



# Full wwPDB EM Validation Report (i)

Nov 16, 2024 – 11:48 pm GMT

PDB ID : 9F16  
EMDB ID : EMD-50123  
Title : Structure of a homomeric LRRC8C point mutation disease mutant  
Authors : Rutz, S.; Quinodoz, M.; Peter, V.; Garavelli, L.; Innes, M.A.; Kellenberger, S.; Peng, Z.; Barone, A.; Campos-Xavier, B.; Unger, S.; Rivolta, C.; Dutzler, R.; Superti-Furga, A.  
Deposited on : 2024-04-18  
Resolution : 4.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

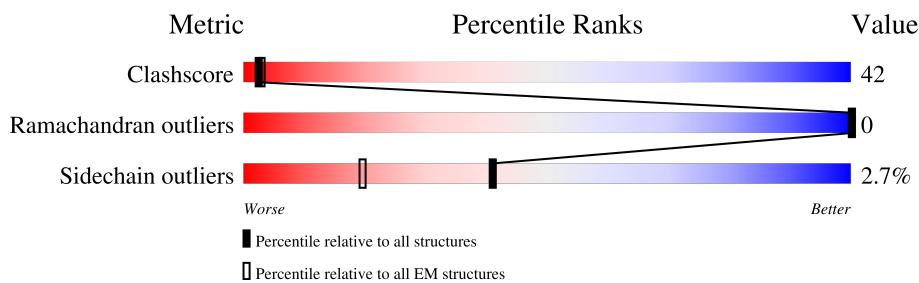
EMDB validation analysis : 0.0.1.dev113  
MolProbit : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
**ELECTRON MICROSCOPY**

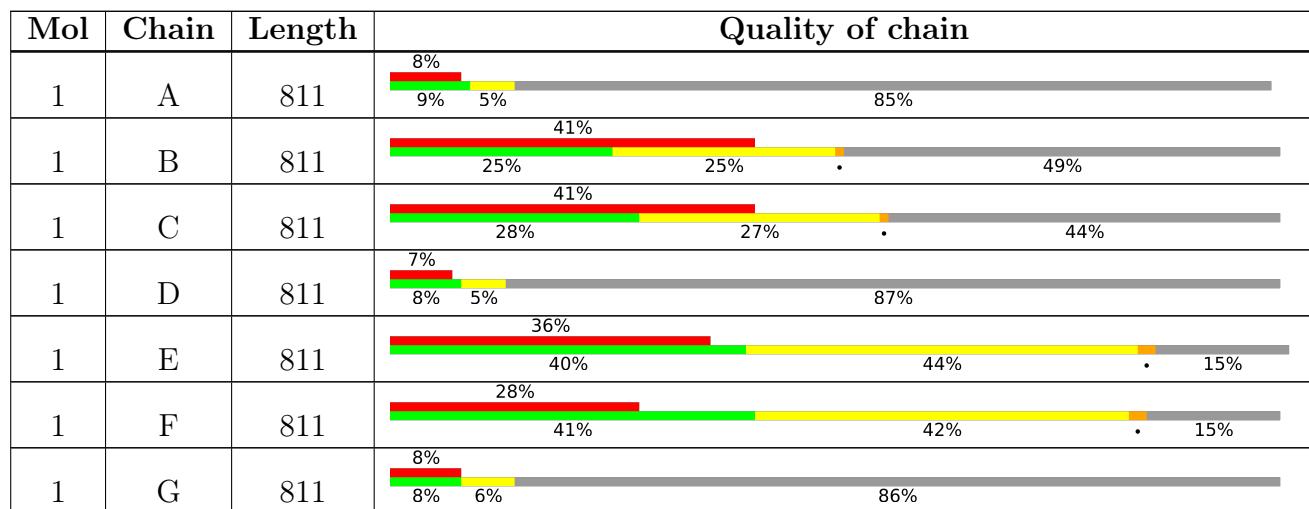
The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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



## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21285 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 Volume-regulated anion channel subunit LRRC8C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	122	Total	C	N	O	S	0	0
			992	650	157	172	13		
1	B	414	Total	C	N	O	S	0	0
			3424	2248	549	601	26		
1	C	458	Total	C	N	O	S	0	0
			3753	2455	609	662	27		
1	D	108	Total	C	N	O	S	0	0
			885	575	143	156	11		
1	E	692	Total	C	N	O	S	0	0
			5642	3676	926	1004	36		
1	F	692	Total	C	N	O	S	0	0
			5642	3676	926	1004	36		
1	G	116	Total	C	N	O	S	0	0
			947	620	151	164	12		

There are 91 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8TDW0
A	1	SER	-	expression tag	UNP Q8TDW0
A	205	GLY	ASP	conflict	UNP Q8TDW0
A	390	LEU	VAL	engineered mutation	UNP Q8TDW0
A	802	ALA	-	expression tag	UNP Q8TDW0
A	803	ASP	-	expression tag	UNP Q8TDW0
A	804	ALA	-	expression tag	UNP Q8TDW0
A	805	LEU	-	expression tag	UNP Q8TDW0
A	806	GLU	-	expression tag	UNP Q8TDW0
A	807	VAL	-	expression tag	UNP Q8TDW0
A	808	LEU	-	expression tag	UNP Q8TDW0
A	809	PHE	-	expression tag	UNP Q8TDW0
A	810	GLN	-	expression tag	UNP Q8TDW0
B	0	MET	-	initiating methionine	UNP Q8TDW0
B	1	SER	-	expression tag	UNP Q8TDW0
B	205	GLY	ASP	conflict	UNP Q8TDW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	390	LEU	VAL	engineered mutation	UNP Q8TDW0
B	802	ALA	-	expression tag	UNP Q8TDW0
B	803	ASP	-	expression tag	UNP Q8TDW0
B	804	ALA	-	expression tag	UNP Q8TDW0
B	805	LEU	-	expression tag	UNP Q8TDW0
B	806	GLU	-	expression tag	UNP Q8TDW0
B	807	VAL	-	expression tag	UNP Q8TDW0
B	808	LEU	-	expression tag	UNP Q8TDW0
B	809	PHE	-	expression tag	UNP Q8TDW0
B	810	GLN	-	expression tag	UNP Q8TDW0
C	0	MET	-	initiating methionine	UNP Q8TDW0
C	1	SER	-	expression tag	UNP Q8TDW0
C	205	GLY	ASP	conflict	UNP Q8TDW0
C	390	LEU	VAL	engineered mutation	UNP Q8TDW0
C	802	ALA	-	expression tag	UNP Q8TDW0
C	803	ASP	-	expression tag	UNP Q8TDW0
C	804	ALA	-	expression tag	UNP Q8TDW0
C	805	LEU	-	expression tag	UNP Q8TDW0
C	806	GLU	-	expression tag	UNP Q8TDW0
C	807	VAL	-	expression tag	UNP Q8TDW0
C	808	LEU	-	expression tag	UNP Q8TDW0
C	809	PHE	-	expression tag	UNP Q8TDW0
C	810	GLN	-	expression tag	UNP Q8TDW0
D	0	MET	-	initiating methionine	UNP Q8TDW0
D	1	SER	-	expression tag	UNP Q8TDW0
D	205	GLY	ASP	conflict	UNP Q8TDW0
D	390	LEU	VAL	engineered mutation	UNP Q8TDW0
D	802	ALA	-	expression tag	UNP Q8TDW0
D	803	ASP	-	expression tag	UNP Q8TDW0
D	804	ALA	-	expression tag	UNP Q8TDW0
D	805	LEU	-	expression tag	UNP Q8TDW0
D	806	GLU	-	expression tag	UNP Q8TDW0
D	807	VAL	-	expression tag	UNP Q8TDW0
D	808	LEU	-	expression tag	UNP Q8TDW0
D	809	PHE	-	expression tag	UNP Q8TDW0
D	810	GLN	-	expression tag	UNP Q8TDW0
E	0	MET	-	initiating methionine	UNP Q8TDW0
E	1	SER	-	expression tag	UNP Q8TDW0
E	205	GLY	ASP	conflict	UNP Q8TDW0
E	390	LEU	VAL	engineered mutation	UNP Q8TDW0
E	802	ALA	-	expression tag	UNP Q8TDW0
E	803	ASP	-	expression tag	UNP Q8TDW0

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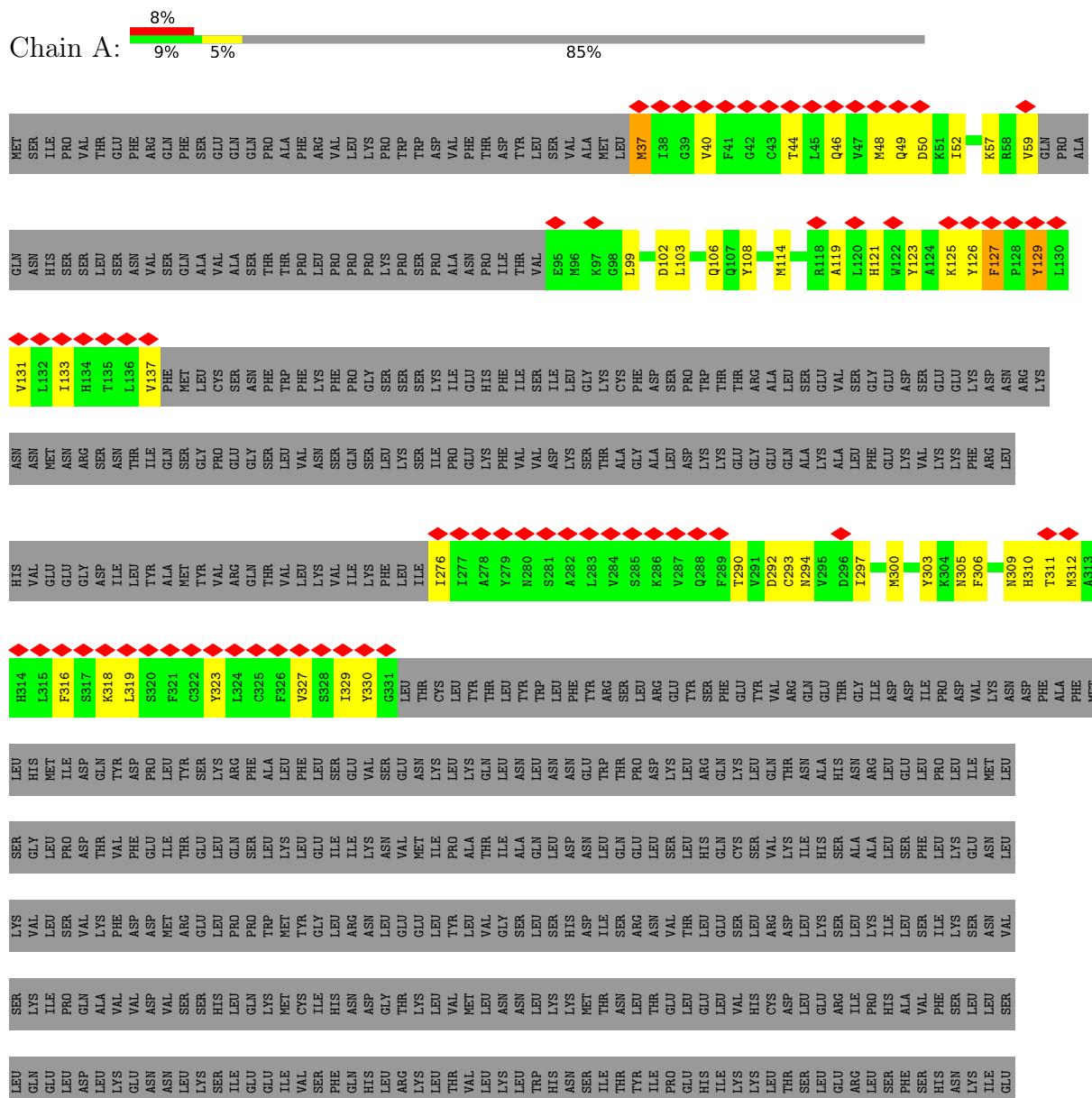
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Chain	Residue	Modelled	Actual	Comment	Reference
E	804	ALA	-	expression tag	UNP Q8TDW0
E	805	LEU	-	expression tag	UNP Q8TDW0
E	806	GLU	-	expression tag	UNP Q8TDW0
E	807	VAL	-	expression tag	UNP Q8TDW0
E	808	LEU	-	expression tag	UNP Q8TDW0
E	809	PHE	-	expression tag	UNP Q8TDW0
E	810	GLN	-	expression tag	UNP Q8TDW0
F	0	MET	-	initiating methionine	UNP Q8TDW0
F	1	SER	-	expression tag	UNP Q8TDW0
F	205	GLY	ASP	conflict	UNP Q8TDW0
F	390	LEU	VAL	engineered mutation	UNP Q8TDW0
F	802	ALA	-	expression tag	UNP Q8TDW0
F	803	ASP	-	expression tag	UNP Q8TDW0
F	804	ALA	-	expression tag	UNP Q8TDW0
F	805	LEU	-	expression tag	UNP Q8TDW0
F	806	GLU	-	expression tag	UNP Q8TDW0
F	807	VAL	-	expression tag	UNP Q8TDW0
F	808	LEU	-	expression tag	UNP Q8TDW0
F	809	PHE	-	expression tag	UNP Q8TDW0
F	810	GLN	-	expression tag	UNP Q8TDW0
G	0	MET	-	initiating methionine	UNP Q8TDW0
G	1	SER	-	expression tag	UNP Q8TDW0
G	205	GLY	ASP	conflict	UNP Q8TDW0
G	390	LEU	VAL	engineered mutation	UNP Q8TDW0
G	802	ALA	-	expression tag	UNP Q8TDW0
G	803	ASP	-	expression tag	UNP Q8TDW0
G	804	ALA	-	expression tag	UNP Q8TDW0
G	805	LEU	-	expression tag	UNP Q8TDW0
G	806	GLU	-	expression tag	UNP Q8TDW0
G	807	VAL	-	expression tag	UNP Q8TDW0
G	808	LEU	-	expression tag	UNP Q8TDW0
G	809	PHE	-	expression tag	UNP Q8TDW0
G	810	GLN	-	expression tag	UNP Q8TDW0

### 3 Residue-property plots

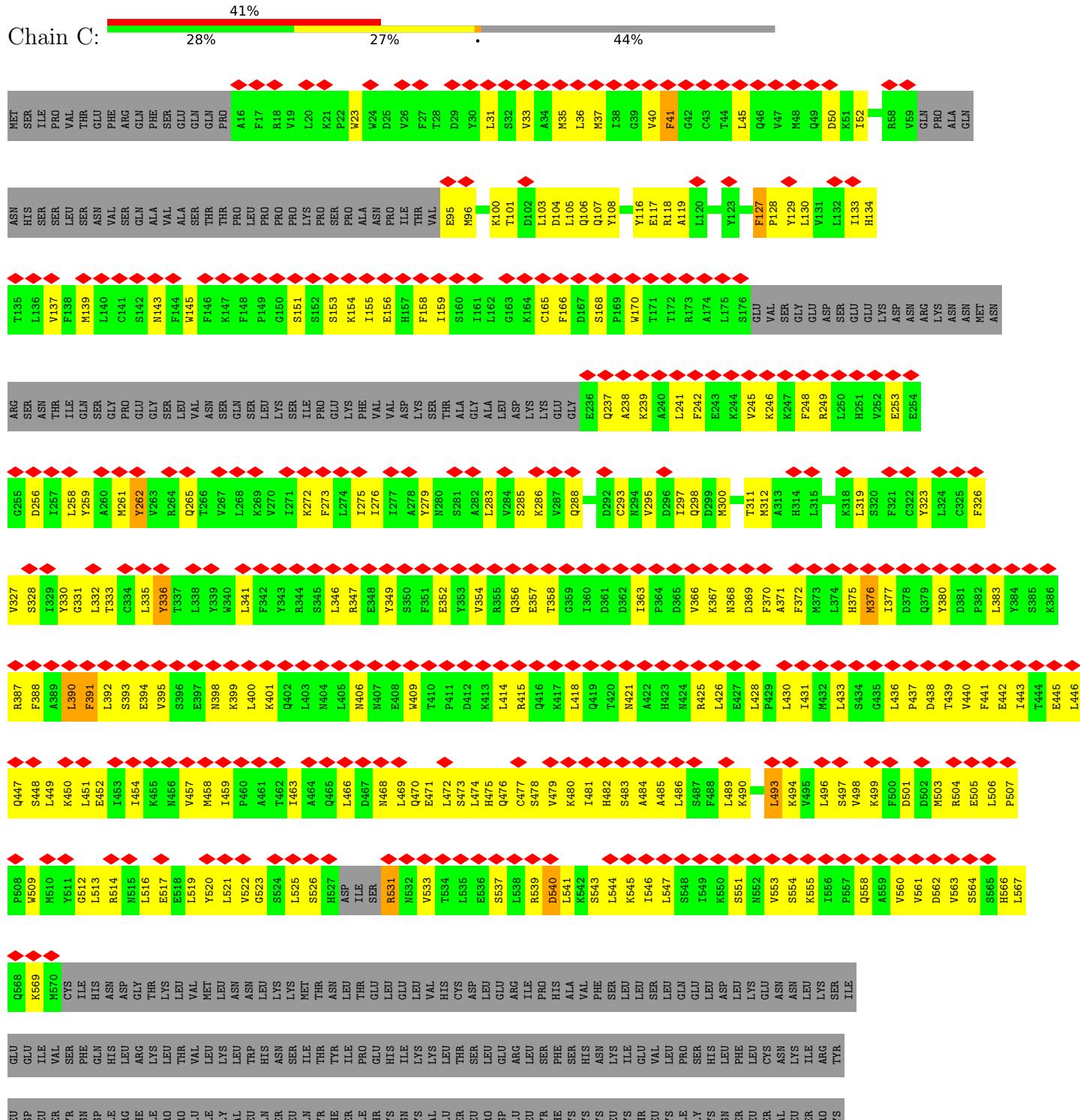
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

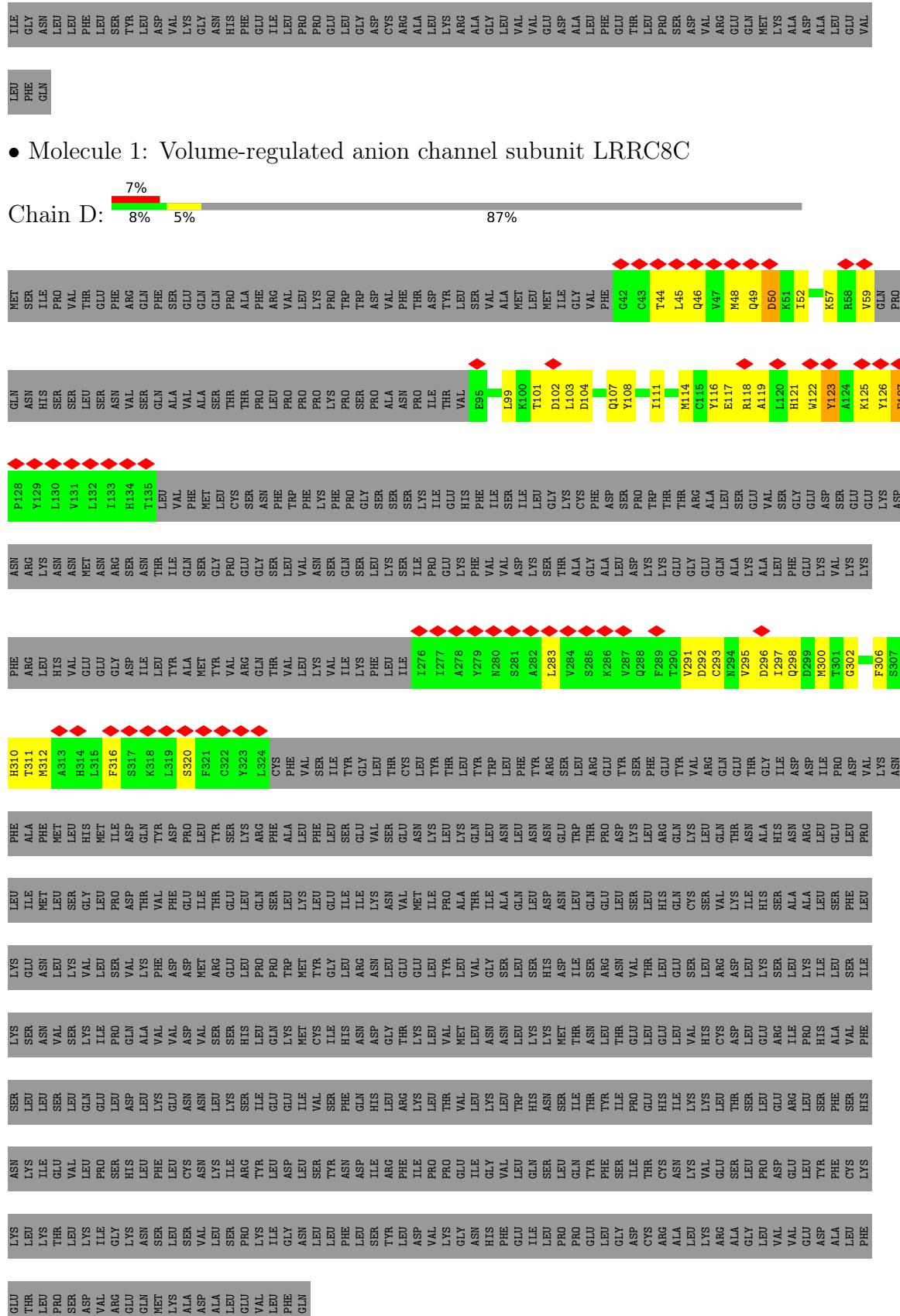
- Molecule 1: Volume-regulated anion channel subunit LRRC8C



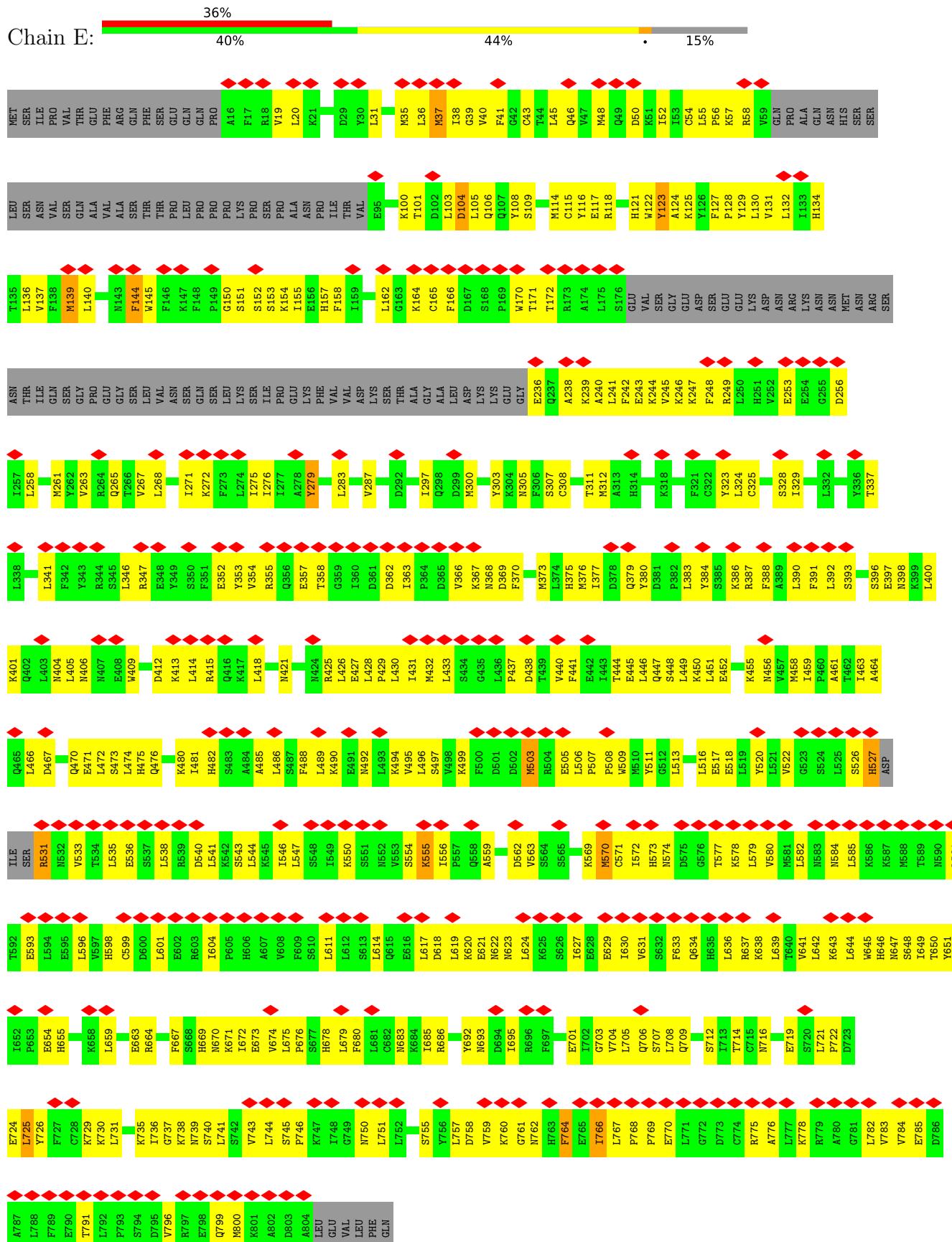
SER	VAL	LEU	LYS	PRO	ALA	ILE	ILE	GLY	HIS
MET	Y126	ASP	ASP	PRO	ALA	ALA	ALA	PRO	
SER	K247	F247	F248	P128	P128	P128	P128	VAL	
ASN	K249	R249	A313	Y129	Y129	Y129	Y129	ASN	
ARG	F250	A313	H314	L130	L130	L130	L130	HIS	
LYS	H315	H315	L315	V131	V131	V131	V131	SER	
ASN	H316	MET	L132	L132	L132	L132	L132	SER	
ASN	V252	ASN	L133	L133	L133	L133	L133	ALA	
ARG	A323	ARG	L134	SER	SER	SER	SER	VAL	
GLN	G324	A324	H134	ASN	ASN	ASN	ASN	ASN	
GLN	A325	PHE	A16	VAL	VAL	VAL	VAL	VAL	
ASP	A326	SER	K21	SER	SER	SER	SER	ILE	
GLU	A327	GLU	F17	GLU	GLU	GLU	GLU	GLU	
GLN	A328	VAL	R18	VAL	VAL	VAL	VAL	VAL	
GLN	A329	PHE	T18	VAL	VAL	VAL	VAL	VAL	
GLN	A330	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A331	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A332	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A333	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A334	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A335	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A336	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A337	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A338	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A339	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A340	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A341	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A342	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A343	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A344	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A345	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A346	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A347	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A348	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A349	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A350	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A351	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A352	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A353	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A354	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A355	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A356	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A357	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A358	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A359	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A360	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A361	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A362	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A363	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A364	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A365	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A366	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A367	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A368	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A369	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A370	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A371	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A372	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A373	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A374	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A375	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A376	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A377	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A378	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A379	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A380	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A381	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A382	ASP	A329	VAL	VAL	VAL	VAL	VAL	
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ALA	A384	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A385	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A386	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A387	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A388	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A389	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A390	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A391	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A392	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A393	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A394	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A395	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A396	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A397	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A398	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A399	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A400	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A401	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A402	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A403	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A404	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A405	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A406	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A407	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A408	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A409	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A410	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A411	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A412	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A413	ASP	A329	VAL	VAL	VAL	VAL	VAL	
ALA	A414	ASP	A329						

