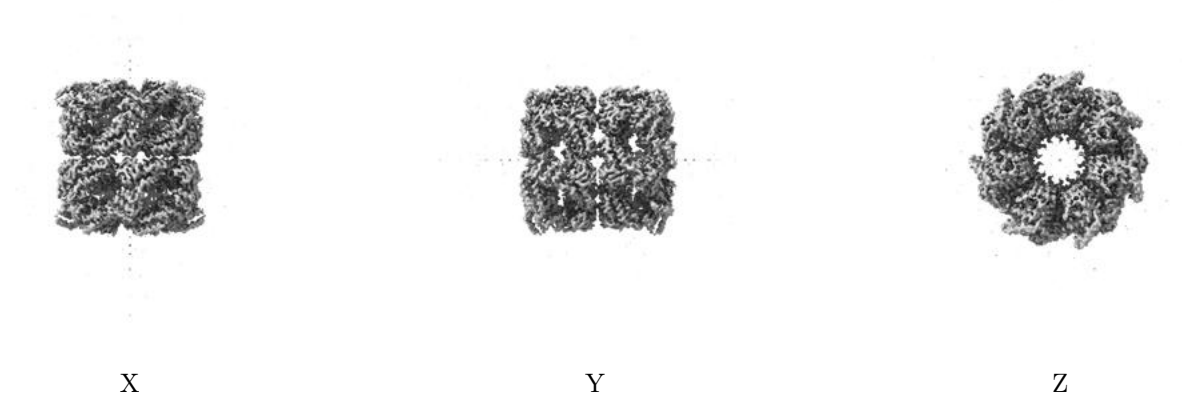


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

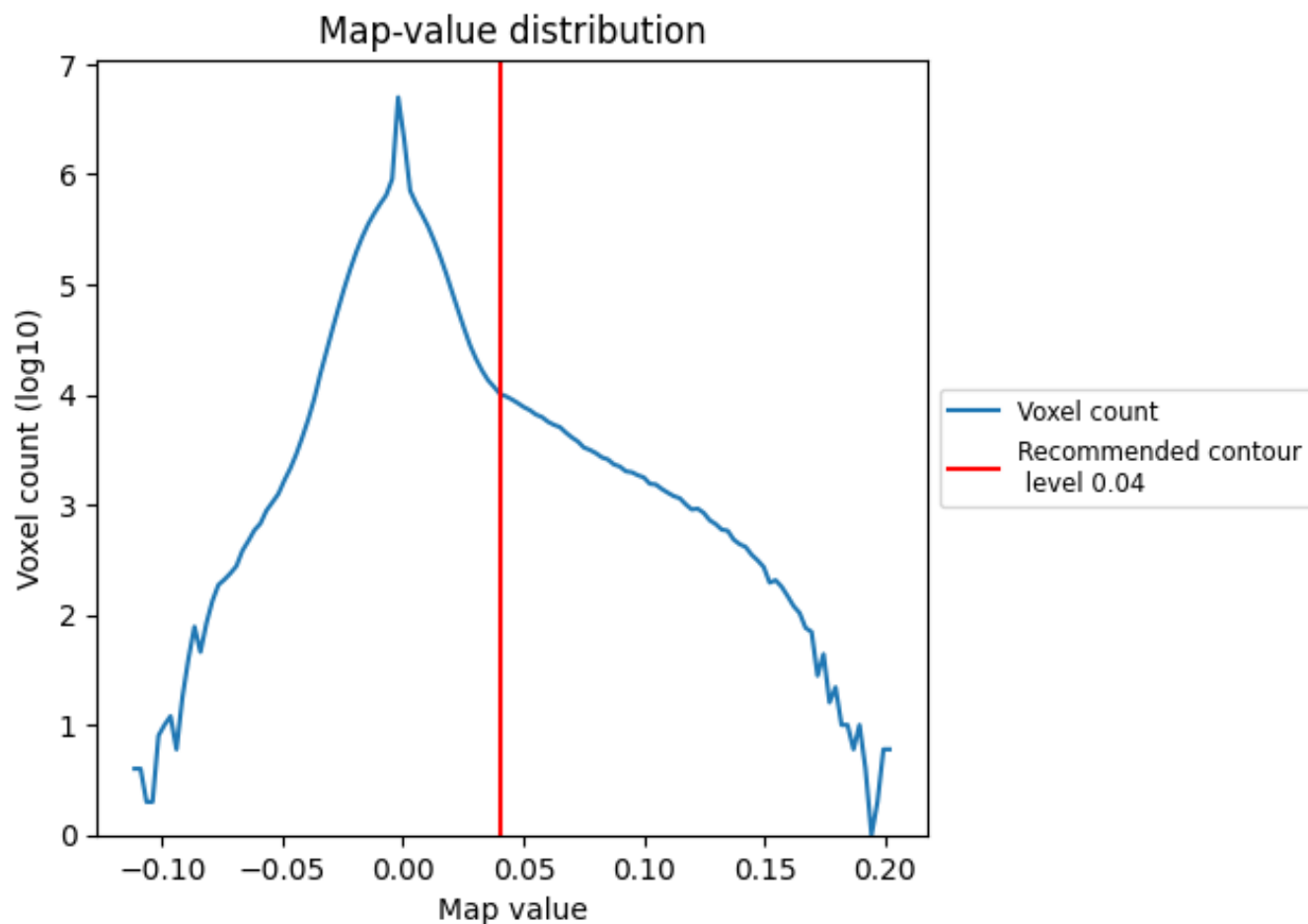
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

