Full wwPDB EM Validation Report ⓘ

Nov 16, 2024 – 11:36 pm GMT

PDB ID	:	8RTS
EMDB ID	:	EMD-19495
Title	:	Structure of a homomeric human LRRC8C Volume-Regulated Anion Channel
Authors	:	Rutz, S.; Quinodoz, M.; Peter, V.; Garavelli, L.; Innes, M.; Kellenberger, S.; Barone, A.; Campos-Xavier, B.; Unger, S.; Rivolta, C.; Dutzler, R.; Superti-Furga, A.
Deposited on	:	2024-01-29
Resolution	:	3.73 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

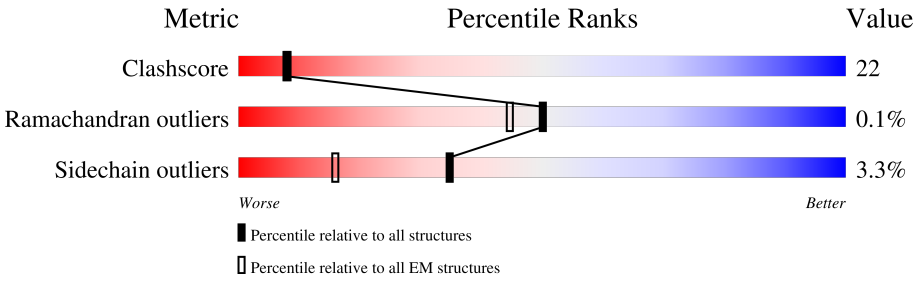
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.73 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.

Mol	Chain	Length	Quality of chain
1	A	811	26% 45% 39% • 15%
1	B	811	27% 43% 41% • 15%
1	C	811	74% 49% 35% • 15%
1	D	811	77% 57% 27% • 15%
1	E	811	72% 47% 36% • 15%
1	F	811	67% 48% 36% • 15%
1	G	811	16% 17% 6% 76%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 35445 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	692	Total 5641	C 3675	N 926	O 1004	S 36	0	0
1	B	692	Total 5641	C 3675	N 926	O 1004	S 36	0	0
1	C	692	Total 5641	C 3675	N 926	O 1004	S 36	0	0
1	D	692	Total 5641	C 3675	N 926	O 1004	S 36	0	0
1	E	692	Total 5641	C 3675	N 926	O 1004	S 36	0	0
1	F	692	Total 5641	C 3675	N 926	O 1004	S 36	0	0
1	G	192	Total 1599	C 1070	N 246	O 265	S 18	0	0

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	variant	UNP Q8TDW0
A	781	ARG	GLY	conflict	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	variant	UNP Q8TDW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	781	ARG	GLY	conflict	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	variant	UNP Q8TDW0
C	781	ARG	GLY	conflict	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	variant	UNP Q8TDW0
D	781	ARG	GLY	conflict	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	variant	UNP Q8TDW0
E	781	ARG	GLY	conflict	UNP Q8TDW0
E	802	ALA	-	expression tag	UNP Q8TDW0
E	803	ASP	-	expression tag	UNP Q8TDW0

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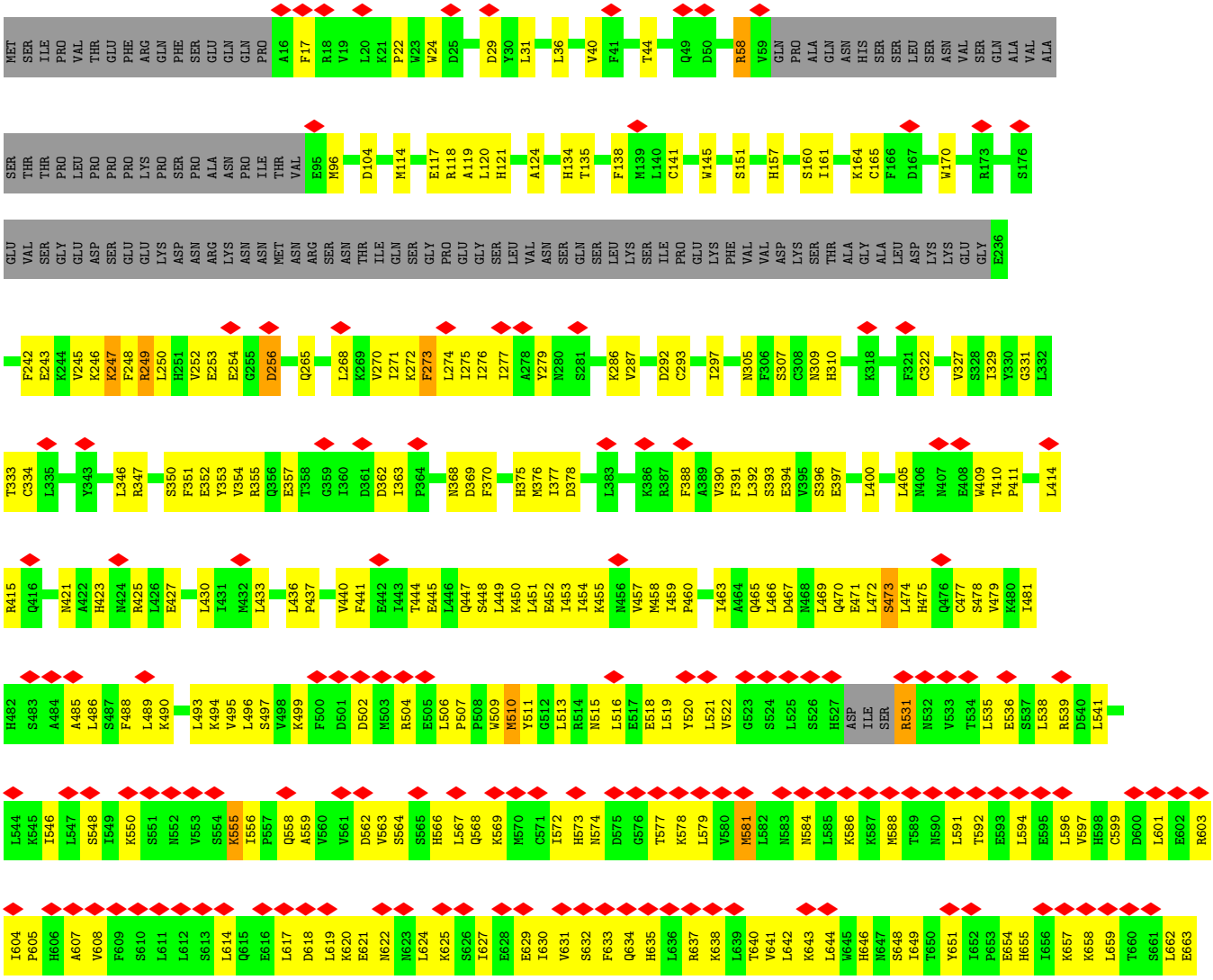
Chain	Residue	Modelled	Actual	Comment	Reference
E	804	ALA	-	expression tag	UNP Q8TDW0
E	805	LEU	-	expression tag	UNP Q8TDW0
E	806	GLU	-	expression tag	UNP Q8TDW0
E	807	VAL	-	expression tag	UNP Q8TDW0
E	808	LEU	-	expression tag	UNP Q8TDW0
E	809	PHE	-	expression tag	UNP Q8TDW0
E	810	GLN	-	expression tag	UNP Q8TDW0
F	0	MET	-	initiating methionine	UNP Q8TDW0
F	1	SER	-	expression tag	UNP Q8TDW0
F	205	GLY	ASP	variant	UNP Q8TDW0
F	781	ARG	GLY	conflict	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	variant	UNP Q8TDW0
G	781	ARG	GLY	conflict	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

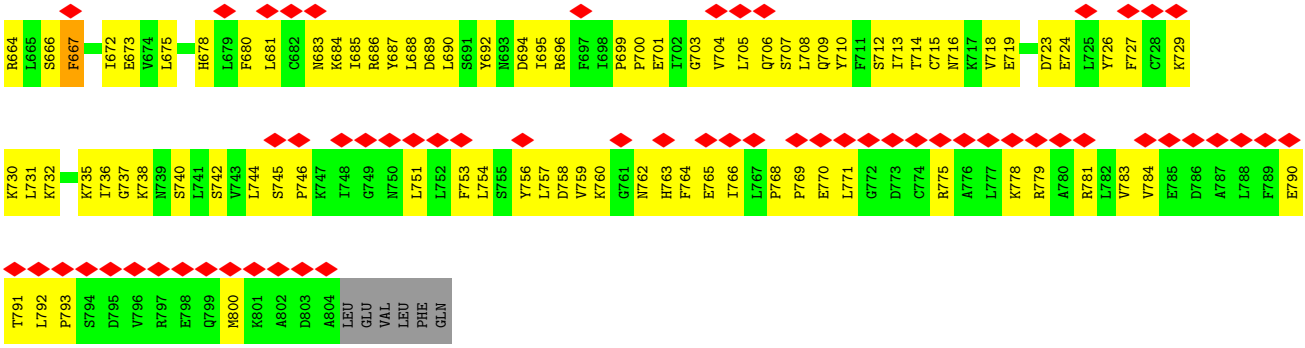
3 Residue-property plots (i)

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

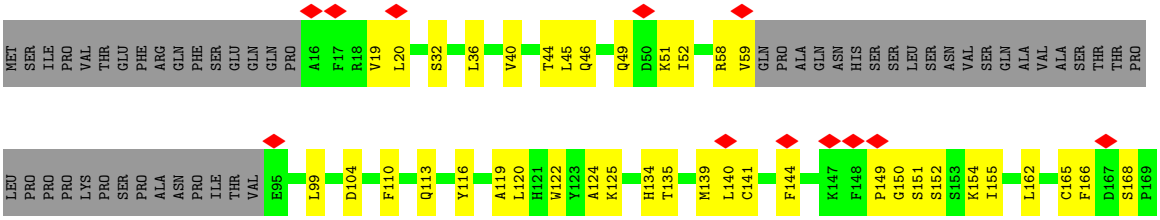
Chain A:

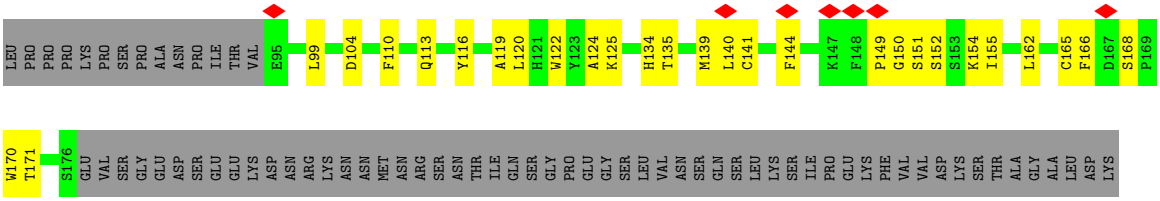


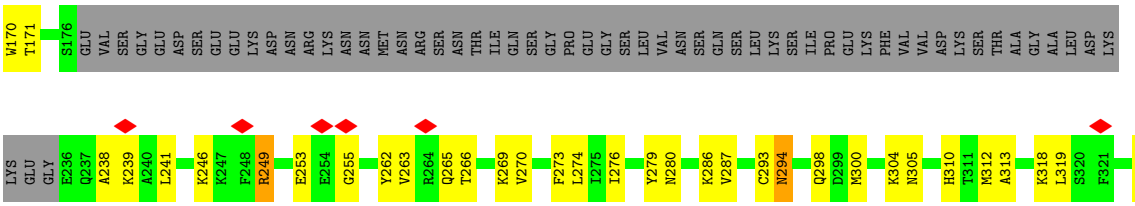


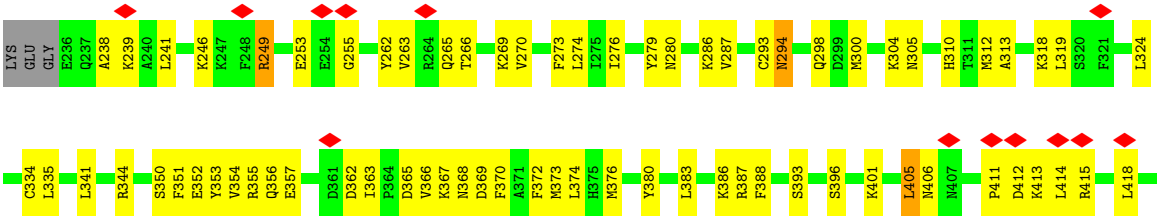
• Molecule 1: Volume-regulated anion channel subunit LRRC8C

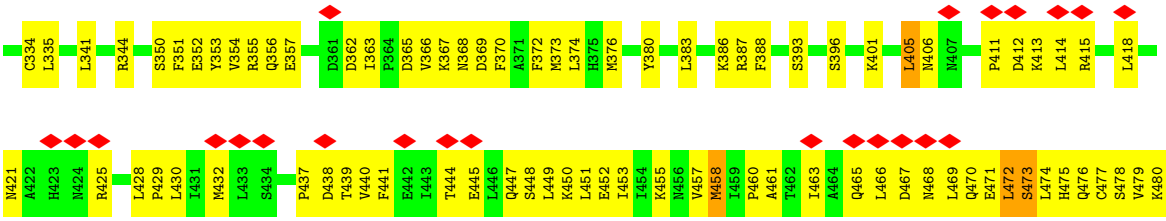
Chain B:

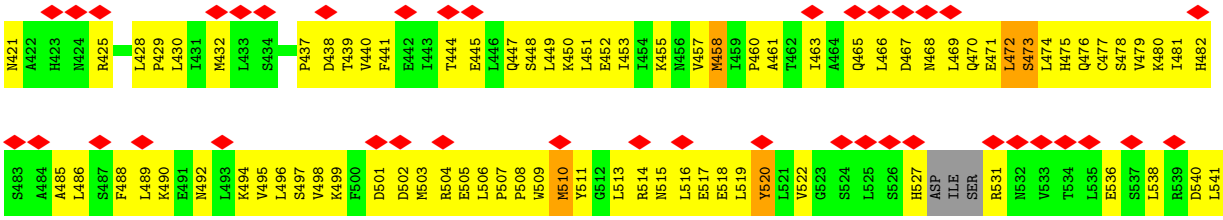


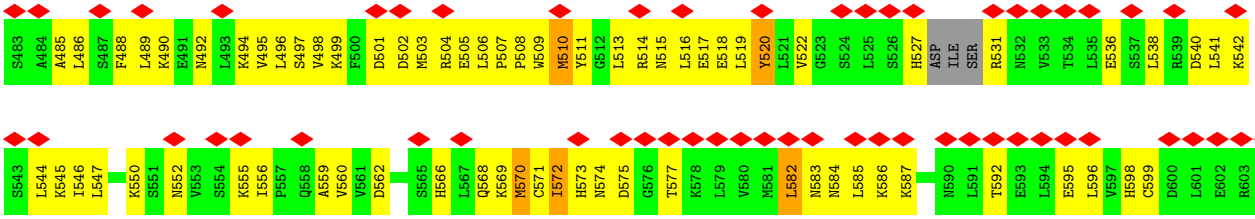


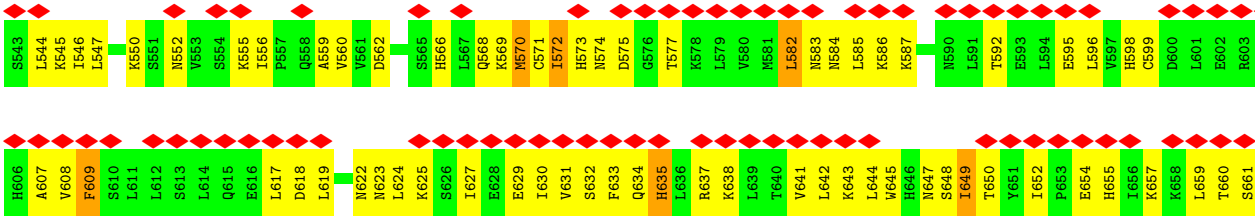


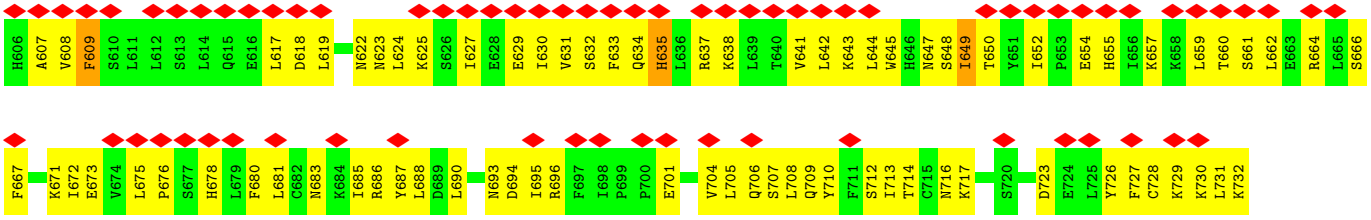


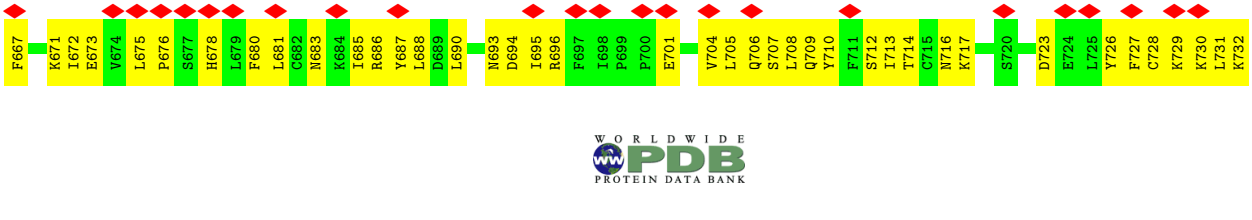


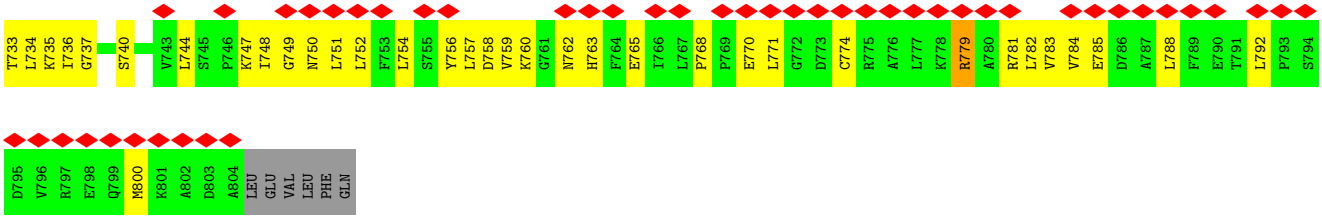




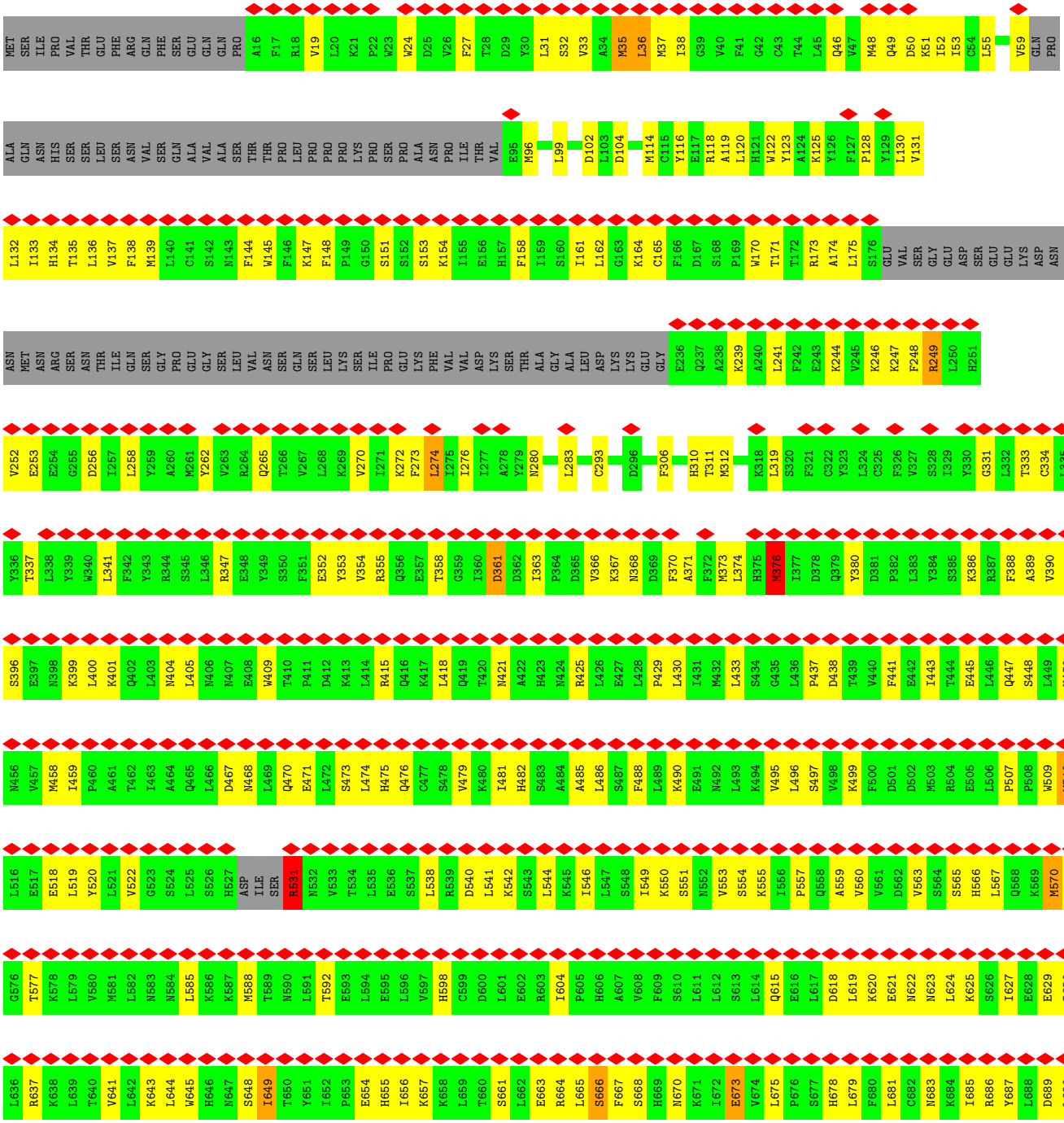


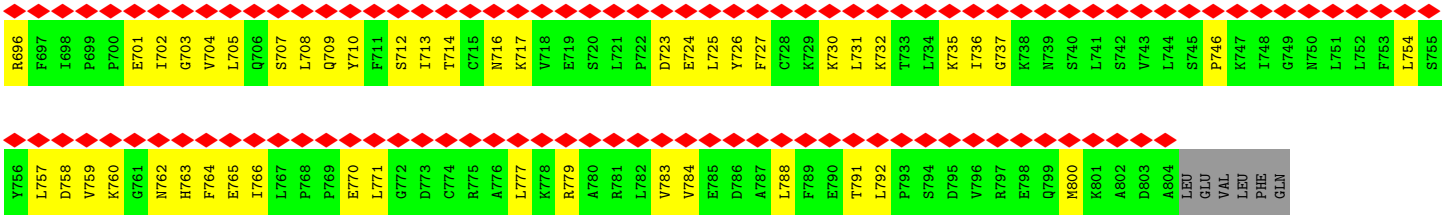






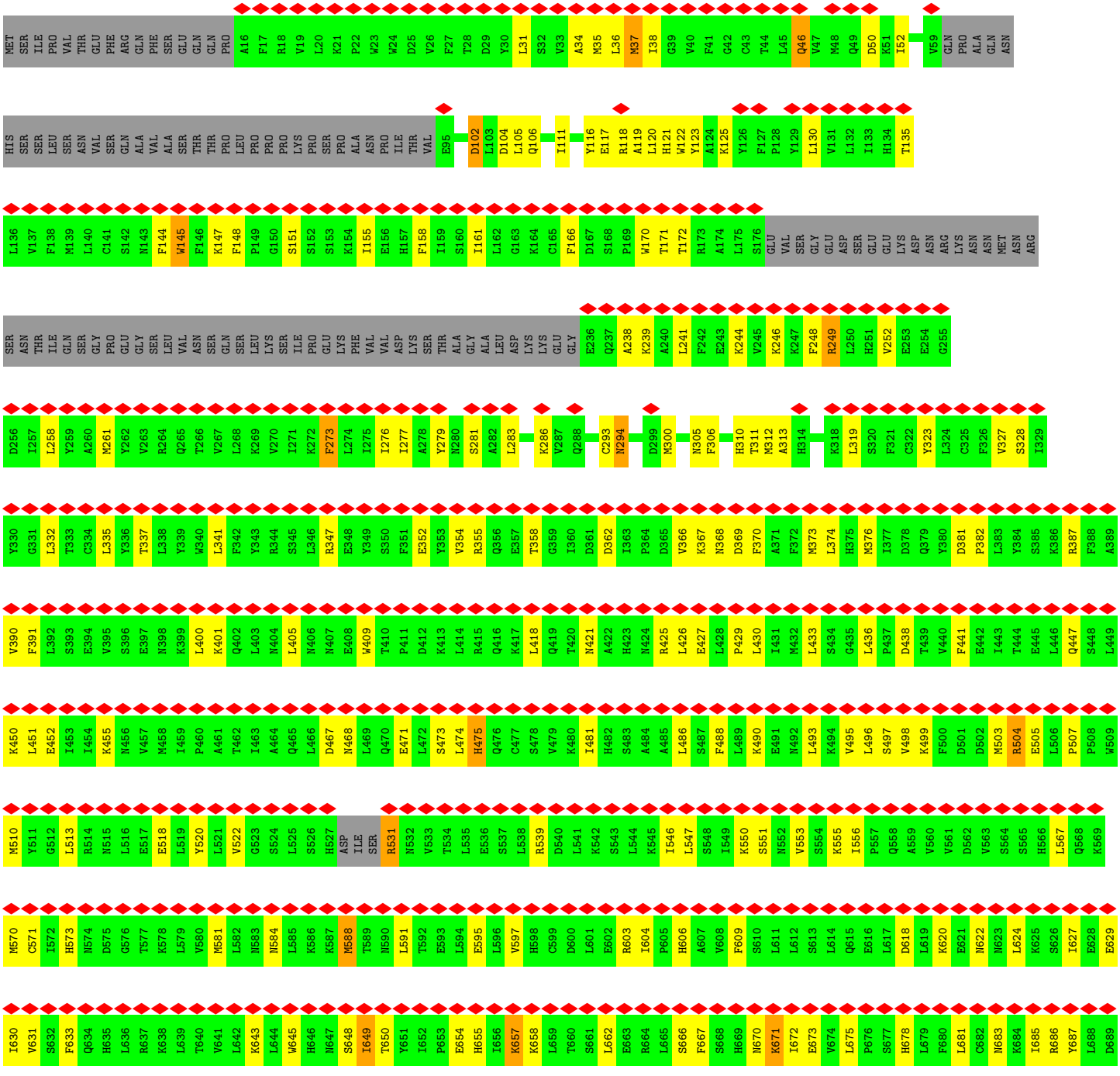
• Molecule 1: Volume-regulated anion channel subunit LRRC8C