- Molecule 1: Volume-regulated anion channel subunit LRRC8C





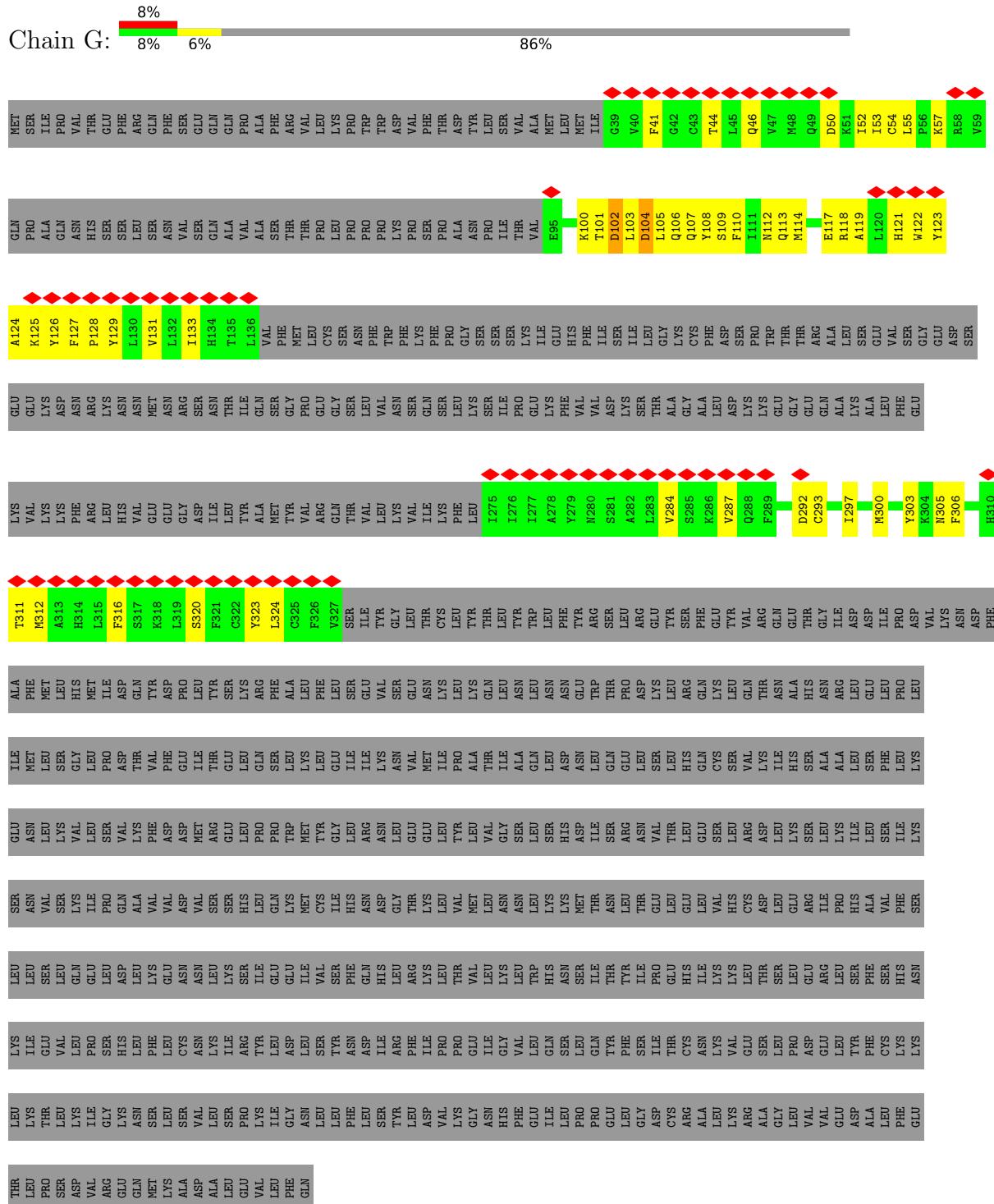
- Molecule 1: Volume-regulated anion channel subunit LRRC8C



- Molecule 1: Volume-regulated anion channel subunit LRRC8C



- Molecule 1: Volume-regulated anion channel subunit LRRC8C



## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180735	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.676	Depositor
Minimum map value	-1.557	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.811	Depositor
Map size (Å)	437.47202, 437.47202, 437.47202	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.29	0/1014	0.45	0/1367
1	B	0.31	0/3509	0.49	0/4745
1	C	0.29	0/3839	0.50	0/5187
1	D	0.29	0/904	0.45	0/1218
1	E	0.31	0/5765	0.51	2/7791 (0.0%)
1	F	0.31	0/5765	0.52	2/7791 (0.0%)
1	G	0.31	0/968	0.51	0/1305
All	All	0.30	0/21764	0.50	4/29404 (0.0%)

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	B	0	1
1	C	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	527	HIS	CB-CA-C	-7.49	95.42	110.40
1	F	527	HIS	CB-CA-C	-7.37	95.66	110.40
1	F	721	LEU	CA-CB-CG	5.53	128.02	115.30
1	E	503	MET	CA-CB-CG	5.29	122.29	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	415	ARG	Sidechain
1	C	531	ARG	Sidechain
1	E	531	ARG	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	992	0	988	42	0
1	B	3424	0	3453	393	0
1	C	3753	0	3803	359	0
1	D	885	0	876	41	0
1	E	5642	0	5768	464	0
1	F	5642	0	5768	479	0
1	G	947	0	942	75	0
All	All	21285	0	21598	1816	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 42.