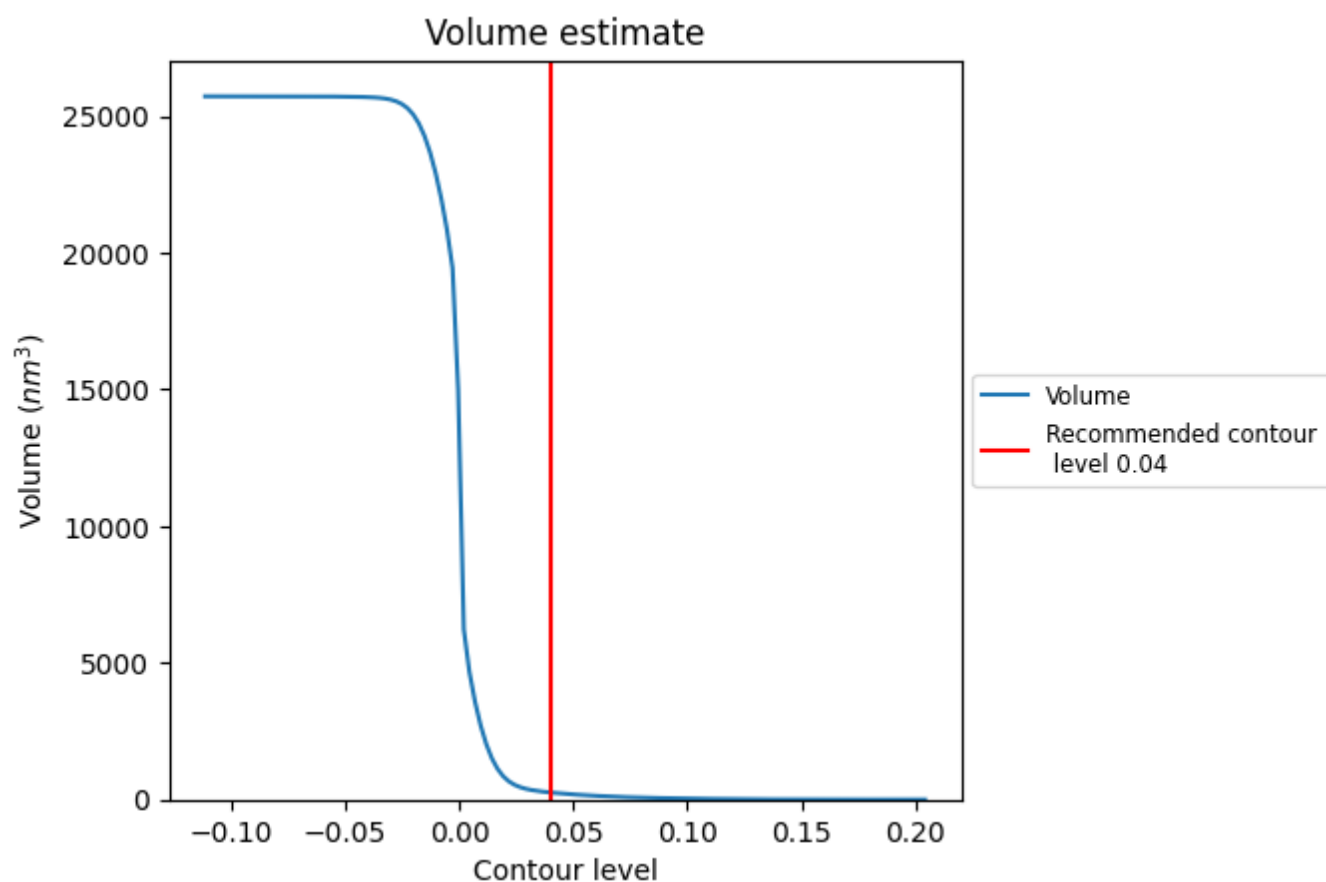
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