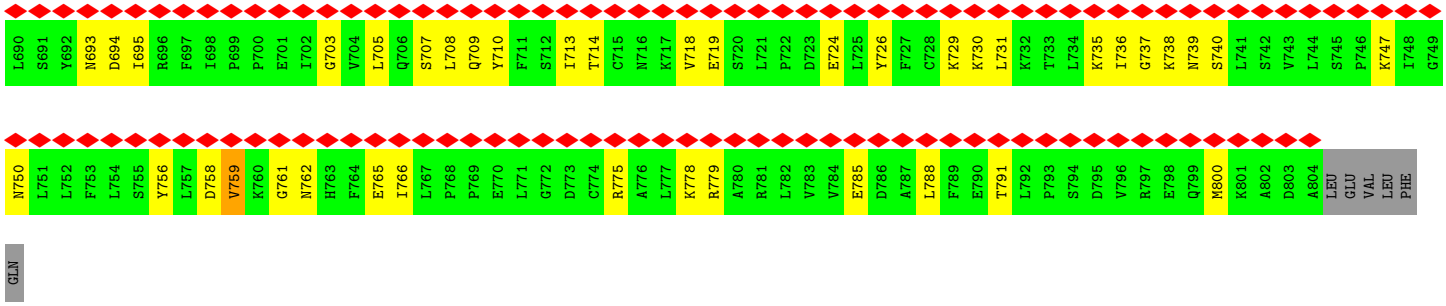




• Molecule 1: Volume-regulated anion channel subunit LRRC8C

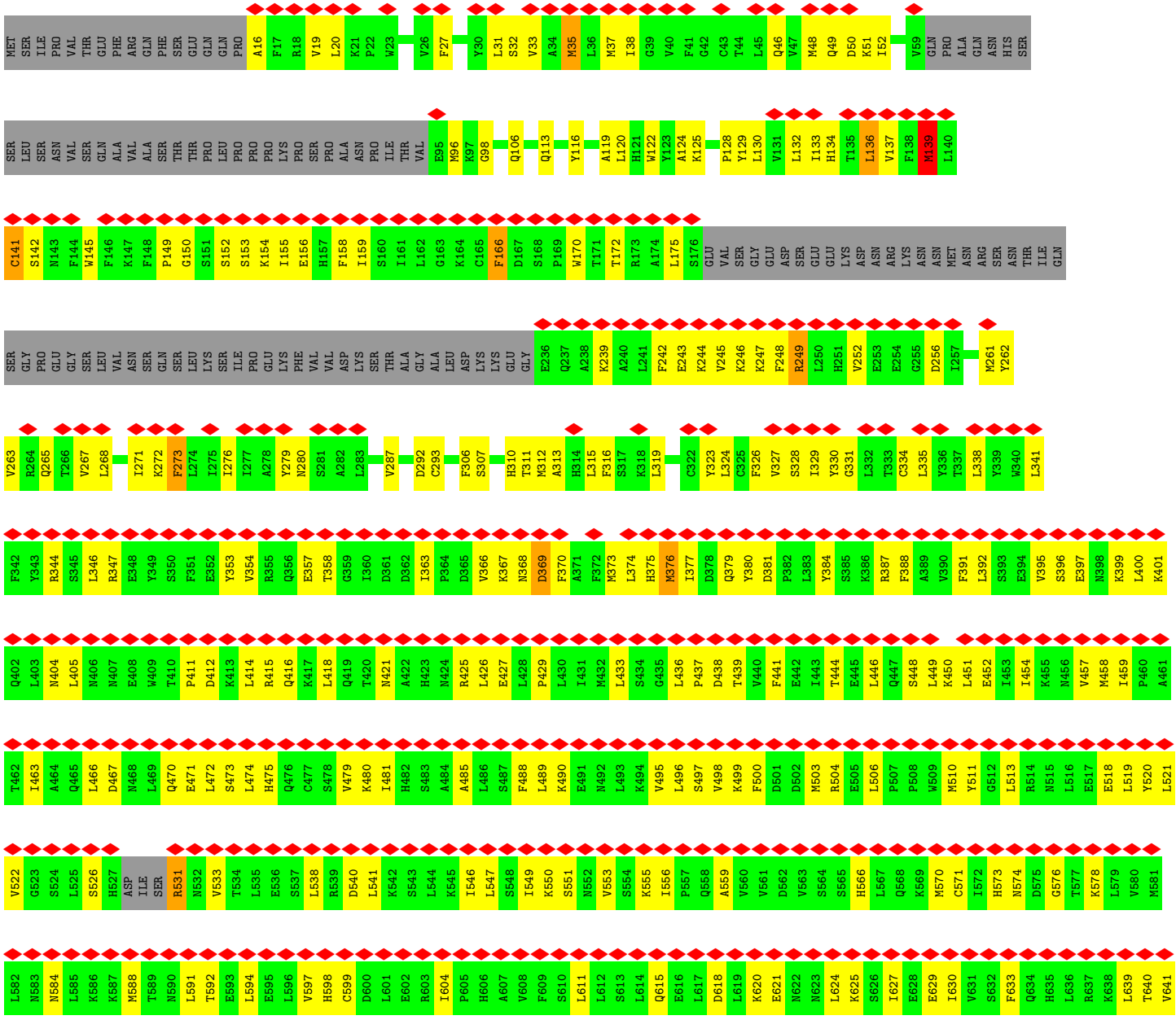
Chain D:





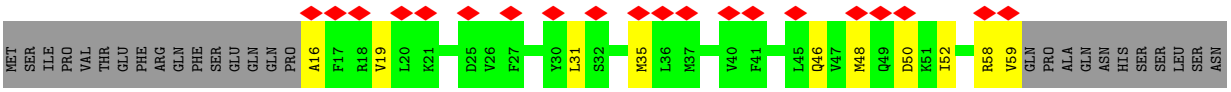
• Molecule 1: Volume-regulated anion channel subunit LRRC8C

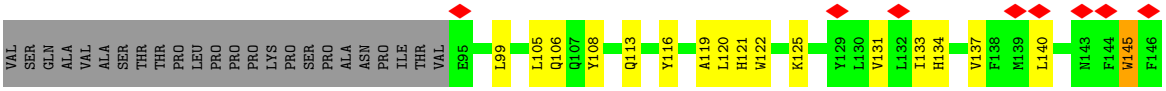
Chain E:

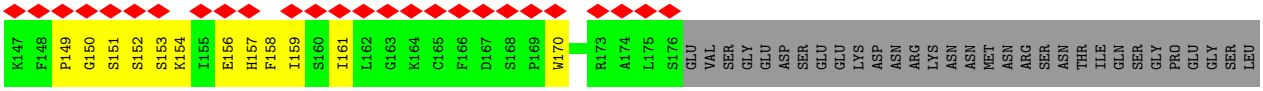


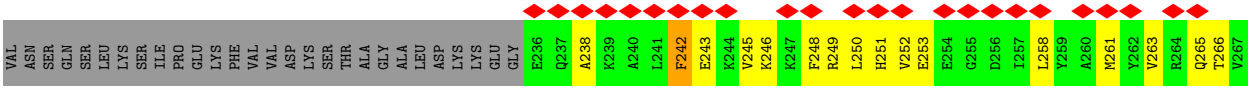
• Molecule 1: Volume-regulated anion channel subunit LRRC8C

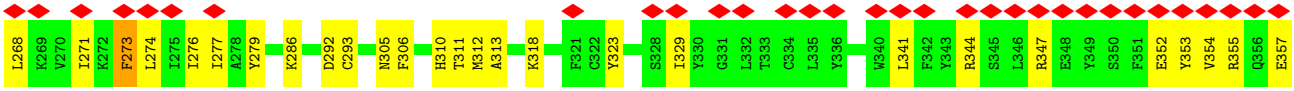
Chain F:

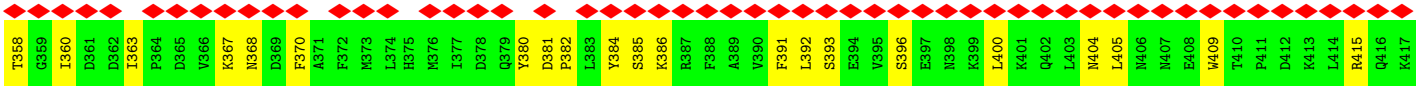


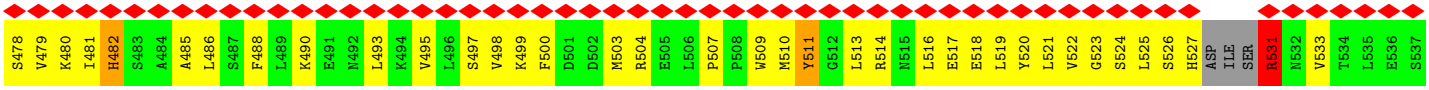


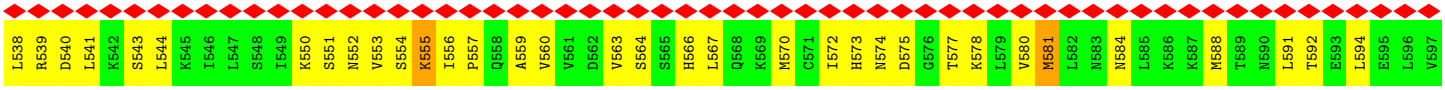


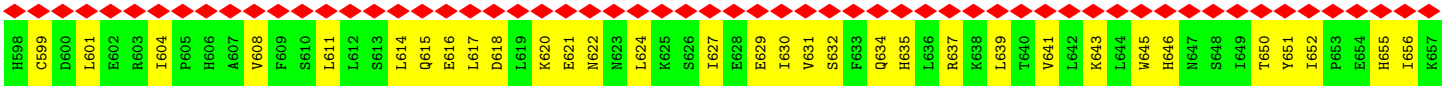


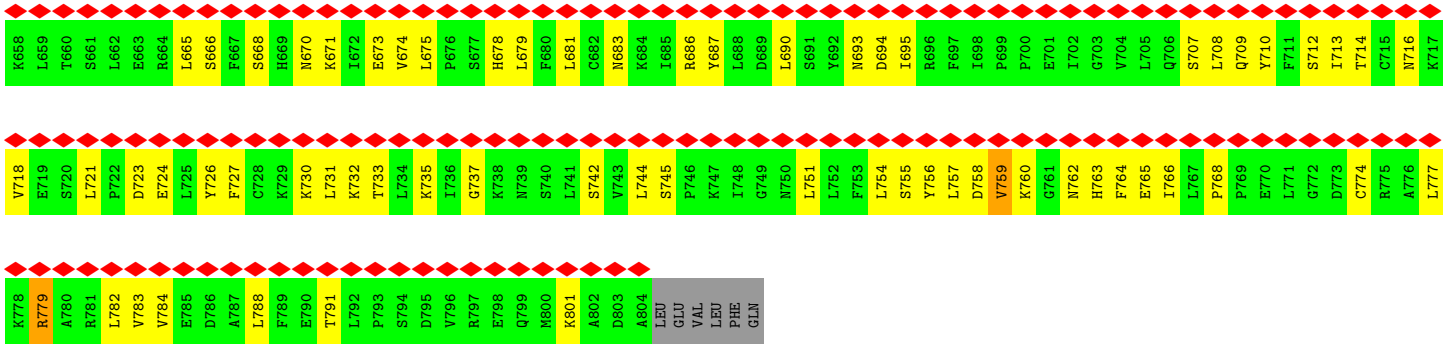






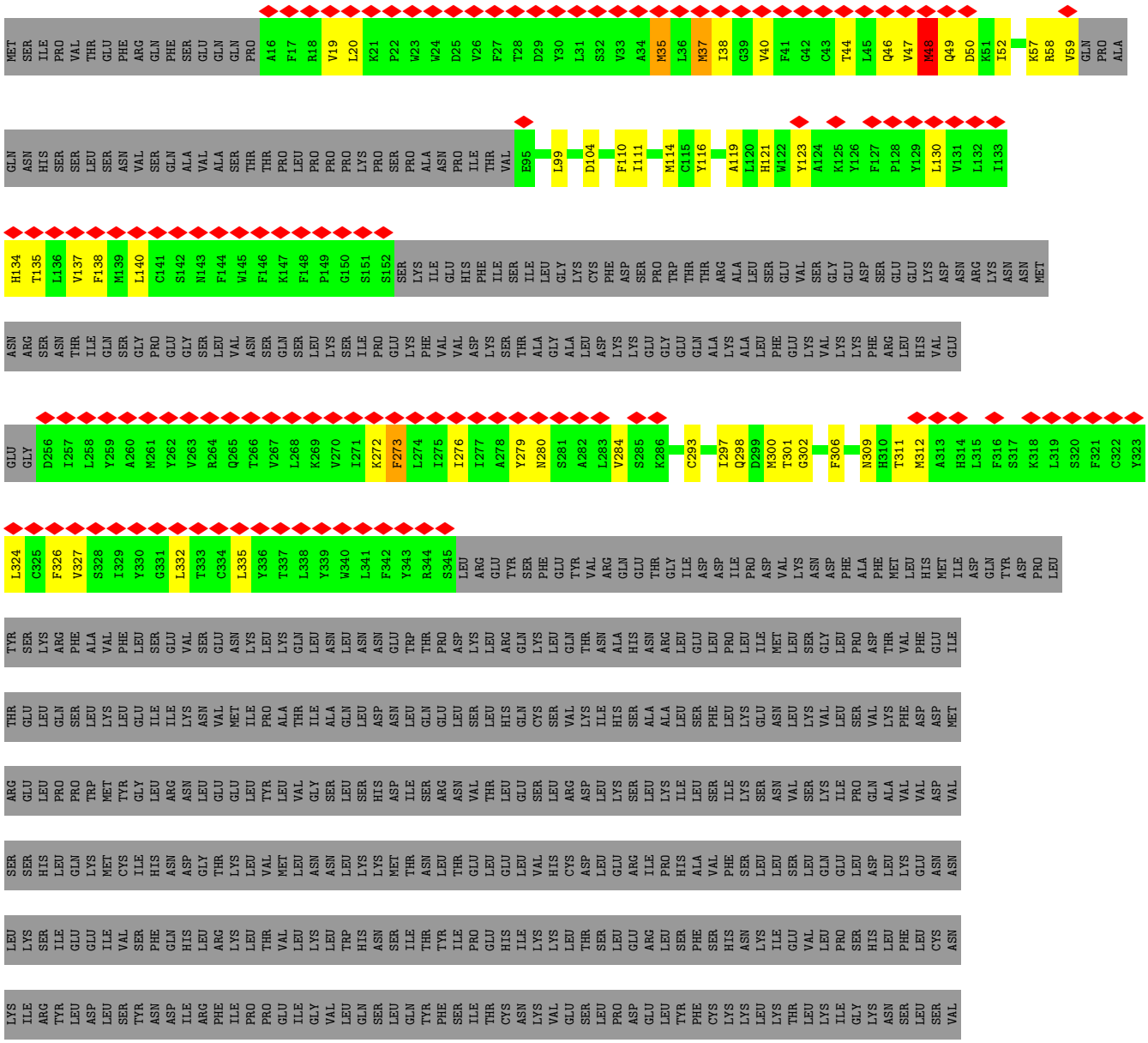






• Molecule 1: Volume-regulated anion channel subunit LRRC8C

Chain G:



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

ALA LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	216564	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 ($e^-/Å^2$)	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	0.756	Depositor
Minimum map value	-0.261	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.175	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

5.1 Standard geometry

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	0.36	0/5764	0.51	0/7790
1	B	0.37	0/5764	0.53	1/7790 (0.0%)
1	C	0.31	0/5764	0.52	3/7790 (0.0%)
1	D	0.30	0/5764	0.47	0/7790
1	E	0.31	0/5764	0.51	2/7790 (0.0%)
1	F	0.32	0/5764	0.50	0/7790
1	G	0.34	0/1645	0.52	1/2227 (0.0%)
All	All	0.33	0/36229	0.51	7/48967 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	36	LEU	CA-CB-CG	9.60	137.39	115.30
1	G	48	MET	CA-CB-CG	6.25	123.92	113.30
1	C	274	LEU	CA-CB-CG	5.71	128.44	115.30
1	B	405	LEU	CA-CB-CG	5.49	127.93	115.30
1	E	136	LEU	CA-CB-CG	5.47	127.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	376	MET	CA-CB-CG	5.31	122.33	113.30
1	E	139	MET	CA-CB-CG	5.03	121.86	113.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	531	ARG	Sidechain
1	B	531	ARG	Sidechain
1	C	531	ARG	Sidechain
1	D	531	ARG	Sidechain
1	E	531	ARG	Sidechain
1	F	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	5641	0	5764	295	0
1	B	5641	0	5764	297	0
1	C	5641	0	5764	220	0
1	D	5641	0	5764	173	0
1	E	5641	0	5764	283	0
1	F	5641	0	5764	276	0
1	G	1599	0	1601	41	0
All	All	35445	0	36185	1575	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 22.