All (1816) 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:B:145:TRP:CZ3	1:B:262:TYR:CD1	1.80	1.67
1:B:27:PHE:CE2	1:B:333:THR:HG21	1.15	1.61
1:B:145:TRP:CZ3	1:B:262:TYR:CE1	1.89	1.58
1:C:418:LEU:CD2	1:C:428:LEU:HD13	1.32	1.57
1:B:162:LEU:CA	1:B:388:PHE:CE1	1.86	1.56
1:B:27:PHE:CE2	1:B:333:THR:CG2	1.81	1.55
1:F:555:LYS:CB	1:F:581:MET:HE3	1.35	1.53
1:B:27:PHE:HE2	1:B:333:THR:CG2	1.08	1.50
1:B:297:ILE:HA	1:B:300:MET:CE	1.36	1.50
1:E:744:LEU:HB2	1:E:764:PHE:CE2	1.44	1.48
1:F:778:LYS:HA	1:F:800:MET:SD	1.51	1.48
1:C:478:SER:C	1:C:480:LYS:HZ1	1.10	1.46
1:B:145:TRP:CH2	1:B:262:TYR:CG	2.04	1.46
1:F:555:LYS:CB	1:F:581:MET:CE	1.84	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:744:LEU:HB2	1:E:764:PHE:CZ	1.51	1.44
1:E:799:GLN:CG	1:E:800:MET:HE1	1.44	1.44
1:B:162:LEU:HA	1:B:388:PHE:CE1	0.90	1.43
1:B:415:ARG:NH2	1:B:416:GLN:HA	1.25	1.43
1:F:132:LEU:O	1:F:136:LEU:CD2	1.66	1.41
1:B:145:TRP:CE3	1:B:262:TYR:CD1	2.10	1.40
1:B:297:ILE:CA	1:B:300:MET:CE	2.01	1.36
1:F:555:LYS:HB2	1:F:581:MET:CE	0.89	1.36
1:F:778:LYS:CA	1:F:800:MET:SD	2.14	1.34
1:B:145:TRP:CZ2	1:B:262:TYR:HB2	1.63	1.34
1:E:130:LEU:HD11	1:E:279:TYR:OH	1.16	1.33
1:B:303:TYR:HA	1:C:96:MET:CE	1.58	1.33
1:B:415:ARG:HH21	1:B:416:GLN:CA	1.41	1.32
1:G:54:CYS:O	1:G:55:LEU:HD23	1.22	1.29
1:C:443:ILE:HG23	1:C:445:GLU:OE2	1.18	1.29
1:B:297:ILE:CA	1:B:300:MET:HE1	1.59	1.25
1:C:489:LEU:HA	1:C:493:LEU:CD1	1.64	1.25
1:B:302:GLY:O	1:C:96:MET:HE2	1.32	1.24
1:B:31:LEU:HB2	1:B:330:TYR:CE1	1.72	1.24
1:F:778:LYS:C	1:F:800:MET:SD	2.17	1.23
1:B:162:LEU:HA	1:B:388:PHE:CZ	1.72	1.23
1:C:478:SER:C	1:C:480:LYS:NZ	1.90	1.23
1:B:297:ILE:C	1:B:300:MET:CE	2.07	1.22
1:F:138:PHE:HE2	1:F:330:TYR:CE1	1.56	1.22
1:B:323:TYR:HA	1:B:326:PHE:CD2	1.75	1.22
1:F:271:ILE:HD12	1:F:272:LYS:N	1.54	1.21
1:C:41:PHE:HE1	1:C:319:LEU:CD1	1.53	1.20
1:E:458:MET:SD	1:E:481:ILE:C	2.19	1.20
1:G:57:LYS:HD3	1:G:305:ASN:OD1	1.39	1.20
1:E:130:LEU:CD1	1:E:279:TYR:OH	1.88	1.19
1:B:145:TRP:CH2	1:B:262:TYR:CD1	2.27	1.19
1:C:376:MET:HE3	1:C:377:ILE:CG1	1.73	1.19
1:F:555:LYS:HB2	1:F:581:MET:HE2	1.25	1.18
1:E:128:PRO:O	1:E:132:LEU:HD22	1.42	1.18
1:G:113:GLN:OE1	1:G:114:MET:CE	1.90	1.18
1:C:478:SER:CA	1:C:480:LYS:HZ1	1.54	1.17
1:E:144:PHE:CD2	1:E:265:GLN:NE2	2.11	1.17
1:F:507:PRO:O	1:F:510:MET:SD	2.02	1.17
1:F:555:LYS:HB2	1:F:581:MET:HE1	1.26	1.17
1:C:346:LEU:CD1	1:C:372:PHE:HB2	1.72	1.16
1:F:48:MET:HG3	1:F:49:GLN:HG2	1.25	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:TYR:HA	1:B:326:PHE:CE2	1.80	1.15
1:E:760:LYS:HG3	1:E:783:VAL:HG12	1.25	1.15
1:F:430:LEU:HD12	1:F:451:LEU:CD1	1.74	1.15
1:E:744:LEU:CB	1:E:764:PHE:CZ	2.29	1.15
1:B:409:TRP:CE3	1:B:437:PRO:HG3	1.80	1.15
1:F:564:SER:CB	1:F:588:MET:CE	2.23	1.14
1:F:48:MET:SD	1:F:49:GLN:NE2	2.20	1.14
1:C:23:TRP:CZ2	1:C:336:TYR:CE1	2.34	1.14
1:C:418:LEU:HD23	1:C:428:LEU:CD1	1.79	1.13
1:C:346:LEU:HD13	1:C:372:PHE:HA	1.14	1.13
1:B:302:GLY:O	1:C:96:MET:CE	1.96	1.13
1:C:346:LEU:HD11	1:C:372:PHE:HB2	1.13	1.13
1:C:482:HIS:CE1	1:C:484:ALA:H	1.66	1.13
1:F:564:SER:HB3	1:F:588:MET:CE	1.76	1.13
1:F:114:MET:CE	1:F:295:VAL:HG11	1.78	1.13
1:B:503:MET:HE1	1:B:506:LEU:HD13	1.16	1.12
1:E:128:PRO:O	1:E:132:LEU:CD2	1.95	1.12
1:B:145:TRP:CZ2	1:B:262:TYR:CB	2.32	1.12
1:G:129:TYR:O	1:G:133:ILE:HG13	1.47	1.12
1:C:376:MET:HE3	1:C:377:ILE:HG12	1.24	1.12
1:C:512:GLY:O	1:C:540:ASP:OD2	1.66	1.12
1:F:777:LEU:O	1:F:800:MET:HE1	1.49	1.12
1:E:144:PHE:HD2	1:E:265:GLN:NE2	1.45	1.11
1:B:297:ILE:C	1:B:300:MET:HE1	1.66	1.10
1:B:370:PHE:HA	1:B:373:MET:HE3	1.32	1.10
1:C:418:LEU:CD2	1:C:428:LEU:CD1	2.28	1.10
1:E:743:VAL:C	1:E:764:PHE:CE1	2.23	1.10
1:E:458:MET:SD	1:E:481:ILE:O	2.09	1.09
1:C:41:PHE:HE1	1:C:319:LEU:HD11	1.11	1.09
1:C:418:LEU:CG	1:C:428:LEU:HD13	1.82	1.09
1:C:443:ILE:CG2	1:C:445:GLU:OE2	1.99	1.09
1:F:564:SER:HB3	1:F:588:MET:HE1	1.13	1.09
1:C:525:LEU:HD23	1:C:553:VAL:HG22	1.32	1.08
1:B:298:GLN:O	1:B:300:MET:SD	2.09	1.08
1:E:376:MET:HE3	1:E:377:ILE:HG12	1.30	1.08
1:F:132:LEU:O	1:F:136:LEU:HD22	0.91	1.08
1:C:525:LEU:HD23	1:C:553:VAL:CG2	1.82	1.08
1:B:28:THR:O	1:B:330:TYR:OH	1.69	1.08
1:B:303:TYR:CA	1:C:96:MET:HE3	1.84	1.08
1:F:138:PHE:CE2	1:F:330:TYR:CE1	2.41	1.07
1:F:240:ALA:O	1:F:243:GLU:OE2	1.71	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TYR:HA	1:A:129:TYR:CD2	1.89	1.07
1:C:376:MET:CE	1:C:377:ILE:CD1	2.32	1.07
1:E:744:LEU:CB	1:E:764:PHE:CE2	2.38	1.07
1:C:531:ARG:HD2	1:C:554:SER:HB3	1.28	1.07
1:F:635:HIS:CE1	1:F:636:LEU:HD21	1.91	1.06
1:B:303:TYR:HA	1:C:96:MET:HE3	1.08	1.06
1:E:799:GLN:HG2	1:E:800:MET:CE	1.85	1.06
1:E:725:LEU:HD12	1:E:726:TYR:N	1.70	1.06
1:C:311:THR:OG1	1:C:312:MET:SD	2.12	1.06
1:C:346:LEU:HD13	1:C:372:PHE:CA	1.85	1.05
1:C:258:LEU:HD12	1:C:261:MET:HE3	1.36	1.04
1:E:376:MET:HE3	1:E:377:ILE:CG1	1.88	1.04
1:F:430:LEU:HD12	1:F:451:LEU:HD11	1.07	1.04
1:G:54:CYS:C	1:G:55:LEU:HD23	1.79	1.04
1:E:725:LEU:HD11	1:E:726:TYR:CE2	1.93	1.03
1:B:145:TRP:CH2	1:B:262:TYR:CD2	2.46	1.03
1:B:415:ARG:NH2	1:B:416:GLN:CA	2.08	1.03
1:B:297:ILE:O	1:B:300:MET:HE2	1.59	1.03
1:B:31:LEU:O	1:B:35:MET:HE3	1.57	1.02
1:B:162:LEU:CA	1:B:388:PHE:CZ	2.34	1.02
1:C:41:PHE:CE1	1:C:319:LEU:HD11	1.94	1.02
1:E:376:MET:CE	1:E:377:ILE:CD1	2.37	1.02
1:E:472:LEU:HD12	1:E:473:SER:H	1.20	1.02
1:B:31:LEU:CB	1:B:330:TYR:CE1	2.43	1.02
1:F:472:LEU:HD12	1:F:473:SER:N	1.73	1.02
1:B:145:TRP:CZ2	1:B:262:TYR:CG	2.48	1.02
1:C:258:LEU:HD12	1:C:261:MET:CE	1.89	1.02
1:C:489:LEU:CA	1:C:493:LEU:CD1	2.37	1.02
1:F:271:ILE:HD12	1:F:272:LYS:H	1.14	1.02
1:F:635:HIS:CE1	1:F:636:LEU:CD2	2.41	1.02
1:F:132:LEU:HD23	1:F:136:LEU:HD21	1.38	1.01
1:F:485:ALA:O	1:F:489:LEU:HG	1.59	1.01
1:B:273:PHE:O	1:B:277:ILE:HG12	1.58	1.01
1:C:376:MET:CE	1:C:377:ILE:HD13	1.89	1.01
1:E:796:VAL:O	1:E:800:MET:HE2	1.60	1.01
1:B:503:MET:CE	1:B:506:LEU:HD13	1.91	1.00
1:E:799:GLN:CG	1:E:800:MET:CE	2.38	1.00
1:C:418:LEU:HD23	1:C:428:LEU:HD13	1.01	1.00
1:B:27:PHE:CE2	1:B:333:THR:HG22	1.94	1.00
1:B:297:ILE:HA	1:B:300:MET:HE3	1.36	1.00
1:C:41:PHE:CE1	1:C:319:LEU:CD1	2.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:ILE:CD1	1:E:489:LEU:HD21	1.93	0.99
1:F:296:ASP:O	1:F:296:ASP:OD2	1.79	0.99
1:B:128:PRO:O	1:B:132:LEU:HD22	1.60	0.99
1:B:474:LEU:HD23	1:B:498:VAL:HG12	1.43	0.99
1:B:297:ILE:CA	1:B:300:MET:HE2	1.91	0.99
1:F:265:GLN:O	1:F:268:LEU:HD12	1.60	0.99
1:F:452:GLU:HG3	1:F:475:HIS:HB2	1.45	0.99
1:F:472:LEU:HD12	1:F:473:SER:H	1.23	0.99
1:C:489:LEU:CA	1:C:493:LEU:HD11	1.91	0.99
1:B:31:LEU:HB2	1:B:330:TYR:HE1	1.08	0.98
1:E:744:LEU:N	1:E:764:PHE:CZ	2.31	0.98
1:F:779:ARG:NH2	1:F:782:LEU:HG	1.78	0.98
1:B:145:TRP:CE2	1:B:262:TYR:HB2	1.98	0.98
1:C:418:LEU:CG	1:C:428:LEU:CD1	2.42	0.98
1:F:452:GLU:CG	1:F:475:HIS:HB2	1.93	0.98
1:C:489:LEU:HA	1:C:493:LEU:HD11	0.98	0.97
1:B:165:CYS:HB3	1:B:388:PHE:CE1	1.99	0.97
1:E:485:ALA:O	1:E:489:LEU:HG	1.63	0.97
1:A:126:TYR:HA	1:A:129:TYR:CE2	1.98	0.97
1:C:33:VAL:HA	1:C:36:LEU:HD23	1.45	0.97
1:E:376:MET:HE1	1:E:377:ILE:CD1	1.93	0.97
1:B:134:HIS:CE1	1:B:276:ILE:CD1	2.47	0.97
1:F:635:HIS:ND1	1:F:636:LEU:CD2	2.28	0.97
1:C:346:LEU:CD1	1:C:372:PHE:CB	2.43	0.97
1:G:113:GLN:OE1	1:G:114:MET:HE1	1.65	0.96
1:B:409:TRP:HE3	1:B:437:PRO:HG3	1.30	0.96
1:E:376:MET:CE	1:E:377:ILE:HD13	1.94	0.96
1:C:418:LEU:HG	1:C:428:LEU:CD1	1.94	0.96
1:B:145:TRP:CE3	1:B:262:TYR:CE1	2.40	0.96
1:E:743:VAL:C	1:E:764:PHE:HE1	1.68	0.96
1:F:779:ARG:N	1:F:800:MET:SD	2.38	0.96
1:B:145:TRP:CE3	1:B:262:TYR:HD1	1.82	0.96
1:B:297:ILE:C	1:B:300:MET:HE2	1.79	0.96
1:F:114:MET:HE2	1:F:295:VAL:HG11	1.48	0.96
1:E:41:PHE:CD1	1:E:45:LEU:HD21	2.01	0.95
1:B:162:LEU:N	1:B:388:PHE:CZ	2.34	0.95
1:E:123:TYR:CE2	1:E:283:LEU:O	2.19	0.95
1:F:123:TYR:CG	1:F:283:LEU:HD13	2.01	0.95
1:B:323:TYR:CA	1:B:326:PHE:CE2	2.49	0.95
1:C:238:ALA:HA	1:C:241:LEU:HG	1.46	0.95
1:C:479:VAL:N	1:C:480:LYS:NZ	2.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:PHE:CD1	1:E:45:LEU:CD2	2.49	0.95
1:C:376:MET:HE1	1:C:377:ILE:CD1	1.94	0.95
1:E:721:LEU:HB3	1:E:725:LEU:HD21	1.44	0.95
1:C:418:LEU:HG	1:C:428:LEU:HD11	1.49	0.95
1:C:489:LEU:O	1:C:493:LEU:CD1	2.13	0.95
1:C:489:LEU:O	1:C:493:LEU:HD12	1.67	0.94
1:B:31:LEU:CB	1:B:330:TYR:HE1	1.80	0.94
1:B:27:PHE:CD2	1:B:333:THR:HG21	2.00	0.94
1:B:145:TRP:CZ3	1:B:262:TYR:CG	2.44	0.94
1:E:300:MET:HE3	1:F:57:LYS:HA	1.50	0.94
1:E:799:GLN:HG2	1:E:800:MET:HE1	0.96	0.94
1:C:346:LEU:HD12	1:C:346:LEU:O	1.68	0.94
1:B:43:CYS:SG	1:B:132:LEU:HD21	2.06	0.93
1:E:744:LEU:HB2	1:E:764:PHE:HE2	1.26	0.93
1:C:145:TRP:HD1	1:C:261:MET:SD	1.90	0.93
1:F:672:ILE:HG23	1:F:695:ILE:HD11	1.49	0.93
1:C:514:ARG:HA	1:C:541:LEU:HA	1.50	0.93
1:F:564:SER:CB	1:F:588:MET:HE1	1.92	0.93
1:C:376:MET:CE	1:C:377:ILE:HG12	1.98	0.93
1:C:479:VAL:C	1:C:480:LYS:HD3	1.89	0.93
1:F:114:MET:CE	1:F:295:VAL:CG1	2.47	0.93
1:B:261:MET:HE1	1:B:264:ARG:HD2	1.47	0.93
1:F:452:GLU:OE2	1:F:475:HIS:ND1	2.02	0.93
1:B:145:TRP:CZ3	1:B:262:TYR:CZ	2.57	0.93
1:C:445:GLU:OE1	1:C:445:GLU:N	2.02	0.93
1:C:478:SER:CA	1:C:480:LYS:NZ	2.28	0.93
1:E:744:LEU:CA	1:E:764:PHE:HZ	1.82	0.92
1:C:482:HIS:ND1	1:C:484:ALA:N	2.17	0.92
1:E:151:SER:O	1:E:155:ILE:HG12	1.69	0.92
1:B:409:TRP:CH2	1:B:433:LEU:HD22	2.04	0.92
1:B:126:TYR:O	1:B:130:LEU:HG	1.67	0.92
1:B:162:LEU:HA	1:B:388:PHE:CD1	2.01	0.92
1:B:322:CYS:HB2	1:B:326:PHE:CZ	2.06	0.91
1:B:35:MET:HE3	1:B:35:MET:N	1.85	0.91
1:E:744:LEU:CA	1:E:764:PHE:CZ	2.53	0.91
1:F:564:SER:CB	1:F:588:MET:HE2	1.98	0.91
1:E:129:TYR:HA	1:E:132:LEU:HD23	1.52	0.91
1:C:23:TRP:HZ2	1:C:336:TYR:CE1	1.77	0.91
1:E:130:LEU:HD11	1:E:279:TYR:CZ	2.05	0.91
1:F:430:LEU:CD1	1:F:451:LEU:HD11	2.00	0.91
1:E:472:LEU:HD12	1:E:473:SER:N	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:725:LEU:HD11	1:E:726:TYR:CD2	2.06	0.91
1:B:165:CYS:HB3	1:B:388:PHE:CD1	2.06	0.91
1:G:54:CYS:O	1:G:55:LEU:CD2	2.16	0.90
1:B:370:PHE:CA	1:B:373:MET:HE3	2.01	0.90
1:E:130:LEU:HD11	1:E:279:TYR:HH	1.34	0.90
1:A:311:THR:OG1	1:A:312:MET:SD	2.30	0.89
1:E:104:ASP:OD1	1:E:106:GLN:N	2.04	0.89
1:F:29:ASP:O	1:F:33:VAL:HG23	1.73	0.89
1:B:162:LEU:HD12	1:B:388:PHE:CZ	2.07	0.89
1:E:131:VAL:HG22	1:E:323:TYR:CE2	2.07	0.88
1:F:133:ILE:HA	1:F:136:LEU:HD23	1.55	0.88
1:B:409:TRP:CH2	1:B:433:LEU:CD2	2.57	0.88
1:C:145:TRP:CD1	1:C:261:MET:SD	2.66	0.88
1:B:162:LEU:HD12	1:B:388:PHE:CE2	2.09	0.88
1:D:48:MET:HG3	1:D:49:GLN:HG2	1.54	0.88
1:F:132:LEU:C	1:F:136:LEU:CD2	2.42	0.88
1:F:474:LEU:HD12	1:F:477:CYS:HB2	1.55	0.88
1:F:635:HIS:ND1	1:F:636:LEU:HD23	1.87	0.88
1:E:744:LEU:HB2	1:E:764:PHE:HZ	1.40	0.87
1:B:498:VAL:CG2	1:B:519:LEU:HD11	2.05	0.87
1:E:123:TYR:HE1	1:E:127:PHE:HD2	1.21	0.87
1:F:507:PRO:HG2	1:F:510:MET:HG3	1.55	0.87
1:C:376:MET:CE	1:C:377:ILE:CG1	2.50	0.87
1:G:117:GLU:OE1	1:G:118:ARG:HG2	1.74	0.87
1:B:503:MET:HE1	1:B:506:LEU:CD1	2.03	0.87
1:C:346:LEU:HD11	1:C:372:PHE:CB	2.02	0.87
1:B:134:HIS:CE1	1:B:276:ILE:HD11	2.10	0.86
1:E:123:TYR:CE1	1:E:127:PHE:HD2	1.92	0.86
1:F:555:LYS:CA	1:F:581:MET:HE3	2.04	0.86
1:F:132:LEU:HD23	1:F:136:LEU:CD2	2.04	0.86
1:B:415:ARG:HH22	1:B:416:GLN:HA	1.40	0.86
1:F:778:LYS:HA	1:F:800:MET:CE	2.05	0.86
1:B:162:LEU:CD1	1:B:388:PHE:CE2	2.59	0.86
1:B:297:ILE:HA	1:B:300:MET:HE1	1.26	0.86
1:C:346:LEU:CD1	1:C:372:PHE:HA	2.04	0.85
1:E:743:VAL:CA	1:E:764:PHE:CE1	2.59	0.85
1:F:555:LYS:CB	1:F:581:MET:HE1	1.90	0.85
1:B:473:SER:HA	1:B:497:SER:HB2	1.57	0.85
1:C:452:GLU:HA	1:C:475:HIS:HB2	1.56	0.85
1:B:162:LEU:HG	1:B:388:PHE:CG	2.12	0.85
1:F:120:LEU:HD21	1:F:310:HIS:CD2	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:LEU:CD2	1:F:136:LEU:HD21	2.06	0.85
1:B:409:TRP:CZ2	1:B:433:LEU:CD2	2.60	0.84
1:E:300:MET:CE	1:F:57:LYS:HA	2.07	0.84
1:E:760:LYS:HE3	1:E:785:GLU:N	1.92	0.84
1:C:363:ILE:HA	1:C:392:LEU:CD2	2.07	0.84
1:E:757:LEU:O	1:E:757:LEU:HD23	1.77	0.84
1:E:799:GLN:CD	1:E:800:MET:HE1	1.97	0.84
1:C:328:SER:O	1:C:332:LEU:CD2	2.24	0.84
1:E:41:PHE:CE1	1:E:45:LEU:HD21	2.13	0.84
1:B:498:VAL:HG22	1:B:519:LEU:HD11	1.58	0.84
1:F:52:ILE:HG21	1:F:116:TYR:HB2	1.60	0.84
1:C:376:MET:HE3	1:C:377:ILE:CD1	2.02	0.84
1:F:138:PHE:CE2	1:F:330:TYR:CZ	2.66	0.84
1:C:418:LEU:HD21	1:C:428:LEU:HD13	1.56	0.84
1:F:782:LEU:CD1	1:F:784:VAL:HG13	2.08	0.84
1:B:145:TRP:HZ3	1:B:262:TYR:CE1	1.59	0.83
1:E:449:LEU:HD12	1:E:450:LYS:N	1.93	0.83
1:B:162:LEU:CA	1:B:388:PHE:HE1	1.54	0.83
1:F:261:MET:SD	1:F:262:TYR:N	2.51	0.83
1:F:473:SER:O	1:F:474:LEU:HD22	1.78	0.83
1:B:31:LEU:O	1:B:35:MET:CE	2.25	0.83
1:E:37:MET:HE3	1:E:38:ILE:N	1.94	0.83
1:F:265:GLN:O	1:F:268:LEU:CD1	2.26	0.83
1:C:346:LEU:CD1	1:C:372:PHE:CA	2.56	0.83
1:F:564:SER:HB2	1:F:588:MET:CE	2.06	0.82
1:B:503:MET:HE3	1:B:506:LEU:HB3	1.61	0.82
1:F:372:PHE:HB3	1:F:373:MET:CE	2.08	0.82
1:B:162:LEU:HG	1:B:388:PHE:CD1	2.14	0.82
1:F:114:MET:HE1	1:F:295:VAL:CG1	2.08	0.82
1:B:145:TRP:HZ3	1:B:262:TYR:CZ	1.93	0.82
1:B:323:TYR:CA	1:B:326:PHE:CD2	2.61	0.82
1:F:271:ILE:CD1	1:F:272:LYS:N	2.40	0.82
1:F:372:PHE:CG	1:F:373:MET:HE1	2.15	0.82
1:B:322:CYS:C	1:B:326:PHE:CE2	2.53	0.81
1:E:41:PHE:HD1	1:E:45:LEU:CD2	1.92	0.81
1:E:757:LEU:HD21	1:E:759:VAL:HG22	1.60	0.81
1:F:624:LEU:HD12	1:F:627:ILE:HG22	1.60	0.81
1:F:635:HIS:CE1	1:F:636:LEU:HD23	2.15	0.81
1:B:28:THR:C	1:B:330:TYR:OH	2.19	0.81
1:E:463:ILE:CD1	1:E:489:LEU:CD2	2.59	0.81
1:F:138:PHE:HE2	1:F:330:TYR:CD1	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:372:PHE:HB3	1:F:373:MET:HE2	1.62	0.81
1:B:33:VAL:O	1:B:37:MET:SD	2.39	0.81
1:B:161:ILE:C	1:B:388:PHE:HZ	1.84	0.81
1:B:323:TYR:N	1:B:326:PHE:CE2	2.48	0.81
1:B:322:CYS:HB2	1:B:326:PHE:HZ	1.45	0.81
1:E:41:PHE:O	1:E:45:LEU:CD2	2.28	0.81
1:B:134:HIS:CE1	1:B:276:ILE:HD12	2.14	0.81
1:B:171:THR:HA	1:B:390:LEU:HD23	1.61	0.81
1:E:376:MET:HE1	1:E:377:ILE:HD11	1.61	0.81
1:F:123:TYR:CB	1:F:283:LEU:HD13	2.10	0.81
1:G:117:GLU:OE1	1:G:118:ARG:N	2.13	0.81
1:E:130:LEU:HD21	1:E:279:TYR:OH	1.80	0.80
1:E:136:LEU:O	1:E:139:MET:HE3	1.80	0.80
1:E:475:HIS:HA	1:E:499:LYS:HB2	1.62	0.80
1:C:376:MET:C	1:C:376:MET:SD	2.60	0.80
1:C:447:GLN:HA	1:C:469:LEU:HA	1.62	0.80
1:E:41:PHE:O	1:E:45:LEU:HD22	1.81	0.80
1:E:570:MET:SD	1:E:571:CYS:N	2.55	0.80
1:B:453:ILE:O	1:B:453:ILE:HG22	1.80	0.80
1:B:460:PRO:HB2	1:B:462:THR:HG23	1.62	0.80
1:F:123:TYR:HB2	1:F:283:LEU:HD13	1.62	0.80
1:B:303:TYR:CA	1:C:96:MET:CE	2.50	0.80
1:C:475:HIS:HA	1:C:499:LYS:HB2	1.61	0.80
1:E:760:LYS:NZ	1:E:785:GLU:HA	1.96	0.80
1:F:486:LEU:HA	1:F:489:LEU:HD12	1.64	0.80
1:F:612:LEU:HG	1:F:635:HIS:CE1	2.17	0.80
1:F:481:ILE:HD12	1:F:486:LEU:HB2	1.64	0.79
1:E:376:MET:HE3	1:E:377:ILE:CD1	2.10	0.79
1:B:322:CYS:C	1:B:326:PHE:CZ	2.55	0.79
1:E:799:GLN:CB	1:E:800:MET:HE1	2.11	0.79
1:C:328:SER:O	1:C:332:LEU:HD22	1.82	0.79
1:C:445:GLU:H	1:C:445:GLU:CD	1.85	0.79
1:F:123:TYR:HB2	1:F:283:LEU:CD1	2.13	0.79
1:E:707:SER:HA	1:E:730:LYS:HD2	1.65	0.79
1:E:725:LEU:CD1	1:E:726:TYR:CD2	2.66	0.79
1:F:777:LEU:O	1:F:800:MET:CE	2.31	0.79
1:B:35:MET:N	1:B:35:MET:CE	2.46	0.78
1:C:363:ILE:HG12	1:C:392:LEU:HD22	1.64	0.78
1:F:239:LYS:O	1:F:243:GLU:OE1	2.01	0.78
1:C:41:PHE:HE1	1:C:319:LEU:HD12	1.48	0.78
1:B:43:CYS:SG	1:B:132:LEU:CD2	2.72	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:564:SER:HB2	1:F:588:MET:HE2	1.64	0.78
1:B:31:LEU:CB	1:B:330:TYR:CD1	2.66	0.78
1:F:458:MET:O	1:F:458:MET:HE3	1.84	0.78
1:B:32:SER:HA	1:B:35:MET:HG2	1.63	0.78
1:F:48:MET:CG	1:F:49:GLN:HG2	2.10	0.78
1:C:23:TRP:CZ2	1:C:336:TYR:HE1	1.95	0.77
1:E:743:VAL:C	1:E:764:PHE:CZ	2.56	0.77
1:F:652:ILE:HG13	1:F:672:ILE:HG12	1.66	0.77
1:C:458:MET:HA	1:C:458:MET:HE3	1.64	0.77
1:E:52:ILE:HD11	1:E:308:CYS:HB3	1.65	0.77
1:E:144:PHE:HD2	1:E:265:GLN:HE21	0.84	0.77
1:E:651:TYR:HA	1:E:672:ILE:HD12	1.65	0.77
1:C:238:ALA:HA	1:C:241:LEU:CG	2.14	0.77
1:B:165:CYS:CB	1:B:388:PHE:CE1	2.67	0.77
1:E:758:ASP:HA	1:E:783:VAL:HB	1.66	0.77
1:E:796:VAL:O	1:E:800:MET:CE	2.33	0.77
1:E:376:MET:CE	1:E:377:ILE:HG12	2.14	0.77
1:E:376:MET:SD	1:E:376:MET:C	2.63	0.77
1:F:557:PRO:HG2	1:F:560:VAL:HG13	1.67	0.77
1:D:52:ILE:HG21	1:D:116:TYR:HB2	1.64	0.77
1:E:725:LEU:HD11	1:E:726:TYR:CZ	2.18	0.77
1:F:452:GLU:OE2	1:F:475:HIS:CE1	2.38	0.77
1:F:779:ARG:HH22	1:F:782:LEU:HG	1.49	0.77
1:B:35:MET:HE3	1:B:35:MET:H	1.48	0.77
1:F:778:LYS:CA	1:F:800:MET:CE	2.62	0.77
1:B:161:ILE:C	1:B:388:PHE:CZ	2.59	0.76
1:B:162:LEU:HG	1:B:388:PHE:CD2	2.19	0.76
1:C:474:LEU:HD12	1:C:498:VAL:HG22	1.67	0.76
1:E:130:LEU:CD2	1:E:279:TYR:OH	2.33	0.76
1:D:50:ASP:O	1:D:50:ASP:OD2	2.03	0.76
1:E:171:THR:HG22	1:E:390:LEU:HD22	1.68	0.76
1:E:311:THR:OG1	1:E:312:MET:SD	2.44	0.76
1:F:36:LEU:O	1:F:40:VAL:HG12	1.85	0.76
1:B:171:THR:HA	1:B:390:LEU:CD2	2.14	0.76
1:F:114:MET:HE2	1:F:295:VAL:CG1	2.12	0.76
1:C:376:MET:HE1	1:C:377:ILE:HD11	1.65	0.76
1:C:468:ASN:O	1:C:468:ASN:OD1	2.02	0.76
1:F:458:MET:HE3	1:F:459:ILE:C	2.05	0.76
1:F:138:PHE:HE2	1:F:330:TYR:CZ	2.02	0.76
1:B:31:LEU:O	1:B:35:MET:HG2	1.84	0.76
1:F:672:ILE:CG2	1:F:695:ILE:HD11	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HD12	1:B:300:MET:HE3	1.66	0.76
1:E:538:LEU:H	1:E:559:ALA:HB1	1.50	0.76
1:F:510:MET:SD	1:F:511:TYR:CD1	2.79	0.76
1:C:23:TRP:HZ2	1:C:336:TYR:CZ	2.03	0.76
1:F:452:GLU:HG2	1:F:475:HIS:HB2	1.68	0.76
1:B:145:TRP:CD2	1:B:262:TYR:CD1	2.73	0.76
1:B:119:ALA:HB2	1:B:293:CYS:HB3	1.68	0.75
1:F:253:GLU:HG2	1:F:367:LYS:HB2	1.67	0.75
1:F:510:MET:CE	1:F:511:TYR:CE1	2.69	0.75
1:C:560:VAL:HA	1:C:563:VAL:HB	1.68	0.75
1:E:122:TRP:HA	1:E:125:LYS:HE2	1.67	0.75
1:F:672:ILE:HG23	1:F:695:ILE:CD1	2.15	0.75
1:E:572:ILE:HG23	1:E:596:LEU:HD23	1.67	0.75
1:B:31:LEU:CD1	1:B:330:TYR:CD1	2.70	0.75
1:E:170:TRP:CZ3	1:E:390:LEU:HD21	2.22	0.75
1:B:27:PHE:CZ	1:B:31:LEU:HD11	2.22	0.75
1:C:479:VAL:N	1:C:480:LYS:HZ3	1.83	0.75
1:E:572:ILE:HG23	1:E:596:LEU:CD2	2.17	0.75
1:E:743:VAL:CA	1:E:764:PHE:HE1	1.98	0.75
1:F:510:MET:HE3	1:F:511:TYR:CE1	2.22	0.75
1:B:411:PRO:HD3	1:B:439:THR:HG21	1.68	0.75
1:B:31:LEU:HB3	1:B:330:TYR:CD1	2.23	0.74
1:E:123:TYR:HE2	1:E:283:LEU:O	1.64	0.74
1:E:526:SER:CB	1:E:531:ARG:HE	2.00	0.74
1:E:721:LEU:HB3	1:E:725:LEU:CD2	2.18	0.74
1:C:478:SER:HB3	1:C:480:LYS:NZ	2.02	0.74
1:E:437:PRO:HB2	1:E:440:VAL:HG23	1.68	0.74
1:B:475:HIS:HA	1:B:499:LYS:HB3	1.67	0.74
1:C:383:LEU:HD12	1:C:383:LEU:O	1.87	0.74
1:C:418:LEU:HA	1:C:428:LEU:HD12	1.69	0.74
1:C:531:ARG:HH11	1:C:554:SER:CB	2.00	0.74
1:E:41:PHE:CD1	1:E:45:LEU:HD23	2.21	0.74
1:F:769:PRO:HG3	1:F:793:PRO:HG2	1.70	0.74
1:F:555:LYS:CD	1:F:581:MET:HE1	2.18	0.74
1:B:46:GLN:HA	1:B:312:MET:HE1	1.70	0.73
1:C:525:LEU:HD23	1:C:553:VAL:HG21	1.70	0.73
1:F:520:TYR:HA	1:F:548:SER:HB3	1.70	0.73
1:C:363:ILE:HA	1:C:392:LEU:HD21	1.69	0.73
1:C:489:LEU:C	1:C:493:LEU:CD1	2.57	0.73
1:E:463:ILE:HD13	1:E:489:LEU:HD21	1.69	0.73
1:C:390:LEU:HD23	1:C:391:PHE:H	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:CYS:SG	1:E:132:LEU:HD21	2.28	0.73
1:F:421:ASN:OD1	1:F:425:ARG:N	2.22	0.73
1:B:162:LEU:CB	1:B:388:PHE:CE1	2.72	0.73
1:B:261:MET:CE	1:B:264:ARG:HD2	2.19	0.73
1:B:449:LEU:HB3	1:B:472:LEU:CD1	2.18	0.73
1:B:300:MET:SD	1:B:300:MET:N	2.61	0.73
1:E:153:SER:OG	1:E:154:LYS:NZ	2.22	0.73
1:E:458:MET:SD	1:E:481:ILE:CA	2.77	0.73
1:E:686:ARG:HA	1:E:708:LEU:HA	1.70	0.73
1:G:52:ILE:C	1:G:53:ILE:HD13	2.09	0.73
1:E:490:LYS:HG2	1:E:513:LEU:HD23	1.70	0.73
1:F:240:ALA:C	1:F:243:GLU:OE2	2.26	0.73
1:C:489:LEU:O	1:C:493:LEU:HD13	1.87	0.72
1:C:531:ARG:CD	1:C:554:SER:HB3	2.14	0.72
1:F:268:LEU:HD12	1:F:269:LYS:H	1.54	0.72
1:E:104:ASP:OD1	1:E:104:ASP:C	2.28	0.72
1:C:33:VAL:HA	1:C:36:LEU:CD2	2.19	0.72
1:F:782:LEU:HD11	1:F:784:VAL:HG13	1.71	0.72
1:B:415:ARG:HH21	1:B:416:GLN:N	1.86	0.72
1:F:766:ILE:HG13	1:F:791:THR:HG21	1.70	0.72
1:C:262:TYR:HE2	1:C:341:LEU:HD11	1.53	0.72
1:C:418:LEU:HA	1:C:428:LEU:CD1	2.20	0.72
1:E:242:PHE:HE2	1:E:400:LEU:HD23	1.55	0.72
1:E:799:GLN:CB	1:E:800:MET:CE	2.68	0.72
1:F:119:ALA:HB2	1:F:293:CYS:HB3	1.70	0.72
1:F:243:GLU:CD	1:F:243:GLU:H	1.92	0.72
1:F:472:LEU:O	1:F:496:LEU:HD12	1.89	0.72
1:C:262:TYR:CE2	1:C:341:LEU:HD11	2.25	0.72
1:B:409:TRP:CZ2	1:B:433:LEU:HD23	2.23	0.72
1:B:441:PHE:CG	1:B:462:THR:OG1	2.42	0.71
1:E:800:MET:HE2	1:E:800:MET:N	2.05	0.71
1:G:57:LYS:CD	1:G:305:ASN:OD1	2.30	0.71
1:F:510:MET:CE	1:F:511:TYR:CD1	2.72	0.71
1:F:429:PRO:HA	1:F:450:LYS:HE3	1.72	0.71
1:B:173:ARG:HH11	1:B:403:LEU:HD21	1.55	0.71
1:B:303:TYR:HA	1:C:96:MET:HE1	1.67	0.71
1:C:436:LEU:HB2	1:C:457:VAL:HG13	1.73	0.71
1:C:480:LYS:HD3	1:C:480:LYS:N	2.04	0.71
1:F:785:GLU:HB2	1:F:788:LEU:HD13	1.72	0.71
1:G:113:GLN:OE1	1:G:114:MET:HE2	1.91	0.71
1:G:312:MET:HB3	1:G:316:PHE:HE1	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:ILE:HG23	1:E:392:LEU:HD23	1.73	0.71
1:F:428:LEU:HD12	1:F:429:PRO:N	2.06	0.71
1:F:775:ARG:NH1	1:F:775:ARG:O	2.21	0.71
1:A:40:VAL:O	1:A:44:THR:OG1	2.09	0.70
1:B:162:LEU:N	1:B:388:PHE:HZ	1.82	0.70
1:C:165:CYS:O	1:C:387:ARG:NH1	2.24	0.70
1:C:496:LEU:CB	1:C:516:LEU:HD21	2.21	0.70
1:E:651:TYR:HA	1:E:672:ILE:CD1	2.21	0.70
1:F:441:PHE:HA	1:F:466:LEU:HD21	1.72	0.70
1:F:555:LYS:CA	1:F:581:MET:CE	2.64	0.70
1:E:725:LEU:CD1	1:E:726:TYR:CG	2.74	0.70
1:B:297:ILE:O	1:B:300:MET:CE	2.27	0.70
1:B:449:LEU:HD12	1:B:450:LYS:N	2.06	0.70
1:C:519:LEU:HD22	1:C:547:LEU:HD12	1.71	0.70
1:G:41:PHE:O	1:G:44:THR:CG2	2.39	0.70
1:B:28:THR:O	1:B:330:TYR:CZ	2.44	0.70
1:B:297:ILE:HD12	1:B:300:MET:CE	2.21	0.70
1:B:415:ARG:HH21	1:B:416:GLN:HA	0.79	0.70
1:C:129:TYR:O	1:C:133:ILE:HG23	1.91	0.70
1:E:572:ILE:CG2	1:E:596:LEU:CD2	2.70	0.70
1:G:119:ALA:HB2	1:G:293:CYS:HB3	1.74	0.70
1:B:323:TYR:HD2	1:B:324:LEU:HD22	1.56	0.70
1:C:478:SER:CB	1:C:480:LYS:NZ	2.54	0.70
1:C:482:HIS:CE1	1:C:484:ALA:N	2.52	0.70
1:B:415:ARG:HA	1:B:418:LEU:HD12	1.73	0.69
1:E:144:PHE:CZ	1:E:261:MET:CE	2.75	0.69
1:C:285:SER:O	1:C:288:GLN:NE2	2.25	0.69
1:C:376:MET:SD	1:C:377:ILE:HD13	2.31	0.69
1:F:458:MET:CE	1:F:458:MET:C	2.61	0.69
1:G:117:GLU:OE1	1:G:118:ARG:CG	2.38	0.69
1:B:376:MET:CE	1:B:377:ILE:HD13	2.23	0.69
1:C:119:ALA:HB2	1:C:293:CYS:HB3	1.75	0.69
1:F:268:LEU:O	1:F:271:ILE:CD1	2.41	0.69
1:F:555:LYS:HB2	1:F:581:MET:HE3	0.70	0.69
1:B:43:CYS:SG	1:B:129:TYR:HD1	2.16	0.69
1:B:449:LEU:HG	1:B:451:LEU:HD11	1.73	0.69
1:E:650:THR:O	1:E:672:ILE:HA	1.91	0.69
1:F:121:HIS:CE1	1:F:283:LEU:HD21	2.27	0.69
1:F:574:ASN:ND2	1:F:577:THR:O	2.25	0.69
1:G:104:ASP:C	1:G:104:ASP:OD2	2.29	0.69
1:E:37:MET:HE1	1:E:38:ILE:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:ASP:O	1:E:373:MET:HG2	1.92	0.69
1:C:52:ILE:HG21	1:C:116:TYR:HB2	1.73	0.69
1:F:271:ILE:O	1:F:275:ILE:HG22	1.93	0.69
1:B:43:CYS:SG	1:B:129:TYR:CD1	2.84	0.69
1:E:618:ASP:HA	1:E:643:LYS:HB2	1.73	0.69
1:C:406:ASN:HD21	1:C:438:ASP:H	1.39	0.69
1:C:478:SER:CB	1:C:480:LYS:HZ1	2.05	0.69
1:D:119:ALA:HB2	1:D:293:CYS:HB3	1.74	0.69
1:B:162:LEU:HG	1:B:388:PHE:CE1	2.27	0.68
1:C:363:ILE:HA	1:C:392:LEU:HD22	1.73	0.68
1:C:445:GLU:HA	1:C:468:ASN:ND2	2.07	0.68
1:C:539:ARG:O	1:C:539:ARG:NH1	2.21	0.68
1:E:41:PHE:CE1	1:E:45:LEU:CD2	2.74	0.68
1:F:684:LYS:O	1:F:686:ARG:NH1	2.25	0.68
1:F:268:LEU:HD12	1:F:269:LYS:N	2.09	0.68
1:C:457:VAL:HB	1:C:479:VAL:HG22	1.74	0.68
1:F:458:MET:SD	1:F:459:ILE:O	2.51	0.68
1:F:747:LYS:O	1:F:750:ASN:HB2	1.94	0.68
1:E:36:LEU:O	1:E:40:VAL:HG12	1.94	0.68
1:E:155:ILE:HD11	1:E:258:LEU:HD11	1.75	0.68
1:B:323:TYR:HA	1:B:326:PHE:HD2	1.52	0.68
1:E:574:ASN:ND2	1:E:577:THR:O	2.26	0.68
1:E:641:VAL:HG13	1:E:664:ARG:HB2	1.74	0.68
1:E:800:MET:HE2	1:E:800:MET:H	1.59	0.68
1:E:114:MET:HG2	1:E:297:ILE:HD11	1.75	0.68
1:E:760:LYS:HZ1	1:E:785:GLU:HA	1.57	0.68
1:G:113:GLN:OE1	1:G:114:MET:HE3	1.92	0.68
1:C:253:GLU:HG2	1:C:367:LYS:HB2	1.75	0.68
1:E:570:MET:HA	1:E:570:MET:HE2	1.76	0.68
1:F:635:HIS:HE1	1:F:636:LEU:HD21	1.53	0.68
1:C:156:GLU:HA	1:C:159:ILE:HD11	1.76	0.67
1:C:523:GLY:O	1:C:551:SER:OG	2.11	0.67
1:G:46:GLN:NE2	1:G:125:LYS:O	2.27	0.67
1:C:482:HIS:ND1	1:C:483:SER:N	2.42	0.67
1:E:170:TRP:HZ3	1:E:390:LEU:HD21	1.57	0.67
1:E:775:ARG:HH21	1:E:778:LYS:HG2	1.59	0.67
1:E:760:LYS:HE2	1:E:785:GLU:OE2	1.95	0.67
1:B:33:VAL:O	1:B:37:MET:HG2	1.95	0.67
1:F:138:PHE:CD2	1:F:330:TYR:CZ	2.82	0.67
1:G:297:ILE:HD13	1:G:306:PHE:HE1	1.60	0.67
1:B:134:HIS:ND1	1:B:276:ILE:HD12	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD12	1:B:330:TYR:CD1	2.29	0.67
1:D:44:THR:C	1:D:48:MET:HE2	2.15	0.67
1:E:650:THR:O	1:E:672:ILE:HD12	1.95	0.67
1:B:127:PHE:HA	1:B:130:LEU:HD12	1.76	0.67
1:B:503:MET:CE	1:B:506:LEU:HB3	2.25	0.67
1:C:346:LEU:HD13	1:C:372:PHE:CB	2.17	0.67
1:E:744:LEU:CB	1:E:764:PHE:HZ	1.88	0.67
1:F:452:GLU:HG3	1:F:475:HIS:CB	2.24	0.67
1:F:635:HIS:ND1	1:F:636:LEU:HD21	2.00	0.67
1:B:162:LEU:CD1	1:B:388:PHE:CZ	2.77	0.67
1:C:541:LEU:HD22	1:C:544:LEU:HB2	1.77	0.67
1:F:261:MET:SD	1:F:261:MET:C	2.73	0.67
1:F:621:GLU:HA	1:F:646:HIS:HB3	1.76	0.67
1:F:555:LYS:CD	1:F:581:MET:CE	2.73	0.66
1:C:376:MET:HE3	1:C:377:ILE:N	2.10	0.66
1:E:757:LEU:HD22	1:E:782:LEU:HD12	1.76	0.66
1:F:166:PHE:O	1:F:387:ARG:NH1	2.29	0.66
1:A:126:TYR:HD1	1:A:129:TYR:CE2	2.14	0.66
1:D:45:LEU:HD23	1:D:48:MET:CE	2.25	0.66
1:F:609:PHE:HA	1:F:636:LEU:HD11	1.77	0.66
1:B:367:LYS:HE3	1:B:368:ASN:H	1.59	0.66
1:E:503:MET:HG2	1:E:506:LEU:HD23	1.78	0.66
1:F:735:LYS:HA	1:F:758:ASP:HB3	1.77	0.66
1:B:243:GLU:HA	1:B:246:LYS:HG2	1.78	0.66
1:C:458:MET:HA	1:C:458:MET:CE	2.25	0.66
1:A:126:TYR:CA	1:A:129:TYR:CD2	2.73	0.66
1:B:166:PHE:HB2	1:B:387:ARG:HD3	1.77	0.66
1:B:453:ILE:HD13	1:B:455:LYS:NZ	2.11	0.66
1:C:458:MET:HE1	1:C:480:LYS:HB2	1.76	0.66
1:B:46:GLN:NE2	1:B:129:TYR:OH	2.29	0.66
1:B:128:PRO:O	1:B:132:LEU:CD2	2.41	0.66
1:B:376:MET:HE1	1:B:377:ILE:HD13	1.77	0.66
1:E:481:ILE:HD12	1:E:486:LEU:HB2	1.78	0.66
1:E:667:PHE:HB3	1:E:693:ASN:HD21	1.61	0.66
1:F:123:TYR:CE2	1:F:127:PHE:HD2	2.13	0.66
1:B:322:CYS:CB	1:B:326:PHE:CZ	2.79	0.66
1:E:37:MET:SD	1:E:37:MET:O	2.54	0.66
1:F:458:MET:HE3	1:F:458:MET:C	2.17	0.66
1:D:59:VAL:HG21	1:D:99:LEU:HD21	1.78	0.66
1:E:55:LEU:CD1	1:E:56:PRO:HD2	2.26	0.66
1:E:37:MET:HE3	1:E:37:MET:C	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:GLY:HA2	1:F:166:PHE:CE2	2.31	0.65
1:F:444:THR:HG22	1:F:466:LEU:HD23	1.77	0.65
1:F:458:MET:O	1:F:458:MET:CE	2.43	0.65
1:B:37:MET:SD	1:B:37:MET:N	2.69	0.65
1:C:33:VAL:O	1:C:36:LEU:HG	1.95	0.65
1:E:130:LEU:CG	1:E:279:TYR:OH	2.44	0.65
1:F:517:GLU:O	1:F:546:ILE:N	2.29	0.65
1:F:782:LEU:HD11	1:F:784:VAL:CG1	2.27	0.65
1:C:421:ASN:OD1	1:C:425:ARG:N	2.30	0.65
1:G:101:THR:OG1	1:G:108:TYR:OH	2.15	0.65
1:E:572:ILE:CG2	1:E:596:LEU:HD23	2.27	0.65
1:G:57:LYS:HG3	1:G:306:PHE:CA	2.25	0.65
1:E:729:LYS:HA	1:E:751:LEU:HD22	1.79	0.65
1:F:296:ASP:OD2	1:F:296:ASP:C	2.32	0.65
1:E:725:LEU:HD12	1:E:726:TYR:CG	2.31	0.65
1:A:119:ALA:HB2	1:A:293:CYS:HB3	1.78	0.65
1:B:239:LYS:HE3	1:B:401:LYS:HG2	1.78	0.65
1:D:45:LEU:HD23	1:D:48:MET:HE3	1.79	0.65
1:F:782:LEU:HD12	1:F:784:VAL:HG13	1.78	0.65
1:C:258:LEU:HD12	1:C:261:MET:HE1	1.78	0.65
1:C:474:LEU:HG	1:C:497:SER:O	1.97	0.65
1:E:604:ILE:HD12	1:E:629:GLU:HB2	1.79	0.65