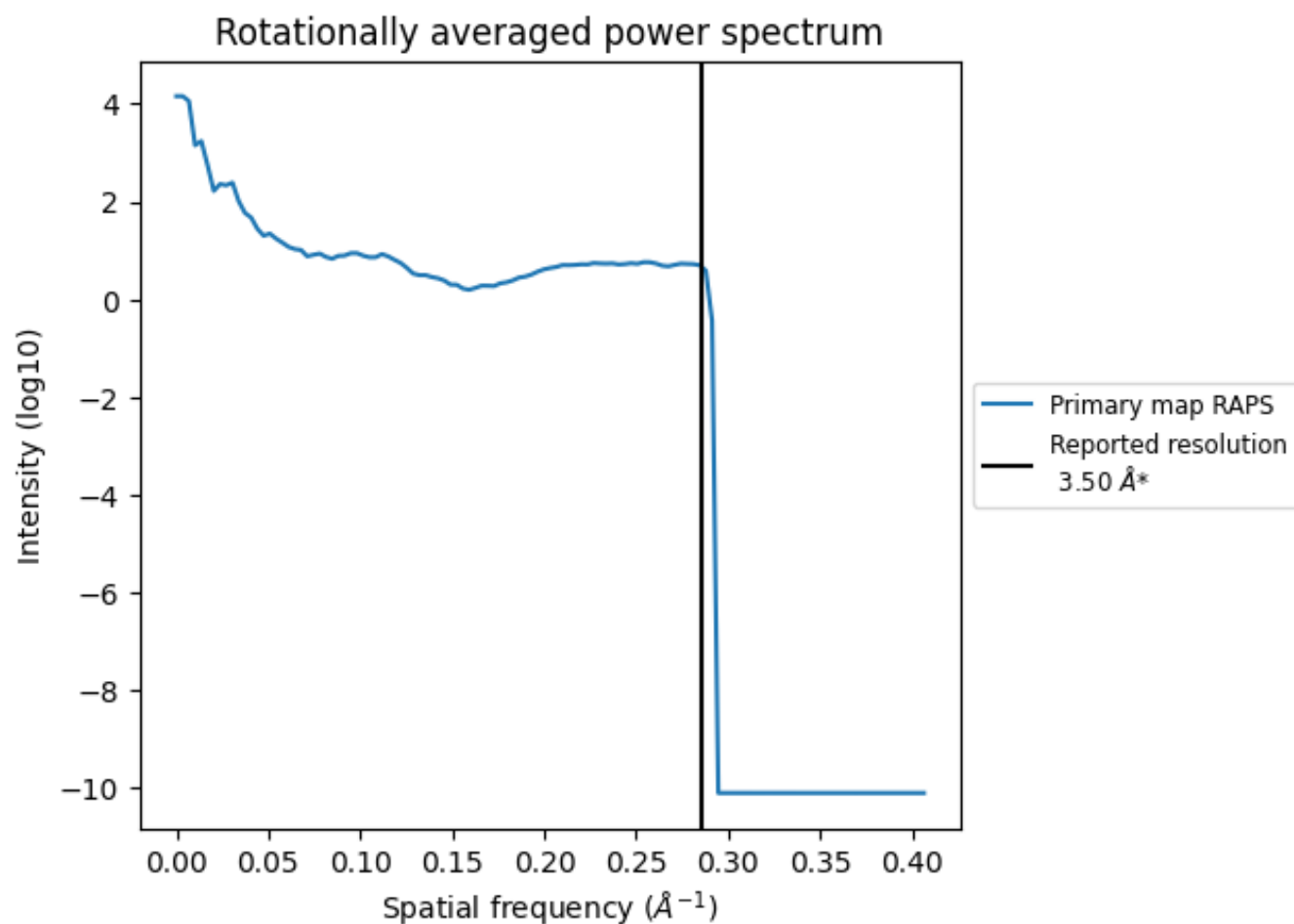
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm³; this corresponds to an approximate mass of 234 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 ⓘ

