Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:45 pm GMT

PDB ID	:	2VOY
EMDB ID	:	EMD-5004
Title	:	CryoEM model of CopA, the copper transporting ATPase from Archaeoglobus fulgidus
Authors	:	Wu, C.-C.; Rice, W.J.; Stokes, D.L.
Deposited on	:	2008-02-25
Resolution	:	18.00 Å(reported)
Based on initial models	:	2B8E, 2HC8, 2EAR

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:

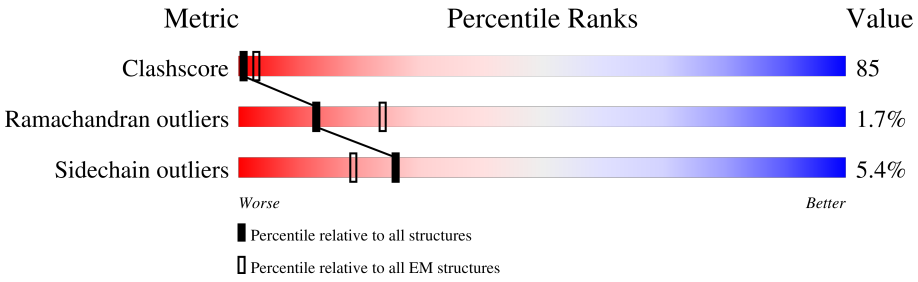
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 18.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	80	21% 42% 49% 9%
2	B	42	24% 26% 67% 5%
3	C	22	14% 82% 18%
4	D	23	13% 83%
5	E	30	27% 40% 60%
6	F	113	20% 75% 22%
7	G	36	42% 78% 19%
8	H	48	19% 33% 56% 10%

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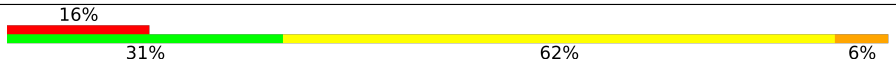
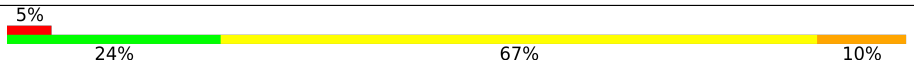
Mol	Chain	Length	Quality of chain
9	I	128	
10	J	118	
11	K	32	
12	L	21	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 5270 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 POTENTIAL COPPER-TRANSPORTING ATPASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	80	615	382	104	126	3	0	0

- Molecule 2 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	42	341	227	52	61	1	0	0

- Molecule 3 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	22	176	123	25	27	1	0	0

- Molecule 4 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	23	176	121	28	26	1	0	0

- Molecule 5 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	30	234	155	38	41	0	0

- Molecule 6 is a protein called CATION-TRANSPORTING ATPASE, P-TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	113	Total	C	N	O	S	0	0
			829	525	138	164	2		

- Molecule 7 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	36	Total	C	N	O	S	0	0
			287	185	47	54	1		

- Molecule 8 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	48	Total	C	N	O	S	0	0
			356	233	64	57	2		

- Molecule 9 is a protein called CATION-TRANSPORTING ATPASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	128	Total	C	N	O	Se	0	0
			959	604	165	188	2		

- Molecule 10 is a protein called CATION-TRANSPORTING ATPASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	118	Total	C	N	O	Se	0	0
			887	553	157	176	1		

- Molecule 11 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	32	Total	C	N	O	S	0	0
			253	163	43	45	2		

- Molecule 12 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

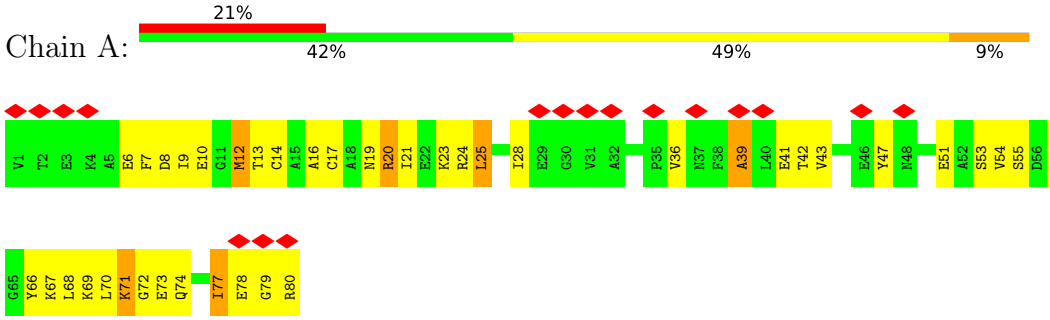
Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	21	Total	C	N	O	0	0
			157	106	24	27		

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.

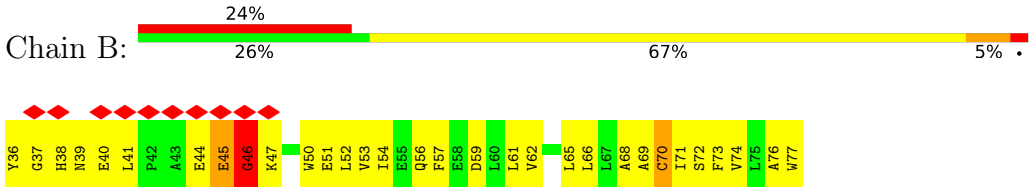
• Molecule 1: POTENTIAL COPPER-TRANSPORTING ATPASE

Chain A:



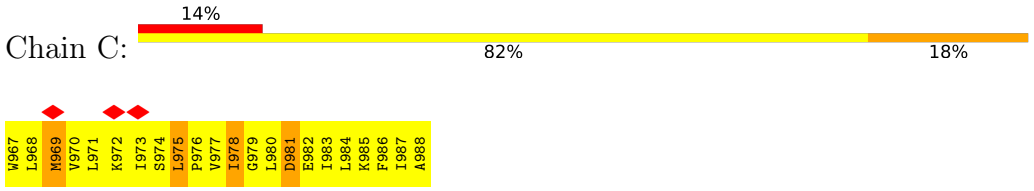
• Molecule 2: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1

Chain B:



• Molecule 3: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1

Chain C:

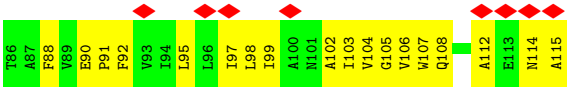


• Molecule 4: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1

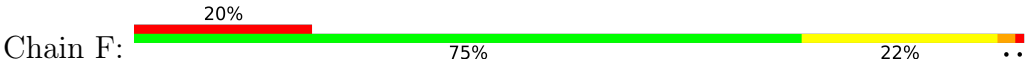
Chain D:

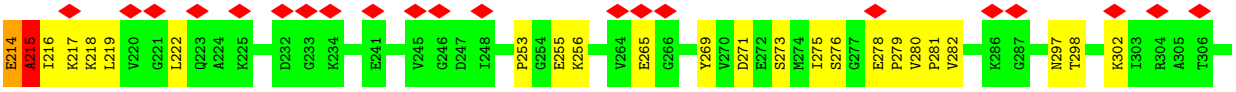
• Molecule 5: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1

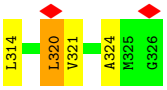
Chain E:



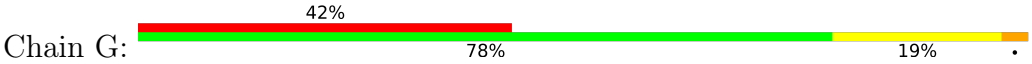
• Molecule 6: CATION-TRANSPORTING ATPASE, P-TYPE

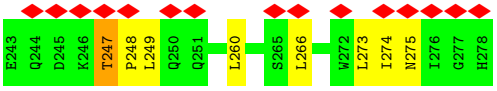




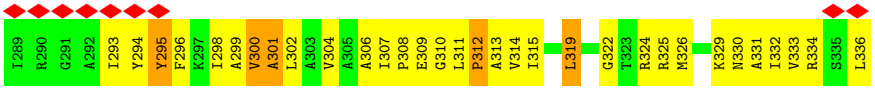


• Molecule 7: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1

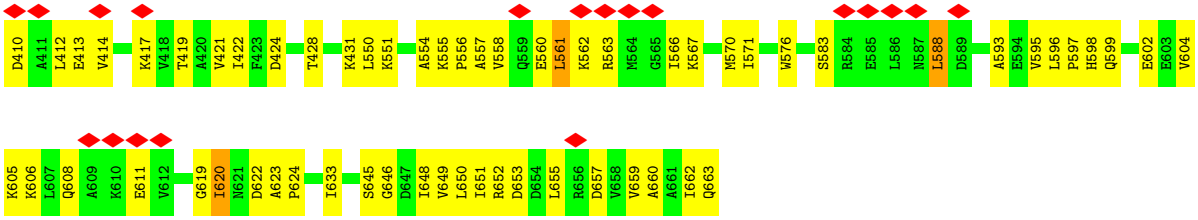




• Molecule 8: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1



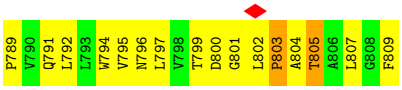
• Molecule 9: CATION-TRANSPORTING ATPASE



• Molecule 10: CATION-TRANSPORTING ATPASE

• Molecule 11: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1

• Molecule 12: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL TUBES	Depositor
Microscope	FEI/PHILIPS CM200FEG/ST	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	900.00	Depositor
Maximum defocus (nm)	2500.00	Depositor
Magnification	51300	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	75.388	Depositor
Minimum map value	-48.614	Depositor
Average map value	0.529	Depositor
Map value standard deviation	4.943	Depositor
Recommended contour level	10.0	Depositor
Map size (Å)	202, 202, 202	wwPDB
Map dimensions	101, 101, 101	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2, 2, 2	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	0.50	0/620	0.87	0/831
2	B	0.30	0/349	0.49	0/475
3	C	0.52	0/179	0.71	0/242
4	D	0.44	0/183	0.56	0/249
5	E	0.31	0/238	0.52	0/326
6	F	0.73	1/835 (0.1%)	0.77	1/1129 (0.1%)
7	G	0.29	0/291	0.49	0/393
8	H	0.30	0/360	0.54	0/487
9	I	0.52	1/962 (0.1%)	0.80	1/1293 (0.1%)
10	J	0.49	1/892 (0.1%)	0.82	3/1202 (0.2%)
11	K	0.48	0/256	0.65	0/344
12	L	0.44	0/161	0.72	0/222
All	All	0.51	3/5326 (0.1%)	0.73	5/7193 (0.1%)

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
2	B	0	3
6	F	0	1
8	H	0	2
9	I	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	215	ALA	C-N	7.47	1.51	1.34
9	I	570	MSE	SE-CE	-5.54	1.62	1.95
10	J	506	MSE	SE-CE	-5.52	1.62	1.95

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	622	ASP	CB-CG-OD1	9.26	126.63	118.30
10	J	497	GLY	O-C-N	6.38	132.91	122.70
10	J	497	GLY	CA-C-N	-5.57	104.95	117.20
10	J	496	ASP	O-C-N	-5.26	114.26	123.20
6	F	215	ALA	CA-C-N	-5.01	106.17	117.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	TYR	Sidechain
2	B	45	GLU	Peptide
2	B	46	GLY	Peptide
2	B	70	CYS	Mainchain
6	F	215	ALA	Mainchain
8	H	301	ALA	Mainchain
8	H	302	LEU	Mainchain
9	I	620	ILE	Mainchain

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	615	0	608	285	0
2	B	341	0	336	267	0
3	C	176	0	196	165	0
4	D	176	0	164	143	0
5	E	234	0	239	89	0
6	F	829	0	874	218	0
7	G	287	0	294	40	0
8	H	356	0	397	74	0
9	I	959	0	999	149	0
10	J	887	0	915	127	0
11	K	253	0	257	40	0
12	L	157	0	163	18	0
All	All	5270	0	5442	913	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 85.