1:B:134:HIS:ND1	1:B:276:ILE:CD1	2.59	0.64
1:B:145:TRP:HH2	1:B:262:TYR:CD2	2.11	0.64
1:B:162:LEU:HG	1:B:388:PHE:CE2	2.32	0.64
1:F:372:PHE:CG	1:F:373:MET:CE	2.80	0.64
1:F:535:LEU:HD11	1:F:538:LEU:HD21	1.79	0.64
1:B:46:GLN:CD	1:B:129:TYR:OH	2.36	0.64
1:E:144:PHE:CE2	1:E:261:MET:HE2	2.31	0.64
1:E:325:CYS:O	1:E:328:SER:OG	2.14	0.64
1:F:564:SER:HG	1:F:587:LYS:HZ2	1.45	0.64
1:C:499:LYS:HG2	1:C:522:VAL:HB	1.77	0.64
1:G:57:LYS:HG3	1:G:306:PHE:HA	1.80	0.64
1:D:44:THR:O	1:D:48:MET:HE2	1.97	0.64
1:E:123:TYR:HE1	1:E:127:PHE:CD2	2.11	0.64
1:B:27:PHE:CZ	1:B:333:THR:CG2	2.72	0.64
1:B:145:TRP:CD2	1:B:262:TYR:HD1	2.13	0.64
1:C:332:LEU:HD13	1:C:335:LEU:HD12	1.78	0.64
1:E:37:MET:SD	1:E:37:MET:C	2.76	0.64
1:E:744:LEU:CD1	1:E:764:PHE:HE2	2.11	0.64
1:F:555:LYS:CG	1:F:581:MET:CE	2.74	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:HIS:CD2	1:G:123:TYR:HB3	2.32	0.64
1:E:300:MET:HE3	1:F:57:LYS:CA	2.27	0.64
1:F:372:PHE:CB	1:F:373:MET:CE	2.76	0.64
1:F:758:ASP:HA	1:F:783:VAL:HB	1.78	0.64
1:C:458:MET:HE3	1:C:480:LYS:O	1.98	0.64
1:C:544:LEU:HB3	1:C:566:HIS:HD2	1.61	0.64
1:E:101:THR:OG1	1:E:108:TYR:OH	2.16	0.64
1:E:744:LEU:N	1:E:764:PHE:CE1	2.58	0.64
1:B:162:LEU:CG	1:B:388:PHE:CZ	2.81	0.63
1:D:311:THR:OG1	1:D:312:MET:SD	2.56	0.63
1:E:238:ALA:HA	1:E:241:LEU:HD13	1.80	0.63
1:E:499:LYS:HA	1:E:522:VAL:HB	1.79	0.63
1:C:439:THR:O	1:C:442:GLU:HG3	1.99	0.63
1:C:494:LYS:C	1:C:516:LEU:HD12	2.18	0.63
1:E:240:ALA:O	1:E:244:LYS:NZ	2.30	0.63
1:F:544:LEU:HD23	1:F:563:VAL:HG21	1.81	0.63
1:B:27:PHE:CD2	1:B:333:THR:CG2	2.71	0.63
1:B:498:VAL:HG22	1:B:519:LEU:CD1	2.26	0.63
1:C:347:ARG:O	1:C:368:ASN:ND2	2.29	0.63
1:C:474:LEU:CD1	1:C:498:VAL:HG22	2.28	0.63
1:C:474:LEU:O	1:C:499:LYS:N	2.30	0.63
1:E:139:MET:C	1:E:139:MET:SD	2.76	0.63
1:E:144:PHE:CZ	1:E:261:MET:HE3	2.33	0.63
1:F:458:MET:SD	1:F:481:ILE:C	2.76	0.63
1:F:475:HIS:HA	1:F:499:LYS:HB2	1.79	0.63
1:F:599:CYS:N	1:F:622:ASN:OD1	2.31	0.63
1:F:490:LYS:HA	1:F:513:LEU:HD13	1.80	0.63
1:B:490:LYS:HG2	1:B:513:LEU:HA	1.80	0.63
1:C:390:LEU:HD23	1:C:391:PHE:N	2.13	0.63
1:E:363:ILE:HD11	1:E:393:SER:HB2	1.81	0.63
1:E:463:ILE:HD12	1:E:489:LEU:CD2	2.27	0.63
1:F:166:PHE:HA	1:F:387:ARG:HG2	1.81	0.63
1:F:264:ARG:O	1:F:268:LEU:HG	1.99	0.63
1:F:510:MET:HA	1:F:513:LEU:HD23	1.81	0.63
1:C:330:TYR:O	1:C:333:THR:OG1	2.16	0.63
1:E:139:MET:SD	1:E:140:LEU:N	2.72	0.63
1:B:129:TYR:HA	1:B:132:LEU:HD23	1.81	0.63
1:F:632:SER:O	1:F:635:HIS:HB3	1.99	0.63
1:E:725:LEU:HD12	1:E:725:LEU:C	2.18	0.63
1:F:548:SER:HA	1:F:571:CYS:HB2	1.81	0.63
1:F:782:LEU:HD11	1:F:784:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:663:GLU:HA	1:F:685:ILE:HA	1.80	0.63
1:F:546:ILE:HG12	1:F:569:LYS:HB3	1.81	0.62
1:F:693:ASN:N	1:F:716:ASN:OD1	2.28	0.62
1:B:133:ILE:HG23	1:B:134:HIS:HD2	1.63	0.62
1:E:37:MET:C	1:E:37:MET:CE	2.67	0.62
1:E:458:MET:HG2	1:E:480:LYS:CB	2.30	0.62
1:C:496:LEU:HB2	1:C:516:LEU:HD21	1.81	0.62
1:E:41:PHE:O	1:E:45:LEU:HD23	1.99	0.62
1:E:300:MET:HE3	1:F:57:LYS:HD2	1.80	0.62
1:E:547:LEU:HB3	1:E:570:MET:HE2	1.81	0.62
1:F:556:ILE:HG22	1:F:581:MET:SD	2.39	0.62
1:F:709:GLN:HG2	1:F:730:LYS:HB3	1.81	0.62
1:C:238:ALA:CA	1:C:241:LEU:HG	2.27	0.62
1:C:450:LYS:HA	1:C:473:SER:HB3	1.80	0.62
1:C:478:SER:HB3	1:C:480:LYS:HZ2	1.63	0.62
1:E:366:VAL:HB	1:E:370:PHE:HB3	1.81	0.62
1:F:458:MET:CE	1:F:459:ILE:C	2.68	0.62
1:F:709:GLN:HA	1:F:731:LEU:HA	1.81	0.62
1:F:48:MET:HE2	1:F:48:MET:HA	1.81	0.62
1:B:31:LEU:HB3	1:B:330:TYR:CE1	2.33	0.62
1:E:719:GLU:HG2	1:E:740:SER:HB3	1.81	0.62
1:E:735:LYS:HA	1:E:758:ASP:HB3	1.81	0.62
1:E:799:GLN:HB3	1:E:800:MET:CE	2.29	0.62
1:F:569:LYS:HD3	1:F:593:GLU:HB2	1.81	0.62
1:B:162:LEU:HA	1:B:388:PHE:HE1	0.79	0.62
1:C:363:ILE:CG1	1:C:392:LEU:HD22	2.30	0.62
1:C:478:SER:C	1:C:480:LYS:CE	2.68	0.62
1:C:519:LEU:HD21	1:C:521:LEU:HD13	1.81	0.62
1:D:296:ASP:C	1:D:296:ASP:OD1	2.37	0.62
1:E:721:LEU:HD11	1:E:741:LEU:HD21	1.81	0.62
1:C:259:TYR:OH	1:C:347:ARG:NH2	2.33	0.62
1:C:468:ASN:O	1:C:468:ASN:CG	2.38	0.62
1:F:347:ARG:O	1:F:368:ASN:ND2	2.30	0.62
1:E:421:ASN:OD1	1:E:425:ARG:N	2.33	0.62
1:F:537:SER:OG	1:F:562:ASP:OD2	2.18	0.62
1:F:757:LEU:HG	1:F:759:VAL:HG22	1.81	0.62
1:B:419:GLN:HE21	1:B:429:PRO:HG2	1.64	0.61
1:C:431:ILE:HA	1:C:452:GLU:HB2	1.81	0.61
1:E:132:LEU:HD22	1:E:132:LEU:H	1.65	0.61
1:F:268:LEU:O	1:F:271:ILE:HD12	2.00	0.61
1:F:452:GLU:CG	1:F:475:HIS:CB	2.76	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:517:GLU:HA	1:F:544:LEU:HA	1.80	0.61
1:C:449:LEU:O	1:C:473:SER:N	2.30	0.61
1:E:144:PHE:CZ	1:E:261:MET:HE2	2.35	0.61
1:E:243:GLU:HA	1:E:246:LYS:HG2	1.80	0.61
1:A:103:LEU:HB2	1:A:108:TYR:CE2	2.35	0.61
1:C:363:ILE:HG23	1:C:392:LEU:HD22	1.82	0.61
1:G:312:MET:HB3	1:G:316:PHE:CE1	2.36	0.61
1:B:52:ILE:HG21	1:B:116:TYR:HB2	1.82	0.61
1:C:328:SER:O	1:C:332:LEU:HD23	1.99	0.61
1:C:547:LEU:HD22	1:C:563:VAL:HG11	1.81	0.61
1:B:162:LEU:HG	1:B:388:PHE:CZ	2.36	0.61
1:B:354:VAL:HA	1:B:357:GLU:HG3	1.83	0.61
1:C:470:GLN:OE1	1:C:494:LYS:N	2.33	0.61
1:E:669:HIS:H	1:E:692:TYR:HB2	1.64	0.61
1:F:330:TYR:O	1:F:333:THR:OG1	2.18	0.61
1:B:27:PHE:CE2	1:B:333:THR:HG23	2.20	0.61
1:B:127:PHE:HA	1:B:130:LEU:CD1	2.31	0.61
1:C:153:SER:OG	1:C:154:LYS:NZ	2.33	0.61
1:E:157:HIS:CE1	1:E:248:PHE:HD1	2.19	0.61
1:E:760:LYS:HE3	1:E:784:VAL:C	2.20	0.61
1:F:686:ARG:HA	1:F:708:LEU:HA	1.83	0.61
1:E:743:VAL:N	1:E:764:PHE:HE1	1.99	0.61
1:F:460:PRO:O	1:F:463:ILE:HG22	2.01	0.61
1:C:482:HIS:H	1:C:485:ALA:HB3	1.65	0.61
1:C:531:ARG:HH11	1:C:554:SER:HB2	1.64	0.61
1:F:137:VAL:HG12	1:F:272:LYS:HZ2	1.66	0.61
1:F:657:LYS:HB2	1:F:681:LEU:HB2	1.82	0.60
1:F:134:HIS:CE1	1:F:276:ILE:HD11	2.36	0.60
1:A:290:THR:HA	1:A:309:ASN:HB3	1.82	0.60
1:F:557:PRO:HG2	1:F:560:VAL:CG1	2.30	0.60
1:B:323:TYR:CD2	1:B:324:LEU:HD22	2.36	0.60
1:B:363:ILE:HG23	1:B:392:LEU:HD22	1.82	0.60
1:G:129:TYR:O	1:G:133:ILE:CG1	2.37	0.60
1:B:503:MET:HE3	1:B:503:MET:HA	1.82	0.60
1:F:381:ASP:HB3	1:F:384:TYR:HD2	1.67	0.60
1:G:41:PHE:O	1:G:44:THR:HG22	2.00	0.60
1:D:103:LEU:HB2	1:D:108:TYR:CZ	2.37	0.60
1:F:617:LEU:HB2	1:F:639:LEU:HD11	1.81	0.60
1:F:766:ILE:HG23	1:F:791:THR:HB	1.84	0.60
1:B:46:GLN:HA	1:B:312:MET:CE	2.32	0.60
1:C:363:ILE:HG12	1:C:392:LEU:CD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:PRO:HA	1:E:450:LYS:HG3	1.84	0.60
1:E:796:VAL:O	1:E:800:MET:HG2	2.02	0.60
1:B:503:MET:HE3	1:B:506:LEU:CB	2.31	0.60
1:F:738:LYS:HG3	1:F:761:GLY:HA3	1.84	0.60
1:E:373:MET:N	1:E:373:MET:SD	2.75	0.60
1:F:555:LYS:HD3	1:F:581:MET:CE	2.32	0.60
1:C:531:ARG:HH11	1:C:554:SER:HB3	1.67	0.59
1:E:239:LYS:HA	1:E:242:PHE:HD2	1.66	0.59
1:B:323:TYR:HA	1:B:326:PHE:HE2	1.62	0.59
1:B:507:PRO:HG2	1:B:510:MET:HG2	1.84	0.59
1:B:503:MET:CE	1:B:503:MET:HA	2.32	0.59
1:E:128:PRO:O	1:E:132:LEU:HD23	1.95	0.59
1:E:144:PHE:CE1	1:E:261:MET:HE3	2.37	0.59
1:E:623:ASN:HA	1:E:647:ASN:HA	1.85	0.59
1:F:652:ILE:HD12	1:F:676:PRO:HD2	1.83	0.59
1:C:541:LEU:CD2	1:C:544:LEU:HB2	2.33	0.59
1:E:430:LEU:HB2	1:E:451:LEU:HA	1.84	0.59
1:E:518:GLU:HG2	1:E:546:ILE:HB	1.83	0.59
1:E:123:TYR:CD2	1:E:283:LEU:O	2.54	0.59
1:F:777:LEU:C	1:F:800:MET:CE	2.71	0.59
1:B:162:LEU:C	1:B:388:PHE:HE1	2.06	0.59
1:B:249:ARG:HA	1:B:370:PHE:CZ	2.37	0.59
1:C:276:ILE:HG21	1:C:327:VAL:HG11	1.85	0.59
1:C:354:VAL:O	1:C:358:THR:OG1	2.20	0.59
1:C:418:LEU:HD21	1:C:446:LEU:HD13	1.84	0.59
1:F:50:ASP:C	1:F:50:ASP:OD2	2.41	0.59
1:F:510:MET:HE1	1:F:511:TYR:CD1	2.38	0.59
1:G:128:PRO:HG3	1:G:316:PHE:HE2	1.68	0.59
1:C:168:SER:O	1:C:387:ARG:NH2	2.28	0.59
1:E:170:TRP:HH2	1:E:396:SER:HB2	1.68	0.59
1:B:31:LEU:HB3	1:B:330:TYR:HD1	1.68	0.59
1:E:746:PRO:HB3	1:E:770:GLU:HG3	1.84	0.59
1:E:800:MET:CE	1:E:800:MET:N	2.65	0.59
1:F:428:LEU:HD12	1:F:428:LEU:C	2.22	0.59
1:F:782:LEU:HD11	1:F:784:VAL:CG2	2.33	0.59
1:E:41:PHE:HD1	1:E:45:LEU:HD21	1.51	0.59
1:E:449:LEU:HD12	1:E:450:LYS:H	1.66	0.59
1:E:455:LYS:NZ	1:E:476:GLN:O	2.28	0.59
1:F:538:LEU:HG	1:F:559:ALA:HB1	1.84	0.59
1:F:766:ILE:HG13	1:F:791:THR:CG2	2.31	0.59
1:B:134:HIS:HE1	1:B:276:ILE:CD1	2.08	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:722:PRO:O	1:E:725:LEU:HG	2.03	0.58
1:E:764:PHE:HD2	1:E:767:LEU:CD2	2.16	0.58
1:C:531:ARG:N	1:C:554:SER:HG	2.00	0.58
1:C:537:SER:OG	1:C:562:ASP:OD2	2.20	0.58
1:F:145:TRP:HD1	1:F:261:MET:CE	2.16	0.58
1:F:723:ASP:HB3	1:F:747:LYS:HD2	1.84	0.58
1:B:122:TRP:HA	1:B:125:LYS:HE2	1.85	0.58
1:B:322:CYS:O	1:B:326:PHE:CE2	2.57	0.58
1:E:591:LEU:HD23	1:E:611:LEU:HD13	1.85	0.58
1:E:663:GLU:HA	1:E:685:ILE:HA	1.84	0.58
1:C:45:LEU:O	1:C:312:MET:HE1	2.03	0.58
1:E:151:SER:O	1:E:155:ILE:CG1	2.48	0.58
1:E:405:LEU:HG	1:E:409:TRP:HD1	1.68	0.58
1:B:150:GLY:O	1:B:154:LYS:NZ	2.35	0.58
1:E:369:ASP:O	1:E:373:MET:SD	2.61	0.58
1:E:236:GLU:O	1:E:404:ASN:ND2	2.36	0.58
1:B:449:LEU:HD12	1:B:450:LYS:H	1.68	0.58
1:E:412:ASP:OD1	1:E:413:LYS:N	2.37	0.58
1:E:604:ILE:HD13	1:E:633:PHE:HE2	1.68	0.58
1:B:162:LEU:CG	1:B:388:PHE:CE1	2.86	0.58
1:C:41:PHE:CE1	1:C:319:LEU:HD12	2.28	0.58
1:B:32:SER:HA	1:B:35:MET:CG	2.30	0.58
1:C:366:VAL:HB	1:C:370:PHE:HB3	1.86	0.58
1:E:249:ARG:HA	1:E:370:PHE:HZ	1.69	0.58
1:F:458:MET:C	1:F:458:MET:SD	2.82	0.58
1:F:779:ARG:NH2	1:F:782:LEU:CG	2.61	0.58
1:B:28:THR:HB	1:B:330:TYR:CZ	2.39	0.58
1:B:170:TRP:CZ2	1:B:400:LEU:HB2	2.38	0.58
1:B:302:GLY:C	1:C:96:MET:CE	2.72	0.58
1:B:409:TRP:CZ3	1:B:433:LEU:HD22	2.39	0.58
1:C:426:LEU:HB3	1:C:446:LEU:HA	1.86	0.58
1:B:31:LEU:HD13	1:B:330:TYR:HD1	1.69	0.57
1:B:33:VAL:O	1:B:37:MET:CG	2.52	0.57
1:E:495:VAL:HG13	1:E:518:GLU:HB2	1.86	0.57
1:A:309:ASN:HD21	1:G:114:MET:CE	2.17	0.57
1:B:354:VAL:HG22	1:B:386:LYS:HE2	1.86	0.57
1:C:392:LEU:C	1:C:392:LEU:HD23	2.24	0.57
1:D:45:LEU:HA	1:D:48:MET:HE3	1.85	0.57
1:C:31:LEU:O	1:C:35:MET:HG3	2.04	0.57
1:C:409:TRP:HE1	1:C:433:LEU:HD21	1.69	0.57
1:C:418:LEU:CA	1:C:428:LEU:CD1	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ARG:HA	1:E:370:PHE:CZ	2.39	0.57
1:E:470:GLN:O	1:E:495:VAL:N	2.33	0.57
1:F:555:LYS:C	1:F:581:MET:HE1	2.25	0.57
1:B:165:CYS:SG	1:B:388:PHE:HA	2.44	0.57
1:F:325:CYS:O	1:F:329:ILE:HG12	2.04	0.57
1:G:41:PHE:O	1:G:44:THR:HG23	2.03	0.57
1:B:453:ILE:O	1:B:453:ILE:CG2	2.53	0.57
1:B:470:GLN:O	1:B:495:VAL:N	2.34	0.57
1:E:757:LEU:HD23	1:E:757:LEU:C	2.24	0.57
1:F:133:ILE:CA	1:F:136:LEU:HD23	2.32	0.57
1:G:117:GLU:C	1:G:117:GLU:CD	2.63	0.57
1:G:101:THR:C	1:G:102:ASP:OD1	2.43	0.57
1:E:245:VAL:HG21	1:E:391:PHE:HB3	1.87	0.57
1:F:137:VAL:HG12	1:F:272:LYS:NZ	2.19	0.57
1:F:276:ILE:O	1:F:280:ASN:ND2	2.31	0.57
1:A:114:MET:HG2	1:A:297:ILE:HD11	1.87	0.57
1:E:571:CYS:HB3	1:E:573:HIS:CE1	2.38	0.57
1:F:673:GLU:O	1:F:695:ILE:HA	2.04	0.57
1:G:52:ILE:O	1:G:53:ILE:HD13	2.04	0.57
1:B:16:ALA:HA	1:B:159:ILE:HD13	1.87	0.57
1:C:273:PHE:HE1	1:C:328:SER:HA	1.68	0.57
1:E:430:LEU:HD12	1:E:451:LEU:HG	1.87	0.57
1:E:799:GLN:CD	1:E:800:MET:CE	2.72	0.57
1:B:272:LYS:O	1:B:276:ILE:HG12	2.04	0.56
1:B:302:GLY:O	1:C:96:MET:HE3	1.99	0.56
1:B:322:CYS:O	1:B:326:PHE:CZ	2.58	0.56
1:C:563:VAL:HG12	1:C:567:LEU:HB2	1.86	0.56
1:F:253:GLU:HB3	1:F:367:LYS:HG3	1.87	0.56
1:C:363:ILE:CA	1:C:392:LEU:HD22	2.35	0.56
1:E:130:LEU:HD21	1:E:279:TYR:HH	1.68	0.56
1:F:555:LYS:HD3	1:F:581:MET:HE2	1.86	0.56
1:B:31:LEU:CD1	1:B:330:TYR:HD1	2.16	0.56
1:B:406:ASN:HD22	1:B:437:PRO:HA	1.71	0.56
1:C:478:SER:O	1:C:480:LYS:HE2	2.05	0.56
1:E:535:LEU:HD11	1:E:538:LEU:HD21	1.86	0.56
1:F:759:VAL:O	1:F:762:ASN:ND2	2.37	0.56
1:C:394:GLU:O	1:C:398:ASN:ND2	2.39	0.56
1:C:479:VAL:O	1:C:480:LYS:HD3	2.06	0.56
1:E:129:TYR:CA	1:E:132:LEU:HD23	2.31	0.56
1:E:376:MET:SD	1:E:377:ILE:HD13	2.46	0.56
1:F:123:TYR:HE2	1:F:127:PHE:HD2	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:541:LEU:O	1:F:566:HIS:NE2	2.33	0.56
1:G:109:SER:HA	1:G:112:ASN:HD22	1.70	0.56
1:B:370:PHE:HA	1:B:373:MET:CE	2.22	0.56
1:C:323:TYR:O	1:C:327:VAL:HG23	2.06	0.56
1:E:55:LEU:HD12	1:E:56:PRO:HD2	1.86	0.56
1:D:114:MET:HG2	1:D:297:ILE:HD11	1.87	0.56
1:E:736:ILE:O	1:E:739:ASN:ND2	2.38	0.56
1:F:430:LEU:HD12	1:F:451:LEU:HD12	1.80	0.56
1:F:673:GLU:HG3	1:F:694:ASP:HB2	1.87	0.56
1:F:739:ASN:N	1:F:761:GLY:O	2.29	0.56
1:A:126:TYR:HD1	1:A:129:TYR:HE2	1.53	0.56
1:B:415:ARG:NH2	1:B:416:GLN:N	2.49	0.56
1:C:50:ASP:HA	1:C:312:MET:SD	2.46	0.56
1:F:114:MET:HE1	1:F:295:VAL:HG11	1.67	0.56
1:B:28:THR:O	1:B:330:TYR:CE1	2.59	0.56
1:D:296:ASP:OD1	1:D:296:ASP:O	2.24	0.56
1:B:245:VAL:HG21	1:B:391:PHE:HB3	1.88	0.56
1:B:449:LEU:HG	1:B:451:LEU:CD1	2.34	0.56
1:C:117:GLU:OE1	1:C:118:ARG:NE	2.32	0.56
1:C:363:ILE:CB	1:C:392:LEU:HD22	2.36	0.56
1:E:425:ARG:NH1	1:E:471:GLU:OE1	2.36	0.56
1:E:437:PRO:HB2	1:E:440:VAL:CG2	2.36	0.56
1:F:354:VAL:O	1:F:358:THR:OG1	2.23	0.56
1:F:458:MET:SD	1:F:459:ILE:N	2.79	0.55
1:F:564:SER:HB2	1:F:588:MET:SD	2.45	0.55
1:F:634:GLN:OE1	1:F:637:ARG:NH1	2.39	0.55
1:C:493:LEU:HD12	1:C:493:LEU:H	1.70	0.55
1:E:52:ILE:HG21	1:E:116:TYR:HB2	1.88	0.55
1:F:325:CYS:O	1:F:328:SER:OG	2.16	0.55
1:F:500:PHE:HD2	1:F:503:MET:H	1.53	0.55
1:C:447:GLN:O	1:C:471:GLU:N	2.34	0.55
1:C:563:VAL:HA	1:C:566:HIS:CE1	2.41	0.55
1:E:570:MET:SD	1:E:570:MET:C	2.85	0.55
1:E:507:PRO:HB2	1:E:509:TRP:NE1	2.21	0.55
1:A:46:GLN:HA	1:A:50:ASP:HB2	1.87	0.55
1:C:156:GLU:HA	1:C:159:ILE:CD1	2.37	0.55
1:C:489:LEU:C	1:C:493:LEU:HD12	2.25	0.55
1:F:271:ILE:HD12	1:F:271:ILE:C	2.25	0.55
1:B:303:TYR:N	1:C:96:MET:HE3	2.21	0.55
1:C:166:PHE:HD1	1:C:387:ARG:HD3	1.72	0.55
1:C:516:LEU:HB3	1:C:541:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ARG:HH11	1:E:305:ASN:ND2	2.04	0.55
1:E:323:TYR:HD1	1:E:324:LEU:HD22	1.71	0.55
1:E:352:GLU:OE1	1:E:355:ARG:NH2	2.40	0.55
1:F:122:TRP:HA	1:F:125:LYS:HE2	1.87	0.55
1:B:46:GLN:O	1:B:50:ASP:HB3	2.07	0.55
1:B:162:LEU:CG	1:B:388:PHE:CE2	2.90	0.55
1:F:499:LYS:HG2	1:F:522:VAL:HB	1.87	0.55
1:F:425:ARG:NH1	1:F:471:GLU:OE1	2.39	0.55
1:F:676:PRO:HB2	1:F:678:HIS:CE1	2.42	0.55
1:G:117:GLU:OE1	1:G:118:ARG:CA	2.55	0.55
1:E:300:MET:CE	1:F:57:LYS:O	2.55	0.55
1:E:624:LEU:O	1:E:648:SER:N	2.40	0.55
1:F:367:LYS:HE3	1:F:368:ASN:H	1.71	0.55
1:F:596:LEU:O	1:F:620:LYS:N	2.40	0.55
1:B:506:LEU:HD23	1:B:506:LEU:C	2.27	0.55
1:F:41:PHE:CD1	1:F:41:PHE:C	2.78	0.55
1:F:751:LEU:HB3	1:F:754:LEU:HB2	1.88	0.55
1:G:103:LEU:HB3	1:G:107:GLN:HE21	1.72	0.55
1:C:496:LEU:HB3	1:C:516:LEU:HD21	1.89	0.54
1:G:53:ILE:HD13	1:G:53:ILE:N	2.22	0.54
1:B:151:SER:HB2	1:B:258:LEU:HD13	1.89	0.54
1:B:165:CYS:CB	1:B:388:PHE:CD1	2.84	0.54
1:C:242:PHE:CD1	1:C:391:PHE:CD2	2.95	0.54
1:E:31:LEU:HD21	1:E:329:ILE:HD11	1.88	0.54
1:E:311:THR:HG1	1:E:312:MET:N	2.03	0.54
1:E:680:PHE:HA	1:E:705:LEU:HD11	1.90	0.54
1:B:302:GLY:C	1:C:96:MET:HE3	2.27	0.54
1:B:503:MET:CE	1:B:503:MET:CA	2.85	0.54
1:E:52:ILE:HD11	1:E:308:CYS:CB	2.34	0.54
1:E:459:ILE:HG22	1:E:481:ILE:HA	1.89	0.54
1:F:120:LEU:HD21	1:F:310:HIS:HD2	1.71	0.54
1:F:372:PHE:CB	1:F:373:MET:HE1	2.37	0.54
1:C:480:LYS:N	1:C:480:LYS:CD	2.69	0.54
1:E:267:VAL:O	1:E:271:ILE:HG12	2.07	0.54
1:F:106:GLN:NE2	1:G:108:TYR:HB3	2.22	0.54
1:F:158:PHE:HB2	1:F:248:PHE:CZ	2.43	0.54
1:F:270:VAL:HG22	1:F:334:CYS:HB3	1.89	0.54
1:F:573:HIS:HB3	1:F:597:VAL:HB	1.88	0.54
1:B:261:MET:CE	1:B:261:MET:HA	2.38	0.54
1:B:474:LEU:N	1:B:497:SER:O	2.38	0.54
1:C:421:ASN:ND2	1:C:471:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:MET:CE	1:C:480:LYS:HB2	2.38	0.54
1:E:172:THR:OG1	1:E:387:ARG:NH1	2.34	0.54
1:C:237:GLN:O	1:C:241:LEU:HG	2.08	0.54
1:E:150:GLY:O	1:E:154:LYS:NZ	2.28	0.54
1:F:523:GLY:O	1:F:551:SER:OG	2.20	0.54
1:B:322:CYS:CB	1:B:326:PHE:HZ	2.16	0.54
1:E:505:GLU:O	1:E:507:PRO:HD3	2.07	0.54
1:F:604:ILE:HD11	1:F:627:ILE:HB	1.90	0.54
1:E:162:LEU:HD13	1:E:388:PHE:CD1	2.43	0.54
1:E:337:THR:O	1:E:341:LEU:N	2.41	0.54
1:E:547:LEU:HB3	1:E:570:MET:CE	2.37	0.54
1:B:337:THR:O	1:B:341:LEU:N	2.40	0.54
1:E:369:ASP:O	1:E:373:MET:CG	2.56	0.54
1:F:31:LEU:O	1:F:35:MET:HG3	2.08	0.54
1:F:57:LYS:HB3	1:F:305:ASN:HB3	1.90	0.54
1:F:123:TYR:HB2	1:F:283:LEU:HD11	1.89	0.54
1:F:430:LEU:HB2	1:F:451:LEU:HD12	1.90	0.54
1:F:486:LEU:HA	1:F:489:LEU:CD1	2.37	0.54
1:C:482:HIS:CG	1:C:483:SER:N	2.76	0.54
1:E:376:MET:HE3	1:E:377:ILE:N	2.23	0.54
1:F:390:LEU:HD12	1:F:391:PHE:N	2.23	0.54
1:B:429:PRO:HA	1:B:450:LYS:HB3	1.90	0.53
1:B:461:ALA:HA	1:B:485:ALA:HB2	1.90	0.53
1:C:376:MET:SD	1:C:377:ILE:N	2.81	0.53
1:C:503:MET:HA	1:C:506:LEU:HB3	1.90	0.53
1:E:472:LEU:HG	1:E:496:LEU:HD13	1.90	0.53
1:E:757:LEU:HD21	1:E:759:VAL:CG2	2.34	0.53
1:F:296:ASP:O	1:F:296:ASP:CG	2.47	0.53
1:A:126:TYR:HA	1:A:129:TYR:HD2	1.60	0.53
1:B:32:SER:CA	1:B:35:MET:HG2	2.35	0.53
1:C:376:MET:CE	1:C:377:ILE:N	2.71	0.53
1:D:104:ASP:H	1:D:107:GLN:HE22	1.56	0.53
1:F:351:PHE:HB3	1:F:354:VAL:HG22	1.90	0.53
1:C:238:ALA:HA	1:C:241:LEU:CD1	2.38	0.53
1:F:510:MET:SD	1:F:511:TYR:CE1	3.01	0.53
1:F:555:LYS:HB3	1:F:581:MET:HE3	1.69	0.53
1:C:474:LEU:N	1:C:497:SER:O	2.39	0.53
1:C:514:ARG:O	1:C:541:LEU:HG	2.08	0.53
1:D:316:PHE:O	1:D:320:SER:N	2.32	0.53
1:E:488:PHE:O	1:E:492:ASN:HB2	2.08	0.53
1:B:45:LEU:O	1:B:312:MET:HE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ASP:H	1:D:107:GLN:NE2	2.07	0.53
1:D:121:HIS:CE1	1:D:123:TYR:HB3	2.43	0.53
1:E:37:MET:CE	1:E:38:ILE:N	2.67	0.53
1:E:244:LYS:HG2	1:E:247:LYS:NZ	2.24	0.53
1:F:615:GLN:O	1:F:640:THR:N	2.41	0.53
1:B:28:THR:HB	1:B:330:TYR:OH	2.08	0.53
1:B:276:ILE:HD13	1:B:279:TYR:HE2	1.73	0.53
1:B:453:ILE:HD13	1:B:455:LYS:HZ3	1.72	0.53
1:B:503:MET:CE	1:B:506:LEU:CD1	2.75	0.53
1:G:104:ASP:OD2	1:G:105:LEU:N	2.42	0.53
1:B:163:GLY:HA2	1:B:166:PHE:CE2	2.43	0.53
1:E:472:LEU:CD1	1:E:473:SER:N	2.67	0.53
1:F:101:THR:OG1	1:F:108:TYR:OH	2.24	0.53
1:B:38:ILE:CD1	1:B:326:PHE:CE2	2.92	0.53
1:B:96:MET:N	1:B:96:MET:SD	2.82	0.53
1:B:124:ALA:HB2	1:B:287:VAL:HG12	1.91	0.53
1:B:346:LEU:HB3	1:B:375:HIS:CD2	2.43	0.53
1:B:474:LEU:CD2	1:B:498:VAL:HG12	2.28	0.53
1:C:430:LEU:HB2	1:C:451:LEU:HA	1.90	0.53
1:E:268:LEU:HA	1:E:271:ILE:HD11	1.90	0.53
1:F:263:VAL:HG22	1:F:341:LEU:HD21	1.91	0.53
1:F:372:PHE:CD1	1:F:373:MET:CE	2.91	0.53
1:A:59:VAL:HG11	1:A:99:LEU:HD21	1.91	0.53
1:C:376:MET:HE3	1:C:377:ILE:CA	2.39	0.53
1:C:481:ILE:HD12	1:C:486:LEU:HB2	1.91	0.53
1:G:117:GLU:OE1	1:G:117:GLU:C	2.48	0.53
1:B:276:ILE:HA	1:B:279:TYR:CE2	2.44	0.53
1:B:413:LYS:O	1:B:417:LYS:HG2	2.09	0.53
1:E:631:VAL:O	1:E:634:GLN:HB2	2.08	0.53
1:G:126:TYR:HA	1:G:129:TYR:HD2	1.74	0.53
1:F:612:LEU:HA	1:F:636:LEU:HD22	1.91	0.52
1:B:131:VAL:HG22	1:B:323:TYR:CE1	2.44	0.52
1:E:158:PHE:O	1:E:162:LEU:HD23	2.09	0.52
1:E:164:LYS:NZ	1:E:244:LYS:HE3	2.23	0.52
1:E:511:TYR:O	1:E:540:ASP:HB2	2.09	0.52
1:F:256:ASP:HA	1:F:369:ASP:HB3	1.90	0.52
1:F:612:LEU:CG	1:F:635:HIS:CE1	2.91	0.52
1:B:31:LEU:HD13	1:B:330:TYR:CD1	2.43	0.52
1:B:395:VAL:HG12	1:B:399:LYS:HE3	1.90	0.52
1:C:134:HIS:CE1	1:C:276:ILE:HD11	2.43	0.52
1:E:685:ILE:O	1:E:707:SER:OG	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:495:VAL:HG22	1:F:518:GLU:HB2	1.90	0.52
1:F:595:GLU:HB2	1:F:618:ASP:HB3	1.91	0.52
1:F:687:TYR:HA	1:F:710:TYR:HB3	1.90	0.52
1:C:170:TRP:CZ2	1:C:400:LEU:HB2	2.43	0.52
1:C:367:LYS:O	1:C:371:ALA:N	2.33	0.52
1:E:415:ARG:NE	1:E:445:GLU:OE2	2.34	0.52
1:E:744:LEU:HA	1:E:764:PHE:HZ	1.73	0.52
1:F:138:PHE:CE2	1:F:330:TYR:CD1	2.89	0.52
1:F:276:ILE:HD13	1:F:279:TYR:HE2	1.74	0.52
1:B:27:PHE:CZ	1:B:31:LEU:CD1	2.92	0.52
1:B:28:THR:CA	1:B:330:TYR:CZ	2.93	0.52
1:E:743:VAL:N	1:E:764:PHE:CE1	2.76	0.52
1:C:23:TRP:CH2	1:C:336:TYR:CE1	2.94	0.52
1:C:133:ILE:HG13	1:C:134:HIS:N	2.23	0.52
1:E:367:LYS:HD3	1:E:368:ASN:H	1.74	0.52
1:E:533:VAL:H	1:E:555:LYS:HE3	1.74	0.52
1:E:617:LEU:HD21	1:E:619:LEU:HG	1.91	0.52
1:F:507:PRO:HG2	1:F:510:MET:CG	2.33	0.52
1:F:733:THR:HG23	1:F:756:TYR:CD1	2.45	0.52
1:G:57:LYS:HD2	1:G:306:PHE:O	2.09	0.52
1:B:273:PHE:CD2	1:B:274:LEU:N	2.78	0.52
1:B:462:THR:O	1:B:465:GLN:HB2	2.10	0.52
1:E:139:MET:HE3	1:E:140:LEU:N	2.25	0.52
1:B:446:LEU:HD11	1:B:466:LEU:HD13	1.92	0.52
1:C:490:LYS:HE3	1:C:513:LEU:HD23	1.91	0.52
1:D:123:TYR:HE2	1:D:283:LEU:O	1.93	0.52
1:E:128:PRO:C	1:E:132:LEU:CD2	2.75	0.52
1:E:527:HIS:O	1:E:531:ARG:HD2	2.09	0.52
1:E:769:PRO:HB3	1:E:796:VAL:HG21	1.91	0.52
1:F:124:ALA:HB2	1:F:287:VAL:HG12	1.92	0.52
1:B:145:TRP:CZ2	1:B:262:TYR:CD1	2.87	0.52
1:B:453:ILE:CD1	1:B:455:LYS:HZ3	2.22	0.52
1:C:139:MET:SD	1:C:143:ASN:ND2	2.83	0.52
1:C:249:ARG:HA	1:C:370:PHE:CZ	2.45	0.52
1:F:145:TRP:N	1:F:265:GLN:HE22	2.08	0.52
1:B:159:ILE:HG13	1:B:160:SER:N	2.25	0.51
1:C:454:ILE:N	1:C:477:CYS:SG	2.69	0.51
1:C:525:LEU:HD21	1:C:533:VAL:CB	2.40	0.51
1:E:458:MET:HG2	1:E:480:LYS:HB3	1.90	0.51
1:E:744:LEU:HD12	1:E:764:PHE:HE2	1.73	0.51
1:F:454:ILE:HG22	1:F:457:VAL:HG21	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:303:TYR:HB3	1:G:306:PHE:HE2	1.74	0.51
1:C:104:ASP:OD2	1:C:107:GLN:NE2	2.39	0.51
1:E:145:TRP:N	1:E:265:GLN:HE22	2.08	0.51
1:E:764:PHE:CD2	1:E:767:LEU:CD2	2.94	0.51
1:F:372:PHE:CD1	1:F:373:MET:HE3	2.45	0.51
1:F:597:VAL:HG13	1:F:620:LYS:HG2	1.92	0.51
1:G:121:HIS:HD2	1:G:123:TYR:HB3	1.75	0.51
1:D:59:VAL:HG11	1:D:99:LEU:HD11	1.91	0.51
1:E:123:TYR:CE1	1:E:127:PHE:CD2	2.85	0.51
1:E:166:PHE:CD1	1:E:387:ARG:HD2	2.46	0.51
1:F:253:GLU:HG3	1:F:370:PHE:CZ	2.45	0.51
1:A:305:ASN:OD1	1:A:306:PHE:N	2.43	0.51
1:B:246:LYS:HA	1:B:249:ARG:HG2	1.92	0.51
1:C:490:LYS:HB3	1:C:514:ARG:HG2	1.91	0.51
1:E:134:HIS:CG	1:E:276:ILE:HD11	2.45	0.51
1:F:248:PHE:CE2	1:F:252:VAL:HG21	2.45	0.51
1:B:59:VAL:HG11	1:B:99:LEU:HD21	1.91	0.51
1:B:113:GLN:HE21	1:C:311:THR:HG22	1.75	0.51
1:B:126:TYR:HB3	1:B:130:LEU:HD21	1.92	0.51
1:B:363:ILE:HD11	1:B:393:SER:HB2	1.92	0.51
1:D:101:THR:OG1	1:D:108:TYR:OH	2.26	0.51
1:E:406:ASN:ND2	1:E:438:ASP:OD2	2.44	0.51
1:F:564:SER:CB	1:F:588:MET:SD	2.97	0.51
1:C:165:CYS:SG	1:C:388:PHE:HA	2.50	0.51
1:A:108:TYR:CG	1:G:106:GLN:OE1	2.64	0.51
1:C:415:ARG:HD2	1:C:418:LEU:HD12	1.93	0.51
1:F:373:MET:CE	1:F:373:MET:N	2.74	0.51
1:F:724:GLU:OE1	1:F:724:GLU:N	2.34	0.51
1:F:777:LEU:C	1:F:800:MET:HE1	2.25	0.51
1:E:709:GLN:HA	1:E:731:LEU:HA	1.93	0.51
1:E:743:VAL:HA	1:E:764:PHE:CE1	2.46	0.51
1:F:458:MET:HE3	1:F:460:PRO:N	2.26	0.51
1:B:31:LEU:HD21	1:B:329:ILE:HD11	1.93	0.50
1:B:52:ILE:HD12	1:B:310:HIS:HB3	1.93	0.50
1:B:149:PRO:HA	1:B:152:SER:HB3	1.92	0.50
1:B:474:LEU:HD23	1:B:498:VAL:CG1	2.29	0.50
1:C:504:ARG:HG3	1:C:505:GLU:H	1.76	0.50
1:E:472:LEU:O	1:E:496:LEU:HA	2.11	0.50
1:C:272:LYS:O	1:C:276:ILE:HG12	2.09	0.50
1:E:725:LEU:HD12	1:E:726:TYR:CD2	2.45	0.50
1:F:276:ILE:HD13	1:F:279:TYR:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:477:CYS:N	1:F:505:GLU:HG2	2.27	0.50
1:B:114:MET:HG2	1:B:295:VAL:HG11	1.94	0.50
1:B:244:LYS:HA	1:B:247:LYS:HE3	1.93	0.50
1:D:45:LEU:HA	1:D:48:MET:CE	2.41	0.50
1:E:55:LEU:HD13	1:E:56:PRO:HD2	1.92	0.50
1:E:458:MET:SD	1:E:481:ILE:N	2.85	0.50
1:E:599:CYS:N	1:E:622:ASN:OD1	2.43	0.50
1:E:634:GLN:OE1	1:E:637:ARG:NH1	2.44	0.50
1:F:556:ILE:CG2	1:F:581:MET:SD	2.99	0.50
1:G:110:PHE:O	1:G:114:MET:HG2	2.11	0.50
1:E:279:TYR:C	1:E:279:TYR:CD2	2.84	0.50
1:E:729:LYS:NZ	1:E:750:ASN:O	2.39	0.50
1:F:123:TYR:CD1	1:F:283:LEU:HD22	2.46	0.50
1:F:474:LEU:CD1	1:F:477:CYS:HB2	2.35	0.50
1:B:419:GLN:NE2	1:B:429:PRO:HG2	2.26	0.50
1:E:458:MET:HE1	1:E:482:HIS:HB2	1.94	0.50
1:F:643:LYS:HB3	1:F:645:TRP:CD1	2.47	0.50
1:C:258:LEU:HA	1:C:261:MET:HE3	1.94	0.50
1:E:121:HIS:ND1	1:E:123:TYR:HB3	2.26	0.50
1:F:578:LYS:HG3	1:F:601:LEU:HD23	1.94	0.50
1:C:238:ALA:HB1	1:C:391:PHE:HZ	1.77	0.50
1:E:579:LEU:HD23	1:E:596:LEU:HD11	1.92	0.50
1:F:273:PHE:CD2	1:F:274:LEU:HD22	2.47	0.50
1:C:470:GLN:OE1	1:C:494:LYS:HG2	2.11	0.50
1:G:57:LYS:HD2	1:G:306:PHE:C	2.32	0.50
1:G:104:ASP:OD2	1:G:106:GLN:N	2.38	0.50
1:B:498:VAL:HG21	1:B:519:LEU:HD11	1.88	0.50
1:B:510:MET:SD	1:B:513:LEU:HD11	2.52	0.50
1:E:347:ARG:O	1:E:368:ASN:HA	2.12	0.50
1:F:268:LEU:HA	1:F:271:ILE:HG13	1.92	0.50
1:B:46:GLN:CA	1:B:312:MET:HE1	2.42	0.49
1:B:161:ILE:O	1:B:388:PHE:CE1	2.65	0.49
1:F:246:LYS:O	1:F:249:ARG:HG2	2.11	0.49
1:F:450:LYS:NZ	1:F:452:GLU:OE1	2.25	0.49
1:G:124:ALA:HB2	1:G:287:VAL:HG11	1.94	0.49
1:C:246:LYS:HA	1:C:249:ARG:HG2	1.93	0.49
1:E:19:VAL:HG12	1:E:380:TYR:CE2	2.47	0.49
1:E:31:LEU:O	1:E:35:MET:HG2	2.11	0.49
1:F:556:ILE:N	1:F:581:MET:HE1	2.26	0.49
1:A:125:LYS:O	1:A:129:TYR:CE2	2.66	0.49
1:C:35:MET:HE1	1:C:326:PHE:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PHE:CD1	1:C:391:PHE:HD2	2.30	0.49
1:C:478:SER:HA	1:C:480:LYS:NZ	2.24	0.49
1:E:494:LYS:HA	1:E:516:LEU:HA	1.94	0.49
1:F:165:CYS:SG	1:F:388:PHE:HA	2.53	0.49
1:B:370:PHE:N	1:B:373:MET:HE3	2.26	0.49
1:C:363:ILE:HD11	1:C:393:SER:HB2	1.93	0.49
1:C:414:LEU:O	1:C:428:LEU:HD11	2.12	0.49
1:A:312:MET:SD	1:A:312:MET:N	2.84	0.49
1:D:298:GLN:HG3	1:D:302:GLY:HA2	1.95	0.49
1:E:268:LEU:HA	1:E:271:ILE:CG1	2.42	0.49
1:E:426:LEU:O	1:E:447:GLN:N	2.45	0.49
1:E:631:VAL:HA	1:E:634:GLN:HG2	1.94	0.49
1:F:652:ILE:CG1	1:F:672:ILE:HG12	2.39	0.49
1:B:34:ALA:HA	1:B:37:MET:HG2	1.94	0.49
1:C:415:ARG:HA	1:C:418:LEU:HD12	1.95	0.49
1:E:516:LEU:HB3	1:E:541:LEU:HD11	1.93	0.49
1:E:725:LEU:CD1	1:E:725:LEU:C	2.81	0.49
1:A:310:HIS:ND1	1:A:312:MET:HG2	2.27	0.49
1:C:101:THR:O	1:C:103:LEU:HG	2.13	0.49
1:C:245:VAL:HG11	1:C:391:PHE:HB3	1.95	0.49
1:E:246:LYS:HA	1:E:249:ARG:HG2	1.95	0.49
1:E:714:THR:HA	1:E:737:GLY:HA3	1.94	0.49
1:E:743:VAL:O	1:E:764:PHE:HE1	1.96	0.49
1:F:717:LYS:O	1:F:719:GLU:HG3	2.13	0.49
1:F:760:LYS:HB2	1:F:783:VAL:HG12	1.95	0.49
1:B:27:PHE:HE2	1:B:333:THR:HG21	0.35	0.49
1:B:449:LEU:CG	1:B:451:LEU:HD11	2.43	0.49
1:B:474:LEU:CD1	1:B:477:CYS:HB2	2.42	0.49
1:C:497:SER:HA	1:C:520:TYR:HB2	1.95	0.49
1:E:463:ILE:HD12	1:E:489:LEU:HD23	1.94	0.49
1:F:20:LEU:HB2	1:F:21:LYS:NZ	2.27	0.49
1:B:133:ILE:HG23	1:B:134:HIS:CD2	2.46	0.49
1:B:145:TRP:CH2	1:B:262:TYR:CE2	3.01	0.49
1:E:405:LEU:HG	1:E:409:TRP:CD1	2.48	0.49
1:F:20:LEU:HB2	1:F:21:LYS:HZ2	1.78	0.49
1:C:312:MET:SD	1:C:312:MET:N	2.86	0.48
1:C:352:GLU:O	1:C:356:GLN:NE2	2.46	0.48
1:F:354:VAL:HG12	1:F:386:LYS:HE2	1.93	0.48
1:F:779:ARG:NH2	1:F:782:LEU:O	2.44	0.48
1:B:323:TYR:CD2	1:B:323:TYR:C	2.86	0.48
1:C:331:GLY:O	1:C:335:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:766:ILE:HD12	1:E:791:THR:HB	1.95	0.48
1:F:363:ILE:HA	1:F:392:LEU:HD22	1.95	0.48
1:B:280:ASN:O	1:B:284:VAL:HG23	2.13	0.48
1:B:376:MET:HE3	1:B:377:ILE:HD13	1.94	0.48
1:C:433:LEU:HB2	1:C:454:ILE:HD13	1.94	0.48
1:C:476:GLN:NE2	1:C:501:ASP:OD1	2.47	0.48
1:C:526:SER:HA	1:C:533:VAL:HA	1.94	0.48
1:F:253:GLU:O	1:F:367:LYS:HE2	2.13	0.48
1:B:323:TYR:CA	1:B:326:PHE:HE2	2.20	0.48
1:B:350:SER:OG	1:B:365:ASP:OD1	2.19	0.48
1:E:639:LEU:HD23	1:E:659:LEU:HD13	1.94	0.48
1:F:114:MET:SD	1:F:295:VAL:HG11	2.52	0.48
1:F:241:LEU:HD12	1:F:244:LYS:HE2	1.95	0.48
1:F:726:TYR:CD2	1:F:747:LYS:HB2	2.48	0.48
1:B:28:THR:HB	1:B:330:TYR:CE2	2.49	0.48
1:B:390:LEU:HD12	1:B:390:LEU:O	2.14	0.48
1:C:498:VAL:HB	1:C:521:LEU:HD12	1.95	0.48
1:F:457:VAL:HB	1:F:479:VAL:HG22	1.95	0.48
1:F:604:ILE:HD13	1:F:633:PHE:HE2	1.79	0.48
1:C:406:ASN:ND2	1:C:438:ASP:H	2.10	0.48