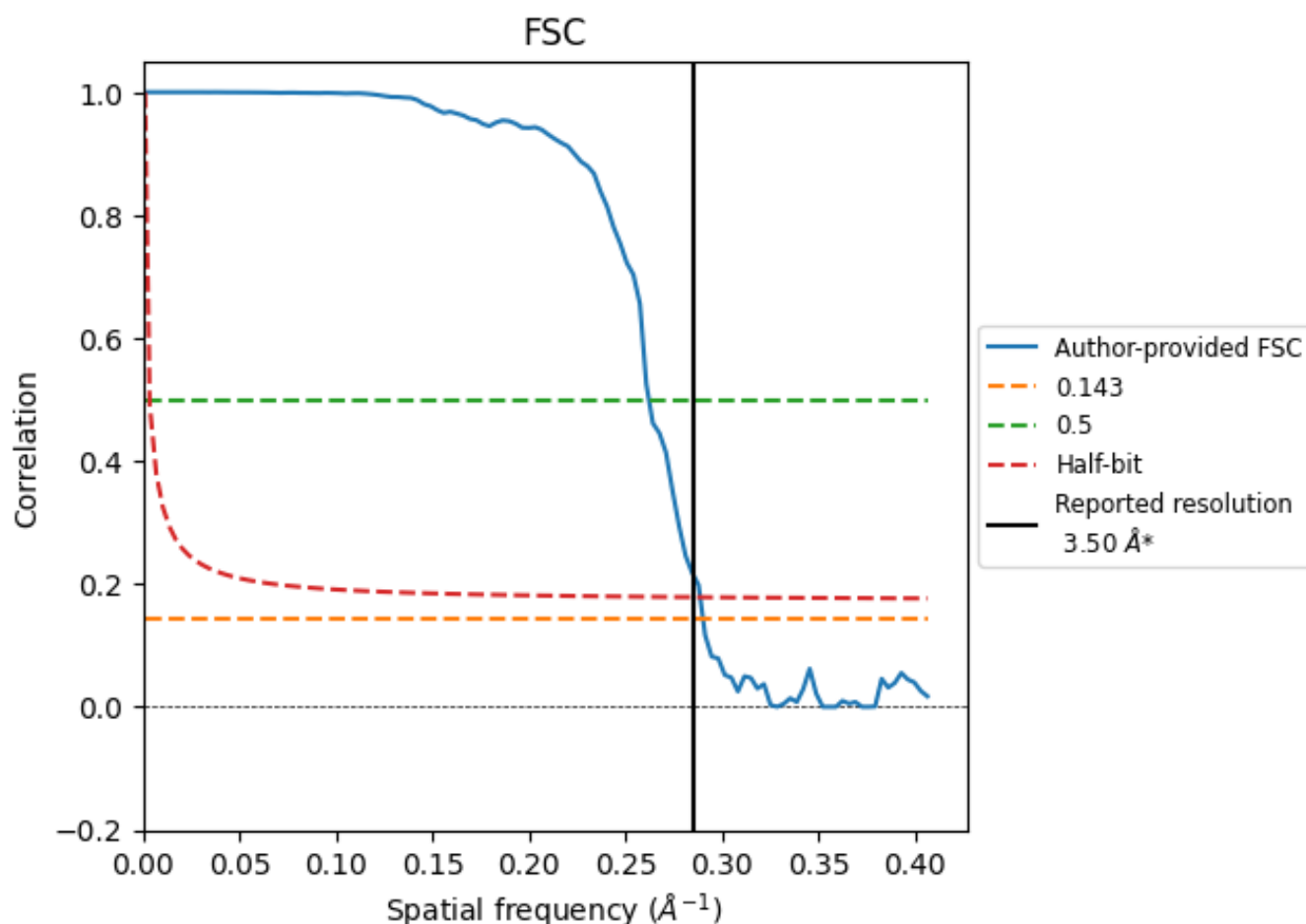


*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.45	3.81	3.46
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