All (913) 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)
3:C:968:LEU:HD21	8:H:296:PHE:CZ	1.17	1.68
3:C:985:LYS:CG	4:D:838:MET:HG2	1.24	1.66
1:A:58:LYS:HB3	6:F:298:THR:CG2	1.19	1.64
1:A:12:MET:SD	10:J:459:ARG:HB3	1.29	1.62
7:G:247:THR:HG21	9:I:410:ASP:CB	1.30	1.61
1:A:71:LYS:HG3	6:F:273:SER:CB	1.32	1.58
7:G:247:THR:CG2	9:I:410:ASP:HB3	1.27	1.56
1:A:77:ILE:CG2	2:B:39:ASN:HB2	1.31	1.56
2:B:77:TRP:CH2	4:D:852:ALA:CB	1.88	1.56
4:D:832:TRP:CE3	5:E:106:VAL:HG13	1.39	1.53
2:B:50:TRP:CE3	3:C:986:PHE:HB3	1.04	1.50
3:C:985:LYS:CE	4:D:838:MET:HG3	1.41	1.49
1:A:71:LYS:NZ	6:F:279:PRO:HB3	1.27	1.49
1:A:77:ILE:CG2	2:B:39:ASN:CB	1.88	1.48
2:B:53:VAL:HG11	3:C:985:LYS:CD	1.00	1.47
7:G:247:THR:CB	9:I:410:ASP:CG	1.81	1.45
2:B:50:TRP:CE3	3:C:986:PHE:CB	1.98	1.44
2:B:41:LEU:N	6:F:214:GLU:HB3	1.30	1.44
2:B:77:TRP:CH2	4:D:852:ALA:HB3	1.41	1.44
2:B:51:GLU:OE1	3:C:986:PHE:CE1	1.66	1.44
1:A:77:ILE:CG2	2:B:39:ASN:N	1.81	1.43
1:A:77:ILE:HG23	2:B:39:ASN:CA	1.43	1.43
7:G:247:THR:HB	9:I:410:ASP:CG	1.15	1.43
2:B:45:GLU:HB3	2:B:47:LYS:CE	1.51	1.41
1:A:74:GLN:HG3	2:B:36:TYR:N	1.36	1.40
7:G:247:THR:CG2	9:I:410:ASP:CB	1.85	1.40
1:A:71:LYS:CA	6:F:273:SER:HB3	1.27	1.40
1:A:71:LYS:CA	6:F:273:SER:CB	1.87	1.38
1:A:69:LYS:CE	6:F:282:VAL:O	1.68	1.38
2:B:41:LEU:CD2	6:F:217:LYS:HB2	1.52	1.38
2:B:51:GLU:CD	3:C:986:PHE:CE1	1.94	1.38
2:B:77:TRP:HH2	4:D:852:ALA:CB	1.09	1.38
4:D:832:TRP:CZ3	5:E:106:VAL:HG13	1.58	1.38
2:B:51:GLU:CD	3:C:986:PHE:HE1	1.27	1.37
2:B:74:VAL:O	3:C:967:TRP:CZ3	1.75	1.36
1:A:77:ILE:HG22	2:B:39:ASN:N	1.34	1.36
1:A:71:LYS:CG	6:F:273:SER:HB2	1.52	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:985:LYS:CG	4:D:838:MET:CG	2.04	1.35
4:D:832:TRP:CZ3	5:E:106:VAL:CG1	2.10	1.34
1:A:12:MET:CB	10:J:485:VAL:HG11	1.58	1.33
4:D:835:PHE:CZ	5:E:102:ALA:O	1.82	1.32
1:A:12:MET:CA	10:J:460:SER:OG	1.78	1.31
3:C:968:LEU:CD2	8:H:296:PHE:CZ	2.10	1.31
1:A:16:ALA:CB	10:J:481:GLU:OE2	1.78	1.31
1:A:12:MET:HB3	10:J:485:VAL:CG1	1.57	1.30
1:A:58:LYS:HG3	6:F:269:TYR:CB	1.44	1.30
2:B:53:VAL:CG1	3:C:985:LYS:HD3	0.83	1.30
1:A:58:LYS:CB	6:F:298:THR:HG21	1.61	1.30
7:G:247:THR:HB	9:I:410:ASP:OD2	1.15	1.30
1:A:67:LYS:HG3	6:F:269:TYR:OH	1.16	1.30
1:A:71:LYS:CG	6:F:273:SER:CB	2.09	1.29
1:A:12:MET:SD	10:J:459:ARG:CB	2.04	1.29
1:A:77:ILE:HG23	2:B:39:ASN:CB	1.52	1.28
1:A:77:ILE:CD1	9:I:620:ILE:N	1.96	1.28
1:A:58:LYS:CG	6:F:269:TYR:HB2	1.39	1.26
1:A:66:TYR:HB3	10:J:485:VAL:O	1.33	1.26
7:G:249:LEU:CB	9:I:413:GLU:OE2	1.82	1.26
2:B:41:LEU:HA	6:F:214:GLU:N	1.50	1.25
2:B:44:GLU:CD	6:F:217:LYS:HZ3	1.37	1.25
3:C:968:LEU:HD21	8:H:296:PHE:CE2	1.69	1.25
1:A:66:TYR:CB	10:J:485:VAL:O	1.82	1.25
1:A:74:GLN:CG	2:B:36:TYR:N	2.00	1.24
1:A:77:ILE:CG2	2:B:39:ASN:CA	2.08	1.24
1:A:77:ILE:HG21	2:B:39:ASN:CB	1.56	1.24
7:G:249:LEU:HB3	9:I:413:GLU:OE2	1.37	1.24
3:C:985:LYS:CE	4:D:838:MET:CG	2.17	1.23
1:A:77:ILE:HD11	9:I:620:ILE:N	1.12	1.23
2:B:77:TRP:CZ3	4:D:849:VAL:O	1.90	1.23
1:A:54:VAL:HB	6:F:297:ASN:CG	1.45	1.22
2:B:53:VAL:CB	3:C:985:LYS:HB3	1.70	1.22
2:B:44:GLU:CD	6:F:217:LYS:NZ	1.92	1.22
2:B:74:VAL:HG12	3:C:967:TRP:CE3	1.73	1.22
1:A:12:MET:HA	10:J:460:SER:OG	1.06	1.21
3:C:985:LYS:HG3	4:D:838:MET:SD	1.80	1.20
1:A:68:LEU:O	6:F:269:TYR:CD1	1.93	1.20
1:A:58:LYS:CB	6:F:298:THR:CG2	2.15	1.20
8:H:332:ILE:O	9:I:649:VAL:N	1.72	1.20
1:A:58:LYS:CG	6:F:269:TYR:CB	1.95	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:985:LYS:HG3	4:D:838:MET:CE	1.71	1.19
1:A:54:VAL:HG21	6:F:297:ASN:OD1	1.41	1.18
1:A:54:VAL:C	6:F:297:ASN:HB3	1.58	1.17
1:A:71:LYS:CB	6:F:279:PRO:HA	1.74	1.17
2:B:46:GLY:N	2:B:47:LYS:HG3	1.57	1.17
1:A:39:ALA:C	10:J:461:GLU:HB2	1.66	1.16
1:A:54:VAL:CG2	6:F:297:ASN:OD1	1.93	1.16
1:A:71:LYS:CB	6:F:273:SER:HB3	1.76	1.16
4:D:835:PHE:CD2	5:E:106:VAL:HG11	1.80	1.16
1:A:58:LYS:HB3	6:F:298:THR:HG23	1.23	1.15
8:H:332:ILE:HB	9:I:649:VAL:HB	1.23	1.15
7:G:247:THR:CB	9:I:410:ASP:CB	2.21	1.15
2:B:46:GLY:H	2:B:47:LYS:CG	1.58	1.15
9:I:663:GLN:O	11:K:751:ARG:N	1.78	1.15
1:A:74:GLN:O	2:B:36:TYR:N	1.61	1.14
2:B:77:TRP:O	4:D:853:ALA:O	1.64	1.14
2:B:74:VAL:CG1	3:C:967:TRP:HE3	1.60	1.14
2:B:41:LEU:HG	6:F:217:LYS:CB	1.76	1.13
2:B:40:GLU:C	6:F:214:GLU:HB3	1.68	1.13
2:B:41:LEU:HG	6:F:217:LYS:HB3	1.20	1.13
2:B:50:TRP:CD2	3:C:986:PHE:HB3	1.80	1.13
2:B:44:GLU:OE2	6:F:217:LYS:HE2	1.48	1.13
7:G:247:THR:CG2	9:I:410:ASP:CG	2.07	1.13
1:A:10:GLU:OE1	10:J:489:ALA:HB2	1.48	1.13
1:A:10:GLU:OE1	10:J:489:ALA:CB	1.97	1.12
4:D:843:TYR:CZ	5:E:92:PHE:CE2	2.37	1.12
8:H:319:LEU:HD13	11:K:757:MET:HE1	1.13	1.12
4:D:839:ALA:HB1	5:E:99:ILE:CG2	1.79	1.12
8:H:319:LEU:CD1	11:K:757:MET:CE	2.26	1.12
2:B:45:GLU:CB	2:B:47:LYS:HE2	1.80	1.12
1:A:14:CYS:N	10:J:459:ARG:HA	1.62	1.12
2:B:50:TRP:NE1	3:C:981:ASP:O	1.83	1.12
1:A:71:LYS:NZ	6:F:279:PRO:CB	2.13	1.11
8:H:319:LEU:HD13	11:K:757:MET:CE	1.81	1.11
2:B:51:GLU:OE1	3:C:986:PHE:CD1	2.02	1.11
6:F:324:ALA:HB1	9:I:605:LYS:HD2	1.24	1.11
1:A:41:GLU:CD	10:J:462:HIS:N	2.05	1.11
1:A:67:LYS:CG	6:F:269:TYR:OH	1.99	1.10
1:A:70:LEU:C	6:F:271:ASP:OD2	1.89	1.10
2:B:50:TRP:CE2	3:C:982:GLU:O	1.90	1.10
2:B:53:VAL:HG11	3:C:985:LYS:CG	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:O	10:J:461:GLU:HB2	1.49	1.10
1:A:71:LYS:HB2	6:F:279:PRO:CA	1.79	1.10
2:B:44:GLU:OE1	6:F:217:LYS:NZ	1.84	1.10
2:B:74:VAL:HG21	3:C:971:LEU:HD23	1.21	1.10
2:B:41:LEU:HD23	6:F:217:LYS:HB2	1.18	1.10
2:B:73:PHE:CE1	4:D:846:ALA:O	2.04	1.10
2:B:53:VAL:HG12	3:C:985:LYS:HD3	1.13	1.10
1:A:13:THR:HG21	10:J:462:HIS:N	1.68	1.09
4:D:832:TRP:CE3	5:E:106:VAL:CG1	2.32	1.08
4:D:835:PHE:CG	5:E:106:VAL:HG11	1.87	1.08
2:B:51:GLU:HA	3:C:986:PHE:CD1	1.89	1.08
1:A:54:VAL:CB	6:F:297:ASN:CG	2.17	1.08
4:D:832:TRP:CZ3	5:E:106:VAL:HG12	1.89	1.08
1:A:71:LYS:HA	6:F:273:SER:CB	1.66	1.08
4:D:835:PHE:CE2	5:E:102:ALA:O	2.06	1.08
2:B:51:GLU:OE1	3:C:986:PHE:HE1	1.10	1.07
5:E:115:ALA:HB1	6:F:214:GLU:OE2	1.55	1.07
8:H:330:ASN:HB3	9:I:652:ARG:H	1.08	1.07
3:C:985:LYS:HG3	4:D:838:MET:CG	1.81	1.07
6:F:275:ILE:HG22	9:I:598:HIS:NE2	1.66	1.07
3:C:985:LYS:HE3	4:D:838:MET:CG	1.81	1.07
7:G:247:THR:HG22	9:I:410:ASP:OD1	1.55	1.07
1:A:41:GLU:CA	10:J:461:GLU:OE2	2.00	1.06
1:A:77:ILE:CG2	2:B:39:ASN:H	1.50	1.06
7:G:248:PRO:HD3	9:I:417:LYS:NZ	1.70	1.06
2:B:53:VAL:CG1	3:C:985:LYS:CD	1.79	1.06
2:B:41:LEU:CG	6:F:217:LYS:HB3	1.85	1.05
1:A:67:LYS:HG3	6:F:269:TYR:CZ	1.91	1.05
3:C:968:LEU:CD2	8:H:296:PHE:CE2	2.33	1.05
2:B:41:LEU:CG	6:F:217:LYS:CB	2.34	1.05
2:B:50:TRP:CB	3:C:984:LEU:O	1.81	1.05
2:B:74:VAL:CG2	3:C:971:LEU:HD23	1.84	1.05
1:A:62:ASP:OD2	6:F:269:TYR:OH	1.75	1.05
2:B:57:PHE:CD2	3:C:982:GLU:OE2	2.09	1.04
1:A:17:CYS:SG	10:J:482:PRO:HG2	1.97	1.04
2:B:77:TRP:CZ3	4:D:852:ALA:N	2.26	1.04
2:B:50:TRP:NE1	3:C:982:GLU:C	1.94	1.04
7:G:248:PRO:HD3	9:I:417:LYS:HZ1	1.20	1.03
1:A:54:VAL:CB	6:F:297:ASN:OD1	2.06	1.03
1:A:73:GLU:HG3	2:B:36:TYR:HA	1.40	1.03
1:A:71:LYS:HZ2	6:F:279:PRO:CB	1.72	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LEU:CD2	6:F:217:LYS:CB	2.35	1.03
6:F:324:ALA:HB2	9:I:605:LYS:NZ	1.71	1.03
1:A:71:LYS:N	6:F:271:ASP:OD2	1.90	1.02
2:B:50:TRP:CZ3	3:C:986:PHE:HB3	1.93	1.02
7:G:248:PRO:HG3	9:I:417:LYS:HE2	1.40	1.02
2:B:41:LEU:N	6:F:214:GLU:CB	2.22	1.01
1:A:16:ALA:HB3	10:J:481:GLU:OE2	0.85	1.01
1:A:41:GLU:HA	10:J:461:GLU:OE2	1.05	1.01
1:A:17:CYS:CA	10:J:459:ARG:NE	2.01	1.00
1:A:69:LYS:HE3	6:F:282:VAL:C	1.81	1.00
8:H:322:GLY:HA2	8:H:325:ARG:HH12	1.27	1.00
2:B:41:LEU:CA	6:F:214:GLU:N	2.23	1.00
6:F:275:ILE:CG2	9:I:598:HIS:NE2	2.22	0.99
7:G:249:LEU:HB2	9:I:413:GLU:OE2	1.57	0.99
2:B:74:VAL:O	3:C:967:TRP:CE3	2.16	0.99
7:G:247:THR:HB	9:I:410:ASP:CB	1.90	0.99
2:B:53:VAL:HB	3:C:985:LYS:CB	1.92	0.99
2:B:77:TRP:C	3:C:967:TRP:HH2	1.64	0.99
2:B:46:GLY:H	2:B:47:LYS:HG3	0.82	0.99
8:H:319:LEU:CD1	11:K:757:MET:HE1	1.88	0.98
8:H:322:GLY:HA2	8:H:325:ARG:NH1	1.78	0.98
2:B:53:VAL:HB	3:C:985:LYS:HB3	1.02	0.98
8:H:319:LEU:CD1	11:K:757:MET:HE3	1.90	0.98
1:A:17:CYS:C	10:J:459:ARG:NE	2.17	0.98
1:A:58:LYS:NZ	6:F:298:THR:OG1	1.97	0.97
2:B:44:GLU:OE2	6:F:217:LYS:CE	2.10	0.97
2:B:66:LEU:HD21	3:C:978:ILE:HG21	1.43	0.97
2:B:74:VAL:HG12	3:C:967:TRP:HE3	0.81	0.97
1:A:71:LYS:CB	6:F:273:SER:CB	2.40	0.97
2:B:41:LEU:H	6:F:214:GLU:HB3	1.28	0.97
3:C:981:ASP:OD2	4:D:838:MET:SD	2.22	0.97
2:B:74:VAL:O	3:C:967:TRP:HZ3	1.41	0.97
2:B:77:TRP:CA	4:D:853:ALA:O	2.13	0.97
3:C:985:LYS:HG3	4:D:838:MET:HG2	1.43	0.97