All (1575) 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:F:531:ARG:HH22	1:F:552:ASN:ND2	1.22	1.33
1:E:766:ILE:HD13	1:E:791:THR:CG2	1.67	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:673:GLU:OE1	1:E:674:VAL:CG2	1.83	1.25
1:A:507:PRO:O	1:A:510:MET:SD	1.99	1.19
1:C:763:HIS:O	1:C:765:GLU:OE2	1.62	1.18
1:A:766:ILE:CD1	1:A:791:THR:HB	1.73	1.18
1:B:673:GLU:HG3	1:B:694:ASP:CB	1.74	1.17
1:F:531:ARG:NH1	1:F:552:ASN:HB2	1.60	1.16
1:B:673:GLU:OE2	1:B:694:ASP:OD2	1.63	1.14
1:B:673:GLU:HG3	1:B:694:ASP:HB2	1.15	1.13
1:E:673:GLU:CD	1:E:674:VAL:HG23	1.65	1.13
1:D:370:PHE:HA	1:D:373:MET:HE3	1.31	1.10
1:C:35:MET:HE2	1:C:135:THR:HG23	1.21	1.08
1:E:370:PHE:HA	1:E:373:MET:HE3	1.36	1.07
1:A:766:ILE:HD13	1:A:791:THR:CB	1.85	1.06
1:E:673:GLU:OE1	1:E:674:VAL:HG23	0.89	1.06
1:C:35:MET:CE	1:C:135:THR:HG23	1.86	1.05
1:D:672:ILE:HD12	1:D:695:ILE:HD11	1.33	1.05
1:F:531:ARG:NH2	1:F:552:ASN:ND2	2.06	1.02
1:B:473:SER:C	1:B:474:LEU:HD23	1.78	1.02
1:F:531:ARG:HH12	1:F:552:ASN:HB2	1.10	1.02
1:B:473:SER:O	1:B:474:LEU:HD23	1.59	1.02
1:F:742:SER:O	1:F:765:GLU:OE2	1.79	0.98
1:B:673:GLU:CG	1:B:694:ASP:HB2	1.94	0.97
1:E:766:ILE:HD13	1:E:791:THR:HG21	1.41	0.97
1:F:671:LYS:HE3	1:F:671:LYS:HA	1.46	0.96
1:A:507:PRO:O	1:A:510:MET:CE	2.14	0.94
1:A:766:ILE:HD13	1:A:791:THR:HB	1.37	0.94
1:F:763:HIS:O	1:F:765:GLU:OE1	1.83	0.94
1:E:766:ILE:HD13	1:E:791:THR:CB	1.98	0.92
1:A:481:ILE:HD13	1:A:486:LEU:HB2	1.50	0.92
1:B:671:LYS:O	1:B:673:GLU:OE1	1.88	0.91
1:A:766:ILE:HD13	1:A:791:THR:CG2	2.02	0.90
1:A:507:PRO:O	1:A:510:MET:HE1	1.72	0.89
1:C:35:MET:HE3	1:C:135:THR:HA	1.53	0.89
1:A:765:GLU:OE2	1:A:765:GLU:N	2.07	0.88
1:E:475:HIS:HA	1:E:499:LYS:HB2	1.55	0.87
1:C:765:GLU:HB2	1:C:766:ILE:HD12	1.57	0.85
1:F:52:ILE:HG21	1:F:116:TYR:HB2	1.55	0.85
1:D:311:THR:OG1	1:D:312:MET:SD	2.35	0.85
1:A:673:GLU:OE2	1:A:673:GLU:N	2.10	0.85
1:D:671:LYS:HD3	1:D:671:LYS:N	1.89	0.85
1:F:531:ARG:HH22	1:F:552:ASN:CG	1.80	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:MET:HE2	1:E:591:LEU:HB2	1.59	0.84
1:E:766:ILE:CD1	1:E:791:THR:CG2	2.56	0.84
1:A:766:ILE:HD12	1:A:791:THR:HB	1.59	0.83
1:E:496:LEU:HD11	1:E:498:VAL:HG23	1.60	0.83
1:B:475:HIS:HA	1:B:499:LYS:HB2	1.58	0.83
1:B:571:CYS:SG	1:B:595:GLU:OE1	2.37	0.83
1:F:531:ARG:HH12	1:F:552:ASN:CB	1.92	0.82
1:B:32:SER:HB3	1:B:139:MET:HE2	1.61	0.82
1:B:547:LEU:HD23	1:B:570:MET:HG2	1.61	0.82
1:C:452:GLU:HA	1:C:475:HIS:HB2	1.62	0.81
1:B:630:ILE:HB	1:B:655:HIS:HB2	1.63	0.81
1:F:671:LYS:O	1:F:673:GLU:OE2	1.98	0.81
1:F:574:ASN:ND2	1:F:577:THR:O	2.13	0.80
1:F:119:ALA:HB2	1:F:293:CYS:HB3	1.61	0.80
1:A:630:ILE:HB	1:A:655:HIS:HB2	1.60	0.80
1:E:766:ILE:HD13	1:E:791:THR:HB	1.64	0.80
1:B:571:CYS:HG	1:B:595:GLU:CD	1.83	0.80
1:A:363:ILE:HG23	1:A:392:LEU:HD23	1.64	0.80
1:A:574:ASN:ND2	1:A:577:THR:O	2.16	0.79
1:E:766:ILE:CD1	1:E:791:THR:HB	2.12	0.79
1:E:625:LYS:HE2	1:E:650:THR:HB	1.65	0.79
1:B:643:LYS:HA	1:B:666:SER:OG	1.83	0.79
1:E:496:LEU:HD12	1:E:497:SER:N	1.98	0.79
1:B:119:ALA:HB2	1:B:293:CYS:HB3	1.65	0.78
1:E:370:PHE:HA	1:E:373:MET:CE	2.12	0.78
1:B:571:CYS:SG	1:B:595:GLU:CD	2.62	0.77
1:E:433:LEU:HB2	1:E:454:ILE:HD13	1.66	0.77
1:A:766:ILE:CD1	1:A:791:THR:CB	2.51	0.77
1:B:671:LYS:O	1:B:673:GLU:CD	2.23	0.77
1:E:588:MET:HE2	1:E:591:LEU:CB	2.15	0.77
1:B:657:LYS:HD2	1:B:681:LEU:HD12	1.67	0.77
1:E:119:ALA:HB2	1:E:293:CYS:HB3	1.66	0.77
1:F:531:ARG:NH1	1:F:552:ASN:CB	2.46	0.77
1:F:311:THR:OG1	1:F:312:MET:SD	2.42	0.77
1:F:531:ARG:NH2	1:F:552:ASN:CG	2.34	0.76
1:A:758:ASP:HA	1:A:783:VAL:HB	1.67	0.76
1:G:59:VAL:HG21	1:G:99:LEU:HD21	1.68	0.76
1:B:758:ASP:HA	1:B:783:VAL:HB	1.67	0.75
1:F:429:PRO:HA	1:F:450:LYS:HB3	1.69	0.75
1:C:475:HIS:HA	1:C:499:LYS:HB2	1.66	0.75
1:E:33:VAL:HG13	1:E:37:MET:HE3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:712:SER:HA	1:E:735:LYS:HB2	1.69	0.75
1:F:541:LEU:O	1:F:566:HIS:NE2	2.20	0.74
1:B:541:LEU:O	1:B:566:HIS:NE2	2.19	0.74
1:D:672:ILE:HD11	1:D:693:ASN:HD22	1.52	0.74
1:F:475:HIS:HA	1:F:499:LYS:HB2	1.67	0.74
1:F:758:ASP:HA	1:F:783:VAL:HB	1.68	0.74
1:F:570:MET:HE3	1:F:588:MET:CE	2.17	0.74
1:C:467:ASP:HA	1:C:488:PHE:HZ	1.53	0.74
1:F:238:ALA:HB1	1:F:391:PHE:HZ	1.53	0.74
1:E:311:THR:OG1	1:E:312:MET:SD	2.46	0.73
1:F:425:ARG:HD3	1:F:447:GLN:HB3	1.70	0.73
1:B:239:LYS:HE3	1:B:401:LYS:HG2	1.71	0.73
1:C:119:ALA:HB2	1:C:293:CYS:HB3	1.70	0.73
1:A:684:LYS:O	1:A:686:ARG:NH1	2.21	0.73
1:A:766:ILE:HD13	1:A:791:THR:HG21	1.69	0.73
1:B:363:ILE:HD11	1:B:393:SER:HB2	1.71	0.73
1:D:119:ALA:HB2	1:D:293:CYS:HB3	1.71	0.73
1:F:474:LEU:HD12	1:F:498:VAL:HG22	1.70	0.73
1:C:757:LEU:HG	1:C:759:VAL:HG13	1.70	0.72
1:E:459:ILE:HB	1:E:481:ILE:HG22	1.71	0.72
1:E:541:LEU:O	1:E:566:HIS:NE2	2.21	0.72
1:F:580:VAL:HG23	1:F:581:MET:CE	2.18	0.72
1:E:474:LEU:HD12	1:E:498:VAL:HG22	1.71	0.72
1:E:588:MET:HG3	1:E:591:LEU:HB2	1.71	0.72
1:A:666:SER:HA	1:A:689:ASP:HB3	1.70	0.72
1:B:36:LEU:HB2	1:B:135:THR:HG21	1.72	0.72
1:A:474:LEU:HD23	1:A:496:LEU:HD11	1.70	0.72
1:B:445:GLU:O	1:B:468:ASN:ND2	2.23	0.72
1:E:52:ILE:HG12	1:E:310:HIS:HB3	1.72	0.72
1:B:696:ARG:HH21	1:B:717:LYS:HD3	1.54	0.72
1:E:452:GLU:HA	1:E:475:HIS:HB2	1.71	0.72
1:B:673:GLU:HG3	1:B:694:ASP:HB3	1.70	0.72
1:D:481:ILE:HD13	1:D:486:LEU:HB2	1.71	0.72
1:F:650:THR:HG22	1:F:671:LYS:CB	2.20	0.72
1:C:531:ARG:N	1:C:554:SER:HG	1.86	0.71
1:D:370:PHE:CA	1:D:373:MET:HE3	2.15	0.71
1:B:32:SER:HB3	1:B:139:MET:CE	2.19	0.71
1:B:495:VAL:HG13	1:B:518:GLU:HB2	1.72	0.71
1:D:595:GLU:HA	1:D:618:ASP:HB3	1.71	0.71
1:A:686:ARG:HA	1:A:708:LEU:HA	1.71	0.71
1:E:779:ARG:HA	1:E:800:MET:HE3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:GLU:HA	1:F:475:HIS:HB2	1.71	0.71
1:B:632:SER:O	1:B:635:HIS:HB3	1.89	0.71
1:E:497:SER:HA	1:E:520:TYR:HB2	1.73	0.71
1:A:588:MET:HB3	1:A:591:LEU:HB2	1.73	0.71
1:E:496:LEU:HD11	1:E:498:VAL:CG2	2.20	0.71
1:E:759:VAL:HG23	1:E:784:VAL:HG12	1.72	0.71
1:E:473:SER:HA	1:E:497:SER:HB2	1.73	0.70
1:C:311:THR:OG1	1:C:312:MET:SD	2.49	0.70
1:B:683:ASN:HA	1:B:705:LEU:HD23	1.73	0.70
1:A:425:ARG:HD3	1:A:447:GLN:HG2	1.73	0.70
1:F:671:LYS:HA	1:F:671:LYS:CE	2.21	0.70
1:B:760:LYS:HB2	1:B:783:VAL:HG12	1.73	0.70
1:C:459:ILE:HB	1:C:481:ILE:HG22	1.72	0.70
1:E:758:ASP:HA	1:E:783:VAL:HB	1.74	0.70
1:A:541:LEU:O	1:A:566:HIS:NE2	2.24	0.69
1:F:686:ARG:HA	1:F:708:LEU:HA	1.74	0.69
1:A:475:HIS:HA	1:A:499:LYS:HB2	1.73	0.69
1:B:707:SER:HA	1:B:730:LYS:HD2	1.72	0.69
1:A:707:SER:HA	1:A:730:LYS:HD2	1.74	0.69
1:A:709:GLN:HA	1:A:731:LEU:HA	1.73	0.69
1:A:604:ILE:HD12	1:A:629:GLU:HB2	1.73	0.69
1:F:490:LYS:HD3	1:F:514:ARG:HH12	1.57	0.69
1:F:760:LYS:CG	1:F:783:VAL:HG12	2.23	0.69
1:E:673:GLU:CD	1:E:674:VAL:CG2	2.49	0.69
1:A:354:VAL:HA	1:A:357:GLU:HB3	1.75	0.69
1:D:672:ILE:HD11	1:D:693:ASN:ND2	2.07	0.69
1:E:312:MET:SD	1:E:312:MET:N	2.66	0.69
1:D:657:LYS:HE3	1:D:681:LEU:HD12	1.75	0.69
1:F:363:ILE:HG12	1:F:392:LEU:HB3	1.75	0.69
1:C:429:PRO:HA	1:C:450:LYS:HB3	1.74	0.69
1:D:52:ILE:HD11	1:D:120:LEU:HD22	1.75	0.69
1:C:270:VAL:O	1:C:274:LEU:HD22	1.93	0.68
1:F:497:SER:HA	1:F:520:TYR:HB2	1.75	0.68
1:B:485:ALA:O	1:B:489:LEU:HG	1.93	0.68
1:A:520:TYR:HA	1:A:548:SER:HB3	1.74	0.68
1:B:574:ASN:ND2	1:B:577:THR:O	2.25	0.68
1:F:618:ASP:HA	1:F:643:LYS:HB2	1.74	0.68
1:A:684:LYS:HG2	1:A:686:ARG:HH12	1.58	0.68
1:B:263:VAL:HG22	1:B:341:LEU:HD13	1.76	0.68
1:F:652:ILE:HG21	1:F:679:LEU:HD13	1.73	0.68
1:C:759:VAL:HG22	1:C:784:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:MET:SD	1:D:312:MET:N	2.67	0.68
1:F:31:LEU:O	1:F:35:MET:HG2	1.93	0.68
1:F:650:THR:HG22	1:F:671:LYS:HB2	1.75	0.68
1:E:149:PRO:HA	1:E:152:SER:HB3	1.74	0.68
1:C:531:ARG:HH12	1:C:577:THR:CG2	2.06	0.67
1:D:122:TRP:HA	1:D:125:LYS:HE2	1.76	0.67
1:D:145:TRP:HD1	1:D:261:MET:HE1	1.59	0.67
1:E:667:PHE:HB3	1:E:672:ILE:HD11	1.76	0.67
1:A:556:ILE:O	1:A:584:ASN:ND2	2.26	0.67
1:A:735:LYS:HA	1:A:758:ASP:HB3	1.75	0.67
1:B:556:ILE:O	1:B:584:ASN:ND2	2.26	0.67
1:B:671:LYS:O	1:B:673:GLU:OE2	2.12	0.67
1:F:481:ILE:HD13	1:F:486:LEU:HB2	1.73	0.67
1:C:522:VAL:HA	1:C:550:LYS:HB2	1.75	0.67
1:C:686:ARG:HA	1:C:708:LEU:HA	1.76	0.67
1:E:766:ILE:HD13	1:E:791:THR:HG22	1.74	0.67
1:F:271:ILE:HA	1:F:274:LEU:HD12	1.77	0.67
1:B:713:ILE:HG13	1:B:736:ILE:HA	1.76	0.67
1:B:522:VAL:HA	1:B:550:LYS:HB2	1.77	0.67
1:E:421:ASN:OD1	1:E:425:ARG:N	2.28	0.67
1:E:438:ASP:HA	1:E:441:PHE:HD2	1.59	0.67
1:C:737:GLY:O	1:C:762:ASN:ND2	2.28	0.67
1:E:618:ASP:HA	1:E:643:LYS:HB2	1.76	0.67
1:C:122:TRP:HA	1:C:125:LYS:HE2	1.77	0.67
1:E:760:LYS:HB2	1:E:783:VAL:HG12	1.77	0.67
1:C:366:VAL:HB	1:C:370:PHE:HB3	1.77	0.66
1:C:544:LEU:HD23	1:C:563:VAL:HG21	1.76	0.66
1:E:32:SER:OG	1:E:330:TYR:OH	2.10	0.66
1:C:46:GLN:NE2	1:C:125:LYS:O	2.26	0.66
1:F:245:VAL:HG11	1:F:391:PHE:HB3	1.78	0.66
1:G:48:MET:SD	1:G:49:GLN:HG2	2.35	0.66
1:B:701:GLU:O	1:B:704:VAL:HG12	1.96	0.66
1:B:150:GLY:O	1:B:154:LYS:NZ	2.25	0.66
1:F:473:SER:HA	1:F:497:SER:HB2	1.77	0.66
1:C:495:VAL:HG13	1:C:518:GLU:HB2	1.77	0.66
1:F:150:GLY:O	1:F:154:LYS:NZ	2.28	0.66
1:B:759:VAL:CG2	1:B:784:VAL:HG12	2.26	0.66
1:B:507:PRO:HB2	1:B:509:TRP:NE1	2.10	0.65
1:C:170:TRP:CD1	1:C:173:ARG:HD2	2.31	0.65
1:A:732:LYS:HA	1:A:754:LEU:HA	1.77	0.65
1:C:151:SER:HB2	1:C:258:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:643:LYS:HA	1:D:666:SER:HB2	1.76	0.65
1:E:738:LYS:HG2	1:E:761:GLY:HA3	1.77	0.65
1:F:591:LEU:HD21	1:F:594:LEU:HB2	1.78	0.65
1:G:40:VAL:O	1:G:44:THR:HG23	1.95	0.65
1:A:712:SER:HA	1:A:735:LYS:HB2	1.77	0.65
1:C:758:ASP:HA	1:C:783:VAL:HB	1.77	0.65
1:D:475:HIS:HA	1:D:499:LYS:HB2	1.78	0.65
1:A:256:ASP:H	1:A:369:ASP:HB2	1.61	0.65
1:B:134:HIS:CD2	1:B:276:ILE:HD11	2.32	0.65
1:E:48:MET:HG3	1:E:49:GLN:HG2	1.77	0.65
1:F:363:ILE:HA	1:F:392:LEU:HD22	1.79	0.65
1:F:765:GLU:CD	1:F:765:GLU:N	2.50	0.65
1:D:713:ILE:HD12	1:D:718:VAL:HG21	1.79	0.65
1:G:48:MET:HE3	1:G:48:MET:H	1.60	0.65
1:B:519:LEU:HD12	1:B:520:TYR:N	2.12	0.65
1:D:279:TYR:HD1	1:D:283:LEU:HD23	1.61	0.64
1:E:49:GLN:O	1:E:51:LYS:NZ	2.29	0.64
1:F:712:SER:HA	1:F:735:LYS:HB2	1.78	0.64
1:E:150:GLY:O	1:E:154:LYS:NZ	2.25	0.64
1:A:40:VAL:O	1:A:44:THR:HG23	1.97	0.64
1:F:570:MET:HE3	1:F:588:MET:HG2	1.79	0.64
1:A:452:GLU:HA	1:A:475:HIS:HB2	1.78	0.64
1:A:490:LYS:HG2	1:A:513:LEU:HA	1.78	0.64
1:E:604:ILE:HD12	1:E:629:GLU:HB2	1.80	0.64
1:E:686:ARG:HA	1:E:708:LEU:HA	1.78	0.64
1:B:686:ARG:HA	1:B:708:LEU:HA	1.79	0.64
1:D:654:GLU:O	1:D:657:LYS:NZ	2.27	0.64
1:F:153:SER:OG	1:F:154:LYS:NZ	2.31	0.64
1:A:447:GLN:HA	1:A:469:LEU:HA	1.79	0.64
1:B:40:VAL:O	1:B:44:THR:HG23	1.98	0.64
1:B:134:HIS:CG	1:B:276:ILE:HD11	2.33	0.64
1:B:490:LYS:HG2	1:B:513:LEU:HA	1.80	0.64
1:F:744:LEU:HD23	1:F:768:PRO:HD2	1.79	0.64
1:A:538:LEU:HG	1:A:559:ALA:HB1	1.80	0.64
1:C:35:MET:HE2	1:C:135:THR:CG2	2.13	0.63
1:C:134:HIS:CG	1:C:276:ILE:HD11	2.34	0.63
1:E:52:ILE:HD11	1:E:120:LEU:HD22	1.80	0.63
1:A:701:GLU:O	1:A:704:VAL:HG12	1.99	0.63
1:A:457:VAL:HB	1:A:479:VAL:HG22	1.81	0.63
1:E:145:TRP:HD1	1:E:261:MET:SD	2.21	0.63
1:E:153:SER:OG	1:E:154:LYS:NZ	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:ALA:HB2	1:G:293:CYS:HB3	1.81	0.63
1:B:541:LEU:HB3	1:B:544:LEU:HD23	1.79	0.63
1:F:673:GLU:HG2	1:F:674:VAL:H	1.63	0.63
1:G:312:MET:SD	1:G:312:MET:N	2.72	0.63
1:F:574:ASN:HD21	1:F:599:CYS:HA	1.64	0.63
1:F:760:LYS:HG2	1:F:783:VAL:HG12	1.81	0.63
1:E:256:ASP:HB2	1:E:367:LYS:HZ1	1.62	0.63
1:F:122:TRP:HA	1:F:125:LYS:HE2	1.81	0.63
1:A:405:LEU:O	1:A:409:TRP:N	2.29	0.62
1:E:490:LYS:HG2	1:E:513:LEU:HA	1.80	0.62
1:E:665:LEU:HB2	1:E:685:ILE:HD13	1.80	0.62
1:B:444:THR:HA	1:B:466:LEU:HG	1.80	0.62
1:B:538:LEU:HG	1:B:559:ALA:HB1	1.79	0.62
1:D:429:PRO:HA	1:D:450:LYS:HB3	1.81	0.62
1:F:438:ASP:HA	1:F:441:PHE:HD2	1.63	0.62
1:A:455:LYS:HD3	1:A:478:SER:H	1.63	0.62
1:A:737:GLY:O	1:A:762:ASN:ND2	2.32	0.62
1:C:373:MET:HA	1:C:376:MET:SD	2.40	0.62
1:B:517:GLU:HA	1:B:544:LEU:HA	1.80	0.62
1:B:641:VAL:HG13	1:B:664:ARG:HB2	1.80	0.62
1:A:675:LEU:HD23	1:A:675:LEU:H	1.65	0.62
1:B:52:ILE:HG21	1:B:116:TYR:HB2	1.80	0.62
1:A:766:ILE:CD1	1:A:791:THR:CG2	2.76	0.62
1:C:732:LYS:HA	1:C:754:LEU:HA	1.82	0.62
1:B:49:GLN:O	1:B:51:LYS:NZ	2.30	0.62
1:A:486:LEU:HD12	1:A:489:LEU:HD12	1.82	0.62
1:B:430:LEU:HD12	1:B:451:LEU:HG	1.81	0.62
1:C:405:LEU:HD21	1:C:437:PRO:HG3	1.82	0.62
1:E:588:MET:HE2	1:E:591:LEU:CD1	2.29	0.62
1:F:687:TYR:HA	1:F:710:TYR:HB3	1.81	0.62
1:E:474:LEU:O	1:E:499:LYS:N	2.30	0.61
1:B:421:ASN:OD1	1:B:425:ARG:N	2.31	0.61
1:B:490:LYS:HD3	1:B:514:ARG:HH12	1.63	0.61
1:E:707:SER:HA	1:E:730:LYS:HD2	1.82	0.61
1:C:135:THR:O	1:C:139:MET:HE3	1.99	0.61
1:E:366:VAL:HB	1:E:370:PHE:HB3	1.81	0.61
1:A:632:SER:O	1:A:635:HIS:HB3	2.00	0.61
1:D:421:ASN:HB3	1:D:427:GLU:HB2	1.81	0.61
1:E:759:VAL:CG2	1:E:784:VAL:HG12	2.31	0.61
1:A:352:GLU:OE1	1:A:355:ARG:NH2	2.32	0.61
1:B:516:LEU:HD12	1:B:517:GLU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:ASN:O	1:C:707:SER:OG	2.19	0.61
1:F:149:PRO:HA	1:F:152:SER:HB3	1.83	0.61
1:D:447:GLN:NE2	1:D:468:ASN:OD1	2.34	0.61
1:C:618:ASP:HA	1:C:643:LYS:HB2	1.83	0.61
1:D:426:LEU:HB3	1:D:447:GLN:H	1.65	0.61
1:A:254:GLU:N	1:A:254:GLU:OE1	2.32	0.61
1:A:597:VAL:HG22	1:A:620:LYS:HB3	1.83	0.61
1:D:631:VAL:HA	1:D:655:HIS:CE1	2.35	0.61
1:E:175:LEU:HD22	1:E:358:THR:HG21	1.82	0.61
1:F:134:HIS:CE1	1:F:276:ILE:HD11	2.35	0.61
1:C:355:ARG:HG3	1:C:361:ASP:HA	1.81	0.60
1:E:733:THR:HG23	1:E:756:TYR:HD2	1.66	0.60
1:A:393:SER:O	1:A:396:SER:OG	2.17	0.60
1:A:447:GLN:OE1	1:A:447:GLN:N	2.31	0.60
1:A:760:LYS:HB2	1:A:783:VAL:HG12	1.82	0.60
1:C:354:VAL:O	1:C:358:THR:OG1	2.16	0.60
1:E:405:LEU:HD21	1:E:437:PRO:HG3	1.84	0.60
1:F:16:ALA:HA	1:F:159:ILE:HD13	1.83	0.60
1:B:470:GLN:O	1:B:495:VAL:N	2.31	0.60
1:B:706:GLN:NE2	1:B:727:PHE:O	2.30	0.60
1:C:630:ILE:HB	1:C:655:HIS:HB2	1.82	0.60
1:C:139:MET:N	1:C:139:MET:HE2	2.17	0.60
1:D:52:ILE:HG12	1:D:310:HIS:HB3	1.82	0.60
1:F:480:LYS:HE3	1:F:504:ARG:HH22	1.67	0.60
1:A:473:SER:O	1:A:474:LEU:HD13	2.02	0.60
1:E:457:VAL:HB	1:E:479:VAL:HG22	1.83	0.60
1:G:48:MET:HG2	1:G:49:GLN:NE2	2.16	0.60
1:G:111:ILE:HD11	1:G:301:THR:HG21	1.84	0.60
1:A:353:TYR:O	1:A:357:GLU:N	2.32	0.60
1:A:778:LYS:HA	1:A:800:MET:HG2	1.84	0.60
1:E:425:ARG:NH1	1:E:471:GLU:OE1	2.34	0.60
1:F:425:ARG:NH1	1:F:471:GLU:OE1	2.27	0.60
1:B:270:VAL:O	1:B:274:LEU:HD22	2.01	0.60
1:C:170:TRP:CE2	1:C:400:LEU:HD13	2.37	0.60
1:A:120:LEU:HD21	1:A:310:HIS:CD2	2.37	0.60
1:A:497:SER:HA	1:A:520:TYR:HB2	1.84	0.60
1:F:630:ILE:HB	1:F:655:HIS:HB2	1.84	0.60
1:B:457:VAL:HB	1:B:479:VAL:HG22	1.83	0.60
1:E:276:ILE:HD13	1:E:279:TYR:HE2	1.67	0.60
1:F:433:LEU:HB2	1:F:454:ILE:HD13	1.84	0.60
1:B:516:LEU:HD12	1:B:517:GLU:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:ILE:O	1:D:633:PHE:HB2	2.01	0.59
1:E:166:PHE:HD1	1:E:387:ARG:HD2	1.67	0.59
1:B:46:GLN:NE2	1:B:125:LYS:O	2.35	0.59
1:B:732:LYS:HA	1:B:754:LEU:HA	1.85	0.59
1:C:709:GLN:HA	1:C:731:LEU:HA	1.83	0.59
1:C:760:LYS:HB2	1:C:783:VAL:HG12	1.83	0.59
1:A:568:GLN:O	1:A:592:THR:N	2.36	0.59
1:C:367:LYS:O	1:C:371:ALA:N	2.28	0.59
1:E:472:LEU:HD12	1:E:473:SER:N	2.17	0.59
1:E:675:LEU:HD23	1:E:675:LEU:H	1.66	0.59
1:A:273:PHE:CE2	1:A:274:LEU:HD23	2.37	0.59
1:A:706:GLN:HG3	1:A:730:LYS:HE3	1.83	0.59
1:B:170:TRP:HH2	1:B:396:SER:HB2	1.66	0.59
1:B:448:SER:HB2	1:B:471:GLU:HB3	1.84	0.59
1:G:44:THR:O	1:G:47:VAL:N	2.36	0.59
1:B:759:VAL:HG22	1:B:784:VAL:HG12	1.84	0.59
1:B:771:LEU:HD12	1:B:792:LEU:HD11	1.84	0.59
1:C:363:ILE:HA	1:C:392:LEU:HD12	1.83	0.59
1:E:427:GLU:HG2	1:E:450:LYS:HD2	1.83	0.59
1:E:597:VAL:HG22	1:E:620:LYS:HB3	1.83	0.59
1:E:673:GLU:OE1	1:E:674:VAL:N	2.35	0.59
1:E:778:LYS:C	1:E:800:MET:CE	2.71	0.59
1:F:683:ASN:O	1:F:707:SER:OG	2.20	0.59
1:C:144:PHE:HA	1:C:147:LYS:HB2	1.85	0.59
1:C:531:ARG:HH12	1:C:577:THR:HG23	1.68	0.59
1:F:59:VAL:HG21	1:F:99:LEU:HD21	1.84	0.59
1:B:496:LEU:HD23	1:B:497:SER:N	2.18	0.59
1:D:354:VAL:O	1:D:358:THR:OG1	2.21	0.59
1:A:539:ARG:HH12	1:A:566:HIS:HE1	1.50	0.59
1:C:48:MET:HG2	1:C:49:GLN:HG2	1.84	0.59
1:C:312:MET:SD	1:C:312:MET:N	2.75	0.59
1:D:366:VAL:HB	1:D:370:PHE:HB3	1.84	0.59
1:D:436:LEU:HD21	1:D:451:LEU:HD21	1.85	0.59
1:D:556:ILE:O	1:D:584:ASN:ND2	2.33	0.59
1:G:44:THR:O	1:G:48:MET:HE3	2.01	0.59
1:A:394:GLU:HA	1:A:397:GLU:HG3	1.84	0.58
1:B:425:ARG:NH1	1:B:471:GLU:OE1	2.30	0.58
1:C:59:VAL:HG11	1:C:99:LEU:HD11	1.85	0.58
1:F:474:LEU:O	1:F:499:LYS:N	2.36	0.58
1:F:707:SER:HA	1:F:730:LYS:HD2	1.85	0.58
1:D:426:LEU:H	1:D:447:GLN:HB3	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:641:VAL:HG13	1:E:664:ARG:HB2	1.84	0.58
1:F:732:LYS:HA	1:F:754:LEU:HA	1.83	0.58
1:A:161:ILE:HD11	1:A:245:VAL:HA	1.86	0.58
1:A:421:ASN:OD1	1:A:425:ARG:N	2.36	0.58
1:B:538:LEU:HB3	1:B:541:LEU:HD12	1.85	0.58
1:A:735:LYS:HG2	1:A:756:TYR:HE2	1.68	0.58
1:E:16:ALA:HA	1:E:159:ILE:HD12	1.86	0.58
1:F:273:PHE:O	1:F:277:ILE:HG22	2.03	0.58
1:F:560:VAL:HA	1:F:563:VAL:HG12	1.85	0.58
1:B:444:THR:HG22	1:B:466:LEU:HD12	1.86	0.58
1:E:709:GLN:HA	1:E:731:LEU:HA	1.85	0.58
1:E:522:VAL:HA	1:E:550:LYS:HB3	1.85	0.58
1:A:114:MET:HG2	1:A:297:ILE:HD11	1.84	0.58
1:A:495:VAL:HG13	1:A:518:GLU:HB2	1.85	0.58
1:A:641:VAL:HG13	1:A:664:ARG:HB2	1.86	0.58
1:C:148:PHE:HD2	1:C:151:SER:H	1.49	0.58
1:E:588:MET:HE2	1:E:591:LEU:HD13	1.84	0.58
1:F:570:MET:HE3	1:F:588:MET:HE3	1.84	0.58
1:F:588:MET:SD	1:F:591:LEU:HB2	2.44	0.58
1:F:673:GLU:HA	1:F:694:ASP:HB2	1.84	0.58
1:E:588:MET:HG3	1:E:588:MET:O	2.03	0.58
1:F:650:THR:HG22	1:F:671:LYS:HB3	1.86	0.58
1:A:744:LEU:HD23	1:A:768:PRO:HD2	1.85	0.58
1:B:735:LYS:HA	1:B:758:ASP:HB3	1.84	0.58
1:E:145:TRP:CD1	1:E:262:TYR:HD1	2.22	0.58
1:F:363:ILE:HG23	1:F:392:LEU:HD13	1.85	0.58
1:F:675:LEU:HD23	1:F:675:LEU:H	1.69	0.58
1:B:673:GLU:OE1	1:B:673:GLU:N	2.37	0.57
1:D:111:ILE:HD13	1:D:306:PHE:HE2	1.69	0.57
1:F:531:ARG:HH22	1:F:552:ASN:HD21	1.39	0.57
1:F:538:LEU:H	1:F:559:ALA:HB1	1.69	0.57
1:D:645:TRP:CD1	1:D:666:SER:HB3	2.40	0.57
1:F:352:GLU:OE1	1:F:355:ARG:NH2	2.37	0.57
1:F:567:LEU:HD23	1:F:570:MET:HE2	1.85	0.57
1:F:617:LEU:HB2	1:F:639:LEU:HD11	1.86	0.57
1:A:124:ALA:HB2	1:A:287:VAL:HG12	1.85	0.57
1:A:459:ILE:HD12	1:A:481:ILE:HG22	1.85	0.57
1:F:474:LEU:N	1:F:497:SER:O	2.34	0.57
1:A:624:LEU:HD23	1:A:627:ILE:HG22	1.85	0.57
1:A:687:TYR:HA	1:A:710:TYR:HB3	1.85	0.57
1:A:715:CYS:SG	1:A:738:LYS:NZ	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:GLN:HA	1:B:731:LEU:HA	1.87	0.57
1:B:712:SER:HA	1:B:735:LYS:HB2	1.86	0.57
1:A:509:TRP:CZ3	1:A:510:MET:HG3	2.39	0.57
1:A:663:GLU:HA	1:A:685:ILE:HA	1.85	0.57
1:A:714:THR:HA	1:A:737:GLY:HA3	1.87	0.57
1:B:124:ALA:HB2	1:B:287:VAL:HG12	1.86	0.57
1:B:604:ILE:HD12	1:B:629:GLU:HB2	1.85	0.57
1:B:662:LEU:HB3	1:B:685:ILE:HG12	1.85	0.57
1:C:470:GLN:O	1:C:495:VAL:N	2.31	0.57
1:E:436:LEU:HD11	1:E:459:ILE:HG12	1.86	0.57
1:E:449:LEU:O	1:E:473:SER:N	2.25	0.57
1:C:52:ILE:HG21	1:C:116:TYR:HB2	1.87	0.57
1:F:381:ASP:OD2	1:F:384:TYR:N	2.37	0.57
1:A:472:LEU:CD2	1:A:474:LEU:HD21	2.35	0.57
1:D:499:LYS:HG2	1:D:522:VAL:HB	1.87	0.57
1:F:764:PHE:HB2	1:F:788:LEU:HD21	1.86	0.57
1:B:353:TYR:O	1:B:357:GLU:N	2.34	0.57
1:B:490:LYS:HB3	1:B:514:ARG:HH12	1.70	0.57
1:C:625:LYS:HG2	1:C:648:SER:HB2	1.85	0.57
1:D:145:TRP:CD1	1:D:261:MET:SD	2.98	0.57
1:E:625:LYS:O	1:E:625:LYS:NZ	2.33	0.57
1:F:539:ARG:NH1	1:F:540:ASP:OD1	2.38	0.57
1:A:485:ALA:O	1:A:489:LEU:HG	2.05	0.57
1:E:412:ASP:OD2	1:E:416:GLN:NE2	2.37	0.57
1:B:59:VAL:HG21	1:B:99:LEU:HD21	1.87	0.56
1:A:430:LEU:HD12	1:A:451:LEU:HG	1.85	0.56
1:F:650:THR:CG2	1:F:671:LYS:HB2	2.35	0.56
1:A:625:LYS:HB2	1:A:648:SER:HB2	1.86	0.56
1:B:166:PHE:HA	1:B:387:ARG:HD2	1.87	0.56
1:B:294:ASN:ND2	1:B:305:ASN:OD1	2.38	0.56
1:B:687:TYR:HA	1:B:710:TYR:HB3	1.87	0.56
1:C:771:LEU:HD12	1:C:792:LEU:HD21	1.88	0.56
1:D:624:LEU:HD23	1:D:627:ILE:HG22	1.87	0.56
1:E:31:LEU:HB2	1:E:330:TYR:HE1	1.70	0.56
1:F:737:GLY:O	1:F:762:ASN:ND2	2.36	0.56
1:A:474:LEU:CD2	1:A:496:LEU:HD11	2.35	0.56
1:B:678:HIS:HA	1:B:681:LEU:HG	1.86	0.56
1:E:52:ILE:HD12	1:E:116:TYR:HA	1.87	0.56
1:F:170:TRP:CZ2	1:F:400:LEU:HB2	2.40	0.56
1:F:450:LYS:HA	1:F:473:SER:HB3	1.86	0.56
1:A:618:ASP:HB2	1:A:643:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:LEU:HD22	1:A:662:LEU:HD22	1.87	0.56
1:C:455:LYS:NZ	1:C:476:GLN:O	2.28	0.56
1:C:620:LYS:HG2	1:C:621:GLU:HG3	1.88	0.56
1:A:31:LEU:HD11	1:A:329:ILE:HG22	1.88	0.56
1:B:499:LYS:HG2	1:B:522:VAL:HB	1.87	0.56
1:C:631:VAL:O	1:C:634:GLN:HB3	2.06	0.56
1:D:683:ASN:O	1:D:707:SER:OG	2.20	0.56
1:E:451:LEU:HD11	1:E:454:ILE:HB	1.88	0.56
1:E:733:THR:HG23	1:E:756:TYR:CD2	2.40	0.56
1:D:738:LYS:HG2	1:D:761:GLY:HA3	1.86	0.56
1:E:172:THR:OG1	1:E:387:ARG:NH1	2.38	0.56
1:A:273:PHE:CD2	1:A:274:LEU:HD23	2.41	0.56
1:A:423:HIS:NE2	1:A:520:TYR:OH	2.38	0.56
1:B:757:LEU:HG	1:B:759:VAL:HG13	1.87	0.56
1:C:759:VAL:CG2	1:C:784:VAL:HG12	2.36	0.56
1:E:426:LEU:HB3	1:E:446:LEU:HA	1.87	0.56
1:E:444:THR:HG22	1:E:466:LEU:HD23	1.87	0.56
1:C:354:VAL:HG12	1:C:386:LYS:HD3	1.88	0.56
1:C:510:MET:HA	1:C:513:LEU:HG	1.87	0.56
1:E:366:VAL:HG11	1:E:374:LEU:HD11	1.86	0.56
1:E:766:ILE:HD12	1:E:791:THR:HB	1.86	0.56
1:D:670:ASN:C	1:D:671:LYS:HD3	2.26	0.55
1:A:134:HIS:CE1	1:A:276:ILE:HD11	2.41	0.55
1:A:161:ILE:HD11	1:A:245:VAL:HG22	1.88	0.55
1:B:568:GLN:O	1:B:592:THR:OG1	2.20	0.55
1:A:249:ARG:HE	1:A:253:GLU:CD	2.09	0.55
1:D:714:THR:HA	1:D:737:GLY:HA3	1.88	0.55
1:E:133:ILE:HA	1:E:136:LEU:HG	1.87	0.55
1:F:765:GLU:OE2	1:F:765:GLU:N	2.39	0.55
1:A:165:CYS:SG	1:A:388:PHE:HA	2.47	0.55
1:A:726:TYR:HA	1:A:751:LEU:HD11	1.89	0.55
1:E:136:LEU:HD12	1:E:137:VAL:N	2.22	0.55
1:B:455:LYS:NZ	1:B:476:GLN:O	2.31	0.55
1:B:694:ASP:O	1:B:696:ARG:NH2	2.40	0.55
1:D:672:ILE:CD1	1:D:695:ILE:HD11	2.23	0.55
1:F:714:THR:HA	1:F:737:GLY:HA3	1.86	0.55
1:C:619:LEU:HD22	1:C:622:ASN:HD22	1.71	0.55
1:E:267:VAL:O	1:E:271:ILE:HG12	2.05	0.55
1:E:732:LYS:HA	1:E:754:LEU:HA	1.88	0.55
1:F:472:LEU:HD12	1:F:473:SER:N	2.21	0.55
1:B:599:CYS:N	1:B:622:ASN:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:ILE:HD12	1:B:676:PRO:HD2	1.88	0.55
1:D:352:GLU:OE1	1:D:355:ARG:NH2	2.40	0.55
1:A:719:GLU:HG2	1:A:740:SER:HB3	1.89	0.55
1:E:427:GLU:OE2	1:E:448:SER:OG	2.16	0.55
1:E:470:GLN:O	1:E:495:VAL:N	2.40	0.55
1:E:495:VAL:HG13	1:E:518:GLU:HB2	1.89	0.55
1:E:551:SER:HB2	1:E:553:VAL:HG23	1.88	0.55
1:C:474:LEU:O	1:C:499:LYS:N	2.37	0.55
1:E:450:LYS:HA	1:E:473:SER:HB3	1.89	0.55
1:G:57:LYS:NZ	1:G:58:ARG:HH21	2.05	0.55
1:A:510:MET:SD	1:A:510:MET:N	2.73	0.55
1:B:673:GLU:O	1:B:695:ILE:HA	2.07	0.55
1:D:604:ILE:HD12	1:D:629:GLU:HB2	1.89	0.55
1:F:621:GLU:HA	1:F:646:HIS:HB3	1.88	0.55
1:C:114:MET:HA	1:C:114:MET:HE2	1.88	0.54
1:C:701:GLU:O	1:C:704:VAL:HG22	2.07	0.54
1:D:367:LYS:HG3	1:D:368:ASN:H	1.72	0.54
1:D:522:VAL:HA	1:D:550:LYS:HB2	1.88	0.54
1:D:672:ILE:HG13	1:D:693:ASN:HB3	1.88	0.54
1:E:441:PHE:HA	1:E:466:LEU:HD21	1.88	0.54
1:E:737:GLY:O	1:E:762:ASN:ND2	2.33	0.54
1:G:276:ILE:O	1:G:280:ASN:ND2	2.34	0.54
1:A:141:CYS:HB2	1:A:268:LEU:HD11	1.89	0.54
1:A:470:GLN:HA	1:A:493:LEU:HA	1.88	0.54
1:D:145:TRP:CD1	1:D:261:MET:HE1	2.41	0.54
1:D:369:ASP:O	1:D:373:MET:HE2	2.07	0.54
1:E:687:TYR:HA	1:E:710:TYR:HB3	1.89	0.54
1:A:449:LEU:HD12	1:A:450:LYS:H	1.73	0.54
1:E:499:LYS:HG3	1:E:522:VAL:HB	1.88	0.54
1:E:547:LEU:HD23	1:E:570:MET:HG2	1.88	0.54
1:E:778:LYS:C	1:E:800:MET:HE1	2.27	0.54
1:F:156:GLU:HA	1:F:159:ILE:HD12	1.88	0.54
1:F:253:GLU:HG2	1:F:367:LYS:HB2	1.89	0.54