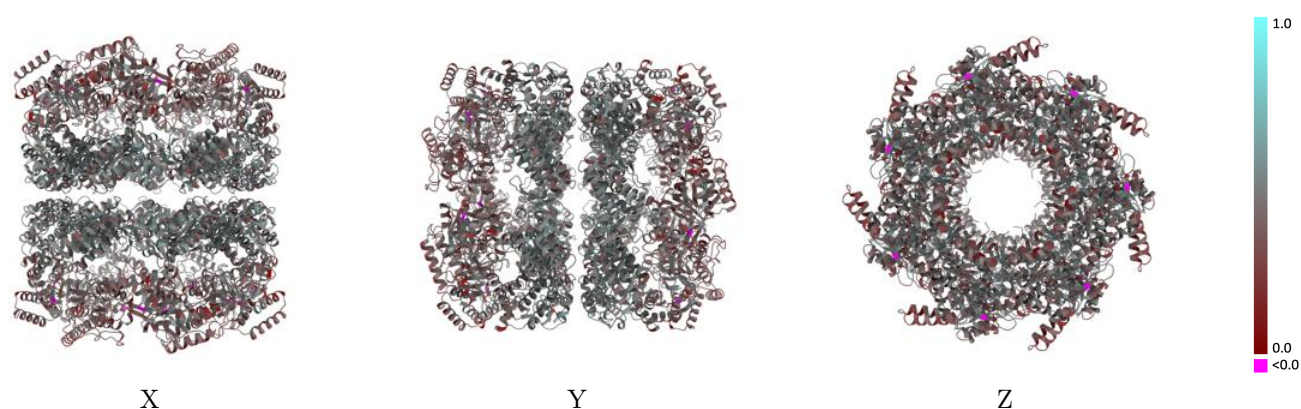
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8750 and PDB model 5W0S. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