3:C:985:LYS:HA	4:D:834:PHE:HE2	1.29	0.96
2:B:45:GLU:CB	2:B:47:LYS:CE	2.38	0.96
3:C:985:LYS:CG	4:D:838:MET:CE	2.43	0.96
4:D:839:ALA:HB1	5:E:99:ILE:HG23	1.46	0.96
1:A:13:THR:HB	10:J:461:GLU:OE1	1.66	0.96
2:B:40:GLU:C	6:F:214:GLU:CB	2.34	0.96
1:A:62:ASP:OD2	6:F:269:TYR:CE2	2.19	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:663:GLN:C	11:K:751:ARG:H	1.70	0.96
1:A:66:TYR:HA	10:J:486:GLU:HA	1.47	0.95
3:C:985:LYS:CD	4:D:838:MET:HG2	1.97	0.95
1:A:58:LYS:HG3	6:F:269:TYR:HB3	1.47	0.95
2:B:53:VAL:HG11	3:C:985:LYS:CE	1.96	0.95
3:C:985:LYS:N	4:D:838:MET:HE3	1.82	0.95
7:G:248:PRO:HD3	9:I:417:LYS:CE	1.96	0.95
5:E:115:ALA:C	6:F:217:LYS:HD3	1.85	0.95
2:B:70:CYS:O	3:C:971:LEU:HD22	1.66	0.95
2:B:77:TRP:CZ2	4:D:852:ALA:CB	2.50	0.94
1:A:62:ASP:OD2	6:F:269:TYR:CZ	2.20	0.94
7:G:248:PRO:CG	9:I:417:LYS:HE2	1.96	0.94
1:A:71:LYS:HZ1	6:F:279:PRO:HB3	1.16	0.94
2:B:41:LEU:HD23	6:F:217:LYS:CB	1.96	0.93
2:B:74:VAL:CG2	3:C:971:LEU:CD2	2.46	0.93
4:D:854:TRP:HB3	5:E:88:PHE:CZ	2.03	0.93
1:A:64:LEU:O	10:J:484:LYS:HA	1.67	0.93
3:C:968:LEU:HD21	8:H:296:PHE:HZ	1.18	0.93
3:C:985:LYS:N	4:D:838:MET:CE	2.31	0.93
3:C:985:LYS:HA	4:D:834:PHE:CE2	2.03	0.93
4:D:843:TYR:OH	5:E:92:PHE:CD2	2.19	0.93
1:A:14:CYS:N	10:J:459:ARG:CA	2.31	0.93
2:B:50:TRP:HE3	3:C:986:PHE:HB3	1.16	0.93
1:A:77:ILE:HD11	9:I:620:ILE:H	1.17	0.93
1:A:66:TYR:CD1	10:J:485:VAL:HB	2.04	0.92
1:A:77:ILE:HG21	2:B:39:ASN:HB2	1.14	0.92
2:B:39:ASN:HB2	9:I:620:ILE:HD13	1.46	0.92
2:B:73:PHE:HE1	4:D:846:ALA:O	1.51	0.92
1:A:77:ILE:HG23	2:B:39:ASN:HA	1.48	0.92
2:B:50:TRP:CD2	3:C:986:PHE:CB	2.35	0.92
3:C:967:TRP:CD1	8:H:293:ILE:HD11	2.05	0.92
2:B:77:TRP:CE3	4:D:850:GLY:O	2.23	0.92
3:C:981:ASP:O	4:D:838:MET:HE3	1.69	0.92
3:C:985:LYS:CD	4:D:838:MET:CG	2.48	0.92
4:D:843:TYR:CZ	5:E:92:PHE:HE2	1.89	0.91
2:B:54:ILE:HB	3:C:982:GLU:O	1.71	0.91
9:I:605:LYS:HA	9:I:608:GLN:HE21	1.35	0.90
1:A:71:LYS:HA	6:F:273:SER:HB3	0.90	0.90
2:B:50:TRP:HB2	3:C:984:LEU:O	1.08	0.90
4:D:839:ALA:HB1	5:E:99:ILE:HG21	1.48	0.90
2:B:39:ASN:HB2	9:I:620:ILE:CD1	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:TRP:C	4:D:853:ALA:O	2.10	0.90
9:I:660:ALA:O	11:K:749:GLU:N	2.04	0.90
1:A:58:LYS:HD3	6:F:269:TYR:H	1.37	0.90
1:A:41:GLU:OE1	10:J:462:HIS:CA	2.20	0.89
6:F:219:LEU:HB3	6:F:314:LEU:HD11	1.55	0.89
8:H:330:ASN:HB3	9:I:652:ARG:N	1.88	0.89
1:A:69:LYS:HE3	6:F:282:VAL:O	0.71	0.89
8:H:330:ASN:HD22	9:I:651:ILE:CG1	1.86	0.89
3:C:985:LYS:HG2	4:D:838:MET:CG	1.79	0.89
6:F:324:ALA:HB1	9:I:605:LYS:CD	2.03	0.89
1:A:41:GLU:OE1	10:J:462:HIS:HA	1.72	0.88
1:A:6:GLU:OE2	2:B:36:TYR:CZ	2.12	0.88
1:A:77:ILE:HG21	2:B:39:ASN:HB3	1.54	0.88
2:B:45:GLU:HB3	2:B:47:LYS:HE2	0.90	0.88
1:A:66:TYR:CD1	10:J:485:VAL:O	2.27	0.88
2:B:45:GLU:HB3	2:B:47:LYS:HE3	1.52	0.88
1:A:70:LEU:C	6:F:271:ASP:CG	2.30	0.88
5:E:90:GLU:HB3	5:E:91:PRO:HD3	1.55	0.88
8:H:330:ASN:CB	9:I:652:ARG:H	1.87	0.88
1:A:66:TYR:CA	10:J:485:VAL:O	2.21	0.88
2:B:74:VAL:HG21	3:C:971:LEU:CD2	2.05	0.87
1:A:13:THR:O	10:J:460:SER:O	1.72	0.87
2:B:54:ILE:HA	3:C:982:GLU:OE1	1.75	0.87
2:B:77:TRP:HA	4:D:853:ALA:O	1.74	0.87
2:B:57:PHE:HD2	3:C:982:GLU:OE2	1.53	0.87
1:A:17:CYS:C	10:J:459:ARG:HE	1.79	0.86
3:C:985:LYS:CG	4:D:838:MET:HE2	2.04	0.86
1:A:71:LYS:HB2	6:F:279:PRO:HA	0.88	0.86
2:B:39:ASN:O	9:I:645:SER:HA	1.74	0.86
9:I:663:GLN:O	11:K:751:ARG:CB	2.24	0.86
2:B:51:GLU:OE2	3:C:986:PHE:CE1	2.28	0.86
4:D:835:PHE:HZ	5:E:102:ALA:O	1.52	0.86
6:F:276:SER:O	9:I:597:PRO:CG	2.24	0.86
2:B:77:TRP:HH2	4:D:852:ALA:HB3	0.69	0.86
8:H:331:ALA:HA	9:I:650:LEU:CA	1.89	0.85
1:A:71:LYS:HD3	6:F:279:PRO:N	1.92	0.85
6:F:324:ALA:HB2	9:I:605:LYS:HZ3	1.41	0.85
7:G:247:THR:CB	9:I:410:ASP:OD2	2.09	0.85
2:B:50:TRP:HE1	3:C:982:GLU:C	1.76	0.85
4:D:843:TYR:CZ	5:E:92:PHE:CD2	2.64	0.85
2:B:77:TRP:C	3:C:967:TRP:CH2	2.50	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:HD3	6:F:279:PRO:CA	2.07	0.85
6:F:276:SER:O	9:I:597:PRO:HG3	1.77	0.85
2:B:70:CYS:O	3:C:975:LEU:HD11	1.75	0.84
3:C:985:LYS:HG2	4:D:838:MET:HG2	0.84	0.84
8:H:326:MET:HE1	9:I:412:LEU:HD21	1.58	0.84
3:C:985:LYS:HE3	4:D:838:MET:HG3	0.86	0.84
4:D:835:PHE:CD2	5:E:106:VAL:CG1	2.61	0.84
8:H:330:ASN:HB2	9:I:657:ASP:OD1	1.78	0.84
1:A:68:LEU:HG	6:F:281:PRO:HG3	1.59	0.84
1:A:14:CYS:H	10:J:459:ARG:HA	1.38	0.84
1:A:71:LYS:CA	6:F:271:ASP:OD2	2.24	0.84
8:H:332:ILE:HB	9:I:649:VAL:CB	2.06	0.84
1:A:13:THR:HG21	10:J:462:HIS:H	1.39	0.83
9:I:663:GLN:O	11:K:751:ARG:HB2	1.78	0.83
4:D:843:TYR:OH	5:E:92:PHE:CE2	2.31	0.83
10:J:470:LYS:O	10:J:474:GLU:HG3	1.77	0.83
2:B:51:GLU:OE2	3:C:986:PHE:HE1	1.59	0.83
6:F:275:ILE:CG2	9:I:598:HIS:CE1	2.60	0.83
1:A:74:GLN:HG2	2:B:36:TYR:N	1.94	0.82
2:B:41:LEU:CG	6:F:217:LYS:HB2	2.04	0.82
4:D:832:TRP:CZ3	5:E:106:VAL:C	2.53	0.82
2:B:77:TRP:HE3	4:D:850:GLY:O	1.63	0.82
8:H:319:LEU:HD12	11:K:757:MET:HE3	1.59	0.82
2:B:41:LEU:HD22	5:E:115:ALA:HB1	1.59	0.82
2:B:77:TRP:HA	4:D:853:ALA:C	2.01	0.82
1:A:6:GLU:OE2	2:B:36:TYR:CE1	2.32	0.81
6:F:324:ALA:CB	9:I:605:LYS:HD2	2.07	0.81
3:C:981:ASP:CG	4:D:838:MET:SD	2.59	0.81
6:F:276:SER:HA	9:I:598:HIS:CD2	2.15	0.81
8:H:331:ALA:CA	9:I:650:LEU:HA	2.06	0.81
1:A:70:LEU:O	6:F:271:ASP:HA	1.81	0.81
1:A:58:LYS:NZ	6:F:298:THR:CB	2.44	0.81
5:E:115:ALA:C	6:F:217:LYS:CD	2.49	0.81
3:C:985:LYS:HE2	4:D:838:MET:CG	2.07	0.81
1:A:12:MET:C	10:J:460:SER:OG	2.17	0.80
1:A:14:CYS:SG	10:J:458:ARG:HB3	2.22	0.80
1:A:66:TYR:N	10:J:485:VAL:O	2.13	0.80
1:A:66:TYR:CG	10:J:485:VAL:O	2.34	0.80
1:A:58:LYS:HB3	6:F:298:THR:HG21	0.81	0.80
1:A:12:MET:CG	10:J:459:ARG:CB	2.59	0.80
1:A:53:SER:OG	6:F:253:PRO:HB3	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:843:TYR:OH	5:E:92:PHE:HD2	1.64	0.80
1:A:54:VAL:HB	6:F:297:ASN:OD1	1.77	0.80
1:A:77:ILE:CB	2:B:39:ASN:HB2	2.11	0.80
2:B:77:TRP:HB3	3:C:967:TRP:HZ3	1.45	0.80
2:B:54:ILE:HG21	3:C:986:PHE:CD1	2.17	0.79
6:F:275:ILE:HG22	9:I:598:HIS:CD2	2.16	0.79
1:A:17:CYS:SG	10:J:482:PRO:CG	2.69	0.79
1:A:39:ALA:C	10:J:461:GLU:CB	2.48	0.79
1:A:58:LYS:CD	6:F:269:TYR:N	2.46	0.79
1:A:68:LEU:HG	6:F:281:PRO:CG	2.12	0.78
1:A:71:LYS:C	6:F:271:ASP:OD2	2.22	0.78
9:I:596:LEU:H	9:I:599:GLN:NE2	1.81	0.78
4:D:832:TRP:HZ3	5:E:106:VAL:C	1.87	0.78
1:A:77:ILE:HG22	2:B:39:ASN:H	0.95	0.78
3:C:985:LYS:HE2	4:D:838:MET:HG3	1.55	0.78
6:F:276:SER:HB2	6:F:278:GLU:OE1	1.84	0.78
6:F:275:ILE:HG23	9:I:598:HIS:CE1	2.19	0.77
2:B:40:GLU:CA	6:F:214:GLU:CB	2.62	0.77
2:B:77:TRP:CZ2	4:D:852:ALA:HB3	2.14	0.77
4:D:840:ILE:O	4:D:844:VAL:HG13	1.84	0.77
1:A:53:SER:OG	6:F:253:PRO:CB	2.33	0.77
1:A:71:LYS:CG	6:F:273:SER:HB3	1.98	0.77
2:B:53:VAL:CB	3:C:985:LYS:CB	2.59	0.77
2:B:44:GLU:OE2	6:F:217:LYS:NZ	2.16	0.77
2:B:54:ILE:CG2	3:C:986:PHE:HD1	1.96	0.77
10:J:458:ARG:HD3	10:J:479:LEU:HD13	1.65	0.77
1:A:77:ILE:HD13	2:B:39:ASN:HB2	1.67	0.77
2:B:41:LEU:HD21	6:F:217:LYS:HB2	1.62	0.77
6:F:324:ALA:HB2	9:I:605:LYS:HZ2	1.46	0.76
2:B:77:TRP:CH2	4:D:852:ALA:N	2.34	0.76
4:D:832:TRP:HE3	5:E:106:VAL:O	1.67	0.76
8:H:326:MET:HE1	8:H:333:VAL:HG21	1.67	0.76
11:K:759:GLN:HE22	11:K:762:ARG:HH11	1.33	0.76
1:A:58:LYS:CD	6:F:269:TYR:H	1.97	0.76
8:H:330:ASN:HD22	9:I:651:ILE:HG13	1.49	0.76
9:I:663:GLN:O	11:K:751:ARG:CA	2.33	0.76
1:A:77:ILE:CG1	2:B:39:ASN:HB2	2.16	0.76
1:A:71:LYS:HZ2	6:F:279:PRO:HB3	0.93	0.76
2:B:40:GLU:O	6:F:214:GLU:N	2.19	0.76
8:H:319:LEU:HB3	8:H:336:LEU:HD12	1.69	0.75
11:K:757:MET:HA	11:K:760:PHE:CE2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:HG3	6:F:269:TYR:CE1	2.21	0.75
7:G:247:THR:CG2	9:I:410:ASP:OD1	2.24	0.75
9:I:595:VAL:HA	9:I:599:GLN:HE21	1.52	0.75
2:B:53:VAL:CG2	3:C:985:LYS:HB3	2.16	0.75
1:A:41:GLU:CD	10:J:462:HIS:H	1.89	0.74
3:C:985:LYS:CA	4:D:838:MET:HE2	2.16	0.74
2:B:50:TRP:NE1	3:C:982:GLU:O	2.10	0.74
2:B:66:LEU:HD11	3:C:978:ILE:HD13	1.69	0.74
1:A:70:LEU:HB2	6:F:297:ASN:HD21	1.51	0.74
2:B:41:LEU:HD22	5:E:115:ALA:CB	2.18	0.74
1:A:71:LYS:HZ1	6:F:279:PRO:CB	1.87	0.74
2:B:40:GLU:C	6:F:214:GLU:N	2.41	0.74
1:A:77:ILE:HG23	2:B:39:ASN:HB2	1.22	0.73
1:A:77:ILE:HD13	2:B:39:ASN:CB	2.18	0.73
8:H:330:ASN:ND2	9:I:651:ILE:HG13	2.02	0.73
1:A:54:VAL:O	6:F:297:ASN:HB3	1.87	0.73
9:I:663:GLN:C	11:K:749:GLU:N	2.42	0.73
4:D:832:TRP:CE3	5:E:106:VAL:O	2.42	0.73
1:A:9:ILE:CA	6:F:280:VAL:CG1	2.62	0.73
5:E:95:LEU:HD23	5:E:95:LEU:O	1.87	0.73
8:H:331:ALA:HA	9:I:650:LEU:HA	1.55	0.73
1:A:14:CYS:CA	10:J:459:ARG:HA	2.05	0.73
2:B:40:GLU:CA	6:F:214:GLU:HB3	2.18	0.73