1:D:295:VAL:HG23	1:D:297:ILE:HG12	1.94	0.48
1:F:670:ASN:O	1:F:693:ASN:HA	2.13	0.48
1:B:459:ILE:HD12	1:B:481:ILE:HG12	1.95	0.48
1:C:347:ARG:O	1:C:368:ASN:HA	2.14	0.48
1:C:558:GLN:O	1:C:561:VAL:HB	2.14	0.48
1:E:725:LEU:HD12	1:E:726:TYR:H	1.65	0.48
1:F:518:GLU:HG2	1:F:546:ILE:HB	1.95	0.48
1:F:544:LEU:HD12	1:F:545:LYS:N	2.29	0.48
1:F:630:ILE:HA	1:F:633:PHE:HD2	1.78	0.48
1:A:103:LEU:HD11	1:A:303:TYR:HE2	1.79	0.48
1:A:127:PHE:CZ	1:A:319:LEU:HD23	2.49	0.48
1:E:162:LEU:HD22	1:E:388:PHE:CE1	2.48	0.48
1:G:105:LEU:N	1:G:105:LEU:CD1	2.76	0.48
1:B:310:HIS:NE2	1:B:313:ALA:HB2	2.29	0.48
1:C:238:ALA:HB1	1:C:391:PHE:CZ	2.48	0.48
1:E:152:SER:HA	1:E:155:ILE:HG12	1.95	0.48
1:E:170:TRP:CZ2	1:E:400:LEU:HB2	2.48	0.48
1:E:472:LEU:HG	1:E:496:LEU:CD1	2.44	0.48
1:E:473:SER:HA	1:E:497:SER:O	2.14	0.48
1:C:134:HIS:ND1	1:C:276:ILE:HD11	2.28	0.48
1:E:123:TYR:CD2	1:E:283:LEU:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ALA:HB1	1:E:391:PHE:HZ	1.78	0.48
1:E:409:TRP:HE1	1:E:433:LEU:HD21	1.78	0.48
1:E:683:ASN:HA	1:E:705:LEU:HD22	1.95	0.48
1:G:316:PHE:O	1:G:320:SER:N	2.32	0.48
1:C:430:LEU:O	1:C:452:GLU:N	2.47	0.47
1:E:104:ASP:OD1	1:E:105:LEU:N	2.46	0.47
1:F:445:GLU:OE1	1:F:445:GLU:N	2.46	0.47
1:F:605:PRO:HG2	1:F:608:VAL:HG23	1.96	0.47
1:F:690:LEU:O	1:F:693:ASN:ND2	2.47	0.47
1:A:48:MET:HB3	1:A:49:GLN:HE21	1.79	0.47
1:A:121:HIS:CE1	1:A:123:TYR:HB3	2.49	0.47
1:C:297:ILE:HG22	1:C:300:MET:HB3	1.95	0.47
1:E:52:ILE:CG2	1:E:116:TYR:HB2	2.44	0.47
1:E:494:LYS:O	1:E:517:GLU:N	2.37	0.47
1:F:149:PRO:HA	1:F:152:SER:HB3	1.96	0.47
1:F:171:THR:HB	1:F:390:LEU:HD21	1.94	0.47
1:G:101:THR:O	1:G:103:LEU:HG	2.14	0.47
1:A:294:ASN:OD1	1:A:305:ASN:ND2	2.47	0.47
1:D:122:TRP:HA	1:D:125:LYS:HE3	1.96	0.47
1:F:452:GLU:HG2	1:F:475:HIS:CB	2.41	0.47
1:F:510:MET:HE3	1:F:511:TYR:CZ	2.48	0.47
1:F:612:LEU:HD11	1:F:635:HIS:HE2	1.79	0.47
1:F:625:LYS:HA	1:F:649:ILE:HA	1.96	0.47
1:B:34:ALA:HB3	1:B:35:MET:CE	2.45	0.47
1:B:475:HIS:ND1	1:B:499:LYS:HE2	2.29	0.47
1:C:367:LYS:HE3	1:C:368:ASN:H	1.79	0.47
1:E:117:GLU:C	1:E:117:GLU:OE1	2.53	0.47
1:B:297:ILE:HA	1:B:300:MET:HE2	1.54	0.47
1:F:132:LEU:O	1:F:136:LEU:HD23	1.92	0.47
1:F:133:ILE:HG13	1:F:134:HIS:N	2.28	0.47
1:F:466:LEU:HB3	1:F:469:LEU:HD13	1.96	0.47
1:F:511:TYR:CZ	1:F:536:GLU:HB2	2.49	0.47
1:B:45:LEU:C	1:B:312:MET:HE1	2.34	0.47
1:B:449:LEU:HB3	1:B:472:LEU:HD13	1.96	0.47
1:C:127:PHE:CD2	1:C:128:PRO:N	2.83	0.47
1:C:145:TRP:N	1:C:265:GLN:HE22	2.13	0.47
1:C:239:LYS:HD2	1:C:401:LYS:HA	1.97	0.47
1:E:415:ARG:HG2	1:E:418:LEU:HD12	1.96	0.47
1:F:123:TYR:CB	1:F:283:LEU:CD1	2.82	0.47
1:F:133:ILE:O	1:F:137:VAL:HG23	2.14	0.47
1:F:145:TRP:CD1	1:F:261:MET:SD	3.08	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:428:LEU:HD12	1:F:429:PRO:CD	2.43	0.47
1:F:643:LYS:HA	1:F:666:SER:HB2	1.96	0.47
1:A:126:TYR:CA	1:A:129:TYR:HD2	2.22	0.47
1:A:276:ILE:HG21	1:A:327:VAL:HG11	1.95	0.47
1:B:27:PHE:CE1	1:B:31:LEU:HD11	2.49	0.47
1:B:101:THR:HG1	1:B:108:TYR:HH	1.49	0.47
1:B:448:SER:HA	1:B:471:GLU:O	2.15	0.47
1:C:253:GLU:HG3	1:C:370:PHE:CD1	2.49	0.47
1:C:431:ILE:N	1:C:431:ILE:HD12	2.30	0.47
1:E:37:MET:CE	1:E:38:ILE:HA	2.42	0.47
1:E:124:ALA:HB2	1:E:287:VAL:HG12	1.96	0.47
1:E:130:LEU:CD1	1:E:279:TYR:HH	2.07	0.47
1:E:139:MET:HE3	1:E:140:LEU:H	1.79	0.47
1:E:170:TRP:CH2	1:E:396:SER:HB2	2.49	0.47
1:E:427:GLU:HB2	1:E:448:SER:HB3	1.97	0.47
1:E:496:LEU:HB3	1:E:516:LEU:HD11	1.97	0.47
1:E:569:LYS:NZ	1:E:593:GLU:OE1	2.37	0.47
1:E:654:GLU:HG3	1:E:678:HIS:CG	2.49	0.47
1:E:725:LEU:CD1	1:E:726:TYR:CD1	2.97	0.47
1:F:243:GLU:CD	1:F:243:GLU:N	2.65	0.47
1:F:352:GLU:HA	1:F:355:ARG:HH21	1.78	0.47
1:F:597:VAL:HG22	1:F:620:LYS:HB3	1.96	0.47
1:A:292:ASP:OD1	1:A:293:CYS:N	2.48	0.47
1:B:461:ALA:O	1:B:464:ALA:HB3	2.15	0.47
1:E:263:VAL:HG22	1:E:341:LEU:HD13	1.96	0.47
1:F:373:MET:HE2	1:F:373:MET:N	2.29	0.47
1:E:36:LEU:O	1:E:36:LEU:HD12	2.15	0.47
1:E:725:LEU:HD11	1:E:726:TYR:CG	2.44	0.47
1:F:627:ILE:HG13	1:F:653:PRO:HG2	1.97	0.47
1:F:650:THR:HA	1:F:672:ILE:N	2.29	0.47
1:C:166:PHE:HA	1:C:387:ARG:NH1	2.30	0.47
1:C:376:MET:HE3	1:C:377:ILE:HD13	1.77	0.47
1:C:472:LEU:HG	1:C:474:LEU:HD21	1.96	0.47
1:E:103:LEU:HD11	1:E:303:TYR:HE2	1.79	0.47
1:E:630:ILE:HB	1:E:655:HIS:HB2	1.97	0.47
1:E:703:GLY:HA3	1:E:724:GLU:HB3	1.96	0.47
1:B:126:TYR:C	1:B:130:LEU:HG	2.34	0.46
1:B:518:GLU:OE1	1:B:520:TYR:OH	2.22	0.46
1:C:463:ILE:HD12	1:C:466:LEU:HD12	1.98	0.46
1:C:517:GLU:O	1:C:545:LYS:N	2.39	0.46
1:F:129:TYR:O	1:F:133:ILE:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HB	1:B:370:PHE:CZ	2.50	0.46
1:B:415:ARG:NH2	1:B:415:ARG:C	2.69	0.46
1:E:376:MET:SD	1:E:377:ILE:N	2.88	0.46
1:F:161:ILE:HG13	1:F:162:LEU:N	2.30	0.46
1:F:535:LEU:HD21	1:F:538:LEU:HD11	1.97	0.46
1:F:779:ARG:CZ	1:F:782:LEU:HD23	2.46	0.46
1:B:503:MET:SD	1:B:506:LEU:HD13	2.55	0.46
1:C:564:SER:HA	1:C:567:LEU:HB3	1.96	0.46
1:D:46:GLN:O	1:D:50:ASP:HB3	2.15	0.46
1:D:52:ILE:HD11	1:D:308:CYS:HB3	1.95	0.46
1:E:764:PHE:HD2	1:E:767:LEU:HD21	1.80	0.46
1:G:54:CYS:C	1:G:55:LEU:CD2	2.68	0.46
1:B:370:PHE:HA	1:B:373:MET:HG2	1.98	0.46
1:E:414:LEU:HD22	1:E:428:LEU:HD21	1.97	0.46
1:E:639:LEU:HD21	1:E:642:LEU:HD12	1.97	0.46
1:F:52:ILE:HD11	1:F:308:CYS:HB3	1.97	0.46
1:F:395:VAL:HG12	1:F:399:LYS:HE3	1.98	0.46
1:B:425:ARG:NH1	1:B:471:GLU:HB2	2.30	0.46
1:C:473:SER:C	1:C:474:LEU:HD23	2.36	0.46
1:D:52:ILE:CG2	1:D:116:TYR:HB2	2.42	0.46
1:E:644:LEU:HD13	1:E:649:ILE:HD13	1.97	0.46
1:F:311:THR:OG1	1:F:312:MET:SD	2.66	0.46
1:F:461:ALA:HB2	1:F:482:HIS:ND1	2.30	0.46
1:F:473:SER:C	1:F:474:LEU:HD22	2.36	0.46
1:B:145:TRP:CE2	1:B:262:TYR:CD1	3.04	0.46
1:F:113:GLN:OE1	1:G:311:THR:HG22	2.15	0.46
1:F:432:MET:HA	1:F:432:MET:CE	2.44	0.46
1:B:162:LEU:N	1:B:388:PHE:CE1	2.62	0.46
1:B:266:THR:HA	1:B:269:LYS:HD2	1.98	0.46
1:C:279:TYR:HD1	1:C:283:LEU:HD12	1.81	0.46
1:C:376:MET:HE3	1:C:377:ILE:CB	2.43	0.46
1:D:127:PHE:C	1:D:127:PHE:CD2	2.89	0.46
1:F:298:GLN:HB2	1:F:304:LYS:HB2	1.97	0.46
1:G:312:MET:O	1:G:316:PHE:HD1	1.98	0.46
1:A:57:LYS:HA	1:G:300:MET:CE	2.45	0.46
1:C:489:LEU:CA	1:C:493:LEU:HD13	2.40	0.46
1:C:560:VAL:O	1:C:564:SER:N	2.32	0.46
1:F:390:LEU:HD12	1:F:390:LEU:C	2.36	0.46
1:B:161:ILE:HG13	1:B:162:LEU:HD12	1.98	0.46
1:B:346:LEU:HD22	1:B:375:HIS:CE1	2.51	0.46
1:B:409:TRP:CZ3	1:B:433:LEU:CD2	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PHE:CG	1:C:391:PHE:CE2	3.04	0.46
1:E:559:ALA:O	1:E:562:ASP:HB2	2.16	0.46
1:F:263:VAL:HG22	1:F:341:LEU:HD11	1.98	0.46
1:A:297:ILE:O	1:A:300:MET:HB2	2.16	0.46
1:C:103:LEU:HB2	1:C:108:TYR:CZ	2.51	0.46
1:C:395:VAL:HG12	1:C:399:LYS:HE3	1.98	0.46
1:C:446:LEU:HG	1:C:469:LEU:HD12	1.98	0.46
1:E:19:VAL:HG23	1:E:20:LEU:HD22	1.97	0.46
1:E:354:VAL:O	1:E:358:THR:OG1	2.27	0.46
1:F:265:GLN:HA	1:F:268:LEU:HD11	1.97	0.46
1:F:398:ASN:HA	1:F:401:LYS:HE2	1.97	0.46
1:F:433:LEU:O	1:F:454:ILE:HG23	2.16	0.46
1:F:507:PRO:HB2	1:F:509:TRP:CE2	2.51	0.46
1:G:123:TYR:O	1:G:127:PHE:N	2.49	0.46
1:E:437:PRO:O	1:E:440:VAL:HG23	2.16	0.45
1:E:693:ASN:N	1:E:716:ASN:OD1	2.40	0.45
1:F:555:LYS:HD2	1:F:581:MET:HE1	1.94	0.45
1:C:332:LEU:HD22	1:C:332:LEU:H	1.81	0.45
1:C:531:ARG:NH1	1:C:554:SER:HB2	2.30	0.45
1:C:544:LEU:HB3	1:C:566:HIS:CD2	2.47	0.45
1:D:117:GLU:OE1	1:D:118:ARG:NE	2.46	0.45
1:E:511:TYR:CE2	1:E:536:GLU:HB2	2.51	0.45
1:B:303:TYR:CD1	1:C:96:MET:CE	3.00	0.45
1:C:346:LEU:CD1	1:C:346:LEU:O	2.53	0.45
1:C:479:VAL:C	1:C:480:LYS:CD	2.76	0.45
1:D:297:ILE:O	1:D:300:MET:HB2	2.16	0.45
1:E:570:MET:HA	1:E:570:MET:CE	2.46	0.45
1:F:272:LYS:HA	1:F:275:ILE:CG2	2.46	0.45
1:F:555:LYS:CG	1:F:581:MET:HE1	2.44	0.45
1:F:616:GLU:HA	1:F:641:VAL:HB	1.98	0.45
1:G:57:LYS:CG	1:G:306:PHE:C	2.85	0.45
1:A:131:VAL:HG23	1:A:323:TYR:CZ	2.51	0.45
1:B:144:PHE:CD2	1:B:144:PHE:O	2.70	0.45
1:B:322:CYS:O	1:B:326:PHE:CD2	2.70	0.45
1:B:418:LEU:HG	1:B:428:LEU:HD13	1.98	0.45
1:C:170:TRP:CD1	1:C:400:LEU:HD13	2.52	0.45
1:C:392:LEU:HD23	1:C:392:LEU:O	2.16	0.45
1:E:46:GLN:O	1:E:50:ASP:HB3	2.16	0.45
1:E:431:ILE:O	1:E:432:MET:SD	2.75	0.45
1:F:268:LEU:O	1:F:271:ILE:HD11	2.14	0.45
1:F:430:LEU:CD1	1:F:451:LEU:CD1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:521:LEU:N	1:F:548:SER:O	2.48	0.45
1:F:538:LEU:HB3	1:F:541:LEU:HD12	1.97	0.45
1:B:411:PRO:CD	1:B:439:THR:HG21	2.42	0.45
1:E:397:GLU:HG2	1:E:401:LYS:HZ3	1.81	0.45
1:E:757:LEU:CD2	1:E:759:VAL:HG22	2.38	0.45
1:F:411:PRO:HA	1:F:414:LEU:HD12	1.99	0.45
1:F:550:LYS:NZ	1:F:573:HIS:HB2	2.32	0.45
1:F:614:LEU:HD11	1:F:616:GLU:O	2.16	0.45
1:E:106:GLN:NE2	1:F:108:TYR:HB3	2.32	0.45
1:E:132:LEU:HD22	1:E:132:LEU:N	2.30	0.45
1:E:238:ALA:HB3	1:E:400:LEU:HD21	1.98	0.45
1:F:510:MET:HE1	1:F:511:TYR:CG	2.51	0.45
1:B:28:THR:HA	1:B:330:TYR:CZ	2.52	0.45
1:B:161:ILE:O	1:B:388:PHE:CZ	2.69	0.45
1:B:239:LYS:HD3	1:B:404:ASN:HD22	1.82	0.45
1:B:414:LEU:HD22	1:B:428:LEU:HD21	1.99	0.45
1:C:449:LEU:HB2	1:C:469:LEU:HD11	1.97	0.45
1:E:241:LEU:HA	1:E:244:LYS:NZ	2.32	0.45
1:E:544:LEU:HB3	1:E:563:VAL:HG21	1.98	0.45
1:F:300:MET:HG2	1:G:57:LYS:HA	1.98	0.45
1:F:507:PRO:O	1:F:510:MET:CG	2.64	0.45
1:F:638:LYS:HD3	1:F:638:LYS:HA	1.79	0.45
1:F:650:THR:HA	1:F:672:ILE:CA	2.47	0.45
1:A:37:MET:N	1:A:37:MET:SD	2.90	0.45
1:B:57:LYS:HB3	1:B:305:ASN:HB3	1.98	0.45
1:B:251:HIS:C	1:B:251:HIS:ND1	2.69	0.45
1:C:151:SER:HB2	1:C:258:LEU:HD13	1.99	0.45
1:C:472:LEU:O	1:C:497:SER:N	2.38	0.45
1:C:513:LEU:O	1:C:541:LEU:HB2	2.17	0.45
1:D:111:ILE:CD1	1:D:297:ILE:HG21	2.47	0.45
1:D:123:TYR:CE2	1:D:283:LEU:O	2.70	0.45
1:E:166:PHE:CE1	1:E:387:ARG:HD2	2.51	0.45
1:E:238:ALA:HB1	1:E:391:PHE:CZ	2.51	0.45
1:E:485:ALA:O	1:E:489:LEU:CG	2.49	0.45
1:E:634:GLN:NE2	1:E:659:LEU:HG	2.31	0.45
1:E:759:VAL:O	1:E:762:ASN:ND2	2.50	0.45
1:B:503:MET:HE3	1:B:503:MET:CA	2.47	0.45
1:C:242:PHE:CD2	1:C:391:PHE:CE2	3.04	0.45
1:C:297:ILE:O	1:C:300:MET:HB3	2.17	0.45
1:C:437:PRO:HB2	1:C:440:VAL:HG23	1.98	0.45
1:C:490:LYS:HG2	1:C:513:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:ALA:HB2	1:E:482:HIS:ND1	2.32	0.45
1:E:712:SER:HA	1:E:735:LYS:HB2	1.98	0.45
1:F:123:TYR:HD1	1:F:283:LEU:HD22	1.82	0.45
1:F:348:GLU:OE2	1:F:365:ASP:HB3	2.17	0.45
1:F:426:LEU:HB3	1:F:446:LEU:HA	1.97	0.45
1:B:153:SER:OG	1:B:154:LYS:NZ	2.40	0.45
1:B:503:MET:CE	1:B:506:LEU:CB	2.93	0.45
1:C:363:ILE:CG2	1:C:392:LEU:HD22	2.44	0.45
1:C:390:LEU:O	1:C:393:SER:N	2.49	0.45
1:E:463:ILE:HD11	1:E:489:LEU:HD21	1.90	0.45
1:E:554:SER:HB2	1:E:580:VAL:HG22	1.99	0.45
1:F:459:ILE:HG22	1:F:481:ILE:HA	1.98	0.45
1:F:557:PRO:O	1:F:584:ASN:ND2	2.50	0.45
1:C:37:MET:HA	1:C:40:VAL:HG12	1.99	0.44
1:E:121:HIS:CE1	1:E:123:TYR:HB3	2.53	0.44
1:E:341:LEU:HA	1:E:341:LEU:HD23	1.83	0.44
1:F:726:TYR:HD1	1:F:751:LEU:HD23	1.82	0.44
1:B:43:CYS:SG	1:B:132:LEU:HD23	2.57	0.44
1:B:137:VAL:HB	1:B:272:LYS:NZ	2.32	0.44
1:B:252:VAL:HB	1:B:370:PHE:CE2	2.51	0.44
1:B:409:TRP:CE2	1:B:433:LEU:HD21	2.52	0.44
1:C:300:MET:HE3	1:D:57:LYS:HA	1.99	0.44
1:F:273:PHE:HD2	1:F:274:LEU:HD22	1.80	0.44
1:F:721:LEU:HB2	1:F:725:LEU:HD21	1.99	0.44
1:B:297:ILE:CG1	1:B:300:MET:HE2	2.48	0.44
1:B:425:ARG:HG2	1:B:447:GLN:HG2	2.00	0.44
1:B:472:LEU:O	1:B:497:SER:N	2.44	0.44
1:F:271:ILE:CD1	1:F:271:ILE:C	2.83	0.44
1:F:458:MET:SD	1:F:481:ILE:O	2.76	0.44
1:F:740:SER:HA	1:F:763:HIS:ND1	2.33	0.44
1:E:246:LYS:O	1:E:249:ARG:HG2	2.17	0.44
1:E:497:SER:HA	1:E:520:TYR:HB2	1.99	0.44
1:F:132:LEU:C	1:F:136:LEU:HD23	2.34	0.44
1:E:452:GLU:HG2	1:E:475:HIS:HB2	1.99	0.44
1:F:121:HIS:ND1	1:F:123:TYR:HB3	2.33	0.44
1:F:157:HIS:ND1	1:F:248:PHE:HD2	2.16	0.44
1:F:283:LEU:HD23	1:F:283:LEU:HA	1.84	0.44
1:G:57:LYS:HD2	1:G:292:ASP:OD2	2.18	0.44
1:G:100:LYS:HG3	1:G:100:LYS:O	2.17	0.44
1:G:297:ILE:O	1:G:297:ILE:HG22	2.17	0.44
1:A:318:LYS:HA	1:A:318:LYS:HD3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ARG:NH2	1:B:305:ASN:OD1	2.51	0.44
1:B:363:ILE:N	1:B:364:PRO:HD3	2.32	0.44
1:E:738:LYS:HA	1:E:761:GLY:HA3	2.00	0.44
1:F:120:LEU:HD12	1:F:120:LEU:HA	1.81	0.44
1:F:452:GLU:HG3	1:F:475:HIS:CG	2.53	0.44
1:F:671:LYS:O	1:F:694:ASP:OD2	2.35	0.44
1:G:57:LYS:NZ	1:G:57:LYS:HB3	2.33	0.44
1:A:309:ASN:HD21	1:G:114:MET:HE1	1.82	0.44
1:B:441:PHE:HA	1:B:466:LEU:HD21	2.00	0.44
1:C:376:MET:SD	1:C:376:MET:O	2.75	0.44
1:E:768:PRO:HA	1:E:769:PRO:HD3	1.92	0.44
1:F:360:ILE:HG13	1:F:360:ILE:O	2.18	0.44
1:B:54:CYS:O	1:B:55:LEU:HD12	2.17	0.44
1:B:157:HIS:CE1	1:B:248:PHE:HB2	2.53	0.44
1:C:425:ARG:HE	1:C:470:GLN:HB3	1.82	0.44
1:F:263:VAL:HG13	1:F:341:LEU:HD21	2.00	0.44
1:B:145:TRP:CZ3	1:B:262:TYR:CE2	3.04	0.44
1:C:452:GLU:O	1:C:454:ILE:HG13	2.18	0.44
1:C:478:SER:O	1:C:480:LYS:CE	2.65	0.44
1:C:525:LEU:CD2	1:C:533:VAL:CB	2.95	0.44
1:E:165:CYS:SG	1:E:388:PHE:HA	2.57	0.44
1:E:427:GLU:HA	1:E:448:SER:O	2.18	0.44
1:E:725:LEU:HD11	1:E:726:TYR:CE1	2.53	0.44
1:G:57:LYS:CD	1:G:306:PHE:C	2.87	0.44
1:B:370:PHE:CD1	1:B:373:MET:CE	3.01	0.43
1:C:127:PHE:HD2	1:C:128:PRO:CD	2.31	0.43
1:C:357:GLU:HG2	1:C:358:THR:N	2.32	0.43
1:E:249:ARG:O	1:E:253:GLU:HG3	2.18	0.43
1:E:507:PRO:HA	1:E:508:PRO:HD3	1.88	0.43
1:F:732:LYS:HA	1:F:754:LEU:HA	2.00	0.43
1:G:122:TRP:HA	1:G:125:LYS:HE2	2.00	0.43
1:B:38:ILE:HD11	1:B:326:PHE:CE2	2.53	0.43
1:B:157:HIS:CE1	1:B:161:ILE:HG21	2.53	0.43
1:B:286:LYS:HA	1:B:286:LYS:HD2	1.78	0.43
1:C:394:GLU:HG3	1:C:398:ASN:HD21	1.83	0.43
1:C:490:LYS:O	1:C:514:ARG:HG3	2.17	0.43
1:F:138:PHE:HD2	1:F:330:TYR:CZ	2.35	0.43
1:G:131:VAL:HG13	1:G:323:TYR:CZ	2.54	0.43
1:C:458:MET:SD	1:C:480:LYS:HB2	2.57	0.43
1:E:103:LEU:HD11	1:E:303:TYR:CE2	2.53	0.43
1:E:430:LEU:O	1:E:452:GLU:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:LEU:HD23	1:F:336:TYR:N	2.33	0.43
1:F:721:LEU:HD21	1:F:743:VAL:O	2.17	0.43
1:B:357:GLU:CD	1:B:358:THR:HG23	2.38	0.43
1:C:104:ASP:N	1:C:107:GLN:OE1	2.51	0.43
1:C:127:PHE:CD2	1:C:127:PHE:C	2.92	0.43
1:E:353:TYR:O	1:E:357:GLU:N	2.31	0.43
1:E:449:LEU:HD21	1:E:451:LEU:HD11	1.99	0.43
1:F:714:THR:HA	1:F:737:GLY:HA3	2.01	0.43
1:B:289:PHE:HD2	1:B:314:HIS:HB2	1.84	0.43
1:B:297:ILE:N	1:B:300:MET:HE1	2.26	0.43
1:C:100:LYS:HE3	1:C:100:LYS:HB2	1.78	0.43
1:C:395:VAL:HA	1:C:398:ASN:HD22	1.84	0.43
1:D:122:TRP:HB2	1:D:126:TYR:CE2	2.54	0.43
1:E:464:ALA:HA	1:E:488:PHE:CE1	2.53	0.43
1:F:669:HIS:HA	1:F:692:TYR:HB2	2.01	0.43
1:C:459:ILE:HB	1:C:481:ILE:HG22	2.00	0.43
1:C:546:ILE:HG12	1:C:569:LYS:HB3	2.00	0.43
1:E:39:GLY:CA	1:E:131:VAL:HG11	2.48	0.43
1:E:362:ASP:OD2	1:E:393:SER:OG	2.21	0.43
1:E:426:LEU:HB3	1:E:447:GLN:H	1.83	0.43
1:E:651:TYR:HE1	1:E:674:VAL:H	1.66	0.43
1:F:476:GLN:N	1:F:499:LYS:O	2.48	0.43
1:F:499:LYS:HA	1:F:522:VAL:HB	1.99	0.43
1:A:52:ILE:HD11	1:A:309:ASN:HA	2.01	0.43
1:B:354:VAL:HG12	1:B:360:ILE:HD11	2.00	0.43
1:C:262:TYR:HE2	1:C:341:LEU:CD1	2.26	0.43
1:F:48:MET:SD	1:F:48:MET:O	2.77	0.43
1:F:110:PHE:CD2	1:G:55:LEU:HD11	2.53	0.43
1:F:369:ASP:O	1:F:373:MET:HE2	2.18	0.43
1:F:432:MET:SD	1:F:453:ILE:O	2.76	0.43
1:A:127:PHE:CD2	1:A:127:PHE:C	2.92	0.43
1:B:46:GLN:NE2	1:B:129:TYR:CZ	2.87	0.43
1:B:481:ILE:HD13	1:B:489:LEU:HD12	2.01	0.43
1:C:494:LYS:C	1:C:516:LEU:CD1	2.87	0.43
1:E:268:LEU:HA	1:E:271:ILE:CD1	2.49	0.43
1:E:268:LEU:HA	1:E:271:ILE:HG12	1.99	0.43
1:E:367:LYS:HD3	1:E:368:ASN:N	2.32	0.43
1:F:158:PHE:HA	1:F:161:ILE:HG12	2.01	0.43
1:F:444:THR:O	1:F:468:ASN:HB3	2.18	0.43
1:F:472:LEU:O	1:F:496:LEU:CD1	2.64	0.43
1:B:170:TRP:NE1	1:B:400:LEU:HD13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ILE:HD13	1:B:277:ILE:N	2.34	0.43
1:B:419:GLN:O	1:B:427:GLU:N	2.37	0.43
1:C:272:LYS:HA	1:C:275:ILE:HG12	2.01	0.43
1:C:363:ILE:CA	1:C:392:LEU:CD2	2.86	0.43
1:C:509:TRP:CE3	1:C:513:LEU:HD21	2.54	0.43
1:E:701:GLU:O	1:E:704:VAL:HG22	2.18	0.43
1:F:240:ALA:CA	1:F:243:GLU:OE2	2.67	0.43
1:F:496:LEU:HD12	1:F:497:SER:H	1.84	0.43
1:B:273:PHE:CD2	1:B:273:PHE:C	2.92	0.43
1:B:441:PHE:CD1	1:B:462:THR:OG1	2.72	0.43
1:C:155:ILE:O	1:C:159:ILE:HG12	2.19	0.43
1:E:782:LEU:HD12	1:E:782:LEU:HA	1.87	0.43
1:F:246:LYS:HB3	1:F:246:LYS:HE2	1.82	0.43
1:F:293:CYS:SG	1:F:306:PHE:HB2	2.59	0.43
1:F:347:ARG:HB3	1:F:368:ASN:ND2	2.33	0.43
1:F:363:ILE:HG12	1:F:392:LEU:HD22	2.01	0.43
1:F:713:ILE:HD12	1:F:718:VAL:HG21	2.00	0.43
1:B:28:THR:CB	1:B:330:TYR:CZ	3.02	0.42
1:B:156:GLU:HA	1:B:159:ILE:HG12	2.00	0.42
1:C:293:CYS:HB2	1:C:295:VAL:HG23	2.01	0.42
1:E:155:ILE:HD13	1:E:155:ILE:N	2.34	0.42
1:E:486:LEU:O	1:E:490:LYS:HG3	2.19	0.42
1:F:329:ILE:HD13	1:F:329:ILE:N	2.34	0.42
1:F:618:ASP:CB	1:F:643:LYS:HB2	2.49	0.42
1:B:113:GLN:NE2	1:C:311:THR:HG22	2.33	0.42
1:C:367:LYS:HE3	1:C:367:LYS:HB3	1.84	0.42
1:C:475:HIS:CD2	1:C:499:LYS:HG3	2.54	0.42
1:E:134:HIS:CE1	1:E:276:ILE:HD11	2.53	0.42
1:E:376:MET:SD	1:E:376:MET:O	2.77	0.42
1:E:415:ARG:HA	1:E:418:LEU:HD12	2.01	0.42
1:F:114:MET:CE	1:F:295:VAL:HG12	2.43	0.42
1:F:164:LYS:HE2	1:F:241:LEU:HD13	2.01	0.42
1:F:249:ARG:HA	1:F:370:PHE:CZ	2.54	0.42
1:F:494:LYS:HB3	1:F:517:GLU:OE1	2.19	0.42
1:G:127:PHE:CD2	1:G:316:PHE:HD2	2.36	0.42
1:C:137:VAL:HG11	1:C:272:LYS:HD2	2.00	0.42
1:E:37:MET:CE	1:E:38:ILE:CA	2.97	0.42
1:E:244:LYS:HA	1:E:247:LYS:HG2	2.01	0.42
1:E:376:MET:HE1	1:E:377:ILE:HD13	1.68	0.42
1:E:627:ILE:O	1:E:630:ILE:HG12	2.19	0.42
1:E:631:VAL:HG13	1:E:655:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:MET:HA	1:F:48:MET:CE	2.48	0.42
1:F:388:PHE:CD2	1:F:388:PHE:C	2.91	0.42
1:F:759:VAL:HG23	1:F:784:VAL:HG12	2.01	0.42
1:F:777:LEU:C	1:F:800:MET:HE3	2.40	0.42
1:A:102:ASP:HB2	1:B:100:LYS:HE2	2.01	0.42
1:C:35:MET:CE	1:C:326:PHE:HB3	2.49	0.42
1:C:545:LYS:O	1:C:569:LYS:N	2.52	0.42
1:E:647:ASN:HB2	1:E:670:ASN:HD21	1.85	0.42
1:E:743:VAL:O	1:E:764:PHE:CE1	2.65	0.42
1:F:381:ASP:HB3	1:F:384:TYR:CD2	2.51	0.42
1:F:555:LYS:CA	1:F:581:MET:HE1	2.43	0.42
1:F:571:CYS:HB3	1:F:573:HIS:NE2	2.34	0.42
1:F:708:LEU:HB3	1:F:731:LEU:HD21	2.00	0.42
1:F:721:LEU:O	1:F:721:LEU:HD12	2.19	0.42
1:C:101:THR:OG1	1:C:108:TYR:OH	2.37	0.42
1:F:347:ARG:O	1:F:368:ASN:HA	2.20	0.42
1:F:654:GLU:HG3	1:F:678:HIS:CD2	2.54	0.42
1:B:406:ASN:ND2	1:B:437:PRO:HA	2.35	0.42
1:C:253:GLU:HB3	1:C:367:LYS:HG3	2.02	0.42
1:C:256:ASP:HA	1:C:369:ASP:HB2	2.02	0.42
1:E:744:LEU:HD12	1:E:764:PHE:CE2	2.53	0.42
1:F:168:SER:O	1:F:171:THR:OG1	2.25	0.42
1:F:240:ALA:HA	1:F:243:GLU:OE2	2.20	0.42
1:F:300:MET:CE	1:G:55:LEU:HD12	2.49	0.42
1:B:402:GLN:OE1	1:B:406:ASN:ND2	2.52	0.42
1:E:130:LEU:CG	1:E:279:TYR:HH	2.30	0.42
1:E:449:LEU:HD12	1:E:449:LEU:C	2.38	0.42
1:E:503:MET:SD	1:E:503:MET:O	2.77	0.42
1:F:429:PRO:CA	1:F:450:LYS:HE3	2.44	0.42
1:F:561:VAL:HG13	1:F:587:LYS:HD2	2.01	0.42
1:F:588:MET:CE	1:F:588:MET:HA	2.50	0.42
1:G:46:GLN:HA	1:G:50:ASP:HB2	2.02	0.42
1:B:488:PHE:O	1:B:492:ASN:HB2	2.20	0.42
1:C:158:PHE:HB2	1:C:248:PHE:CZ	2.55	0.42
1:D:102:ASP:HB2	1:E:100:LYS:HE3	2.02	0.42
1:E:375:HIS:O	1:E:379:GLN:HG2	2.20	0.42
1:E:620:LYS:HA	1:E:645:TRP:HB2	2.02	0.42
1:F:50:ASP:OD2	1:F:50:ASP:O	2.37	0.42
1:A:329:ILE:HG13	1:A:330:TYR:N	2.33	0.42
1:B:170:TRP:CZ3	1:B:390:LEU:HD11	2.55	0.42
1:B:322:CYS:O	1:B:326:PHE:CE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:TYR:HD2	1:B:375:HIS:CE1	2.37	0.42
1:E:54:CYS:SG	1:E:115:CYS:HB3	2.60	0.42
1:E:578:LYS:HA	1:E:599:CYS:O	2.20	0.42
1:E:676:PRO:HG2	1:E:679:LEU:HD23	2.00	0.42
1:B:56:PRO:HB3	1:B:303:TYR:CG	2.55	0.42
1:B:453:ILE:HD13	1:B:455:LYS:HZ1	1.84	0.42
1:C:428:LEU:HD12	1:C:428:LEU:HA	1.71	0.42
1:E:106:GLN:O	1:E:109:SER:OG	2.32	0.42
1:E:256:ASP:H	1:E:369:ASP:HB3	1.85	0.42
1:E:458:MET:HG2	1:E:480:LYS:HB2	2.01	0.42
1:E:550:LYS:HD2	1:E:550:LYS:HA	1.92	0.42
1:E:760:LYS:HZ2	1:E:785:GLU:HA	1.82	0.42
1:F:170:TRP:CE2	1:F:400:LEU:HD13	2.54	0.42
1:F:432:MET:CE	1:F:432:MET:CA	2.97	0.42
1:F:556:ILE:O	1:F:584:ASN:ND2	2.53	0.42
1:B:289:PHE:CD2	1:B:314:HIS:HB2	2.55	0.41
1:E:41:PHE:HE1	1:E:45:LEU:HD21	1.76	0.41
1:E:778:LYS:O	1:E:782:LEU:N	2.48	0.41
1:F:54:CYS:O	1:F:55:LEU:HD12	2.20	0.41
1:F:145:TRP:CD1	1:F:261:MET:CE	3.00	0.41
1:F:570:MET:HE3	1:F:572:ILE:HG12	2.02	0.41
1:F:634:GLN:O	1:F:637:ARG:NE	2.53	0.41
1:F:711:PHE:HB3	1:F:734:LEU:HD12	2.01	0.41
1:B:50:ASP:HA	1:B:312:MET:SD	2.60	0.41
1:B:107:GLN:O	1:B:111:ILE:HG12	2.20	0.41
1:B:251:HIS:ND1	1:B:251:HIS:O	2.54	0.41
1:C:441:PHE:HA	1:C:466:LEU:HD21	2.02	0.41
1:D:111:ILE:HD11	1:D:306:PHE:CZ	2.54	0.41
1:E:137:VAL:HB	1:E:272:LYS:HZ1	1.84	0.41
1:E:614:LEU:HB3	1:E:636:LEU:HD13	2.01	0.41
1:E:659:LEU:HD23	1:E:659:LEU:HA	1.96	0.41
1:F:355:ARG:HG3	1:F:361:ASP:HA	2.02	0.41
1:F:672:ILE:HD12	1:F:672:ILE:HA	1.84	0.41
1:G:102:ASP:OD1	1:G:102:ASP:N	2.53	0.41
1:G:117:GLU:OE1	1:G:118:ARG:CD	2.67	0.41
1:A:309:ASN:OD1	1:G:113:GLN:OE1	2.38	0.41
1:C:101:THR:HG1	1:C:108:TYR:HH	1.67	0.41
1:C:106:GLN:OE1	1:D:108:TYR:CG	2.73	0.41
1:C:262:TYR:CD2	1:C:262:TYR:C	2.94	0.41
1:C:349:TYR:HD1	1:C:375:HIS:CE1	2.38	0.41
1:E:57:LYS:HD3	1:E:307:SER:OG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:LEU:CD2	1:E:132:LEU:H	2.33	0.41
1:E:398:ASN:HA	1:E:401:LYS:HE2	2.01	0.41
1:E:426:LEU:HB3	1:E:446:LEU:HA	2.01	0.41
1:E:526:SER:CB	1:E:531:ARG:NE	2.77	0.41
1:F:511:TYR:CE2	1:F:536:GLU:HB2	2.55	0.41
1:F:538:LEU:HD12	1:F:560:VAL:HA	2.02	0.41
1:B:165:CYS:HB2	1:B:388:PHE:CE1	2.53	0.41
1:D:291:VAL:HG23	1:D:308:CYS:HB2	2.03	0.41
1:E:383:LEU:HA	1:E:386:LYS:HB3	2.02	0.41
1:E:507:PRO:HB2	1:E:509:TRP:CE2	2.55	0.41
1:F:569:LYS:NZ	1:F:595:GLU:OE1	2.52	0.41
1:B:293:CYS:SG	1:B:306:PHE:HB2	2.60	0.41
1:E:272:LYS:O	1:E:275:ILE:HG12	2.21	0.41
1:E:346:LEU:HB3	1:E:375:HIS:CD2	2.56	0.41
1:E:646:HIS:HA	1:E:669:HIS:O	2.20	0.41
1:B:134:HIS:ND1	1:B:276:ILE:HD11	2.29	0.41
1:B:168:SER:O	1:B:171:THR:OG1	2.30	0.41
1:B:425:ARG:HD2	1:B:471:GLU:OE1	2.21	0.41
1:C:286:LYS:HA	1:C:286:LYS:HD2	1.82	0.41
1:C:473:SER:HA	1:C:497:SER:HB3	2.02	0.41
1:C:563:VAL:O	1:C:566:HIS:N	2.45	0.41
1:E:467:ASP:HA	1:E:488:PHE:HZ	1.85	0.41
1:E:675:LEU:H	1:E:675:LEU:HD23	1.85	0.41
1:E:726:TYR:CZ	1:E:745:SER:HB3	2.55	0.41
1:F:597:VAL:HA	1:F:620:LYS:HB3	2.01	0.41
1:B:337:THR:HA	1:B:340:TRP:HB3	2.03	0.41
1:B:347:ARG:O	1:B:368:ASN:HA	2.20	0.41
1:B:463:ILE:HD12	1:B:466:LEU:HD12	2.02	0.41
1:E:58:ARG:HD2	1:E:305:ASN:ND2	2.36	0.41
1:E:130:LEU:CD2	1:E:279:TYR:HH	2.30	0.41
1:E:170:TRP:CD2	1:E:400:LEU:HD22	2.56	0.41
1:E:474:LEU:HD23	1:E:474:LEU:HA	1.90	0.41
1:E:511:TYR:CD2	1:E:536:GLU:HB2	2.56	0.41
1:F:238:ALA:HB1	1:F:391:PHE:HZ	1.85	0.41
1:F:643:LYS:HB3	1:F:645:TRP:HD1	1.84	0.41
1:A:127:PHE:CD2	1:A:316:PHE:CE2	3.09	0.41
1:B:346:LEU:HD22	1:B:375:HIS:CD2	2.55	0.41
1:C:158:PHE:HB2	1:C:248:PHE:HZ	1.86	0.41
1:E:242:PHE:CE2	1:E:400:LEU:HD23	2.44	0.41
1:E:444:THR:HA	1:E:466:LEU:HG	2.03	0.41
1:E:654:GLU:HA	1:E:678:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLN:NE2	1:B:108:TYR:HB3	2.36	0.41
1:B:130:LEU:O	1:B:133:ILE:HG22	2.21	0.41
1:B:418:LEU:HD22	1:B:426:LEU:HG	2.03	0.41
1:B:425:ARG:HH11	1:B:471:GLU:HB2	1.86	0.41
1:B:453:ILE:HD13	1:B:453:ILE:HA	1.85	0.41
1:C:41:PHE:CD2	1:C:45:LEU:HD13	2.56	0.41
1:C:239:LYS:HE3	1:C:401:LYS:HG2	2.02	0.41
1:C:517:GLU:HA	1:C:543:SER:O	2.21	0.41
1:E:164:LYS:HZ3	1:E:244:LYS:HE3	1.85	0.41
1:E:543:SER:O	1:E:543:SER:OG	2.35	0.41
1:E:578:LYS:NZ	1:E:601:LEU:O	2.52	0.41
1:E:582:LEU:HD23	1:E:585:LEU:HD23	2.01	0.41
1:F:48:MET:SD	1:F:48:MET:C	2.99	0.41
1:F:273:PHE:CZ	1:F:331:GLY:HA3	2.56	0.41
1:F:618:ASP:OD1	1:F:619:LEU:N	2.54	0.41
1:F:644:LEU:HD23	1:F:644:LEU:HA	1.83	0.41
1:B:149:PRO:HB2	1:C:380:TYR:CE1	2.56	0.41
1:B:171:THR:HA	1:B:390:LEU:HD21	2.01	0.41
1:C:95:GLU:HG2	1:C:96:MET:N	2.36	0.41
1:C:298:GLN:C	1:C:300:MET:H	2.22	0.41
1:C:433:LEU:HD23	1:C:433:LEU:HA	1.98	0.41
1:C:448:SER:HA	1:C:471:GLU:O	2.21	0.41
1:C:474:LEU:HB2	1:C:498:VAL:HA	2.02	0.41
1:E:433:LEU:HD23	1:E:433:LEU:HA	1.89	0.41
1:E:646:HIS:HD2	1:E:669:HIS:HB2	1.86	0.41
1:E:673:GLU:O	1:E:695:ILE:HD13	2.21	0.41
1:F:276:ILE:HA	1:F:279:TYR:CE2	2.56	0.41
1:F:782:LEU:CD1	1:F:784:VAL:CG1	2.86	0.41
1:G:284:VAL:HG21	1:G:324:LEU:HD11	2.03	0.41
1:A:133:ILE:O	1:A:137:VAL:HG13	2.21	0.40
1:B:376:MET:CE	1:B:377:ILE:CD1	2.97	0.40
1:C:137:VAL:HB	1:C:272:LYS:HZ2	1.86	0.40
1:C:425:ARG:NE	1:C:470:GLN:HB3	2.36	0.40
1:E:54:CYS:O	1:E:55:LEU:HD22	2.21	0.40
1:E:127:PHE:HB3	1:E:128:PRO:HD3	2.03	0.40
1:E:683:ASN:O	1:E:707:SER:OG	2.23	0.40
1:E:766:ILE:HA	1:E:791:THR:HG21	2.02	0.40
1:F:367:LYS:HE3	1:F:367:LYS:HB3	1.88	0.40
1:F:424:ASN:O	1:F:424:ASN:ND2	2.54	0.40
1:F:461:ALA:HB2	1:F:482:HIS:CE1	2.56	0.40
1:F:712:SER:HA	1:F:735:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:TYR:HD1	1:B:30:TYR:HA	1.74	0.40
1:B:126:TYR:CB	1:B:130:LEU:HD21	2.51	0.40
1:B:253:GLU:HG2	1:B:367:LYS:HB2	2.03	0.40
1:B:303:TYR:CD1	1:C:96:MET:HE1	2.56	0.40
1:E:463:ILE:CD1	1:E:489:LEU:HD23	2.48	0.40
1:E:663:GLU:CD	1:E:686:ARG:HH12	2.24	0.40
1:F:277:ILE:HD13	1:F:277:ILE:HA	1.93	0.40
1:F:654:GLU:HG3	1:F:678:HIS:NE2	2.36	0.40
1:B:351:PHE:C	1:B:353:TYR:H	2.25	0.40
1:D:310:HIS:CE1	1:D:312:MET:H	2.39	0.40
1:E:117:GLU:OE1	1:E:118:ARG:HA	2.21	0.40
1:E:380:TYR:HE2	1:E:384:TYR:CE2	2.39	0.40
1:E:598:HIS:ND1	1:E:621:GLU:OE1	2.54	0.40
1:E:673:GLU:C	1:E:695:ILE:HD13	2.42	0.40
1:E:735:LYS:HE2	1:E:735:LYS:HB3	1.85	0.40
1:F:246:LYS:HA	1:F:249:ARG:HG2	2.03	0.40
1:F:286:LYS:HA	1:F:286:LYS:HD2	1.79	0.40
1:F:512:GLY:HA2	1:F:540:ASP:OD2	2.21	0.40
1:B:297:ILE:HD12	1:B:300:MET:HE2	2.00	0.40
1:C:105:LEU:HD12	1:C:106:GLN:N	2.37	0.40
1:C:421:ASN:HD21	1:C:425:ARG:HB2	1.87	0.40
1:E:441:PHE:HA	1:E:466:LEU:HD11	2.04	0.40
1:E:556:ILE:HG23	1:E:584:ASN:HB2	2.03	0.40
1:E:638:LYS:HA	1:E:638:LYS:HD3	1.92	0.40
1:E:706:GLN:NE2	1:E:729:LYS:H	2.20	0.40
1:F:144:PHE:HA	1:F:147:LYS:HB2	2.04	0.40
1:F:415:ARG:HA	1:F:418:LEU:HD12	2.03	0.40
1:F:547:LEU:O	1:F:571:CYS:N	2.54	0.40
1:F:625:LYS:HE3	1:F:625:LYS:HB2	1.85	0.40
1:C:127:PHE:O	1:C:130:LEU:HG	2.22	0.40
1:C:506:LEU:HD12	1:C:507:PRO:HD2	2.04	0.40
1:E:458:MET:SD	1:E:482:HIS:N	2.88	0.40
1:E:755:SER:HB3	1:E:776:ALA:HB1	2.03	0.40
1:F:136:LEU:HD22	1:F:136:LEU:H	1.87	0.40
1:F:519:LEU:O	1:F:548:SER:N	2.53	0.40
1:F:569:LYS:HZ3	1:F:593:GLU:HB3	1.87	0.40
1:F:673:GLU:HA	1:F:694:ASP:C	2.41	0.40
1:F:726:TYR:HA	1:F:751:LEU:HD21	2.04	0.40
1:F:778:LYS:N	1:F:800:MET:CE	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	116/811 (14%)	109 (94%)	7 (6%)	0	100 100
1	B	408/811 (50%)	383 (94%)	25 (6%)	0	100 100
1	C	450/811 (56%)	418 (93%)	32 (7%)	0	100 100
1	D	102/811 (13%)	97 (95%)	5 (5%)	0	100 100
1	E	684/811 (84%)	640 (94%)	44 (6%)	0	100 100
1	F	684/811 (84%)	629 (92%)	55 (8%)	0	100 100
1	G	110/811 (14%)	104 (94%)	6 (6%)	0	100 100
All	All	2554/5677 (45%)	2380 (93%)	174 (7%)	0	100 100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	112/756 (15%)	109 (97%)	3 (3%)	40 60
1	B	384/756 (51%)	371 (97%)	13 (3%)	32 53
1	C	422/756 (56%)	412 (98%)	10 (2%)	44 63
1	D	100/756 (13%)	96 (96%)	4 (4%)	27 48
1	E	642/756 (85%)	628 (98%)	14 (2%)	47 66
1	F	642/756 (85%)	624 (97%)	18 (3%)	38 59
1	G	107/756 (14%)	105 (98%)	2 (2%)	52 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2409/5292 (46%)	2345 (97%)	64 (3%)	41 60