1:F:405:LEU:HG	1:F:409:TRP:HD1	1.72	0.54
1:F:526:SER:CB	1:F:531:ARG:HE	2.20	0.54
1:A:119:ALA:HB2	1:A:293:CYS:HB3	1.89	0.54
1:A:574:ASN:HD21	1:A:599:CYS:HA	1.72	0.54
1:E:598:HIS:ND1	1:E:621:GLU:OE1	2.36	0.54
1:B:425:ARG:HD3	1:B:447:GLN:HB2	1.88	0.54
1:B:516:LEU:HG	1:B:544:LEU:HD11	1.90	0.54
1:D:620:LYS:HZ3	1:D:643:LYS:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:MET:O	1:E:316:PHE:N	2.28	0.54
1:F:449:LEU:O	1:F:473:SER:N	2.30	0.54
1:A:463:ILE:HD11	1:A:485:ALA:HA	1.89	0.54
1:A:506:LEU:HG	1:A:510:MET:HE1	1.89	0.54
1:E:766:ILE:CD1	1:E:791:THR:CB	2.73	0.54
1:F:360:ILE:HD12	1:F:393:SER:HB2	1.90	0.54
1:F:580:VAL:HG23	1:F:581:MET:SD	2.48	0.54
1:C:352:GLU:HA	1:C:355:ARG:HH21	1.73	0.54
1:C:687:TYR:HA	1:C:710:TYR:HB3	1.89	0.54
1:D:490:LYS:HG2	1:D:513:LEU:HA	1.90	0.54
1:D:673:GLU:HA	1:D:694:ASP:HB2	1.90	0.54
1:D:686:ARG:HA	1:D:708:LEU:HA	1.89	0.54
1:F:421:ASN:OD1	1:F:425:ARG:N	2.40	0.54
1:F:592:THR:O	1:F:615:GLN:N	2.37	0.54
1:B:471:GLU:HA	1:B:495:VAL:O	2.07	0.54
1:C:735:LYS:HA	1:C:758:ASP:HB3	1.90	0.54
1:E:485:ALA:O	1:E:489:LEU:HG	2.08	0.54
1:E:591:LEU:HD21	1:E:594:LEU:HB2	1.90	0.54
1:C:128:PRO:O	1:C:132:LEU:HD22	2.07	0.54
1:E:310:HIS:NE2	1:E:313:ALA:HB2	2.23	0.54
1:C:153:SER:OG	1:C:154:LYS:NZ	2.35	0.53
1:E:170:TRP:CZ2	1:E:400:LEU:HB2	2.44	0.53
1:C:366:VAL:HG21	1:C:374:LEU:HD22	1.90	0.53
1:D:675:LEU:HD22	1:D:695:ILE:HD12	1.90	0.53
1:F:671:LYS:HE3	1:F:671:LYS:CA	2.26	0.53
1:B:113:GLN:HG3	1:C:53:ILE:HD12	1.89	0.53
1:B:624:LEU:HD23	1:B:627:ILE:HG22	1.89	0.53
1:B:643:LYS:CA	1:B:666:SER:OG	2.56	0.53
1:B:659:LEU:HB2	1:B:662:LEU:HG	1.91	0.53
1:F:788:LEU:O	1:F:791:THR:OG1	2.26	0.53
1:A:430:LEU:O	1:A:452:GLU:N	2.39	0.53
1:A:452:GLU:HG3	1:A:475:HIS:HB2	1.89	0.53
1:B:449:LEU:HD12	1:B:450:LYS:H	1.73	0.53
1:B:637:ARG:NH1	1:B:660:THR:H	2.06	0.53
1:A:145:TRP:O	1:A:151:SER:OG	2.23	0.53
1:A:790:GLU:OE2	1:B:732:LYS:NZ	2.31	0.53
1:E:624:LEU:HD23	1:E:627:ILE:HG22	1.89	0.53
1:F:531:ARG:N	1:F:554:SER:HG	2.06	0.53
1:C:499:LYS:HA	1:C:522:VAL:HB	1.91	0.53
1:C:541:LEU:O	1:C:566:HIS:NE2	2.42	0.53
1:D:347:ARG:O	1:D:368:ASN:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:526:SER:HA	1:E:533:VAL:HA	1.89	0.53
1:G:46:GLN:O	1:G:50:ASP:HB3	2.08	0.53
1:D:467:ASP:HA	1:D:488:PHE:HZ	1.73	0.53
1:E:766:ILE:CD1	1:E:791:THR:HG22	2.35	0.53
1:F:511:TYR:O	1:F:540:ASP:HB2	2.07	0.53
1:B:757:LEU:HD23	1:B:782:LEU:HD12	1.89	0.53
1:C:675:LEU:HD22	1:C:695:ILE:HD12	1.89	0.53
1:E:503:MET:HE3	1:E:506:LEU:HB3	1.89	0.53
1:F:480:LYS:HA	1:F:509:TRP:HZ2	1.74	0.53
1:F:557:PRO:HG2	1:F:560:VAL:HG23	1.90	0.53
1:D:766:ILE:HG23	1:D:791:THR:HB	1.91	0.53
1:E:673:GLU:OE2	1:E:674:VAL:CG2	2.57	0.53
1:F:131:VAL:HG22	1:F:323:TYR:CZ	2.44	0.53
1:B:546:ILE:HG12	1:B:569:LYS:HB3	1.91	0.53
1:D:671:LYS:N	1:D:671:LYS:CD	2.66	0.53
1:D:735:LYS:HA	1:D:758:ASP:HB3	1.89	0.53
1:A:430:LEU:HB2	1:A:451:LEU:HA	1.90	0.52
1:A:558:GLN:NE2	1:A:562:ASP:OD1	2.43	0.52
1:F:393:SER:O	1:F:396:SER:OG	2.20	0.52
1:F:466:LEU:HB3	1:F:469:LEU:HD23	1.90	0.52
1:B:104:ASP:OD1	1:B:104:ASP:N	2.42	0.52
1:B:170:TRP:CH2	1:B:396:SER:HB2	2.44	0.52
1:C:249:ARG:HA	1:C:370:PHE:CZ	2.44	0.52
1:D:455:LYS:HD2	1:D:504:ARG:HH12	1.74	0.52
1:A:678:HIS:HA	1:A:681:LEU:HG	1.92	0.52
1:C:788:LEU:O	1:C:791:THR:OG1	2.24	0.52
1:D:155:ILE:HD11	1:D:258:LEU:HD11	1.91	0.52
1:D:474:LEU:HD12	1:D:498:VAL:HG22	1.91	0.52
1:B:519:LEU:HD12	1:B:520:TYR:H	1.72	0.52
1:C:239:LYS:HE3	1:C:401:LYS:HG2	1.91	0.52
1:D:104:ASP:N	1:D:104:ASP:OD1	2.36	0.52
1:E:276:ILE:HD13	1:E:279:TYR:CE2	2.44	0.52
1:E:683:ASN:O	1:E:707:SER:OG	2.20	0.52
1:A:630:ILE:O	1:A:633:PHE:HB2	2.09	0.52
1:B:352:GLU:OE1	1:B:355:ARG:NE	2.42	0.52
1:B:596:LEU:HB2	1:B:619:LEU:HD23	1.92	0.52
1:C:690:LEU:O	1:C:716:ASN:ND2	2.29	0.52
1:E:427:GLU:HB2	1:E:448:SER:HB3	1.91	0.52
1:E:663:GLU:HA	1:E:685:ILE:HA	1.91	0.52
1:F:632:SER:O	1:F:635:HIS:HB3	2.10	0.52
1:D:507:PRO:O	1:D:510:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:PHE:CG	1:E:373:MET:HE3	2.45	0.52
1:F:567:LEU:HD23	1:F:588:MET:HE3	1.90	0.52
1:A:449:LEU:HG	1:A:451:LEU:HD11	1.91	0.52
1:B:246:LYS:O	1:B:249:ARG:HG3	2.10	0.52
1:B:351:PHE:C	1:B:353:TYR:H	2.13	0.52
1:B:538:LEU:HD12	1:B:560:VAL:HA	1.91	0.52
1:C:712:SER:HA	1:C:735:LYS:HB2	1.92	0.52
1:D:121:HIS:CD2	1:D:286:LYS:HG2	2.44	0.52
1:D:474:LEU:HB2	1:D:498:VAL:HA	1.91	0.52
1:D:618:ASP:HA	1:D:643:LYS:HB2	1.92	0.52
1:F:421:ASN:HB3	1:F:427:GLU:HB2	1.92	0.52
1:A:104:ASP:OD1	1:A:104:ASP:N	2.34	0.52
1:B:168:SER:O	1:B:171:THR:OG1	2.19	0.52
1:C:531:ARG:HH12	1:C:577:THR:HG21	1.72	0.52
1:C:643:LYS:HA	1:C:666:SER:HB3	1.91	0.52
1:E:673:GLU:CD	1:E:673:GLU:C	2.67	0.52
1:F:779:ARG:HG3	1:F:801:LYS:HG2	1.92	0.52
1:B:448:SER:HA	1:B:471:GLU:O	2.10	0.52
1:E:312:MET:O	1:E:315:LEU:HB3	2.10	0.52
1:E:346:LEU:HB3	1:E:375:HIS:CD2	2.45	0.52
1:G:332:LEU:HD23	1:G:335:LEU:HD12	1.92	0.52
1:B:714:THR:HA	1:B:737:GLY:HA3	1.92	0.51
1:E:106:GLN:NE2	1:F:108:TYR:HB3	2.25	0.51
1:E:588:MET:CE	1:E:591:LEU:HD13	2.39	0.51
1:F:19:VAL:HA	1:F:380:TYR:CE1	2.45	0.51
1:A:451:LEU:HB3	1:A:454:ILE:HD13	1.91	0.51
1:C:695:ILE:HB	1:C:716:ASN:HD22	1.75	0.51
1:D:121:HIS:CE1	1:D:123:TYR:HB3	2.46	0.51
1:D:455:LYS:HD2	1:D:504:ARG:HH22	1.75	0.51
1:F:622:ASN:HB3	1:F:624:LEU:HD13	1.92	0.51
1:A:249:ARG:NE	1:A:253:GLU:OE2	2.38	0.51
1:B:165:CYS:SG	1:B:388:PHE:HA	2.50	0.51
1:C:120:LEU:HD21	1:C:310:HIS:CD2	2.45	0.51
1:B:734:LEU:HB2	1:B:754:LEU:HD11	1.93	0.51
1:D:145:TRP:HD1	1:D:261:MET:CE	2.21	0.51
1:E:556:ILE:O	1:E:584:ASN:ND2	2.40	0.51
1:E:703:GLY:HA3	1:E:724:GLU:HB3	1.91	0.51
1:G:104:ASP:OD1	1:G:104:ASP:N	2.43	0.51
1:B:238:ALA:HA	1:B:241:LEU:HG	1.93	0.51
1:B:504:ARG:NE	1:B:504:ARG:O	2.44	0.51
1:B:518:GLU:HG2	1:B:546:ILE:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:VAL:O	1:C:135:THR:OG1	2.18	0.51
1:C:352:GLU:OE1	1:C:355:ARG:NH2	2.44	0.51
1:E:521:LEU:HD23	1:E:549:ILE:HG12	1.93	0.51
1:A:36:LEU:HB2	1:A:135:THR:HG21	1.91	0.51
1:A:352:GLU:HA	1:A:355:ARG:HH21	1.75	0.51
1:B:510:MET:HA	1:B:513:LEU:HG	1.91	0.51
1:B:545:LYS:O	1:B:569:LYS:N	2.43	0.51
1:B:650:THR:O	1:B:672:ILE:HA	2.10	0.51
1:B:733:THR:HA	1:B:756:TYR:HB3	1.91	0.51
1:D:571:CYS:HB3	1:D:573:HIS:CE1	2.45	0.51
1:D:709:GLN:HA	1:D:731:LEU:HA	1.91	0.51
1:F:724:GLU:HA	1:F:727:PHE:CD2	2.46	0.51
1:D:438:ASP:HA	1:D:441:PHE:HD2	1.76	0.51
1:D:726:TYR:O	1:D:729:LYS:NZ	2.40	0.51
1:E:33:VAL:CG1	1:E:37:MET:HE3	2.39	0.51
1:E:451:LEU:O	1:E:475:HIS:N	2.38	0.51
1:G:111:ILE:HD13	1:G:306:PHE:HE2	1.75	0.51
1:A:242:PHE:HE1	1:A:391:PHE:HA	1.75	0.51
1:A:276:ILE:HG21	1:A:327:VAL:HG21	1.93	0.51
1:A:683:ASN:OD1	1:A:683:ASN:N	2.41	0.51
1:E:363:ILE:HG23	1:E:392:LEU:HD13	1.93	0.51
1:C:395:VAL:HG12	1:C:399:LYS:HE3	1.93	0.51
1:D:145:TRP:HD1	1:D:261:MET:SD	2.34	0.51
1:D:373:MET:O	1:D:376:MET:HG3	2.11	0.51
1:F:516:LEU:HD21	1:F:519:LEU:HD13	1.93	0.51
1:A:455:LYS:O	1:A:457:VAL:HG23	2.11	0.50
1:C:644:LEU:HD13	1:C:649:ILE:HD13	1.91	0.50
1:E:366:VAL:HG21	1:E:374:LEU:HD12	1.93	0.50
1:A:117:GLU:OE1	1:A:118:ARG:NE	2.44	0.50
1:A:423:HIS:HE2	1:A:520:TYR:HH	1.51	0.50
1:C:585:LEU:HD12	1:C:588:MET:HG2	1.93	0.50
1:C:630:ILE:HA	1:C:633:PHE:HB2	1.93	0.50
1:F:759:VAL:HG22	1:F:784:VAL:HG12	1.92	0.50
1:A:449:LEU:O	1:A:473:SER:N	2.43	0.50
1:C:158:PHE:HA	1:C:161:ILE:HG22	1.92	0.50
1:D:123:TYR:CD2	1:D:283:LEU:HB3	2.47	0.50
1:D:276:ILE:HA	1:D:279:TYR:CE2	2.46	0.50
1:E:246:LYS:O	1:E:249:ARG:HG3	2.10	0.50
1:F:405:LEU:O	1:F:409:TRP:N	2.35	0.50
1:F:415:ARG:HA	1:F:418:LEU:HD12	1.91	0.50
1:F:614:LEU:HD21	1:F:617:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ARG:NH2	1:A:562:ASP:O	2.44	0.50
1:C:415:ARG:HA	1:C:418:LEU:HD12	1.94	0.50
1:C:604:ILE:HD12	1:C:629:GLU:HB2	1.92	0.50
1:D:655:HIS:CE1	1:D:658:LYS:HD2	2.47	0.50
1:D:703:GLY:HA3	1:D:724:GLU:HB3	1.93	0.50
1:E:129:TYR:O	1:E:133:ILE:HG23	2.11	0.50
1:E:673:GLU:OE1	1:E:674:VAL:CB	2.58	0.50
1:F:467:ASP:HA	1:F:488:PHE:CZ	2.46	0.50
1:F:631:VAL:HA	1:F:634:GLN:HG2	1.92	0.50
1:B:467:ASP:OD1	1:B:492:ASN:ND2	2.45	0.50
1:B:630:ILE:O	1:B:633:PHE:HB2	2.12	0.50
1:B:723:ASP:HB3	1:B:747:LYS:HD2	1.93	0.50
1:E:714:THR:HA	1:E:737:GLY:HA3	1.92	0.50
1:F:507:PRO:HG2	1:F:510:MET:HE3	1.92	0.50
1:F:709:GLN:HA	1:F:731:LEU:HA	1.94	0.50
1:B:735:LYS:HG2	1:B:756:TYR:HE2	1.76	0.50
1:E:395:VAL:HG12	1:E:399:LYS:HE3	1.93	0.50
1:A:347:ARG:O	1:A:368:ASN:HA	2.12	0.50
1:A:449:LEU:HD12	1:A:450:LYS:N	2.27	0.50
1:B:280:ASN:HB3	1:B:324:LEU:HD21	1.94	0.50
1:B:644:LEU:HD13	1:B:649:ILE:HD13	1.93	0.50
1:B:723:ASP:HA	1:B:726:TYR:CD2	2.47	0.50
1:C:624:LEU:HD23	1:C:627:ILE:HG22	1.94	0.50
1:C:675:LEU:HD23	1:C:675:LEU:H	1.76	0.50
1:F:433:LEU:H	1:F:454:ILE:HG12	1.77	0.50
1:F:451:LEU:HD11	1:F:454:ILE:HB	1.94	0.50
1:A:486:LEU:HG	1:A:490:LYS:HE3	1.94	0.50
1:A:579:LEU:HB3	1:A:601:LEU:HD21	1.93	0.50
1:B:693:ASN:N	1:B:716:ASN:OD1	2.37	0.50
1:E:496:LEU:HD12	1:E:497:SER:H	1.72	0.50
1:C:519:LEU:HD12	1:C:520:TYR:N	2.27	0.50
1:D:603:ARG:NH1	1:D:629:GLU:OE2	2.45	0.50
1:F:133:ILE:O	1:F:137:VAL:HG23	2.11	0.50
1:F:360:ILE:O	1:F:360:ILE:HG13	2.11	0.50
1:A:22:PRO:HG3	1:A:376:MET:HE1	1.94	0.49
1:B:496:LEU:CD2	1:B:498:VAL:HG23	2.42	0.49
1:C:246:LYS:O	1:C:249:ARG:HG3	2.11	0.49
1:C:253:GLU:HG2	1:C:367:LYS:HB2	1.94	0.49
1:D:144:PHE:HA	1:D:147:LYS:HB2	1.93	0.49
1:E:627:ILE:O	1:E:630:ILE:HG12	2.12	0.49
1:F:444:THR:HG22	1:F:466:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:SER:HB3	1:A:352:GLU:HG2	1.93	0.49
1:A:564:SER:HA	1:A:567:LEU:HB3	1.93	0.49
1:B:623:ASN:HA	1:B:647:ASN:HA	1.93	0.49
1:E:145:TRP:CD1	1:E:261:MET:SD	3.05	0.49
1:E:326:PHE:HA	1:E:329:ILE:HD12	1.94	0.49
1:F:766:ILE:HG13	1:F:766:ILE:O	2.12	0.49
1:A:619:LEU:HB2	1:A:644:LEU:HD23	1.93	0.49
1:A:759:VAL:HB	1:A:764:PHE:HE2	1.77	0.49
1:B:362:ASP:OD1	1:B:362:ASP:N	2.43	0.49
1:B:441:PHE:HB3	1:B:465:GLN:OE1	2.13	0.49
1:B:654:GLU:HA	1:B:678:HIS:CD2	2.47	0.49
1:C:136:LEU:O	1:C:136:LEU:HD23	2.12	0.49
1:F:113:GLN:HB3	1:G:309:ASN:HD21	1.78	0.49
1:B:570:MET:CE	1:B:572:ILE:HG22	2.43	0.49
1:B:749:GLY:HA3	1:B:770:GLU:HB3	1.93	0.49
1:B:751:LEU:HB3	1:B:754:LEU:HB2	1.94	0.49
1:F:570:MET:CE	1:F:588:MET:CE	2.90	0.49
1:C:347:ARG:O	1:C:368:ASN:HA	2.11	0.49
1:D:421:ASN:OD1	1:D:425:ARG:N	2.44	0.49
1:D:518:GLU:HG2	1:D:546:ILE:HB	1.94	0.49
1:D:551:SER:HB2	1:D:553:VAL:HG23	1.95	0.49
1:E:327:VAL:O	1:E:330:TYR:HB2	2.12	0.49
1:E:347:ARG:O	1:E:368:ASN:HA	2.13	0.49
1:E:498:VAL:HG12	1:E:500:PHE:HD1	1.77	0.49
1:F:525:LEU:H	1:F:551:SER:HB3	1.78	0.49
1:A:134:HIS:CD2	1:A:276:ILE:HD11	2.48	0.49
1:A:535:LEU:HD21	1:A:538:LEU:HD11	1.93	0.49
1:B:729:LYS:NZ	1:B:750:ASN:O	2.40	0.49
1:B:744:LEU:HD21	1:B:748:ILE:HG21	1.94	0.49
1:C:622:ASN:HB3	1:C:624:LEU:HD13	1.94	0.49
1:C:764:PHE:HB2	1:C:788:LEU:HD21	1.93	0.49
1:F:441:PHE:HA	1:F:466:LEU:HD21	1.95	0.49
1:F:588:MET:HG3	1:F:591:LEU:HB2	1.95	0.49
1:A:265:GLN:O	1:A:268:LEU:HG	2.12	0.49
1:B:369:ASP:O	1:B:373:MET:HG2	2.13	0.49
1:B:631:VAL:O	1:B:634:GLN:HG2	2.12	0.49
1:C:649:ILE:HG21	1:C:667:PHE:HE1	1.78	0.49
1:E:405:LEU:HD11	1:E:433:LEU:HD22	1.94	0.49
1:E:411:PRO:HA	1:E:414:LEU:HD12	1.93	0.49
1:F:151:SER:HB2	1:F:258:LEU:HD13	1.95	0.49
1:A:170:TRP:NE1	1:A:400:LEU:HD13	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PHE:HA	1:A:466:LEU:HD11	1.94	0.49
1:B:262:TYR:O	1:B:266:THR:HG23	2.13	0.49
1:B:735:LYS:HG2	1:B:756:TYR:CE2	2.48	0.49
1:C:46:GLN:O	1:C:50:ASP:HB3	2.13	0.49
1:F:405:LEU:HG	1:F:409:TRP:CD1	2.47	0.49
1:A:246:LYS:O	1:A:249:ARG:HG3	2.13	0.49
1:A:574:ASN:OD1	1:A:574:ASN:N	2.46	0.49
1:B:452:GLU:HA	1:B:475:HIS:HB2	1.95	0.49
1:F:643:LYS:HA	1:F:666:SER:HB2	1.95	0.49
1:A:759:VAL:HG22	1:A:784:VAL:HG12	1.95	0.48
1:B:415:ARG:HG2	1:B:418:LEU:HD12	1.95	0.48
1:B:496:LEU:HD21	1:B:498:VAL:HG23	1.96	0.48
1:C:668:SER:O	1:C:670:ASN:ND2	2.46	0.48
1:C:705:LEU:HB3	1:C:708:LEU:HB2	1.95	0.48
1:D:249:ARG:HA	1:D:370:PHE:CZ	2.47	0.48
1:E:639:LEU:HD21	1:E:642:LEU:HD13	1.95	0.48
1:E:591:LEU:HD23	1:E:611:LEU:HD13	1.96	0.48
1:F:353:TYR:O	1:F:357:GLU:N	2.47	0.48
1:F:556:ILE:O	1:F:584:ASN:ND2	2.44	0.48
1:A:723:ASP:HA	1:A:726:TYR:HD2	1.77	0.48
1:C:675:LEU:HD12	1:C:679:LEU:HD23	1.95	0.48
1:E:449:LEU:HG	1:E:472:LEU:HD13	1.94	0.48
1:E:778:LYS:O	1:E:800:MET:HE1	2.13	0.48
1:F:248:PHE:CZ	1:F:252:VAL:HG21	2.49	0.48
1:B:494:LYS:NZ	1:B:515:ASN:HB3	2.28	0.48
1:D:497:SER:HA	1:D:520:TYR:HB2	1.95	0.48
1:D:719:GLU:HG2	1:D:740:SER:HB3	1.95	0.48
1:A:726:TYR:CZ	1:A:745:SER:HB3	2.48	0.48
1:B:428:LEU:HD12	1:B:429:PRO:HD2	1.95	0.48
1:A:450:LYS:HA	1:A:473:SER:HB3	1.95	0.48
1:B:387:ARG:HG3	1:B:387:ARG:HH11	1.78	0.48
1:B:511:TYR:HA	1:B:541:LEU:HD21	1.96	0.48
1:B:149:PRO:HA	1:B:152:SER:HB3	1.94	0.48
1:C:551:SER:HB2	1:C:553:VAL:HG23	1.96	0.48
1:C:766:ILE:HD12	1:C:766:ILE:N	2.29	0.48
1:D:248:PHE:CE2	1:D:252:VAL:HG21	2.48	0.48
1:E:244:LYS:HA	1:E:247:LYS:HG2	1.95	0.48
1:E:256:ASP:N	1:E:369:ASP:OD2	2.44	0.48
1:E:436:LEU:HD12	1:E:459:ILE:HA	1.96	0.48
1:F:620:LYS:HG2	1:F:621:GLU:HG3	1.95	0.48
1:F:757:LEU:HB3	1:F:782:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:THR:OG1	1:G:312:MET:SD	2.69	0.48
1:A:713:ILE:HG13	1:A:736:ILE:HA	1.94	0.48
1:B:460:PRO:O	1:B:463:ILE:HG22	2.14	0.48
1:C:641:VAL:HG13	1:C:664:ARG:HB2	1.95	0.48
1:F:526:SER:CB	1:F:531:ARG:NE	2.76	0.48
1:A:248:PHE:O	1:A:252:VAL:HG22	2.13	0.48
1:A:441:PHE:HB3	1:A:465:GLN:OE1	2.13	0.48
1:A:445:GLU:OE1	1:A:445:GLU:N	2.42	0.48
1:A:458:MET:HE2	1:A:458:MET:HA	1.94	0.48
1:A:494:LYS:NZ	1:A:515:ASN:HB3	2.29	0.48
1:B:740:SER:HA	1:B:763:HIS:CE1	2.49	0.48
1:C:405:LEU:HG	1:C:409:TRP:HD1	1.79	0.48
1:C:707:SER:HA	1:C:730:LYS:HD2	1.96	0.48
1:E:276:ILE:HA	1:E:279:TYR:CE2	2.49	0.48
1:E:576:GLY:HA2	1:E:598:HIS:HD2	1.78	0.48
1:E:640:THR:O	1:E:663:GLU:N	2.40	0.48
1:F:170:TRP:HH2	1:F:396:SER:HB2	1.79	0.48
1:A:96:MET:SD	1:A:96:MET:N	2.87	0.48
1:B:45:LEU:HB3	1:B:312:MET:HE1	1.95	0.48
1:C:145:TRP:NE1	1:C:262:TYR:HB2	2.29	0.48
1:C:765:GLU:N	1:C:765:GLU:CD	2.67	0.48
1:D:765:GLU:OE1	1:D:765:GLU:HA	2.13	0.48
1:A:134:HIS:CG	1:A:276:ILE:HD11	2.49	0.47
1:A:654:GLU:HG2	1:A:657:LYS:HD3	1.94	0.47
1:A:771:LEU:HD12	1:A:792:LEU:HD11	1.95	0.47
1:B:372:PHE:CE1	1:B:376:MET:HE2	2.48	0.47
1:C:170:TRP:HZ3	1:C:396:SER:HB2	1.79	0.47
1:C:272:LYS:HB3	1:C:272:LYS:HE2	1.59	0.47
1:C:273:PHE:CD2	1:C:274:LEU:HD13	2.50	0.47
1:D:117:GLU:OE1	1:D:118:ARG:HG2	2.14	0.47
1:E:265:GLN:O	1:E:268:LEU:HG	2.13	0.47
1:F:265:GLN:O	1:F:268:LEU:HG	2.14	0.47
1:F:455:LYS:HD3	1:F:477:CYS:HA	1.96	0.47
1:B:625:LYS:HB2	1:B:648:SER:HB2	1.96	0.47
1:B:675:LEU:H	1:B:675:LEU:HD23	1.78	0.47
1:D:539:ARG:O	1:D:539:ARG:NH1	2.37	0.47
1:D:707:SER:HA	1:D:730:LYS:HD2	1.95	0.47
1:G:37:MET:SD	1:G:38:ILE:N	2.87	0.47
1:B:643:LYS:HB3	1:B:645:TRP:CD1	2.49	0.47
1:B:757:LEU:N	1:B:781:ARG:O	2.46	0.47
1:C:657:LYS:HD2	1:C:681:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:HG13	1:D:116:TYR:HD2	1.78	0.47
1:D:172:THR:OG1	1:D:387:ARG:NH1	2.41	0.47
1:D:294:ASN:ND2	1:D:305:ASN:OD1	2.47	0.47
1:E:243:GLU:O	1:E:246:LYS:HG2	2.14	0.47
1:F:544:LEU:HG	1:F:567:LEU:HD13	1.96	0.47
1:A:453:ILE:N	1:A:477:CYS:SG	2.87	0.47
1:A:680:PHE:HA	1:A:705:LEU:HD21	1.96	0.47
1:B:583:ASN:OD1	1:B:584:ASN:N	2.47	0.47
1:B:667:PHE:HB2	1:B:690:LEU:HD23	1.97	0.47
1:C:476:GLN:N	1:C:499:LYS:O	2.37	0.47
1:D:161:ILE:HD13	1:D:244:LYS:HG2	1.96	0.47
1:D:241:LEU:HD23	1:D:391:PHE:HE2	1.80	0.47
1:E:37:MET:SD	1:E:37:MET:N	2.88	0.47
1:E:496:LEU:CD1	1:E:498:VAL:HG23	2.40	0.47
1:E:630:ILE:HG21	1:E:656:ILE:HA	1.97	0.47
1:E:663:GLU:O	1:E:686:ARG:N	2.37	0.47
1:G:298:GLN:HG3	1:G:302:GLY:HA2	1.97	0.47
1:A:654:GLU:OE2	1:A:657:LYS:NZ	2.37	0.47
1:A:724:GLU:HA	1:A:727:PHE:CD2	2.49	0.47
1:B:45:LEU:C	1:B:312:MET:HE2	2.35	0.47
1:B:286:LYS:HD2	1:B:286:LYS:HA	1.68	0.47
1:B:609:PHE:O	1:B:635:HIS:NE2	2.39	0.47
1:C:145:TRP:N	1:C:265:GLN:HE22	2.11	0.47
1:D:452:GLU:HG2	1:D:475:HIS:HB2	1.95	0.47
1:F:531:ARG:CZ	1:F:552:ASN:O	2.62	0.47
1:A:425:ARG:CD	1:A:447:GLN:HG2	2.41	0.47
1:A:663:GLU:O	1:A:686:ARG:N	2.35	0.47
1:B:571:CYS:HB3	1:B:573:HIS:CE1	2.49	0.47
1:C:170:TRP:CD2	1:C:400:LEU:HD13	2.50	0.47
1:D:300:MET:SD	1:E:307:SER:HB2	2.55	0.47
1:E:732:LYS:O	1:E:755:SER:OG	2.27	0.47
1:F:452:GLU:O	1:F:454:ILE:HG13	2.14	0.47
1:A:273:PHE:O	1:A:277:ILE:HG22	2.15	0.47
1:A:605:PRO:HG2	1:A:608:VAL:HG23	1.96	0.47
1:B:122:TRP:HA	1:B:125:LYS:HE2	1.96	0.47
1:B:511:TYR:O	1:B:540:ASP:HB2	2.15	0.47
1:B:514:ARG:HG2	1:B:542:LYS:HG2	1.97	0.47
1:B:559:ALA:HA	1:B:562:ASP:OD2	2.15	0.47
1:C:165:CYS:HB3	1:C:388:PHE:HD1	1.79	0.47
1:C:430:LEU:HD22	1:C:433:LEU:HD11	1.97	0.47
1:C:557:PRO:HG2	1:C:560:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:LEU:O	1:D:499:LYS:N	2.42	0.47
1:D:675:LEU:H	1:D:675:LEU:HD23	1.79	0.47
1:D:759:VAL:O	1:D:762:ASN:ND2	2.45	0.47
1:E:130:LEU:HD21	1:E:279:TYR:OH	2.14	0.47
1:E:136:LEU:HA	1:E:139:MET:SD	2.54	0.47
1:E:411:PRO:HG3	1:E:439:THR:HB	1.96	0.47
1:F:360:ILE:HD11	1:F:363:ILE:HD12	1.95	0.47
1:F:418:LEU:HB3	1:F:426:LEU:HD11	1.96	0.47
1:G:46:GLN:HA	1:G:50:ASP:HB2	1.96	0.47
1:A:683:ASN:O	1:A:707:SER:OG	2.22	0.47
1:A:688:LEU:HB2	1:A:708:LEU:HD11	1.96	0.47
1:B:36:LEU:O	1:B:36:LEU:HD12	2.15	0.47
1:D:171:THR:HB	1:D:390:VAL:HG21	1.97	0.47
1:D:588:MET:SD	1:D:591:LEU:HB2	2.55	0.47
1:F:134:HIS:CG	1:F:276:ILE:HD11	2.50	0.47
1:F:495:VAL:HG13	1:F:518:GLU:HB2	1.96	0.47
1:F:533:VAL:H	1:F:555:LYS:HE3	1.80	0.47
1:F:604:ILE:HD12	1:F:629:GLU:HB2	1.97	0.47
1:A:256:ASP:N	1:A:369:ASP:HB2	2.29	0.47
1:B:501:ASP:H	1:B:505:GLU:CD	2.18	0.47
1:B:680:PHE:CD2	1:B:701:GLU:HB2	2.50	0.47
1:D:170:TRP:NE1	1:D:400:LEU:HD13	2.30	0.47
1:D:735:LYS:HG2	1:D:756:TYR:HE2	1.78	0.47
1:A:411:PRO:HA	1:A:414:LEU:HD12	1.96	0.47
1:A:703:GLY:HA3	1:A:724:GLU:HB3	1.97	0.47
1:B:457:VAL:O	1:B:479:VAL:HA	2.14	0.47
1:B:631:VAL:HA	1:B:634:GLN:NE2	2.30	0.47
1:B:765:GLU:O	1:B:788:LEU:HD22	2.15	0.47
1:C:170:TRP:CZ3	1:C:396:SER:HB2	2.50	0.47
1:D:687:TYR:HA	1:D:710:TYR:HB3	1.96	0.47
1:E:128:PRO:O	1:E:132:LEU:HD23	2.15	0.47
1:F:723:ASP:HA	1:F:726:TYR:HD2	1.80	0.47
1:G:134:HIS:CE1	1:G:276:ILE:HD11	2.50	0.47
1:A:479:VAL:O	1:A:507:PRO:HG3	2.14	0.46
1:A:556:ILE:HG23	1:A:584:ASN:HB2	1.97	0.46
1:A:757:LEU:N	1:A:781:ARG:O	2.33	0.46
1:B:489:LEU:HB2	1:B:513:LEU:HD22	1.97	0.46
1:B:740:SER:HA	1:B:763:HIS:HE1	1.80	0.46
1:E:124:ALA:HB2	1:E:287:VAL:HG12	1.97	0.46
1:E:571:CYS:HB3	1:E:573:HIS:CE1	2.50	0.46
1:F:471:GLU:HA	1:F:495:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LYS:HA	1:A:522:VAL:HB	1.96	0.46
1:B:503:MET:SD	1:B:506:LEU:HD22	2.55	0.46
1:C:270:VAL:HG22	1:C:334:CYS:HB3	1.96	0.46
1:C:415:ARG:NH2	1:C:445:GLU:OE2	2.48	0.46
1:E:796:VAL:O	1:E:800:MET:HB2	2.15	0.46
1:F:344:ARG:HA	1:F:344:ARG:NE	2.30	0.46
1:F:591:LEU:HD23	1:F:611:LEU:HD13	1.96	0.46
1:F:643:LYS:HB3	1:F:645:TRP:CD1	2.50	0.46
1:A:493:LEU:HD21	1:A:496:LEU:HB2	1.96	0.46
1:B:450:LYS:HA	1:B:473:SER:HB3	1.97	0.46
1:D:622:ASN:HB3	1:D:624:LEU:HD13	1.97	0.46
1:E:141:CYS:O	1:E:265:GLN:NE2	2.49	0.46
1:E:498:VAL:HG11	1:E:506:LEU:HD12	1.97	0.46
1:F:580:VAL:HG23	1:F:581:MET:HE3	1.94	0.46
1:A:729:LYS:HA	1:A:751:LEU:HD22	1.98	0.46
1:A:746:PRO:HB3	1:A:770:GLU:HG3	1.97	0.46
1:F:570:MET:CE	1:F:588:MET:HE3	2.45	0.46
1:F:673:GLU:OE2	1:F:673:GLU:N	2.48	0.46
1:A:425:ARG:HD2	1:A:471:GLU:OE1	2.16	0.46
1:A:584:ASN:O	1:A:588:MET:HE2	2.16	0.46
1:A:634:GLN:HB2	1:A:637:ARG:NH2	2.31	0.46
1:B:414:LEU:HD11	1:B:439:THR:OG1	2.16	0.46
1:B:473:SER:O	1:B:474:LEU:CD2	2.48	0.46
1:C:703:GLY:HA3	1:C:724:GLU:HB3	1.98	0.46
1:D:130:LEU:HD11	1:D:279:TYR:OH	2.15	0.46
1:E:521:LEU:O	1:E:550:LYS:N	2.39	0.46
1:F:352:GLU:HA	1:F:355:ARG:HH21	1.81	0.46
1:A:272:LYS:HE2	1:A:272:LYS:HB3	1.69	0.46
1:A:535:LEU:HD11	1:A:538:LEU:HD21	1.98	0.46
1:A:769:PRO:HB3	1:A:793:PRO:HG2	1.97	0.46
1:B:362:ASP:C	1:B:363:ILE:HD12	2.35	0.46
1:B:490:LYS:HB3	1:B:514:ARG:HH22	1.81	0.46
1:B:627:ILE:O	1:B:630:ILE:HG12	2.16	0.46
1:C:363:ILE:HG21	1:C:389:ALA:HB1	1.97	0.46
1:C:702:ILE:HG13	1:C:705:LEU:HD12	1.97	0.46
1:E:38:ILE:HG12	1:E:319:LEU:HD21	1.97	0.46
1:F:242:PHE:CD2	1:F:400:LEU:HD23	2.51	0.46
1:F:735:LYS:HG2	1:F:756:TYR:HE2	1.81	0.46
1:A:273:PHE:CZ	1:A:331:GLY:HA3	2.50	0.46
1:A:489:LEU:HB2	1:A:513:LEU:HD22	1.98	0.46
1:A:673:GLU:O	1:A:695:ILE:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:SER:O	1:A:765:GLU:OE2	2.34	0.46
1:B:351:PHE:O	1:B:353:TYR:N	2.49	0.46
1:B:688:LEU:HB2	1:B:708:LEU:HD11	1.98	0.46
1:D:430:LEU:HD12	1:D:451:LEU:HG	1.97	0.46
1:E:276:ILE:O	1:E:280:ASN:ND2	2.42	0.46
1:F:249:ARG:HE	1:F:250:LEU:HG	1.80	0.46
1:A:436:LEU:HD12	1:A:460:PRO:HD3	1.97	0.46
1:E:480:LYS:NZ	1:E:504:ARG:HH22	2.14	0.46
1:F:678:HIS:HA	1:F:681:LEU:HG	1.98	0.46
1:A:708:LEU:HD23	1:A:731:LEU:HD21	1.98	0.46
1:B:541:LEU:HB3	1:B:544:LEU:CD2	2.46	0.46
1:C:663:GLU:HA	1:C:685:ILE:HA	1.98	0.46
1:C:713:ILE:HG13	1:C:736:ILE:HA	1.97	0.46
1:D:34:ALA:O	1:D:37:MET:HG3	2.16	0.46
1:D:499:LYS:HE2	1:D:522:VAL:HG21	1.96	0.46
1:E:35:MET:O	1:E:38:ILE:HG22	2.16	0.46
1:E:273:PHE:CZ	1:E:331:GLY:HA3	2.50	0.46
1:E:760:LYS:HB3	1:E:760:LYS:HE3	1.48	0.46
1:F:474:LEU:HB2	1:F:498:VAL:HA	1.98	0.46
1:A:723:ASP:HA	1:A:726:TYR:CD2	2.50	0.46
1:B:575:ASP:OD1	1:B:575:ASP:N	2.41	0.46
1:B:672:ILE:HG13	1:B:695:ILE:HD11	1.98	0.46
1:C:673:GLU:HA	1:C:694:ASP:HB2	1.98	0.46
1:E:33:VAL:O	1:E:37:MET:HG2	2.15	0.46
1:A:471:GLU:HA	1:A:495:VAL:O	2.15	0.45
1:A:759:VAL:CG2	1:A:784:VAL:HG12	2.46	0.45
1:C:164:LYS:HE2	1:C:241:LEU:HD13	1.98	0.45
1:C:405:LEU:HG	1:C:409:TRP:CD1	2.52	0.45
1:D:31:LEU:O	1:D:35:MET:HG2	2.16	0.45
1:E:152:SER:HA	1:E:155:ILE:HG12	1.98	0.45
1:E:538:LEU:HG	1:E:559:ALA:HB1	1.98	0.45
1:F:358:THR:HB	1:F:360:ILE:HG23	1.99	0.45
1:F:490:LYS:HD3	1:F:514:ARG:NH1	2.28	0.45
1:F:526:SER:CB	1:F:531:ARG:NH2	2.79	0.45
1:A:640:THR:O	1:A:663:GLU:N	2.37	0.45
1:A:735:LYS:HG2	1:A:756:TYR:CE2	2.49	0.45
1:B:486:LEU:HD11	1:B:490:LYS:HE3	1.97	0.45
1:B:688:LEU:H	1:B:710:TYR:HD1	1.64	0.45
1:C:337:THR:O	1:C:341:LEU:N	2.48	0.45
1:E:467:ASP:HA	1:E:488:PHE:CZ	2.51	0.45
1:F:354:VAL:HG22	1:F:386:LYS:HE2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:PRO:O	1:F:385:SER:OG	2.21	0.45
1:F:578:LYS:NZ	1:F:601:LEU:HA	2.30	0.45
1:A:657:LYS:HD2	1:A:681:LEU:HD12	1.98	0.45
1:B:45:LEU:O	1:B:312:MET:HE2	2.15	0.45
1:C:293:CYS:SG	1:C:306:PHE:HB2	2.56	0.45
1:C:665:LEU:HB2	1:C:685:ILE:HD13	1.98	0.45
1:F:624:LEU:HD23	1:F:627:ILE:HG22	1.98	0.45
1:F:759:VAL:O	1:F:762:ASN:ND2	2.43	0.45
1:A:292:ASP:OD1	1:A:293:CYS:N	2.50	0.45
1:B:672:ILE:HG13	1:B:695:ILE:CD1	2.47	0.45
1:B:696:ARG:HG3	1:B:717:LYS:O	2.15	0.45
1:C:36:LEU:HD12	1:C:135:THR:CG2	2.46	0.45
1:C:400:LEU:HA	1:C:400:LEU:HD12	1.72	0.45
1:C:654:GLU:OE2	1:C:657:LYS:NZ	2.42	0.45
1:D:785:GLU:HB2	1:D:788:LEU:HD13	1.98	0.45
1:E:757:LEU:N	1:E:781:ARG:O	2.36	0.45
1:F:551:SER:HB2	1:F:553:VAL:HG23	1.97	0.45
1:G:273:PHE:HD1	1:G:327:VAL:HG12	1.80	0.45
1:E:19:VAL:HG22	1:E:380:TYR:CE2	2.52	0.45
1:F:493:LEU:HD23	1:F:516:LEU:HD13	1.97	0.45
1:F:510:MET:SD	1:F:510:MET:N	2.89	0.45
1:A:247:LYS:HB3	1:A:247:LYS:HE3	1.72	0.45
1:A:410:THR:O	1:A:414:LEU:HG	2.17	0.45
1:A:538:LEU:HB3	1:A:541:LEU:HD12	1.99	0.45
1:A:673:GLU:HA	1:A:694:ASP:HB2	1.99	0.45
1:B:350:SER:HB3	1:B:352:GLU:HG2	1.97	0.45
1:B:617:LEU:HB3	1:B:642:LEU:HD23	1.99	0.45
1:C:746:PRO:HB3	1:C:770:GLU:HG3	1.98	0.45
1:C:777:LEU:HG	1:C:800:MET:HE1	1.98	0.45
1:E:764:PHE:HB2	1:E:788:LEU:HD21	1.97	0.45