2:B:44:GLU:CD	6:F:217:LYS:HZ1	1.91	0.72
2:B:74:VAL:CG1	3:C:967:TRP:CE3	2.50	0.72
2:B:74:VAL:HB	3:C:971:LEU:HD21	1.71	0.72
2:B:53:VAL:CB	3:C:985:LYS:HD3	2.08	0.72
2:B:40:GLU:CA	6:F:214:GLU:HB2	2.20	0.72
4:D:839:ALA:CB	5:E:99:ILE:HG23	2.19	0.72
7:G:247:THR:HG22	9:I:410:ASP:CB	2.11	0.72
10:J:454:ALA:O	10:J:458:ARG:HG2	1.89	0.72
1:A:17:CYS:O	10:J:459:ARG:NH1	2.23	0.71
1:A:17:CYS:SG	10:J:482:PRO:HD2	2.30	0.71
8:H:326:MET:CE	8:H:333:VAL:HG21	2.19	0.71
3:C:967:TRP:NE1	8:H:293:ILE:HD11	2.04	0.71
4:D:846:ALA:HB3	5:E:95:LEU:CD1	2.20	0.71
1:A:58:LYS:HD3	6:F:269:TYR:N	2.04	0.71
10:J:490:GLY:O	10:J:504:ARG:NH2	2.23	0.71
4:D:835:PHE:CE1	5:E:106:VAL:HB	2.25	0.70
9:I:595:VAL:HG13	9:I:599:GLN:HG3	1.73	0.70
9:I:431:LYS:HE2	9:I:551:LYS:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:764:LEU:HD21	12:L:804:ALA:HB2	1.74	0.70
1:A:12:MET:CG	10:J:459:ARG:HB3	2.20	0.70
7:G:247:THR:HG22	9:I:410:ASP:CG	1.92	0.70
7:G:248:PRO:CD	9:I:417:LYS:CE	2.69	0.70
2:B:54:ILE:HG21	3:C:986:PHE:HB2	1.73	0.70
2:B:74:VAL:HG11	3:C:970:VAL:HB	1.73	0.70
1:A:12:MET:CG	10:J:459:ARG:HB2	2.21	0.69
1:A:41:GLU:CD	10:J:462:HIS:CA	2.60	0.69
1:A:74:GLN:C	2:B:36:TYR:N	2.45	0.69
2:B:53:VAL:HG22	4:D:835:PHE:HD1	1.57	0.69
4:D:835:PHE:CE2	5:E:106:VAL:CG1	2.75	0.69
6:F:276:SER:O	9:I:597:PRO:HG2	1.91	0.69
7:G:266:LEU:HD13	7:G:266:LEU:O	1.92	0.69
1:A:10:GLU:CD	10:J:489:ALA:HB2	2.12	0.69
1:A:17:CYS:HA	10:J:459:ARG:NE	2.04	0.69
1:A:39:ALA:O	10:J:461:GLU:CB	2.37	0.69
1:A:62:ASP:HB2	6:F:269:TYR:HE2	1.56	0.69
1:A:66:TYR:HD1	10:J:485:VAL:O	1.73	0.69
5:E:114:ASN:OD1	6:F:217:LYS:NZ	2.24	0.69
1:A:10:GLU:OE1	10:J:489:ALA:HB3	1.90	0.69
1:A:58:LYS:HD2	6:F:269:TYR:N	2.08	0.68
2:B:51:GLU:N	3:C:986:PHE:O	2.27	0.68
6:F:324:ALA:CB	9:I:605:LYS:CD	2.67	0.68
9:I:652:ARG:HD3	9:I:657:ASP:OD1	1.94	0.68
11:K:759:GLN:HE22	11:K:762:ARG:NH1	1.90	0.68
1:A:7:PHE:CE2	1:A:57:LEU:HD11	2.28	0.68
1:A:58:LYS:HZ2	6:F:298:THR:CB	2.02	0.68
3:C:979:GLY:O	3:C:983:ILE:HG13	1.93	0.68
1:A:10:GLU:N	6:F:280:VAL:HG11	2.08	0.68
1:A:68:LEU:O	6:F:269:TYR:CG	2.46	0.68
2:B:73:PHE:CZ	4:D:846:ALA:O	2.47	0.68
7:G:248:PRO:CD	9:I:417:LYS:NZ	2.54	0.68
1:A:58:LYS:CB	6:F:298:THR:HG23	2.01	0.68
1:A:41:GLU:OE2	10:J:462:HIS:N	2.23	0.68
5:E:115:ALA:O	6:F:217:LYS:HD3	1.93	0.68
1:A:77:ILE:CD1	2:B:39:ASN:HB2	2.24	0.67
1:A:62:ASP:OD2	6:F:269:TYR:HE2	1.78	0.67
3:C:985:LYS:CA	4:D:838:MET:CE	2.72	0.67
4:D:833:LEU:HD11	4:D:837:TYR:CE2	2.28	0.67
8:H:330:ASN:HD22	9:I:651:ILE:HG12	1.59	0.67
12:L:801:GLY:O	12:L:805:THR:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:CYS:SG	10:J:482:PRO:CD	2.83	0.67
1:A:77:ILE:CD1	9:I:619:GLY:C	2.61	0.67
1:A:53:SER:HG	6:F:253:PRO:HB3	1.55	0.67
1:A:58:LYS:CA	6:F:298:THR:HG21	2.24	0.67
2:B:74:VAL:HG22	3:C:970:VAL:CG1	2.25	0.67
6:F:320:LEU:HD21	9:I:602:GLU:OE1	1.94	0.67
1:A:12:MET:CB	10:J:459:ARG:C	2.59	0.67
2:B:77:TRP:HZ3	4:D:852:ALA:N	1.89	0.67
2:B:50:TRP:HE1	3:C:981:ASP:C	1.94	0.66
7:G:247:THR:CB	9:I:410:ASP:HB2	2.22	0.66
8:H:333:VAL:HG22	9:I:648:ILE:HG23	1.78	0.66
2:B:41:LEU:N	6:F:214:GLU:N	2.41	0.66
1:A:9:ILE:HA	6:F:280:VAL:HG13	1.75	0.66
4:D:835:PHE:CE2	5:E:102:ALA:C	2.67	0.66
7:G:247:THR:OG1	9:I:413:GLU:CB	2.44	0.66
2:B:54:ILE:CG2	3:C:986:PHE:CD1	2.76	0.66
8:H:322:GLY:CA	8:H:325:ARG:HH12	2.06	0.66
7:G:248:PRO:CD	9:I:417:LYS:HE2	2.25	0.66
10:J:461:GLU:CD	10:J:461:GLU:H	1.98	0.66
1:A:71:LYS:HD3	6:F:279:PRO:HA	1.77	0.66
2:B:40:GLU:HA	6:F:214:GLU:CB	2.26	0.66
1:A:58:LYS:HD3	6:F:298:THR:OG1	1.96	0.65
1:A:62:ASP:HB2	6:F:269:TYR:CE2	2.30	0.65
2:B:39:ASN:OD1	9:I:623:ALA:HB2	1.96	0.65
4:D:846:ALA:CB	5:E:95:LEU:CD1	2.74	0.65
1:A:7:PHE:HB3	6:F:281:PRO:HD3	1.79	0.65
1:A:67:LYS:CD	6:F:269:TYR:OH	2.44	0.65
2:B:77:TRP:CZ3	4:D:850:GLY:C	2.70	0.65
1:A:9:ILE:HA	6:F:280:VAL:CG1	2.25	0.65
1:A:9:ILE:C	6:F:280:VAL:HG21	1.90	0.65
1:A:77:ILE:HD11	9:I:619:GLY:C	2.08	0.65
9:I:410:ASP:HB2	9:I:413:GLU:HB2	1.77	0.65
1:A:69:LYS:CD	6:F:269:TYR:CA	2.71	0.65
11:K:749:GLU:O	11:K:753:ILE:HG12	1.97	0.65
8:H:308:PRO:HG3	11:K:768:ASN:CG	2.17	0.64
10:J:458:ARG:NH1	10:J:469:VAL:HG13	2.12	0.64
1:A:54:VAL:O	6:F:298:THR:CG2	2.45	0.64
1:A:12:MET:HB2	10:J:459:ARG:HB2	1.79	0.64
1:A:12:MET:HB2	10:J:459:ARG:C	2.16	0.64
1:A:14:CYS:N	10:J:459:ARG:C	2.42	0.64
1:A:58:LYS:HZ3	6:F:298:THR:CB	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:HD2	6:F:269:TYR:CA	2.01	0.64
2:B:53:VAL:HG22	4:D:835:PHE:CD1	2.33	0.64
9:I:431:LYS:HD3	9:I:551:LYS:HG2	1.80	0.64
1:A:17:CYS:O	10:J:459:ARG:CZ	2.45	0.63
1:A:28:ILE:HD11	1:A:57:LEU:HB3	1.80	0.63
2:B:45:GLU:CB	2:B:47:LYS:HE3	2.18	0.63
1:A:69:LYS:HD3	6:F:269:TYR:HB3	1.79	0.63
1:A:71:LYS:N	6:F:271:ASP:CG	2.49	0.63
4:D:834:PHE:HE2	4:D:838:MET:HE2	1.61	0.63
4:D:835:PHE:CZ	5:E:102:ALA:C	2.70	0.63
10:J:502:ASN:ND2	10:J:504:ARG:HB2	2.14	0.63
10:J:502:ASN:HD22	10:J:505:LEU:H	1.47	0.63
4:D:843:TYR:CE1	5:E:92:PHE:CD2	2.86	0.63
4:D:843:TYR:CE2	5:E:92:PHE:HE2	2.17	0.62
1:A:39:ALA:O	10:J:461:GLU:O	2.16	0.62
2:B:77:TRP:CZ3	4:D:851:ALA:C	2.72	0.62
12:L:795:VAL:HA	12:L:799:THR:OG1	2.00	0.62
1:A:54:VAL:C	6:F:297:ASN:CB	2.43	0.62
1:A:66:TYR:CA	10:J:486:GLU:HA	2.26	0.62
1:A:69:LYS:CD	6:F:269:TYR:HB3	2.29	0.62
2:B:70:CYS:C	3:C:975:LEU:HD11	2.19	0.62
2:B:50:TRP:CE3	3:C:986:PHE:CA	2.75	0.62
2:B:54:ILE:CG2	3:C:986:PHE:HB2	2.30	0.62
3:C:984:LEU:HA	3:C:987:ILE:HG12	1.80	0.62
4:D:843:TYR:HA	5:E:95:LEU:HD21	1.82	0.61
8:H:324:ARG:HG3	8:H:325:ARG:N	2.14	0.61
2:B:57:PHE:HD2	3:C:982:GLU:CD	2.03	0.61
2:B:77:TRP:CZ3	4:D:850:GLY:O	2.54	0.61
1:A:41:GLU:N	10:J:461:GLU:CB	2.58	0.61
8:H:306:ALA:HB2	11:K:772:VAL:CG2	2.31	0.61
2:B:76:ALA:O	4:D:854:TRP:HA	2.01	0.61
1:A:12:MET:CB	10:J:459:ARG:HB2	2.31	0.61
2:B:77:TRP:CA	4:D:853:ALA:C	2.61	0.61
9:I:557:ALA:O	9:I:561:LEU:HD22	2.01	0.60
1:A:9:ILE:O	6:F:280:VAL:HG21	2.00	0.60
2:B:74:VAL:CG2	3:C:971:LEU:HD21	2.31	0.60
1:A:54:VAL:O	6:F:298:THR:HG22	2.02	0.60
2:B:46:GLY:CA	2:B:47:LYS:HG3	2.31	0.60
8:H:299:ALA:C	8:H:301:ALA:H	2.04	0.60
9:I:422:ILE:HG21	9:I:571:ILE:HG13	1.81	0.60
2:B:74:VAL:HG23	3:C:971:LEU:CD2	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:832:TRP:CE3	5:E:106:VAL:C	2.75	0.60
2:B:44:GLU:OE1	5:E:114:ASN:HB3	2.01	0.60
4:D:832:TRP:CZ3	5:E:107:TRP:N	2.70	0.60
2:B:53:VAL:CG1	3:C:985:LYS:CE	2.67	0.60
1:A:12:MET:HA	10:J:460:SER:HG	1.56	0.59
2:B:41:LEU:CD2	5:E:115:ALA:C	2.71	0.59
3:C:985:LYS:HA	4:D:838:MET:HE2	1.83	0.59
7:G:247:THR:OG1	9:I:413:GLU:HB3	2.03	0.59
1:A:41:GLU:CG	10:J:461:GLU:C	2.67	0.59
11:K:757:MET:O	11:K:761:ILE:HG13	2.03	0.59
1:A:9:ILE:C	6:F:280:VAL:HG11	2.21	0.59
1:A:77:ILE:HG22	2:B:38:HIS:C	2.20	0.59
1:A:8:ASP:O	6:F:281:PRO:HD2	2.03	0.59
9:I:431:LYS:HE2	9:I:551:LYS:CB	2.33	0.59
2:B:51:GLU:HA	3:C:986:PHE:HD1	1.59	0.58
9:I:421:VAL:HG23	9:I:566:ILE:HG21	1.84	0.58
2:B:71:ILE:HA	3:C:971:LEU:CD1	2.32	0.58
2:B:77:TRP:HZ3	4:D:850:GLY:C	2.06	0.58
1:A:17:CYS:SG	10:J:482:PRO:O	2.61	0.58
1:A:55:SER:HB2	6:F:253:PRO:HB3	1.85	0.58
1:A:71:LYS:HZ1	6:F:279:PRO:CG	2.15	0.58
2:B:77:TRP:HA	4:D:854:TRP:HA	1.86	0.58
2:B:52:LEU:HB3	5:E:106:VAL:HG23	1.86	0.58
10:J:434:PRO:HG3	10:J:463:PRO:HB2	1.85	0.58
8:H:332:ILE:HD11	9:I:651:ILE:CG2	2.34	0.57
1:A:66:TYR:HB3	10:J:485:VAL:C	2.17	0.57
2:B:74:VAL:CB	3:C:971:LEU:HD21	2.34	0.57
8:H:329:LYS:O	8:H:330:ASN:HB2	2.04	0.57
3:C:968:LEU:CD2	8:H:296:PHE:HZ	1.85	0.57
4:D:832:TRP:HE3	5:E:106:VAL:HG13	1.49	0.57
1:A:70:LEU:O	6:F:271:ASP:OD2	2.20	0.57
1:A:71:LYS:CD	6:F:279:PRO:HA	2.34	0.57
2:B:61:LEU:HD21	7:G:260:LEU:HD23	1.86	0.57
10:J:458:ARG:CD	10:J:479:LEU:HD13	2.34	0.57
11:K:756:ASN:O	11:K:757:MET:C	2.42	0.57
2:B:66:LEU:HD21	3:C:978:ILE:HD13	1.87	0.57
1:A:77:ILE:O	2:B:36:TYR:C	2.43	0.57
9:I:550:LEU:N	10:J:432:GLY:N	2.52	0.57
4:D:846:ALA:HB3	5:E:95:LEU:HD13	1.86	0.57
9:I:596:LEU:H	9:I:599:GLN:HE21	1.51	0.57
10:J:502:ASN:HD21	10:J:504:ARG:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:985:LYS:HG3	4:D:838:MET:HE3	1.79	0.56
6:F:218:LYS:O	6:F:222:LEU:HG	2.05	0.56
2:B:74:VAL:HG22	3:C:970:VAL:HG12	1.87	0.56
1:A:69:LYS:HD3	6:F:269:TYR:CB	2.35	0.56
2:B:77:TRP:CH2	4:D:849:VAL:O	2.53	0.56
2:B:77:TRP:HB3	3:C:967:TRP:CZ3	2.35	0.56
8:H:311:LEU:C	8:H:313:ALA:H	2.08	0.56
4:D:835:PHE:CE2	5:E:106:VAL:HG11	2.32	0.56
1:A:53:SER:OG	6:F:253:PRO:HB2	2.04	0.56
2:B:41:LEU:HB2	6:F:214:GLU:OE2	2.04	0.56
2:B:50:TRP:CD1	3:C:981:ASP:O	2.58	0.56