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	MET
1	A	127	PHE
1	A	129	TYR
1	B	27	PHE
1	B	50	ASP
1	B	144	PHE
1	B	251	HIS
1	B	273	PHE
1	B	300	MET
1	B	326	PHE
1	B	330	TYR
1	B	372	PHE
1	B	388	PHE
1	B	415	ARG
1	B	473	SER
1	B	503	MET
1	C	41	PHE
1	C	127	PHE
1	C	262	TYR
1	C	336	TYR
1	C	376	MET
1	C	390	LEU
1	C	391	PHE
1	C	493	LEU
1	C	540	ASP
1	C	555	LYS
1	D	50	ASP
1	D	123	TYR
1	D	127	PHE
1	D	292	ASP
1	E	37	MET
1	E	48	MET
1	E	104	ASP
1	E	123	TYR
1	E	139	MET
1	E	144	PHE
1	E	279	TYR

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Mol	Chain	Res	Type
1	E	456	ASN
1	E	555	LYS
1	E	570	MET
1	E	671	LYS
1	E	725	LEU
1	E	764	PHE
1	E	766	ILE
1	F	41	PHE
1	F	138	PHE
1	F	261	MET
1	F	268	LEU
1	F	283	LEU
1	F	296	ASP
1	F	299	ASP
1	F	388	PHE
1	F	391	PHE
1	F	450	LYS
1	F	458	MET
1	F	510	MET
1	F	531	ARG
1	F	555	LYS
1	F	581	MET
1	F	666	SER
1	F	759	VAL
1	F	765	GLU
1	G	102	ASP
1	G	104	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	GLN
1	B	134	HIS
1	B	375	HIS
1	B	404	ASN
1	B	419	GLN
1	C	288	GLN
1	C	398	ASN
1	C	406	ASN
1	C	566	HIS
1	E	375	HIS
1	E	670	ASN