1:F:693:ASN:N	1:F:716:ASN:OD1	2.38	0.45
1:A:24:TRP:HB2	1:A:333:THR:HG23	1.99	0.45
1:A:444:THR:OG1	1:A:466:LEU:HA	2.17	0.45
1:A:559:ALA:O	1:A:562:ASP:HB2	2.16	0.45
1:B:354:VAL:HG13	1:B:386:LYS:HD3	1.97	0.45
1:B:366:VAL:HB	1:B:370:PHE:HB3	1.98	0.45
1:C:35:MET:HE3	1:C:135:THR:HG23	1.88	0.45
1:E:370:PHE:CA	1:E:373:MET:HE3	2.26	0.45
1:A:415:ARG:NH2	1:A:445:GLU:OE2	2.33	0.45
1:B:350:SER:HA	1:B:365:ASP:OD1	2.16	0.45
1:C:170:TRP:HE3	1:C:391:PHE:HE1	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:LYS:HB2	1:D:400:LEU:HG	1.99	0.45
1:E:122:TRP:HA	1:E:125:LYS:HE2	1.99	0.45
1:E:737:GLY:N	1:E:758:ASP:O	2.42	0.45
1:F:293:CYS:SG	1:F:306:PHE:HB2	2.57	0.45
1:A:596:LEU:HB2	1:A:619:LEU:HD23	1.99	0.45
1:B:474:LEU:HD23	1:B:474:LEU:N	2.23	0.45
1:C:134:HIS:CD2	1:C:276:ILE:HD11	2.52	0.45
1:C:137:VAL:HB	1:C:272:LYS:HZ1	1.82	0.45
1:C:373:MET:O	1:C:376:MET:SD	2.75	0.45
1:D:481:ILE:CD1	1:D:486:LEU:HB2	2.45	0.45
1:E:245:VAL:HG21	1:E:391:PHE:HB3	1.99	0.45
1:E:474:LEU:N	1:E:497:SER:O	2.47	0.45
1:F:170:TRP:CH2	1:F:396:SER:HB2	2.52	0.45
1:F:268:LEU:HA	1:F:271:ILE:HG12	1.99	0.45
1:F:426:LEU:HB3	1:F:446:LEU:HA	1.98	0.45
1:F:499:LYS:HA	1:F:522:VAL:HB	1.99	0.45
1:G:49:GLN:O	1:G:311:THR:OG1	2.35	0.45
1:A:160:SER:O	1:A:164:LYS:HG2	2.17	0.45
1:A:427:GLU:HB2	1:A:448:SER:HB3	1.98	0.45
1:B:683:ASN:OD1	1:B:683:ASN:N	2.50	0.45
1:C:175:LEU:HD22	1:C:358:THR:HG21	1.98	0.45
1:C:714:THR:HA	1:C:737:GLY:HA3	1.99	0.45
1:D:105:LEU:HD12	1:D:105:LEU:HA	1.80	0.45
1:D:645:TRP:HD1	1:D:666:SER:HB3	1.81	0.45
1:F:425:ARG:HH12	1:F:495:VAL:HG21	1.82	0.45
1:B:120:LEU:HD21	1:B:310:HIS:CE1	2.51	0.44
1:B:638:LYS:HA	1:B:638:LYS:HD3	1.79	0.44
1:B:649:ILE:HG21	1:B:667:PHE:HE1	1.83	0.44
1:B:759:VAL:O	1:B:762:ASN:ND2	2.48	0.44
1:D:258:LEU:HD12	1:D:261:MET:CE	2.47	0.44
1:E:19:VAL:HG12	1:E:20:LEU:HD22	1.99	0.44
1:F:46:GLN:HG3	1:F:50:ASP:HB2	1.99	0.44
1:F:510:MET:O	1:F:513:LEU:HG	2.17	0.44
1:G:276:ILE:HD13	1:G:279:TYR:CE2	2.52	0.44
1:B:367:LYS:HD3	1:B:368:ASN:N	2.32	0.44
1:B:461:ALA:HB2	1:B:482:HIS:ND1	2.32	0.44
1:C:35:MET:CE	1:C:135:THR:CG2	2.77	0.44
1:C:433:LEU:HB2	1:C:454:ILE:HD13	1.99	0.44
1:E:158:PHE:CZ	1:E:373:MET:HG3	2.53	0.44
1:E:376:MET:SD	1:E:377:ILE:N	2.91	0.44
1:E:719:GLU:HG2	1:E:740:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ASP:HA	1:A:488:PHE:CE2	2.52	0.44
1:A:649:ILE:HD13	1:A:667:PHE:HE1	1.82	0.44
1:B:461:ALA:HB2	1:B:482:HIS:CE1	2.51	0.44
1:B:696:ARG:HB2	1:B:696:ARG:CZ	2.47	0.44
1:C:518:GLU:HG2	1:C:546:ILE:HD12	1.99	0.44
1:C:567:LEU:HD21	1:C:570:MET:HB3	1.98	0.44
1:D:620:LYS:HD2	1:D:645:TRP:HB2	1.99	0.44
1:E:463:ILE:HD12	1:E:466:LEU:HB2	1.99	0.44
1:A:276:ILE:HD13	1:A:279:TYR:HE1	1.82	0.44
1:B:367:LYS:HD3	1:B:368:ASN:H	1.81	0.44
1:C:637:ARG:O	1:C:661:SER:OG	2.32	0.44
1:D:148:PHE:HD2	1:D:151:SER:H	1.65	0.44
1:D:158:PHE:HA	1:D:161:ILE:HG22	1.99	0.44
1:D:246:LYS:O	1:D:249:ARG:HG3	2.17	0.44
1:D:310:HIS:NE2	1:D:313:ALA:HB2	2.33	0.44
1:D:597:VAL:HA	1:D:620:LYS:HB2	2.00	0.44
1:D:627:ILE:O	1:D:630:ILE:HG12	2.18	0.44
1:G:52:ILE:HG21	1:G:116:TYR:HB2	1.99	0.44
1:G:121:HIS:ND1	1:G:123:TYR:HB3	2.33	0.44
1:A:273:PHE:CE1	1:A:331:GLY:HA3	2.52	0.44
1:B:527:HIS:HA	1:B:552:ASN:HD21	1.82	0.44
1:B:605:PRO:HG2	1:B:608:VAL:HG23	1.98	0.44
1:B:752:LEU:HA	1:B:774:CYS:HA	1.99	0.44
1:C:33:VAL:HA	1:C:36:LEU:HD13	2.00	0.44
1:D:277:ILE:O	1:D:281:SER:OG	2.30	0.44
1:D:294:ASN:OD1	1:D:294:ASN:N	2.50	0.44
1:E:654:GLU:HA	1:E:678:HIS:CD2	2.53	0.44
1:F:52:ILE:CG2	1:F:116:TYR:HB2	2.38	0.44
1:F:120:LEU:HD21	1:F:310:HIS:CE1	2.52	0.44
1:F:158:PHE:HA	1:F:161:ILE:HG22	1.99	0.44
1:F:452:GLU:HG2	1:F:475:HIS:ND1	2.33	0.44
1:F:713:ILE:HD12	1:F:718:VAL:HG21	1.99	0.44
1:A:425:ARG:HB3	1:A:448:SER:HB2	1.98	0.44
1:B:411:PRO:HG3	1:B:439:THR:HB	1.99	0.44
1:B:744:LEU:HD23	1:B:768:PRO:HD2	2.00	0.44
1:C:161:ILE:HD13	1:C:244:LYS:HG2	1.99	0.44
1:C:353:TYR:HD2	1:C:386:LYS:HE2	1.83	0.44
1:C:550:LYS:HD2	1:C:573:HIS:HB2	1.98	0.44
1:E:133:ILE:HG13	1:E:134:HIS:N	2.32	0.44
1:E:331:GLY:O	1:E:335:LEU:HG	2.17	0.44
1:F:630:ILE:HG22	1:F:634:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:HIS:O	1:A:161:ILE:HG22	2.17	0.44
1:A:614:LEU:HD21	1:A:617:LEU:HB2	2.00	0.44
1:B:49:GLN:O	1:B:51:LYS:N	2.51	0.44
1:B:481:ILE:HD12	1:B:486:LEU:HB2	1.99	0.44
1:C:450:LYS:HA	1:C:473:SER:HB3	1.99	0.44
1:C:565:SER:OG	1:C:566:HIS:ND1	2.49	0.44
1:C:630:ILE:HG21	1:C:656:ILE:HA	2.00	0.44
1:C:735:LYS:HB3	1:C:735:LYS:HE2	1.85	0.44
1:D:654:GLU:HG3	1:D:678:HIS:CE1	2.52	0.44
1:E:31:LEU:CB	1:E:330:TYR:HE1	2.31	0.44
1:E:367:LYS:HZ3	1:E:368:ASN:HB2	1.83	0.44
1:E:496:LEU:HD23	1:E:519:LEU:HD13	1.99	0.44
1:E:630:ILE:O	1:E:633:PHE:HB2	2.18	0.44
1:A:346:LEU:HD22	1:A:375:HIS:CD2	2.53	0.44
1:A:740:SER:HA	1:A:763:HIS:CE1	2.53	0.44
1:B:634:GLN:HB2	1:B:637:ARG:CZ	2.47	0.44
1:B:744:LEU:HD21	1:B:771:LEU:HD21	1.99	0.44
1:C:24:TRP:HB2	1:C:333:THR:HG23	1.99	0.44
1:D:352:GLU:HA	1:D:355:ARG:HH21	1.83	0.44
1:D:430:LEU:HD13	1:D:433:LEU:HD12	2.00	0.44
1:E:156:GLU:O	1:E:159:ILE:HG12	2.17	0.44
1:E:244:LYS:HG3	1:E:247:LYS:NZ	2.33	0.44
1:F:482:HIS:H	1:F:485:ALA:HB3	1.82	0.44
1:G:130:LEU:HD11	1:G:279:TYR:OH	2.17	0.44
1:A:511:TYR:CD2	1:A:536:GLU:HB2	2.53	0.44
1:A:631:VAL:O	1:A:634:GLN:HG2	2.17	0.44
1:A:631:VAL:HG13	1:A:655:HIS:CG	2.52	0.44
1:B:467:ASP:HA	1:B:488:PHE:CE2	2.53	0.44
1:B:723:ASP:HA	1:B:726:TYR:HD2	1.82	0.44
1:C:171:THR:HA	1:C:390:VAL:HG11	2.00	0.44
1:E:740:SER:HA	1:E:763:HIS:CE1	2.52	0.44
1:F:470:GLN:HA	1:F:493:LEU:HA	1.99	0.44
1:F:564:SER:HA	1:F:588:MET:HE1	1.98	0.44
1:F:575:ASP:N	1:F:575:ASP:OD1	2.48	0.44
1:F:673:GLU:HG2	1:F:674:VAL:N	2.32	0.44
1:F:675:LEU:HD22	1:F:695:ILE:HG23	1.99	0.44
1:F:735:LYS:HG2	1:F:756:TYR:CE2	2.52	0.44
1:A:268:LEU:O	1:A:271:ILE:HG22	2.18	0.43
1:A:427:GLU:HA	1:A:448:SER:O	2.18	0.43
1:E:113:GLN:NE2	1:F:311:THR:HG22	2.33	0.43
1:F:318:LYS:HA	1:F:318:LYS:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:774:CYS:HB3	1:F:777:LEU:HB3	2.00	0.43
1:G:37:MET:HA	1:G:40:VAL:HG12	2.00	0.43
1:G:272:LYS:HE2	1:G:272:LYS:HB3	1.73	0.43
1:A:270:VAL:HG23	1:A:334:CYS:HB3	1.99	0.43
1:A:425:ARG:NH1	1:A:471:GLU:OE1	2.42	0.43
1:A:522:VAL:HA	1:A:550:LYS:HB2	2.00	0.43
1:A:637:ARG:NH1	1:A:658:LYS:O	2.46	0.43
1:B:141:CYS:SG	1:B:269:LYS:HG3	2.58	0.43
1:B:490:LYS:HB3	1:B:514:ARG:NH1	2.32	0.43
1:B:502:ASP:C	1:B:504:ARG:H	2.21	0.43
1:C:135:THR:O	1:C:139:MET:CE	2.64	0.43
1:C:683:ASN:N	1:C:683:ASN:OD1	2.52	0.43
1:E:427:GLU:HG3	1:E:449:LEU:CA	2.48	0.43
1:E:624:LEU:O	1:E:649:ILE:HG13	2.18	0.43
1:F:656:ILE:HD11	1:F:665:LEU:HD11	2.00	0.43
1:G:52:ILE:HA	1:G:52:ILE:HD12	1.83	0.43
1:A:121:HIS:CG	1:A:286:LYS:HG2	2.53	0.43
1:E:242:PHE:CE2	1:E:400:LEU:HD23	2.52	0.43
1:E:592:THR:O	1:E:615:GLN:N	2.40	0.43
1:A:351:PHE:O	1:A:353:TYR:N	2.51	0.43
1:A:414:LEU:HD13	1:A:440:VAL:HG12	2.00	0.43
1:A:441:PHE:HA	1:A:466:LEU:HD21	2.00	0.43
1:A:759:VAL:HB	1:A:764:PHE:CE2	2.53	0.43
1:B:134:HIS:CE1	1:B:276:ILE:HD11	2.53	0.43
1:B:609:PHE:HB3	1:B:635:HIS:HD2	1.83	0.43
1:D:38:ILE:HG23	1:D:319:LEU:HD21	2.01	0.43
1:D:425:ARG:HD3	1:D:447:GLN:HG3	2.01	0.43
1:E:642:LEU:HD12	1:E:642:LEU:HA	1.81	0.43
1:F:249:ARG:HD2	1:F:253:GLU:OE1	2.19	0.43
1:A:390:VAL:HG13	1:A:391:PHE:CD1	2.54	0.43
1:A:452:GLU:HG3	1:A:475:HIS:CB	2.49	0.43
1:A:578:LYS:HA	1:A:599:CYS:O	2.18	0.43
1:B:120:LEU:HD21	1:B:310:HIS:CG	2.54	0.43
1:B:294:ASN:HD22	1:B:304:LYS:NZ	2.17	0.43
1:B:458:MET:HA	1:B:480:LYS:O	2.18	0.43
1:C:702:ILE:HD13	1:C:725:LEU:HD13	2.00	0.43
1:D:401:LYS:O	1:D:405:LEU:HG	2.19	0.43
1:D:726:TYR:HB2	1:D:747:LYS:HE3	2.01	0.43
1:E:650:THR:OG1	1:E:671:LYS:HB2	2.18	0.43
1:F:140:LEU:HD12	1:F:140:LEU:HA	1.78	0.43
1:F:459:ILE:HG12	1:F:480:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PHE:C	1:A:353:TYR:H	2.22	0.43
1:A:539:ARG:HH12	1:A:566:HIS:CE1	2.32	0.43
1:A:620:LYS:HG3	1:A:646:HIS:CD2	2.54	0.43
1:A:729:LYS:HB3	1:A:753:PHE:HD2	1.84	0.43
1:B:45:LEU:HB3	1:B:312:MET:CE	2.49	0.43
1:B:162:LEU:HD12	1:B:162:LEU:O	2.18	0.43
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.76	0.43
1:C:713:ILE:HD11	1:C:736:ILE:HD12	2.01	0.43
1:D:151:SER:HB2	1:D:258:LEU:HD13	2.01	0.43
1:D:705:LEU:HB3	1:D:708:LEU:HB2	1.99	0.43
1:D:736:ILE:O	1:D:739:ASN:ND2	2.52	0.43
1:E:373:MET:HA	1:E:376:MET:HG3	2.00	0.43
1:E:798:GLU:HB3	1:E:804:ALA:HB2	2.00	0.43
1:F:560:VAL:O	1:F:564:SER:N	2.52	0.43
1:A:437:PRO:O	1:A:440:VAL:HG22	2.18	0.43
1:B:511:TYR:CE2	1:B:536:GLU:HB2	2.53	0.43
1:C:35:MET:HE3	1:C:135:THR:CA	2.36	0.43
1:C:496:LEU:HD12	1:C:497:SER:N	2.34	0.43
1:C:511:TYR:O	1:C:540:ASP:HB3	2.19	0.43
1:C:644:LEU:HD22	1:C:649:ILE:HD11	2.00	0.43
1:D:369:ASP:C	1:D:373:MET:HE2	2.39	0.43
1:D:370:PHE:O	1:D:374:LEU:HG	2.18	0.43
1:E:248:PHE:O	1:E:252:VAL:HG23	2.19	0.43
1:E:427:GLU:HA	1:E:448:SER:O	2.18	0.43
1:A:272:LYS:O	1:A:275:ILE:HG22	2.19	0.43
1:A:732:LYS:HE2	1:A:732:LYS:HB3	1.90	0.43
1:B:414:LEU:HB3	1:B:428:LEU:HD22	2.01	0.43
1:C:538:LEU:HG	1:C:559:ALA:HB1	2.01	0.43
1:E:263:VAL:HG22	1:E:341:LEU:HD13	1.99	0.43
1:F:503:MET:HE1	1:F:524:SER:O	2.18	0.43
1:F:782:LEU:HG	1:F:784:VAL:HG13	2.01	0.43
1:A:243:GLU:O	1:A:246:LYS:HG2	2.19	0.43
1:A:550:LYS:NZ	1:A:573:HIS:HB2	2.34	0.43
1:E:170:TRP:HH2	1:E:396:SER:HB2	1.84	0.43
1:F:58:ARG:HH12	1:F:305:ASN:HD22	1.66	0.43
1:F:263:VAL:O	1:F:266:THR:OG1	2.29	0.43
1:F:470:GLN:O	1:F:495:VAL:N	2.40	0.43
1:F:517:GLU:HA	1:F:543:SER:O	2.19	0.43
1:A:621:GLU:HG3	1:A:646:HIS:HD2	1.84	0.43
1:A:667:PHE:HB2	1:A:690:LEU:HD23	2.01	0.43
1:B:406:ASN:ND2	1:B:438:ASP:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:ASP:H	1:B:505:GLU:CD	2.23	0.43
1:B:713:ILE:HD11	1:B:736:ILE:HD12	2.01	0.43
1:C:138:PHE:CB	1:C:139:MET:HE2	2.49	0.43
1:D:273:PHE:HE1	1:D:328:SER:HA	1.83	0.43
1:D:421:ASN:ND2	1:D:471:GLU:OE1	2.51	0.43
1:E:759:VAL:O	1:E:762:ASN:ND2	2.52	0.43
1:F:292:ASP:OD1	1:F:293:CYS:N	2.52	0.43
1:F:418:LEU:HD22	1:F:426:LEU:HG	2.01	0.43
1:F:723:ASP:HA	1:F:726:TYR:CD2	2.53	0.43
1:A:594:LEU:HB3	1:A:614:LEU:HD13	2.01	0.42
1:B:151:SER:O	1:B:155:ILE:HG12	2.19	0.42
1:B:547:LEU:O	1:B:571:CYS:N	2.52	0.42
1:C:482:HIS:H	1:C:485:ALA:HB3	1.84	0.42
1:E:511:TYR:O	1:E:540:ASP:HB2	2.19	0.42
1:E:713:ILE:HG13	1:E:736:ILE:HA	2.01	0.42
1:F:145:TRP:HA	1:F:261:MET:HE1	2.01	0.42
1:F:527:HIS:N	1:F:531:ARG:HH21	2.17	0.42
1:A:706:GLN:NE2	1:A:727:PHE:O	2.40	0.42
1:B:110:PHE:CD2	1:C:55:LEU:HD12	2.54	0.42
1:B:447:GLN:HA	1:B:469:LEU:HA	2.00	0.42
1:B:624:LEU:O	1:B:648:SER:N	2.52	0.42
1:F:709:GLN:HG2	1:F:730:LYS:HB3	2.01	0.42
1:A:692:TYR:N	1:A:716:ASN:OD1	2.52	0.42
1:A:712:SER:HB2	1:A:735:LYS:HD3	2.01	0.42
1:A:736:ILE:HB	1:A:759:VAL:HA	2.01	0.42
1:B:19:VAL:HA	1:B:380:TYR:CD2	2.54	0.42
1:B:489:LEU:HD13	1:B:509:TRP:CZ3	2.54	0.42
1:B:583:ASN:O	1:B:587:LYS:HE2	2.20	0.42
1:B:729:LYS:HA	1:B:751:LEU:HD23	2.01	0.42
1:C:273:PHE:CZ	1:C:331:GLY:HA3	2.54	0.42
1:C:549:ILE:HB	1:C:572:ILE:HA	2.00	0.42
1:D:36:LEU:HB2	1:D:135:THR:HG21	2.01	0.42
1:D:567:LEU:HD23	1:D:588:MET:CE	2.50	0.42
1:E:436:LEU:HG	1:E:457:VAL:HG13	2.01	0.42
1:E:496:LEU:HD23	1:E:519:LEU:CD1	2.50	0.42
1:E:518:GLU:HG2	1:E:546:ILE:HB	2.00	0.42
1:E:588:MET:HE2	1:E:591:LEU:CA	2.47	0.42
1:F:531:ARG:CZ	1:F:552:ASN:CG	2.87	0.42
1:F:570:MET:HE3	1:F:588:MET:CG	2.49	0.42
1:A:425:ARG:HH12	1:A:495:VAL:HG21	1.84	0.42
1:A:586:LYS:HG2	1:A:607:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:HA	1:B:120:LEU:HD12	1.79	0.42
1:B:246:LYS:HE2	1:B:246:LYS:HB3	1.76	0.42
1:B:657:LYS:HD3	1:B:678:HIS:HB2	2.00	0.42
1:C:447:GLN:HA	1:C:468:ASN:O	2.18	0.42
1:C:507:PRO:HB2	1:C:509:TRP:NE1	2.34	0.42
1:E:480:LYS:HZ3	1:E:504:ARG:HH22	1.68	0.42
1:E:588:MET:CG	1:E:591:LEU:HB2	2.45	0.42
1:F:347:ARG:O	1:F:368:ASN:HA	2.20	0.42
1:G:35:MET:HE2	1:G:135:THR:HA	2.00	0.42
1:A:250:LEU:HD12	1:A:250:LEU:O	2.20	0.42
1:B:449:LEU:HD12	1:B:450:LYS:N	2.33	0.42
1:B:469:LEU:HD11	1:B:472:LEU:HD22	2.01	0.42
1:C:138:PHE:HB2	1:C:139:MET:HE2	2.01	0.42
1:C:421:ASN:OD1	1:C:425:ARG:N	2.47	0.42
1:D:310:HIS:CE1	1:D:313:ALA:HB2	2.53	0.42
1:E:353:TYR:CE1	1:E:354:VAL:HG23	2.54	0.42
1:E:693:ASN:N	1:E:716:ASN:OD1	2.39	0.42
1:E:736:ILE:O	1:E:739:ASN:ND2	2.52	0.42
1:A:696:ARG:O	1:A:718:VAL:HA	2.20	0.42
1:B:32:SER:CB	1:B:139:MET:CE	2.95	0.42
1:B:140:LEU:HD12	1:B:140:LEU:HA	1.79	0.42
1:C:130:LEU:HA	1:C:133:ILE:HG22	2.02	0.42
1:D:662:LEU:HG	1:D:685:ILE:HG12	2.02	0.42
1:E:20:LEU:HD12	1:E:145:TRP:CH2	2.55	0.42
1:E:141:CYS:SG	1:E:268:LEU:HD11	2.59	0.42
1:F:31:LEU:HD11	1:F:329:ILE:HG22	2.02	0.42
1:F:634:GLN:HB3	1:F:637:ARG:NH2	2.34	0.42
1:G:19:VAL:HG23	1:G:20:LEU:HD22	2.02	0.42
1:G:37:MET:SD	1:G:38:ILE:HG13	2.59	0.42
1:A:546:ILE:HA	1:A:569:LYS:O	2.20	0.42
1:B:708:LEU:HD23	1:B:731:LEU:HD21	2.00	0.42
1:C:248:PHE:CE1	1:C:252:VAL:HG21	2.55	0.42
1:C:448:SER:HB2	1:C:471:GLU:HB3	2.02	0.42
1:D:675:LEU:HD22	1:D:695:ILE:HG23	2.02	0.42
1:E:141:CYS:SG	1:E:142:SER:N	2.93	0.42
1:E:158:PHE:CE1	1:E:373:MET:SD	3.12	0.42
1:E:239:LYS:HB2	1:E:400:LEU:HG	2.02	0.42
1:E:576:GLY:HA2	1:E:598:HIS:CD2	2.55	0.42
1:E:650:THR:O	1:E:672:ILE:HA	2.20	0.42
1:F:134:HIS:ND1	1:F:276:ILE:HD11	2.35	0.42
1:F:500:PHE:HE1	1:F:521:LEU:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:608:VAL:HG11	1:F:617:LEU:HD21	2.02	0.42
1:G:137:VAL:HG12	1:G:272:LYS:NZ	2.33	0.42
1:A:511:TYR:CE2	1:A:536:GLU:HB2	2.54	0.42
1:B:505:GLU:CD	1:B:505:GLU:H	2.23	0.42
1:C:592:THR:O	1:C:615:GLN:N	2.45	0.42
1:D:493:LEU:HD21	1:D:496:LEU:HD13	2.01	0.42
1:E:363:ILE:HA	1:E:392:LEU:HD22	2.01	0.42
1:E:713:ILE:HD12	1:E:718:VAL:HG21	2.01	0.42
1:F:441:PHE:CZ	1:F:460:PRO:HD2	2.55	0.42
1:A:141:CYS:CB	1:A:268:LEU:HD11	2.49	0.42
1:B:383:LEU:HD11	1:B:387:ARG:NH2	2.34	0.42
1:B:662:LEU:HD13	1:B:685:ILE:HD11	2.01	0.42
1:B:728:CYS:HB2	1:B:731:LEU:HD12	2.01	0.42
1:C:170:TRP:CH2	1:C:174:ALA:HB2	2.55	0.42
1:F:469:LEU:HD13	1:F:469:LEU:HA	1.91	0.42
1:A:516:LEU:HD21	1:A:519:LEU:HB2	2.02	0.42
1:A:599:CYS:N	1:A:622:ASN:OD1	2.53	0.42
1:B:412:ASP:OD1	1:B:413:LYS:N	2.53	0.42
1:B:582:LEU:O	1:B:585:LEU:HB3	2.20	0.42
1:C:247:LYS:O	1:C:247:LYS:HD3	2.20	0.42
1:C:571:CYS:HB3	1:C:573:HIS:CE1	2.54	0.42
1:E:451:LEU:HD12	1:E:452:GLU:N	2.34	0.42
1:E:578:LYS:HA	1:E:599:CYS:O	2.20	0.42
1:E:643:LYS:HB3	1:E:645:TRP:HD1	1.85	0.42
1:F:145:TRP:N	1:F:265:GLN:HE22	2.18	0.42
1:F:347:ARG:HB3	1:F:368:ASN:OD1	2.20	0.42
1:F:436:LEU:HD23	1:F:436:LEU:HA	1.81	0.42
1:F:490:LYS:HB3	1:F:514:ARG:HH12	1.85	0.42
1:F:616:GLU:HA	1:F:641:VAL:HB	2.02	0.42
1:A:768:PRO:HA	1:A:769:PRO:HD3	1.95	0.41
1:B:437:PRO:O	1:B:440:VAL:HG13	2.20	0.41
1:B:453:ILE:N	1:B:477:CYS:SG	2.93	0.41
1:D:547:LEU:HD23	1:D:570:MET:SD	2.60	0.41
1:E:46:GLN:O	1:E:50:ASP:HB3	2.19	0.41
1:E:381:ASP:OD2	1:E:384:TYR:N	2.49	0.41
1:E:723:ASP:HA	1:E:726:TYR:CD2	2.55	0.41
1:F:263:VAL:HG22	1:F:341:LEU:HD13	2.01	0.41
1:F:690:LEU:O	1:F:716:ASN:ND2	2.37	0.41
1:A:433:LEU:C	1:A:454:ILE:HG23	2.41	0.41
1:B:455:LYS:HD3	1:B:478:SER:H	1.84	0.41
1:C:32:SER:O	1:C:36:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:PHE:HB2	1:C:248:PHE:CZ	2.55	0.41
1:D:765:GLU:HG3	1:D:766:ILE:HD12	2.02	0.41
1:E:293:CYS:SG	1:E:306:PHE:HB2	2.60	0.41
1:F:105:LEU:HD23	1:F:105:LEU:HA	1.74	0.41
1:F:243:GLU:O	1:F:246:LYS:HG2	2.20	0.41
1:F:724:GLU:HA	1:F:727:PHE:CE2	2.54	0.41
1:F:732:LYS:O	1:F:755:SER:OG	2.26	0.41
1:F:735:LYS:HE2	1:F:735:LYS:HB3	1.80	0.41
1:F:759:VAL:HB	1:F:764:PHE:HE2	1.85	0.41
1:G:284:VAL:HG21	1:G:324:LEU:HD21	2.00	0.41
1:A:246:LYS:HB3	1:A:246:LYS:HE2	1.72	0.41
1:A:726:TYR:OH	1:A:745:SER:HB3	2.20	0.41
1:A:775:ARG:H	1:A:775:ARG:HG3	1.72	0.41
1:B:319:LEU:HD23	1:B:319:LEU:HA	1.75	0.41
1:C:724:GLU:HA	1:C:727:PHE:CD2	2.55	0.41
1:D:606:HIS:HA	1:D:609:PHE:CE2	2.55	0.41
1:E:120:LEU:HD21	1:E:310:HIS:CE1	2.54	0.41
1:E:573:HIS:ND1	1:E:597:VAL:HB	2.35	0.41
1:E:652:ILE:HD11	1:E:672:ILE:HD13	2.02	0.41
1:E:654:GLU:HG3	1:E:678:HIS:CG	2.55	0.41
1:E:779:ARG:CA	1:E:800:MET:HE3	2.44	0.41
1:F:526:SER:HA	1:F:533:VAL:HA	2.02	0.41
1:F:668:SER:O	1:F:670:ASN:ND2	2.53	0.41
1:F:735:LYS:HA	1:F:758:ASP:HB3	2.02	0.41
1:A:634:GLN:NE2	1:A:658:LYS:HD3	2.35	0.41
1:B:637:ARG:HA	1:B:637:ARG:HD3	1.80	0.41
1:B:785:GLU:H	1:B:785:GLU:HG2	1.68	0.41
1:C:438:ASP:HA	1:C:441:PHE:HD2	1.85	0.41
1:C:643:LYS:HB3	1:C:645:TRP:HD1	1.86	0.41
1:C:759:VAL:O	1:C:762:ASN:ND2	2.53	0.41
1:D:46:GLN:HA	1:D:50:ASP:HB2	2.03	0.41
1:E:334:CYS:O	1:E:338:LEU:N	2.34	0.41
1:E:375:HIS:O	1:E:379:GLN:HG2	2.20	0.41
1:F:457:VAL:HB	1:F:479:VAL:HG13	2.02	0.41
1:A:58:ARG:NH1	1:A:305:ASN:HD22	2.19	0.41
1:A:121:HIS:CD2	1:A:286:LYS:HG2	2.55	0.41
1:A:157:HIS:CE1	1:A:248:PHE:HD1	2.37	0.41
1:A:502:ASP:C	1:A:504:ARG:H	2.23	0.41
1:C:451:LEU:O	1:C:475:HIS:N	2.52	0.41
1:C:479:VAL:O	1:C:507:PRO:HB3	2.21	0.41
1:C:481:ILE:HD12	1:C:486:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:666:SER:HA	1:C:689:ASP:HB3	2.02	0.41
1:C:696:ARG:HH21	1:C:717:LYS:NZ	2.18	0.41
1:D:409:TRP:CZ2	1:D:433:LEU:HD21	2.55	0.41
1:E:448:SER:HA	1:E:471:GLU:O	2.21	0.41
1:E:499:LYS:HA	1:E:522:VAL:HB	2.03	0.41
1:F:454:ILE:HG22	1:F:457:VAL:CG2	2.51	0.41
1:A:242:PHE:CE1	1:A:391:PHE:HA	2.54	0.41
1:A:672:ILE:HG13	1:A:695:ILE:HD11	2.02	0.41
1:A:765:GLU:HG2	1:A:766:ILE:H	1.86	0.41
1:B:270:VAL:HG23	1:B:334:CYS:HB3	2.02	0.41
1:B:630:ILE:HG22	1:B:659:LEU:HD21	2.02	0.41
1:B:779:ARG:N	1:B:800:MET:HB3	2.36	0.41
1:F:121:HIS:CG	1:F:286:LYS:HG2	2.56	0.41
1:F:310:HIS:NE2	1:F:313:ALA:HB2	2.35	0.41
1:F:392:LEU:HD23	1:F:392:LEU:O	2.21	0.41
1:F:523:GLY:O	1:F:551:SER:OG	2.26	0.41
1:A:346:LEU:HD22	1:A:375:HIS:CG	2.56	0.41
1:A:430:LEU:N	1:A:450:LYS:HZ2	2.19	0.41
1:B:144:PHE:HB3	1:B:265:GLN:HE21	1.86	0.41
1:B:318:LYS:H	1:B:318:LYS:HG2	1.57	0.41
1:D:418:LEU:HB3	1:D:426:LEU:HD11	2.03	0.41
1:D:496:LEU:O	1:D:520:TYR:N	2.49	0.41
1:F:46:GLN:HG3	1:F:50:ASP:CB	2.51	0.41
1:A:273:PHE:CE2	1:A:274:LEU:CD2	3.03	0.41
1:A:307:SER:CB	1:G:300:MET:CE	2.99	0.41
1:A:729:LYS:HB3	1:A:753:PHE:CD2	2.55	0.41
1:B:255:GLY:O	1:B:367:LYS:NZ	2.53	0.41
1:B:516:LEU:O	1:B:544:LEU:HD22	2.19	0.41
1:B:637:ARG:O	1:B:661:SER:OG	2.22	0.41
1:D:252:VAL:HB	1:D:370:PHE:HE1	1.85	0.41
1:D:778:LYS:NZ	1:D:800:MET:HA	2.36	0.41
1:E:683:ASN:OD1	1:E:683:ASN:N	2.53	0.41
1:F:733:THR:HG23	1:F:756:TYR:HD2	1.86	0.41
1:A:309:ASN:HB3	1:G:110:PHE:HE1	1.86	0.41
1:A:520:TYR:O	1:A:521:LEU:HD13	2.21	0.41
1:A:603:ARG:HD3	1:A:603:ARG:HA	1.92	0.41
1:A:634:GLN:HE22	1:A:658:LYS:HD3	1.85	0.41
1:A:680:PHE:CD1	1:A:701:GLU:HB2	2.56	0.41
1:C:27:PHE:O	1:C:31:LEU:HG	2.21	0.41
1:C:49:GLN:O	1:C:51:LYS:NZ	2.53	0.41
1:C:104:ASP:OD1	1:C:104:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:TYR:HB2	1:C:283:LEU:HD13	2.03	0.41
1:C:499:LYS:HG2	1:C:522:VAL:HB	2.02	0.41
1:C:632:SER:HA	1:C:635:HIS:CD2	2.56	0.41
1:C:654:GLU:HG3	1:C:678:HIS:CG	2.56	0.41
1:C:656:ILE:HD11	1:C:665:LEU:HD11	2.02	0.41
1:C:723:ASP:HA	1:C:726:TYR:HD2	1.85	0.41
1:D:102:ASP:OD1	1:E:98:GLY:HA3	2.19	0.41
1:D:147:LYS:HD3	1:D:147:LYS:HA	1.95	0.41
1:D:323:TYR:O	1:D:327:VAL:HG23	2.21	0.41
1:D:332:LEU:O	1:D:335:LEU:HB2	2.21	0.41
1:E:134:HIS:O	1:E:272:LYS:NZ	2.54	0.41
1:E:353:TYR:O	1:E:357:GLU:N	2.46	0.41
1:E:397:GLU:HG2	1:E:401:LYS:NZ	2.36	0.41
1:E:496:LEU:O	1:E:520:TYR:N	2.54	0.41
1:F:449:LEU:HD23	1:F:472:LEU:HD13	2.03	0.41
1:F:550:LYS:NZ	1:F:573:HIS:HB2	2.36	0.41
1:F:751:LEU:HB3	1:F:754:LEU:HB2	2.03	0.41
1:A:510:MET:HA	1:A:513:LEU:HG	2.02	0.41
1:A:563:VAL:HG13	1:A:567:LEU:HB2	2.03	0.41
1:A:638:LYS:HA	1:A:638:LYS:HD3	1.92	0.41
1:A:699:PRO:HA	1:A:700:PRO:HD3	1.96	0.41
1:A:759:VAL:O	1:A:762:ASN:ND2	2.52	0.41
1:B:383:LEU:HD11	1:B:387:ARG:HH21	1.85	0.41
1:C:99:LEU:HD12	1:C:99:LEU:HA	1.84	0.41
1:D:172:THR:HG1	1:D:387:ARG:HH12	1.67	0.41
1:D:337:THR:O	1:D:341:LEU:N	2.53	0.41
1:D:649:ILE:HG21	1:D:667:PHE:HE1	1.86	0.41
1:E:273:PHE:HE1	1:E:328:SER:HA	1.87	0.41
1:E:280:ASN:HB2	1:E:324:LEU:HD11	2.03	0.41
1:E:415:ARG:HA	1:E:418:LEU:HD12	2.03	0.41
1:E:675:LEU:HD22	1:E:695:ILE:HD12	2.02	0.41
1:A:659:LEU:HB3	1:A:662:LEU:HG	2.03	0.40
1:B:508:PRO:O	1:B:511:TYR:HD1	2.04	0.40
1:B:586:LYS:HG2	1:B:607:ALA:HA	2.03	0.40
1:B:712:SER:HB2	1:B:735:LYS:HD3	2.02	0.40
1:C:38:ILE:HG13	1:C:319:LEU:HD21	2.03	0.40
1:C:55:LEU:HA	1:C:55:LEU:HD23	1.73	0.40
1:D:171:THR:HA	1:D:390:VAL:HG11	2.02	0.40
1:E:397:GLU:HG2	1:E:401:LYS:HZ3	1.85	0.40
1:F:252:VAL:HB	1:F:370:PHE:CZ	2.56	0.40
1:F:427:GLU:HA	1:F:448:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:LYS:HA	1:F:509:TRP:CZ2	2.56	0.40
1:F:721:LEU:HD23	1:F:721:LEU:HA	1.89	0.40
1:A:555:LYS:HB2	1:A:581:MET:CE	2.51	0.40
1:A:713:ILE:HD11	1:A:736:ILE:HD12	2.03	0.40
1:B:249:ARG:HE	1:B:253:GLU:CD	2.23	0.40
1:B:335:LEU:HD23	1:B:335:LEU:HA	1.77	0.40
1:B:405:LEU:HD12	1:B:406:ASN:N	2.36	0.40
1:C:418:LEU:HD11	1:C:443:ILE:HG21	2.04	0.40
1:D:300:MET:HE3	1:D:300:MET:HB3	1.98	0.40
1:E:497:SER:HB3	1:E:499:LYS:HZ2	1.86	0.40
1:E:735:LYS:HE2	1:E:735:LYS:HB3	1.85	0.40
1:F:500:PHE:CE1	1:F:521:LEU:HD12	2.55	0.40
1:F:665:LEU:HD21	1:F:679:LEU:HD11	2.03	0.40
1:A:377:ILE:HA	1:A:377:ILE:HD13	1.82	0.40
1:A:620:LYS:HG3	1:A:646:HIS:HD2	1.86	0.40
1:B:32:SER:HB3	1:B:139:MET:SD	2.61	0.40
1:B:355:ARG:HH22	1:B:356:GLN:HE21	1.69	0.40
1:B:556:ILE:HG23	1:B:584:ASN:HB2	2.02	0.40
1:B:595:GLU:HA	1:B:618:ASP:HB3	2.03	0.40
1:C:276:ILE:O	1:C:280:ASN:HB2	2.22	0.40
1:D:238:ALA:HB1	1:D:391:PHE:CZ	2.56	0.40
1:D:504:ARG:HD3	1:D:505:GLU:HG3	2.02	0.40
1:D:648:SER:HA	1:D:671:LYS:NZ	2.36	0.40
1:E:38:ILE:HD13	1:E:323:TYR:HB2	2.03	0.40
1:E:429:PRO:HA	1:E:450:LYS:HG2	2.02	0.40
1:F:120:LEU:HA	1:F:120:LEU:HD12	1.81	0.40
1:F:478:SER:HB3	1:F:504:ARG:CZ	2.52	0.40
1:F:490:LYS:HG2	1:F:513:LEU:HA	2.03	0.40
1:G:114:MET:HG3	1:G:297:ILE:HD11	2.02	0.40
1:G:140:LEU:HD12	1:G:140:LEU:HA	1.97	0.40
1:A:447:GLN:CA	1:A:469:LEU:HA	2.47	0.40
1:A:683:ASN:HA	1:A:705:LEU:HD23	2.04	0.40
1:C:490:LYS:HG2	1:C:513:LEU:HA	2.02	0.40
1:D:381:ASP:HA	1:D:382:PRO:HD3	1.98	0.40
1:D:495:VAL:HG22	1:D:518:GLU:HB2	2.04	0.40
1:E:120:LEU:HA	1:E:120:LEU:HD12	1.81	0.40
1:E:418:LEU:HD22	1:E:426:LEU:HG	2.03	0.40
1:E:475:HIS:N	1:E:475:HIS:CD2	2.89	0.40
1:F:415:ARG:HG3	1:F:443:ILE:HD13	2.04	0.40
1:F:726:TYR:CZ	1:F:745:SER:HB3	2.56	0.40
1:G:44:THR:O	1:G:48:MET:CE	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:HE2	1:A:370:PHE:HE1	1.69	0.40
1:A:744:LEU:HD21	1:A:771:LEU:HD21	2.03	0.40
1:B:294:ASN:OD1	1:B:294:ASN:N	2.53	0.40
1:B:298:GLN:C	1:B:300:MET:H	2.25	0.40
1:B:312:MET:O	1:B:313:ALA:C	2.60	0.40
1:B:518:GLU:HA	1:B:546:ILE:O	2.22	0.40
1:C:19:VAL:HA	1:C:380:TYR:CE1	2.57	0.40
1:C:162:LEU:HA	1:C:388:PHE:CD1	2.56	0.40
1:C:538:LEU:HD12	1:C:560:VAL:HA	2.04	0.40
1:C:540:ASP:O	1:C:542:LYS:N	2.54	0.40
1:D:735:LYS:HE2	1:D:735:LYS:HB3	1.94	0.40
1:E:292:ASP:OD1	1:E:293:CYS:N	2.55	0.40
1:E:418:LEU:HB3	1:E:426:LEU:HD11	2.03	0.40
1:F:458:MET:SD	1:F:459:ILE:N	2.95	0.40
1:F:637:ARG:HD3	1:F:637:ARG:HA	1.90	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	684/811 (84%)	631 (92%)	53 (8%)	0	100	100
1	B	684/811 (84%)	630 (92%)	53 (8%)	1 (0%)	48	78
1	C	684/811 (84%)	648 (95%)	35 (5%)	1 (0%)	48	78
1	D	684/811 (84%)	647 (95%)	36 (5%)	1 (0%)	48	78
1	E	684/811 (84%)	646 (94%)	37 (5%)	1 (0%)	48	78
1	F	684/811 (84%)	641 (94%)	43 (6%)	0	100	100
1	G	186/811 (23%)	177 (95%)	9 (5%)	0	100	100
All	All	4290/5677 (76%)	4020 (94%)	266 (6%)	4 (0%)	50	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	649	ILE
1	B	649	ILE
1	C	649	ILE
1	D	649	ILE