4:D:832:TRP:HZ3	5:E:106:VAL:CG1	2.06	0.56
6:F:214:GLU:OE1	6:F:215:ALA:HB3	2.05	0.56
1:A:73:GLU:HG3	2:B:36:TYR:HD2	1.70	0.56
2:B:41:LEU:CB	6:F:217:LYS:HB3	2.35	0.56
1:A:12:MET:CA	10:J:485:VAL:HG11	2.34	0.56
7:G:247:THR:CB	9:I:410:ASP:OD1	2.43	0.56
11:K:760:PHE:CD1	11:K:760:PHE:C	2.79	0.56
1:A:14:CYS:H	10:J:459:ARG:CA	2.09	0.56
4:D:832:TRP:HZ3	5:E:107:TRP:N	2.03	0.56
1:A:9:ILE:CA	6:F:280:VAL:HG11	2.35	0.55
9:I:604:VAL:O	9:I:608:GLN:HG3	2.05	0.55
3:C:984:LEU:HB2	4:D:838:MET:HE1	1.87	0.55
8:H:333:VAL:HA	9:I:648:ILE:HA	1.88	0.55
1:A:17:CYS:HA	10:J:459:ARG:CZ	2.37	0.55
2:B:41:LEU:HD23	5:E:115:ALA:C	2.27	0.55
2:B:71:ILE:HA	3:C:971:LEU:HD11	1.88	0.55
4:D:835:PHE:CE2	5:E:106:VAL:HG12	2.40	0.55
1:A:17:CYS:CA	10:J:459:ARG:CZ	2.79	0.55
1:A:71:LYS:NZ	6:F:279:PRO:CG	2.70	0.55
4:D:854:TRP:CB	5:E:88:PHE:CZ	2.85	0.55
2:B:70:CYS:O	3:C:975:LEU:CD1	2.51	0.55
4:D:835:PHE:CD1	5:E:106:VAL:HG21	2.41	0.55
9:I:431:LYS:CD	9:I:551:LYS:HG2	2.36	0.55
10:J:446:GLU:O	10:J:449:LEU:HB3	2.07	0.55
4:D:832:TRP:CH2	5:E:106:VAL:HG12	2.41	0.55
9:I:431:LYS:HE2	9:I:551:LYS:CA	2.35	0.55
2:B:65:LEU:CD2	8:H:307:ILE:HD12	2.36	0.54
3:C:968:LEU:O	3:C:972:LYS:HG2	2.07	0.54
2:B:50:TRP:CZ2	3:C:983:ILE:CG1	2.68	0.54
1:A:17:CYS:O	10:J:459:ARG:NE	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:O	2:B:37:GLY:N	2.40	0.54
2:B:44:GLU:CD	6:F:217:LYS:CE	2.64	0.54
4:D:854:TRP:CB	5:E:88:PHE:CE1	2.90	0.54
10:J:502:ASN:ND2	10:J:505:LEU:H	2.04	0.54
2:B:51:GLU:CA	3:C:986:PHE:CD1	2.79	0.54
12:L:800:ASP:C	12:L:803:PRO:HD2	2.27	0.54
3:C:968:LEU:HD23	8:H:296:PHE:CE2	2.38	0.54
9:I:424:ASP:O	9:I:428:THR:HB	2.08	0.54
1:A:73:GLU:CG	2:B:36:TYR:HA	2.27	0.54
2:B:51:GLU:OE1	3:C:986:PHE:HD1	1.84	0.54
9:I:410:ASP:OD2	9:I:414:VAL:HG23	2.08	0.54
2:B:40:GLU:HA	6:F:214:GLU:HB2	1.85	0.54
2:B:77:TRP:CE3	4:D:849:VAL:O	2.57	0.54
10:J:499:LEU:HB3	10:J:506:MSE:HE1	1.89	0.54
10:J:454:ALA:O	10:J:458:ARG:CD	2.55	0.54
1:A:6:GLU:CG	2:B:36:TYR:CZ	2.63	0.53
7:G:248:PRO:CG	9:I:417:LYS:CE	2.81	0.53
1:A:54:VAL:CG1	6:F:297:ASN:OD1	2.56	0.53
1:A:62:ASP:CG	6:F:269:TYR:OH	2.44	0.53
1:A:71:LYS:HG3	6:F:273:SER:HB2	0.57	0.53
5:E:104:VAL:HG12	5:E:104:VAL:O	2.08	0.53
5:E:103:ILE:C	5:E:105:GLY:H	2.11	0.53
3:C:974:SER:C	3:C:976:PRO:HD2	2.29	0.53
6:F:276:SER:CB	6:F:278:GLU:OE1	2.56	0.53
10:J:455:ILE:O	10:J:458:ARG:HG2	2.09	0.53
11:K:754:TYR:HA	11:K:757:MET:HB3	1.90	0.53
12:L:804:ALA:O	12:L:807:LEU:HB2	2.08	0.53
1:A:10:GLU:OE1	10:J:489:ALA:N	2.41	0.53
1:A:20:ARG:HB3	10:J:459:ARG:NH1	2.24	0.53
7:G:275:ASN:N	7:G:275:ASN:HD22	2.06	0.53
9:I:623:ALA:N	9:I:624:PRO:HD2	2.24	0.53
4:D:843:TYR:CE1	5:E:92:PHE:CE2	2.96	0.52
9:I:419:THR:OG1	9:I:611:GLU:HB3	2.09	0.52
1:A:41:GLU:CG	10:J:462:HIS:N	2.71	0.52
7:G:248:PRO:CD	9:I:417:LYS:HZ1	2.06	0.52
10:J:473:LEU:CD1	10:J:473:LEU:N	2.71	0.52
1:A:62:ASP:CB	6:F:269:TYR:HE2	2.20	0.52
2:B:39:ASN:CG	9:I:620:ILE:HA	2.29	0.52
2:B:77:TRP:HA	4:D:854:TRP:CA	2.39	0.52
9:I:560:GLU:CG	9:I:659:VAL:HG11	2.39	0.52
9:I:663:GLN:HB3	11:K:749:GLU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:758:LYS:HG2	11:K:759:GLN:N	2.23	0.52
1:A:12:MET:HB3	10:J:485:VAL:CB	2.32	0.52
1:A:74:GLN:CA	2:B:36:TYR:CE2	2.92	0.52
1:A:69:LYS:CD	6:F:269:TYR:CB	2.87	0.52
2:B:74:VAL:HG22	3:C:970:VAL:HG11	1.91	0.52
9:I:422:ILE:CG2	9:I:571:ILE:HG13	2.39	0.52
2:B:77:TRP:CE3	4:D:850:GLY:C	2.82	0.52
8:H:311:LEU:N	8:H:312:PRO:HD2	2.25	0.52
10:J:454:ALA:O	10:J:458:ARG:CG	2.56	0.52
3:C:985:LYS:CB	4:D:838:MET:CE	2.87	0.52
4:D:843:TYR:CE2	5:E:92:PHE:CE2	2.93	0.52
2:B:40:GLU:HA	6:F:214:GLU:HB3	1.90	0.52
2:B:41:LEU:HG	6:F:217:LYS:CA	2.39	0.52
4:D:846:ALA:HB3	5:E:95:LEU:HD11	1.92	0.52
10:J:486:GLU:HB3	10:J:494:VAL:HB	1.91	0.52
2:B:70:CYS:HB3	3:C:975:LEU:CD1	1.79	0.52
8:H:310:GLY:O	8:H:314:VAL:HG23	2.09	0.52
1:A:71:LYS:CE	6:F:279:PRO:HG3	2.40	0.51
2:B:41:LEU:HD23	6:F:217:LYS:HD2	1.92	0.51
9:I:558:VAL:O	9:I:562:LYS:HG3	2.10	0.51
4:D:854:TRP:HB3	5:E:88:PHE:CE2	2.44	0.51
2:B:39:ASN:HB3	9:I:645:SER:OG	2.11	0.51
3:C:986:PHE:C	3:C:988:ALA:N	2.63	0.51
8:H:294:TYR:O	8:H:298:ILE:HG23	2.11	0.51
1:A:58:LYS:NZ	6:F:298:THR:HB	2.26	0.51
9:I:633:ILE:CD1	9:I:662:ILE:HD11	2.41	0.51
1:A:71:LYS:HE3	6:F:279:PRO:HG3	1.93	0.51
1:A:73:GLU:CG	2:B:36:TYR:HD2	2.23	0.51
2:B:59:ASP:O	2:B:62:VAL:HG12	2.10	0.51
2:B:66:LEU:CD2	3:C:978:ILE:HG21	2.30	0.51
3:C:974:SER:O	3:C:976:PRO:N	2.44	0.51
1:A:12:MET:HB2	10:J:459:ARG:CB	2.40	0.50
2:B:41:LEU:HB2	5:E:115:ALA:HB1	1.93	0.50
2:B:77:TRP:HZ3	4:D:849:VAL:O	1.81	0.50
11:K:766:SER:O	11:K:769:VAL:HB	2.10	0.50
2:B:56:GLN:HA	2:B:56:GLN:NE2	2.25	0.50
4:D:834:PHE:CE2	4:D:838:MET:HE2	2.44	0.50
5:E:115:ALA:C	6:F:217:LYS:HD2	2.30	0.50
8:H:308:PRO:HG3	11:K:768:ASN:OD1	2.11	0.50
2:B:74:VAL:CG2	3:C:970:VAL:CG1	2.89	0.50
8:H:330:ASN:ND2	9:I:651:ILE:CG1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:443:ASN:HD22	10:J:541:GLU:CD	2.15	0.50
12:L:795:VAL:O	12:L:800:ASP:HB2	2.11	0.50
1:A:54:VAL:O	6:F:298:THR:HG23	2.10	0.50
4:D:835:PHE:HE2	5:E:102:ALA:C	2.15	0.50
9:I:410:ASP:HB2	9:I:413:GLU:CB	2.41	0.50
4:D:835:PHE:CE2	5:E:103:ILE:HA	2.47	0.50
4:D:836:ARG:O	4:D:840:ILE:HG12	2.12	0.50
1:A:68:LEU:O	6:F:269:TYR:HD1	1.78	0.50
10:J:497:GLY:O	10:J:536:ARG:HA	2.10	0.50
2:B:41:LEU:HD23	6:F:217:LYS:CD	2.42	0.50
8:H:325:ARG:HH11	8:H:325:ARG:HB3	1.77	0.50
8:H:330:ASN:CB	9:I:657:ASP:OD1	2.54	0.50
1:A:12:MET:HB3	10:J:485:VAL:HG11	0.67	0.50
1:A:74:GLN:C	2:B:36:TYR:CE2	2.74	0.50
3:C:977:VAL:O	3:C:980:LEU:HB3	2.12	0.50
9:I:410:ASP:OD2	9:I:410:ASP:O	2.30	0.50
1:A:71:LYS:CG	6:F:279:PRO:HA	2.39	0.49
2:B:74:VAL:CG1	3:C:970:VAL:HB	2.41	0.49
4:D:839:ALA:O	5:E:99:ILE:HD13	2.11	0.49
2:B:77:TRP:HA	4:D:854:TRP:N	2.28	0.49
10:J:448:GLU:OE2	10:J:448:GLU:HA	2.12	0.49
1:A:58:LYS:CB	6:F:269:TYR:HB2	2.30	0.49
9:I:410:ASP:HB2	9:I:413:GLU:CG	2.42	0.49
10:J:483:GLU:HG3	10:J:484:LYS:H	1.77	0.49
5:E:97:ILE:HD11	12:L:797:LEU:HD11	1.93	0.49
3:C:971:LEU:HB3	3:C:975:LEU:HD12	1.94	0.49
4:D:839:ALA:CB	5:E:99:ILE:CG2	2.70	0.49
2:B:41:LEU:HD22	6:F:214:GLU:OE2	2.13	0.49
3:C:985:LYS:CB	4:D:838:MET:HE2	2.42	0.49
3:C:981:ASP:O	3:C:985:LYS:N	2.45	0.49
1:A:70:LEU:HB2	6:F:297:ASN:ND2	2.22	0.49
10:J:503:LYS:HG3	10:J:513:VAL:HG21	1.95	0.48
1:A:71:LYS:CD	6:F:279:PRO:CA	2.85	0.48
8:H:301:ALA:HA	12:L:789:PRO:HG3	1.95	0.48
1:A:12:MET:HB2	10:J:459:ARG:CA	2.44	0.48
3:C:969:MET:O	3:C:972:LYS:HG3	2.13	0.48
8:H:319:LEU:HD11	11:K:757:MET:CE	2.34	0.48
1:A:7:PHE:HB2	1:A:68:LEU:HD11	1.94	0.48
6:F:324:ALA:CB	9:I:605:LYS:NZ	2.61	0.48
9:I:602:GLU:O	9:I:606:LYS:HG3	2.12	0.48
12:L:792:LEU:O	12:L:796:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:848:THR:O	4:D:851:ALA:HB3	2.14	0.48
4:D:846:ALA:CB	5:E:95:LEU:HD11	2.42	0.48
1:A:79:GLY:O	2:B:38:HIS:CD2	2.66	0.48
2:B:39:ASN:O	9:I:645:SER:CA	2.55	0.48
4:D:835:PHE:CD1	5:E:106:VAL:HG11	2.42	0.48
6:F:216:ILE:HG13	6:F:321:VAL:HG11	1.95	0.48
2:B:70:CYS:SG	3:C:978:ILE:CD1	3.02	0.47
2:B:74:VAL:CG2	3:C:970:VAL:HG12	2.44	0.47
4:D:854:TRP:HB3	5:E:88:PHE:CE1	2.46	0.47
8:H:314:VAL:HG13	12:L:805:THR:HG22	1.96	0.47
10:J:494:VAL:HG21	10:J:509:PHE:CZ	2.48	0.47
1:A:58:LYS:HZ3	6:F:298:THR:HG21	1.78	0.47
4:D:854:TRP:HB2	5:E:88:PHE:CE1	2.50	0.47
9:I:560:GLU:HG2	9:I:659:VAL:HG11	1.96	0.47
1:A:70:LEU:O	6:F:271:ASP:CA	2.58	0.47
2:B:72:SER:C	5:E:91:PRO:HG3	2.34	0.47
7:G:247:THR:CA	9:I:410:ASP:CG	2.73	0.47
9:I:567:LYS:HD2	9:I:611:GLU:OE2	2.13	0.47
1:A:77:ILE:HG23	2:B:39:ASN:N	1.77	0.47
2:B:66:LEU:CD1	3:C:978:ILE:HD13	2.42	0.47
1:A:77:ILE:HD13	9:I:619:GLY:C	2.33	0.47
2:B:57:PHE:CD2	3:C:982:GLU:CD	2.81	0.47
2:B:57:PHE:HE2	3:C:985:LYS:NZ	2.12	0.47
2:B:70:CYS:SG	3:C:978:ILE:HD12	2.55	0.47
3:C:977:VAL:O	3:C:980:LEU:N	2.47	0.47
2:B:40:GLU:C	6:F:214:GLU:CA	2.82	0.47
8:H:308:PRO:C	8:H:310:GLY:H	2.18	0.46
9:I:595:VAL:CG1	9:I:599:GLN:HG3	2.42	0.46
2:B:53:VAL:HG12	3:C:985:LYS:CD	1.95	0.46
9:I:596:LEU:O	9:I:599:GLN:HG2	2.16	0.46
10:J:536:ARG:NH1	10:J:537:ASN:HD22	2.12	0.46
4:D:832:TRP:HZ3	5:E:106:VAL:CA	2.29	0.46
11:K:758:LYS:O	11:K:761:ILE:HB	2.15	0.46
11:K:759:GLN:NE2	11:K:762:ARG:HH11	2.07	0.46
1:A:71:LYS:HD3	6:F:278:GLU:C	2.34	0.46
8:H:334:ARG:CD	9:I:646:GLY:O	2.63	0.46
1:A:71:LYS:HZ1	6:F:279:PRO:HG3	1.81	0.46
5:E:90:GLU:HB3	5:E:91:PRO:CD	2.36	0.46
8:H:332:ILE:CB	9:I:649:VAL:HB	2.17	0.46
9:I:410:ASP:HB2	9:I:413:GLU:HG3	1.96	0.46