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Mol	Chain	Res	Type
1	E	678	HIS
1	F	106	GLN
1	F	310	HIS
1	F	492	ASN
1	F	678	HIS
1	G	106	GLN
1	G	112	ASN
1	G	121	HIS

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no 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.

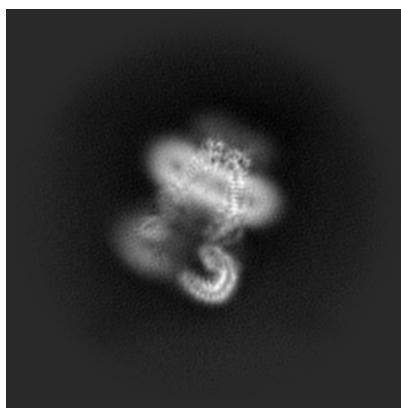
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-50123. These allow visual inspection of the internal detail of the map and identification of artifacts.

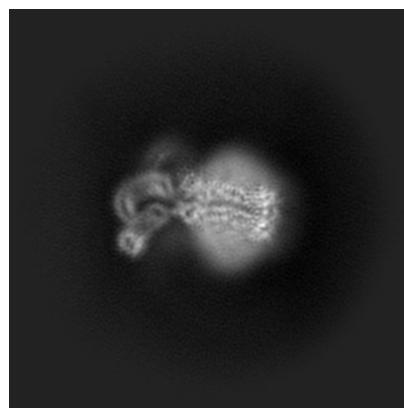
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections (i)

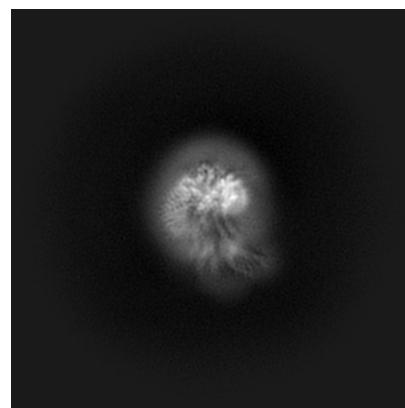
#### 6.1.1 Primary map



X

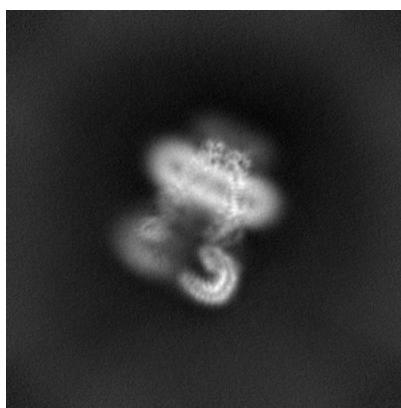


Y

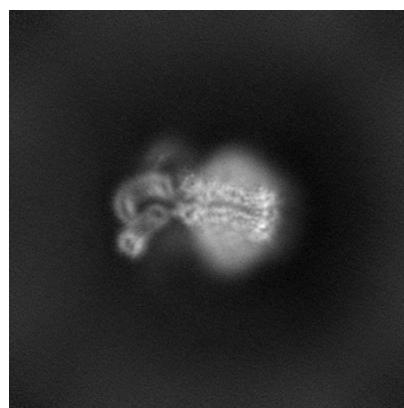


Z

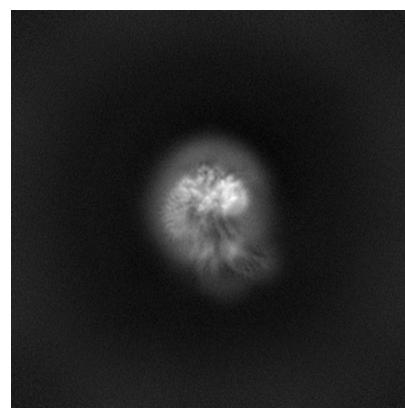
#### 6.1.2 Raw map



X



Y

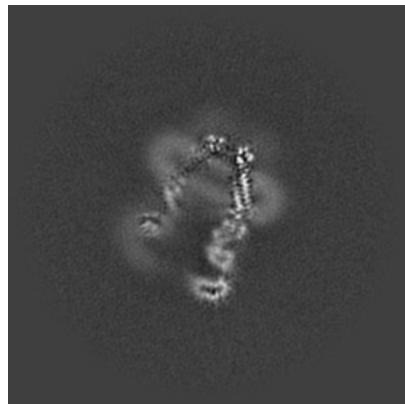


Z

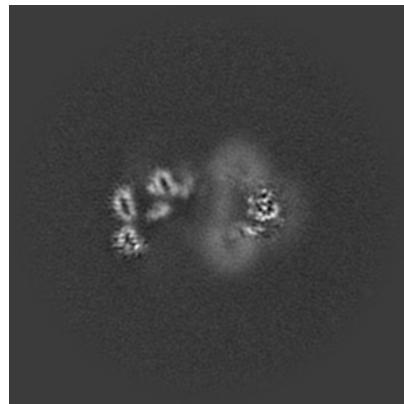
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [\(i\)](#)

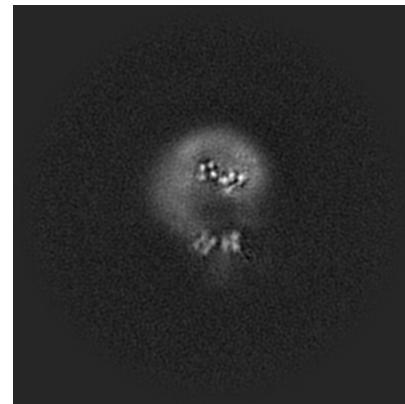
### 6.2.1 Primary map



X Index: 168



Y Index: 168

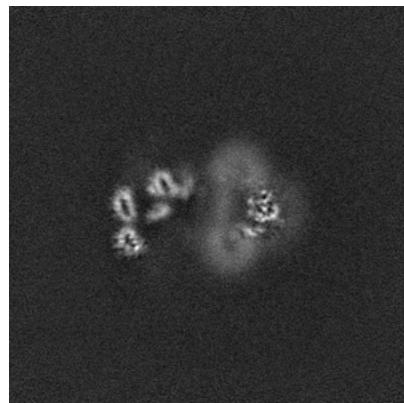


Z Index: 168

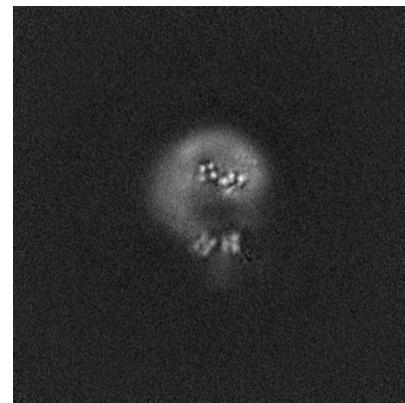
### 6.2.2 Raw map



X Index: 168



Y Index: 168



Z Index: 168

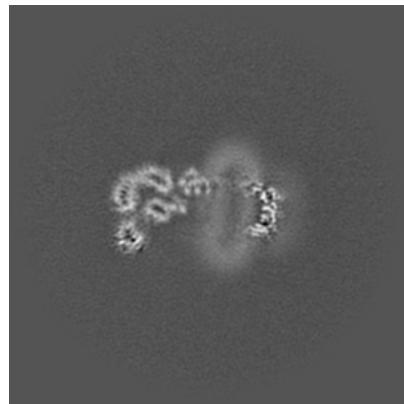
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

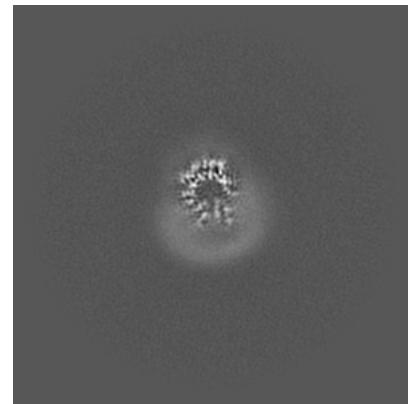
### 6.3.1 Primary map



X Index: 165



Y Index: 178

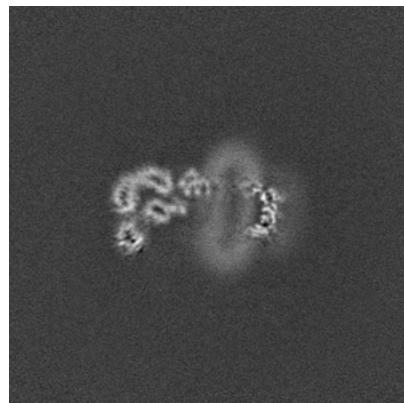


Z Index: 208

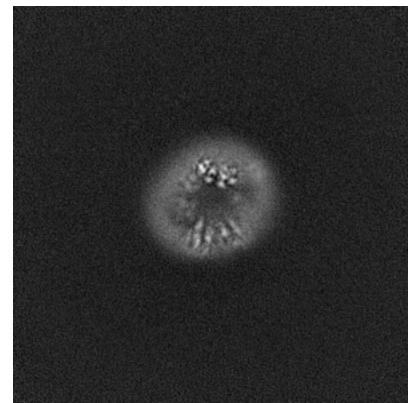
### 6.3.2 Raw map



X Index: 165



Y Index: 178

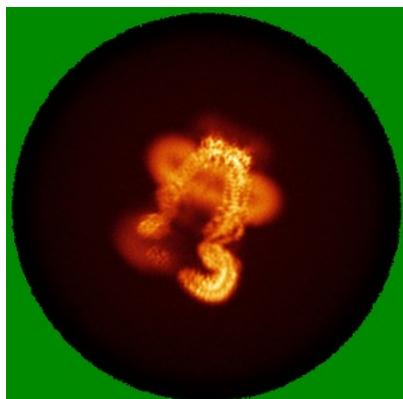


Z Index: 190

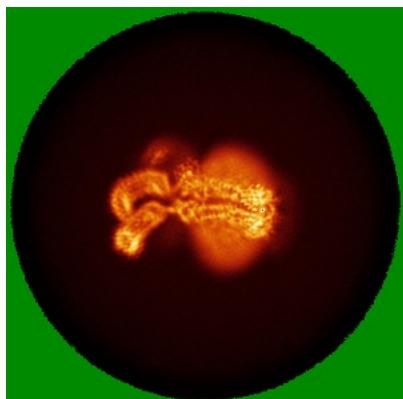
The images above show the largest variance slices of the map in three orthogonal directions.