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	642/757 (85%)	622 (97%)	20 (3%)	35	58
1	B	642/757 (85%)	621 (97%)	21 (3%)	33	57
1	C	642/757 (85%)	621 (97%)	21 (3%)	33	57
1	D	642/757 (85%)	617 (96%)	25 (4%)	27	53
1	E	642/757 (85%)	618 (96%)	24 (4%)	29	54
1	F	642/757 (85%)	624 (97%)	18 (3%)	38	60
1	G	178/757 (24%)	172 (97%)	6 (3%)	32	56
All	All	4030/5299 (76%)	3895 (97%)	135 (3%)	35	57

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	29	ASP
1	A	58	ARG
1	A	138	PHE
1	A	247	LYS
1	A	249	ARG
1	A	256	ASP
1	A	273	PHE
1	A	322	CYS
1	A	362	ASP
1	A	378	ASP
1	A	473	SER

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Mol	Chain	Res	Type
1	A	510	MET
1	A	531	ARG
1	A	555	LYS
1	A	572	ILE
1	A	581	MET
1	A	651	TYR
1	A	667	PHE
1	A	779	ARG
1	B	20	LEU
1	B	58	ARG
1	B	249	ARG
1	B	273	PHE
1	B	279	TYR
1	B	294	ASN
1	B	344	ARG
1	B	432	MET
1	B	458	MET
1	B	472	LEU
1	B	473	SER
1	B	510	MET
1	B	520	TYR
1	B	555	LYS
1	B	570	MET
1	B	572	ILE
1	B	582	LEU
1	B	598	HIS
1	B	609	PHE
1	B	635	HIS
1	B	779	ARG
1	C	35	MET
1	C	37	MET
1	C	96	MET
1	C	102	ASP
1	C	118	ARG
1	C	249	ARG
1	C	256	ASP
1	C	361	ASP
1	C	376	MET
1	C	404	ASN
1	C	458	MET
1	C	510	MET
1	C	531	ARG