9:I:551:LYS:HE2	9:I:653:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:502:ASN:OD1	10:J:504:ARG:NH2	2.48	0.46
2:B:54:ILE:HG21	3:C:986:PHE:CB	2.43	0.45
2:B:73:PHE:CD1	4:D:850:GLY:HA3	2.22	0.45
3:C:975:LEU:HB2	3:C:976:PRO:HD3	1.98	0.45
3:C:984:LEU:CA	3:C:987:ILE:HG12	2.46	0.45
11:K:771:GLU:O	11:K:774:CYS:HB3	2.17	0.45
12:L:791:GLN:O	12:L:794:TRP:N	2.50	0.45
1:A:71:LYS:HZ2	6:F:279:PRO:CA	2.26	0.45
4:D:843:TYR:HA	5:E:95:LEU:CD2	2.45	0.45
8:H:295:TYR:CD1	8:H:295:TYR:N	2.85	0.45
8:H:333:VAL:HG13	9:I:648:ILE:HG12	1.98	0.45
10:J:524:LEU:O	10:J:527:GLU:HB2	2.16	0.45
1:A:71:LYS:HA	6:F:273:SER:CA	2.41	0.45
2:B:40:GLU:N	6:F:214:GLU:HB2	2.31	0.45
2:B:70:CYS:CB	3:C:975:LEU:CD1	2.61	0.45
6:F:255:GLU:HG2	6:F:256:LYS:N	2.32	0.45
8:H:332:ILE:HD11	9:I:651:ILE:HG22	1.97	0.45
2:B:77:TRP:CZ2	4:D:852:ALA:HB1	2.44	0.45
9:I:561:LEU:CD2	9:I:659:VAL:HG22	2.46	0.45
9:I:633:ILE:HD11	9:I:662:ILE:HD11	1.99	0.45
10:J:464:ILE:HD13	10:J:464:ILE:O	2.17	0.45
1:A:58:LYS:HZ3	6:F:298:THR:CG2	2.30	0.45
1:A:67:LYS:HE3	6:F:269:TYR:HH	1.82	0.45
12:L:803:PRO:O	12:L:807:LEU:HG	2.17	0.45
1:A:24:ARG:HG3	1:A:64:LEU:HD11	1.99	0.45
3:C:969:MET:O	3:C:973:ILE:HG13	2.17	0.45
9:I:431:LYS:HE2	9:I:551:LYS:HB3	1.98	0.44
10:J:472:ALA:HA	10:J:477:ILE:HD12	1.99	0.44
2:B:73:PHE:CD1	4:D:850:GLY:CA	2.71	0.44
8:H:322:GLY:O	8:H:326:MET:HG3	2.18	0.44
8:H:315:ILE:O	8:H:319:LEU:HB2	2.16	0.44
11:K:767:SER:O	11:K:771:GLU:HG3	2.17	0.44
12:L:802:LEU:N	12:L:803:PRO:HD2	2.33	0.44
1:A:41:GLU:OE2	10:J:461:GLU:OE1	2.36	0.44
1:A:54:VAL:HG11	6:F:297:ASN:OD1	2.18	0.44
2:B:41:LEU:HD11	6:F:215:ALA:HB3	1.96	0.44
8:H:311:LEU:O	8:H:313:ALA:N	2.51	0.44
11:K:754:TYR:O	11:K:758:LYS:HB3	2.17	0.44
1:A:14:CYS:SG	10:J:458:ARG:CB	2.99	0.44
2:B:65:LEU:HD11	8:H:307:ILE:HG21	2.00	0.44
3:C:968:LEU:HD23	3:C:968:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ALA:C	2:B:71:ILE:H	2.21	0.44
7:G:248:PRO:HB3	9:I:417:LYS:HZ3	1.82	0.44
10:J:450:LEU:HD21	10:J:472:ALA:HA	2.00	0.44
2:B:54:ILE:HG21	3:C:986:PHE:CG	2.51	0.44
3:C:967:TRP:HA	3:C:970:VAL:HG23	1.99	0.44
1:A:77:ILE:HA	9:I:620:ILE:HG23	1.33	0.43
2:B:51:GLU:OE2	3:C:986:PHE:CZ	2.70	0.43
2:B:53:VAL:CG2	3:C:985:LYS:CB	2.92	0.43
8:H:304:VAL:HG21	12:L:789:PRO:HB3	2.00	0.43
9:I:563:ARG:HH11	9:I:563:ARG:HG2	1.83	0.43
1:A:58:LYS:HA	1:A:68:LEU:HD23	2.00	0.43
2:B:51:GLU:N	3:C:988:ALA:HB3	2.33	0.43
4:D:844:VAL:CG2	4:D:845:GLY:N	2.81	0.43
1:A:12:MET:CB	10:J:459:ARG:CB	2.95	0.43
1:A:53:SER:CB	6:F:253:PRO:HB2	2.48	0.43
1:A:58:LYS:HZ3	6:F:298:THR:HB	1.84	0.43
1:A:36:VAL:HG12	1:A:43:VAL:HG13	2.01	0.43
8:H:326:MET:HE2	9:I:412:LEU:HD11	2.01	0.43
2:B:65:LEU:HD21	8:H:307:ILE:HD12	1.98	0.43
2:B:57:PHE:HE2	3:C:985:LYS:HZ2	1.65	0.43
2:B:68:ALA:HA	8:H:300:VAL:HG12	2.00	0.43
1:A:70:LEU:CB	6:F:297:ASN:HD21	2.28	0.43
2:B:53:VAL:O	2:B:56:GLN:HB3	2.18	0.43
2:B:72:SER:OG	5:E:91:PRO:HG3	2.19	0.43
6:F:214:GLU:HG2	6:F:215:ALA:N	2.33	0.43
10:J:502:ASN:HD22	10:J:502:ASN:C	2.22	0.43
1:A:20:ARG:HB3	10:J:459:ARG:HH12	1.84	0.43
4:D:835:PHE:CZ	5:E:106:VAL:HB	2.54	0.43
10:J:464:ILE:HD13	10:J:464:ILE:C	2.38	0.43
10:J:518:GLU:O	10:J:522:GLU:HG3	2.18	0.43
1:A:71:LYS:O	6:F:273:SER:N	2.44	0.43
2:B:53:VAL:HG21	3:C:985:LYS:CB	2.49	0.43
2:B:66:LEU:HD11	3:C:978:ILE:CD1	2.46	0.43
3:C:967:TRP:O	3:C:970:VAL:HB	2.19	0.43
9:I:410:ASP:CG	9:I:410:ASP:O	2.57	0.43
12:L:809:PHE:CD1	12:L:809:PHE:N	2.81	0.43
1:A:21:ILE:HG22	1:A:25:LEU:HD12	2.00	0.42
12:L:801:GLY:C	12:L:803:PRO:HD2	2.40	0.42
1:A:42:THR:HG22	6:F:279:PRO:CB	2.49	0.42
1:A:73:GLU:HG3	2:B:36:TYR:CD2	2.53	0.42
2:B:41:LEU:N	6:F:214:GLU:CA	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:306:ALA:HB2	11:K:772:VAL:HG21	2.01	0.42
9:I:583:SER:HA	9:I:588:LEU:HD22	2.01	0.42
10:J:438:ASP:HB2	10:J:545:ALA:HB3	2.00	0.42
9:I:554:ALA:HA	9:I:655:LEU:HD12	2.01	0.42
4:D:840:ILE:O	4:D:843:TYR:HB3	2.20	0.42
8:H:326:MET:HE3	8:H:333:VAL:HG21	1.97	0.42
9:I:663:GLN:C	11:K:750:GLY:N	2.73	0.42
1:A:67:LYS:CG	6:F:269:TYR:CE1	2.98	0.42
1:A:69:LYS:HD2	6:F:269:TYR:HB3	2.01	0.42
2:B:38:HIS:O	2:B:40:GLU:N	2.52	0.42
3:C:969:MET:SD	3:C:972:LYS:HD2	2.59	0.42
4:D:835:PHE:CE1	5:E:106:VAL:CB	3.00	0.42
2:B:41:LEU:CD2	6:F:214:GLU:OE2	2.66	0.42
5:E:97:ILE:CD1	12:L:797:LEU:HD11	2.50	0.42
2:B:66:LEU:HD13	5:E:98:LEU:HD13	2.01	0.42
2:B:53:VAL:CG1	3:C:985:LYS:CB	2.96	0.41
1:A:61:VAL:HA	1:A:64:LEU:HD12	2.01	0.41
1:A:62:ASP:CG	6:F:269:TYR:HH	2.12	0.41
9:I:419:THR:OG1	9:I:611:GLU:CB	2.69	0.41
10:J:521:LEU:HD12	10:J:533:ILE:HD11	2.02	0.41
1:A:70:LEU:C	6:F:271:ASP:HA	2.34	0.41
9:I:410:ASP:O	9:I:414:VAL:HG23	2.21	0.41
4:D:832:TRP:O	4:D:835:PHE:HB3	2.20	0.41
12:L:802:LEU:N	12:L:803:PRO:CD	2.83	0.41
1:A:6:GLU:CG	2:B:36:TYR:CE2	3.03	0.41
5:E:103:ILE:C	5:E:105:GLY:N	2.73	0.41
6:F:278:GLU:HA	6:F:279:PRO:HD3	1.97	0.41
10:J:434:PRO:O	10:J:467:ALA:HB2	2.21	0.41
1:A:7:PHE:CB	1:A:68:LEU:HD11	2.51	0.41
5:E:106:VAL:O	5:E:106:VAL:HG22	2.21	0.41
10:J:441:PRO:HB3	10:J:446:GLU:HA	2.02	0.41
1:A:14:CYS:H	10:J:459:ARG:C	2.21	0.41
1:A:62:ASP:CB	6:F:269:TYR:CE2	3.01	0.41
1:A:70:LEU:N	6:F:271:ASP:HA	2.35	0.41
9:I:562:LYS:HE2	9:I:562:LYS:HB3	1.93	0.41
11:K:752:ALA:O	11:K:753:ILE:C	2.58	0.41
1:A:66:TYR:HD1	10:J:485:VAL:HB	1.72	0.41
1:A:71:LYS:NZ	6:F:279:PRO:HG3	2.35	0.41
5:E:99:ILE:O	5:E:103:ILE:HG13	2.21	0.41
7:G:247:THR:OG1	9:I:413:GLU:CG	2.69	0.41
8:H:330:ASN:CB	9:I:652:ARG:N	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:CB	2:B:36:TYR:OH	2.41	0.40
4:D:846:ALA:O	4:D:850:GLY:N	2.54	0.40
6:F:265:GLU:HB3	6:F:302:LYS:HB2	2.03	0.40
7:G:273:LEU:C	7:G:273:LEU:HD23	2.42	0.40
8:H:299:ALA:C	8:H:301:ALA:N	2.70	0.40
9:I:576:TRP:CD2	9:I:593:ALA:HB3	2.56	0.40
11:K:751:ARG:O	11:K:752:ALA:C	2.59	0.40
11:K:759:GLN:O	11:K:762:ARG:N	2.54	0.40
1:A:10:GLU:OE1	10:J:489:ALA:CA	2.66	0.40
11:K:754:TYR:O	11:K:758:LYS:CB	2.69	0.40
1:A:78:GLU:N	2:B:38:HIS:HA	2.36	0.40
3:C:986:PHE:O	3:C:988:ALA:N	2.54	0.40
7:G:247:THR:HG21	9:I:410:ASP:HB3	0.46	0.40
7:G:274:ILE:HD13	7:G:274:ILE:HA	1.93	0.40
9:I:555:LYS:N	9:I:556:PRO:HD2	2.37	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	78/80 (98%)	65 (83%)	10 (13%)	3 (4%)	3 24
2	B	40/42 (95%)	29 (72%)	10 (25%)	1 (2%)	5 32
3	C	20/22 (91%)	13 (65%)	5 (25%)	2 (10%)	0 9
4	D	21/23 (91%)	19 (90%)	2 (10%)	0	100 100
5	E	28/30 (93%)	16 (57%)	11 (39%)	1 (4%)	3 25
6	F	111/113 (98%)	109 (98%)	2 (2%)	0	100 100
7	G	34/36 (94%)	28 (82%)	6 (18%)	0	100 100
8	H	46/48 (96%)	39 (85%)	4 (9%)	3 (6%)	1 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	I	122/128 (95%)	118 (97%)	4 (3%)	0	100 100
10	J	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
11	K	30/32 (94%)	23 (77%)	7 (23%)	0	100 100
12	L	19/21 (90%)	13 (68%)	5 (26%)	1 (5%)	2 19
All	All	665/693 (96%)	582 (88%)	72 (11%)	11 (2%)	13 42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ALA
1	A	77	ILE
8	H	300	VAL
8	H	309	GLU
2	B	46	GLY
3	C	975	LEU
5	E	112	ALA
8	H	312	PRO
1	A	72	GLY
12	L	803	PRO
3	C	978	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	66/66 (100%)	56 (85%)	10 (15%)	3 14
2	B	36/36 (100%)	36 (100%)	0	100 100
3	C	20/20 (100%)	18 (90%)	2 (10%)	7 26
4	D	13/13 (100%)	12 (92%)	1 (8%)	13 37
5	E	24/24 (100%)	23 (96%)	1 (4%)	30 54
6	F	91/91 (100%)	89 (98%)	2 (2%)	52 71
7	G	33/33 (100%)	32 (97%)	1 (3%)	41 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	35/35 (100%)	33 (94%)	2 (6%)	20 45
9	I	102/100 (102%)	100 (98%)	2 (2%)	55 74
10	J	93/92 (101%)	88 (95%)	5 (5%)	22 47
11	K	27/27 (100%)	24 (89%)	3 (11%)	6 22
12	L	17/17 (100%)	16 (94%)	1 (6%)	19 45
All	All	557/554 (100%)	527 (95%)	30 (5%)	26 47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	19	ASN
1	A	20	ARG
1	A	23	LYS
1	A	25	LEU
1	A	51	GLU
1	A	58	LYS
1	A	59	GLU
1	A	71	LYS
1	A	80	ARG
3	C	969	MET
3	C	981	ASP
4	D	844	VAL
5	E	108	GLN
6	F	214	GLU
6	F	320	LEU
7	G	247	THR
8	H	295	TYR
8	H	319	LEU
9	I	561	LEU
9	I	588	LEU
10	J	461	GLU
10	J	464	ILE
10	J	478	GLU
10	J	481	GLU
10	J	502	ASN
11	K	760	PHE
11	K	767	SER
11	K	778	THR
12	L	805	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	38	HIS
2	B	56	GLN
5	E	101	ASN
6	F	316	GLN
7	G	250	GLN
7	G	275	ASN
9	I	587	ASN
9	I	599	GLN
9	I	608	GLN
9	I	628	GLN
10	J	443	ASN
10	J	462	HIS
10	J	515	ASN
10	J	537	ASN
11	K	759	GLN
11	K	768	ASN
12	L	796	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	636:GLY	C	645:SER	N	12.26
1	I	431:LYS	C	550:LEU	N	7.12