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

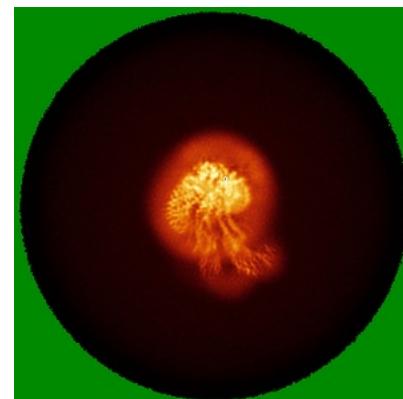
### 6.4.1 Primary map



X

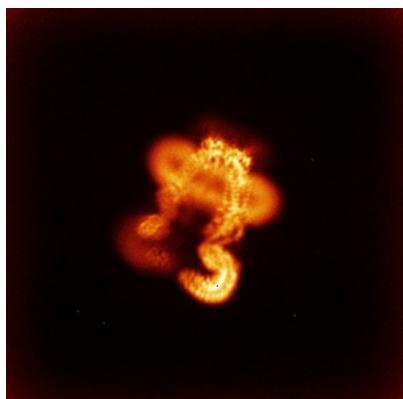


Y

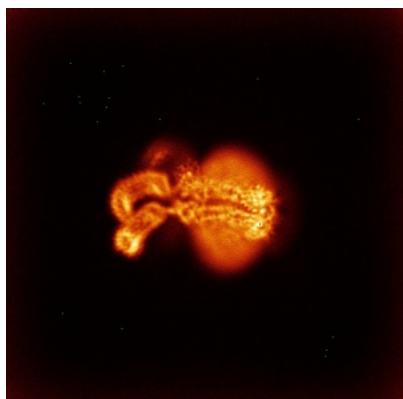


Z

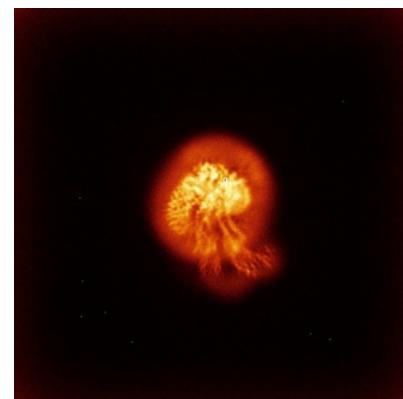
### 6.4.2 Raw map



X



Y

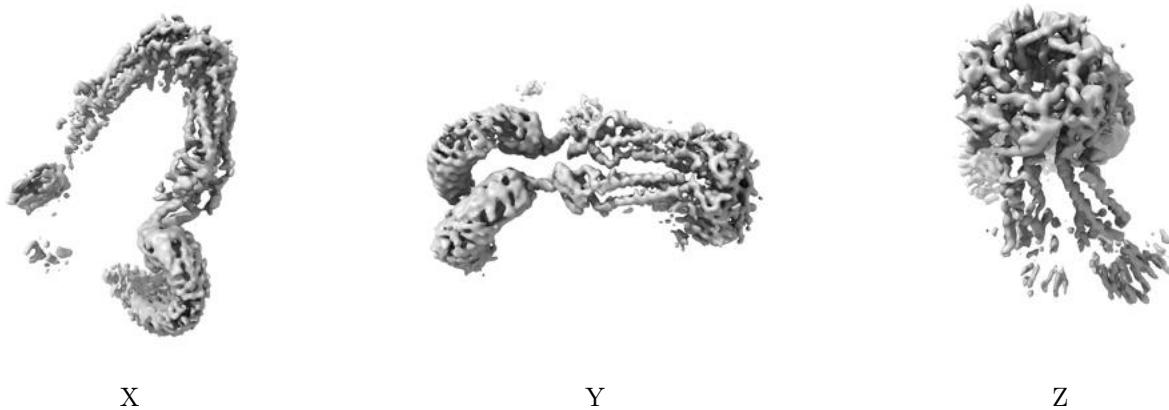


Z

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

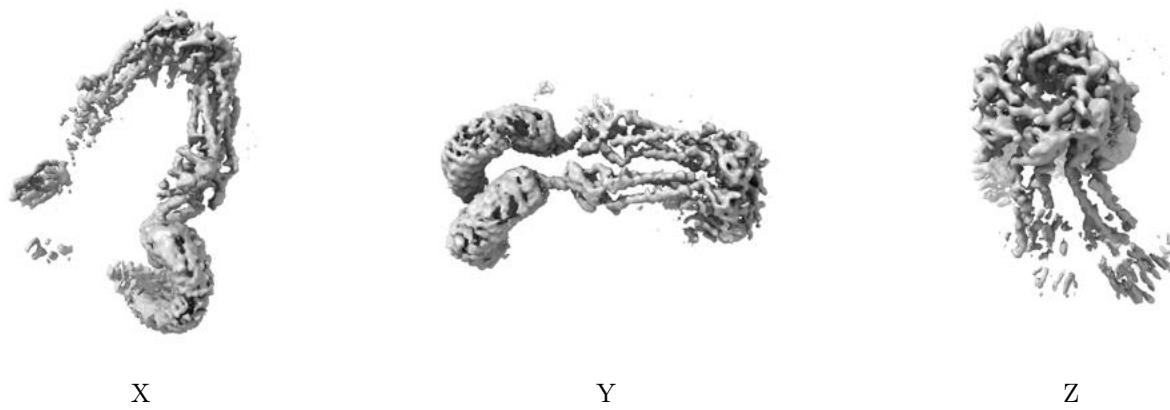
## 6.5 Orthogonal surface views [\(i\)](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.811. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

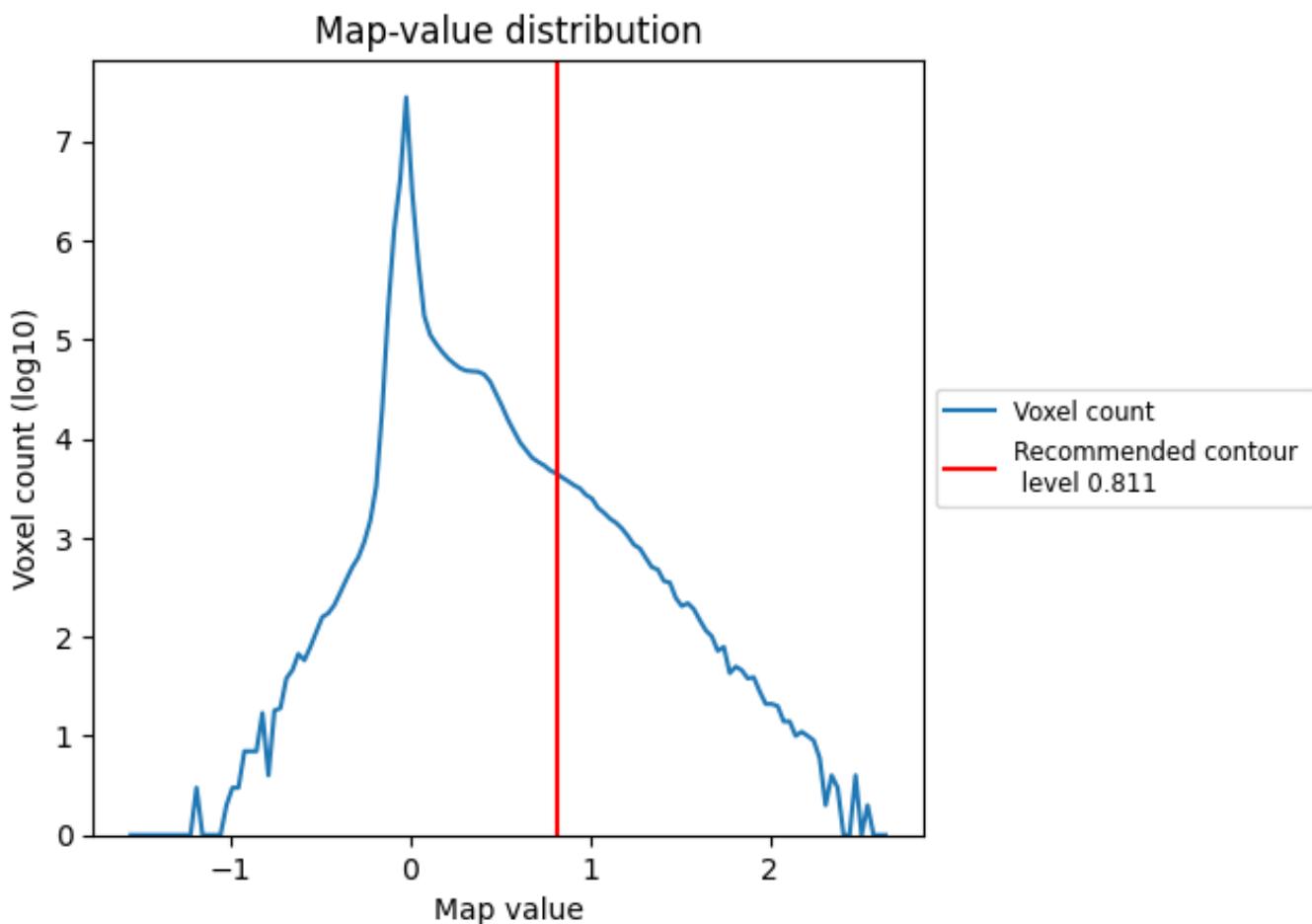
## 6.6 Mask visualisation [\(i\)](#)

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

## 7 Map analysis (i)

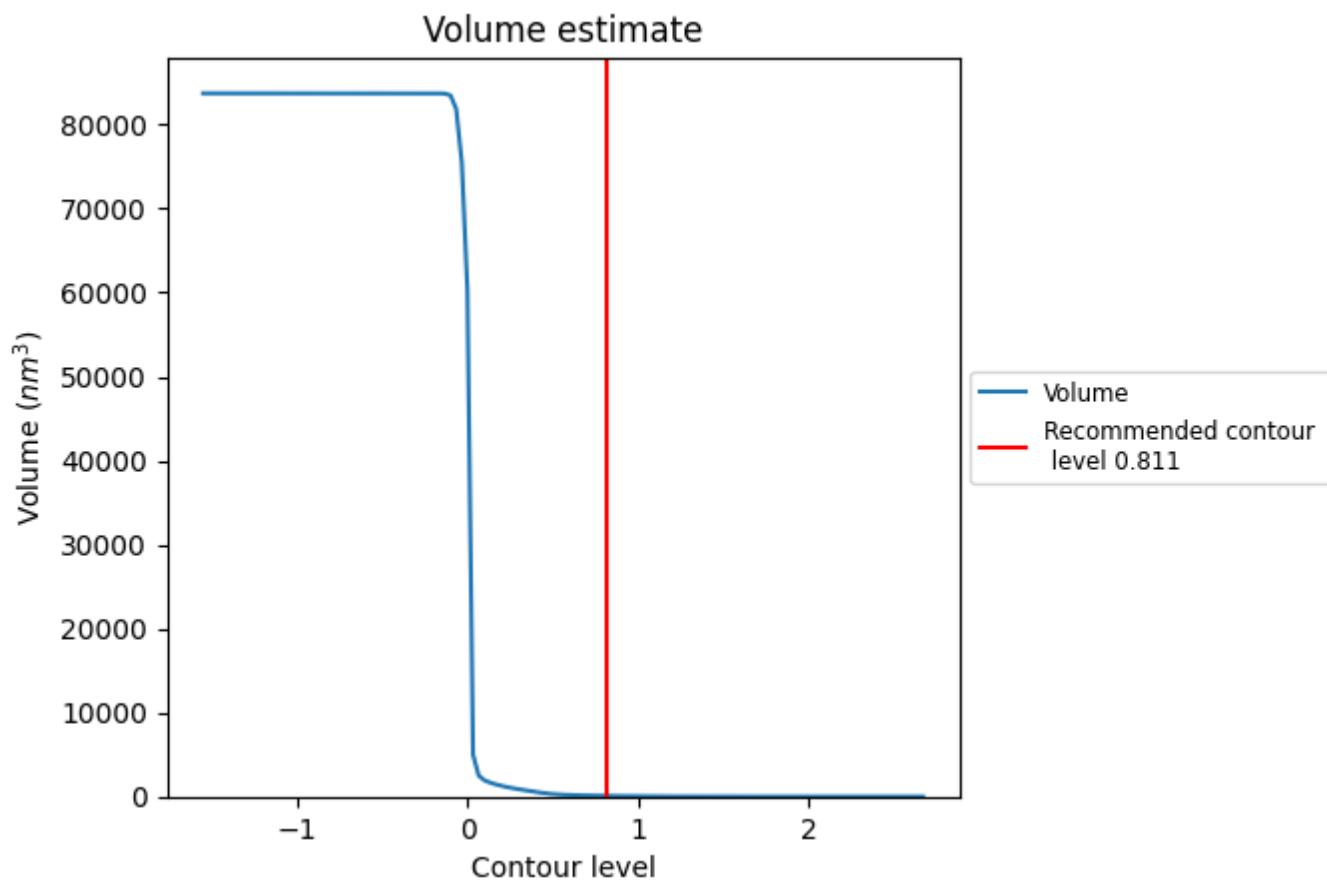
This section contains the results of statistical analysis of the map.

### 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.

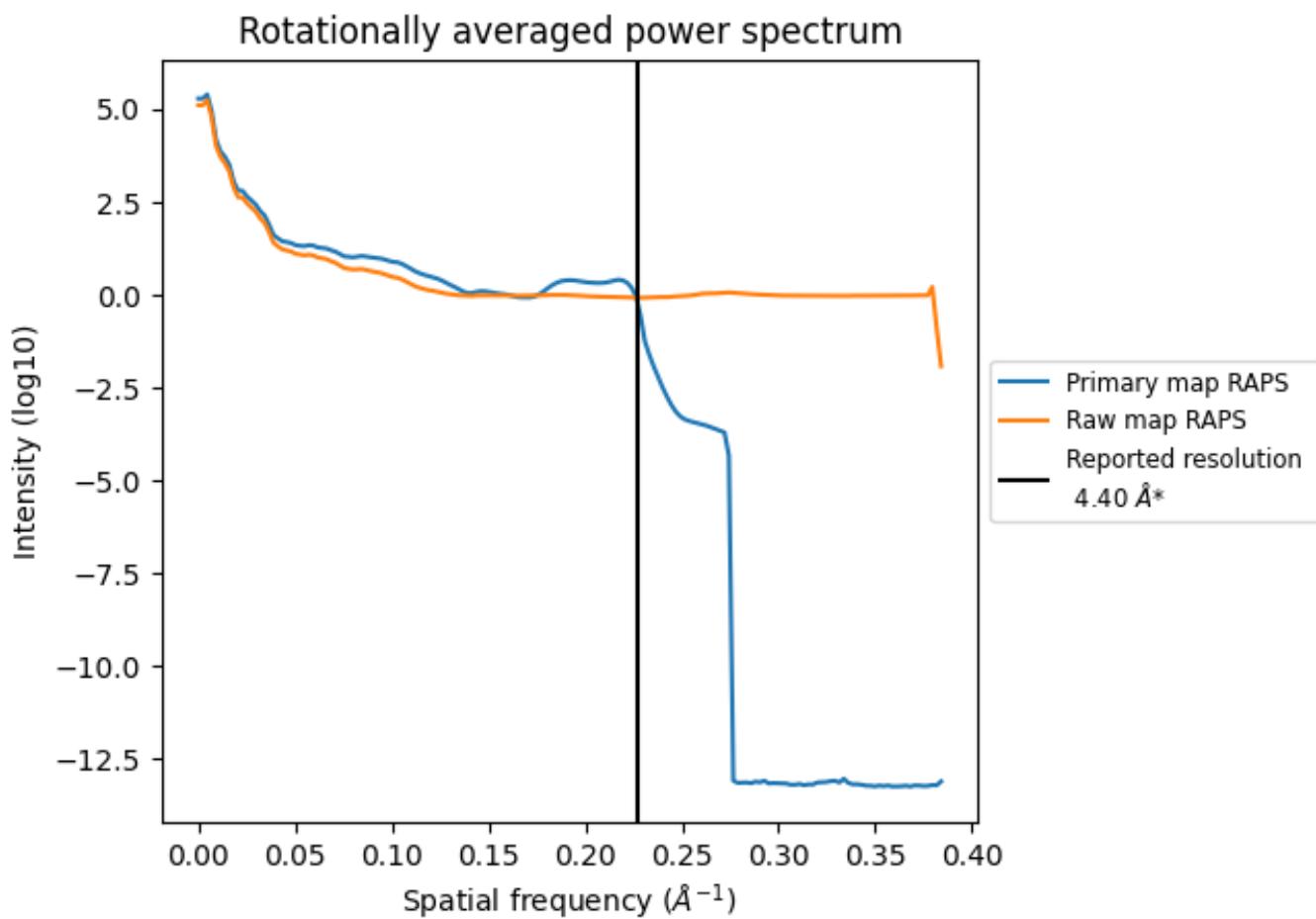
## 7.2 Volume estimate (i)



The volume at the recommended contour level is 85 nm<sup>3</sup>; this corresponds to an approximate mass of 77 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 [\(i\)](#)

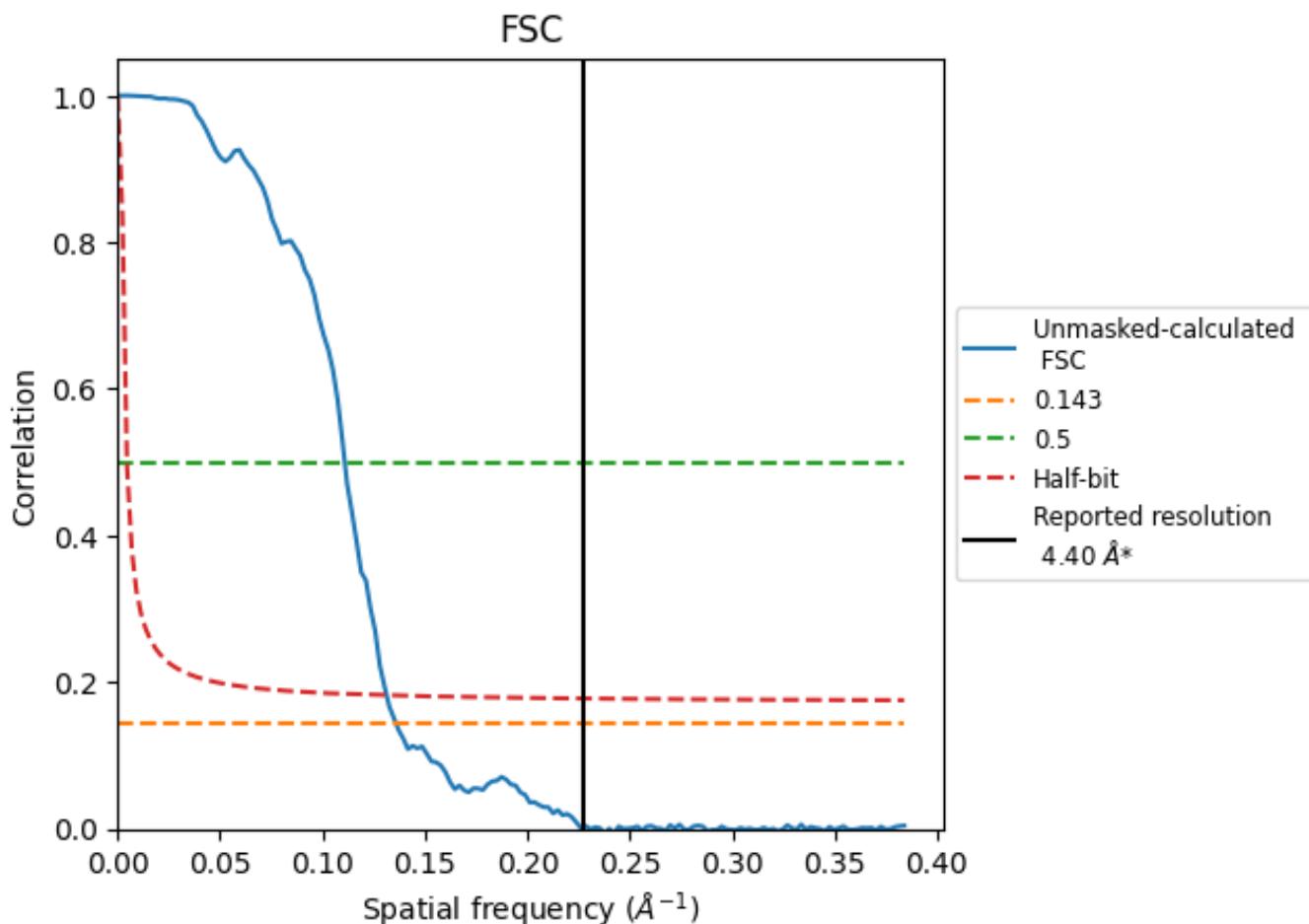


\*Reported resolution corresponds to spatial frequency of  $0.227 \text{\AA}^{-1}$

## 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  $0.227 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [\(i\)](#)

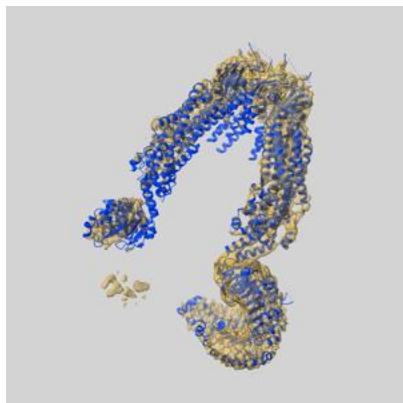
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.36	9.02	7.62

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.36 differs from the reported value 4.4 by more than 10 %

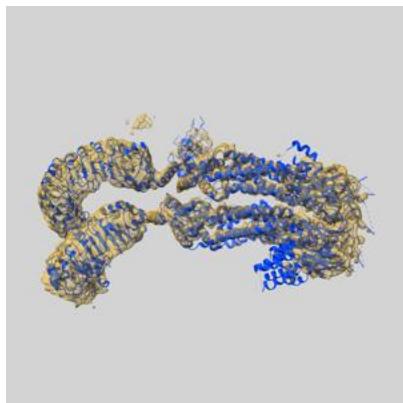
## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-50123 and PDB model 9F16. Per-residue inclusion information can be found in section [3](#) on page [6](#).

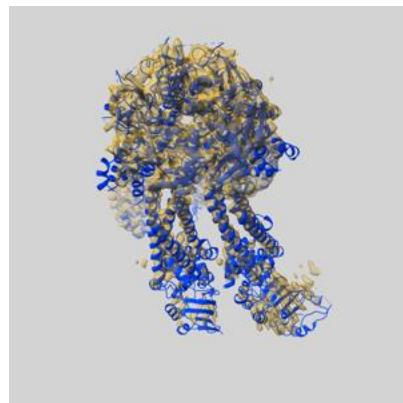
### 9.1 Map-model overlay (i)



X



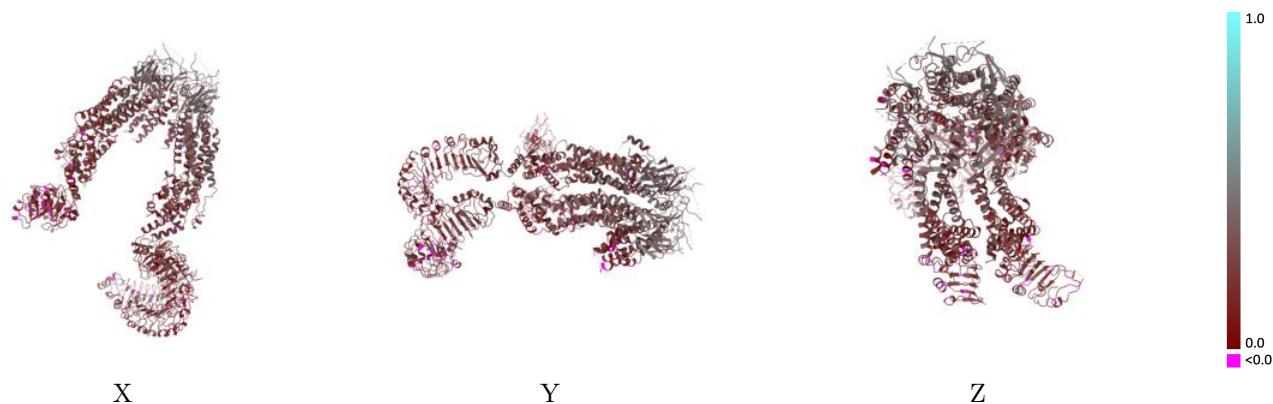
Y



Z

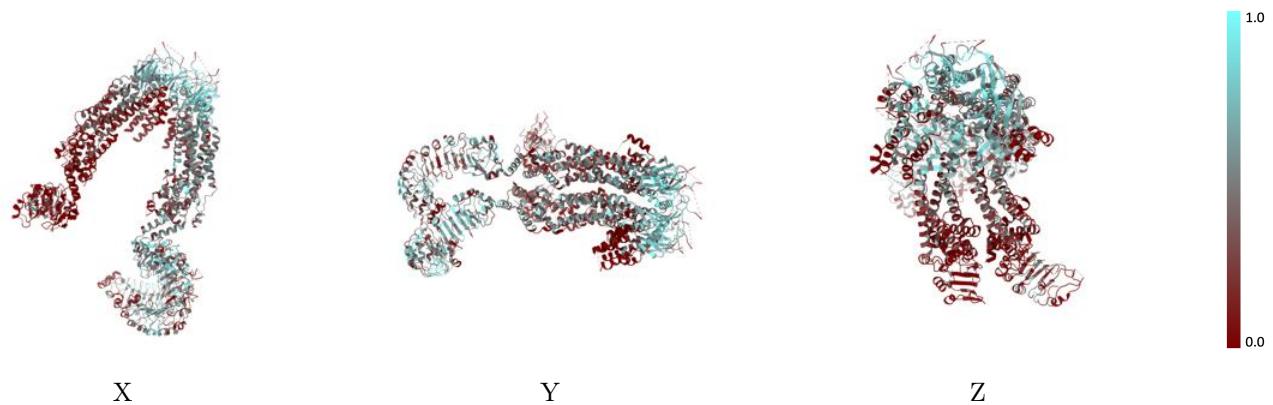
The images above show the 3D surface view of the map at the recommended contour level 0.811 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



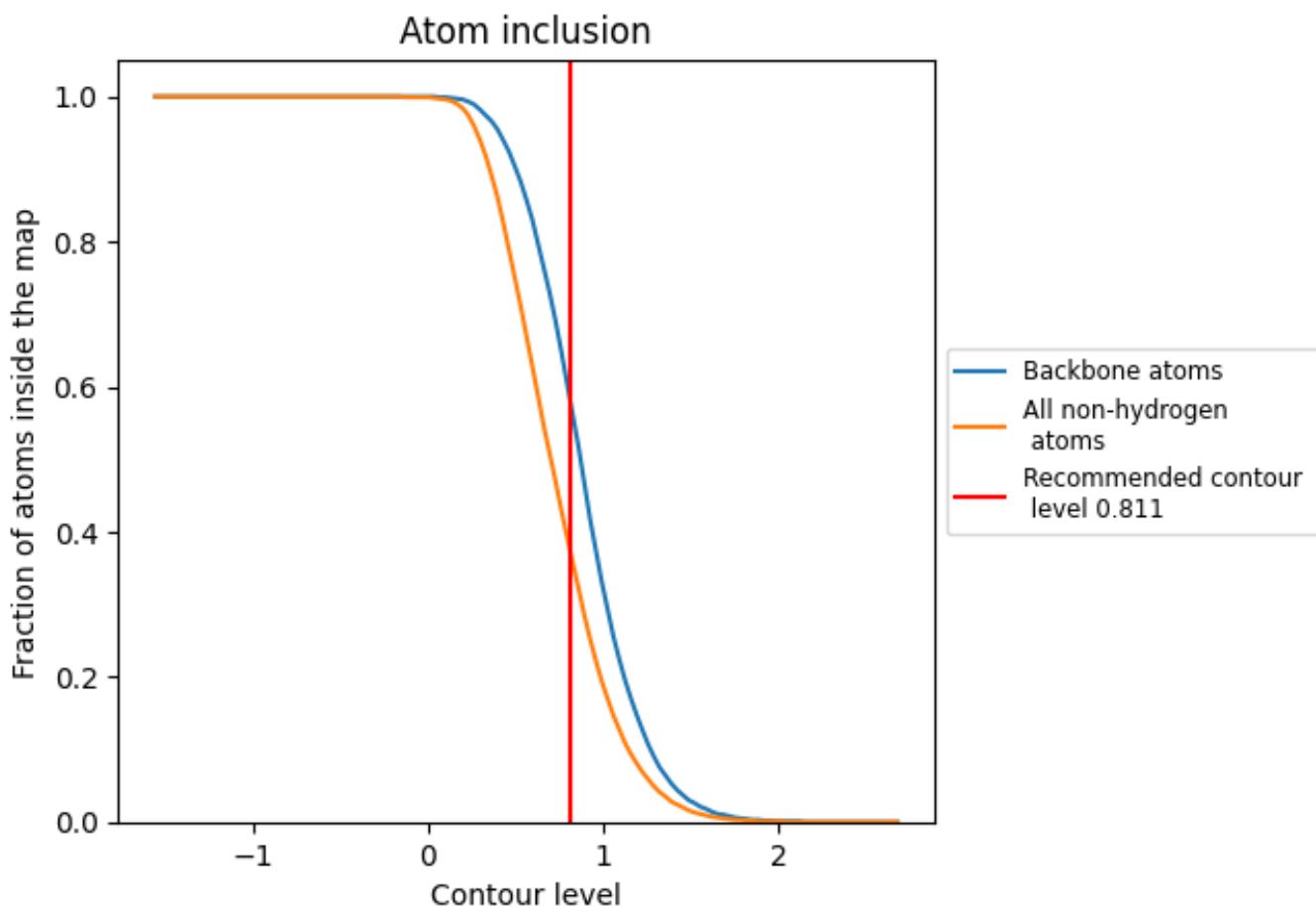
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.811).

## 9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 58% of all backbone atoms, 37% 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 (0.811) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3710	0.2510
A	0.3310	0.2870
B	0.1950	0.2370
C	0.2420	0.2350
D	0.3750	0.3210
E	0.4480	0.2450
F	0.5020	0.2560
G	0.3230	0.2710