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Mol	Chain	Res	Type
1	C	555	LYS
1	C	570	MET
1	C	572	ILE
1	C	598	HIS
1	C	623	ASN
1	C	666	SER
1	C	673	GLU
1	C	779	ARG
1	D	37	MET
1	D	46	GLN
1	D	102	ASP
1	D	106	GLN
1	D	145	TRP
1	D	166	PHE
1	D	249	ARG
1	D	273	PHE
1	D	294	ASN
1	D	362	ASP
1	D	473	SER
1	D	475	HIS
1	D	503	MET
1	D	504	ARG
1	D	531	ARG
1	D	555	LYS
1	D	581	MET
1	D	588	MET
1	D	650	THR
1	D	657	LYS
1	D	671	LYS
1	D	750	ASN
1	D	759	VAL
1	D	775	ARG
1	D	779	ARG
1	E	27	PHE
1	E	35	MET
1	E	96	MET
1	E	139	MET
1	E	141	CYS
1	E	166	PHE
1	E	249	ARG
1	E	273	PHE
1	E	344	ARG

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Mol	Chain	Res	Type
1	E	369	ASP
1	E	376	MET
1	E	388	PHE
1	E	404	ASN
1	E	458	MET
1	E	510	MET
1	E	531	ARG
1	E	555	LYS
1	E	574	ASN
1	E	666	SER
1	E	672	ILE
1	E	756	TYR
1	E	760	LYS
1	E	779	ARG
1	E	800	MET
1	F	48	MET
1	F	106	GLN
1	F	145	TRP
1	F	157	HIS
1	F	242	PHE
1	F	251	HIS
1	F	273	PHE
1	F	279	TYR
1	F	404	ASN
1	F	482	HIS
1	F	511	TYR
1	F	531	ARG
1	F	555	LYS
1	F	572	ILE
1	F	581	MET
1	F	651	TYR
1	F	759	VAL
1	F	779	ARG
1	G	35	MET
1	G	37	MET
1	G	48	MET
1	G	138	PHE
1	G	273	PHE
1	G	326	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	A	646	HIS
1	B	265	GLN
1	B	294	ASN
1	B	305	ASN
1	B	406	ASN
1	C	265	GLN
1	C	310	HIS
1	C	375	HIS
1	C	402	GLN
1	D	49	GLN
1	D	655	HIS
1	E	375	HIS
1	E	406	ASN
1	F	305	ASN
1	G	134	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

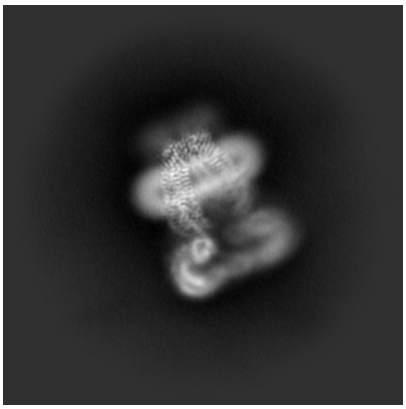
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19495. These allow visual inspection of the internal detail of the map and identification of artifacts.

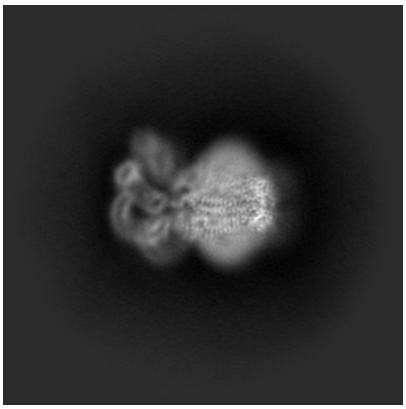
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

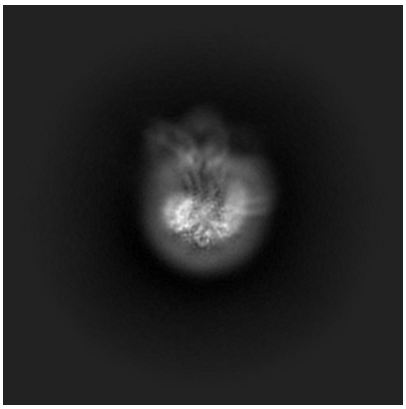
6.1.1 Primary map



X

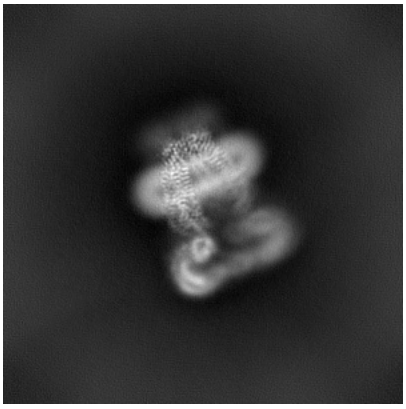


Y

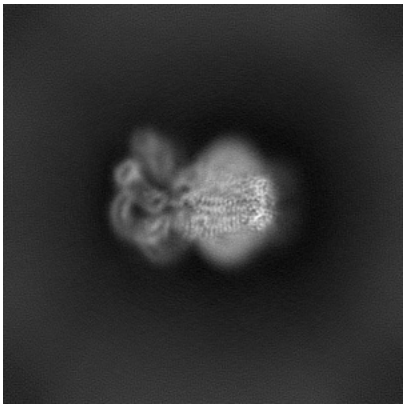


Z

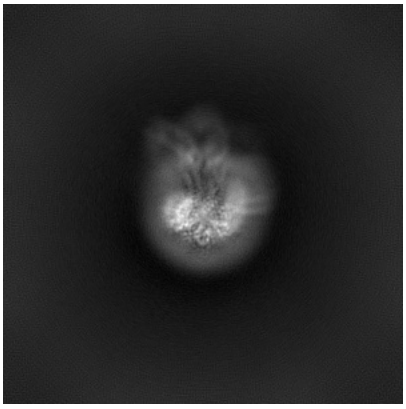
6.1.2 Raw map



X



Y



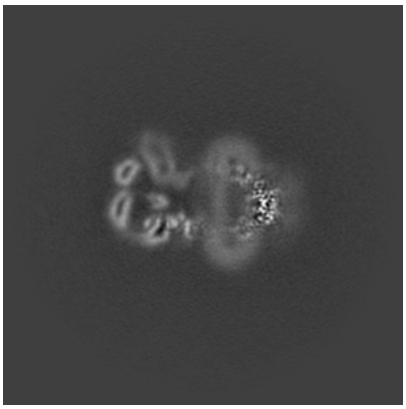
Z

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

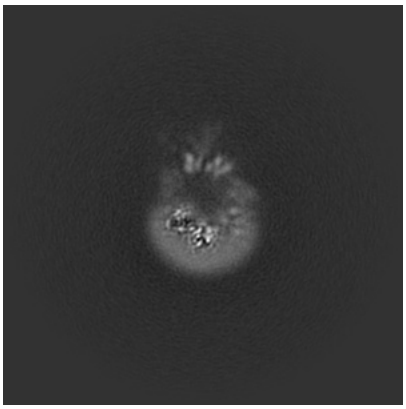
6.2 Central slices (i)

6.2.1 Primary map

X Index: 168



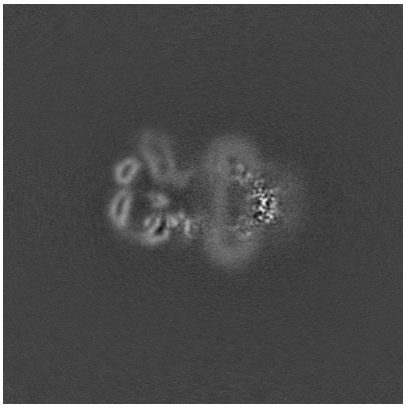
Y Index: 168



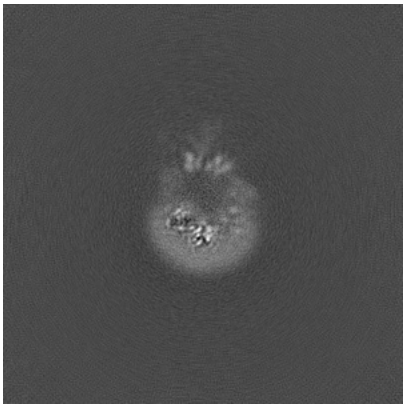
Z Index: 168

6.2.2 Raw map

X Index: 168



Y Index: 168



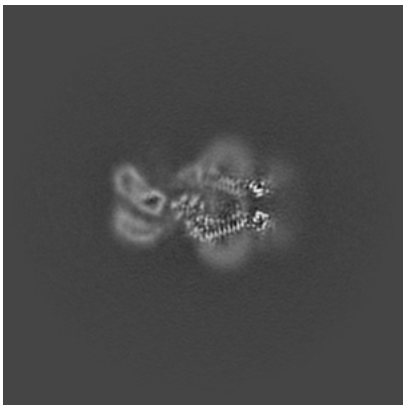
Z Index: 168

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

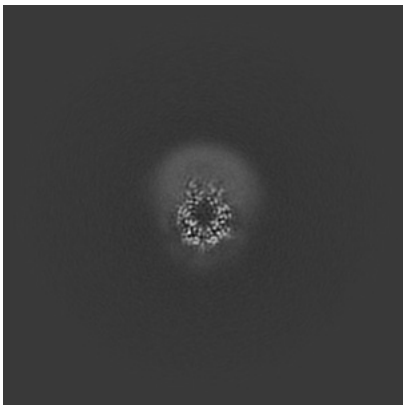
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 154



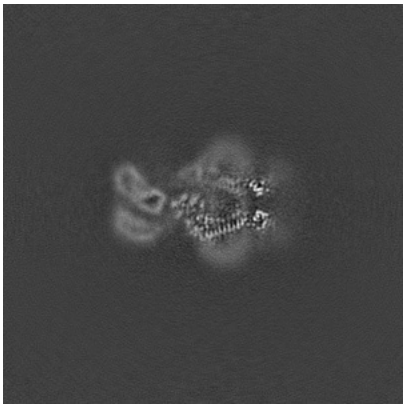
Y Index: 152



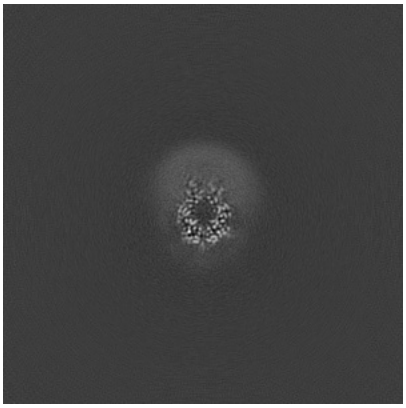
Z Index: 213

6.3.2 Raw map

X Index: 154



Y Index: 152

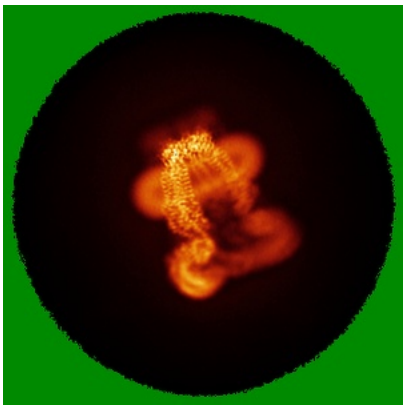


Z Index: 213

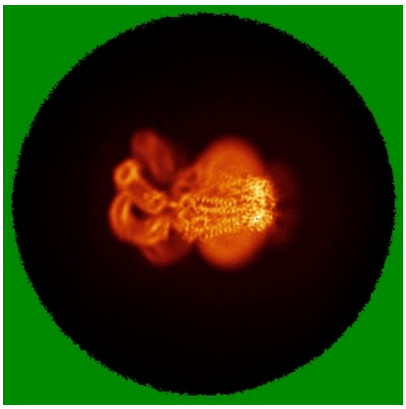
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