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5004. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map

X

Y

Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 50

Y Index: 50

Z Index: 50

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: 50

Y Index: 47

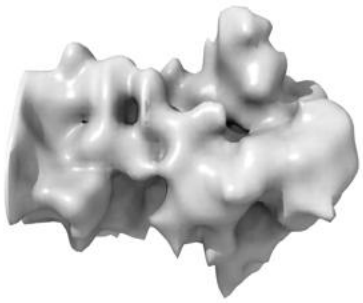
Z Index: 57

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

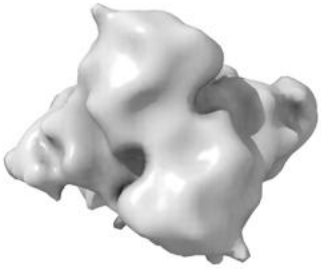
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

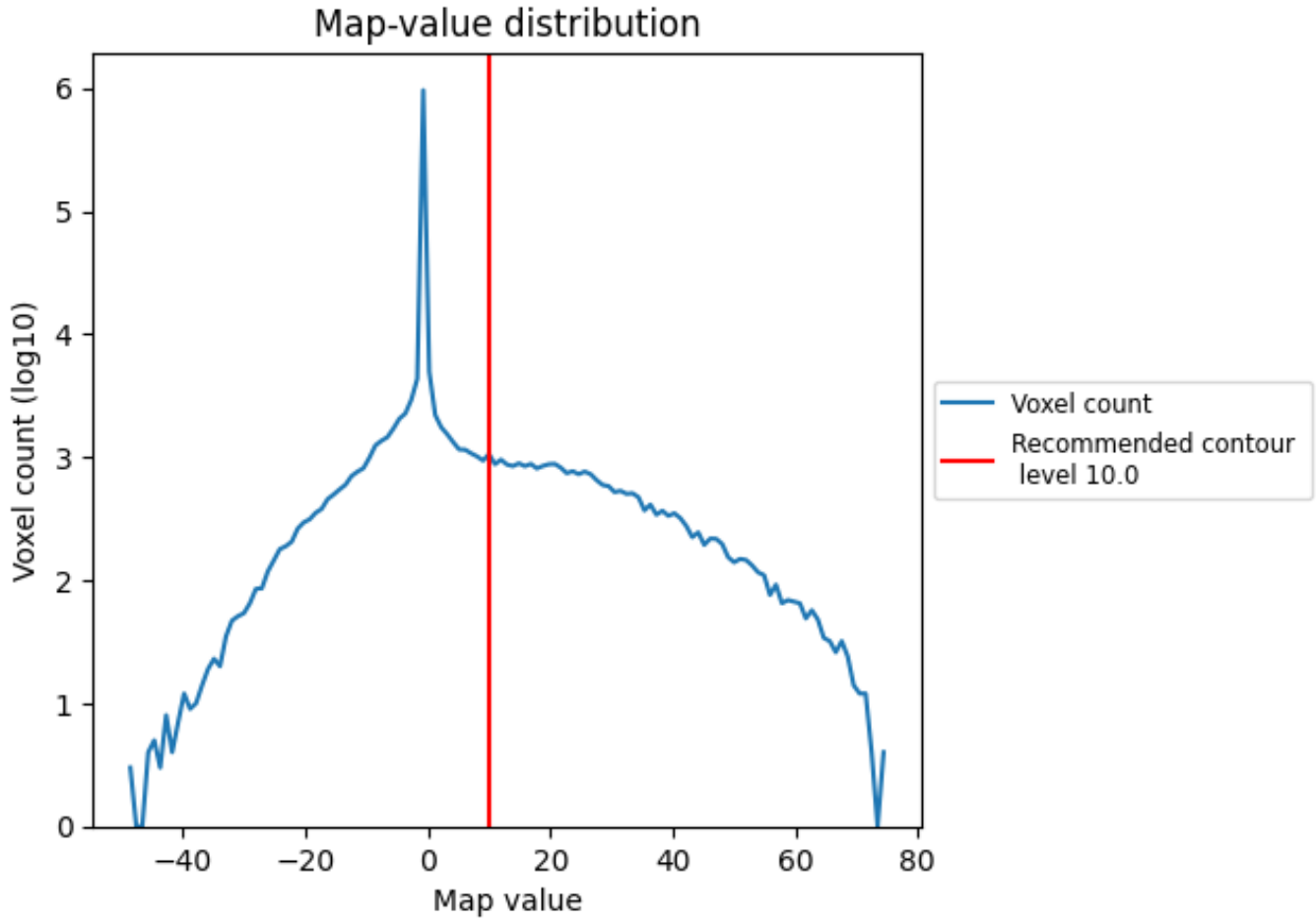
6.5 Mask visualisation (i)

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

7 Map analysis

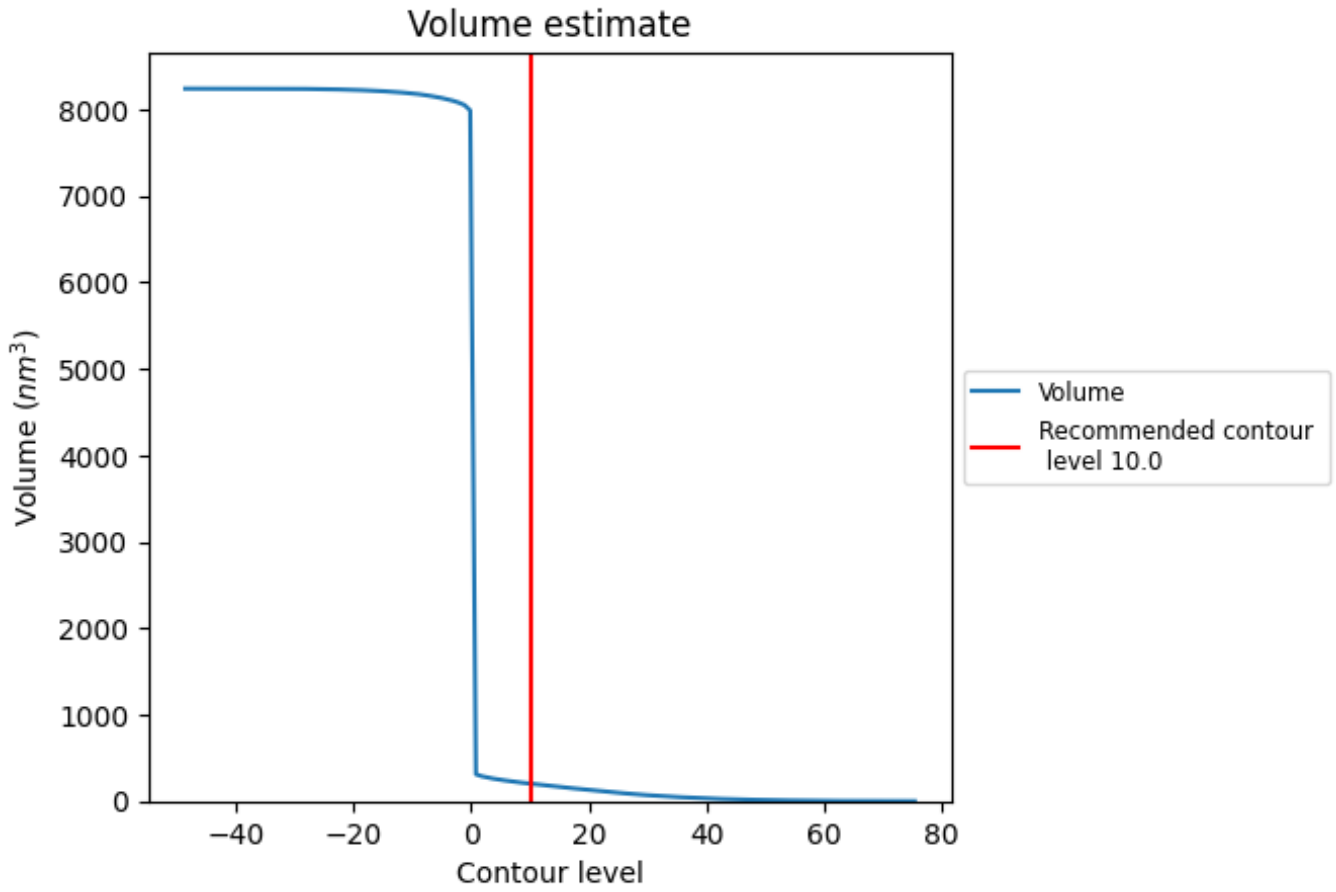
This section contains the results of statistical analysis of the map.