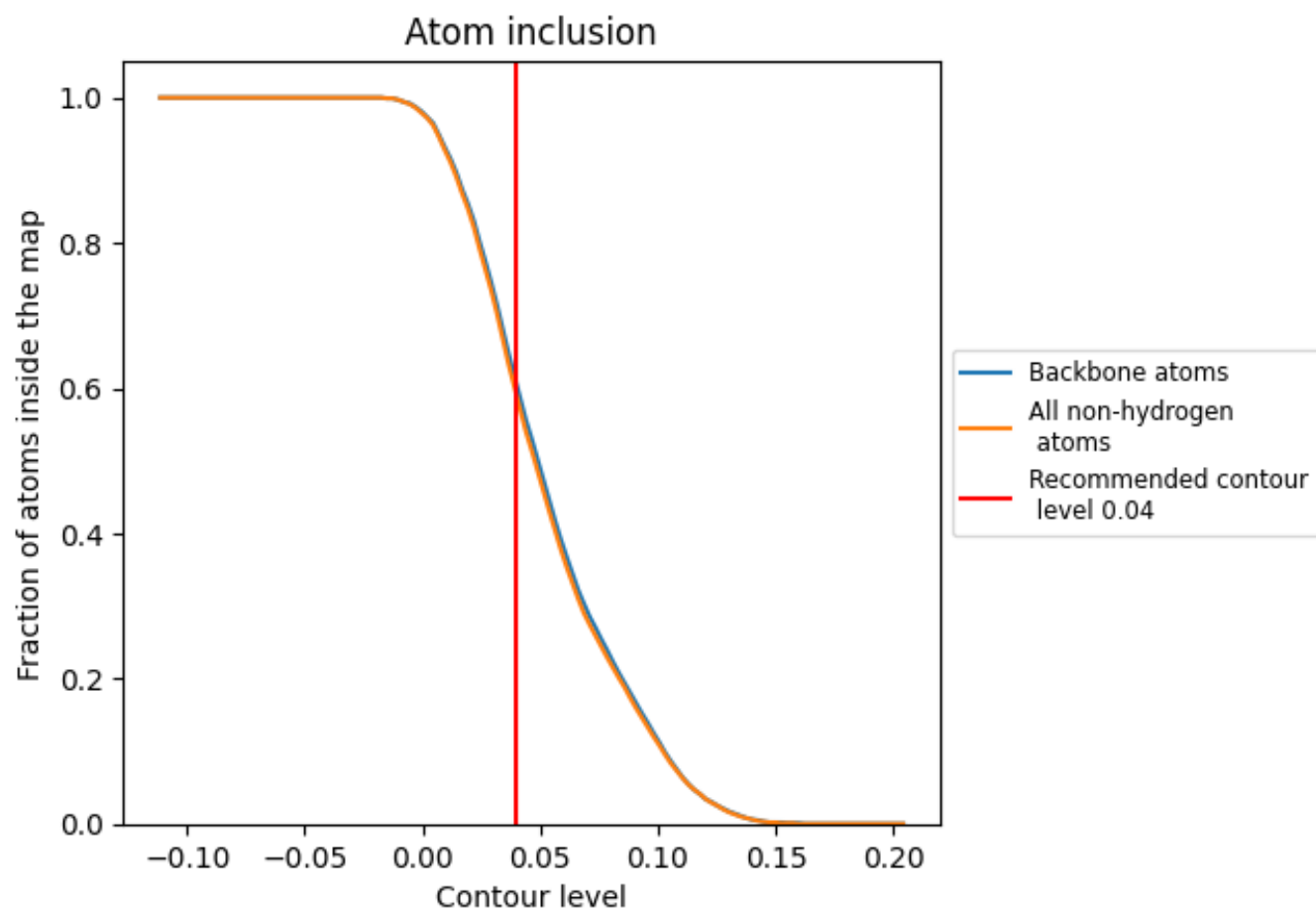


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 59% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5900	0.4240
A	0.5960	0.4250
B	0.5970	0.4240
C	0.5960	0.4230
D	0.5960	0.4230
E	0.5950	0.4240
F	0.5940	0.4250
G	0.5960	0.4240
H	0.5960	0.4250
I	0.5960	0.4260
J	0.5960	0.4230
K	0.5960	0.4230
L	0.5960	0.4230
M	0.5930	0.4230
N	0.5950	0.4260

1.0

0.0

<0.0