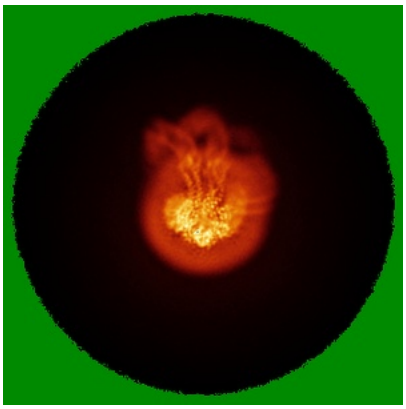
6.4.1 Primary map



X

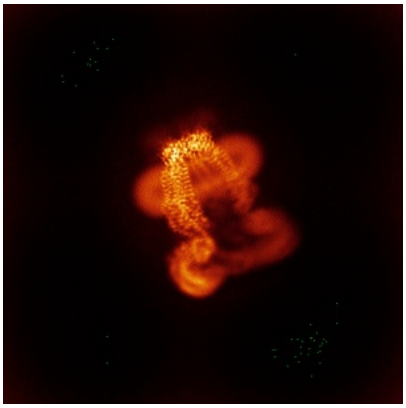


Y

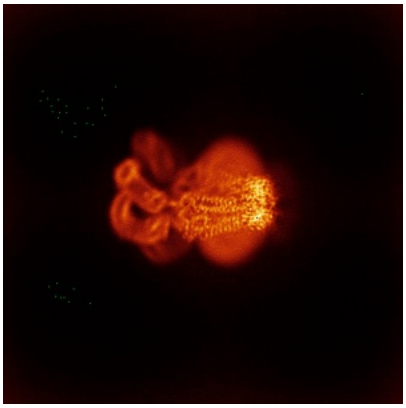


Z

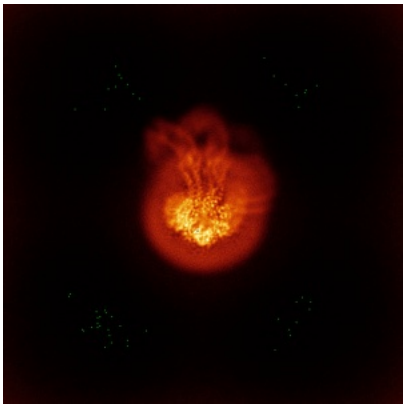
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

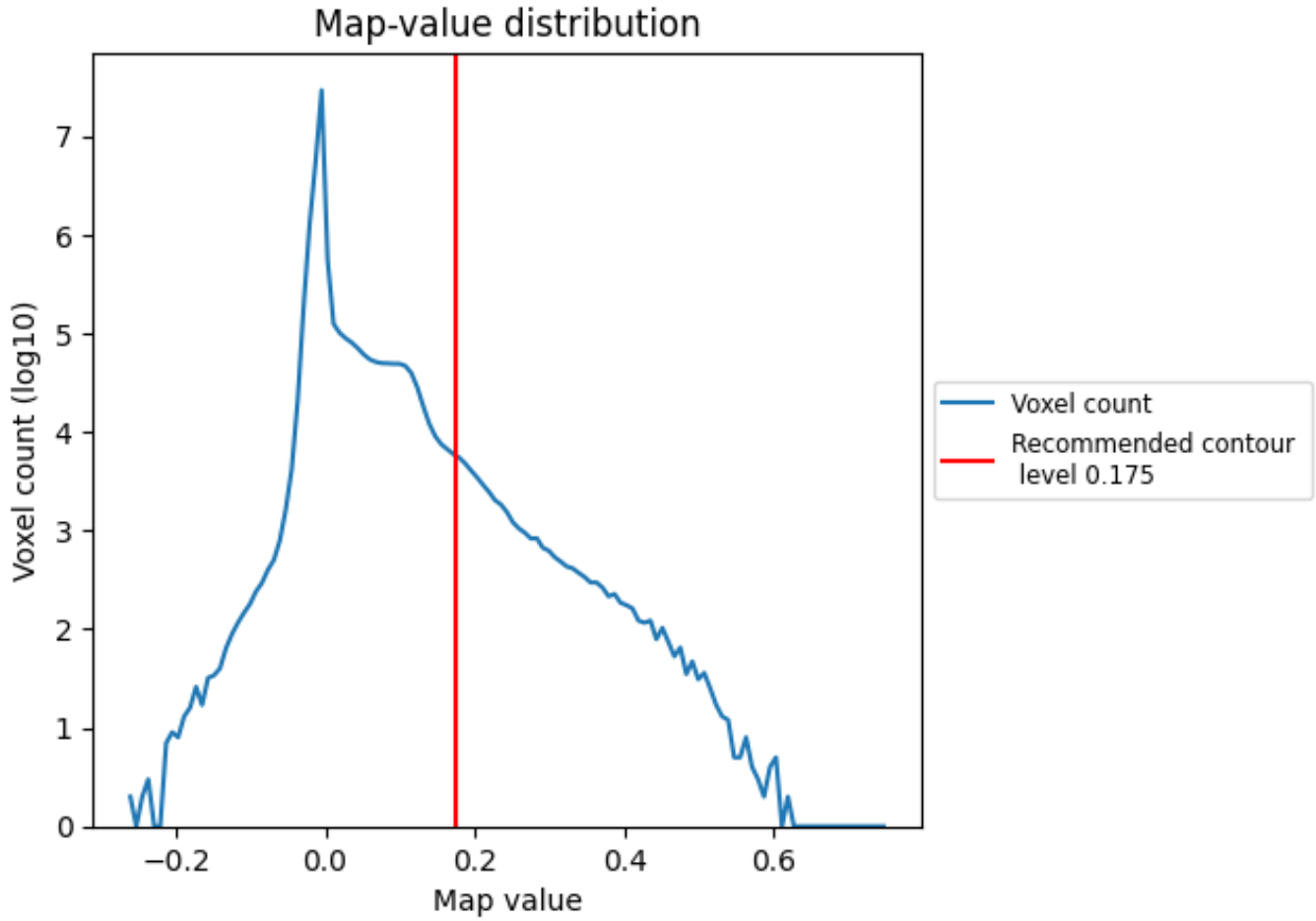
6.6 Mask visualisation (i)

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

7 Map analysis

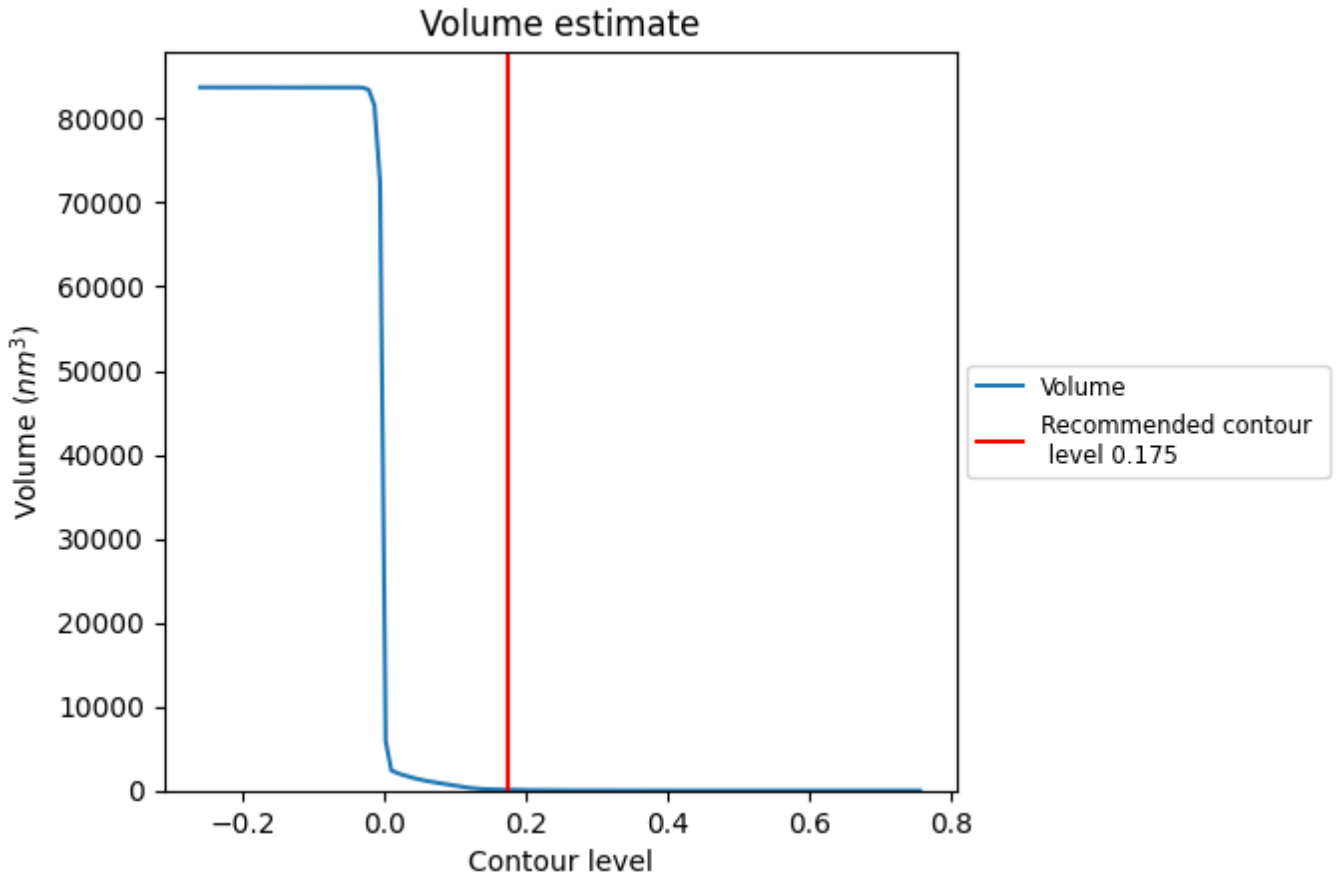
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

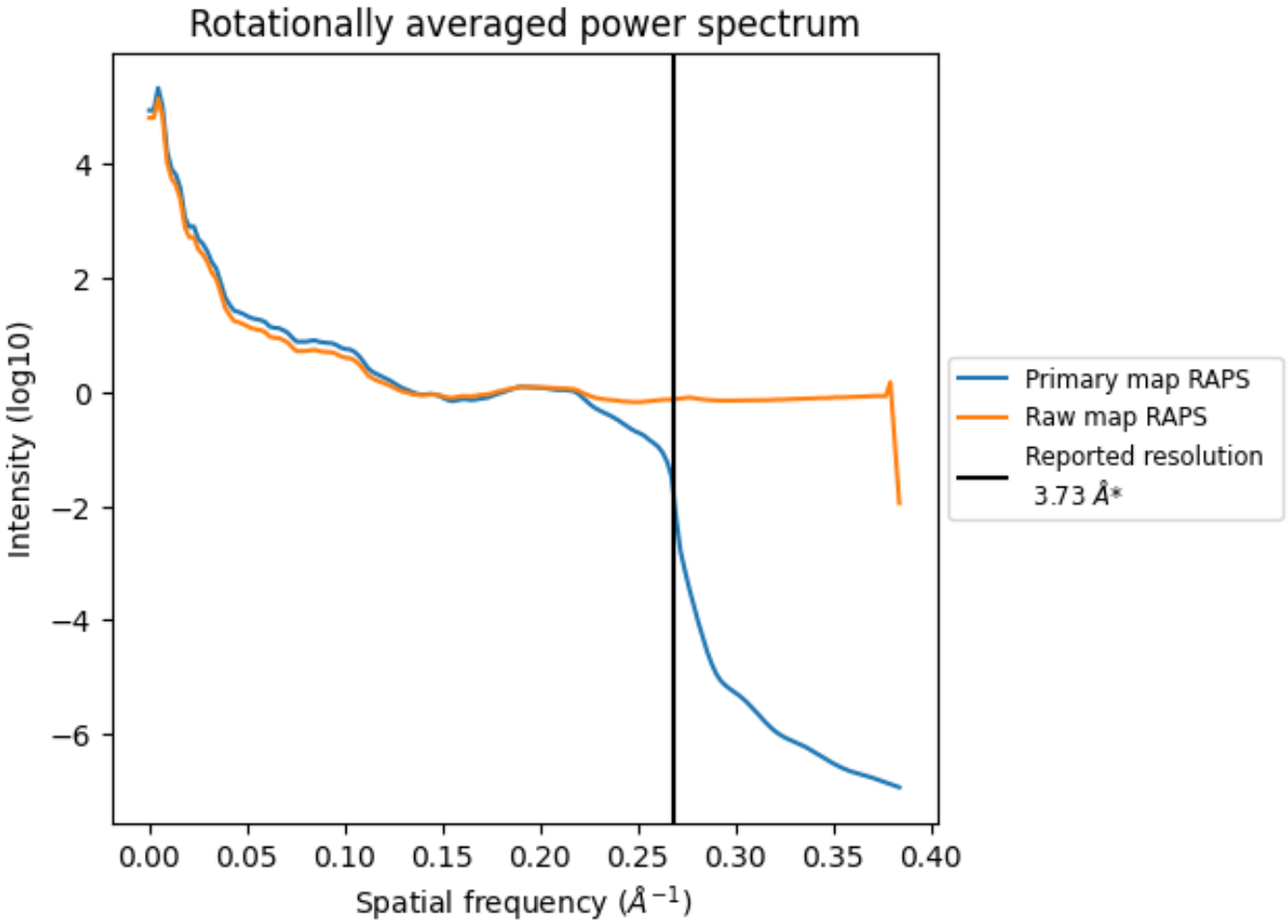
7.2 Volume estimate



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 86 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)

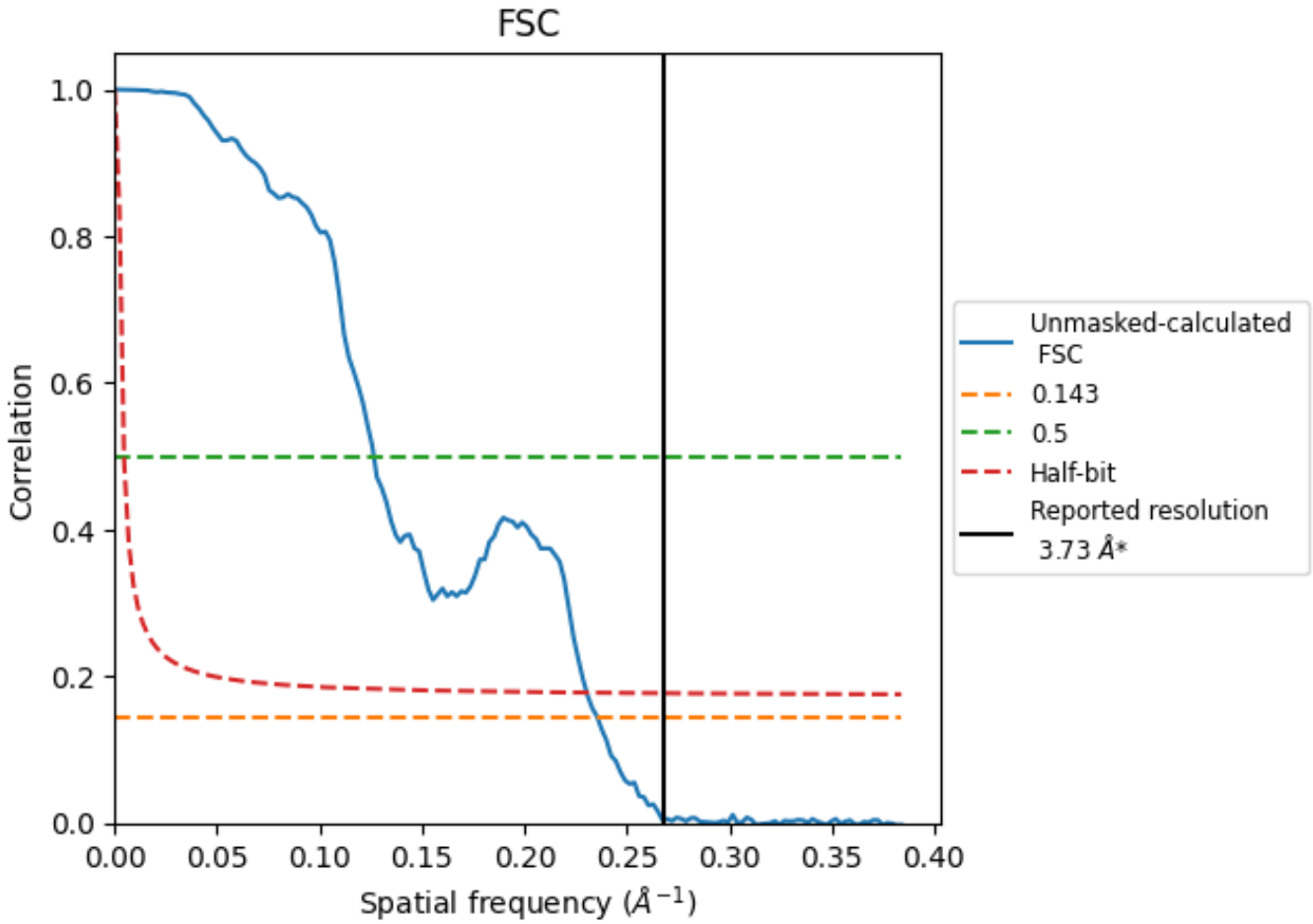


*Reported resolution corresponds to spatial frequency of 0.268 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.268 Å^{-1}

8.2 Resolution estimates (i)

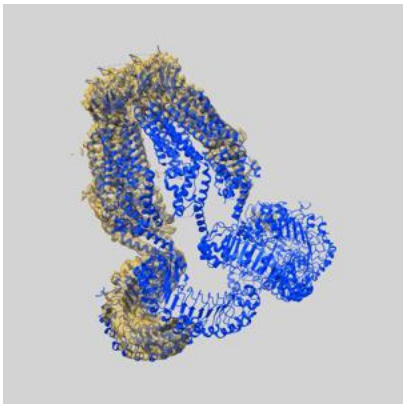
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.91	4.34

*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 4.24 differs from the reported value 3.73 by more than 10 %

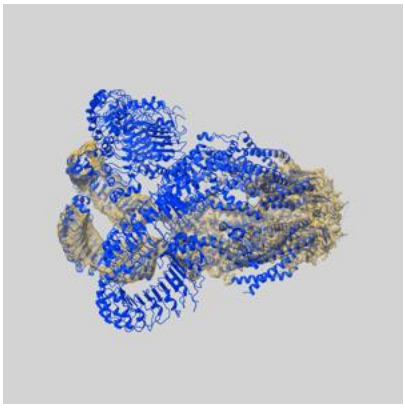
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19495 and PDB model 8RTS. Per-residue inclusion information can be found in section 3 on page 6.

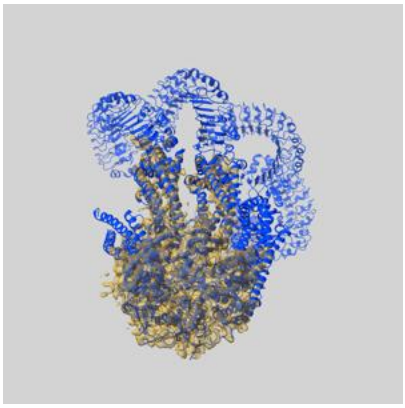
9.1 Map-model overlay



X



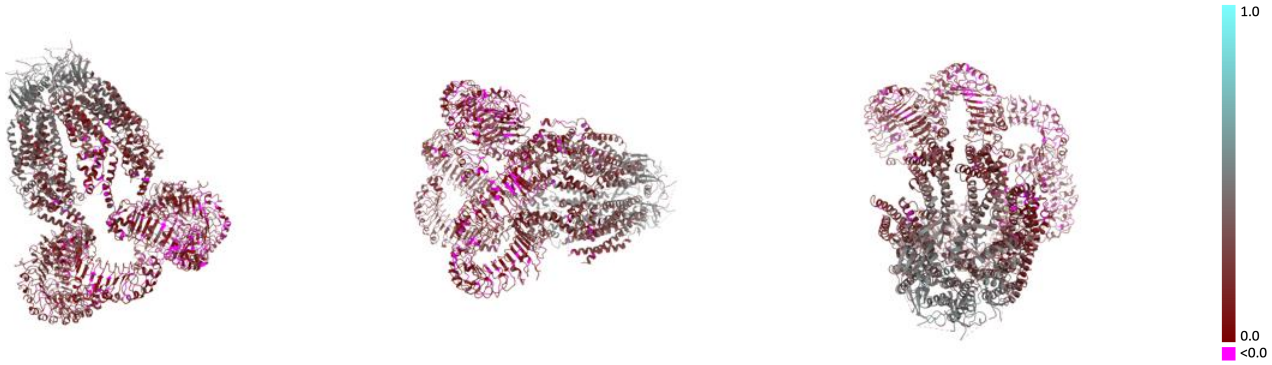
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.175 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.

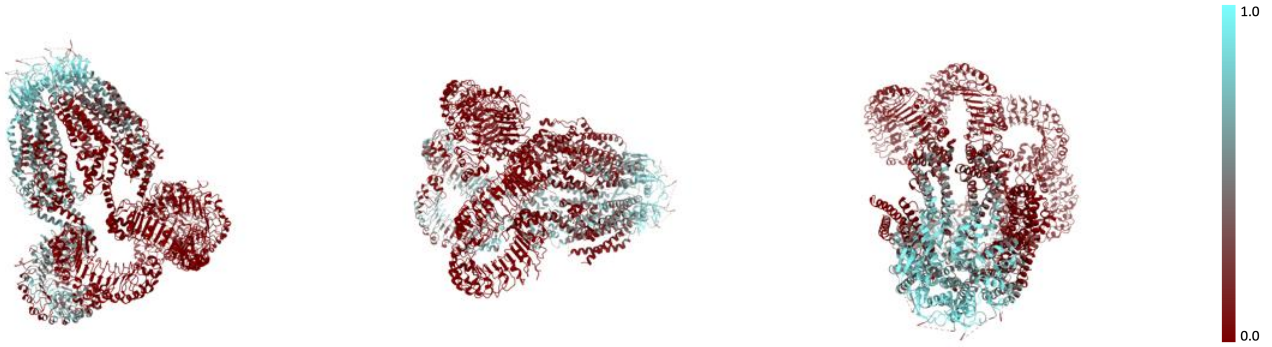
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

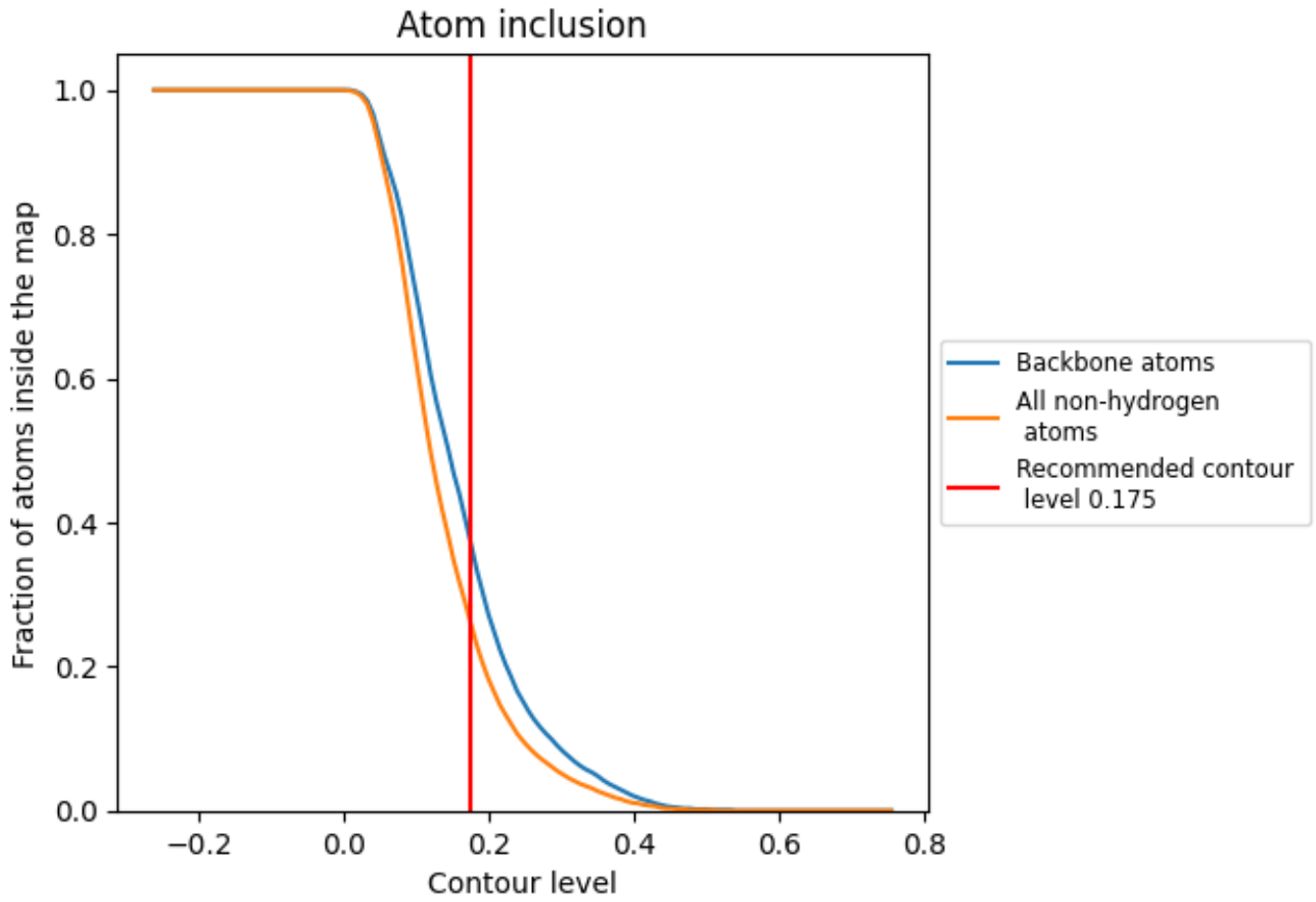
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.175).

9.4 Atom inclusion (i)



At the recommended contour level, 37% of all backbone atoms, 26% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2620	0.2250
A	0.5320	0.2850
B	0.5110	0.2810
C	0.1200	0.1990
D	0.0810	0.1600
E	0.1410	0.1940
F	0.1800	0.2150
G	0.2770	0.2860