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.

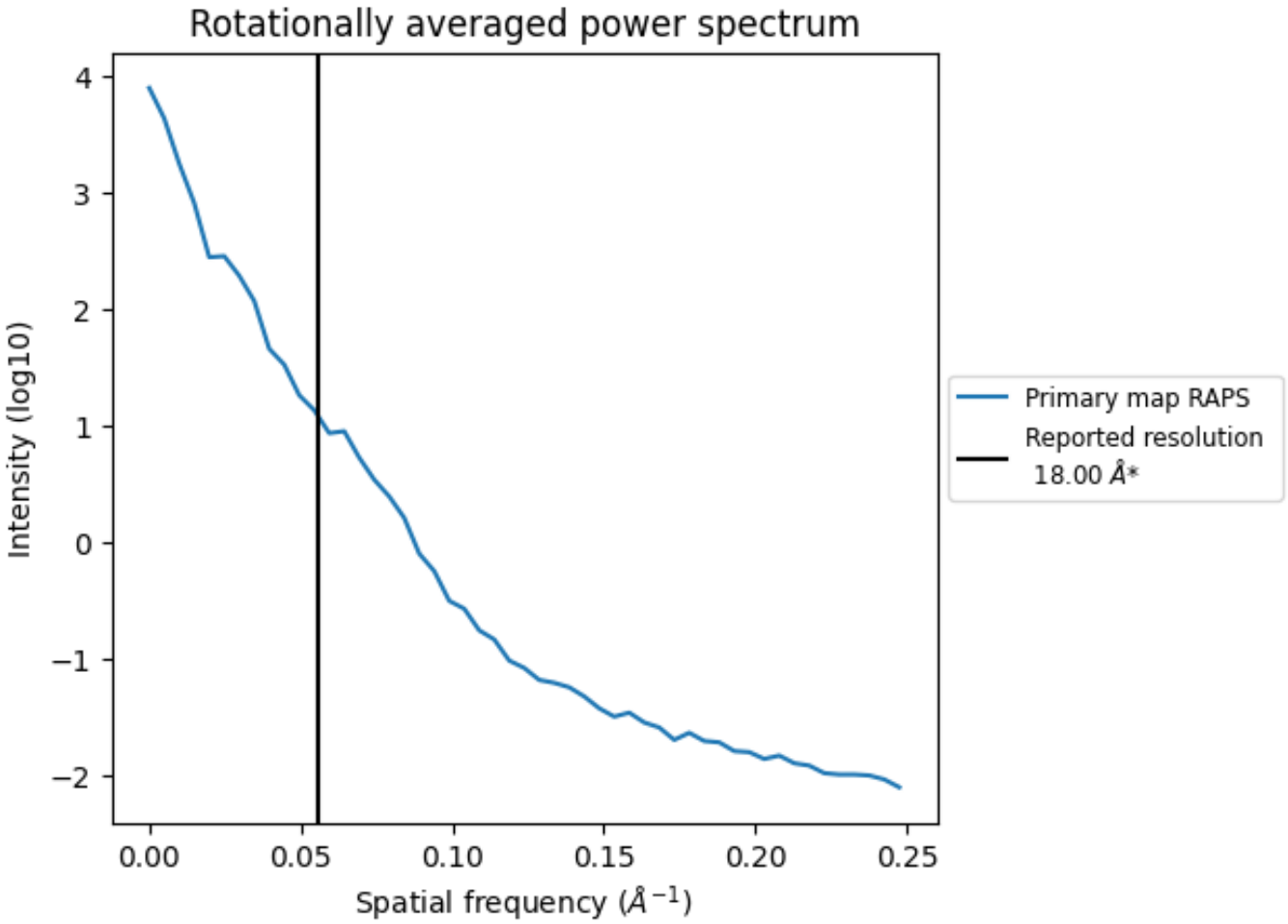
7.2 Volume estimate (i)



The volume at the recommended contour level is 203 nm^3; this corresponds to an approximate mass of 183 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 0.056 Å^{-1}

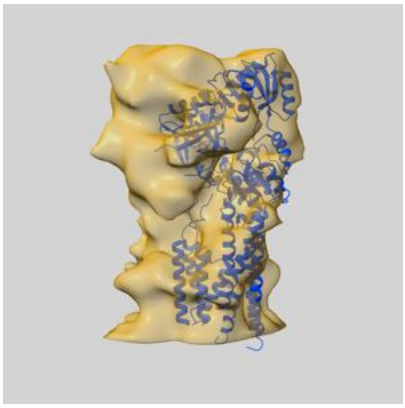
8 Fourier-Shell correlation (i)

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

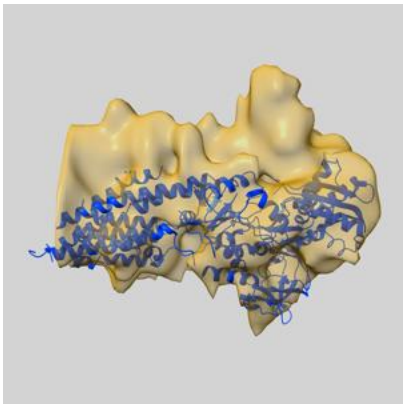
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-5004 and PDB model 2VOY. Per-residue inclusion information can be found in section 3 on page 6.

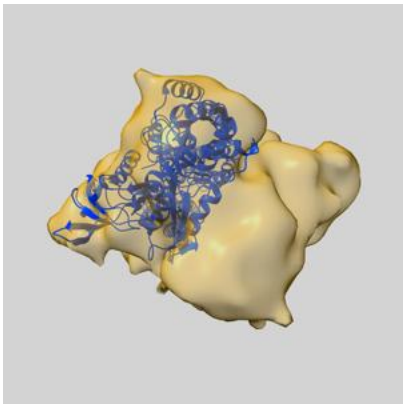
9.1 Map-model overlay



X



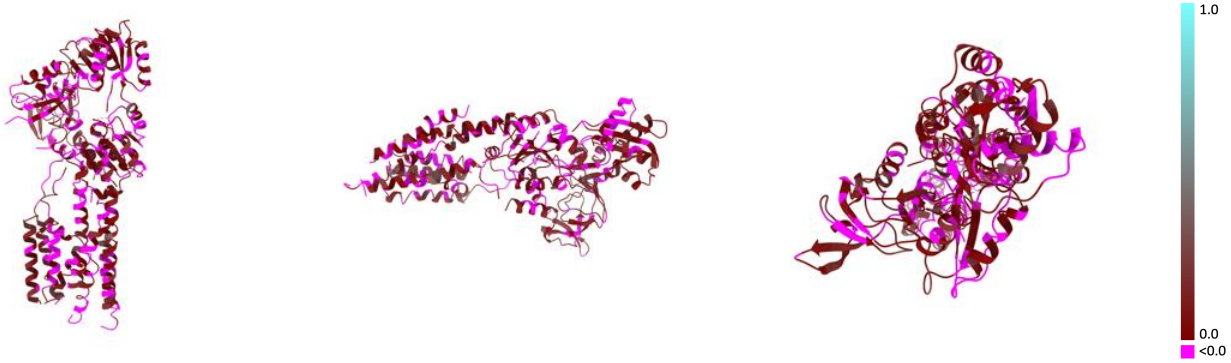
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0 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.

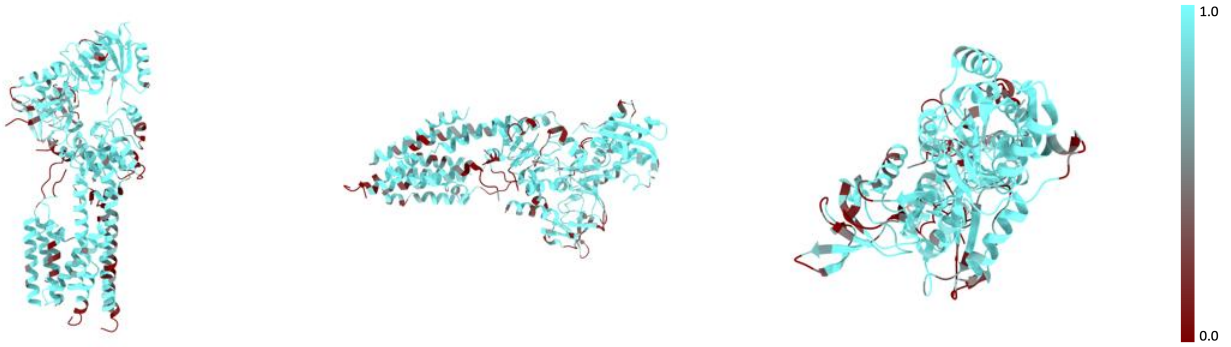
9.2 Q-score mapped to coordinate model



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.

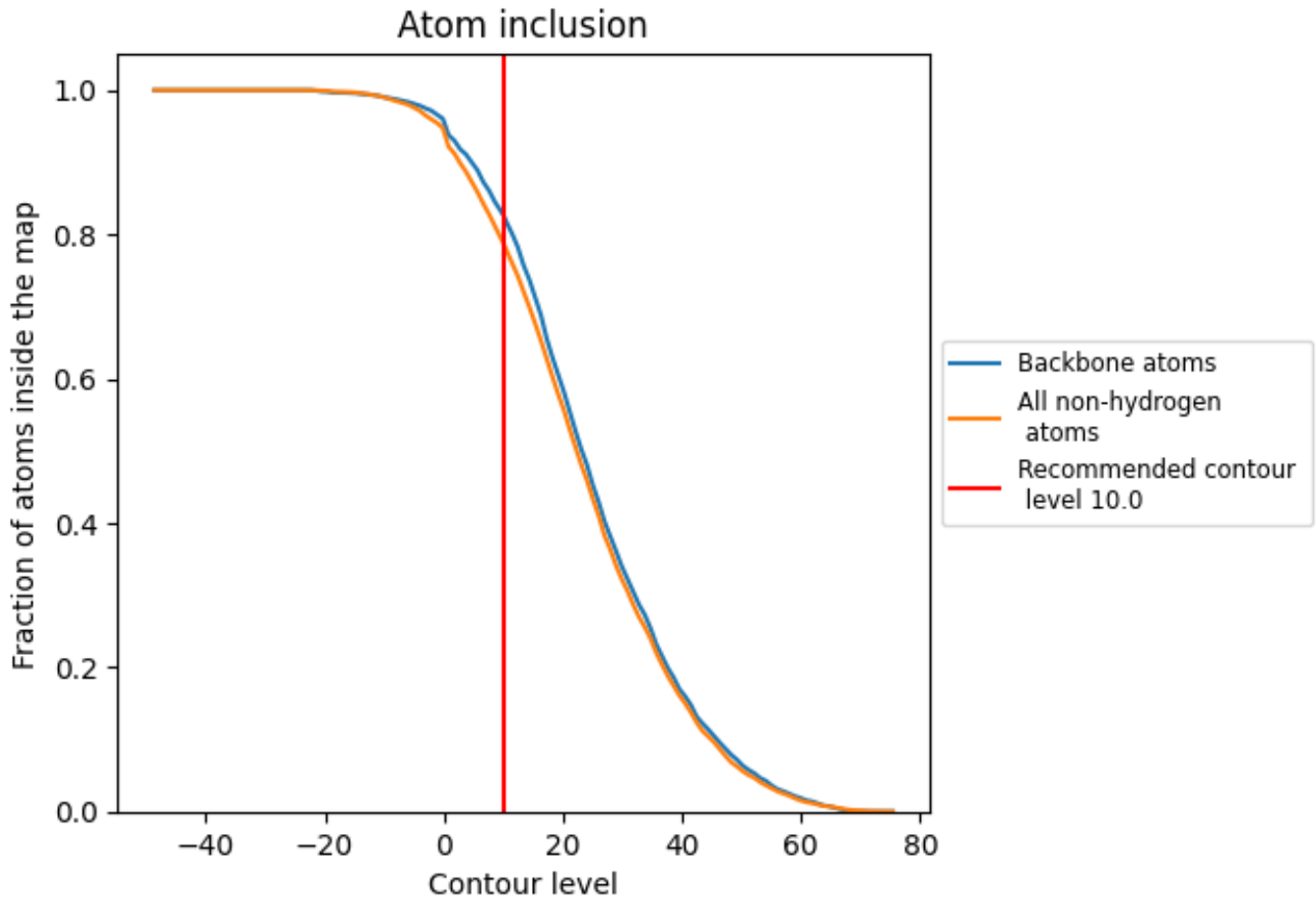
9.3 Atom inclusion mapped to coordinate model



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 (10.0).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7874	0.0410
A	0.7381	0.0140
B	0.7589	0.0670
C	0.8057	0.0640
D	0.9353	0.1190
E	0.7619	-0.0070
F	0.7293	0.0520
G	0.4930	0.0500
H	0.8237	-0.0010
I	0.8133	0.0450
J	0.9104	0.0490
K	0.7449	0.0430
L	0.8846	0.0080